



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 26, 2014 – 10:49 PM GMT

PDB ID : 2EX5  
Title : Group I Intron-encoded Homing Endonuclease I-CeuI Complexed With DNA  
Authors : Spiegel, P.C.; Stoddard, B.L.  
Deposited on : 2005-11-07  
Resolution : 2.20 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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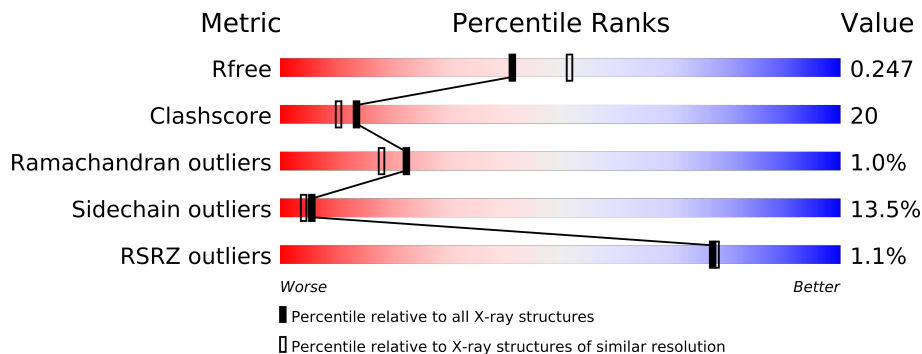
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance





The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 66092                       | 2938 (2.20-2.20)                                      |
| Clashscore            | 79885                       | 3751 (2.20-2.20)                                      |
| Ramachandran outliers | 78287                       | 3681 (2.20-2.20)                                      |
| Sidechain outliers    | 78261                       | 3682 (2.20-2.20)                                      |
| RSRZ outliers         | 66119                       | 2939 (2.20-2.20)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 1   | X     | 26     |  |
| 2   | Y     | 26     |  |
| 3   | A     | 207    |  |
| 3   | B     | 207    |  |

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4664 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a DNA chain called I-CeuI DNA target site.

| Mol | Chain | Residues | Atoms |     |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 1   | X     | 26       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 535   | 254 | 106 | 150 | 25 |         |         |       |

- Molecule 2 is a DNA chain called I-CeuI DNA target site, complimentary strand.

| Mol | Chain | Residues | Atoms |     |    |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|---------|-------|
| 2   | Y     | 26       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 525   | 252 | 90 | 158 | 25 |         |         |       |

- Molecule 3 is a protein called DNA endonuclease I-CeuI.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3   | A     | 207      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1669  | 1071 | 286 | 311 | 1 |         |         |       |
| 3   | B     | 207      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1669  | 1071 | 286 | 311 | 1 |         |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment    | Reference  |
|-------|---------|----------|--------|------------|------------|
| A     | 93      | ARG      | GLN    | ENGINEERED | UNP P32761 |
| B     | 93      | ARG      | GLN    | ENGINEERED | UNP P32761 |

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 4   | X     | 1        | Total | Ca | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 4   | B     | 1        | Total | Ca | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 4   | A     | 1        | Total | Ca | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 5 is water.

| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 5   | A     | 118      | Total<br>118 | O<br>118 | 0       | 0       |
| 5   | B     | 78       | Total<br>78  | O<br>78  | 0       | 0       |
| 5   | X     | 27       | Total<br>27  | O<br>27  | 0       | 0       |
| 5   | Y     | 40       | Total<br>40  | O<br>40  | 0       | 0       |

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: I-CeuI DNA target site

Chain X: 

G601 G602 A603 T604 A605 A606 C607 G608 G609 T610 G611 G612 T613 A614 A615 G616 G617 T618 A619 G620 G621 A623 A624 G625 G626

- Molecule 2: I-CeuI DNA target site, complimentary strand

Chain Y: 

G701 C702 T703 T704 C705 G706 C707 T708 A709 C710 C711 C712 T713 A714 G715 G716 A717 C718 C719 G720 T721 A722 A723 T724 C725 C726

- Molecule 3: DNA endonuclease I-CeuI

Chain A: 

I5 L12 P13 Q14 D15 E16 T23 A26 V27 K28 K31 K32 F33 D39 R41 L43 D47 E48 Q50 E54 L57 G61 N70 I71 K74 K75 L76 A77 T78 L83 N90 V91 T92 A93 H94 N96 G97 V98 L101 Y102 L103 E106 E107 F108 K109 K116 T122 V124 L125 T126 T127 D128 N129 R130 Q131 S132 L133 E134 K136 P139 F140 Q143 V144 V146 K153 V154 K155 K161 A162 L163 L164 E165 L166 F167 N168 H169 D170 A171 Q173 D174 L175 Q177 L178 V179 N180 K181 L182 L183 P184 I185 Q188 M189 R190 K191 S196 N197 Q207 R211

- Molecule 3: DNA endonuclease I-CeuI

Chain B: 

I5 L6 K7 E10 Q14 L17 L20 K21 K22 V27 K28 K31 Q45 V49 Q50 S53 L57 F58 L59 F62 N70 T73 L76 S79 K80 F81 G82 V85 N90 R93 H94 N95 N96 G97 V98 L101 Y102 L103 A104 L105 E106 R114 K116 A121 T122 L123 V124 L125 T126 T127 L133 K136 Y144 V145 S149 K153 V154 K155 R156 L164 E165 L166 F167 A171 H172 Q173 D174 L175 E176 Q177 L178 V179 I182 L183 P184 I185 W186 D187 Q188 K191 Q192 Q195 S196 N197 E198 P201 N202 L203 E204 A205 A206 Q207 D208 F209 A210 R211

## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 21 21 21  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 50.23Å 69.18Å 169.41Å<br>90.00° 90.00° 90.00°               | Depositor        |
| Resolution (Å)  | 20.00 – 2.20<br>19.83 – 2.20                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 96.0 (20.00-2.20)<br>96.4 (19.83-2.20)                      | Depositor<br>EDS |
| $R_{merge}$   | 0.08  | Depositor        |
| $R_{sym}$   | 0.08  | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 3.10 (at 2.21Å)   | Xtriage          |
| Refinement program  | CNS   | Depositor        |
| R, $R_{free}$   | 0.219 , 0.231<br>0.237 , 0.247                              | Depositor<br>DCC |
| $R_{free}$ test set   | 2959 reflections (10.00%)                                   | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 37.7  | Xtriage          |
| Anisotropy  | 0.445   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.33 , 42.9   | EDS              |
| Estimated twinning fraction   | No twinning to report.                                      | Xtriage          |
| L-test for twinning   | $\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$ | Xtriage          |
| Outliers  | 0 of 30529 reflections                                      | Xtriage          |
| $F_o, F_c$ correlation  | 0.95  | EDS              |
| Total number of atoms   | 4664  | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 43.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.70% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section:  
CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths |                | Bond angles |                 |
|-----|-------|--------------|----------------|-------------|-----------------|
|     |       | RMSZ         | # $ Z  > 5$    | RMSZ        | # $ Z  > 5$     |
| 1   | X     | 2.23         | 24/602 (4.0%)  | 3.33        | 122/928 (13.1%) |
| 2   | Y     | 2.41         | 29/586 (4.9%)  | 3.54        | 135/902 (15.0%) |
| 3   | A     | 1.46         | 12/1697 (0.7%) | 1.21        | 9/2283 (0.4%)   |
| 3   | B     | 1.24         | 4/1697 (0.2%)  | 1.15        | 9/2283 (0.4%)   |
| All | All   | 1.66         | 69/4582 (1.5%) | 2.09        | 275/6396 (4.3%) |

All (69) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | X     | 606 | DA   | N7-C5   | 9.68  | 1.45        | 1.39     |
| 2   | Y     | 714 | DA   | N3-C4   | 9.52  | 1.40        | 1.34     |
| 1   | X     | 609 | DG   | C6-N1   | 8.65  | 1.45        | 1.39     |
| 2   | Y     | 701 | DG   | C8-N7   | 8.27  | 1.35        | 1.30     |
| 1   | X     | 618 | DT   | N1-C6   | 8.00  | 1.43        | 1.38     |
| 2   | Y     | 706 | DG   | N7-C5   | 7.96  | 1.44        | 1.39     |
| 1   | X     | 604 | DT   | C5-C7   | 7.92  | 1.54        | 1.50     |
| 1   | X     | 611 | DC   | C2-N3   | 7.88  | 1.42        | 1.35     |
| 3   | A     | 91  | VAL  | CB-CG1  | 7.84  | 1.69        | 1.52     |
| 2   | Y     | 721 | DT   | N3-C4   | -7.42 | 1.32        | 1.38     |
| 3   | A     | 140 | PHE  | CG-CD1  | 7.34  | 1.49        | 1.38     |
| 2   | Y     | 716 | DG   | O3'-P   | -7.23 | 1.52        | 1.61     |
| 2   | Y     | 714 | DA   | N1-C2   | 7.22  | 1.40        | 1.34     |
| 1   | X     | 611 | DC   | C2-O2   | 7.21  | 1.30        | 1.24     |
| 1   | X     | 606 | DA   | N9-C8   | 7.12  | 1.43        | 1.37     |
| 2   | Y     | 704 | DT   | C1'-N1  | 7.10  | 1.58        | 1.49     |
| 2   | Y     | 701 | DG   | C6-N1   | 7.09  | 1.44        | 1.39     |
| 2   | Y     | 720 | DG   | C5-C4   | -7.03 | 1.33        | 1.38     |
| 3   | B     | 106 | GLU  | CG-CD   | -6.99 | 1.41        | 1.51     |
| 2   | Y     | 714 | DA   | C2-N3   | 6.91  | 1.39        | 1.33     |
| 2   | Y     | 716 | DG   | C3'-O3' | 6.84  | 1.52        | 1.44     |
| 3   | B     | 191 | LYS  | CE-NZ   | 6.80  | 1.66        | 1.49     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | Y     | 707 | DC   | N3-C4   | 6.54  | 1.38        | 1.33     |
| 2   | Y     | 708 | DT   | C5-C7   | 6.50  | 1.53        | 1.50     |
| 1   | X     | 626 | DC   | C1'-N1  | 6.48  | 1.57        | 1.49     |
| 2   | Y     | 718 | DC   | C1'-N1  | 6.46  | 1.57        | 1.49     |
| 1   | X     | 612 | DC   | C3'-O3' | -6.43 | 1.35        | 1.44     |
| 1   | X     | 612 | DC   | C4-C5   | 6.42  | 1.48        | 1.43     |
| 3   | A     | 134 | GLU  | CB-CG   | -6.39 | 1.40        | 1.52     |
| 1   | X     | 609 | DG   | C2-N2   | 6.31  | 1.40        | 1.34     |
| 3   | A     | 140 | PHE  | CE2-CZ  | 6.25  | 1.49        | 1.37     |
| 2   | Y     | 702 | DC   | C3'-O3' | -6.22 | 1.35        | 1.44     |
| 1   | X     | 611 | DC   | N1-C6   | 6.09  | 1.40        | 1.37     |
| 2   | Y     | 708 | DT   | N1-C6   | -6.09 | 1.33        | 1.38     |
| 1   | X     | 609 | DG   | N7-C5   | 6.08  | 1.42        | 1.39     |
| 1   | X     | 607 | DC   | N1-C6   | -5.98 | 1.33        | 1.37     |
| 2   | Y     | 718 | DC   | C5-C6   | 5.92  | 1.39        | 1.34     |
| 3   | A     | 165 | GLU  | CG-CD   | 5.87  | 1.60        | 1.51     |
| 2   | Y     | 716 | DG   | C6-N1   | 5.78  | 1.43        | 1.39     |
| 2   | Y     | 710 | DC   | C2-N3   | 5.70  | 1.40        | 1.35     |
| 3   | A     | 98  | VAL  | CB-CG1  | 5.69  | 1.64        | 1.52     |
| 1   | X     | 614 | DA   | N7-C5   | 5.59  | 1.42        | 1.39     |
| 3   | A     | 26  | ALA  | CA-CB   | 5.55  | 1.64        | 1.52     |
| 1   | X     | 609 | DG   | C2-N3   | 5.50  | 1.37        | 1.32     |
| 2   | Y     | 713 | DT   | C1'-N1  | 5.45  | 1.56        | 1.49     |
| 2   | Y     | 716 | DG   | C5'-C4' | 5.45  | 1.57        | 1.51     |
| 2   | Y     | 719 | DC   | C1'-N1  | 5.43  | 1.56        | 1.49     |
| 2   | Y     | 715 | DG   | N7-C5   | 5.41  | 1.42        | 1.39     |
| 1   | X     | 606 | DA   | O4'-C1' | 5.39  | 1.48        | 1.42     |
| 2   | Y     | 716 | DG   | C4'-C3' | -5.37 | 1.47        | 1.52     |
| 3   | A     | 140 | PHE  | CE1-CZ  | 5.33  | 1.47        | 1.37     |
| 1   | X     | 616 | DG   | P-OP2   | 5.33  | 1.58        | 1.49     |
| 3   | B     | 7   | LYS  | CD-CE   | 5.31  | 1.64        | 1.51     |
| 2   | Y     | 717 | DA   | C3'-C2' | 5.26  | 1.58        | 1.52     |
| 3   | A     | 161 | LYS  | CE-NZ   | 5.24  | 1.62        | 1.49     |
| 2   | Y     | 704 | DT   | N1-C2   | 5.24  | 1.42        | 1.38     |
| 3   | A     | 91  | VAL  | CB-CG2  | -5.22 | 1.41        | 1.52     |
| 2   | Y     | 701 | DG   | N9-C8   | 5.21  | 1.41        | 1.37     |
| 3   | A     | 33  | PHE  | CD1-CE1 | 5.20  | 1.49        | 1.39     |
| 1   | X     | 601 | DC   | C2-N3   | 5.14  | 1.39        | 1.35     |
| 3   | A     | 155 | LYS  | CD-CE   | 5.12  | 1.64        | 1.51     |
| 1   | X     | 611 | DC   | N3-C4   | 5.09  | 1.37        | 1.33     |
| 1   | X     | 607 | DC   | N3-C4   | -5.06 | 1.30        | 1.33     |
| 1   | X     | 613 | DT   | N1-C2   | 5.06  | 1.42        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | X     | 607 | DC   | C3'-O3' | -5.06 | 1.37        | 1.44     |
| 2   | Y     | 717 | DA   | N7-C5   | 5.06  | 1.42        | 1.39     |
| 3   | B     | 62  | PHE  | CE1-CZ  | 5.05  | 1.47        | 1.37     |
| 2   | Y     | 714 | DA   | C3'-C2' | 5.04  | 1.58        | 1.52     |
| 1   | X     | 616 | DG   | N1-C2   | -5.00 | 1.33        | 1.37     |

All (275) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 2   | Y     | 708 | DT   | C6-C5-C7    | -16.84 | 112.80      | 122.90   |
| 1   | X     | 607 | DC   | O4'-C1'-N1  | 16.67  | 119.67      | 108.00   |
| 1   | X     | 601 | DC   | O4'-C1'-N1  | -15.76 | 96.97       | 108.00   |
| 2   | Y     | 704 | DT   | O4'-C1'-N1  | 12.31  | 116.62      | 108.00   |
| 1   | X     | 603 | DA   | O4'-C1'-N9  | 12.20  | 116.54      | 108.00   |
| 2   | Y     | 715 | DG   | C5-C6-N1    | 12.16  | 117.58      | 111.50   |
| 1   | X     | 613 | DT   | C6-C5-C7    | -12.03 | 115.68      | 122.90   |
| 2   | Y     | 704 | DT   | N3-C2-O2    | -12.03 | 115.08      | 122.30   |
| 1   | X     | 604 | DT   | N3-C2-O2    | -11.99 | 115.11      | 122.30   |
| 2   | Y     | 718 | DC   | N1-C2-O2    | -11.59 | 111.95      | 118.90   |
| 1   | X     | 602 | DG   | N3-C2-N2    | -11.27 | 112.01      | 119.90   |
| 2   | Y     | 701 | DG   | N3-C4-N9    | -11.17 | 119.30      | 126.00   |
| 1   | X     | 615 | DA   | P-O5'-C5'   | -10.75 | 103.70      | 120.90   |
| 1   | X     | 607 | DC   | O5'-P-OP1   | -10.75 | 96.03       | 105.70   |
| 2   | Y     | 724 | DT   | C6-C5-C7    | -10.74 | 116.45      | 122.90   |
| 2   | Y     | 708 | DT   | C4-C5-C7    | 10.66  | 125.40      | 119.00   |
| 2   | Y     | 709 | DA   | N1-C2-N3    | -10.66 | 123.97      | 129.30   |
| 2   | Y     | 720 | DG   | P-O3'-C3'   | 10.32  | 132.09      | 119.70   |
| 2   | Y     | 715 | DG   | C5-C6-O6    | -10.28 | 122.43      | 128.60   |
| 2   | Y     | 721 | DT   | C5-C6-N1    | -10.04 | 117.67      | 123.70   |
| 2   | Y     | 726 | DG   | O4'-C1'-N9  | 10.00  | 115.00      | 108.00   |
| 2   | Y     | 726 | DG   | N1-C6-O6    | -9.89  | 113.96      | 119.90   |
| 2   | Y     | 713 | DT   | C6-C5-C7    | -9.88  | 116.97      | 122.90   |
| 1   | X     | 614 | DA   | C5-C6-N6    | 9.80   | 131.54      | 123.70   |
| 2   | Y     | 716 | DG   | C2-N3-C4    | 9.67   | 116.73      | 111.90   |
| 2   | Y     | 716 | DG   | O4'-C1'-C2' | -9.66  | 98.17       | 105.90   |
| 2   | Y     | 703 | DT   | N3-C4-O4    | 9.62   | 125.67      | 119.90   |
| 1   | X     | 606 | DA   | O4'-C1'-C2' | -9.54  | 98.26       | 105.90   |
| 2   | Y     | 723 | DA   | C5'-C4'-C3' | -9.46  | 97.07       | 114.10   |
| 2   | Y     | 722 | DT   | P-O3'-C3'   | 9.45   | 131.04      | 119.70   |
| 1   | X     | 608 | DG   | P-O3'-C3'   | 9.39   | 130.97      | 119.70   |
| 2   | Y     | 710 | DC   | O4'-C1'-N1  | 9.25   | 114.48      | 108.00   |
| 1   | X     | 609 | DG   | C2-N3-C4    | 9.24   | 116.52      | 111.90   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | X     | 618 | DT   | O4'-C4'-C3' | -9.21 | 100.47      | 106.00   |
| 1   | X     | 623 | DA   | O4'-C4'-C3' | -9.15 | 100.51      | 106.00   |
| 1   | X     | 622 | DG   | N3-C2-N2    | -9.14 | 113.50      | 119.90   |
| 1   | X     | 612 | DC   | O4'-C1'-N1  | 9.11  | 114.38      | 108.00   |
| 1   | X     | 617 | DG   | O4'-C1'-C2' | -9.07 | 98.64       | 105.90   |
| 2   | Y     | 716 | DG   | N3-C2-N2    | -9.05 | 113.56      | 119.90   |
| 2   | Y     | 714 | DA   | P-O3'-C3'   | 9.04  | 130.54      | 119.70   |
| 1   | X     | 602 | DG   | N1-C6-O6    | 8.97  | 125.28      | 119.90   |
| 1   | X     | 613 | DT   | O4'-C1'-N1  | 8.96  | 114.28      | 108.00   |
| 2   | Y     | 704 | DT   | O4'-C1'-C2' | -8.93 | 98.75       | 105.90   |
| 2   | Y     | 715 | DG   | C5'-C4'-O4' | -8.86 | 92.46       | 109.30   |
| 2   | Y     | 716 | DG   | C5-C6-O6    | -8.76 | 123.34      | 128.60   |
| 2   | Y     | 712 | DT   | N3-C4-O4    | 8.72  | 125.14      | 119.90   |
| 1   | X     | 609 | DG   | N1-C6-O6    | -8.64 | 114.71      | 119.90   |
| 1   | X     | 614 | DA   | C5'-C4'-C3' | -8.64 | 98.54       | 114.10   |
| 2   | Y     | 716 | DG   | C8-N9-C4    | -8.63 | 102.95      | 106.40   |
| 1   | X     | 614 | DA   | N1-C6-N6    | -8.57 | 113.46      | 118.60   |
| 2   | Y     | 712 | DT   | C5-C4-O4    | -8.48 | 118.96      | 124.90   |
| 1   | X     | 602 | DG   | O4'-C1'-N9  | 8.48  | 113.94      | 108.00   |
| 2   | Y     | 716 | DG   | N1-C2-N2    | 8.46  | 123.82      | 116.20   |
| 1   | X     | 604 | DT   | P-O3'-C3'   | 8.42  | 129.80      | 119.70   |
| 2   | Y     | 724 | DT   | C4-C5-C7    | 8.34  | 124.00      | 119.00   |
| 2   | Y     | 703 | DT   | C5-C4-O4    | -8.31 | 119.08      | 124.90   |
| 2   | Y     | 701 | DG   | N9-C4-C5    | 8.27  | 108.71      | 105.40   |
| 2   | Y     | 715 | DG   | O5'-P-OP1   | -8.27 | 98.26       | 105.70   |
| 2   | Y     | 713 | DT   | O4'-C1'-N1  | 8.23  | 113.76      | 108.00   |
| 2   | Y     | 717 | DA   | O4'-C1'-N9  | 8.22  | 113.75      | 108.00   |
| 2   | Y     | 705 | DC   | N3-C4-N4    | -8.19 | 112.26      | 118.00   |
| 1   | X     | 611 | DC   | OP1-P-OP2   | 8.16  | 131.84      | 119.60   |
| 1   | X     | 606 | DA   | C5-N7-C8    | -7.96 | 99.92       | 103.90   |
| 2   | Y     | 721 | DT   | O4'-C1'-C2' | 7.95  | 112.26      | 105.90   |
| 1   | X     | 615 | DA   | O4'-C1'-N9  | -7.87 | 102.49      | 108.00   |
| 2   | Y     | 712 | DT   | O4'-C1'-N1  | -7.83 | 102.52      | 108.00   |
| 1   | X     | 611 | DC   | O5'-P-OP2   | -7.82 | 98.66       | 105.70   |
| 2   | Y     | 715 | DG   | P-O5'-C5'   | 7.82  | 133.41      | 120.90   |
| 1   | X     | 618 | DT   | P-O5'-C5'   | 7.79  | 133.36      | 120.90   |
| 1   | X     | 605 | DA   | O3'-P-O5'   | 7.77  | 118.77      | 104.00   |
| 2   | Y     | 709 | DA   | C2-N3-C4    | 7.76  | 114.48      | 110.60   |
| 2   | Y     | 715 | DG   | C6-N1-C2    | -7.76 | 120.44      | 125.10   |
| 1   | X     | 620 | DG   | N3-C2-N2    | -7.75 | 114.48      | 119.90   |
| 1   | X     | 609 | DG   | O4'-C1'-N9  | 7.74  | 113.42      | 108.00   |
| 2   | Y     | 726 | DG   | N9-C4-C5    | 7.73  | 108.49      | 105.40   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | Y     | 722 | DT   | N3-C2-O2    | -7.68 | 117.69      | 122.30   |
| 1   | X     | 617 | DG   | O4'-C1'-N9  | -7.68 | 102.63      | 108.00   |
| 2   | Y     | 714 | DA   | O3'-P-O5'   | 7.67  | 118.58      | 104.00   |
| 1   | X     | 618 | DT   | O4'-C1'-N1  | 7.67  | 113.37      | 108.00   |
| 2   | Y     | 706 | DG   | N1-C6-O6    | -7.61 | 115.33      | 119.90   |
| 2   | Y     | 724 | DT   | O4'-C1'-N1  | -7.61 | 102.67      | 108.00   |
| 2   | Y     | 701 | DG   | C8-N9-C1'   | 7.60  | 136.88      | 127.00   |
| 1   | X     | 602 | DG   | C5-C6-O6    | -7.59 | 124.05      | 128.60   |
| 3   | B     | 156 | ARG  | NE-CZ-NH2   | -7.57 | 116.52      | 120.30   |
| 2   | Y     | 716 | DG   | C6-N1-C2    | -7.56 | 120.56      | 125.10   |
| 2   | Y     | 719 | DC   | N3-C4-C5    | -7.51 | 118.89      | 121.90   |
| 2   | Y     | 718 | DC   | P-O5'-C5'   | 7.42  | 132.77      | 120.90   |
| 1   | X     | 613 | DT   | C4-C5-C7    | 7.41  | 123.44      | 119.00   |
| 1   | X     | 619 | DA   | N1-C2-N3    | -7.41 | 125.60      | 129.30   |
| 1   | X     | 606 | DA   | C1'-O4'-C4' | -7.38 | 102.72      | 110.10   |
| 2   | Y     | 715 | DG   | N3-C4-N9    | 7.35  | 130.41      | 126.00   |
| 2   | Y     | 726 | DG   | C5-C6-O6    | 7.33  | 133.00      | 128.60   |
| 1   | X     | 611 | DC   | C5-C6-N1    | 7.30  | 124.65      | 121.00   |
| 1   | X     | 609 | DG   | C5-C6-N1    | 7.29  | 115.15      | 111.50   |
| 1   | X     | 613 | DT   | N3-C2-O2    | -7.28 | 117.93      | 122.30   |
| 2   | Y     | 705 | DC   | C5-C4-N4    | 7.25  | 125.28      | 120.20   |
| 2   | Y     | 705 | DC   | C6-N1-C1'   | 7.25  | 129.50      | 120.80   |
| 3   | B     | 98  | VAL  | CB-CA-C     | -7.22 | 97.68       | 111.40   |
| 2   | Y     | 711 | DC   | P-O3'-C3'   | 7.19  | 128.33      | 119.70   |
| 2   | Y     | 715 | DG   | N9-C4-C5    | -7.17 | 102.53      | 105.40   |
| 1   | X     | 618 | DT   | C5-C6-N1    | -7.15 | 119.41      | 123.70   |
| 2   | Y     | 723 | DA   | P-O5'-C5'   | -7.12 | 109.50      | 120.90   |
| 2   | Y     | 715 | DG   | O4'-C1'-C2' | 7.12  | 111.60      | 105.90   |
| 2   | Y     | 719 | DC   | C2-N3-C4    | 7.12  | 123.46      | 119.90   |
| 2   | Y     | 705 | DC   | C2-N1-C1'   | -7.00 | 111.10      | 118.80   |
| 2   | Y     | 721 | DT   | C4-C5-C6    | 6.94  | 122.17      | 118.00   |
| 3   | B     | 156 | ARG  | NE-CZ-NH1   | 6.94  | 123.77      | 120.30   |
| 1   | X     | 607 | DC   | O5'-P-OP2   | 6.93  | 119.02      | 110.70   |
| 1   | X     | 602 | DG   | N1-C2-N2    | 6.93  | 122.44      | 116.20   |
| 2   | Y     | 716 | DG   | P-O5'-C5'   | 6.92  | 131.96      | 120.90   |
| 2   | Y     | 701 | DG   | O4'-C4'-C3' | -6.85 | 101.76      | 104.50   |
| 2   | Y     | 709 | DA   | O4'-C1'-C2' | -6.83 | 100.44      | 105.90   |
| 2   | Y     | 720 | DG   | O4'-C1'-C2' | 6.83  | 111.36      | 105.90   |
| 1   | X     | 605 | DA   | O4'-C1'-N9  | -6.82 | 103.22      | 108.00   |
| 1   | X     | 610 | DT   | N3-C2-O2    | -6.80 | 118.22      | 122.30   |
| 2   | Y     | 707 | DC   | C4-C5-C6    | 6.79  | 120.80      | 117.40   |
| 2   | Y     | 701 | DG   | N3-C4-C5    | 6.79  | 132.00      | 128.60   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | X     | 609 | DG   | C6-C5-N7    | 6.76  | 134.46      | 130.40   |
| 2   | Y     | 716 | DG   | C5-C6-N1    | 6.73  | 114.86      | 111.50   |
| 2   | Y     | 716 | DG   | O4'-C4'-C3' | -6.68 | 101.83      | 104.50   |
| 1   | X     | 620 | DG   | P-O3'-C3'   | 6.56  | 127.57      | 119.70   |
| 3   | B     | 133 | LEU  | CA-CB-CG    | 6.55  | 130.36      | 115.30   |
| 1   | X     | 610 | DT   | C6-C5-C7    | -6.52 | 118.99      | 122.90   |
| 2   | Y     | 702 | DC   | C6-N1-C2    | 6.51  | 122.91      | 120.30   |
| 2   | Y     | 714 | DA   | O4'-C4'-C3' | -6.51 | 101.90      | 104.50   |
| 1   | X     | 609 | DG   | N3-C2-N2    | 6.50  | 124.45      | 119.90   |
| 2   | Y     | 715 | DG   | C4-C5-N7    | 6.50  | 113.40      | 110.80   |
| 3   | B     | 105 | LEU  | CB-CG-CD1   | 6.50  | 122.05      | 111.00   |
| 2   | Y     | 704 | DT   | N1-C2-O2    | 6.47  | 128.27      | 123.10   |
| 1   | X     | 618 | DT   | C2-N3-C4    | -6.46 | 123.33      | 127.20   |
| 3   | A     | 12  | LEU  | CA-CB-CG    | 6.46  | 130.15      | 115.30   |
| 2   | Y     | 717 | DA   | O4'-C1'-C2' | -6.43 | 100.76      | 105.90   |
| 1   | X     | 615 | DA   | O4'-C4'-C3' | 6.42  | 109.85      | 106.00   |
| 2   | Y     | 712 | DT   | N1-C2-O2    | -6.40 | 117.98      | 123.10   |
| 1   | X     | 603 | DA   | P-O5'-C5'   | -6.38 | 110.70      | 120.90   |
| 2   | Y     | 716 | DG   | C5'-C4'-O4' | 6.37  | 121.40      | 109.30   |
| 2   | Y     | 719 | DC   | C6-N1-C2    | -6.32 | 117.77      | 120.30   |
| 2   | Y     | 720 | DG   | O4'-C1'-N9  | -6.28 | 103.60      | 108.00   |
| 1   | X     | 614 | DA   | C5'-C4'-O4' | -6.26 | 97.40       | 109.30   |
| 1   | X     | 607 | DC   | C4-C5-C6    | 6.24  | 120.52      | 117.40   |
| 1   | X     | 602 | DG   | O4'-C4'-C3' | -6.22 | 102.01      | 104.50   |
| 1   | X     | 614 | DA   | O5'-P-OP1   | -6.20 | 100.12      | 105.70   |
| 2   | Y     | 712 | DT   | P-O3'-C3'   | 6.16  | 127.10      | 119.70   |
| 1   | X     | 619 | DA   | OP1-P-OP2   | -6.16 | 110.36      | 119.60   |
| 2   | Y     | 710 | DC   | N1-C2-O2    | -6.14 | 115.22      | 118.90   |
| 1   | X     | 626 | DC   | N3-C2-O2    | -6.12 | 117.61      | 121.90   |
| 1   | X     | 606 | DA   | C4-C5-N7    | 6.11  | 113.76      | 110.70   |
| 1   | X     | 620 | DG   | C5-C6-O6    | -6.10 | 124.94      | 128.60   |
| 1   | X     | 609 | DG   | N1-C2-N3    | -6.10 | 120.24      | 123.90   |
| 2   | Y     | 721 | DT   | N3-C2-O2    | 6.08  | 125.95      | 122.30   |
| 1   | X     | 625 | DG   | C5-C6-O6    | -6.08 | 124.95      | 128.60   |
| 2   | Y     | 712 | DT   | N1-C2-N3    | 6.08  | 118.25      | 114.60   |
| 1   | X     | 604 | DT   | N1-C2-O2    | 6.07  | 127.95      | 123.10   |
| 1   | X     | 601 | DC   | P-O3'-C3'   | 6.05  | 126.96      | 119.70   |
| 2   | Y     | 703 | DT   | O4'-C1'-C2' | -6.03 | 101.08      | 105.90   |
| 2   | Y     | 704 | DT   | P-O3'-C3'   | 6.03  | 126.93      | 119.70   |
| 1   | X     | 609 | DG   | C4-C5-C6    | -6.02 | 115.19      | 118.80   |
| 1   | X     | 612 | DC   | C5-C4-N4    | 6.02  | 124.41      | 120.20   |
| 1   | X     | 605 | DA   | C5-C6-N1    | -6.01 | 114.69      | 117.70   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | Y     | 726 | DG   | O4'-C4'-C3' | 6.01  | 109.61      | 106.00   |
| 1   | X     | 614 | DA   | C5-N7-C8    | 6.01  | 106.91      | 103.90   |
| 3   | A     | 103 | LEU  | CA-CB-CG    | 6.01  | 129.11      | 115.30   |
| 1   | X     | 613 | DT   | O4'-C1'-C2' | -5.99 | 101.11      | 105.90   |
| 1   | X     | 617 | DG   | N1-C6-O6    | -5.97 | 116.32      | 119.90   |
| 1   | X     | 606 | DA   | OP1-P-O3'   | 5.96  | 118.32      | 105.20   |
| 1   | X     | 615 | DA   | O5'-P-OP2   | -5.94 | 100.35      | 105.70   |
| 2   | Y     | 720 | DG   | O5'-P-OP1   | -5.94 | 100.35      | 105.70   |
| 2   | Y     | 708 | DT   | O4'-C1'-N1  | -5.93 | 103.85      | 108.00   |
| 1   | X     | 612 | DC   | N3-C4-N4    | -5.92 | 113.85      | 118.00   |
| 1   | X     | 612 | DC   | C4'-C3'-C2' | 5.89  | 108.40      | 103.10   |
| 3   | A     | 57  | LEU  | CA-CB-CG    | 5.88  | 128.82      | 115.30   |
| 3   | B     | 95  | VAL  | CB-CA-C     | -5.88 | 100.23      | 111.40   |
| 2   | Y     | 702 | DC   | C4'-C3'-C2' | 5.86  | 108.38      | 103.10   |
| 1   | X     | 615 | DA   | O3'-P-O5'   | -5.84 | 92.90       | 104.00   |
| 2   | Y     | 704 | DT   | N3-C4-O4    | 5.83  | 123.40      | 119.90   |
| 2   | Y     | 715 | DG   | C1'-O4'-C4' | -5.83 | 104.27      | 110.10   |
| 1   | X     | 622 | DG   | C5-C6-O6    | -5.82 | 125.11      | 128.60   |
| 1   | X     | 625 | DG   | C5'-C4'-O4' | -5.81 | 98.27       | 109.30   |
| 1   | X     | 604 | DT   | O4'-C1'-N1  | 5.81  | 112.06      | 108.00   |
| 1   | X     | 612 | DC   | C2-N1-C1'   | -5.79 | 112.43      | 118.80   |
| 2   | Y     | 701 | DG   | C4-N9-C1'   | -5.79 | 118.98      | 126.50   |
| 1   | X     | 603 | DA   | N1-C2-N3    | -5.79 | 126.41      | 129.30   |
| 2   | Y     | 723 | DA   | C5-C6-N6    | 5.79  | 128.33      | 123.70   |
| 2   | Y     | 712 | DT   | C2-N3-C4    | -5.78 | 123.73      | 127.20   |
| 1   | X     | 618 | DT   | OP2-P-O3'   | 5.77  | 117.90      | 105.20   |
| 1   | X     | 615 | DA   | P-O3'-C3'   | 5.76  | 126.61      | 119.70   |
| 2   | Y     | 710 | DC   | N3-C2-O2    | 5.76  | 125.93      | 121.90   |
| 2   | Y     | 721 | DT   | C5'-C4'-C3' | -5.76 | 103.73      | 114.10   |
| 1   | X     | 610 | DT   | C2-N3-C4    | -5.76 | 123.75      | 127.20   |
| 2   | Y     | 701 | DG   | C8-N9-C4    | -5.76 | 104.10      | 106.40   |
| 2   | Y     | 706 | DG   | C2-N3-C4    | 5.76  | 114.78      | 111.90   |
| 3   | A     | 41  | ARG  | NE-CZ-NH1   | 5.75  | 123.18      | 120.30   |
| 2   | Y     | 721 | DT   | O4'-C4'-C3' | 5.75  | 109.45      | 106.00   |
| 1   | X     | 604 | DT   | C1'-O4'-C4' | -5.74 | 104.36      | 110.10   |
| 1   | X     | 606 | DA   | O5'-P-OP1   | -5.73 | 100.54      | 105.70   |
| 3   | A     | 164 | LEU  | CA-CB-CG    | 5.72  | 128.46      | 115.30   |
| 1   | X     | 616 | DG   | O4'-C1'-N9  | 5.71  | 112.00      | 108.00   |
| 1   | X     | 613 | DT   | C4'-C3'-C2' | -5.70 | 97.97       | 103.10   |
| 1   | X     | 614 | DA   | C6-C5-N7    | 5.70  | 136.29      | 132.30   |
| 2   | Y     | 723 | DA   | N1-C6-N6    | -5.69 | 115.19      | 118.60   |
| 1   | X     | 614 | DA   | N7-C8-N9    | -5.66 | 110.97      | 113.80   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | X     | 612 | DC   | C6-N1-C1'   | 5.66  | 127.59      | 120.80   |
| 2   | Y     | 721 | DT   | C2-N1-C1'   | -5.65 | 109.15      | 118.20   |
| 1   | X     | 614 | DA   | N3-C4-N9    | -5.65 | 122.88      | 127.40   |
| 2   | Y     | 705 | DC   | C4'-C3'-C2' | 5.64  | 108.18      | 103.10   |
| 2   | Y     | 716 | DG   | C1'-O4'-C4' | 5.63  | 115.73      | 110.10   |
| 1   | X     | 611 | DC   | N1-C2-N3    | -5.62 | 115.26      | 119.20   |
| 1   | X     | 623 | DA   | C3'-C2'-C1' | -5.61 | 95.77       | 102.50   |
| 2   | Y     | 719 | DC   | O4'-C1'-N1  | -5.60 | 104.08      | 108.00   |
| 3   | B     | 136 | LYS  | CD-CE-NZ    | 5.59  | 124.56      | 111.70   |
| 1   | X     | 606 | DA   | O3'-P-O5'   | -5.59 | 93.38       | 104.00   |
| 2   | Y     | 718 | DC   | O4'-C1'-C2' | 5.58  | 110.36      | 105.90   |
| 1   | X     | 625 | DG   | O4'-C1'-N9  | 5.58  | 111.91      | 108.00   |
| 1   | X     | 604 | DT   | C5-C6-N1    | -5.56 | 120.36      | 123.70   |
| 1   | X     | 618 | DT   | N3-C4-C5    | 5.55  | 118.53      | 115.20   |
| 2   | Y     | 706 | DG   | N1-C2-N3    | -5.55 | 120.57      | 123.90   |
| 2   | Y     | 718 | DC   | C2-N3-C4    | -5.55 | 117.13      | 119.90   |
| 1   | X     | 621 | DC   | C6-N1-C2    | 5.54  | 122.51      | 120.30   |
| 2   | Y     | 721 | DT   | C6-C5-C7    | -5.53 | 119.58      | 122.90   |
| 3   | B     | 27  | VAL  | CB-CA-C     | -5.53 | 100.90      | 111.40   |
| 1   | X     | 616 | DG   | P-O5'-C5'   | 5.52  | 129.74      | 120.90   |
| 2   | Y     | 712 | DT   | N1-C1'-C2'  | 5.51  | 123.08      | 112.60   |
| 2   | Y     | 703 | DT   | O4'-C1'-N1  | -5.49 | 104.16      | 108.00   |
| 2   | Y     | 710 | DC   | OP1-P-OP2   | -5.49 | 111.37      | 119.60   |
| 2   | Y     | 719 | DC   | C5-C6-N1    | 5.48  | 123.74      | 121.00   |
| 1   | X     | 610 | DT   | N1-C2-N3    | 5.47  | 117.88      | 114.60   |
| 1   | X     | 619 | DA   | C2-N3-C4    | 5.47  | 113.33      | 110.60   |
| 3   | A     | 164 | LEU  | CB-CG-CD1   | 5.46  | 120.28      | 111.00   |
| 1   | X     | 605 | DA   | P-O3'-C3'   | 5.45  | 126.25      | 119.70   |
| 2   | Y     | 726 | DG   | C8-N9-C4    | -5.45 | 104.22      | 106.40   |
| 2   | Y     | 724 | DT   | OP1-P-O3'   | 5.42  | 117.12      | 105.20   |
| 2   | Y     | 719 | DC   | C5-C4-N4    | 5.41  | 123.99      | 120.20   |
| 1   | X     | 614 | DA   | C5-C6-N1    | -5.41 | 115.00      | 117.70   |
| 1   | X     | 624 | DA   | C3'-C2'-C1' | -5.40 | 96.02       | 102.50   |
| 1   | X     | 626 | DC   | C6-N1-C2    | -5.39 | 118.14      | 120.30   |
| 3   | A     | 131 | GLN  | CA-CB-CG    | 5.37  | 125.20      | 113.40   |
| 1   | X     | 622 | DG   | C6-N1-C2    | -5.36 | 121.88      | 125.10   |
| 1   | X     | 614 | DA   | N3-C4-C5    | 5.36  | 130.55      | 126.80   |
| 2   | Y     | 721 | DT   | N1-C2-O2    | -5.35 | 118.82      | 123.10   |
| 2   | Y     | 705 | DC   | N1-C1'-C2'  | 5.33  | 122.73      | 112.60   |
| 3   | A     | 74  | LYS  | CD-CE-NZ    | -5.33 | 99.44       | 111.70   |
| 2   | Y     | 721 | DT   | C6-N1-C2    | 5.32  | 123.96      | 121.30   |
| 1   | X     | 618 | DT   | N3-C4-O4    | -5.31 | 116.71      | 119.90   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | X     | 614 | DA   | C6-N1-C2    | 5.31  | 121.78      | 118.60   |
| 2   | Y     | 720 | DG   | OP2-P-O3'   | 5.31  | 116.88      | 105.20   |
| 2   | Y     | 707 | DC   | C2-N3-C4    | -5.28 | 117.26      | 119.90   |
| 1   | X     | 625 | DG   | P-O5'-C5'   | -5.28 | 112.46      | 120.90   |
| 3   | B     | 187 | ASP  | CB-CG-OD2   | -5.27 | 113.56      | 118.30   |
| 1   | X     | 606 | DA   | C6-C5-N7    | -5.26 | 128.61      | 132.30   |
| 2   | Y     | 719 | DC   | OP2-P-O3'   | 5.24  | 116.74      | 105.20   |
| 2   | Y     | 726 | DG   | C4-C5-N7    | -5.24 | 108.70      | 110.80   |
| 1   | X     | 619 | DA   | C6-N1-C2    | 5.24  | 121.74      | 118.60   |
| 1   | X     | 621 | DC   | O4'-C1'-C2' | -5.24 | 101.71      | 105.90   |
| 2   | Y     | 723 | DA   | OP1-P-OP2   | 5.22  | 127.43      | 119.60   |
| 2   | Y     | 718 | DC   | O5'-P-OP2   | -5.22 | 101.00      | 105.70   |
| 2   | Y     | 721 | DT   | C4'-C3'-C2' | 5.18  | 107.77      | 103.10   |
| 2   | Y     | 723 | DA   | C5'-C4'-O4' | 5.18  | 119.14      | 109.30   |
| 1   | X     | 608 | DG   | C8-N9-C4    | -5.17 | 104.33      | 106.40   |
| 2   | Y     | 717 | DA   | N1-C6-N6    | -5.17 | 115.50      | 118.60   |
| 2   | Y     | 720 | DG   | N7-C8-N9    | -5.17 | 110.52      | 113.10   |
| 1   | X     | 621 | DC   | C1'-O4'-C4' | -5.16 | 104.94      | 110.10   |
| 1   | X     | 613 | DT   | OP1-P-O3'   | 5.16  | 116.55      | 105.20   |
| 2   | Y     | 718 | DC   | N1-C1'-C2'  | 5.15  | 122.39      | 112.60   |
| 1   | X     | 602 | DG   | P-O3'-C3'   | -5.15 | 113.53      | 119.70   |
| 3   | A     | 134 | GLU  | OE1-CD-OE2  | 5.14  | 129.47      | 123.30   |
| 2   | Y     | 719 | DC   | OP1-P-OP2   | -5.13 | 111.90      | 119.60   |
| 1   | X     | 602 | DG   | C8-N9-C4    | -5.12 | 104.35      | 106.40   |
| 1   | X     | 611 | DC   | N1-C1'-C2'  | 5.11  | 122.31      | 112.60   |
| 2   | Y     | 708 | DT   | O4'-C1'-C2' | -5.10 | 101.82      | 105.90   |
| 2   | Y     | 718 | DC   | N3-C2-O2    | 5.08  | 125.45      | 121.90   |
| 1   | X     | 615 | DA   | N1-C6-N6    | 5.06  | 121.64      | 118.60   |
| 2   | Y     | 710 | DC   | C5-C4-N4    | -5.06 | 116.66      | 120.20   |
| 1   | X     | 612 | DC   | N1-C1'-C2'  | 5.04  | 122.18      | 112.60   |
| 2   | Y     | 721 | DT   | P-O5'-C5'   | -5.03 | 112.85      | 120.90   |
| 2   | Y     | 706 | DG   | C4-C5-C6    | -5.02 | 115.79      | 118.80   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the

chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | X     | 535   | 0        | 292      | 20      | 0            |
| 2   | Y     | 525   | 0        | 295      | 30      | 1            |
| 3   | A     | 1669  | 0        | 1717     | 58      | 0            |
| 3   | B     | 1669  | 0        | 1717     | 73      | 0            |
| 4   | A     | 1     | 0        | 0        | 0       | 0            |
| 4   | B     | 1     | 0        | 0        | 0       | 0            |
| 4   | X     | 1     | 0        | 0        | 0       | 0            |
| 5   | A     | 118   | 0        | 0        | 11      | 0            |
| 5   | B     | 78    | 0        | 0        | 11      | 0            |
| 5   | X     | 27    | 0        | 0        | 2       | 0            |
| 5   | Y     | 40    | 0        | 0        | 6       | 1            |
| All | All   | 4664  | 0        | 4021     | 166     | 1            |

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 20.

All (166) close contacts within the same asymmetric unit are listed below.

| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 3:B:22:LYS:HD3   | 5:B:1213:HOH:O   | 1.40        | 1.20     |
| 2:Y:721:DT:H2''  | 2:Y:722:DT:H5'   | 1.21        | 1.11     |
| 3:B:73:THR:HG22  | 3:B:85:VAL:HG22  | 1.40        | 1.01     |
| 2:Y:722:DT:O4    | 5:Y:1236:HOH:O   | 1.84        | 0.95     |
| 3:B:53:SER:O     | 3:B:57:LEU:HD22  | 1.70        | 0.92     |
| 3:B:156:ARG:HH21 | 3:B:156:ARG:HG2  | 1.34        | 0.90     |
| 2:Y:721:DT:H2''  | 2:Y:722:DT:C5'   | 2.02        | 0.90     |
| 3:B:174:ASP:OD1  | 3:B:175:LEU:N    | 2.08        | 0.86     |
| 3:A:94:HIS:HD2   | 3:A:96:ASN:H     | 1.16        | 0.86     |
| 3:A:170:ASP:O    | 3:A:173:GLN:NE2  | 2.07        | 0.86     |
| 2:Y:721:DT:C2'   | 2:Y:722:DT:H5'   | 2.07        | 0.83     |
| 3:A:163:LEU:CD2  | 3:A:185:ILE:HG21 | 2.09        | 0.81     |
| 3:A:170:ASP:HB3  | 3:A:173:GLN:NE2  | 1.96        | 0.80     |
| 3:A:163:LEU:HD21 | 3:A:185:ILE:CG2  | 2.12        | 0.80     |
| 3:B:98:VAL:HG13  | 3:B:123:LEU:HD12 | 1.64        | 0.79     |
| 3:B:195:GLN:O    | 3:B:198:GLU:HG2  | 1.81        | 0.79     |
| 1:X:602:DG:H2''  | 1:X:603:DA:C8    | 2.18        | 0.79     |
| 2:Y:723:DA:H2''  | 2:Y:724:DT:H5''  | 1.67        | 0.77     |
| 1:X:606:DA:OP2   | 5:X:1109:HOH:O   | 2.02        | 0.77     |
| 3:A:127:ILE:HG22 | 3:A:133:LEU:HD13 | 1.66        | 0.77     |
| 3:A:71:ILE:HD12  | 3:A:189:MET:SD   | 2.25        | 0.76     |
| 3:A:170:ASP:C    | 3:A:173:GLN:HE22 | 1.88        | 0.76     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 3:A:129:ASN:HD22 | 3:A:132:SER:H    | 1.33        | 0.76     |
| 3:A:163:LEU:HD21 | 3:A:185:ILE:HG21 | 1.64        | 0.75     |
| 3:B:197:ASN:HD22 | 3:B:197:ASN:H    | 1.34        | 0.75     |
| 3:A:94:HIS:CD2   | 3:A:96:ASN:H     | 2.03        | 0.74     |
| 1:X:601:DC:H2''  | 1:X:602:DG:O5'   | 1.87        | 0.74     |
| 3:B:166:LEU:HD22 | 3:B:182:ILE:HG13 | 1.71        | 0.72     |
| 2:Y:723:DA:H2''  | 2:Y:724:DT:C5'   | 2.21        | 0.71     |
| 1:X:612:DC:OP1   | 5:X:1042:HOH:O   | 2.08        | 0.71     |
| 3:A:76:LEU:HD22  | 3:A:78:THR:HG22  | 1.73        | 0.71     |
| 3:B:201:PRO:HG3  | 5:B:1115:HOH:O   | 1.91        | 0.70     |
| 3:B:73:THR:CG2   | 3:B:85:VAL:HG22  | 2.20        | 0.70     |
| 3:A:196:SER:O    | 5:A:1204:HOH:O   | 2.08        | 0.70     |
| 3:B:156:ARG:HH21 | 3:B:156:ARG:CG   | 1.98        | 0.70     |
| 3:A:49:VAL:HG12  | 3:A:50:GLN:O     | 1.91        | 0.69     |
| 3:A:76:LEU:CD2   | 3:A:78:THR:HG22  | 2.23        | 0.69     |
| 3:B:179:VAL:HA   | 3:B:183:LEU:HD23 | 1.75        | 0.69     |
| 2:Y:706:DG:H4'   | 3:B:28:LYS:HE3   | 1.74        | 0.68     |
| 3:B:179:VAL:HG23 | 3:B:207:GLN:HG2  | 1.74        | 0.68     |
| 3:B:156:ARG:NH2  | 3:B:156:ARG:HG2  | 2.08        | 0.68     |
| 3:A:170:ASP:CA   | 3:A:173:GLN:HE22 | 2.07        | 0.67     |
| 1:X:612:DC:N4    | 2:Y:715:DG:O6    | 2.19        | 0.67     |
| 3:B:174:ASP:CG   | 3:B:175:LEU:H    | 1.97        | 0.67     |
| 3:B:179:VAL:CG2  | 3:B:207:GLN:HG2  | 2.25        | 0.66     |
| 3:B:175:LEU:O    | 3:B:179:VAL:HG12 | 1.96        | 0.66     |
| 3:B:174:ASP:CG   | 3:B:175:LEU:N    | 2.49        | 0.66     |
| 3:A:188:GLN:NE2  | 5:A:1128:HOH:O   | 2.29        | 0.65     |
| 2:Y:723:DA:C2'   | 2:Y:724:DT:H5''  | 2.26        | 0.65     |
| 3:B:156:ARG:CG   | 3:B:156:ARG:NH2  | 2.54        | 0.63     |
| 3:B:20:LEU:HD11  | 3:B:114:ARG:HA   | 1.80        | 0.62     |
| 3:B:76:LEU:HB3   | 3:B:79:SER:OG    | 2.00        | 0.61     |
| 3:B:192:GLN:HE21 | 3:B:195:GLN:NE2  | 1.99        | 0.61     |
| 3:A:129:ASN:ND2  | 3:A:132:SER:H    | 2.00        | 0.60     |
| 3:B:127:ILE:HG22 | 3:B:133:LEU:HD13 | 1.83        | 0.60     |
| 3:A:12:LEU:HD22  | 3:A:13:PRO:HD2   | 1.83        | 0.60     |
| 3:B:204:GLU:HA   | 3:B:207:GLN:HB2  | 1.84        | 0.59     |
| 3:B:98:VAL:HG13  | 3:B:123:LEU:CD1  | 2.32        | 0.59     |
| 1:X:612:DC:N3    | 2:Y:715:DG:N1    | 2.42        | 0.59     |
| 3:A:179:VAL:HG13 | 3:A:207:GLN:HG2  | 1.86        | 0.58     |
| 2:Y:709:DA:H1'   | 2:Y:710:DC:H5''  | 1.85        | 0.57     |
| 1:X:621:DC:H2''  | 1:X:622:DG:C8    | 2.39        | 0.57     |
| 3:B:105:LEU:HD13 | 3:B:125:LEU:HD13 | 1.86        | 0.56     |
| 3:B:6:LEU:HD13   | 3:B:10:GLU:HG2   | 1.86        | 0.56     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 3:B:95:VAL:O     | 3:B:98:VAL:HG22  | 2.05        | 0.56     |
| 3:A:143:GLN:NE2  | 3:A:144:TYR:CZ   | 2.73        | 0.56     |
| 3:A:166:LEU:HD22 | 5:A:1091:HOH:O   | 2.05        | 0.56     |
| 1:X:616:DG:O6    | 3:B:116:LYS:CE   | 2.54        | 0.55     |
| 1:X:602:DG:H2''  | 1:X:603:DA:H8    | 1.70        | 0.55     |
| 2:Y:703:DT:H5''  | 3:B:173:GLN:HE22 | 1.72        | 0.55     |
| 1:X:614:DA:H5''  | 1:X:614:DA:C8    | 2.41        | 0.55     |
| 1:X:602:DG:OP1   | 1:X:602:DG:H4'   | 2.07        | 0.55     |
| 3:A:94:HIS:HD2   | 3:A:96:ASN:N     | 1.95        | 0.54     |
| 3:B:188:GLN:HG3  | 5:B:1158:HOH:O   | 2.07        | 0.54     |
| 3:B:95:VAL:CG2   | 3:B:121:ALA:HB1  | 2.37        | 0.54     |
| 5:A:1166:HOH:O   | 3:B:49:VAL:HG21  | 2.08        | 0.54     |
| 2:Y:712:DT:H4'   | 3:B:192:GLN:HG2  | 1.89        | 0.54     |
| 2:Y:722:DT:C7    | 5:Y:1236:HOH:O   | 2.55        | 0.53     |
| 2:Y:723:DA:H1'   | 2:Y:724:DT:H5''  | 1.89        | 0.53     |
| 3:A:90:ASN:ND2   | 5:A:1032:HOH:O   | 2.41        | 0.53     |
| 2:Y:722:DT:H71   | 5:Y:1236:HOH:O   | 2.07        | 0.53     |
| 3:A:28:LYS:O     | 3:A:31:LYS:HE2   | 2.09        | 0.53     |
| 3:B:59:LEU:HD13  | 3:B:103:LEU:HD13 | 1.91        | 0.53     |
| 3:A:161:LYS:O    | 3:A:165:GLU:HG3  | 2.09        | 0.53     |
| 3:A:170:ASP:CB   | 3:A:173:GLN:NE2  | 2.71        | 0.52     |
| 3:A:170:ASP:HB3  | 3:A:173:GLN:CD   | 2.29        | 0.52     |
| 2:Y:705:DC:H2''  | 2:Y:706:DG:O5'   | 2.09        | 0.52     |
| 1:X:625:DG:H2''  | 1:X:626:DC:C5    | 2.44        | 0.52     |
| 3:A:18:GLU:HG3   | 5:A:1181:HOH:O   | 2.09        | 0.52     |
| 2:Y:711:DC:H3'   | 5:Y:1074:HOH:O   | 2.10        | 0.51     |
| 3:A:163:LEU:HD22 | 3:A:185:ILE:HG21 | 1.92        | 0.51     |
| 3:B:116:LYS:HG3  | 5:B:1225:HOH:O   | 2.11        | 0.51     |
| 3:A:75:LYS:CE    | 5:A:1136:HOH:O   | 2.58        | 0.51     |
| 3:A:170:ASP:HB3  | 3:A:173:GLN:HE22 | 1.72        | 0.51     |
| 2:Y:709:DA:H2''  | 2:Y:710:DC:H5'   | 1.92        | 0.51     |
| 3:A:170:ASP:O    | 3:A:173:GLN:CD   | 2.49        | 0.51     |
| 3:B:81:PHE:CE2   | 3:B:175:LEU:HD23 | 2.46        | 0.50     |
| 3:A:170:ASP:CB   | 3:A:173:GLN:HE22 | 2.24        | 0.50     |
| 3:B:172:HIS:H    | 3:B:172:HIS:CD2  | 2.27        | 0.50     |
| 3:B:105:LEU:HD13 | 3:B:125:LEU:CD1  | 2.41        | 0.50     |
| 3:A:163:LEU:HD21 | 3:A:185:ILE:HG22 | 1.94        | 0.50     |
| 1:X:619:DA:C2    | 2:Y:709:DA:C2    | 2.99        | 0.50     |
| 3:A:57:LEU:HD13  | 3:A:144:TYR:HD2  | 1.75        | 0.50     |
| 2:Y:703:DT:OP1   | 3:B:80:LYS:HB2   | 2.12        | 0.49     |
| 3:B:156:ARG:NH2  | 5:B:1135:HOH:O   | 2.43        | 0.49     |
| 3:B:95:VAL:HG23  | 3:B:121:ALA:HB1  | 1.95        | 0.49     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 3:A:71:ILE:CD1   | 3:A:189:MET:SD   | 3.00        | 0.49     |
| 3:B:62:PHE:HZ    | 3:B:93:ARG:HD3   | 1.78        | 0.49     |
| 1:X:618:DT:H4'   | 3:B:195:GLN:HE22 | 1.78        | 0.49     |
| 3:B:22:LYS:NZ    | 5:B:1213:HOH:O   | 2.43        | 0.48     |
| 3:B:202:ASN:ND2  | 3:B:205:ALA:H    | 2.10        | 0.48     |
| 3:B:171:ALA:HB1  | 3:B:177:GLN:HB3  | 1.96        | 0.48     |
| 3:A:23:ILE:HD12  | 3:A:43:LEU:HD22  | 1.96        | 0.47     |
| 3:A:108:PHE:O    | 3:A:136:LYS:HE3  | 2.14        | 0.47     |
| 3:B:14:GLN:HA    | 3:B:17:LEU:HD12  | 1.96        | 0.47     |
| 3:A:127:ILE:CG2  | 3:A:133:LEU:HD13 | 2.42        | 0.47     |
| 3:A:106:GLU:OE1  | 3:A:109:LYS:NZ   | 2.47        | 0.47     |
| 3:B:122:THR:CG2  | 5:B:1010:HOH:O   | 2.63        | 0.47     |
| 3:A:75:LYS:HE2   | 5:A:1136:HOH:O   | 2.13        | 0.47     |
| 3:A:93:ARG:NH2   | 5:A:1051:HOH:O   | 2.22        | 0.47     |
| 3:A:146:VAL:HG13 | 3:A:154:VAL:HG22 | 1.96        | 0.47     |
| 2:Y:718:DC:C2'   | 2:Y:719:DC:H5'   | 2.45        | 0.46     |
| 3:A:77:ALA:HA    | 5:A:1066:HOH:O   | 2.14        | 0.46     |
| 3:B:167:PHE:HD1  | 3:B:172:HIS:CD2  | 2.33        | 0.46     |
| 2:Y:703:DT:OP1   | 3:B:173:GLN:OE1  | 2.34        | 0.46     |
| 3:A:28:LYS:NZ    | 5:A:1106:HOH:O   | 2.49        | 0.46     |
| 3:A:47:ASP:O     | 3:A:49:VAL:HG23  | 2.16        | 0.46     |
| 3:B:166:LEU:HD23 | 3:B:171:ALA:CB   | 2.45        | 0.46     |
| 1:X:614:DA:H5'   | 1:X:614:DA:H2'   | 1.42        | 0.45     |
| 2:Y:704:DT:H3'   | 5:Y:1151:HOH:O   | 2.14        | 0.45     |
| 1:X:601:DC:C2'   | 1:X:602:DG:O5'   | 2.61        | 0.45     |
| 3:A:23:ILE:HG12  | 3:A:39:ASP:HB3   | 1.99        | 0.45     |
| 3:A:180:ASN:O    | 3:A:184:PRO:HG2  | 2.17        | 0.45     |
| 3:B:188:GLN:CG   | 5:B:1158:HOH:O   | 2.65        | 0.45     |
| 3:B:188:GLN:HG3  | 3:B:188:GLN:O    | 2.16        | 0.45     |
| 3:B:7:LYS:O      | 3:B:10:GLU:HB3   | 2.17        | 0.44     |
| 2:Y:723:DA:H2''  | 2:Y:724:DT:H5'   | 1.98        | 0.44     |
| 1:X:617:DG:H1'   | 1:X:618:DT:H5''  | 1.99        | 0.44     |
| 2:Y:723:DA:C1'   | 2:Y:724:DT:H5''  | 2.47        | 0.44     |
| 2:Y:706:DG:H5''  | 3:B:28:LYS:HG3   | 1.99        | 0.44     |
| 3:B:57:LEU:HD13  | 3:B:144:TYR:HD2  | 1.82        | 0.44     |
| 2:Y:721:DT:H2'   | 2:Y:722:DT:C6    | 2.53        | 0.44     |
| 3:B:155:LYS:HE3  | 3:B:188:GLN:OE1  | 2.18        | 0.43     |
| 3:B:6:LEU:CD1    | 3:B:10:GLU:O     | 2.66        | 0.43     |
| 5:Y:1187:HOH:O   | 3:A:153:LYS:HE3  | 2.17        | 0.43     |
| 3:B:153:LYS:HG2  | 5:B:1127:HOH:O   | 2.18        | 0.43     |
| 3:A:197:ASN:HD22 | 3:A:197:ASN:H    | 1.66        | 0.43     |
| 1:X:616:DG:O6    | 3:B:116:LYS:HE3  | 2.18        | 0.43     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 3:B:22:LYS:CD    | 5:B:1213:HOH:O   | 2.23        | 0.43     |
| 3:B:90:ASN:HA    | 3:B:125:LEU:O    | 2.17        | 0.43     |
| 3:A:146:VAL:O    | 3:A:146:VAL:CG1  | 2.66        | 0.43     |
| 3:B:122:THR:HG22 | 5:B:1010:HOH:O   | 2.18        | 0.42     |
| 3:A:177:GLN:HE21 | 3:A:181:LYS:HD2  | 1.84        | 0.42     |
| 3:A:61:GLY:HA3   | 3:B:58:PHE:O     | 2.19        | 0.42     |
| 3:B:179:VAL:HG22 | 3:B:207:GLN:HG2  | 1.99        | 0.41     |
| 1:X:608:DG:H2''  | 1:X:609:DG:O5'   | 2.20        | 0.41     |
| 3:A:171:ALA:HB1  | 3:A:177:GLN:HB3  | 2.03        | 0.41     |
| 1:X:611:DC:H5'   | 3:A:197:ASN:HB3  | 2.02        | 0.41     |
| 3:B:82:GLY:HA3   | 3:B:209:PHE:HE2  | 1.86        | 0.41     |
| 2:Y:720:DG:H2''  | 2:Y:721:DT:O5'   | 2.21        | 0.41     |
| 3:B:73:THR:HG23  | 3:B:186:TRP:CD1  | 2.56        | 0.41     |
| 3:B:145:VAL:HG12 | 3:B:149:SER:HB2  | 2.03        | 0.41     |
| 2:Y:716:DG:O6    | 3:A:116:LYS:CE   | 2.69        | 0.40     |
| 3:A:168:ASN:HA   | 3:A:168:ASN:HD22 | 1.53        | 0.40     |
| 3:B:174:ASP:C    | 3:B:174:ASP:OD1  | 2.60        | 0.40     |
| 3:B:209:PHE:C    | 3:B:211:ARG:H    | 2.24        | 0.40     |

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1         | Atom-2                | Distance(Å) | Clash(Å) |
|----------------|-----------------------|-------------|----------|
| 2:Y:701:DG:O5' | 5:Y:1234:HOH:O[2_674] | 1.80        | 0.40     |

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 3   | A     | 205/207 (99%) | 198 (97%) | 7 (3%)  | 0        | 100         | 100 |
| 3   | B     | 205/207 (99%) | 185 (90%) | 16 (8%) | 4 (2%)   | 11          | 6   |
| All | All   | 410/414 (99%) | 383 (93%) | 23 (6%) | 4 (1%)   | 22          | 18  |

All (4) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | B     | 204 | GLU  |
| 3   | B     | 203 | LEU  |
| 3   | B     | 96  | ASN  |
| 3   | B     | 184 | PRO  |

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |   |
|-----|-------|----------------|-----------|----------|-------------|---|
| 3   | A     | 185/185 (100%) | 159 (86%) | 26 (14%) | 5           | 4 |
| 3   | B     | 185/185 (100%) | 161 (87%) | 24 (13%) | 6           | 5 |
| All | All   | 370/370 (100%) | 320 (86%) | 50 (14%) | 6           | 4 |

All (50) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | A     | 14  | GLN  |
| 3   | A     | 15  | ASP  |
| 3   | A     | 47  | ASP  |
| 3   | A     | 48  | GLU  |
| 3   | A     | 50  | GLN  |
| 3   | A     | 54  | GLU  |
| 3   | A     | 57  | LEU  |
| 3   | A     | 70  | ASN  |
| 3   | A     | 83  | LEU  |
| 3   | A     | 90  | ASN  |
| 3   | A     | 101 | LEU  |
| 3   | A     | 103 | LEU  |
| 3   | A     | 107 | VAL  |
| 3   | A     | 122 | THR  |
| 3   | A     | 123 | LEU  |
| 3   | A     | 125 | LEU  |
| 3   | A     | 133 | LEU  |
| 3   | A     | 139 | PRO  |
| 3   | A     | 143 | GLN  |
| 3   | A     | 153 | LYS  |
| 3   | A     | 164 | LEU  |
| 3   | A     | 173 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | A     | 175 | LEU  |
| 3   | A     | 183 | LEU  |
| 3   | A     | 191 | LYS  |
| 3   | A     | 197 | ASN  |
| 3   | B     | 7   | LYS  |
| 3   | B     | 14  | GLN  |
| 3   | B     | 20  | LEU  |
| 3   | B     | 27  | VAL  |
| 3   | B     | 31  | LYS  |
| 3   | B     | 45  | GLN  |
| 3   | B     | 57  | LEU  |
| 3   | B     | 70  | ASN  |
| 3   | B     | 90  | ASN  |
| 3   | B     | 95  | VAL  |
| 3   | B     | 98  | VAL  |
| 3   | B     | 101 | LEU  |
| 3   | B     | 103 | LEU  |
| 3   | B     | 105 | LEU  |
| 3   | B     | 106 | GLU  |
| 3   | B     | 122 | THR  |
| 3   | B     | 124 | VAL  |
| 3   | B     | 133 | LEU  |
| 3   | B     | 156 | ARG  |
| 3   | B     | 164 | LEU  |
| 3   | B     | 166 | LEU  |
| 3   | B     | 174 | ASP  |
| 3   | B     | 196 | SER  |
| 3   | B     | 197 | ASN  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | A     | 50  | GLN  |
| 3   | A     | 70  | ASN  |
| 3   | A     | 90  | ASN  |
| 3   | A     | 94  | HIS  |
| 3   | A     | 129 | ASN  |
| 3   | A     | 159 | ASN  |
| 3   | A     | 168 | ASN  |
| 3   | A     | 173 | GLN  |
| 3   | A     | 177 | GLN  |
| 3   | A     | 192 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | A     | 193 | GLN  |
| 3   | A     | 197 | ASN  |
| 3   | B     | 14  | GLN  |
| 3   | B     | 159 | ASN  |
| 3   | B     | 168 | ASN  |
| 3   | B     | 172 | HIS  |
| 3   | B     | 173 | GLN  |
| 3   | B     | 180 | ASN  |
| 3   | B     | 195 | GLN  |
| 3   | B     | 197 | ASN  |
| 3   | B     | 202 | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2      | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|--------------|-----------------------|-------|
| 1   | X     | 26/26 (100%)   | -0.17  | 0 100 100    | 38, 48, 71, 86        | 0     |
| 2   | Y     | 26/26 (100%)   | -0.18  | 0 100 100    | 28, 49, 61, 62        | 0     |
| 3   | A     | 207/207 (100%) | -0.26  | 2 (0%) 79 80 | 21, 34, 53, 62        | 0     |
| 3   | B     | 207/207 (100%) | 0.04   | 3 (1%) 72 72 | 20, 44, 72, 77        | 0     |
| All | All   | 466/466 (100%) | -0.12  | 5 (1%) 77 78 | 20, 40, 66, 86        | 0     |

All (5) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 3   | B     | 204 | GLU  | 2.5  |
| 3   | A     | 49  | VAL  | 2.5  |
| 3   | A     | 50  | GLN  | 2.1  |
| 3   | B     | 14  | GLN  | 2.0  |
| 3   | B     | 50  | GLN  | 2.0  |

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSR  | LLDF  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|-------|----------------------------|-------|
| 4   | CA   | B     | 803 | 1/1   | 0.10 | -0.55 | 51,51,51,51                | 0     |
| 4   | CA   | X     | 802 | 1/1   | 0.06 | -2.55 | 36,36,36,36                | 0     |
| 4   | CA   | A     | 801 | 1/1   | 0.05 | -3.23 | 34,34,34,34                | 0     |

## 6.5 Other polymers ⓘ

There are no such residues in this entry.