APPENDIX A

NMR RESONANCE ASSIGNMENTS

**Table A-1:** Resonance assignments for the *R-BD-N3-dU* modified oligonucleotide 5′-$G^{1}C^{2}T^{3}A^{4}G^{5}C^{6}X^{7}A^{8}G^{9}T^{10}C^{11}C^{12}$-3’·5’-$G^{13}G^{14}A^{15}C^{16}T^{17}A^{18}G^{19}C^{20}T^{21}A^{22}G^{23}C^{24}$-3′.

| Primary Strand | | | Complementary Strand | | |
|---|---|---|---|---|---|
| Residue | Atom | Chemical Shift (ppm) | Residue | Atom | Chemical Shift (ppm) |
| G1 | H1' | 5.852 | G13 | H1' | 5.495 |
| G1 | H2' | 2.527 | G13 | H2' | 2.37 |
| G1 | H2" | 2.635 | G13 | H2" | 2.55 |
| G1 | H3' | 4.694 | G13 | H3' | 4.676 |
| G1 | H4' | 4.11 | G13 | H4' | 4.031 |
| G1 | H5' | 3.585 | G13 | H5' | 3.513 |
| G1 | H5" | 3.583 | G13 | H5" | 3.507 |
| G1 | H8 | 7.837 | G13 | H8 | 7.701 |
| C2 | H1' | 5.908 | G14 | H1' | 5.457 |
| C2 | H2' | 1.977 | G14 | H2' | 2.571 |
| C2 | H2" | 2.355 | G14 | H2" | 2.66 |
| C2 | H3' | 4.683 | G14 | H3' | 4.89 |
| C2 | H5 | 5.212 | G14 | H4' | 4.236 |
| C2 | H5' | 4.098 | G14 | H5' | 3.926 |
| C2 | H6 | 7.386 | G14 | H5" | 4.021 |
| T3 | CH3 | 1.51 | G14 | H8 | 7.711 |
| T3 | H1' | 5.359 | A15 | H1' | 6.144 |
| T3 | H2' | 2.022 | A15 | H2 | 7.808 |
| T3 | H2" | 2.27 | A15 | H2' | 2.578 |
| T3 | H3' | 4.727 | A15 | H2" | 2.787 |
| T3 | H4' | 3.995 | A15 | H3' | 4.928 |
| T3 | H5' | 3.91 | A15 | H4' | 4.355 |
| T3 | H6 | 7.278 | A15 | H5' | 4.115 |
| T3 | M7 | 1.514 | A15 | H5" | 4.098 |
| A4 | H1' | 5.917 | A15 | H8 | 8.08 |
| A4 | H2' | 2.62 | C16 | H1' | 5.702 |
| A4 | H2" | 2.758 | C16 | H2' | 1.657 |
| A4 | H3' | 4.92 | C16 | H2" | 2.194 |
| A4 | H4' | 4.273 | C16 | H3' | 4.615 |
| A4 | H5' | 3.894 | C16 | H4' | 3.965 |
| A4 | H5" | 4.001 | C16 | H5 | 5.115 |
| A4 | H8 | 8.076 | C16 | H5' | 4.02 |
| G5 | H1' | 5.535 | C16 | H5" | 4.187 |
| G5 | H2' | 2.296 | C16 | H6 | 7.111 |
| G5 | H2" | 2.436 | T17 | CH3 | 1.505 |
| G5 | H3' | 4.82 | T17 | H1' | 5.846 |
| G5 | H4' | 4.178 | T17 | H2' | 1.661 |
| G5 | H8 | 7.514 | T17 | H2" | 1.75 |

**Table A-1:** Continued

| Primary Strand | | | Complementary Strand | | |
|---|---|---|---|---|---|
| Residue | Atom | Chemical Shift (ppm) | Residue | Atom | Chemical Shift (ppm) |
| C6 | H1' | 5.877 | T17 | H3' | 4.673 |
| C6 | H2' | 2.003 | T17 | H4' | 3.885 |
| C6 | H2'' | 2.087 | T17 | H5' | 3.959 |
| C6 | H3' | 4.646 | T17 | H6 | 7.083 |
| C6 | H4' | 3.949 | T17 | M7 | 1.453 |
| C6 | H5 | 5.283 | A18 | H1' | 5.505 |
| C6 | H6 | 7.235 | A18 | H2 | 7.487 |
| X7 | H1' | 5.606 | A18 | H2' | 2.303 |
| X7 | Hγ | 4.9 | A18 | H2'' | 2.37 |
| X7 | Hδ' | 4.479 | A18 | H3' | 4.748 |
| X7 | Hδ | 4.351 | A18 | H4' | 4.035 |
| X7 | Hα' | 2.936 | A18 | H5' | 3.718 |
| X7 | Hα | 2.822 | A18 | H5'' | 3.846 |
| X7 | H2' | 1.125 | A18 | H8 | 7.925 |
| X7 | H2'' | 1.79 | T18 | CH3 | 1.239 |
| X7 | H3' | 4.477 | T18 | H1' | 5.553 |
| X7 | H4' | 3.952 | T18 | H2' | 1.458 |
| X7 | H5 | 5.186 | T18 | H2'' | 1.715 |
| X7 | H5' | 3.795 | T18 | H3' | 4.519 |
| X7 | H5'' | 3.906 | T18 | H4' | 3.9 |
| X7 | H6 | 7.047 | T18 | H5' | 3.742 |
| X7 | Hβ | 3.185 | T18 | H5'' | 3.801 |
| A8 | H1' | 5.692 | T18 | H6 | 6.949 |
| A8 | H2 | 7.455 | T18 | M7 | 1.283 |
| A8 | H2' | 2.673 | G19 | H1' | 5.583 |
| A8 | H2'' | 2.691 | G19 | H2' | 2.497 |
| A8 | H3' | 4.829 | G19 | H2'' | 2.545 |
| A8 | H4' | 4.158 | G19 | H3' | 4.801 |
| A8 | H5' | 3.74 | G19 | H4' | 4.188 |
| A8 | H5'' | 3.883 | G19 | H5' | 3.751 |
| A8 | H8 | 8.176 | G19 | H5'' | 3.843 |
| G9 | H1' | 5.757 | G19 | H8 | 7.771 |
| G9 | H2' | 2.376 | C20 | H1' | 5.773 |
| G9 | H2'' | 2.551 | C20 | H2' | 1.885 |
| G9 | H3' | 4.683 | C20 | H2'' | 2.288 |
| G9 | H4' | 4.238 | C20 | H3' | 4.575 |
| G9 | H5' | 4.047 | C20 | H4' | 4.054 |
| G9 | H8 | 7.523 | C20 | H5 | 5.164 |
| T10 | CH3 | 1.128 | C20 | H5' | 3.97 |
| T10 | H1' | 5.951 | C20 | H5'' | 3.887 |
| T10 | H2' | 2.037 | C20 | H6 | 7.271 |
| T10 | H2'' | 2.388 | T21 | CH3 | 1.486 |
| T10 | H3' | 4.713 | T21 | H1' | 5.341 |
| T10 | H4' | 4.099 | T21 | H2' | 1.991 |
| T10 | H6 | 7.184 | T21 | H2'' | 2.239 |

**Table A-1:** Continued

| Primary Strand | | | Complementary Strand | | |
|---|---|---|---|---|---|
| Residue | Atom | Chemical Shift (ppm) | Residue | Atom | Chemical Shift (ppm) |
| T10 | M7 | 1.134 | T21 | H3' | 4.704 |
| C11 | H1' | 5.913 | T21 | H4' | 3.973 |
| C11 | H2' | 2.065 | T21 | H5' | 3.885 |
| C11 | H2'' | 2.341 | T21 | H6 | 7.255 |
| C11 | H3' | 4.686 | T21 | M7 | 1.491 |
| C11 | H5 | 5.558 | A22 | H1' | 5.904 |
| C11 | H6 | 7.456 | A22 | H2' | 2.61 |
| C12 | H1' | 6.085 | A22 | H2'' | 2.745 |
| C12 | H2' | 2.119 | A22 | H3' | 4.901 |
| C12 | H2'' | 2.138 | A22 | H4' | 4.264 |
| C12 | H3' | 4.416 | A22 | H5' | 3.869 |
| C12 | H4' | 3.886 | A22 | H5'' | 3.985 |
| C12 | H5 | 5.596 | A22 | H8 | 8.075 |
| C12 | H5' | 4.024 | G23 | H1' | 5.634 |
| C12 | H6 | 7.496 | G23 | H2' | 2.324 |
| | | | G23 | H2'' | 2.487 |
| | | | G23 | H3' | 4.8 |
| | | | G23 | H4' | 4.206 |
| | | | G23 | H5' | 4.076 |
| | | | G23 | H8 | 7.543 |
| | | | C24 | H1' | 5.951 |
| | | | C24 | H2' | 1.968 |
| | | | C24 | H2'' | 2.037 |
| | | | C24 | H3' | 4.297 |
| | | | C24 | H4' | 3.888 |
| | | | C24 | H5 | 5.156 |
| | | | C24 | H5' | 4.082 |
| | | | C24 | H5'' | 4.048 |
| | | | C24 | H6 | 7.219 |

**Table A-2:** Resonance assignments for the *S-BD-N3-dU* modified oligonucleotide 5′-$G^{1}C^{2}T^{3}A^{4}G^{5}C^{6}X^{7}A^{8}G^{9}T^{10}C^{11}C^{12}$-3’·5’-$G^{13}G^{14}A^{15}C^{16}T^{17}A^{18}G^{19}C^{20}T^{21}A^{22}G^{23}C^{24}$-3′.

| Primary Strand | | | Complementary Strand | | |
|---|---|---|---|---|---|
| Residue | Atom | Chemical Shift (ppm) | Residue | Atom | Chemical Shift (ppm) |
| G1 | H1' | 5.845 | G13 | H1' | 5.493 |
| G1 | H2' | 2.521 | G13 | H2' | 2.369 |
| G1 | H2'' | 2.631 | G13 | H2'' | 2.551 |
| G1 | H3' | 4.691 | G13 | H3' | 4.675 |
| G1 | H4' | 4.111 | G13 | H4' | 4.031 |
| G1 | H5' | 3.585 | G13 | H5' | 3.513 |
| G1 | H5'' | 3.583 | G13 | H5'' | 3.507 |
| G1 | H8 | 7.831 | G13 | H8 | 7.698 |
| C2 | H1' | 5.903 | G14 | H1' | 5.454 |
| C2 | H2' | 1.973 | G14 | H2' | 2.568 |
| C2 | H2'' | 2.349 | G14 | H2'' | 2.654 |
| C2 | H3' | 4.68 | G14 | H3' | 4.887 |
| C2 | H5 | 5.204 | G14 | H4' | 4.233 |
| C2 | H5' | 4.098 | G14 | H5' | 3.926 |
| C2 | H6 | 7.38 | G14 | H5'' | 4.021 |
| T3 | CH3 | 1.506 | G14 | H8 | 7.705 |
| T3 | H1' | 5.348 | A15 | H1' | 6.137 |
| T3 | H2' | 2.015 | A15 | H2 | 7.795 |
| T3 | H2'' | 2.258 | A15 | H2' | 2.575 |
| T3 | H3' | 4.72 | A15 | H2'' | 2.78 |
| T3 | H4' | 3.995 | A15 | H3' | 4.923 |
| T3 | H5' | 3.91 | A15 | H4' | 4.353 |
| T3 | H6 | 7.274 | A15 | H5' | 4.115 |
| T3 | M7 | 1.514 | A15 | H5'' | 4.098 |
| A4 | H1' | 5.91 | A15 | H8 | 8.076 |
| A4 | H2' | 2.607 | C16 | H1' | 5.678 |
| A4 | H2'' | 2.754 | C16 | H2' | 1.689 |
| A4 | H3' | 4.917 | C16 | H2'' | 2.214 |
| A4 | H4' | 4.269 | C16 | H3' | 4.599 |
| A4 | H5' | 3.894 | C16 | H4' | 3.965 |
| A4 | H5'' | 4.001 | C16 | H5 | 5.108 |
| A4 | H8 | 8.065 | C16 | H5' | 4.02 |
| G5 | H1' | 5.507 | C16 | H5'' | 4.187 |
| G5 | H2' | 2.306 | C16 | H6 | 7.119 |
| G5 | H2'' | 2.42 | T17 | CH3 | 1.464 |
| G5 | H3' | 4.813 | T17 | H1' | 5.826 |
| G5 | H4' | 4.179 | T17 | H2' | 1.589 |
| G5 | H8 | 7.524 | T17 | H2'' | 1.773 |
| C6 | H1' | 5.848 | T17 | H3' | 4.628 |
| C6 | H2' | 1.942 | T17 | H4' | 3.885 |
| C6 | H2'' | 2.086 | T17 | H5' | 3.959 |
| C6 | H3' | 4.605 | T17 | H6 | 7.043 |
| C6 | H4' | 3.949 | T17 | M7 | 1.453 |

**Table A-2:** Continued

| Primary Strand | | | Complementary Strand | | |
|---|---|---|---|---|---|
| Residue | Atom | Chemical Shift (ppm) | Residue | Atom | Chemical Shift (ppm) |
| C6 | H5 | 5.28 | A18 | H1' | 5.518 |
| C6 | H6 | 7.243 | A18 | H2 | 7.507 |
| X7 | H1' | 5.513 | A18 | H2' | 2.214 |
| X7 | Hγ | 5.089 | A18 | H2" | 2.314 |
| X7 | Hδ' | 4.539 | A18 | H3' | 4.769 |
| X7 | Hδ | 4.351 | A18 | H4' | 4.045 |
| X7 | Hα' | 3.000 | A18 | H5' | 3.731 |
| X7 | Hα | 2.552 | A18 | H5" | 3.851 |
| X7 | H2' | 1.074 | A18 | H8 | 7.899 |
| X7 | H2" | 1.73 | T18 | CH3 | 1.239 |
| X7 | H3' | 4.466 | T18 | H1' | 5.553 |
| X7 | H4' | 3.908 | T18 | H2' | 1.458 |
| X7 | H5 | 5.195 | T18 | H2" | 1.715 |
| X7 | H5' | 3.794 | T18 | H3' | 4.519 |
| X7 | H5" | 3.906 | T18 | H4' | 3.9 |
| X7 | H6 | 7.013 | T18 | H5' | 3.742 |
| X7 | Hβ | 3.498 | T18 | H5" | 3.801 |
| A8 | H1' | 5.782 | T18 | H6 | 6.949 |
| A8 | H2 | 7.456 | T18 | M7 | 1.283 |
| A8 | H2' | 2.704 | G19 | H1' | 5.582 |
| A8 | H2" | 2.727 | G19 | H2' | 2.507 |
| A8 | H3' | 4.834 | G19 | H2" | 2.534 |
| A8 | H4' | 4.177 | G19 | H3' | 4.793 |
| A8 | H5' | 3.729 | G19 | H4' | 4.186 |
| A8 | H5" | 3.88 | G19 | H5' | 3.751 |
| A8 | H8 | 8.129 | G19 | H5" | 3.843 |
| G9 | H1' | 5.716 | G19 | H8 | 7.749 |
| G9 | H2' | 2.356 | C20 | H1' | 5.741 |
| G9 | H2" | 2.537 | C20 | H2' | 1.862 |
| G9 | H3' | 4.691 | C20 | H2" | 2.274 |
| G9 | H4' | 4.215 | C20 | H3' | 4.559 |
| G9 | H5' | 4.047 | C20 | H4' | 4.04 |
| G9 | H8 | 7.499 | C20 | H5 | 5.144 |
| T10 | CH3 | 1.12 | C20 | H5' | 3.962 |
| T10 | H1' | 5.931 | C20 | H5" | 3.887 |
| T10 | H2' | 2.022 | C20 | H6 | 7.244 |
| T10 | H2" | 2.378 | T21 | CH3 | 1.477 |
| T10 | H3' | 4.697 | T21 | H1' | 5.327 |
| T10 | H4' | 4.099 | T21 | H2' | 1.984 |
| T10 | H6 | 7.157 | T21 | H2" | 2.237 |
| T10 | M7 | 1.134 | T21 | H3' | 4.692 |
| C11 | H1' | 5.905 | T21 | H4' | 3.973 |
| C11 | H2' | 2.053 | T21 | H5' | 3.885 |
| C11 | H2" | 2.333 | T21 | H6 | 7.251 |
| C11 | H3' | 4.683 | T21 | M7 | 1.491 |

**Table A-2:** Continued

| Primary Strand | | | Complementary Strand | | |
|---|---|---|---|---|---|
| Residue | Atom | Chemical Shift (ppm) | Residue | Atom | Chemical Shift (ppm) |
| C11 | H5 | 5.546 | A22 | H1' | 5.901 |
| C11 | H6 | 7.445 | A22 | H2' | 2.61 |
| C12 | H1' | 6.075 | A22 | H2'' | 2.742 |
| C12 | H2' | 2.118 | A22 | H3' | 4.898 |
| C12 | H2'' | 2.135 | A22 | H4' | 4.255 |
| C12 | H3' | 4.413 | A22 | H5' | 3.869 |
| C12 | H4' | 3.879 | A22 | H5'' | 3.985 |
| C12 | H5 | 5.566 | A22 | H8 | 8.072 |
| C12 | H5' | 4.022 | G23 | H1' | 5.629 |
| C12 | H6 | 7.48 | G23 | H2' | 2.318 |
| | | | G23 | H2'' | 2.482 |
| | | | G23 | H3' | 4.798 |
| | | | G23 | H4' | 4.204 |
| | | | G23 | H5' | 4.076 |
| | | | G23 | H8 | 7.538 |
| | | | C24 | H1' | 5.94 |
| | | | C24 | H2' | 1.969 |
| | | | C24 | H2'' | 2.034 |
| | | | C24 | H3' | 4.294 |
| | | | C24 | H4' | 3.883 |
| | | | C24 | H5 | 5.124 |
| | | | C24 | H5' | 4.082 |
| | | | C24 | H5'' | 4.048 |
| | | | C24 | H6 | 7.201 |

**Table A-3:** Resonance assignments for the *R-N3-dU* modified oligonucleotide 5′-$G^{1}C^{2}T^{3}A^{4}G^{5}C^{6}X^{7}A^{8}G^{9}T^{10}C^{11}C^{12}$-3′·5′-$G^{13}G^{14}A^{15}C^{16}T^{17}T^{18}G^{19}C^{20}T^{21}A^{22}G^{23}C^{24}$-3′.

| Primary Strand | | | Complementary Strand | | |
|---|---|---|---|---|---|
| Residue | Atom | Chemical Shift (ppm) | Residue | Atom | Chemical Shift (ppm) |
| G1 | H1' | 5.844 | G13 | H1' | 5.479 |
| G1 | H2' | 2.52 | G13 | H2' | 2.36 |
| G1 | H2" | 2.629 | G13 | H2" | 2.539 |
| G1 | H3' | 4.684 | G13 | H3' | 4.667 |
| G1 | H4' | 4.102 | G13 | H4' | 4.022 |
| G1 | H5' | 3.571 | G13 | H5' | 3.496 |
| G1 | H5" | 3.583 | G13 | H5" | 3.507 |
| G1 | H8 | 7.83 | G13 | H8 | 7.691 |
| C2 | H1' | 5.904 | G14 | H1' | 5.436 |
| C2 | H2' | 1.971 | G14 | H2' | 2.558 |
| C2 | H2" | 2.349 | G14 | H2" | 2.65 |
| C2 | H3' | 4.68 | G14 | H3' | 4.878 |
| C2 | H5 | 5.206 | G14 | H4' | 4.222 |
| C2 | H6 | 7.38 | G14 | H5' | 3.912 |
| T3 | CH3 | 1.511 | G14 | H5" | 3.996 |
| T3 | H1' | 5.345 | G14 | H8 | 7.706 |
| T3 | H2' | 2.025 | A15 | H1' | 6.138 |
| T3 | H2" | 2.261 | A15 | H2 | 7.818 |
| T3 | H3' | 4.717 | A15 | H2' | 2.562 |
| T3 | H4' | 3.989 | A15 | H2" | 2.776 |
| T3 | H6 | 7.284 | A15 | H3' | 4.922 |
| T3 | M7 | 1.514 | A15 | H4' | 4.344 |
| A4 | H1' | 5.925 | A15 | H5' | 4.03 |
| A4 | H2' | 2.613 | A15 | H5" | 4.098 |
| A4 | H2" | 2.753 | A15 | H8 | 8.074 |
| A4 | H3' | 4.916 | C16 | H1' | 5.729 |
| A4 | H4' | 4.271 | C16 | H2' | 1.664 |
| A4 | H5' | 3.884 | C16 | H2" | 2.183 |
| A4 | H5" | 3.994 | C16 | H3' | 4.63 |
| A4 | H8 | 8.076 | C16 | H4' | 3.955 |
| G5 | H1' | 5.531 | C16 | H5 | 5.128 |
| G5 | H2' | 2.262 | C16 | H5' | 4.176 |
| G5 | H2" | 2.417 | C16 | H6 | 7.104 |
| G5 | H3' | 4.814 | T17 | CH3 | 1.425 |
| G5 | H4' | 4.16 | T17 | H1' | 6.007 |
| G5 | H8 | 7.509 | T17 | H2' | 1.975 |
| C6 | H1' | 5.838 | T17 | H2" | 2.155 |
| C6 | H2' | 1.977 | T17 | H3' | 4.726 |
| C6 | H2" | 2.001 | T17 | H4' | 3.914 |
| C6 | H3' | 4.627 | T17 | H6 | 7.145 |
| C6 | H4' | 3.948 | T17 | M7 | 1.453 |
| C6 | H5 | 5.256 | T18 | CH3 | 1.239 |
| C6 | H6 | 7.227 | T18 | H1' | 5.553 |

**Table A-3:** Continued

| Primary Strand | | | Complementary Strand | | |
|---|---|---|---|---|---|
| Residue | Atom | Chemical Shift (ppm) | Residue | Atom | Chemical Shift (ppm) |
| X7 | H1' | 5.568 | T18 | H2' | 1.458 |
| X7 | Hγ | 5.101 | T18 | H2" | 1.715 |
| X7 | Hδ' | 4.479 | T18 | H3' | 4.519 |
| X7 | Hδ | 4.555 | T18 | H4' | 3.9 |
| X7 | Hα' | 3.099 | T18 | H5' | 3.742 |
| X7 | Hα | 3.008 | T18 | H5" | 3.801 |
| X7 | H2' | 0.869 | T18 | H6 | 6.949 |
| X7 | H2" | 1.579 | T18 | M7 | 1.283 |
| X7 | H3' | 4.45 | G19 | H1' | 5.654 |
| X7 | H4' | 3.942 | G19 | H2' | 2.566 |
| X7 | H5 | 5 | G19 | H2" | 2.58 |
| X7 | H5' | 3.789 | G19 | H3' | 4.766 |
| X7 | H5" | 3.906 | G19 | H4' | 4.143 |
| X7 | H6 | 6.953 | G19 | H5' | 3.751 |
| X7 | Hβ | 3.389 | G19 | H5" | 3.843 |
| A8 | H1' | 5.681 | G19 | H8 | 7.843 |
| A8 | H2 | 7.514 | C20 | H1' | 5.786 |
| A8 | H2' | 2.682 | C20 | H2' | 1.897 |
| A8 | H2" | 2.694 | C20 | H2" | 2.291 |
| A8 | H3' | 4.811 | C20 | H3' | 4.558 |
| A8 | H4' | 4.144 | C20 | H4' | 4.046 |
| A8 | H5' | 3.686 | C20 | H5 | 5.219 |
| A8 | H5" | 3.844 | C20 | H5' | 3.877 |
| A8 | H8 | 8.14 | C20 | H5" | 3.96 |
| G9 | H1' | 5.742 | C20 | H6 | 7.304 |
| G9 | H2' | 2.383 | T21 | CH3 | 1.484 |
| G9 | H2" | 2.542 | T21 | H1' | 5.33 |
| G9 | H3' | 4.688 | T21 | H2' | 1.994 |
| G9 | H4' | 4.229 | T21 | H2" | 2.236 |
| G9 | H8 | 7.537 | T21 | H3' | 4.693 |
| T10 | CH3 | 1.121 | T21 | H4' | 3.966 |
| T10 | H1' | 5.96 | T21 | H6 | 7.265 |
| T10 | H2' | 2.034 | T21 | M7 | 1.491 |
| T10 | H2" | 2.388 | A22 | H1' | 5.902 |
| T10 | H3' | 4.713 | A22 | H2' | 2.614 |
| T10 | H4' | 4.105 | A22 | H2" | 2.743 |
| T10 | H6 | 7.182 | A22 | H3' | 4.895 |
| T10 | M7 | 1.134 | A22 | H4' | 4.26 |
| C11 | H1' | 5.907 | A22 | H5' | 3.865 |
| C11 | H2' | 2.06 | A22 | H5" | 3.974 |
| C11 | H2" | 2.333 | A22 | H8 | 8.072 |
| C11 | H3' | 4.681 | G23 | H1' | 5.625 |
| C11 | H5 | 5.555 | G23 | H2' | 2.318 |
| C11 | H6 | 7.451 | G23 | H2" | 2.479 |
| C12 | H1' | 6.074 | G23 | H3' | 4.795 |

**Table A-3:** Continued

| Primary Strand | | | Complementary Strand | | |
|---|---|---|---|---|---|
| Residue | Atom | Chemical Shift (ppm) | Residue | Atom | Chemical Shift (ppm) |
| C12 | H2' | 2.115 | G23 | H4' | 4.201 |
| C12 | H2'' | 2.127 | G23 | H5' | 4.076 |
| C12 | H3' | 4.409 | G23 | H8 | 7.54 |
| C12 | H4' | 3.875 | C24 | H1' | 5.939 |
| C12 | H5 | 5.581 | C24 | H2' | 1.96 |
| C12 | H5' | 4.021 | C24 | H2'' | 2.028 |
| C12 | H6 | 7.483 | C24 | H3' | 4.288 |
| | | | C24 | H4' | 3.88 |
| | | | C24 | H5 | 5.137 |
| | | | C24 | H6 | 7.203 |

**Table A-4:** Resonance assignments for the *S-BD-N3-dU* modified oligonucleotide 5′-$G^{1}C^{2}T^{3}A^{4}G^{5}C^{6}X^{7}A^{8}G^{9}T^{10}C^{11}C^{12}$-3′·5′-$G^{13}G^{14}A^{15}C^{16}T^{17}T^{18}G^{19}C^{20}T^{21}A^{22}G^{23}C^{24}$-3′.

| Primary Strand | | | Complementary Strand | | |
|---|---|---|---|---|---|
| Residue | Atom | Chemical Shift (ppm) | Residue | Atom | Chemical Shift (ppm) |
| G1 | H1' | 5.83 | G13 | H1' | 5.48 |
| G1 | H2' | 2.511 | G13 | H2' | 2.362 |
| G1 | H2" | 2.623 | G13 | H2" | 2.548 |
| G1 | H3' | 4.684 | G13 | H3' | 4.668 |
| G1 | H4' | 4.109 | G13 | H4' | 4.03 |
| G1 | H8 | 7.82 | G13 | H8 | 7.687 |
| C2 | H1' | 5.898 | G14 | H1' | 5.439 |
| C2 | H2' | 1.97 | G14 | H2' | 2.556 |
| C2 | H2" | 2.344 | G14 | H2" | 2.65 |
| C2 | H3' | 4.679 | G14 | H3' | 4.882 |
| C2 | H5 | 5.189 | G14 | H4' | 4.221 |
| C2 | H6 | 7.373 | G14 | H8 | 7.699 |
| T3 | CH3 | 1.511 | A15 | H1' | 6.134 |
| T3 | H1' | 5.343 | A15 | H2 | 7.816 |
| T3 | H2' | 2.018 | A15 | H2' | 2.56 |
| T3 | H2" | 2.26 | A15 | H2" | 2.773 |
| T3 | H3' | 4.717 | A15 | H3' | 4.921 |
| T3 | H4' | 3.984 | A15 | H4' | 4.342 |
| T3 | H6 | 7.278 | A15 | H5' | 4.021 |
| A4 | H1' | 5.919 | A15 | H5" | 4.1 |
| A4 | H2' | 2.6 | A15 | H8 | 8.07 |
| A4 | H2" | 2.742 | C16 | H1' | 5.712 |
| A4 | H3' | 4.913 | C16 | H2' | 1.675 |
| A4 | H4' | 4.264 | C16 | H2" | 2.193 |
| A4 | H5' | 3.894 | C16 | H3' | 4.619 |
| A4 | H8 | 8.071 | C16 | H4' | 3.948 |
| G5 | H1' | 5.51 | C16 | H5 | 5.148 |
| G5 | H2' | 2.253 | C16 | H5' | 4.174 |
| G5 | H2" | 2.403 | C16 | H6 | 7.114 |
| G5 | H3' | 4.811 | T17 | CH3 | 1.425 |
| G5 | H4' | 4.156 | T17 | H1' | 6.005 |
| G5 | H8 | 7.503 | T17 | H2' | 1.978 |
| C6 | H1' | 5.79 | T17 | H2" | 2.112 |
| C6 | H2' | 1.981 | T17 | H3' | 4.705 |
| C6 | H2" | 2 | T17 | H4' | 3.918 |
| C6 | H3' | 4.604 | T17 | H6 | 7.121 |
| C6 | H4' | 3.967 | T18 | CH3 | 1.239 |
| C6 | H5 | 5.233 | T18 | H1' | 5.596 |
| C6 | H6 | 7.244 | T18 | H2' | 1.405 |
| X7 | H1' | 5.607 | T18 | H2" | 1.679 |
| X7 | Hγ | 5.194 | T18 | H3' | 4.514 |
| X7 | Hα' | 3.192 | T18 | H4' | 3.934 |
| X7 | Hα | 2.852 | T18 | H5' | 3.742 |

**Table A-4:** Continued

| Primary Strand | | | Complementary Strand | | |
|---|---|---|---|---|---|
| Residue | Atom | Chemical Shift (ppm) | Residue | Atom | Chemical Shift (ppm) |
| X7 | H2' | 0.53 | T18 | H5'' | 3.801 |
| X7 | H2'' | 1.389 | T18 | H6 | 6.936 |
| X7 | H3' | 4.402 | G19 | H1' | 5.68 |
| X7 | H4' | 3.917 | G19 | H2' | 2.58 |
| X7 | H5 | 4.884 | G19 | H2'' | 2.6 |
| X7 | H5' | 3.789 | G19 | H3' | 4.769 |
| X7 | H5'' | 3.906 | G19 | H4' | 4.153 |
| X7 | H6 | 6.829 | G19 | H5' | 3.745 |
| X7 | Hβ | 3.559 | G19 | H5'' | 3.846 |
| A8 | H1' | 5.762 | G19 | H8 | 7.838 |
| A8 | H2 | 7.512 | C20 | H1' | 5.763 |
| A8 | H2' | 2.723 | C20 | H2' | 1.886 |
| A8 | H2'' | 2.746 | C20 | H2'' | 2.287 |
| A8 | H3' | 4.813 | C20 | H3' | 4.543 |
| A8 | H4' | 4.151 | C20 | H4' | 4.046 |
| A8 | H5' | 3.817 | C20 | H5 | 5.199 |
| A8 | H5'' | 3.649 | C20 | H5' | 3.877 |
| A8 | H8 | 8.118 | C20 | H5'' | 3.96 |
| G9 | H1' | 5.698 | C20 | H6 | 7.288 |
| G9 | H2' | 2.353 | T21 | CH3 | 1.484 |
| G9 | H2'' | 2.522 | T21 | H1' | 5.323 |
| G9 | H3' | 4.688 | T21 | H2' | 1.993 |
| G9 | H4' | 4.204 | T21 | H2'' | 2.241 |
| G9 | H8 | 7.508 | T21 | H3' | 4.693 |
| T10 | CH3 | 1.121 | T21 | H4' | 3.969 |
| T10 | H1' | 5.958 | T21 | H6 | 7.269 |
| T10 | H2' | 2.029 | A22 | H1' | 5.903 |
| T10 | H2'' | 2.385 | A22 | H2' | 2.611 |
| T10 | H3' | 4.705 | A22 | H2'' | 2.747 |
| T10 | H6 | 7.171 | A22 | H3' | 4.895 |
| C11 | H1' | 5.901 | A22 | H4' | 4.261 |
| C11 | H2' | 2.045 | A22 | H5' | 3.864 |
| C11 | H2'' | 2.329 | A22 | H8 | 8.071 |
| C11 | H3' | 4.681 | G23 | H1' | 5.619 |
| C11 | H5 | 5.541 | G23 | H2' | 2.307 |
| C11 | H6 | 7.442 | G23 | H2'' | 2.474 |
| C12 | H1' | 6.058 | G23 | H3' | 4.795 |
| C12 | H2' | 2.119 | G23 | H4' | 4.199 |
| C12 | H2'' | 2.14 | G23 | H5' | 4.076 |
| C12 | H3' | 4.409 | G23 | H8 | 7.529 |
| C12 | H4' | 3.864 | C24 | H1' | 5.917 |
| C12 | H5 | 5.506 | C24 | H2' | 1.97 |
| C12 | H5' | 4.021 | C24 | H2'' | 2.032 |
| C12 | H6 | 7.452 | C24 | H3' | 4.283 |
| | | | C24 | H4' | 3.87 |

**Table A-4:** Continued

| Primary Strand | | | Complementary Strand | | |
|---|---|---|---|---|---|
| Residue | Atom | Chemical Shift (ppm) | Residue | Atom | Chemical Shift (ppm) |
| | | | C24 | H5 | 5.057 |
| | | | C24 | H6 | 7.165 |

**Table A-5:** Resonance assignments for the *R-BD-N3-dU* modified oligonucleotide 5′-$G^{1}C^{2}T^{3}A^{4}G^{5}C^{6}X^{7}A^{8}G^{9}T^{10}C^{11}C^{12}$-3′·5′-$G^{13}G^{14}A^{15}C^{16}T^{17}G^{18}G^{19}C^{20}T^{21}A^{22}G^{23}C^{24}$-3′.

| Primary Strand | | | Complementary Strand | | |
|---|---|---|---|---|---|
| Residue | Atom | Chemical Shift (ppm) | Residue | Atom | Chemical Shift (ppm) |
| G1 | H1' | 5.865 | G13 | H1' | 5.498 |
| G1 | H2' | 2.528 | G13 | H2' | 2.358 |
| G1 | H2" | 2.635 | G13 | H2" | 2.525 |
| G1 | H3' | 4.692 | G13 | H3' | 4.667 |
| G1 | H4' | 4.106 | G13 | H4' | 4.016 |
| G1 | H5' | 3.584 | G13 | H5' | 3.505 |
| G1 | H5" | 3.583 | G13 | H5" | 3.507 |
| G1 | H8 | 7.839 | G13 | H8 | 7.69 |
| C2 | H1' | 5.914 | G14 | H1' | 5.449 |
| C2 | H2' | 1.982 | G14 | H2' | 2.572 |
| C2 | H2" | 2.359 | G14 | H2" | 2.657 |
| C2 | H3' | 4.682 | G14 | H3' | 4.881 |
| C2 | H4' | 4.1 | G14 | H4' | 4.23 |
| C2 | H5 | 5.228 | G14 | H5' | 3.915 |
| C2 | H5' | 4.098 | G14 | H5" | 4.021 |
| C2 | H6 | 7.392 | G14 | H8 | 7.718 |
| T3 | CH3 | 1.515 | A15 | H1' | 6.139 |
| T3 | H1' | 5.368 | A15 | H2 | 7.795 |
| T3 | H2' | 2.018 | A15 | H2' | 2.57 |
| T3 | H2" | 2.268 | A15 | H2" | 2.779 |
| T3 | H3' | 4.724 | A15 | H3' | 4.92 |
| T3 | H4' | 3.992 | A15 | H4' | 4.349 |
| T3 | H5' | 3.91 | A15 | H5' | 4.102 |
| T3 | H6 | 7.281 | A15 | H5" | 4.098 |
| T3 | M7 | 1.514 | A15 | H8 | 8.078 |
| A4 | H1' | 5.914 | C16 | H1' | 5.699 |
| A4 | H2' | 2.607 | C16 | H2' | 1.663 |
| A4 | H2" | 2.751 | C16 | H2" | 2.189 |
| A4 | H3' | 4.909 | C16 | H3' | 4.604 |
| A4 | H4' | 4.271 | C16 | H4' | 4.178 |
| A4 | H5' | 3.907 | C16 | H5 | 5.105 |
| A4 | H5" | 4.001 | C16 | H5' | 4.02 |
| A4 | H8 | 8.069 | C16 | H5" | 4.187 |
| G5 | H1' | 5.537 | C16 | H6 | 7.11 |
| G5 | H2' | 2.289 | T17 | CH3 | 1.478 |
| G5 | H2" | 2.436 | T17 | H1' | 5.866 |
| G5 | H3' | 4.809 | T17 | H2' | 1.673 |
| G5 | H4' | 4.178 | T17 | H2" | 1.847 |
| G5 | H8 | 7.504 | T17 | H3' | 4.613 |
| C6 | H1' | 5.846 | T17 | H4' | 3.919 |
| C6 | H2' | 1.993 | T17 | H5' | 3.959 |
| C6 | H2" | 2.101 | T17 | H6 | 7.024 |
| C6 | H3' | 4.624 | T17 | M7 | 1.453 |

**Table A-5:** Continued

| Primary Strand | | | Complementary Strand | | |
|---|---|---|---|---|---|
| Residue | Atom | Chemical Shift (ppm) | Residue | Atom | Chemical Shift (ppm) |
| C6 | H4' | 3.962 | A18 | H1' | 5.518 |
| C6 | H5 | 5.23 | A18 | H2 | 7.507 |
| C6 | H6 | 7.204 | A18 | H2' | 2.214 |
| X7 | H1' | 5.628 | A18 | H2" | 2.314 |
| X7 | Hγ | 5.127 | A18 | H3' | 4.769 |
| X7 | Hδ' | 4.465 | A18 | H4' | 4.045 |
| X7 | Hδ | 4.351 | A18 | H5' | 3.731 |
| X7 | Hα' | 3.13 | A18 | H5" | 3.851 |
| X7 | Hα | 3.002 | A18 | H8 | 7.899 |
| X7 | H2' | 1.035 | G18 | H1' | 5.044 |
| X7 | H2" | 1.752 | G18 | H2' | 2.138 |
| X7 | H3' | 4.423 | G18 | H2" | 2.28 |
| X7 | H4' | 3.951 | G18 | H3' | 4.683 |
| X7 | H5 | 5.172 | G18 | H4' | 3.934 |
| X7 | H5' | 3.764 | G18 | H5' | 3.819 |
| X7 | H5" | 3.906 | G18 | H8 | 7.601 |
| X7 | H6 | 7.037 | T18 | CH3 | 1.239 |
| X7 | Hβ | 3.408 | T18 | H1' | 5.553 |
| A8 | H1' | 5.715 | T18 | H2' | 1.458 |
| A8 | H2 | 7.511 | T18 | H2" | 1.715 |
| A8 | H2' | 2.675 | T18 | H3' | 4.519 |
| A8 | H2" | 2.699 | T18 | H4' | 3.9 |
| A8 | H3' | 4.826 | T18 | H5' | 3.742 |
| A8 | H4' | 4.163 | T18 | H5" | 3.801 |
| A8 | H5' | 3.729 | T18 | H6 | 6.949 |
| A8 | H5" | 3.88 | T18 | M7 | 1.283 |
| A8 | H8 | 8.164 | G19 | H1' | 5.736 |
| G9 | H1' | 5.76 | G19 | H2' | 2.565 |
| G9 | H2' | 2.377 | G19 | H2" | 2.597 |
| G9 | H2" | 2.554 | G19 | H3' | 4.821 |
| G9 | H3' | 4.689 | G19 | H4' | 4.193 |
| G9 | H4' | 4.24 | G19 | H5' | 3.751 |
| G9 | H5' | 4.047 | G19 | H5" | 3.843 |
| G9 | H8 | 7.53 | G19 | H8 | 7.784 |
| T10 | CH3 | 1.136 | C20 | H1' | 5.796 |
| T10 | H1' | 5.954 | C20 | H2' | 1.911 |
| T10 | H2' | 2.039 | C20 | H2" | 2.299 |
| T10 | H2" | 2.391 | C20 | H3' | 4.596 |
| T10 | H3' | 4.715 | C20 | H4' | 4.058 |
| T10 | H4' | 4.099 | C20 | H5 | 5.184 |
| T10 | H6 | 7.186 | C20 | H5' | 3.962 |
| T10 | M7 | 1.134 | C20 | H5" | 3.887 |
| C11 | H1' | 5.924 | C20 | H6 | 7.297 |
| C11 | H2' | 2.079 | T21 | CH3 | 1.496 |
| C11 | H2" | 2.345 | T21 | H1' | 5.353 |

**Table A-5:** Continued

| Primary Strand | | | Complementary Strand | | |
|---|---|---|---|---|---|
| Residue | Atom | Chemical Shift (ppm) | Residue | Atom | Chemical Shift (ppm) |
| C11 | H3' | 4.688 | T21 | H2' | 1.993 |
| C11 | H5 | 5.566 | T21 | H2" | 2.245 |
| C11 | H6 | 7.466 | T21 | H3' | 4.594 |
| C12 | H1' | 6.093 | T21 | H4' | 3.975 |
| C12 | H2' | 2.115 | T21 | H5' | 3.885 |
| C12 | H2" | 2.13 | T21 | H6 | 7.267 |
| C12 | H3' | 4.416 | T21 | M7 | 1.491 |
| C12 | H4' | 4.018 | A22 | H1' | 5.909 |
| C12 | H5 | 5.645 | A22 | H2' | 2.614 |
| C12 | H5' | 3.892 | A22 | H2" | 2.739 |
| C12 | H6 | 7.527 | A22 | H3' | 4.901 |
| | | | A22 | H4' | 4.264 |
| | | | A22 | H5' | 3.882 |
| | | | A22 | H5" | 3.985 |
| | | | A22 | H8 | 8.079 |
| | | | G23 | H1' | 5.643 |
| | | | G23 | H2' | 2.33 |
| | | | G23 | H2" | 2.49 |
| | | | G23 | H3' | 4.797 |
| | | | G23 | H4' | 4.205 |
| | | | G23 | H5' | 4.076 |
| | | | G23 | H8 | 7.549 |
| | | | C24 | H1' | 5.965 |
| | | | C24 | H2' | 1.965 |
| | | | C24 | H2" | 2.029 |
| | | | C24 | H3' | 4.301 |
| | | | C24 | H4' | 4.078 |
| | | | C24 | H5 | 5.209 |
| | | | C24 | H5' | 3.891 |
| | | | C24 | H5" | 4.048 |
| | | | C24 | H6 | 7.249 |

**Table A-6:** Resonance assignments for the *S-BD-N3-dU* modified oligonucleotide 5′-$G^{1}C^{2}T^{3}A^{4}G^{5}C^{6}X^{7}A^{8}G^{9}T^{10}C^{11}C^{12}$-3′·5′-$G^{13}G^{14}A^{15}C^{16}T^{17}G^{18}G^{19}C^{20}T^{21}A^{22}G^{23}C^{24}$-3′.

| Primary Strand | | | Complementary Strand | | |
|---|---|---|---|---|---|
| Residue | Atom | Chemical Shift (ppm) | Residue | Atom | Chemical Shift (ppm) |
| G1 | H1' | 5.857 | G13 | H1' | 5.493 |
| G1 | H2' | 2.525 | G13 | H2' | 2.362 |
| G1 | H2" | 2.635 | G13 | H2" | 2.536 |
| G1 | H3' | 4.691 | G13 | H3' | 4.67 |
| G1 | H4' | 4.106 | G13 | H4' | 4.022 |
| G1 | H5' | 3.583 | G13 | H5' | 3.507 |
| G1 | H5" | 3.583 | G13 | H5" | 3.507 |
| G1 | H8 | 7.837 | G13 | H8 | 7.693 |
| C2 | H1' | 5.911 | G14 | H1' | 5.452 |
| C2 | H2' | 1.976 | G14 | H2' | 2.566 |
| C2 | H2" | 2.355 | G14 | H2" | 2.655 |
| C2 | H3' | 4.679 | G14 | H3' | 4.881 |
| C2 | H4' | 4.1 | G14 | H4' | 4.23 |
| C2 | H5 | 5.218 | G14 | H5' | 3.915 |
| C2 | H5' | 4.098 | G14 | H5" | 4.021 |
| C2 | H6 | 7.387 | G14 | H8 | 7.714 |
| T3 | CH3 | 1.511 | A15 | H1' | 6.135 |
| T3 | H1' | 5.361 | A15 | H2 | 7.795 |
| T3 | H2' | 2.014 | A15 | H2' | 2.566 |
| T3 | H2" | 2.261 | A15 | H2" | 2.776 |
| T3 | H3' | 4.717 | A15 | H3' | 4.918 |
| T3 | H4' | 3.99 | A15 | H4' | 4.348 |
| T3 | H5' | 3.91 | A15 | H5' | 4.102 |
| T3 | H6 | 7.275 | A15 | H5" | 4.098 |
| T3 | M7 | 1.514 | A15 | H8 | 8.074 |
| A4 | H1' | 5.908 | C16 | H1' | 5.691 |
| A4 | H2' | 2.596 | C16 | H2' | 1.683 |
| A4 | H2" | 2.737 | C16 | H2" | 2.19 |
| A4 | H3' | 4.91 | C16 | H3' | 4.599 |
| A4 | H4' | 4.263 | C16 | H4' | 4.178 |
| A4 | H5' | 3.907 | C16 | H5 | 5.109 |
| A4 | H5" | 4.001 | C16 | H5' | 4.173 |
| A4 | H8 | 8.063 | C16 | H5" | 4.187 |
| G5 | H1' | 5.52 | C16 | H6 | 7.119 |
| G5 | H2' | 2.291 | T17 | CH3 | 1.465 |
| G5 | H2" | 2.429 | T17 | H1' | 5.863 |
| G5 | H3' | 4.805 | T17 | H2' | 1.678 |
| G5 | H4' | 4.178 | T17 | H2" | 1.89 |
| G5 | H8 | 7.505 | T17 | H3' | 4.608 |
| C6 | H1' | 5.824 | T17 | H4' | 3.928 |
| C6 | H2' | 1.986 | T17 | H5' | 3.847 |
| C6 | H2" | 2.12 | T17 | H6 | 7.017 |
| C6 | H3' | 4.601 | T17 | M7 | 1.453 |

**Table A-6:** Continued

| Primary Strand | | | Complementary Strand | | |
|---|---|---|---|---|---|
| Residue | Atom | Chemical Shift (ppm) | Residue | Atom | Chemical Shift (ppm) |
| C6 | H4' | 3.984 | A18 | H1' | 5.518 |
| C6 | H5 | 5.206 | A18 | H2 | 7.507 |
| C6 | H6 | 7.202 | A18 | H2' | 2.214 |
| X7 | H1' | 5.658 | A18 | H2" | 2.314 |
| X7 | Hγ | 5.247 | A18 | H3' | 4.769 |
| X7 | Hδ' | 4.465 | A18 | H4' | 4.045 |
| X7 | Hδ | 4.351 | A18 | H5' | 3.731 |
| X7 | Hα' | 3.25 | A18 | H5" | 3.851 |
| X7 | Hα | 2.918 | A18 | H8 | 7.899 |
| X7 | H2' | 0.919 | G18 | H1' | 5.028 |
| X7 | H2" | 1.656 | G18 | H2' | 2.142 |
| X7 | H3' | 4.412 | G18 | H2" | 2.244 |
| X7 | H4' | 3.915 | G18 | H3' | 4.685 |
| X7 | H5 | 5.142 | G18 | H4' | 3.939 |
| X7 | H5' | 3.843 | G18 | H5' | 3.825 |
| X7 | H5" | 3.769 | G18 | H5" | 3.714 |
| X7 | H6 | 6.987 | G18 | H8 | 7.603 |
| X7 | Hβ | 3.59 | T18 | CH3 | 1.239 |
| A8 | H1' | 5.773 | T18 | H1' | 5.553 |
| A8 | H2 | 7.524 | T18 | H2' | 1.458 |
| A8 | H2' | 2.699 | T18 | H2" | 1.715 |
| A8 | H2" | 2.725 | T18 | H3' | 4.519 |
| A8 | H3' | 4.827 | T18 | H4' | 3.9 |
| A8 | H4' | 4.173 | T18 | H5' | 3.742 |
| A8 | H5' | 3.729 | T18 | H5" | 3.801 |
| A8 | H5" | 3.88 | T18 | H6 | 6.949 |
| A8 | H8 | 8.133 | T18 | M7 | 1.283 |
| G9 | H1' | 5.722 | G19 | H1' | 5.75 |
| G9 | H2' | 2.365 | G19 | H2' | 2.578 |
| G9 | H2" | 2.543 | G19 | H2" | 2.599 |
| G9 | H3' | 4.689 | G19 | H3' | 4.828 |
| G9 | H4' | 4.221 | G19 | H4' | 4.202 |
| G9 | H5' | 4.047 | G19 | H5' | 3.751 |
| G9 | H8 | 7.515 | G19 | H5" | 3.843 |
| T10 | CH3 | 1.13 | G19 | H8 | 7.772 |
| T10 | H1' | 5.946 | C20 | H1' | 5.787 |
| T10 | H2' | 2.032 | C20 | H2' | 1.898 |
| T10 | H2" | 2.383 | C20 | H2" | 2.293 |
| T10 | H3' | 4.708 | C20 | H3' | 4.592 |
| T10 | H4' | 4.099 | C20 | H4' | 4.179 |
| T10 | H6 | 7.169 | C20 | H5 | 5.164 |
| T10 | M7 | 1.134 | C20 | H5' | 3.962 |
| C11 | H1' | 5.917 | C20 | H5" | 3.887 |
| C11 | H2' | 2.07 | C20 | H6 | 7.278 |
| C11 | H2" | 2.345 | T21 | CH3 | 1.49 |

**Table A-6:** Continued

| Primary Strand | | | Complementary Strand | | |
|---|---|---|---|---|---|
| Residue | Atom | Chemical Shift (ppm) | Residue | Atom | Chemical Shift (ppm) |
| C11 | H3' | 4.686 | T21 | H1' | 5.345 |
| C11 | H5 | 5.559 | T21 | H2' | 1.995 |
| C11 | H6 | 7.46 | T21 | H2'' | 2.241 |
| C12 | H1' | 6.087 | T21 | H3' | 4.591 |
| C12 | H2' | 2.114 | T21 | H4' | 3.973 |
| C12 | H2'' | 2.131 | T21 | H5' | 3.885 |
| C12 | H3' | 4.416 | T21 | H6 | 7.261 |
| C12 | H4' | 4.018 | T21 | M7 | 1.491 |
| C12 | H5 | 5.621 | A22 | H1' | 5.907 |
| C12 | H5' | 3.888 | A22 | H2' | 2.613 |
| C12 | H6 | 7.511 | A22 | H2'' | 2.75 |
| | | | A22 | H3' | 4.899 |
| | | | A22 | H4' | 4.264 |
| | | | A22 | H5' | 3.884 |
| | | | A22 | H5'' | 3.985 |
| | | | A22 | H8 | 8.074 |
| | | | G23 | H1' | 5.637 |
| | | | G23 | H2' | 2.325 |
| | | | G23 | H2'' | 2.489 |
| | | | G23 | H3' | 4.797 |
| | | | G23 | H4' | 4.203 |
| | | | G23 | H5' | 4.076 |
| | | | G23 | H8 | 7.546 |
| | | | C24 | H1' | 5.955 |
| | | | C24 | H2' | 1.964 |
| | | | C24 | H2'' | 2.03 |
| | | | C24 | H3' | 4.299 |
| | | | C24 | H4' | 4.08 |
| | | | C24 | H5 | 5.182 |
| | | | C24 | H5' | 3.886 |
| | | | C24 | H5'' | 4.048 |
| | | | C24 | H6 | 7.232 |

APPENDIX B

EXPERIMENTAL DISTANCE RESTRAINT FILES

**Table B-1:** Distance restraints used for the *R-N3-dU* modified sequence, 5′-$G^{1}C^{2}T^{3}A^{4}G^{5}C^{6}X^{7}A^{8}G^{9}T^{10}C^{11}C^{12}$-3′·5′-$G^{13}G^{14}A^{15}C^{16}T^{17}A^{18}G^{19}C^{20}T^{21}A^{22}G^{23}C^{24}$-3′.

| | Residue Number | Residue Name | Atom Name | Residue Number | Residue Name | Atom Name | Lower Bound | Upper Bound |
|---|---|---|---|---|---|---|---|---|
| Class 1 | 2 | CYT | H6 | 1 | GUA | H2'1 | 3.32 | 4.32 |
| | 2 | CYT | H6 | 1 | GUA | H2'2 | 1.80 | 3.10 |
| | 2 | CYT | H5 | 1 | GUA | H8 | 3.23 | 4.76 |
| | 2 | CYT | H5 | 2 | CYT | H6 | 1.72 | 2.49 |
| | 2 | CYT | H3' | 2 | CYT | H6 | 3.53 | 4.48 |
| | 2 | CYT | H2'2 | 2 | CYT | H2'1 | 1.53 | 2.40 |
| | 3 | THY | M7 | 2 | CYT | H6 | 3.20 | 4.16 |
| | 3 | THY | M7 | 2 | CYT | H5 | 3.91 | 4.94 |
| | 3 | THY | H2'2 | 3 | THY | H2'1 | 1.65 | 2.25 |
| | 6 | CYT | H6 | 5 | GUA | H1' | 1.87 | 3.16 |
| | 6 | CYT | H6 | 6 | CYT | H1' | 3.05 | 4.20 |
| | 6 | CYT | H5 | 5 | GUA | H8 | 3.47 | 4.31 |
| | 7 | UBX | H6 | 7 | UBX | H1' | 2.96 | 4.21 |
| | 7 | UBX | H5 | 7 | UBX | H6 | 1.69 | 2.52 |
| | 7 | UBX | H2'2 | 7 | UBX | H2'1 | 1.61 | 2.35 |
| | 7 | UBX | H9 | 7 | UBX | H15 | 1.86 | 2.56 |
| | 7 | UBX | H9 | 7 | UBX | H14 | 1.79 | 2.81 |
| | 9 | GUA | H8 | 8 | ADE | H1' | 3.26 | 4.56 |
| | 9 | GUA | H8 | 9 | GUA | H1' | 3.14 | 4.22 |
| | 10 | THY | H2'2 | 10 | THY | H2'1 | 1.70 | 2.26 |
| | 11 | CYT | H2'2 | 11 | CYT | H2'1 | 1.57 | 2.23 |
| | 12 | CYT | H6 | 12 | CYT | H1' | 3.03 | 4.46 |
| | 14 | GUA | H3' | 14 | GUA | H8 | 3.82 | 5.13 |
| | 16 | CYT | H5 | 16 | CYT | H6 | 1.77 | 2.72 |
| | 16 | CYT | H2'1 | 16 | CYT | H1' | 2.45 | 3.12 |
| | 16 | CYT | H2'2 | 16 | CYT | H2'1 | 1.75 | 2.44 |
| | 20 | CYT | H2'2 | 20 | CYT | H2'1 | 1.58 | 2.34 |
| | 21 | THY | H2'2 | 21 | THY | H2'1 | 1.57 | 1.99 |
| | 23 | GUA | H1' | 23 | GUA | H4' | 2.95 | 4.28 |
| | 23 | GUA | H2'1 | 23 | GUA | H1' | 2.52 | 4.10 |
| | 24 | CYT | H3' | 24 | CYT | H6 | 3.44 | 4.35 |
| | 1 | GUA | H2'2 | 1 | GUA | H2'1 | 1.62 | 2.05 |
| | 5 | GUA | H2'2 | 5 | GUA | H2'1 | 1.79 | 2.99 |
| | 9 | GUA | H2'1 | 9 | GUA | H4' | 3.32 | 4.39 |
| | 14 | GUA | H2'2 | 14 | GUA | H2'1 | 1.57 | 2.16 |
| | 15 | ADE | H2'2 | 15 | ADE | H2'1 | 1.87 | 2.29 |
| | 17 | THY | H2'2 | 17 | THY | H2'1 | 1.77 | 2.39 |

**Table B-1:** Continued

| | Residue Number | Residue Name | Atom Name | Residue Number | Residue Name | Atom Name | Lower Bound | Upper Bound |
|---|---|---|---|---|---|---|---|---|
| | 20 | CYT | H3' | 20 | CYT | H1' | 3.31 | 4.51 |
| | 22 | ADE | H2'2 | 22 | ADE | H2'1 | 1.53 | 1.88 |
| | 23 | GUA | H2'2 | 23 | GUA | H2'1 | 1.61 | 2.27 |
| Class 2 | 1 | GUA | H8 | 1 | GUA | H1' | 3.64 | 4.3 |
| | 1 | GUA | H2'1 | 1 | GUA | H1' | 2.77 | 3.39 |
| | 1 | GUA | H2'2 | 1 | GUA | H1' | 1.8 | 2.72 |
| | 1 | GUA | H2'2 | 1 | GUA | H8 | 3.48 | 4.29 |
| | 2 | CYT | H5 | 1 | GUA | H2'1 | 2.65 | 3.64 |
| | 2 | CYT | H5 | 1 | GUA | H2'2 | 2.27 | 3.24 |
| | 2 | CYT | H2'2 | 2 | CYT | H6 | 2.88 | 3.71 |
| | 3 | THY | H6 | 2 | CYT | H1' | 2.08 | 3.47 |
| | 3 | THY | H6 | 3 | THY | H1' | 2.77 | 4.13 |
| | 5 | GUA | H1' | 5 | GUA | H4' | 2.75 | 3.96 |
| | 5 | GUA | H3' | 5 | GUA | H8 | 4.04 | 4.7 |
| | 6 | CYT | H5 | 5 | GUA | H2'1 | 2.36 | 3.6 |
| | 6 | CYT | H5 | 5 | GUA | H2'2 | 2.31 | 3.73 |
| | 7 | UBX | H1' | 7 | UBX | H4' | 3.04 | 4.1 |
| | 7 | UBX | H3' | 7 | UBX | H4' | 2.1 | 2.82 |
| | 7 | UBX | H2'1 | 7 | UBX | H1' | 2.35 | 3.84 |
| | 8 | ADE | H1' | 8 | ADE | H4' | 2.64 | 3.82 |
| | 8 | ADE | H8 | 8 | ADE | H1' | 3.47 | 4.47 |
| | 8 | ADE | H3' | 8 | ADE | H5'1 | 3.54 | 4.49 |
| | 9 | GUA | H1' | 9 | GUA | H4' | 3.18 | 4.19 |
| | 9 | GUA | H3' | 9 | GUA | H8 | 4.18 | 4.86 |
| | 9 | GUA | H2'1 | 9 | GUA | H1' | 2.43 | 3.36 |
| | 9 | GUA | H2'2 | 9 | GUA | H1' | 1.69 | 2.63 |
| | 10 | THY | H6 | 9 | GUA | H1' | 2.01 | 3.35 |
| | 10 | THY | H6 | 9 | GUA | H2'2 | 1.8 | 2.51 |
| | 10 | THY | H6 | 10 | THY | H1' | 2.95 | 3.75 |
| | 10 | THY | M7 | 9 | GUA | H8 | 2.89 | 4.17 |
| | 12 | CYT | H1' | 12 | CYT | H4' | 2.82 | 3.87 |
| | 12 | CYT | H5 | 12 | CYT | H6 | 1.71 | 2.48 |
| | 12 | CYT | H3' | 12 | CYT | H4' | 2.19 | 2.85 |
| | 12 | CYT | H3' | 12 | CYT | H6 | 3.48 | 4.43 |
| | 13 | GUA | H3' | 13 | GUA | H8 | 3.83 | 4.88 |
| | 14 | GUA | H1' | 14 | GUA | H4' | 2.71 | 3.95 |
| | 14 | GUA | H2'2 | 14 | GUA | H1' | 1.8 | 2.56 |
| | 15 | ADE | H1' | 15 | ADE | H4' | 3.04 | 3.9 |
| | 15 | ADE | H8 | 14 | GUA | H1' | 2.18 | 3.37 |
| | 15 | ADE | H8 | 15 | ADE | H1' | 3.43 | 4.35 |
| | 15 | ADE | H2'1 | 15 | ADE | H1' | 2.78 | 3.68 |
| | 15 | ADE | H2'2 | 15 | ADE | H1' | 1.99 | 2.58 |
| | 16 | CYT | H6 | 15 | ADE | H1' | 2.07 | 3.05 |
| | 16 | CYT | H5 | 15 | ADE | H8 | 3.06 | 4.4 |
| | 16 | CYT | H2'2 | 16 | CYT | H1' | 2 | 2.58 |
| | 17 | THY | H6 | 17 | THY | H1' | 3.03 | 4.02 |

**Table B-1:** Continued

| | Residue Number | Residue Name | Atom Name | Residue Number | Residue Name | Atom Name | Lower Bound | Upper Bound |
|---|---|---|---|---|---|---|---|---|
| | 17 | THY | M7 | 16 | CYT | H5 | 3.43 | 4.45 |
| | 17 | THY | H3' | 17 | THY | H6 | 3.79 | 4.59 |
| | 18 | ADE | H8 | 18 | ADE | H1' | 3.53 | 4.7 |
| | 18 | ADE | H3' | 18 | ADE | H8 | 3.8 | 4.95 |
| | 19 | GUA | H1' | 19 | GUA | H4' | 3.2 | 3.89 |
| | 19 | GUA | H3' | 19 | GUA | H8 | 3.72 | 4.78 |
| | 20 | CYT | H6 | 19 | GUA | H1' | 2.1 | 3.21 |
| | 20 | CYT | H2'1 | 20 | CYT | H3' | 2.1 | 3.02 |
| | 20 | CYT | H2'2 | 20 | CYT | H1' | 1.91 | 2.45 |
| | 20 | CYT | H2'2 | 20 | CYT | H3' | 2.19 | 3.25 |
| | 21 | THY | M7 | 20 | CYT | H5 | 3.39 | 4.86 |
| | 21 | THY | M7 | 20 | CYT | H3' | 3.82 | 4.48 |
| | 21 | THY | M7 | 20 | CYT | H2'2 | 2.74 | 4.14 |
| | 23 | GUA | H8 | 22 | ADE | H1' | 2.01 | 3.44 |
| | 23 | GUA | H8 | 23 | GUA | H1' | 3.2 | 4.36 |
| | 23 | GUA | H2'2 | 23 | GUA | H1' | 1.99 | 2.46 |
| | 24 | CYT | H6 | 23 | GUA | H1' | 2.4 | 3.58 |
| | 24 | CYT | H6 | 24 | CYT | H1' | 3.4 | 4.5 |
| | 24 | CYT | H5 | 23 | GUA | H8 | 3.2 | 4.61 |
| | 6 | CYT | H2'1 | 6 | CYT | H5 | 3.83 | 4.69 |
| | 7 | UBX | H3' | 7 | UBX | H1' | 3.04 | 4.05 |
| | 7 | UBX | H2'1 | 7 | UBX | H5 | 3.48 | 4.75 |
| | 8 | ADE | H3' | 8 | ADE | H1' | 2.95 | 4.19 |
| | 8 | ADE | H2'2 | 8 | ADE | H4' | 3.15 | 4.51 |
| | 14 | GUA | H2'2 | 14 | GUA | H4' | 3.53 | 4.42 |
| | 15 | ADE | H3' | 15 | ADE | H1' | 3.4 | 4.46 |
| | 15 | ADE | H2'1 | 15 | ADE | H4' | 3.19 | 4.37 |
| | 15 | ADE | H2'2 | 15 | ADE | H4' | 3.55 | 4.56 |
| | 16 | CYT | H5 | 15 | ADE | H2'1 | 2.71 | 3.75 |
| | 16 | CYT | H5 | 15 | ADE | H2'2 | 2.57 | 3.29 |
| | 16 | CYT | H3' | 16 | CYT | H1' | 3.38 | 4.43 |
| | 16 | CYT | H2'1 | 16 | CYT | H5 | 3.53 | 4.75 |
| | 18 | ADE | H3' | 18 | ADE | H5'1 | 3.52 | 4.21 |
| | 20 | CYT | H2'1 | 20 | CYT | H5 | 3.88 | 4.86 |
| | 23 | GUA | H2'1 | 23 | GUA | H4' | 3.24 | 4.5 |
| | 23 | GUA | H2'2 | 23 | GUA | H4' | 3.72 | 4.59 |
| | 8 | ADE | H8 | 7 | UBX | H1' | 4.84 | 5.58 |
| | 13 | GUA | H3' | 13 | GUA | H1' | 3.21 | 4.27 |
| | 17 | THY | M7 | 17 | THY | H1' | 5.56 | 6.47 |
| | 20 | CYT | H2'1 | 20 | CYT | H4' | 3.12 | 4.3 |
| Class 3 | 1 | GUA | H2'1 | 1 | GUA | H8 | 1.69 | 2.56 |
| | 2 | CYT | H6 | 1 | GUA | H1' | 2.69 | 3.18 |
| | 2 | CYT | H6 | 2 | CYT | H1' | 3.36 | 4.48 |
| | 3 | THY | H3' | 3 | THY | H6 | 3.47 | 4.58 |
| | 3 | THY | H2'1 | 3 | THY | H1' | 2.35 | 3.52 |
| | 3 | THY | H2'2 | 3 | THY | H1' | 1.88 | 2.61 |

**Table B-1:** Continued

| Residue Number | Residue Name | Atom Name | Residue Number | Residue Name | Atom Name | Lower Bound | Upper Bound |
|---|---|---|---|---|---|---|---|
| 5 | GUA | H8 | 4 | ADE | H1' | 2.48 | 3.18 |
| 5 | GUA | H2'1 | 5 | GUA | H3' | 1.92 | 3.13 |
| 6 | CYT | H6 | 5 | GUA | H2'2 | 1.8 | 2.54 |
| 6 | CYT | H5 | 6 | CYT | H6 | 1.73 | 2.43 |
| 6 | CYT | H3' | 6 | CYT | H6 | 3.49 | 4.56 |
| 7 | UBX | H3' | 7 | UBX | H6 | 3.08 | 4.4 |
| 7 | UBX | H2'1 | 7 | UBX | H6 | 1.79 | 2.69 |
| 7 | UBX | H2'2 | 7 | UBX | H1' | 1.89 | 2.61 |
| 7 | UBX | H2'2 | 7 | UBX | H6 | 2.53 | 3.9 |
| 7 | UBX | H2'2 | 7 | UBX | H3' | 1.94 | 3.46 |
| 8 | ADE | H5'1 | 7 | UBX | H1' | 3.28 | 4.58 |
| 8 | ADE | H2 | 7 | UBX | H15 | 3.59 | 4.11 |
| 8 | ADE | H2 | 7 | UBX | H14 | 3.28 | 4.02 |
| 8 | ADE | H3' | 8 | ADE | H8 | 3.51 | 4.99 |
| 10 | THY | M7 | 10 | THY | H6 | 2.3 | 3.32 |
| 11 | CYT | H5 | 10 | THY | M7 | 4.1 | 6.02 |
| 11 | CYT | H5 | 10 | THY | H2'1 | 2.56 | 4.06 |
| 11 | CYT | H5 | 11 | CYT | H6 | 1.76 | 2.53 |
| 11 | CYT | H3' | 11 | CYT | H6 | 3.51 | 4.69 |
| 12 | CYT | H3' | 12 | CYT | H5'1 | 3.44 | 4.2 |
| 12 | CYT | H3' | 12 | CYT | H1' | 3.07 | 4.16 |
| 13 | GUA | H2'2 | 13 | GUA | H1' | 1.6 | 2.9 |
| 15 | ADE | H3' | 15 | ADE | H4' | 1.79 | 2.68 |
| 16 | CYT | H6 | 15 | ADE | H2'1 | 3.03 | 4.3 |
| 16 | CYT | H6 | 15 | ADE | H2'2 | 1.8 | 2.55 |
| 16 | CYT | H3' | 16 | CYT | H6 | 3.67 | 4.51 |
| 16 | CYT | H2'1 | 16 | CYT | H3' | 2.03 | 2.85 |
| 16 | CYT | H2'2 | 16 | CYT | H6 | 2.65 | 3.75 |
| 16 | CYT | H2'2 | 16 | CYT | H3' | 2.1 | 3.12 |
| 17 | THY | M7 | 16 | CYT | H6 | 2.82 | 3.76 |
| 17 | THY | H3' | 17 | THY | H1' | 3.65 | 4.56 |
| 17 | THY | H2'2 | 17 | THY | H1' | 1.59 | 2.54 |
| 19 | GUA | H8 | 19 | GUA | H1' | 3.43 | 4.91 |
| 20 | CYT | H5 | 19 | GUA | H1' | 3.24 | 4.28 |
| 20 | CYT | H5 | 19 | GUA | H8 | 3.12 | 4.73 |
| 20 | CYT | H5 | 20 | CYT | H6 | 1.71 | 2.58 |
| 21 | THY | H6 | 21 | THY | H1' | 3.08 | 4.55 |
| 23 | GUA | H8 | 22 | ADE | H2'2 | 2.03 | 2.68 |
| 23 | GUA | H3' | 23 | GUA | H1' | 3.66 | 4.27 |
| 23 | GUA | H3' | 23 | GUA | H8 | 3.57 | 4.85 |
| 23 | GUA | H2'2 | 23 | GUA | H8 | 2.82 | 4.56 |
| 24 | CYT | H5 | 24 | CYT | H6 | 1.76 | 2.61 |
| 24 | CYT | H2'1 | 24 | CYT | H3' | 1.69 | 2.53 |
| 24 | CYT | H2'2 | 24 | CYT | H3' | 2.48 | 3.1 |
| 1 | GUA | H3' | 1 | GUA | H8 | 4.03 | 5.15 |
| 2 | CYT | H5 | 1 | GUA | H1' | 3.06 | 4.58 |

**Table B-1:** Continued

| | Residue Number | Residue Name | Atom Name | Residue Number | Residue Name | Atom Name | Lower Bound | Upper Bound |
|---|---|---|---|---|---|---|---|---|
| | 4 | ADE | H3' | 4 | ADE | H1' | 3.3 | 4.39 |
| | 5 | GUA | H8 | 4 | ADE | H3' | 4.37 | 5.07 |
| | 7 | UBX | H5 | 6 | CYT | H2'2 | 5.06 | 6.17 |
| | 7 | UBX | H11 | 7 | UBX | H14 | 2.98 | 4.35 |
| | 7 | UBX | H11 | 7 | UBX | H9 | 1.95 | 3.04 |
| | 9 | GUA | H3' | 9 | GUA | H1' | 3.46 | 4.61 |
| | 10 | THY | H3' | 10 | THY | H1' | 3.39 | 4.27 |
| | 12 | CYT | H6 | 12 | CYT | H4' | 4.19 | 4.75 |
| | 16 | CYT | H6 | 16 | CYT | H1' | 3.1 | 4.24 |
| | 17 | THY | M7 | 16 | CYT | H2'2 | 2.65 | 3.63 |
| | 17 | THY | H2'1 | 17 | THY | H3' | 2 | 2.74 |
| | 17 | THY | H2'2 | 17 | THY | H3' | 1.96 | 3.26 |
| | 20 | CYT | H3' | 20 | CYT | H4' | 1.82 | 3.01 |
| | 23 | GUA | H8 | 22 | ADE | H3' | 4.46 | 5.43 |
| | 24 | CYT | H4' | 23 | GUA | H1' | 3.32 | 4.41 |
| | 24 | CYT | H6 | 24 | CYT | H4' | 4.18 | 4.81 |
| | 24 | CYT | H5 | 23 | GUA | H1' | 3.36 | 4.57 |
| | 24 | CYT | H3' | 24 | CYT | H1' | 3.1 | 4.38 |
| | 24 | CYT | H2'1 | 24 | CYT | H5 | 3.49 | 4.68 |
| | 1 | GUA | H8 | 1 | GUA | H4' | 4.14 | 5.53 |
| | 6 | CYT | H2'2 | 6 | CYT | H5 | 4.89 | 5.78 |
| | 7 | UBX | H5'1 | 6 | CYT | H2'1 | 3.9 | 4.84 |
| | 7 | UBX | H2'2 | 7 | UBX | H4' | 3.67 | 4.55 |
| | 14 | GUA | H8 | 14 | GUA | H4' | 4.34 | 5.56 |
| | 16 | CYT | H5 | 15 | ADE | H1' | 3.39 | 4.51 |
| | 18 | ADE | H8 | 17 | THY | H1' | 4.26 | 5.46 |
| | 18 | ADE | H3' | 18 | ADE | H1' | 3.51 | 4.3 |
| | 23 | GUA | H8 | 23 | GUA | H4' | 4.06 | 5.41 |
| | 2 | CYT | H2'2 | 2 | CYT | H5 | 5.03 | 5.76 |
| | 6 | CYT | H5 | 5 | GUA | H1' | 3.16 | 4.17 |
| | 7 | UBX | H5'1 | 6 | CYT | H1' | 3.5 | 4.51 |
| | 18 | ADE | H1' | 18 | ADE | H5'1 | 3.91 | 4.92 |
| | 20 | CYT | H6 | 19 | GUA | H3' | 4.23 | 4.94 |
| | 24 | CYT | H6 | 23 | GUA | H3' | 4.35 | 5.05 |
| Class 4 | 1 | GUA | H8 | 1 | GUA | H5'1 | 3.2 | 4.08 |
| | 1 | GUA | H2'1 | 1 | GUA | H5'1 | 2.93 | 4.42 |
| | 2 | CYT | H2'1 | 2 | CYT | H6 | 1.86 | 2.56 |
| | 4 | ADE | H8 | 4 | ADE | H1' | 3.31 | 4.07 |
| | 5 | GUA | H8 | 5 | GUA | H1' | 2.97 | 4.3 |
| | 5 | GUA | H2'2 | 5 | GUA | H1' | 1.76 | 2.81 |
| | 5 | GUA | H2'2 | 5 | GUA | H8 | 2.75 | 4.29 |
| | 8 | ADE | H4' | 8 | ADE | H5'1 | 2.08 | 3.02 |
| | 8 | ADE | H8 | 7 | UBX | H2'1 | 4.07 | 5.01 |
| | 8 | ADE | H8 | 7 | UBX | H2'2 | 3.56 | 4.5 |
| | 8 | ADE | H3' | 8 | ADE | H5'2 | 1.62 | 3.08 |
| | 9 | GUA | H2'2 | 9 | GUA | H8 | 3.07 | 4.23 |

**Table B-1:** Continued

| | Residue Number | Residue Name | Atom Name | Residue Number | Residue Name | Atom Name | Lower Bound | Upper Bound |
|---|---|---|---|---|---|---|---|---|
| | 10 | THY | M7 | 9 | GUA | H2'2 | 2.52 | 3.41 |
| | 11 | CYT | H6 | 10 | THY | H2'2 | 1.94 | 2.65 |
| | 11 | CYT | H5 | 10 | THY | H6 | 3.34 | 4.41 |
| | 11 | CYT | H2'2 | 11 | CYT | H6 | 2.41 | 3.81 |
| | 12 | CYT | H6 | 11 | CYT | H1' | 2.1 | 3.55 |
| | 14 | GUA | H3' | 14 | GUA | H4' | 1.82 | 2.76 |
| | 14 | GUA | H2'1 | 14 | GUA | H1' | 2.44 | 3.25 |
| | 14 | GUA | H2'2 | 14 | GUA | H8 | 3.15 | 4.42 |
| | 17 | THY | H6 | 16 | CYT | H2'2 | 2.38 | 3.42 |
| | 17 | THY | M7 | 17 | THY | H6 | 2.83 | 4.23 |
| | 17 | THY | H2'1 | 17 | THY | H1' | 2.23 | 3.71 |
| | 18 | ADE | H2'2 | 18 | ADE | H8 | 2.86 | 4.21 |
| | 19 | GUA | H8 | 18 | ADE | H2'1 | 3.28 | 4.01 |
| | 20 | CYT | H3' | 20 | CYT | H6 | 3.5 | 4.54 |
| | 21 | THY | H2'2 | 21 | THY | H1' | 2.01 | 2.47 |
| | 22 | ADE | H3' | 22 | ADE | H4' | 1.78 | 3.13 |
| | 2 | CYT | H2'1 | 2 | CYT | H5 | 3.57 | 4.87 |
| | 5 | GUA | H3' | 5 | GUA | H4' | 1.76 | 2.73 |
| | 5 | GUA | H3' | 5 | GUA | H1' | 3.36 | 4.37 |
| | 7 | UBX | H5 | 6 | CYT | H2'1 | 4.54 | 5.76 |
| | 10 | THY | H3' | 10 | THY | H6 | 3.31 | 4.38 |
| | 11 | CYT | H6 | 10 | THY | H1' | 2.04 | 3.02 |
| | 11 | CYT | H6 | 11 | CYT | H1' | 3.06 | 4.64 |
| | 16 | CYT | H2'1 | 16 | CYT | H4' | 3 | 4.05 |
| | 18 | ADE | H3' | 18 | ADE | H5'2 | 2.78 | 3.49 |
| | 22 | ADE | H3' | 22 | ADE | H1' | 3.27 | 4.39 |
| | 24 | CYT | H5 | 23 | GUA | H2'1 | 2.49 | 4.07 |
| | 5 | GUA | H2'1 | 5 | GUA | H4' | 3.04 | 4.52 |
| | 5 | GUA | H2'2 | 5 | GUA | H4' | 3.22 | 4.21 |
| | 7 | UBX | H2'1 | 7 | UBX | H4' | 2.83 | 4.23 |
| | 7 | UBX | H2'2 | 7 | UBX | H5'1 | 4.27 | 5.1 |
| | 7 | UBX | H2'2 | 7 | UBX | H5 | 4.41 | 5.52 |
| | 8 | ADE | H8 | 8 | ADE | H4' | 4 | 4.97 |
| | 8 | ADE | H2 | 7 | UBX | H11 | 5.45 | 6.07 |
| | 10 | THY | H2'1 | 10 | THY | M7 | 3.79 | 5.53 |
| | 19 | GUA | H8 | 19 | GUA | H4' | 4.02 | 4.91 |
| | 6 | CYT | H6 | 5 | GUA | H3' | 4.3 | 5 |
| | 7 | UBX | H1' | 7 | UBX | H5'1 | 3.42 | 4.99 |
| Class 5 | 1 | GUA | H4' | 1 | GUA | H5'1 | 2.15 | 2.87 |
| | 2 | CYT | H3' | 2 | CYT | H1' | 2.94 | 4.49 |
| | 2 | CYT | H2'1 | 2 | CYT | H1' | 2.47 | 3.41 |
| | 2 | CYT | H2'1 | 2 | CYT | H3' | 1.99 | 2.79 |
| | 3 | THY | H6 | 2 | CYT | H2'2 | 1.8 | 2.44 |
| | 3 | THY | M7 | 2 | CYT | H3' | 4 | 4.89 |
| | 3 | THY | M7 | 2 | CYT | H2'1 | 2.59 | 3.48 |
| | 3 | THY | M7 | 3 | THY | H6 | 2.57 | 3 |

**Table B-1:** Continued

| Residue Number | Residue Name | Atom Name | Residue Number | Residue Name | Atom Name | Lower Bound | Upper Bound |
|---|---|---|---|---|---|---|---|
| 4 | ADE | H3' | 4 | ADE | H4' | 1.81 | 2.74 |
| 5 | GUA | H8 | 4 | ADE | H2'1 | 2.85 | 4.19 |
| 5 | GUA | H8 | 4 | ADE | H2'2 | 2.12 | 2.98 |
| 5 | GUA | H2'1 | 5 | GUA | H1' | 2.26 | 3.23 |
| 5 | GUA | H2'1 | 5 | GUA | H8 | 1.69 | 2.88 |
| 5 | GUA | H2'2 | 5 | GUA | H3' | 1.77 | 3.2 |
| 6 | CYT | H2'1 | 6 | CYT | H1' | 2.34 | 3.19 |
| 6 | CYT | H2'1 | 6 | CYT | H3' | 1.94 | 2.81 |
| 6 | CYT | H2'2 | 6 | CYT | H1' | 1.57 | 2.34 |
| 6 | CYT | H2'2 | 6 | CYT | H6 | 2.45 | 3.95 |
| 6 | CYT | H2'2 | 6 | CYT | H3' | 2.07 | 3.67 |
| 7 | UBX | H4' | 6 | CYT | H1' | 3.44 | 4.89 |
| 7 | UBX | H2'1 | 7 | UBX | H3' | 1.99 | 3.31 |
| 7 | UBX | H14 | 7 | UBX | H15 | 1.75 | 2.13 |
| 8 | ADE | H8 | 7 | UBX | H3' | 4.12 | 5.19 |
| 8 | ADE | H2'1 | 8 | ADE | H1' | 1.88 | 3.25 |
| 8 | ADE | H2'1 | 8 | ADE | H8 | 1.79 | 3.07 |
| 8 | ADE | H2'2 | 8 | ADE | H1' | 1.62 | 2.77 |
| 8 | ADE | H2'2 | 8 | ADE | H8 | 2.72 | 4.41 |
| 9 | GUA | H8 | 8 | ADE | H2'1 | 3.2 | 4.51 |
| 9 | GUA | H2'1 | 9 | GUA | H8 | 1.66 | 2.7 |
| 10 | THY | M7 | 9 | GUA | H1' | 3.4 | 5.14 |
| 10 | THY | M7 | 9 | GUA | H2'1 | 2.48 | 3.9 |
| 10 | THY | H2'1 | 10 | THY | H6 | 1.95 | 2.7 |
| 10 | THY | H2'2 | 10 | THY | H1' | 1.88 | 2.46 |
| 11 | CYT | H6 | 10 | THY | H2'1 | 3.14 | 4.02 |
| 11 | CYT | H2'1 | 11 | CYT | H1' | 2.11 | 3.3 |
| 11 | CYT | H2'1 | 11 | CYT | H6 | 1.9 | 2.87 |
| 11 | CYT | H2'1 | 11 | CYT | H3' | 2.2 | 2.86 |
| 12 | CYT | H6 | 11 | CYT | H2'1 | 3.1 | 4.09 |
| 12 | CYT | H5 | 11 | CYT | H2'1 | 2.45 | 3.7 |
| 12 | CYT | H2'1 | 12 | CYT | H1' | 2.28 | 3.48 |
| 12 | CYT | H2'1 | 12 | CYT | H6 | 1.83 | 2.5 |
| 12 | CYT | H2'1 | 12 | CYT | H3' | 2.05 | 3.2 |
| 12 | CYT | H2'2 | 12 | CYT | H1' | 1.77 | 2.77 |
| 12 | CYT | H2'2 | 12 | CYT | H6 | 2.51 | 3.87 |
| 12 | CYT | H2'2 | 12 | CYT | H3' | 2.05 | 3.27 |
| 13 | GUA | H4' | 13 | GUA | H5'1 | 1.64 | 2.88 |
| 13 | GUA | H8 | 13 | GUA | H5'1 | 2.8 | 4.47 |
| 13 | GUA | H8 | 13 | GUA | H1' | 2.99 | 4.44 |
| 13 | GUA | H3' | 13 | GUA | H5'1 | 3.45 | 4.04 |
| 13 | GUA | H2'1 | 13 | GUA | H5'1 | 3.11 | 4.25 |
| 13 | GUA | H2'1 | 13 | GUA | H1' | 2.42 | 3.62 |
| 13 | GUA | H2'1 | 13 | GUA | H8 | 1.6 | 2.6 |
| 13 | GUA | H2'2 | 13 | GUA | H8 | 2.67 | 4.49 |
| 14 | GUA | H8 | 13 | GUA | H1' | 2.25 | 3.46 |

**Table B-1:** Continued

| Residue Number | Residue Name | Atom Name | Residue Number | Residue Name | Atom Name | Lower Bound | Upper Bound |
|---|---|---|---|---|---|---|---|
| 14 | GUA | H8 | 14 | GUA | H1' | 3.03 | 4.73 |
| 14 | GUA | H2'1 | 14 | GUA | H8 | 1.62 | 2.54 |
| 14 | GUA | H2'2 | 14 | GUA | H3' | 1.61 | 3.14 |
| 16 | CYT | H1' | 15 | ADE | H2 | 3.97 | 5.4 |
| 16 | CYT | H2'1 | 16 | CYT | H6 | 1.8 | 2.77 |
| 17 | THY | M7 | 16 | CYT | H3' | 3.82 | 5.5 |
| 17 | THY | H2'1 | 17 | THY | H6 | 1.58 | 2.54 |
| 17 | THY | H2'2 | 17 | THY | H6 | 2.85 | 4.08 |
| 18 | ADE | H4' | 18 | ADE | H5'1 | 1.74 | 2.5 |
| 18 | ADE | H8 | 17 | THY | H2'1 | 3.86 | 5.12 |
| 18 | ADE | H8 | 17 | THY | H2'2 | 3.47 | 5.56 |
| 18 | ADE | H2'1 | 18 | ADE | H1' | 2.15 | 3.53 |
| 18 | ADE | H2'1 | 18 | ADE | H8 | 1.87 | 2.7 |
| 18 | ADE | H2'1 | 18 | ADE | H3' | 1.77 | 3.13 |
| 18 | ADE | H2'2 | 18 | ADE | H1' | 1.92 | 2.54 |
| 18 | ADE | H2'2 | 18 | ADE | H3' | 1.64 | 2.78 |
| 19 | GUA | H8 | 18 | ADE | H1' | 4.19 | 5.04 |
| 19 | GUA | H8 | 18 | ADE | H2'2 | 2.04 | 4.05 |
| 19 | GUA | H3' | 19 | GUA | H1' | 3.41 | 4.13 |
| 19 | GUA | H2'1 | 19 | GUA | H1' | 2.47 | 3.82 |
| 19 | GUA | H2'1 | 19 | GUA | H8 | 1.73 | 2.58 |
| 19 | GUA | H2'2 | 19 | GUA | H1' | 1.82 | 3.32 |
| 19 | GUA | H2'2 | 19 | GUA | H8 | 2.79 | 3.81 |
| 19 | GUA | H2'2 | 19 | GUA | H3' | 2.33 | 3.24 |
| 20 | CYT | H1' | 20 | CYT | H4' | 2.91 | 3.72 |
| 20 | CYT | H6 | 19 | GUA | H2'1 | 2.7 | 4.53 |
| 20 | CYT | H6 | 19 | GUA | H2'2 | 1.95 | 3.03 |
| 20 | CYT | H5 | 19 | GUA | H2'1 | 2.25 | 3.79 |
| 20 | CYT | H2'1 | 20 | CYT | H1' | 2.25 | 3.93 |
| 20 | CYT | H2'1 | 20 | CYT | H6 | 1.8 | 2.62 |
| 21 | THY | H6 | 20 | CYT | H2'1 | 2.96 | 4.23 |
| 21 | THY | M7 | 20 | CYT | H2'1 | 2.32 | 4.13 |
| 21 | THY | M7 | 21 | THY | H6 | 1.95 | 3.13 |
| 21 | THY | H2'1 | 21 | THY | H1' | 2.37 | 3.73 |
| 22 | ADE | H8 | 22 | ADE | H1' | 2.92 | 4.48 |
| 22 | ADE | H2'2 | 22 | ADE | H3' | 1.93 | 3.05 |
| 23 | GUA | H8 | 22 | ADE | H2'1 | 3.19 | 4.23 |
| 23 | GUA | H2'1 | 23 | GUA | H8 | 2.05 | 2.42 |
| 23 | GUA | H2'1 | 23 | GUA | H3' | 2.09 | 2.92 |
| 23 | GUA | H2'2 | 23 | GUA | H3' | 2.22 | 2.84 |
| 24 | CYT | H6 | 23 | GUA | H2'1 | 3.18 | 4.12 |
| 24 | CYT | H6 | 23 | GUA | H2'2 | 2.55 | 3.86 |
| 24 | CYT | H2'1 | 24 | CYT | H1' | 2.57 | 3.41 |
| 24 | CYT | H2'2 | 24 | CYT | H1' | 1.68 | 2.62 |
| 1 | GUA | H2'2 | 1 | GUA | H5'1 | 4.31 | 5.41 |
| 2 | CYT | H2'2 | 2 | CYT | H1' | 1.92 | 2.89 |

**Table B-1:** Continued

| Residue Number | Residue Name | Atom Name | Residue Number | Residue Name | Atom Name | Lower Bound | Upper Bound |
|---|---|---|---|---|---|---|---|
| 3 | THY | M7 | 2 | CYT | H1' | 3.23 | 5.05 |
| 4 | ADE | H1' | 4 | ADE | H4' | 2.7 | 3.69 |
| 4 | ADE | H8 | 3 | THY | H1' | 2.46 | 3.21 |
| 4 | ADE | H8 | 3 | THY | H2'1 | 2.96 | 4.16 |
| 4 | ADE | H2'1 | 4 | ADE | H3' | 1.88 | 2.81 |
| 4 | ADE | H2'2 | 4 | ADE | H3' | 2.34 | 3.28 |
| 6 | CYT | H3' | 6 | CYT | H1' | 2.86 | 4.09 |
| 7 | UBX | H5'1 | 6 | CYT | H2'2 | 3.5 | 4.28 |
| 7 | UBX | H6 | 6 | CYT | H2'1 | 4.12 | 5.15 |
| 7 | UBX | H6 | 6 | CYT | H2'2 | 4.41 | 5.59 |
| 7 | UBX | H3' | 7 | UBX | H5'1 | 3.16 | 4.1 |
| 7 | UBX | H2'1 | 7 | UBX | H5'1 | 3.06 | 4.12 |
| 7 | UBX | H11 | 7 | UBX | H15 | 2.43 | 2.85 |
| 8 | ADE | H2 | 7 | UBX | H9 | 4.71 | 5.21 |
| 9 | GUA | H1' | 8 | ADE | H2 | 4.18 | 5.5 |
| 10 | THY | H6 | 9 | GUA | H2'1 | 2.99 | 4.12 |
| 10 | THY | H2'2 | 10 | THY | H6 | 2.44 | 4.18 |
| 11 | CYT | H5 | 10 | THY | H2'2 | 2.21 | 3.68 |
| 11 | CYT | H2'1 | 11 | CYT | H5 | 3.8 | 5.07 |
| 11 | CYT | H2'2 | 11 | CYT | H1' | 1.78 | 2.53 |
| 12 | CYT | H5 | 11 | CYT | H2'2 | 2.5 | 3.77 |
| 14 | GUA | H3' | 14 | GUA | H1' | 3.27 | 4.88 |
| 15 | ADE | H8 | 15 | ADE | H4' | 4.66 | 5.66 |
| 15 | ADE | H2'1 | 15 | ADE | H3' | 2.07 | 3.16 |
| 15 | ADE | H2'2 | 15 | ADE | H3' | 2.68 | 3.3 |
| 16 | CYT | H6 | 15 | ADE | H3' | 4.67 | 5.67 |
| 17 | THY | H6 | 16 | CYT | H1' | 2.43 | 3.71 |
| 17 | THY | M7 | 16 | CYT | H1' | 3.45 | 5.19 |
| 18 | ADE | H8 | 17 | THY | H3' | 4.44 | 5.04 |
| 18 | ADE | H2 | 7 | UBX | H15 | 5.03 | 5.54 |
| 18 | ADE | H2 | 7 | UBX | H14 | 5.03 | 5.51 |
| 18 | ADE | H2 | 7 | UBX | H9 | 4.51 | 5.01 |
| 18 | ADE | H3' | 18 | ADE | H4' | 2.36 | 3.05 |
| 19 | GUA | H3' | 19 | GUA | H4' | 1.6 | 2.85 |
| 20 | CYT | H6 | 20 | CYT | H1' | 3.27 | 4.49 |
| 20 | CYT | H5 | 19 | GUA | H2'2 | 2.07 | 3.67 |
| 20 | CYT | H3' | 20 | CYT | H5'1 | 2.88 | 4.2 |
| 21 | THY | H6 | 20 | CYT | H1' | 2.21 | 3.14 |
| 21 | THY | M7 | 20 | CYT | H1' | 2.89 | 5.04 |
| 22 | ADE | H1' | 22 | ADE | H4' | 3.08 | 3.97 |
| 22 | ADE | H8 | 21 | THY | H2'1 | 2.8 | 4.36 |
| 24 | CYT | H2'1 | 24 | CYT | H4' | 3.01 | 4.07 |
| 24 | CYT | H2'2 | 24 | CYT | H4' | 3.54 | 4.29 |
| 3 | THY | H3' | 3 | THY | H1' | 3.19 | 4.43 |
| 3 | THY | H2'1 | 3 | THY | M7 | 3.06 | 4.19 |
| 4 | ADE | H2'1 | 4 | ADE | H1' | 2.52 | 3.48 |

**Table B-1:** Continued

| Residue Number | Residue Name | Atom Name | Residue Number | Residue Name | Atom Name | Lower Bound | Upper Bound |
|---|---|---|---|---|---|---|---|
| 4 | ADE | H2'2 | 4 | ADE | H1' | 2.07 | 2.44 |
| 7 | UBX | H13 | 7 | UBX | H11 | 1.83 | 2.7 |
| 8 | ADE | H2'1 | 8 | ADE | H3' | 2.1 | 3.09 |
| 8 | ADE | H2'2 | 8 | ADE | H3' | 2.12 | 3.16 |
| 9 | GUA | H2'2 | 9 | GUA | H4' | 3.28 | 4.51 |
| 12 | CYT | H2'1 | 12 | CYT | H5 | 3.64 | 5.05 |
| 12 | CYT | H2'2 | 12 | CYT | H5 | 4.79 | 5.52 |
| 14 | GUA | H2'1 | 14 | GUA | H4' | 3.15 | 4.23 |
| 19 | GUA | H8 | 18 | ADE | H3' | 4.14 | 5.52 |
| 21 | THY | H3' | 21 | THY | H6 | 3.57 | 4.42 |
| 22 | ADE | H8 | 21 | THY | H1' | 2.51 | 3.52 |
| 22 | ADE | H2'1 | 22 | ADE | H1' | 1.88 | 3.16 |
| 22 | ADE | H2'2 | 22 | ADE | H1' | 1.97 | 2.54 |
| 24 | CYT | H5 | 23 | GUA | H2'2 | 2.46 | 3.12 |
| 1 | GUA | H1' | 1 | GUA | H5'1 | 3.89 | 4.84 |
| 4 | ADE | H3' | 4 | ADE | H8 | 3.76 | 4.77 |
| 11 | CYT | H3' | 11 | CYT | H1' | 3.43 | 4.15 |
| 12 | CYT | H6 | 11 | CYT | H3' | 3.7 | 4.93 |
| 13 | GUA | H1' | 13 | GUA | H5'1 | 3.76 | 5.03 |
| 4 | ADE | H5'1 | 3 | THY | H1' | 1.85 | 3.32 |
| 6 | CYT | H5'1 | 5 | GUA | H1' | 1.85 | 3.32 |
| 10 | THY | H5'1 | 9 | GUA | H1' | 1.85 | 3.32 |
| 8 | ADE | H8 | 7 | UBX | H6 | 5 | 5.49 |
| 22 | ADE | H8 | 21 | THY | H6 | 4.49 | 5.21 |
| 18 | ADE | H8 | 17 | THY | H6 | 4.52 | 5.89 |
| 5 | GUA | H8 | 4 | ADE | H8 | 4.81 | 5.38 |
| 4 | ADE | H8 | 3 | THY | H6 | 4.78 | 5.39 |
| 15 | ADE | H8 | 14 | GUA | H8 | 4.44 | 5.4 |
| 16 | CYT | H6 | 15 | ADE | H8 | 4.76 | 5.14 |
| 2 | CYT | H6 | 1 | GUA | H8 | 4.76 | 5.14 |
| 12 | CYT | H6 | 11 | CYT | H6 | 4.76 | 5.14 |
| 5 | GUA | H5'1 | 4 | ADE | H1' | 1.76 | 3.14 |
| 22 | ADE | H5'1 | 21 | THY | H1' | 2.21 | 3.14 |
| 21 | THY | H5'1 | 20 | CYT | H1' | 2.12 | 3.32 |
| 18 | THY | H5'1 | 17 | CYT | H4' | 3.12 | 4.32 |
| 14 | GUA | H8 | 13 | GUA | H8 | 4.62 | 5.32 |
| 23 | GUA | H5'1 | 23 | GUA | H3' | 3.62 | 4.32 |
| 19 | GUA | H5'1 | 19 | GUA | H3' | 3.62 | 4.32 |
| 19 | GUA | H5'1 | 18 | GUA | H1' | 1.62 | 3.32 |
| 17 | GUA | H5'1 | 17 | GUA | H3' | 3.62 | 4.32 |
| 17 | GUA | H5'1 | 16 | GUA | H1' | 1.62 | 3.32 |
| 16 | CYT | H5'1 | 16 | CYT | H3' | 3.62 | 4.32 |
| 3 | THY | H5'1 | 3 | THY | H3' | 3.62 | 4.32 |
| 9 | GUA | H5'1 | 8 | ADE | H3' | 4.12 | 4.82 |
| 19 | GUA | H5'1 | 18 | ADE | H3' | 4.12 | 4.82 |
| 3 | THY | H6 | 2 | CYT | H6 | 4.62 | 5.32 |

**Table B-1:** Continued

| Residue Number | Residue Name | Atom Name | Residue Number | Residue Name | Atom Name | Lower Bound | Upper Bound |
|---|---|---|---|---|---|---|---|
| 23 | GUA | H5'1 | 22 | ADE | H2'2 | 3.3 | 4.32 |
| 24 | CYT | H6 | 23 | GUA | H8 | 4.72 | 5.32 |
| 7 | UBX | H5'1 | 6 | CYT | H4' | 3.52 | 4.32 |
| 7 | UBX | H6 | 6 | CYT | H1' | 5.02 | 5.82 |
| 7 | UBX | H6 | 6 | CYT | H3' | 5.32 | 5.82 |
| 4 | ADE | H5'1 | 3 | THY | H3' | 4.32 | 4.92 |
| 18 | ADE | H5'1 | 18 | ADE | H2'1 | 4.32 | 5.02 |
| 9 | GUA | H8 | 8 | ADE | H8 | 4.72 | 5.32 |
| 19 | GUA | H8 | 18 | ADE | H8 | 4.72 | 5.32 |
| 19 | GUA | H1' | 18 | ADE | H1' | 4.82 | 5.32 |
| 24 | CYT | H1' | 23 | GUA | H1' | 4.82 | 5.22 |
| 2 | CYT | H1' | 1 | GUA | H1' | 4.82 | 5.32 |
| 14 | GUA | H1' | 13 | GUA | H1' | 4.82 | 5.32 |
| 15 | ADE | H1' | 14 | GUA | H1' | 4.82 | 5.32 |
| 16 | CYT | H1' | 15 | ADE | H1' | 4.82 | 5.32 |
| 22 | ADE | H1' | 21 | THY | H1' | 4.82 | 5.32 |
| 23 | GUA | H1' | 22 | ADE | H1' | 4.82 | 5.32 |
| 3 | THY | H1' | 2 | CYT | H1' | 4.82 | 5.32 |
| 4 | ADE | H1' | 3 | THY | H1' | 4.72 | 5.22 |
| 5 | GUA | H1' | 4 | ADE | H1' | 4.82 | 5.32 |
| 11 | CYT | H1' | 10 | THY | H1' | 4.82 | 5.32 |
| 12 | CYT | H1' | 11 | CYT | H1' | 4.82 | 5.32 |
| 4 | ADE | H5'1 | 3 | THY | H2'2 | 3.52 | 4.02 |
| 9 | GUA | H5'1 | 8 | ADE | H2'2 | 3.52 | 4.32 |
| 19 | GUA | H5'1 | 18 | ADE | H2'2 | 3.52 | 4.32 |
| 8 | ADE | H5'1 | 7 | UBX | H2'2 | 4.52 | 5.32 |
| 18 | ADE | H5'1 | 17 | THY | H4' | 3.52 | 4.52 |
| 7 | UBX | H6 | 6 | CYT | H6 | 5.52 | 6.32 |
| 6 | CYT | H6 | 5 | GUA | H8 | 4.82 | 5.32 |
| 9 | GUA | H1' | 8 | ADE | H1' | 4.82 | 5.32 |
| 20 | CYT | H1' | 19 | GUA | H1' | 4.82 | 5.22 |
| 21 | THY | H1' | 20 | CYT | H1' | 4.82 | 5.22 |
| 18 | ADE | H1' | 17 | THY | H1' | 5.7 | 6.3 |
| 7 | UBX | H12 | 6 | CYT | H2'2 | 6.3 | 7.3 |
| 9 | GUA | H5'1 | 9 | GUA | H3' | 3.5 | 4.3 |
| 16 | CYT | H5'1 | 15 | ADE | H3' | 4.1 | 4.9 |
| 23 | GUA | H8 | 22 | ADE | H8 | 4.5 | 5.4 |
| 1 | GUA | H5'1 | 1 | GUA | H3' | 3.5 | 4.3 |
| 17 | THY | H5'1 | 16 | CYT | H3' | 4.1 | 4.9 |
| 22 | ADE | H5'1 | 21 | THY | H3' | 4.1 | 4.9 |
| 18 | ADE | H5'1 | 17 | THY | H5'1 | 5.1 | 5.9 |
| 4 | ADE | H4' | 3 | THY | H1' | 4.5 | 4.9 |
| 18 | ADE | H4' | 17 | THY | H1' | 4.8 | 5.5 |
| 4 | ADE | H3' | 4 | ADE | H5'1 | 3.5 | 4.2 |
| 4 | ADE | H2' | 3 | THY | H2'2 | 3.5 | 4.2 |
| 4 | ADE | H3' | 3 | THY | H2'2 | 4.7 | 5.4 |

**Table B-1:** Continued

| Residue Number | Residue Name | Atom Name | Residue Number | Residue Name | Atom Name | Lower Bound | Upper Bound |
|---|---|---|---|---|---|---|---|
| 14 | GUA | H5'1 | 13 | GUA | H3' | 4.2 | 4.9 |
| 6 | CYT | H5'1 | 5 | GUA | H3' | 4.2 | 4.9 |
| 24 | CYT | H2'1 | 23 | GUA | H1' | 4.6 | 5.1 |
| 23 | GUA | H2'1 | 22 | ADE | H1' | 4.6 | 5.1 |
| 22 | ADE | H2'1 | 21 | THY | H1' | 4.6 | 5.1 |
| 21 | THY | H2'1 | 20 | CYT | H1' | 4.6 | 5.1 |
| 20 | CYT | H2'1 | 19 | GUA | H1' | 4.6 | 5.1 |
| 19 | GUA | H2'1 | 18 | ADE | H1' | 4.6 | 5.1 |
| 17 | THY | H2'1 | 16 | CYT | H1' | 4.6 | 5.1 |
| 16 | CYT | H2'1 | 15 | ADE | H1' | 4.6 | 5.1 |
| 15 | ADE | H2'1 | 14 | GUA | H1' | 4.6 | 5.1 |
| 14 | GUA | H2'1 | 13 | GUA | H1' | 4.6 | 5.1 |
| 12 | CYT | H2'1 | 11 | CYT | H1' | 4.6 | 5.1 |
| 11 | CYT | H2'1 | 10 | THY | H1' | 4.6 | 5.1 |
| 10 | THY | H2'1 | 9 | GUA | H1' | 4.6 | 5.1 |
| 9 | GUA | H2'1 | 8 | ADE | H1' | 4.6 | 5.1 |
| 7 | UBX | H2'1 | 6 | CYT | H1' | 4.6 | 5.1 |
| 6 | CYT | H2'1 | 5 | GUA | H1' | 4.6 | 5.1 |
| 5 | GUA | H2'1 | 4 | ADE | H1' | 4.6 | 5.1 |
| 4 | ADE | H2'1 | 3 | THY | H1' | 4.6 | 5.1 |
| 3 | THY | H2'1 | 2 | CYT | H1' | 4.6 | 5.1 |
| 2 | CYT | H2'1 | 1 | GUA | H1' | 4.6 | 5.1 |
| 4 | ADE | H3' | 3 | THY | H3' | 6.8 | 7.3 |
| 11 | CYT | H3' | 11 | CYT | H5'1 | 3.4 | 4.1 |
| 3 | THY | H2'1 | 2 | CYT | H2'2 | 3.4 | 4.1 |
| 8 | ADE | H3' | 7 | UBX | H3' | 6.8 | 7.3 |
| 17 | THY | H4' | 16 | CYT | H4' | 5.8 | 6.3 |
| 14 | GUA | H3' | 14 | GUA | H5'1 | 3.5 | 4.3 |
| 7 | UBX | H1' | 6 | CYT | H1' | 5 | 6 |
| 8 | ADE | H1' | 7 | UBX | H1' | 5 | 6 |
| 7 | UBX | H3' | 7 | UBX | H5'1 | 3.5 | 4.3 |
| 20 | CYT | H3' | 20 | CYT | H5'1 | 3.5 | 4.3 |
| 7 | UBX | H4' | 6 | CYT | H4' | 5.8 | 6.3 |
| 8 | ADE | H4' | 7 | UBX | H4' | 5.8 | 6.3 |
| 17 | THY | H3' | 16 | CYT | H3' | 6.3 | 7.1 |
| 14 | GUA | H2'1 | 13 | GUA | H2'2 | 3.5 | 4.3 |
| 7 | UBX | H3' | 6 | CYT | H3' | 6.3 | 7.1 |
| 2 | CYT | H4' | 1 | GUA | H4' | 5.8 | 6.3 |
| 23 | GUA | H4' | 22 | ADE | H4' | 5.8 | 6.3 |
| 15 | ADE | H3' | 15 | ADE | H5'1 | 3.5 | 4.3 |
| 18 | ADE | H2 | 17 | THY | H1' | 7.5 | 9.3 |

**Table B-2:** Distance restraints used for the *S-N3-dU* modified oligonucleotide 5′-$G^{1}C^{2}T^{3}A^{4}G^{5}C^{6}X^{7}A^{8}G^{9}T^{10}C^{11}C^{12}$-3′·5′-$G^{13}G^{14}A^{15}C^{16}T^{17}A^{18}G^{19}C^{20}T^{21}A^{22}G^{23}C^{24}$-3′.

| | Residue Number | Residue Name | Atom Number | Residue Number | Residue Name | Atom Number | Lower Bound | Upper Bound |
|---|---|---|---|---|---|---|---|---|
| Class 1 | 1 | GUA | H8 | 1 | GUA | H1' | 3.47 | 4.21 |
| | 2 | CYT | H6 | 1 | GUA | H1' | 2.28 | 3.39 |
| | 2 | CYT | H6 | 1 | GUA | H2'1 | 3.17 | 3.90 |
| | 2 | CYT | H6 | 1 | GUA | H2'2 | 2.05 | 2.97 |
| | 2 | CYT | H5 | 1 | GUA | H1' | 3.20 | 4.14 |
| | 2 | CYT | H5 | 1 | GUA | H8 | 3.65 | 4.63 |
| | 2 | CYT | H2'2 | 2 | CYT | H6 | 3.35 | 4.32 |
| | 3 | THY | M7 | 2 | CYT | H6 | 3.07 | 4.84 |
| | 3 | THY | M7 | 2 | CYT | H5 | 3.51 | 4.56 |
| | 6 | CYT | H6 | 5 | GUA | H1' | 2.35 | 3.32 |
| | 6 | CYT | H5 | 5 | GUA | H8 | 3.14 | 4.47 |
| | 7 | UBX | H6 | 7 | UBX | H1' | 3.40 | 4.19 |
| | 7 | UBX | H2'2 | 7 | UBX | H6 | 3.40 | 4.19 |
| | 9 | GUA | H8 | 8 | ADE | H1' | 3.19 | 3.51 |
| | 10 | THY | M7 | 9 | GUA | H8 | 2.56 | 4.20 |
| | 15 | ADE | H8 | 14 | GUA | H1' | 2.68 | 3.10 |
| Class 2 | 1 | GUA | H3' | 1 | GUA | H8 | 4.14 | 4.70 |
| | 1 | GUA | H2'1 | 1 | GUA | H1' | 2.86 | 3.33 |
| | 1 | GUA | H2'2 | 1 | GUA | H1' | 1.70 | 2.55 |
| | 1 | GUA | H2'2 | 1 | GUA | H8 | 3.09 | 4.11 |
| | 2 | CYT | H6 | 2 | CYT | H1' | 3.35 | 3.99 |
| | 2 | CYT | H5 | 1 | GUA | H2'1 | 2.90 | 3.97 |
| | 2 | CYT | H5 | 1 | GUA | H2'2 | 2.69 | 3.03 |
| | 2 | CYT | H5 | 2 | CYT | H6 | 1.81 | 2.43 |
| | 2 | CYT | H3' | 2 | CYT | H1' | 3.53 | 4.45 |
| | 3 | THY | H6 | 2 | CYT | H1' | 2.04 | 3.00 |
| | 3 | THY | H6 | 3 | THY | H1' | 3.22 | 3.90 |
| | 3 | THY | H5'1 | 3 | THY | H3' | 3.32 | 4.10 |
| | 3 | THY | M7 | 2 | CYT | H2'2 | 2.61 | 3.44 |
| | 5 | GUA | H8 | 5 | GUA | H1' | 3.34 | 4.49 |
| | 6 | CYT | H6 | 6 | CYT | H1' | 3.04 | 3.97 |
| | 6 | CYT | H5 | 5 | GUA | H2'2 | 2.57 | 3.57 |
| | 6 | CYT | H5 | 6 | CYT | H6 | 1.80 | 2.52 |
| | 6 | CYT | H2'1 | 6 | CYT | H1' | 2.70 | 3.28 |
| | 6 | CYT | H2'1 | 6 | CYT | H3' | 1.80 | 2.75 |
| | 6 | CYT | H2'2 | 6 | CYT | H3' | 2.17 | 3.50 |
| | 7 | UBX | H5 | 7 | UBX | H6 | 1.80 | 2.76 |
| | 7 | UBX | H3' | 7 | UBX | H4' | 1.82 | 3.26 |
| | 7 | UBX | H3' | 7 | UBX | H6 | 3.85 | 4.57 |
| | 7 | UBX | H2'1 | 7 | UBX | H1' | 2.30 | 3.24 |
| | 7 | UBX | H2'1 | 7 | UBX | H6 | 1.84 | 2.35 |
| | 7 | UBX | H2'2 | 7 | UBX | H1' | 1.90 | 2.85 |
| | 7 | UBX | H2'2 | 7 | UBX | H3' | 1.80 | 3.17 |
| | 8 | ADE | H3' | 8 | ADE | H8 | 4.14 | 4.75 |

**Table B-2:** Continued

| Residue Number | Residue Name | Atom Number | Residue Number | Residue Name | Atom Number | Lower Bound | Upper Bound |
|---|---|---|---|---|---|---|---|
| 9 | GUA | H1' | 9 | GUA | H4' | 2.80 | 4.10 |
| 9 | GUA | H8 | 9 | GUA | H1' | 3.13 | 4.77 |
| 9 | GUA | H8 | 8 | ADE | H8 | 4.73 | 5.27 |
| 9 | GUA | H2'1 | 9 | GUA | H1' | 2.68 | 3.50 |
| 9 | GUA | H2'2 | 9 | GUA | H1' | 1.80 | 2.68 |
| 10 | THY | H6 | 9 | GUA | H1' | 2.06 | 3.36 |
| 10 | THY | H6 | 10 | THY | H1' | 3.14 | 4.01 |
| 12 | CYT | H6 | 11 | CYT | H1' | 2.26 | 3.25 |
| 12 | CYT | H6 | 11 | CYT | H6 | 4.76 | 5.25 |
| 12 | CYT | H6 | 12 | CYT | H1' | 3.24 | 4.17 |
| 12 | CYT | H3' | 12 | CYT | H6 | 3.87 | 4.26 |
| 13 | GUA | H3' | 13 | GUA | H8 | 4.10 | 4.69 |
| 14 | GUA | H5'1 | 13 | GUA | H3' | 3.90 | 4.79 |
| 14 | GUA | H1' | 14 | GUA | H4' | 2.92 | 4.24 |
| 14 | GUA | H3' | 14 | GUA | H8 | 4.12 | 4.81 |
| 15 | ADE | H8 | 15 | ADE | H1' | 3.28 | 4.25 |
| 15 | ADE | H3' | 15 | ADE | H4' | 1.85 | 2.71 |
| 15 | ADE | H2'1 | 15 | ADE | H1' | 2.44 | 3.38 |
| 15 | ADE | H2'2 | 15 | ADE | H1' | 1.76 | 2.52 |
| 16 | CYT | H6 | 15 | ADE | H2'1 | 2.93 | 3.97 |
| 16 | CYT | H6 | 15 | ADE | H2'2 | 1.86 | 2.76 |
| 16 | CYT | H5 | 15 | ADE | H8 | 3.47 | 4.06 |
| 16 | CYT | H5 | 15 | ADE | H2'2 | 2.71 | 3.55 |
| 16 | CYT | H3' | 16 | CYT | H6 | 3.89 | 4.55 |
| 16 | CYT | H3' | 16 | CYT | H5'1 | 3.31 | 4.25 |
| 16 | CYT | H2'1 | 16 | CYT | H1' | 2.30 | 3.12 |
| 16 | CYT | H2'2 | 16 | CYT | H1' | 1.84 | 2.70 |
| 16 | CYT | H2'2 | 16 | CYT | H6 | 3.45 | 3.75 |
| 16 | CYT | H2'2 | 16 | CYT | H3' | 2.08 | 2.87 |
| 17 | THY | H6 | 16 | CYT | H2'2 | 2.17 | 3.63 |
| 17 | THY | H6 | 17 | THY | H1' | 3.21 | 4.58 |
| 17 | THY | M7 | 16 | CYT | H6 | 2.62 | 4.52 |
| 17 | THY | M7 | 16 | CYT | H5 | 3.71 | 4.61 |
| 17 | THY | M7 | 17 | THY | H6 | 2.01 | 3.28 |
| 17 | THY | H2'1 | 17 | THY | H1' | 1.83 | 3.22 |
| 17 | THY | H2'2 | 17 | THY | H1' | 1.93 | 2.63 |
| 17 | THY | H2'2 | 17 | THY | H3' | 1.90 | 3.22 |
| 18 | ADE | H3' | 18 | ADE | H5'1 | 3.32 | 4.07 |
| 18 | ADE | H3' | 18 | ADE | H8 | 3.86 | 4.50 |
| 19 | GUA | H5'1 | 18 | ADE | H3' | 3.96 | 4.90 |
| 19 | GUA | H1' | 19 | GUA | H4' | 3.01 | 4.52 |
| 19 | GUA | H8 | 18 | ADE | H2'1 | 3.14 | 4.01 |
| 19 | GUA | H3' | 19 | GUA | H8 | 4.18 | 4.71 |
| 19 | GUA | H5'1 | 19 | GUA | H3' | 3.49 | 4.45 |
| 20 | CYT | H5'1 | 19 | GUA | H3' | 4.20 | 5.05 |
| 20 | CYT | H5'1 | 20 | CYT | H3' | 3.45 | 4.25 |

**Table B-2:** Continued

| | Residue Number | Residue Name | Atom Number | Residue Number | Residue Name | Atom Number | Lower Bound | Upper Bound |
|---|---|---|---|---|---|---|---|---|
| | 20 | CYT | H6 | 19 | GUA | H1' | 2.00 | 3.05 |
| | 20 | CYT | H5 | 20 | CYT | H6 | 1.87 | 2.79 |
| | 20 | CYT | H2'1 | 20 | CYT | H1' | 2.33 | 3.43 |
| | 20 | CYT | H2'1 | 20 | CYT | H3' | 2.10 | 3.15 |
| | 20 | CYT | H2'2 | 20 | CYT | H3' | 2.11 | 3.59 |
| | 21 | THY | M7 | 20 | CYT | H5 | 3.79 | 4.97 |
| | 23 | GUA | H8 | 23 | GUA | H1' | 3.18 | 4.12 |
| | 23 | GUA | H2'1 | 23 | GUA | H1' | 2.60 | 3.10 |
| | 23 | GUA | H2'2 | 23 | GUA | H1' | 1.99 | 2.63 |
| | 24 | CYT | H6 | 23 | GUA | H1' | 2.32 | 3.14 |
| | 24 | CYT | H6 | 23 | GUA | H2'1 | 3.10 | 4.05 |
| | 24 | CYT | H6 | 23 | GUA | H2'2 | 1.86 | 2.78 |
| | 24 | CYT | H5 | 24 | CYT | H6 | 1.78 | 2.51 |
| | 24 | CYT | H3' | 24 | CYT | H6 | 3.80 | 4.57 |
| | 1 | GUA | H3' | 1 | GUA | H1' | 3.30 | 4.38 |
| | 3 | THY | M7 | 2 | CYT | H1' | 3.47 | 4.95 |
| | 7 | UBX | H3' | 7 | UBX | H1' | 3.41 | 4.16 |
| | 10 | THY | M7 | 9 | GUA | H1' | 3.29 | 4.51 |
| | 11 | CYT | H5 | 10 | THY | H6 | 2.63 | 4.21 |
| | 11 | CYT | H5 | 10 | THY | M7 | 3.99 | 5.40 |
| | 13 | GUA | H3' | 13 | GUA | H1' | 3.42 | 4.48 |
| | 21 | THY | M7 | 20 | CYT | H1' | 3.15 | 4.23 |
| | 24 | CYT | H5 | 23 | GUA | H1' | 3.20 | 4.15 |
| Class 3 | 1 | GUA | H2'1 | 1 | GUA | H8 | 1.72 | 2.39 |
| | 3 | THY | H6 | 2 | CYT | H2'2 | 1.82 | 2.53 |
| | 3 | THY | M7 | 3 | THY | H6 | 2.51 | 3.93 |
| | 3 | THY | H2'1 | 3 | THY | H1' | 2.32 | 3.63 |
| | 5 | GUA | H2'2 | 5 | GUA | H1' | 1.69 | 2.79 |
| | 6 | CYT | H6 | 5 | GUA | H2'2 | 1.80 | 2.63 |
| | 6 | CYT | H2'2 | 6 | CYT | H1' | 1.80 | 2.72 |
| | 6 | CYT | H2'2 | 6 | CYT | H6 | 3.30 | 3.79 |
| | 7 | UBX | H2'1 | 7 | UBX | H3' | 2.02 | 2.93 |
| | 8 | ADE | H3' | 8 | ADE | H5'2 | 2.39 | 3.21 |
| | 8 | ADE | H3' | 8 | ADE | H1' | 3.18 | 4.34 |
| | 9 | GUA | H3' | 9 | GUA | H8 | 4.09 | 4.85 |
| | 9 | GUA | H2'2 | 9 | GUA | H8 | 3.21 | 4.22 |
| | 10 | THY | H6 | 9 | GUA | H2'2 | 1.86 | 2.87 |
| | 10 | THY | M7 | 9 | GUA | H2'2 | 3.01 | 4.08 |
| | 10 | THY | M7 | 10 | THY | H6 | 2.29 | 3.20 |
| | 11 | CYT | H5 | 11 | CYT | H6 | 1.73 | 2.46 |
| | 12 | CYT | H6 | 11 | CYT | H2'1 | 2.75 | 4.02 |
| | 12 | CYT | H5 | 12 | CYT | H6 | 1.80 | 2.46 |
| | 12 | CYT | H3' | 12 | CYT | H5'1 | 2.93 | 4.49 |
| | 12 | CYT | H3' | 12 | CYT | H4' | 2.25 | 3.12 |
| | 13 | GUA | H2'2 | 13 | GUA | H1' | 1.53 | 2.36 |
| | 14 | GUA | H3' | 14 | GUA | H1' | 3.01 | 4.45 |

**Table B-2:** Continued

| Residue Number | Residue Name | Atom Number | Residue Number | Residue Name | Atom Number | Lower Bound | Upper Bound |
|---|---|---|---|---|---|---|---|
| 14 | GUA | H3' | 14 | GUA | H1' | 3.01 | 4.45 |
| 14 | GUA | H2'1 | 14 | GUA | H1' | 2.59 | 3.55 |
| 14 | GUA | H2'2 | 14 | GUA | H1' | 1.80 | 2.63 |
| 14 | GUA | H2'2 | 14 | GUA | H8 | 3.14 | 3.81 |
| 15 | ADE | H1' | 15 | ADE | H4' | 3.16 | 3.77 |
| 16 | CYT | H1' | 15 | ADE | H2 | 4.33 | 4.93 |
| 16 | CYT | H6 | 15 | ADE | H1' | 2.24 | 3.42 |
| 16 | CYT | H2'1 | 16 | CYT | H6 | 1.90 | 2.50 |
| 17 | THY | H6 | 16 | CYT | H2'1 | 3.04 | 4.29 |
| 17 | THY | M7 | 16 | CYT | H3' | 4.13 | 5.29 |
| 17 | THY | M7 | 16 | CYT | H2'2 | 2.70 | 3.90 |
| 17 | THY | H2'1 | 17 | THY | H6 | 1.84 | 2.78 |
| 17 | THY | H2'1 | 17 | THY | H3' | 2.07 | 2.81 |
| 17 | THY | H2'2 | 17 | THY | H6 | 2.83 | 3.69 |
| 18 | ADE | H8 | 18 | ADE | H1' | 3.69 | 4.50 |
| 18 | ADE | H2'1 | 18 | ADE | H1' | 2.34 | 3.18 |
| 18 | ADE | H2'1 | 18 | ADE | H3' | 2.04 | 3.07 |
| 18 | ADE | H2'2 | 18 | ADE | H8 | 3.19 | 4.22 |
| 19 | GUA | H8 | 18 | ADE | H2'2 | 2.07 | 3.25 |
| 19 | GUA | H8 | 19 | GUA | H1' | 3.27 | 4.32 |
| 20 | CYT | H2'2 | 20 | CYT | H1' | 2.00 | 2.98 |
| 21 | THY | H6 | 20 | CYT | H1' | 2.86 | 4.16 |
| 21 | THY | M7 | 20 | CYT | H3' | 3.51 | 4.64 |
| 21 | THY | H3' | 21 | THY | H6 | 3.37 | 4.47 |
| 23 | GUA | H2'2 | 23 | GUA | H8 | 2.93 | 3.93 |
| 24 | CYT | H3' | 24 | CYT | H1' | 2.97 | 4.34 |
| 24 | CYT | H2'1 | 24 | CYT | H4' | 3.28 | 4.26 |
| 24 | CYT | H2'1 | 24 | CYT | H3' | 1.80 | 3.18 |
| 24 | CYT | H2'2 | 24 | CYT | H4' | 3.28 | 4.35 |
| 24 | CYT | H2'2 | 24 | CYT | H3' | 2.19 | 3.08 |
| 1 | GUA | H8 | 1 | GUA | H4' | 4.54 | 5.40 |
| 6 | CYT | H5 | 5 | GUA | H2'1 | 2.81 | 3.35 |
| 6 | CYT | H2'1 | 6 | CYT | H5 | 3.42 | 4.63 |
| 7 | UBX | H11 | 7 | UBX | H14 | 2.94 | 3.86 |
| 15 | ADE | H2'1 | 15 | ADE | H4' | 3.30 | 4.05 |
| 15 | ADE | H2'2 | 15 | ADE | H4' | 3.56 | 4.33 |
| 16 | CYT | H2'1 | 16 | CYT | H5 | 3.64 | 4.87 |
| 17 | THY | H6 | 16 | CYT | H1' | 2.58 | 3.44 |
| 17 | THY | M7 | 16 | CYT | H1' | 4.32 | 5.86 |
| 20 | CYT | H2'1 | 20 | CYT | H5 | 3.58 | 4.78 |
| 8 | ADE | H4' | 8 | ADE | H5'1 | 1.81 | 2.80 |
| 9 | GUA | H3' | 9 | GUA | H1' | 3.30 | 4.17 |
| 12 | CYT | H1' | 12 | CYT | H4' | 3.36 | 4.22 |
| 6 | CYT | H5 | 5 | GUA | H1' | 3.22 | 4.34 |
| 14 | GUA | H8 | 14 | GUA | H5'1 | 3.19 | 3.84 |
| 14 | GUA | H2'2 | 14 | GUA | H4' | 3.48 | 4.35 |

**Table B-2:** Continued

| | Residue Number | Residue Name | Atom Number | Residue Number | Residue Name | Atom Number | Lower Bound | Upper Bound |
|---|---|---|---|---|---|---|---|---|
| | 16 | CYT | H2'2 | 16 | CYT | H4' | 3.56 | 4.48 |
| | 21 | THY | H3' | 21 | THY | H1' | 3.17 | 4.37 |
| | 24 | CYT | H6 | 24 | CYT | H4' | 4.24 | 5.33 |
| Class 4 | 2 | CYT | H2'1 | 2 | CYT | H1' | 2.30 | 3.56 |
| | 2 | CYT | H2'1 | 2 | CYT | H6 | 1.83 | 2.32 |
| | 3 | THY | H2'2 | 3 | THY | H1' | 1.73 | 2.44 |
| | 3 | THY | H2'2 | 3 | THY | H6 | 2.71 | 3.80 |
| | 5 | GUA | H8 | 4 | ADE | H1' | 2.71 | 3.08 |
| | 5 | GUA | H3' | 5 | GUA | H1' | 3.62 | 4.07 |
| | 5 | GUA | H3' | 5 | GUA | H8 | 4.18 | 4.86 |
| | 5 | GUA | H2'2 | 5 | GUA | H8 | 2.98 | 4.07 |
| | 8 | ADE | H1' | 8 | ADE | H4' | 2.92 | 4.43 |
| | 8 | ADE | H2 | 7 | UBX | H15 | 3.91 | 5.37 |
| | 10 | THY | M7 | 9 | GUA | H2'1 | 2.46 | 3.64 |
| | 10 | THY | H3' | 10 | THY | H6 | 3.60 | 4.54 |
| | 11 | CYT | H2'1 | 11 | CYT | H1' | 2.95 | 3.26 |
| | 11 | CYT | H2'2 | 11 | CYT | H6 | 2.92 | 3.83 |
| | 12 | CYT | H6 | 11 | CYT | H2'2 | 1.80 | 2.42 |
| | 14 | GUA | H3' | 14 | GUA | H4' | 1.80 | 2.97 |
| | 18 | ADE | H3' | 18 | ADE | H1' | 3.41 | 4.26 |
| | 20 | CYT | H3' | 20 | CYT | H4' | 2.25 | 3.07 |
| | 21 | THY | M7 | 20 | CYT | H2'1 | 2.34 | 3.44 |
| | 21 | THY | M7 | 20 | CYT | H2'2 | 2.50 | 4.48 |
| | 22 | ADE | H1' | 22 | ADE | H4' | 3.31 | 4.25 |
| | 23 | GUA | H8 | 22 | ADE | H1' | 2.51 | 3.18 |
| | 23 | GUA | H3' | 23 | GUA | H8 | 3.59 | 4.74 |
| | 24 | CYT | H6 | 24 | CYT | H1' | 3.58 | 4.59 |
| | 24 | CYT | H2'1 | 24 | CYT | H1' | 2.30 | 3.44 |
| | 24 | CYT | H2'2 | 24 | CYT | H1' | 1.87 | 2.65 |
| | 24 | CYT | H2'2 | 24 | CYT | H6 | 2.99 | 3.63 |
| | 3 | THY | H3' | 3 | THY | H6 | 3.63 | 4.47 |
| | 7 | UBX | H2'1 | 7 | UBX | H5'1 | 3.29 | 4.68 |
| | 7 | UBX | H2'1 | 7 | UBX | H4' | 3.49 | 4.45 |
| | 7 | UBX | H2'1 | 7 | UBX | H5 | 3.79 | 4.89 |
| | 19 | GUA | H8 | 18 | ADE | H1' | 3.71 | 4.48 |
| | 24 | CYT | H4' | 23 | GUA | H1' | 3.78 | 4.58 |
| | 24 | CYT | H5 | 23 | GUA | H2'1 | 2.84 | 3.92 |
| | 15 | ADE | H8 | 15 | ADE | H4' | 4.54 | 5.31 |
| | 22 | ADE | H8 | 21 | THY | H6 | 4.48 | 5.20 |
| | 23 | GUA | H8 | 23 | GUA | H4' | 4.57 | 5.55 |
| | 3 | THY | H3' | 3 | THY | H1' | 3.47 | 4.38 |
| | 20 | CYT | H2'1 | 20 | CYT | H4' | 2.98 | 4.27 |
| Class 5 | 2 | CYT | H2'2 | 2 | CYT | H1' | 2.06 | 3.02 |
| | 4 | ADE | H1' | 4 | ADE | H4' | 2.91 | 3.87 |
| | 1 | GUA | H5'1 | 1 | GUA | H3' | 3.41 | 4.37 |
| | 4 | ADE | H8 | 3 | THY | H6 | 4.77 | 5.32 |

**Table B-2:** Continued

| Residue Number | Residue Name | Atom Number | Residue Number | Residue Name | Atom Number | Lower Bound | Upper Bound |
|---|---|---|---|---|---|---|---|
| 4 | ADE | H8 | 4 | ADE | H1' | 3.47 | 4.32 |
| 4 | ADE | H3' | 4 | ADE | H8 | 3.78 | 4.72 |
| 4 | ADE | H2'2 | 4 | ADE | H3' | 2.14 | 2.79 |
| 5 | GUA | H8 | 4 | ADE | H2'1 | 3.07 | 4.53 |
| 5 | GUA | H8 | 4 | ADE | H8 | 4.77 | 5.23 |
| 5 | GUA | H8 | 4 | ADE | H2'2 | 1.75 | 2.82 |
| 5 | GUA | H2'1 | 5 | GUA | H1' | 2.51 | 3.64 |
| 5 | GUA | H2'1 | 5 | GUA | H8 | 1.80 | 2.45 |
| 5 | GUA | H2'1 | 5 | GUA | H3' | 1.99 | 2.92 |
| 5 | GUA | H2'2 | 5 | GUA | H3' | 2.17 | 3.16 |
| 8 | ADE | H3' | 8 | ADE | H4' | 1.80 | 3.18 |
| 8 | ADE | H2'1 | 8 | ADE | H1' | 2.01 | 3.57 |
| 8 | ADE | H2'1 | 8 | ADE | H8 | 1.80 | 2.82 |
| 8 | ADE | H2'1 | 8 | ADE | H3' | 2.46 | 2.57 |
| 8 | ADE | H2'2 | 8 | ADE | H1' | 1.83 | 3.20 |
| 8 | ADE | H2'2 | 8 | ADE | H8 | 2.80 | 3.92 |
| 8 | ADE | H2'2 | 8 | ADE | H3' | 2.30 | 3.37 |
| 9 | GUA | H8 | 8 | ADE | H2'1 | 2.74 | 3.94 |
| 9 | GUA | H8 | 8 | ADE | H2'2 | 1.80 | 3.08 |
| 9 | GUA | H2'1 | 9 | GUA | H8 | 1.80 | 3.00 |
| 10 | THY | H6 | 9 | GUA | H2'1 | 2.91 | 3.90 |
| 10 | THY | H2'1 | 10 | THY | H6 | 1.80 | 2.49 |
| 10 | THY | H2'2 | 10 | THY | H6 | 2.90 | 4.17 |
| 11 | CYT | H6 | 10 | THY | H1' | 1.86 | 3.21 |
| 11 | CYT | H6 | 10 | THY | H2'1 | 3.12 | 4.15 |
| 11 | CYT | H6 | 10 | THY | H2'2 | 1.96 | 2.68 |
| 11 | CYT | H6 | 11 | CYT | H1' | 3.32 | 4.12 |
| 11 | CYT | H5 | 10 | THY | H2'1 | 3.15 | 3.30 |
| 11 | CYT | H5 | 10 | THY | H2'2 | 1.96 | 2.52 |
| 11 | CYT | H2'1 | 11 | CYT | H6 | 1.81 | 2.76 |
| 11 | CYT | H2'1 | 11 | CYT | H5 | 2.90 | 4.68 |
| 11 | CYT | H2'2 | 11 | CYT | H1' | 1.80 | 2.69 |
| 12 | CYT | H2'1 | 12 | CYT | H1' | 1.80 | 3.31 |
| 12 | CYT | H2'1 | 12 | CYT | H6 | 1.80 | 2.67 |
| 12 | CYT | H2'1 | 12 | CYT | H3' | 2.15 | 2.75 |
| 12 | CYT | H2'2 | 12 | CYT | H1' | 2.08 | 2.68 |
| 12 | CYT | H2'2 | 12 | CYT | H6 | 2.64 | 3.68 |
| 12 | CYT | H2'2 | 12 | CYT | H3' | 2.08 | 3.67 |
| 13 | GUA | H8 | 13 | GUA | H1' | 3.27 | 4.44 |
| 13 | GUA | H2'1 | 13 | GUA | H1' | 2.59 | 3.39 |
| 13 | GUA | H2'1 | 13 | GUA | H8 | 1.60 | 2.42 |
| 14 | GUA | H5'1 | 13 | GUA | H1' | 2.50 | 3.32 |
| 14 | GUA | H8 | 13 | GUA | H1' | 2.37 | 3.75 |
| 14 | GUA | H8 | 14 | GUA | H1' | 2.95 | 4.33 |
| 14 | GUA | H2'1 | 14 | GUA | H8 | 1.80 | 2.53 |
| 15 | ADE | H3' | 15 | ADE | H1' | 3.22 | 4.60 |

**Table B-2:** Continued

| Residue Number | Residue Name | Atom Number | Residue Number | Residue Name | Atom Number | Lower Bound | Upper Bound |
|---|---|---|---|---|---|---|---|
| 15 | ADE | H2'2 | 15 | ADE | H3' | 2.05 | 2.78 |
| 16 | CYT | H6 | 16 | CYT | H1' | 2.94 | 4.33 |
| 16 | CYT | H5 | 16 | CYT | H6 | 1.84 | 2.56 |
| 16 | CYT | H3' | 16 | CYT | H1' | 3.15 | 4.43 |
| 18 | ADE | H1' | 18 | ADE | H5'1 | 3.35 | 4.55 |
| 18 | ADE | H2'2 | 18 | ADE | H1' | 1.91 | 2.87 |
| 18 | ADE | H2'2 | 18 | ADE | H3' | 2.17 | 3.25 |
| 19 | GUA | H3' | 19 | GUA | H4' | 1.80 | 3.17 |
| 19 | GUA | H3' | 19 | GUA | H1' | 3.29 | 4.36 |
| 19 | GUA | H2'1 | 19 | GUA | H1' | 1.80 | 3.35 |
| 19 | GUA | H2'1 | 19 | GUA | H8 | 1.88 | 2.47 |
| 19 | GUA | H2'1 | 19 | GUA | H3' | 2.10 | 3.12 |
| 19 | GUA | H2'2 | 19 | GUA | H1' | 2.15 | 2.99 |
| 19 | GUA | H2'2 | 19 | GUA | H3' | 2.09 | 3.20 |
| 20 | CYT | H6 | 19 | GUA | H2'2 | 1.93 | 2.71 |
| 20 | CYT | H5 | 19 | GUA | H1' | 2.81 | 4.31 |
| 20 | CYT | H5 | 19 | GUA | H8 | 3.38 | 4.32 |
| 20 | CYT | H3' | 20 | CYT | H1' | 3.00 | 4.38 |
| 20 | CYT | H2'1 | 20 | CYT | H6 | 1.75 | 2.36 |
| 21 | THY | M7 | 21 | THY | H6 | 1.91 | 3.91 |
| 21 | THY | H2'1 | 21 | THY | H1' | 2.30 | 3.21 |
| 21 | THY | H2'2 | 21 | THY | H1' | 1.95 | 2.67 |
| 22 | ADE | H8 | 22 | ADE | H1' | 2.89 | 4.26 |
| 22 | ADE | H8 | 21 | THY | H6 | 4.89 | 5.26 |
| 22 | ADE | H3' | 22 | ADE | H4' | 1.87 | 3.36 |
| 22 | ADE | H2'2 | 22 | ADE | H3' | 1.94 | 3.29 |
| 23 | GUA | H8 | 22 | ADE | H2'1 | 2.69 | 4.03 |
| 23 | GUA | H8 | 22 | ADE | H2'1 | 4.69 | 5.33 |
| 23 | GUA | H3' | 23 | GUA | H1' | 3.44 | 4.22 |
| 23 | GUA | H2'1 | 23 | GUA | H8 | 1.80 | 2.73 |
| 23 | GUA | H2'1 | 23 | GUA | H3' | 1.85 | 2.63 |
| 23 | GUA | H2'2 | 23 | GUA | H3' | 2.12 | 2.94 |
| 24 | CYT | H5 | 23 | GUA | H8 | 2.44 | 4.07 |
| 24 | CYT | H2'1 | 24 | CYT | H6 | 1.80 | 2.70 |
| 2 | CYT | H2'1 | 2 | CYT | H5 | 3.46 | 4.43 |
| 3 | THY | H6 | 2 | CYT | H3' | 3.88 | 5.19 |
| 4 | ADE | H8 | 3 | THY | H1' | 1.98 | 3.16 |
| 4 | ADE | H3' | 4 | ADE | H1' | 3.34 | 4.29 |
| 4 | ADE | H2'1 | 4 | ADE | H1' | 2.10 | 3.43 |
| 4 | ADE | H2'1 | 4 | ADE | H8 | 1.80 | 2.64 |
| 4 | ADE | H2'1 | 4 | ADE | H3' | 1.80 | 2.79 |
| 4 | ADE | H2'2 | 4 | ADE | H1' | 2.00 | 2.95 |
| 4 | ADE | H2'2 | 4 | ADE | H8 | 3.04 | 4.10 |
| 5 | GUA | H8 | 4 | ADE | H3' | 4.37 | 5.28 |
| 6 | CYT | H6 | 5 | GUA | H3' | 3.78 | 5.23 |
| 6 | CYT | H3' | 6 | CYT | H1' | 3.34 | 4.04 |

**Table B-2:** Continued

| Residue Number | Residue Name | Atom Number | Residue Number | Residue Name | Atom Number | Lower Bound | Upper Bound |
|---|---|---|---|---|---|---|---|
| 6 | CYT | H5' | 6 | CYT | H3' | 3.34 | 4.04 |
| 9 | GUA | H1' | 8 | ADE | H2 | 3.86 | 4.96 |
| 9 | GUA | H8 | 8 | ADE | H3' | 3.90 | 5.30 |
| 10 | THY | H2'1 | 10 | THY | M7 | 4.01 | 5.44 |
| 11 | CYT | H3' | 11 | CYT | H1' | 2.81 | 4.03 |
| 12 | CYT | H5 | 11 | CYT | H2'1 | 2.21 | 3.55 |
| 12 | CYT | H2'1 | 12 | CYT | H4' | 2.83 | 4.33 |
| 12 | CYT | H2'1 | 12 | CYT | H5 | 3.80 | 4.77 |
| 12 | CYT | H2'2 | 12 | CYT | H4' | 2.80 | 4.38 |
| 12 | CYT | H2'2 | 12 | CYT | H5 | 4.38 | 5.54 |
| 14 | GUA | H2'1 | 14 | GUA | H3' | 1.84 | 2.61 |
| 14 | GUA | H2'2 | 14 | GUA | H3' | 1.84 | 3.17 |
| 15 | ADE | H2'1 | 15 | ADE | H8 | 1.95 | 2.51 |
| 16 | CYT | H6 | 15 | ADE | H3' | 4.25 | 5.16 |
| 16 | CYT | H5 | 15 | ADE | H1' | 3.48 | 4.52 |
| 16 | CYT | H5 | 15 | ADE | H2'1 | 2.58 | 3.78 |
| 16 | CYT | H2'1 | 16 | CYT | H3' | 2.01 | 2.75 |
| 17 | THY | H3' | 17 | THY | H1' | 3.09 | 4.68 |
| 17 | THY | H3' | 17 | THY | M7 | 4.42 | 7.30 |
| 17 | THY | H2'2 | 17 | THY | M7 | 5.42 | 6.03 |
| 18 | ADE | H3' | 18 | ADE | H5'2 | 1.57 | 3.32 |
| 20 | CYT | H6 | 19 | GUA | H3' | 3.31 | 5.11 |
| 20 | CYT | H6 | 20 | CYT | H1' | 3.25 | 4.15 |
| 20 | CYT | H5 | 19 | GUA | H2'1 | 2.34 | 3.56 |
| 20 | CYT | H5 | 19 | GUA | H2'2 | 2.60 | 3.72 |
| 21 | THY | M7 | 20 | CYT | H6 | 2.74 | 4.55 |
| 21 | THY | H2'2 | 21 | THY | H6 | 2.87 | 4.20 |
| 22 | ADE | H8 | 21 | THY | H1' | 2.25 | 3.10 |
| 22 | ADE | H3' | 22 | ADE | H1' | 3.02 | 4.42 |
| 22 | ADE | H2'1 | 22 | ADE | H1' | 2.27 | 3.15 |
| 22 | ADE | H2'1 | 22 | ADE | H8 | 1.77 | 2.52 |
| 22 | ADE | H2'1 | 22 | ADE | H3' | 2.17 | 3.07 |
| 22 | ADE | H2'2 | 22 | ADE | H1' | 1.80 | 2.38 |
| 22 | ADE | H2'2 | 22 | ADE | H8 | 2.85 | 4.37 |
| 23 | GUA | H8 | 22 | ADE | H3' | 4.56 | 5.49 |
| 23 | GUA | H3' | 23 | GUA | H4' | 1.90 | 3.25 |
| 24 | CYT | H6 | 23 | GUA | H3' | 3.49 | 5.36 |
| 24 | CYT | H3' | 24 | CYT | H4' | 1.80 | 2.71 |
| 2 | CYT | H6 | 1 | GUA | H8 | 4.20 | 5.49 |
| 3 | THY | M7 | 2 | CYT | H2'1 | 1.94 | 3.04 |
| 3 | THY | H2'1 | 3 | THY | H6 | 1.80 | 3.34 |
| 5 | GUA | H8 | 5 | GUA | H4' | 4.26 | 5.22 |
| 6 | CYT | H5 | 5 | GUA | H3' | 4.69 | 5.97 |
| 6 | CYT | H2'1 | 6 | CYT | H6 | 1.84 | 2.83 |
| 10 | THY | H2'2 | 10 | THY | M7 | 3.81 | 5.46 |
| 12 | CYT | H6 | 11 | CYT | H3' | 3.90 | 5.25 |

**Table B-2:** Continued

| Residue Number | Residue Name | Atom Number | Residue Number | Residue Name | Atom Number | Lower Bound | Upper Bound |
|---|---|---|---|---|---|---|---|
| 15 | ADE | H8 | 14 | GUA | H8 | 4.61 | 5.40 |
| 15 | ADE | H2'1 | 15 | ADE | H3' | 1.98 | 3.29 |
| 20 | CYT | H6 | 19 | GUA | H8 | 4.21 | 5.39 |
| 21 | THY | H6 | 21 | THY | H1' | 3.47 | 4.26 |
| 21 | THY | H2'1 | 21 | THY | H6 | 1.86 | 2.22 |
| 21 | THY | H2'1 | 21 | THY | M7 | 2.67 | 4.66 |
| 22 | ADE | H8 | 22 | ADE | H4' | 4.44 | 5.31 |
| 1 | GUA | H2'2 | 1 | GUA | H4' | 3.52 | 4.29 |
| 3 | THY | H2'2 | 3 | THY | H3' | 2.06 | 2.91 |
| 4 | ADE | H8 | 3 | THY | H2'1 | 3.18 | 4.27 |
| 5 | GUA | H2'1 | 5 | GUA | H4' | 3.24 | 4.23 |
| 10 | THY | M7 | 9 | GUA | H4' | 4.61 | 6.35 |
| 14 | GUA | H4' | 14 | GUA | H5'1 | 1.78 | 2.87 |
| 18 | ADE | H4' | 18 | ADE | H5'1 | 1.96 | 2.56 |
| 18 | ADE | H3' | 18 | ADE | H4' | 2.23 | 2.83 |
| 18 | ADE | H2'1 | 18 | ADE | H4' | 2.98 | 4.22 |
| 21 | THY | H2'2 | 21 | THY | M7 | 4.07 | 5.56 |
| 22 | ADE | H8 | 21 | THY | M7 | 5.87 | 6.86 |
| 22 | ADE | H8 | 21 | THY | H2'1 | 2.84 | 3.99 |
| 23 | GUA | H2'1 | 23 | GUA | H4' | 3.03 | 4.32 |
| 24 | CYT | H5 | 23 | GUA | H2'2 | 2.27 | 3.48 |
| 7 | UBX | H9 | 7 | UBX | H14 | 2.12 | 3.08 |
| 17 | THY | H6 | 7 | UBX | H12 | 6.11 | 8.37 |
| 17 | THY | H1' | 7 | UBX | H12 | 5.91 | 7.37 |
| 17 | THY | H1' | 7 | UBX | H13 | 5.91 | 7.37 |
| 18 | ADE | H8 | 7 | UBX | H12 | 6.11 | 8.37 |
| 17 | THY | H2'2 | 7 | UBX | H12 | 6.11 | 8.37 |
| 7 | UBX | H12 | 7 | UBX | H11 | 2.11 | 3.37 |
| 7 | UBX | H12 | 7 | UBX | H14 | 4.51 | 5.37 |
| 7 | UBX | H12 | 7 | UBX | H15 | 4.51 | 5.37 |
| 8 | ADE | H8 | 7 | UBX | H2'2 | 2.86 | 3.50 |
| 8 | ADE | H2 | 7 | UBX | H9 | 3.02 | 4.00 |
| 8 | ADE | H2 | 7 | UBX | H13 | 6.22 | 7.28 |
| 18 | ADE | H1' | 7 | UBX | H13 | 5.97 | 7.25 |
| 18 | ADE | H2 | 7 | UBX | H9 | 3.07 | 4.00 |
| 18 | ADE | H8 | 17 | THY | H2'1 | 4.46 | 5.44 |
| 18 | ADE | H8 | 17 | THY | H2'2 | 3.03 | 4.51 |
| 7 | UBX | H5 | 6 | CYT | H2'1 | 3.58 | 4.50 |
| 7 | UBX | H11 | 7 | UBX | H15 | 2.93 | 3.95 |
| 18 | ADE | H8 | 17 | THY | H1' | 4.54 | 5.57 |
| 7 | UBX | H5 | 6 | CYT | H3' | 4.81 | 5.64 |
| 8 | ADE | H8 | 7 | UBX | H1' | 4.80 | 5.50 |
| 7 | UBX | H6 | 6 | CYT | H1' | 4.66 | 5.96 |
| 7 | UBX | H6 | 6 | CYT | H2'1 | 4.73 | 5.53 |
| 7 | UBX | H6 | 6 | CYT | H2'2 | 3.23 | 5.05 |
| 17 | THY | H1' | 7 | UBX | H9 | 5.00 | 6.00 |

**Table B-2:** Continued

| Residue Number | Residue Name | Atom Number | Residue Number | Residue Name | Atom Number | Lower Bound | Upper Bound |
|---|---|---|---|---|---|---|---|
| 18 | ADE | H1' | 7 | UBX | H9 | 5.50 | 6.50 |
| 7 | UBX | H13 | 7 | UBX | H11 | 2.00 | 3.38 |
| 18 | ADE | H2 | 7 | UBX | H11 | 5.50 | 6.38 |
| 18 | ADE | H2 | 7 | UBX | H13 | 6.50 | 7.38 |
| 18 | ADE | H2 | 7 | UBX | H14 | 3.91 | 4.97 |
| 18 | ADE | H2 | 7 | UBX | H15 | 3.91 | 4.97 |
| 8 | ADE | H8 | 7 | UBX | H3' | 5.16 | 5.71 |
| 8 | ADE | H5'1 | 7 | UBX | H5'1 | 5.16 | 5.81 |
| 8 | ADE | H5'1 | 8 | ADE | H3' | 3.66 | 5.01 |
| 7 | UBX | H5'1 | 6 | CYT | H1' | 2.37 | 3.84 |
| 7 | UBX | H5 | 6 | CYT | H1' | 4.37 | 5.34 |
| 8 | ADE | H2 | 7 | UBX | H14 | 3.91 | 5.37 |
| 23 | GUA | H3'1 | 22 | ADE | H1' | 4.95 | 5.25 |
| 17 | THY | H5'1 | 16 | CYT | H3' | 3.95 | 5.25 |
| 14 | GUA | H5'1 | 13 | CYT | H2'2 | 2.70 | 4.10 |
| 17 | THY | H6 | 16 | CYT | H6 | 4.50 | 5.50 |
| 21 | THY | H6 | 20 | CYT | H6 | 4.50 | 5.50 |
| 12 | CYT | H1' | 11 | CYT | H1' | 4.50 | 5.50 |
| 13 | GUA | H3' | 13 | GUA | H5'1 | 3.27 | 4.32 |
| 21 | THY | H3' | 21 | THY | H5'1 | 3.27 | 4.32 |
| 19 | GUA | H8 | 18 | ADE | H4'1 | 5.87 | 6.32 |
| 19 | GUA | H8 | 18 | ADE | H8 | 4.87 | 5.32 |
| 18 | ADE | H8 | 17 | THY | H6 | 5.07 | 5.52 |
| 4 | ADE | H5'1 | 4 | ADE | H3' | 4.07 | 5.02 |
| 3 | THY | H1' | 2 | CYT | H1' | 4.75 | 5.25 |
| 4 | ADE | H1' | 3 | THY | H1' | 4.75 | 5.25 |
| 6 | CYT | H1' | 5 | GUA | H1' | 4.75 | 5.25 |
| 14 | GUA | H1' | 13 | GUA | H1' | 4.75 | 5.25 |
| 18 | ADE | H1' | 17 | THY | H1' | 4.75 | 5.50 |
| 19 | GUA | H1' | 18 | ADE | H1' | 4.75 | 5.25 |
| 20 | CYT | H1' | 19 | GUA | H1' | 4.75 | 5.25 |
| 21 | THY | H1' | 20 | CYT | H1' | 4.75 | 5.25 |
| 23 | GUA | H1' | 22 | ADE | H1' | 4.75 | 5.25 |
| 24 | CYT | H1' | 23 | GUA | H1' | 4.75 | 5.25 |
| 8 | ADE | H8 | 7 | UBX | H6 | 5.50 | 6.25 |
| 7 | UBX | H5'1 | 6 | CYT | H3' | 5.00 | 6.00 |
| 10 | THY | H3' | 10 | THY | H5'1 | 3.42 | 4.26 |
| 22 | ADE | H5'1 | 21 | THY | H2'2 | 3.18 | 4.46 |
| 4 | ADE | H5'1 | 3 | THY | H3' | 3.18 | 4.46 |
| 7 | UBX | H1' | 6 | CYT | H1' | 5.00 | 5.66 |
| 18 | ADE | H5'1 | 17 | THY | H3' | 4.50 | 5.50 |
| 7 | UBX | H6 | 6 | CYT | H6 | 5.00 | 5.96 |
| 22 | ADE | H5'1 | 22 | ADE | H3' | 3.50 | 4.20 |
| 16 | CYT | H5'1 | 15 | ADE | H3' | 4.00 | 5.00 |
| 9 | GUA | H3' | 9 | GUA | H5'1 | 3.50 | 4.00 |
| 18 | ADE | H2 | 7 | UBX | H6 | 6.50 | 8.00 |

**Table B-2:** Continued

| Residue Number | Residue Name | Atom Number | Residue Number | Residue Name | Atom Number | Lower Bound | Upper Bound |
|---|---|---|---|---|---|---|---|
| 17 | THY | H1' | 16 | CYT | H1' | 4.70 | 5.46 |
| 24 | CYT | H3' | 24 | CYT | H5'1 | 3.42 | 4.26 |
| 2 | CYT | H3' | 2 | CYT | H5'1 | 3.42 | 4.26 |
| 5 | GUA | H3' | 5 | GUA | H5'1 | 3.42 | 4.26 |
| 11 | CYT | H3' | 11 | CYT | H5'1 | 3.42 | 4.26 |
| 14 | GUA | H3' | 14 | GUA | H5'1 | 3.42 | 4.26 |
| 15 | ADE | H3' | 15 | ADE | H5'1 | 3.42 | 4.26 |
| 17 | THY | H3' | 17 | THY | H5'1 | 3.42 | 4.26 |
| 23 | GUA | H3' | 23 | GUA | H5'1 | 3.42 | 4.26 |
| 7 | UBX | H3' | 7 | UBX | H5'1 | 3.42 | 4.26 |
| 18 | ADE | H8 | 17 | THY | H5'2 | 6.82 | 7.36 |
| 8 | ADE | H8 | 8 | ADE | H5'1 | 3.22 | 3.86 |
| 7 | UBX | H6 | 7 | UBX | H5'1 | 3.02 | 3.66 |
| 4 | ADE | H3' | 3 | THY | H3' | 6.80 | 7.30 |
| 4 | ADE | H3' | 4 | ADE | H5'1 | 3.40 | 4.30 |
| 4 | ADE | H2'1 | 3 | THY | H2'2 | 3.60 | 4.20 |
| 23 | GUA | H2'1 | 22 | ADE | H2'2 | 3.60 | 4.20 |
| 23 | GUA | H8 | 22 | ADE | H8 | 4.80 | 5.20 |
| 7 | UBX | H4' | 6 | CYT | H4' | 5.80 | 7.30 |
| 3 | THY | H4' | 2 | CYT | H4' | 5.80 | 6.30 |
| 14 | GUA | H4' | 13 | GUA | H4' | 5.80 | 6.30 |
| 14 | GUA | H2'1 | 13 | GUA | H2'2 | 3.60 | 4.20 |
| 14 | GUA | H8 | 13 | GUA | H8 | 4.80 | 5.20 |
| 6 | CYT | H3' | 6 | CYT | H5'1 | 3.60 | 4.30 |
| 23 | GUA | H3' | 23 | GUA | H5'1 | 3.60 | 4.30 |
| 6 | CYT | H3' | 6 | CYT | H6 | 3.79 | 4.50 |
| 2 | CYT | H3' | 2 | CYT | H6 | 3.79 | 4.50 |
| 11 | CYT | H3' | 11 | CYT | H6 | 3.79 | 4.50 |
| 17 | THY | H3' | 17 | THY | H6 | 3.79 | 4.50 |
| 15 | ADE | H3' | 15 | ADE | H8 | 4.19 | 4.70 |
| 22 | ADE | H3' | 22 | ADE | H8 | 4.19 | 4.70 |
| 4 | ADE | H3' | 4 | ADE | H8 | 4.19 | 4.70 |
| 7 | UBX | H2'1 | 6 | CYT | H2'2 | 3.40 | 4.30 |
| 16 | CYT | H4' | 15 | GUA | H4' | 5.80 | 6.30 |
| 8 | ADE | H5'1 | 7 | UBX | H2'2 | 3.20 | 4.10 |
| 7 | UBX | H1' | 7 | UBX | H9 | 5.00 | 6.80 |
| 10 | THY | H4' | 9 | GUA | H4' | 5.80 | 6.30 |
| 6 | CYT | H4' | 5 | GUA | H4' | 5.80 | 6.30 |
| 7 | UBX | H3' | 6 | CYT | H3' | 6.50 | 7.30 |
| 19 | GUA | H1' | 18 | ADE | H2 | 4.50 | 6.30 |
| 18 | ADE | H5'1 | 17 | THY | H4' | 3.70 | 4.30 |
| 20 | CYT | H5'1 | 19 | GUA | H4' | 3.70 | 4.30 |
| 20 | CYT | H3' | 20 | CYT | H6 | 4.10 | 4.70 |
| 9 | GUA | H8 | 9 | GUA | H5'1 | 3.22 | 3.86 |
| 19 | GUA | H8 | 19 | GUA | H5'1 | 3.22 | 3.86 |
| 18 | ADE | H8 | 18 | ADE | H5'1 | 3.22 | 3.86 |

**Table B-2:** Continued

| Residue Number | Residue Name | Atom Number | Residue Number | Residue Name | Atom Number | Lower Bound | Upper Bound |
|---|---|---|---|---|---|---|---|
| 17 | THY | H6 | 17 | THY | H5'1 | 3.02 | 3.66 |
| 17 | THY | H2'1 | 16 | CYT | H2'2 | 3.50 | 4.30 |
| 6 | CYT | H6 | 5 | GUA | H8 | 4.75 | 5.25 |
| 16 | CYT | H6 | 15 | ADE | H8 | 4.75 | 5.25 |
| 2 | CYT | H6 | 2 | CYT | H5'1 | 3.02 | 3.66 |
| 3 | THY | H6 | 3 | THY | H5'1 | 3.02 | 3.66 |
| 6 | CYT | H6 | 6 | CYT | H5'1 | 3.02 | 3.66 |
| 10 | THY | H6 | 10 | THY | H5'1 | 3.02 | 3.66 |
| 11 | CYT | H6 | 11 | CYT | H5'1 | 3.02 | 3.66 |
| 12 | CYT | H6 | 12 | CYT | H5'1 | 3.02 | 3.66 |
| 16 | CYT | H6 | 16 | CYT | H5'1 | 3.02 | 3.66 |
| 20 | CYT | H6 | 20 | CYT | H5'1 | 3.02 | 3.66 |
| 21 | THY | H6 | 21 | THY | H5'1 | 3.02 | 3.66 |
| 24 | CYT | H6 | 24 | CYT | H5'1 | 3.02 | 3.66 |
| 1 | GUA | H8 | 1 | GUA | H5'1 | 3.22 | 3.86 |
| 4 | ADE | H8 | 4 | ADE | H5'1 | 3.22 | 3.86 |
| 5 | GUA | H8 | 5 | GUA | H5'1 | 3.22 | 3.86 |
| 13 | GUA | H8 | 13 | GUA | H5'1 | 3.22 | 3.86 |
| 15 | ADE | H8 | 15 | ADE | H5'1 | 3.22 | 3.86 |
| 22 | ADE | H8 | 22 | ADE | H5'1 | 3.22 | 3.86 |
| 23 | GUA | H8 | 23 | GUA | H5'1 | 3.22 | 3.86 |
| 18 | ADE | H8 | 17 | THY | H3' | 4.63 | 5.14 |
| 17 | THY | H2'1 | 17 | THY | H5'1 | 3.63 | 4.14 |
| 7 | UBX | H5'1 | 6 | CYT | H6 | 5.13 | 5.84 |
| 8 | ADE | H1' | 7 | UBX | H1' | 5.13 | 5.84 |
| 18 | ADE | H5'1 | 17 | THY | H1' | 2.63 | 3.84 |

**Table B-3:** Distance restraints used for the *R-N3-dU* modified oligonucleotide 5′-$G^{1}C^{2}T^{3}A^{4}G^{5}C^{6}X^{7}A^{8}G^{9}T^{10}C^{11}C^{12}$-3′·5′-$G^{13}G^{14}A^{15}C^{16}T^{17}T^{18}G^{19}C^{20}T^{21}A^{22}G^{23}C^{24}$-3′.

| | Residue Number | Residue Name | Atom Number | Residue Number | Residue Name | Atom Number | Lower Bound | Upper Bound |
|---|---|---|---|---|---|---|---|---|
| Class 1 | 1 | GUA | H8 | 1 | GUA | H1' | 3.63 | 4.44 |
| | 2 | CYT | H6 | 2 | CYT | H1' | 3.41 | 4.36 |
| | 6 | CYT | H6 | 6 | CYT | H1' | 3.34 | 4.32 |
| | 16 | CYT | H2'2 | 16 | CYT | H2'1 | 1.6 | 2.44 |
| | 19 | GUA | H8 | 19 | GUA | H1' | 3.51 | 4.45 |
| Class 2 | 1 | GUA | H2'2 | 1 | GUA | H1' | 1.7 | 2.4 |
| | 2 | CYT | H6 | 1 | GUA | H1' | 2.21 | 2.98 |
| | 2 | CYT | H6 | 1 | GUA | H2'1 | 3.12 | 3.92 |
| | 2 | CYT | H6 | 1 | GUA | H2'2 | 2.05 | 2.69 |
| | 2 | CYT | H5 | 2 | CYT | H6 | 1.81 | 2.4 |
| | 2 | CYT | H2'2 | 2 | CYT | H6 | 2.8 | 3.97 |
| | 5 | GUA | H8 | 5 | GUA | H1' | 3.41 | 4.32 |
| | 5 | GUA | H3' | 5 | GUA | H8 | 4.07 | 4.7 |
| | 6 | CYT | H6 | 5 | GUA | H1' | 2.36 | 3.14 |
| | 7 | UBX | H3' | 7 | UBX | H4' | 1.94 | 2.7 |
| | 8 | ADE | H2 | 7 | UBX | H15 | 2.87 | 3.89 |
| | 8 | ADE | H2 | 7 | UBX | H14 | 2.8 | 3.87 |
| | 9 | GUA | H2'1 | 9 | GUA | H1' | 2.71 | 3.38 |
| | 9 | GUA | H2'2 | 9 | GUA | H1' | 1.67 | 2.56 |
| | 10 | THY | H6 | 10 | THY | H1' | 3.3 | 4.21 |
| | 11 | CYT | H6 | 11 | CYT | H1' | 3.22 | 4.19 |
| | 12 | CYT | H6 | 12 | CYT | H1' | 3.3 | 4.39 |
| | 12 | CYT | H3' | 12 | CYT | H1' | 3.72 | 4.55 |
| | 13 | GUA | H2'2 | 13 | GUA | H1' | 1.55 | 2.46 |
| | 14 | GUA | H1' | 14 | GUA | H4' | 3.01 | 3.98 |
| | 14 | GUA | H8 | 14 | GUA | H1' | 3.54 | 4.2 |
| | 14 | GUA | H3' | 14 | GUA | H8 | 3.73 | 4.71 |
| | 14 | GUA | H2'2 | 14 | GUA | H1' | 1.65 | 2.43 |
| | 15 | ADE | H3' | 15 | ADE | H4' | 2.38 | 3.17 |
| | 15 | ADE | H2'2 | 15 | ADE | H1' | 1.7 | 2.41 |
| | 16 | CYT | H1' | 15 | ADE | H2 | 3.98 | 4.82 |
| | 16 | CYT | H6 | 15 | ADE | H2'2 | 1.89 | 2.52 |
| | 16 | CYT | H6 | 16 | CYT | H1' | 3.14 | 4.15 |
| | 16 | CYT | H5 | 15 | ADE | H8 | 3.41 | 4.14 |
| | 16 | CYT | H2'1 | 16 | CYT | H1' | 2.43 | 3.16 |
| | 16 | CYT | H2'1 | 16 | CYT | H6 | 1.88 | 2.68 |
| | 17 | THY | M7 | 16 | CYT | H5 | 3.29 | 3.99 |
| | 18 | THY | H1' | 18 | THY | H4' | 2.86 | 4.03 |
| | 18 | THY | M7 | 18 | THY | H6 | 2.8 | 3.87 |
| | 18 | THY | H2'1 | 18 | THY | H1' | 2.74 | 3.51 |
| | 18 | THY | H2'1 | 18 | THY | H6 | 1.65 | 2.41 |
| | 18 | THY | H2'1 | 18 | THY | H3' | 1.91 | 2.88 |
| | 18 | THY | H2'2 | 18 | THY | H1' | 1.8 | 2.49 |
| | 18 | THY | H2'2 | 18 | THY | H3' | 2.43 | 3.29 |

**Table B-3:** Continued

| | Residue Number | Residue Name | Atom Number | Residue Number | Residue Name | Atom Number | Lower Bound | Upper Bound |
|---|---|---|---|---|---|---|---|---|
| | 20 | CYT | H6 | 20 | CYT | H1' | 3.17 | 3.92 |
| | 23 | GUA | H1' | 23 | GUA | H4' | 3.1 | 3.96 |
| | 23 | GUA | H2'1 | 23 | GUA | H1' | 2.46 | 3.41 |
| | 23 | GUA | H2'2 | 23 | GUA | H1' | 1.8 | 2.56 |
| | 3 | THY | M7 | 2 | CYT | H1' | 3.75 | 5.13 |
| | 5 | GUA | H3' | 5 | GUA | H1' | 3.4 | 4.1 |
| | 6 | CYT | H3' | 6 | CYT | H1' | 3.52 | 4.21 |
| | 7 | UBX | H3' | 7 | UBX | H1' | 3.47 | 4.11 |
| | 7 | UBX | H2'2 | 7 | UBX | H4' | 3.68 | 4.23 |
| | 8 | ADE | H2 | 7 | UBX | H9 | 3.65 | 4.8 |
| | 8 | ADE | H2 | 7 | UBX | H12 | 3.86 | 5.13 |
| | 18 | THY | H1' | 7 | UBX | H12 | 4.86 | 6.13 |
| | 8 | ADE | H2 | 7 | UBX | H13 | 4.25 | 5.46 |
| | 17 | THY | H6 | 7 | UBX | H12 | 6.06 | 7.13 |
| | 17 | THY | H6 | 7 | UBX | H13 | 6.05 | 7.06 |
| | 8 | ADE | H3' | 8 | ADE | H1' | 3.42 | 4.32 |
| | 14 | GUA | H3' | 14 | GUA | H1' | 3.22 | 4.07 |
| | 16 | CYT | H5 | 15 | ADE | H2'1 | 2.47 | 3.58 |
| | 16 | CYT | H5 | 15 | ADE | H2'2 | 2.37 | 3.23 |
| | 23 | GUA | H3' | 23 | GUA | H1' | 3.45 | 4.27 |
| | 23 | GUA | H2'2 | 23 | GUA | H4' | 3.68 | 4.44 |
| | 24 | CYT | H6 | 23 | GUA | H2'1 | 2.74 | 3.77 |
| | 24 | CYT | H5 | 23 | GUA | H2'2 | 2.85 | 3.29 |
| | 20 | CYT | H3' | 20 | CYT | H1' | 3.42 | 4.1 |
| Class 3 | 1 | GUA | H2'1 | 1 | GUA | H1' | 2.99 | 3.32 |
| | 2 | CYT | H5 | 1 | GUA | H8 | 3.12 | 4.34 |
| | 2 | CYT | H5 | 1 | GUA | H2'1 | 2.64 | 3.52 |
| | 2 | CYT | H5 | 1 | GUA | H2'2 | 2.4 | 3.25 |
| | 2 | CYT | H2'1 | 2 | CYT | H1' | 2.96 | 3.29 |
| | 3 | THY | M7 | 2 | CYT | H6 | 3.26 | 4.58 |
| | 5 | GUA | H1' | 5 | GUA | H4' | 2.91 | 3.78 |
| | 5 | GUA | H8 | 4 | ADE | H2'1 | 3.13 | 3.98 |
| | 5 | GUA | H8 | 4 | ADE | H2'2 | 1.88 | 2.85 |
| | 5 | GUA | H2'1 | 5 | GUA | H1' | 2.43 | 3.57 |
| | 5 | GUA | H2'2 | 5 | GUA | H8 | 2.91 | 4.41 |
| | 5 | GUA | H2'2 | 5 | GUA | H3' | 2.04 | 3.16 |
| | 6 | CYT | H5 | 5 | GUA | H8 | 2.95 | 4.17 |
| | 6 | CYT | H5 | 6 | CYT | H6 | 1.74 | 2.41 |
| | 7 | UBX | H5 | 7 | UBX | H6 | 1.73 | 2.51 |
| | 7 | UBX | H3' | 7 | UBX | H6 | 3.45 | 4.32 |
| | 7 | UBX | H2'1 | 7 | UBX | H1' | 2.12 | 3.37 |
| | 7 | UBX | H2'1 | 7 | UBX | H3' | 1.83 | 2.79 |
| | 7 | UBX | H2'2 | 7 | UBX | H1' | 1.81 | 2.55 |
| | 7 | UBX | H2'2 | 7 | UBX | H3' | 1.94 | 3.25 |
| | 8 | ADE | H3' | 8 | ADE | H5'1 | 3.1 | 4.23 |
| | 9 | GUA | H8 | 8 | ADE | H1' | 3.6 | 4.63 |

**Table B-3:** Continued

| Residue Number | Residue Name | Atom Number | Residue Number | Residue Name | Atom Number | Lower Bound | Upper Bound |
|---|---|---|---|---|---|---|---|
| 10 | THY | H6 | 9 | GUA | H2'2 | 1.95 | 2.47 |
| 10 | THY | M7 | 9 | GUA | H1' | 3.67 | 4.6 |
| 10 | THY | H2'2 | 10 | THY | H1' | 1.75 | 2.4 |
| 11 | CYT | H5 | 10 | THY | M7 | 4.41 | 5.2 |
| 11 | CYT | H3' | 11 | CYT | H6 | 3.48 | 4.39 |
| 12 | CYT | H1' | 12 | CYT | H4' | 3.14 | 4.24 |
| 12 | CYT | H6 | 11 | CYT | H2'2 | 1.97 | 2.43 |
| 13 | GUA | H2'1 | 13 | GUA | H1' | 2.51 | 3.39 |
| 14 | GUA | H2'1 | 14 | GUA | H1' | 2.58 | 3.47 |
| 15 | ADE | H1' | 15 | ADE | H4' | 3.08 | 4.04 |
| 15 | ADE | H8 | 14 | GUA | H1' | 2.48 | 3.16 |
| 15 | ADE | H2'1 | 15 | ADE | H1' | 2.31 | 3.36 |
| 16 | CYT | H5 | 16 | CYT | H6 | 1.66 | 2.5 |
| 16 | CYT | H2'2 | 16 | CYT | H1' | 1.8 | 2.67 |
| 16 | CYT | H2'2 | 16 | CYT | H6 | 2.64 | 3.73 |
| 17 | THY | H6 | 16 | CYT | H2'1 | 3.16 | 4.25 |
| 17 | THY | M7 | 17 | THY | H6 | 1.8 | 3.56 |
| 18 | THY | M7 | 17 | THY | H6 | 3.22 | 4.62 |
| 18 | THY | H3' | 18 | THY | H4' | 1.8 | 2.68 |
| 18 | THY | H2'2 | 18 | THY | H6 | 2.73 | 3.54 |
| 19 | GUA | H4' | 19 | GUA | H5'1 | 1.8 | 2.7 |
| 19 | GUA | H3' | 19 | GUA | H5'1 | 3.14 | 4 |
| 19 | GUA | H3' | 19 | GUA | H8 | 3.8 | 4.84 |
| 20 | CYT | H1' | 20 | CYT | H4' | 2.93 | 3.9 |
| 20 | CYT | H5 | 19 | GUA | H8 | 3.4 | 4.5 |
| 20 | CYT | H3' | 20 | CYT | H6 | 3.54 | 4.2 |
| 20 | CYT | H2'1 | 20 | CYT | H1' | 2.86 | 3.33 |
| 20 | CYT | H2'2 | 20 | CYT | H1' | 1.8 | 2.49 |
| 23 | GUA | H8 | 22 | ADE | H2'1 | 3.11 | 3.9 |
| 23 | GUA | H8 | 22 | ADE | H2'2 | 2.02 | 2.7 |
| 23 | GUA | H3' | 23 | GUA | H8 | 3.87 | 4.82 |
| 23 | GUA | H2'1 | 23 | GUA | H3' | 1.75 | 3.28 |
| 24 | CYT | H6 | 23 | GUA | H2'2 | 2.06 | 2.86 |
| 24 | CYT | H6 | 24 | CYT | H1' | 3.4 | 3.9 |
| 24 | CYT | H5 | 24 | CYT | H6 | 1.84 | 2.58 |
| 24 | CYT | H3' | 24 | CYT | H6 | 3.45 | 4.4 |
| 24 | CYT | H2'1 | 24 | CYT | H3' | 2.22 | 2.91 |
| 1 | GUA | H8 | 1 | GUA | H4' | 4.44 | 5.24 |
| 2 | CYT | H5 | 1 | GUA | H1' | 3.31 | 4.25 |
| 2 | CYT | H2'1 | 2 | CYT | H5 | 3.95 | 4.56 |
| 5 | GUA | H8 | 4 | ADE | H3' | 4.67 | 5.28 |
| 5 | GUA | H2'2 | 5 | GUA | H4' | 3.8 | 4.31 |
| 6 | CYT | H6 | 6 | CYT | H5' | 2.59 | 3.55 |
| 7 | UBX | H9 | 7 | UBX | H15 | 1.82 | 2.99 |
| 7 | UBX | H9 | 7 | UBX | H14 | 1.82 | 3.04 |
| 9 | GUA | H2'1 | 9 | GUA | H4' | 3.37 | 4.22 |

**Table B-3:** Continued

| | Residue Number | Residue Name | Atom Number | Residue Number | Residue Name | Atom Number | Lower Bound | Upper Bound |
|---|---|---|---|---|---|---|---|---|
| | 10 | THY | M7 | 9 | GUA | H2'2 | 1.94 | 4.1 |
| | 11 | CYT | H5 | 10 | THY | H6 | 3.25 | 3.96 |
| | 13 | GUA | H8 | 13 | GUA | H4' | 4.26 | 5.32 |
| | 14 | GUA | H8 | 14 | GUA | H4' | 4.54 | 5.33 |
| | 14 | GUA | H2'2 | 14 | GUA | H4' | 3.41 | 4.4 |
| | 15 | ADE | H8 | 15 | ADE | H4' | 4.42 | 5.3 |
| | 15 | ADE | H3' | 15 | ADE | H1' | 3.22 | 4.19 |
| | 15 | ADE | H2'1 | 15 | ADE | H4' | 3.17 | 4.13 |
| | 15 | ADE | H2'2 | 15 | ADE | H4' | 3.75 | 4.28 |
| | 18 | THY | H3' | 18 | THY | H1' | 3.53 | 4.44 |
| | 18 | THY | H2'1 | 18 | THY | H4' | 3.42 | 4.11 |
| | 18 | THY | H2'2 | 18 | THY | H4' | 3.26 | 4.25 |
| | 19 | GUA | H8 | 19 | GUA | H4' | 4.36 | 5.19 |
| | 19 | GUA | H3' | 19 | GUA | H1' | 3.36 | 4.45 |
| | 21 | THY | M7 | 20 | CYT | H1' | 3.72 | 4.32 |
| | 23 | GUA | H8 | 22 | ADE | H3' | 4.74 | 5.27 |
| | 24 | CYT | H2'2 | 24 | CYT | H3' | 2.39 | 3.51 |
| | 18 | THY | M7 | 17 | THY | H1' | 3.72 | 5.18 |
| | 19 | GUA | H8 | 18 | THY | H3' | 4.4 | 5.48 |
| | 20 | CYT | H2'1 | 20 | CYT | H4' | 3.25 | 4.19 |
| | 7 | UBX | H2'1 | 7 | UBX | H4' | 2.93 | 3.93 |
| | 8 | ADE | H5'1 | 7 | UBX | H1' | 2.04 | 3.75 |
| | 8 | ADE | H8 | 7 | UBX | H2'1 | 4.53 | 5.34 |
| | 3 | THY | H6 | 2 | CYT | H1' | 1.88 | 2.97 |
| | 5 | GUA | H8 | 4 | ADE | H1' | 2.43 | 3.4 |
| | 10 | THY | H6 | 9 | GUA | H1' | 2.45 | 3.24 |
| | 21 | THY | H6 | 20 | CYT | H1' | 1.97 | 3.45 |
| | 23 | GUA | H8 | 22 | ADE | H1' | 2.52 | 3.13 |
| | 24 | CYT | H6 | 23 | GUA | H1' | 2.21 | 2.95 |
| Class 4 | 2 | CYT | H2'1 | 2 | CYT | H6 | 1.67 | 2.32 |
| | 3 | THY | H6 | 2 | CYT | H2'2 | 1.62 | 2.62 |
| | 3 | THY | H6 | 3 | THY | H1' | 3.45 | 4.02 |
| | 3 | THY | M7 | 2 | CYT | H5 | 3.36 | 4.39 |
| | 4 | ADE | H3' | 4 | ADE | H4' | 1.95 | 2.89 |
| | 5 | GUA | H2'1 | 5 | GUA | H8 | 1.86 | 2.55 |
| | 5 | GUA | H2'1 | 5 | GUA | H3' | 1.82 | 3.01 |
| | 5 | GUA | H2'2 | 5 | GUA | H1' | 1.62 | 2.43 |
| | 6 | CYT | H6 | 5 | GUA | H2'2 | 1.89 | 2.42 |
| | 7 | UBX | H2'1 | 7 | UBX | H6 | 1.77 | 2.57 |
| | 7 | UBX | H2'2 | 7 | UBX | H6 | 3.13 | 3.7 |
| | 8 | ADE | H4' | 8 | ADE | H5'1 | 1.63 | 2.91 |
| | 8 | ADE | H3' | 8 | ADE | H5'2 | 1.82 | 3.15 |
| | 10 | THY | M7 | 9 | GUA | H8 | 2.63 | 3.83 |
| | 10 | THY | M7 | 10 | THY | H6 | 2.87 | 3.91 |
| | 10 | THY | H2'2 | 10 | THY | H6 | 2.8 | 3.54 |
| | 11 | CYT | H6 | 10 | THY | H2'2 | 1.8 | 2.56 |

**Table B-3:** Continued

| Residue Number | Residue Name | Atom Number | Residue Number | Residue Name | Atom Number | Lower Bound | Upper Bound |
|---|---|---|---|---|---|---|---|
| 11 | CYT | H2'2 | 11 | CYT | H6 | 2.53 | 3.79 |
| 12 | CYT | H5 | 12 | CYT | H6 | 1.69 | 2.76 |
| 13 | GUA | H3' | 13 | GUA | H8 | 3.3 | 4.51 |
| 14 | GUA | H3' | 14 | GUA | H5'1 | 3.56 | 4.27 |
| 14 | GUA | H2'2 | 14 | GUA | H8 | 3.36 | 4.11 |
| 15 | ADE | H3' | 15 | ADE | H5'2 | 2.18 | 3.17 |
| 16 | CYT | H6 | 15 | ADE | H2'1 | 2.76 | 4.16 |
| 16 | CYT | H2'1 | 16 | CYT | H3' | 1.88 | 2.77 |
| 17 | THY | M7 | 16 | CYT | H6 | 2.93 | 4.74 |
| 17 | THY | H2'1 | 17 | THY | H1' | 1.88 | 3.23 |
| 17 | THY | H2'2 | 17 | THY | H1' | 1.92 | 2.54 |
| 18 | THY | H3' | 18 | THY | H6 | 2.82 | 4.36 |
| 19 | GUA | H1' | 19 | GUA | H4' | 2.76 | 3.98 |
| 19 | GUA | H8 | 18 | THY | H2'2 | 1.8 | 2.88 |
| 20 | CYT | H6 | 19 | GUA | H1' | 2.13 | 3.34 |
| 20 | CYT | H5 | 20 | CYT | H6 | 1.63 | 2.57 |
| 20 | CYT | H3' | 20 | CYT | H4' | 1.71 | 3.04 |
| 20 | CYT | H2'1 | 20 | CYT | H6 | 1.79 | 2.76 |
| 20 | CYT | H2'1 | 20 | CYT | H3' | 1.86 | 2.67 |
| 23 | GUA | H2'2 | 23 | GUA | H8 | 2.95 | 3.97 |
| 23 | GUA | H2'2 | 23 | GUA | H3' | 1.82 | 3.21 |
| 24 | CYT | H5 | 23 | GUA | H8 | 3.48 | 4.31 |
| 3 | THY | M7 | 2 | CYT | H2'2 | 2.3 | 3.56 |
| 3 | THY | H3' | 3 | THY | H6 | 3.51 | 4.31 |
| 5 | GUA | H2'1 | 5 | GUA | H4' | 3.53 | 3.97 |
| 6 | CYT | H5 | 5 | GUA | H2'1 | 2.42 | 3.55 |
| 6 | CYT | H5 | 5 | GUA | H2'2 | 2.21 | 3.46 |
| 8 | ADE | H3' | 8 | ADE | H8 | 3.79 | 4.7 |
| 12 | CYT | H6 | 11 | CYT | H1' | 2.47 | 3.15 |
| 12 | CYT | H5 | 11 | CYT | H2'1 | 2.59 | 3.57 |
| 14 | GUA | H8 | 13 | GUA | H3' | 4.64 | 5.28 |
| 15 | ADE | H4' | 15 | ADE | H5'1 | 1.81 | 2.84 |
| 15 | ADE | H4' | 15 | ADE | H5'2 | 1.8 | 2.42 |
| 16 | CYT | H3' | 16 | CYT | H1' | 3.28 | 4.55 |
| 16 | CYT | H2'1 | 16 | CYT | H4' | 2.92 | 3.97 |
| 16 | CYT | H2'2 | 16 | CYT | H3' | 1.81 | 2.93 |
| 17 | THY | M7 | 16 | CYT | H3' | 4.4 | 5.72 |
| 17 | THY | H3' | 17 | THY | H6 | 2.83 | 4.3 |
| 20 | CYT | H5 | 19 | GUA | H1' | 3.04 | 4.01 |
| 20 | CYT | H2'2 | 20 | CYT | H3' | 2.23 | 3.09 |
| 21 | THY | M7 | 20 | CYT | H3' | 3.94 | 5.3 |
| 23 | GUA | H2'1 | 23 | GUA | H4' | 2.96 | 4.01 |
| 8 | ADE | H2 | 8 | ADE | H1' | 3.68 | 5.11 |
| 9 | GUA | H1' | 8 | ADE | H2 | 4.14 | 5.32 |
| 12 | CYT | H5 | 11 | CYT | H2'2 | 2.13 | 3.46 |
| 16 | CYT | H5'1 | 15 | ADE | H1' | 1.8 | 2.54 |

**Table B-3:** Continued

| | Residue Number | Residue Name | Atom Number | Residue Number | Residue Name | Atom Number | Lower Bound | Upper Bound |
|---|---|---|---|---|---|---|---|---|
| | 16 | CYT | H2'1 | 16 | CYT | H5 | 3.8 | 4.74 |
| | 18 | THY | H6 | 17 | THY | H2'2 | 3.34 | 4.25 |
| | 6 | CYT | H6 | 5 | GUA | H2'1 | 2.81 | 3.96 |
| Class 5 | 1 | GUA | H3' | 1 | GUA | H8 | 3.82 | 4.79 |
| | 1 | GUA | H2'1 | 1 | GUA | H8 | 1.69 | 2.41 |
| | 1 | GUA | H2'2 | 1 | GUA | H8 | 3.29 | 4 |
| | 3 | THY | M7 | 3 | THY | H6 | 2.54 | 3.75 |
| | 3 | THY | H2'1 | 3 | THY | H1' | 2.54 | 3.47 |
| | 3 | THY | H2'2 | 3 | THY | H1' | 1.64 | 2.56 |
| | 4 | ADE | H4' | 4 | ADE | H5'1 | 1.93 | 2.71 |
| | 4 | ADE | H3' | 4 | ADE | H5'1 | 3.41 | 4.45 |
| | 4 | ADE | H3' | 4 | ADE | H5'2 | 2.48 | 2.98 |
| | 4 | ADE | H2'1 | 4 | ADE | H1' | 2.36 | 3.4 |
| | 4 | ADE | H2'2 | 4 | ADE | H1' | 1.88 | 2.77 |
| | 4 | ADE | H2'2 | 4 | ADE | H3' | 1.87 | 2.76 |
| | 5 | GUA | H3' | 5 | GUA | H4' | 2.3 | 2.98 |
| | 6 | CYT | H2'1 | 6 | CYT | H1' | 2.42 | 3.21 |
| | 6 | CYT | H2'2 | 6 | CYT | H1' | 1.91 | 2.64 |
| | 7 | UBX | H6 | 7 | UBX | H1' | 3.2 | 3.93 |
| | 8 | ADE | H8 | 7 | UBX | H3' | 4.58 | 5.27 |
| | 8 | ADE | H8 | 7 | UBX | H2'2 | 4.38 | 5.12 |
| | 8 | ADE | H3' | 8 | ADE | H4' | 2 | 3.16 |
| | 8 | ADE | H2'1 | 8 | ADE | H1' | 2.33 | 3.34 |
| | 8 | ADE | H2'1 | 8 | ADE | H3' | 2.02 | 2.85 |
| | 8 | ADE | H2'2 | 8 | ADE | H1' | 1.82 | 2.78 |
| | 8 | ADE | H2'2 | 8 | ADE | H3' | 2.24 | 3.14 |
| | 9 | GUA | H2'1 | 9 | GUA | H8 | 1.64 | 2.61 |
| | 9 | GUA | H2'2 | 9 | GUA | H8 | 3.66 | 4.11 |
| | 10 | THY | H2'1 | 10 | THY | H6 | 1.69 | 2.44 |
| | 11 | CYT | H6 | 10 | THY | H1' | 2.21 | 3.18 |
| | 11 | CYT | H5 | 11 | CYT | H6 | 1.76 | 2.59 |
| | 11 | CYT | H2'1 | 11 | CYT | H1' | 2.56 | 3.2 |
| | 12 | CYT | H2'1 | 12 | CYT | H1' | 2.83 | 3.17 |
| | 12 | CYT | H2'1 | 12 | CYT | H6 | 1.8 | 2.33 |
| | 12 | CYT | H2'2 | 12 | CYT | H1' | 1.75 | 2.68 |
| | 12 | CYT | H2'2 | 12 | CYT | H6 | 2.42 | 3.99 |
| | 12 | CYT | H2'2 | 12 | CYT | H3' | 1.8 | 3.29 |
| | 13 | GUA | H8 | 13 | GUA | H1' | 3.35 | 4.23 |
| | 13 | GUA | H2'1 | 13 | GUA | H8 | 1.61 | 2.33 |
| | 14 | GUA | H8 | 13 | GUA | H1' | 2.32 | 2.94 |
| | 14 | GUA | H8 | 13 | GUA | H2'1 | 3.02 | 4.21 |
| | 14 | GUA | H3' | 14 | GUA | H5'2 | 1.68 | 3.35 |
| | 14 | GUA | H3' | 14 | GUA | H4' | 1.82 | 2.98 |
| | 14 | GUA | H2'1 | 14 | GUA | H3' | 1.69 | 3.18 |
| | 14 | GUA | H2'2 | 14 | GUA | H3' | 2.29 | 3.17 |
| | 15 | ADE | H3' | 15 | ADE | H5'1 | 3.39 | 4.04 |

**Table B-3:** Continued

| Residue Number | Residue Name | Atom Number | Residue Number | Residue Name | Atom Number | Lower Bound | Upper Bound |
|---|---|---|---|---|---|---|---|
| 15 | ADE | H2'1 | 15 | ADE | H3' | 1.75 | 2.84 |
| 15 | ADE | H2'2 | 15 | ADE | H3' | 2.57 | 3.37 |
| 16 | CYT | H3' | 16 | CYT | H6 | 3.44 | 4.13 |
| 17 | THY | H6 | 16 | CYT | H2'2 | 2.02 | 2.85 |
| 17 | THY | H2'2 | 17 | THY | H6 | 2.82 | 3.54 |
| 18 | THY | H6 | 18 | THY | H1' | 3.46 | 4.15 |
| 19 | GUA | H8 | 18 | THY | H2'1 | 3.43 | 4.4 |
| 19 | GUA | H3' | 19 | GUA | H5'2 | 2.2 | 3.08 |
| 19 | GUA | H3' | 19 | GUA | H4' | 1.87 | 2.63 |
| 21 | THY | H6 | 20 | CYT | H2'1 | 3.04 | 4.23 |
| 21 | THY | H6 | 21 | THY | H1' | 3.35 | 4.19 |
| 21 | THY | M7 | 20 | CYT | H6 | 3 | 4.88 |
| 21 | THY | M7 | 20 | CYT | H5 | 3.58 | 5.3 |
| 21 | THY | M7 | 21 | THY | H6 | 2.28 | 3.51 |
| 21 | THY | H2'1 | 21 | THY | H1' | 2.57 | 3.19 |
| 21 | THY | H2'2 | 21 | THY | H1' | 1.62 | 2.48 |
| 21 | THY | H2'2 | 21 | THY | H6 | 3.06 | 3.69 |
| 22 | ADE | H4' | 22 | ADE | H5'1 | 1.61 | 2.74 |
| 22 | ADE | H1' | 22 | ADE | H4' | 3.07 | 4.01 |
| 22 | ADE | H3' | 22 | ADE | H5'1 | 3.37 | 3.95 |
| 22 | ADE | H3' | 22 | ADE | H5'2 | 2.36 | 3.47 |
| 22 | ADE | H3' | 22 | ADE | H4' | 1.93 | 3.21 |
| 22 | ADE | H2'1 | 22 | ADE | H1' | 2.26 | 3.46 |
| 22 | ADE | H2'2 | 22 | ADE | H1' | 1.8 | 2.56 |
| 22 | ADE | H2'2 | 22 | ADE | H3' | 2.3 | 3.09 |
| 23 | GUA | H2'1 | 23 | GUA | H8 | 1.72 | 2.29 |
| 24 | CYT | H3' | 24 | CYT | H4' | 1.81 | 2.74 |
| 24 | CYT | H2'1 | 24 | CYT | H1' | 2.97 | 3.35 |
| 24 | CYT | H2'2 | 24 | CYT | H1' | 1.57 | 2.6 |
| 3 | THY | H2'1 | 3 | THY | H6 | 1.7 | 2.24 |
| 4 | ADE | H8 | 3 | THY | H1' | 2.4 | 3.08 |
| 4 | ADE | H8 | 3 | THY | H2'2 | 2.12 | 2.88 |
| 4 | ADE | H8 | 4 | ADE | H1' | 3.32 | 4.1 |
| 4 | ADE | H3' | 4 | ADE | H8 | 3.75 | 4.84 |
| 4 | ADE | H2'1 | 4 | ADE | H3' | 2.02 | 2.68 |
| 5 | GUA | H3' | 5 | GUA | H5'2 | 2.46 | 3.2 |
| 5 | GUA | H3' | 5 | GUA | H5'1 | 3.22 | 4.38 |
| 6 | CYT | H2'1 | 6 | CYT | H6 | 1.87 | 2.55 |
| 6 | CYT | H2'1 | 6 | CYT | H3' | 2.03 | 2.68 |
| 6 | CYT | H2'2 | 6 | CYT | H6 | 2.8 | 3.88 |
| 6 | CYT | H2'2 | 6 | CYT | H3' | 2.37 | 3 |
| 8 | ADE | H2'1 | 8 | ADE | H8 | 1.91 | 2.38 |
| 8 | ADE | H2'2 | 8 | ADE | H8 | 2.87 | 3.91 |
| 9 | GUA | H8 | 8 | ADE | H2'1 | 3.31 | 4.39 |
| 9 | GUA | H8 | 8 | ADE | H2'2 | 2.14 | 2.97 |
| 10 | THY | H3' | 10 | THY | H6 | 3.75 | 4.34 |

**Table B-3:** Continued

| Residue Number | Residue Name | Atom Number | Residue Number | Residue Name | Atom Number | Lower Bound | Upper Bound |
|---|---|---|---|---|---|---|---|
| 11 | CYT | H5 | 10 | THY | H2'1 | 2.61 | 3.69 |
| 11 | CYT | H5 | 10 | THY | H2'2 | 2.48 | 3.49 |
| 11 | CYT | H2'1 | 11 | CYT | H6 | 1.79 | 2.43 |
| 11 | CYT | H2'1 | 11 | CYT | H5 | 3.78 | 4.73 |
| 12 | CYT | H6 | 11 | CYT | H2'1 | 3.04 | 3.82 |
| 12 | CYT | H2'1 | 12 | CYT | H3' | 1.7 | 3.14 |
| 13 | GUA | H2'2 | 13 | GUA | H8 | 3.11 | 3.98 |
| 14 | GUA | H2'1 | 14 | GUA | H8 | 1.7 | 2.51 |
| 17 | THY | M7 | 6 | CYT | H5 | 4.05 | 4.82 |
| 17 | THY | M7 | 16 | CYT | H1' | 3.17 | 5.09 |
| 17 | THY | H2'1 | 17 | THY | H6 | 1.73 | 2.53 |
| 19 | GUA | H2'1 | 19 | GUA | H1' | 1.84 | 3.32 |
| 19 | GUA | H2'1 | 19 | GUA | H8 | 1.85 | 2.75 |
| 19 | GUA | H2'2 | 19 | GUA | H1' | 1.88 | 2.79 |
| 19 | GUA | H2'2 | 19 | GUA | H8 | 2.74 | 3.89 |
| 20 | CYT | H6 | 19 | GUA | H2'1 | 3.16 | 3.76 |
| 20 | CYT | H6 | 19 | GUA | H2'2 | 1.8 | 2.86 |
| 20 | CYT | H2'1 | 20 | CYT | H5 | 3.79 | 4.55 |
| 20 | CYT | H2'2 | 20 | CYT | H6 | 2.87 | 3.69 |
| 21 | THY | H6 | 20 | CYT | H2'2 | 1.98 | 2.62 |
| 21 | THY | H2'1 | 21 | THY | H6 | 1.53 | 2.32 |
| 22 | ADE | H8 | 21 | THY | H1' | 2.38 | 3.21 |
| 22 | ADE | H8 | 21 | THY | H2'2 | 1.8 | 2.87 |
| 22 | ADE | H5'1 | 21 | THY | H1' | 1.86 | 3.01 |
| 22 | ADE | H8 | 21 | THY | H2'1 | 3.35 | 4.2 |
| 22 | ADE | H8 | 22 | ADE | H1' | 3.3 | 4.02 |
| 22 | ADE | H3' | 22 | ADE | H8 | 3.86 | 4.81 |
| 22 | ADE | H2'1 | 22 | ADE | H3' | 1.85 | 2.87 |
| 23 | GUA | H3' | 23 | GUA | H5'1 | 3.69 | 4.3 |
| 23 | GUA | H3' | 23 | GUA | H5'2 | 2.4 | 3.21 |
| 24 | CYT | H6 | 24 | CYT | H4' | 4.4 | 5.06 |
| 24 | CYT | H2'1 | 24 | CYT | H6 | 1.8 | 2.34 |
| 24 | CYT | H2'2 | 24 | CYT | H6 | 2.53 | 3.5 |
| 1 | GUA | H8 | 1 | GUA | H5'1 | 3.18 | 3.84 |
| 1 | GUA | H8 | 1 | GUA | H5'2 | 4 | 4.73 |
| 2 | CYT | H6 | 1 | GUA | H8 | 4.64 | 5.25 |
| 3 | THY | H6 | 2 | CYT | H2'1 | 3.16 | 3.82 |
| 3 | THY | H6 | 3 | THY | H4' | 3.92 | 4.81 |
| 3 | THY | H2'2 | 3 | THY | H6 | 2.98 | 3.53 |
| 4 | ADE | H4' | 4 | ADE | H5'2 | 1.68 | 2.47 |
| 4 | ADE | H3' | 4 | ADE | H1' | 3.42 | 4.16 |
| 5 | GUA | H8 | 4 | ADE | H8 | 4.47 | 5.3 |
| 6 | CYT | H6 | 5 | GUA | H8 | 4.79 | 5.25 |
| 7 | UBX | H2'1 | 7 | UBX | H5 | 3.88 | 4.48 |
| 9 | GUA | H8 | 8 | ADE | H8 | 4.55 | 5.5 |
| 10 | THY | M7 | 9 | GUA | H2'1 | 2.47 | 3.41 |

**Table B-3:** Continued

| Residue Number | Residue Name | Atom Number | Residue Number | Residue Name | Atom Number | Lower Bound | Upper Bound |
|---|---|---|---|---|---|---|---|
| 11 | CYT | H6 | 10 | THY | H2'1 | 3.09 | 3.85 |
| 12 | CYT | H2'1 | 12 | CYT | H5 | 3.61 | 4.41 |
| 12 | CYT | H2'2 | 12 | CYT | H5 | 5.06 | 5.56 |
| 13 | GUA | H8 | 13 | GUA | H5'2 | 3.62 | 5.09 |
| 14 | GUA | H8 | 13 | GUA | H2'2 | 1.88 | 2.75 |
| 15 | ADE | H8 | 14 | GUA | H8 | 4.6 | 5.17 |
| 15 | ADE | H8 | 14 | GUA | H3' | 4.54 | 5.39 |
| 15 | ADE | H8 | 14 | GUA | H2'1 | 3.07 | 3.99 |
| 15 | ADE | H3' | 15 | ADE | H8 | 3.72 | 4.77 |
| 15 | ADE | H2'1 | 15 | ADE | H8 | 1.69 | 2.41 |
| 16 | CYT | H6 | 15 | ADE | H8 | 4.68 | 5.37 |
| 19 | GUA | H2'1 | 19 | GUA | H3' | 1.8 | 2.78 |
| 19 | GUA | H2'2 | 19 | GUA | H3' | 1.82 | 2.86 |
| 21 | THY | H6 | 21 | THY | H4' | 3.78 | 5.02 |
| 21 | THY | M7 | 20 | CYT | H2'2 | 2.51 | 3.88 |
| 22 | ADE | H4' | 22 | ADE | H5'2 | 1.76 | 2.46 |
| 22 | ADE | H3' | 22 | ADE | H1' | 3.34 | 4.29 |
| 10 | THY | H2'1 | 10 | THY | H1' | 2.43 | 3.23 |
| 12 | CYT | H3' | 12 | CYT | H4' | 1.8 | 3.09 |
| 14 | GUA | H4' | 14 | GUA | H5'1 | 1.84 | 2.65 |
| 15 | ADE | H2'2 | 15 | ADE | H8 | 3.4 | 4.09 |
| 22 | ADE | H2'1 | 22 | ADE | H4' | 3.26 | 3.97 |
| 22 | ADE | H2'2 | 22 | ADE | H4' | 3.33 | 4.25 |
| 6 | CYT | H3' | 7 | UBX | H6 | 4.9 | 6 |
| 6 | CYT | H1' | 7 | UBX | H6 | 5 | 6 |
| 17 | THY | H1' | 7 | UBX | H12 | 5.1 | 6.49 |
| 17 | THY | H1' | 7 | UBX | H11 | 5.1 | 6.49 |
| 17 | THY | M7 | 7 | UBX | H5 | 3.75 | 6.22 |
| 18 | THY | M7 | 7 | UBX | H5 | 3.12 | 5.56 |
| 18 | THY | M7 | 6 | CYT | H5 | 3.8 | 6.37 |
| 13 | GUA | H5'1 | 13 | GUA | H3' | 3.5 | 4.3 |
| 13 | GUA | H4' | 13 | GUA | H1' | 3 | 4 |
| 4 | ADE | H8 | 3 | CYT | H6 | 4.75 | 5.25 |
| 14 | GUA | H5'1 | 13 | GUA | H2'2 | 3.7 | 4.1 |
| 4 | ADE | H5'1 | 3 | CYT | H2'2 | 3.7 | 4.1 |
| 21 | THY | H3' | 21 | THY | H5'1 | 3.5 | 4.1 |
| 6 | CYT | H3' | 6 | CYT | H5'1 | 3.5 | 4.1 |
| 20 | CYT | H3' | 20 | CYT | H5'1 | 3.5 | 4.1 |
| 12 | CYT | H1' | 11 | CYT | H1' | 4.75 | 5.25 |
| 2 | CYT | H3' | 2 | CYT | H5'1 | 3.5 | 4.1 |
| 2 | CYT | H1' | 1 | GUA | H1' | 4.75 | 5.25 |
| 4 | ADE | H1' | 3 | THY | H1' | 4.75 | 5.25 |
| 5 | GUA | H1' | 4 | ADE | H1' | 4.75 | 5.25 |
| 9 | GUA | H3' | 9 | CYT | H5'1 | 3.5 | 4.1 |
| 7 | UBX | H3' | 7 | UBX | H5'1 | 3.5 | 4.1 |
| 18 | THY | H3' | 18 | THY | H5'1 | 3.5 | 4.1 |

**Table B-3:** Continued

| Residue Number | Residue Name | Atom Number | Residue Number | Residue Name | Atom Number | Lower Bound | Upper Bound |
|---|---|---|---|---|---|---|---|
| 1 | GUA | H3' | 1 | GUA | H5'1 | 3.5 | 4.1 |
| 3 | THY | H3' | 3 | THY | H5'1 | 3.5 | 4.1 |
| 10 | THY | H3' | 10 | THY | H5'1 | 3.5 | 4.1 |
| 11 | CYT | H3' | 11 | CYT | H5'1 | 3.5 | 4.1 |
| 12 | CYT | H3' | 12 | CYT | H5'1 | 3.5 | 4.1 |
| 16 | CYT | H3' | 16 | CYT | H5'1 | 3.5 | 4.1 |
| 17 | THY | H3' | 17 | THY | H5'1 | 3.5 | 4.1 |
| 24 | CYT | H3' | 24 | CYT | H5'1 | 3.5 | 4.1 |
| 3 | THY | H1' | 2 | CYT | H1' | 4.75 | 5.25 |
| 6 | CYT | H1' | 5 | GUA | H1' | 4.75 | 5.25 |
| 7 | UBX | H1' | 6 | CYT | H1' | 5 | 6 |
| 8 | ADE | H1' | 7 | UBX | H1' | 5 | 6 |
| 9 | GUA | H1' | 8 | ADE | H1' | 4.75 | 5.75 |
| 10 | THY | H1' | 9 | GUA | H1' | 4.75 | 5.25 |
| 11 | CYT | H1' | 10 | THY | H1' | 4.75 | 5.25 |
| 14 | GUA | H1' | 13 | GUA | H1' | 4.75 | 5.25 |
| 15 | ADE | H1' | 14 | GUA | H1' | 4.75 | 5.25 |
| 16 | CYT | H1' | 15 | ADE | H1' | 4.75 | 5.25 |
| 17 | THY | H1' | 16 | CYT | H1' | 5 | 6 |
| 18 | THY | H1' | 17 | THY | H1' | 5 | 6 |
| 19 | GUA | H1' | 18 | THY | H1' | 4.75 | 5.75 |
| 20 | CYT | H1' | 19 | GUA | H1' | 4.75 | 5.25 |
| 21 | THY | H1' | 20 | CYT | H1' | 4.75 | 5.25 |
| 22 | ADE | H1' | 21 | THY | H1' | 4.75 | 5.25 |
| 23 | GUA | H1' | 22 | ADE | H1' | 4.75 | 5.25 |
| 24 | CYT | H1' | 23 | GUA | H1' | 4.75 | 5.25 |
| 3 | THY | H6 | 2 | CYT | H6 | 4.68 | 5.37 |
| 7 | UBX | H6 | 6 | CYT | H6 | 5.18 | 6.37 |
| 8 | ADE | H8 | 7 | UBX | H6 | 5.18 | 5.87 |
| 10 | THY | H6 | 9 | GUA | H8 | 4.68 | 5.37 |
| 11 | CYT | H6 | 10 | THY | H6 | 4.68 | 5.37 |
| 12 | CYT | H6 | 11 | CYT | H6 | 4.68 | 5.37 |
| 14 | GUA | H8 | 13 | GUA | H8 | 4.68 | 5.37 |
| 17 | THY | H6 | 16 | CYT | H6 | 5.18 | 5.87 |
| 18 | THY | H6 | 17 | THY | H6 | 5.18 | 6.37 |
| 19 | GUA | H8 | 18 | THY | H6 | 5.18 | 5.87 |
| 20 | CYT | H6 | 19 | GUA | H8 | 4.68 | 5.37 |
| 21 | THY | H6 | 20 | CYT | H6 | 4.68 | 5.37 |
| 22 | ADE | H8 | 21 | THY | H6 | 4.68 | 5.37 |
| 23 | GUA | H8 | 22 | ADE | H8 | 4.68 | 5.37 |
| 24 | CYT | H6 | 23 | GUA | H8 | 4.68 | 5.37 |
| 5 | GUA | H3' | 4 | ADE | H3' | 6.18 | 7.17 |
| 8 | ADE | H2 | 7 | UBX | H11 | 6.18 | 7.17 |
| 17 | THY | H2'1 | 16 | CYT | H2'2 | 3.58 | 4.17 |
| 17 | THY | H3' | 16 | CYT | H3' | 6.38 | 7.17 |
| 14 | GUA | H4' | 13 | GUA | H4' | 5.88 | 6.37 |

**Table B-3:** Continued

| Residue Number | Residue Name | Atom Number | Residue Number | Residue Name | Atom Number | Lower Bound | Upper Bound |
|---|---|---|---|---|---|---|---|
| 8 | ADE | H8 | 7 | UBX | H1' | 4.58 | 5.57 |
| 7 | UBX | H12 | 7 | UBX | H15 | 4.58 | 5.57 |
| 7 | UBX | H12 | 7 | UBX | H14 | 4.58 | 5.57 |
| 19 | GUA | H4' | 18 | THY | H4' | 5.88 | 6.37 |
| 18 | THY | H4' | 17 | THY | H4' | 5.88 | 6.37 |
| 17 | THY | H4' | 16 | CYT | H4' | 5.88 | 6.37 |
| 2 | CYT | H6 | 2 | CYT | H5'1 | 3.18 | 3.84 |
| 3 | THY | H6 | 3 | THY | H5'1 | 3.18 | 3.84 |
| 4 | ADE | H8 | 4 | ADE | H5'1 | 3.18 | 3.84 |
| 5 | GUA | H8 | 5 | GUA | H5'1 | 3.18 | 3.84 |
| 6 | CYT | H6 | 6 | CYT | H5'1 | 3.18 | 3.84 |
| 7 | UBX | H6 | 7 | UBX | H5'1 | 3.18 | 3.84 |
| 8 | ADE | H8 | 8 | ADE | H5'1 | 3.18 | 3.84 |
| 9 | GUA | H8 | 9 | GUA | H5'1 | 3.18 | 3.84 |
| 10 | THY | H6 | 10 | THY | H5'1 | 3.18 | 3.84 |
| 11 | CYT | H6 | 11 | CYT | H5'1 | 3.18 | 3.84 |
| 12 | CYT | H6 | 12 | CYT | H5'1 | 3.18 | 3.84 |
| 13 | GUA | H8 | 13 | GUA | H5'1 | 3.18 | 3.84 |
| 14 | GUA | H8 | 14 | GUA | H5'1 | 3.18 | 3.84 |
| 15 | ADE | H8 | 15 | ADE | H5'1 | 3.18 | 3.84 |
| 16 | CYT | H6 | 16 | CYT | H5'1 | 3.18 | 3.84 |
| 17 | THY | H6 | 17 | THY | H5'1 | 3.18 | 3.84 |
| 18 | THY | H6 | 18 | THY | H5'1 | 3.18 | 3.84 |
| 19 | GUA | H8 | 19 | GUA | H5'1 | 3.18 | 3.84 |
| 20 | CYT | H6 | 20 | CYT | H5'1 | 3.18 | 3.84 |
| 21 | THY | H6 | 21 | THY | H5'1 | 3.18 | 3.84 |
| 22 | ADE | H8 | 22 | ADE | H5'1 | 3.18 | 3.84 |
| 23 | GUA | H8 | 23 | GUA | H5'1 | 3.18 | 3.84 |
| 24 | CYT | H6 | 24 | CYT | H5'1 | 3.18 | 3.84 |
| 21 | THY | H5'1 | 20 | CYT | H3' | 4.18 | 4.84 |
| 4 | ADE | H5'1 | 3 | THY | H3' | 4.18 | 4.84 |
| 9 | GUA | H8 | 8 | ADE | H8 | 4.68 | 5.34 |
| 16 | CYT | H4' | 15 | ADE | H4' | 5.88 | 6.37 |
| 2 | CYT | H6 | 1 | GUA | H3' | 4.64 | 5.39 |
| 3 | THY | H6 | 2 | CYT | H3' | 4.64 | 5.39 |
| 4 | ADE | H8 | 3 | THY | H3' | 4.64 | 5.39 |
| 6 | CYT | H6 | 5 | GUA | H3' | 4.64 | 5.39 |
| 10 | THY | H6 | 9 | GUA | H3' | 4.64 | 5.39 |
| 11 | CYT | H6 | 10 | THY | H3' | 4.64 | 5.39 |
| 12 | CYT | H6 | 11 | CYT | H3' | 4.64 | 5.39 |
| 16 | CYT | H6 | 15 | GUA | H3' | 4.64 | 5.39 |
| 20 | CYT | H6 | 19 | GUA | H3' | 4.64 | 5.39 |
| 21 | THY | H6 | 20 | CYT | H3' | 4.64 | 5.39 |
| 22 | ADE | H8 | 21 | THY | H3' | 4.64 | 5.39 |
| 24 | CYT | H6 | 23 | GUA | H3' | 4.64 | 5.39 |
| 18 | THY | H6 | 17 | THY | H3' | 4.94 | 5.59 |

**Table B-3:** Continued

| Residue Number | Residue Name | Atom Number | Residue Number | Residue Name | Atom Number | Lower Bound | Upper Bound |
|---|---|---|---|---|---|---|---|
| 17 | THY | H6 | 16 | CYT | H3' | 4.64 | 5.39 |
| 9 | GUA | H8 | 8 | ADE | H3' | 4.64 | 5.39 |
| 18 | THY | M7 | 17 | THY | H2'2 | 3.51 | 4.88 |
| 7 | UBX | H5 | 6 | CYT | H6 | 4.7 | 6 |
| 24 | CYT | H5'1 | 23 | GUA | H3' | 4.18 | 4.84 |
| 23 | GUA | H5'1 | 22 | CYT | H3' | 4.18 | 4.84 |
| 19 | GUA | H3' | 19 | GUA | H5'1 | 3.68 | 4.24 |
| 17 | THY | H1' | 7 | UBX | H9 | 5.07 | 6.09 |
| 17 | THY | H1' | 7 | UBX | H14 | 5.57 | 6.59 |
| 17 | THY | H1' | 7 | UBX | H15 | 5.57 | 6.59 |
| 18 | THY | H1' | 7 | UBX | H9 | 6.57 | 7.59 |
| 18 | THY | H1' | 7 | UBX | H14 | 5.57 | 6.59 |
| 18 | THY | H1' | 7 | UBX | H15 | 5.57 | 6.59 |
| 17 | THY | H6 | 7 | UBX | H9 | 6.07 | 7.59 |
| 17 | THY | H6 | 7 | UBX | H14 | 5.57 | 6.59 |
| 17 | THY | H6 | 7 | UBX | H15 | 5.57 | 6.59 |
| 8 | ADE | H5'1 | 7 | UBX | H2'2 | 3.27 | 3.89 |
| 7 | UBX | H5'1 | 6 | CYT | H2'2 | 3.27 | 3.89 |
| 17 | THY | H2'1 | 7 | UBX | H13 | 5.57 | 7.59 |
| 18 | THY | H1' | 7 | UBX | H13 | 5.57 | 7.59 |
| 18 | THY | H1' | 7 | UBX | H11 | 5.57 | 7.59 |
| 7 | UBX | H2'1 | 6 | CYT | H2'2 | 3.47 | 4.59 |
| 8 | ADE | H2'1 | 7 | UBX | H2'2 | 3.47 | 4.59 |
| 8 | ADE | H8 | 7 | UBX | H5 | 5.97 | 7.09 |
| 18 | THY | H6 | 17 | THY | H1' | 3.97 | 5.09 |
| 19 | GUA | H8 | 18 | THY | H1' | 3.97 | 5.09 |
| 7 | UBX | H6 | 6 | CYT | H2'2 | 2.97 | 4.59 |
| 5 | GUA | H2'1 | 4 | ADE | H2'2 | 3.47 | 4.19 |
| 18 | THY | H5'1 | 17 | THY | H2'2 | 3.17 | 3.79 |
| 18 | THY | H5'1 | 17 | THY | H1' | 2.37 | 3.79 |
| 17 | THY | H2'1 | 16 | CYT | H3' | 5.87 | 6.39 |

**Table B-4:** Distance restraints used for the *S-N3-dU* modified oligonucleotide 5′-$G^{1}C^{2}T^{3}A^{4}G^{5}C^{6}X^{7}A^{8}G^{9}T^{10}C^{11}C^{12}$-3′·5′-$G^{13}G^{14}A^{15}C^{16}T^{17}T^{18}G^{19}C^{20}T^{21}A^{22}G^{23}C^{24}$-3′.

| | Residue Number | Residue Name | Atom Number | Residue Number | Residue Name | Atom Number | Lower Bound | Upper Bound |
|---|---|---|---|---|---|---|---|---|
| Class 1 | 2 | CYT | H5 | 1 | GUA | H1' | 3.43 | 4.13 |
| | 2 | CYT | H2'2 | 2 | CYT | H2'1 | 1.41 | 2.64 |
| | 7 | UBX | H2'2 | 7 | UBX | H2'1 | 1.57 | 2.50 |
| | 12 | CYT | H6 | 12 | CYT | H1' | 3.31 | 4.21 |
| | 16 | CYT | H2'2 | 16 | CYT | H2'1 | 1.56 | 2.43 |
| | 18 | THY | H2'2 | 18 | THY | H2'1 | 1.46 | 2.28 |
| | 20 | CYT | H2'2 | 20 | CYT | H2'1 | 1.60 | 2.65 |
| | 2 | CYT | H2'2 | 2 | CYT | H5 | 4.81 | 5.73 |
| | 3 | THY | H2'2 | 3 | THY | H2'1 | 1.80 | 2.61 |
| | 10 | THY | H2'2 | 10 | THY | H2'1 | 1.78 | 2.43 |
| | 21 | THY | H2'2 | 21 | THY | H2'1 | 1.80 | 2.78 |
| Class 2 | 1 | GUA | H8 | 1 | GUA | H1' | 3.36 | 4.40 |
| | 1 | GUA | H2'1 | 1 | GUA | H1' | 2.45 | 3.33 |
| | 1 | GUA | H2'2 | 1 | GUA | H1' | 1.67 | 2.82 |
| | 2 | CYT | H6 | 1 | GUA | H2'1 | 3.31 | 3.98 |
| | 2 | CYT | H6 | 1 | GUA | H2'2 | 1.88 | 3.00 |
| | 2 | CYT | H5 | 2 | CYT | H6 | 1.65 | 2.98 |
| | 2 | CYT | H3' | 2 | CYT | H6 | 3.48 | 4.20 |
| | 2 | CYT | H2'2 | 2 | CYT | H6 | 2.84 | 3.88 |
| | 3 | THY | M7 | 2 | CYT | H1' | 3.58 | 5.16 |
| | 3 | THY | M7 | 2 | CYT | H6 | 2.28 | 3.75 |
| | 5 | GUA | H3' | 5 | GUA | H1' | 3.49 | 4.52 |
| | 6 | CYT | H6 | 5 | GUA | H1' | 2.67 | 3.38 |
| | 6 | CYT | H6 | 5 | GUA | H2'2 | 1.80 | 2.76 |
| | 6 | CYT | H5 | 5 | GUA | H8 | 3.61 | 4.49 |
| | 6 | CYT | H5 | 5 | GUA | H2'1 | 2.83 | 3.40 |
| | 6 | CYT | H5 | 5 | GUA | H2'2 | 2.41 | 3.43 |
| | 6 | CYT | H3' | 6 | CYT | H1' | 3.46 | 4.38 |
| | 6 | CYT | H3' | 6 | CYT | H6 | 3.58 | 4.30 |
| | 7 | UBX | H6 | 7 | UBX | H1' | 3.11 | 3.99 |
| | 7 | UBX | H5 | 7 | UBX | H6 | 1.56 | 2.66 |
| | 7 | UBX | H3' | 7 | UBX | H6 | 3.21 | 4.67 |
| | 7 | UBX | H2'1 | 7 | UBX | H1' | 2.32 | 3.22 |
| | 7 | UBX | H2'1 | 7 | UBX | H6 | 1.74 | 2.54 |
| | 7 | UBX | H2'1 | 7 | UBX | H3' | 2.06 | 3.19 |
| | 7 | UBX | H2'2 | 7 | UBX | H6 | 2.73 | 4.06 |
| | 7 | UBX | H2'2 | 7 | UBX | H3' | 2.45 | 3.55 |
| | 7 | UBX | H14 | 7 | UBX | H15 | 1.56 | 2.28 |
| | 7 | UBX | H9 | 7 | UBX | H15 | 2.28 | 3.36 |
| | 7 | UBX | H9 | 7 | UBX | H14 | 2.58 | 4.10 |
| | 8 | ADE | H8 | 8 | ADE | H1' | 3.44 | 4.26 |
| | 8 | ADE | H3' | 8 | ADE | H1' | 3.54 | 4.36 |
| | 9 | GUA | H3' | 9 | GUA | H8 | 3.83 | 4.70 |
| | 10 | THY | H6 | 9 | GUA | H1' | 2.34 | 3.43 |

**Table B-4:** Continued

| | Residue Number | Residue Name | Atom Number | Residue Number | Residue Name | Atom Number | Lower Bound | Upper Bound |
|---|---|---|---|---|---|---|---|---|
| | 10 | THY | M7 | 9 | GUA | H1' | 3.37 | 5.09 |
| | 10 | THY | M7 | 9 | GUA | H8 | 2.45 | 4.06 |
| | 12 | CYT | H3' | 12 | CYT | H1' | 3.49 | 4.24 |
| | 12 | CYT | H3' | 12 | CYT | H6 | 3.48 | 4.66 |
| | 14 | GUA | H1' | 14 | GUA | H4' | 3.35 | 4.51 |
| | 15 | ADE | H1' | 15 | ADE | H4' | 3.11 | 4.31 |
| | 15 | ADE | H8 | 14 | GUA | H1' | 2.61 | 3.38 |
| | 15 | ADE | H3' | 15 | ADE | H4' | 1.80 | 2.71 |
| | 15 | ADE | H3' | 15 | ADE | H1' | 3.40 | 4.56 |
| | 15 | ADE | H2'2 | 15 | ADE | H1' | 1.71 | 2.82 |
| | 16 | CYT | H5'1 | 15 | ADE | H1' | 1.80 | 3.25 |
| | 16 | CYT | H6 | 15 | ADE | H1' | 2.15 | 3.18 |
| | 16 | CYT | H6 | 15 | ADE | H2'1 | 3.28 | 4.59 |
| | 16 | CYT | H6 | 15 | ADE | H2'2 | 1.80 | 2.34 |
| | 16 | CYT | H5 | 15 | ADE | H2'1 | 2.45 | 3.53 |
| | 16 | CYT | H5 | 15 | ADE | H2'2 | 2.56 | 3.41 |
| | 16 | CYT | H5 | 16 | CYT | H6 | 1.65 | 2.78 |
| | 16 | CYT | H3' | 16 | CYT | H1' | 3.32 | 4.35 |
| | 16 | CYT | H2'1 | 16 | CYT | H1' | 2.64 | 3.41 |
| | 16 | CYT | H2'2 | 16 | CYT | H1' | 1.61 | 2.71 |
| | 17 | THY | H6 | 17 | THY | H1' | 3.26 | 4.04 |
| | 17 | THY | M7 | 16 | CYT | H5 | 3.49 | 4.86 |
| | 18 | THY | H6 | 18 | THY | H1' | 3.42 | 4.15 |
| | 18 | THY | M7 | 17 | THY | H6 | 3.40 | 4.69 |
| | 18 | THY | H3' | 18 | THY | H6 | 3.50 | 4.47 |
| | 20 | CYT | H6 | 19 | GUA | H1' | 2.68 | 3.59 |
| | 20 | CYT | H3' | 20 | CYT | H1' | 3.36 | 4.42 |
| | 24 | CYT | H6 | 23 | GUA | H1' | 2.94 | 3.99 |
| | 24 | CYT | H5 | 23 | GUA | H2'2 | 2.21 | 3.59 |
| | 24 | CYT | H5 | 24 | CYT | H6 | 1.70 | 2.62 |
| | 24 | CYT | H3' | 24 | CYT | H6 | 3.67 | 4.24 |
| | 6 | CYT | H5 | 5 | GUA | H1' | 3.15 | 4.14 |
| | 7 | UBX | H3' | 7 | UBX | H1' | 3.25 | 4.03 |
| | 9 | GUA | H8 | 8 | ADE | H8 | 4.75 | 5.27 |
| | 11 | CYT | H5 | 10 | THY | M7 | 4.03 | 5.12 |
| | 15 | ADE | H2'1 | 15 | ADE | H4' | 3.45 | 4.37 |
| | 15 | ADE | H2'2 | 15 | ADE | H4' | 3.82 | 4.41 |
| | 16 | CYT | H2'1 | 16 | CYT | H5 | 3.76 | 4.77 |
| Class 3 | 1 | GUA | H3' | 1 | GUA | H1' | 3.64 | 4.30 |
| | 1 | GUA | H3' | 1 | GUA | H8 | 3.80 | 4.53 |
| | 2 | CYT | H6 | 1 | GUA | H1' | 2.10 | 3.38 |
| | 2 | CYT | H6 | 2 | CYT | H1' | 3.20 | 4.24 |
| | 2 | CYT | H2'1 | 2 | CYT | H6 | 1.78 | 2.43 |
| | 2 | CYT | H2'1 | 2 | CYT | H5 | 3.77 | 4.67 |
| | 3 | THY | H6 | 2 | CYT | H1' | 1.96 | 3.22 |
| | 3 | THY | M7 | 2 | CYT | H2'2 | 2.57 | 3.96 |
| | 5 | GUA | H8 | 5 | GUA | H1' | 3.36 | 4.12 |

**Table B-4:** Continued

| Residue Number | Residue Name | Atom Number | Residue Number | Residue Name | Atom Number | Lower Bound | Upper Bound |
|---|---|---|---|---|---|---|---|
| 5 | GUA | H3' | 5 | GUA | H8 | 3.42 | 4.74 |
| 6 | CYT | H5 | 6 | CYT | H6 | 1.75 | 3.06 |
| 8 | ADE | H1' | 8 | ADE | H4' | 3.28 | 4.06 |
| 8 | ADE | H8 | 7 | UBX | H3' | 4.42 | 5.48 |
| 8 | ADE | H2 | 7 | UBX | H9 | 3.72 | 5.29 |
| 8 | ADE | H3' | 8 | ADE | H5'1 | 3.53 | 4.01 |
| 8 | ADE | H3' | 8 | ADE | H5'2 | 1.84 | 3.22 |
| 8 | ADE | H3' | 8 | ADE | H8 | 3.82 | 4.93 |
| 9 | GUA | H8 | 8 | ADE | H1' | 2.59 | 3.83 |
| 9 | GUA | H8 | 9 | GUA | H1' | 3.35 | 4.23 |
| 10 | THY | M7 | 9 | GUA | H2'2 | 2.57 | 4.15 |
| 10 | THY | M7 | 10 | THY | H6 | 1.57 | 3.47 |
| 11 | CYT | H6 | 10 | THY | H1' | 2.40 | 3.45 |
| 11 | CYT | H5 | 10 | THY | H6 | 3.46 | 4.48 |
| 12 | CYT | H1' | 12 | CYT | H4' | 3.17 | 4.40 |
| 12 | CYT | H5 | 12 | CYT | H6 | 1.59 | 2.64 |
| 13 | GUA | H3' | 13 | GUA | H1' | 3.35 | 4.65 |
| 14 | GUA | H3' | 14 | GUA | H1' | 3.25 | 4.56 |
| 14 | GUA | H3' | 14 | GUA | H8 | 3.76 | 5.00 |
| 14 | GUA | H2'1 | 14 | GUA | H1' | 2.73 | 3.25 |
| 14 | GUA | H2'2 | 14 | GUA | H1' | 1.66 | 2.55 |
| 15 | ADE | H2'1 | 15 | ADE | H1' | 2.42 | 3.49 |
| 16 | CYT | H5 | 15 | ADE | H8 | 3.47 | 4.48 |
| 16 | CYT | H3' | 16 | CYT | H5'1 | 3.43 | 4.64 |
| 16 | CYT | H2'1 | 16 | CYT | H3' | 2.17 | 3.29 |
| 17 | THY | M7 | 16 | CYT | H3' | 4.25 | 6.46 |
| 17 | THY | M7 | 16 | CYT | H2'2 | 2.65 | 3.78 |
| 17 | THY | H3' | 17 | THY | H6 | 3.51 | 4.35 |
| 17 | THY | H2'1 | 17 | THY | H1' | 2.78 | 3.59 |
| 17 | THY | H2'1 | 17 | THY | H6 | 1.80 | 2.37 |
| 17 | THY | H2'2 | 17 | THY | H1' | 1.93 | 2.89 |
| 18 | THY | M7 | 17 | THY | H2'1 | 2.67 | 4.24 |
| 18 | THY | M7 | 18 | THY | H6 | 1.80 | 3.17 |
| 18 | THY | H2'1 | 18 | THY | H6 | 1.80 | 2.44 |
| 18 | THY | H2'1 | 18 | THY | H3' | 2.12 | 3.24 |
| 18 | THY | H2'2 | 18 | THY | H1' | 1.78 | 2.56 |
| 18 | THY | H2'2 | 18 | THY | H6 | 2.68 | 4.11 |
| 18 | THY | H2'2 | 18 | THY | H3' | 2.39 | 3.41 |
| 19 | GUA | H8 | 19 | GUA | H1' | 3.22 | 4.04 |
| 19 | GUA | H3' | 19 | GUA | H5'1 | 3.51 | 4.48 |
| 19 | GUA | H3' | 19 | GUA | H1' | 3.27 | 4.25 |
| 19 | GUA | H3' | 19 | GUA | H8 | 3.87 | 5.08 |
| 20 | CYT | H5 | 19 | GUA | H1' | 3.42 | 4.57 |
| 20 | CYT | H2'1 | 20 | CYT | H3' | 2.09 | 3.13 |
| 20 | CYT | H2'2 | 20 | CYT | H3' | 2.23 | 3.15 |
| 21 | THY | M7 | 20 | CYT | H3' | 3.99 | 5.82 |
| 23 | GUA | H8 | 23 | GUA | H1' | 3.45 | 4.29 |

**Table B-4:** Continued

| | Residue Number | Residue Name | Atom Number | Residue Number | Residue Name | Atom Number | Lower Bound | Upper Bound |
|---|---|---|---|---|---|---|---|---|
| | 23 | GUA | H3' | 23 | GUA | H1' | 3.28 | 4.60 |
| | 23 | GUA | H2'1 | 23 | GUA | H1' | 2.54 | 3.48 |
| | 23 | GUA | H2'2 | 23 | GUA | H1' | 1.68 | 3.05 |
| | 24 | CYT | H5 | 23 | GUA | H8 | 3.22 | 4.51 |
| | 1 | GUA | H8 | 1 | GUA | H4' | 4.42 | 5.66 |
| | 2 | CYT | H6 | 1 | GUA | H8 | 4.39 | 5.11 |
| | 5 | GUA | H2'1 | 5 | GUA | H4' | 3.42 | 4.55 |
| | 5 | GUA | H2'2 | 5 | GUA | H4' | 3.75 | 4.66 |
| | 7 | UBX | H2'1 | 7 | UBX | H4' | 3.30 | 4.40 |
| | 9 | GUA | H3' | 9 | GUA | H1' | 3.26 | 4.42 |
| | 12 | CYT | H1' | 12 | CYT | H5'1 | 3.87 | 5.04 |
| | 17 | THY | M7 | 16 | CYT | H1' | 3.40 | 5.29 |
| | 18 | THY | H3' | 18 | THY | H1' | 3.14 | 4.37 |
| | 20 | CYT | H2'1 | 20 | CYT | H5 | 3.89 | 4.53 |
| | 21 | THY | M7 | 20 | CYT | H1' | 3.65 | 4.93 |
| | 24 | CYT | H6 | 23 | GUA | H3' | 4.44 | 4.99 |
| | 14 | GUA | H8 | 14 | GUA | H4' | 4.64 | 5.36 |
| | 18 | THY | H6 | 17 | THY | H1' | 4.59 | 5.67 |
| Class 4 | 2 | CYT | H5 | 1 | GUA | H2'1 | 2.85 | 3.58 |
| | 3 | THY | H6 | 3 | THY | H1' | 3.39 | 4.18 |
| | 3 | THY | M7 | 2 | CYT | H3' | 4.42 | 5.96 |
| | 3 | THY | H3' | 3 | THY | H1' | 3.26 | 4.55 |
| | 4 | ADE | H3' | 4 | ADE | H4' | 1.98 | 3.33 |
| | 5 | GUA | H8 | 4 | ADE | H1' | 2.34 | 3.41 |
| | 5 | GUA | H2'1 | 5 | GUA | H1' | 1.79 | 3.40 |
| | 5 | GUA | H2'1 | 5 | GUA | H3' | 1.87 | 2.95 |
| | 5 | GUA | H2'2 | 5 | GUA | H1' | 1.62 | 2.80 |
| | 6 | CYT | H6 | 6 | CYT | H1' | 3.39 | 4.22 |
| | 7 | UBX | H3' | 7 | UBX | H5'1 | 3.54 | 4.25 |
| | 7 | UBX | H3' | 7 | UBX | H5'2 | 2.42 | 3.19 |
| | 9 | GUA | H2'1 | 9 | GUA | H1' | 2.53 | 3.62 |
| | 10 | THY | H2'2 | 10 | THY | H1' | 1.80 | 2.78 |
| | 12 | CYT | H3' | 12 | CYT | H4' | 1.82 | 2.73 |
| | 13 | GUA | H1' | 13 | GUA | H4' | 3.35 | 4.06 |
| | 13 | GUA | H2'1 | 13 | GUA | H1' | 2.33 | 3.68 |
| | 14 | GUA | H2'2 | 14 | GUA | H8 | 3.23 | 3.87 |
| | 15 | ADE | H3' | 15 | ADE | H5'2 | 2.23 | 3.44 |
| | 16 | CYT | H2'1 | 16 | CYT | H4' | 3.33 | 4.55 |
| | 16 | CYT | H2'2 | 16 | CYT | H3' | 2.34 | 3.29 |
| | 17 | THY | H1' | 17 | THY | H4' | 2.93 | 4.25 |
| | 17 | THY | H2'2 | 17 | THY | H6 | 2.85 | 3.97 |
| | 18 | THY | H3' | 18 | THY | H4' | 2.30 | 2.87 |
| | 19 | GUA | H5'1 | 18 | THY | H1' | 1.76 | 3.42 |
| | 19 | GUA | H8 | 18 | THY | H2'2 | 2.37 | 3.55 |
| | 20 | CYT | H6 | 20 | CYT | H1' | 3.27 | 4.23 |
| | 20 | CYT | H3' | 20 | CYT | H4' | 1.74 | 2.84 |
| | 20 | CYT | H3' | 20 | CYT | H6 | 3.53 | 4.26 |

**Table B-4:** Continued

| | Residue Number | Residue Name | Atom Number | Residue Number | Residue Name | Atom Number | Lower Bound | Upper Bound |
|---|---|---|---|---|---|---|---|---|
| | 20 | CYT | H2'1 | 20 | CYT | H1' | 2.23 | 3.43 |
| | 21 | THY | H6 | 20 | CYT | H2'1 | 3.17 | 4.18 |
| | 21 | THY | M7 | 20 | CYT | H5 | 3.62 | 5.07 |
| | 21 | THY | M7 | 20 | CYT | H2'1 | 2.30 | 4.06 |
| | 21 | THY | M7 | 20 | CYT | H2'2 | 2.30 | 4.06 |
| | 23 | GUA | H1' | 23 | GUA | H4' | 2.95 | 4.00 |
| | 23 | GUA | H8 | 22 | ADE | H1' | 2.03 | 3.75 |
| | 23 | GUA | H8 | 22 | ADE | H2'1 | 3.31 | 4.16 |
| | 23 | GUA | H8 | 22 | ADE | H2'2 | 1.79 | 3.01 |
| | 12 | CYT | H6 | 11 | CYT | H6 | 4.50 | 5.50 |
| | 23 | GUA | H3' | 23 | GUA | H8 | 3.77 | 4.83 |
| | 24 | CYT | H6 | 24 | CYT | H4' | 4.24 | 5.01 |
| | 24 | CYT | H2'1 | 24 | CYT | H3' | 1.80 | 3.05 |
| | 5 | GUA | H8 | 4 | ADE | H3' | 4.46 | 5.15 |
| | 7 | UBX | H2'1 | 7 | UBX | H5 | 3.69 | 5.06 |
| | 7 | UBX | H11 | 7 | UBX | H15 | 2.07 | 4.06 |
| | 7 | UBX | H11 | 7 | UBX | H14 | 2.34 | 3.60 |
| | 8 | ADE | H2 | 7 | UBX | H15 | 3.45 | 4.30 |
| | 8 | ADE | H2 | 7 | UBX | H14 | 3.45 | 4.30 |
| | 10 | THY | H3' | 10 | THY | H1' | 3.34 | 4.27 |
| | 14 | GUA | H5'1 | 13 | GUA | H1' | 1.80 | 2.68 |
| | 15 | ADE | H1' | 15 | ADE | H5'1 | 3.91 | 4.72 |
| | 17 | THY | H3' | 17 | THY | H1' | 3.21 | 4.61 |
| | 17 | THY | H2'1 | 17 | THY | M7 | 3.98 | 5.08 |
| | 8 | ADE | H8 | 8 | ADE | H5'1 | 3.21 | 3.82 |
| | 8 | ADE | H8 | 8 | ADE | H4' | 4.31 | 5.72 |
| | 11 | CYT | H5 | 10 | THY | H1' | 3.00 | 4.24 |
| | 16 | CYT | H6 | 15 | ADE | H3' | 4.26 | 5.37 |
| | 18 | THY | H6 | 18 | THY | H4' | 3.46 | 5.37 |
| | 18 | THY | M7 | 17 | THY | H1' | 3.27 | 5.50 |
| | 19 | GUA | H8 | 18 | THY | H3' | 4.30 | 5.43 |
| | 19 | GUA | H8 | 19 | GUA | H4' | 4.12 | 5.45 |
| Class 5 | 1 | GUA | H1' | 1 | GUA | H4' | 2.74 | 4.22 |
| | 1 | GUA | H2'1 | 1 | GUA | H8 | 1.57 | 2.70 |
| | 1 | GUA | H2'2 | 1 | GUA | H8 | 3.19 | 4.24 |
| | 2 | CYT | H5 | 1 | GUA | H8 | 3.48 | 4.68 |
| | 2 | CYT | H5 | 1 | GUA | H2'2 | 2.44 | 3.62 |
| | 2 | CYT | H3' | 2 | CYT | H1' | 3.26 | 4.57 |
| | 2 | CYT | H3' | 2 | CYT | H5 | 5.83 | 6.81 |
| | 2 | CYT | H2'1 | 2 | CYT | H1' | 2.63 | 3.45 |
| | 2 | CYT | H2'2 | 2 | CYT | H1' | 1.77 | 2.41 |
| | 3 | THY | H1' | 3 | THY | H4' | 2.81 | 3.90 |
| | 3 | THY | H6 | 2 | CYT | H2'1 | 3.32 | 4.12 |
| | 3 | THY | H6 | 2 | CYT | H2'2 | 1.77 | 2.61 |
| | 3 | THY | M7 | 2 | CYT | H5 | 3.37 | 4.86 |
| | 3 | THY | M7 | 2 | CYT | H2'1 | 2.58 | 3.50 |
| | 3 | THY | M7 | 3 | THY | H6 | 2.56 | 4.05 |

**Table B-4:** Continued

| Residue Number | Residue Name | Atom Number | Residue Number | Residue Name | Atom Number | Lower Bound | Upper Bound |
|---|---|---|---|---|---|---|---|
| 3 | THY | H3' | 3 | THY | H6 | 3.50 | 4.50 |
| 3 | THY | H2'1 | 3 | THY | H1' | 2.40 | 3.49 |
| 3 | THY | H2'1 | 3 | THY | H6 | 1.37 | 2.32 |
| 3 | THY | H2'1 | 3 | THY | M7 | 3.89 | 5.25 |
| 3 | THY | H2'2 | 3 | THY | H1' | 1.52 | 2.73 |
| 3 | THY | H2'2 | 3 | THY | H6 | 2.74 | 3.81 |
| 21 | THY | H3' | 21 | THY | H5'1 | 3.50 | 4.10 |
| 6 | CYT | H3' | 6 | CYT | H5'1 | 3.50 | 4.10 |
| 20 | CYT | H3' | 20 | CYT | H5'1 | 3.50 | 4.10 |
| 2 | CYT | H3' | 2 | CYT | H5'1 | 3.50 | 4.10 |
| 9 | GUA | H3' | 9 | CYT | H5'1 | 3.50 | 4.10 |
| 18 | THY | H3' | 18 | THY | H5'1 | 3.50 | 4.10 |
| 1 | GUA | H3' | 1 | GUA | H5'1 | 3.50 | 4.10 |
| 3 | THY | H3' | 3 | THY | H5'1 | 3.50 | 4.10 |
| 10 | THY | H3' | 10 | THY | H5'1 | 3.50 | 4.10 |
| 11 | CYT | H3' | 11 | CYT | H5'1 | 3.50 | 4.10 |
| 12 | CYT | H3' | 12 | CYT | H5'1 | 3.50 | 4.10 |
| 17 | THY | H3' | 17 | THY | H5'1 | 3.50 | 4.10 |
| 24 | CYT | H3' | 24 | CYT | H5'1 | 3.50 | 4.10 |
| 23 | GUA | H3' | 23 | GUA | H5'1 | 3.50 | 4.10 |
| 22 | ADE | H3' | 22 | ADE | H5'1 | 3.50 | 4.10 |
| 15 | ADE | H3' | 15 | ADE | H5'1 | 3.50 | 4.10 |
| 14 | GUA | H3' | 14 | GUA | H5'1 | 3.50 | 4.10 |
| 13 | GUA | H3' | 13 | GUA | H5'1 | 3.50 | 4.10 |
| 5 | GUA | H3' | 5 | GUA | H5'1 | 3.50 | 4.10 |
| 4 | ADE | H3' | 4 | ADE | H5'1 | 3.50 | 4.10 |
| 3 | THY | H1' | 2 | CYT | H1' | 4.75 | 5.25 |
| 6 | CYT | H1' | 5 | GUA | H1' | 4.75 | 5.25 |
| 7 | UBX | H1' | 6 | CYT | H1' | 5.00 | 5.50 |
| 8 | ADE | H1' | 7 | UBX | H1' | 5.50 | 6.50 |
| 9 | GUA | H1' | 8 | ADE | H1' | 4.75 | 5.75 |
| 10 | THY | H1' | 9 | GUA | H1' | 4.75 | 5.25 |
| 11 | CYT | H1' | 10 | THY | H1' | 4.75 | 5.25 |
| 14 | GUA | H1' | 13 | GUA | H1' | 4.75 | 5.25 |
| 15 | ADE | H1' | 14 | GUA | H1' | 4.75 | 5.25 |
| 16 | CYT | H1' | 15 | ADE | H1' | 4.75 | 5.25 |
| 17 | THY | H1' | 16 | CYT | H1' | 5.00 | 6.00 |
| 18 | THY | H1' | 17 | THY | H1' | 5.00 | 6.00 |
| 19 | GUA | H1' | 18 | THY | H1' | 4.75 | 5.75 |
| 20 | CYT | H1' | 19 | GUA | H1' | 4.75 | 5.25 |
| 21 | THY | H1' | 20 | CYT | H1' | 4.75 | 5.25 |
| 22 | ADE | H1' | 21 | THY | H1' | 4.75 | 5.25 |
| 23 | GUA | H1' | 22 | ADE | H1' | 4.75 | 5.25 |
| 24 | CYT | H1' | 23 | GUA | H1' | 4.75 | 5.25 |
| 12 | CYT | H1' | 11 | CYT | H1' | 4.75 | 5.25 |
| 2 | CYT | H1' | 1 | GUA | H1' | 4.75 | 5.25 |
| 4 | ADE | H1' | 3 | THY | H1' | 4.75 | 5.25 |

**Table B-4:** Continued

| Residue Number | Residue Name | Atom Number | Residue Number | Residue Name | Atom Number | Lower Bound | Upper Bound |
|---|---|---|---|---|---|---|---|
| 5 | GUA | H1' | 4 | ADE | H1' | 4.75 | 5.25 |
| 3 | THY | H6 | 2 | CYT | H6 | 4.68 | 5.37 |
| 7 | UBX | H6 | 6 | CYT | H6 | 5.18 | 6.37 |
| 8 | ADE | H8 | 7 | UBX | H6 | 5.18 | 6.37 |
| 10 | THY | H6 | 9 | GUA | H8 | 4.68 | 5.37 |
| 11 | CYT | H6 | 10 | THY | H6 | 4.68 | 5.37 |
| 14 | GUA | H8 | 13 | GUA | H8 | 4.68 | 5.37 |
| 17 | THY | H6 | 16 | CYT | H6 | 4.68 | 5.37 |
| 18 | THY | H6 | 17 | THY | H6 | 5.18 | 6.37 |
| 19 | GUA | H8 | 18 | THY | H6 | 5.18 | 5.87 |
| 20 | CYT | H6 | 19 | GUA | H8 | 4.68 | 5.37 |
| 21 | THY | H6 | 20 | CYT | H6 | 4.68 | 5.37 |
| 22 | ADE | H8 | 21 | THY | H6 | 4.68 | 5.37 |
| 23 | GUA | H8 | 22 | ADE | H8 | 4.68 | 5.37 |
| 24 | CYT | H6 | 23 | GUA | H8 | 4.68 | 5.37 |
| 15 | ADE | H8 | 14 | GUA | H8 | 4.60 | 5.17 |
| 16 | CYT | H6 | 15 | ADE | H8 | 4.68 | 5.37 |
| 5 | GUA | H8 | 4 | ADE | H8 | 4.47 | 5.30 |
| 6 | CYT | H6 | 5 | GUA | H8 | 4.79 | 5.25 |
| 4 | ADE | H8 | 3 | THY | H6 | 4.68 | 5.37 |
| 14 | GUA | H8 | 13 | GUA | H1' | 2.60 | 3.17 |
| 12 | CYT | H6 | 11 | CYT | H1' | 2.40 | 3.17 |
| 13 | GUA | H3' | 13 | GUA | H8 | 4.10 | 4.87 |
| 2 | CYT | H5'1 | 1 | GUA | H8 | 5.80 | 6.20 |
| 3 | THY | H5'1 | 2 | CYT | H6 | 5.80 | 6.20 |
| 4 | ADE | H5'1 | 3 | GUA | H8 | 5.80 | 6.20 |
| 5 | GUA | H5'1 | 4 | ADE | H8 | 5.80 | 6.20 |
| 6 | CYT | H5'1 | 5 | GUA | H8 | 5.80 | 6.20 |
| 9 | GUA | H5'1 | 8 | ADE | H8 | 5.80 | 6.20 |
| 10 | THY | H5'1 | 9 | GUA | H8 | 5.80 | 6.20 |
| 11 | CYT | H5'1 | 10 | THY | H6 | 5.80 | 6.20 |
| 12 | CYT | H5'1 | 11 | CYT | H6 | 5.80 | 6.20 |
| 14 | GUA | H5'1 | 13 | GUA | H8 | 5.80 | 6.20 |
| 15 | ADE | H5'1 | 14 | GUA | H8 | 5.80 | 6.20 |
| 16 | CYT | H5'1 | 15 | ADE | H8 | 5.80 | 6.20 |
| 19 | GUA | H5'1 | 18 | THY | H6 | 5.80 | 6.20 |
| 20 | CYT | H5'1 | 19 | GUA | H8 | 5.80 | 6.20 |
| 21 | THY | H5'1 | 20 | CYT | H6 | 5.80 | 6.20 |
| 22 | ADE | H5'1 | 21 | THY | H6 | 5.80 | 6.20 |
| 23 | GUA | H5'1 | 22 | ADE | H8 | 5.80 | 6.20 |
| 24 | CYT | H5'1 | 23 | GUA | H8 | 5.80 | 6.20 |
| 24 | CYT | H6 | 23 | GUA | H2'1 | 3.31 | 3.98 |
| 23 | GUA | H8 | 22 | ADE | H2'1 | 3.31 | 3.98 |
| 22 | ADE | H8 | 21 | THY | H2'1 | 3.31 | 3.98 |
| 12 | CYT | H6 | 11 | CYT | H2'1 | 3.31 | 3.98 |
| 10 | THY | H6 | 9 | GUA | H2'1 | 3.31 | 3.98 |
| 4 | ADE | H8 | 3 | THY | H1' | 2.03 | 3.75 |

**Table B-4:** Continued

| Residue Number | Residue Name | Atom Number | Residue Number | Residue Name | Atom Number | Lower Bound | Upper Bound |
|---|---|---|---|---|---|---|---|
| 7 | UBX | H6 | 6 | CYT | H1' | 5.03 | 5.75 |
| 8 | ADE | H8 | 7 | UBX | H1' | 5.03 | 5.75 |
| 17 | THY | H6 | 16 | CYT | H1' | 3.03 | 3.75 |
| 19 | GUA | H8 | 18 | THY | H1' | 4.03 | 4.75 |
| 21 | THY | H6 | 20 | CYT | H1' | 2.03 | 3.75 |
| 22 | ADE | H8 | 21 | THY | H1' | 2.03 | 3.75 |
| 22 | ADE | H8 | 21 | THY | H3' | 4.73 | 5.25 |
| 23 | GUA | H8 | 22 | ADE | H3' | 4.73 | 5.25 |
| 21 | THY | H6 | 20 | CYT | H3' | 4.73 | 5.25 |
| 20 | CYT | H6 | 19 | GUA | H3' | 4.73 | 5.25 |
| 18 | THY | H6 | 17 | THY | H3' | 5.03 | 6.05 |
| 18 | THY | H6 | 17 | THY | H2'1 | 4.03 | 5.05 |
| 18 | THY | H6 | 17 | THY | H2'2 | 3.03 | 4.05 |
| 19 | GUA | H8 | 18 | THY | H2'1 | 4.03 | 5.05 |
| 19 | GUA | H8 | 18 | THY | H2'2 | 3.03 | 4.05 |
| 15 | ADE | H8 | 14 | GUA | H3' | 4.73 | 5.25 |
| 14 | GUA | H8 | 13 | GUA | H3' | 4.73 | 5.25 |
| 12 | CYT | H6 | 11 | CYT | H3' | 4.73 | 5.25 |
| 11 | CYT | H6 | 10 | THY | H3' | 4.73 | 5.25 |
| 10 | THY | H6 | 9 | GUA | H3' | 4.73 | 5.25 |
| 7 | UBX | H6 | 6 | CYT | H3' | 5.03 | 6.05 |
| 6 | CYT | H6 | 5 | GUA | H3' | 4.73 | 5.25 |
| 4 | ADE | H8 | 3 | THY | H3' | 4.73 | 5.25 |
| 3 | THY | H6 | 2 | CYT | H3' | 4.73 | 5.25 |
| 2 | CYT | H6 | 1 | GUA | H3' | 4.73 | 5.25 |
| 2 | CYT | H6 | 2 | CYT | H5'1 | 3.18 | 3.84 |
| 3 | THY | H6 | 3 | THY | H5'1 | 3.18 | 3.84 |
| 4 | ADE | H8 | 4 | ADE | H5'1 | 3.18 | 3.84 |
| 5 | GUA | H8 | 5 | GUA | H5'1 | 3.18 | 3.84 |
| 6 | CYT | H6 | 6 | CYT | H5'1 | 3.18 | 3.84 |
| 7 | UBX | H6 | 7 | UBX | H5'1 | 3.18 | 3.84 |
| 9 | GUA | H8 | 9 | GUA | H5'1 | 3.38 | 3.84 |
| 10 | THY | H6 | 10 | THY | H5'1 | 3.18 | 3.84 |
| 11 | CYT | H6 | 11 | CYT | H5'1 | 3.18 | 3.84 |
| 12 | CYT | H6 | 12 | CYT | H5'1 | 3.18 | 3.84 |
| 13 | GUA | H8 | 13 | GUA | H5'1 | 3.18 | 3.84 |
| 14 | GUA | H8 | 14 | GUA | H5'1 | 3.18 | 3.84 |
| 15 | ADE | H8 | 15 | ADE | H5'1 | 3.18 | 3.84 |
| 16 | CYT | H6 | 16 | CYT | H5'1 | 3.18 | 3.84 |
| 17 | THY | H6 | 17 | THY | H5'1 | 3.18 | 3.84 |
| 18 | THY | H6 | 18 | THY | H5'1 | 3.18 | 3.84 |
| 19 | GUA | H8 | 19 | GUA | H5'1 | 3.18 | 3.84 |
| 20 | CYT | H6 | 20 | CYT | H5'1 | 3.18 | 3.84 |
| 21 | THY | H6 | 21 | THY | H5'1 | 3.18 | 3.84 |
| 22 | ADE | H8 | 22 | ADE | H5'1 | 3.18 | 3.84 |
| 23 | GUA | H8 | 23 | GUA | H5'1 | 3.18 | 3.84 |
| 24 | CYT | H6 | 24 | CYT | H5'1 | 3.18 | 3.84 |

**Table B-4:** Continued

| Residue Number | Residue Name | Atom Number | Residue Number | Residue Name | Atom Number | Lower Bound | Upper Bound |
|---|---|---|---|---|---|---|---|
| 1 | GUA | H8 | 1 | GUA | H5'1 | 3.18 | 3.84 |
| 9 | GUA | H2'1 | 8 | ADE | H2'2 | 3.58 | 4.34 |
| 8 | ADE | H2'1 | 7 | UBX | H2'2 | 3.58 | 4.34 |
| 7 | UBX | H2'1 | 6 | CYT | H2'2 | 3.58 | 4.34 |
| 17 | THY | H2'1 | 16 | CYT | H2'2 | 3.58 | 4.34 |
| 18 | THY | H2'1 | 17 | THY | H2'2 | 3.58 | 4.34 |
| 20 | CYT | H2'1 | 19 | GUA | H2'2 | 3.58 | 4.34 |
| 17 | THY | H1' | 8 | ADE | H2 | 6.08 | 7.34 |
| 14 | GUA | H2'1 | 13 | GUA | H2'2 | 3.58 | 4.34 |
| 7 | UBX | H5 | 6 | CYT | H2'2 | 2.90 | 3.90 |
| 7 | UBX | H5 | 6 | CYT | H2'1 | 3.20 | 4.20 |
| 7 | UBX | H5 | 6 | CYT | H1' | 4.90 | 5.60 |
| 7 | UBX | H5 | 6 | CYT | H6 | 4.70 | 5.50 |
| 17 | THY | H1' | 7 | UBX | H9 | 5.07 | 6.09 |
| 17 | THY | H1' | 7 | UBX | H14 | 5.57 | 6.59 |
| 17 | THY | H1' | 7 | UBX | H15 | 5.57 | 6.59 |
| 18 | THY | H1' | 7 | UBX | H9 | 6.57 | 7.59 |
| 18 | THY | H1' | 7 | UBX | H14 | 5.57 | 6.59 |
| 18 | THY | H1' | 7 | UBX | H15 | 5.57 | 6.59 |
| 17 | THY | H6 | 7 | UBX | H9 | 5.57 | 6.59 |
| 17 | THY | H6 | 7 | UBX | H14 | 5.57 | 6.59 |
| 17 | THY | H6 | 7 | UBX | H15 | 5.57 | 6.59 |
| 9 | GUA | H1' | 8 | ADE | H2 | 4.37 | 5.09 |
| 8 | ADE | H2 | 7 | UBX | H5 | 5.37 | 6.59 |
| 7 | UBX | H3' | 6 | CYT | H3' | 6.40 | 7.00 |
| 24 | CYT | H2'1 | 23 | GUA | H1' | 4.80 | 5.20 |
| 8 | ADE | H5'1 | 7 | UBX | H2'2 | 3.07 | 3.89 |
| 7 | UBX | H5'1 | 6 | CYT | H2'2 | 3.00 | 3.80 |
| 21 | THY | H5'1 | 21 | THY | H3' | 3.60 | 4.10 |
| 9 | GUA | H4' | 8 | ADE | H4' | 5.87 | 6.39 |
| 5 | GUA | H2'1 | 4 | ADE | H2'2 | 3.58 | 4.14 |
| 4 | ADE | H2'1 | 3 | THY | H2'2 | 3.58 | 4.14 |
| 12 | CYT | H2'1 | 11 | CYT | H2'2 | 3.58 | 4.14 |
| 16 | CYT | H3' | 15 | ADE | H3' | 6.38 | 6.84 |
| 16 | CYT | H4' | 15 | ADE | H4' | 5.88 | 6.34 |

**Table B-5:** Distance restraints used for the *R-N3-dU* modified oligonucleotide 5′-$G^{1}C^{2}T^{3}A^{4}G^{5}C^{6}X^{7}A^{8}G^{9}T^{10}C^{11}C^{12}$-3′·5′-$G^{13}G^{14}A^{15}C^{16}T^{17}G^{18}G^{19}C^{20}T^{21}A^{22}G^{23}C^{24}$-3′.

| | Residue Number | Residue Name | Atom Number | Residue Number | Residue Name | Atom Number | Lower Bound | Upper Bound |
|---|---|---|---|---|---|---|---|---|
| Class 1 | 1 | GUA | H8 | 1 | GUA | H1' | 3.15 | 4.73 |
| | 1 | GUA | H2'1 | 1 | GUA | H1' | 2.23 | 3.75 |
| | 1 | GUA | H2'1 | 1 | GUA | H8 | 1.86 | 2.52 |
| | 1 | GUA | H2'2 | 1 | GUA | H1' | 1.97 | 2.49 |
| | 2 | CYT | H6 | 1 | GUA | H2'2 | 2.07 | 3.47 |
| | 2 | CYT | H5 | 2 | CYT | H6 | 1.94 | 2.78 |
| | 2 | CYT | H2'1 | 2 | CYT | H6 | 1.91 | 2.87 |
| | 2 | CYT | H2'2 | 2 | CYT | H6 | 2.85 | 4.34 |
| | 3 | THY | M7 | 2 | CYT | H6 | 3.22 | 4.04 |
| | 3 | THY | M7 | 2 | CYT | H5 | 3.67 | 4.52 |
| | 3 | THY | M7 | 2 | CYT | H2'2 | 1.89 | 3.82 |
| | 3 | THY | M7 | 3 | THY | H6 | 2.58 | 3.32 |
| | 5 | GUA | H3' | 5 | GUA | H1' | 3.18 | 4.17 |
| | 5 | GUA | H2'1 | 5 | GUA | H1' | 2.19 | 3.69 |
| | 5 | GUA | H2'1 | 5 | GUA | H8 | 1.86 | 2.85 |
| | 6 | CYT | H5 | 6 | CYT | H6 | 1.97 | 2.52 |
| | 6 | CYT | H2'1 | 6 | CYT | H1' | 2.14 | 3.72 |
| | 6 | CYT | H2'1 | 6 | CYT | H6 | 1.76 | 2.53 |
| | 6 | CYT | H2'1 | 6 | CYT | H3' | 1.82 | 2.78 |
| | 6 | CYT | H2'2 | 6 | CYT | H1' | 1.87 | 2.70 |
| | 6 | CYT | H2'2 | 6 | CYT | H6 | 2.96 | 4.27 |
| | 6 | CYT | H2'2 | 6 | CYT | H3' | 2.16 | 3.43 |
| | 7 | UBX | H1' | 7 | UBX | H4' | 2.80 | 3.38 |
| | 7 | UBX | H5 | 7 | UBX | H6 | 2.44 | 2.98 |
| | 7 | UBX | H3' | 7 | UBX | H4' | 2.39 | 3.11 |
| | 7 | UBX | H2'2 | 7 | UBX | H3' | 2.50 | 3.38 |
| | 7 | UBX | H2'2 | 7 | UBX | H2'1 | 1.88 | 2.68 |
| | 8 | ADE | H3' | 8 | ADE | H1' | 3.23 | 4.64 |
| | 9 | GUA | H2'1 | 9 | GUA | H8 | 1.84 | 2.38 |
| | 10 | THY | M7 | 10 | THY | H6 | 2.71 | 3.61 |
| | 10 | THY | H2'1 | 10 | THY | H6 | 1.84 | 2.56 |
| | 10 | THY | H2'2 | 10 | THY | H1' | 1.89 | 2.66 |
| | 10 | THY | H2'2 | 10 | THY | H2'1 | 1.61 | 2.45 |
| | 11 | CYT | H5 | 10 | THY | H2'1 | 2.58 | 4.41 |
| | 11 | CYT | H5 | 11 | CYT | H6 | 1.92 | 2.61 |
| | 11 | CYT | H2'1 | 11 | CYT | H6 | 1.78 | 2.75 |
| | 11 | CYT | H2'2 | 11 | CYT | H1' | 1.82 | 2.45 |
| | 11 | CYT | H2'2 | 11 | CYT | H2'1 | 1.60 | 2.74 |
| | 12 | CYT | H5 | 12 | CYT | H6 | 1.80 | 2.57 |
| | 12 | CYT | H3' | 12 | CYT | H4' | 2.33 | 3.26 |
| | 12 | CYT | H2'2 | 12 | CYT | H1' | 1.71 | 2.72 |
| | 13 | GUA | H4' | 13 | GUA | H5'1 | 1.76 | 2.87 |
| | 13 | GUA | H2'1 | 13 | GUA | H8 | 1.78 | 2.46 |
| | 13 | GUA | H2'2 | 13 | GUA | H1' | 1.86 | 2.72 |
| | 13 | GUA | H2'2 | 13 | GUA | H3' | 2.26 | 2.85 |

**Table B-5:** Continued

| Residue Number | Residue Name | Atom Number | Residue Number | Residue Name | Atom Number | Lower Bound | Upper Bound |
|---|---|---|---|---|---|---|---|
| 14 | GUA | H3' | 14 | GUA | H4' | 1.81 | 2.73 |
| 14 | GUA | H2'1 | 14 | GUA | H8 | 1.75 | 2.77 |
| 14 | GUA | H2'1 | 14 | GUA | H3' | 1.86 | 3.22 |
| 14 | GUA | H2'2 | 14 | GUA | H1' | 1.84 | 3.11 |
| 14 | GUA | H2'2 | 14 | GUA | H8 | 3.11 | 4.02 |
| 15 | ADE | H8 | 15 | ADE | H1' | 2.93 | 4.63 |
| 15 | ADE | H3' | 15 | ADE | H4' | 2.32 | 3.31 |
| 15 | ADE | H2'1 | 15 | ADE | H1' | 2.23 | 3.68 |
| 15 | ADE | H2'1 | 15 | ADE | H3' | 1.98 | 2.80 |
| 15 | ADE | H2'2 | 15 | ADE | H1' | 1.86 | 2.80 |
| 16 | CYT | H6 | 15 | ADE | H8 | 4.66 | 5.53 |
| 16 | CYT | H6 | 15 | ADE | H2'1 | 2.85 | 4.43 |
| 16 | CYT | H6 | 15 | ADE | H2'2 | 1.89 | 2.63 |
| 16 | CYT | H5 | 16 | CYT | H6 | 1.98 | 2.79 |
| 16 | CYT | H3' | 16 | CYT | H4' | 2.25 | 3.49 |
| 16 | CYT | H3' | 16 | CYT | H6 | 2.80 | 4.45 |
| 16 | CYT | H2'1 | 16 | CYT | H1' | 2.29 | 3.88 |
| 16 | CYT | H2'2 | 16 | CYT | H1' | 2.04 | 2.74 |
| 16 | CYT | H2'2 | 16 | CYT | H2'1 | 1.68 | 2.70 |
| 17 | THY | H6 | 17 | THY | H1' | 2.96 | 4.20 |
| 17 | THY | M7 | 17 | THY | H6 | 2.81 | 3.38 |
| 17 | THY | H2'1 | 17 | THY | H1' | 2.41 | 3.23 |
| 17 | THY | H2'1 | 17 | THY | H6 | 1.68 | 2.54 |
| 17 | THY | H2'1 | 17 | THY | H3' | 1.87 | 2.85 |
| 17 | THY | H2'2 | 17 | THY | H1' | 2.15 | 2.87 |
| 17 | THY | H2'2 | 17 | THY | H3' | 2.37 | 3.32 |
| 17 | THY | H2'2 | 17 | THY | H2'1 | 1.71 | 2.86 |
| 18 | GUA | H2'1 | 18 | GUA | H1' | 2.11 | 3.31 |
| 18 | GUA | H2'2 | 18 | GUA | H8 | 2.60 | 4.15 |
| 19 | GUA | H1' | 19 | GUA | H4' | 1.93 | 3.69 |
| 19 | GUA | H8 | 19 | GUA | H1' | 3.40 | 4.26 |
| 19 | GUA | H2'2 | 19 | GUA | H1' | 1.72 | 2.59 |
| 20 | CYT | H6 | 19 | GUA | H1' | 2.38 | 3.79 |
| 20 | CYT | H5 | 20 | CYT | H6 | 2.06 | 2.64 |
| 20 | CYT | H2'1 | 20 | CYT | H3' | 1.92 | 2.69 |
| 20 | CYT | H2'2 | 20 | CYT | H1' | 1.97 | 2.58 |
| 20 | CYT | H2'2 | 20 | CYT | H2'1 | 1.59 | 2.50 |
| 21 | THY | H2'1 | 21 | THY | H6 | 1.78 | 2.59 |
| 21 | THY | H2'2 | 21 | THY | H1' | 1.89 | 2.67 |
| 23 | GUA | H2'1 | 23 | GUA | H8 | 1.79 | 2.57 |
| 23 | GUA | H2'1 | 23 | GUA | H3' | 1.91 | 2.83 |
| 23 | GUA | H2'2 | 23 | GUA | H1' | 1.92 | 2.69 |
| 23 | GUA | H2'2 | 23 | GUA | H3' | 1.94 | 2.73 |
| 24 | CYT | H6 | 23 | GUA | H2'2 | 1.99 | 2.69 |
| 24 | CYT | H5 | 24 | CYT | H6 | 1.89 | 2.50 |
| 24 | CYT | H2'1 | 24 | CYT | H6 | 1.87 | 2.65 |
| 24 | CYT | H2'1 | 24 | CYT | H3' | 1.88 | 2.80 |

**Table B-5:** Continued

| | Residue Number | Residue Name | Atom Number | Residue Number | Residue Name | Atom Number | Lower Bound | Upper Bound |
|---|---|---|---|---|---|---|---|---|
| | 24 | CYT | H2'2 | 24 | CYT | H1' | 1.67 | 2.48 |
| | 24 | CYT | H2'2 | 24 | CYT | H6 | 2.19 | 4.02 |
| | 2 | CYT | H2'2 | 2 | CYT | H1' | 2.07 | 2.48 |
| | 5 | GUA | H8 | 5 | GUA | H4' | 4.01 | 5.18 |
| | 18 | GUA | H2'2 | 18 | GUA | H2'1 | 1.54 | 1.86 |
| Class 2 | 1 | GUA | H2'2 | 1 | GUA | H8 | 3.16 | 4.85 |
| | 2 | CYT | H6 | 1 | GUA | H2'1 | 2.91 | 3.78 |
| | 2 | CYT | H6 | 2 | CYT | H1' | 2.96 | 4.44 |
| | 2 | CYT | H5 | 1 | GUA | H8 | 2.88 | 4.15 |
| | 2 | CYT | H3' | 2 | CYT | H6 | 3.12 | 4.05 |
| | 2 | CYT | H2'1 | 2 | CYT | H1' | 2.10 | 3.86 |
| | 3 | THY | H3' | 3 | THY | H1' | 3.47 | 4.58 |
| | 2 | CYT | H2'2 | 2 | CYT | H2'1 | 1.52 | 2.32 |
| | 2 | CYT | H1' | 3 | THY | M7 | 3.35 | 4.39 |
| | 4 | ADE | H3' | 4 | ADE | H4' | 2.25 | 3.88 |
| | 5 | GUA | H1' | 5 | GUA | H4' | 2.55 | 3.92 |
| | 5 | GUA | H8 | 4 | ADE | H2'1 | 2.27 | 4.20 |
| | 5 | GUA | H8 | 5 | GUA | H1' | 2.82 | 4.43 |
| | 5 | GUA | H2'1 | 5 | GUA | H3' | 1.99 | 3.59 |
| | 5 | GUA | H2'2 | 5 | GUA | H4' | 3.82 | 4.87 |
| | 5 | GUA | H2'2 | 5 | GUA | H8 | 3.19 | 4.15 |
| | 6 | CYT | H6 | 5 | GUA | H2'2 | 1.84 | 3.36 |
| | 6 | CYT | H5 | 5 | GUA | H8 | 2.79 | 4.00 |
| | 6 | CYT | H3' | 6 | CYT | H1' | 3.17 | 4.86 |
| | 7 | UBX | H6 | 7 | UBX | H1' | 2.74 | 3.98 |
| | 7 | UBX | H3' | 7 | UBX | H5'1 | 2.96 | 4.48 |
| | 7 | UBX | H2'1 | 7 | UBX | H1' | 2.74 | 3.86 |
| | 7 | UBX | H2'1 | 7 | UBX | H3' | 2.22 | 3.06 |
| | 7 | UBX | H2'2 | 7 | UBX | H1' | 1.83 | 2.81 |
| | 7 | UBX | H2'2 | 7 | UBX | H5 | 4.82 | 5.88 |
| | 8 | ADE | H1' | 8 | ADE | H4' | 3.05 | 4.29 |
| | 8 | ADE | H8 | 7 | UBX | H1' | 3.85 | 4.50 |
| | 8 | ADE | H8 | 8 | ADE | H1' | 3.34 | 4.85 |
| | 8 | ADE | H3' | 8 | ADE | H8 | 3.56 | 4.92 |
| | 8 | ADE | H2'1 | 8 | ADE | H1' | 1.93 | 3.61 |
| | 8 | ADE | H2'1 | 8 | ADE | H8 | 1.84 | 3.12 |
| | 8 | ADE | H2'2 | 8 | ADE | H8 | 2.83 | 4.02 |
| | 9 | GUA | H8 | 9 | GUA | H4' | 3.75 | 5.42 |
| | 9 | GUA | H2'1 | 9 | GUA | H1' | 2.70 | 3.78 |
| | 9 | GUA | H2'2 | 9 | GUA | H1' | 1.80 | 2.93 |
| | 9 | GUA | H2'2 | 9 | GUA | H8 | 2.54 | 3.87 |
| | 10 | THY | H6 | 9 | GUA | H1' | 1.82 | 3.22 |
| | 10 | THY | H3' | 10 | THY | H1' | 3.74 | 5.40 |
| | 10 | THY | H2'1 | 10 | THY | M7 | 3.33 | 5.06 |
| | 10 | THY | H2'2 | 10 | THY | H6 | 2.45 | 3.98 |
| | 11 | CYT | H5 | 10 | THY | H6 | 2.95 | 4.63 |
| | 11 | CYT | H5 | 10 | THY | M7 | 3.68 | 5.09 |

**Table B-5:** Continued

| Residue Number | Residue Name | Atom Number | Residue Number | Residue Name | Atom Number | Lower Bound | Upper Bound |
|---|---|---|---|---|---|---|---|
| 11 | CYT | H5 | 10 | THY | H2'2 | 2.17 | 3.20 |
| 11 | CYT | H2'1 | 11 | CYT | H1' | 1.98 | 3.91 |
| 11 | CYT | H2'1 | 11 | CYT | H5 | 3.60 | 4.87 |
| 11 | CYT | H2'2 | 11 | CYT | H6 | 2.30 | 4.25 |
| 12 | CYT | H1' | 12 | CYT | H5'1 | 4.19 | 5.26 |
| 12 | CYT | H6 | 12 | CYT | H1' | 3.30 | 4.37 |
| 12 | CYT | H5 | 11 | CYT | H6 | 3.37 | 4.57 |
| 12 | CYT | H5 | 11 | CYT | H2'1 | 2.10 | 3.97 |
| 12 | CYT | H3' | 12 | CYT | H5'1 | 2.76 | 4.42 |
| 12 | CYT | H3' | 12 | CYT | H1' | 2.99 | 4.42 |
| 12 | CYT | H2'1 | 12 | CYT | H1' | 2.37 | 3.93 |
| 12 | CYT | H2'1 | 12 | CYT | H3' | 2.02 | 3.18 |
| 12 | CYT | H2'2 | 12 | CYT | H6 | 2.86 | 3.78 |
| 12 | CYT | H2'2 | 12 | CYT | H3' | 1.95 | 3.80 |
| 13 | GUA | H8 | 13 | GUA | H5'1 | 2.31 | 3.72 |
| 13 | GUA | H2'1 | 13 | GUA | H5'1 | 3.00 | 4.61 |
| 13 | GUA | H2'1 | 13 | GUA | H1' | 2.21 | 4.28 |
| 13 | GUA | H2'2 | 13 | GUA | H8 | 2.99 | 4.35 |
| 14 | GUA | H1' | 14 | GUA | H4' | 2.71 | 3.47 |
| 14 | GUA | H8 | 13 | GUA | H2'1 | 2.41 | 4.04 |
| 14 | GUA | H8 | 13 | GUA | H2'2 | 2.28 | 2.71 |
| 14 | GUA | H3' | 14 | GUA | H1' | 3.63 | 4.52 |
| 14 | GUA | H2'1 | 14 | GUA | H1' | 2.08 | 3.76 |
| 14 | GUA | H2'2 | 14 | GUA | H3' | 1.99 | 3.60 |
| 15 | ADE | H5'1 | 14 | GUA | H1' | 2.58 | 4.28 |
| 15 | ADE | H1' | 15 | ADE | H4' | 2.79 | 3.45 |
| 15 | ADE | H8 | 15 | ADE | H4' | 3.93 | 5.71 |
| 15 | ADE | H3' | 15 | ADE | H1' | 3.18 | 4.53 |
| 15 | ADE | H2'1 | 15 | ADE | H4' | 2.82 | 4.23 |
| 16 | CYT | H4' | 15 | ADE | H1' | 2.94 | 4.80 |
| 16 | CYT | H6 | 16 | CYT | H4' | 3.78 | 5.51 |
| 16 | CYT | H6 | 16 | CYT | H1' | 3.02 | 4.73 |
| 16 | CYT | H5 | 15 | ADE | H1' | 3.29 | 4.59 |
| 16 | CYT | H5 | 15 | ADE | H8 | 3.02 | 4.59 |
| 16 | CYT | H3' | 16 | CYT | H1' | 3.29 | 4.65 |
| 16 | CYT | H2'1 | 16 | CYT | H6 | 1.85 | 2.78 |
| 16 | CYT | H2'1 | 16 | CYT | H5 | 3.56 | 5.15 |
| 16 | CYT | H2'1 | 16 | CYT | H3' | 2.12 | 3.03 |
| 16 | CYT | H2'2 | 16 | CYT | H6 | 2.58 | 4.01 |
| 16 | CYT | H2'2 | 16 | CYT | H3' | 2.18 | 3.45 |
| 17 | THY | H3' | 17 | THY | H1' | 3.25 | 4.72 |
| 18 | GUA | H8 | 18 | GUA | H1' | 2.72 | 4.17 |
| 18 | GUA | H2'1 | 18 | GUA | H8 | 1.82 | 2.73 |
| 19 | GUA | H8 | 19 | GUA | H4' | 4.08 | 5.78 |
| 19 | GUA | H3' | 19 | GUA | H8 | 3.75 | 5.45 |
| 19 | GUA | H2'2 | 19 | GUA | H3' | 1.74 | 2.98 |
| 20 | CYT | H6 | 20 | CYT | H1' | 3.39 | 4.10 |

**Table B-5:** Continued

| | Residue Number | Residue Name | Atom Number | Residue Number | Residue Name | Atom Number | Lower Bound | Upper Bound |
|---|---|---|---|---|---|---|---|---|
| | 20 | CYT | H6 | 20 | CYT | H1' | 3.39 | 4.10 |
| | 20 | CYT | H2'1 | 20 | CYT | H1' | 2.10 | 4.17 |
| | 20 | CYT | H2'1 | 20 | CYT | H6 | 1.91 | 2.72 |
| | 20 | CYT | H2'2 | 20 | CYT | H6 | 2.01 | 3.67 |
| | 20 | CYT | H2'2 | 20 | CYT | H3' | 2.26 | 3.66 |
| | 21 | THY | H6 | 20 | CYT | H1' | 1.82 | 3.34 |
| | 21 | THY | M7 | 20 | CYT | H5 | 3.77 | 4.61 |
| | 21 | THY | M7 | 20 | CYT | H2'1 | 2.73 | 3.89 |
| | 21 | THY | M7 | 21 | THY | H6 | 2.61 | 3.35 |
| | 22 | ADE | H2'2 | 22 | ADE | H3' | 1.80 | 2.71 |
| | 23 | GUA | H1' | 23 | GUA | H4' | 2.51 | 3.20 |
| | 23 | GUA | H8 | 22 | ADE | H2'1 | 2.33 | 4.07 |
| | 23 | GUA | H8 | 22 | ADE | H2'2 | 2.26 | 2.93 |
| | 23 | GUA | H2'1 | 23 | GUA | H1' | 2.65 | 3.74 |
| | 23 | GUA | H2'2 | 23 | GUA | H8 | 3.06 | 4.53 |
| | 6 | CYT | H5 | 5 | GUA | H1' | 2.99 | 4.13 |
| | 9 | GUA | H2'1 | 9 | GUA | H4' | 3.20 | 4.46 |
| | 11 | CYT | H6 | 10 | THY | H6 | 4.36 | 5.63 |
| | 24 | CYT | H5 | 23 | GUA | H1' | 2.90 | 4.63 |
| | 3 | THY | H2'1 | 3 | THY | M7 | 3.89 | 5.61 |
| | 12 | CYT | H6 | 11 | CYT | H3' | 3.57 | 5.11 |
| Class 3 | 2 | CYT | H5 | 1 | GUA | H1' | 2.96 | 4.69 |
| | 3 | THY | H6 | 3 | THY | H1' | 2.98 | 4.03 |
| | 3 | THY | H2'1 | 3 | THY | H1' | 2.21 | 3.91 |
| | 3 | THY | H2'2 | 3 | THY | H1' | 2.08 | 2.86 |
| | 4 | ADE | H5'1 | 3 | THY | H1' | 2.24 | 3.14 |
| | 4 | ADE | H8 | 3 | THY | H1' | 2.13 | 3.48 |
| | 4 | ADE | H8 | 3 | THY | H2'1 | 3.08 | 4.30 |
| | 4 | ADE | H8 | 3 | THY | H2'2 | 1.82 | 3.08 |
| | 5 | GUA | H8 | 4 | ADE | H1' | 2.32 | 3.46 |
| | 5 | GUA | H8 | 4 | ADE | H2'2 | 1.86 | 3.24 |
| | 5 | GUA | H2'2 | 5 | GUA | H1' | 1.93 | 2.57 |
| | 7 | UBX | H3' | 7 | UBX | H1' | 3.10 | 4.87 |
| | 7 | UBX | H2'1 | 7 | UBX | H4' | 3.32 | 5.09 |
| | 8 | ADE | H2'2 | 8 | ADE | H3' | 2.11 | 3.21 |
| | 12 | CYT | H6 | 11 | CYT | H1' | 2.36 | 3.35 |
| | 13 | GUA | H2'2 | 13 | GUA | H5'1 | 4.18 | 5.30 |
| | 14 | GUA | H8 | 13 | GUA | H3' | 4.34 | 5.12 |
| | 14 | GUA | H3' | 14 | GUA | H5'1 | 2.71 | 4.18 |
| | 15 | ADE | H8 | 14 | GUA | H1' | 2.01 | 3.69 |
| | 15 | ADE | H2'2 | 15 | ADE | H4' | 3.05 | 4.77 |
| | 16 | CYT | H2'2 | 16 | CYT | H5 | 4.98 | 5.62 |
| | 20 | CYT | H1' | 20 | CYT | H4' | 2.40 | 3.58 |
| | 20 | CYT | H6 | 19 | GUA | H8 | 4.90 | 5.52 |
| | 20 | CYT | H2'1 | 20 | CYT | H4' | 2.75 | 4.16 |
| | 21 | THY | H6 | 21 | THY | H1' | 3.33 | 4.42 |
| | 23 | GUA | H8 | 22 | ADE | H8 | 4.94 | 5.30 |

**Table B-5:** Continued

| | Residue Number | Residue Name | Atom Number | Residue Number | Residue Name | Atom Number | Lower Bound | Upper Bound |
|---|---|---|---|---|---|---|---|---|
| | 23 | GUA | H8 | 23 | GUA | H1' | 3.37 | 4.54 |
| | 23 | GUA | H2'2 | 23 | GUA | H4' | 3.66 | 4.78 |
| | 24 | CYT | H6 | 23 | GUA | H2'1 | 2.86 | 3.92 |
| | 24 | CYT | H3' | 24 | CYT | H1' | 3.53 | 4.45 |
| | 24 | CYT | H2'1 | 24 | CYT | H1' | 2.55 | 3.57 |
| | 24 | CYT | H2'2 | 24 | CYT | H3' | 2.27 | 3.30 |
| | 2 | CYT | H2'1 | 2 | CYT | H3' | 1.94 | 2.78 |
| | 10 | THY | H6 | 9 | GUA | H8 | 3.90 | 5.09 |
| | 15 | ADE | H8 | 14 | GUA | H8 | 3.99 | 5.39 |
| | 18 | GUA | H8 | 17 | THY | H1' | 4.34 | 5.14 |
| | 24 | CYT | H6 | 23 | GUA | H8 | 4.47 | 5.49 |
| | 18 | GUA | H8 | 17 | THY | H6 | 4.91 | 5.57 |
| | 10 | THY | H2'1 | 10 | THY | H1' | 2.06 | 3.21 |
| Class 4 | 1 | GUA | H4' | 1 | GUA | H5'1 | 1.76 | 2.71 |
| | 1 | GUA | H1' | 1 | GUA | H5'1 | 3.68 | 5.08 |
| | 1 | GUA | H1' | 1 | GUA | H4' | 2.32 | 3.92 |
| | 1 | GUA | H8 | 1 | GUA | H5'1 | 3.27 | 4.25 |
| | 1 | GUA | H8 | 1 | GUA | H4' | 4.05 | 5.66 |
| | 1 | GUA | H3' | 1 | GUA | H1' | 3.39 | 5.27 |
| | 1 | GUA | H2'1 | 1 | GUA | H5'1 | 2.97 | 4.40 |
| | 1 | GUA | H2'1 | 1 | GUA | H3' | 1.93 | 2.82 |
| | 1 | GUA | H2'2 | 1 | GUA | H5'1 | 4.08 | 5.23 |
| | 1 | GUA | H2'2 | 1 | GUA | H4' | 3.37 | 4.50 |
| | 2 | CYT | H6 | 1 | GUA | H1' | 2.72 | 3.40 |
| | 2 | CYT | H3' | 2 | CYT | H5'1 | 3.59 | 4.27 |
| | 2 | CYT | H6 | 2 | CYT | H4' | 3.99 | 4.86 |
| | 2 | CYT | H5 | 1 | GUA | H2'1 | 2.16 | 3.32 |
| | 2 | CYT | H5 | 1 | GUA | H2'2 | 2.14 | 3.32 |
| | 2 | CYT | H3' | 2 | CYT | H1' | 3.15 | 5.03 |
| | 2 | CYT | H2'1 | 1 | GUA | H1' | 3.62 | 5.04 |
| | 2 | CYT | H2'1 | 2 | CYT | H5 | 3.13 | 4.83 |
| | 3 | THY | H1' | 3 | THY | H4' | 2.40 | 4.09 |
| | 3 | THY | H6 | 2 | CYT | H1' | 1.89 | 3.40 |
| | 3 | THY | H6 | 2 | CYT | H2'2 | 1.80 | 3.02 |
| | 3 | THY | M7 | 2 | CYT | H3' | 4.57 | 5.59 |
| | 3 | THY | M7 | 2 | CYT | H2'1 | 2.27 | 3.36 |
| | 3 | THY | H3' | 3 | THY | H5'1 | 3.59 | 4.27 |
| | 3 | THY | H3' | 3 | THY | H6 | 3.56 | 5.24 |
| | 3 | THY | H2'1 | 3 | THY | H6 | 1.65 | 2.48 |
| | 3 | THY | H2'2 | 3 | THY | H6 | 2.79 | 4.01 |
| | 3 | THY | H2'2 | 3 | THY | H3' | 2.42 | 3.36 |
| | 4 | ADE | H1' | 4 | ADE | H4' | 2.81 | 4.16 |
| | 4 | ADE | H3' | 4 | ADE | H5'1 | 3.59 | 4.27 |
| | 4 | ADE | H8 | 4 | ADE | H1' | 2.91 | 4.09 |
| | 4 | ADE | H3' | 4 | ADE | H1' | 3.58 | 4.76 |
| | 4 | ADE | H3' | 4 | ADE | H8 | 2.95 | 4.83 |
| | 4 | ADE | H2'1 | 4 | ADE | H4' | 3.16 | 4.29 |

**Table B-5:** Continued

| Residue Number | Residue Name | Atom Number | Residue Number | Residue Name | Atom Number | Lower Bound | Upper Bound |
|---|---|---|---|---|---|---|---|
| 4 | ADE | H2'1 | 4 | ADE | H1' | 2.13 | 3.21 |
| 4 | ADE | H2'1 | 4 | ADE | H3' | 1.78 | 3.28 |
| 4 | ADE | H2'2 | 4 | ADE | H4' | 3.44 | 5.39 |
| 4 | ADE | H2'2 | 4 | ADE | H1' | 1.96 | 3.20 |
| 4 | ADE | H2'2 | 4 | ADE | H3' | 2.06 | 3.50 |
| 5 | GUA | H8 | 4 | ADE | H8 | 4.56 | 6.25 |
| 5 | GUA | H8 | 4 | ADE | H3' | 3.89 | 5.63 |
| 5 | GUA | H3' | 5 | GUA | H5'1 | 3.59 | 4.27 |
| 5 | GUA | H3' | 5 | GUA | H8 | 3.44 | 5.27 |
| 5 | GUA | H2'1 | 5 | GUA | H4' | 3.31 | 4.38 |
| 5 | GUA | H2'2 | 5 | GUA | H3' | 1.98 | 2.85 |
| 6 | CYT | H1' | 6 | CYT | H4' | 2.18 | 3.82 |
| 6 | CYT | H6 | 5 | GUA | H1' | 1.84 | 3.20 |
| 6 | CYT | H6 | 5 | GUA | H3' | 3.55 | 5.43 |
| 6 | CYT | H6 | 5 | GUA | H2'1 | 3.11 | 4.20 |
| 6 | CYT | H6 | 6 | CYT | H1' | 2.91 | 4.23 |
| 6 | CYT | H5 | 5 | GUA | H2'1 | 2.51 | 3.91 |
| 6 | CYT | H5 | 5 | GUA | H2'2 | 1.88 | 2.95 |
| 6 | CYT | H3' | 6 | CYT | H6 | 3.41 | 5.24 |
| 6 | CYT | H2'2 | 6 | CYT | H5 | 3.92 | 5.78 |
| 7 | UBX | H6 | 6 | CYT | H1' | 4.21 | 5.38 |
| 7 | UBX | H6 | 6 | CYT | H2'1 | 4.14 | 5.56 |
| 7 | UBX | H6 | 6 | CYT | H2'2 | 3.87 | 5.09 |
| 7 | UBX | H6 | 7 | UBX | H4' | 4.39 | 5.30 |
| 7 | UBX | H5 | 6 | CYT | H2'1 | 4.22 | 5.22 |
| 7 | UBX | H5 | 6 | CYT | H2'2 | 4.37 | 5.49 |
| 7 | UBX | H3' | 7 | UBX | H6 | 3.40 | 4.69 |
| 7 | UBX | H2'1 | 7 | UBX | H6 | 1.88 | 3.04 |
| 7 | UBX | H2'1 | 7 | UBX | H5 | 3.29 | 5.05 |
| 7 | UBX | H2'2 | 7 | UBX | H4' | 3.41 | 5.24 |
| 7 | UBX | H2'2 | 7 | UBX | H6 | 2.41 | 4.35 |
| 7 | UBX | H9 | 7 | UBX | H15 | 1.82 | 3.83 |
| 7 | UBX | H9 | 7 | UBX | H14 | 1.92 | 3.05 |
| 7 | UBX | H11 | 7 | UBX | H15 | 2.38 | 4.45 |
| 7 | UBX | H11 | 7 | UBX | H14 | 2.58 | 4.51 |
| 7 | UBX | H11 | 7 | UBX | H9 | 2.48 | 3.77 |
| 8 | ADE | H8 | 7 | UBX | H3' | 4.51 | 5.48 |
| 8 | ADE | H8 | 7 | UBX | H2'1 | 3.71 | 5.12 |
| 8 | ADE | H8 | 7 | UBX | H2'2 | 3.16 | 4.63 |
| 8 | ADE | H8 | 8 | ADE | H4' | 4.26 | 5.43 |
| 8 | ADE | H2 | 7 | UBX | H15 | 2.59 | 3.64 |
| 8 | ADE | H2 | 7 | UBX | H14 | 2.62 | 3.88 |
| 8 | ADE | H2 | 7 | UBX | H9 | 4.18 | 5.06 |
| 8 | ADE | H2 | 7 | UBX | H11 | 6.18 | 8.06 |
| 8 | ADE | H2'1 | 8 | ADE | H3' | 2.00 | 3.23 |
| 8 | ADE | H2'2 | 8 | ADE | H1' | 1.85 | 3.22 |

**Table B-5:** Continued

| Residue Number | Residue Name | Atom Number | Residue Number | Residue Name | Atom Number | Lower Bound | Upper Bound |
|---|---|---|---|---|---|---|---|
| 9 | GUA | H1' | 9 | GUA | H4' | 2.88 | 3.86 |
| 9 | GUA | H8 | 8 | ADE | H1' | 1.67 | 3.51 |
| 9 | GUA | H8 | 8 | ADE | H8 | 4.86 | 5.32 |
| 9 | GUA | H8 | 8 | ADE | H3' | 4.50 | 5.46 |
| 9 | GUA | H8 | 8 | ADE | H2'1 | 3.04 | 5.36 |
| 9 | GUA | H8 | 8 | ADE | H2'2 | 2.14 | 3.98 |
| 9 | GUA | H8 | 9 | GUA | H1' | 3.08 | 4.39 |
| 9 | GUA | H3' | 9 | GUA | H1' | 3.65 | 4.63 |
| 9 | GUA | H3' | 9 | GUA | H5'1 | 3.65 | 4.33 |
| 9 | GUA | H3' | 9 | GUA | H8 | 4.17 | 4.86 |
| 10 | THY | H6 | 9 | GUA | H2'1 | 1.95 | 3.70 |
| 10 | THY | H6 | 9 | GUA | H2'2 | 1.88 | 2.76 |
| 10 | THY | H3' | 10 | THY | H5'1 | 3.65 | 4.33 |
| 10 | THY | H6 | 10 | THY | H1' | 2.93 | 4.73 |
| 10 | THY | M7 | 9 | GUA | H1' | 3.72 | 4.32 |
| 10 | THY | M7 | 9 | GUA | H8 | 2.93 | 3.70 |
| 10 | THY | M7 | 9 | GUA | H2'1 | 2.83 | 3.44 |
| 10 | THY | M7 | 9 | GUA | H2'2 | 2.16 | 3.49 |
| 10 | THY | H3' | 10 | THY | H6 | 3.73 | 4.86 |
| 11 | CYT | H6 | 10 | THY | H1' | 1.91 | 3.61 |
| 11 | CYT | H6 | 10 | THY | H2'1 | 3.06 | 4.09 |
| 11 | CYT | H6 | 10 | THY | H2'2 | 1.83 | 2.86 |
| 11 | CYT | H3' | 11 | CYT | H5'1 | 3.65 | 4.33 |
| 11 | CYT | H6 | 11 | CYT | H1' | 3.25 | 4.50 |
| 11 | CYT | H3' | 11 | CYT | H6 | 3.33 | 4.36 |
| 12 | CYT | H1' | 12 | CYT | H4' | 3.22 | 4.69 |
| 12 | CYT | H6 | 11 | CYT | H2'1 | 2.86 | 4.26 |
| 12 | CYT | H3' | 12 | CYT | H6 | 3.16 | 4.12 |
| 12 | CYT | H3' | 12 | CYT | H5 | 4.98 | 6.44 |
| 12 | CYT | H2'1 | 12 | CYT | H6 | 1.88 | 2.59 |
| 12 | CYT | H2'1 | 12 | CYT | H5 | 3.35 | 4.43 |
| 12 | CYT | H2'2 | 12 | CYT | H5 | 5.35 | 6.26 |
| 13 | GUA | H1' | 13 | GUA | H5'1 | 3.63 | 5.21 |
| 13 | GUA | H1' | 13 | GUA | H4' | 2.36 | 3.22 |
| 13 | GUA | H8 | 13 | GUA | H4' | 3.52 | 5.32 |
| 13 | GUA | H8 | 13 | GUA | H1' | 3.11 | 4.53 |
| 13 | GUA | H3' | 13 | GUA | H1' | 3.00 | 4.57 |
| 13 | GUA | H3' | 13 | GUA | H8 | 3.74 | 5.32 |
| 14 | GUA | H5'1 | 13 | GUA | H1' | 1.88 | 3.37 |
| 14 | GUA | H8 | 13 | GUA | H1' | 1.83 | 3.33 |
| 14 | GUA | H8 | 14 | GUA | H4' | 3.40 | 5.76 |
| 14 | GUA | H8 | 14 | GUA | H1' | 3.55 | 4.59 |
| 14 | GUA | H3' | 14 | GUA | H8 | 3.52 | 4.84 |
| 15 | ADE | H3' | 15 | ADE | H8 | 3.40 | 5.35 |
| 15 | ADE | H2'2 | 15 | ADE | H3' | 2.58 | 3.00 |
| 16 | CYT | H1' | 16 | CYT | H4' | 2.60 | 3.75 |

**Table B-5:** Continued

| Residue Number | Residue Name | Atom Number | Residue Number | Residue Name | Atom Number | Lower Bound | Upper Bound |
|---|---|---|---|---|---|---|---|
| 16 | CYT | H6 | 15 | ADE | H1' | 1.77 | 3.10 |
| 16 | CYT | H6 | 15 | ADE | H3' | 4.30 | 5.08 |
| 16 | CYT | H5 | 15 | ADE | H2'1 | 2.54 | 3.56 |
| 16 | CYT | H5 | 15 | ADE | H2'2 | 2.69 | 3.13 |
| 17 | THY | H1' | 17 | THY | H4' | 2.37 | 3.48 |
| 17 | THY | H6 | 16 | CYT | H1' | 3.15 | 4.38 |
| 17 | THY | H6 | 16 | CYT | H2'2 | 3.00 | 4.41 |
| 17 | THY | H6 | 17 | THY | H4' | 4.05 | 5.33 |
| 17 | THY | M7 | 16 | CYT | H1' | 2.97 | 4.36 |
| 17 | THY | M7 | 16 | CYT | H6 | 3.47 | 4.48 |
| 17 | THY | M7 | 16 | CYT | H5 | 3.70 | 4.62 |
| 17 | THY | M7 | 16 | CYT | H2'2 | 2.50 | 3.46 |
| 17 | THY | H3' | 17 | THY | H6 | 3.46 | 4.73 |
| 17 | THY | H2'2 | 17 | THY | H6 | 2.61 | 4.11 |
| 18 | GUA | H1' | 18 | GUA | H5'1 | 3.63 | 4.76 |
| 18 | GUA | H1' | 18 | GUA | H4' | 2.99 | 3.93 |
| 18 | GUA | H8 | 17 | THY | H3' | 4.24 | 5.30 |
| 18 | GUA | H8 | 17 | THY | H2'1 | 3.87 | 4.63 |
| 18 | GUA | H8 | 17 | THY | H2'2 | 2.90 | 4.61 |
| 18 | GUA | H8 | 18 | GUA | H4' | 3.43 | 5.22 |
| 18 | GUA | H3' | 18 | GUA | H8 | 3.85 | 4.74 |
| 18 | GUA | H2'2 | 18 | GUA | H1' | 1.63 | 2.74 |
| 19 | GUA | H8 | 18 | GUA | H1' | 3.52 | 4.63 |
| 19 | GUA | H8 | 18 | GUA | H2'1 | 3.92 | 4.44 |
| 19 | GUA | H8 | 18 | GUA | H2'2 | 2.92 | 3.61 |
| 19 | GUA | H3' | 19 | GUA | H1' | 3.18 | 4.62 |
| 19 | GUA | H2'1 | 19 | GUA | H1' | 2.38 | 3.21 |
| 19 | GUA | H2'1 | 19 | GUA | H3' | 1.85 | 2.96 |
| 19 | GUA | H2'2 | 19 | GUA | H8 | 2.78 | 4.24 |
| 20 | CYT | H6 | 19 | GUA | H3' | 3.65 | 5.25 |
| 20 | CYT | H6 | 19 | GUA | H2'1 | 2.91 | 4.38 |
| 20 | CYT | H6 | 19 | GUA | H2'2 | 1.96 | 2.31 |
| 20 | CYT | H6 | 20 | CYT | H4' | 4.63 | 5.39 |
| 20 | CYT | H5 | 19 | GUA | H1' | 1.82 | 3.54 |
| 20 | CYT | H5 | 19 | GUA | H8 | 3.30 | 4.08 |
| 20 | CYT | H5 | 19 | GUA | H2'1 | 2.27 | 3.45 |
| 20 | CYT | H5 | 19 | GUA | H2'2 | 2.49 | 3.19 |
| 20 | CYT | H3' | 20 | CYT | H1' | 3.31 | 4.22 |
| 20 | CYT | H3' | 20 | CYT | H6 | 3.48 | 5.01 |
| 20 | CYT | H2'1 | 20 | CYT | H5 | 3.70 | 5.14 |
| 20 | CYT | H2'2 | 20 | CYT | H5 | 4.78 | 5.73 |
| 21 | THY | H1' | 21 | THY | H4' | 2.70 | 4.45 |
| 21 | THY | H6 | 20 | CYT | H2'1 | 2.93 | 3.74 |
| 21 | THY | H6 | 20 | CYT | H2'2 | 1.85 | 2.50 |
| 21 | THY | M7 | 20 | CYT | H1' | 3.66 | 4.95 |
| 21 | THY | M7 | 20 | CYT | H6 | 3.09 | 4.17 |

**Table B-5:** Continued

| Residue Number | Residue Name | Atom Number | Residue Number | Residue Name | Atom Number | Lower Bound | Upper Bound |
|---|---|---|---|---|---|---|---|
| 21 | THY | M7 | 20 | CYT | H2'2 | 1.81 | 3.48 |
| 21 | THY | H3' | 21 | THY | H6 | 3.10 | 4.67 |
| 21 | THY | H2'1 | 21 | THY | H1' | 2.40 | 3.87 |
| 21 | THY | H2'2 | 21 | THY | H6 | 2.51 | 3.72 |
| 22 | ADE | H5'1 | 21 | THY | H1' | 2.66 | 3.85 |
| 22 | ADE | H1' | 22 | ADE | H4' | 2.48 | 3.29 |
| 22 | ADE | H8 | 21 | THY | H1' | 2.46 | 3.65 |
| 22 | ADE | H3' | 22 | ADE | H5'1 | 3.51 | 4.49 |
| 22 | ADE | H8 | 21 | THY | H2'1 | 2.71 | 4.46 |
| 22 | ADE | H8 | 21 | THY | H2'2 | 1.85 | 2.58 |
| 22 | ADE | H8 | 22 | ADE | H1' | 3.02 | 5.05 |
| 22 | ADE | H3' | 22 | ADE | H4' | 1.91 | 3.49 |
| 22 | ADE | H3' | 22 | ADE | H1' | 3.26 | 4.73 |
| 22 | ADE | H3' | 22 | ADE | H8 | 3.80 | 4.40 |
| 22 | ADE | H2'1 | 22 | ADE | H4' | 3.25 | 4.63 |
| 22 | ADE | H2'1 | 22 | ADE | H1' | 1.88 | 3.75 |
| 22 | ADE | H2'1 | 22 | ADE | H3' | 2.30 | 3.19 |
| 22 | ADE | H2'2 | 22 | ADE | H4' | 3.51 | 5.07 |
| 23 | GUA | H8 | 22 | ADE | H1' | 2.78 | 3.34 |
| 23 | GUA | H8 | 22 | ADE | H3' | 4.07 | 5.37 |
| 23 | GUA | H8 | 23 | GUA | H4' | 4.33 | 5.40 |
| 23 | GUA | H3' | 23 | GUA | H1' | 3.09 | 4.63 |
| 23 | GUA | H3' | 23 | GUA | H8 | 3.96 | 5.09 |
| 23 | GUA | H2'1 | 23 | GUA | H4' | 3.29 | 4.32 |
| 24 | CYT | H1' | 24 | CYT | H5'1 | 4.27 | 4.98 |
| 24 | CYT | H6 | 23 | GUA | H1' | 2.26 | 3.54 |
| 24 | CYT | H6 | 23 | GUA | H3' | 3.92 | 5.60 |
| 24 | CYT | H6 | 24 | CYT | H4' | 3.67 | 5.24 |
| 24 | CYT | H6 | 24 | CYT | H1' | 2.89 | 4.46 |
| 24 | CYT | H5 | 23 | GUA | H8 | 3.24 | 4.72 |
| 24 | CYT | H5 | 23 | GUA | H2'2 | 1.79 | 3.39 |
| 24 | CYT | H3' | 24 | CYT | H6 | 3.37 | 4.44 |
| 24 | CYT | H3' | 24 | CYT | H5'1 | 3.57 | 4.44 |
| 2 | CYT | H6 | 1 | GUA | H8 | 4.93 | 5.30 |
| 3 | THY | M7 | 2 | CYT | H1' | 3.52 | 4.64 |
| 4 | ADE | H8 | 3 | THY | H6 | 4.54 | 5.34 |
| 8 | ADE | H2 | 8 | ADE | H1' | 3.50 | 5.04 |
| 8 | ADE | H2'1 | 8 | ADE | H4' | 3.07 | 4.31 |
| 8 | ADE | H2'2 | 8 | ADE | H4' | 3.40 | 4.32 |
| 9 | GUA | H1' | 8 | ADE | H2 | 4.26 | 4.96 |
| 9 | GUA | H2'2 | 9 | GUA | H4' | 3.75 | 4.56 |
| 10 | THY | H6 | 9 | GUA | H3' | 4.00 | 5.15 |
| 11 | CYT | H5 | 10 | THY | H1' | 3.10 | 4.72 |
| 17 | THY | H1' | 7 | UBX | H9 | 4.13 | 5.15 |
| 22 | ADE | H8 | 21 | THY | H6 | 4.33 | 5.55 |
| 6 | CYT | H1' | 5 | GUA | H1' | 4.29 | 5.19 |

**Table B-5:** Continued

| Residue Number | Residue Name | Atom Number | Residue Number | Residue Name | Atom Number | Lower Bound | Upper Bound |
|---|---|---|---|---|---|---|---|
| 7 | UBX | H5 | 7 | UBX | H1' | 4.83 | 5.70 |
| 10 | THY | H6 | 10 | THY | H4' | 4.06 | 4.88 |
| 17 | THY | M7 | 16 | CYT | H3' | 4.37 | 5.35 |
| 21 | THY | H6 | 20 | CYT | H3' | 3.96 | 5.31 |
| 24 | CYT | H3' | 24 | CYT | H5 | 5.67 | 6.57 |
| 7 | UBX | H2'2 | 7 | UBX | H5'1 | 3.96 | 5.18 |
| 8 | ADE | H5'1 | 8 | ADE | H3' | 3.46 | 4.18 |
| 16 | CYT | H5'1 | 16 | CYT | H3' | 3.46 | 4.18 |
| 8 | ADE | H1' | 7 | UBX | H1' | 4.96 | 6.18 |
| 8 | ADE | H8 | 7 | UBX | H5 | 5.96 | 7.18 |
| 7 | UBX | H3' | 7 | UBX | H5'1 | 3.66 | 4.18 |
| 1 | GUA | H3' | 1 | GUA | H8 | 3.96 | 4.68 |
| 1 | GUA | H3' | 1 | GUA | H5'1 | 3.46 | 4.18 |
| 13 | GUA | H3' | 13 | GUA | H8 | 3.96 | 4.68 |
| 17 | THY | H3' | 17 | THY | H5'1 | 3.46 | 4.18 |
| 12 | CYT | H6 | 11 | CYT | H6 | 4.76 | 5.38 |
| 4 | ADE | H8 | 3 | THY | H6 | 4.76 | 5.38 |
| 5 | GUA | H8 | 4 | ADE | H8 | 4.76 | 5.38 |
| 19 | GUA | H8 | 18 | GUA | H8 | 4.76 | 5.38 |
| 17 | THY | H6 | 16 | CYT | H6 | 4.76 | 5.38 |
| 21 | THY | H6 | 20 | CYT | H6 | 4.76 | 5.38 |
| 18 | GUA | H3' | 18 | GUA | H5'1 | 3.46 | 4.18 |
| 7 | UBX | H2'1 | 6 | CYT | H3' | 5.76 | 6.68 |
| 24 | CYT | H6 | 23 | GUA | H8 | 4.76 | 5.38 |
| 24 | CYT | H1' | 23 | GUA | H1' | 4.76 | 5.38 |
| 2 | CYT | H2'1 | 1 | GUA | H2'2 | 3.76 | 4.28 |
| 3 | THY | H2'1 | 2 | CYT | H2'2 | 3.76 | 4.28 |
| 4 | ADE | H2'1 | 3 | THY | H2'2 | 3.76 | 4.28 |
| 5 | GUA | H2'1 | 4 | ADE | H2'2 | 3.76 | 4.28 |
| 6 | CYT | H2'1 | 5 | GUA | H2'2 | 3.76 | 4.28 |
| 9 | GUA | H2'1 | 8 | ADE | H2'2 | 3.76 | 4.28 |
| 10 | THY | H2'1 | 9 | GUA | H2'2 | 3.76 | 4.28 |
| 11 | CYT | H2'1 | 10 | THY | H2'2 | 3.76 | 4.28 |
| 12 | CYT | H2'1 | 11 | CYT | H2'2 | 3.76 | 4.28 |
| 14 | GUA | H2'1 | 13 | GUA | H2'2 | 3.76 | 4.28 |
| 15 | ADE | H2'1 | 14 | GUA | H2'2 | 3.76 | 4.28 |
| 16 | CYT | H2'1 | 15 | ADE | H2'2 | 3.76 | 4.28 |
| 17 | THY | H2'1 | 16 | CYT | H2'2 | 3.76 | 4.28 |
| 20 | CYT | H2'1 | 19 | GUA | H2'2 | 3.76 | 4.28 |
| 21 | THY | H2'1 | 20 | CYT | H2'2 | 3.76 | 4.28 |
| 22 | ADE | H2'1 | 21 | THY | H2'2 | 3.76 | 4.28 |
| 23 | GUA | H2'1 | 22 | ADE | H2'2 | 3.76 | 4.28 |
| 24 | CYT | H2'1 | 23 | GUA | H2'2 | 3.76 | 4.28 |
| 6 | CYT | H3' | 6 | CYT | H5'1 | 3.36 | 4.28 |
| 7 | UBX | H1' | 6 | CYT | H1' | 5.06 | 5.78 |
| 7 | UBX | H5'1 | 6 | CYT | H2'1 | 4.06 | 4.98 |

**Table B-5:** Continued

| Residue Number | Residue Name | Atom Number | Residue Number | Residue Name | Atom Number | Lower Bound | Upper Bound |
|---|---|---|---|---|---|---|---|
| 7 | UBX | H5 | 6 | CYT | H5 | 4.56 | 5.48 |
| 18 | GUA | H1' | 7 | UBX | 2H1 | 5.56 | 7.48 |
| 18 | GUA | H8 | 7 | UBX | 2H1 | 5.56 | 7.48 |
| 18 | GUA | H8 | 7 | UBX | H9 | 5.56 | 7.48 |
| 18 | GUA | H8 | 7 | UBX | 1H1 | 5.56 | 7.48 |
| 18 | GUA | H8 | 7 | UBX | 2H1 | 5.56 | 7.48 |
| 18 | GUA | H1' | 7 | UBX | 3H1 | 5.56 | 7.48 |
| 18 | GUA | H1' | 7 | UBX | H9 | 5.56 | 7.48 |
| 17 | THY | H1' | 7 | UBX | 2H1 | 5.56 | 7.48 |
| 17 | THY | H6 | 7 | UBX | 2H1 | 5.56 | 7.48 |
| 4 | ADE | H8 | 3 | THY | H3' | 4.56 | 5.28 |
| 5 | GUA | H3' | 4 | ADE | H1' | 5.36 | 5.98 |
| 11 | CYT | H6 | 10 | THY | H6 | 4.76 | 5.28 |
| 5 | GUA | H5'1 | 4 | ADE | H4' | 3.56 | 4.28 |
| 5 | GUA | H5'1 | 4 | ADE | H3' | 4.56 | 5.28 |
| 4 | ADE | H5'1 | 3 | THY | H3' | 4.56 | 5.28 |
| 18 | GUA | H5'1 | 17 | THY | H3' | 4.56 | 5.28 |
| 18 | GUA | H5'1 | 17 | THY | H2'2 | 4.56 | 5.28 |
| 18 | GUA | H1' | 17 | THY | H1' | 4.86 | 5.78 |
| 19 | GUA | H1' | 18 | GUA | H1' | 4.86 | 5.78 |
| 20 | CYT | H3' | 20 | CYT | H5'1 | 3.36 | 4.28 |
| 15 | ADE | H3' | 15 | ADE | H5'1 | 3.36 | 4.28 |
| 21 | THY | H3' | 21 | THY | H5'1 | 3.36 | 4.28 |
| 19 | GUA | H3' | 19 | GUA | H5'1 | 3.36 | 4.28 |
| 7 | UBX | H5'1 | 6 | CYT | H3' | 4.56 | 5.28 |
| 8 | ADE | H4' | 7 | UBX | H4' | 6.26 | 6.98 |
| 5 | GUA | H2'1 | 4 | ADE | H3' | 5.56 | 6.28 |
| 4 | ADE | H2'1 | 3 | THY | H3' | 5.56 | 6.28 |
| 18 | GUA | H2'1 | 17 | THY | H3' | 5.56 | 6.28 |
| 13 | GUA | H3' | 13 | GUA | H5'1 | 3.36 | 4.28 |
| 12 | CYT | H1' | 11 | CYT | H1' | 4.76 | 5.28 |
| 23 | GUA | H3' | 23 | GUA | H5'1 | 3.36 | 4.28 |
| 8 | ADE | H1' | 7 | UBX | H1' | 5.06 | 5.78 |
| 6 | CYT | H5'1 | 5 | GUA | H1' | 3.06 | 3.78 |

**Table B-6:** Distance restraints used for the *S-N3-dU* modified oligonucleotide 5′-$G^{1}C^{2}T^{3}A^{4}G^{5}C^{6}X^{7}A^{8}G^{9}T^{10}C^{11}C^{12}$-3′·5′-$G^{13}G^{14}A^{15}C^{16}T^{17}G^{18}G^{19}C^{20}T^{21}A^{22}G^{23}C^{24}$-3′.

| | Residue Number | Residue Name | Atom Number | Residue Number | Residue Name | Atom Number | Lower Bound | Upper Bound |
|---|---|---|---|---|---|---|---|---|
| Class 1 | 1 | GUA | H2'1 | 1 | GUA | H5'1 | 3.01 | 4.35 |
| | 1 | GUA | H2'1 | 1 | GUA | H8 | 1.95 | 2.68 |
| | 1 | GUA | H2'2 | 1 | GUA | H1' | 2.00 | 2.50 |
| | 2 | CYT | H5 | 2 | CYT | H6 | 2.07 | 2.55 |
| | 3 | THY | H6 | 2 | CYT | H6 | 4.82 | 5.34 |
| | 3 | THY | H2'2 | 3 | THY | H1' | 1.97 | 2.70 |
| | 4 | ADE | H8 | 3 | THY | H6 | 4.87 | 5.30 |
| | 4 | ADE | H2'1 | 4 | ADE | H8 | 1.81 | 3.20 |
| | 4 | ADE | H2'2 | 4 | ADE | H3' | 2.02 | 2.84 |
| | 5 | GUA | H1' | 5 | GUA | H4' | 2.32 | 3.50 |
| | 5 | GUA | H8 | 4 | ADE | H2'2 | 2.09 | 2.80 |
| | 5 | GUA | H2'2 | 5 | GUA | H1' | 1.80 | 2.52 |
| | 6 | CYT | H5 | 5 | GUA | H2'1 | 2.67 | 3.44 |
| | 6 | CYT | H5 | 6 | CYT | H6 | 2.10 | 2.63 |
| | 6 | CYT | H2'1 | 6 | CYT | H1' | 2.75 | 3.65 |
| | 6 | CYT | H2'1 | 6 | CYT | H6 | 1.68 | 2.49 |
| | 6 | CYT | H2'1 | 6 | CYT | H3' | 2.11 | 2.93 |
| | 6 | CYT | H2'2 | 6 | CYT | H1' | 1.90 | 2.46 |
| | 7 | UBX | H3' | 7 | UBX | H1' | 3.17 | 4.40 |
| | 7 | UBX | H3' | 7 | UBX | H6 | 2.85 | 4.36 |
| | 7 | UBX | H2'1 | 7 | UBX | H4' | 3.08 | 3.90 |
| | 7 | UBX | H2'1 | 7 | UBX | H3' | 2.29 | 3.33 |
| | 7 | UBX | H2'2 | 7 | UBX | H3' | 2.58 | 3.58 |
| | 7 | UBX | H2'2 | 7 | UBX | H2'1 | 1.78 | 2.92 |
| | 8 | ADE | H1' | 8 | ADE | H4' | 2.53 | 3.41 |
| | 8 | ADE | H2'1 | 8 | ADE | H3' | 2.09 | 2.86 |
| | 8 | ADE | H5'1 | 7 | UBX | H4' | 4.49 | 5.36 |
| | 9 | GUA | H2'1 | 9 | GUA | H8 | 1.88 | 2.31 |
| | 9 | GUA | H2'2 | 9 | GUA | H1' | 1.93 | 2.64 |
| | 9 | GUA | H2'2 | 9 | GUA | H8 | 3.18 | 3.79 |
| | 10 | THY | M7 | 10 | THY | H6 | 2.66 | 3.44 |
| | 10 | THY | H2'1 | 10 | THY | H1' | 2.23 | 3.39 |
| | 10 | THY | H2'2 | 10 | THY | H1' | 1.73 | 2.50 |
| | 10 | THY | H2'2 | 10 | THY | H6 | 2.16 | 3.87 |
| | 11 | CYT | H6 | 10 | THY | H1' | 1.70 | 3.20 |
| | 11 | CYT | H5 | 11 | CYT | H6 | 1.98 | 2.51 |
| | 11 | CYT | H2'1 | 11 | CYT | H1' | 1.65 | 3.20 |
| | 11 | CYT | H2'1 | 11 | CYT | H6 | 1.87 | 2.71 |
| | 11 | CYT | H2'2 | 11 | CYT | H1' | 1.79 | 2.53 |
| | 12 | CYT | H6 | 12 | CYT | H5'1 | 2.41 | 4.22 |
| | 12 | CYT | H5 | 12 | CYT | H6 | 1.85 | 2.47 |
| | 12 | CYT | H2'1 | 12 | CYT | H6 | 1.86 | 2.33 |
| | 12 | CYT | H2'1 | 12 | CYT | H3' | 2.32 | 3.37 |
| | 12 | CYT | H2'2 | 12 | CYT | H1' | 1.64 | 2.56 |

**Table B-6:** Continued

| Residue Number | Residue Name | Atom Number | Residue Number | Residue Name | Atom Number | Lower Bound | Upper Bound |
|---|---|---|---|---|---|---|---|
| 12 | CYT | H2'2 | 12 | CYT | H3' | 1.87 | 2.89 |
| 13 | GUA | H4' | 13 | GUA | H5'1 | 1.76 | 2.85 |
| 13 | GUA | H1' | 13 | GUA | H5'1 | 3.63 | 5.17 |
| 13 | GUA | H8 | 13 | GUA | H5'1 | 2.27 | 3.81 |
| 13 | GUA | H2'1 | 13 | GUA | H8 | 1.81 | 2.50 |
| 13 | GUA | H2'2 | 13 | GUA | H3' | 1.91 | 2.77 |
| 14 | GUA | H3' | 14 | GUA | H4' | 2.00 | 2.97 |
| 14 | GUA | H2'1 | 14 | GUA | H4' | 3.39 | 4.48 |
| 14 | GUA | H2'1 | 14 | GUA | H1' | 1.89 | 3.47 |
| 14 | GUA | H2'1 | 14 | GUA | H8 | 1.57 | 3.11 |
| 14 | GUA | H2'2 | 14 | GUA | H1' | 1.83 | 2.70 |
| 14 | GUA | H2'2 | 14 | GUA | H8 | 3.11 | 4.36 |
| 15 | ADE | H1' | 15 | ADE | H4' | 2.66 | 3.41 |
| 15 | ADE | H8 | 15 | ADE | H1' | 3.46 | 4.47 |
| 15 | ADE | H3' | 15 | ADE | H4' | 2.15 | 2.94 |
| 15 | ADE | H2'1 | 15 | ADE | H3' | 1.89 | 2.53 |
| 15 | ADE | H2'2 | 15 | ADE | H4' | 2.92 | 5.15 |
| 15 | ADE | H2'2 | 15 | ADE | H1' | 1.96 | 2.55 |
| 16 | CYT | H5 | 15 | ADE | H8 | 3.60 | 4.32 |
| 16 | CYT | H2'1 | 15 | ADE | H2'2 | 3.61 | 4.25 |
| 16 | CYT | H5 | 16 | CYT | H6 | 2.06 | 2.86 |
| 16 | CYT | H2'1 | 16 | CYT | H1' | 1.91 | 3.25 |
| 16 | CYT | H2'1 | 16 | CYT | H3' | 1.95 | 2.82 |
| 16 | CYT | H2'2 | 16 | CYT | H1' | 2.06 | 2.77 |
| 16 | CYT | H2'2 | 16 | CYT | H2'1 | 1.65 | 2.52 |
| 17 | THY | H2'1 | 17 | THY | H3' | 2.24 | 3.07 |
| 17 | THY | H2'2 | 17 | THY | H2'1 | 1.80 | 2.73 |
| 18 | GUA | H1' | 18 | GUA | H4' | 2.82 | 4.29 |
| 18 | GUA | H2'1 | 18 | GUA | H1' | 2.57 | 3.35 |
| 19 | GUA | H3' | 19 | GUA | H5'1 | 3.57 | 4.35 |
| 20 | CYT | H5 | 20 | CYT | H6 | 2.10 | 2.68 |
| 20 | CYT | H3' | 20 | CYT | H1' | 2.92 | 4.34 |
| 20 | CYT | H2'1 | 20 | CYT | H6 | 1.84 | 2.62 |
| 20 | CYT | H2'1 | 20 | CYT | H3' | 2.05 | 2.72 |
| 20 | CYT | H2'2 | 20 | CYT | H1' | 2.01 | 2.63 |
| 21 | THY | H6 | 20 | CYT | H6 | 4.71 | 5.33 |
| 20 | CYT | H2'2 | 20 | CYT | H2'1 | 1.74 | 2.69 |
| 21 | THY | M7 | 21 | THY | H6 | 2.41 | 3.47 |
| 21 | THY | H2'2 | 21 | THY | H1' | 1.96 | 2.74 |
| 22 | ADE | H1' | 22 | ADE | H4' | 2.35 | 3.63 |
| 22 | ADE | H2'1 | 22 | ADE | H8 | 1.63 | 2.29 |
| 22 | ADE | H2'1 | 22 | ADE | H3' | 2.33 | 2.83 |
| 22 | ADE | H2'2 | 22 | ADE | H3' | 2.36 | 2.85 |
| 23 | GUA | H2'1 | 23 | GUA | H8 | 1.78 | 2.72 |
| 23 | GUA | H2'1 | 23 | GUA | H3' | 2.13 | 2.89 |
| 23 | GUA | H2'2 | 23 | GUA | H1' | 1.79 | 2.69 |

**Table B-6:** Continued

| | Residue Number | Residue Name | Atom Number | Residue Number | Residue Name | Atom Number | Lower Bound | Upper Bound |
|---|---|---|---|---|---|---|---|---|
| | 24 | CYT | H1' | 23 | GUA | H1' | 4.79 | 5.39 |
| | 24 | CYT | H5 | 24 | CYT | H6 | 1.98 | 2.97 |
| | 24 | CYT | H2'1 | 24 | CYT | H3' | 2.11 | 3.04 |
| | 1 | GUA | H2'2 | 1 | GUA | H4' | 2.81 | 4.18 |
| | 2 | CYT | H2'2 | 2 | CYT | H1' | 1.87 | 2.40 |
| | 6 | CYT | H2'2 | 6 | CYT | H2'1 | 1.62 | 2.34 |
| | 14 | GUA | H8 | 13 | GUA | H2'2 | 1.93 | 2.75 |
| | 21 | THY | H6 | 20 | CYT | H2'2 | 1.83 | 3.12 |
| | 2 | CYT | H2'2 | 2 | CYT | H2'1 | 1.64 | 2.17 |
| | 2 | CYT | H2'1 | 1 | GUA | H2'2 | 3.64 | 4.17 |
| | 2 | CYT | H3' | 1 | GUA | H2'2 | 4.84 | 5.27 |
| | 3 | THY | H2'2 | 3 | THY | H2'1 | 1.76 | 2.40 |
| | 3 | THY | H2'1 | 2 | CYT | H2'2 | 3.64 | 4.17 |
| | 3 | THY | H3' | 2 | CYT | H2'2 | 4.84 | 5.27 |
| | 8 | ADE | H4' | 8 | ADE | H5'1 | 2.33 | 3.15 |
| | 10 | THY | H2'2 | 10 | THY | H2'1 | 1.63 | 2.32 |
| | 11 | CYT | H2'1 | 11 | CYT | H3' | 2.08 | 2.54 |
| | 11 | CYT | H2'2 | 11 | CYT | H2'1 | 1.80 | 2.48 |
| | 16 | CYT | H2'2 | 16 | CYT | H4' | 2.66 | 4.19 |
| | 21 | THY | H2'2 | 21 | THY | H2'1 | 1.62 | 2.06 |
| | 24 | CYT | H2'2 | 24 | CYT | H2'1 | 1.80 | 2.19 |
| Class 2 | 1 | GUA | H4' | 1 | GUA | H5'1 | 1.85 | 2.60 |
| | 1 | GUA | H8 | 1 | GUA | H5'1 | 2.44 | 3.75 |
| | 1 | GUA | H8 | 1 | GUA | H1' | 2.92 | 4.57 |
| | 1 | GUA | H2'1 | 1 | GUA | H1' | 2.14 | 3.69 |
| | 1 | GUA | H2'2 | 1 | GUA | H8 | 2.38 | 3.95 |
| | 2 | CYT | H6 | 1 | GUA | H1' | 2.19 | 3.42 |
| | 2 | CYT | H6 | 1 | GUA | H2'2 | 1.89 | 2.98 |
| | 2 | CYT | H5 | 1 | GUA | H1' | 2.85 | 4.75 |
| | 2 | CYT | H5 | 1 | GUA | H2'1 | 2.69 | 3.87 |
| | 2 | CYT | H5 | 1 | GUA | H2'2 | 2.37 | 3.63 |
| | 2 | CYT | H3' | 2 | CYT | H1' | 3.17 | 4.89 |
| | 2 | CYT | H2'1 | 2 | CYT | H1' | 1.99 | 3.71 |
| | 2 | CYT | H2'1 | 2 | CYT | H6 | 1.84 | 2.63 |
| | 2 | CYT | H2'2 | 2 | CYT | H6 | 2.74 | 4.21 |
| | 3 | THY | H1' | 3 | THY | H4' | 2.43 | 3.56 |
| | 3 | THY | H6 | 2 | CYT | H2'2 | 1.88 | 2.87 |
| | 3 | THY | M7 | 2 | CYT | H1' | 3.42 | 4.72 |
| | 3 | THY | M7 | 2 | CYT | H6 | 3.46 | 4.36 |
| | 3 | THY | M7 | 2 | CYT | H5 | 3.27 | 5.24 |
| | 3 | THY | M7 | 3 | THY | H6 | 2.47 | 3.82 |
| | 3 | THY | H2'1 | 3 | THY | H1' | 2.48 | 3.71 |
| | 3 | THY | H2'1 | 3 | THY | H6 | 1.88 | 3.02 |
| | 4 | ADE | H5'1 | 3 | THY | H1' | 2.18 | 3.38 |
| | 4 | ADE | H2'1 | 3 | THY | H2'2 | 3.68 | 4.38 |
| | 4 | ADE | H1' | 3 | THY | H1' | 4.78 | 5.18 |

**Table B-6:** Continued

| Residue Number | Residue Name | Atom Number | Residue Number | Residue Name | Atom Number | Lower Bound | Upper Bound |
|---|---|---|---|---|---|---|---|
| 4 | ADE | H3' | 3 | THY | H2'2 | 4.88 | 5.28 |
| 4 | ADE | H1' | 4 | ADE | H4' | 2.69 | 3.77 |
| 4 | ADE | H3' | 4 | ADE | H1' | 2.95 | 4.62 |
| 4 | ADE | H2'1 | 4 | ADE | H1' | 2.03 | 3.99 |
| 4 | ADE | H2'1 | 4 | ADE | H3' | 1.80 | 2.85 |
| 4 | ADE | H2'2 | 4 | ADE | H8 | 3.47 | 3.92 |
| 5 | GUA | H8 | 4 | ADE | H1' | 1.71 | 3.16 |
| 5 | GUA | H1' | 4 | ADE | H1' | 4.71 | 5.16 |
| 5 | GUA | H2'1 | 4 | ADE | H2'2 | 3.41 | 4.16 |
| 5 | GUA | H3' | 4 | ADE | H2'2 | 4.81 | 5.26 |
| 5 | GUA | H2'1 | 5 | GUA | H1' | 2.52 | 3.84 |
| 5 | GUA | H2'1 | 5 | GUA | H8 | 1.92 | 2.62 |
| 5 | GUA | H2'1 | 5 | GUA | H3' | 2.06 | 3.29 |
| 5 | GUA | H2'2 | 5 | GUA | H8 | 3.12 | 4.65 |
| 6 | CYT | H5 | 6 | CYT | H5'1 | 4.82 | 5.72 |
| 6 | CYT | H6 | 5 | GUA | H1' | 2.62 | 3.22 |
| 6 | CYT | H3' | 5 | GUA | H2'2 | 4.82 | 5.22 |
| 6 | CYT | H6 | 5 | GUA | H2'1 | 2.37 | 3.96 |
| 6 | CYT | H2'1 | 5 | GUA | H2'2 | 3.37 | 3.96 |
| 6 | CYT | H5 | 5 | GUA | H8 | 3.57 | 4.33 |
| 6 | CYT | H5 | 5 | GUA | H2'2 | 2.50 | 3.52 |
| 6 | CYT | H3' | 6 | CYT | H6 | 3.61 | 4.58 |
| 6 | CYT | H2'2 | 6 | CYT | H3' | 2.30 | 3.43 |
| 7 | UBX | H6 | 7 | UBX | H1' | 2.71 | 3.98 |
| 7 | UBX | H5 | 7 | UBX | H6 | 2.13 | 2.50 |
| 7 | UBX | H2'1 | 7 | UBX | H1' | 2.60 | 3.45 |
| 7 | UBX | H2'1 | 7 | UBX | H6 | 1.83 | 2.89 |
| 7 | UBX | H2'2 | 7 | UBX | H1' | 1.92 | 2.95 |
| 7 | UBX | H2'2 | 7 | UBX | H5 | 4.89 | 5.76 |
| 7 | UBX | H14 | 7 | UBX | H15 | 1.57 | 2.40 |
| 8 | ADE | H8 | 8 | ADE | H1' | 2.95 | 4.84 |
| 8 | ADE | H2'2 | 8 | ADE | H1' | 1.94 | 2.87 |
| 8 | ADE | H2'2 | 8 | ADE | H3' | 1.70 | 3.81 |
| 9 | GUA | H1' | 9 | GUA | H4' | 2.56 | 4.52 |
| 9 | GUA | H8 | 8 | ADE | H1' | 2.63 | 4.24 |
| 9 | GUA | H2'1 | 9 | GUA | H1' | 2.25 | 3.79 |
| 10 | THY | H2'1 | 9 | GUA | H2'2 | 3.31 | 4.01 |
| 10 | THY | H6 | 9 | GUA | H1' | 1.81 | 3.51 |
| 10 | THY | H6 | 9 | GUA | H8 | 4.41 | 5.24 |
| 10 | THY | H6 | 9 | GUA | H2'2 | 1.82 | 2.42 |
| 10 | THY | H2'1 | 10 | THY | M7 | 3.21 | 5.61 |
| 11 | CYT | H6 | 10 | THY | H6 | 4.69 | 5.65 |
| 11 | CYT | H5 | 10 | THY | M7 | 3.99 | 5.45 |
| 11 | CYT | H5 | 10 | THY | H2'1 | 2.87 | 4.38 |
| 11 | CYT | H2'1 | 10 | CYT | H2'2 | 3.53 | 4.37 |
| 11 | CYT | H2'1 | 11 | CYT | H5 | 3.53 | 4.37 |

**Table B-6:** Continued

| Residue Number | Residue Name | Atom Number | Residue Number | Residue Name | Atom Number | Lower Bound | Upper Bound |
|---|---|---|---|---|---|---|---|
| 11 | CYT | H2'2 | 11 | CYT | H6 | 2.55 | 3.95 |
| 12 | CYT | H6 | 11 | CYT | H1' | 2.16 | 2.87 |
| 12 | CYT | H5 | 11 | CYT | H2'1 | 2.27 | 3.81 |
| 12 | CYT | H5 | 11 | CYT | H2'2 | 2.23 | 3.68 |
| 12 | CYT | H2'1 | 11 | CYT | H2'2 | 3.53 | 4.38 |
| 12 | CYT | H3' | 12 | CYT | H1' | 3.14 | 4.38 |
| 12 | CYT | H2'1 | 12 | CYT | H1' | 1.95 | 3.57 |
| 12 | CYT | H2'1 | 12 | CYT | H5 | 3.27 | 5.13 |
| 12 | CYT | H2'2 | 12 | CYT | H6 | 2.82 | 4.20 |
| 13 | GUA | H8 | 13 | GUA | H1' | 3.18 | 4.08 |
| 13 | GUA | H3' | 13 | GUA | H5'1 | 2.85 | 4.68 |
| 13 | GUA | H3' | 13 | GUA | H8 | 3.68 | 5.23 |
| 13 | GUA | H2'1 | 13 | GUA | H1' | 2.54 | 3.87 |
| 13 | GUA | H2'2 | 13 | GUA | H1' | 1.84 | 3.01 |
| 14 | GUA | H5'1 | 13 | GUA | H1' | 2.35 | 4.12 |
| 14 | GUA | H1' | 14 | GUA | H5'1 | 3.89 | 4.54 |
| 14 | GUA | H1' | 14 | GUA | H4' | 2.43 | 3.61 |
| 14 | GUA | H8 | 13 | GUA | H1' | 2.29 | 3.20 |
| 14 | GUA | H2'1 | 14 | GUA | H3' | 1.73 | 3.14 |
| 15 | ADE | H8 | 14 | GUA | H1' | 2.45 | 3.74 |
| 15 | ADE | H8 | 14 | GUA | H3' | 3.90 | 5.00 |
| 15 | ADE | H3' | 15 | ADE | H8 | 3.56 | 5.01 |
| 15 | ADE | H2'1 | 15 | ADE | H4' | 3.20 | 4.67 |
| 15 | ADE | H2'1 | 15 | ADE | H1' | 2.76 | 3.67 |
| 15 | ADE | H2'2 | 15 | ADE | H8 | 2.87 | 3.97 |
| 15 | ADE | H2'2 | 15 | ADE | H3' | 2.55 | 3.49 |
| 16 | CYT | H6 | 15 | ADE | H1' | 1.88 | 3.29 |
| 16 | CYT | H6 | 15 | ADE | H2'1 | 3.33 | 3.90 |
| 16 | CYT | H6 | 15 | ADE | H2'2 | 1.86 | 2.72 |
| 16 | CYT | H6 | 16 | CYT | H1' | 3.33 | 4.60 |
| 16 | CYT | H5 | 15 | ADE | H1' | 3.35 | 4.09 |
| 16 | CYT | H5 | 15 | ADE | H2'1 | 2.73 | 3.65 |
| 16 | CYT | H5 | 15 | ADE | H2'2 | 2.57 | 3.56 |
| 16 | CYT | H3' | 16 | CYT | H6 | 2.84 | 4.37 |
| 16 | CYT | H2'1 | 16 | CYT | H6 | 1.87 | 2.91 |
| 16 | CYT | H2'2 | 16 | CYT | H6 | 2.51 | 4.31 |
| 16 | CYT | H2'2 | 16 | CYT | H3' | 2.14 | 3.64 |
| 17 | THY | H6 | 17 | THY | H5'1 | 2.89 | 3.97 |
| 17 | THY | H6 | 17 | THY | H4' | 3.07 | 4.73 |
| 17 | THY | H6 | 17 | THY | H1' | 2.97 | 4.56 |
| 17 | THY | M7 | 17 | THY | H6 | 2.74 | 3.57 |
| 17 | THY | H3' | 17 | THY | H1' | 3.03 | 4.44 |
| 17 | THY | H2'1 | 17 | THY | H6 | 1.88 | 2.84 |
| 17 | THY | H2'2 | 17 | THY | H1' | 2.08 | 3.26 |
| 17 | THY | H2'2 | 17 | THY | H6 | 2.96 | 4.00 |
| 18 | GUA | H8 | 18 | GUA | H4' | 3.87 | 5.19 |

**Table B-6:** Continued

| Residue Number | Residue Name | Atom Number | Residue Number | Residue Name | Atom Number | Lower Bound | Upper Bound |
|---|---|---|---|---|---|---|---|
| 18 | GUA | H8 | 18 | GUA | H1' | 2.76 | 4.04 |
| 18 | GUA | H2'1 | 18 | GUA | H8 | 1.88 | 2.49 |
| 18 | GUA | H2'2 | 18 | GUA | H1' | 1.82 | 2.99 |
| 18 | GUA | H2'2 | 18 | GUA | H8 | 2.00 | 3.88 |
| 18 | GUA | H8 | 7 | UBX | H13 | 6.00 | 7.88 |
| 18 | GUA | H1' | 7 | UBX | H12 | 6.00 | 7.88 |
| 20 | CYT | H6 | 19 | GUA | H1' | 2.10 | 3.20 |
| 20 | CYT | H6 | 19 | GUA | H2'1 | 2.72 | 4.10 |
| 20 | CYT | H6 | 20 | CYT | H1' | 2.81 | 4.40 |
| 20 | CYT | H5 | 19 | GUA | H8 | 3.20 | 4.56 |
| 20 | CYT | H3' | 20 | CYT | H6 | 3.18 | 4.74 |
| 20 | CYT | H2'1 | 20 | CYT | H1' | 2.28 | 3.92 |
| 20 | CYT | H2'2 | 20 | CYT | H4' | 3.56 | 4.48 |
| 20 | CYT | H2'2 | 20 | CYT | H3' | 2.27 | 3.50 |
| 21 | THY | H1' | 21 | THY | H4' | 2.59 | 3.40 |
| 21 | THY | H3' | 21 | THY | H6 | 3.47 | 4.93 |
| 21 | THY | H2'2 | 21 | THY | H6 | 2.88 | 3.67 |
| 22 | ADE | H5'1 | 21 | THY | H1' | 1.82 | 3.34 |
| 22 | ADE | H8 | 21 | THY | H1' | 2.16 | 3.56 |
| 22 | ADE | H2'1 | 22 | ADE | H1' | 1.83 | 4.15 |
| 22 | ADE | H2'2 | 22 | ADE | H4' | 3.80 | 4.37 |
| 22 | ADE | H2'2 | 22 | ADE | H1' | 1.82 | 3.15 |
| 22 | ADE | H2'2 | 22 | ADE | H8 | 3.17 | 4.10 |
| 23 | GUA | H8 | 22 | ADE | H2'1 | 3.43 | 4.05 |
| 23 | GUA | H8 | 22 | ADE | H2'2 | 1.88 | 2.99 |
| 23 | GUA | H3' | 23 | GUA | H1' | 3.21 | 4.61 |
| 23 | GUA | H2'1 | 23 | GUA | H1' | 2.51 | 3.77 |
| 23 | GUA | H2'2 | 23 | GUA | H4' | 3.20 | 4.51 |
| 23 | GUA | H2'2 | 23 | GUA | H8 | 2.76 | 4.39 |
| 23 | GUA | H2'2 | 23 | GUA | H3' | 2.16 | 3.38 |
| 24 | CYT | H6 | 23 | GUA | H1' | 2.25 | 2.73 |
| 24 | CYT | H6 | 24 | CYT | H1' | 2.78 | 4.31 |
| 24 | CYT | H5 | 23 | GUA | H2'2 | 2.35 | 3.27 |
| 24 | CYT | H3' | 24 | CYT | H1' | 3.51 | 4.16 |
| 24 | CYT | H2'1 | 24 | CYT | H1' | 2.04 | 3.27 |
| 24 | CYT | H2'1 | 24 | CYT | H6 | 1.91 | 2.58 |
| 24 | CYT | H2'2 | 24 | CYT | H1' | 1.74 | 3.44 |
| 24 | CYT | H2'2 | 24 | CYT | H6 | 2.66 | 4.02 |
| 24 | CYT | H2'2 | 24 | CYT | H3' | 2.36 | 3.41 |
| 1 | GUA | H1' | 1 | GUA | H4' | 2.66 | 3.22 |
| 2 | CYT | H6 | 1 | GUA | H8 | 4.74 | 5.27 |
| 3 | THY | H6 | 2 | CYT | H3' | 4.26 | 5.21 |
| 10 | THY | M7 | 9 | GUA | H1' | 3.86 | 5.16 |
| 12 | CYT | H6 | 11 | CYT | H3' | 3.14 | 4.82 |
| 14 | GUA | H3' | 13 | GUA | H2'2 | 4.84 | 5.22 |
| 13 | GUA | H3' | 13 | GUA | H5'1 | 3.54 | 4.22 |

**Table B-6:** Continued

| | Residue Number | Residue Name | Atom Number | Residue Number | Residue Name | Atom Number | Lower Bound | Upper Bound |
|---|---|---|---|---|---|---|---|---|
| | 15 | ADE | H1' | 14 | GUA | H1' | 4.84 | 5.22 |
| | 16 | CYT | H1' | 16 | CYT | H4' | 2.45 | 3.24 |
| | 16 | CYT | H3' | 15 | ADE | H2'2 | 5.05 | 5.54 |
| | 17 | THY | H1' | 17 | THY | H4' | 2.61 | 3.96 |
| | 19 | GUA | H2'2 | 19 | GUA | H3' | 1.83 | 2.81 |
| | 21 | THY | H6 | 20 | CYT | H3' | 4.04 | 5.59 |
| | 20 | CYT | H3' | 20 | CYT | H2'1 | 2.02 | 2.54 |
| | 20 | CYT | H3' | 20 | CYT | H2'2 | 2.28 | 3.38 |
| | 22 | ADE | H3' | 21 | THY | H2'2 | 4.88 | 5.28 |
| | 23 | GUA | H3' | 22 | ADE | H2'2 | 4.88 | 5.28 |
| | 24 | CYT | H4' | 23 | GUA | H1' | 3.05 | 4.83 |
| | 1 | GUA | H3' | 1 | GUA | H5'1 | 3.10 | 4.41 |
| | 2 | CYT | H6 | 2 | CYT | H5'2 | 3.82 | 4.49 |
| | 2 | CYT | H6 | 2 | CYT | H4' | 3.46 | 4.90 |
| | 2 | CYT | H2'1 | 2 | CYT | H3' | 2.17 | 2.96 |
| | 3 | THY | M7 | 2 | CYT | H2'1 | 2.48 | 3.65 |
| | 3 | THY | H2'2 | 3 | THY | H3' | 2.10 | 2.84 |
| | 10 | THY | H6 | 10 | THY | H4' | 3.58 | 4.87 |
| | 15 | ADE | H5'1 | 14 | GUA | H1' | 2.86 | 3.55 |
| | 17 | THY | H5'1 | 16 | CYT | H3' | 4.13 | 4.87 |
| | 17 | THY | H1' | 16 | CYT | H1' | 4.63 | 5.37 |
| | 17 | THY | H3' | 16 | CYT | H2'2 | 4.83 | 5.27 |
| | 7 | UBX | H4' | 6 | CYT | H1' | 5.03 | 6.07 |
| | 7 | UBX | H1' | 6 | CYT | H2'2 | 5.83 | 6.77 |
| Class 3 | 2 | CYT | H3' | 2 | CYT | H6 | 3.53 | 4.66 |
| | 3 | THY | H2'2 | 3 | THY | H6 | 2.45 | 4.04 |
| | 4 | ADE | H3' | 4 | ADE | H8 | 3.63 | 4.87 |
| | 4 | ADE | H5'1 | 3 | THY | H3' | 4.13 | 4.87 |
| | 5 | GUA | H3' | 5 | GUA | H1' | 3.45 | 4.38 |
| | 5 | GUA | H2'2 | 5 | GUA | H3' | 2.07 | 3.42 |
| | 16 | CYT | H3' | 16 | CYT | H1' | 3.04 | 4.33 |
| | 17 | THY | H2'2 | 17 | THY | H3' | 2.10 | 3.49 |
| | 19 | GUA | H1' | 19 | GUA | H4' | 2.24 | 3.37 |
| | 20 | CYT | H2'2 | 20 | CYT | H6 | 2.96 | 4.53 |
| | 21 | THY | H6 | 21 | THY | H1' | 2.95 | 4.45 |
| | 21 | THY | H2'1 | 21 | THY | H1' | 2.29 | 3.78 |
| | 22 | ADE | H2'1 | 22 | ADE | H4' | 3.03 | 4.48 |
| | 22 | ADE | H8 | 21 | THY | H6 | 4.73 | 5.28 |
| | 23 | GUA | H1' | 23 | GUA | H4' | 2.30 | 3.40 |
| | 23 | GUA | H8 | 22 | ADE | H1' | 2.63 | 3.28 |
| | 23 | GUA | H2'1 | 23 | GUA | H4' | 3.53 | 4.39 |
| | 24 | CYT | H6 | 23 | GUA | H8 | 4.56 | 5.87 |
| | 24 | CYT | H3' | 24 | CYT | H6 | 3.49 | 4.47 |
| | 9 | GUA | H8 | 9 | GUA | H4' | 4.60 | 5.82 |
| | 2 | CYT | H6 | 2 | CYT | H5'1 | 3.02 | 4.34 |
| | 3 | THY | H2'1 | 3 | THY | M7 | 3.64 | 5.09 |

**Table B-6:** Continued

| | Residue Number | Residue Name | Atom Number | Residue Number | Residue Name | Atom Number | Lower Bound | Upper Bound |
|---|---|---|---|---|---|---|---|---|
| | 6 | CYT | H6 | 6 | CYT | H4' | 3.24 | 4.87 |
| | 6 | CYT | H2'2 | 6 | CYT | H4' | 2.94 | 4.17 |
| | 8 | ADE | H8 | 8 | ADE | H4' | 4.16 | 5.48 |
| | 11 | CYT | H2'1 | 11 | CYT | H4' | 3.00 | 4.21 |
| | 13 | GUA | H1' | 13 | GUA | H4' | 2.76 | 3.55 |
| Class 4 | 1 | GUA | H1' | 1 | GUA | H5'1 | 3.46 | 4.88 |
| | 1 | GUA | H2'2 | 1 | GUA | H5'1 | 4.16 | 5.17 |
| | 2 | CYT | H6 | 1 | GUA | H2'1 | 3.03 | 4.42 |
| | 2 | CYT | H2'1 | 1 | GUA | H1' | 3.73 | 4.42 |
| | 2 | CYT | H6 | 2 | CYT | H1' | 2.95 | 4.28 |
| | 2 | CYT | H5 | 1 | GUA | H8 | 3.03 | 4.38 |
| | 2 | CYT | H2'1 | 2 | CYT | H5 | 3.38 | 4.48 |
| | 2 | CYT | H2'2 | 2 | CYT | H5 | 4.96 | 5.55 |
| | 3 | THY | H6 | 2 | CYT | H1' | 1.78 | 3.33 |
| | 3 | THY | H2'1 | 2 | CYT | H1' | 3.73 | 4.42 |
| | 3 | THY | H6 | 3 | THY | H1' | 3.25 | 4.47 |
| | 3 | THY | M7 | 2 | CYT | H3' | 4.66 | 5.59 |
| | 3 | THY | M7 | 2 | CYT | H2'2 | 2.47 | 3.89 |
| | 3 | THY | H3' | 3 | THY | H6 | 3.20 | 4.71 |
| | 3 | THY | H2'2 | 3 | THY | M7 | 5.53 | 6.30 |
| | 4 | ADE | H8 | 3 | THY | H1' | 1.95 | 3.72 |
| | 4 | ADE | H2'1 | 3 | THY | H1' | 3.73 | 4.42 |
| | 4 | ADE | H8 | 3 | THY | H2'1 | 3.10 | 4.06 |
| | 4 | ADE | H8 | 3 | THY | H2'2 | 1.85 | 3.36 |
| | 4 | ADE | H3' | 4 | ADE | H5'1 | 3.59 | 4.43 |
| | 4 | ADE | H8 | 4 | ADE | H1' | 3.19 | 4.43 |
| | 4 | ADE | H2'1 | 4 | ADE | H4' | 3.09 | 4.74 |
| | 4 | ADE | H2'2 | 4 | ADE | H4' | 3.62 | 4.25 |
| | 4 | ADE | H2'2 | 4 | ADE | H1' | 1.81 | 3.26 |
| | 4 | ADE | H2'2 | 4 | ADE | H8 | 3.21 | 4.61 |
| | 5 | GUA | H8 | 4 | ADE | H8 | 4.67 | 5.54 |
| | 5 | GUA | H2'1 | 4 | ADE | H1' | 3.73 | 4.42 |
| | 5 | GUA | H8 | 4 | ADE | H3' | 3.71 | 5.41 |
| | 5 | GUA | H8 | 4 | ADE | H2'1 | 2.92 | 4.04 |
| | 5 | GUA | H8 | 5 | GUA | H4' | 4.32 | 5.72 |
| | 5 | GUA | H8 | 5 | GUA | H1' | 3.49 | 4.57 |
| | 5 | GUA | H3' | 5 | GUA | H8 | 3.65 | 5.36 |
| | 5 | GUA | H2'2 | 5 | GUA | H4' | 3.28 | 4.94 |
| | 6 | CYT | H1' | 6 | CYT | H4' | 2.25 | 3.54 |
| | 6 | CYT | H6 | 5 | GUA | H8 | 4.52 | 5.36 |
| | 6 | CYT | H2'1 | 5 | GUA | H1' | 3.73 | 4.42 |
| | 6 | CYT | H6 | 5 | GUA | H3' | 4.08 | 5.12 |
| | 6 | CYT | H5'1 | 5 | GUA | H3' | 4.12 | 5.07 |
| | 6 | CYT | H6 | 5 | GUA | H2'2 | 1.81 | 3.17 |
| | 6 | CYT | H6 | 6 | CYT | H1' | 3.33 | 4.44 |
| | 6 | CYT | H5 | 5 | GUA | H1' | 2.88 | 4.65 |

**Table B-6:** Continued

| Residue Number | Residue Name | Atom Number | Residue Number | Residue Name | Atom Number | Lower Bound | Upper Bound |
|---|---|---|---|---|---|---|---|
| 6 | CYT | H3' | 6 | CYT | H1' | 3.10 | 4.62 |
| 6 | CYT | H3' | 6 | CYT | H5'1 | 3.30 | 4.22 |
| 6 | CYT | H2'1 | 6 | CYT | H5 | 3.39 | 5.20 |
| 6 | CYT | H2'2 | 6 | CYT | H6 | 2.56 | 3.77 |
| 6 | CYT | H2'2 | 6 | CYT | H5 | 4.84 | 5.76 |
| 7 | UBX | H2'1 | 6 | CYT | H1' | 4.53 | 5.42 |
| 7 | UBX | H4' | 6 | CYT | H2'2 | 5.52 | 6.86 |
| 7 | UBX | H5'1 | 6 | CYT | H1' | 3.02 | 4.26 |
| 7 | UBX | H6 | 6 | CYT | H1' | 4.21 | 5.87 |
| 7 | UBX | H6 | 6 | CYT | H3' | 4.64 | 5.91 |
| 7 | UBX | H6 | 6 | CYT | H2'1 | 3.02 | 4.33 |
| 7 | UBX | H6 | 6 | CYT | H2'2 | 2.97 | 4.52 |
| 7 | UBX | H6 | 7 | UBX | H5'1 | 2.90 | 4.17 |
| 7 | UBX | H6 | 7 | UBX | H5'2 | 3.37 | 4.83 |
| 7 | UBX | H6 | 7 | UBX | H4' | 3.75 | 5.20 |
| 7 | UBX | H5 | 6 | CYT | H2'1 | 4.73 | 5.30 |
| 7 | UBX | H5 | 6 | CYT | H2'2 | 4.12 | 5.38 |
| 7 | UBX | H1' | 6 | CYT | H1' | 4.92 | 5.78 |
| 7 | UBX | H2'1 | 7 | UBX | H5 | 3.80 | 4.45 |
| 7 | UBX | H2'2 | 7 | UBX | H6 | 1.98 | 3.66 |
| 7 | UBX | H3' | 7 | UBX | H5'1 | 3.58 | 4.16 |
| 7 | UBX | H2'1 | 7 | UBX | H5'1 | 3.58 | 4.16 |
| 7 | UBX | H9 | 7 | UBX | H15 | 2.17 | 3.02 |
| 7 | UBX | H9 | 7 | UBX | H14 | 2.10 | 4.48 |
| 7 | UBX | H11 | 7 | UBX | H15 | 2.58 | 4.44 |
| 7 | UBX | H11 | 7 | UBX | H14 | 2.86 | 4.30 |
| 7 | UBX | H11 | 7 | UBX | H9 | 2.29 | 3.30 |
| 8 | ADE | H1' | 7 | UBX | H1' | 5.03 | 6.12 |
| 8 | ADE | H2'1 | 7 | UBX | H1' | 4.53 | 5.12 |
| 8 | ADE | H8 | 7 | UBX | H1' | 4.09 | 4.85 |
| 8 | ADE | H8 | 7 | UBX | H3' | 4.85 | 5.49 |
| 8 | ADE | H8 | 7 | UBX | H2'1 | 3.25 | 4.53 |
| 8 | ADE | H8 | 7 | UBX | H2'2 | 2.86 | 4.40 |
| 8 | ADE | H2 | 7 | UBX | H15 | 5.30 | 6.07 |
| 8 | ADE | H2 | 7 | UBX | H14 | 5.05 | 6.06 |
| 8 | ADE | H2 | 7 | UBX | H9 | 3.01 | 4.07 |
| 8 | ADE | H5'1 | 7 | UBX | H1' | 3.40 | 4.65 |
| 8 | ADE | H8 | 7 | UBX | H6 | 5.50 | 6.45 |
| 8 | ADE | H3' | 8 | ADE | H1' | 3.51 | 4.68 |
| 8 | ADE | H3' | 8 | ADE | H8 | 3.61 | 5.00 |
| 8 | ADE | H2'1 | 8 | ADE | H1' | 2.18 | 3.61 |
| 8 | ADE | H2'1 | 8 | ADE | H8 | 1.80 | 3.18 |
| 8 | ADE | H2'2 | 8 | ADE | H4' | 3.66 | 4.47 |
| 8 | ADE | H2'2 | 8 | ADE | H8 | 2.71 | 3.59 |
| 9 | GUA | H8 | 8 | ADE | H8 | 4.74 | 5.24 |
| 9 | GUA | H2'1 | 8 | ADE | H1' | 3.74 | 4.44 |

**Table B-6:** Continued

| Residue Number | Residue Name | Atom Number | Residue Number | Residue Name | Atom Number | Lower Bound | Upper Bound |
|---|---|---|---|---|---|---|---|
| 9 | GUA | H8 | 8 | ADE | H4' | 5.74 | 6.24 |
| 9 | GUA | H8 | 8 | ADE | H2'1 | 3.39 | 4.25 |
| 9 | GUA | H1' | 8 | ADE | H1' | 4.59 | 5.45 |
| 9 | GUA | H5'1 | 8 | ADE | H1' | 2.89 | 3.86 |
| 9 | GUA | H5'1 | 9 | GUA | H8 | 3.39 | 3.86 |
| 9 | GUA | H8 | 9 | GUA | H1' | 2.81 | 4.62 |
| 9 | GUA | H2'1 | 9 | GUA | H4' | 3.48 | 4.51 |
| 9 | GUA | H2'2 | 9 | GUA | H4' | 3.08 | 4.59 |
| 10 | THY | H1' | 9 | GUA | H1' | 4.74 | 5.24 |
| 10 | THY | H5'1 | 9 | GUA | H3' | 3.94 | 5.24 |
| 10 | THY | H2'1 | 9 | GUA | H1' | 3.74 | 4.44 |
| 10 | THY | H6 | 9 | GUA | H2'1 | 2.94 | 4.54 |
| 10 | THY | H6 | 10 | THY | H1' | 2.53 | 4.31 |
| 10 | THY | M7 | 9 | GUA | H8 | 2.92 | 3.99 |
| 10 | THY | M7 | 9 | GUA | H2'1 | 2.19 | 3.75 |
| 10 | THY | M7 | 9 | GUA | H2'2 | 1.89 | 3.69 |
| 10 | THY | H3' | 10 | THY | H6 | 3.24 | 5.17 |
| 10 | THY | H2'1 | 10 | THY | H6 | 1.99 | 2.88 |
| 10 | THY | H2'2 | 10 | THY | M7 | 5.27 | 6.36 |
| 11 | CYT | H2'1 | 10 | THY | H1' | 3.74 | 4.44 |
| 11 | CYT | H1' | 10 | THY | H1' | 4.73 | 5.28 |
| 11 | CYT | H6 | 10 | THY | H2'1 | 2.93 | 3.68 |
| 11 | CYT | H6 | 10 | THY | H2'2 | 1.80 | 2.48 |
| 11 | CYT | H6 | 11 | CYT | H1' | 3.22 | 4.16 |
| 11 | CYT | H5 | 10 | THY | H6 | 3.82 | 4.60 |
| 11 | CYT | H5 | 10 | THY | H2'2 | 2.33 | 3.14 |
| 11 | CYT | H3' | 11 | CYT | H6 | 3.24 | 4.54 |
| 11 | CYT | H2'2 | 11 | CYT | H5 | 4.50 | 6.44 |
| 11 | CYT | H3' | 11 | CYT | H5'1 | 3.64 | 4.24 |
| 12 | CYT | H1' | 12 | CYT | H5'1 | 4.28 | 4.97 |
| 12 | CYT | H2'1 | 11 | CYT | H1' | 3.74 | 4.44 |
| 12 | CYT | H6 | 11 | CYT | H2'1 | 3.13 | 4.12 |
| 12 | CYT | H6 | 12 | CYT | H1' | 2.70 | 4.53 |
| 12 | CYT | H5 | 11 | CYT | H6 | 3.72 | 4.63 |
| 12 | CYT | H3' | 12 | CYT | H6 | 2.92 | 4.46 |
| 12 | CYT | H3' | 12 | CYT | H5 | 5.31 | 6.31 |
| 12 | CYT | H2'2 | 12 | CYT | H5 | 4.73 | 6.23 |
| 13 | GUA | H8 | 13 | GUA | H4' | 3.74 | 5.48 |
| 13 | GUA | H3' | 13 | GUA | H1' | 3.44 | 4.22 |
| 13 | GUA | H2'1 | 13 | GUA | H5'1 | 3.18 | 4.06 |
| 13 | GUA | H2'2 | 13 | GUA | H5'1 | 4.00 | 5.27 |
| 13 | GUA | H2'2 | 13 | GUA | H8 | 2.82 | 4.22 |
| 14 | GUA | H2'1 | 13 | CYT | H1' | 3.74 | 4.44 |
| 14 | GUA | H8 | 13 | GUA | H3' | 4.13 | 5.77 |
| 14 | GUA | H8 | 13 | GUA | H2'1 | 3.24 | 4.20 |
| 14 | GUA | H8 | 14 | GUA | H4' | 4.38 | 5.25 |

**Table B-6:** Continued

| Residue Number | Residue Name | Atom Number | Residue Number | Residue Name | Atom Number | Lower Bound | Upper Bound |
|---|---|---|---|---|---|---|---|
| 14 | GUA | H8 | 14 | GUA | H1' | 3.24 | 4.76 |
| 14 | GUA | H3' | 14 | GUA | H1' | 3.23 | 4.29 |
| 14 | GUA | H3' | 14 | GUA | H8 | 3.61 | 5.19 |
| 14 | GUA | H2'2 | 14 | GUA | H4' | 3.16 | 4.81 |
| 14 | GUA | H2'2 | 14 | GUA | H3' | 2.03 | 3.51 |
| 15 | ADE | H2'1 | 14 | GUA | H1' | 3.74 | 4.44 |
| 15 | ADE | H8 | 14 | GUA | H8 | 4.72 | 5.27 |
| 15 | ADE | H3' | 14 | GUA | H2'2 | 4.82 | 5.27 |
| 15 | ADE | H8 | 15 | ADE | H4' | 3.72 | 5.60 |
| 15 | ADE | H3' | 15 | ADE | H1' | 3.27 | 4.54 |
| 15 | ADE | H2'1 | 15 | ADE | H8 | 1.81 | 3.07 |
| 16 | CYT | H5'1 | 15 | ADE | H1' | 3.13 | 3.68 |
| 16 | CYT | H2'1 | 15 | ADE | H1' | 3.74 | 4.44 |
| 16 | CYT | H6 | 15 | ADE | H8 | 4.76 | 5.26 |
| 16 | CYT | H6 | 15 | ADE | H3' | 4.58 | 5.19 |
| 16 | CYT | H2'1 | 16 | CYT | H5 | 3.79 | 5.11 |
| 17 | THY | H6 | 16 | CYT | H1' | 3.38 | 4.25 |
| 17 | THY | H2'1 | 16 | CYT | H1' | 3.74 | 4.74 |
| 17 | THY | H3' | 17 | THY | H5'1 | 3.46 | 3.96 |
| 17 | THY | H6 | 16 | CYT | H2'2 | 1.96 | 2.56 |
| 17 | THY | M7 | 16 | CYT | H1' | 3.48 | 5.39 |
| 17 | THY | M7 | 16 | CYT | H6 | 3.69 | 5.22 |
| 17 | THY | M7 | 16 | CYT | H5 | 3.49 | 4.40 |
| 17 | THY | M7 | 16 | CYT | H2'2 | 3.39 | 5.73 |
| 17 | THY | H3' | 17 | THY | H6 | 2.59 | 4.53 |
| 17 | THY | H2'1 | 17 | THY | H1' | 2.42 | 3.96 |
| 18 | GUA | H2'1 | 17 | THY | H1' | 4.24 | 4.94 |
| 18 | GUA | H5'1 | 17 | THY | H1' | 3.41 | 4.36 |
| 18 | GUA | H1' | 18 | GUA | H5'1 | 3.33 | 5.03 |
| 18 | GUA | H8 | 17 | THY | H3' | 4.84 | 5.41 |
| 18 | GUA | H8 | 17 | THY | H1' | 3.64 | 5.01 |
| 18 | GUA | H8 | 17 | THY | H2'1 | 4.15 | 4.62 |
| 18 | GUA | H8 | 17 | THY | H2'2 | 3.16 | 4.16 |
| 18 | GUA | H2'1 | 17 | THY | H2'2 | 3.61 | 4.56 |
| 18 | GUA | H8 | 17 | THY | H6 | 4.81 | 5.66 |
| 18 | GUA | H3' | 17 | THY | H3' | 6.61 | 7.06 |
| 18 | GUA | H8 | 18 | GUA | H5'1 | 3.25 | 4.00 |
| 18 | GUA | H8 | 18 | GUA | H5'2 | 3.74 | 5.49 |
| 18 | GUA | H3' | 18 | GUA | H8 | 3.43 | 5.24 |
| 18 | GUA | H3' | 18 | GUA | H5'1 | 3.43 | 4.24 |
| 19 | GUA | H2'1 | 18 | GUA | H1' | 3.74 | 4.64 |
| 19 | GUA | H8 | 18 | GUA | H1' | 3.65 | 4.56 |
| 19 | GUA | H8 | 18 | GUA | H2'1 | 3.46 | 4.55 |
| 19 | GUA | H8 | 18 | GUA | H2'2 | 2.49 | 3.55 |
| 19 | GUA | H8 | 19 | GUA | H4' | 3.65 | 5.22 |
| 19 | GUA | H8 | 19 | GUA | H1' | 3.02 | 4.32 |

**Table B-6:** Continued

| Residue Number | Residue Name | Atom Number | Residue Number | Residue Name | Atom Number | Lower Bound | Upper Bound |
|---|---|---|---|---|---|---|---|
| 19 | GUA | H3' | 19 | GUA | H1' | 3.02 | 4.60 |
| 19 | GUA | H3' | 19 | GUA | H8 | 3.29 | 4.85 |
| 19 | GUA | H2'1 | 19 | GUA | H4' | 2.98 | 4.60 |
| 19 | GUA | H2'1 | 19 | GUA | H1' | 2.67 | 3.57 |
| 19 | GUA | H2'1 | 19 | GUA | H8 | 1.83 | 2.76 |
| 19 | GUA | H2'1 | 19 | GUA | H3' | 2.14 | 3.55 |
| 19 | GUA | H2'2 | 19 | GUA | H4' | 3.24 | 4.54 |
| 19 | GUA | H2'2 | 19 | GUA | H8 | 2.88 | 3.72 |
| 20 | CYT | H2'1 | 19 | GUA | H1' | 3.74 | 4.44 |
| 20 | CYT | H6 | 19 | GUA | H8 | 4.47 | 5.43 |
| 20 | CYT | H6 | 19 | GUA | H3' | 3.95 | 5.21 |
| 20 | CYT | H6 | 19 | GUA | H2'2 | 1.81 | 2.70 |
| 20 | CYT | H5 | 19 | GUA | H1' | 3.46 | 4.55 |
| 20 | CYT | H5 | 19 | GUA | H2'1 | 2.60 | 4.09 |
| 20 | CYT | H5 | 19 | GUA | H2'2 | 2.52 | 3.42 |
| 20 | CYT | H2'1 | 20 | CYT | H5 | 3.56 | 5.27 |
| 21 | THY | H2'1 | 20 | GUA | H1' | 3.74 | 4.44 |
| 21 | THY | H6 | 20 | CYT | H1' | 2.50 | 3.72 |
| 21 | THY | M7 | 20 | CYT | H1' | 3.78 | 4.19 |
| 21 | THY | M7 | 20 | CYT | H6 | 3.10 | 4.17 |
| 21 | THY | M7 | 20 | CYT | H5 | 3.50 | 4.85 |
| 21 | THY | M7 | 20 | CYT | H2'1 | 1.82 | 3.45 |
| 21 | THY | M7 | 20 | CYT | H2'2 | 2.07 | 3.93 |
| 21 | THY | H2'1 | 21 | THY | H6 | 1.71 | 2.56 |
| 21 | THY | H2'2 | 21 | THY | M7 | 5.66 | 6.58 |
| 22 | ADE | H2'1 | 21 | THY | H1' | 3.74 | 4.44 |
| 22 | ADE | H8 | 21 | THY | H2'1 | 3.14 | 4.59 |
| 22 | ADE | H8 | 21 | THY | H2'2 | 1.85 | 2.93 |
| 22 | ADE | H8 | 22 | ADE | H1' | 3.35 | 4.35 |
| 22 | ADE | H3' | 22 | ADE | H1' | 3.23 | 4.69 |
| 22 | ADE | H3' | 22 | ADE | H8 | 3.71 | 4.87 |
| 23 | GUA | H2'1 | 22 | ADE | H1' | 3.74 | 4.44 |
| 23 | GUA | H8 | 22 | ADE | H4' | 5.66 | 6.02 |
| 23 | GUA | H8 | 22 | ADE | H8 | 4.89 | 5.37 |
| 23 | GUA | H8 | 22 | ADE | H3' | 4.62 | 5.34 |
| 23 | GUA | H8 | 23 | GUA | H4' | 4.56 | 5.34 |
| 23 | GUA | H8 | 23 | GUA | H1' | 2.96 | 4.30 |
| 23 | GUA | H3' | 23 | GUA | H8 | 3.73 | 5.13 |
| 24 | CYT | H2'1 | 23 | GUA | H1' | 3.74 | 4.44 |
| 24 | CYT | H1' | 24 | CYT | H5'1 | 4.01 | 5.21 |
| 24 | CYT | H6 | 23 | GUA | H8 | 4.76 | 5.36 |
| 24 | CYT | H6 | 23 | GUA | H3' | 3.76 | 5.36 |
| 24 | CYT | H6 | 24 | CYT | H5'1 | 2.76 | 3.85 |
| 24 | CYT | H6 | 24 | CYT | H4' | 3.58 | 5.11 |
| 24 | CYT | H5 | 23 | GUA | H1' | 2.82 | 4.05 |
| 24 | CYT | H5 | 23 | GUA | H8 | 2.79 | 4.49 |

**Table B-6:** Continued

| Residue Number | Residue Name | Atom Number | Residue Number | Residue Name | Atom Number | Lower Bound | Upper Bound |
|---|---|---|---|---|---|---|---|
| 24 | CYT | H5 | 23 | GUA | H2'1 | 3.74 | 4.94 |
| 24 | CYT | H2'1 | 24 | CYT | H5 | 3.69 | 4.66 |
| 5 | GUA | H2'1 | 5 | GUA | H4' | 2.86 | 4.56 |
| 9 | GUA | H8 | 8 | ADE | H2'2 | 2.57 | 3.43 |
| 1 | GUA | H8 | 1 | GUA | H4' | 4.11 | 5.55 |
| 8 | ADE | H3' | 8 | ADE | H5'1 | 3.64 | 4.27 |
| 9 | GUA | H8 | 8 | ADE | H3' | 3.94 | 5.44 |
| 17 | THY | H6 | 16 | CYT | H2'1 | 2.74 | 4.16 |
| 17 | THY | M7 | 16 | CYT | H3' | 3.73 | 5.18 |
| 17 | THY | H2'1 | 17 | THY | M7 | 3.98 | 4.97 |
| 10 | THY | H1' | 10 | THY | H4' | 2.41 | 3.37 |
| 12 | CYT | H2'2 | 12 | CYT | H5'1 | 4.33 | 5.34 |
| 16 | CYT | H3' | 16 | CYT | H5'1 | 3.19 | 3.99 |
| 21 | THY | H6 | 20 | CYT | H2'1 | 3.29 | 4.53 |
| 21 | THY | H3' | 21 | THY | H5'1 | 3.59 | 4.23 |
| 23 | GUA | H1' | 22 | ADE | H1' | 4.79 | 5.23 |
| 24 | CYT | H2'1 | 23 | GUA | H2'2 | 3.70 | 4.21 |
| 24 | CYT | H2'1 | 24 | CYT | H5'1 | 2.90 | 4.71 |
| 24 | CYT | H2'2 | 24 | CYT | H5'1 | 4.45 | 5.39 |
| 19 | GUA | H2'1 | 18 | GUA | H2'2 | 3.70 | 4.21 |
| 19 | GUA | H8 | 18 | GUA | H4' | 5.75 | 6.39 |
| 19 | GUA | H8 | 19 | GUA | H5'1 | 2.95 | 4.39 |
| 19 | GUA | H5'1 | 18 | GUA | H1' | 2.75 | 3.79 |
| 19 | GUA | H5'1 | 7 | UBX | H13 | 5.85 | 7.79 |
| 19 | GUA | H8 | 18 | GUA | H8 | 4.75 | 5.39 |
| 22 | ADE | H8 | 21 | THY | M7 | 5.48 | 6.57 |
| 20 | CYT | H1' | 19 | GUA | H1' | 4.75 | 5.39 |
| 17 | THY | H1' | 7 | UBX | H12 | 6.25 | 8.39 |
| 17 | THY | H1' | 7 | UBX | H13 | 6.25 | 8.39 |
| 17 | THY | H1' | 7 | UBX | H11 | 6.25 | 8.39 |

# APPENDIX C

## TORSION ANGLE AND EMPIRICAL RESTRAINT FILES

**File C-1:** Restraints used for structural determination, including torsion angle, B-N-hydroxy angle, and Watson-Crick distance restraints.

```
# 2 CYT ALPHA:  (1 DG5 O3')-(2 DC P)-(2 DC O5')-(2 DC C5') -90.0 -30.0
 &rst     iat =    31,    32,    35,    36,
        r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,
        rk2 =   2.0, rk3 =   2.0,                     &end
# 3 THY ALPHA:  (2 DC O3')-(3 DT P)-(3 DT O5')-(3 DT C5') -90.0 -30.0
 &rst     iat =    61,    62,    65,    66,
        r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,&end
# 4 ADE ALPHA:  (3 DT O3')-(4 DA P)-(4 DA O5')-(4 DA C5') -90.0 -30.0
 &rst     iat =    93,    94,    97,    98,
        r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,&end
# 5 GUA ALPHA:  (4 DA O3')-(5 DG P)-(5 DG O5')-(5 DG C5') -90.0 -30.0
 &rst     iat =   125,   126,   129,   130,
        r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,&end
# 6 CYT ALPHA:  (5 DG O3')-(6 DC P)-(6 DC O5')-(6 DC C5') -120.0   0.0
 &rst     iat =   158,   159,   162,   163,
        r1 = -121.0, r2 = -120.0, r3 =   0.0, r4 =   1.0,&end
# 9 GUA ALPHA:  (8 DA O3')-(9 DG P)-(9 DG O5')-(9 DG C5') -120.0   0.0
 &rst     iat =   260,   261,   264,   265,
        r1 = -121.0, r2 = -120.0, r3 =   0.0, r4 =   1.0,&end
# 10 THY ALPHA:  (9 DG O3')-(10 DT P)-(10 DT O5')-(10 DT C5') -90.0 -
30.0
 &rst     iat =   293,   294,   297,   298,
        r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,&end
# 11 CYT ALPHA:  (10 DT O3')-(11 DC P)-(11 DC O5')-(11 DC C5') -90.0 -
30.0
 &rst     iat =   325,   326,   329,   330,
        r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,&end
# 12 CYT ALPHA:  (11 DC O3')-(12 DC3 P)-(12 DC3 O5')-(12 DC3 C5') -
120.0   0.0
 &rst     iat =   355,   356,   359,   360,
        r1 = -121.0, r2 = -120.0, r3 =   0.0, r4 =   1.0,&end
# 14 GUA ALPHA:  (13 DG5 O3')-(14 DG P)-(14 DG O5')-(14 DG C5') -90.0 -
30.0
 &rst     iat =   417,   418,   421,   422,
        r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,&end
# 15 ADE ALPHA:  (14 DG O3')-(15 DA P)-(15 DA O5')-(15 DA C5') -90.0 -
30.0
 &rst     iat =   450,   451,   454,   455,
        r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,&end
# 16 CYT ALPHA:  (15 DA O3')-(16 DC P)-(16 DC O5')-(16 DC C5') -120.0
0.0
 &rst     iat =   482,   483,   486,   487,
        r1 = -121.0, r2 = -120.0, r3 =   0.0, r4 =   1.0,&end
```

```
# 19 GUA ALPHA:  (18 DA O3')-(19 DG P)-(19 DG O5')-(19 DG C5') -120.0
0.0
 &rst     iat =   576,   577,   580,   581,
        r1 = -121.0, r2 = -120.0, r3 =   0.0, r4 =   1.0,&end
# 20 CYT ALPHA:  (19 DG O3')-(20 DC P)-(20 DC O5')-(20 DC C5') -90.0 -
30.0
 &rst     iat =   609,   610,   613,   614,
        r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,&end
# 21 THY ALPHA:  (20 DC O3')-(21 DT P)-(21 DT O5')-(21 DT C5') -90.0 -
30.0
 &rst     iat =   639,   640,   643,   644,
        r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,&end
# 22 ADE ALPHA:  (21 DT O3')-(22 DA P)-(22 DA O5')-(22 DA C5') -90.0 -
30.0
 &rst     iat =   671,   672,   675,   676,
        r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,&end
# 23 GUA ALPHA:  (22 DA O3')-(23 DG P)-(23 DG O5')-(23 DG C5') -90.0 -
30.0
 &rst     iat =   703,   704,   707,   708,
        r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,&end
# 24 CYT ALPHA:  (23 DG O3')-(24 DC3 P)-(24 DC3 O5')-(24 DC3 C5') -
120.0   0.0
 &rst     iat =   736,   737,   740,   741,
        r1 = -121.0, r2 = -120.0, r3 =   0.0, r4 =   1.0,&end
# 2 CYT BETA:  (2 DC P)-(2 DC O5')-(2 DC C5')-(2 DC C4') 150.0 210.0
 &rst     iat =    32,    35,    36,    39,
        r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,&end
# 3 THY BETA:  (3 DT P)-(3 DT O5')-(3 DT C5')-(3 DT C4') 150.0 210.0
 &rst     iat =    62,    65,    66,    69,
        r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,&end
# 4 ADE BETA:  (4 DA P)-(4 DA O5')-(4 DA C5')-(4 DA C4') 150.0 210.0
 &rst     iat =    94,    97,    98,   101,
        r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,&end
# 5 GUA BETA:  (5 DG P)-(5 DG O5')-(5 DG C5')-(5 DG C4') 150.0 210.0
 &rst     iat =   126,   129,   130,   133,
        r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,&end
# 6 CYT BETA:  (6 DC P)-(6 DC O5')-(6 DC C5')-(6 DC C4') 120.0 240.0
 &rst     iat =   159,   162,   163,   166,
        r1 = 119.0, r2 = 120.0, r3 = 240.0, r4 = 241.0,&end
# 9 GUA BETA:  (9 DG P)-(9 DG O5')-(9 DG C5')-(9 DG C4') 120.0 240.0
 &rst     iat =   261,   264,   265,   268,
        r1 = 119.0, r2 = 120.0, r3 = 240.0, r4 = 241.0,&end
# 10 THY BETA:  (10 DT P)-(10 DT O5')-(10 DT C5')-(10 DT C4') 150.0
210.0
 &rst     iat =   294,   297,   298,   301,
        r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,&end
# 11 CYT BETA:  (11 DC P)-(11 DC O5')-(11 DC C5')-(11 DC C4') 150.0
210.0
 &rst     iat =   326,   329,   330,   333,
        r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,&end
# 12 CYT BETA:  (12 DC3 P)-(12 DC3 O5')-(12 DC3 C5')-(12 DC3 C4') 120.0
240.0
 &rst     iat =   356,   359,   360,   363,
        r1 = 119.0, r2 = 120.0, r3 = 240.0, r4 = 241.0,&end
# 14 GUA BETA:  (14 DG P)-(14 DG O5')-(14 DG C5')-(14 DG C4') 150.0
210.0
 &rst     iat =   418,   421,   422,   425,
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```
        r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,&end
# 15 ADE BETA:  (15 DA P)-(15 DA O5')-(15 DA C5')-(15 DA C4') 120.0
240.0
 &rst     iat =   451,   454,   455,   458,
        r1 = 119.0, r2 = 120.0, r3 = 240.0, r4 = 241.0,&end
# 16 CYT BETA:  (16 DC P)-(16 DC O5')-(16 DC C5')-(16 DC C4') 120.0
240.0
 &rst     iat =   483,   486,   487,   490,
        r1 = 119.0, r2 = 120.0, r3 = 240.0, r4 = 241.0,&end
# 19 GUA BETA:  (19 DG P)-(19 DG O5')-(19 DG C5')-(19 DG C4') 150.0
210.0
 &rst     iat =   577,   580,   581,   584,
        r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,&end
# 20 CYT BETA:  (20 DC P)-(20 DC O5')-(20 DC C5')-(20 DC C4') 150.0
210.0
 &rst     iat =   610,   613,   614,   617,
        r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,&end
# 21 THY BETA:  (21 DT P)-(21 DT O5')-(21 DT C5')-(21 DT C4') 150.0
210.0
 &rst     iat =   640,   643,   644,   647,
        r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,&end
# 22 ADE BETA:  (22 DA P)-(22 DA O5')-(22 DA C5')-(22 DA C4') 150.0
210.0
 &rst     iat =   672,   675,   676,   679,
        r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,&end
# 23 GUA BETA:  (23 DG P)-(23 DG O5')-(23 DG C5')-(23 DG C4') 150.0
210.0
 &rst     iat =   704,   707,   708,   711,
        r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,&end
# 24 CYT BETA:  (24 DC3 P)-(24 DC3 O5')-(24 DC3 C5')-(24 DC3 C4') 120.0
240.0
 &rst     iat =   737,   740,   741,   744,
        r1 = 119.0, r2 = 120.0, r3 = 240.0, r4 = 241.0,&end
# 1 GUA GAMMA:  (1 DG5 O5')-(1 DG5 C5')-(1 DG5 C4')-(1 DG5 C3')   0.0
120.0
 &rst     iat =     2,     3,     6,    26,
        r1 =  -1.0, r2 =   0.0, r3 = 120.0, r4 = 121.0,&end
# 2 CYT GAMMA:  (2 DC O5')-(2 DC C5')-(2 DC C4')-(2 DC C3')  30.0  90.0
 &rst     iat =    35,    36,    39,    56,
        r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,&end

# 3 THY GAMMA:  (3 DT O5')-(3 DT C5')-(3 DT C4')-(3 DT C3')  30.0  90.0
 &rst     iat =    65,    66,    69,    88,
        r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,
      &end
# 4 ADE GAMMA:  (4 DA O5')-(4 DA C5')-(4 DA C4')-(4 DA C3')  30.0  90.0
 &rst     iat =    97,    98,   101,   120,
        r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,&end
# 5 GUA GAMMA:  (5 DG O5')-(5 DG C5')-(5 DG C4')-(5 DG C3')  30.0  90.0
 &rst     iat =   129,   130,   133,   153,
        r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,&end
# 6 CYT GAMMA:  (6 DC O5')-(6 DC C5')-(6 DC C4')-(6 DC C3')   0.0 120.0
 &rst     iat =   162,   163,   166,   183,
        r1 =  -1.0, r2 =   0.0, r3 = 120.0, r4 = 121.0,&end
# 9 GUA GAMMA:  (9 DG O5')-(9 DG C5')-(9 DG C4')-(9 DG C3')   0.0 120.0
 &rst     iat =   264,   265,   268,   288,
        r1 =  -1.0, r2 =   0.0, r3 = 120.0, r4 = 121.0,&end
```

```
# 10 THY GAMMA:  (10 DT O5')-(10 DT C5')-(10 DT C4')-(10 DT C3')  30.0
90.0
 &rst     iat =   297,   298,   301,   320,
        r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,&end
# 11 CYT GAMMA:  (11 DC O5')-(11 DC C5')-(11 DC C4')-(11 DC C3')  30.0
90.0
 &rst     iat =   329,   330,   333,   350,
        r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,&end
# 12 CYT GAMMA:  (12 DC3 O5')-(12 DC3 C5')-(12 DC3 C4')-(12 DC3 C3')
0.0 120.0
 &rst     iat =   359,   360,   363,   380,
        r1 =  -1.0, r2 =   0.0, r3 = 120.0, r4 = 121.0,&end
# 13 GUA GAMMA:  (13 DG5 O5')-(13 DG5 C5')-(13 DG5 C4')-(13 DG5 C3')
0.0 120.0
 &rst     iat =   388,   389,   392,   412,
        r1 =  -1.0, r2 =   0.0, r3 = 120.0, r4 = 121.0,&end
# 14 GUA GAMMA:  (14 DG O5')-(14 DG C5')-(14 DG C4')-(14 DG C3')  30.0
90.0
 &rst     iat =   421,   422,   425,   445,
        r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,&end
# 15 ADE GAMMA:  (15 DA O5')-(15 DA C5')-(15 DA C4')-(15 DA C3')  30.0
90.0
 &rst     iat =   454,   455,   458,   477,
        r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,&end
# 16 CYT GAMMA:  (16 DC O5')-(16 DC C5')-(16 DC C4')-(16 DC C3')   0.0
120.0
 &rst     iat =   486,   487,   490,   507,
        r1 =  -1.0, r2 =   0.0, r3 = 120.0, r4 = 121.0,&end
# 19 GUA GAMMA:  (19 DG O5')-(19 DG C5')-(19 DG C4')-(19 DG C3')   0.0
120.0
 &rst     iat =   580,   581,   584,   604,
        r1 =  -1.0, r2 =   0.0, r3 = 120.0, r4 = 121.0,&end
# 20 CYT GAMMA:  (20 DC O5')-(20 DC C5')-(20 DC C4')-(20 DC C3')  30.0
90.0
 &rst     iat =   613,   614,   617,   634,
        r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,&end
# 21 THY GAMMA:  (21 DT O5')-(21 DT C5')-(21 DT C4')-(21 DT C3')  30.0
90.0
 &rst     iat =   643,   644,   647,   666,
        r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,&end
# 22 ADE GAMMA:  (22 DA O5')-(22 DA C5')-(22 DA C4')-(22 DA C3')  30.0
90.0
 &rst     iat =   675,   676,   679,   698,
        r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,&end
# 23 GUA GAMMA:  (23 DG O5')-(23 DG C5')-(23 DG C4')-(23 DG C3')  30.0
90.0
 &rst     iat =   707,   708,   711,   731,
        r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,&end
# 24 CYT GAMMA:  (24 DC3 O5')-(24 DC3 C5')-(24 DC3 C4')-(24 DC3 C3')
0.0 120.0
 &rst     iat =   740,   741,   744,   761,
        r1 =  -1.0, r2 =   0.0, r3 = 120.0, r4 = 121.0,&end
# 1 GUA EPSILN:  (1 DG5 C4')-(1 DG5 C3')-(1 DG5 O3')-(2 DC P) 120.0
240.0
 &rst     iat =     6,    26,    31,    32,
        r1 = 119.0, r2 = 120.0, r3 = 240.0, r4 = 241.0,&end
```

```
# 2 CYT EPSILN:  (2 DC C4')-(2 DC C3')-(2 DC O3')-(3 DT P) 150.0 210.0
 &rst     iat =    39,    56,    61,    62,
        r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,&end
# 3 THY EPSILN:  (3 DT C4')-(3 DT C3')-(3 DT O3')-(4 DA P) 150.0 210.0
 &rst     iat =    69,    88,    93,    94,
        r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,&end
# 4 ADE EPSILN:  (4 DA C4')-(4 DA C3')-(4 DA O3')-(5 DG P) 150.0 210.0
 &rst     iat =   101,   120,   125,   126,
        r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,&end
# 5 GUA EPSILN:  (5 DG C4')-(5 DG C3')-(5 DG O3')-(6 DC P) 150.0 210.0
 &rst     iat =   133,   153,   158,   159,
        r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,&end
# 6 CYT EPSILN:  (6 DC C4')-(6 DC C3')-(6 DC O3')-(7 DX P) 120.0 240.0
 &rst     iat =   166,   183,   188,   189,
        r1 = 119.0, r2 = 120.0, r3 = 240.0, r4 = 241.0,&end
# 9 GUA EPSILN:  (9 DG C4')-(9 DG C3')-(9 DG O3')-(10 DT P) 120.0 240.0
 &rst     iat =   268,   288,   293,   294,
        r1 = 119.0, r2 = 120.0, r3 = 240.0, r4 = 241.0,&end
# 10 THY EPSILN:  (10 DT C4')-(10 DT C3')-(10 DT O3')-(11 DC P) 150.0
210.0
 &rst     iat =   301,   320,   325,   326,
        r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,&end
# 11 CYT EPSILN:  (11 DC C4')-(11 DC C3')-(11 DC O3')-(12 DC3 P) 150.0
210.0
 &rst     iat =   333,   350,   355,   356,
        r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,&end
# 13 GUA EPSILN:  (13 DG5 C4')-(13 DG5 C3')-(13 DG5 O3')-(14 DG P)
120.0 240.0
 &rst     iat =   392,   412,   417,   418,
        r1 = 119.0, r2 = 120.0, r3 = 240.0, r4 = 241.0,&end
# 14 GUA EPSILN:  (14 DG C4')-(14 DG C3')-(14 DG O3')-(15 DA P) 150.0
210.0
 &rst     iat =   425,   445,   450,   451,
        r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,&end
# 15 ADE EPSILN:  (15 DA C4')-(15 DA C3')-(15 DA O3')-(16 DC P) 150.0
210.0
 &rst     iat =   458,   477,   482,   483,
        r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,&end
# 16 CYT EPSILN:  (16 DC C4')-(16 DC C3')-(16 DC O3')-(17 DT P) 120.0
240.0
 &rst     iat =   490,   507,   512,   513,
        r1 = 119.0, r2 = 120.0, r3 = 240.0, r4 = 241.0,&end
# 19 GUA EPSILN:  (19 DG C4')-(19 DG C3')-(19 DG O3')-(20 DC P) 120.0
240.0
 &rst     iat =   584,   604,   609,   610,
        r1 = 119.0, r2 = 120.0, r3 = 240.0, r4 = 241.0,&end
# 20 CYT EPSILN:  (20 DC C4')-(20 DC C3')-(20 DC O3')-(21 DT P) 150.0
210.0
 &rst     iat =   617,   634,   639,   640,
        r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,&end
# 21 THY EPSILN:  (21 DT C4')-(21 DT C3')-(21 DT O3')-(22 DA P) 150.0
210.0
 &rst     iat =   647,   666,   671,   672,
        r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,&end
```

```
# 22 ADE EPSILN:  (22 DA C4')-(22 DA C3')-(22 DA O3')-(23 DG P) 150.0
210.0
 &rst     iat =   679,   698,   703,   704,
        r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,&end
# 23 GUA EPSILN:  (23 DG C4')-(23 DG C3')-(23 DG O3')-(24 DC3 P) 150.0
210.0
 &rst     iat =   711,   731,   736,   737,
        r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,&end
# 1 GUA ZETA:  (1 DG5 C3')-(1 DG5 O3')-(2 DC P)-(2 DC O5') -150.0 -30.0
 &rst     iat =    26,    31,    32,    35,
        r1 = -151.0, r2 = -150.0, r3 = -30.0, r4 = -29.0,&end
# 2 CYT ZETA:  (2 DC C3')-(2 DC O3')-(3 DT P)-(3 DT O5') -120.0 -60.0
 &rst     iat =    56,    61,    62,    65,
        r1 = -121.0, r2 = -120.0, r3 = -60.0, r4 = -59.0,&end
# 3 THY ZETA:  (3 DT C3')-(3 DT O3')-(4 DA P)-(4 DA O5') -120.0 -60.0
 &rst     iat =    88,    93,    94,    97,
        r1 = -121.0, r2 = -120.0, r3 = -60.0, r4 = -59.0,&end
# 4 ADE ZETA:  (4 DA C3')-(4 DA O3')-(5 DG P)-(5 DG O5') -120.0 -60.0
 &rst     iat =   120,   125,   126,   129,
        r1 = -121.0, r2 = -120.0, r3 = -60.0, r4 = -59.0,&end
# 5 GUA ZETA:  (5 DG C3')-(5 DG O3')-(6 DC P)-(6 DC O5') -120.0 -60.0
 &rst     iat =   153,   158,   159,   162,
        r1 = -121.0, r2 = -120.0, r3 = -60.0, r4 = -59.0,&end
# 6 CYT ZETA:  (6 DC C3')-(6 DC O3')-(7 DX P)-(7 DX O5') -150.0 -30.0
 &rst     iat =   183,   188,   189,   192,
        r1 = -151.0, r2 = -150.0, r3 = -30.0, r4 = -29.0,&end
# 8 ADE ZETA:  (8 DA C3')-(8 DA O3')-(9 DG P)-(9 DG O5') -150.0 -30.0
 &rst     iat =   255,   260,   261,   264,
        r1 = -151.0, r2 = -150.0, r3 = -30.0, r4 = -29.0,&end
# 9 GUA ZETA:  (9 DG C3')-(9 DG O3')-(10 DT P)-(10 DT O5') -150.0 -30.0
 &rst     iat =   288,   293,   294,   297,
        r1 = -151.0, r2 = -150.0, r3 = -30.0, r4 = -29.0,&end
# 10 THY ZETA:  (10 DT C3')-(10 DT O3')-(11 DC P)-(11 DC O5') -120.0 -
60.0
 &rst     iat =   320,   325,   326,   329,
        r1 = -121.0, r2 = -120.0, r3 = -60.0, r4 = -59.0,&end
# 11 CYT ZETA:  (11 DC C3')-(11 DC O3')-(12 DC3 P)-(12 DC3 O5') -120.0
-60.0
 &rst     iat =   350,   355,   356,   359,
        r1 = -121.0, r2 = -120.0, r3 = -60.0, r4 = -59.0,&end
# 13 GUA ZETA:  (13 DG5 C3')-(13 DG5 O3')-(14 DG P)-(14 DG O5') -150.0
-30.0
 &rst     iat =   412,   417,   418,   421,
        r1 = -151.0, r2 = -150.0, r3 = -30.0, r4 = -29.0,&end
# 14 GUA ZETA:  (14 DG C3')-(14 DG O3')-(15 DA P)-(15 DA O5') -120.0 -
60.0
 &rst     iat =   445,   450,   451,   454,
        r1 = -121.0, r2 = -120.0, r3 = -60.0, r4 = -59.0,&end
# 15 ADE ZETA:  (15 DA C3')-(15 DA O3')-(16 DC P)-(16 DC O5') -120.0 -
60.0
 &rst     iat =   477,   482,   483,   486,
        r1 = -121.0, r2 = -120.0, r3 = -60.0, r4 = -59.0,&end
# 16 CYT ZETA:  (16 DC C3')-(16 DC O3')-(17 DT P)-(17 DT O5') -150.0 -
30.0
 &rst     iat =   507,   512,   513,   516,
        r1 = -151.0, r2 = -150.0, r3 = -30.0, r4 = -29.0,&end
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# 17 THY ZETA:  (17 DT C3')-(17 DT O3')-(18 DA P)-(18 DA O5') -150.0 -
30.0
 &rst     iat =   539,   544,   545,   548,
        r1 = -151.0, r2 = -150.0, r3 = -30.0, r4 = -29.0,&end
# 19 GUA ZETA:  (19 DG C3')-(19 DG O3')-(20 DC P)-(20 DC O5') -150.0 -
30.0
 &rst     iat =   604,   609,   610,   613,
        r1 = -151.0, r2 = -150.0, r3 = -30.0, r4 = -29.0,&end
# 20 CYT ZETA:  (20 DC C3')-(20 DC O3')-(21 DT P)-(21 DT O5') -120.0 -
60.0
 &rst     iat =   634,   639,   640,   643,
        r1 = -121.0, r2 = -120.0, r3 = -60.0, r4 = -59.0,&end
# 21 THY ZETA:  (21 DT C3')-(21 DT O3')-(22 DA P)-(22 DA O5') -120.0 -
60.0
 &rst     iat =   666,   671,   672,   675,
        r1 = -121.0, r2 = -120.0, r3 = -60.0, r4 = -59.0,&end
# 22 ADE ZETA:  (22 DA C3')-(22 DA O3')-(23 DG P)-(23 DG O5') -120.0 -
60.0
 &rst     iat =   698,   703,   704,   707,
        r1 = -121.0, r2 = -120.0, r3 = -60.0, r4 = -59.0,&end
# 23 GUA ZETA:  (23 DG C3')-(23 DG O3')-(24 DC3 P)-(24 DC3 O5') -120.0
-60.0
 &rst     iat =   731,   736,   737,   740,
        r1 = -121.0, r2 = -120.0, r3 = -60.0, r4 = -59.0,&end
# 767 atoms read from pdb file R-N3-dUdA.amb.pdb.
# 1 GUA CHI:  (1 DG5 O4')-(1 DG5 C1')-(1 DG5 N9)-(1 DG5 C4) -470.0 -
150.0
 &rst     iat =     8,     9,    11,    25,
        r1 = -471.0, r2 = -470.0, r3 = -150.0, r4 = -149.0,
        rk2 =   2.0, rk3 =   2.0,                      &end
# 2 CYT CHI:  (2 DC O4')-(2 DC C1')-(2 DC N1)-(2 DC C2) -470.0 -150.0
 &rst     iat =    41,    42,    44,    54,
        r1 = -471.0, r2 = -470.0, r3 = -150.0, r4 = -149.0,&end
# 3 THY CHI:  (3 DT O4')-(3 DT C1')-(3 DT N1)-(3 DT C2) -470.0 -150.0
 &rst     iat =    71,    72,    74,    86,
        r1 = -471.0, r2 = -470.0, r3 = -150.0, r4 = -149.0,&end
# 4 ADE CHI:  (4 DA O4')-(4 DA C1')-(4 DA N9)-(4 DA C4) -470.0 -150.0
 &rst     iat =   103,   104,   106,   119,
        r1 = -471.0, r2 = -470.0, r3 = -150.0, r4 = -149.0,&end
# 5 GUA CHI:  (5 DG O4')-(5 DG C1')-(5 DG N9)-(5 DG C4) -470.0 -150.0
 &rst     iat =   135,   136,   138,   152,
        r1 = -471.0, r2 = -470.0, r3 = -150.0, r4 = -149.0,&end
# 6 CYT CHI:  (6 DC O4')-(6 DC C1')-(6 DC N1)-(6 DC C2) -470.0 -150.0
 &rst     iat =   168,   169,   171,   181,
        r1 = -471.0, r2 = -470.0, r3 = -150.0, r4 = -149.0,&end
# 7 UBX CHI:  (7 DX O4')-(7 DX C1')-(7 DX N1)-(7 DX C4) -470.0 -150.0
 &rst     iat =   198,   199,   201,   206,
        r1 = -471.0, r2 = -470.0, r3 = -150.0, r4 = -149.0,&end
# 8 ADE CHI:  (8 DA O4')-(8 DA C1')-(8 DA N9)-(8 DA C4) -470.0 -150.0
 &rst     iat =   238,   239,   241,   254,
        r1 = -471.0, r2 = -470.0, r3 = -150.0, r4 = -149.0,&end
# 9 GUA CHI:  (9 DG O4')-(9 DG C1')-(9 DG N9)-(9 DG C4) -470.0 -150.0
 &rst     iat =   270,   271,   273,   287,
        r1 = -471.0, r2 = -470.0, r3 = -150.0, r4 = -149.0,&end
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# 10 THY CHI:  (10 DT O4')-(10 DT C1')-(10 DT N1)-(10 DT C2) -470.0 -
150.0
 &rst     iat =   303,   304,   306,   318,
        r1 = -471.0, r2 = -470.0, r3 = -150.0, r4 = -149.0,&end
# 11 CYT CHI:  (11 DC O4')-(11 DC C1')-(11 DC N1)-(11 DC C2) -470.0 -
150.0
 &rst     iat =   335,   336,   338,   348,
        r1 = -471.0, r2 = -470.0, r3 = -150.0, r4 = -149.0,&end
# 12 CYT CHI:  (12 DC3 O4')-(12 DC3 C1')-(12 DC3 N1)-(12 DC3 C2) -470.0
-150.0
 &rst     iat =   365,   366,   368,   378,
        r1 = -471.0, r2 = -470.0, r3 = -150.0, r4 = -149.0,&end
# 13 GUA CHI:  (13 DG5 O4')-(13 DG5 C1')-(13 DG5 N9)-(13 DG5 C4) -470.0
-150.0
 &rst     iat =   394,   395,   397,   411,
        r1 = -471.0, r2 = -470.0, r3 = -150.0, r4 = -149.0,&end
# 14 GUA CHI:  (14 DG O4')-(14 DG C1')-(14 DG N9)-(14 DG C4) -470.0 -
150.0
 &rst     iat =   427,   428,   430,   444,
        r1 = -471.0, r2 = -470.0, r3 = -150.0, r4 = -149.0,&end
# 15 ADE CHI:  (15 DA O4')-(15 DA C1')-(15 DA N9)-(15 DA C4) -470.0 -
150.0
 &rst     iat =   460,   461,   463,   476,
        r1 = -471.0, r2 = -470.0, r3 = -150.0, r4 = -149.0,&end
# 16 CYT CHI:  (16 DC O4')-(16 DC C1')-(16 DC N1)-(16 DC C2) -470.0 -
150.0
 &rst     iat =   492,   493,   495,   505,
        r1 = -471.0, r2 = -470.0, r3 = -150.0, r4 = -149.0,&end
# 17 THY CHI:  (17 DT O4')-(17 DT C1')-(17 DT N1)-(17 DT C2) -470.0 -
150.0
 &rst     iat =   522,   523,   525,   537,
        r1 = -471.0, r2 = -470.0, r3 = -150.0, r4 = -149.0,&end
# 18 ADE CHI:  (18 DA O4')-(18 DA C1')-(18 DA N9)-(18 DA C4) -470.0 -
150.0
 &rst     iat =   554,   555,   557,   570,
        r1 = -471.0, r2 = -470.0, r3 = -150.0, r4 = -149.0,&end
# 19 GUA CHI:  (19 DG O4')-(19 DG C1')-(19 DG N9)-(19 DG C4) -470.0 -
150.0
 &rst     iat =   586,   587,   589,   603,
        r1 = -471.0, r2 = -470.0, r3 = -150.0, r4 = -149.0,&end
# 20 CYT CHI:  (20 DC O4')-(20 DC C1')-(20 DC N1)-(20 DC C2) -470.0 -
150.0
 &rst     iat =   619,   620,   622,   632,
        r1 = -471.0, r2 = -470.0, r3 = -150.0, r4 = -149.0,&end
# 21 THY CHI:  (21 DT O4')-(21 DT C1')-(21 DT N1)-(21 DT C2) -470.0 -
150.0
 &rst     iat =   649,   650,   652,   664,
        r1 = -471.0, r2 = -470.0, r3 = -150.0, r4 = -149.0,&end
# 22 ADE CHI:  (22 DA O4')-(22 DA C1')-(22 DA N9)-(22 DA C4) -470.0 -
150.0
 &rst     iat =   681,   682,   684,   697,
        r1 = -471.0, r2 = -470.0, r3 = -150.0, r4 = -149.0,&end
# 23 GUA CHI:  (23 DG O4')-(23 DG C1')-(23 DG N9)-(23 DG C4) -470.0 -
150.0
 &rst     iat =   713,   714,   716,   730,
        r1 = -471.0, r2 = -470.0, r3 = -150.0, r4 = -149.0,&end
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# 24 CYT CHI:  (24 DC3 O4')-(24 DC3 C1')-(24 DC3 N1)-(24 DC3 C2) -470.0
-150.0
 &rst     iat =   746,   747,   749,   759,
        r1 = -471.0, r2 = -470.0, r3 = -150.0, r4 = -149.0,&end
# 767 atoms read from pdb file dUdAmod_B2.amb.pdb.
# 1 GUA NU0:  (1 DG5 C4')-(1 DG5 O4')-(1 DG5 C1')-(1 DG5 C2') -44.7 -
14.7
 &rst     iat =     6,     8,     9,    28,
        r1 = -45.7, r2 = -44.7, r3 = -14.7, r4 = -13.7,
        rk2 =   2.0, rk3 =   2.0,                     &end
# 1 GUA NU1:  (1 DG5 O4')-(1 DG5 C1')-(1 DG5 C2')-(1 DG5 C3')  18.1
48.1
 &rst     iat =     8,     9,    28,    26,
        r1 =  17.1, r2 =  18.1, r3 =  48.1, r4 =  49.1,&end
# 1 GUA NU2:  (1 DG5 C1')-(1 DG5 C2')-(1 DG5 C3')-(1 DG5 C4') -37.2  -
6.7
 &rst     iat =     9,    28,    26,     6,
        r1 = -38.2, r2 = -37.2, r3 =  -6.7, r4 =  -5.7,&end
# 1 GUA NU3:  (1 DG5 C2')-(1 DG5 C3')-(1 DG5 C4')-(1 DG5 O4')-16.9
24.2
 &rst     iat =    28,    26,     6,     8,
        r1 = -17.9, r2 = -16.9, r3 =  24.2, r4 =  25.2,&end
# 1 GUA NU4:  (1 DG5 C3')-(1 DG5 C4')-(1 DG5 O4')-(1 DG5 C1')  -1.9
34.0
 &rst     iat =    26,     6,     8,     9,
        r1 =  -2.9, r2 =  -1.9, r3 =  34.0, r4 =  35.0,&end
# 2 CYT NU0:  (2 DC C4')-(2 DC O4')-(2 DC C1')-(2 DC C2') -44.7 -14.7
 &rst     iat =    39,    41,    42,    58,
        r1 = -45.7, r2 = -44.7, r3 = -14.7, r4 = -13.7,&end
# 2 CYT NU1:  (2 DC O4')-(2 DC C1')-(2 DC C2')-(2 DC C3')  18.1  48.1
 &rst     iat =    41,    42,    58,    56,
        r1 =  17.1, r2 =  18.1, r3 =  48.1, r4 =  49.1,&end
# 2 CYT NU2:  (2 DC C1')-(2 DC C2')-(2 DC C3')-(2 DC C4') -37.2  -6.7
 &rst     iat =    42,    58,    56,    39,
        r1 = -38.2, r2 = -37.2, r3 =  -6.7, r4 =  -5.7,&end
# 2 CYT NU3:  (2 DC C2')-(2 DC C3')-(2 DC C4')-(2 DC O4') -16.9  24.2
 &rst     iat =    58,    56,    39,    41,
        r1 = -17.9, r2 = -16.9, r3 =  24.2, r4 =  25.2,&end
# 2 CYT NU4:  (2 DC C3')-(2 DC C4')-(2 DC O4')-(2 DC C1')  -1.9  34.0
 &rst     iat =    56,    39,    41,    42,
        r1 =  -2.9, r2 =  -1.9, r3 =  34.0, r4 =  35.0,&end
# 3 THY NU0:  (3 DT C4')-(3 DT O4')-(3 DT C1')-(3 DT C2') -52.1 -22.1
 &rst     iat =    69,    71,    72,    90,
        r1 = -53.1, r2 = -52.1, r3 = -22.1, r4 = -21.1,&end
# 3 THY NU1:  (3 DT O4')-(3 DT C1')-(3 DT C2')-(3 DT C3')  15.0  45.0
 &rst     iat =    71,    72,    90,    88,
        r1 =  14.0, r2 =  15.0, r3 =  45.0, r4 =  46.0,&end
# 3 THY NU2:  (3 DT C1')-(3 DT C2')-(3 DT C3')-(3 DT C4') -27.4   2.6
 &rst     iat =    72,    90,    88,    69,
        r1 = -28.4, r2 = -27.4, r3 =   2.6, r4 =   3.6,&end
# 3 THY NU3:  (3 DT C2')-(3 DT C3')-(3 DT C4')-(3 DT O4') -25.0   5.0
 &rst     iat =    90,    88,    69,    71,
        r1 = -26.0, r2 = -25.0, r3 =   5.0, r4 =   6.0,&end
# 3 THY NU4:  (3 DT C3')-(3 DT C4')-(3 DT O4')-(3 DT C1')  13.5  43.5
 &rst     iat =    88,    69,    71,    72,
        r1 =  12.5, r2 =  13.5, r3 =  43.5, r4 =  44.5,&end
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# 4 ADE NU0:  (4 DA C4')-(4 DA O4')-(4 DA C1')-(4 DA C2') -41.1 -11.1
 &rst     iat =   101,   103,   104,   122,
        r1 = -42.1, r2 = -41.1, r3 = -11.1, r4 = -10.1,&end
# 4 ADE NU1:  (4 DA O4')-(4 DA C1')-(4 DA C2')-(4 DA C3')  22.2  52.2
 &rst     iat =   103,   104,   122,   120,
        r1 =  21.2, r2 =  22.2, r3 =  52.2, r4 =  53.2,&end
# 4 ADE NU2:  (4 DA C1')-(4 DA C2')-(4 DA C3')-(4 DA C4') -49.2 -19.2
 &rst     iat =   104,   122,   120,   101,
        r1 = -50.2, r2 = -49.2, r3 = -19.2, r4 = -18.2,&end
# 4 ADE NU3:  (4 DA C2')-(4 DA C3')-(4 DA C4')-(4 DA O4')   3.1  33.1
 &rst     iat =   122,   120,   101,   103,
        r1 =   2.1, r2 =   3.1, r3 =  33.1, r4 =  34.1,&end
# 4 ADE NU4:  (4 DA C3')-(4 DA C4')-(4 DA O4')-(4 DA C1') -10.0  20.0
 &rst     iat =   120,   101,   103,   104,
        r1 = -11.0, r2 = -10.0, r3 =  20.0, r4 =  21.0,&end
# 5 GUA NU0:  (5 DG C4')-(5 DG O4')-(5 DG C1')-(5 DG C2') -41.1 -11.1
 &rst     iat =   133,   135,   136,   155,
        r1 = -42.1, r2 = -41.1, r3 = -11.1, r4 = -10.1,&end
# 5 GUA NU1:  (5 DG O4')-(5 DG C1')-(5 DG C2')-(5 DG C3')  22.2  52.2
 &rst     iat =   135,   136,   155,   153,
        r1 =  21.2, r2 =  22.2, r3 =  52.2, r4 =  53.2,&end
# 5 GUA NU2:  (5 DG C1')-(5 DG C2')-(5 DG C3')-(5 DG C4') -49.2 -19.2
 &rst     iat =   136,   155,   153,   133,
        r1 = -50.2, r2 = -49.2, r3 = -19.2, r4 = -18.2,&end
# 5 GUA NU3:  (5 DG C2')-(5 DG C3')-(5 DG C4')-(5 DG O4')   3.1  33.1
 &rst     iat =   155,   153,   133,   135,
        r1 =   2.1, r2 =   3.1, r3 =  33.1, r4 =  34.1,&end
# 5 GUA NU4:  (5 DG C3')-(5 DG C4')-(5 DG O4')-(5 DG C1') -10.0  20.0
 &rst     iat =   153,   133,   135,   136,
        r1 = -11.0, r2 = -10.0, r3 =  20.0, r4 =  21.0,&end
# 6 CYT NU0:  (6 DC C4')-(6 DC O4')-(6 DC C1')-(6 DC C2') -45.3 -15.3
 &rst     iat =   166,   168,   169,   185,
        r1 = -46.3, r2 = -45.3, r3 = -15.3, r4 = -14.3,&end
# 6 CYT NU1:  (6 DC O4')-(6 DC C1')-(6 DC C2')-(6 DC C3')  22.5  52.5
 &rst     iat =   168,   169,   185,   183,
        r1 =  21.5, r2 =  22.5, r3 =  52.5, r4 =  53.5,&end
# 6 CYT NU2:  (6 DC C1')-(6 DC C2')-(6 DC C3')-(6 DC C4') -44.1 -14.1
 &rst     iat =   169,   185,   183,   166,  r1 = -45.1, r2 = -44.1, r3
= -14.1, r4 = -13.1,&end
# 6 CYT NU3:  (6 DC C2')-(6 DC C3')-(6 DC C4')-(6 DC O4')  -4.6  25.4
 &rst     iat =   185,   183,   166,   168,
        r1 =  -5.6, r2 =  -4.6, r3 =  25.4, r4 =  26.4,&end
# 6 CYT NU4:  (6 DC C3')-(6 DC C4')-(6 DC O4')-(6 DC C1')  -2.7  27.3
 &rst     iat =   183,   166,   168,   169,
        r1 =  -3.7, r2 =  -2.7, r3 =  27.3, r4 =  28.3,&end
# 7 UBX NU0:  (7 DX C4')-(7 DX O4')-(7 DX C1')-(7 DX C2') -33.3  -3.3
 &rst     iat =   196,   198,   199,   214,
        r1 = -34.3, r2 = -33.3, r3 =  -3.3, r4 =  -2.3,&end
# 7 UBX NU1:  (7 DX O4')-(7 DX C1')-(7 DX C2')-(7 DX C3')  17.6  47.6
 &rst     iat =   198,   199,   214,   212,
        r1 =  16.6, r2 =  17.6, r3 =  47.6, r4 =  48.6,&end
# 7 UBX NU2:  (7 DX C1')-(7 DX C2')-(7 DX C3')-(7 DX C4') -49.8 -19.8
 &rst     iat =   199,   214,   212,   196,
        r1 = -50.8, r2 = -49.8, r3 = -19.8, r4 = -18.8,&end
# 7 UBX NU3:  (7 DX C2')-(7 DX C3')-(7 DX C4')-(7 DX O4')   8.3  38.3
 &rst     iat =   214,   212,   196,   198,
        r1 =   7.3, r2 =   8.3, r3 =  38.3, r4 =  39.3,&end
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# 7 UBX NU4:  (7 DX C3')-(7 DX C4')-(7 DX O4')-(7 DX C1') -18.1  11.9
 &rst     iat =   212,   196,   198,   199,
        r1 = -19.1, r2 = -18.1, r3 =  11.9, r4 =  12.9,&end
# 8 ADE NU0:  (8 DA C4')-(8 DA O4')-(8 DA C1')-(8 DA C2') -33.3  -3.3
 &rst     iat =   236,   238,   239,   257,
        r1 = -34.3, r2 = -33.3, r3 =  -3.3, r4 =  -2.3,&end
# 8 ADE NU1:  (8 DA O4')-(8 DA C1')-(8 DA C2')-(8 DA C3')  17.6  47.6
 &rst     iat =   238,   239,   257,   255,
        r1 =  16.6, r2 =  17.6, r3 =  47.6, r4 =  48.6,&end
# 8 ADE NU2:  (8 DA C1')-(8 DA C2')-(8 DA C3')-(8 DA C4') -49.8 -19.8
 &rst     iat =   239,   257,   255,   236,
        r1 = -50.8, r2 = -49.8, r3 = -19.8, r4 = -18.8,&end
# 8 ADE NU3:  (8 DA C2')-(8 DA C3')-(8 DA C4')-(8 DA O4')   8.3  38.3
 &rst     iat =   257,   255,   236,   238,
        r1 =   7.3, r2 =   8.3, r3 =  38.3, r4 =  39.3,&end
# 8 ADE NU4:  (8 DA C3')-(8 DA C4')-(8 DA O4')-(8 DA C1') -18.1  11.9
 &rst     iat =   255,   236,   238,   239,
        r1 = -19.1, r2 = -18.1, r3 =  11.9, r4 =  12.9,&end
# 9 GUA NU0:  (9 DG C4')-(9 DG O4')-(9 DG C1')-(9 DG C2') -43.9 -13.9
 &rst     iat =   268,   270,   271,   290,
        r1 = -44.9, r2 = -43.9, r3 = -13.9, r4 = -12.9,&end
# 9 GUA NU1:  (9 DG O4')-(9 DG C1')-(9 DG C2')-(9 DG C3')  22.2  52.2
 &rst     iat =   270,   271,   290,   288,
        r1 =  21.2, r2 =  22.2, r3 =  52.2, r4 =  53.2,&end

# 9 GUA NU2:  (9 DG C1')-(9 DG C2')-(9 DG C3')-(9 DG C4') -44.6 -14.6
 &rst     iat =   271,   290,   288,   268,
        r1 = -45.6, r2 = -44.6, r3 = -14.6, r4 = -13.6,&end
# 9 GUA NU3:  (9 DG C2')-(9 DG C3')-(9 DG C4')-(9 DG O4')  -3.2  26.8
 &rst     iat =   290,   288,   268,   270,
        r1 =  -4.2, r2 =  -3.2, r3 =  26.8, r4 =  27.8,&end
# 9 GUA NU4:  (9 DG C3')-(9 DG C4')-(9 DG O4')-(9 DG C1')  -4.4  25.6
 &rst     iat =   288,   268,   270,   271,
        r1 =  -5.4, r2 =  -4.4, r3 =  25.6, r4 =  26.6,&end
# 10 THY NU0:  (10 DT C4')-(10 DT O4')-(10 DT C1')-(10 DT C2') -52.1 -
22.1
 &rst     iat =   301,   303,   304,   322,
        r1 = -53.1, r2 = -52.1, r3 = -22.1, r4 = -21.1,&end
# 10 THY NU1:  (10 DT O4')-(10 DT C1')-(10 DT C2')-(10 DT C3')  15.0
45.0
 &rst     iat =   303,   304,   322,   320,
        r1 =  14.0, r2 =  15.0, r3 =  45.0, r4 =  46.0,&end
# 10 THY NU2:  (10 DT C1')-(10 DT C2')-(10 DT C3')-(10 DT C4') -27.4
2.6
 &rst     iat =   304,   322,   320,   301,
        r1 = -28.4, r2 = -27.4, r3 =   2.6, r4 =   3.6,&end
# 10 THY NU3:  (10 DT C2')-(10 DT C3')-(10 DT C4')-(10 DT O4') -25.0
5.0
 &rst     iat =   322,   320,   301,   303,
        r1 = -26.0, r2 = -25.0, r3 =   5.0, r4 =   6.0,&end
# 10 THY NU4:  (10 DT C3')-(10 DT C4')-(10 DT O4')-(10 DT C1')  13.5
43.5
 &rst     iat =   320,   301,   303,   304,
        r1 =  12.5, r2 =  13.5, r3 =  43.5, r4 =  44.5,&end
# 11 CYT NU0:  (11 DC C4')-(11 DC O4')-(11 DC C1')-(11 DC C2') -44.7 -
14.7
 &rst     iat =   333,   335,   336,   352,
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        r1 = -45.7, r2 = -44.7, r3 = -14.7, r4 = -13.7,&end
# 11 CYT NU1:  (11 DC O4')-(11 DC C1')-(11 DC C2')-(11 DC C3')  18.1
48.1
 &rst     iat =   335,   336,   352,   350,
        r1 =  17.1, r2 =  18.1, r3 =  48.1, r4 =  49.1,&end
# 11 CYT NU2:  (11 DC C1')-(11 DC C2')-(11 DC C3')-(11 DC C4') -37.2  -
6.7
 &rst     iat =   336,   352,   350,   333,
        r1 = -38.2, r2 = -37.2, r3 =  -6.7, r4 =  -5.7,&end
# 11 CYT NU3:  (11 DC C2')-(11 DC C3')-(11 DC C4')-(11 DC O4') -16.9
24.2
 &rst     iat =   352,   350,   333,   335,
        r1 = -17.9, r2 = -16.9, r3 =  24.2, r4 =  25.2,&end
# 11 CYT NU4:  (11 DC C3')-(11 DC C4')-(11 DC O4')-(11 DC C1')  -1.9
34.0
 &rst     iat =   350,   333,   335,   336,
        r1 =  -2.9, r2 =  -1.9, r3 =  34.0, r4 =  35.0,&end
# 13 GUA NU0:  (13 DG5 C4')-(13 DG5 O4')-(13 DG5 C1')-(13 DG5 C2') -
43.9 -13.9
 &rst     iat =   392,   394,   395,   414,
        r1 = -44.9, r2 = -43.9, r3 = -13.9, r4 = -12.9,&end
# 13 GUA NU1:  (13 DG5 O4')-(13 DG5 C1')-(13 DG5 C2')-(13 DG5 C3')
22.2  52.2
 &rst     iat =   394,   395,   414,   412,
        r1 =  21.2, r2 =  22.2, r3 =  52.2, r4 =  53.2,&end
# 13 GUA NU2:  (13 DG5 C1')-(13 DG5 C2')-(13 DG5 C3')-(13 DG5 C4') -
44.6 -14.6
 &rst     iat =   395,   414,   412,   392,
        r1 = -45.6, r2 = -44.6, r3 = -14.6, r4 = -13.6,&end
# 13 GUA NU3:  (13 DG5 C2')-(13 DG5 C3')-(13 DG5 C4')-(13 DG5 O4')  -
3.2  26.8
 &rst     iat =   414,   412,   392,   394,
        r1 =  -4.2, r2 =  -3.2, r3 =  26.8, r4 =  27.8,&end
# 13 GUA NU4:  (13 DG5 C3')-(13 DG5 C4')-(13 DG5 O4')-(13 DG5 C1')  -
4.4  25.6
 &rst     iat =   412,   392,   394,   395,
        r1 =  -5.4, r2 =  -4.4, r3 =  25.6, r4 =  26.6,&end
# 14 GUA NU0:  (14 DG C4')-(14 DG O4')-(14 DG C1')-(14 DG C2') -43.9 -
13.9
 &rst     iat =   425,   427,   428,   447,
        r1 = -44.9, r2 = -43.9, r3 = -13.9, r4 = -12.9,&end
# 14 GUA NU1:  (14 DG O4')-(14 DG C1')-(14 DG C2')-(14 DG C3')  22.2
52.2
 &rst     iat =   427,   428,   447,   445,
        r1 =  21.2, r2 =  22.2, r3 =  52.2, r4 =  53.2,&end
# 14 GUA NU2:  (14 DG C1')-(14 DG C2')-(14 DG C3')-(14 DG C4') -44.6 -
14.6
 &rst     iat =   428,   447,   445,   425,
        r1 = -45.6, r2 = -44.6, r3 = -14.6, r4 = -13.6,&end
# 14 GUA NU3:  (14 DG C2')-(14 DG C3')-(14 DG C4')-(14 DG O4')  -3.2
26.8
 &rst     iat =   447,   445,   425,   427,
        r1 =  -4.2, r2 =  -3.2, r3 =  26.8, r4 =  27.8,&end
# 14 GUA NU4:  (14 DG C3')-(14 DG C4')-(14 DG O4')-(14 DG C1')  -4.4
25.6
 &rst     iat =   445,   425,   427,   428,
        r1 =  -5.4, r2 =  -4.4, r3 =  25.6, r4 =  26.6,&end
```

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# 15 ADE NU0:  (15 DA C4')-(15 DA O4')-(15 DA C1')-(15 DA C2') -43.9 -
13.9
 &rst     iat =   458,   460,   461,   479,
        r1 = -44.9, r2 = -43.9, r3 = -13.9, r4 = -12.9,&end
# 15 ADE NU1:  (15 DA O4')-(15 DA C1')-(15 DA C2')-(15 DA C3')  22.2
52.2
 &rst     iat =   460,   461,   479,   477,
        r1 =  21.2, r2 =  22.2, r3 =  52.2, r4 =  53.2,&end
# 15 ADE NU2:  (15 DA C1')-(15 DA C2')-(15 DA C3')-(15 DA C4') -44.6 -
14.6
 &rst     iat =   461,   479,   477,   458,
        r1 = -45.6, r2 = -44.6, r3 = -14.6, r4 = -13.6,&end
# 15 ADE NU3:  (15 DA C2')-(15 DA C3')-(15 DA C4')-(15 DA O4')  -3.2
26.8
 &rst     iat =   479,   477,   458,   460,
        r1 =  -4.2, r2 =  -3.2, r3 =  26.8, r4 =  27.8,&end
# 15 ADE NU4:  (15 DA C3')-(15 DA C4')-(15 DA O4')-(15 DA C1')  -4.4
25.6
 &rst     iat =   477,   458,   460,   461,
        r1 =  -5.4, r2 =  -4.4, r3 =  25.6, r4 =  26.6,&end
# 16 CYT NU0:  (16 DC C4')-(16 DC O4')-(16 DC C1')-(16 DC C2') -52.1 -
22.1
 &rst     iat =   490,   492,   493,   509,
        r1 = -53.1, r2 = -52.1, r3 = -22.1, r4 = -21.1,&end
# 16 CYT NU1:  (16 DC O4')-(16 DC C1')-(16 DC C2')-(16 DC C3')  15.0
45.0
 &rst     iat =   492,   493,   509,   507,
        r1 =  14.0, r2 =  15.0, r3 =  45.0, r4 =  46.0,&end
# 16 CYT NU2:  (16 DC C1')-(16 DC C2')-(16 DC C3')-(16 DC C4') -27.4
2.6
 &rst     iat =   493,   509,   507,   490,
        r1 = -28.4, r2 = -27.4, r3 =   2.6, r4 =   3.6,&end
# 16 CYT NU3:  (16 DC C2')-(16 DC C3')-(16 DC C4')-(16 DC O4') -25.0
5.0
 &rst     iat =   509,   507,   490,   492,
        r1 = -26.0, r2 = -25.0, r3 =   5.0, r4 =   6.0,&end
# 16 CYT NU4:  (16 DC C3')-(16 DC C4')-(16 DC O4')-(16 DC C1')  13.5
43.5
 &rst     iat =   507,   490,   492,   493,
        r1 =  12.5, r2 =  13.5, r3 =  43.5, r4 =  44.5,&end
# 17 THY NU0:  (17 DT C4')-(17 DT O4')-(17 DT C1')-(17 DT C2') -38.5  -
5.4
 &rst     iat =   520,   522,   523,   541,
        r1 = -39.5, r2 = -38.5, r3 =  -5.4, r4 =  -4.4,&end
# 17 THY NU1:  (17 DT O4')-(17 DT C1')-(17 DT C2')-(17 DT C3')  15.6
45.6
 &rst     iat =   522,   523,   541,   539,
        r1 =  14.6, r2 =  15.6, r3 =  45.6, r4 =  46.6,&end
# 17 THY NU2:  (17 DT C1')-(17 DT C2')-(17 DT C3')-(17 DT C4') -38.5
0.0
 &rst     iat =   523,   541,   539,   520,
        r1 = -39.5, r2 = -38.5, r3 =   0.0, r4 =   1.0,&end
# 17 THY NU3:  (17 DT C2')-(17 DT C3')-(17 DT C4')-(17 DT O4') -22.6
34.6
 &rst     iat =   541,   539,   520,   522,
        r1 = -23.6, r2 = -22.6, r3 =  34.6, r4 =  35.6,&end
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# 17 THY NU4:  (17 DT C3')-(17 DT C4')-(17 DT O4')-(17 DT C1') -18.0
36.6
 &rst     iat =   539,   520,   522,   523,
        r1 = -19.0, r2 = -18.0, r3 =  36.6, r4 =  37.6,&end
# 18 ADE NU0:  (18 DA C4')-(18 DA O4')-(18 DA C1')-(18 DA C2') -38.5  -
5.4
 &rst     iat =   552,   554,   555,   573,
        r1 = -39.5, r2 = -38.5, r3 =  -5.4, r4 =  -4.4,&end
# 18 ADE NU1:  (18 DA O4')-(18 DA C1')-(18 DA C2')-(18 DA C3')  15.6
45.6
 &rst     iat =   554,   555,   573,   571,
        r1 =  14.6, r2 =  15.6, r3 =  45.6, r4 =  46.6,&end
# 18 ADE NU2:  (18 DA C1')-(18 DA C2')-(18 DA C3')-(18 DA C4') -38.5
0.0
 &rst     iat =   555,   573,   571,   552,
        r1 = -39.5, r2 = -38.5, r3 =   0.0, r4 =   1.0,&end
# 18 ADE NU3:  (18 DA C2')-(18 DA C3')-(18 DA C4')-(18 DA O4') -22.6
34.6
 &rst     iat =   573,   571,   552,   554,
        r1 = -23.6, r2 = -22.6, r3 =  34.6, r4 =  35.6,&end
# 18 ADE NU4:  (18 DA C3')-(18 DA C4')-(18 DA O4')-(18 DA C1') -18.0
36.6
 &rst     iat =   571,   552,   554,   555,
        r1 = -19.0, r2 = -18.0, r3 =  36.6, r4 =  37.6,&end
# 19 GUA NU0:  (19 DG C4')-(19 DG O4')-(19 DG C1')-(19 DG C2') -43.9 -
13.9
 &rst     iat =   584,   586,   587,   606,
        r1 = -44.9, r2 = -43.9, r3 = -13.9, r4 = -12.9,&end
# 19 GUA NU1:  (19 DG O4')-(19 DG C1')-(19 DG C2')-(19 DG C3')  22.2
52.2
 &rst     iat =   586,   587,   606,   604,
        r1 =  21.2, r2 =  22.2, r3 =  52.2, r4 =  53.2,&end
# 19 GUA NU2:  (19 DG C1')-(19 DG C2')-(19 DG C3')-(19 DG C4') -44.6 -
14.6
 &rst     iat =   587,   606,   604,   584,
        r1 = -45.6, r2 = -44.6, r3 = -14.6, r4 = -13.6,&end
# 19 GUA NU3:  (19 DG C2')-(19 DG C3')-(19 DG C4')-(19 DG O4')  -3.2
26.8
 &rst     iat =   606,   604,   584,   586,
        r1 =  -4.2, r2 =  -3.2, r3 =  26.8, r4 =  27.8,&end
# 19 GUA NU4:  (19 DG C3')-(19 DG C4')-(19 DG O4')-(19 DG C1')  -4.4
25.6
 &rst     iat =   604,   584,   586,   587,
        r1 =  -5.4, r2 =  -4.4, r3 =  25.6, r4 =  26.6,&end
# 20 CYT NU0:  (20 DC C4')-(20 DC O4')-(20 DC C1')-(20 DC C2') -52.1 -
22.1
 &rst     iat =   617,   619,   620,   636,
        r1 = -53.1, r2 = -52.1, r3 = -22.1, r4 = -21.1,&end
# 20 CYT NU1:  (20 DC O4')-(20 DC C1')-(20 DC C2')-(20 DC C3')  15.0
45.0
 &rst     iat =   619,   620,   636,   634,
        r1 =  14.0, r2 =  15.0, r3 =  45.0, r4 =  46.0,&end
# 20 CYT NU2:  (20 DC C1')-(20 DC C2')-(20 DC C3')-(20 DC C4') -27.4
2.6
 &rst     iat =   620,   636,   634,   617,
        r1 = -28.4, r2 = -27.4, r3 =   2.6, r4 =   3.6,&end
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# 20 CYT NU3:  (20 DC C2')-(20 DC C3')-(20 DC C4')-(20 DC O4') -25.0
5.0
 &rst     iat =   636,   634,   617,   619,
        r1 = -26.0, r2 = -25.0, r3 =   5.0, r4 =   6.0,&end
# 20 CYT NU4:  (20 DC C3')-(20 DC C4')-(20 DC O4')-(20 DC C1')  13.5
43.5
 &rst     iat =   634,   617,   619,   620,
        r1 =  12.5, r2 =  13.5, r3 =  43.5, r4 =  44.5,&end
# 21 THY NU0:  (21 DT C4')-(21 DT O4')-(21 DT C1')-(21 DT C2') -52.1 -
22.1
 &rst     iat =   647,   649,   650,   668,
        r1 = -53.1, r2 = -52.1, r3 = -22.1, r4 = -21.1,&end
# 21 THY NU1:  (21 DT O4')-(21 DT C1')-(21 DT C2')-(21 DT C3')  15.0
45.0
 &rst     iat =   649,   650,   668,   666,
        r1 =  14.0, r2 =  15.0, r3 =  45.0, r4 =  46.0,&end
# 21 THY NU2:  (21 DT C1')-(21 DT C2')-(21 DT C3')-(21 DT C4') -27.4
2.6
 &rst     iat =   650,   668,   666,   647,
        r1 = -28.4, r2 = -27.4, r3 =   2.6, r4 =   3.6,&end
# 21 THY NU3:  (21 DT C2')-(21 DT C3')-(21 DT C4')-(21 DT O4') -25.0
5.0
 &rst     iat =   668,   666,   647,   649,
        r1 = -26.0, r2 = -25.0, r3 =   5.0, r4 =   6.0,&end
# 21 THY NU4:  (21 DT C3')-(21 DT C4')-(21 DT O4')-(21 DT C1')  13.5
43.5
 &rst     iat =   666,   647,   649,   650,
        r1 =  12.5, r2 =  13.5, r3 =  43.5, r4 =  44.5,&end
# 22 ADE NU0:  (22 DA C4')-(22 DA O4')-(22 DA C1')-(22 DA C2') -43.9 -
13.9
 &rst     iat =   679,   681,   682,   700,
        r1 = -44.9, r2 = -43.9, r3 = -13.9, r4 = -12.9,&end
# 22 ADE NU1:  (22 DA O4')-(22 DA C1')-(22 DA C2')-(22 DA C3')  22.2
52.2
 &rst     iat =   681,   682,   700,   698,
        r1 =  21.2, r2 =  22.2, r3 =  52.2, r4 =  53.2,&end
# 22 ADE NU2:  (22 DA C1')-(22 DA C2')-(22 DA C3')-(22 DA C4') -44.6 -
14.6
 &rst     iat =   682,   700,   698,   679,
        r1 = -45.6, r2 = -44.6, r3 = -14.6, r4 = -13.6,&end
# 22 ADE NU3:  (22 DA C2')-(22 DA C3')-(22 DA C4')-(22 DA O4')  -3.2
26.8
 &rst     iat =   700,   698,   679,   681,
        r1 =  -4.2, r2 =  -3.2, r3 =  26.8, r4 =  27.8,&end
# 22 ADE NU4:  (22 DA C3')-(22 DA C4')-(22 DA O4')-(22 DA C1')  -4.4
25.6
 &rst     iat =   698,   679,   681,   682,
        r1 =  -5.4, r2 =  -4.4, r3 =  25.6, r4 =  26.6,&end
# 23 GUA NU0:  (23 DG C4')-(23 DG O4')-(23 DG C1')-(23 DG C2') -44.7 -
14.7
 &rst     iat =   711,   713,   714,   733,
        r1 = -45.7, r2 = -44.7, r3 = -14.7, r4 = -13.7,&end
# 23 GUA NU1:  (23 DG O4')-(23 DG C1')-(23 DG C2')-(23 DG C3')  18.1
48.1
 &rst     iat =   713,   714,   733,   731,
        r1 =  17.1, r2 =  18.1, r3 =  48.1, r4 =  49.1,&end
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# 23 GUA NU2:  (23 DG C1')-(23 DG C2')-(23 DG C3')-(23 DG C4') -37.2  -
6.7
 &rst     iat =   714,   733,   731,   711,
        r1 = -38.2, r2 = -37.2, r3 =  -6.7, r4 =  -5.7,&end
# 23 GUA NU3:  (23 DG C2')-(23 DG C3')-(23 DG C4')-(23 DG O4') -16.9
24.2
 &rst     iat =   733,   731,   711,   713,
        r1 = -17.9, r2 = -16.9, r3 =  24.2, r4 =  25.2,&end
# 23 GUA NU4:  (23 DG C3')-(23 DG C4')-(23 DG O4')-(23 DG C1')  -1.9
34.0
 &rst     iat =   731,   711,   713,   714,
        r1 =  -2.9, r2 =  -1.9, r3 =  34.0, r4 =  35.0,&end
#   1  GUA  H1     24  CYT  N3      1.84   2.04
 &rst
  ixpk= 0, nxpk= 0, iat=  19, 758, r1= 1.34, r2= 1.84, r3= 2.04, r4=
2.54,
      rk2=20.0, rk3=20.0, ir6=1, ialtd=0,
 &end
#   1  GUA  H22    24  CYT  O2      1.75   1.95
 &rst
  ixpk= 0, nxpk= 0, iat=  23, 760, r1= 1.25, r2= 1.75, r3= 1.95, r4=
2.45,  &end
#   1  GUA  N1     24  CYT  N3      2.85   3.05
 &rst
  ixpk= 0, nxpk= 0, iat=  18, 758, r1= 2.35, r2= 2.85, r3= 3.05, r4=
3.55,  &end
#   1  GUA  O6     24  CYT  H42     1.80   2.00
 &rst
  ixpk= 0, nxpk= 0, iat=  17, 757, r1= 1.30, r2= 1.80, r3= 2.00, r4=
2.50,  &end
#   1  GUA  O6     24  CYT  N4      2.81   3.01
 &rst
  ixpk= 0, nxpk= 0, iat=  17, 755, r1= 2.31, r2= 2.81, r3= 3.01, r4=
3.51,  &end
#   2  CYT  H42    23  GUA  O6      1.80   2.00
 &rst
  ixpk= 0, nxpk= 0, iat=  52, 722, r1= 1.30, r2= 1.80, r3= 2.00, r4=
2.50,  &end
#   2  CYT  N3     23  GUA  H1      1.84   2.04
 &rst
  ixpk= 0, nxpk= 0, iat=  53, 724, r1= 1.34, r2= 1.84, r3= 2.04, r4=
2.54,  &end
#   2  CYT  N3     23  GUA  N1      2.85   3.05
 &rst
  ixpk= 0, nxpk= 0, iat=  53, 723, r1= 2.35, r2= 2.85, r3= 3.05, r4=
3.55,  &end
#   2  CYT  N4     23  GUA  O6      2.81   3.01
 &rst
  ixpk= 0, nxpk= 0, iat=  50, 722, r1= 2.31, r2= 2.81, r3= 3.01, r4=
3.51,  &end
#   2  CYT  O2     23  GUA  H22     1.75   1.95
 &rst
  ixpk= 0, nxpk= 0, iat=  55, 728, r1= 1.25, r2= 1.75, r3= 1.95, r4=
2.45,  &end
#   3  THY  H3     22  ADE  N1      1.71   1.91
 &rst
```

```
  ixpk= 0, nxpk= 0, iat=  85, 693, r1= 1.21, r2= 1.71, r3= 1.91, r4=
2.41,  &end
#   3  THY  N3     22  ADE  N1      2.72   2.92
 &rst
  ixpk= 0, nxpk= 0, iat=  84, 693, r1= 2.22, r2= 2.72, r3= 2.92, r4=
3.42,  &end
#   3  THY  O4     22  ADE  H61     1.84   2.04
 &rst
  ixpk= 0, nxpk= 0, iat=  83, 691, r1= 1.34, r2= 1.84, r3= 2.04, r4=
2.54,  &end
#   4  ADE  H61    21  THY  O4      1.84   2.04
 &rst
  ixpk= 0, nxpk= 0, iat= 113, 661, r1= 1.34, r2= 1.84, r3= 2.04, r4=
2.54,  &end
#   4  ADE  N1     21  THY  H3      1.71   1.91
 &rst
  ixpk= 0, nxpk= 0, iat= 115, 663, r1= 1.21, r2= 1.71, r3= 1.91, r4=
2.41,  &end
#   4  ADE  N1     21  THY  N3      2.72   2.92
 &rst
  ixpk= 0, nxpk= 0, iat= 115, 662, r1= 2.22, r2= 2.72, r3= 2.92, r4=
3.42,  &end
#   5  GUA  H1     20  CYT  N3      1.84   2.04
 &rst
  ixpk= 0, nxpk= 0, iat= 146, 631, r1= 1.34, r2= 1.84, r3= 2.04, r4=
2.54,  &end
#   5  GUA  H22    20  CYT  O2      1.75   1.95
 &rst
  ixpk= 0, nxpk= 0, iat= 150, 633, r1= 1.25, r2= 1.75, r3= 1.95, r4=
2.45,  &end
#   5  GUA  N1     20  CYT  N3      2.85   3.05
 &rst
  ixpk= 0, nxpk= 0, iat= 145, 631, r1= 2.35, r2= 2.85, r3= 3.05, r4=
3.55,  &end
#   5  GUA  O6     20  CYT  H42     1.80   2.00
 &rst
  ixpk= 0, nxpk= 0, iat= 144, 630, r1= 1.30, r2= 1.80, r3= 2.00, r4=
2.50,  &end
#   5  GUA  O6     20  CYT  N4      2.81   3.01
 &rst
  ixpk= 0, nxpk= 0, iat= 144, 628, r1= 2.31, r2= 2.81, r3= 3.01, r4=
3.51,  &end
#   6  CYT  H42    19  GUA  O6      1.80   2.00
 &rst
  ixpk= 0, nxpk= 0, iat= 179, 595, r1= 1.30, r2= 1.80, r3= 2.00, r4=
2.50,  &end
#   6  CYT  N3     19  GUA  H1      1.84   2.04
 &rst
  ixpk= 0, nxpk= 0, iat= 180, 597, r1= 1.34, r2= 1.84, r3= 2.04, r4=
2.54,  &end
#   6  CYT  N3     19  GUA  N1      2.85   3.05
 &rst
  ixpk= 0, nxpk= 0, iat= 180, 596, r1= 2.35, r2= 2.85, r3= 3.05, r4=
3.55,  &end
#   6  CYT  N4     19  GUA  O6      2.81   3.01
 &rst
```

```
  ixpk= 0, nxpk= 0, iat= 177, 595, r1= 2.31, r2= 2.81, r3= 3.01, r4=
3.51,  &end
#   6  CYT  O2     19  GUA  H22     1.75   1.95
 &rst
  ixpk= 0, nxpk= 0, iat= 182, 601, r1= 1.25, r2= 1.75, r3= 1.95, r4=
2.45,  &end
#   9  GUA  H1     16  CYT  N3      1.84   2.04
 &rst
  ixpk= 0, nxpk= 0, iat= 281, 504, r1= 1.34, r2= 1.84, r3= 2.04, r4=
2.54,  &end
#
#   9  GUA  H22    16  CYT  O2      1.75   1.95
 &rst
  ixpk= 0, nxpk= 0, iat= 285, 506, r1= 1.25, r2= 1.75, r3= 1.95, r4=
2.45,  &end
#
#   9  GUA  N1     16  CYT  N3      2.85   3.05
 &rst
  ixpk= 0, nxpk= 0, iat= 280, 504, r1= 2.35, r2= 2.85, r3= 3.05, r4=
3.55,  &end
#   9  GUA  O6     16  CYT  H42     1.80   2.00
 &rst
  ixpk= 0, nxpk= 0, iat= 279, 503, r1= 1.30, r2= 1.80, r3= 2.00, r4=
2.50,  &end
#   9  GUA  O6     16  CYT  N4      2.81   3.01
 &rst
  ixpk= 0, nxpk= 0, iat= 279, 501, r1= 2.31, r2= 2.81, r3= 3.01, r4=
3.51,  &end
#  10  THY  H3     15  ADE  N1      1.71   1.91
 &rst
  ixpk= 0, nxpk= 0, iat= 317, 472, r1= 1.21, r2= 1.71, r3= 1.91, r4=
2.41,  &end
#  10  THY  N3     15  ADE  N1      2.72   2.92
 &rst
  ixpk= 0, nxpk= 0, iat= 316, 472, r1= 2.22, r2= 2.72, r3= 2.92, r4=
3.42,  &end
#  10  THY  O4     15  ADE  H61     1.84   2.04
 &rst
  ixpk= 0, nxpk= 0, iat= 315, 470, r1= 1.34, r2= 1.84, r3= 2.04, r4=
2.54,  &end
#  11  CYT  H42    14  GUA  O6      1.80   2.00
 &rst
  ixpk= 0, nxpk= 0, iat= 346, 436, r1= 1.30, r2= 1.80, r3= 2.00, r4=
2.50,  &end
#  11  CYT  N3     14  GUA  H1      1.84   2.04
 &rst
  ixpk= 0, nxpk= 0, iat= 347, 438, r1= 1.34, r2= 1.84, r3= 2.04, r4=
2.54,  &end
#  11  CYT  N3     14  GUA  N1      2.85   3.05
 &rst
  ixpk= 0, nxpk= 0, iat= 347, 437, r1= 2.35, r2= 2.85, r3= 3.05, r4=
3.55,  &end
#  11  CYT  N4     14  GUA  O6      2.81   3.01
 &rst
  ixpk= 0, nxpk= 0, iat= 344, 436, r1= 2.31, r2= 2.81, r3= 3.01, r4=
3.51,  &end
#  11  CYT  O2     14  GUA  H22     1.75   1.95
```

```
 &rst
  ixpk= 0, nxpk= 0, iat= 349, 442, r1= 1.25, r2= 1.75, r3= 1.95, r4=
2.45,  &end
#  12  CYT  H42    13  GUA  O6      1.80   2.00
 &rst
  ixpk= 0, nxpk= 0, iat= 376, 403, r1= 1.30, r2= 1.80, r3= 2.00, r4=
2.50,  &end
#  12  CYT  N3     13  GUA  H1      1.84   2.04
 &rst
  ixpk= 0, nxpk= 0, iat= 377, 405, r1= 1.34, r2= 1.84, r3= 2.04, r4=
2.54,  &end
#  12  CYT  N3     13  GUA  N1      2.85   3.05
 &rst
  ixpk= 0, nxpk= 0, iat= 377, 404, r1= 2.35, r2= 2.85, r3= 3.05, r4=
3.55,  &end
#  12  CYT  N4     13  GUA  O6      2.81   3.01
 &rst
  ixpk= 0, nxpk= 0, iat= 374, 403, r1= 2.31, r2= 2.81, r3= 3.01, r4=
3.51,  &end
#  12  CYT  O2     13  GUA  H22     1.75   1.95
 &rst
  ixpk= 0, nxpk= 0, iat= 379, 409, r1= 1.25, r2= 1.75, r3= 1.95, r4=
2.45,  &end
```

# APPENDIX D

## MOLECULAR DYNAMICS INPUT FILES

**File D-1:** An example of a Generalized Born rMD input file usin the simulated annealing protocol.

```
simulated annealing protocol, 20 ps

 &cntrl
    nstlim=20000, pencut=-0.001, nmropt=1,
    ntpr=200, ntt=1, ntwx=200, ntc=2
    cut=10.0, ntb=0, vlimit=10,rgbmax=12.0,
    igb=1, saltcon=0.2, offset=0.13,
 /
 &ewald
    eedmeth=5,
 &end
#
#Simple simulated annealing algorithm:
#
#from steps 0 to 5000: heat the system to 600K
#from steps 5001-18000: re-cool to low temperatures with long tautp
#from steps 18001-20000: final cooling with short tautp
#
 &wt type='TEMP0', istep1=0,istep2=5000,value1=600.,
            value2=600.,    /
 &wt type='TEMP0', istep1=5001, istep2=18000, value1=600.0,
            value2=100.0,     /
 &wt type='TEMP0', istep1=18001, istep2=20000, value1=0.0,
            value2=0.0,     /

 &wt type='TAUTP', istep1=0,istep2=5000,value1=0.4,
            value2=0.4,     /
 &wt type='TAUTP', istep1=5001,istep2=18000,value1=1.0,
            value2=0.5,     /
 &wt type='TAUTP', istep1=18001,istep2=19000,value1=1.0,
            value2=1.0,     /
 &wt type='TAUTP', istep1=19001,istep2=20000,value1=0.1,
            value2=0.05,    /

 &wt type='REST', istep1=0,istep2=3000,value1=0.1,
            value2=1.0,  /
 &wt type='REST', istep1=3001,istep2=20000,value1=1.0,
            value2=1.0,  /

 &wt type='END'  /
LISTOUT=POUT
DISANG=RST.file
```

# APPENDIX E

## PDB COORDINATE FILES

**File E-1**: Average structure coordinate file of the rMD refined *R*-BD-N3-dU modified 5′ -$G^{1}C^{2}T^{3}A^{4}G^{5}C^{6}X^{7}A^{8}G^{9}T^{10}C^{11}C^{12}$- 3′·5′ - $G^{13}G^{14}A^{15}C^{16}T^{17}A^{18}G^{19}C^{20}T^{21}A^{22}G^{23}C^{24}$ -3′.

```
ATOM      1  H5T DG5     1       0.273  -3.843  -3.927
ATOM      2  O5* DG5     1       0.947  -3.579  -3.294
ATOM      3  C5* DG5     1       2.234  -3.772  -3.866
ATOM      4 1H5* DG5     1       2.313  -3.187  -4.785
ATOM      5 2H5* DG5     1       2.357  -4.827  -4.118
ATOM      6  C4* DG5     1       3.385  -3.359  -2.931
ATOM      7  H4* DG5     1       4.326  -3.629  -3.412
ATOM      8  O4* DG5     1       3.363  -1.950  -2.737
ATOM      9  C1* DG5     1       3.248  -1.677  -1.350
ATOM     10  H1* DG5     1       4.241  -1.480  -0.937
ATOM     11  N9  DG5     1       2.370  -0.507  -1.134
ATOM     12  C8  DG5     1       1.021  -0.391  -1.359
ATOM     13  H8  DG5     1       0.433  -1.195  -1.782
ATOM     14  N7  DG5     1       0.521   0.768  -1.029
ATOM     15  C5  DG5     1       1.626   1.487  -0.559
ATOM     16  C6  DG5     1       1.753   2.831  -0.061
ATOM     17  O6  DG5     1       0.899   3.706   0.071
ATOM     18  N1  DG5     1       3.048   3.157   0.300
ATOM     19  H1  DG5     1       3.195   4.096   0.654
ATOM     20  C2  DG5     1       4.105   2.302   0.212
ATOM     21  N2  DG5     1       5.274   2.736   0.614
ATOM     22 1H2  DG5     1       6.030   2.076   0.606
ATOM     23 2H2  DG5     1       5.378   3.692   0.972
ATOM     24  N3  DG5     1       4.026   1.054  -0.242
ATOM     25  C4  DG5     1       2.761   0.705  -0.620
ATOM     26  C3* DG5     1       3.344  -4.025  -1.549
ATOM     27  H3* DG5     1       2.748  -4.939  -1.554
ATOM     28  C2* DG5     1       2.687  -2.941  -0.705
ATOM     29 1H2* DG5     1       1.606  -3.004  -0.818
ATOM     30 2H2* DG5     1       2.947  -3.011   0.347
ATOM     31  O3* DG5     1       4.679  -4.308  -1.158
ATOM     32  P   DC      2       5.062  -4.933   0.281
ATOM     33  O1P DC      2       6.196  -5.860   0.094
ATOM     34  O2P DC      2       3.822  -5.388   0.947
ATOM     35  O5* DC      2       5.594  -3.618   1.051
ATOM     36  C5* DC      2       6.771  -2.956   0.612
ATOM     37 1H5* DC      2       6.591  -2.507  -0.364
ATOM     38 2H5* DC      2       7.571  -3.692   0.507
ATOM     39  C4* DC      2       7.248  -1.871   1.585
ATOM     40  H4* DC      2       8.208  -1.499   1.228
ATOM     41  O4* DC      2       6.328  -0.785   1.620
ATOM     42  C1* DC      2       5.904  -0.571   2.957
ATOM     43  H1* DC      2       6.516   0.220   3.403
ATOM     44  N1  DC      2       4.465  -0.189   2.947
ATOM     45  C6  DC      2       3.513  -1.056   2.465
```

```
ATOM     46  H6  DC      2       3.828  -2.032   2.111
ATOM     47  C5  DC      2       2.208  -0.687   2.410
ATOM     48  H5  DC      2       1.469  -1.368   2.019
ATOM     49  C4  DC      2       1.884   0.627   2.860
ATOM     50  N4  DC      2       0.660   1.084   2.768
ATOM     51 1H4  DC      2      -0.058   0.531   2.344
ATOM     52 2H4  DC      2       0.495   2.050   3.068
ATOM     53  N3  DC      2       2.789   1.470   3.326
ATOM     54  C2  DC      2       4.089   1.088   3.382
ATOM     55  O2  DC      2       4.904   1.897   3.821
ATOM     56  C3* DC      2       7.438  -2.388   3.015
ATOM     57  H3* DC      2       7.486  -3.479   3.046
ATOM     58  C2* DC      2       6.182  -1.874   3.709
ATOM     59 1H2* DC      2       5.386  -2.604   3.569
ATOM     60 2H2* DC      2       6.340  -1.705   4.771
ATOM     61  O3* DC      2       8.635  -1.827   3.530
ATOM     62  P   DT      3       9.177  -2.147   5.016
ATOM     63  O1P DT      3      10.654  -2.151   4.982
ATOM     64  O2P DT      3       8.435  -3.306   5.557
ATOM     65  O5* DT      3       8.688  -0.825   5.795
ATOM     66  C5* DT      3       9.250   0.437   5.477
ATOM     67 1H5* DT      3       9.048   0.672   4.431
ATOM     68 2H5* DT      3      10.331   0.390   5.619
ATOM     69  C4* DT      3       8.690   1.559   6.354
ATOM     70  H4* DT      3       9.235   2.475   6.124
ATOM     71  O4* DT      3       7.315   1.766   6.062
ATOM     72  C1* DT      3       6.605   1.827   7.284
ATOM     73  H1* DT      3       6.636   2.854   7.662
ATOM     74  N1  DT      3       5.199   1.393   7.069
ATOM     75  C6  DT      3       4.897   0.090   6.722
ATOM     76  H6  DT      3       5.704  -0.619   6.607
ATOM     77  C5  DT      3       3.613  -0.302   6.504
ATOM     78  C7  DT      3       3.320  -1.745   6.133
ATOM     79 1H7  DT      3       2.662  -2.178   6.885
ATOM     80 2H7  DT      3       2.806  -1.776   5.173
ATOM     81 3H7  DT      3       4.236  -2.333   6.075
ATOM     82  C4  DT      3       2.516   0.655   6.625
ATOM     83  O4  DT      3       1.324   0.425   6.451
ATOM     84  N3  DT      3       2.901   1.931   6.971
ATOM     85  H3  DT      3       2.172   2.629   7.081
ATOM     86  C2  DT      3       4.190   2.349   7.218
ATOM     87  O2  DT      3       4.389   3.509   7.563
ATOM     88  C3* DT      3       8.825   1.279   7.856
ATOM     89  H3* DT      3       9.495   0.440   8.055
ATOM     90  C2* DT      3       7.391   0.944   8.251
ATOM     91 1H2* DT      3       7.220  -0.114   8.066
ATOM     92 2H2* DT      3       7.173   1.180   9.289
ATOM     93  O3* DT      3       9.309   2.462   8.467
ATOM     94  P   DA      4       9.583   2.580  10.052
ATOM     95  O1P DA      4      10.826   3.354  10.249
ATOM     96  O2P DA      4       9.424   1.247  10.672
ATOM     97  O5* DA      4       8.338   3.498  10.489
ATOM     98  C5* DA      4       8.247   4.838  10.033
ATOM     99 1H5* DA      4       8.128   4.849   8.949
ATOM    100 2H5* DA      4       9.172   5.359  10.283
ATOM    101  C4* DA      4       7.080   5.597  10.671
ATOM    102  H4* DA      4       7.160   6.645  10.384
```

```
ATOM    103  O4* DA      4       5.842   5.090  10.191
ATOM    104  C1* DA      4       5.031   4.739  11.297
ATOM    105  H1* DA      4       4.388   5.583  11.565
ATOM    106  N9  DA      4       4.211   3.564  10.940
ATOM    107  C8  DA      4       4.624   2.285  10.661
ATOM    108  H8  DA      4       5.665   1.995  10.694
ATOM    109  N7  DA      4       3.662   1.465  10.331
ATOM    110  C5  DA      4       2.521   2.273  10.425
ATOM    111  C6  DA      4       1.143   2.064  10.202
ATOM    112  N6  DA      4       0.636   0.921   9.770
ATOM    113 1H6  DA      4      -0.361   0.856   9.566
ATOM    114 2H6  DA      4       1.260   0.153   9.597
ATOM    115  N1  DA      4       0.261   3.052  10.399
ATOM    116  C2  DA      4       0.722   4.239  10.781
ATOM    117  H2  DA      4      -0.019   5.014  10.924
ATOM    118  N3  DA      4       1.986   4.590  10.991
ATOM    119  C4  DA      4       2.845   3.550  10.799
ATOM    120  C3* DA      4       7.069   5.510  12.200
ATOM    121  H3* DA      4       8.034   5.190  12.598
ATOM    122  C2* DA      4       5.994   4.457  12.447
ATOM    123 1H2* DA      4       6.438   3.466  12.354
ATOM    124 2H2* DA      4       5.515   4.561  13.417
ATOM    125  O3* DA      4       6.727   6.794  12.693
ATOM    126  P   DG      5       6.572   7.114  14.263
ATOM    127  O1P DG      5       7.078   8.481  14.507
ATOM    128  O2P DG      5       7.094   5.973  15.044
ATOM    129  O5* DG      5       4.971   7.128  14.399
ATOM    130  C5* DG      5       4.203   8.145  13.773
ATOM    131 1H5* DG      5       4.186   7.980  12.695
ATOM    132 2H5* DG      5       4.670   9.112  13.968
ATOM    133  C4* DG      5       2.768   8.200  14.308
ATOM    134  H4* DG      5       2.302   9.117  13.946
ATOM    135  O4* DG      5       2.023   7.089  13.835
ATOM    136  C1* DG      5       1.516   6.358  14.938
ATOM    137  H1* DG      5       0.480   6.655  15.119
ATOM    138  N9  DG      5       1.578   4.915  14.611
ATOM    139  C8  DG      5       2.681   4.104  14.511
ATOM    140  H8  DG      5       3.683   4.461  14.714
ATOM    141  N7  DG      5       2.420   2.883  14.132
ATOM    142  C5  DG      5       1.031   2.882  13.952
ATOM    143  C6  DG      5       0.126   1.855  13.508
ATOM    144  O6  DG      5       0.358   0.705  13.139
ATOM    145  N1  DG      5      -1.196   2.260  13.495
ATOM    146  H1  DG      5      -1.875   1.588  13.155
ATOM    147  C2  DG      5      -1.618   3.501  13.863
ATOM    148  N2  DG      5      -2.905   3.738  13.806
ATOM    149 1H2  DG      5      -3.198   4.676  13.997
ATOM    150 2H2  DG      5      -3.553   3.037  13.431
ATOM    151  N3  DG      5      -0.809   4.482  14.265
ATOM    152  C4  DG      5       0.508   4.115  14.280
ATOM    153  C3* DG      5       2.722   8.197  15.838
ATOM    154  H3* DG      5       3.694   8.461  16.263
ATOM    155  C2* DG      5       2.364   6.750  16.150
ATOM    156 1H2* DG      5       3.279   6.162  16.200
ATOM    157 2H2* DG      5       1.811   6.661  17.080
ATOM    158  O3* DG      5       1.735   9.119  16.269
ATOM    159  P   DC      6       1.562   9.512  17.825
```

```
ATOM    160  O1P DC      6       1.133  10.925  17.901
ATOM    161  O2P DC      6       2.755   9.048  18.565
ATOM    162  O5* DC      6       0.327   8.574  18.237
ATOM    163  C5* DC      6      -0.992   8.889  17.829
ATOM    164 1H5* DC      6      -1.018   9.019  16.746
ATOM    165 2H5* DC      6      -1.301   9.820  18.307
ATOM    166  C4* DC      6      -1.965   7.775  18.220
ATOM    167  H4* DC      6      -2.978   8.089  17.968
ATOM    168  O4* DC      6      -1.668   6.599  17.493
ATOM    169  C1* DC      6      -2.064   5.485  18.262
ATOM    170  H1* DC      6      -3.103   5.240  18.018
ATOM    171  N1  DC      6      -1.160   4.354  17.925
ATOM    172  C6  DC      6       0.201   4.474  18.077
ATOM    173  H6  DC      6       0.602   5.403  18.467
ATOM    174  C5  DC      6       1.023   3.454  17.725
ATOM    175  H5  DC      6       2.091   3.558  17.835
ATOM    176  C4  DC      6       0.411   2.270  17.215
ATOM    177  N4  DC      6       1.140   1.254  16.826
ATOM    178 1H4  DC      6       2.122   1.382  16.667
ATOM    179 2H4  DC      6       0.639   0.436  16.463
ATOM    180  N3  DC      6      -0.896   2.147  17.060
ATOM    181  C2  DC      6      -1.706   3.179  17.403
ATOM    182  O2  DC      6      -2.918   3.047  17.240
ATOM    183  C3* DC      6      -1.930   7.426  19.710
ATOM    184  H3* DC      6      -0.999   7.777  20.161
ATOM    185  C2* DC      6      -1.988   5.897  19.737
ATOM    186 1H2* DC      6      -1.091   5.515  20.224
ATOM    187 2H2* DC      6      -2.869   5.535  20.267
ATOM    188  O3* DC      6      -3.048   8.013  20.351
ATOM    189  P   DX      7      -3.158   8.098  21.958
ATOM    190  O1P DX      7      -4.051   9.228  22.290
ATOM    191  O2P DX      7      -1.796   8.034  22.527
ATOM    192  O5* DX      7      -3.918   6.730  22.333
ATOM    193  C5* DX      7      -5.270   6.524  21.960
ATOM    194 1H5* DX      7      -5.336   6.360  20.884
ATOM    195 2H5* DX      7      -5.844   7.418  22.210
ATOM    196  C4* DX      7      -5.896   5.340  22.705
ATOM    197  H4* DX      7      -6.971   5.364  22.520
ATOM    198  O4* DX      7      -5.399   4.087  22.243
ATOM    199  C1* DX      7      -5.341   3.239  23.375
ATOM    200  H1* DX      7      -6.359   2.958  23.660
ATOM    201  N1  DX      7      -4.538   2.006  23.112
ATOM    202  C6  DX      7      -3.177   2.065  22.932
ATOM    203  H6  DX      7      -2.673   3.021  22.998
ATOM    204  C5  DX      7      -2.466   0.945  22.652
ATOM    205  H5  DX      7      -1.399   1.004  22.510
ATOM    206  C4  DX      7      -3.089  -0.356  22.523
ATOM    207  O4  DX      7      -2.462  -1.382  22.259
ATOM    208  N3  DX      7      -4.475  -0.363  22.709
ATOM    209  C11 DX      7      -5.198  -1.680  22.570
ATOM    210  C2  DX      7      -5.221   0.785  23.016
ATOM    211  O2  DX      7      -6.439   0.725  23.195
ATOM    212  C3* DX      7      -5.674   5.401  24.225
ATOM    213  H3* DX      7      -5.159   6.315  24.530
ATOM    214  C2* DX      7      -4.804   4.170  24.458
ATOM    215 1H2* DX      7      -3.762   4.431  24.280
ATOM    216 2H2* DX      7      -4.935   3.763  25.454
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ATOM    217  O3* DX      7      -6.945   5.299  24.852
ATOM    218  C12 DX      7      -5.804  -1.953  21.182
ATOM    219  C9  DX      7      -7.108  -1.192  20.990
ATOM    220  C10 DX      7      -7.569  -0.601  19.895
ATOM    221  O12 DX      7      -4.910  -1.596  20.158
ATOM    222  H15 DX      7      -5.995  -1.730  23.314
ATOM    223  H14 DX      7      -4.513  -2.496  22.799
ATOM    224  H9  DX      7      -6.021  -3.017  21.103
ATOM    225 1H1  DX      7      -7.765  -1.070  21.838
ATOM    226 2H1  DX      7      -6.971  -0.643  18.992
ATOM    227 3H1  DX      7      -8.512  -0.074  19.932
ATOM    228  H10 DX      7      -4.089  -2.106  20.243
ATOM    229  P   DA      8      -7.157   5.445  26.450
ATOM    230  O1P DA      8      -8.295   6.357  26.689
ATOM    231  O2P DA      8      -5.850   5.692  27.094
ATOM    232  O5* DA      8      -7.614   3.953  26.844
ATOM    233  C5* DA      8      -8.831   3.419  26.354
ATOM    234 1H5* DA      8      -8.821   3.451  25.264
ATOM    235 2H5* DA      8      -9.659   4.035  26.709
ATOM    236  C4* DA      8      -9.063   1.967  26.793
ATOM    237  H4* DA      8      -9.989   1.628  26.328
ATOM    238  O4* DA      8      -7.998   1.141  26.338
ATOM    239  C1* DA      8      -7.241   0.678  27.447
ATOM    240  H1* DA      8      -7.416  -0.396  27.559
ATOM    241  N9  DA      8      -5.797   0.921  27.209
ATOM    242  C8  DA      8      -5.059   2.065  27.419
ATOM    243  H8  DA      8      -5.491   2.997  27.765
ATOM    244  N7  DA      8      -3.793   1.954  27.125
ATOM    245  C5  DA      8      -3.686   0.630  26.699
ATOM    246  C6  DA      8      -2.615  -0.159  26.236
ATOM    247  N6  DA      8      -1.380   0.298  26.124
ATOM    248 1H6  DA      8      -0.646  -0.313  25.764
ATOM    249 2H6  DA      8      -1.192   1.236  26.430
ATOM    250  N1  DA      8      -2.810  -1.433  25.874
ATOM    251  C2  DA      8      -4.042  -1.925  25.973
ATOM    252  H2  DA      8      -4.164  -2.958  25.679
ATOM    253  N3  DA      8      -5.141  -1.304  26.391
ATOM    254  C4  DA      8      -4.896  -0.009  26.740
ATOM    255  C3* DA      8      -9.190   1.774  28.306
ATOM    256  H3* DA      8      -9.500   2.692  28.809
ATOM    257  C2* DA      8      -7.765   1.398  28.693
ATOM    258 1H2* DA      8      -7.218   2.317  28.891
ATOM    259 2H2* DA      8      -7.718   0.763  29.573
ATOM    260  O3* DA      8     -10.145   0.748  28.525
ATOM    261  P   DG      9     -10.452   0.123  29.979
ATOM    262  O1P DG      9     -11.868  -0.298  30.013
ATOM    263  O2P DG      9      -9.915   1.030  31.017
ATOM    264  O5* DG      9      -9.533  -1.196  29.914
ATOM    265  C5* DG      9      -9.834  -2.222  28.982
ATOM    266 1H5* DG      9      -9.761  -1.825  27.968
ATOM    267 2H5* DG      9     -10.859  -2.558  29.148
ATOM    268  C4* DG      9      -8.899  -3.426  29.110
ATOM    269  H4* DG      9      -9.267  -4.212  28.450
ATOM    270  O4* DG      9      -7.584  -3.066  28.702
ATOM    271  C1* DG      9      -6.672  -3.455  29.713
ATOM    272  H1* DG      9      -6.315  -4.470  29.512
ATOM    273  N9  DG      9      -5.528  -2.514  29.752
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ATOM    274  C8  DG      9      -5.503  -1.213  30.187
ATOM    275  H8  DG      9      -6.384  -0.707  30.557
ATOM    276  N7  DG      9      -4.333  -0.642  30.112
ATOM    277  C5  DG      9      -3.508  -1.642  29.587
ATOM    278  C6  DG      9      -2.109  -1.646  29.257
ATOM    279  O6  DG      9      -1.280  -0.744  29.341
ATOM    280  N1  DG      9      -1.669  -2.858  28.757
ATOM    281  H1  DG      9      -0.694  -2.911  28.483
ATOM    282  C2  DG      9      -2.472  -3.940  28.568
ATOM    283  N2  DG      9      -1.921  -5.012  28.054
ATOM    284 1H2  DG      9      -2.517  -5.806  27.911
ATOM    285 2H2  DG      9      -0.918  -5.042  27.840
ATOM    286  N3  DG      9      -3.770  -3.976  28.867
ATOM    287  C4  DG      9      -4.236  -2.794  29.369
ATOM    288  C3* DG      9      -8.832  -3.985  30.537
ATOM    289  H3* DG      9      -9.644  -3.603  31.162
ATOM    290  C2* DG      9      -7.482  -3.457  31.006
ATOM    291 1H2* DG      9      -7.618  -2.446  31.388
ATOM    292 2H2* DG      9      -7.031  -4.087  31.766
ATOM    293  O3* DG      9      -8.894  -5.399  30.453
ATOM    294  P   DT     10      -8.799  -6.366  31.741
ATOM    295  O1P DT     10      -9.774  -7.465  31.576
ATOM    296  O2P DT     10      -8.792  -5.544  32.970
ATOM    297  O5* DT     10      -7.322  -6.962  31.539
ATOM    298  C5* DT     10      -7.024  -7.779  30.418
ATOM    299 1H5* DT     10      -7.181  -7.208  29.502
ATOM    300 2H5* DT     10      -7.699  -8.636  30.412
ATOM    301  C4* DT     10      -5.579  -8.288  30.442
ATOM    302  H4* DT     10      -5.429  -8.936  29.579
ATOM    303  O4* DT     10      -4.684  -7.185  30.354
ATOM    304  C1* DT     10      -3.815  -7.216  31.472
ATOM    305  H1* DT     10      -2.917  -7.776  31.192
ATOM    306  N1  DT     10      -3.454  -5.828  31.872
ATOM    307  C6  DT     10      -4.365  -4.989  32.490
ATOM    308  H6  DT     10      -5.374  -5.343  32.663
ATOM    309  C5  DT     10      -4.021  -3.724  32.857
ATOM    310  C7  DT     10      -5.033  -2.846  33.573
ATOM    311 1H7  DT     10      -5.302  -2.006  32.933
ATOM    312 2H7  DT     10      -5.929  -3.409  33.839
ATOM    313 3H7  DT     10      -4.581  -2.447  34.482
ATOM    314  C4  DT     10      -2.681  -3.211  32.584
ATOM    315  O4  DT     10      -2.254  -2.090  32.840
ATOM    316  N3  DT     10      -1.836  -4.112  31.978
ATOM    317  H3  DT     10      -0.877  -3.816  31.826
ATOM    318  C2  DT     10      -2.145  -5.403  31.622
ATOM    319  O2  DT     10      -1.271  -6.114  31.136
ATOM    320  C3* DT     10      -5.238  -9.078  31.712
ATOM    321  H3* DT     10      -6.134  -9.455  32.210
ATOM    322  C2* DT     10      -4.542  -8.018  32.553
ATOM    323 1H2* DT     10      -5.297  -7.430  33.069
ATOM    324 2H2* DT     10      -3.860  -8.448  33.279
ATOM    325  O3* DT     10      -4.381 -10.149  31.346
ATOM    326  P   DC     11      -3.786 -11.207  32.412
ATOM    327  O1P DC     11      -3.848 -12.556  31.813
ATOM    328  O2P DC     11      -4.386 -10.947  33.738
ATOM    329  O5* DC     11      -2.246 -10.741  32.465
ATOM    330  C5* DC     11      -1.408 -10.895  31.330
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ATOM    331 1H5* DC     11      -1.811 -10.307  30.504
ATOM    332 2H5* DC     11      -1.401 -11.946  31.033
ATOM    333  C4* DC     11       0.035 -10.448  31.595
ATOM    334  H4* DC     11       0.624 -10.645  30.698
ATOM    335  O4* DC     11       0.056  -9.054  31.865
ATOM    336  C1* DC     11       0.678  -8.834  33.118
ATOM    337  H1* DC     11       1.745  -8.647  32.949
ATOM    338  N1  DC     11       0.035  -7.668  33.783
ATOM    339  C6  DC     11      -1.275  -7.722  34.198
ATOM    340  H6  DC     11      -1.839  -8.632  34.024
ATOM    341  C5  DC     11      -1.858  -6.648  34.791
ATOM    342  H5  DC     11      -2.889  -6.695  35.102
ATOM    343  C4  DC     11      -1.054  -5.479  34.949
ATOM    344  N4  DC     11      -1.538  -4.390  35.491
ATOM    345 1H4  DC     11      -2.494  -4.335  35.778
ATOM    346 2H4  DC     11      -0.901  -3.587  35.545
ATOM    347  N3  DC     11       0.205  -5.417  34.559
ATOM    348  C2  DC     11       0.776  -6.495  33.967
ATOM    349  O2  DC     11       1.958  -6.407  33.640
ATOM    350  C3* DC     11       0.698 -11.167  32.775
ATOM    351  H3* DC     11       0.189 -12.102  33.017
ATOM    352  C2* DC     11       0.543 -10.146  33.895
ATOM    353 1H2* DC     11      -0.442 -10.261  34.341
ATOM    354 2H2* DC     11       1.305 -10.253  34.661
ATOM    355  O3* DC     11       2.055 -11.412  32.444
ATOM    356  P   DC3    12       3.067 -12.154  33.454
ATOM    357  O1P DC3    12       4.066 -12.898  32.659
ATOM    358  O2P DC3    12       2.279 -12.842  34.499
ATOM    359  O5* DC3    12       3.807 -10.903  34.143
ATOM    360  C5* DC3    12       4.719 -10.104  33.409
ATOM    361 1H5* DC3    12       4.191  -9.582  32.609
ATOM    362 2H5* DC3    12       5.480 -10.747  32.964
ATOM    363  C4* DC3    12       5.410  -9.081  34.316
ATOM    364  H4* DC3    12       6.210  -8.599  33.754
ATOM    365  O4* DC3    12       4.470  -8.097  34.720
ATOM    366  C1* DC3    12       4.654  -7.863  36.099
ATOM    367  H1* DC3    12       5.489  -7.165  36.221
ATOM    368  N1  DC3    12       3.413  -7.301  36.695
ATOM    369  C6  DC3    12       2.225  -7.990  36.649
ATOM    370  H6  DC3    12       2.208  -8.967  36.184
ATOM    371  C5  DC3    12       1.091  -7.445  37.160
ATOM    372  H5  DC3    12       0.160  -7.986  37.111
ATOM    373  C4  DC3    12       1.197  -6.138  37.727
ATOM    374  N4  DC3    12       0.150  -5.522  38.217
ATOM    375 1H4  DC3    12      -0.758  -5.934  38.158
ATOM    376 2H4  DC3    12       0.297  -4.566  38.557
ATOM    377  N3  DC3    12       2.340  -5.478  37.800
ATOM    378  C2  DC3    12       3.467  -6.041  37.299
ATOM    379  O2  DC3    12       4.522  -5.418  37.408
ATOM    380  C3* DC3    12       6.004  -9.717  35.585
ATOM    381  H3* DC3    12       5.991 -10.809  35.526
ATOM    382  C2* DC3    12       5.068  -9.216  36.679
ATOM    383 1H2* DC3    12       4.216  -9.891  36.762
ATOM    384 2H2* DC3    12       5.569  -9.106  37.641
ATOM    385  O3* DC3    12       7.317  -9.236  35.821
ATOM    386  H3T DC3    12       7.717  -9.738  36.536
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ATOM    387  H5T DG5    13       1.267   4.971  41.682
ATOM    388  O5* DG5    13       1.916   4.508  41.145
ATOM    389  C5* DG5    13       3.199   4.630  41.745
ATOM    390 1H5* DG5    13       3.179   4.179  42.739
ATOM    391 2H5* DG5    13       3.441   5.689  41.854
ATOM    392  C4* DG5    13       4.323   3.961  40.932
ATOM    393  H4* DG5    13       5.273   4.199  41.413
ATOM    394  O4* DG5    13       4.157   2.548  40.939
ATOM    395  C1* DG5    13       3.974   2.087  39.609
ATOM    396  H1* DG5    13       4.906   1.641  39.249
ATOM    397  N9  DG5    13       2.892   1.078  39.589
ATOM    398  C8  DG5    13       1.573   1.229  39.937
ATOM    399  H8  DG5    13       1.174   2.168  40.295
ATOM    400  N7  DG5    13       0.859   0.143  39.819
ATOM    401  C5  DG5    13       1.771  -0.805  39.344
ATOM    402  C6  DG5    13       1.619  -2.198  39.018
ATOM    403  O6  DG5    13       0.625  -2.921  39.081
ATOM    404  N1  DG5    13       2.795  -2.785  38.585
ATOM    405  H1  DG5    13       2.741  -3.764  38.324
ATOM    406  C2  DG5    13       3.985  -2.129  38.484
ATOM    407  N2  DG5    13       5.012  -2.801  38.027
ATOM    408 1H2  DG5    13       5.855  -2.279  37.877
ATOM    409 2H2  DG5    13       4.907  -3.777  37.728
ATOM    410  N3  DG5    13       4.167  -0.847  38.791
ATOM    411  C4  DG5    13       3.021  -0.236  39.211
ATOM    412  C3* DG5    13       4.400   4.418  39.472
ATOM    413  H3* DG5    13       3.914   5.385  39.327
ATOM    414  C2* DG5    13       3.646   3.308  38.751
ATOM    415 1H2* DG5    13       2.578   3.525  38.773
ATOM    416 2H2* DG5    13       3.974   3.182  37.722
ATOM    417  O3* DG5    13       5.769   4.492  39.108
ATOM    418  P   DG     14       6.252   4.999  37.653
ATOM    419  O1P DG     14       7.597   5.594  37.800
ATOM    420  O2P DG     14       5.154   5.780  37.046
ATOM    421  O5* DG     14       6.395   3.604  36.856
ATOM    422  C5* DG     14       7.412   2.679  37.204
ATOM    423 1H5* DG     14       7.265   2.347  38.232
ATOM    424 2H5* DG     14       8.379   3.182  37.140
ATOM    425  C4* DG     14       7.445   1.455  36.282
ATOM    426  H4* DG     14       8.359   0.901  36.498
ATOM    427  O4* DG     14       6.334   0.598  36.532
ATOM    428  C1* DG     14       5.760   0.241  35.287
ATOM    429  H1* DG     14       6.281  -0.626  34.871
ATOM    430  N9  DG     14       4.320  -0.064  35.441
ATOM    431  C8  DG     14       3.303   0.783  35.803
ATOM    432  H8  DG     14       3.471   1.825  36.031
ATOM    433  N7  DG     14       2.127   0.221  35.862
ATOM    434  C5  DG     14       2.378  -1.103  35.492
ATOM    435  C6  DG     14       1.498  -2.231  35.361
ATOM    436  O6  DG     14       0.289  -2.310  35.566
ATOM    437  N1  DG     14       2.144  -3.376  34.935
ATOM    438  H1  DG     14       1.556  -4.187  34.769
ATOM    439  C2  DG     14       3.479  -3.454  34.682
ATOM    440  N2  DG     14       3.937  -4.590  34.214
ATOM    441 1H2  DG     14       4.902  -4.604  33.938
ATOM    442 2H2  DG     14       3.290  -5.348  33.968
ATOM    443  N3  DG     14       4.329  -2.435  34.811
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ATOM    444  C4  DG     14       3.718  -1.281  35.220
ATOM    445  C3* DG     14       7.444   1.813  34.789
ATOM    446  H3* DG     14       7.644   2.873  34.621
ATOM    447  C2* DG     14       6.016   1.449  34.394
ATOM    448 1H2* DG     14       5.354   2.274  34.658
ATOM    449 2H2* DG     14       5.915   1.212  33.338
ATOM    450  O3* DG     14       8.437   1.010  34.169
ATOM    451  P   DA     15       8.712   0.999  32.579
ATOM    452  O1P DA     15      10.170   0.908  32.359
ATOM    453  O2P DA     15       7.923   2.069  31.934
ATOM    454  O5* DA     15       8.053  -0.418  32.192
ATOM    455  C5* DA     15       8.595  -1.626  32.704
ATOM    456 1H5* DA     15       8.383  -1.694  33.772
ATOM    457 2H5* DA     15       9.678  -1.612  32.572
ATOM    458  C4* DA     15       8.052  -2.878  32.002
ATOM    459  H4* DA     15       8.610  -3.738  32.374
ATOM    460  O4* DA     15       6.672  -3.067  32.294
ATOM    461  C1* DA     15       5.926  -2.971  31.090
ATOM    462  H1* DA     15       5.662  -3.976  30.748
ATOM    463  N9  DA     15       4.701  -2.189  31.348
ATOM    464  C8  DA     15       4.576  -0.853  31.643
ATOM    465  H8  DA     15       5.429  -0.187  31.688
ATOM    466  N7  DA     15       3.349  -0.468  31.877
ATOM    467  C5  DA     15       2.614  -1.650  31.731
ATOM    468  C6  DA     15       1.253  -1.997  31.884
ATOM    469  N6  DA     15       0.320  -1.154  32.294
ATOM    470 1H6  DA     15      -0.631  -1.496  32.444
ATOM    471 2H6  DA     15       0.581  -0.210  32.523
ATOM    472  N1  DA     15       0.841  -3.250  31.659
ATOM    473  C2  DA     15       1.744  -4.156  31.297
ATOM    474  H2  DA     15       1.373  -5.157  31.122
ATOM    475  N3  DA     15       3.049  -3.979  31.132
ATOM    476  C4  DA     15       3.425  -2.694  31.378
ATOM    477  C3* DA     15       8.202  -2.828  30.480
ATOM    478  H3* DA     15       8.996  -2.146  30.168
ATOM    479  C2* DA     15       6.832  -2.318  30.049
ATOM    480 1H2* DA     15       6.812  -1.233  30.127
ATOM    481 2H2* DA     15       6.575  -2.612  29.035
ATOM    482  O3* DA     15       8.481  -4.148  30.044
ATOM    483  P   DC     16       8.618  -4.544  28.488
ATOM    484  O1P DC     16       9.564  -5.675  28.381
ATOM    485  O2P DC     16       8.832  -3.313  27.698
ATOM    486  O5* DC     16       7.128  -5.088  28.197
ATOM    487  C5* DC     16       6.664  -6.273  28.827
ATOM    488 1H5* DC     16       6.544  -6.097  29.897
ATOM    489 2H5* DC     16       7.406  -7.061  28.688
ATOM    490  C4* DC     16       5.337  -6.763  28.243
ATOM    491  H4* DC     16       5.130  -7.752  28.653
ATOM    492  O4* DC     16       4.277  -5.896  28.610
ATOM    493  C1* DC     16       3.503  -5.590  27.467
ATOM    494  H1* DC     16       2.694  -6.323  27.371
ATOM    495  N1  DC     16       2.968  -4.213  27.644
ATOM    496  C6  DC     16       3.827  -3.156  27.836
ATOM    497  H6  DC     16       4.894  -3.334  27.769
ATOM    498  C5  DC     16       3.348  -1.926  28.148
ATOM    499  H5  DC     16       4.029  -1.109  28.325
ATOM    500  C4  DC     16       1.933  -1.794  28.278
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ATOM    501  N4  DC     16       1.406  -0.671  28.696
ATOM    502 1H4  DC     16       1.998   0.092  28.962
ATOM    503 2H4  DC     16       0.397  -0.664  28.872
ATOM    504  N3  DC     16       1.094  -2.795  28.073
ATOM    505  C2  DC     16       1.586  -4.016  27.744
ATOM    506  O2  DC     16       0.779  -4.922  27.542
ATOM    507  C3* DC     16       5.369  -6.871  26.715
ATOM    508  H3* DC     16       6.380  -6.726  26.328
ATOM    509  C2* DC     16       4.447  -5.738  26.272
ATOM    510 1H2* DC     16       5.048  -4.842  26.125
ATOM    511 2H2* DC     16       3.907  -5.977  25.358
ATOM    512  O3* DC     16       4.889  -8.155  26.363
ATOM    513  P   DT     17       4.938  -8.702  24.850
ATOM    514  O1P DT     17       5.104 -10.170  24.896
ATOM    515  O2P DT     17       5.874  -7.864  24.070
ATOM    516  O5* DT     17       3.442  -8.369  24.373
ATOM    517  C5* DT     17       2.344  -9.095  24.896
ATOM    518 1H5* DT     17       2.338  -9.017  25.984
ATOM    519 2H5* DT     17       2.445 -10.145  24.619
ATOM    520  C4* DT     17       1.021  -8.560  24.352
ATOM    521  H4* DT     17       0.221  -9.222  24.684
ATOM    522  O4* DT     17       0.760  -7.266  24.864
ATOM    523  C1* DT     17       0.032  -6.552  23.889
ATOM    524  H1* DT     17      -1.026  -6.822  23.963
ATOM    525  N1  DT     17       0.224  -5.098  24.139
ATOM    526  C6  DT     17       1.482  -4.537  24.060
ATOM    527  H6  DT     17       2.321  -5.169  23.801
ATOM    528  C5  DT     17       1.683  -3.220  24.326
ATOM    529  C7  DT     17       3.083  -2.639  24.225
ATOM    530 1H7  DT     17       3.351  -2.181  25.177
ATOM    531 2H7  DT     17       3.814  -3.406  23.973
ATOM    532 3H7  DT     17       3.093  -1.861  23.462
ATOM    533  C4  DT     17       0.568  -2.369  24.724
ATOM    534  O4  DT     17       0.641  -1.177  25.006
ATOM    535  N3  DT     17      -0.656  -3.004  24.792
ATOM    536  H3  DT     17      -1.457  -2.453  25.088
ATOM    537  C2  DT     17      -0.888  -4.335  24.518
ATOM    538  O2  DT     17      -2.023  -4.792  24.624
ATOM    539  C3* DT     17       0.976  -8.488  22.821
ATOM    540  H3* DT     17       1.958  -8.703  22.393
ATOM    541  C2* DT     17       0.572  -7.039  22.540
ATOM    542 1H2* DT     17       1.460  -6.486  22.239
ATOM    543 2H2* DT     17      -0.186  -6.957  21.763
ATOM    544  O3* DT     17       0.020  -9.428  22.367
ATOM    545  P   DA     18      -0.050  -9.899  20.826
ATOM    546  O1P DA     18      -0.749 -11.200  20.776
ATOM    547  O2P DA     18       1.291  -9.748  20.222
ATOM    548  O5* DA     18      -1.014  -8.783  20.194
ATOM    549  C5* DA     18      -2.374  -8.694  20.585
ATOM    550 1H5* DA     18      -2.437  -8.441  21.644
ATOM    551 2H5* DA     18      -2.858  -9.658  20.421
ATOM    552  C4* DA     18      -3.104  -7.631  19.764
ATOM    553  H4* DA     18      -4.161  -7.655  20.029
ATOM    554  O4* DA     18      -2.607  -6.338  20.065
ATOM    555  C1* DA     18      -2.559  -5.565  18.884
ATOM    556  H1* DA     18      -3.462  -4.954  18.804
ATOM    557  N9  DA     18      -1.363  -4.699  18.973
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ATOM    558  C8  DA     18      -0.040  -5.076  19.011
ATOM    559  H8  DA     18       0.270  -6.113  19.003
ATOM    560  N7  DA     18       0.803  -4.078  19.063
ATOM    561  C5  DA     18      -0.035  -2.958  19.069
ATOM    562  C6  DA     18       0.184  -1.562  19.099
ATOM    563  N6  DA     18       1.369  -0.980  19.094
ATOM    564 1H6  DA     18       1.362   0.020  18.972
ATOM    565 2H6  DA     18       2.192  -1.553  19.025
ATOM    566  N1  DA     18      -0.839  -0.707  19.102
ATOM    567  C2  DA     18      -2.067  -1.208  19.077
ATOM    568  H2  DA     18      -2.867  -0.481  19.073
ATOM    569  N3  DA     18      -2.435  -2.489  19.045
ATOM    570  C4  DA     18      -1.354  -3.324  19.034
ATOM    571  C3* DA     18      -2.985  -7.880  18.258
ATOM    572  H3* DA     18      -2.249  -8.660  18.045
ATOM    573  C2* DA     18      -2.498  -6.541  17.705
ATOM    574 1H2* DA     18      -1.476  -6.665  17.347
ATOM    575 2H2* DA     18      -3.127  -6.189  16.891
ATOM    576  O3* DA     18      -4.257  -8.277  17.777
ATOM    577  P   DG     19      -4.516  -8.708  16.242
ATOM    578  O1P DG     19      -5.550  -9.763  16.221
ATOM    579  O2P DG     19      -3.217  -8.917  15.568
ATOM    580  O5* DG     19      -5.168  -7.360  15.671
ATOM    581  C5* DG     19      -6.401  -6.896  16.192
ATOM    582 1H5* DG     19      -6.308  -6.753  17.270
ATOM    583 2H5* DG     19      -7.172  -7.643  16.005
ATOM    584  C4* DG     19      -6.819  -5.572  15.556
ATOM    585  H4* DG     19      -7.808  -5.314  15.935
ATOM    586  O4* DG     19      -5.905  -4.549  15.932
ATOM    587  C1* DG     19      -5.396  -3.935  14.762
ATOM    588  H1* DG     19      -5.997  -3.049  14.539
ATOM    589  N9  DG     19      -3.983  -3.537  14.972
ATOM    590  C8  DG     19      -2.838  -4.293  14.874
ATOM    591  H8  DG     19      -2.848  -5.349  14.642
ATOM    592  N7  DG     19      -1.737  -3.631  15.108
ATOM    593  C5  DG     19      -2.181  -2.338  15.392
ATOM    594  C6  DG     19      -1.465  -1.141  15.746
ATOM    595  O6  DG     19      -0.258  -0.961  15.894
ATOM    596  N1  DG     19      -2.296  -0.058  15.963
ATOM    597  H1  DG     19      -1.852   0.792  16.294
ATOM    598  C2  DG     19      -3.651  -0.094  15.837
ATOM    599  N2  DG     19      -4.316   1.009  16.093
ATOM    600 1H2  DG     19      -5.308   0.980  15.952
ATOM    601 2H2  DG     19      -3.831   1.842  16.442
ATOM    602  N3  DG     19      -4.346  -1.175  15.492
ATOM    603  C4  DG     19      -3.556  -2.273  15.300
ATOM    604  C3* DG     19      -6.883  -5.637  14.025
ATOM    605  H3* DG     19      -6.908  -6.667  13.662
ATOM    606  C2* DG     19      -5.579  -4.948  13.634
ATOM    607 1H2* DG     19      -4.785  -5.693  13.637
ATOM    608 2H2* DG     19      -5.625  -4.465  12.661
ATOM    609  O3* DG     19      -8.060  -4.950  13.641
ATOM    610  P   DC     20      -8.475  -4.657  12.111
ATOM    611  O1P DC     20      -9.918  -4.932  11.956
ATOM    612  O2P DC     20      -7.488  -5.270  11.197
ATOM    613  O5* DC     20      -8.252  -3.066  12.112
ATOM    614  C5* DC     20      -9.031  -2.246  12.970
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ATOM    615 1H5* DC     20      -8.845  -2.525  14.008
ATOM    616 2H5* DC     20     -10.088  -2.407  12.752
ATOM    617  C4* DC     20      -8.713  -0.761  12.800
ATOM    618  H4* DC     20      -9.402  -0.191  13.424
ATOM    619  O4* DC     20      -7.382  -0.505  13.233
ATOM    620  C1* DC     20      -6.677   0.140  12.190
ATOM    621  H1* DC     20      -6.746   1.223  12.339
ATOM    622  N1  DC     20      -5.256  -0.306  12.197
ATOM    623  C6  DC     20      -4.917  -1.612  11.928
ATOM    624  H6  DC     20      -5.706  -2.334  11.743
ATOM    625  C5  DC     20      -3.613  -1.995  11.914
ATOM    626  H5  DC     20      -3.355  -3.021  11.709
ATOM    627  C4  DC     20      -2.635  -0.996  12.206
ATOM    628  N4  DC     20      -1.365  -1.305  12.292
ATOM    629 1H4  DC     20      -1.069  -2.256  12.186
ATOM    630 2H4  DC     20      -0.715  -0.562  12.567
ATOM    631  N3  DC     20      -2.951   0.257  12.487
ATOM    632  C2  DC     20      -4.256   0.628  12.489
ATOM    633  O2  DC     20      -4.516   1.799  12.753
ATOM    634  C3* DC     20      -8.865  -0.287  11.351
ATOM    635  H3* DC     20      -9.425  -1.004  10.747
ATOM    636  C2* DC     20      -7.414  -0.208  10.896
ATOM    637 1H2* DC     20      -7.120  -1.181  10.508
ATOM    638 2H2* DC     20      -7.263   0.551  10.135
ATOM    639  O3* DC     20      -9.527   0.966  11.365
ATOM    640  P   DT     21      -9.836   1.812  10.026
ATOM    641  O1P DT     21     -11.185   2.403  10.148
ATOM    642  O2P DT     21      -9.470   1.004   8.842
ATOM    643  O5* DT     21      -8.747   2.983  10.188
ATOM    644  C5* DT     21      -8.831   3.888  11.277
ATOM    645 1H5* DT     21      -8.766   3.334  12.214
ATOM    646 2H5* DT     21      -9.794   4.399  11.242
ATOM    647  C4* DT     21      -7.714   4.935  11.245
ATOM    648  H4* DT     21      -7.864   5.620  12.080
ATOM    649  O4* DT     21      -6.454   4.295  11.395
ATOM    650  C1* DT     21      -5.619   4.674  10.315
ATOM    651  H1* DT     21      -5.048   5.559  10.612
ATOM    652  N1  DT     21      -4.699   3.555   9.975
ATOM    653  C6  DT     21      -5.165   2.394   9.386
ATOM    654  H6  DT     21      -6.225   2.292   9.192
ATOM    655  C5  DT     21      -4.318   1.380   9.064
ATOM    656  C7  DT     21      -4.862   0.126   8.398
ATOM    657 1H7  DT     21      -4.676  -0.737   9.038
ATOM    658 2H7  DT     21      -5.930   0.214   8.206
ATOM    659 3H7  DT     21      -4.343  -0.030   7.453
ATOM    660  C4  DT     21      -2.890   1.491   9.349
ATOM    661  O4  DT     21      -2.032   0.648   9.104
ATOM    662  N3  DT     21      -2.512   2.670   9.951
ATOM    663  H3  DT     21      -1.526   2.801  10.152
ATOM    664  C2  DT     21      -3.342   3.719  10.269
ATOM    665  O2  DT     21      -2.866   4.732  10.774
ATOM    666  C3* DT     21      -7.688   5.747   9.947
ATOM    667  H3* DT     21      -8.632   5.671   9.403
ATOM    668  C2* DT     21      -6.552   5.087   9.176
ATOM    669 1H2* DT     21      -6.951   4.231   8.636
ATOM    670 2H2* DT     21      -6.072   5.769   8.480
ATOM    671  O3* DT     21      -7.414   7.097  10.280
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ATOM    672  P   DA     22      -7.336   8.264   9.169
ATOM    673  O1P DA     22      -7.889   9.499   9.763
ATOM    674  O2P DA     22      -7.873   7.742   7.894
ATOM    675  O5* DA     22      -5.743   8.440   9.019
ATOM    676  C5* DA     22      -4.983   8.987  10.084
ATOM    677 1H5* DA     22      -5.046   8.327  10.950
ATOM    678 2H5* DA     22      -5.405   9.956  10.355
ATOM    679  C4* DA     22      -3.511   9.189   9.715
ATOM    680  H4* DA     22      -3.033   9.739  10.526
ATOM    681  O4* DA     22      -2.863   7.932   9.583
ATOM    682  C1* DA     22      -2.143   7.914   8.366
ATOM    683  H1* DA     22      -1.125   8.281   8.532
ATOM    684  N9  DA     22      -2.115   6.529   7.850
ATOM    685  C8  DA     22      -3.170   5.752   7.439
ATOM    686  H8  DA     22      -4.188   6.114   7.440
ATOM    687  N7  DA     22      -2.841   4.543   7.068
ATOM    688  C5  DA     22      -1.450   4.539   7.226
ATOM    689  C6  DA     22      -0.436   3.580   7.010
ATOM    690  N6  DA     22      -0.672   2.351   6.579
ATOM    691 1H6  DA     22       0.098   1.686   6.502
ATOM    692 2H6  DA     22      -1.620   2.082   6.385
ATOM    693  N1  DA     22       0.848   3.876   7.248
ATOM    694  C2  DA     22       1.136   5.091   7.706
ATOM    695  H2  DA     22       2.183   5.296   7.888
ATOM    696  N3  DA     22       0.292   6.084   7.966
ATOM    697  C4  DA     22      -1.000   5.741   7.701
ATOM    698  C3* DA     22      -3.311   9.975   8.413
ATOM    699  H3* DA     22      -4.235  10.456   8.083
ATOM    700  C2* DA     22      -2.885   8.878   7.443
ATOM    701 1H2* DA     22      -3.779   8.410   7.030
ATOM    702 2H2* DA     22      -2.250   9.249   6.641
ATOM    703  O3* DA     22      -2.304  10.945   8.653
ATOM    704  P   DG     23      -1.796  11.982   7.526
ATOM    705  O1P DG     23      -1.509  13.276   8.182
ATOM    706  O2P DG     23      -2.710  11.918   6.365
ATOM    707  O5* DG     23      -0.397  11.301   7.116
ATOM    708  C5* DG     23       0.666  11.233   8.053
ATOM    709 1H5* DG     23       0.355  10.636   8.912
ATOM    710 2H5* DG     23       0.898  12.242   8.399
ATOM    711  C4* DG     23       1.937  10.619   7.458
ATOM    712  H4* DG     23       2.737  10.709   8.194
ATOM    713  O4* DG     23       1.723   9.239   7.186
ATOM    714  C1* DG     23       2.134   8.978   5.857
ATOM    715  H1* DG     23       3.200   8.735   5.848
ATOM    716  N9  DG     23       1.359   7.854   5.286
ATOM    717  C8  DG     23       0.030   7.808   4.948
ATOM    718  H8  DG     23      -0.638   8.643   5.109
ATOM    719  N7  DG     23      -0.353   6.675   4.423
ATOM    720  C5  DG     23       0.812   5.900   4.422
ATOM    721  C6  DG     23       1.063   4.553   3.985
ATOM    722  O6  DG     23       0.286   3.723   3.515
ATOM    723  N1  DG     23       2.383   4.168   4.127
ATOM    724  H1  DG     23       2.617   3.225   3.835
ATOM    725  C2  DG     23       3.362   4.970   4.628
ATOM    726  N2  DG     23       4.586   4.502   4.619
ATOM    727 1H2  DG     23       5.292   5.087   5.023
ATOM    728 2H2  DG     23       4.782   3.542   4.314
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ATOM    729  N3  DG     23       3.165   6.216   5.058
ATOM    730  C4  DG     23       1.867   6.625   4.935
ATOM    731  C3* DG     23       2.393  11.297   6.159
ATOM    732  H3* DG     23       1.919  12.271   6.018
ATOM    733  C2* DG     23       1.915  10.293   5.115
ATOM    734 1H2* DG     23       0.855  10.458   4.922
ATOM    735 2H2* DG     23       2.479  10.350   4.188
ATOM    736  O3* DG     23       3.806  11.430   6.218
ATOM    737  P   DC3    24       4.692  12.058   5.024
ATOM    738  O1P DC3    24       5.751  12.903   5.614
ATOM    739  O2P DC3    24       3.798  12.597   3.977
ATOM    740  O5* DC3    24       5.382  10.725   4.444
ATOM    741  C5* DC3    24       6.291   9.980   5.240
ATOM    742 1H5* DC3    24       5.756   9.526   6.076
ATOM    743 2H5* DC3    24       7.048  10.655   5.643
ATOM    744  C4* DC3    24       6.997   8.884   4.433
ATOM    745  H4* DC3    24       7.769   8.437   5.060
ATOM    746  O4* DC3    24       6.057   7.883   4.070
ATOM    747  C1* DC3    24       6.073   7.722   2.665
ATOM    748  H1* DC3    24       6.755   6.901   2.424
ATOM    749  N1  DC3    24       4.696   7.414   2.193
ATOM    750  C6  DC3    24       3.669   8.311   2.372
ATOM    751  H6  DC3    24       3.883   9.260   2.853
ATOM    752  C5  DC3    24       2.407   7.999   1.981
ATOM    753  H5  DC3    24       1.603   8.699   2.142
ATOM    754  C4  DC3    24       2.205   6.712   1.399
ATOM    755  N4  DC3    24       1.006   6.295   1.078
ATOM    756 1H4  DC3    24       0.200   6.838   1.322
ATOM    757 2H4  DC3    24       0.926   5.338   0.719
ATOM    758  N3  DC3    24       3.187   5.846   1.211
ATOM    759  C2  DC3    24       4.445   6.173   1.598
ATOM    760  O2  DC3    24       5.343   5.354   1.399
ATOM    761  C3* DC3    24       7.646   9.419   3.150
ATOM    762  H3* DC3    24       7.759  10.506   3.191
ATOM    763  C2* DC3    24       6.651   9.011   2.072
ATOM    764 1H2* DC3    24       5.891   9.786   1.974
ATOM    765 2H2* DC3    24       7.130   8.830   1.110
ATOM    766  O3* DC3    24       8.896   8.788   2.920
ATOM    767  H3T DC3    24       9.345   9.229   2.195
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END
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**File E-2**: Average structure of rMD refined *S*-BD-N3-dU modified duplex 5′ - $G^{1}C^{2}T^{3}A^{4}G^{5}C^{6}X^{7}A^{8}G^{9}T^{10}C^{11}C^{12}$- 3′·5′ - $G^{13}G^{14}A^{15}C^{16}T^{17}A^{18}G^{19}C^{20}T^{21}A^{22}G^{23}C^{24}$ -3′.

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REMARK
ATOM      1  H5T DG5     1      -0.063  -4.215  -3.799
ATOM      2  O5* DG5     1       0.649  -3.863  -3.225
ATOM      3  C5* DG5     1       1.887  -3.863  -3.938
ATOM      4 1H5* DG5     1       1.786  -3.256  -4.841
ATOM      5 2H5* DG5     1       2.119  -4.884  -4.249
ATOM      6  C4* DG5     1       3.084  -3.326  -3.126
ATOM      7  H4* DG5     1       3.982  -3.470  -3.731
ATOM      8  O4* DG5     1       2.918  -1.931  -2.877
ATOM      9  C1* DG5     1       2.909  -1.705  -1.474
ATOM     10  H1* DG5     1       3.903  -1.378  -1.153
ATOM     11  N9  DG5     1       1.908  -0.669  -1.130
ATOM     12  C8  DG5     1       0.541  -0.715  -1.275
ATOM     13  H8  DG5     1       0.038  -1.575  -1.706
ATOM     14  N7  DG5     1      -0.081   0.361  -0.866
ATOM     15  C5  DG5     1       0.959   1.188  -0.411
ATOM     16  C6  DG5     1       0.953   2.514   0.156
ATOM     17  O6  DG5     1       0.001   3.267   0.374
ATOM     18  N1  DG5     1       2.212   2.981   0.478
ATOM     19  H1  DG5     1       2.272   3.906   0.878
ATOM     20  C2  DG5     1       3.351   2.273   0.284
ATOM     21  N2  DG5     1       4.474   2.831   0.641
ATOM     22 1H2  DG5     1       5.322   2.301   0.525
ATOM     23 2H2  DG5     1       4.476   3.764   1.047
ATOM     24  N3  DG5     1       3.410   1.054  -0.241
ATOM     25  C4  DG5     1       2.178   0.560  -0.571
ATOM     26  C3* DG5     1       3.291  -4.027  -1.772
ATOM     27  H3* DG5     1       2.797  -5.000  -1.755
ATOM     28  C2* DG5     1       2.604  -3.051  -0.821
ATOM     29 1H2* DG5     1       1.533  -3.250  -0.809
ATOM     30 2H2* DG5     1       2.994  -3.110   0.189
ATOM     31  O3* DG5     1       4.689  -4.172  -1.523
ATOM     32  P   DC      2       5.289  -4.840  -0.180
ATOM     33  O1P DC      2       6.542  -5.546  -0.547
ATOM     34  O2P DC      2       4.217  -5.601   0.508
ATOM     35  O5* DC      2       5.668  -3.563   0.734
ATOM     36  C5* DC      2       6.699  -2.662   0.335
ATOM     37 1H5* DC      2       6.399  -2.152  -0.582
ATOM     38 2H5* DC      2       7.606  -3.229   0.121
ATOM     39  C4* DC      2       7.052  -1.604   1.393
ATOM     40  H4* DC      2       7.952  -1.089   1.051
ATOM     41  O4* DC      2       6.002  -0.647   1.501
ATOM     42  C1* DC      2       5.603  -0.534   2.857
ATOM     43  H1* DC      2       6.141   0.297   3.327
ATOM     44  N1  DC      2       4.131  -0.307   2.907
ATOM     45  C6  DC      2       3.260  -1.248   2.417
ATOM     46  H6  DC      2       3.661  -2.166   2.005
ATOM     47  C5  DC      2       1.922  -1.022   2.440
ATOM     48  H5  DC      2       1.240  -1.761   2.049
ATOM     49  C4  DC      2       1.484   0.216   2.981
ATOM     50  N4  DC      2       0.220   0.521   2.994
ATOM     51 1H4  DC      2      -0.457  -0.125   2.630
ATOM     52 2H4  DC      2      -0.040   1.427   3.370
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ATOM     53  N3  DC      2       2.298   1.137   3.448
ATOM     54  C2  DC      2       3.631   0.895   3.423
ATOM     55  O2  DC      2       4.362   1.774   3.877
ATOM     56  C3* DC      2       7.330  -2.186   2.791
ATOM     57  H3* DC      2       7.464  -3.269   2.745
ATOM     58  C2* DC      2       6.043  -1.834   3.535
ATOM     59 1H2* DC      2       5.322  -2.635   3.373
ATOM     60 2H2* DC      2       6.195  -1.699   4.602
ATOM     61  O3* DC      2       8.497  -1.567   3.323
ATOM     62  P   DT      3       9.065  -1.866   4.804
ATOM     63  O1P DT      3      10.544  -1.750   4.759
ATOM     64  O2P DT      3       8.460  -3.115   5.327
ATOM     65  O5* DT      3       8.480  -0.622   5.644
ATOM     66  C5* DT      3       8.864   0.711   5.321
ATOM     67 1H5* DT      3       8.526   0.953   4.312
ATOM     68 2H5* DT      3       9.953   0.785   5.338
ATOM     69  C4* DT      3       8.304   1.762   6.289
ATOM     70  H4* DT      3       8.783   2.715   6.056
ATOM     71  O4* DT      3       6.902   1.901   6.092
ATOM     72  C1* DT      3       6.257   1.861   7.352
ATOM     73  H1* DT      3       6.210   2.873   7.766
ATOM     74  N1  DT      3       4.890   1.293   7.191
ATOM     75  C6  DT      3       4.713  -0.004   6.752
ATOM     76  H6  DT      3       5.583  -0.610   6.538
ATOM     77  C5  DT      3       3.467  -0.519   6.567
ATOM     78  C7  DT      3       3.319  -1.958   6.106
ATOM     79 1H7  DT      3       4.279  -2.471   6.082
ATOM     80 2H7  DT      3       2.655  -2.489   6.788
ATOM     81 3H7  DT      3       2.869  -1.982   5.115
ATOM     82  C4  DT      3       2.282   0.297   6.819
ATOM     83  O4  DT      3       1.111  -0.051   6.680
ATOM     84  N3  DT      3       2.542   1.573   7.259
ATOM     85  H3  DT      3       1.749   2.166   7.451
ATOM     86  C2  DT      3       3.788   2.112   7.478
ATOM     87  O2  DT      3       3.873   3.258   7.917
ATOM     88  C3* DT      3       8.564   1.434   7.770
ATOM     89  H3* DT      3       9.267   0.604   7.872
ATOM     90  C2* DT      3       7.172   1.022   8.245
ATOM     91 1H2* DT      3       7.044  -0.043   8.059
ATOM     92 2H2* DT      3       7.006   1.229   9.298
ATOM     93  O3* DT      3       9.076   2.595   8.414
ATOM     94  P   DA      4       9.434   2.654   9.987
ATOM     95  O1P DA      4      10.654   3.483  10.150
ATOM     96  O2P DA      4       9.415   1.285  10.557
ATOM     97  O5* DA      4       8.176   3.471  10.575
ATOM     98  C5* DA      4       7.929   4.810  10.157
ATOM     99 1H5* DA      4       7.710   4.822   9.088
ATOM    100 2H5* DA      4       8.828   5.407  10.321
ATOM    101  C4* DA      4       6.771   5.494  10.899
ATOM    102  H4* DA      4       6.776   6.548  10.612
ATOM    103  O4* DA      4       5.530   4.923  10.501
ATOM    104  C1* DA      4       4.839   4.463  11.650
ATOM    105  H1* DA      4       4.116   5.218  11.974
ATOM    106  N9  DA      4       4.142   3.202  11.315
ATOM    107  C8  DA      4       4.693   1.980  11.009
ATOM    108  H8  DA      4       5.764   1.818  11.006
ATOM    109  N7  DA      4       3.823   1.050  10.709
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ATOM    110  C5  DA      4       2.597   1.722  10.855
ATOM    111  C6  DA      4       1.238   1.360  10.702
ATOM    112  N6  DA      4       0.822   0.170  10.314
ATOM    113 1H6  DA      4      -0.171   0.003  10.201
ATOM    114 2H6  DA      4       1.500  -0.550  10.125
ATOM    115  N1  DA      4       0.257   2.234  10.938
ATOM    116  C2  DA      4       0.591   3.466  11.301
ATOM    117  H2  DA      4      -0.229   4.149  11.482
ATOM    118  N3  DA      4       1.812   3.962  11.464
ATOM    119  C4  DA      4       2.781   3.028  11.228
ATOM    120  C3* DA      4       6.881   5.403  12.429
ATOM    121  H3* DA      4       7.892   5.127  12.736
ATOM    122  C2* DA      4       5.893   4.280  12.740
ATOM    123 1H2* DA      4       6.405   3.324  12.633
ATOM    124 2H2* DA      4       5.464   4.355  13.735
ATOM    125  O3* DA      4       6.519   6.663  12.985
ATOM    126  P   DG      5       6.482   6.954  14.570
ATOM    127  O1P DG      5       6.959   8.342  14.792
ATOM    128  O2P DG      5       7.147   5.845  15.297
ATOM    129  O5* DG      5       4.903   6.895  14.884
ATOM    130  C5* DG      5       4.014   7.857  14.322
ATOM    131 1H5* DG      5       3.951   7.712  13.242
ATOM    132 2H5* DG      5       4.410   8.857  14.504
ATOM    133  C4* DG      5       2.597   7.810  14.915
ATOM    134  H4* DG      5       2.079   8.719  14.602
ATOM    135  O4* DG      5       1.882   6.686  14.409
ATOM    136  C1* DG      5       1.427   5.886  15.489
ATOM    137  H1* DG      5       0.381   6.119  15.709
ATOM    138  N9  DG      5       1.561   4.457  15.118
ATOM    139  C8  DG      5       2.715   3.733  14.942
ATOM    140  H8  DG      5       3.695   4.172  15.090
ATOM    141  N7  DG      5       2.529   2.494  14.572
ATOM    142  C5  DG      5       1.133   2.385  14.499
ATOM    143  C6  DG      5       0.283   1.282  14.133
ATOM    144  O6  DG      5       0.597   0.151  13.762
ATOM    145  N1  DG      5      -1.063   1.571  14.210
ATOM    146  H1  DG      5      -1.707   0.838  13.952
ATOM    147  C2  DG      5      -1.555   2.776  14.583
ATOM    148  N2  DG      5      -2.853   2.891  14.643
ATOM    149 1H2  DG      5      -3.237   3.780  14.908
ATOM    150 2H2  DG      5      -3.450   2.109  14.382
ATOM    151  N3  DG      5      -0.813   3.833  14.912
ATOM    152  C4  DG      5       0.532   3.578  14.849
ATOM    153  C3* DG      5       2.591   7.747  16.450
ATOM    154  H3* DG      5       3.570   8.010  16.858
ATOM    155  C2* DG      5       2.290   6.270  16.693
ATOM    156 1H2* DG      5       3.230   5.720  16.691
ATOM    157 2H2* DG      5       1.775   6.095  17.632
ATOM    158  O3* DG      5       1.602   8.640  16.948
ATOM    159  P   DC      6       1.278   8.810  18.519
ATOM    160  O1P DC      6       0.875  10.218  18.757
ATOM    161  O2P DC      6       2.385   8.234  19.321
ATOM    162  O5* DC      6      -0.017   7.867  18.684
ATOM    163  C5* DC      6      -1.222   8.165  17.983
ATOM    164 1H5* DC      6      -1.057   8.055  16.910
ATOM    165 2H5* DC      6      -1.499   9.202  18.175
ATOM    166  C4* DC      6      -2.405   7.279  18.396
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ATOM    167  H4* DC      6      -3.311   7.728  17.985
ATOM    168  O4* DC      6      -2.263   5.979  17.840
ATOM    169  C1* DC      6      -2.447   4.993  18.842
ATOM    170  H1* DC      6      -3.472   4.611  18.787
ATOM    171  N1  DC      6      -1.457   3.907  18.576
ATOM    172  C6  DC      6      -0.111   4.172  18.631
ATOM    173  H6  DC      6       0.219   5.163  18.923
ATOM    174  C5  DC      6       0.790   3.216  18.297
ATOM    175  H5  DC      6       1.846   3.434  18.332
ATOM    176  C4  DC      6       0.282   1.956  17.891
ATOM    177  N4  DC      6       1.107   1.028  17.505
ATOM    178 1H4  DC      6       2.092   1.217  17.496
ATOM    179 2H4  DC      6       0.745   0.122  17.231
ATOM    180  N3  DC      6      -1.003   1.670  17.823
ATOM    181  C2  DC      6      -1.894   2.636  18.169
ATOM    182  O2  DC      6      -3.089   2.338  18.109
ATOM    183  C3* DC      6      -2.568   7.165  19.919
ATOM    184  H3* DC      6      -1.841   7.804  20.425
ATOM    185  C2* DC      6      -2.259   5.692  20.197
ATOM    186 1H2* DC      6      -1.229   5.622  20.544
ATOM    187 2H2* DC      6      -2.917   5.267  20.953
ATOM    188  O3* DC      6      -3.884   7.553  20.288
ATOM    189  P   DX      7      -4.322   7.781  21.824
ATOM    190  O1P DX      7      -5.267   8.925  21.864
ATOM    191  O2P DX      7      -3.115   7.822  22.686
ATOM    192  O5* DX      7      -5.133   6.435  22.165
ATOM    193  C5* DX      7      -6.321   6.106  21.454
ATOM    194 1H5* DX      7      -6.056   5.780  20.446
ATOM    195 2H5* DX      7      -6.946   6.994  21.360
ATOM    196  C4* DX      7      -7.164   5.011  22.126
ATOM    197  H4* DX      7      -8.176   5.079  21.722
ATOM    198  O4* DX      7      -6.626   3.738  21.793
ATOM    199  C1* DX      7      -6.417   3.005  22.986
ATOM    200  H1* DX      7      -7.336   2.469  23.241
ATOM    201  N1  DX      7      -5.317   2.023  22.759
ATOM    202  C6  DX      7      -3.996   2.412  22.752
ATOM    203  H6  DX      7      -3.731   3.439  22.964
ATOM    204  C5  DX      7      -3.019   1.527  22.443
ATOM    205  H5  DX      7      -1.988   1.844  22.437
ATOM    206  C4  DX      7      -3.307   0.154  22.100
ATOM    207  O4  DX      7      -2.433  -0.676  21.856
ATOM    208  N3  DX      7      -4.662  -0.180  22.052
ATOM    209  C11 DX      7      -5.042  -1.536  21.491
ATOM    210  C2  DX      7      -5.684   0.717  22.394
ATOM    211  O2  DX      7      -6.871   0.371  22.353
ATOM    212  C3* DX      7      -7.234   5.112  23.663
ATOM    213  H3* DX      7      -6.940   6.105  24.009
ATOM    214  C2* DX      7      -6.208   4.057  24.076
ATOM    215 1H2* DX      7      -5.215   4.498  24.034
ATOM    216 2H2* DX      7      -6.395   3.658  25.067
ATOM    217  O3* DX      7      -8.566   4.816  24.078
ATOM    218  C12 DX      7      -4.744  -2.711  22.427
ATOM    219  C9  DX      7      -5.211  -4.016  21.813
ATOM    220  C10 DX      7      -5.031  -5.243  22.283
ATOM    221  O12 DX      7      -5.449  -2.526  23.624
ATOM    222  H15 DX      7      -4.497  -1.703  20.562
ATOM    223  H14 DX      7      -6.101  -1.574  21.242
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ATOM    224  H9  DX      7      -3.676  -2.773  22.632
ATOM    225 1H1  DX      7      -5.771  -3.990  20.890
ATOM    226 2H1  DX      7      -4.490  -5.368  23.212
ATOM    227 3H1  DX      7      -5.440  -6.089  21.748
ATOM    228  H10 DX      7      -5.198  -1.649  23.958
ATOM    229  P   DA      8      -9.032   4.769  25.626
ATOM    230  O1P DA      8     -10.469   5.134  25.678
ATOM    231  O2P DA      8      -8.068   5.534  26.454
ATOM    232  O5* DA      8      -8.893   3.207  25.999
ATOM    233  C5* DA      8      -9.646   2.230  25.289
ATOM    234 1H5* DA      8      -9.459   2.345  24.220
ATOM    235 2H5* DA      8     -10.711   2.397  25.459
ATOM    236  C4* DA      8      -9.313   0.778  25.661
ATOM    237  H4* DA      8      -9.875   0.143  24.974
ATOM    238  O4* DA      8      -7.926   0.532  25.455
ATOM    239  C1* DA      8      -7.307   0.195  26.685
ATOM    240  H1* DA      8      -7.064  -0.872  26.678
ATOM    241  N9  DA      8      -6.055   0.983  26.811
ATOM    242  C8  DA      8      -5.863   2.261  27.293
ATOM    243  H8  DA      8      -6.675   2.873  27.671
ATOM    244  N7  DA      8      -4.629   2.693  27.213
ATOM    245  C5  DA      8      -3.954   1.602  26.642
ATOM    246  C6  DA      8      -2.616   1.340  26.251
ATOM    247  N6  DA      8      -1.612   2.190  26.338
ATOM    248 1H6  DA      8      -0.708   1.877  26.024
ATOM    249 2H6  DA      8      -1.770   3.114  26.711
ATOM    250  N1  DA      8      -2.264   0.166  25.728
ATOM    251  C2  DA      8      -3.205  -0.748  25.561
ATOM    252  H2  DA      8      -2.884  -1.691  25.138
ATOM    253  N3  DA      8      -4.496  -0.649  25.851
ATOM    254  C4  DA      8      -4.811   0.560  26.401
ATOM    255  C3* DA      8      -9.679   0.370  27.097
ATOM    256  H3* DA      8     -10.384   1.077  27.540
ATOM    257  C2* DA      8      -8.324   0.456  27.800
ATOM    258 1H2* DA      8      -8.222   1.459  28.207
ATOM    259 2H2* DA      8      -8.213  -0.266  28.607
ATOM    260  O3* DA      8     -10.265  -0.927  27.027
ATOM    261  P   DG      9     -10.606  -1.857  28.302
ATOM    262  O1P DG      9     -11.854  -2.603  28.004
ATOM    263  O2P DG      9     -10.529  -1.059  29.551
ATOM    264  O5* DG      9      -9.371  -2.892  28.263
ATOM    265  C5* DG      9      -9.173  -3.717  27.117
ATOM    266 1H5* DG      9      -9.026  -3.085  26.239
ATOM    267 2H5* DG      9     -10.068  -4.317  26.949
ATOM    268  C4* DG      9      -7.974  -4.670  27.216
ATOM    269  H4* DG      9      -8.014  -5.332  26.349
ATOM    270  O4* DG      9      -6.762  -3.925  27.154
ATOM    271  C1* DG      9      -5.943  -4.277  28.254
ATOM    272  H1* DG      9      -5.251  -5.072  27.961
ATOM    273  N9  DG      9      -5.181  -3.082  28.686
ATOM    274  C8  DG      9      -5.631  -1.964  29.348
ATOM    275  H8  DG      9      -6.666  -1.850  29.652
ATOM    276  N7  DG      9      -4.715  -1.056  29.561
ATOM    277  C5  DG      9      -3.560  -1.618  28.995
ATOM    278  C6  DG      9      -2.212  -1.120  28.870
ATOM    279  O6  DG      9      -1.743  -0.037  29.220
ATOM    280  N1  DG      9      -1.355  -2.002  28.245
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ATOM    281  H1  DG      9      -0.404  -1.699  28.100
ATOM    282  C2  DG      9      -1.740  -3.194  27.734
ATOM    283  N2  DG      9      -0.835  -3.901  27.116
ATOM    284 1H2  DG      9      -1.109  -4.794  26.748
ATOM    285 2H2  DG      9       0.137  -3.601  27.113
ATOM    286  N3  DG      9      -2.972  -3.688  27.806
ATOM    287  C4  DG      9      -3.842  -2.856  28.456
ATOM    288  C3* DG      9      -7.959  -5.534  28.488
ATOM    289  H3* DG      9      -8.925  -5.510  28.996
ATOM    290  C2* DG      9      -6.893  -4.820  29.321
ATOM    291 1H2* DG      9      -7.370  -4.006  29.867
ATOM    292 2H2* DG      9      -6.384  -5.480  30.018
ATOM    293  O3* DG      9      -7.633  -6.868  28.105
ATOM    294  P   DT     10      -7.345  -8.066  29.148
ATOM    295  O1P DT     10      -7.801  -9.334  28.526
ATOM    296  O2P DT     10      -7.862  -7.698  30.489
ATOM    297  O5* DT     10      -5.734  -8.072  29.195
ATOM    298  C5* DT     10      -4.984  -8.307  28.006
ATOM    299 1H5* DT     10      -5.243  -7.552  27.261
ATOM    300 2H5* DT     10      -5.251  -9.283  27.598
ATOM    301  C4* DT     10      -3.464  -8.270  28.209
ATOM    302  H4* DT     10      -2.999  -8.522  27.253
ATOM    303  O4* DT     10      -3.060  -6.955  28.576
ATOM    304  C1* DT     10      -2.232  -7.037  29.722
ATOM    305  H1* DT     10      -1.193  -7.168  29.404
ATOM    306  N1  DT     10      -2.378  -5.793  30.528
ATOM    307  C6  DT     10      -3.573  -5.477  31.142
ATOM    308  H6  DT     10      -4.407  -6.162  31.062
ATOM    309  C5  DT     10      -3.730  -4.303  31.812
ATOM    310  C7  DT     10      -5.060  -4.011  32.482
ATOM    311 1H7  DT     10      -5.631  -4.924  32.643
ATOM    312 2H7  DT     10      -4.890  -3.540  33.448
ATOM    313 3H7  DT     10      -5.642  -3.324  31.872
ATOM    314  C4  DT     10      -2.630  -3.345  31.904
ATOM    315  O4  DT     10      -2.651  -2.246  32.456
ATOM    316  N3  DT     10      -1.471  -3.745  31.288
ATOM    317  H3  DT     10      -0.675  -3.129  31.358
ATOM    318  C2  DT     10      -1.280  -4.925  30.611
ATOM    319  O2  DT     10      -0.176  -5.156  30.126
ATOM    320  C3* DT     10      -2.949  -9.255  29.273
ATOM    321  H3* DT     10      -3.714  -9.988  29.538
ATOM    322  C2* DT     10      -2.669  -8.313  30.442
ATOM    323 1H2* DT     10      -3.592  -8.165  30.999
ATOM    324 2H2* DT     10      -1.899  -8.689  31.108
ATOM    325  O3* DT     10      -1.789  -9.903  28.758
ATOM    326  P   DC     11      -0.920 -10.989  29.580
ATOM    327  O1P DC     11      -0.554 -12.085  28.648
ATOM    328  O2P DC     11      -1.610 -11.329  30.849
ATOM    329  O5* DC     11       0.412 -10.151  29.934
ATOM    330  C5* DC     11       1.266  -9.677  28.895
ATOM    331 1H5* DC     11       0.689  -9.047  28.216
ATOM    332 2H5* DC     11       1.641 -10.528  28.323
ATOM    333  C4* DC     11       2.472  -8.862  29.389
ATOM    334  H4* DC     11       3.064  -8.591  28.512
ATOM    335  O4* DC     11       2.018  -7.667  30.019
ATOM    336  C1* DC     11       2.532  -7.609  31.340
ATOM    337  H1* DC     11       3.449  -7.010  31.338
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ATOM    338  N1  DC     11       1.513  -6.998  32.241
ATOM    339  C6  DC     11       0.318  -7.629  32.492
ATOM    340  H6  DC     11       0.122  -8.590  32.030
ATOM    341  C5  DC     11      -0.611  -7.042  33.289
ATOM    342  H5  DC     11      -1.552  -7.535  33.477
ATOM    343  C4  DC     11      -0.291  -5.770  33.833
ATOM    344  N4  DC     11      -1.148  -5.133  34.575
ATOM    345 1H4  DC     11      -2.034  -5.549  34.796
ATOM    346 2H4  DC     11      -0.875  -4.215  34.913
ATOM    347  N3  DC     11       0.844  -5.147  33.609
ATOM    348  C2  DC     11       1.765  -5.745  32.815
ATOM    349  O2  DC     11       2.825  -5.142  32.648
ATOM    350  C3* DC     11       3.384  -9.610  30.375
ATOM    351  H3* DC     11       3.217 -10.689  30.326
ATOM    352  C2* DC     11       2.906  -9.046  31.710
ATOM    353 1H2* DC     11       2.040  -9.618  32.039
ATOM    354 2H2* DC     11       3.671  -9.084  32.479
ATOM    355  O3* DC     11       4.743  -9.299  30.070
ATOM    356  P   DC3    12       6.000  -9.833  30.933
ATOM    357  O1P DC3    12       7.126 -10.081  29.999
ATOM    358  O2P DC3    12       5.557 -10.935  31.823
ATOM    359  O5* DC3    12       6.369  -8.558  31.852
ATOM    360  C5* DC3    12       6.826  -7.342  31.263
ATOM    361 1H5* DC3    12       6.038  -6.926  30.633
ATOM    362 2H5* DC3    12       7.686  -7.553  30.627
ATOM    363  C4* DC3    12       7.248  -6.276  32.288
ATOM    364  H4* DC3    12       7.690  -5.441  31.741
ATOM    365  O4* DC3    12       6.103  -5.808  32.993
ATOM    366  C1* DC3    12       6.338  -5.918  34.387
ATOM    367  H1* DC3    12       6.752  -4.972  34.750
ATOM    368  N1  DC3    12       5.053  -6.227  35.073
ATOM    369  C6  DC3    12       4.341  -7.356  34.753
ATOM    370  H6  DC3    12       4.762  -8.050  34.036
ATOM    371  C5  DC3    12       3.124  -7.578  35.312
ATOM    372  H5  DC3    12       2.560  -8.460  35.051
ATOM    373  C4  DC3    12       2.640  -6.599  36.223
ATOM    374  N4  DC3    12       1.471  -6.730  36.779
ATOM    375 1H4  DC3    12       0.896  -7.524  36.560
ATOM    376 2H4  DC3    12       1.153  -5.974  37.377
ATOM    377  N3  DC3    12       3.318  -5.525  36.570
ATOM    378  C2  DC3    12       4.540  -5.327  36.017
ATOM    379  O2  DC3    12       5.169  -4.337  36.393
ATOM    380  C3* DC3    12       8.270  -6.786  33.320
ATOM    381  H3* DC3    12       8.723  -7.726  32.989
ATOM    382  C2* DC3    12       7.406  -7.003  34.557
ATOM    383 1H2* DC3    12       6.974  -8.002  34.520
ATOM    384 2H2* DC3    12       7.966  -6.874  35.484
ATOM    385  O3* DC3    12       9.274  -5.808  33.588
ATOM    386  H3T DC3    12       9.973  -6.205  34.147
TER
ATOM    387  H5T DG5    13      -2.332   2.625  43.072
ATOM    388  O5* DG5    13      -1.686   2.530  42.341
ATOM    389  C5* DG5    13      -0.371   2.798  42.829
ATOM    390 1H5* DG5    13      -0.095   2.040  43.564
ATOM    391 2H5* DG5    13      -0.367   3.766  43.335
ATOM    392  C4* DG5    13       0.708   2.829  41.729
ATOM    393  H4* DG5    13       1.601   3.283  42.163
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ATOM    394  O4* DG5    13       1.037   1.503  41.323
ATOM    395  C1* DG5    13       0.955   1.411  39.910
ATOM    396  H1* DG5    13       1.934   1.611  39.466
ATOM    397  N9  DG5    13       0.507   0.045  39.547
ATOM    398  C8  DG5    13      -0.710  -0.550  39.784
ATOM    399  H8  DG5    13      -1.533  -0.017  40.247
ATOM    400  N7  DG5    13      -0.771  -1.812  39.443
ATOM    401  C5  DG5    13       0.507  -2.073  38.925
ATOM    402  C6  DG5    13       1.101  -3.279  38.402
ATOM    403  O6  DG5    13       0.615  -4.407  38.289
ATOM    404  N1  DG5    13       2.407  -3.114  37.985
ATOM    405  H1  DG5    13       2.865  -3.917  37.580
ATOM    406  C2  DG5    13       3.086  -1.945  38.078
ATOM    407  N2  DG5    13       4.312  -1.932  37.634
ATOM    408 1H2  DG5    13       4.806  -1.056  37.644
ATOM    409 2H2  DG5    13       4.709  -2.762  37.201
ATOM    410  N3  DG5    13       2.591  -0.813  38.569
ATOM    411  C4  DG5    13       1.290  -0.937  38.977
ATOM    412  C3* DG5    13       0.310   3.631  40.478
ATOM    413  H3* DG5    13      -0.570   4.250  40.666
ATOM    414  C2* DG5    13      -0.012   2.514  39.486
ATOM    415 1H2* DG5    13      -1.044   2.199  39.634
ATOM    416 2H2* DG5    13       0.137   2.811  38.451
ATOM    417  O3* DG5    13       1.418   4.444  40.110
ATOM    418  P   DG     14       1.419   5.441  38.844
ATOM    419  O1P DG     14       2.123   6.686  39.240
ATOM    420  O2P DG     14       0.051   5.537  38.275
ATOM    421  O5* DG     14       2.350   4.629  37.813
ATOM    422  C5* DG     14       3.705   4.334  38.142
ATOM    423 1H5* DG     14       3.731   3.684  39.018
ATOM    424 2H5* DG     14       4.223   5.259  38.401
ATOM    425  C4* DG     14       4.491   3.656  37.012
ATOM    426  H4* DG     14       5.540   3.636  37.314
ATOM    427  O4* DG     14       4.046   2.313  36.841
ATOM    428  C1* DG     14       3.579   2.141  35.512
ATOM    429  H1* DG     14       4.362   1.676  34.907
ATOM    430  N9  DG     14       2.382   1.268  35.531
ATOM    431  C8  DG     14       1.111   1.557  35.968
ATOM    432  H8  DG     14       0.835   2.542  36.326
ATOM    433  N7  DG     14       0.286   0.543  35.940
ATOM    434  C5  DG     14       1.070  -0.499  35.421
ATOM    435  C6  DG     14       0.766  -1.880  35.147
ATOM    436  O6  DG     14      -0.281  -2.500  35.341
ATOM    437  N1  DG     14       1.821  -2.579  34.598
ATOM    438  H1  DG     14       1.641  -3.528  34.307
ATOM    439  C2  DG     14       3.039  -2.038  34.355
ATOM    440  N2  DG     14       3.924  -2.794  33.769
ATOM    441 1H2  DG     14       4.798  -2.371  33.514
ATOM    442 2H2  DG     14       3.653  -3.704  33.404
ATOM    443  N3  DG     14       3.377  -0.778  34.614
ATOM    444  C4  DG     14       2.347  -0.053  35.149
ATOM    445  C3* DG     14       4.382   4.379  35.660
ATOM    446  H3* DG     14       4.051   5.413  35.786
ATOM    447  C2* DG     14       3.307   3.542  34.968
ATOM    448 1H2* DG     14       2.327   3.900  35.280
ATOM    449 2H2* DG     14       3.374   3.579  33.886
ATOM    450  O3* DG     14       5.668   4.339  35.049
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ATOM    451  P   DA     15       5.986   4.865  33.559
ATOM    452  O1P DA     15       7.314   5.527  33.581
ATOM    453  O2P DA     15       4.821   5.612  33.025
ATOM    454  O5* DA     15       6.119   3.474  32.759
ATOM    455  C5* DA     15       7.107   2.519  33.139
ATOM    456 1H5* DA     15       6.908   2.177  34.155
ATOM    457 2H5* DA     15       8.087   3.000  33.136
ATOM    458  C4* DA     15       7.188   1.288  32.223
ATOM    459  H4* DA     15       8.042   0.697  32.559
ATOM    460  O4* DA     15       6.014   0.488  32.344
ATOM    461  C1* DA     15       5.335   0.440  31.097
ATOM    462  H1* DA     15       5.499  -0.535  30.626
ATOM    463  N9  DA     15       3.888   0.645  31.338
ATOM    464  C8  DA     15       3.248   1.786  31.761
ATOM    465  H8  DA     15       3.773   2.725  31.894
ATOM    466  N7  DA     15       1.974   1.631  32.021
ATOM    467  C5  DA     15       1.761   0.276  31.716
ATOM    468  C6  DA     15       0.654  -0.604  31.791
ATOM    469  N6  DA     15      -0.532  -0.283  32.273
ATOM    470 1H6  DA     15      -1.257  -0.990  32.309
ATOM    471 2H6  DA     15      -0.698   0.659  32.588
ATOM    472  N1  DA     15       0.756  -1.879  31.415
ATOM    473  C2  DA     15       1.929  -2.306  30.966
ATOM    474  H2  DA     15       1.976  -3.344  30.662
ATOM    475  N3  DA     15       3.057  -1.613  30.856
ATOM    476  C4  DA     15       2.910  -0.319  31.262
ATOM    477  C3* DA     15       7.387   1.633  30.740
ATOM    478  H3* DA     15       7.766   2.650  30.616
ATOM    479  C2* DA     15       5.954   1.528  30.218
ATOM    480 1H2* DA     15       5.457   2.484  30.374
ATOM    481 2H2* DA     15       5.904   1.272  29.165
ATOM    482  O3* DA     15       8.312   0.694  30.201
ATOM    483  P   DC     16       8.626   0.527  28.630
ATOM    484  O1P DC     16      10.015   0.025  28.490
ATOM    485  O2P DC     16       8.228   1.761  27.907
ATOM    486  O5* DC     16       7.612  -0.660  28.234
ATOM    487  C5* DC     16       7.672  -1.909  28.918
ATOM    488 1H5* DC     16       7.437  -1.758  29.972
ATOM    489 2H5* DC     16       8.688  -2.303  28.856
ATOM    490  C4* DC     16       6.718  -2.973  28.361
ATOM    491  H4* DC     16       6.913  -3.900  28.904
ATOM    492  O4* DC     16       5.367  -2.600  28.591
ATOM    493  C1* DC     16       4.646  -2.647  27.371
ATOM    494  H1* DC     16       4.165  -3.626  27.272
ATOM    495  N1  DC     16       3.627  -1.560  27.407
ATOM    496  C6  DC     16       4.003  -0.251  27.591
ATOM    497  H6  DC     16       5.056   0.006  27.541
ATOM    498  C5  DC     16       3.071   0.691  27.885
ATOM    499  H5  DC     16       3.370   1.713  28.061
ATOM    500  C4  DC     16       1.721   0.261  27.987
ATOM    501  N4  DC     16       0.792   1.085  28.377
ATOM    502 1H4  DC     16       1.034   2.026  28.629
ATOM    503 2H4  DC     16      -0.140   0.712  28.528
ATOM    504  N3  DC     16       1.329  -0.972  27.757
ATOM    505  C2  DC     16       2.268  -1.898  27.443
ATOM    506  O2  DC     16       1.866  -3.035  27.194
ATOM    507  C3* DC     16       6.902  -3.229  26.861
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ATOM    508  H3* DC     16       7.834  -2.787  26.500
ATOM    509  C2* DC     16       5.690  -2.514  26.260
ATOM    510 1H2* DC     16       5.951  -1.471  26.086
ATOM    511 2H2* DC     16       5.354  -2.969  25.331
ATOM    512  O3* DC     16       6.910  -4.637  26.665
ATOM    513  P   DT     17       7.174  -5.322  25.235
ATOM    514  O1P DT     17       7.878  -6.608  25.468
ATOM    515  O2P DT     17       7.784  -4.331  24.315
ATOM    516  O5* DT     17       5.681  -5.634  24.725
ATOM    517  C5* DT     17       4.862  -6.591  25.392
ATOM    518 1H5* DT     17       4.588  -6.215  26.379
ATOM    519 2H5* DT     17       5.419  -7.519  25.529
ATOM    520  C4* DT     17       3.586  -6.927  24.609
ATOM    521  H4* DT     17       3.174  -7.852  25.016
ATOM    522  O4* DT     17       2.637  -5.884  24.793
ATOM    523  C1* DT     17       2.108  -5.512  23.535
ATOM    524  H1* DT     17       1.236  -6.137  23.318
ATOM    525  N1  DT     17       1.719  -4.070  23.578
ATOM    526  C6  DT     17       2.676  -3.073  23.641
ATOM    527  H6  DT     17       3.723  -3.344  23.649
ATOM    528  C5  DT     17       2.324  -1.763  23.721
ATOM    529  C7  DT     17       3.410  -0.701  23.776
ATOM    530 1H7  DT     17       4.402  -1.142  23.677
ATOM    531 2H7  DT     17       3.255   0.011  22.965
ATOM    532 3H7  DT     17       3.342  -0.161  24.720
ATOM    533  C4  DT     17       0.916  -1.367  23.749
ATOM    534  O4  DT     17       0.486  -0.217  23.825
ATOM    535  N3  DT     17       0.023  -2.414  23.688
ATOM    536  H3  DT     17      -0.951  -2.178  23.679
ATOM    537  C2  DT     17       0.352  -3.750  23.615
ATOM    538  O2  DT     17      -0.551  -4.587  23.582
ATOM    539  C3* DT     17       3.835  -7.119  23.100
ATOM    540  H3* DT     17       4.905  -7.136  22.886
ATOM    541  C2* DT     17       3.193  -5.864  22.513
ATOM    542 1H2* DT     17       3.956  -5.091  22.444
ATOM    543 2H2* DT     17       2.763  -6.045  21.534
ATOM    544  O3* DT     17       3.238  -8.325  22.635
ATOM    545  P   DA     18       3.460  -8.882  21.131
ATOM    546  O1P DA     18       3.494 -10.364  21.193
ATOM    547  O2P DA     18       4.597  -8.167  20.500
ATOM    548  O5* DA     18       2.113  -8.436  20.370
ATOM    549  C5* DA     18       0.850  -8.922  20.806
ATOM    550 1H5* DA     18       0.699  -8.642  21.849
ATOM    551 2H5* DA     18       0.844 -10.011  20.747
ATOM    552  C4* DA     18      -0.337  -8.389  19.992
ATOM    553  H4* DA     18      -1.235  -8.844  20.413
ATOM    554  O4* DA     18      -0.443  -6.976  20.136
ATOM    555  C1* DA     18      -0.204  -6.338  18.891
ATOM    556  H1* DA     18      -1.131  -5.860  18.561
ATOM    557  N9  DA     18       0.836  -5.292  19.071
ATOM    558  C8  DA     18       2.210  -5.408  19.036
ATOM    559  H8  DA     18       2.713  -6.354  18.864
ATOM    560  N7  DA     18       2.857  -4.295  19.271
ATOM    561  C5  DA     18       1.820  -3.369  19.467
ATOM    562  C6  DA     18       1.760  -1.987  19.774
ATOM    563  N6  DA     18       2.803  -1.202  19.969
ATOM    564 1H6  DA     18       2.629  -0.233  20.179
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ATOM    565 2H6  DA     18       3.734  -1.582  19.893
ATOM    566  N1  DA     18       0.594  -1.357  19.904
ATOM    567  C2  DA     18      -0.515  -2.061  19.732
ATOM    568  H2  DA     18      -1.443  -1.512  19.800
ATOM    569  N3  DA     18      -0.628  -3.355  19.447
ATOM    570  C4  DA     18       0.591  -3.962  19.334
ATOM    571  C3* DA     18      -0.283  -8.733  18.495
ATOM    572  H3* DA     18       0.449  -9.523  18.306
ATOM    573  C2* DA     18       0.174  -7.417  17.870
ATOM    574 1H2* DA     18       1.249  -7.468  17.715
ATOM    575 2H2* DA     18      -0.309  -7.224  16.916
ATOM    576  O3* DA     18      -1.578  -9.155  18.086
ATOM    577  P   DG     19      -1.937  -9.658  16.593
ATOM    578  O1P DG     19      -2.610 -10.977  16.697
ATOM    579  O2P DG     19      -0.755  -9.522  15.707
ATOM    580  O5* DG     19      -3.028  -8.554  16.158
ATOM    581  C5* DG     19      -4.265  -8.458  16.858
ATOM    582 1H5* DG     19      -4.065  -8.352  17.925
ATOM    583 2H5* DG     19      -4.828  -9.382  16.717
ATOM    584  C4* DG     19      -5.155  -7.280  16.433
ATOM    585  H4* DG     19      -6.094  -7.374  16.982
ATOM    586  O4* DG     19      -4.537  -6.051  16.804
ATOM    587  C1* DG     19      -4.285  -5.279  15.639
ATOM    588  H1* DG     19      -5.048  -4.499  15.554
ATOM    589  N9  DG     19      -2.947  -4.648  15.745
ATOM    590  C8  DG     19      -1.709  -5.200  15.511
ATOM    591  H8  DG     19      -1.581  -6.233  15.208
ATOM    592  N7  DG     19      -0.707  -4.383  15.708
ATOM    593  C5  DG     19      -1.332  -3.188  16.095
ATOM    594  C6  DG     19      -0.794  -1.901  16.458
ATOM    595  O6  DG     19       0.380  -1.541  16.534
ATOM    596  N1  DG     19      -1.759  -0.969  16.785
ATOM    597  H1  DG     19      -1.454  -0.054  17.080
ATOM    598  C2  DG     19      -3.087  -1.228  16.776
ATOM    599  N2  DG     19      -3.888  -0.260  17.129
ATOM    600 1H2  DG     19      -4.876  -0.440  17.106
ATOM    601 2H2  DG     19      -3.524   0.648  17.412
ATOM    602  N3  DG     19      -3.633  -2.396  16.448
ATOM    603  C4  DG     19      -2.702  -3.344  16.119
ATOM    604  C3* DG     19      -5.476  -7.222  14.930
ATOM    605  H3* DG     19      -5.338  -8.197  14.457
ATOM    606  C2* DG     19      -4.423  -6.228  14.447
ATOM    607 1H2* DG     19      -3.496  -6.768  14.261
ATOM    608 2H2* DG     19      -4.716  -5.703  13.542
ATOM    609  O3* DG     19      -6.826  -6.785  14.791
ATOM    610  P   DC     20      -7.528  -6.428  13.383
ATOM    611  O1P DC     20      -8.940  -6.882  13.449
ATOM    612  O2P DC     20      -6.677  -6.899  12.262
ATOM    613  O5* DC     20      -7.506  -4.815  13.407
ATOM    614  C5* DC     20      -8.233  -4.101  14.406
ATOM    615 1H5* DC     20      -7.871  -4.394  15.393
ATOM    616 2H5* DC     20      -9.288  -4.375  14.344
ATOM    617  C4* DC     20      -8.134  -2.572  14.293
ATOM    618  H4* DC     20      -8.794  -2.142  15.049
ATOM    619  O4* DC     20      -6.798  -2.154  14.564
ATOM    620  C1* DC     20      -6.335  -1.349  13.493
ATOM    621  H1* DC     20      -6.521  -0.294  13.726
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ATOM    622  N1  DC     20      -4.878  -1.592  13.286
ATOM    623  C6  DC     20      -4.418  -2.829  12.904
ATOM    624  H6  DC     20      -5.129  -3.635  12.759
ATOM    625  C5  DC     20      -3.089  -3.039  12.728
ATOM    626  H5  DC     20      -2.729  -4.013  12.435
ATOM    627  C4  DC     20      -2.220  -1.942  12.967
ATOM    628  N4  DC     20      -0.931  -2.088  12.880
ATOM    629 1H4  DC     20      -0.542  -2.982  12.642
ATOM    630 2H4  DC     20      -0.352  -1.288  13.115
ATOM    631  N3  DC     20      -2.634  -0.753  13.347
ATOM    632  C2  DC     20      -3.964  -0.552  13.507
ATOM    633  O2  DC     20      -4.313   0.578  13.845
ATOM    634  C3* DC     20      -8.552  -2.025  12.918
ATOM    635  H3* DC     20      -9.088  -2.783  12.342
ATOM    636  C2* DC     20      -7.196  -1.730  12.287
ATOM    637 1H2* DC     20      -6.840  -2.642  11.812
ATOM    638 2H2* DC     20      -7.238  -0.930  11.553
ATOM    639  O3* DC     20      -9.366  -0.868  13.090
ATOM    640  P   DT     21      -9.958  -0.010  11.855
ATOM    641  O1P DT     21     -11.283   0.522  12.261
ATOM    642  O2P DT     21      -9.861  -0.808  10.608
ATOM    643  O5* DT     21      -8.922   1.220  11.752
ATOM    644  C5* DT     21      -8.801   2.154  12.821
ATOM    645 1H5* DT     21      -8.481   1.632  13.724
ATOM    646 2H5* DT     21      -9.776   2.603  13.020
ATOM    647  C4* DT     21      -7.805   3.287  12.538
ATOM    648  H4* DT     21      -7.879   4.005  13.356
ATOM    649  O4* DT     21      -6.483   2.760  12.516
ATOM    650  C1* DT     21      -5.824   3.227  11.353
ATOM    651  H1* DT     21      -5.339   4.182  11.578
ATOM    652  N1  DT     21      -4.816   2.220  10.918
ATOM    653  C6  DT     21      -5.201   0.988  10.422
ATOM    654  H6  DT     21      -6.254   0.751  10.348
ATOM    655  C5  DT     21      -4.280   0.064  10.038
ATOM    656  C7  DT     21      -4.765  -1.261   9.474
ATOM    657 1H7  DT     21      -3.923  -1.854   9.119
ATOM    658 2H7  DT     21      -5.273  -1.832  10.247
ATOM    659 3H7  DT     21      -5.440  -1.084   8.636
ATOM    660  C4  DT     21      -2.852   0.348  10.155
ATOM    661  O4  DT     21      -1.926  -0.399   9.848
ATOM    662  N3  DT     21      -2.552   1.587  10.667
ATOM    663  H3  DT     21      -1.575   1.819  10.768
ATOM    664  C2  DT     21      -3.459   2.549  11.041
ATOM    665  O2  DT     21      -3.041   3.635  11.443
ATOM    666  C3* DT     21      -8.060   4.029  11.213
ATOM    667  H3* DT     21      -9.035   3.764  10.796
ATOM    668  C2* DT     21      -6.933   3.492  10.334
ATOM    669 1H2* DT     21      -7.275   2.574   9.860
ATOM    670 2H2* DT     21      -6.617   4.198   9.571
ATOM    671  O3* DT     21      -7.988   5.432  11.447
ATOM    672  P   DA     22      -8.170   6.538  10.285
ATOM    673  O1P DA     22      -8.913   7.688  10.859
ATOM    674  O2P DA     22      -8.691   5.892   9.055
ATOM    675  O5* DA     22      -6.648   6.994  10.016
ATOM    676  C5* DA     22      -5.903   7.648  11.040
ATOM    677 1H5* DA     22      -5.807   6.983  11.900
ATOM    678 2H5* DA     22      -6.445   8.538  11.363
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ATOM    679  C4* DA     22      -4.497   8.086  10.607
ATOM    680  H4* DA     22      -4.085   8.696  11.413
ATOM    681  O4* DA     22      -3.659   6.948  10.436
ATOM    682  C1* DA     22      -3.047   7.005   9.159
ATOM    683  H1* DA     22      -2.059   7.468   9.237
ATOM    684  N9  DA     22      -2.927   5.628   8.627
ATOM    685  C8  DA     22      -3.935   4.770   8.253
ATOM    686  H8  DA     22      -4.980   5.047   8.321
ATOM    687  N7  DA     22      -3.526   3.602   7.826
ATOM    688  C5  DA     22      -2.128   3.717   7.913
ATOM    689  C6  DA     22      -1.036   2.868   7.611
ATOM    690  N6  DA     22      -1.151   1.638   7.148
ATOM    691 1H6  DA     22      -0.316   1.090   6.981
ATOM    692 2H6  DA     22      -2.069   1.255   6.990
ATOM    693  N1  DA     22       0.225   3.272   7.778
ATOM    694  C2  DA     22       0.429   4.488   8.268
ATOM    695  H2  DA     22       1.463   4.782   8.400
ATOM    696  N3  DA     22      -0.484   5.388   8.618
ATOM    697  C4  DA     22      -1.756   4.941   8.406
ATOM    698  C3* DA     22      -4.475   8.914   9.312
ATOM    699  H3* DA     22      -5.478   9.246   9.036
ATOM    700  C2* DA     22      -3.951   7.891   8.304
ATOM    701 1H2* DA     22      -4.797   7.325   7.917
ATOM    702 2H2* DA     22      -3.407   8.344   7.477
ATOM    703  O3* DA     22      -3.625  10.036   9.523
ATOM    704  P   DG     23      -3.228  11.089   8.370
ATOM    705  O1P DG     23      -3.019  12.413   9.008
ATOM    706  O2P DG     23      -4.184  10.979   7.241
ATOM    707  O5* DG     23      -1.799  10.517   7.897
ATOM    708  C5* DG     23      -0.713  10.433   8.816
ATOM    709 1H5* DG     23      -0.955   9.722   9.607
ATOM    710 2H5* DG     23      -0.558  11.409   9.279
ATOM    711  C4* DG     23       0.609  10.007   8.162
ATOM    712  H4* DG     23       1.408  10.170   8.889
ATOM    713  O4* DG     23       0.569   8.622   7.832
ATOM    714  C1* DG     23       0.962   8.467   6.479
ATOM    715  H1* DG     23       2.048   8.343   6.420
ATOM    716  N9  DG     23       0.290   7.289   5.883
ATOM    717  C8  DG     23      -1.048   7.096   5.640
ATOM    718  H8  DG     23      -1.791   7.846   5.885
ATOM    719  N7  DG     23      -1.341   5.936   5.112
ATOM    720  C5  DG     23      -0.090   5.312   4.983
ATOM    721  C6  DG     23       0.288   4.019   4.469
ATOM    722  O6  DG     23      -0.425   3.121   4.018
ATOM    723  N1  DG     23       1.649   3.789   4.500
ATOM    724  H1  DG     23       1.976   2.906   4.139
ATOM    725  C2  DG     23       2.553   4.682   4.967
ATOM    726  N2  DG     23       3.814   4.364   4.871
ATOM    727 1H2  DG     23       4.490   5.027   5.208
ATOM    728 2H2  DG     23       4.092   3.460   4.495
ATOM    729  N3  DG     23       2.254   5.879   5.463
ATOM    730  C4  DG     23       0.912   6.140   5.446
ATOM    731  C3* DG     23       0.935  10.801   6.885
ATOM    732  H3* DG     23       0.309  11.692   6.801
ATOM    733  C2* DG     23       0.578   9.781   5.805
ATOM    734 1H2* DG     23      -0.495   9.819   5.618
ATOM    735 2H2* DG     23       1.119   9.943   4.878
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ATOM    736  O3* DG     23       2.313  11.163   6.912
ATOM    737  P   DC3    24       3.043  11.978   5.727
ATOM    738  O1P DC3    24       4.018  12.911   6.345
ATOM    739  O2P DC3    24       2.026  12.522   4.794
ATOM    740  O5* DC3    24       3.859  10.815   4.967
ATOM    741  C5* DC3    24       4.895  10.098   5.635
ATOM    742 1H5* DC3    24       4.472   9.557   6.484
ATOM    743 2H5* DC3    24       5.629  10.807   6.021
ATOM    744  C4* DC3    24       5.633   9.095   4.734
ATOM    745  H4* DC3    24       6.477   8.694   5.299
ATOM    746  O4* DC3    24       4.757   8.027   4.392
ATOM    747  C1* DC3    24       4.742   7.877   2.983
ATOM    748  H1* DC3    24       5.505   7.144   2.700
ATOM    749  N1  DC3    24       3.391   7.420   2.552
ATOM    750  C6  DC3    24       2.276   8.181   2.805
ATOM    751  H6  DC3    24       2.399   9.140   3.294
ATOM    752  C5  DC3    24       1.044   7.719   2.469
ATOM    753  H5  DC3    24       0.167   8.312   2.680
ATOM    754  C4  DC3    24       0.975   6.439   1.857
ATOM    755  N4  DC3    24      -0.171   5.910   1.545
ATOM    756 1H4  DC3    24      -1.024   6.401   1.748
ATOM    757 2H4  DC3    24      -0.163   4.982   1.133
ATOM    758  N3  DC3    24       2.030   5.698   1.592
ATOM    759  C2  DC3    24       3.254   6.176   1.924
ATOM    760  O2  DC3    24       4.223   5.470   1.641
ATOM    761  C3* DC3    24       6.162   9.722   3.431
ATOM    762  H3* DC3    24       6.159  10.814   3.494
ATOM    763  C2* DC3    24       5.150   9.234   2.401
ATOM    764 1H2* DC3    24       4.309   9.927   2.369
ATOM    765 2H2* DC3    24       5.585   9.129   1.406
ATOM    766  O3* DC3    24       7.464   9.235   3.110
ATOM    767  H3T DC3    24       7.833   9.760   2.370
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END
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**File E-3**: Average structure of rMD refined *R*-BD-N3-dU modified duplex 5′ - $G^{1}C^{2}T^{3}A^{4}G^{5}C^{6}X^{7}A^{8}G^{9}T^{10}C^{11}C^{12}$- 3′·5′ - $G^{13}G^{14}A^{15}C^{16}T^{17}T^{18}G^{19}C^{20}T^{21}A^{22}G^{23}C^{24}$ -3′.

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REMARK
ATOM      1  H5T DG5      1      -2.956  -8.103  -3.152
ATOM      2  O5* DG5      1      -2.147  -7.944  -2.622
ATOM      3  C5* DG5      1      -0.999  -8.357  -3.365
ATOM      4 1H5* DG5      1      -0.969  -7.823  -4.317
ATOM      5 2H5* DG5      1      -1.081  -9.424  -3.586
ATOM      6  C4* DG5      1       0.343  -8.122  -2.640
ATOM      7  H4* DG5      1       1.128  -8.561  -3.260
ATOM      8  O4* DG5      1       0.596  -6.724  -2.510
ATOM      9  C1* DG5      1       0.680  -6.383  -1.132
ATOM     10  H1* DG5      1       1.731  -6.275  -0.848
ATOM     11  N9  DG5      1      -0.034  -5.106  -0.889
ATOM     12  C8  DG5      1      -1.385  -4.853  -0.947
ATOM     13  H8  DG5      1      -2.106  -5.625  -1.195
ATOM     14  N7  DG5      1      -1.713  -3.610  -0.702
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ATOM     15  C5  DG5     1      -0.478  -2.987  -0.462
ATOM     16  C6  DG5     1      -0.138  -1.619  -0.157
ATOM     17  O6  DG5     1      -0.874  -0.637  -0.044
ATOM     18  N1  DG5     1       1.218  -1.411   0.004
ATOM     19  H1  DG5     1       1.518  -0.471   0.211
ATOM     20  C2  DG5     1       2.150  -2.386  -0.123
ATOM     21  N2  DG5     1       3.398  -2.045   0.039
ATOM     22 1H2  DG5     1       4.096  -2.766  -0.026
ATOM     23 2H2  DG5     1       3.641  -1.085   0.274
ATOM     24  N3  DG5     1       1.889  -3.657  -0.414
ATOM     25  C4  DG5     1       0.552  -3.900  -0.572
ATOM     26  C3* DG5     1       0.422  -8.750  -1.238
ATOM     27  H3* DG5     1      -0.320  -9.542  -1.120
ATOM     28  C2* DG5     1       0.083  -7.554  -0.352
ATOM     29 1H2* DG5     1      -1.000  -7.466  -0.273
ATOM     30 2H2* DG5     1       0.509  -7.635   0.642
ATOM     31  O3* DG5     1       1.736  -9.269  -1.041
ATOM     32  P   DC      2       2.243  -9.922   0.347
ATOM     33  O1P DC      2       3.227 -10.983   0.017
ATOM     34  O2P DC      2       1.070 -10.270   1.186
ATOM     35  O5* DC      2       3.026  -8.695   1.043
ATOM     36  C5* DC      2       4.194  -8.147   0.437
ATOM     37 1H5* DC      2       3.939  -7.747  -0.546
ATOM     38 2H5* DC      2       4.929  -8.940   0.295
ATOM     39  C4* DC      2       4.858  -7.031   1.257
ATOM     40  H4* DC      2       5.789  -6.763   0.753
ATOM     41  O4* DC      2       4.019  -5.880   1.291
ATOM     42  C1* DC      2       3.850  -5.463   2.636
ATOM     43  H1* DC      2       4.608  -4.711   2.882
ATOM     44  N1  DC      2       2.478  -4.901   2.793
ATOM     45  C6  DC      2       1.368  -5.688   2.603
ATOM     46  H6  DC      2       1.503  -6.738   2.368
ATOM     47  C5  DC      2       0.125  -5.152   2.687
ATOM     48  H5  DC      2      -0.744  -5.771   2.528
ATOM     49  C4  DC      2       0.035  -3.763   2.973
ATOM     50  N4  DC      2      -1.121  -3.169   3.016
ATOM     51 1H4  DC      2      -1.961  -3.694   2.852
ATOM     52 2H4  DC      2      -1.129  -2.168   3.179
ATOM     53  N3  DC      2       1.081  -2.988   3.157
ATOM     54  C2  DC      2       2.316  -3.538   3.075
ATOM     55  O2  DC      2       3.269  -2.784   3.262
ATOM     56  C3* DC      2       5.192  -7.442   2.701
ATOM     57  H3* DC      2       5.094  -8.522   2.833
ATOM     58  C2* DC      2       4.113  -6.705   3.492
ATOM     59 1H2* DC      2       3.234  -7.345   3.552
ATOM     60 2H2* DC      2       4.437  -6.441   4.495
ATOM     61  O3* DC      2       6.521  -7.028   3.001
ATOM     62  P   DT      3       7.214  -7.243   4.443
ATOM     63  O1P DT      3       8.669  -7.441   4.227
ATOM     64  O2P DT      3       6.457  -8.263   5.210
ATOM     65  O5* DT      3       6.991  -5.807   5.141
ATOM     66  C5* DT      3       7.593  -4.639   4.591
ATOM     67 1H5* DT      3       7.275  -4.519   3.554
ATOM     68 2H5* DT      3       8.677  -4.756   4.600
ATOM     69  C4* DT      3       7.241  -3.356   5.353
ATOM     70  H4* DT      3       7.816  -2.540   4.909
ATOM     71  O4* DT      3       5.856  -3.062   5.205
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ATOM     72  C1* DT      3       5.344  -2.685   6.471
ATOM     73  H1* DT      3       5.534  -1.620   6.636
ATOM     74  N1  DT      3       3.885  -2.977   6.537
ATOM     75  C6  DT      3       3.416  -4.268   6.389
ATOM     76  H6  DT      3       4.129  -5.068   6.239
ATOM     77  C5  DT      3       2.085  -4.541   6.420
ATOM     78  C7  DT      3       1.615  -5.978   6.266
ATOM     79 1H7  DT      3       2.449  -6.648   6.057
ATOM     80 2H7  DT      3       1.124  -6.294   7.186
ATOM     81 3H7  DT      3       0.889  -6.039   5.454
ATOM     82  C4  DT      3       1.112  -3.464   6.594
ATOM     83  O4  DT      3      -0.112  -3.578   6.610
ATOM     84  N3  DT      3       1.658  -2.213   6.749
ATOM     85  H3  DT      3       1.017  -1.443   6.873
ATOM     86  C2  DT      3       2.999  -1.912   6.752
ATOM     87  O2  DT      3       3.349  -0.750   6.953
ATOM     88  C3* DT      3       7.569  -3.417   6.856
ATOM     89  H3* DT      3       8.146  -4.312   7.100
ATOM     90  C2* DT      3       6.174  -3.483   7.474
ATOM     91 1H2* DT      3       5.857  -4.525   7.512
ATOM     92 2H2* DT      3       6.132  -3.052   8.470
ATOM     93  O3* DT      3       8.293  -2.242   7.204
ATOM     94  P   DA      4       8.838  -1.934   8.692
ATOM     95  O1P DA      4      10.222  -1.412   8.574
ATOM     96  O2P DA      4       8.585  -3.101   9.573
ATOM     97  O5* DA      4       7.871  -0.731   9.153
ATOM     98  C5* DA      4       7.897   0.517   8.465
ATOM     99 1H5* DA      4       7.624   0.361   7.420
ATOM    100 2H5* DA      4       8.912   0.916   8.489
ATOM    101  C4* DA      4       6.960   1.581   9.056
ATOM    102  H4* DA      4       7.139   2.510   8.512
ATOM    103  O4* DA      4       5.599   1.203   8.867
ATOM    104  C1* DA      4       4.946   1.131  10.125
ATOM    105  H1* DA      4       4.355   2.039  10.287
ATOM    106  N9  DA      4       4.068  -0.060  10.143
ATOM    107  C8  DA      4       4.434  -1.385  10.090
ATOM    108  H8  DA      4       5.473  -1.688  10.036
ATOM    109  N7  DA      4       3.433  -2.228  10.094
ATOM    110  C5  DA      4       2.317  -1.377  10.176
ATOM    111  C6  DA      4       0.916  -1.571  10.219
ATOM    112  N6  DA      4       0.319  -2.747  10.156
ATOM    113 1H6  DA      4      -0.693  -2.791  10.145
ATOM    114 2H6  DA      4       0.881  -3.580  10.095
ATOM    115  N1  DA      4       0.076  -0.538  10.316
ATOM    116  C2  DA      4       0.592   0.684  10.355
ATOM    117  H2  DA      4      -0.118   1.499  10.434
ATOM    118  N3  DA      4       1.873   1.028  10.301
ATOM    119  C4  DA      4       2.694  -0.059  10.212
ATOM    120  C3* DA      4       7.190   1.842  10.553
ATOM    121  H3* DA      4       8.155   1.446  10.877
ATOM    122  C2* DA      4       6.046   1.053  11.184
ATOM    123 1H2* DA      4       6.373   0.024  11.331
ATOM    124 2H2* DA      4       5.718   1.467  12.133
ATOM    125  O3* DA      4       7.133   3.247  10.778
ATOM    126  P   DG      5       7.257   3.918  12.239
ATOM    127  O1P DG      5       7.910   5.241  12.081
ATOM    128  O2P DG      5       7.844   2.938  13.186
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ATOM    129  O5* DG      5       5.712   4.150  12.631
ATOM    130  C5* DG      5       4.891   5.022  11.859
ATOM    131 1H5* DG      5       4.783   4.624  10.848
ATOM    132 2H5* DG      5       5.376   5.997  11.786
ATOM    133  C4* DG      5       3.493   5.238  12.456
ATOM    134  H4* DG      5       3.021   6.056  11.909
ATOM    135  O4* DG      5       2.699   4.066  12.295
ATOM    136  C1* DG      5       2.146   3.702  13.549
ATOM    137  H1* DG      5       1.155   4.152  13.666
ATOM    138  N9  DG      5       2.044   2.224  13.625
ATOM    139  C8  DG      5       3.066   1.306  13.661
ATOM    140  H8  DG      5       4.107   1.605  13.669
ATOM    141  N7  DG      5       2.675   0.059  13.659
ATOM    142  C5  DG      5       1.276   0.159  13.638
ATOM    143  C6  DG      5       0.250  -0.853  13.613
ATOM    144  O6  DG      5       0.368  -2.077  13.569
ATOM    145  N1  DG      5      -1.031  -0.341  13.623
ATOM    146  H1  DG      5      -1.792  -1.002  13.587
ATOM    147  C2  DG      5      -1.312   0.983  13.639
ATOM    148  N2  DG      5      -2.573   1.319  13.675
ATOM    149 1H2  DG      5      -2.799   2.298  13.666
ATOM    150 2H2  DG      5      -3.298   0.606  13.661
ATOM    151  N3  DG      5      -0.403   1.957  13.640
ATOM    152  C4  DG      5       0.882   1.482  13.639
ATOM    153  C3* DG      5       3.529   5.603  13.949
ATOM    154  H3* DG      5       4.542   5.868  14.264
ATOM    155  C2* DG      5       3.090   4.291  14.596
ATOM    156 1H2* DG      5       3.966   3.657  14.730
ATOM    157 2H2* DG      5       2.596   4.441  15.552
ATOM    158  O3* DG      5       2.643   6.692  14.183
ATOM    159  P   DC      6       2.439   7.368  15.634
ATOM    160  O1P DC      6       2.262   8.828  15.438
ATOM    161  O2P DC      6       3.499   6.892  16.558
ATOM    162  O5* DC      6       1.034   6.736  16.105
ATOM    163  C5* DC      6      -0.168   7.044  15.405
ATOM    164 1H5* DC      6      -0.080   6.719  14.367
ATOM    165 2H5* DC      6      -0.321   8.124  15.410
ATOM    166  C4* DC      6      -1.411   6.385  16.019
ATOM    167  H4* DC      6      -2.288   6.776  15.499
ATOM    168  O4* DC      6      -1.364   4.981  15.815
ATOM    169  C1* DC      6      -1.701   4.310  17.014
ATOM    170  H1* DC      6      -2.764   4.047  16.992
ATOM    171  N1  DC      6      -0.850   3.088  17.093
ATOM    172  C6  DC      6       0.520   3.189  17.085
ATOM    173  H6  DC      6       0.974   4.175  17.085
ATOM    174  C5  DC      6       1.287   2.070  17.046
ATOM    175  H5  DC      6       2.363   2.150  17.024
ATOM    176  C4  DC      6       0.612   0.820  17.013
ATOM    177  N4  DC      6       1.283  -0.287  16.890
ATOM    178 1H4  DC      6       2.284  -0.264  16.836
ATOM    179 2H4  DC      6       0.757  -1.154  16.858
ATOM    180  N3  DC      6      -0.699   0.697  17.034
ATOM    181  C2  DC      6      -1.451   1.823  17.087
ATOM    182  O2  DC      6      -2.674   1.677  17.134
ATOM    183  C3* DC      6      -1.569   6.675  17.520
ATOM    184  H3* DC      6      -0.751   7.312  17.863
ATOM    185  C2* DC      6      -1.464   5.294  18.168
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ATOM    186 1H2* DC      6      -0.463   5.181  18.584
ATOM    187 2H2* DC      6      -2.202   5.153  18.959
ATOM    188  O3* DC      6      -2.819   7.314  17.755
ATOM    189  P   DX      7      -3.158   8.076  19.139
ATOM    190  O1P DX      7      -3.955   9.283  18.805
ATOM    191  O2P DX      7      -1.914   8.241  19.931
ATOM    192  O5* DX      7      -4.107   7.040  19.922
ATOM    193  C5* DX      7      -5.398   6.705  19.421
ATOM    194 1H5* DX      7      -5.297   6.217  18.450
ATOM    195 2H5* DX      7      -5.986   7.615  19.287
ATOM    196  C4* DX      7      -6.162   5.772  20.370
ATOM    197  H4* DX      7      -7.154   5.595  19.948
ATOM    198  O4* DX      7      -5.481   4.528  20.463
ATOM    199  C1* DX      7      -5.560   4.057  21.796
ATOM    200  H1* DX      7      -6.470   3.462  21.911
ATOM    201  N1  DX      7      -4.347   3.237  22.104
ATOM    202  C6  DX      7      -3.101   3.814  22.051
ATOM    203  H6  DX      7      -3.011   4.855  21.759
ATOM    204  C5  DX      7      -1.993   3.090  22.329
ATOM    205  H5  DX      7      -1.021   3.555  22.274
ATOM    206  C4  DX      7      -2.060   1.691  22.691
ATOM    207  O4  DX      7      -1.050   1.016  22.895
ATOM    208  N3  DX      7      -3.350   1.140  22.766
ATOM    209  C11 DX      7      -3.440  -0.338  23.145
ATOM    210  C2  DX      7      -4.499   1.872  22.404
ATOM    211  O2  DX      7      -5.609   1.335  22.335
ATOM    212  C3* DX      7      -6.334   6.362  21.781
ATOM    213  H3* DX      7      -5.782   7.301  21.861
ATOM    214  C2* DX      7      -5.690   5.305  22.678
ATOM    215 1H2* DX      7      -4.716   5.672  22.999
ATOM    216 2H2* DX      7      -6.299   5.087  23.549
ATOM    217  O3* DX      7      -7.713   6.580  22.069
ATOM    218  C12 DX      7      -4.652  -0.862  23.936
ATOM    219  C9  DX      7      -4.384  -2.285  24.412
ATOM    220  C10 DX      7      -4.287  -2.758  25.652
ATOM    221  O12 DX      7      -4.877  -0.031  25.042
ATOM    222  H15 DX      7      -2.575  -0.592  23.757
ATOM    223  H14 DX      7      -3.365  -0.932  22.235
ATOM    224  H9  DX      7      -5.537  -0.885  23.301
ATOM    225 1H1  DX      7      -4.270  -3.058  23.665
ATOM    226 2H1  DX      7      -4.101  -3.813  25.800
ATOM    227 3H1  DX      7      -4.391  -2.082  26.491
ATOM    228  H10 DX      7      -5.060   0.847  24.671
ATOM    229  P   DA      8      -8.219   7.437  23.350
ATOM    230  O1P DA      8      -9.556   7.992  23.020
ATOM    231  O2P DA      8      -7.145   8.370  23.768
ATOM    232  O5* DA      8      -8.405   6.333  24.511
ATOM    233  C5* DA      8      -9.383   5.310  24.375
ATOM    234 1H5* DA      8      -9.382   4.958  23.342
ATOM    235 2H5* DA      8     -10.373   5.720  24.583
ATOM    236  C4* DA      8      -9.143   4.084  25.269
ATOM    237  H4* DA      8      -9.797   3.301  24.880
ATOM    238  O4* DA      8      -7.801   3.622  25.145
ATOM    239  C1* DA      8      -7.122   3.741  26.386
ATOM    240  H1* DA      8      -6.830   2.737  26.712
ATOM    241  N9  DA      8      -5.893   4.567  26.236
ATOM    242  C8  DA      8      -5.745   5.939  26.240
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ATOM    243  H8  DA      8      -6.590   6.615  26.300
ATOM    244  N7  DA      8      -4.505   6.355  26.163
ATOM    245  C5  DA      8      -3.779   5.155  26.085
ATOM    246  C6  DA      8      -2.407   4.814  25.977
ATOM    247  N6  DA      8      -1.404   5.673  25.929
ATOM    248 1H6  DA      8      -0.470   5.303  25.861
ATOM    249 2H6  DA      8      -1.592   6.663  25.978
ATOM    250  N1  DA      8      -2.012   3.545  25.904
ATOM    251  C2  DA      8      -2.941   2.600  25.944
ATOM    252  H2  DA      8      -2.597   1.577  25.880
ATOM    253  N3  DA      8      -4.255   2.759  26.052
ATOM    254  C4  DA      8      -4.615   4.070  26.118
ATOM    255  C3* DA      8      -9.479   4.265  26.758
ATOM    256  H3* DA      8     -10.010   5.204  26.927
ATOM    257  C2* DA      8      -8.099   4.315  27.417
ATOM    258 1H2* DA      8      -7.870   5.353  27.651
ATOM    259 2H2* DA      8      -8.051   3.737  28.337
ATOM    260  O3* DA      8     -10.306   3.167  27.140
ATOM    261  P   DG      9     -10.709   2.795  28.659
ATOM    262  O1P DG      9     -12.065   2.192  28.638
ATOM    263  O2P DG      9     -10.451   3.954  29.549
ATOM    264  O5* DG      9      -9.641   1.631  28.986
ATOM    265  C5* DG      9      -9.590   0.465  28.167
ATOM    266 1H5* DG      9      -9.462   0.764  27.125
ATOM    267 2H5* DG      9     -10.535  -0.074  28.247
ATOM    268  C4* DG      9      -8.450  -0.500  28.512
ATOM    269  H4* DG      9      -8.543  -1.364  27.851
ATOM    270  O4* DG      9      -7.195   0.125  28.261
ATOM    271  C1* DG      9      -6.356  -0.097  29.379
ATOM    272  H1* DG      9      -5.814  -1.039  29.254
ATOM    273  N9  DG      9      -5.393   1.020  29.512
ATOM    274  C8  DG      9      -5.635   2.344  29.791
ATOM    275  H8  DG      9      -6.636   2.722  29.968
ATOM    276  N7  DG      9      -4.564   3.096  29.810
ATOM    277  C5  DG      9      -3.525   2.192  29.534
ATOM    278  C6  DG      9      -2.099   2.371  29.417
ATOM    279  O6  DG      9      -1.429   3.400  29.520
ATOM    280  N1  DG      9      -1.417   1.199  29.154
ATOM    281  H1  DG      9      -0.419   1.260  29.019
ATOM    282  C2  DG      9      -2.016  -0.007  29.017
ATOM    283  N2  DG      9      -1.250  -1.049  28.858
ATOM    284 1H2  DG      9      -1.684  -1.955  28.886
ATOM    285 2H2  DG      9      -0.238  -0.940  28.839
ATOM    286  N3  DG      9      -3.322  -0.224  29.114
ATOM    287  C4  DG      9      -4.029   0.919  29.365
ATOM    288  C3* DG      9      -8.470  -0.999  29.967
ATOM    289  H3* DG      9      -9.407  -0.739  30.463
ATOM    290  C2* DG      9      -7.299  -0.225  30.570
ATOM    291 1H2* DG      9      -7.651   0.757  30.890
ATOM    292 2H2* DG      9      -6.830  -0.746  31.401
ATOM    293  O3* DG      9      -8.291  -2.413  29.947
ATOM    294  P   DT     10      -8.195  -3.328  31.272
ATOM    295  O1P DT     10      -8.900  -4.605  30.997
ATOM    296  O2P DT     10      -8.593  -2.531  32.460
ATOM    297  O5* DT     10      -6.613  -3.625  31.358
ATOM    298  C5* DT     10      -5.957  -4.334  30.309
ATOM    299 1H5* DT     10      -6.071  -3.783  29.374
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ATOM    300 2H5* DT     10      -6.432  -5.308  30.184
ATOM    301  C4* DT     10      -4.459  -4.564  30.553
ATOM    302  H4* DT     10      -4.081  -5.170  29.727
ATOM    303  O4* DT     10      -3.765  -3.320  30.556
ATOM    304  C1* DT     10      -2.951  -3.262  31.715
ATOM    305  H1* DT     10      -1.976  -3.706  31.490
ATOM    306  N1  DT     10      -2.793  -1.847  32.151
ATOM    307  C6  DT     10      -3.886  -1.098  32.546
ATOM    308  H6  DT     10      -4.866  -1.560  32.548
ATOM    309  C5  DT     10      -3.750   0.205  32.909
ATOM    310  C7  DT     10      -4.974   0.990  33.354
ATOM    311 1H7  DT     10      -5.090   1.872  32.724
ATOM    312 2H7  DT     10      -5.876   0.381  33.298
ATOM    313 3H7  DT     10      -4.831   1.321  34.383
ATOM    314  C4  DT     10      -2.439   0.854  32.869
ATOM    315  O4  DT     10      -2.192   2.028  33.135
ATOM    316  N3  DT     10      -1.405   0.038  32.479
ATOM    317  H3  DT     10      -0.479   0.441  32.462
ATOM    318  C2  DT     10      -1.508  -1.287  32.132
ATOM    319  O2  DT     10      -0.488  -1.905  31.834
ATOM    320  C3* DT     10      -4.153  -5.297  31.871
ATOM    321  H3* DT     10      -5.057  -5.741  32.295
ATOM    322  C2* DT     10      -3.646  -4.152  32.745
ATOM    323 1H2* DT     10      -4.499  -3.648  33.196
ATOM    324 2H2* DT     10      -2.963  -4.486  33.520
ATOM    325  O3* DT     10      -3.174  -6.301  31.617
ATOM    326  P   DC     11      -2.602  -7.300  32.751
ATOM    327  O1P DC     11      -2.482  -8.651  32.149
ATOM    328  O2P DC     11      -3.388  -7.139  33.999
ATOM    329  O5* DC     11      -1.120  -6.718  33.007
ATOM    330  C5* DC     11      -0.135  -6.766  31.977
ATOM    331 1H5* DC     11      -0.510  -6.244  31.095
ATOM    332 2H5* DC     11       0.044  -7.806  31.700
ATOM    333  C4* DC     11       1.211  -6.137  32.370
ATOM    334  H4* DC     11       1.893  -6.267  31.528
ATOM    335  O4* DC     11       1.038  -4.743  32.604
ATOM    336  C1* DC     11       1.555  -4.419  33.883
ATOM    337  H1* DC     11       2.602  -4.113  33.777
ATOM    338  N1  DC     11       0.748  -3.317  34.480
ATOM    339  C6  DC     11      -0.570  -3.505  34.825
ATOM    340  H6  DC     11      -1.026  -4.476  34.662
ATOM    341  C5  DC     11      -1.294  -2.480  35.342
ATOM    342  H5  DC     11      -2.331  -2.628  35.604
ATOM    343  C4  DC     11      -0.635  -1.231  35.495
ATOM    344  N4  DC     11      -1.275  -0.197  35.954
ATOM    345 1H4  DC     11      -2.236  -0.277  36.234
ATOM    346 2H4  DC     11      -0.758   0.675  36.014
ATOM    347  N3  DC     11       0.620  -1.025  35.167
ATOM    348  C2  DC     11       1.334  -2.056  34.656
ATOM    349  O2  DC     11       2.512  -1.829  34.381
ATOM    350  C3* DC     11       1.856  -6.762  33.619
ATOM    351  H3* DC     11       1.398  -7.725  33.857
ATOM    352  C2* DC     11       1.523  -5.723  34.686
ATOM    353 1H2* DC     11       0.529  -5.933  35.077
ATOM    354 2H2* DC     11       2.239  -5.718  35.502
ATOM    355  O3* DC     11       3.256  -6.916  33.391
ATOM    356  P   DC3    12       4.274  -7.524  34.488
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ATOM    357  O1P DC3    12       5.310  -8.304  33.765
ATOM    358  O2P DC3    12       3.500  -8.191  35.564
ATOM    359  O5* DC3    12       4.967  -6.205  35.108
ATOM    360  C5* DC3    12       5.814  -5.384  34.308
ATOM    361 1H5* DC3    12       5.247  -4.997  33.459
ATOM    362 2H5* DC3    12       6.635  -5.986  33.917
ATOM    363  C4* DC3    12       6.417  -4.193  35.070
ATOM    364  H4* DC3    12       7.125  -3.695  34.406
ATOM    365  O4* DC3    12       5.384  -3.276  35.411
ATOM    366  C1* DC3    12       5.520  -2.932  36.778
ATOM    367  H1* DC3    12       6.200  -2.077  36.864
ATOM    368  N1  DC3    12       4.183  -2.601  37.339
ATOM    369  C6  DC3    12       3.164  -3.520  37.316
ATOM    370  H6  DC3    12       3.361  -4.506  36.912
ATOM    371  C5  DC3    12       1.933  -3.185  37.780
ATOM    372  H5  DC3    12       1.130  -3.906  37.756
ATOM    373  C4  DC3    12       1.765  -1.863  38.274
ATOM    374  N4  DC3    12       0.611  -1.462  38.721
ATOM    375 1H4  DC3    12      -0.178  -2.083  38.703
ATOM    376 2H4  DC3    12       0.538  -0.494  39.014
ATOM    377  N3  DC3    12       2.734  -0.974  38.331
ATOM    378  C2  DC3    12       3.961  -1.329  37.880
ATOM    379  O2  DC3    12       4.859  -0.492  37.986
ATOM    380  C3* DC3    12       7.157  -4.584  36.366
ATOM    381  H3* DC3    12       7.327  -5.663  36.414
ATOM    382  C2* DC3    12       6.181  -4.138  37.450
ATOM    383 1H2* DC3    12       5.462  -4.936  37.639
ATOM    384 2H2* DC3    12       6.682  -3.858  38.377
ATOM    385  O3* DC3    12       8.383  -3.866  36.489
ATOM    386  H3T DC3    12       8.897  -4.223  37.241
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ATOM    387  H5T DG5    13      -0.373   9.193  41.841
ATOM    388  O5* DG5    13       0.319   8.928  41.199
ATOM    389  C5* DG5    13       1.602   9.322  41.689
ATOM    390 1H5* DG5    13       1.763   8.888  42.678
ATOM    391 2H5* DG5    13       1.625  10.409  41.796
ATOM    392  C4* DG5    13       2.781   8.907  40.785
ATOM    393  H4* DG5    13       3.685   9.349  41.210
ATOM    394  O4* DG5    13       2.928   7.488  40.786
ATOM    395  C1* DG5    13       2.729   6.988  39.471
ATOM    396  H1* DG5    13       3.698   6.741  39.027
ATOM    397  N9  DG5    13       1.882   5.773  39.525
ATOM    398  C8  DG5    13       0.545   5.668  39.828
ATOM    399  H8  DG5    13      -0.060   6.533  40.077
ATOM    400  N7  DG5    13       0.080   4.444  39.810
ATOM    401  C5  DG5    13       1.202   3.676  39.462
ATOM    402  C6  DG5    13       1.372   2.254  39.289
ATOM    403  O6  DG5    13       0.546   1.347  39.414
ATOM    404  N1  DG5    13       2.659   1.893  38.944
ATOM    405  H1  DG5    13       2.833   0.911  38.788
ATOM    406  C2  DG5    13       3.679   2.773  38.804
ATOM    407  N2  DG5    13       4.844   2.292  38.473
ATOM    408 1H2  DG5    13       5.597   2.941  38.320
ATOM    409 2H2  DG5    13       4.954   1.296  38.296
ATOM    410  N3  DG5    13       3.577   4.089  38.962
ATOM    411  C4  DG5    13       2.308   4.484  39.290
ATOM    412  C3* DG5    13       2.657   9.368  39.323
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ATOM    413  H3* DG5    13       1.959  10.204  39.232
ATOM    414  C2* DG5    13       2.094   8.115  38.656
ATOM    415 1H2* DG5    13       1.010   8.115  38.763
ATOM    416 2H2* DG5    13       2.349   8.045  37.602
ATOM    417  O3* DG5    13       3.950   9.747  38.857
ATOM    418  P   DG     14       4.254  10.210  37.341
ATOM    419  O1P DG     14       5.319  11.243  37.386
ATOM    420  O2P DG     14       2.978  10.528  36.655
ATOM    421  O5* DG     14       4.867   8.868  36.689
ATOM    422  C5* DG     14       6.094   8.325  37.169
ATOM    423 1H5* DG     14       5.973   8.015  38.208
ATOM    424 2H5* DG     14       6.862   9.099  37.138
ATOM    425  C4* DG     14       6.611   7.126  36.357
ATOM    426  H4* DG     14       7.617   6.899  36.714
ATOM    427  O4* DG     14       5.786   5.984  36.576
ATOM    428  C1* DG     14       5.321   5.500  35.325
ATOM    429  H1* DG     14       5.970   4.692  34.974
ATOM    430  N9  DG     14       3.935   5.003  35.481
ATOM    431  C8  DG     14       2.798   5.726  35.748
ATOM    432  H8  DG     14       2.814   6.805  35.840
ATOM    433  N7  DG     14       1.719   5.004  35.900
ATOM    434  C5  DG     14       2.177   3.694  35.697
ATOM    435  C6  DG     14       1.489   2.429  35.734
ATOM    436  O6  DG     14       0.306   2.195  35.984
ATOM    437  N1  DG     14       2.302   1.352  35.447
ATOM    438  H1  DG     14       1.858   0.448  35.385
ATOM    439  C2  DG     14       3.624   1.456  35.170
ATOM    440  N2  DG     14       4.253   0.359  34.851
ATOM    441 1H2  DG     14       5.215   0.435  34.575
ATOM    442 2H2  DG     14       3.733  -0.506  34.723
ATOM    443  N3  DG     14       4.308   2.597  35.144
ATOM    444  C4  DG     14       3.528   3.688  35.419
ATOM    445  C3* DG     14       6.679   7.394  34.845
ATOM    446  H3* DG     14       6.624   8.463  34.630
ATOM    447  C2* DG     14       5.423   6.677  34.357
ATOM    448 1H2* DG     14       4.571   7.347  34.464
ATOM    449 2H2* DG     14       5.500   6.348  33.325
ATOM    450  O3* DG     14       7.895   6.848  34.342
ATOM    451  P   DA     15       8.308   6.883  32.783
ATOM    452  O1P DA     15       9.780   7.054  32.703
ATOM    453  O2P DA     15       7.435   7.839  32.057
ATOM    454  O5* DA     15       7.937   5.391  32.301
ATOM    455  C5* DA     15       8.620   4.265  32.846
ATOM    456 1H5* DA     15       8.411   4.192  33.915
ATOM    457 2H5* DA     15       9.695   4.406  32.724
ATOM    458  C4* DA     15       8.246   2.934  32.181
ATOM    459  H4* DA     15       8.923   2.174  32.575
ATOM    460  O4* DA     15       6.911   2.561  32.512
ATOM    461  C1* DA     15       6.154   2.393  31.324
ATOM    462  H1* DA     15       6.075   1.328  31.081
ATOM    463  N9  DA     15       4.806   2.965  31.548
ATOM    464  C8  DA     15       4.453   4.289  31.674
ATOM    465  H8  DA     15       5.175   5.090  31.565
ATOM    466  N7  DA     15       3.192   4.492  31.959
ATOM    467  C5  DA     15       2.675   3.187  32.005
ATOM    468  C6  DA     15       1.401   2.628  32.272
ATOM    469  N6  DA     15       0.329   3.325  32.596
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ATOM    470 1H6  DA     15      -0.536   2.835  32.796
ATOM    471 2H6  DA     15       0.389   4.329  32.646
ATOM    472  N1  DA     15       1.205   1.310  32.252
ATOM    473  C2  DA     15       2.238   0.530  31.960
ATOM    474  H2  DA     15       2.042  -0.535  31.942
ATOM    475  N3  DA     15       3.485   0.900  31.688
ATOM    476  C4  DA     15       3.643   2.254  31.738
ATOM    477  C3* DA     15       8.383   2.957  30.651
ATOM    478  H3* DA     15       8.970   3.818  30.320
ATOM    479  C2* DA     15       6.927   3.103  30.211
ATOM    480 1H2* DA     15       6.681   4.163  30.179
ATOM    481 2H2* DA     15       6.733   2.660  29.238
ATOM    482  O3* DA     15       9.015   1.745  30.253
ATOM    483  P   DC     16       9.267   1.333  28.717
ATOM    484  O1P DC     16      10.473   0.470  28.666
ATOM    485  O2P DC     16       9.211   2.544  27.861
ATOM    486  O5* DC     16       7.973   0.426  28.413
ATOM    487  C5* DC     16       7.766  -0.797  29.114
ATOM    488 1H5* DC     16       7.743  -0.607  30.189
ATOM    489 2H5* DC     16       8.593  -1.479  28.906
ATOM    490  C4* DC     16       6.458  -1.489  28.716
ATOM    491  H4* DC     16       6.418  -2.457  29.219
ATOM    492  O4* DC     16       5.350  -0.716  29.150
ATOM    493  C1* DC     16       4.329  -0.793  28.175
ATOM    494  H1* DC     16       3.699  -1.667  28.372
ATOM    495  N1  DC     16       3.535   0.466  28.244
ATOM    496  C6  DC     16       4.146   1.687  28.087
ATOM    497  H6  DC     16       5.204   1.719  27.848
ATOM    498  C5  DC     16       3.438   2.832  28.255
ATOM    499  H5  DC     16       3.923   3.790  28.143
ATOM    500  C4  DC     16       2.064   2.702  28.593
ATOM    501  N4  DC     16       1.337   3.759  28.813
ATOM    502 1H4  DC     16       1.752   4.672  28.754
ATOM    503 2H4  DC     16       0.363   3.622  29.060
ATOM    504  N3  DC     16       1.455   1.546  28.743
ATOM    505  C2  DC     16       2.170   0.409  28.560
ATOM    506  O2  DC     16       1.569  -0.660  28.681
ATOM    507  C3* DC     16       6.336  -1.723  27.203
ATOM    508  H3* DC     16       7.182  -1.274  26.677
ATOM    509  C2* DC     16       5.044  -0.992  26.834
ATOM    510 1H2* DC     16       5.309  -0.036  26.383
ATOM    511 2H2* DC     16       4.425  -1.562  26.142
ATOM    512  O3* DC     16       6.294  -3.120  26.948
ATOM    513  P   DT     17       6.312  -3.731  25.456
ATOM    514  O1P DT     17       7.171  -4.942  25.467
ATOM    515  O2P DT     17       6.602  -2.656  24.477
ATOM    516  O5* DT     17       4.783  -4.189  25.261
ATOM    517  C5* DT     17       4.218  -5.200  26.090
ATOM    518 1H5* DT     17       4.029  -4.794  27.086
ATOM    519 2H5* DT     17       4.926  -6.024  26.191
ATOM    520  C4* DT     17       2.913  -5.782  25.530
ATOM    521  H4* DT     17       2.730  -6.734  26.032
ATOM    522  O4* DT     17       1.841  -4.901  25.825
ATOM    523  C1* DT     17       1.185  -4.519  24.630
ATOM    524  H1* DT     17       0.298  -5.149  24.510
ATOM    525  N1  DT     17       0.762  -3.096  24.813
ATOM    526  C6  DT     17       1.594  -2.022  24.537
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ATOM    527  H6  DT     17       2.548  -2.176  24.055
ATOM    528  C5  DT     17       1.265  -0.759  24.923
ATOM    529  C7  DT     17       2.222   0.378  24.593
ATOM    530 1H7  DT     17       2.584   0.276  23.569
ATOM    531 2H7  DT     17       1.709   1.336  24.682
ATOM    532 3H7  DT     17       3.058   0.371  25.289
ATOM    533  C4  DT     17       0.015  -0.498  25.636
ATOM    534  O4  DT     17      -0.362   0.579  26.091
ATOM    535  N3  DT     17      -0.787  -1.600  25.813
ATOM    536  H3  DT     17      -1.639  -1.464  26.322
ATOM    537  C2  DT     17      -0.469  -2.890  25.457
ATOM    538  O2  DT     17      -1.262  -3.792  25.728
ATOM    539  C3* DT     17       2.958  -6.023  24.012
ATOM    540  H3* DT     17       3.986  -5.965  23.647
ATOM    541  C2* DT     17       2.131  -4.856  23.469
ATOM    542 1H2* DT     17       2.813  -4.043  23.242
ATOM    543 2H2* DT     17       1.574  -5.128  22.574
ATOM    544  O3* DT     17       2.420  -7.306  23.721
ATOM    545  P   DT     18       2.512  -7.981  22.257
ATOM    546  O1P DT     18       2.740  -9.436  22.437
ATOM    547  O2P DT     18       3.450  -7.206  21.408
ATOM    548  O5* DT     18       1.028  -7.764  21.685
ATOM    549  C5* DT     18      -0.098  -8.294  22.376
ATOM    550 1H5* DT     18      -0.118  -7.897  23.392
ATOM    551 2H5* DT     18      -0.009  -9.380  22.438
ATOM    552  C4* DT     18      -1.433  -7.948  21.702
ATOM    553  H4* DT     18      -2.231  -8.377  22.311
ATOM    554  O4* DT     18      -1.591  -6.533  21.660
ATOM    555  C1* DT     18      -1.723  -6.115  20.310
ATOM    556  H1* DT     18      -2.789  -5.992  20.093
ATOM    557  N1  DT     18      -1.015  -4.810  20.135
ATOM    558  C6  DT     18       0.365  -4.734  20.069
ATOM    559  H6  DT     18       0.955  -5.641  20.107
ATOM    560  C5  DT     18       1.005  -3.535  20.001
ATOM    561  C7  DT     18       2.523  -3.508  19.938
ATOM    562 1H7  DT     18       2.912  -2.957  20.795
ATOM    563 2H7  DT     18       2.937  -4.517  19.942
ATOM    564 3H7  DT     18       2.837  -2.996  19.028
ATOM    565  C4  DT     18       0.246  -2.284  20.012
ATOM    566  O4  DT     18       0.709  -1.145  19.993
ATOM    567  N3  DT     18      -1.120  -2.440  20.071
ATOM    568  H3  DT     18      -1.674  -1.604  20.089
ATOM    569  C2  DT     18      -1.792  -3.641  20.128
ATOM    570  O2  DT     18      -3.021  -3.630  20.168
ATOM    571  C3* DT     18      -1.554  -8.500  20.273
ATOM    572  H3* DT     18      -0.830  -9.300  20.100
ATOM    573  C2* DT     18      -1.217  -7.270  19.437
ATOM    574 1H2* DT     18      -0.141  -7.236  19.287
ATOM    575 2H2* DT     18      -1.714  -7.290  18.474
ATOM    576  O3* DT     18      -2.880  -8.977  20.070
ATOM    577  P   DG     19      -3.350  -9.759  18.736
ATOM    578  O1P DG     19      -4.060 -10.993  19.156
ATOM    579  O2P DG     19      -2.212  -9.872  17.791
ATOM    580  O5* DG     19      -4.422  -8.737  18.105
ATOM    581  C5* DG     19      -5.625  -8.429  18.804
ATOM    582 1H5* DG     19      -5.374  -8.098  19.813
ATOM    583 2H5* DG     19      -6.232  -9.331  18.891
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ATOM    584  C4* DG     19      -6.479  -7.329  18.149
ATOM    585  H4* DG     19      -7.362  -7.194  18.777
ATOM    586  O4* DG     19      -5.752  -6.104  18.117
ATOM    587  C1* DG     19      -5.488  -5.744  16.767
ATOM    588  H1* DG     19      -6.138  -4.909  16.490
ATOM    589  N9  DG     19      -4.071  -5.319  16.637
ATOM    590  C8  DG     19      -2.942  -6.087  16.472
ATOM    591  H8  DG     19      -2.977  -7.168  16.396
ATOM    592  N7  DG     19      -1.824  -5.410  16.464
ATOM    593  C5  DG     19      -2.245  -4.082  16.614
ATOM    594  C6  DG     19      -1.504  -2.851  16.704
ATOM    595  O6  DG     19      -0.286  -2.671  16.709
ATOM    596  N1  DG     19      -2.305  -1.735  16.830
ATOM    597  H1  DG     19      -1.843  -0.840  16.893
ATOM    598  C2  DG     19      -3.657  -1.781  16.888
ATOM    599  N2  DG     19      -4.290  -0.648  17.013
ATOM    600 1H2  DG     19      -5.294  -0.670  17.036
ATOM    601 2H2  DG     19      -3.773   0.228  17.044
ATOM    602  N3  DG     19      -4.385  -2.892  16.832
ATOM    603  C4  DG     19      -3.620  -4.019  16.697
ATOM    604  C3* DG     19      -6.945  -7.638  16.718
ATOM    605  H3* DG     19      -6.955  -8.714  16.528
ATOM    606  C2* DG     19      -5.854  -6.952  15.899
ATOM    607 1H2* DG     19      -5.017  -7.639  15.797
ATOM    608 2H2* DG     19      -6.190  -6.653  14.911
ATOM    609  O3* DG     19      -8.252  -7.092  16.550
ATOM    610  P   DC     20      -9.034  -7.035  15.138
ATOM    611  O1P DC     20     -10.489  -7.127  15.419
ATOM    612  O2P DC     20      -8.424  -8.005  14.195
ATOM    613  O5* DC     20      -8.703  -5.539  14.631
ATOM    614  C5* DC     20      -9.169  -4.412  15.369
ATOM    615 1H5* DC     20      -8.812  -4.480  16.398
ATOM    616 2H5* DC     20     -10.260  -4.423  15.390
ATOM    617  C4* DC     20      -8.714  -3.062  14.796
ATOM    618  H4* DC     20      -9.180  -2.276  15.393
ATOM    619  O4* DC     20      -7.300  -2.936  14.915
ATOM    620  C1* DC     20      -6.781  -2.427  13.700
ATOM    621  H1* DC     20      -6.800  -1.331  13.722
ATOM    622  N1  DC     20      -5.389  -2.929  13.517
ATOM    623  C6  DC     20      -5.138  -4.276  13.408
ATOM    624  H6  DC     20      -5.968  -4.972  13.446
ATOM    625  C5  DC     20      -3.866  -4.725  13.269
ATOM    626  H5  DC     20      -3.672  -5.784  13.190
ATOM    627  C4  DC     20      -2.830  -3.754  13.255
ATOM    628  N4  DC     20      -1.585  -4.119  13.181
ATOM    629 1H4  DC     20      -1.353  -5.095  13.150
ATOM    630 2H4  DC     20      -0.877  -3.396  13.245
ATOM    631  N3  DC     20      -3.042  -2.460  13.374
ATOM    632  C2  DC     20      -4.319  -2.023  13.497
ATOM    633  O2  DC     20      -4.478  -0.806  13.580
ATOM    634  C3* DC     20      -9.108  -2.845  13.324
ATOM    635  H3* DC     20      -9.761  -3.647  12.972
ATOM    636  C2* DC     20      -7.754  -2.908  12.621
ATOM    637 1H2* DC     20      -7.562  -3.942  12.341
ATOM    638 2H2* DC     20      -7.714  -2.278  11.737
ATOM    639  O3* DC     20      -9.761  -1.585  13.197
ATOM    640  P   DT     21     -10.316  -1.010  11.792
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ATOM    641  O1P DT     21     -11.558  -0.245  12.069
ATOM    642  O2P DT     21     -10.358  -2.104  10.790
ATOM    643  O5* DT     21      -9.161   0.029  11.364
ATOM    644  C5* DT     21      -8.900   1.181  12.160
ATOM    645 1H5* DT     21      -8.690   0.871  13.185
ATOM    646 2H5* DT     21      -9.786   1.817  12.175
ATOM    647  C4* DT     21      -7.714   2.018  11.664
ATOM    648  H4* DT     21      -7.633   2.891  12.314
ATOM    649  O4* DT     21      -6.512   1.262  11.773
ATOM    650  C1* DT     21      -5.787   1.396  10.564
ATOM    651  H1* DT     21      -5.160   2.292  10.618
ATOM    652  N1  DT     21      -4.951   0.183  10.342
ATOM    653  C6  DT     21      -5.534  -1.056  10.158
ATOM    654  H6  DT     21      -6.613  -1.132  10.163
ATOM    655  C5  DT     21      -4.777  -2.171   9.984
ATOM    656  C7  DT     21      -5.460  -3.512   9.772
ATOM    657 1H7  DT     21      -5.154  -4.205  10.555
ATOM    658 2H7  DT     21      -6.546  -3.410   9.782
ATOM    659 3H7  DT     21      -5.150  -3.925   8.812
ATOM    660  C4  DT     21      -3.318  -2.086  10.000
ATOM    661  O4  DT     21      -2.527  -3.019   9.874
ATOM    662  N3  DT     21      -2.816  -0.819  10.179
ATOM    663  H3  DT     21      -1.812  -0.718  10.203
ATOM    664  C2  DT     21      -3.557   0.328  10.339
ATOM    665  O2  DT     21      -2.972   1.404  10.453
ATOM    666  C3* DT     21      -7.855   2.509  10.212
ATOM    667  H3* DT     21      -8.866   2.343   9.833
ATOM    668  C2* DT     21      -6.848   1.620   9.487
ATOM    669 1H2* DT     21      -7.341   0.690   9.211
ATOM    670 2H2* DT     21      -6.431   2.088   8.601
ATOM    671  O3* DT     21      -7.527   3.895  10.175
ATOM    672  P   DA     22      -7.558   4.791   8.832
ATOM    673  O1P DA     22      -8.217   6.080   9.155
ATOM    674  O2P DA     22      -8.074   3.985   7.698
ATOM    675  O5* DA     22      -5.989   5.063   8.586
ATOM    676  C5* DA     22      -5.231   5.806   9.537
ATOM    677 1H5* DA     22      -5.276   5.305  10.506
ATOM    678 2H5* DA     22      -5.672   6.797   9.653
ATOM    679  C4* DA     22      -3.753   5.984   9.161
ATOM    680  H4* DA     22      -3.298   6.612   9.930
ATOM    681  O4* DA     22      -3.089   4.724   9.155
ATOM    682  C1* DA     22      -2.541   4.486   7.868
ATOM    683  H1* DA     22      -1.469   4.710   7.878
ATOM    684  N9  DA     22      -2.759   3.068   7.508
ATOM    685  C8  DA     22      -3.947   2.424   7.254
ATOM    686  H8  DA     22      -4.899   2.943   7.288
ATOM    687  N7  DA     22      -3.829   1.147   6.988
ATOM    688  C5  DA     22      -2.438   0.950   7.051
ATOM    689  C6  DA     22      -1.576  -0.159   6.874
ATOM    690  N6  DA     22      -1.979  -1.387   6.607
ATOM    691 1H6  DA     22      -1.290  -2.130   6.547
ATOM    692 2H6  DA     22      -2.963  -1.570   6.497
ATOM    693  N1  DA     22      -0.252  -0.032   6.979
ATOM    694  C2  DA     22       0.238   1.164   7.276
ATOM    695  H2  DA     22       1.317   1.232   7.356
ATOM    696  N3  DA     22      -0.435   2.286   7.497
ATOM    697  C4  DA     22      -1.781   2.112   7.363
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ATOM    698  C3* DA     22      -3.529   6.654   7.797
ATOM    699  H3* DA     22      -4.427   7.177   7.459
ATOM    700  C2* DA     22      -3.240   5.447   6.907
ATOM    701 1H2* DA     22      -4.186   5.032   6.559
ATOM    702 2H2* DA     22      -2.614   5.689   6.051
ATOM    703  O3* DA     22      -2.442   7.563   7.937
ATOM    704  P   DG     23      -1.812   8.402   6.714
ATOM    705  O1P DG     23      -1.311   9.690   7.255
ATOM    706  O2P DG     23      -2.771   8.424   5.582
ATOM    707  O5* DG     23      -0.546   7.492   6.300
ATOM    708  C5* DG     23       0.527   7.282   7.215
ATOM    709 1H5* DG     23       0.164   6.732   8.085
ATOM    710 2H5* DG     23       0.896   8.250   7.559
ATOM    711  C4* DG     23       1.715   6.519   6.609
ATOM    712  H4* DG     23       2.540   6.570   7.322
ATOM    713  O4* DG     23       1.373   5.151   6.406
ATOM    714  C1* DG     23       1.683   4.796   5.068
ATOM    715  H1* DG     23       2.706   4.413   5.012
ATOM    716  N9  DG     23       0.732   3.762   4.597
ATOM    717  C8  DG     23      -0.623   3.873   4.396
ATOM    718  H8  DG     23      -1.151   4.806   4.550
ATOM    719  N7  DG     23      -1.209   2.762   4.032
ATOM    720  C5  DG     23      -0.152   1.841   3.970
ATOM    721  C6  DG     23      -0.121   0.438   3.638
ATOM    722  O6  DG     23      -1.051  -0.315   3.348
ATOM    723  N1  DG     23       1.147  -0.108   3.665
ATOM    724  H1  DG     23       1.233  -1.088   3.443
ATOM    725  C2  DG     23       2.262   0.593   3.979
ATOM    726  N2  DG     23       3.404  -0.029   3.889
ATOM    727 1H2  DG     23       4.235   0.484   4.124
ATOM    728 2H2  DG     23       3.437  -1.014   3.636
ATOM    729  N3  DG     23       2.283   1.880   4.315
ATOM    730  C4  DG     23       1.041   2.454   4.295
ATOM    731  C3* DG     23       2.190   7.104   5.268
ATOM    732  H3* DG     23       1.777   8.102   5.103
ATOM    733  C2* DG     23       1.599   6.101   4.279
ATOM    734 1H2* DG     23       0.560   6.365   4.079
ATOM    735 2H2* DG     23       2.154   6.056   3.348
ATOM    736  O3* DG     23       3.615   7.148   5.266
ATOM    737  P   DC3    24       4.485   7.699   4.023
ATOM    738  O1P DC3    24       5.674   8.398   4.573
ATOM    739  O2P DC3    24       3.599   8.428   3.082
ATOM    740  O5* DC3    24       4.976   6.341   3.306
ATOM    741  C5* DC3    24       5.865   5.448   3.974
ATOM    742 1H5* DC3    24       5.403   5.100   4.900
ATOM    743 2H5* DC3    24       6.781   5.979   4.235
ATOM    744  C4* DC3    24       6.248   4.219   3.134
ATOM    745  H4* DC3    24       7.003   3.660   3.687
ATOM    746  O4* DC3    24       5.104   3.393   2.953
ATOM    747  C1* DC3    24       4.984   3.076   1.577
ATOM    748  H1* DC3    24       5.549   2.161   1.374
ATOM    749  N1  DC3    24       3.546   2.893   1.240
ATOM    750  C6  DC3    24       2.651   3.924   1.389
ATOM    751  H6  DC3    24       3.016   4.890   1.718
ATOM    752  C5  DC3    24       1.331   3.721   1.150
ATOM    753  H5  DC3    24       0.627   4.529   1.279
ATOM    754  C4  DC3    24       0.937   2.416   0.753
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ATOM    755  N4  DC3    24      -0.318   2.130   0.568
ATOM    756 1H4  DC3    24      -1.020   2.831   0.729
ATOM    757 2H4  DC3    24      -0.552   1.170   0.334
ATOM    758  N3  DC3    24       1.777   1.417   0.586
ATOM    759  C2  DC3    24       3.094   1.639   0.811
ATOM    760  O2  DC3    24       3.861   0.694   0.614
ATOM    761  C3* DC3    24       6.818   4.561   1.742
ATOM    762  H3* DC3    24       7.078   5.621   1.672
ATOM    763  C2* DC3    24       5.653   4.225   0.817
ATOM    764 1H2* DC3    24       4.997   5.093   0.736
ATOM    765 2H2* DC3    24       5.982   3.913  -0.176
ATOM    766  O3* DC3    24       7.939   3.736   1.435
ATOM    767  H3T DC3    24       8.367   4.058   0.616
TER
END
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**File E-4**: Average structure of rMD refined *S*-BD-N3-dU modified duplex 5′ - $G^{1}C^{2}T^{3}A^{4}G^{5}C^{6}X^{7}A^{8}G^{9}T^{10}C^{11}C^{12}$- 3′·5′ - $G^{13}G^{14}A^{15}C^{16}T^{17}T^{18}G^{19}C^{20}T^{21}A^{22}G^{23}C^{24}$ -3′.

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REMARK
ATOM      1  H5T DG5     1       0.723  -4.481  -4.674
ATOM      2  O5* DG5     1       1.422  -4.200  -4.076
ATOM      3  C5* DG5     1       2.680  -4.341  -4.722
ATOM      4 1H5* DG5     1       2.697  -3.728  -5.623
ATOM      5 2H5* DG5     1       2.814  -5.384  -5.016
ATOM      6  C4* DG5     1       3.871  -3.930  -3.836
ATOM      7  H4* DG5     1       4.789  -4.157  -4.377
ATOM      8  O4* DG5     1       3.830  -2.530  -3.581
ATOM      9  C1* DG5     1       3.717  -2.309  -2.182
ATOM     10  H1* DG5     1       4.698  -2.047  -1.775
ATOM     11  N9  DG5     1       2.754  -1.214  -1.932
ATOM     12  C8  DG5     1       1.401  -1.200  -2.161
ATOM     13  H8  DG5     1       0.879  -2.041  -2.598
ATOM     14  N7  DG5     1       0.811  -0.088  -1.821
ATOM     15  C5  DG5     1       1.853   0.707  -1.333
ATOM     16  C6  DG5     1       1.867   2.048  -0.813
ATOM     17  O6  DG5     1       0.944   2.849  -0.678
ATOM     18  N1  DG5     1       3.125   2.466  -0.421
ATOM     19  H1  DG5     1       3.192   3.400  -0.028
ATOM     20  C2  DG5     1       4.246   1.696  -0.502
ATOM     21  N2  DG5     1       5.366   2.206  -0.048
ATOM     22 1H2  DG5     1       6.170   1.605  -0.051
ATOM     23 2H2  DG5     1       5.388   3.155   0.341
ATOM     24  N3  DG5     1       4.273   0.455  -0.986
ATOM     25  C4  DG5     1       3.045   0.016  -1.391
ATOM     26  C3* DG5     1       3.928  -4.644  -2.483
ATOM     27  H3* DG5     1       3.377  -5.587  -2.493
ATOM     28  C2* DG5     1       3.262  -3.630  -1.564
ATOM     29 1H2* DG5     1       2.180  -3.747  -1.624
ATOM     30 2H2* DG5     1       3.577  -3.730  -0.531
ATOM     31  O3* DG5     1       5.292  -4.875  -2.172
ATOM     32  P   DC      2       5.761  -5.556  -0.787
ATOM     33  O1P DC      2       7.013  -6.299  -1.039
ATOM     34  O2P DC      2       4.592  -6.234  -0.186
ATOM     35  O5* DC      2       6.104  -4.247   0.095
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ATOM     36  C5* DC      2       7.199  -3.409  -0.249
ATOM     37 1H5* DC      2       6.992  -2.905  -1.194
ATOM     38 2H5* DC      2       8.087  -4.029  -0.381
ATOM     39  C4* DC      2       7.502  -2.357   0.827
ATOM     40  H4* DC      2       8.448  -1.879   0.568
ATOM     41  O4* DC      2       6.486  -1.359   0.856
ATOM     42  C1* DC      2       6.049  -1.179   2.193
ATOM     43  H1* DC      2       6.657  -0.403   2.672
ATOM     44  N1  DC      2       4.608  -0.802   2.186
ATOM     45  C6  DC      2       3.674  -1.654   1.651
ATOM     46  H6  DC      2       4.012  -2.600   1.246
ATOM     47  C5  DC      2       2.362  -1.309   1.609
ATOM     48  H5  DC      2       1.640  -1.982   1.176
ATOM     49  C4  DC      2       2.009  -0.031   2.136
ATOM     50  N4  DC      2       0.774   0.400   2.075
ATOM     51 1H4  DC      2       0.065  -0.147   1.629
ATOM     52 2H4  DC      2       0.582   1.336   2.445
ATOM     53  N3  DC      2       2.898   0.801   2.652
ATOM     54  C2  DC      2       4.207   0.444   2.686
ATOM     55  O2  DC      2       5.007   1.246   3.163
ATOM     56  C3* DC      2       7.639  -2.944   2.238
ATOM     57  H3* DC      2       7.730  -4.033   2.216
ATOM     58  C2* DC      2       6.329  -2.513   2.889
ATOM     59 1H2* DC      2       5.570  -3.260   2.658
ATOM     60 2H2* DC      2       6.418  -2.402   3.966
ATOM     61  O3* DC      2       8.781  -2.368   2.850
ATOM     62  P   DT      3       9.241  -2.740   4.352
ATOM     63  O1P DT      3      10.718  -2.710   4.409
ATOM     64  O2P DT      3       8.497  -3.938   4.798
ATOM     65  O5* DT      3       8.675  -1.463   5.153
ATOM     66  C5* DT      3       9.217  -0.175   4.912
ATOM     67 1H5* DT      3       9.027   0.113   3.877
ATOM     68 2H5* DT      3      10.296  -0.212   5.070
ATOM     69  C4* DT      3       8.626   0.887   5.841
ATOM     70  H4* DT      3       9.175   1.816   5.684
ATOM     71  O4* DT      3       7.259   1.110   5.524
ATOM     72  C1* DT      3       6.514   1.114   6.726
ATOM     73  H1* DT      3       6.528   2.122   7.150
ATOM     74  N1  DT      3       5.120   0.676   6.457
ATOM     75  C6  DT      3       4.856  -0.594   5.984
ATOM     76  H6  DT      3       5.688  -1.260   5.792
ATOM     77  C5  DT      3       3.583  -1.007   5.749
ATOM     78  C7  DT      3       3.332  -2.416   5.247
ATOM     79 1H7  DT      3       4.268  -2.958   5.113
ATOM     80 2H7  DT      3       2.708  -2.946   5.967
ATOM     81 3H7  DT      3       2.795  -2.372   4.300
ATOM     82  C4  DT      3       2.457  -0.106   5.978
ATOM     83  O4  DT      3       1.270  -0.365   5.805
ATOM     84  N3  DT      3       2.805   1.147   6.433
ATOM     85  H3  DT      3       2.055   1.808   6.614
ATOM     86  C2  DT      3       4.083   1.582   6.702
ATOM     87  O2  DT      3       4.253   2.713   7.143
ATOM     88  C3* DT      3       8.722   0.517   7.326
ATOM     89  H3* DT      3       9.374  -0.344   7.490
ATOM     90  C2* DT      3       7.274   0.187   7.674
ATOM     91 1H2* DT      3       7.093  -0.863   7.448
ATOM     92 2H2* DT      3       7.037   0.389   8.716
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ATOM     93  O3* DT      3       9.222   1.651   8.013
ATOM     94  P   DA      4       9.450   1.678   9.609
ATOM     95  O1P DA      4      10.672   2.460   9.889
ATOM     96  O2P DA      4       9.298   0.309  10.146
ATOM     97  O5* DA      4       8.175   2.552  10.052
ATOM     98  C5* DA      4       8.064   3.902   9.628
ATOM     99 1H5* DA      4       7.935   3.937   8.545
ATOM    100 2H5* DA      4       8.986   4.428   9.882
ATOM    101  C4* DA      4       6.898   4.636  10.291
ATOM    102  H4* DA      4       6.970   5.693  10.030
ATOM    103  O4* DA      4       5.663   4.137   9.804
ATOM    104  C1* DA      4       4.848   3.771  10.900
ATOM    105  H1* DA      4       4.200   4.609  11.172
ATOM    106  N9  DA      4       4.041   2.595  10.519
ATOM    107  C8  DA      4       4.475   1.334  10.186
ATOM    108  H8  DA      4       5.523   1.070  10.184
ATOM    109  N7  DA      4       3.522   0.503   9.859
ATOM    110  C5  DA      4       2.369   1.282  10.007
ATOM    111  C6  DA      4       0.991   1.045   9.818
ATOM    112  N6  DA      4       0.510  -0.107   9.380
ATOM    113 1H6  DA      4      -0.488  -0.197   9.193
ATOM    114 2H6  DA      4       1.153  -0.854   9.186
ATOM    115  N1  DA      4       0.091   2.009  10.053
ATOM    116  C2  DA      4       0.536   3.198  10.451
ATOM    117  H2  DA      4      -0.216   3.955  10.625
ATOM    118  N3  DA      4       1.797   3.570  10.647
ATOM    119  C4  DA      4       2.673   2.555  10.409
ATOM    120  C3* DA      4       6.898   4.511  11.816
ATOM    121  H3* DA      4       7.859   4.159  12.197
ATOM    122  C2* DA      4       5.804   3.474  12.050
ATOM    123 1H2* DA      4       6.236   2.478  11.955
ATOM    124 2H2* DA      4       5.319   3.576  13.019
ATOM    125  O3* DA      4       6.596   5.792  12.340
ATOM    126  P   DG      5       6.425   6.072  13.914
ATOM    127  O1P DG      5       6.901   7.442  14.197
ATOM    128  O2P DG      5       6.963   4.920  14.670
ATOM    129  O5* DG      5       4.821   6.056  14.022
ATOM    130  C5* DG      5       4.052   7.052  13.364
ATOM    131 1H5* DG      5       4.080   6.887  12.286
ATOM    132 2H5* DG      5       4.486   8.033  13.573
ATOM    133  C4* DG      5       2.596   7.070  13.839
ATOM    134  H4* DG      5       2.123   7.975  13.454
ATOM    135  O4* DG      5       1.898   5.939  13.340
ATOM    136  C1* DG      5       1.283   5.256  14.416
ATOM    137  H1* DG      5       0.261   5.615  14.543
ATOM    138  N9  DG      5       1.285   3.806  14.125
ATOM    139  C8  DG      5       2.367   2.966  14.036
ATOM    140  H8  DG      5       3.381   3.304  14.207
ATOM    141  N7  DG      5       2.072   1.741  13.702
ATOM    142  C5  DG      5       0.684   1.769  13.541
ATOM    143  C6  DG      5      -0.242   0.749  13.144
ATOM    144  O6  DG      5      -0.026  -0.414  12.821
ATOM    145  N1  DG      5      -1.556   1.174  13.128
ATOM    146  H1  DG      5      -2.254   0.497  12.838
ATOM    147  C2  DG      5      -1.951   2.435  13.454
ATOM    148  N2  DG      5      -3.245   2.668  13.447
ATOM    149 1H2  DG      5      -3.537   3.602  13.666
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ATOM    150 2H2  DG      5      -3.913   1.950  13.136
ATOM    151  N3  DG      5      -1.119   3.415  13.818
ATOM    152  C4  DG      5       0.191   3.023  13.833
ATOM    153  C3* DG      5       2.481   7.066  15.365
ATOM    154  H3* DG      5       3.429   7.330  15.841
ATOM    155  C2* DG      5       2.104   5.617  15.654
ATOM    156 1H2* DG      5       3.016   5.024  15.710
ATOM    157 2H2* DG      5       1.532   5.510  16.572
ATOM    158  O3* DG      5       1.476   7.990  15.736
ATOM    159  P   DC      6       1.133   8.298  17.278
ATOM    160  O1P DC      6       0.745   9.720  17.395
ATOM    161  O2P DC      6       2.209   7.740  18.125
ATOM    162  O5* DC      6      -0.175   7.382  17.464
ATOM    163  C5* DC      6      -1.393   7.725  16.824
ATOM    164 1H5* DC      6      -1.277   7.635  15.743
ATOM    165 2H5* DC      6      -1.647   8.759  17.066
ATOM    166  C4* DC      6      -2.540   6.822  17.286
ATOM    167  H4* DC      6      -3.477   7.245  16.924
ATOM    168  O4* DC      6      -2.396   5.530  16.727
ATOM    169  C1* DC      6      -2.742   4.555  17.689
ATOM    170  H1* DC      6      -3.799   4.295  17.574
ATOM    171  N1  DC      6      -1.868   3.377  17.430
ATOM    172  C6  DC      6      -0.501   3.504  17.510
ATOM    173  H6  DC      6      -0.081   4.462  17.795
ATOM    174  C5  DC      6       0.309   2.461  17.199
ATOM    175  H5  DC      6       1.381   2.573  17.251
ATOM    176  C4  DC      6      -0.321   1.252  16.782
ATOM    177  N4  DC      6       0.402   0.228  16.399
ATOM    178 1H4  DC      6       1.395   0.316  16.311
ATOM    179 2H4  DC      6      -0.096  -0.608  16.080
ATOM    180  N3  DC      6      -1.634   1.123  16.678
ATOM    181  C2  DC      6      -2.436   2.170  16.999
ATOM    182  O2  DC      6      -3.655   2.024  16.895
ATOM    183  C3* DC      6      -2.628   6.700  18.812
ATOM    184  H3* DC      6      -1.798   7.225  19.292
ATOM    185  C2* DC      6      -2.530   5.195  19.070
ATOM    186 1H2* DC      6      -1.540   4.977  19.470
ATOM    187 2H2* DC      6      -3.286   4.854  19.777
ATOM    188  O3* DC      6      -3.859   7.252  19.242
ATOM    189  P   DX      7      -4.144   7.604  20.794
ATOM    190  O1P DX      7      -5.048   8.773  20.836
ATOM    191  O2P DX      7      -2.860   7.624  21.528
ATOM    192  O5* DX      7      -4.968   6.307  21.264
ATOM    193  C5* DX      7      -6.242   6.025  20.710
ATOM    194 1H5* DX      7      -6.142   5.855  19.635
ATOM    195 2H5* DX      7      -6.899   6.883  20.870
ATOM    196  C4* DX      7      -6.867   4.789  21.364
ATOM    197  H4* DX      7      -7.848   4.625  20.919
ATOM    198  O4* DX      7      -6.074   3.638  21.113
ATOM    199  C1* DX      7      -6.129   2.800  22.252
ATOM    200  H1* DX      7      -7.023   2.172  22.183
ATOM    201  N1  DX      7      -4.893   1.967  22.317
ATOM    202  C6  DX      7      -3.662   2.573  22.283
ATOM    203  H6  DX      7      -3.609   3.656  22.237
ATOM    204  C5  DX      7      -2.529   1.832  22.280
ATOM    205  H5  DX      7      -1.563   2.315  22.247
ATOM    206  C4  DX      7      -2.556   0.385  22.291
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ATOM    207  O4  DX      7      -1.529  -0.289  22.231
ATOM    208  N3  DX      7      -3.832  -0.198  22.338
ATOM    209  C11 DX      7      -3.872  -1.704  22.119
ATOM    210  C2  DX      7      -5.013   0.569  22.378
ATOM    211  O2  DX      7      -6.123   0.040  22.488
ATOM    212  C3* DX      7      -7.050   4.942  22.880
ATOM    213  H3* DX      7      -6.605   5.877  23.231
ATOM    214  C2* DX      7      -6.293   3.743  23.445
ATOM    215 1H2* DX      7      -5.327   4.083  23.815
ATOM    216 2H2* DX      7      -6.855   3.255  24.236
ATOM    217  O3* DX      7      -8.435   4.907  23.195
ATOM    218  C12 DX      7      -4.962  -2.614  22.714
ATOM    219  C9  DX      7      -6.011  -2.928  21.667
ATOM    220  C10 DX      7      -6.385  -4.121  21.225
ATOM    221  O12 DX      7      -5.574  -2.033  23.817
ATOM    222  H15 DX      7      -2.945  -2.119  22.509
ATOM    223  H14 DX      7      -3.843  -1.872  21.044
ATOM    224  H9  DX      7      -4.495  -3.548  23.025
ATOM    225 1H1  DX      7      -6.544  -2.111  21.203
ATOM    226 2H1  DX      7      -5.914  -5.003  21.637
ATOM    227 3H1  DX      7      -7.151  -4.187  20.464
ATOM    228  H10 DX      7      -5.867  -1.154  23.472
ATOM    229  P   DA      8      -9.012   5.359  24.643
ATOM    230  O1P DA      8     -10.367   5.917  24.447
ATOM    231  O2P DA      8      -7.978   6.147  25.346
ATOM    232  O5* DA      8      -9.163   3.961  25.424
ATOM    233  C5* DA      8     -10.108   3.001  24.991
ATOM    234 1H5* DA      8      -9.989   2.853  23.916
ATOM    235 2H5* DA      8     -11.116   3.379  25.173
ATOM    236  C4* DA      8      -9.938   1.641  25.676
ATOM    237  H4* DA      8     -10.613   0.948  25.174
ATOM    238  O4* DA      8      -8.610   1.170  25.495
ATOM    239  C1* DA      8      -7.923   1.158  26.736
ATOM    240  H1* DA      8      -7.673   0.117  26.967
ATOM    241  N9  DA      8      -6.663   1.943  26.639
ATOM    242  C8  DA      8      -6.431   3.289  26.839
ATOM    243  H8  DA      8      -7.217   4.004  27.048
ATOM    244  N7  DA      8      -5.182   3.648  26.704
ATOM    245  C5  DA      8      -4.543   2.451  26.376
ATOM    246  C6  DA      8      -3.215   2.095  26.055
ATOM    247  N6  DA      8      -2.193   2.929  25.993
ATOM    248 1H6  DA      8      -1.314   2.524  25.725
ATOM    249 2H6  DA      8      -2.339   3.903  26.198
ATOM    250  N1  DA      8      -2.904   0.842  25.736
ATOM    251  C2  DA      8      -3.870  -0.067  25.739
ATOM    252  H2  DA      8      -3.583  -1.076  25.480
ATOM    253  N3  DA      8      -5.156   0.119  26.018
ATOM    254  C4  DA      8      -5.434   1.413  26.328
ATOM    255  C3* DA      8     -10.263   1.606  27.174
ATOM    256  H3* DA      8     -10.871   2.461  27.476
ATOM    257  C2* DA      8      -8.877   1.683  27.813
ATOM    258 1H2* DA      8      -8.680   2.725  28.054
ATOM    259 2H2* DA      8      -8.791   1.092  28.723
ATOM    260  O3* DA      8     -10.983   0.403  27.402
ATOM    261  P   DG      9     -11.303  -0.211  28.863
ATOM    262  O1P DG      9     -12.626  -0.870  28.810
ATOM    263  O2P DG      9     -11.015   0.804  29.899
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ATOM    264  O5* DG      9     -10.168  -1.353  28.902
ATOM    265  C5* DG      9     -10.191  -2.386  27.927
ATOM    266 1H5* DG      9     -10.107  -1.947  26.932
ATOM    267 2H5* DG      9     -11.148  -2.908  27.991
ATOM    268  C4* DG      9      -9.065  -3.408  28.093
ATOM    269  H4* DG      9      -9.242  -4.215  27.380
ATOM    270  O4* DG      9      -7.811  -2.808  27.791
ATOM    271  C1* DG      9      -6.885  -3.183  28.790
ATOM    272  H1* DG      9      -6.420  -4.137  28.526
ATOM    273  N9  DG      9      -5.850  -2.137  28.946
ATOM    274  C8  DG      9      -5.995  -0.855  29.412
ATOM    275  H8  DG      9      -6.955  -0.444  29.691
ATOM    276  N7  DG      9      -4.879  -0.183  29.491
ATOM    277  C5  DG      9      -3.914  -1.080  29.020
ATOM    278  C6  DG      9      -2.492  -0.948  28.836
ATOM    279  O6  DG      9      -1.751   0.008  29.062
ATOM    280  N1  DG      9      -1.904  -2.089  28.320
ATOM    281  H1  DG      9      -0.911  -2.042  28.116
ATOM    282  C2  DG      9      -2.580  -3.232  28.028
ATOM    283  N2  DG      9      -1.883  -4.254  27.597
ATOM    284 1H2  DG      9      -2.378  -5.120  27.494
ATOM    285 2H2  DG      9      -0.860  -4.200  27.532
ATOM    286  N3  DG      9      -3.889  -3.398  28.199
ATOM    287  C4  DG      9      -4.507  -2.281  28.686
ATOM    288  C3* DG      9      -8.984  -4.024  29.496
ATOM    289  H3* DG      9      -9.859  -3.779  30.102
ATOM    290  C2* DG      9      -7.724  -3.366  30.051
ATOM    291 1H2* DG      9      -7.996  -2.402  30.483
ATOM    292 2H2* DG      9      -7.215  -3.980  30.791
ATOM    293  O3* DG      9      -8.868  -5.429  29.336
ATOM    294  P   DT     10      -8.662  -6.452  30.568
ATOM    295  O1P DT     10      -9.447  -7.674  30.298
ATOM    296  O2P DT     10      -8.827  -5.719  31.842
ATOM    297  O5* DT     10      -7.101  -6.798  30.380
ATOM    298  C5* DT     10      -6.652  -7.426  29.189
ATOM    299 1H5* DT     10      -6.811  -6.755  28.344
ATOM    300 2H5* DT     10      -7.238  -8.332  29.023
ATOM    301  C4* DT     10      -5.170  -7.810  29.242
ATOM    302  H4* DT     10      -4.931  -8.348  28.322
ATOM    303  O4* DT     10      -4.361  -6.642  29.309
ATOM    304  C1* DT     10      -3.493  -6.753  30.422
ATOM    305  H1* DT     10      -2.558  -7.216  30.091
ATOM    306  N1  DT     10      -3.231  -5.403  30.991
ATOM    307  C6  DT     10      -4.247  -4.661  31.562
ATOM    308  H6  DT     10      -5.248  -5.075  31.585
ATOM    309  C5  DT     10      -4.015  -3.415  32.056
ATOM    310  C7  DT     10      -5.157  -2.645  32.691
ATOM    311 1H7  DT     10      -5.488  -1.865  32.005
ATOM    312 2H7  DT     10      -5.989  -3.310  32.927
ATOM    313 3H7  DT     10      -4.804  -2.169  33.608
ATOM    314  C4  DT     10      -2.680  -2.825  31.993
ATOM    315  O4  DT     10      -2.344  -1.713  32.392
ATOM    316  N3  DT     10      -1.724  -3.633  31.418
ATOM    317  H3  DT     10      -0.776  -3.271  31.375
ATOM    318  C2  DT     10      -1.927  -4.897  30.914
ATOM    319  O2  DT     10      -0.979  -5.515  30.447
ATOM    320  C3* DT     10      -4.820  -8.710  30.432
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ATOM    321  H3* DT     10      -5.710  -9.167  30.871
ATOM    322  C2* DT     10      -4.177  -7.717  31.392
ATOM    323 1H2* DT     10      -4.961  -7.227  31.967
ATOM    324 2H2* DT     10      -3.470  -8.192  32.064
ATOM    325  O3* DT     10      -3.928  -9.711  29.965
ATOM    326  P   DC     11      -3.287 -10.841  30.922
ATOM    327  O1P DC     11      -3.222 -12.106  30.162
ATOM    328  O2P DC     11      -3.952 -10.791  32.242
ATOM    329  O5* DC     11      -1.791 -10.265  31.085
ATOM    330  C5* DC     11      -0.928 -10.196  29.960
ATOM    331 1H5* DC     11      -1.359  -9.526  29.215
ATOM    332 2H5* DC     11      -0.844 -11.190  29.517
ATOM    333  C4* DC     11       0.477  -9.695  30.318
ATOM    334  H4* DC     11       1.084  -9.722  29.413
ATOM    335  O4* DC     11       0.401  -8.352  30.775
ATOM    336  C1* DC     11       1.048  -8.251  32.030
ATOM    337  H1* DC     11       2.100  -7.995  31.864
ATOM    338  N1  DC     11       0.369  -7.204  32.844
ATOM    339  C6  DC     11      -0.934  -7.365  33.252
ATOM    340  H6  DC     11      -1.459  -8.269  32.965
ATOM    341  C5  DC     11      -1.559  -6.401  33.977
ATOM    342  H5  DC     11      -2.584  -6.537  34.286
ATOM    343  C4  DC     11      -0.810  -5.222  34.271
ATOM    344  N4  DC     11      -1.339  -4.232  34.944
ATOM    345 1H4  DC     11      -2.291  -4.259  35.252
ATOM    346 2H4  DC     11      -0.740  -3.412  35.092
ATOM    347  N3  DC     11       0.443  -5.057  33.885
ATOM    348  C2  DC     11       1.058  -6.027  33.165
ATOM    349  O2  DC     11       2.232  -5.841  32.849
ATOM    350  C3* DC     11       1.182 -10.525  31.396
ATOM    351  H3* DC     11       0.724 -11.508  31.519
ATOM    352  C2* DC     11       0.981  -9.657  32.633
ATOM    353 1H2* DC     11       0.000  -9.876  33.052
ATOM    354 2H2* DC     11       1.744  -9.822  33.389
ATOM    355  O3* DC     11       2.546 -10.652  31.022
ATOM    356  P   DC3    12       3.642 -11.403  31.941
ATOM    357  O1P DC3    12       4.624 -12.067  31.059
ATOM    358  O2P DC3    12       2.948 -12.164  32.999
ATOM    359  O5* DC3    12       4.363 -10.144  32.634
ATOM    360  C5* DC3    12       5.134  -9.240  31.860
ATOM    361 1H5* DC3    12       4.480  -8.694  31.176
ATOM    362 2H5* DC3    12       5.860  -9.801  31.268
ATOM    363  C4* DC3    12       5.887  -8.244  32.748
ATOM    364  H4* DC3    12       6.562  -7.658  32.122
ATOM    365  O4* DC3    12       4.959  -7.370  33.372
ATOM    366  C1* DC3    12       5.266  -7.289  34.749
ATOM    367  H1* DC3    12       6.016  -6.505  34.892
ATOM    368  N1  DC3    12       4.027  -6.980  35.516
ATOM    369  C6  DC3    12       2.933  -7.808  35.438
ATOM    370  H6  DC3    12       3.002  -8.699  34.827
ATOM    371  C5  DC3    12       1.782  -7.493  36.087
ATOM    372  H5  DC3    12       0.922  -8.138  36.005
ATOM    373  C4  DC3    12       1.769  -6.275  36.833
ATOM    374  N4  DC3    12       0.685  -5.871  37.449
ATOM    375 1H4  DC3    12      -0.168  -6.387  37.373
ATOM    376 2H4  DC3    12       0.726  -4.952  37.902
ATOM    377  N3  DC3    12       2.825  -5.485  36.938
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ATOM    378  C2  DC3    12       3.971  -5.816  36.291
ATOM    379  O2  DC3    12       4.944  -5.072  36.420
ATOM    380  C3* DC3    12       6.705  -8.937  33.850
ATOM    381  H3* DC3    12       6.777 -10.012  33.670
ATOM    382  C2* DC3    12       5.891  -8.641  35.106
ATOM    383 1H2* DC3    12       5.134  -9.413  35.226
ATOM    384 2H2* DC3    12       6.515  -8.575  35.999
ATOM    385  O3* DC3    12       7.994  -8.356  33.963
ATOM    386  H3T DC3    12       8.541  -8.910  34.526
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ATOM    387  H5T DG5    13       0.648   4.295  42.080
ATOM    388  O5* DG5    13       1.274   4.003  41.411
ATOM    389  C5* DG5    13       2.599   4.211  41.880
ATOM    390 1H5* DG5    13       2.759   3.632  42.791
ATOM    391 2H5* DG5    13       2.733   5.268  42.118
ATOM    392  C4* DG5    13       3.674   3.806  40.854
ATOM    393  H4* DG5    13       4.644   4.114  41.247
ATOM    394  O4* DG5    13       3.686   2.392  40.686
ATOM    395  C1* DG5    13       3.422   2.074  39.328
ATOM    396  H1* DG5    13       4.360   1.838  38.818
ATOM    397  N9  DG5    13       2.504   0.915  39.263
ATOM    398  C8  DG5    13       1.198   0.840  39.673
ATOM    399  H8  DG5    13       0.680   1.680  40.112
ATOM    400  N7  DG5    13       0.650  -0.332  39.506
ATOM    401  C5  DG5    13       1.668  -1.097  38.927
ATOM    402  C6  DG5    13       1.709  -2.475  38.513
ATOM    403  O6  DG5    13       0.840  -3.345  38.572
ATOM    404  N1  DG5    13       2.936  -2.845  37.992
ATOM    405  H1  DG5    13       3.012  -3.797  37.650
ATOM    406  C2  DG5    13       4.006  -2.010  37.881
ATOM    407  N2  DG5    13       5.094  -2.495  37.336
ATOM    408 1H2  DG5    13       5.833  -1.841  37.155
ATOM    409 2H2  DG5    13       5.115  -3.454  36.971
ATOM    410  N3  DG5    13       4.011  -0.736  38.266
ATOM    411  C4  DG5    13       2.810  -0.335  38.779
ATOM    412  C3* DG5    13       3.498   4.442  39.471
ATOM    413  H3* DG5    13       2.872   5.336  39.504
ATOM    414  C2* DG5    13       2.813   3.324  38.695
ATOM    415 1H2* DG5    13       1.739   3.373  38.874
ATOM    416 2H2* DG5    13       3.001   3.378  37.626
ATOM    417  O3* DG5    13       4.791   4.764  38.988
ATOM    418  P   DG     14       5.042   5.396  37.528
ATOM    419  O1P DG     14       6.205   6.303  37.612
ATOM    420  O2P DG     14       3.750   5.879  36.993
ATOM    421  O5* DG     14       5.475   4.076  36.711
ATOM    422  C5* DG     14       6.677   3.392  37.035
ATOM    423 1H5* DG     14       6.581   2.929  38.019
ATOM    424 2H5* DG     14       7.494   4.115  37.073
ATOM    425  C4* DG     14       7.043   2.311  36.009
ATOM    426  H4* DG     14       8.054   1.967  36.231
ATOM    427  O4* DG     14       6.154   1.202  36.103
ATOM    428  C1* DG     14       5.564   0.973  34.834
ATOM    429  H1* DG     14       6.134   0.212  34.295
ATOM    430  N9  DG     14       4.163   0.532  35.007
ATOM    431  C8  DG     14       3.100   1.260  35.477
ATOM    432  H8  DG     14       3.196   2.297  35.767
ATOM    433  N7  DG     14       1.982   0.594  35.559
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ATOM    434  C5  DG     14       2.324  -0.677  35.089
ATOM    435  C6  DG     14       1.540  -1.870  34.939
ATOM    436  O6  DG     14       0.358  -2.070  35.214
ATOM    437  N1  DG     14       2.254  -2.926  34.404
ATOM    438  H1  DG     14       1.727  -3.771  34.211
ATOM    439  C2  DG     14       3.570  -2.864  34.058
ATOM    440  N2  DG     14       4.092  -3.921  33.484
ATOM    441 1H2  DG     14       5.031  -3.828  33.144
ATOM    442 2H2  DG     14       3.498  -4.716  33.218
ATOM    443  N3  DG     14       4.335  -1.781  34.202
ATOM    444  C4  DG     14       3.655  -0.716  34.726
ATOM    445  C3* DG     14       7.016   2.820  34.565
ATOM    446  H3* DG     14       7.061   3.911  34.515
ATOM    447  C2* DG     14       5.668   2.298  34.082
ATOM    448 1H2* DG     14       4.890   2.996  34.391
ATOM    449 2H2* DG     14       5.631   2.163  33.005
ATOM    450  O3* DG     14       8.121   2.248  33.885
ATOM    451  P   DA     15       8.389   2.467  32.311
ATOM    452  O1P DA     15       9.849   2.521  32.095
ATOM    453  O2P DA     15       7.516   3.551  31.815
ATOM    454  O5* DA     15       7.845   1.073  31.725
ATOM    455  C5* DA     15       8.491  -0.143  32.064
ATOM    456 1H5* DA     15       8.315  -0.370  33.116
ATOM    457 2H5* DA     15       9.564  -0.025  31.911
ATOM    458  C4* DA     15       8.016  -1.320  31.207
ATOM    459  H4* DA     15       8.660  -2.173  31.423
ATOM    460  O4* DA     15       6.677  -1.668  31.536
ATOM    461  C1* DA     15       5.864  -1.555  30.379
ATOM    462  H1* DA     15       5.712  -2.547  29.943
ATOM    463  N9  DA     15       4.566  -0.962  30.772
ATOM    464  C8  DA     15       4.294   0.328  31.160
ATOM    465  H8  DA     15       5.053   1.098  31.188
ATOM    466  N7  DA     15       3.050   0.537  31.501
ATOM    467  C5  DA     15       2.460  -0.721  31.330
ATOM    468  C6  DA     15       1.163  -1.242  31.538
ATOM    469  N6  DA     15       0.156  -0.535  32.027
ATOM    470 1H6  DA     15      -0.751  -0.983  32.164
ATOM    471 2H6  DA     15       0.315   0.424  32.285
ATOM    472  N1  DA     15       0.897  -2.528  31.280
ATOM    473  C2  DA     15       1.880  -3.293  30.816
ATOM    474  H2  DA     15       1.627  -4.323  30.608
ATOM    475  N3  DA     15       3.138  -2.941  30.571
ATOM    476  C4  DA     15       3.370  -1.632  30.865
ATOM    477  C3* DA     15       8.084  -1.031  29.705
ATOM    478  H3* DA     15       8.746  -0.191  29.481
ATOM    479  C2* DA     15       6.634  -0.686  29.383
ATOM    480 1H2* DA     15       6.479   0.375  29.578
ATOM    481 2H2* DA     15       6.366  -0.907  28.351
ATOM    482  O3* DA     15       8.552  -2.207  29.072
ATOM    483  P   DC     16       8.715  -2.328  27.474
ATOM    484  O1P DC     16       9.854  -3.226  27.183
ATOM    485  O2P DC     16       8.652  -0.976  26.880
ATOM    486  O5* DC     16       7.348  -3.101  27.130
ATOM    487  C5* DC     16       7.154  -4.440  27.561
ATOM    488 1H5* DC     16       7.216  -4.489  28.650
ATOM    489 2H5* DC     16       7.941  -5.068  27.138
ATOM    490  C4* DC     16       5.793  -4.979  27.116
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ATOM    491  H4* DC     16       5.730  -6.035  27.382
ATOM    492  O4* DC     16       4.746  -4.285  27.774
ATOM    493  C1* DC     16       3.636  -4.188  26.903
ATOM    494  H1* DC     16       2.993  -5.064  27.039
ATOM    495  N1  DC     16       2.909  -2.928  27.218
ATOM    496  C6  DC     16       3.596  -1.739  27.285
ATOM    497  H6  DC     16       4.660  -1.744  27.069
ATOM    498  C5  DC     16       2.961  -0.595  27.642
ATOM    499  H5  DC     16       3.513   0.329  27.711
ATOM    500  C4  DC     16       1.568  -0.689  27.937
ATOM    501  N4  DC     16       0.901   0.356  28.358
ATOM    502 1H4  DC     16       1.372   1.221  28.533
ATOM    503 2H4  DC     16      -0.088   0.218  28.591
ATOM    504  N3  DC     16       0.891  -1.821  27.854
ATOM    505  C2  DC     16       1.534  -2.958  27.485
ATOM    506  O2  DC     16       0.871  -3.991  27.383
ATOM    507  C3* DC     16       5.575  -4.855  25.607
ATOM    508  H3* DC     16       6.345  -4.221  25.161
ATOM    509  C2* DC     16       4.206  -4.188  25.482
ATOM    510 1H2* DC     16       4.353  -3.174  25.112
ATOM    511 2H2* DC     16       3.547  -4.733  24.808
ATOM    512  O3* DC     16       5.609  -6.140  25.017
ATOM    513  P   DT     17       5.631  -6.328  23.415
ATOM    514  O1P DT     17       6.443  -7.522  23.099
ATOM    515  O2P DT     17       5.943  -5.025  22.790
ATOM    516  O5* DT     17       4.091  -6.668  23.110
ATOM    517  C5* DT     17       3.527  -7.891  23.551
ATOM    518 1H5* DT     17       3.545  -7.933  24.643
ATOM    519 2H5* DT     17       4.119  -8.720  23.157
ATOM    520  C4* DT     17       2.084  -8.042  23.067
ATOM    521  H4* DT     17       1.750  -9.055  23.298
ATOM    522  O4* DT     17       1.251  -7.123  23.752
ATOM    523  C1* DT     17       0.343  -6.561  22.828
ATOM    524  H1* DT     17      -0.530  -7.215  22.753
ATOM    525  N1  DT     17      -0.056  -5.219  23.330
ATOM    526  C6  DT     17       0.859  -4.186  23.402
ATOM    527  H6  DT     17       1.864  -4.341  23.033
ATOM    528  C5  DT     17       0.525  -2.990  23.954
ATOM    529  C7  DT     17       1.555  -1.878  23.994
ATOM    530 1H7  DT     17       1.568  -1.428  24.987
ATOM    531 2H7  DT     17       2.548  -2.255  23.748
ATOM    532 3H7  DT     17       1.263  -1.111  23.274
ATOM    533  C4  DT     17      -0.800  -2.780  24.531
ATOM    534  O4  DT     17      -1.195  -1.784  25.124
ATOM    535  N3  DT     17      -1.663  -3.846  24.396
ATOM    536  H3  DT     17      -2.566  -3.750  24.823
ATOM    537  C2  DT     17      -1.360  -5.058  23.814
ATOM    538  O2  DT     17      -2.226  -5.923  23.750
ATOM    539  C3* DT     17       1.932  -7.815  21.557
ATOM    540  H3* DT     17       2.905  -7.643  21.091
ATOM    541  C2* DT     17       1.060  -6.566  21.472
ATOM    542 1H2* DT     17       1.710  -5.702  21.353
ATOM    543 2H2* DT     17       0.350  -6.613  20.649
ATOM    544  O3* DT     17       1.309  -8.951  20.987
ATOM    545  P   DT     18       1.283  -9.199  19.392
ATOM    546  O1P DT     18       1.308 -10.658  19.157
ATOM    547  O2P DT     18       2.289  -8.324  18.756
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ATOM    548  O5* DT     18      -0.176  -8.646  19.004
ATOM    549  C5* DT     18      -1.342  -9.303  19.473
ATOM    550 1H5* DT     18      -1.432  -9.156  20.551
ATOM    551 2H5* DT     18      -1.254 -10.373  19.274
ATOM    552  C4* DT     18      -2.609  -8.787  18.783
ATOM    553  H4* DT     18      -3.438  -9.435  19.066
ATOM    554  O4* DT     18      -2.898  -7.458  19.205
ATOM    555  C1* DT     18      -3.159  -6.684  18.048
ATOM    556  H1* DT     18      -4.203  -6.830  17.753
ATOM    557  N1  DT     18      -2.896  -5.244  18.307
ATOM    558  C6  DT     18      -1.622  -4.783  18.577
ATOM    559  H6  DT     18      -0.808  -5.496  18.632
ATOM    560  C5  DT     18      -1.383  -3.460  18.778
ATOM    561  C7  DT     18       0.026  -2.998  19.092
ATOM    562 1H7  DT     18       0.433  -2.490  18.217
ATOM    563 2H7  DT     18      -0.005  -2.290  19.924
ATOM    564 3H7  DT     18       0.661  -3.842  19.362
ATOM    565  C4  DT     18      -2.471  -2.487  18.718
ATOM    566  O4  DT     18      -2.390  -1.273  18.867
ATOM    567  N3  DT     18      -3.714  -3.029  18.474
ATOM    568  H3  DT     18      -4.489  -2.395  18.426
ATOM    569  C2  DT     18      -3.987  -4.366  18.290
ATOM    570  O2  DT     18      -5.150  -4.718  18.141
ATOM    571  C3* DT     18      -2.499  -8.786  17.250
ATOM    572  H3* DT     18      -1.657  -9.387  16.899
ATOM    573  C2* DT     18      -2.282  -7.306  16.963
ATOM    574 1H2* DT     18      -1.230  -7.062  17.100
ATOM    575 2H2* DT     18      -2.607  -7.035  15.966
ATOM    576  O3* DT     18      -3.723  -9.276  16.720
ATOM    577  P   DG     19      -3.990  -9.454  15.135
ATOM    578  O1P DG     19      -4.756 -10.701  14.935
ATOM    579  O2P DG     19      -2.726  -9.228  14.403
ATOM    580  O5* DG     19      -4.962  -8.210  14.824
ATOM    581  C5* DG     19      -6.269  -8.166  15.372
ATOM    582 1H5* DG     19      -6.198  -8.137  16.460
ATOM    583 2H5* DG     19      -6.802  -9.074  15.088
ATOM    584  C4* DG     19      -7.084  -6.952  14.902
ATOM    585  H4* DG     19      -8.061  -7.008  15.383
ATOM    586  O4* DG     19      -6.446  -5.747  15.304
ATOM    587  C1* DG     19      -5.991  -5.039  14.161
ATOM    588  H1* DG     19      -6.634  -4.168  14.011
ATOM    589  N9  DG     19      -4.593  -4.591  14.382
ATOM    590  C8  DG     19      -3.423  -5.292  14.209
ATOM    591  H8  DG     19      -3.396  -6.328  13.889
ATOM    592  N7  DG     19      -2.345  -4.622  14.506
ATOM    593  C5  DG     19      -2.827  -3.376  14.909
ATOM    594  C6  DG     19      -2.141  -2.207  15.382
ATOM    595  O6  DG     19      -0.941  -2.024  15.568
ATOM    596  N1  DG     19      -2.992  -1.166  15.694
ATOM    597  H1  DG     19      -2.568  -0.335  16.096
ATOM    598  C2  DG     19      -4.344  -1.225  15.573
ATOM    599  N2  DG     19      -5.027  -0.177  15.964
ATOM    600 1H2  DG     19      -6.020  -0.217  15.836
ATOM    601 2H2  DG     19      -4.549   0.668  16.303
ATOM    602  N3  DG     19      -5.017  -2.291  15.142
ATOM    603  C4  DG     19      -4.204  -3.345  14.827
ATOM    604  C3* DG     19      -7.301  -6.875  13.387
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ATOM    605  H3* DG     19      -7.235  -7.856  12.913
ATOM    606  C2* DG     19      -6.143  -5.979  12.962
ATOM    607 1H2* DG     19      -5.264  -6.604  12.821
ATOM    608 2H2* DG     19      -6.344  -5.439  12.040
ATOM    609  O3* DG     19      -8.584  -6.306  13.166
ATOM    610  P   DC     20      -9.129  -5.889  11.706
ATOM    611  O1P DC     20     -10.597  -6.067  11.691
ATOM    612  O2P DC     20      -8.287  -6.532  10.675
ATOM    613  O5* DC     20      -8.804  -4.309  11.720
ATOM    614  C5* DC     20      -9.479  -3.456  12.632
ATOM    615 1H5* DC     20      -9.261  -3.773  13.653
ATOM    616 2H5* DC     20     -10.554  -3.545  12.469
ATOM    617  C4* DC     20      -9.079  -1.984  12.480
ATOM    618  H4* DC     20      -9.704  -1.398  13.153
ATOM    619  O4* DC     20      -7.718  -1.803  12.854
ATOM    620  C1* DC     20      -7.070  -1.020  11.869
ATOM    621  H1* DC     20      -7.187   0.042  12.114
ATOM    622  N1  DC     20      -5.630  -1.401  11.816
ATOM    623  C6  DC     20      -5.262  -2.673  11.449
ATOM    624  H6  DC     20      -6.036  -3.391  11.211
ATOM    625  C5  DC     20      -3.955  -3.032  11.415
ATOM    626  H5  DC     20      -3.678  -4.036  11.139
ATOM    627  C4  DC     20      -2.997  -2.044  11.785
ATOM    628  N4  DC     20      -1.723  -2.343  11.850
ATOM    629 1H4  DC     20      -1.420  -3.288  11.716
ATOM    630 2H4  DC     20      -1.081  -1.618  12.187
ATOM    631  N3  DC     20      -3.336  -0.821  12.161
ATOM    632  C2  DC     20      -4.648  -0.472  12.191
ATOM    633  O2  DC     20      -4.926   0.670  12.552
ATOM    634  C3* DC     20      -9.269  -1.437  11.061
ATOM    635  H3* DC     20      -9.839  -2.127  10.434
ATOM    636  C2* DC     20      -7.831  -1.311  10.572
ATOM    637 1H2* DC     20      -7.538  -2.261  10.128
ATOM    638 2H2* DC     20      -7.711  -0.514   9.844
ATOM    639  O3* DC     20      -9.933  -0.187  11.147
ATOM    640  P   DT     21     -10.297   0.697   9.846
ATOM    641  O1P DT     21     -11.597   1.358  10.084
ATOM    642  O2P DT     21     -10.082  -0.125   8.636
ATOM    643  O5* DT     21      -9.137   1.812   9.914
ATOM    644  C5* DT     21      -9.118   2.745  10.983
ATOM    645 1H5* DT     21      -9.026   2.209  11.929
ATOM    646 2H5* DT     21     -10.060   3.296  10.986
ATOM    647  C4* DT     21      -7.962   3.743  10.870
ATOM    648  H4* DT     21      -8.061   4.464  11.682
ATOM    649  O4* DT     21      -6.722   3.063  11.009
ATOM    650  C1* DT     21      -5.864   3.476   9.963
ATOM    651  H1* DT     21      -5.332   4.380  10.276
ATOM    652  N1  DT     21      -4.901   2.390   9.641
ATOM    653  C6  DT     21      -5.332   1.201   9.085
ATOM    654  H6  DT     21      -6.391   1.053   8.923
ATOM    655  C5  DT     21      -4.452   0.227   8.740
ATOM    656  C7  DT     21      -4.962  -1.059   8.113
ATOM    657 1H7  DT     21      -4.525  -1.915   8.632
ATOM    658 2H7  DT     21      -6.048  -1.118   8.168
ATOM    659 3H7  DT     21      -4.649  -1.094   7.068
ATOM    660  C4  DT     21      -3.023   0.403   8.974
ATOM    661  O4  DT     21      -2.138  -0.404   8.702
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ATOM    662  N3  DT     21      -2.678   1.599   9.565
ATOM    663  H3  DT     21      -1.694   1.764   9.749
ATOM    664  C2  DT     21      -3.544   2.616   9.898
ATOM    665  O2  DT     21      -3.100   3.653  10.378
ATOM    666  C3* DT     21      -7.943   4.514   9.545
ATOM    667  H3* DT     21      -8.881   4.408   8.996
ATOM    668  C2* DT     21      -6.788   3.852   8.803
ATOM    669 1H2* DT     21      -7.169   2.976   8.281
ATOM    670 2H2* DT     21      -6.306   4.523   8.097
ATOM    671  O3* DT     21      -7.698   5.878   9.844
ATOM    672  P   DA     22      -7.600   7.016   8.703
ATOM    673  O1P DA     22      -8.229   8.246   9.225
ATOM    674  O2P DA     22      -8.037   6.443   7.411
ATOM    675  O5* DA     22      -6.007   7.248   8.650
ATOM    676  C5* DA     22      -5.334   7.817   9.762
ATOM    677 1H5* DA     22      -5.411   7.145  10.619
ATOM    678 2H5* DA     22      -5.816   8.761  10.016
ATOM    679  C4* DA     22      -3.853   8.092   9.481
ATOM    680  H4* DA     22      -3.446   8.641  10.332
ATOM    681  O4* DA     22      -3.146   6.867   9.355
ATOM    682  C1* DA     22      -2.409   6.886   8.147
ATOM    683  H1* DA     22      -1.401   7.268   8.337
ATOM    684  N9  DA     22      -2.346   5.520   7.594
ATOM    685  C8  DA     22      -3.376   4.733   7.140
ATOM    686  H8  DA     22      -4.403   5.068   7.150
ATOM    687  N7  DA     22      -3.010   3.554   6.714
ATOM    688  C5  DA     22      -1.620   3.580   6.887
ATOM    689  C6  DA     22      -0.578   2.664   6.633
ATOM    690  N6  DA     22      -0.778   1.455   6.135
ATOM    691 1H6  DA     22       0.013   0.824   6.002
ATOM    692 2H6  DA     22      -1.718   1.170   5.924
ATOM    693  N1  DA     22       0.695   2.983   6.901
ATOM    694  C2  DA     22       0.944   4.182   7.422
ATOM    695  H2  DA     22       1.981   4.407   7.633
ATOM    696  N3  DA     22       0.069   5.137   7.718
ATOM    697  C4  DA     22      -1.209   4.770   7.423
ATOM    698  C3* DA     22      -3.609   8.918   8.213
ATOM    699  H3* DA     22      -4.520   9.410   7.865
ATOM    700  C2* DA     22      -3.149   7.851   7.226
ATOM    701 1H2* DA     22      -4.025   7.378   6.782
ATOM    702 2H2* DA     22      -2.502   8.245   6.444
ATOM    703  O3* DA     22      -2.610   9.877   8.515
ATOM    704  P   DG     23      -2.037  10.916   7.424
ATOM    705  O1P DG     23      -1.754  12.196   8.107
ATOM    706  O2P DG     23      -2.904  10.886   6.227
ATOM    707  O5* DG     23      -0.636  10.212   7.062
ATOM    708  C5* DG     23       0.382  10.105   8.046
ATOM    709 1H5* DG     23       0.053   9.430   8.838
ATOM    710 2H5* DG     23       0.557  11.090   8.483
ATOM    711  C4* DG     23       1.706   9.592   7.470
ATOM    712  H4* DG     23       2.470   9.677   8.243
ATOM    713  O4* DG     23       1.576   8.224   7.105
ATOM    714  C1* DG     23       2.026   8.066   5.773
ATOM    715  H1* DG     23       3.098   7.853   5.774
ATOM    716  N9  DG     23       1.290   6.963   5.116
ATOM    717  C8  DG     23      -0.045   6.891   4.805
ATOM    718  H8  DG     23      -0.739   7.686   5.044
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ATOM    719  N7  DG     23      -0.400   5.784   4.210
ATOM    720  C5  DG     23       0.791   5.056   4.128
ATOM    721  C6  DG     23       1.074   3.752   3.591
ATOM    722  O6  DG     23       0.314   2.933   3.078
ATOM    723  N1  DG     23       2.410   3.406   3.675
ATOM    724  H1  DG     23       2.670   2.498   3.307
ATOM    725  C2  DG     23       3.373   4.203   4.213
ATOM    726  N2  DG     23       4.613   3.780   4.143
ATOM    727 1H2  DG     23       5.311   4.374   4.553
ATOM    728 2H2  DG     23       4.838   2.850   3.770
ATOM    729  N3  DG     23       3.146   5.409   4.734
ATOM    730  C4  DG     23       1.833   5.781   4.668
ATOM    731  C3* DG     23       2.170  10.375   6.235
ATOM    732  H3* DG     23       1.647  11.330   6.140
ATOM    733  C2* DG     23       1.787   9.420   5.109
ATOM    734 1H2* DG     23       0.733   9.557   4.869
ATOM    735 2H2* DG     23       2.394   9.558   4.219
ATOM    736  O3* DG     23       3.570  10.583   6.345
ATOM    737  P   DC3    24       4.436  11.342   5.215
ATOM    738  O1P DC3    24       5.533  12.082   5.874
ATOM    739  O2P DC3    24       3.518  12.035   4.286
ATOM    740  O5* DC3    24       5.075  10.086   4.435
ATOM    741  C5* DC3    24       6.009   9.234   5.081
ATOM    742 1H5* DC3    24       5.512   8.688   5.885
ATOM    743 2H5* DC3    24       6.804   9.842   5.517
ATOM    744  C4* DC3    24       6.638   8.234   4.102
ATOM    745  H4* DC3    24       7.452   7.717   4.610
ATOM    746  O4* DC3    24       5.668   7.278   3.701
ATOM    747  C1* DC3    24       5.719   7.140   2.296
ATOM    748  H1* DC3    24       6.480   6.394   2.047
ATOM    749  N1  DC3    24       4.384   6.723   1.785
ATOM    750  C6  DC3    24       3.273   7.496   2.017
ATOM    751  H6  DC3    24       3.389   8.418   2.574
ATOM    752  C5  DC3    24       2.049   7.094   1.587
ATOM    753  H5  DC3    24       1.180   7.698   1.792
ATOM    754  C4  DC3    24       1.978   5.845   0.899
ATOM    755  N4  DC3    24       0.828   5.357   0.506
ATOM    756 1H4  DC3    24      -0.027   5.820   0.745
ATOM    757 2H4  DC3    24       0.839   4.431   0.068
ATOM    758  N3  DC3    24       3.043   5.096   0.663
ATOM    759  C2  DC3    24       4.260   5.510   1.097
ATOM    760  O2  DC3    24       5.232   4.793   0.860
ATOM    761  C3* DC3    24       7.193   8.908   2.837
ATOM    762  H3* DC3    24       7.231   9.994   2.953
ATOM    763  C2* DC3    24       6.181   8.504   1.772
ATOM    764 1H2* DC3    24       5.364   9.226   1.765
ATOM    765 2H2* DC3    24       6.628   8.425   0.780
ATOM    766  O3* DC3    24       8.472   8.389   2.508
ATOM    767  H3T DC3    24       8.864   8.931   1.817
TER
END
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**File E-5**: Average structure of rMD refined *R*-BD-N3-dU modified duplex 5′ - $G^{1}C^{2}T^{3}A^{4}G^{5}C^{6}X^{7}A^{8}G^{9}T^{10}C^{11}C^{12}$- 3′·5′ - $G^{13}G^{14}A^{15}C^{16}T^{17}G^{18}G^{19}C^{20}T^{21}A^{22}G^{23}C^{24}$ -3′.

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REMARK
ATOM      1  H5T DG5     1       2.278  -6.110  -1.747
ATOM      2  O5* DG5     1       2.933  -5.645  -1.185
ATOM      3  C5* DG5     1       4.247  -5.859  -1.704
ATOM      4 1H5* DG5     1       4.296  -5.498  -2.733
ATOM      5 2H5* DG5     1       4.456  -6.931  -1.717
ATOM      6  C4* DG5     1       5.363  -5.165  -0.895
ATOM      7  H4* DG5     1       6.319  -5.476  -1.320
ATOM      8  O4* DG5     1       5.247  -3.748  -1.016
ATOM      9  C1* DG5     1       5.102  -3.178   0.278
ATOM     10  H1* DG5     1       6.073  -2.815   0.628
ATOM     11  N9  DG5     1       4.136  -2.054   0.230
ATOM     12  C8  DG5     1       2.792  -2.091  -0.057
ATOM     13  H8  DG5     1       2.282  -3.017  -0.301
ATOM     14  N7  DG5     1       2.202  -0.924  -0.029
ATOM     15  C5  DG5     1       3.240  -0.040   0.309
ATOM     16  C6  DG5     1       3.260   1.392   0.489
ATOM     17  O6  DG5     1       2.344   2.208   0.369
ATOM     18  N1  DG5     1       4.503   1.886   0.830
ATOM     19  H1  DG5     1       4.580   2.882   0.972
ATOM     20  C2  DG5     1       5.607   1.115   0.974
ATOM     21  N2  DG5     1       6.719   1.713   1.301
ATOM     22 1H2  DG5     1       7.540   1.147   1.430
ATOM     23 2H2  DG5     1       6.734   2.720   1.448
ATOM     24  N3  DG5     1       5.644  -0.204   0.805
ATOM     25  C4  DG5     1       4.424  -0.729   0.473
ATOM     26  C3* DG5     1       5.359  -5.516   0.603
ATOM     27  H3* DG5     1       4.794  -6.433   0.788
ATOM     28  C2* DG5     1       4.642  -4.308   1.197
ATOM     29 1H2* DG5     1       3.565  -4.458   1.129
ATOM     30 2H2* DG5     1       4.919  -4.126   2.231
ATOM     31  O3* DG5     1       6.703  -5.660   1.060
ATOM     32  P   DC      2       7.088  -6.027   2.586
ATOM     33  O1P DC      2       8.315  -6.862   2.554
ATOM     34  O2P DC      2       5.887  -6.551   3.281
ATOM     35  O5* DC      2       7.461  -4.593   3.229
ATOM     36  C5* DC      2       8.609  -3.873   2.787
ATOM     37 1H5* DC      2       8.498  -3.628   1.729
ATOM     38 2H5* DC      2       9.491  -4.505   2.893
ATOM     39  C4* DC      2       8.866  -2.572   3.565
ATOM     40  H4* DC      2       9.827  -2.175   3.232
ATOM     41  O4* DC      2       7.855  -1.616   3.264
ATOM     42  C1* DC      2       7.334  -1.094   4.474
ATOM     43  H1* DC      2       7.897  -0.197   4.755
ATOM     44  N1  DC      2       5.892  -0.773   4.279
ATOM     45  C6  DC      2       4.988  -1.757   3.959
ATOM     46  H6  DC      2       5.335  -2.780   3.877
ATOM     47  C5  DC      2       3.686  -1.444   3.737
ATOM     48  H5  DC      2       2.979  -2.217   3.479
ATOM     49  C4  DC      2       3.319  -0.076   3.844
ATOM     50  N4  DC      2       2.103   0.308   3.592
ATOM     51 1H4  DC      2       1.406  -0.367   3.334
ATOM     52 2H4  DC      2       1.905   1.302   3.648
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ATOM     53  N3  DC      2       4.167   0.884   4.143
ATOM     54  C2  DC      2       5.462   0.556   4.371
ATOM     55  O2  DC      2       6.223   1.477   4.663
ATOM     56  C3* DC      2       8.923  -2.761   5.092
ATOM     57  H3* DC      2       8.980  -3.821   5.350
ATOM     58  C2* DC      2       7.586  -2.169   5.534
ATOM     59 1H2* DC      2       6.831  -2.952   5.499
ATOM     60 2H2* DC      2       7.625  -1.745   6.535
ATOM     61  O3* DC      2      10.053  -2.063   5.611
ATOM     62  P   DT      3      10.455  -2.076   7.176
ATOM     63  O1P DT      3      11.933  -1.983   7.266
ATOM     64  O2P DT      3       9.767  -3.205   7.850
ATOM     65  O5* DT      3       9.821  -0.698   7.722
ATOM     66  C5* DT      3      10.326   0.558   7.278
ATOM     67 1H5* DT      3      10.281   0.604   6.188
ATOM     68 2H5* DT      3      11.370   0.653   7.578
ATOM     69  C4* DT      3       9.551   1.757   7.843
ATOM     70  H4* DT      3      10.056   2.666   7.512
ATOM     71  O4* DT      3       8.227   1.763   7.323
ATOM     72  C1* DT      3       7.341   2.087   8.377
ATOM     73  H1* DT      3       7.303   3.175   8.493
ATOM     74  N1  DT      3       5.985   1.547   8.077
ATOM     75  C6  DT      3       5.762   0.185   7.992
ATOM     76  H6  DT      3       6.584  -0.496   8.169
ATOM     77  C5  DT      3       4.535  -0.308   7.677
ATOM     78  C7  DT      3       4.329  -1.813   7.629
ATOM     79 1H7  DT      3       4.181  -2.130   6.597
ATOM     80 2H7  DT      3       5.183  -2.341   8.056
ATOM     81 3H7  DT      3       3.434  -2.072   8.196
ATOM     82  C4  DT      3       3.419   0.598   7.411
ATOM     83  O4  DT      3       2.268   0.280   7.119
ATOM     84  N3  DT      3       3.723   1.935   7.512
ATOM     85  H3  DT      3       2.972   2.594   7.368
ATOM     86  C2  DT      3       4.942   2.459   7.867
ATOM     87  O2  DT      3       5.050   3.677   7.999
ATOM     88  C3* DT      3       9.470   1.781   9.381
ATOM     89  H3* DT      3      10.091   0.996   9.817
ATOM     90  C2* DT      3       7.989   1.498   9.630
ATOM     91 1H2* DT      3       7.847   0.420   9.685
ATOM     92 2H2* DT      3       7.615   1.967  10.536
ATOM     93  O3* DT      3       9.880   3.061   9.853
ATOM     94  P   DA      4       9.967   3.434  11.422
ATOM     95  O1P DA      4      11.103   4.371  11.606
ATOM     96  O2P DA      4       9.932   2.186  12.225
ATOM     97  O5* DA      4       8.592   4.236  11.678
ATOM     98  C5* DA      4       8.376   5.518  11.094
ATOM     99 1H5* DA      4       8.414   5.435  10.006
ATOM    100 2H5* DA      4       9.173   6.193  11.409
ATOM    101  C4* DA      4       7.035   6.154  11.492
ATOM    102  H4* DA      4       7.040   7.186  11.134
ATOM    103  O4* DA      4       5.958   5.466  10.866
ATOM    104  C1* DA      4       4.946   5.239  11.831
ATOM    105  H1* DA      4       4.273   6.101  11.879
ATOM    106  N9  DA      4       4.191   4.019  11.464
ATOM    107  C8  DA      4       4.652   2.727  11.364
ATOM    108  H8  DA      4       5.678   2.464  11.589
ATOM    109  N7  DA      4       3.760   1.863  10.951
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ATOM    110  C5  DA      4       2.610   2.657  10.797
ATOM    111  C6  DA      4       1.276   2.417  10.386
ATOM    112  N6  DA      4       0.812   1.248   9.984
ATOM    113 1H6  DA      4      -0.143   1.178   9.653
ATOM    114 2H6  DA      4       1.434   0.458   9.952
ATOM    115  N1  DA      4       0.371   3.398  10.363
ATOM    116  C2  DA      4       0.762   4.617  10.711
ATOM    117  H2  DA      4       0.005   5.391  10.674
ATOM    118  N3  DA      4       1.975   5.005  11.091
ATOM    119  C4  DA      4       2.860   3.966  11.118
ATOM    120  C3* DA      4       6.783   6.167  13.010
ATOM    121  H3* DA      4       7.681   5.875  13.560
ATOM    122  C2* DA      4       5.690   5.109  13.157
ATOM    123 1H2* DA      4       6.156   4.128  13.243
ATOM    124 2H2* DA      4       5.036   5.290  14.009
ATOM    125  O3* DA      4       6.367   7.474  13.396
ATOM    126  P   DG      5       6.062   7.886  14.925
ATOM    127  O1P DG      5       6.514   9.286  15.120
ATOM    128  O2P DG      5       6.583   6.835  15.834
ATOM    129  O5* DG      5       4.453   7.854  14.984
ATOM    130  C5* DG      5       3.676   8.791  14.243
ATOM    131 1H5* DG      5       3.846   8.644  13.175
ATOM    132 2H5* DG      5       3.995   9.802  14.499
ATOM    133  C4* DG      5       2.168   8.691  14.522
ATOM    134  H4* DG      5       1.687   9.559  14.066
ATOM    135  O4* DG      5       1.636   7.512  13.925
ATOM    136  C1* DG      5       0.877   6.815  14.898
ATOM    137  H1* DG      5      -0.158   7.168  14.881
ATOM    138  N9  DG      5       0.915   5.363  14.608
ATOM    139  C8  DG      5       1.980   4.497  14.677
ATOM    140  H8  DG      5       2.961   4.815  15.011
ATOM    141  N7  DG      5       1.712   3.279  14.282
ATOM    142  C5  DG      5       0.353   3.340  13.936
ATOM    143  C6  DG      5      -0.551   2.345  13.413
ATOM    144  O6  DG      5      -0.332   1.170  13.121
ATOM    145  N1  DG      5      -1.833   2.815  13.211
ATOM    146  H1  DG      5      -2.505   2.171  12.822
ATOM    147  C2  DG      5      -2.220   4.085  13.477
ATOM    148  N2  DG      5      -3.472   4.385  13.269
ATOM    149 1H2  DG      5      -3.768   5.326  13.463
ATOM    150 2H2  DG      5      -4.108   3.698  12.871
ATOM    151  N3  DG      5      -1.426   5.040  13.950
ATOM    152  C4  DG      5      -0.143   4.609  14.155
ATOM    153  C3* DG      5       1.824   8.670  16.022
ATOM    154  H3* DG      5       2.680   8.976  16.627
ATOM    155  C2* DG      5       1.502   7.192  16.239
ATOM    156 1H2* DG      5       2.429   6.643  16.403
ATOM    157 2H2* DG      5       0.819   7.030  17.069
ATOM    158  O3* DG      5       0.716   9.535  16.254
ATOM    159  P   DC      6       0.108   9.822  17.722
ATOM    160  O1P DC      6      -0.239  11.263  17.798
ATOM    161  O2P DC      6       1.008   9.248  18.752
ATOM    162  O5* DC      6      -1.257   8.964  17.713
ATOM    163  C5* DC      6      -2.335   9.322  16.852
ATOM    164 1H5* DC      6      -2.000   9.285  15.814
ATOM    165 2H5* DC      6      -2.644  10.346  17.069
ATOM    166  C4* DC      6      -3.566   8.414  17.000
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ATOM    167  H4* DC      6      -4.364   8.832  16.383
ATOM    168  O4* DC      6      -3.256   7.109  16.523
ATOM    169  C1* DC      6      -3.597   6.158  17.515
ATOM    170  H1* DC      6      -4.616   5.802  17.328
ATOM    171  N1  DC      6      -2.627   5.026  17.439
ATOM    172  C6  DC      6      -1.306   5.198  17.778
ATOM    173  H6  DC      6      -0.970   6.169  18.126
ATOM    174  C5  DC      6      -0.430   4.170  17.657
ATOM    175  H5  DC      6       0.607   4.309  17.920
ATOM    176  C4  DC      6      -0.936   2.938  17.163
ATOM    177  N4  DC      6      -0.145   1.921  16.990
ATOM    178 1H4  DC      6       0.834   2.008  17.198
ATOM    179 2H4  DC      6      -0.539   1.073  16.597
ATOM    180  N3  DC      6      -2.191   2.749  16.817
ATOM    181  C2  DC      6      -3.058   3.783  16.950
ATOM    182  O2  DC      6      -4.229   3.570  16.628
ATOM    183  C3* DC      6      -4.074   8.304  18.448
ATOM    184  H3* DC      6      -3.604   9.069  19.070
ATOM    185  C2* DC      6      -3.600   6.909  18.853
ATOM    186 1H2* DC      6      -2.600   6.995  19.273
ATOM    187 2H2* DC      6      -4.258   6.433  19.578
ATOM    188  O3* DC      6      -5.493   8.433  18.473
ATOM    189  P   DX      7      -6.309   8.770  19.826
ATOM    190  O1P DX      7      -7.659   9.242  19.428
ATOM    191  O2P DX      7      -5.476   9.650  20.683
ATOM    192  O5* DX      7      -6.469   7.352  20.572
ATOM    193  C5* DX      7      -7.272   6.319  20.013
ATOM    194 1H5* DX      7      -6.886   6.049  19.028
ATOM    195 2H5* DX      7      -8.293   6.684  19.890
ATOM    196  C4* DX      7      -7.320   5.058  20.884
ATOM    197  H4* DX      7      -8.047   4.380  20.430
ATOM    198  O4* DX      7      -6.065   4.388  20.910
ATOM    199  C1* DX      7      -6.035   3.663  22.124
ATOM    200  H1* DX      7      -6.707   2.803  22.046
ATOM    201  N1  DX      7      -4.655   3.212  22.462
ATOM    202  C6  DX      7      -3.649   4.128  22.669
ATOM    203  H6  DX      7      -3.855   5.183  22.534
ATOM    204  C5  DX      7      -2.410   3.723  23.039
ATOM    205  H5  DX      7      -1.632   4.451  23.214
ATOM    206  C4  DX      7      -2.077   2.325  23.185
ATOM    207  O4  DX      7      -0.962   1.928  23.529
ATOM    208  N3  DX      7      -3.099   1.431  22.858
ATOM    209  C11 DX      7      -2.727  -0.016  22.622
ATOM    210  C2  DX      7      -4.413   1.835  22.583
ATOM    211  O2  DX      7      -5.319   1.004  22.444
ATOM    212  C3* DX      7      -7.754   5.301  22.345
ATOM    213  H3* DX      7      -7.802   6.369  22.570
ATOM    214  C2* DX      7      -6.628   4.635  23.141
ATOM    215 1H2* DX      7      -5.902   5.399  23.420
ATOM    216 2H2* DX      7      -6.979   4.112  24.029
ATOM    217  O3* DX      7      -9.020   4.687  22.554
ATOM    218  C12 DX      7      -2.081  -0.284  21.256
ATOM    219  C9  DX      7      -2.909   0.291  20.119
ATOM    220  C10 DX      7      -4.072  -0.136  19.643
ATOM    221  O12 DX      7      -0.798   0.289  21.234
ATOM    222  H15 DX      7      -3.610  -0.651  22.694
ATOM    223  H14 DX      7      -2.042  -0.362  23.395
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ATOM    224  H9  DX      7      -1.962  -1.350  21.122
ATOM    225 1H1  DX      7      -2.515   1.136  19.572
ATOM    226 2H1  DX      7      -4.563  -0.969  20.127
ATOM    227 3H1  DX      7      -4.527   0.384  18.811
ATOM    228  H10 DX      7      -0.729   0.780  22.073
ATOM    229  P   DA      8      -9.848   4.793  23.939
ATOM    230  O1P DA      8     -11.231   5.221  23.616
ATOM    231  O2P DA      8      -9.070   5.568  24.938
ATOM    232  O5* DA      8      -9.881   3.253  24.410
ATOM    233  C5* DA      8     -10.567   2.279  23.628
ATOM    234 1H5* DA      8     -10.200   2.315  22.601
ATOM    235 2H5* DA      8     -11.633   2.513  23.613
ATOM    236  C4* DA      8     -10.392   0.845  24.143
ATOM    237  H4* DA      8     -10.981   0.191  23.497
ATOM    238  O4* DA      8      -9.024   0.461  24.042
ATOM    239  C1* DA      8      -8.623  -0.127  25.266
ATOM    240  H1* DA      8      -8.787  -1.209  25.226
ATOM    241  N9  DA      8      -7.187   0.158  25.501
ATOM    242  C8  DA      8      -6.589   1.330  25.910
ATOM    243  H8  DA      8      -7.153   2.241  26.078
ATOM    244  N7  DA      8      -5.292   1.250  26.075
ATOM    245  C5  DA      8      -5.019  -0.086  25.731
ATOM    246  C6  DA      8      -3.853  -0.889  25.667
ATOM    247  N6  DA      8      -2.634  -0.486  25.970
ATOM    248 1H6  DA      8      -1.862  -1.121  25.803
ATOM    249 2H6  DA      8      -2.485   0.465  26.266
ATOM    250  N1  DA      8      -3.909  -2.165  25.273
ATOM    251  C2  DA      8      -5.093  -2.666  24.949
ATOM    252  H2  DA      8      -5.102  -3.704  24.643
ATOM    253  N3  DA      8      -6.269  -2.051  24.965
ATOM    254  C4  DA      8      -6.162  -0.750  25.365
ATOM    255  C3* DA      8     -10.863   0.642  25.593
ATOM    256  H3* DA      8     -11.396   1.522  25.961
ATOM    257  C2* DA      8      -9.538   0.470  26.335
ATOM    258 1H2* DA      8      -9.188   1.455  26.642
ATOM    259 2H2* DA      8      -9.614  -0.181  27.204
ATOM    260  O3* DA      8     -11.715  -0.499  25.626
ATOM    261  P   DG      9     -12.370  -1.091  26.977
ATOM    262  O1P DG      9     -13.728  -1.590  26.649
ATOM    263  O2P DG      9     -12.210  -0.114  28.082
ATOM    264  O5* DG      9     -11.414  -2.354  27.261
ATOM    265  C5* DG      9     -11.360  -3.437  26.337
ATOM    266 1H5* DG      9     -11.080  -3.064  25.351
ATOM    267 2H5* DG      9     -12.348  -3.894  26.258
ATOM    268  C4* DG      9     -10.358  -4.525  26.740
ATOM    269  H4* DG      9     -10.464  -5.353  26.036
ATOM    270  O4* DG      9      -9.029  -4.023  26.647
ATOM    271  C1* DG      9      -8.312  -4.471  27.782
ATOM    272  H1* DG      9      -7.918  -5.476  27.601
ATOM    273  N9  DG      9      -7.198  -3.542  28.083
ATOM    274  C8  DG      9      -7.252  -2.234  28.504
ATOM    275  H8  DG      9      -8.191  -1.707  28.630
ATOM    276  N7  DG      9      -6.083  -1.696  28.741
ATOM    277  C5  DG      9      -5.180  -2.727  28.440
ATOM    278  C6  DG      9      -3.739  -2.789  28.484
ATOM    279  O6  DG      9      -2.930  -1.927  28.829
ATOM    280  N1  DG      9      -3.227  -4.000  28.064
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ATOM    281  H1  DG      9      -2.223  -4.083  28.015
ATOM    282  C2  DG      9      -3.992  -5.038  27.647
ATOM    283  N2  DG      9      -3.382  -6.116  27.246
ATOM    284 1H2  DG      9      -3.943  -6.889  26.935
ATOM    285 2H2  DG      9      -2.366  -6.154  27.230
ATOM    286  N3  DG      9      -5.320  -5.041  27.619
ATOM    287  C4  DG      9      -5.860  -3.852  28.022
ATOM    288  C3* DG      9     -10.582  -5.068  28.164
ATOM    289  H3* DG      9     -11.495  -4.659  28.602
ATOM    290  C2* DG      9      -9.350  -4.540  28.898
ATOM    291 1H2* DG      9      -9.569  -3.543  29.281
ATOM    292 2H2* DG      9      -9.028  -5.191  29.709
ATOM    293  O3* DG      9     -10.657  -6.488  28.099
ATOM    294  P   DT     10     -10.887  -7.428  29.391
ATOM    295  O1P DT     10     -11.765  -8.555  28.988
ATOM    296  O2P DT     10     -11.280  -6.593  30.553
ATOM    297  O5* DT     10      -9.405  -8.000  29.651
ATOM    298  C5* DT     10      -8.770  -8.823  28.676
ATOM    299 1H5* DT     10      -8.717  -8.289  27.726
ATOM    300 2H5* DT     10      -9.364  -9.726  28.524
ATOM    301  C4* DT     10      -7.349  -9.244  29.072
ATOM    302  H4* DT     10      -6.973  -9.918  28.299
ATOM    303  O4* DT     10      -6.505  -8.099  29.124
ATOM    304  C1* DT     10      -5.744  -8.157  30.317
ATOM    305  H1* DT     10      -4.836  -8.742  30.135
ATOM    306  N1  DT     10      -5.399  -6.777  30.761
ATOM    307  C6  DT     10      -6.384  -5.882  31.137
ATOM    308  H6  DT     10      -7.420  -6.197  31.108
ATOM    309  C5  DT     10      -6.076  -4.613  31.517
ATOM    310  C7  DT     10      -7.193  -3.681  31.955
ATOM    311 1H7  DT     10      -8.092  -4.244  32.213
ATOM    312 2H7  DT     10      -6.871  -3.114  32.830
ATOM    313 3H7  DT     10      -7.418  -2.976  31.157
ATOM    314  C4  DT     10      -4.684  -4.162  31.534
ATOM    315  O4  DT     10      -4.271  -3.044  31.838
ATOM    316  N3  DT     10      -3.768  -5.115  31.157
ATOM    317  H3  DT     10      -2.793  -4.853  31.192
ATOM    318  C2  DT     10      -4.048  -6.406  30.781
ATOM    319  O2  DT     10      -3.118  -7.159  30.498
ATOM    320  C3* DT     10      -7.283  -9.972  30.426
ATOM    321  H3* DT     10      -8.285 -10.202  30.795
ATOM    322  C2* DT     10      -6.613  -8.926  31.313
ATOM    323 1H2* DT     10      -7.384  -8.290  31.745
ATOM    324 2H2* DT     10      -6.018  -9.370  32.104
ATOM    325  O3* DT     10      -6.522 -11.167  30.281
ATOM    326  P   DC     11      -6.270 -12.208  31.491
ATOM    327  O1P DC     11      -6.306 -13.581  30.928
ATOM    328  O2P DC     11      -7.167 -11.876  32.626
ATOM    329  O5* DC     11      -4.756 -11.872  31.928
ATOM    330  C5* DC     11      -3.673 -12.126  31.038
ATOM    331 1H5* DC     11      -3.852 -11.607  30.094
ATOM    332 2H5* DC     11      -3.620 -13.196  30.829
ATOM    333  C4* DC     11      -2.311 -11.672  31.582
ATOM    334  H4* DC     11      -1.551 -11.953  30.851
ATOM    335  O4* DC     11      -2.306 -10.255  31.725
ATOM    336  C1* DC     11      -1.836  -9.928  33.020
ATOM    337  H1* DC     11      -0.745  -9.831  32.989
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ATOM    338  N1  DC     11      -2.460  -8.650  33.468
ATOM    339  C6  DC     11      -3.805  -8.567  33.742
ATOM    340  H6  DC     11      -4.426  -9.447  33.619
ATOM    341  C5  DC     11      -4.349  -7.392  34.148
ATOM    342  H5  DC     11      -5.406  -7.329  34.359
ATOM    343  C4  DC     11      -3.474  -6.280  34.275
ATOM    344  N4  DC     11      -3.924  -5.124  34.664
ATOM    345 1H4  DC     11      -4.892  -5.008  34.899
ATOM    346 2H4  DC     11      -3.245  -4.373  34.750
ATOM    347  N3  DC     11      -2.189  -6.331  34.009
ATOM    348  C2  DC     11      -1.658  -7.507  33.597
ATOM    349  O2  DC     11      -0.448  -7.520  33.372
ATOM    350  C3* DC     11      -1.938 -12.302  32.936
ATOM    351  H3* DC     11      -2.597 -13.140  33.174
ATOM    352  C2* DC     11      -2.177 -11.138  33.895
ATOM    353 1H2* DC     11      -3.225 -11.143  34.189
ATOM    354 2H2* DC     11      -1.551 -11.191  34.781
ATOM    355  O3* DC     11      -0.580 -12.733  32.893
ATOM    356  P   DC3    12       0.165 -13.441  34.139
ATOM    357  O1P DC3    12       1.117 -14.441  33.595
ATOM    358  O2P DC3    12      -0.847 -13.884  35.131
ATOM    359  O5* DC3    12       1.009 -12.229  34.785
ATOM    360  C5* DC3    12       2.092 -11.634  34.075
ATOM    361 1H5* DC3    12       1.725 -11.211  33.138
ATOM    362 2H5* DC3    12       2.828 -12.403  33.833
ATOM    363  C4* DC3    12       2.805 -10.526  34.867
ATOM    364  H4* DC3    12       3.692 -10.227  34.306
ATOM    365  O4* DC3    12       1.944  -9.399  34.992
ATOM    366  C1* DC3    12       2.009  -8.939  36.330
ATOM    367  H1* DC3    12       2.870  -8.270  36.438
ATOM    368  N1  DC3    12       0.748  -8.237  36.693
ATOM    369  C6  DC3    12      -0.468  -8.861  36.560
ATOM    370  H6  DC3    12      -0.492  -9.880  36.190
ATOM    371  C5  DC3    12      -1.611  -8.204  36.881
ATOM    372  H5  DC3    12      -2.567  -8.693  36.773
ATOM    373  C4  DC3    12      -1.482  -6.867  37.348
ATOM    374  N4  DC3    12      -2.530  -6.172  37.678
ATOM    375 1H4  DC3    12      -3.447  -6.568  37.582
ATOM    376 2H4  DC3    12      -2.377  -5.214  37.976
ATOM    377  N3  DC3    12      -0.326  -6.257  37.507
ATOM    378  C2  DC3    12       0.807  -6.931  37.195
ATOM    379  O2  DC3    12       1.874  -6.347  37.391
ATOM    380  C3* DC3    12       3.234 -10.961  36.284
ATOM    381  H3* DC3    12       3.108 -12.038  36.427
ATOM    382  C2* DC3    12       2.263 -10.191  37.172
ATOM    383 1H2* DC3    12       1.352 -10.775  37.301
ATOM    384 2H2* DC3    12       2.695  -9.943  38.142
ATOM    385  O3* DC3    12       4.569 -10.561  36.593
ATOM    386  H3T DC3    12       5.202 -11.185  36.181
TER
ATOM    387  H5T DG5    13      -0.938   4.723  40.825
ATOM    388  O5* DG5    13      -0.283   4.149  40.374
ATOM    389  C5* DG5    13       0.945   4.158  41.104
ATOM    390 1H5* DG5    13       0.766   3.807  42.123
ATOM    391 2H5* DG5    13       1.317   5.183  41.167
ATOM    392  C4* DG5    13       2.053   3.284  40.481
ATOM    393  H4* DG5    13       2.966   3.455  41.055
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ATOM    394  O4* DG5    13       1.702   1.906  40.583
ATOM    395  C1* DG5    13       1.662   1.337  39.282
ATOM    396  H1* DG5    13       2.598   0.805  39.087
ATOM    397  N9  DG5    13       0.521   0.399  39.174
ATOM    398  C8  DG5    13      -0.822   0.664  39.296
ATOM    399  H8  DG5    13      -1.193   1.656  39.534
ATOM    400  N7  DG5    13      -1.596  -0.376  39.113
ATOM    401  C5  DG5    13      -0.689  -1.413  38.840
ATOM    402  C6  DG5    13      -0.889  -2.811  38.545
ATOM    403  O6  DG5    13      -1.939  -3.453  38.474
ATOM    404  N1  DG5    13       0.287  -3.501  38.322
ATOM    405  H1  DG5    13       0.209  -4.481  38.093
ATOM    406  C2  DG5    13       1.517  -2.938  38.400
ATOM    407  N2  DG5    13       2.544  -3.701  38.148
ATOM    408 1H2  DG5    13       3.456  -3.275  38.150
ATOM    409 2H2  DG5    13       2.407  -4.669  37.868
ATOM    410  N3  DG5    13       1.754  -1.663  38.687
ATOM    411  C4  DG5    13       0.608  -0.945  38.889
ATOM    412  C3* DG5    13       2.344   3.593  39.002
ATOM    413  H3* DG5    13       1.973   4.583  38.728
ATOM    414  C2* DG5    13       1.546   2.499  38.298
ATOM    415 1H2* DG5    13       0.509   2.820  38.195
ATOM    416 2H2* DG5    13       1.947   2.243  37.320
ATOM    417  O3* DG5    13       3.749   3.505  38.775
ATOM    418  P   DG     14       4.428   3.757  37.332
ATOM    419  O1P DG     14       5.798   4.280  37.560
ATOM    420  O2P DG     14       3.495   4.545  36.487
ATOM    421  O5* DG     14       4.542   2.272  36.711
ATOM    422  C5* DG     14       5.400   1.297  37.298
ATOM    423 1H5* DG     14       5.063   1.075  38.312
ATOM    424 2H5* DG     14       6.411   1.702  37.360
ATOM    425  C4* DG     14       5.470  -0.016  36.502
ATOM    426  H4* DG     14       6.280  -0.615  36.923
ATOM    427  O4* DG     14       4.254  -0.748  36.633
ATOM    428  C1* DG     14       3.850  -1.177  35.343
ATOM    429  H1* DG     14       4.325  -2.133  35.101
ATOM    430  N9  DG     14       2.377  -1.319  35.286
ATOM    431  C8  DG     14       1.418  -0.360  35.502
ATOM    432  H8  DG     14       1.676   0.666  35.734
ATOM    433  N7  DG     14       0.189  -0.799  35.430
ATOM    434  C5  DG     14       0.347  -2.157  35.114
ATOM    435  C6  DG     14      -0.617  -3.205  34.898
ATOM    436  O6  DG     14      -1.846  -3.157  34.962
ATOM    437  N1  DG     14      -0.046  -4.417  34.569
ATOM    438  H1  DG     14      -0.676  -5.177  34.355
ATOM    439  C2  DG     14       1.290  -4.624  34.481
ATOM    440  N2  DG     14       1.687  -5.806  34.098
ATOM    441 1H2  DG     14       2.672  -5.944  33.955
ATOM    442 2H2  DG     14       1.006  -6.510  33.825
ATOM    443  N3  DG     14       2.219  -3.697  34.693
ATOM    444  C4  DG     14       1.685  -2.476  35.006
ATOM    445  C3* DG     14       5.747   0.189  35.002
ATOM    446  H3* DG     14       6.052   1.217  34.793
ATOM    447  C2* DG     14       4.377  -0.107  34.394
ATOM    448 1H2* DG     14       3.759   0.790  34.445
ATOM    449 2H2* DG     14       4.436  -0.464  33.370
ATOM    450  O3* DG     14       6.759  -0.725  34.591
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ATOM    451  P   DA     15       7.328  -0.795  33.083
ATOM    452  O1P DA     15       8.778  -1.105  33.157
ATOM    453  O2P DA     15       6.894   0.411  32.335
ATOM    454  O5* DA     15       6.561  -2.073  32.468
ATOM    455  C5* DA     15       6.792  -3.382  32.984
ATOM    456 1H5* DA     15       6.393  -3.450  33.997
ATOM    457 2H5* DA     15       7.867  -3.560  33.034
ATOM    458  C4* DA     15       6.178  -4.506  32.132
ATOM    459  H4* DA     15       6.579  -5.452  32.499
ATOM    460  O4* DA     15       4.761  -4.525  32.283
ATOM    461  C1* DA     15       4.152  -4.360  31.012
ATOM    462  H1* DA     15       3.861  -5.338  30.615
ATOM    463  N9  DA     15       2.955  -3.503  31.170
ATOM    464  C8  DA     15       2.891  -2.157  31.447
ATOM    465  H8  DA     15       3.781  -1.545  31.538
ATOM    466  N7  DA     15       1.677  -1.693  31.611
ATOM    467  C5  DA     15       0.881  -2.834  31.411
ATOM    468  C6  DA     15      -0.509  -3.104  31.442
ATOM    469  N6  DA     15      -1.447  -2.221  31.729
ATOM    470 1H6  DA     15      -2.416  -2.518  31.729
ATOM    471 2H6  DA     15      -1.188  -1.267  31.923
ATOM    472  N1  DA     15      -0.981  -4.328  31.203
ATOM    473  C2  DA     15      -0.112  -5.291  30.926
ATOM    474  H2  DA     15      -0.531  -6.270  30.731
ATOM    475  N3  DA     15       1.210  -5.196  30.856
ATOM    476  C4  DA     15       1.649  -3.932  31.122
ATOM    477  C3* DA     15       6.500  -4.385  30.633
ATOM    478  H3* DA     15       7.355  -3.725  30.468
ATOM    479  C2* DA     15       5.216  -3.755  30.097
ATOM    480 1H2* DA     15       5.273  -2.675  30.222
ATOM    481 2H2* DA     15       5.038  -3.993  29.052
ATOM    482  O3* DA     15       6.769  -5.683  30.109
ATOM    483  P   DC     16       7.135  -5.956  28.561
ATOM    484  O1P DC     16       8.095  -7.087  28.511
ATOM    485  O2P DC     16       7.505  -4.675  27.908
ATOM    486  O5* DC     16       5.728  -6.450  27.950
ATOM    487  C5* DC     16       5.143  -7.678  28.374
ATOM    488 1H5* DC     16       4.964  -7.642  29.451
ATOM    489 2H5* DC     16       5.838  -8.495  28.176
ATOM    490  C4* DC     16       3.815  -7.998  27.672
ATOM    491  H4* DC     16       3.516  -9.007  27.964
ATOM    492  O4* DC     16       2.817  -7.083  28.107
ATOM    493  C1* DC     16       2.131  -6.595  26.970
ATOM    494  H1* DC     16       1.317  -7.286  26.722
ATOM    495  N1  DC     16       1.592  -5.241  27.279
ATOM    496  C6  DC     16       2.424  -4.180  27.543
ATOM    497  H6  DC     16       3.497  -4.323  27.483
ATOM    498  C5  DC     16       1.903  -2.975  27.892
ATOM    499  H5  DC     16       2.557  -2.144  28.108
ATOM    500  C4  DC     16       0.487  -2.877  27.977
ATOM    501  N4  DC     16      -0.081  -1.777  28.376
ATOM    502 1H4  DC     16       0.481  -0.982  28.620
ATOM    503 2H4  DC     16      -1.091  -1.784  28.481
ATOM    504  N3  DC     16      -0.327  -3.882  27.739
ATOM    505  C2  DC     16       0.206  -5.072  27.378
ATOM    506  O2  DC     16      -0.583  -5.986  27.137
ATOM    507  C3* DC     16       3.892  -7.936  26.135
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ATOM    508  H3* DC     16       4.931  -7.876  25.806
ATOM    509  C2* DC     16       3.145  -6.639  25.826
ATOM    510 1H2* DC     16       3.846  -5.807  25.880
ATOM    511 2H2* DC     16       2.658  -6.657  24.852
ATOM    512  O3* DC     16       3.254  -9.084  25.578
ATOM    513  P   DT     17       3.344  -9.455  24.008
ATOM    514  O1P DT     17       3.478 -10.929  23.901
ATOM    515  O2P DT     17       4.374  -8.601  23.364
ATOM    516  O5* DT     17       1.907  -9.025  23.413
ATOM    517  C5* DT     17       0.735  -9.803  23.651
ATOM    518 1H5* DT     17       0.511  -9.811  24.719
ATOM    519 2H5* DT     17       0.917 -10.832  23.335
ATOM    520  C4* DT     17      -0.498  -9.288  22.885
ATOM    521  H4* DT     17      -1.291 -10.033  22.969
ATOM    522  O4* DT     17      -0.934  -8.072  23.484
ATOM    523  C1* DT     17      -1.049  -7.078  22.482
ATOM    524  H1* DT     17      -2.063  -7.118  22.072
ATOM    525  N1  DT     17      -0.825  -5.735  23.107
ATOM    526  C6  DT     17       0.434  -5.168  23.222
ATOM    527  H6  DT     17       1.301  -5.694  22.853
ATOM    528  C5  DT     17       0.612  -3.957  23.814
ATOM    529  C7  DT     17       2.012  -3.371  23.901
ATOM    530 1H7  DT     17       2.301  -3.275  24.946
ATOM    531 2H7  DT     17       2.737  -3.997  23.380
ATOM    532 3H7  DT     17       2.013  -2.375  23.456
ATOM    533  C4  DT     17      -0.525  -3.217  24.358
ATOM    534  O4  DT     17      -0.488  -2.117  24.906
ATOM    535  N3  DT     17      -1.736  -3.854  24.233
ATOM    536  H3  DT     17      -2.541  -3.368  24.598
ATOM    537  C2  DT     17      -1.951  -5.074  23.631
ATOM    538  O2  DT     17      -3.100  -5.518  23.579
ATOM    539  C3* DT     17      -0.212  -9.031  21.393
ATOM    540  H3* DT     17       0.737  -9.494  21.111
ATOM    541  C2* DT     17      -0.093  -7.511  21.360
ATOM    542 1H2* DT     17       0.941  -7.255  21.576
ATOM    543 2H2* DT     17      -0.382  -7.099  20.396
ATOM    544  O3* DT     17      -1.261  -9.491  20.539
ATOM    545  P   DG     18      -0.930 -10.123  19.084
ATOM    546  O1P DG     18      -0.825 -11.595  19.242
ATOM    547  O2P DG     18       0.221  -9.387  18.506
ATOM    548  O5* DG     18      -2.208  -9.785  18.154
ATOM    549  C5* DG     18      -3.388 -10.585  18.148
ATOM    550 1H5* DG     18      -3.704 -10.751  19.179
ATOM    551 2H5* DG     18      -3.160 -11.557  17.708
ATOM    552  C4* DG     18      -4.581  -9.966  17.380
ATOM    553  H4* DG     18      -5.440 -10.620  17.544
ATOM    554  O4* DG     18      -4.875  -8.680  17.910
ATOM    555  C1* DG     18      -4.431  -7.689  16.985
ATOM    556  H1* DG     18      -5.308  -7.188  16.570
ATOM    557  N9  DG     18      -3.634  -6.689  17.720
ATOM    558  C8  DG     18      -2.275  -6.591  17.913
ATOM    559  H8  DG     18      -1.563  -7.255  17.435
ATOM    560  N7  DG     18      -1.926  -5.662  18.765
ATOM    561  C5  DG     18      -3.150  -5.110  19.166
ATOM    562  C6  DG     18      -3.476  -4.114  20.151
ATOM    563  O6  DG     18      -2.726  -3.509  20.913
ATOM    564  N1  DG     18      -4.828  -3.844  20.251
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ATOM    565  H1  DG     18      -5.112  -3.201  20.963
ATOM    566  C2  DG     18      -5.770  -4.444  19.480
ATOM    567  N2  DG     18      -7.007  -4.041  19.603
ATOM    568 1H2  DG     18      -7.265  -3.317  20.255
ATOM    569 2H2  DG     18      -7.687  -4.449  18.981
ATOM    570  N3  DG     18      -5.526  -5.394  18.586
ATOM    571  C4  DG     18      -4.193  -5.694  18.485
ATOM    572  C3* DG     18      -4.425  -9.743  15.864
ATOM    573  H3* DG     18      -3.825 -10.528  15.399
ATOM    574  C2* DG     18      -3.707  -8.396  15.839
ATOM    575 1H2* DG     18      -2.650  -8.544  16.047
ATOM    576 2H2* DG     18      -3.812  -7.860  14.897
ATOM    577  O3* DG     18      -5.743  -9.693  15.306
ATOM    578  P   DG     19      -6.069  -9.263  13.786
ATOM    579  O1P DG     19      -7.396  -9.830  13.440
ATOM    580  O2P DG     19      -4.905  -9.614  12.935
ATOM    581  O5* DG     19      -6.201  -7.648  13.824
ATOM    582  C5* DG     19      -7.288  -6.999  14.485
ATOM    583 1H5* DG     19      -7.198  -7.125  15.564
ATOM    584 2H5* DG     19      -8.225  -7.462  14.173
ATOM    585  C4* DG     19      -7.392  -5.496  14.163
ATOM    586  H4* DG     19      -8.345  -5.140  14.561
ATOM    587  O4* DG     19      -6.349  -4.747  14.782
ATOM    588  C1* DG     19      -5.960  -3.735  13.868
ATOM    589  H1* DG     19      -6.687  -2.917  13.881
ATOM    590  N9  DG     19      -4.617  -3.205  14.203
ATOM    591  C8  DG     19      -3.411  -3.863  14.200
ATOM    592  H8  DG     19      -3.319  -4.900  13.895
ATOM    593  N7  DG     19      -2.404  -3.143  14.622
ATOM    594  C5  DG     19      -2.985  -1.899  14.910
ATOM    595  C6  DG     19      -2.425  -0.676  15.433
ATOM    596  O6  DG     19      -1.272  -0.437  15.796
ATOM    597  N1  DG     19      -3.344   0.347  15.552
ATOM    598  H1  DG     19      -3.015   1.222  15.930
ATOM    599  C2  DG     19      -4.652   0.226  15.223
ATOM    600  N2  DG     19      -5.406   1.276  15.396
ATOM    601 1H2  DG     19      -6.379   1.206  15.150
ATOM    602 2H2  DG     19      -5.015   2.136  15.776
ATOM    603  N3  DG     19      -5.223  -0.886  14.765
ATOM    604  C4  DG     19      -4.336  -1.922  14.628
ATOM    605  C3* DG     19      -7.361  -5.188  12.652
ATOM    606  H3* DG     19      -7.359  -6.106  12.061
ATOM    607  C2* DG     19      -6.034  -4.441  12.517
ATOM    608 1H2* DG     19      -5.222  -5.163  12.416
ATOM    609 2H2* DG     19      -6.029  -3.743  11.685
ATOM    610  O3* DG     19      -8.483  -4.374  12.316
ATOM    611  P   DC     20      -8.891  -4.013  10.794
ATOM    612  O1P DC     20     -10.319  -4.371  10.606
ATOM    613  O2P DC     20      -7.883  -4.576   9.861
ATOM    614  O5* DC     20      -8.752  -2.407  10.760
ATOM    615  C5* DC     20      -9.650  -1.581  11.497
ATOM    616 1H5* DC     20      -9.628  -1.873  12.548
ATOM    617 2H5* DC     20     -10.665  -1.735  11.126
ATOM    618  C4* DC     20      -9.329  -0.079  11.409
ATOM    619  H4* DC     20     -10.114   0.454  11.950
ATOM    620  O4* DC     20      -8.080   0.182  12.045
ATOM    621  C1* DC     20      -7.216   0.839  11.132
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ATOM    622  H1* DC     20      -7.268   1.920  11.307
ATOM    623  N1  DC     20      -5.823   0.343  11.331
ATOM    624  C6  DC     20      -5.490  -0.964  11.069
ATOM    625  H6  DC     20      -6.264  -1.652  10.745
ATOM    626  C5  DC     20      -4.209  -1.387  11.220
ATOM    627  H5  DC     20      -3.948  -2.412  11.009
ATOM    628  C4  DC     20      -3.259  -0.435  11.675
ATOM    629  N4  DC     20      -2.023  -0.781  11.883
ATOM    630 1H4  DC     20      -1.730  -1.724  11.705
ATOM    631 2H4  DC     20      -1.388  -0.077  12.244
ATOM    632  N3  DC     20      -3.558   0.813  11.964
ATOM    633  C2  DC     20      -4.838   1.225  11.797
ATOM    634  O2  DC     20      -5.081   2.401  12.065
ATOM    635  C3* DC     20      -9.274   0.469   9.972
ATOM    636  H3* DC     20      -9.734  -0.232   9.272
ATOM    637  C2* DC     20      -7.769   0.563   9.731
ATOM    638 1H2* DC     20      -7.421  -0.393   9.341
ATOM    639 2H2* DC     20      -7.506   1.354   9.033
ATOM    640  O3* DC     20      -9.939   1.730   9.921
ATOM    641  P   DT     21     -10.105   2.588   8.561
ATOM    642  O1P DT     21     -11.392   3.323   8.641
ATOM    643  O2P DT     21      -9.856   1.708   7.392
ATOM    644  O5* DT     21      -8.900   3.656   8.656
ATOM    645  C5* DT     21      -8.903   4.664   9.662
ATOM    646 1H5* DT     21      -8.997   4.197  10.644
ATOM    647 2H5* DT     21      -9.763   5.318   9.515
ATOM    648  C4* DT     21      -7.633   5.528   9.661
ATOM    649  H4* DT     21      -7.756   6.302  10.422
ATOM    650  O4* DT     21      -6.509   4.729  10.010
ATOM    651  C1* DT     21      -5.434   5.083   9.161
ATOM    652  H1* DT     21      -4.924   5.960   9.573
ATOM    653  N1  DT     21      -4.491   3.936   9.045
ATOM    654  C6  DT     21      -4.886   2.748   8.457
ATOM    655  H6  DT     21      -5.895   2.660   8.077
ATOM    656  C5  DT     21      -4.036   1.692   8.366
ATOM    657  C7  DT     21      -4.508   0.413   7.693
ATOM    658 1H7  DT     21      -5.470   0.560   7.199
ATOM    659 2H7  DT     21      -3.771   0.104   6.950
ATOM    660 3H7  DT     21      -4.596  -0.379   8.436
ATOM    661  C4  DT     21      -2.676   1.789   8.891
ATOM    662  O4  DT     21      -1.814   0.913   8.859
ATOM    663  N3  DT     21      -2.364   2.995   9.472
ATOM    664  H3  DT     21      -1.429   3.108   9.833
ATOM    665  C2  DT     21      -3.196   4.086   9.560
ATOM    666  O2  DT     21      -2.766   5.123  10.063
ATOM    667  C3* DT     21      -7.345   6.218   8.315
ATOM    668  H3* DT     21      -8.168   6.061   7.614
ATOM    669  C2* DT     21      -6.089   5.488   7.840
ATOM    670 1H2* DT     21      -6.393   4.618   7.260
ATOM    671 2H2* DT     21      -5.434   6.119   7.244
ATOM    672  O3* DT     21      -7.131   7.610   8.531
ATOM    673  P   DA     22      -6.865   8.655   7.328
ATOM    674  O1P DA     22      -7.443   9.963   7.726
ATOM    675  O2P DA     22      -7.294   8.045   6.046
ATOM    676  O5* DA     22      -5.258   8.789   7.309
ATOM    677  C5* DA     22      -4.565   9.422   8.381
ATOM    678 1H5* DA     22      -4.780   8.898   9.314
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ATOM    679 2H5* DA     22      -4.920  10.449   8.480
ATOM    680  C4* DA     22      -3.043   9.463   8.182
ATOM    681  H4* DA     22      -2.623  10.092   8.969
ATOM    682  O4* DA     22      -2.494   8.156   8.312
ATOM    683  C1* DA     22      -1.541   7.967   7.282
ATOM    684  H1* DA     22      -0.567   8.357   7.594
ATOM    685  N9  DA     22      -1.438   6.524   6.969
ATOM    686  C8  DA     22      -2.411   5.685   6.475
ATOM    687  H8  DA     22      -3.408   6.036   6.240
ATOM    688  N7  DA     22      -2.034   4.439   6.334
ATOM    689  C5  DA     22      -0.691   4.476   6.746
ATOM    690  C6  DA     22       0.349   3.519   6.854
ATOM    691  N6  DA     22       0.221   2.236   6.571
ATOM    692 1H6  DA     22       1.001   1.610   6.729
ATOM    693 2H6  DA     22      -0.673   1.888   6.267
ATOM    694  N1  DA     22       1.569   3.866   7.270
ATOM    695  C2  DA     22       1.777   5.132   7.606
ATOM    696  H2  DA     22       2.776   5.377   7.945
ATOM    697  N3  DA     22       0.907   6.135   7.580
ATOM    698  C4  DA     22      -0.320   5.738   7.130
ATOM    699  C3* DA     22      -2.610  10.038   6.820
ATOM    700  H3* DA     22      -3.464  10.448   6.277
ATOM    701  C2* DA     22      -2.064   8.798   6.113
ATOM    702 1H2* DA     22      -2.887   8.286   5.614
ATOM    703 2H2* DA     22      -1.277   9.031   5.397
ATOM    704  O3* DA     22      -1.628  11.048   7.037
ATOM    705  P   DG     23      -0.975  11.918   5.844
ATOM    706  O1P DG     23      -0.809  13.310   6.332
ATOM    707  O2P DG     23      -1.732  11.686   4.589
ATOM    708  O5* DG     23       0.484  11.251   5.685
ATOM    709  C5* DG     23       1.451  11.362   6.726
ATOM    710 1H5* DG     23       1.062  10.903   7.636
ATOM    711 2H5* DG     23       1.636  12.417   6.932
ATOM    712  C4* DG     23       2.797  10.704   6.384
ATOM    713  H4* DG     23       3.504  10.962   7.176
ATOM    714  O4* DG     23       2.654   9.287   6.348
ATOM    715  C1* DG     23       3.237   8.805   5.149
ATOM    716  H1* DG     23       4.298   8.593   5.312
ATOM    717  N9  DG     23       2.542   7.573   4.707
ATOM    718  C8  DG     23       1.244   7.423   4.282
ATOM    719  H8  DG     23       0.557   8.260   4.228
ATOM    720  N7  DG     23       0.915   6.196   3.968
ATOM    721  C5  DG     23       2.097   5.474   4.194
ATOM    722  C6  DG     23       2.412   4.076   4.038
ATOM    723  O6  DG     23       1.687   3.150   3.671
ATOM    724  N1  DG     23       3.719   3.766   4.353
ATOM    725  H1  DG     23       3.999   2.801   4.262
ATOM    726  C2  DG     23       4.632   4.678   4.764
ATOM    727  N2  DG     23       5.853   4.261   4.952
ATOM    728 1H2  DG     23       6.538   4.932   5.249
ATOM    729 2H2  DG     23       6.082   3.276   4.839
ATOM    730  N3  DG     23       4.389   5.974   4.932
ATOM    731  C4  DG     23       3.099   6.315   4.635
ATOM    732  C3* DG     23       3.382  11.169   5.039
ATOM    733  H3* DG     23       2.853  12.049   4.664
ATOM    734  C2* DG     23       3.111   9.955   4.153
ATOM    735 1H2* DG     23       2.095  10.018   3.762
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ATOM    736 2H2* DG     23       3.821   9.868   3.336
ATOM    737  O3* DG     23       4.768  11.457   5.205
ATOM    738  P   DC3    24       5.707  12.008   4.011
ATOM    739  O1P DC3    24       6.716  12.919   4.608
ATOM    740  O2P DC3    24       4.853  12.513   2.908
ATOM    741  O5* DC3    24       6.459  10.678   3.498
ATOM    742  C5* DC3    24       7.391   9.999   4.337
ATOM    743 1H5* DC3    24       6.900   9.713   5.269
ATOM    744 2H5* DC3    24       8.214  10.672   4.581
ATOM    745  C4* DC3    24       7.978   8.735   3.691
ATOM    746  H4* DC3    24       8.735   8.332   4.366
ATOM    747  O4* DC3    24       6.951   7.764   3.521
ATOM    748  C1* DC3    24       7.074   7.209   2.224
ATOM    749  H1* DC3    24       7.811   6.400   2.255
ATOM    750  N1  DC3    24       5.753   6.695   1.765
ATOM    751  C6  DC3    24       4.677   7.536   1.620
ATOM    752  H6  DC3    24       4.804   8.593   1.821
ATOM    753  C5  DC3    24       3.469   7.040   1.248
ATOM    754  H5  DC3    24       2.621   7.700   1.144
ATOM    755  C4  DC3    24       3.383   5.640   1.020
ATOM    756  N4  DC3    24       2.251   5.086   0.698
ATOM    757 1H4  DC3    24       1.420   5.646   0.630
ATOM    758 2H4  DC3    24       2.238   4.077   0.587
ATOM    759  N3  DC3    24       4.401   4.816   1.143
ATOM    760  C2  DC3    24       5.603   5.326   1.507
ATOM    761  O2  DC3    24       6.542   4.532   1.587
ATOM    762  C3* DC3    24       8.632   8.985   2.317
ATOM    763  H3* DC3    24       8.726  10.056   2.115
ATOM    764  C2* DC3    24       7.642   8.335   1.355
ATOM    765 1H2* DC3    24       6.875   9.062   1.087
ATOM    766 2H2* DC3    24       8.125   7.947   0.457
ATOM    767  O3* DC3    24       9.899   8.336   2.222
ATOM    768  H3T DC3    24      10.330   8.586   1.379
TER
END
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**File E-6**: Average structure of rMD refined *S*-BD-N3-dU modified duplex 5′ - $G^{1}C^{2}T^{3}A^{4}G^{5}C^{6}X^{7}A^{8}G^{9}T^{10}C^{11}C^{12}$- 3′·5′ - $G^{13}G^{14}A^{15}C^{16}T^{17}G^{18}G^{19}C^{20}T^{21}A^{22}G^{23}C^{24}$ -3′.

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REMARK
ATOM      1  H5T DG5      1      -0.123  -5.561  -2.469
ATOM      2  O5* DG5      1       0.629  -5.240  -1.929
ATOM      3  C5* DG5      1       1.859  -5.547  -2.587
ATOM      4 1H5* DG5      1       1.859  -5.103  -3.585
ATOM      5 2H5* DG5      1       1.942  -6.629  -2.704
ATOM      6  C4* DG5      1       3.113  -5.049  -1.839
ATOM      7  H4* DG5      1       3.986  -5.413  -2.386
ATOM      8  O4* DG5      1       3.144  -3.623  -1.824
ATOM      9  C1* DG5      1       3.155  -3.171  -0.476
ATOM     10  H1* DG5      1       4.180  -2.927  -0.182
ATOM     11  N9  DG5      1       2.298  -1.971  -0.337
ATOM     12  C8  DG5      1       0.938  -1.862  -0.509
ATOM     13  H8  DG5      1       0.326  -2.711  -0.798
ATOM     14  N7  DG5      1       0.464  -0.658  -0.313
ATOM     15  C5  DG5      1       1.603   0.092   0.021
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ATOM     16  C6  DG5     1       1.775   1.489   0.343
ATOM     17  O6  DG5     1       0.935   2.391   0.386
ATOM     18  N1  DG5     1       3.082   1.832   0.627
ATOM     19  H1  DG5     1       3.263   2.795   0.869
ATOM     20  C2  DG5     1       4.115   0.957   0.594
ATOM     21  N2  DG5     1       5.299   1.411   0.896
ATOM     22 1H2  DG5     1       6.064   0.758   0.907
ATOM     23 2H2  DG5     1       5.422   2.385   1.162
ATOM     24  N3  DG5     1       4.012  -0.331   0.285
ATOM     25  C4  DG5     1       2.727  -0.709   0.010
ATOM     26  C3* DG5     1       3.211  -5.541  -0.384
ATOM     27  H3* DG5     1       2.582  -6.420  -0.224
ATOM     28  C2* DG5     1       2.667  -4.337   0.380
ATOM     29 1H2* DG5     1       1.578  -4.383   0.399
ATOM     30 2H2* DG5     1       3.044  -4.279   1.396
ATOM     31  O3* DG5     1       4.573  -5.840  -0.090
ATOM     32  P   DC      2       5.085  -6.326   1.362
ATOM     33  O1P DC      2       6.255  -7.215   1.154
ATOM     34  O2P DC      2       3.930  -6.836   2.141
ATOM     35  O5* DC      2       5.596  -4.955   2.044
ATOM     36  C5* DC      2       6.703  -4.240   1.500
ATOM     37 1H5* DC      2       6.451  -3.884   0.499
ATOM     38 2H5* DC      2       7.556  -4.916   1.410
ATOM     39  C4* DC      2       7.148  -3.039   2.350
ATOM     40  H4* DC      2       8.081  -2.665   1.925
ATOM     41  O4* DC      2       6.177  -1.999   2.284
ATOM     42  C1* DC      2       5.860  -1.570   3.597
ATOM     43  H1* DC      2       6.518  -0.740   3.879
ATOM     44  N1  DC      2       4.431  -1.147   3.633
ATOM     45  C6  DC      2       3.428  -2.033   3.321
ATOM     46  H6  DC      2       3.690  -3.058   3.088
ATOM     47  C5  DC      2       2.136  -1.619   3.288
ATOM     48  H5  DC      2       1.351  -2.315   3.032
ATOM     49  C4  DC      2       1.883  -0.253   3.579
ATOM     50  N4  DC      2       0.678   0.231   3.503
ATOM     51 1H4  DC      2      -0.088  -0.366   3.248
ATOM     52 2H4  DC      2       0.559   1.224   3.674
ATOM     53  N3  DC      2       2.825   0.614   3.882
ATOM     54  C2  DC      2       4.109   0.185   3.923
ATOM     55  O2  DC      2       4.960   1.020   4.227
ATOM     56  C3* DC      2       7.393  -3.387   3.828
ATOM     57  H3* DC      2       7.402  -4.469   3.978
ATOM     58  C2* DC      2       6.175  -2.759   4.507
ATOM     59 1H2* DC      2       5.365  -3.488   4.503
ATOM     60 2H2* DC      2       6.376  -2.444   5.528
ATOM     61  O3* DC      2       8.636  -2.823   4.236
ATOM     62  P   DT      3       9.240  -3.001   5.722
ATOM     63  O1P DT      3      10.721  -2.987   5.618
ATOM     64  O2P DT      3       8.580  -4.151   6.388
ATOM     65  O5* DT      3       8.766  -1.647   6.453
ATOM     66  C5* DT      3       9.244  -0.382   6.009
ATOM     67 1H5* DT      3       8.991  -0.244   4.956
ATOM     68 2H5* DT      3      10.331  -0.354   6.104
ATOM     69  C4* DT      3       8.662   0.793   6.805
ATOM     70  H4* DT      3       9.169   1.702   6.473
ATOM     71  O4* DT      3       7.273   0.930   6.531
ATOM     72  C1* DT      3       6.606   1.219   7.745
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ATOM     73  H1* DT      3       6.680   2.291   7.951
ATOM     74  N1  DT      3       5.181   0.801   7.638
ATOM     75  C6  DT      3       4.838  -0.525   7.440
ATOM     76  H6  DT      3       5.618  -1.276   7.421
ATOM     77  C5  DT      3       3.546  -0.894   7.238
ATOM     78  C7  DT      3       3.232  -2.368   7.052
ATOM     79 1H7  DT      3       3.432  -2.663   6.027
ATOM     80 2H7  DT      3       3.831  -2.971   7.732
ATOM     81 3H7  DT      3       2.181  -2.558   7.262
ATOM     82  C4  DT      3       2.480   0.109   7.230
ATOM     83  O4  DT      3       1.280  -0.088   7.049
ATOM     84  N3  DT      3       2.902   1.398   7.457
ATOM     85  H3  DT      3       2.196   2.118   7.482
ATOM     86  C2  DT      3       4.195   1.795   7.691
ATOM     87  O2  DT      3       4.418   2.978   7.944
ATOM     88  C3* DT      3       8.846   0.663   8.327
ATOM     89  H3* DT      3       9.453  -0.210   8.577
ATOM     90  C2* DT      3       7.407   0.475   8.812
ATOM     91 1H2* DT      3       7.177  -0.590   8.809
ATOM     92 2H2* DT      3       7.236   0.886   9.804
ATOM     93  O3* DT      3       9.467   1.850   8.807
ATOM     94  P   DA      4       9.813   2.100  10.362
ATOM     95  O1P DA      4      11.046   2.923  10.432
ATOM     96  O2P DA      4       9.770   0.809  11.093
ATOM     97  O5* DA      4       8.566   3.000  10.839
ATOM     98  C5* DA      4       8.355   4.294  10.284
ATOM     99 1H5* DA      4       8.184   4.210   9.209
ATOM    100 2H5* DA      4       9.249   4.900  10.437
ATOM    101  C4* DA      4       7.168   5.038  10.911
ATOM    102  H4* DA      4       7.199   6.070  10.556
ATOM    103  O4* DA      4       5.940   4.456  10.489
ATOM    104  C1* DA      4       5.100   4.292  11.617
ATOM    105  H1* DA      4       4.507   5.198  11.778
ATOM    106  N9  DA      4       4.210   3.133  11.376
ATOM    107  C8  DA      4       4.553   1.811  11.205
ATOM    108  H8  DA      4       5.577   1.466  11.289
ATOM    109  N7  DA      4       3.551   1.024  10.901
ATOM    110  C5  DA      4       2.456   1.906  10.904
ATOM    111  C6  DA      4       1.066   1.778  10.658
ATOM    112  N6  DA      4       0.463   0.660  10.298
ATOM    113 1H6  DA      4      -0.528   0.676  10.084
ATOM    114 2H6  DA      4       1.007  -0.180  10.190
ATOM    115  N1  DA      4       0.245   2.824  10.765
ATOM    116  C2  DA      4       0.769   4.001  11.083
ATOM    117  H2  DA      4       0.075   4.829  11.157
ATOM    118  N3  DA      4       2.046   4.287  11.309
ATOM    119  C4  DA      4       2.845   3.185  11.207
ATOM    120  C3* DA      4       7.199   5.048  12.448
ATOM    121  H3* DA      4       8.147   4.659  12.825
ATOM    122  C2* DA      4       6.050   4.100  12.796
ATOM    123 1H2* DA      4       6.432   3.079  12.819
ATOM    124 2H2* DA      4       5.574   4.342  13.744
ATOM    125  O3* DA      4       7.006   6.387  12.889
ATOM    126  P   DG      5       7.001   6.810  14.443
ATOM    127  O1P DG      5       7.585   8.170  14.552
ATOM    128  O2P DG      5       7.581   5.713  15.258
ATOM    129  O5* DG      5       5.426   6.898  14.756
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ATOM    130  C5* DG      5       4.613   7.885  14.126
ATOM    131 1H5* DG      5       4.625   7.737  13.045
ATOM    132 2H5* DG      5       5.023   8.874  14.338
ATOM    133  C4* DG      5       3.156   7.863  14.613
ATOM    134  H4* DG      5       2.665   8.767  14.245
ATOM    135  O4* DG      5       2.477   6.728  14.084
ATOM    136  C1* DG      5       1.779   6.089  15.139
ATOM    137  H1* DG      5       0.787   6.536  15.252
ATOM    138  N9  DG      5       1.647   4.643  14.842
ATOM    139  C8  DG      5       2.633   3.687  14.785
ATOM    140  H8  DG      5       3.671   3.915  14.996
ATOM    141  N7  DG      5       2.214   2.499  14.435
ATOM    142  C5  DG      5       0.834   2.679  14.257
ATOM    143  C6  DG      5      -0.208   1.763  13.864
ATOM    144  O6  DG      5      -0.125   0.573  13.559
ATOM    145  N1  DG      5      -1.462   2.337  13.825
ATOM    146  H1  DG      5      -2.227   1.752  13.525
ATOM    147  C2  DG      5      -1.707   3.632  14.133
ATOM    148  N2  DG      5      -2.951   4.025  14.099
ATOM    149 1H2  DG      5      -3.146   4.988  14.310
ATOM    150 2H2  DG      5      -3.681   3.391  13.784
ATOM    151  N3  DG      5      -0.782   4.520  14.490
ATOM    152  C4  DG      5       0.478   3.985  14.529
ATOM    153  C3* DG      5       3.041   7.827  16.146
ATOM    154  H3* DG      5       4.008   8.023  16.615
ATOM    155  C2* DG      5       2.601   6.384  16.392
ATOM    156 1H2* DG      5       3.484   5.748  16.435
ATOM    157 2H2* DG      5       2.015   6.275  17.301
ATOM    158  O3* DG      5       2.084   8.791  16.572
ATOM    159  P   DC      6       1.809   9.117  18.128
ATOM    160  O1P DC      6       1.606  10.582  18.259
ATOM    161  O2P DC      6       2.848   8.462  18.962
ATOM    162  O5* DC      6       0.407   8.374  18.403
ATOM    163  C5* DC      6      -0.806   8.872  17.844
ATOM    164 1H5* DC      6      -0.744   8.848  16.754
ATOM    165 2H5* DC      6      -0.949   9.908  18.155
ATOM    166  C4* DC      6      -2.039   8.070  18.286
ATOM    167  H4* DC      6      -2.929   8.609  17.956
ATOM    168  O4* DC      6      -2.022   6.801  17.648
ATOM    169  C1* DC      6      -2.333   5.793  18.588
ATOM    170  H1* DC      6      -3.408   5.587  18.550
ATOM    171  N1  DC      6      -1.547   4.579  18.219
ATOM    172  C6  DC      6      -0.175   4.577  18.295
ATOM    173  H6  DC      6       0.337   5.475  18.624
ATOM    174  C5  DC      6       0.527   3.469  17.949
ATOM    175  H5  DC      6       1.604   3.468  18.011
ATOM    176  C4  DC      6      -0.214   2.343  17.500
ATOM    177  N4  DC      6       0.401   1.255  17.140
ATOM    178 1H4  DC      6       1.403   1.215  17.172
ATOM    179 2H4  DC      6      -0.158   0.467  16.832
ATOM    180  N3  DC      6      -1.524   2.338  17.365
ATOM    181  C2  DC      6      -2.213   3.448  17.726
ATOM    182  O2  DC      6      -3.439   3.408  17.600
ATOM    183  C3* DC      6      -2.124   7.871  19.809
ATOM    184  H3* DC      6      -1.284   8.373  20.296
ATOM    185  C2* DC      6      -2.001   6.356  19.978
ATOM    186 1H2* DC      6      -0.978   6.129  20.272
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ATOM    187 2H2* DC      6      -2.686   5.968  20.732
ATOM    188  O3* DC      6      -3.351   8.392  20.310
ATOM    189  P   DX      7      -3.618   8.611  21.890
ATOM    190  O1P DX      7      -4.434   9.842  22.045
ATOM    191  O2P DX      7      -2.333   8.515  22.625
ATOM    192  O5* DX      7      -4.522   7.345  22.308
ATOM    193  C5* DX      7      -5.858   7.211  21.835
ATOM    194 1H5* DX      7      -5.858   7.158  20.745
ATOM    195 2H5* DX      7      -6.435   8.088  22.134
ATOM    196  C4* DX      7      -6.561   5.965  22.393
ATOM    197  H4* DX      7      -7.601   5.994  22.059
ATOM    198  O4* DX      7      -5.956   4.774  21.891
ATOM    199  C1* DX      7      -6.025   3.822  22.935
ATOM    200  H1* DX      7      -7.060   3.479  23.026
ATOM    201  N1  DX      7      -5.131   2.645  22.714
ATOM    202  C6  DX      7      -3.766   2.742  22.856
ATOM    203  H6  DX      7      -3.311   3.716  22.993
ATOM    204  C5  DX      7      -2.988   1.631  22.836
ATOM    205  H5  DX      7      -1.919   1.721  22.967
ATOM    206  C4  DX      7      -3.541   0.306  22.657
ATOM    207  O4  DX      7      -2.863  -0.723  22.701
ATOM    208  N3  DX      7      -4.922   0.268  22.425
ATOM    209  C11 DX      7      -5.550  -1.064  22.073
ATOM    210  C2  DX      7      -5.736   1.409  22.438
ATOM    211  O2  DX      7      -6.949   1.322  22.218
ATOM    212  C3* DX      7      -6.553   5.888  23.935
ATOM    213  H3* DX      7      -6.076   6.772  24.365
ATOM    214  C2* DX      7      -5.710   4.639  24.185
ATOM    215 1H2* DX      7      -4.660   4.927  24.220
ATOM    216 2H2* DX      7      -5.992   4.111  25.093
ATOM    217  O3* DX      7      -7.885   5.745  24.423
ATOM    218  C12 DX      7      -5.981  -1.897  23.275
ATOM    219  C9  DX      7      -6.347  -3.300  22.833
ATOM    220  C10 DX      7      -6.835  -4.284  23.579
ATOM    221  O12 DX      7      -7.110  -1.301  23.863
ATOM    222  H15 DX      7      -4.823  -1.662  21.529
ATOM    223  H14 DX      7      -6.415  -0.926  21.423
ATOM    224  H9  DX      7      -5.158  -1.944  23.982
ATOM    225 1H1  DX      7      -6.217  -3.572  21.795
ATOM    226 2H1  DX      7      -7.004  -4.101  24.632
ATOM    227 3H1  DX      7      -7.065  -5.235  23.120
ATOM    228  H10 DX      7      -6.914  -0.351  23.908
ATOM    229  P   DA      8      -8.254   5.818  25.997
ATOM    230  O1P DA      8      -9.659   6.280  26.107
ATOM    231  O2P DA      8      -7.197   6.584  26.703
ATOM    232  O5* DA      8      -8.182   4.288  26.504
ATOM    233  C5* DA      8      -9.130   3.322  26.061
ATOM    234 1H5* DA      8      -9.111   3.272  24.971
ATOM    235 2H5* DA      8     -10.130   3.632  26.368
ATOM    236  C4* DA      8      -8.872   1.912  26.613
ATOM    237  H4* DA      8      -9.689   1.274  26.270
ATOM    238  O4* DA      8      -7.651   1.397  26.086
ATOM    239  C1* DA      8      -6.933   0.786  27.143
ATOM    240  H1* DA      8      -7.250  -0.256  27.261
ATOM    241  N9  DA      8      -5.484   0.852  26.855
ATOM    242  C8  DA      8      -4.677   1.964  26.786
ATOM    243  H8  DA      8      -5.053   2.965  26.964
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ATOM    244  N7  DA      8      -3.432   1.712  26.469
ATOM    245  C5  DA      8      -3.424   0.313  26.340
ATOM    246  C6  DA      8      -2.443  -0.659  26.023
ATOM    247  N6  DA      8      -1.178  -0.396  25.765
ATOM    248 1H6  DA      8      -0.570  -1.159  25.527
ATOM    249 2H6  DA      8      -0.858   0.559  25.771
ATOM    250  N1  DA      8      -2.736  -1.959  25.982
ATOM    251  C2  DA      8      -3.981  -2.321  26.253
ATOM    252  H2  DA      8      -4.188  -3.384  26.218
ATOM    253  N3  DA      8      -5.007  -1.539  26.571
ATOM    254  C4  DA      8      -4.662  -0.219  26.589
ATOM    255  C3* DA      8      -8.813   1.824  28.151
ATOM    256  H3* DA      8      -9.127   2.761  28.618
ATOM    257  C2* DA      8      -7.324   1.574  28.389
ATOM    258 1H2* DA      8      -6.810   2.534  28.417
ATOM    259 2H2* DA      8      -7.117   1.016  29.300
ATOM    260  O3* DA      8      -9.658   0.752  28.562
ATOM    261  P   DG      9      -9.802   0.241  30.087
ATOM    262  O1P DG      9     -11.221  -0.135  30.309
ATOM    263  O2P DG      9      -9.169   1.218  31.008
ATOM    264  O5* DG      9      -8.914  -1.105  30.071
ATOM    265  C5* DG      9      -9.281  -2.193  29.225
ATOM    266 1H5* DG      9      -9.237  -1.872  28.183
ATOM    267 2H5* DG      9     -10.310  -2.483  29.443
ATOM    268  C4* DG      9      -8.400  -3.442  29.381
ATOM    269  H4* DG      9      -8.845  -4.230  28.770
ATOM    270  O4* DG      9      -7.087  -3.184  28.895
ATOM    271  C1* DG      9      -6.144  -3.531  29.894
ATOM    272  H1* DG      9      -5.787  -4.553  29.730
ATOM    273  N9  DG      9      -5.005  -2.585  29.843
ATOM    274  C8  DG      9      -4.995  -1.242  30.136
ATOM    275  H8  DG      9      -5.884  -0.719  30.473
ATOM    276  N7  DG      9      -3.838  -0.659  29.960
ATOM    277  C5  DG      9      -3.013  -1.700  29.510
ATOM    278  C6  DG      9      -1.630  -1.718  29.102
ATOM    279  O6  DG      9      -0.824  -0.790  29.044
ATOM    280  N1  DG      9      -1.188  -2.962  28.700
ATOM    281  H1  DG      9      -0.242  -3.027  28.355
ATOM    282  C2  DG      9      -1.980  -4.058  28.639
ATOM    283  N2  DG      9      -1.451  -5.156  28.175
ATOM    284 1H2  DG      9      -2.024  -5.981  28.147
ATOM    285 2H2  DG      9      -0.477  -5.174  27.882
ATOM    286  N3  DG      9      -3.257  -4.095  29.010
ATOM    287  C4  DG      9      -3.722  -2.882  29.438
ATOM    288  C3* DG      9      -8.298  -3.952  30.828
ATOM    289  H3* DG      9      -9.056  -3.489  31.464
ATOM    290  C2* DG      9      -6.900  -3.477  31.220
ATOM    291 1H2* DG      9      -6.969  -2.453  31.586
ATOM    292 2H2* DG      9      -6.437  -4.108  31.974
ATOM    293  O3* DG      9      -8.458  -5.367  30.817
ATOM    294  P   DT     10      -8.341  -6.290  32.135
ATOM    295  O1P DT     10      -9.260  -7.443  31.969
ATOM    296  O2P DT     10      -8.465  -5.442  33.347
ATOM    297  O5* DT     10      -6.825  -6.825  32.036
ATOM    298  C5* DT     10      -6.418  -7.633  30.935
ATOM    299 1H5* DT     10      -6.592  -7.092  30.003
ATOM    300 2H5* DT     10      -7.020  -8.543  30.914
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ATOM    301  C4* DT     10      -4.939  -8.037  30.987
ATOM    302  H4* DT     10      -4.749  -8.709  30.147
ATOM    303  O4* DT     10      -4.117  -6.884  30.838
ATOM    304  C1* DT     10      -3.105  -6.912  31.828
ATOM    305  H1* DT     10      -2.254  -7.487  31.451
ATOM    306  N1  DT     10      -2.696  -5.516  32.150
ATOM    307  C6  DT     10      -3.582  -4.631  32.738
ATOM    308  H6  DT     10      -4.571  -4.978  33.014
ATOM    309  C5  DT     10      -3.240  -3.331  32.946
ATOM    310  C7  DT     10      -4.243  -2.392  33.599
ATOM    311 1H7  DT     10      -5.180  -2.906  33.827
ATOM    312 2H7  DT     10      -3.816  -1.997  34.524
ATOM    313 3H7  DT     10      -4.444  -1.551  32.931
ATOM    314  C4  DT     10      -1.927  -2.834  32.538
ATOM    315  O4  DT     10      -1.516  -1.678  32.625
ATOM    316  N3  DT     10      -1.100  -3.783  31.990
ATOM    317  H3  DT     10      -0.168  -3.489  31.740
ATOM    318  C2  DT     10      -1.407  -5.105  31.786
ATOM    319  O2  DT     10      -0.553  -5.847  31.306
ATOM    320  C3* DT     10      -4.541  -8.757  32.287
ATOM    321  H3* DT     10      -5.424  -9.020  32.876
ATOM    322  C2* DT     10      -3.711  -7.688  32.997
ATOM    323 1H2* DT     10      -4.381  -7.067  33.589
ATOM    324 2H2* DT     10      -2.947  -8.117  33.639
ATOM    325  O3* DT     10      -3.803  -9.930  31.951
ATOM    326  P   DC     11      -3.222 -10.958  33.052
ATOM    327  O1P DC     11      -3.292 -12.327  32.482
ATOM    328  O2P DC     11      -3.865 -10.694  34.363
ATOM    329  O5* DC     11      -1.674 -10.520  33.147
ATOM    330  C5* DC     11      -0.807 -10.680  32.028
ATOM    331 1H5* DC     11      -1.229 -10.159  31.166
ATOM    332 2H5* DC     11      -0.731 -11.739  31.778
ATOM    333  C4* DC     11       0.608 -10.137  32.270
ATOM    334  H4* DC     11       1.210 -10.371  31.389
ATOM    335  O4* DC     11       0.557  -8.722  32.424
ATOM    336  C1* DC     11       1.324  -8.359  33.557
ATOM    337  H1* DC     11       2.370  -8.231  33.257
ATOM    338  N1  DC     11       0.788  -7.091  34.131
ATOM    339  C6  DC     11      -0.455  -7.039  34.717
ATOM    340  H6  DC     11      -1.050  -7.942  34.782
ATOM    341  C5  DC     11      -0.940  -5.862  35.191
ATOM    342  H5  DC     11      -1.920  -5.823  35.641
ATOM    343  C4  DC     11      -0.115  -4.715  35.050
ATOM    344  N4  DC     11      -0.525  -3.550  35.456
ATOM    345 1H4  DC     11      -1.420  -3.453  35.898
ATOM    346 2H4  DC     11       0.099  -2.762  35.308
ATOM    347  N3  DC     11       1.076  -4.739  34.494
ATOM    348  C2  DC     11       1.550  -5.918  34.028
ATOM    349  O2  DC     11       2.680  -5.903  33.537
ATOM    350  C3* DC     11       1.303 -10.736  33.506
ATOM    351  H3* DC     11       0.746 -11.595  33.890
ATOM    352  C2* DC     11       1.246  -9.570  34.491
ATOM    353 1H2* DC     11       0.296  -9.611  35.020
ATOM    354 2H2* DC     11       2.064  -9.588  35.206
ATOM    355  O3* DC     11       2.630 -11.121  33.155
ATOM    356  P   DC3    12       3.661 -11.797  34.198
ATOM    357  O1P DC3    12       4.515 -12.749  33.445
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ATOM    358  O2P DC3    12       2.912 -12.291  35.380
ATOM    359  O5* DC3    12       4.571 -10.549  34.662
ATOM    360  C5* DC3    12       5.443  -9.901  33.739
ATOM    361 1H5* DC3    12       4.864  -9.527  32.892
ATOM    362 2H5* DC3    12       6.166 -10.624  33.359
ATOM    363  C4* DC3    12       6.218  -8.726  34.354
ATOM    364  H4* DC3    12       6.930  -8.366  33.609
ATOM    365  O4* DC3    12       5.319  -7.668  34.672
ATOM    366  C1* DC3    12       5.670  -7.161  35.946
ATOM    367  H1* DC3    12       6.484  -6.437  35.832
ATOM    368  N1  DC3    12       4.485  -6.525  36.582
ATOM    369  C6  DC3    12       3.322  -7.231  36.764
ATOM    370  H6  DC3    12       3.290  -8.272  36.465
ATOM    371  C5  DC3    12       2.233  -6.623  37.300
ATOM    372  H5  DC3    12       1.316  -7.176  37.437
ATOM    373  C4  DC3    12       2.362  -5.252  37.651
ATOM    374  N4  DC3    12       1.357  -4.599  38.157
ATOM    375 1H4  DC3    12       0.474  -5.058  38.287
ATOM    376 2H4  DC3    12       1.485  -3.607  38.325
ATOM    377  N3  DC3    12       3.474  -4.562  37.509
ATOM    378  C2  DC3    12       4.558  -5.187  36.991
ATOM    379  O2  DC3    12       5.597  -4.529  36.915
ATOM    380  C3* DC3    12       6.993  -9.093  35.635
ATOM    381  H3* DC3    12       6.987 -10.173  35.804
ATOM    382  C2* DC3    12       6.204  -8.368  36.721
ATOM    383 1H2* DC3    12       5.392  -9.010  37.065
ATOM    384 2H2* DC3    12       6.828  -8.064  37.562
ATOM    385  O3* DC3    12       8.328  -8.591  35.593
ATOM    386  H3T DC3    12       8.818  -8.902  36.381
TER
ATOM    387  H5T DG5    13       2.519   6.434  40.064
ATOM    388  O5* DG5    13       3.145   5.926  39.505
ATOM    389  C5* DG5    13       4.473   6.084  40.009
ATOM    390 1H5* DG5    13       4.508   5.754  41.050
ATOM    391 2H5* DG5    13       4.739   7.143  39.987
ATOM    392  C4* DG5    13       5.546   5.304  39.220
ATOM    393  H4* DG5    13       6.518   5.582  39.634
ATOM    394  O4* DG5    13       5.362   3.900  39.394
ATOM    395  C1* DG5    13       5.114   3.297  38.132
ATOM    396  H1* DG5    13       6.027   2.811  37.774
ATOM    397  N9  DG5    13       4.034   2.291  38.265
ATOM    398  C8  DG5    13       2.713   2.487  38.594
ATOM    399  H8  DG5    13       2.313   3.474  38.804
ATOM    400  N7  DG5    13       2.002   1.390  38.650
ATOM    401  C5  DG5    13       2.926   0.385  38.320
ATOM    402  C6  DG5    13       2.790  -1.046  38.214
ATOM    403  O6  DG5    13       1.800  -1.754  38.411
ATOM    404  N1  DG5    13       3.958  -1.686  37.848
ATOM    405  H1  DG5    13       3.921  -2.690  37.749
ATOM    406  C2  DG5    13       5.135  -1.047  37.643
ATOM    407  N2  DG5    13       6.160  -1.775  37.298
ATOM    408 1H2  DG5    13       7.023  -1.301  37.092
ATOM    409 2H2  DG5    13       6.051  -2.775  37.149
ATOM    410  N3  DG5    13       5.318   0.265  37.750
ATOM    411  C4  DG5    13       4.171   0.933  38.086
ATOM    412  C3* DG5    13       5.561   5.594  37.709
ATOM    413  H3* DG5    13       5.070   6.544  37.488
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ATOM    414  C2* DG5    13       4.749   4.421  37.164
ATOM    415 1H2* DG5    13       3.688   4.661  37.225
ATOM    416 2H2* DG5    13       5.005   4.171  36.138
ATOM    417  O3* DG5    13       6.913   5.612  37.259
ATOM    418  P   DG     14       7.331   5.853  35.718
ATOM    419  O1P DG     14       8.663   6.507  35.707
ATOM    420  O2P DG     14       6.207   6.510  35.006
ATOM    421  O5* DG     14       7.491   4.353  35.144
ATOM    422  C5* DG     14       8.514   3.489  35.633
ATOM    423 1H5* DG     14       8.357   3.305  36.698
ATOM    424 2H5* DG     14       9.482   3.979  35.515
ATOM    425  C4* DG     14       8.579   2.137  34.905
ATOM    426  H4* DG     14       9.487   1.628  35.238
ATOM    427  O4* DG     14       7.458   1.329  35.252
ATOM    428  C1* DG     14       6.887   0.808  34.063
ATOM    429  H1* DG     14       7.363  -0.143  33.805
ATOM    430  N9  DG     14       5.432   0.607  34.256
ATOM    431  C8  DG     14       4.468   1.552  34.512
ATOM    432  H8  DG     14       4.699   2.609  34.558
ATOM    433  N7  DG     14       3.273   1.064  34.720
ATOM    434  C5  DG     14       3.456  -0.318  34.560
ATOM    435  C6  DG     14       2.534  -1.420  34.665
ATOM    436  O6  DG     14       1.339  -1.411  34.961
ATOM    437  N1  DG     14       3.108  -2.644  34.390
ATOM    438  H1  DG     14       2.498  -3.448  34.398
ATOM    439  C2  DG     14       4.414  -2.814  34.078
ATOM    440  N2  DG     14       4.801  -4.021  33.774
ATOM    441 1H2  DG     14       5.753  -4.145  33.478
ATOM    442 2H2  DG     14       4.120  -4.773  33.698
ATOM    443  N3  DG     14       5.310  -1.834  34.001
ATOM    444  C4  DG     14       4.770  -0.601  34.251
ATOM    445  C3* DG     14       8.628   2.263  33.372
ATOM    446  H3* DG     14       8.820   3.294  33.067
ATOM    447  C2* DG     14       7.213   1.836  32.983
ATOM    448 1H2* DG     14       6.548   2.697  33.057
ATOM    449 2H2* DG     14       7.161   1.408  31.985
ATOM    450  O3* DG     14       9.645   1.398  32.874
ATOM    451  P   DA     15       9.996   1.254  31.306
ATOM    452  O1P DA     15      11.456   1.014  31.186
ATOM    453  O2P DA     15       9.394   2.385  30.558
ATOM    454  O5* DA     15       9.219  -0.098  30.896
ATOM    455  C5* DA     15       9.593  -1.350  31.465
ATOM    456 1H5* DA     15       9.456  -1.314  32.546
ATOM    457 2H5* DA     15      10.651  -1.530  31.267
ATOM    458  C4* DA     15       8.802  -2.546  30.911
ATOM    459  H4* DA     15       9.259  -3.454  31.308
ATOM    460  O4* DA     15       7.447  -2.492  31.349
ATOM    461  C1* DA     15       6.594  -2.612  30.223
ATOM    462  H1* DA     15       6.334  -3.664  30.064
ATOM    463  N9  DA     15       5.369  -1.816  30.459
ATOM    464  C8  DA     15       5.245  -0.451  30.568
ATOM    465  H8  DA     15       6.087   0.217  30.428
ATOM    466  N7  DA     15       4.042  -0.038  30.877
ATOM    467  C5  DA     15       3.316  -1.239  30.958
ATOM    468  C6  DA     15       1.978  -1.580  31.274
ATOM    469  N6  DA     15       1.049  -0.718  31.641
ATOM    470 1H6  DA     15       0.133  -1.067  31.900
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ATOM    471 2H6  DA     15       1.270   0.263  31.681
ATOM    472  N1  DA     15       1.566  -2.848  31.265
ATOM    473  C2  DA     15       2.446  -3.789  30.950
ATOM    474  H2  DA     15       2.077  -4.807  30.946
ATOM    475  N3  DA     15       3.729  -3.631  30.642
ATOM    476  C4  DA     15       4.108  -2.321  30.675
ATOM    477  C3* DA     15       8.808  -2.628  29.376
ATOM    478  H3* DA     15       9.576  -1.979  28.949
ATOM    479  C2* DA     15       7.411  -2.115  29.033
ATOM    480 1H2* DA     15       7.432  -1.026  29.002
ATOM    481 2H2* DA     15       7.038  -2.506  28.090
ATOM    482  O3* DA     15       9.029  -3.983  28.995
ATOM    483  P   DC     16       9.119  -4.467  27.459
ATOM    484  O1P DC     16      10.136  -5.546  27.383
ATOM    485  O2P DC     16       9.265  -3.284  26.576
ATOM    486  O5* DC     16       7.663  -5.113  27.207
ATOM    487  C5* DC     16       7.261  -6.293  27.899
ATOM    488 1H5* DC     16       7.242  -6.096  28.973
ATOM    489 2H5* DC     16       7.991  -7.082  27.715
ATOM    490  C4* DC     16       5.881  -6.816  27.473
ATOM    491  H4* DC     16       5.736  -7.792  27.941
ATOM    492  O4* DC     16       4.865  -5.936  27.940
ATOM    493  C1* DC     16       3.978  -5.647  26.875
ATOM    494  H1* DC     16       3.174  -6.392  26.862
ATOM    495  N1  DC     16       3.425  -4.276  27.071
ATOM    496  C6  DC     16       4.252  -3.179  27.083
ATOM    497  H6  DC     16       5.313  -3.318  26.907
ATOM    498  C5  DC     16       3.748  -1.946  27.339
ATOM    499  H5  DC     16       4.402  -1.087  27.360
ATOM    500  C4  DC     16       2.354  -1.854  27.595
ATOM    501  N4  DC     16       1.815  -0.713  27.909
ATOM    502 1H4  DC     16       2.391   0.107  27.981
ATOM    503 2H4  DC     16       0.840  -0.713  28.190
ATOM    504  N3  DC     16       1.539  -2.887  27.590
ATOM    505  C2  DC     16       2.057  -4.113  27.331
ATOM    506  O2  DC     16       1.272  -5.062  27.347
ATOM    507  C3* DC     16       5.725  -6.978  25.951
ATOM    508  H3* DC     16       6.692  -6.872  25.452
ATOM    509  C2* DC     16       4.804  -5.812  25.596
ATOM    510 1H2* DC     16       5.416  -4.933  25.400
ATOM    511 2H2* DC     16       4.175  -6.021  24.734
ATOM    512  O3* DC     16       5.156  -8.251  25.661
ATOM    513  P   DT     17       4.995  -8.812  24.154
ATOM    514  O1P DT     17       5.023 -10.295  24.216
ATOM    515  O2P DT     17       5.965  -8.117  23.271
ATOM    516  O5* DT     17       3.510  -8.346  23.734
ATOM    517  C5* DT     17       2.362  -8.911  24.359
ATOM    518 1H5* DT     17       2.392  -8.710  25.432
ATOM    519 2H5* DT     17       2.373  -9.992  24.214
ATOM    520  C4* DT     17       1.040  -8.371  23.792
ATOM    521  H4* DT     17       0.231  -8.978  24.203
ATOM    522  O4* DT     17       0.829  -7.021  24.192
ATOM    523  C1* DT     17       0.197  -6.352  23.115
ATOM    524  H1* DT     17      -0.867  -6.608  23.103
ATOM    525  N1  DT     17       0.386  -4.879  23.223
ATOM    526  C6  DT     17       1.651  -4.352  23.388
ATOM    527  H6  DT     17       2.492  -5.030  23.464
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ATOM    528  C5  DT     17       1.848  -3.009  23.458
ATOM    529  C7  DT     17       3.260  -2.476  23.640
ATOM    530 1H7  DT     17       3.983  -3.287  23.734
ATOM    531 2H7  DT     17       3.526  -1.857  22.782
ATOM    532 3H7  DT     17       3.301  -1.854  24.533
ATOM    533  C4  DT     17       0.716  -2.086  23.357
ATOM    534  O4  DT     17       0.774  -0.859  23.408
ATOM    535  N3  DT     17      -0.516  -2.687  23.204
ATOM    536  H3  DT     17      -1.320  -2.083  23.116
ATOM    537  C2  DT     17      -0.740  -4.045  23.128
ATOM    538  O2  DT     17      -1.889  -4.462  22.980
ATOM    539  C3* DT     17       0.957  -8.430  22.256
ATOM    540  H3* DT     17       1.858  -8.880  21.835
ATOM    541  C2* DT     17       0.858  -6.952  21.875
ATOM    542 1H2* DT     17       1.864  -6.554  21.742
ATOM    543 2H2* DT     17       0.263  -6.788  20.977
ATOM    544  O3* DT     17      -0.197  -9.168  21.867
ATOM    545  P   DG     18      -0.455  -9.638  20.342
ATOM    546  O1P DG     18      -0.872 -11.062  20.370
ATOM    547  O2P DG     18       0.706  -9.252  19.503
ATOM    548  O5* DG     18      -1.714  -8.741  19.882
ATOM    549  C5* DG     18      -3.017  -8.976  20.407
ATOM    550 1H5* DG     18      -3.023  -8.775  21.480
ATOM    551 2H5* DG     18      -3.280 -10.025  20.258
ATOM    552  C4* DG     18      -4.104  -8.122  19.734
ATOM    553  H4* DG     18      -5.074  -8.492  20.073
ATOM    554  O4* DG     18      -3.974  -6.760  20.132
ATOM    555  C1* DG     18      -4.034  -5.947  18.973
ATOM    556  H1* DG     18      -5.075  -5.697  18.747
ATOM    557  N9  DG     18      -3.252  -4.706  19.175
ATOM    558  C8  DG     18      -1.908  -4.566  19.426
ATOM    559  H8  DG     18      -1.250  -5.422  19.526
ATOM    560  N7  DG     18      -1.508  -3.325  19.544
ATOM    561  C5  DG     18      -2.682  -2.581  19.346
ATOM    562  C6  DG     18      -2.935  -1.160  19.335
ATOM    563  O6  DG     18      -2.154  -0.225  19.512
ATOM    564  N1  DG     18      -4.252  -0.833  19.067
ATOM    565  H1  DG     18      -4.484   0.141  19.055
ATOM    566  C2  DG     18      -5.227  -1.753  18.855
ATOM    567  N2  DG     18      -6.441  -1.323  18.638
ATOM    568 1H2  DG     18      -6.648  -0.342  18.571
ATOM    569 2H2  DG     18      -7.140  -2.018  18.433
ATOM    570  N3  DG     18      -5.048  -3.068  18.878
ATOM    571  C4  DG     18      -3.750  -3.425  19.118
ATOM    572  C3* DG     18      -4.069  -8.184  18.195
ATOM    573  H3* DG     18      -3.413  -8.987  17.849
ATOM    574  C2* DG     18      -3.483  -6.817  17.846
ATOM    575 1H2* DG     18      -2.396  -6.869  17.897
ATOM    576 2H2* DG     18      -3.797  -6.459  16.869
ATOM    577  O3* DG     18      -5.393  -8.380  17.704
ATOM    578  P   DG     19      -5.747  -8.513  16.133
ATOM    579  O1P DG     19      -6.858  -9.487  15.998
ATOM    580  O2P DG     19      -4.499  -8.742  15.363
ATOM    581  O5* DG     19      -6.306  -7.046  15.765
ATOM    582  C5* DG     19      -7.497  -6.554  16.374
ATOM    583 1H5* DG     19      -7.356  -6.507  17.455
ATOM    584 2H5* DG     19      -8.315  -7.248  16.173
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ATOM    585  C4* DG     19      -7.925  -5.163  15.881
ATOM    586  H4* DG     19      -8.877  -4.931  16.362
ATOM    587  O4* DG     19      -6.971  -4.181  16.278
ATOM    588  C1* DG     19      -6.521  -3.473  15.132
ATOM    589  H1* DG     19      -7.079  -2.537  15.037
ATOM    590  N9  DG     19      -5.074  -3.184  15.270
ATOM    591  C8  DG     19      -4.015  -4.059  15.215
ATOM    592  H8  DG     19      -4.151  -5.117  15.016
ATOM    593  N7  DG     19      -2.850  -3.515  15.450
ATOM    594  C5  DG     19      -3.160  -2.165  15.669
ATOM    595  C6  DG     19      -2.332  -1.037  16.017
ATOM    596  O6  DG     19      -1.119  -0.994  16.220
ATOM    597  N1  DG     19      -3.039   0.138  16.177
ATOM    598  H1  DG     19      -2.529   0.942  16.512
ATOM    599  C2  DG     19      -4.377   0.239  16.011
ATOM    600  N2  DG     19      -4.934   1.384  16.291
ATOM    601 1H2  DG     19      -5.926   1.469  16.150
ATOM    602 2H2  DG     19      -4.379   2.164  16.635
ATOM    603  N3  DG     19      -5.181  -0.767  15.684
ATOM    604  C4  DG     19      -4.516  -1.953  15.535
ATOM    605  C3* DG     19      -8.118  -5.071  14.358
ATOM    606  H3* DG     19      -8.179  -6.063  13.906
ATOM    607  C2* DG     19      -6.834  -4.363  13.931
ATOM    608 1H2* DG     19      -6.057  -5.113  13.787
ATOM    609 2H2* DG     19      -6.950  -3.782  13.019
ATOM    610  O3* DG     19      -9.316  -4.340  14.111
ATOM    611  P   DC     20      -9.819  -3.901  12.642
ATOM    612  O1P DC     20     -11.303  -3.918  12.643
ATOM    613  O2P DC     20      -9.093  -4.684  11.611
ATOM    614  O5* DC     20      -9.323  -2.369  12.576
ATOM    615  C5* DC     20      -9.830  -1.413  13.503
ATOM    616 1H5* DC     20      -9.605  -1.738  14.520
ATOM    617 2H5* DC     20     -10.915  -1.354  13.402
ATOM    618  C4* DC     20      -9.257  -0.003  13.313
ATOM    619  H4* DC     20      -9.771   0.658  14.014
ATOM    620  O4* DC     20      -7.869   0.007  13.627
ATOM    621  C1* DC     20      -7.172   0.708  12.613
ATOM    622  H1* DC     20      -7.132   1.774  12.867
ATOM    623  N1  DC     20      -5.799   0.141  12.492
ATOM    624  C6  DC     20      -5.606  -1.180  12.164
ATOM    625  H6  DC     20      -6.470  -1.804  11.957
ATOM    626  C5  DC     20      -4.352  -1.698  12.126
ATOM    627  H5  DC     20      -4.203  -2.738  11.880
ATOM    628  C4  DC     20      -3.277  -0.826  12.446
ATOM    629  N4  DC     20      -2.056  -1.269  12.501
ATOM    630 1H4  DC     20      -1.863  -2.234  12.303
ATOM    631 2H4  DC     20      -1.334  -0.619  12.796
ATOM    632  N3  DC     20      -3.437   0.438  12.772
ATOM    633  C2  DC     20      -4.692   0.945  12.794
ATOM    634  O2  DC     20      -4.800   2.134  13.092
ATOM    635  C3* DC     20      -9.449   0.556  11.893
ATOM    636  H3* DC     20     -10.089  -0.100  11.298
ATOM    637  C2* DC     20      -8.020   0.547  11.350
ATOM    638 1H2* DC     20      -7.838  -0.414  10.871
ATOM    639 2H2* DC     20      -7.837   1.350  10.640
ATOM    640  O3* DC     20     -10.027   1.853  11.991
ATOM    641  P   DT     21     -10.377   2.768  10.708
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ATOM    642  O1P DT     21     -11.583   3.570  11.032
ATOM    643  O2P DT     21     -10.382   1.927   9.486
ATOM    644  O5* DT     21      -9.107   3.757  10.643
ATOM    645  C5* DT     21      -8.854   4.674  11.703
ATOM    646 1H5* DT     21      -8.785   4.130  12.647
ATOM    647 2H5* DT     21      -9.685   5.378  11.778
ATOM    648  C4* DT     21      -7.558   5.472  11.514
ATOM    649  H4* DT     21      -7.492   6.196  12.329
ATOM    650  O4* DT     21      -6.438   4.598  11.595
ATOM    651  C1* DT     21      -5.525   4.949  10.572
ATOM    652  H1* DT     21      -4.891   5.770  10.921
ATOM    653  N1  DT     21      -4.697   3.763  10.215
ATOM    654  C6  DT     21      -5.271   2.632   9.665
ATOM    655  H6  DT     21      -6.336   2.621   9.479
ATOM    656  C5  DT     21      -4.522   1.534   9.374
ATOM    657  C7  DT     21      -5.193   0.310   8.773
ATOM    658 1H7  DT     21      -6.268   0.459   8.666
ATOM    659 2H7  DT     21      -4.760   0.107   7.793
ATOM    660 3H7  DT     21      -5.010  -0.555   9.410
ATOM    661  C4  DT     21      -3.086   1.522   9.650
ATOM    662  O4  DT     21      -2.305   0.596   9.440
ATOM    663  N3  DT     21      -2.595   2.681  10.200
ATOM    664  H3  DT     21      -1.609   2.713  10.409
ATOM    665  C2  DT     21      -3.322   3.811  10.484
ATOM    666  O2  DT     21      -2.739   4.794  10.939
ATOM    667  C3* DT     21      -7.487   6.236  10.180
ATOM    668  H3* DT     21      -8.437   6.176   9.643
ATOM    669  C2* DT     21      -6.396   5.473   9.430
ATOM    670 1H2* DT     21      -6.860   4.659   8.877
ATOM    671 2H2* DT     21      -5.830   6.105   8.750
ATOM    672  O3* DT     21      -7.153   7.594  10.447
ATOM    673  P   DA     22      -7.004   8.710   9.291
ATOM    674  O1P DA     22      -7.447  10.011   9.851
ATOM    675  O2P DA     22      -7.637   8.215   8.043
ATOM    676  O5* DA     22      -5.410   8.764   9.066
ATOM    677  C5* DA     22      -4.548   9.234  10.099
ATOM    678 1H5* DA     22      -4.667   8.610  10.986
ATOM    679 2H5* DA     22      -4.828  10.255  10.363
ATOM    680  C4* DA     22      -3.066   9.235   9.699
ATOM    681  H4* DA     22      -2.511   9.746  10.489
ATOM    682  O4* DA     22      -2.583   7.900   9.603
ATOM    683  C1* DA     22      -1.811   7.782   8.422
ATOM    684  H1* DA     22      -0.772   8.065   8.622
ATOM    685  N9  DA     22      -1.878   6.384   7.941
ATOM    686  C8  DA     22      -2.977   5.680   7.507
ATOM    687  H8  DA     22      -3.963   6.127   7.451
ATOM    688  N7  DA     22      -2.735   4.431   7.194
ATOM    689  C5  DA     22      -1.352   4.321   7.419
ATOM    690  C6  DA     22      -0.396   3.282   7.294
ATOM    691  N6  DA     22      -0.669   2.047   6.917
ATOM    692 1H6  DA     22       0.070   1.353   6.914
ATOM    693 2H6  DA     22      -1.620   1.797   6.703
ATOM    694  N1  DA     22       0.893   3.491   7.567
ATOM    695  C2  DA     22       1.257   4.696   7.985
ATOM    696  H2  DA     22       2.309   4.829   8.203
ATOM    697  N3  DA     22       0.482   5.758   8.176
ATOM    698  C4  DA     22      -0.823   5.504   7.866
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ATOM    699  C3* DA     22      -2.787   9.952   8.366
ATOM    700  H3* DA     22      -3.680  10.466   8.002
ATOM    701  C2* DA     22      -2.424   8.784   7.447
ATOM    702 1H2* DA     22      -3.339   8.385   7.010
ATOM    703 2H2* DA     22      -1.725   9.064   6.662
ATOM    704  O3* DA     22      -1.727  10.882   8.562
ATOM    705  P   DG     23      -1.174  11.851   7.397
ATOM    706  O1P DG     23      -0.800  13.146   8.018
ATOM    707  O2P DG     23      -2.126  11.852   6.258
ATOM    708  O5* DG     23       0.172  11.095   6.935
ATOM    709  C5* DG     23       1.275  10.971   7.828
ATOM    710 1H5* DG     23       0.954  10.457   8.735
ATOM    711 2H5* DG     23       1.623  11.967   8.108
ATOM    712  C4* DG     23       2.460  10.202   7.227
ATOM    713  H4* DG     23       3.292  10.274   7.931
ATOM    714  O4* DG     23       2.122   8.827   7.065
ATOM    715  C1* DG     23       2.542   8.418   5.776
ATOM    716  H1* DG     23       3.594   8.116   5.807
ATOM    717  N9  DG     23       1.714   7.289   5.292
ATOM    718  C8  DG     23       0.379   7.277   4.964
ATOM    719  H8  DG     23      -0.244   8.159   5.053
ATOM    720  N7  DG     23      -0.066   6.117   4.555
ATOM    721  C5  DG     23       1.071   5.295   4.604
ATOM    722  C6  DG     23       1.265   3.904   4.276
ATOM    723  O6  DG     23       0.447   3.075   3.875
ATOM    724  N1  DG     23       2.566   3.474   4.443
ATOM    725  H1  DG     23       2.766   2.511   4.222
ATOM    726  C2  DG     23       3.573   4.271   4.875
ATOM    727  N2  DG     23       4.772   3.759   4.901
ATOM    728 1H2  DG     23       5.522   4.349   5.215
ATOM    729 2H2  DG     23       4.924   2.786   4.650
ATOM    730  N3  DG     23       3.442   5.552   5.203
ATOM    731  C4  DG     23       2.163   6.011   5.048
ATOM    732  C3* DG     23       2.925  10.751   5.866
ATOM    733  H3* DG     23       2.460  11.715   5.646
ATOM    734  C2* DG     23       2.415   9.670   4.914
ATOM    735 1H2* DG     23       1.370   9.870   4.676
ATOM    736 2H2* DG     23       3.000   9.600   4.000
ATOM    737  O3* DG     23       4.345  10.876   5.889
ATOM    738  P   DC3    24       5.216  11.402   4.635
ATOM    739  O1P DC3    24       6.324  12.236   5.166
ATOM    740  O2P DC3    24       4.313  11.982   3.610
ATOM    741  O5* DC3    24       5.840  10.036   4.050
ATOM    742  C5* DC3    24       6.752   9.263   4.826
ATOM    743 1H5* DC3    24       6.264   8.943   5.748
ATOM    744 2H5* DC3    24       7.609   9.881   5.096
ATOM    745  C4* DC3    24       7.274   8.015   4.096
ATOM    746  H4* DC3    24       8.029   7.549   4.731
ATOM    747  O4* DC3    24       6.205   7.094   3.903
ATOM    748  C1* DC3    24       6.216   6.662   2.554
ATOM    749  H1* DC3    24       6.871   5.789   2.468
ATOM    750  N1  DC3    24       4.832   6.331   2.120
ATOM    751  C6  DC3    24       3.833   7.271   2.181
ATOM    752  H6  DC3    24       4.071   8.267   2.540
ATOM    753  C5  DC3    24       2.568   6.944   1.813
ATOM    754  H5  DC3    24       1.781   7.680   1.869
ATOM    755  C4  DC3    24       2.343   5.610   1.379
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ATOM    756  N4  DC3    24       1.148   5.208   1.061
ATOM    757 1H4  DC3    24       0.370   5.840   1.134
ATOM    758 2H4  DC3    24       1.033   4.232   0.809
ATOM    759  N3  DC3    24       3.286   4.696   1.305
ATOM    760  C2  DC3    24       4.547   5.040   1.659
ATOM    761  O2  DC3    24       5.414   4.172   1.549
ATOM    762  C3* DC3    24       7.903   8.312   2.722
ATOM    763  H3* DC3    24       8.077   9.382   2.589
ATOM    764  C2* DC3    24       6.840   7.808   1.753
ATOM    765 1H2* DC3    24       6.118   8.605   1.566
ATOM    766 2H2* DC3    24       7.261   7.457   0.811
ATOM    767  O3* DC3    24       9.108   7.571   2.546
ATOM    768  H3T DC3    24       9.525   7.817   1.694
TER
END
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