



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:25 PM GMT

PDB ID : 1OUQ  
Title : Crystal structure of wild-type Cre recombinase-loxP synapse  
Authors : Ennifar, E.; Meyer, J.E.W.; Buchholz, F.; Stewart, A.F.; Suck, D.  
Deposited on : 2003-03-25  
Resolution : 3.20 Å(reported)

This is a Full wwPDB X-ray Structure 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/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

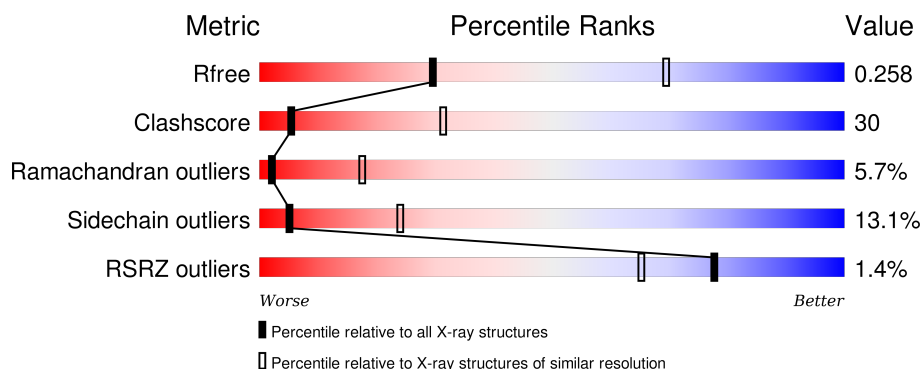
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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.





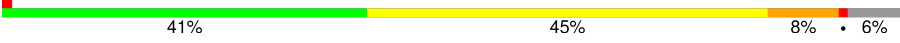
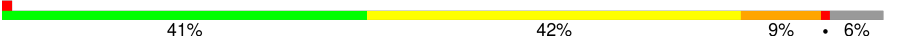

| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 91344                       | 1124 (3.24-3.16)                                      |
| Clashscore            | 102246                      | 1024 (3.22-3.18)                                      |
| Ramachandran outliers | 100387                      | 1004 (3.22-3.18)                                      |
| Sidechain outliers    | 100360                      | 1003 (3.22-3.18)                                      |
| RSRZ outliers         | 91569                       | 1129 (3.24-3.16)                                      |

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 1   | C     | 16     | <div> <div>44%</div> <div>56%</div> </div>                               |
| 1   | G     | 16     | <div> <div>50%</div> <div>38%</div> <div>13%</div> </div>                |
| 2   | X     | 21     | <div> <div>19%</div> <div>71%</div> <div>10%</div> <div>19%</div> </div> |
| 2   | Y     | 21     | <div> <div>14%</div> <div>38%</div> <div>43%</div> <div>19%</div> </div> |
| 3   | D     | 37     | <div> <div>22%</div> <div>65%</div> <div>14%</div> </div>                |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 3   | H     | 37     |  |
| 4   | A     | 343    |  |
| 4   | B     | 343    |  |
| 4   | E     | 343    |  |
| 4   | F     | 343    |  |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 5   | MG   | A     | 344 | -         | -        | -       | X                |
| 5   | MG   | A     | 347 | -         | -        | -       | X                |

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13296 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 loxP DNA.

| Mol | Chain | Residues | Atoms |     |    |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|----|---------|---------|-------|
| 1   | C     | 16       | Total | C   | N  | O  | P  | 0       | 0       | 0     |
|     |       |          | 326   | 156 | 59 | 95 | 16 |         |         |       |
| 1   | G     | 16       | Total | C   | N  | O  | P  | 0       | 0       | 0     |
|     |       |          | 326   | 156 | 59 | 95 | 16 |         |         |       |

- Molecule 2 is a DNA chain called loxP DNA.

| Mol | Chain | Residues | Atoms |     |    |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|---------|-------|
| 2   | X     | 21       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 428   | 207 | 75 | 126 | 20 |         |         |       |
| 2   | Y     | 21       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 428   | 207 | 75 | 126 | 20 |         |         |       |

- Molecule 3 is a DNA chain called loxP DNA.

| Mol | Chain | Residues | Atoms |     |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 3   | D     | 37       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 756   | 364 | 137 | 219 | 36 |         |         |       |
| 3   | H     | 37       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 756   | 364 | 137 | 219 | 36 |         |         |       |

- Molecule 4 is a protein called Cre recombinase.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 4   | A     | 332      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2620  | 1629 | 497 | 479 | 15 |         |         |       |
| 4   | B     | 322      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2550  | 1584 | 486 | 465 | 15 |         |         |       |
| 4   | E     | 321      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2544  | 1581 | 485 | 463 | 15 |         |         |       |
| 4   | F     | 322      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2550  | 1584 | 486 | 465 | 15 |         |         |       |

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 5   | H     | 1        | Total<br>1 | Mg<br>1 | 0       | 0       |
| 5   | A     | 4        | Total<br>4 | Mg<br>4 | 0       | 0       |
| 5   | D     | 1        | Total<br>1 | Mg<br>1 | 0       | 0       |
| 5   | F     | 1        | Total<br>1 | Mg<br>1 | 0       | 0       |

- Molecule 6 is IODIDE ION (three-letter code: IOD) (formula: I).

| Mol | Chain | Residues | Atoms      |        | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|---------|---------|
| 6   | C     | 1        | Total<br>1 | I<br>1 | 0       | 0       |
| 6   | F     | 1        | Total<br>1 | I<br>1 | 0       | 0       |

- Molecule 7 is water.

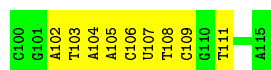
| Mol | Chain | Residues | Atoms      |        | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|---------|---------|
| 7   | A     | 2        | Total<br>2 | O<br>2 | 0       | 0       |
| 7   | F     | 1        | Total<br>1 | O<br>1 | 0       | 0       |

### 3 Residue-property plots [i](#)

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: loxP DNA

Chain C: 



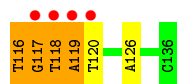
- Molecule 1: loxP DNA

Chain G: 



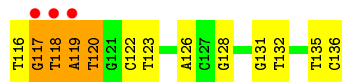
- Molecule 2: loxP DNA

Chain X: 



- Molecule 2: loxP DNA

Chain Y: 



- Molecule 3: loxP DNA

Chain D: 



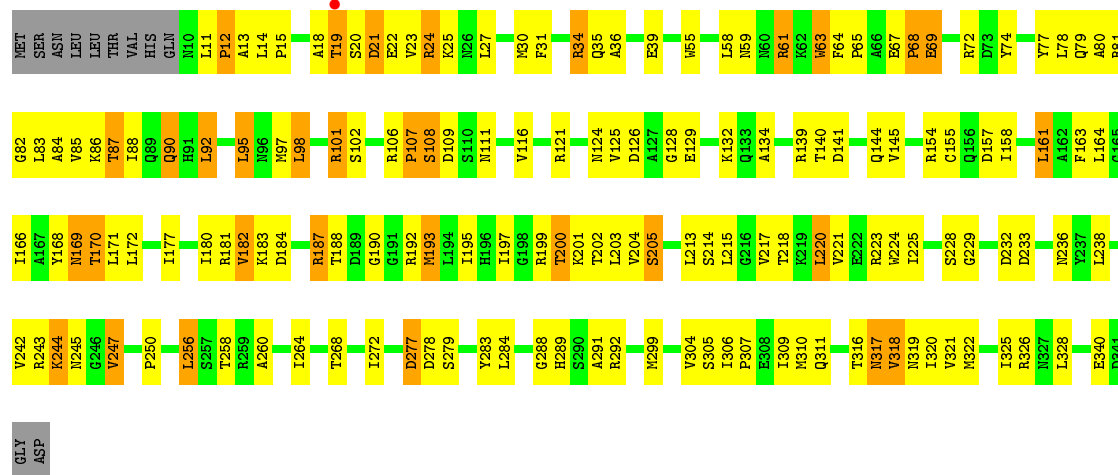
- Molecule 3: loxP DNA

Chain H: 



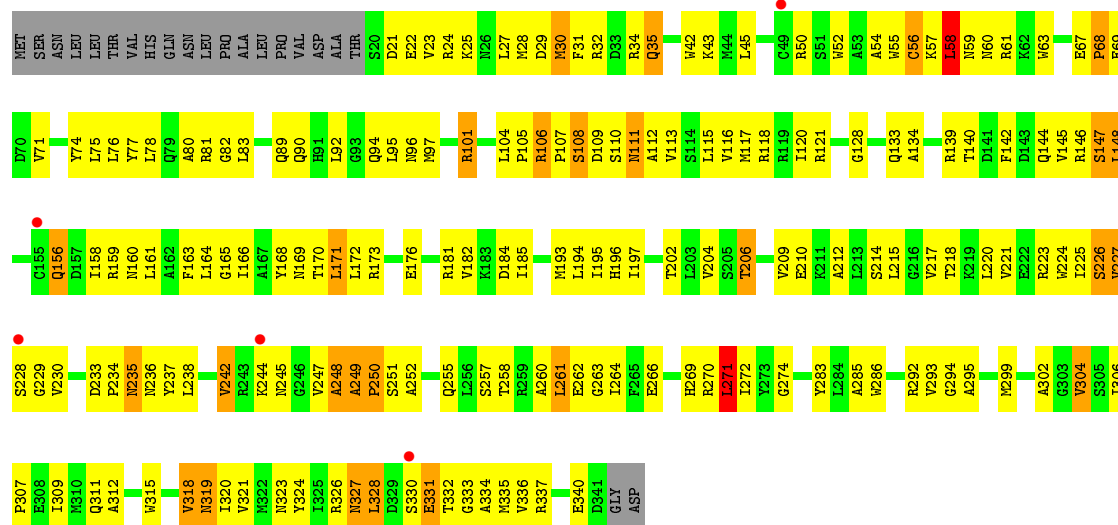
• Molecule 4: Cre recombinase

Chain A: 50% 37% 9%



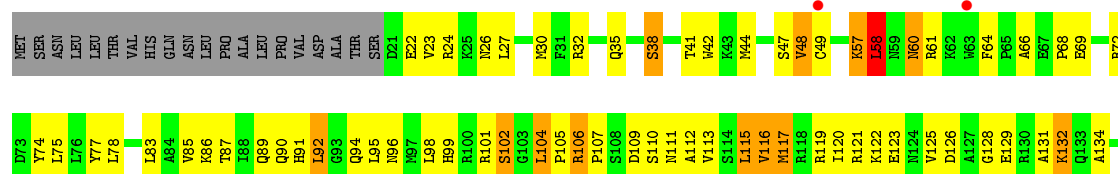
• Molecule 4: Cre recombinase

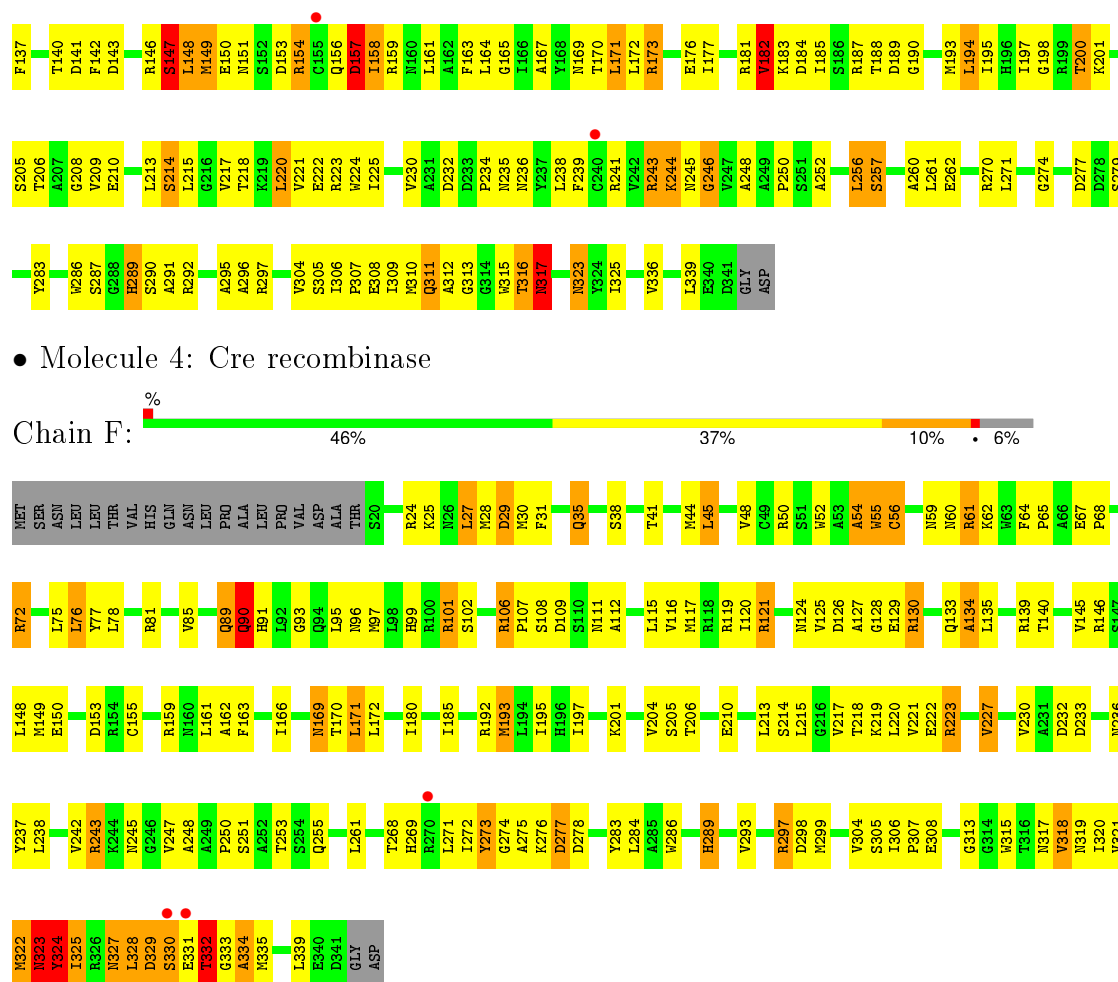
Chain B: 41% 45% 8% 6%



• Molecule 4: Cre recombinase

Chain E: 41% 42% 9% 6%







## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 21 21 21  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 109.50 Å   165.60 Å   193.70 Å<br>90.00°   90.00°   90.00°  | Depositor        |
| Resolution (Å)  | 8.00 – 3.20<br>49.29 – 3.20                                 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 94.7 (8.00-3.20)<br>99.1 (49.29-3.20)                       | Depositor<br>EDS |
| $R_{merge}$   | (Not available)   | Depositor        |
| $R_{sym}$   | 0.15  | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.10 (at 3.19 Å)  | Xtriage          |
| Refinement program  | CNS 1.1   | Depositor        |
| R, $R_{free}$   | 0.210   ,   0.264<br>0.208   ,   0.258                      | Depositor<br>DCC |
| $R_{free}$ test set   | 2754 reflections (5.34%)                                    | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 76.0  | Xtriage          |
| Anisotropy  | 0.356   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.30 , 63.3   | EDS              |
| Estimated twinning fraction   | No twinning to report.                                      | Xtriage          |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$ | Xtriage          |
| Outliers  | 0 of 58248 reflections                                      | Xtriage          |
| $F_o, F_c$ correlation  | 0.92  | EDS              |
| Total number of atoms   | 13296   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 57.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.22% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, IOD, UMP, A3P

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   | C     | 0.76         | 0/316          | 0.90        | 0/483           |
| 1   | G     | 0.78         | 0/316          | 0.97        | 1/483 (0.2%)    |
| 2   | X     | 1.21         | 2/479 (0.4%)   | 1.34        | 7/738 (0.9%)    |
| 2   | Y     | 1.17         | 6/479 (1.3%)   | 1.42        | 9/738 (1.2%)    |
| 3   | D     | 0.88         | 0/848          | 0.95        | 0/1307          |
| 3   | H     | 0.71         | 0/848          | 0.87        | 0/1307          |
| 4   | A     | 0.73         | 1/2663 (0.0%)  | 0.85        | 1/3595 (0.0%)   |
| 4   | B     | 0.57         | 0/2591         | 0.79        | 0/3493          |
| 4   | E     | 0.57         | 0/2585         | 0.79        | 2/3485 (0.1%)   |
| 4   | F     | 0.65         | 0/2591         | 0.84        | 2/3493 (0.1%)   |
| All | All   | 0.72         | 9/13716 (0.1%) | 0.89        | 22/19122 (0.1%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | G     | 0                   | 2                   |
| 2   | X     | 0                   | 1                   |
| 3   | D     | 0                   | 5                   |
| 3   | H     | 0                   | 1                   |
| All | All   | 0                   | 9                   |

All (9) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 2   | X     | 120 | DT   | C5-C7   | 8.43 | 1.55        | 1.50     |
| 2   | Y     | 120 | DT   | C5-C7   | 8.40 | 1.55        | 1.50     |
| 2   | Y     | 118 | DT   | C5-C7   | 7.68 | 1.54        | 1.50     |
| 2   | Y     | 119 | DA   | C5'-C4' | 6.60 | 1.58        | 1.51     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | X     | 118 | DT   | C5-C7   | 6.04  | 1.53        | 1.50     |
| 2   | Y     | 118 | DT   | C5'-C4' | 5.69  | 1.57        | 1.51     |
| 2   | Y     | 117 | DG   | C5'-C4' | 5.68  | 1.57        | 1.51     |
| 4   | A     | 155 | CYS  | CB-SG   | -5.10 | 1.73        | 1.81     |
| 2   | Y     | 117 | DG   | P-O5'   | 5.08  | 1.64        | 1.59     |

All (22) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 2   | Y     | 118 | DT   | O4'-C4'-C3' | -11.85 | 98.89       | 106.00   |
| 2   | Y     | 117 | DG   | O4'-C4'-C3' | -10.62 | 99.63       | 106.00   |
| 4   | E     | 105 | PRO  | CA-N-CD     | -8.19  | 100.04      | 111.50   |
| 4   | F     | 324 | TYR  | CB-CG-CD2   | 7.54   | 125.53      | 121.00   |
| 2   | Y     | 119 | DA   | O4'-C4'-C3' | -6.90  | 101.74      | 104.50   |
| 2   | Y     | 117 | DG   | O5'-P-OP2   | -6.51  | 99.84       | 105.70   |
| 2   | Y     | 119 | DA   | OP1-P-OP2   | -6.29  | 110.17      | 119.60   |
| 2   | X     | 119 | DA   | O4'-C1'-C2' | 6.16   | 110.83      | 105.90   |
| 2   | Y     | 118 | DT   | C6-C5-C7    | -5.99  | 119.31      | 122.90   |
| 2   | X     | 120 | DT   | C4'-C3'-C2' | 5.92   | 108.43      | 103.10   |
| 1   | G     | 114 | DA   | C4'-C3'-C2' | 5.89   | 108.41      | 103.10   |
| 2   | X     | 120 | DT   | O4'-C4'-C3' | -5.83  | 102.17      | 104.50   |
| 2   | Y     | 118 | DT   | C6-N1-C2    | 5.81   | 124.20      | 121.30   |
| 2   | X     | 120 | DT   | C2'-C3'-O3' | -5.61  | 94.08       | 112.60   |
| 2   | Y     | 119 | DA   | C3'-C2'-C1' | -5.47  | 95.93       | 102.50   |
| 2   | X     | 116 | DT   | C5'-C4'-C3' | 5.41   | 123.84      | 114.10   |
| 2   | X     | 120 | DT   | O4'-C1'-N1  | 5.39   | 111.78      | 108.00   |
| 2   | Y     | 119 | DA   | C4'-C3'-C2' | 5.38   | 107.94      | 103.10   |
| 2   | X     | 120 | DT   | N1-C1'-C2'  | 5.38   | 122.82      | 112.60   |
| 4   | A     | 107 | PRO  | CA-N-CD     | -5.24  | 104.17      | 111.50   |
| 4   | F     | 76  | LEU  | CA-CB-CG    | -5.23  | 103.28      | 115.30   |
| 4   | E     | 317 | ASN  | N-CA-C      | -5.17  | 97.06       | 111.00   |

There are no chirality outliers.

All (9) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 3   | D     | 116 | DC   | Sidechain |
| 3   | D     | 117 | DA   | Sidechain |
| 3   | D     | 118 | DT   | Sidechain |
| 3   | D     | 119 | DA   | Sidechain |
| 3   | D     | 126 | DA   | Sidechain |
| 1   | G     | 105 | DA   | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | G     | 106 | DC   | Sidechain |
| 3   | H     | 105 | DA   | Sidechain |
| 2   | X     | 117 | DG   | Sidechain |

## 5.2 Too-close contacts [i](#)

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 hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | C     | 326   | 0        | 178      | 12      | 0            |
| 1   | G     | 326   | 0        | 178      | 8       | 0            |
| 2   | X     | 428   | 0        | 241      | 10      | 0            |
| 2   | Y     | 428   | 0        | 241      | 36      | 0            |
| 3   | D     | 756   | 0        | 421      | 34      | 0            |
| 3   | H     | 756   | 0        | 421      | 34      | 0            |
| 4   | A     | 2620  | 0        | 2643     | 163     | 0            |
| 4   | B     | 2550  | 0        | 2570     | 190     | 0            |
| 4   | E     | 2544  | 0        | 2566     | 183     | 0            |
| 4   | F     | 2550  | 0        | 2570     | 161     | 0            |
| 5   | A     | 4     | 0        | 0        | 0       | 0            |
| 5   | D     | 1     | 0        | 0        | 0       | 0            |
| 5   | F     | 1     | 0        | 0        | 0       | 0            |
| 5   | H     | 1     | 0        | 0        | 0       | 0            |
| 6   | C     | 1     | 0        | 0        | 0       | 0            |
| 6   | F     | 1     | 0        | 0        | 0       | 0            |
| 7   | A     | 2     | 0        | 0        | 0       | 0            |
| 7   | F     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 13296 | 0        | 12029    | 755     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 30.

All (755) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:C:105:DA:H2"  | 1:C:106:DC:H5"   | 1.20                     | 1.15              |
| 4:E:193:MET:HG3 | 4:E:218:THR:HG23 | 1.22                     | 1.12              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:B:35:GLN:HA    | 4:B:35:GLN:HE21  | 1.04                     | 1.10              |
| 3:H:105:DA:H2"   | 3:H:106:DC:H5"   | 1.35                     | 1.09              |
| 4:A:15:PRO:HB2   | 4:A:18:ALA:HB3   | 1.34                     | 1.08              |
| 4:A:299:MET:HE1  | 4:A:309:ILE:HA   | 1.36                     | 1.06              |
| 4:A:72:ARG:HG3   | 4:A:116:VAL:HG21 | 1.38                     | 1.00              |
| 4:A:181:ARG:HH11 | 4:A:199:ARG:HH22 | 1.11                     | 0.97              |
| 4:B:134:ALA:HA   | 4:B:283:TYR:CD2  | 2.01                     | 0.96              |
| 4:B:35:GLN:HA    | 4:B:35:GLN:NE2   | 1.83                     | 0.94              |
| 4:B:194:LEU:HD13 | 4:B:212:ALA:HB2  | 1.48                     | 0.94              |
| 4:E:121:ARG:O    | 4:E:125:VAL:HG12 | 1.67                     | 0.93              |
| 3:D:122:DT:H5"   | 4:B:97:MET:HE2   | 1.50                     | 0.93              |
| 3:H:134:DA:H2"   | 3:H:135:DT:C5'   | 1.99                     | 0.93              |
| 4:B:58:LEU:O     | 4:B:58:LEU:HD12  | 1.69                     | 0.93              |
| 4:E:317:ASN:HD22 | 4:E:317:ASN:H    | 1.16                     | 0.92              |
| 4:F:245:ASN:OD1  | 4:F:247:VAL:HG23 | 1.69                     | 0.91              |
| 4:E:200:THR:HG22 | 4:E:201:LYS:H    | 1.34                     | 0.90              |
| 4:E:146:ARG:O    | 4:E:150:GLU:HB2  | 1.73                     | 0.89              |
| 2:X:116:DT:H5"   | 4:B:173:ARG:NH2  | 1.88                     | 0.89              |
| 1:G:105:DA:H2"   | 1:G:106:DC:H5"   | 1.53                     | 0.89              |
| 4:A:15:PRO:HB2   | 4:A:18:ALA:CB    | 2.03                     | 0.88              |
| 4:A:15:PRO:CB    | 4:A:18:ALA:HB3   | 2.04                     | 0.87              |
| 4:F:193:MET:HB3  | 4:F:213:LEU:HD12 | 1.56                     | 0.87              |
| 1:G:115:A3P:O2P  | 2:Y:116:DT:H5'   | 1.75                     | 0.87              |
| 4:F:134:ALA:HA   | 4:F:283:TYR:CD2  | 2.10                     | 0.86              |
| 4:A:188:THR:HG22 | 4:A:190:GLY:H    | 1.39                     | 0.85              |
| 4:E:243:ARG:HG2  | 4:E:243:ARG:HH11 | 1.41                     | 0.85              |
| 4:A:181:ARG:NH1  | 4:A:199:ARG:HH22 | 1.75                     | 0.84              |
| 4:A:305:SER:HB2  | 4:A:307:PRO:HD2  | 1.59                     | 0.84              |
| 4:E:154:ARG:HB3  | 4:E:154:ARG:HH11 | 1.40                     | 0.84              |
| 4:E:188:THR:HG22 | 4:E:190:GLY:H    | 1.45                     | 0.82              |
| 4:F:163:PHE:CE1  | 4:F:261:LEU:HD13 | 2.15                     | 0.82              |
| 4:B:215:LEU:O    | 4:B:218:THR:HG22 | 1.79                     | 0.81              |
| 2:Y:118:DT:H3    | 3:H:119:DA:H61   | 1.28                     | 0.81              |
| 4:A:134:ALA:HA   | 4:A:283:TYR:CD2  | 2.15                     | 0.81              |
| 3:H:134:DA:H2"   | 3:H:135:DT:H5'   | 1.61                     | 0.81              |
| 4:F:121:ARG:HG3  | 4:F:121:ARG:HH11 | 1.42                     | 0.81              |
| 4:E:58:LEU:HD12  | 4:E:58:LEU:O     | 1.81                     | 0.80              |
| 4:A:325:ILE:HB   | 4:A:328:LEU:HD12 | 1.64                     | 0.80              |
| 3:H:134:DA:H2"   | 3:H:135:DT:H5"   | 1.62                     | 0.80              |
| 4:E:271:LEU:O    | 4:E:271:LEU:HD23 | 1.82                     | 0.79              |
| 4:B:113:VAL:O    | 4:B:116:VAL:HG12 | 1.81                     | 0.79              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:A:72:ARG:CG    | 4:A:116:VAL:HG21 | 2.13                     | 0.79              |
| 4:A:139:ARG:HG3  | 4:A:139:ARG:O    | 1.80                     | 0.79              |
| 4:B:106:ARG:O    | 4:B:109:ASP:HB2  | 1.83                     | 0.79              |
| 2:Y:131:DG:H2"   | 2:Y:132:DT:C5'   | 2.13                     | 0.78              |
| 4:E:117:MET:HE3  | 4:E:120:ILE:HD12 | 1.65                     | 0.78              |
| 4:A:243:ARG:HH11 | 4:A:243:ARG:HG2  | 1.48                     | 0.78              |
| 2:Y:118:DT:H72   | 4:F:319:ASN:ND2  | 1.98                     | 0.78              |
| 1:C:105:DA:C2'   | 1:C:106:DC:H5"   | 2.10                     | 0.78              |
| 4:B:35:GLN:CA    | 4:B:35:GLN:HE21  | 1.93                     | 0.78              |
| 4:B:182:VAL:HG23 | 4:B:236:ASN:O    | 1.84                     | 0.78              |
| 3:D:132:DT:H2"   | 3:D:133:DT:H5"   | 1.67                     | 0.77              |
| 2:Y:117:DG:H5"   | 4:F:320:ILE:HD11 | 1.67                     | 0.76              |
| 4:B:258:THR:HA   | 4:B:261:LEU:HD12 | 1.66                     | 0.76              |
| 4:B:185:ILE:HD13 | 4:B:193:MET:CE   | 2.15                     | 0.76              |
| 4:A:19:THR:HG22  | 4:A:23:VAL:HG23  | 1.66                     | 0.76              |
| 3:H:105:DA:C2'   | 3:H:106:DC:H5"   | 2.14                     | 0.76              |
| 2:X:117:DG:OP2   | 4:B:320:ILE:HG13 | 1.86                     | 0.76              |
| 2:X:116:DT:C5'   | 4:B:173:ARG:NH2  | 2.48                     | 0.76              |
| 4:A:299:MET:CE   | 4:A:309:ILE:HA   | 2.16                     | 0.75              |
| 4:F:317:ASN:ND2  | 4:F:319:ASN:H    | 1.84                     | 0.75              |
| 4:E:148:LEU:O    | 4:E:149:MET:HB2  | 1.84                     | 0.75              |
| 4:E:171:LEU:HD23 | 4:E:171:LEU:N    | 2.01                     | 0.74              |
| 4:E:48:VAL:HG21  | 4:E:91:HIS:HA    | 1.68                     | 0.74              |
| 4:F:130:ARG:HH11 | 4:F:130:ARG:HB3  | 1.51                     | 0.74              |
| 4:F:297:ARG:HG2  | 4:F:297:ARG:HH11 | 1.51                     | 0.74              |
| 4:F:62:LYS:HB2   | 4:F:62:LYS:NZ    | 2.02                     | 0.74              |
| 4:A:90:GLN:HE21  | 4:A:90:GLN:HA    | 1.52                     | 0.73              |
| 4:F:317:ASN:HD22 | 4:F:319:ASN:H    | 1.35                     | 0.73              |
| 4:F:243:ARG:HG2  | 4:F:243:ARG:HH11 | 1.53                     | 0.73              |
| 4:E:74:TYR:O     | 4:E:77:TYR:HB3   | 1.89                     | 0.73              |
| 4:A:166:ILE:O    | 4:A:170:THR:HG23 | 1.89                     | 0.73              |
| 4:A:145:VAL:HG22 | 4:A:272:ILE:HD11 | 1.71                     | 0.73              |
| 2:Y:131:DG:H2"   | 2:Y:132:DT:H5"   | 1.70                     | 0.73              |
| 4:F:52:TRP:O     | 4:F:56:CYS:HB2   | 1.89                     | 0.73              |
| 4:E:122:LYS:O    | 4:E:126:ASP:HB2  | 1.89                     | 0.73              |
| 4:F:163:PHE:HE1  | 4:F:261:LEU:HD13 | 1.51                     | 0.72              |
| 4:B:315:TRP:CZ2  | 4:B:324:TYR:CE2  | 2.78                     | 0.72              |
| 2:Y:135:DT:H2"   | 2:Y:136:DC:C6    | 2.25                     | 0.72              |
| 4:F:230:VAL:HG12 | 4:F:250:PRO:HB3  | 1.71                     | 0.72              |
| 4:A:181:ARG:HH11 | 4:A:199:ARG:NH2  | 1.86                     | 0.71              |
| 4:A:187:ARG:HH11 | 4:A:187:ARG:HB3  | 1.56                     | 0.71              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:B:315:TRP:CZ2  | 4:B:324:TYR:CD2  | 2.78                     | 0.71              |
| 1:C:102:DA:H2"   | 1:C:103:DT:H5"   | 1.73                     | 0.71              |
| 2:Y:117:DG:H5"   | 4:F:320:ILE:CD1  | 2.20                     | 0.71              |
| 4:E:32:ARG:HD2   | 4:F:72:ARG:HH21  | 1.55                     | 0.70              |
| 4:B:193:MET:HE1  | 4:B:221:VAL:HG11 | 1.74                     | 0.70              |
| 4:B:233:ASP:O    | 4:B:236:ASN:HB2  | 1.90                     | 0.70              |
| 4:E:317:ASN:HD22 | 4:E:317:ASN:N    | 1.87                     | 0.70              |
| 4:A:161:LEU:HD22 | 4:A:220:LEU:CD1  | 2.22                     | 0.70              |
| 4:F:323:ASN:CG   | 4:F:324:TYR:N    | 2.45                     | 0.70              |
| 4:B:204:VAL:CG2  | 4:E:125:VAL:HG11 | 2.22                     | 0.70              |
| 4:A:27:LEU:HD13  | 4:A:102:SER:CB   | 2.22                     | 0.70              |
| 4:A:217:VAL:O    | 4:A:221:VAL:HG23 | 1.92                     | 0.69              |
| 4:B:204:VAL:HG22 | 4:E:125:VAL:HG11 | 1.74                     | 0.69              |
| 4:B:261:LEU:HA   | 4:B:264:ILE:HD12 | 1.73                     | 0.69              |
| 4:B:147:SER:O    | 4:B:148:LEU:HB2  | 1.91                     | 0.69              |
| 4:E:159:ARG:HB2  | 4:E:224:TRP:CE3  | 2.27                     | 0.69              |
| 4:F:329:ASP:HA   | 4:F:332:THR:HG23 | 1.75                     | 0.69              |
| 4:A:243:ARG:NH1  | 4:A:243:ARG:HG2  | 2.08                     | 0.69              |
| 4:E:159:ARG:HB2  | 4:E:224:TRP:CZ3  | 2.27                     | 0.69              |
| 2:Y:128:DG:H1    | 3:H:109:DC:H42   | 1.41                     | 0.69              |
| 2:X:126:DA:OP1   | 4:A:288:GLY:N    | 2.25                     | 0.68              |
| 4:B:328:LEU:O    | 4:B:332:THR:HG23 | 1.93                     | 0.68              |
| 4:A:19:THR:HG22  | 4:A:23:VAL:CG2   | 2.24                     | 0.68              |
| 4:E:182:VAL:HG23 | 4:E:234:PRO:O    | 1.93                     | 0.68              |
| 4:B:326:ARG:HH11 | 4:B:326:ARG:HG3  | 1.59                     | 0.68              |
| 4:E:169:ASN:OD1  | 4:F:339:LEU:HD12 | 1.94                     | 0.68              |
| 4:E:117:MET:HA   | 4:E:117:MET:CE   | 2.24                     | 0.68              |
| 4:A:23:VAL:O     | 4:A:27:LEU:HB2   | 1.94                     | 0.68              |
| 4:A:27:LEU:CD1   | 4:A:102:SER:HB3  | 2.24                     | 0.67              |
| 4:E:305:SER:OG   | 4:E:308:GLU:HG3  | 1.94                     | 0.67              |
| 3:D:115:DG:H2"   | 3:D:116:DC:O4'   | 1.95                     | 0.67              |
| 2:Y:118:DT:H3    | 3:H:119:DA:N6    | 1.92                     | 0.67              |
| 4:E:209:VAL:O    | 4:E:210:GLU:HG3  | 1.94                     | 0.67              |
| 4:A:192:ARG:HB3  | 4:A:215:LEU:HD23 | 1.77                     | 0.67              |
| 4:B:245:ASN:OD1  | 4:B:247:VAL:HG23 | 1.94                     | 0.67              |
| 4:A:139:ARG:HB2  | 4:A:168:TYR:OH   | 1.95                     | 0.67              |
| 3:D:120:DC:H3'   | 4:B:106:ARG:NH2  | 2.10                     | 0.67              |
| 4:E:75:LEU:HD11  | 4:E:92:LEU:HG    | 1.78                     | 0.66              |
| 4:B:330:SER:C    | 4:B:332:THR:H    | 1.98                     | 0.66              |
| 4:A:27:LEU:HD13  | 4:A:102:SER:HB3  | 1.78                     | 0.66              |
| 4:E:181:ARG:HB2  | 4:E:236:ASN:O    | 1.94                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:F:313:GLY:HA3  | 4:F:315:TRP:CZ3  | 2.31                     | 0.66              |
| 3:D:101:DG:H2"   | 3:D:102:DA:C8    | 2.30                     | 0.66              |
| 4:E:134:ALA:HA   | 4:E:283:TYR:CD2  | 2.30                     | 0.66              |
| 4:E:170:THR:OG1  | 4:E:172:LEU:HD12 | 1.95                     | 0.66              |
| 1:C:102:DA:H2"   | 1:C:103:DT:C5'   | 2.26                     | 0.66              |
| 4:F:215:LEU:O    | 4:F:218:THR:HG22 | 1.96                     | 0.66              |
| 4:F:148:LEU:HD23 | 4:F:148:LEU:O    | 1.95                     | 0.66              |
| 4:E:183:LYS:HG2  | 4:E:234:PRO:HB2  | 1.78                     | 0.66              |
| 4:B:206:THR:HB   | 4:E:131:ALA:HB2  | 1.78                     | 0.66              |
| 4:A:14:LEU:HD12  | 4:A:19:THR:HG23  | 1.78                     | 0.65              |
| 4:E:317:ASN:ND2  | 4:E:317:ASN:H    | 1.93                     | 0.65              |
| 4:B:172:LEU:HD21 | 4:B:197:ILE:HG13 | 1.77                     | 0.65              |
| 4:E:107:PRO:O    | 4:E:113:VAL:HG21 | 1.96                     | 0.65              |
| 2:Y:117:DG:H3'   | 4:F:317:ASN:HB2  | 1.78                     | 0.65              |
| 4:B:134:ALA:HA   | 4:B:283:TYR:HD2  | 1.57                     | 0.65              |
| 1:G:105:DA:C2'   | 1:G:106:DC:H5"   | 2.25                     | 0.65              |
| 4:E:313:GLY:HA3  | 4:E:315:TRP:CZ3  | 2.33                     | 0.64              |
| 4:F:172:LEU:HD21 | 4:F:197:ILE:HG13 | 1.79                     | 0.64              |
| 4:B:257:SER:O    | 4:B:260:ALA:HB3  | 1.97                     | 0.64              |
| 3:H:106:DC:H2'   | 3:H:107:DT:H72   | 1.80                     | 0.64              |
| 4:A:161:LEU:HD22 | 4:A:220:LEU:HD11 | 1.80                     | 0.64              |
| 2:X:116:DT:H5"   | 4:B:173:ARG:HH22 | 1.59                     | 0.64              |
| 4:B:185:ILE:HD11 | 4:B:238:LEU:HD22 | 1.79                     | 0.64              |
| 2:Y:131:DG:H2"   | 2:Y:132:DT:H5'   | 1.78                     | 0.64              |
| 1:C:103:DT:H2"   | 1:C:104:DA:C8    | 2.33                     | 0.64              |
| 4:A:121:ARG:O    | 4:A:125:VAL:HG23 | 1.97                     | 0.64              |
| 2:Y:119:DA:H61   | 3:H:118:DT:H3    | 1.46                     | 0.64              |
| 4:B:295:ALA:O    | 4:B:299:MET:HG3  | 1.98                     | 0.64              |
| 4:B:330:SER:O    | 4:B:332:THR:N    | 2.31                     | 0.63              |
| 4:F:146:ARG:O    | 4:F:150:GLU:HB2  | 1.98                     | 0.63              |
| 3:D:108:DT:H2"   | 3:D:109:DC:H5'   | 1.79                     | 0.63              |
| 4:B:146:ARG:O    | 4:B:148:LEU:N    | 2.31                     | 0.63              |
| 4:B:315:TRP:HZ2  | 4:B:324:TYR:CE2  | 2.16                     | 0.63              |
| 4:A:307:PRO:HG3  | 4:B:306:ILE:CD1  | 2.29                     | 0.63              |
| 2:Y:117:DG:H3'   | 4:F:317:ASN:CB   | 2.29                     | 0.63              |
| 3:H:106:DC:H2'   | 3:H:107:DT:C7    | 2.29                     | 0.63              |
| 4:E:197:ILE:HG22 | 4:E:209:VAL:C    | 2.20                     | 0.63              |
| 4:A:101:ARG:CZ   | 4:B:115:LEU:HD21 | 2.29                     | 0.63              |
| 4:E:148:LEU:H    | 4:E:148:LEU:HD23 | 1.64                     | 0.62              |
| 4:E:217:VAL:O    | 4:E:221:VAL:HG23 | 1.99                     | 0.62              |
| 4:F:193:MET:CB   | 4:F:213:LEU:HD12 | 2.27                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:E:117:MET:HA   | 4:E:117:MET:HE3  | 1.80                     | 0.62              |
| 4:A:15:PRO:CG    | 4:A:18:ALA:HB3   | 2.27                     | 0.62              |
| 4:E:317:ASN:ND2  | 4:E:317:ASN:N    | 2.48                     | 0.62              |
| 4:A:11:LEU:HD13  | 4:A:14:LEU:HD21  | 1.81                     | 0.62              |
| 4:B:166:ILE:O    | 4:B:170:THR:HG23 | 2.00                     | 0.62              |
| 4:E:110:SER:OG   | 4:E:113:VAL:HG23 | 1.99                     | 0.62              |
| 4:F:306:ILE:N    | 4:F:307:PRO:HD2  | 2.15                     | 0.62              |
| 2:Y:122:DC:H2''  | 2:Y:123:DT:H5'   | 1.81                     | 0.62              |
| 4:F:242:VAL:O    | 4:F:242:VAL:HG23 | 1.99                     | 0.62              |
| 4:E:143:ASP:O    | 4:E:146:ARG:HG2  | 1.99                     | 0.62              |
| 4:B:228:SER:OG   | 4:B:230:VAL:HG13 | 2.00                     | 0.62              |
| 4:F:297:ARG:HG2  | 4:F:297:ARG:NH1  | 2.15                     | 0.62              |
| 4:B:89:GLN:HG2   | 4:B:117:MET:HE2  | 1.81                     | 0.62              |
| 4:A:106:ARG:O    | 4:A:109:ASP:HB2  | 2.00                     | 0.62              |
| 4:B:169:ASN:OD1  | 4:E:339:LEU:HD12 | 1.99                     | 0.62              |
| 2:Y:117:DG:C2'   | 2:Y:118:DT:H71   | 2.28                     | 0.62              |
| 4:A:197:ILE:O    | 4:A:197:ILE:HG13 | 1.99                     | 0.62              |
| 4:A:318:VAL:HG23 | 4:A:319:ASN:N    | 2.13                     | 0.62              |
| 2:Y:135:DT:H2''  | 2:Y:136:DC:H6    | 1.64                     | 0.61              |
| 4:B:96:ASN:HD21  | 4:B:108:SER:HB2  | 1.64                     | 0.61              |
| 4:E:116:VAL:O    | 4:E:119:ARG:HB3  | 2.00                     | 0.61              |
| 4:E:85:VAL:HG23  | 4:E:129:GLU:OE2  | 2.00                     | 0.61              |
| 3:H:102:DA:H2''  | 3:H:103:DT:O5'   | 2.00                     | 0.61              |
| 4:E:74:TYR:CE1   | 4:E:78:LEU:HD11  | 2.36                     | 0.61              |
| 4:F:272:ILE:C    | 4:F:273:TYR:HD1  | 2.04                     | 0.61              |
| 4:F:325:ILE:CG2  | 4:F:327:ASN:ND2  | 2.64                     | 0.61              |
| 4:B:236:ASN:ND2  | 4:B:250:PRO:HB3  | 2.16                     | 0.61              |
| 1:C:108:DT:H2''  | 1:C:109:DC:H5'   | 1.81                     | 0.61              |
| 2:Y:123:DT:H3'   | 4:E:38:SER:OG    | 2.01                     | 0.61              |
| 4:E:311:GLN:HG3  | 4:E:312:ALA:N    | 2.14                     | 0.61              |
| 4:F:333:GLY:O    | 4:F:334:ALA:HB3  | 1.99                     | 0.61              |
| 4:B:330:SER:C    | 4:B:332:THR:N    | 2.54                     | 0.61              |
| 4:F:323:ASN:CG   | 4:F:324:TYR:H    | 2.05                     | 0.60              |
| 4:B:89:GLN:HG2   | 4:B:117:MET:CE   | 2.31                     | 0.60              |
| 4:A:164:LEU:HD11 | 4:A:268:THR:HG21 | 1.84                     | 0.60              |
| 4:B:194:LEU:HD13 | 4:B:212:ALA:CB   | 2.27                     | 0.60              |
| 4:E:158:ILE:HD13 | 4:E:223:ARG:HG2  | 1.83                     | 0.60              |
| 4:E:169:ASN:ND2  | 4:E:213:LEU:HA   | 2.17                     | 0.60              |
| 4:F:214:SER:O    | 4:F:218:THR:HB   | 2.02                     | 0.60              |
| 4:F:272:ILE:HG22 | 4:F:273:TYR:CD1  | 2.37                     | 0.60              |
| 4:E:78:LEU:N     | 4:E:78:LEU:HD12  | 2.17                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:B:94:GLN:HA    | 4:B:94:GLN:OE1   | 2.02                     | 0.59              |
| 4:F:320:ILE:HD12 | 4:F:320:ILE:N    | 2.17                     | 0.59              |
| 4:E:200:THR:HG22 | 4:E:201:LYS:N    | 2.14                     | 0.59              |
| 4:E:154:ARG:NH1  | 4:E:154:ARG:HB3  | 2.12                     | 0.59              |
| 4:E:72:ARG:HE    | 4:E:116:VAL:HG13 | 1.67                     | 0.59              |
| 4:E:193:MET:CG   | 4:E:218:THR:HG23 | 2.15                     | 0.59              |
| 4:A:11:LEU:HD22  | 4:A:12:PRO:HD3   | 1.84                     | 0.59              |
| 4:A:20:SER:O     | 4:A:21:ASP:HB2   | 2.03                     | 0.59              |
| 4:B:30:MET:SD    | 4:B:101:ARG:HG2  | 2.43                     | 0.59              |
| 4:A:169:ASN:HD22 | 4:A:169:ASN:C    | 2.03                     | 0.58              |
| 4:A:181:ARG:HB2  | 4:A:236:ASN:O    | 2.02                     | 0.58              |
| 4:E:243:ARG:CG   | 4:E:243:ARG:HH11 | 2.13                     | 0.58              |
| 4:B:29:ASP:O     | 4:B:32:ARG:HB3   | 2.02                     | 0.58              |
| 4:F:180:ILE:HD13 | 4:F:195:ILE:HG21 | 1.85                     | 0.58              |
| 4:F:320:ILE:O    | 4:F:321:VAL:C    | 2.41                     | 0.58              |
| 3:D:120:DC:H3'   | 4:B:106:ARG:HH21 | 1.67                     | 0.58              |
| 4:F:62:LYS:HB2   | 4:F:62:LYS:HZ3   | 1.68                     | 0.58              |
| 4:B:61:ARG:HG2   | 4:B:61:ARG:HH11  | 1.67                     | 0.58              |
| 4:F:72:ARG:HH11  | 4:F:72:ARG:CG    | 2.16                     | 0.58              |
| 4:A:161:LEU:HD13 | 4:A:220:LEU:HD11 | 1.85                     | 0.58              |
| 4:F:242:VAL:HG12 | 4:F:248:ALA:HA   | 1.86                     | 0.58              |
| 4:E:106:ARG:HD3  | 4:E:109:ASP:OD2  | 2.03                     | 0.58              |
| 4:F:126:ASP:C    | 4:F:128:GLY:H    | 2.06                     | 0.58              |
| 4:B:236:ASN:HD21 | 4:B:250:PRO:HB3  | 1.69                     | 0.57              |
| 4:B:45:LEU:HD23  | 4:B:45:LEU:C     | 2.23                     | 0.57              |
| 4:E:171:LEU:HD23 | 4:E:171:LEU:H    | 1.67                     | 0.57              |
| 4:F:121:ARG:NH1  | 4:F:121:ARG:HG3  | 2.14                     | 0.57              |
| 2:Y:122:DC:H2''  | 2:Y:123:DT:C5'   | 2.35                     | 0.57              |
| 4:A:299:MET:HE2  | 4:A:304:VAL:HG11 | 1.87                     | 0.57              |
| 4:A:193:MET:HE1  | 4:A:221:VAL:HB   | 1.86                     | 0.57              |
| 4:A:22:GLU:C     | 4:A:24:ARG:H     | 2.08                     | 0.57              |
| 4:E:163:PHE:CE2  | 4:E:261:LEU:HD22 | 2.40                     | 0.57              |
| 4:F:320:ILE:O    | 4:F:323:ASN:N    | 2.38                     | 0.57              |
| 4:F:149:MET:HE3  | 4:F:161:LEU:HB2  | 1.87                     | 0.57              |
| 4:B:238:LEU:O    | 4:B:238:LEU:HD12 | 2.05                     | 0.57              |
| 4:B:22:GLU:O     | 4:B:25:LYS:N     | 2.33                     | 0.57              |
| 4:F:325:ILE:HG22 | 4:F:327:ASN:ND2  | 2.19                     | 0.57              |
| 4:B:116:VAL:O    | 4:B:120:ILE:HG13 | 2.05                     | 0.57              |
| 1:G:111:DT:OP2   | 4:F:50:ARG:NH1   | 2.38                     | 0.56              |
| 4:F:323:ASN:O    | 4:F:325:ILE:N    | 2.38                     | 0.56              |
| 4:A:106:ARG:O    | 4:A:109:ASP:CB   | 2.53                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:F:217:VAL:O    | 4:F:221:VAL:HG23 | 2.05                     | 0.56              |
| 4:B:74:TYR:O     | 4:B:77:TYR:HB3   | 2.06                     | 0.56              |
| 4:B:226:SER:OG   | 4:B:227:VAL:N    | 2.39                     | 0.56              |
| 4:F:97:MET:O     | 4:F:101:ARG:HB2  | 2.05                     | 0.56              |
| 4:B:161:LEU:HD23 | 4:B:220:LEU:HD13 | 1.88                     | 0.56              |
| 4:B:306:ILE:N    | 4:B:307:PRO:HD2  | 2.20                     | 0.56              |
| 4:B:306:ILE:HG21 | 4:B:318:VAL:HG13 | 1.86                     | 0.56              |
| 3:D:112:DA:OP1   | 4:A:81:ARG:NH2   | 2.39                     | 0.56              |
| 2:Y:117:DG:C8    | 2:Y:118:DT:H73   | 2.40                     | 0.56              |
| 4:A:170:THR:OG1  | 4:A:172:LEU:HG   | 2.06                     | 0.56              |
| 4:A:22:GLU:C     | 4:A:24:ARG:N     | 2.55                     | 0.56              |
| 4:E:96:ASN:OD1   | 4:E:106:ARG:HB2  | 2.06                     | 0.56              |
| 4:B:96:ASN:ND2   | 4:B:108:SER:HB2  | 2.21                     | 0.56              |
| 4:A:27:LEU:HD13  | 4:A:102:SER:HB2  | 1.86                     | 0.56              |
| 4:E:142:PHE:CZ   | 4:E:165:GLY:HA2  | 2.40                     | 0.56              |
| 4:B:168:TYR:CD2  | 4:B:168:TYR:C    | 2.79                     | 0.56              |
| 4:E:22:GLU:HG3   | 4:E:23:VAL:N     | 2.20                     | 0.56              |
| 2:Y:117:DG:H2''  | 2:Y:118:DT:H71   | 1.87                     | 0.56              |
| 4:A:11:LEU:CD2   | 4:A:12:PRO:HD3   | 2.36                     | 0.56              |
| 4:A:27:LEU:O     | 4:A:31:PHE:HD1   | 1.88                     | 0.56              |
| 1:C:102:DA:C2'   | 1:C:103:DT:H5''  | 2.35                     | 0.56              |
| 4:A:193:MET:CE   | 4:A:221:VAL:HB   | 2.35                     | 0.56              |
| 3:D:114:DA:H5''  | 4:A:132:LYS:O    | 2.05                     | 0.56              |
| 4:F:297:ARG:CG   | 4:F:297:ARG:HH11 | 2.18                     | 0.55              |
| 4:B:209:VAL:HG22 | 4:B:210:GLU:N    | 2.21                     | 0.55              |
| 2:Y:117:DG:H2'   | 2:Y:118:DT:H71   | 1.89                     | 0.55              |
| 4:F:243:ARG:HG2  | 4:F:243:ARG:NH1  | 2.21                     | 0.55              |
| 4:B:214:SER:HA   | 4:E:336:VAL:HG13 | 1.89                     | 0.55              |
| 4:F:323:ASN:ND2  | 4:F:324:TYR:N    | 2.55                     | 0.55              |
| 4:F:121:ARG:O    | 4:F:125:VAL:HG23 | 2.06                     | 0.55              |
| 4:A:161:LEU:HD22 | 4:A:220:LEU:HD12 | 1.88                     | 0.55              |
| 4:F:313:GLY:HA3  | 4:F:315:TRP:CE3  | 2.42                     | 0.55              |
| 3:D:122:DT:OP2   | 4:B:101:ARG:NH1  | 2.39                     | 0.55              |
| 2:Y:118:DT:H72   | 4:F:319:ASN:CG   | 2.27                     | 0.55              |
| 4:E:169:ASN:HD22 | 4:E:213:LEU:HA   | 1.72                     | 0.55              |
| 3:D:135:DT:H1'   | 4:B:244:LYS:HD3  | 1.89                     | 0.55              |
| 3:D:133:DT:H2'   | 3:D:134:DA:C8    | 2.41                     | 0.55              |
| 2:Y:119:DA:H2''  | 2:Y:120:DT:O5'   | 2.06                     | 0.55              |
| 4:A:192:ARG:HH11 | 4:B:331:GLU:HA   | 1.72                     | 0.55              |
| 4:F:272:ILE:HG22 | 4:F:273:TYR:CE1  | 2.42                     | 0.55              |
| 3:H:113:DT:C7    | 4:E:87:THR:HG23  | 2.37                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:111:DT:OP2   | 4:B:50:ARG:NH2   | 2.35                     | 0.55              |
| 4:A:55:TRP:O     | 4:A:59:ASN:HB2   | 2.07                     | 0.54              |
| 4:E:92:LEU:HD12  | 4:E:117:MET:SD   | 2.47                     | 0.54              |
| 4:E:270:ARG:HA   | 4:E:274:GLY:O    | 2.07                     | 0.54              |
| 4:A:72:ARG:CD    | 4:A:116:VAL:HG21 | 2.37                     | 0.54              |
| 4:B:45:LEU:O     | 4:B:45:LEU:HD23  | 2.07                     | 0.54              |
| 2:X:116:DT:C5'   | 4:B:173:ARG:HH21 | 2.20                     | 0.54              |
| 4:A:168:TYR:HA   | 4:A:291:ALA:HB1  | 1.89                     | 0.54              |
| 4:B:315:TRP:HE1  | 4:B:324:TYR:HE2  | 1.56                     | 0.54              |
| 4:F:126:ASP:C    | 4:F:128:GLY:N    | 2.61                     | 0.54              |
| 4:B:159:ARG:HB2  | 4:B:224:TRP:CZ3  | 2.42                     | 0.54              |
| 4:F:317:ASN:ND2  | 4:F:319:ASN:OD1  | 2.41                     | 0.54              |
| 3:H:109:DC:H2''  | 3:H:110:DG:C8    | 2.43                     | 0.54              |
| 4:B:111:ASN:O    | 4:B:115:LEU:HG   | 2.08                     | 0.54              |
| 4:B:195:ILE:HG22 | 4:B:196:HIS:N    | 2.22                     | 0.54              |
| 4:A:90:GLN:HE21  | 4:A:90:GLN:CA    | 2.17                     | 0.54              |
| 4:A:304:VAL:HG12 | 4:A:309:ILE:HG13 | 1.89                     | 0.54              |
| 4:A:233:ASP:O    | 4:A:236:ASN:HB2  | 2.08                     | 0.54              |
| 4:F:48:VAL:HG21  | 4:F:91:HIS:HA    | 1.89                     | 0.54              |
| 4:E:182:VAL:O    | 4:E:185:ILE:N    | 2.37                     | 0.54              |
| 2:X:116:DT:C5'   | 4:B:173:ARG:HH22 | 2.18                     | 0.54              |
| 4:A:101:ARG:NH1  | 4:B:115:LEU:HD21 | 2.22                     | 0.54              |
| 4:B:204:VAL:O    | 4:B:204:VAL:HG13 | 2.09                     | 0.53              |
| 4:A:307:PRO:HG3  | 4:B:306:ILE:HD13 | 1.88                     | 0.53              |
| 4:B:31:PHE:HD1   | 4:B:42:TRP:CH2   | 2.26                     | 0.53              |
| 4:A:83:LEU:HD22  | 4:A:87:THR:HG21  | 1.90                     | 0.53              |
| 4:B:261:LEU:HA   | 4:B:264:ILE:CD1  | 2.36                     | 0.53              |
| 4:E:304:VAL:HG12 | 4:E:309:ILE:HG13 | 1.88                     | 0.53              |
| 3:D:117:DA:H2''  | 3:D:118:DT:OP2   | 2.08                     | 0.53              |
| 4:A:171:LEU:O    | 4:A:292:ARG:NH1  | 2.42                     | 0.53              |
| 4:B:248:ALA:O    | 4:B:249:ALA:HB2  | 2.08                     | 0.53              |
| 4:B:234:PRO:C    | 4:B:236:ASN:H    | 2.10                     | 0.53              |
| 4:B:315:TRP:NE1  | 4:B:324:TYR:HE2  | 2.07                     | 0.53              |
| 4:B:31:PHE:HD1   | 4:B:42:TRP:HH2   | 1.55                     | 0.53              |
| 3:H:116:DC:OP1   | 4:E:292:ARG:NH2  | 2.42                     | 0.53              |
| 4:F:272:ILE:CG2  | 4:F:273:TYR:CE1  | 2.92                     | 0.53              |
| 4:F:237:TYR:CE1  | 4:F:255:GLN:HB3  | 2.43                     | 0.53              |
| 4:A:11:LEU:HD22  | 4:A:12:PRO:CD    | 2.39                     | 0.52              |
| 4:E:60:ASN:O     | 4:E:61:ARG:HD3   | 2.09                     | 0.52              |
| 4:B:235:ASN:HD22 | 4:B:235:ASN:N    | 2.07                     | 0.52              |
| 4:B:299:MET:O    | 4:B:304:VAL:HG23 | 2.10                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:B:234:PRO:O    | 4:B:236:ASN:N    | 2.30                     | 0.52              |
| 4:E:172:LEU:HD23 | 4:E:176:GLU:OE2  | 2.09                     | 0.52              |
| 3:H:118:DT:H2"   | 3:H:119:DA:C8    | 2.44                     | 0.52              |
| 3:H:117:DA:H4'   | 3:H:118:DT:OP1   | 2.09                     | 0.52              |
| 4:B:320:ILE:HA   | 4:B:323:ASN:HB2  | 1.92                     | 0.52              |
| 4:A:317:ASN:O    | 4:A:319:ASN:N    | 2.42                     | 0.52              |
| 4:A:126:ASP:C    | 4:A:128:GLY:H    | 2.13                     | 0.52              |
| 4:F:268:THR:O    | 4:F:268:THR:HG22 | 2.10                     | 0.52              |
| 4:E:78:LEU:HB3   | 4:E:83:LEU:HD12  | 1.92                     | 0.52              |
| 4:E:287:SER:H    | 4:E:290:SER:HG   | 1.58                     | 0.52              |
| 4:A:229:GLY:O    | 4:A:250:PRO:HG2  | 2.10                     | 0.52              |
| 4:A:326:ARG:HD3  | 4:F:210:GLU:HG3  | 1.91                     | 0.52              |
| 4:F:24:ARG:O     | 4:F:28:MET:HB2   | 2.10                     | 0.52              |
| 4:F:146:ARG:HA   | 4:F:161:LEU:HD11 | 1.92                     | 0.52              |
| 4:A:59:ASN:O     | 4:A:61:ARG:HD3   | 2.09                     | 0.52              |
| 3:D:119:DA:P     | 4:B:121:ARG:HH22 | 2.33                     | 0.52              |
| 3:D:112:DA:H1'   | 3:D:113:DT:H5"   | 1.92                     | 0.51              |
| 4:A:201:LYS:HG3  | 4:A:202:THR:OG1  | 2.09                     | 0.51              |
| 4:E:245:ASN:OD1  | 4:E:246:GLY:N    | 2.42                     | 0.51              |
| 4:B:251:SER:OG   | 4:B:252:ALA:N    | 2.42                     | 0.51              |
| 3:D:125:DT:H2"   | 3:D:126:DA:O5'   | 2.11                     | 0.51              |
| 4:B:226:SER:O    | 4:B:228:SER:N    | 2.43                     | 0.51              |
| 3:H:118:DT:H2"   | 3:H:119:DA:N7    | 2.25                     | 0.51              |
| 3:H:113:DT:H71   | 4:E:87:THR:HG23  | 1.93                     | 0.51              |
| 4:F:335:MET:HE3  | 4:F:335:MET:HA   | 1.93                     | 0.51              |
| 4:B:332:THR:HG22 | 4:B:333:GLY:H    | 1.75                     | 0.51              |
| 3:D:123:DT:C2    | 3:D:124:DA:C8    | 2.98                     | 0.51              |
| 3:H:116:DC:H5"   | 4:E:173:ARG:HH22 | 1.76                     | 0.51              |
| 4:F:55:TRP:CD1   | 4:F:56:CYS:N     | 2.79                     | 0.51              |
| 4:E:137:PHE:CE2  | 4:E:141:ASP:HB3  | 2.46                     | 0.51              |
| 4:F:45:LEU:O     | 4:F:45:LEU:HD23  | 2.10                     | 0.51              |
| 4:B:185:ILE:HD13 | 4:B:193:MET:HE3  | 1.93                     | 0.51              |
| 4:A:141:ASP:O    | 4:A:145:VAL:HG23 | 2.11                     | 0.51              |
| 3:H:103:DT:H2"   | 3:H:104:DA:C8    | 2.46                     | 0.51              |
| 4:E:101:ARG:HA   | 4:F:111:ASN:HD21 | 1.76                     | 0.51              |
| 4:A:124:ASN:ND2  | 4:A:129:GLU:OE2  | 2.43                     | 0.51              |
| 2:Y:117:DG:C2'   | 2:Y:118:DT:C7    | 2.89                     | 0.51              |
| 4:E:197:ILE:HG12 | 4:E:197:ILE:O    | 2.11                     | 0.51              |
| 4:F:322:MET:HA   | 4:F:322:MET:CE   | 2.40                     | 0.51              |
| 4:A:154:ARG:HH11 | 4:A:154:ARG:HG3  | 1.76                     | 0.51              |
| 4:F:25:LYS:HD3   | 4:F:29:ASP:OD1   | 2.10                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:H:108:DT:H2"   | 3:H:109:DC:C5'   | 2.41                     | 0.51              |
| 4:F:170:THR:O    | 4:F:171:LEU:HB2  | 2.10                     | 0.50              |
| 4:F:331:GLU:O    | 4:F:332:THR:OG1  | 2.29                     | 0.50              |
| 4:B:90:GLN:HE21  | 4:B:94:GLN:HG2   | 1.74                     | 0.50              |
| 4:B:214:SER:OG   | 4:B:217:VAL:HG23 | 2.11                     | 0.50              |
| 4:A:192:ARG:HE   | 4:A:215:LEU:CD2  | 2.24                     | 0.50              |
| 4:E:163:PHE:HE2  | 4:E:261:LEU:HD13 | 1.76                     | 0.50              |
| 4:E:256:LEU:HD22 | 4:E:260:ALA:CB   | 2.41                     | 0.50              |
| 4:B:80:ALA:C     | 4:B:82:GLY:H     | 2.14                     | 0.50              |
| 4:B:249:ALA:N    | 4:B:250:PRO:HD3  | 2.26                     | 0.50              |
| 4:B:249:ALA:H    | 4:B:250:PRO:HD3  | 1.76                     | 0.50              |
| 4:E:126:ASP:C    | 4:E:128:GLY:H    | 2.15                     | 0.50              |
| 4:E:156:GLN:C    | 4:E:158:ILE:H    | 2.15                     | 0.50              |
| 4:B:156:GLN:HB3  | 4:B:242:VAL:HG11 | 1.92                     | 0.50              |
| 4:B:110:SER:O    | 4:B:112:ALA:N    | 2.44                     | 0.50              |
| 4:E:195:ILE:HD11 | 4:E:213:LEU:HD21 | 1.94                     | 0.50              |
| 4:F:116:VAL:HG13 | 4:F:117:MET:N    | 2.26                     | 0.50              |
| 4:B:293:VAL:HG22 | 4:B:294:GLY:N    | 2.25                     | 0.50              |
| 4:E:85:VAL:HG23  | 4:E:129:GLU:CD   | 2.32                     | 0.50              |
| 4:F:115:LEU:O    | 4:F:116:VAL:C    | 2.48                     | 0.50              |
| 4:A:34:ARG:C     | 4:A:36:ALA:H     | 2.15                     | 0.50              |
| 4:A:30:MET:HA    | 4:B:115:LEU:HD12 | 1.93                     | 0.50              |
| 3:H:101:DG:H2"   | 3:H:102:DA:OP2   | 2.11                     | 0.50              |
| 4:B:263:GLY:HA2  | 4:B:266:GLU:HG3  | 1.94                     | 0.50              |
| 4:E:297:ARG:HA   | 4:E:325:ILE:HG22 | 1.94                     | 0.50              |
| 4:B:193:MET:HE1  | 4:B:221:VAL:CG1  | 2.41                     | 0.50              |
| 4:F:126:ASP:O    | 4:F:128:GLY:N    | 2.45                     | 0.49              |
| 4:E:163:PHE:CD1  | 4:E:164:LEU:HD23 | 2.47                     | 0.49              |
| 4:E:68:PRO:HG2   | 4:E:69:GLU:H     | 1.77                     | 0.49              |
| 4:E:182:VAL:O    | 4:E:183:LYS:C    | 2.48                     | 0.49              |
| 4:A:34:ARG:O     | 4:A:36:ALA:N     | 2.45                     | 0.49              |
| 3:H:134:DA:C8    | 3:H:135:DT:H72   | 2.48                     | 0.49              |
| 4:E:113:VAL:O    | 4:E:116:VAL:HG23 | 2.11                     | 0.49              |
| 4:A:192:ARG:HE   | 4:A:215:LEU:HD21 | 1.77                     | 0.49              |
| 4:B:28:MET:O     | 4:B:29:ASP:C     | 2.50                     | 0.49              |
| 4:E:173:ARG:HG2  | 4:E:173:ARG:HH11 | 1.77                     | 0.49              |
| 4:F:106:ARG:O    | 4:F:109:ASP:HB2  | 2.13                     | 0.49              |
| 4:A:158:ILE:HD11 | 4:A:223:ARG:CZ   | 2.42                     | 0.49              |
| 4:A:13:ALA:O     | 4:A:15:PRO:N     | 2.46                     | 0.49              |
| 4:A:72:ARG:HD2   | 4:A:116:VAL:HG21 | 1.94                     | 0.49              |
| 4:F:204:VAL:O    | 4:F:204:VAL:HG13 | 2.13                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:A:195:ILE:HD12 | 4:A:213:LEU:HD21 | 1.95                     | 0.49              |
| 4:B:258:THR:HA   | 4:B:261:LEU:CD1  | 2.38                     | 0.49              |
| 4:F:331:GLU:C    | 4:F:332:THR:OG1  | 2.50                     | 0.49              |
| 4:E:197:ILE:CG2  | 4:E:209:VAL:HA   | 2.43                     | 0.49              |
| 2:Y:119:DA:N6    | 3:H:118:DT:H3    | 2.08                     | 0.49              |
| 4:E:90:GLN:HE21  | 4:E:94:GLN:HG2   | 1.78                     | 0.49              |
| 4:E:156:GLN:O    | 4:E:158:ILE:N    | 2.46                     | 0.49              |
| 4:E:289:HIS:O    | 4:E:290:SER:C    | 2.51                     | 0.49              |
| 4:A:320:ILE:O    | 4:A:322:MET:N    | 2.46                     | 0.49              |
| 4:E:154:ARG:HG3  | 4:E:157:ASP:HB2  | 1.94                     | 0.49              |
| 4:B:226:SER:O    | 4:B:229:GLY:N    | 2.46                     | 0.49              |
| 4:A:145:VAL:HG22 | 4:A:272:ILE:CD1  | 2.42                     | 0.49              |
| 4:F:218:THR:CG2  | 4:F:219:LYS:N    | 2.75                     | 0.49              |
| 4:B:45:LEU:CD2   | 4:B:45:LEU:C     | 2.81                     | 0.49              |
| 4:A:107:PRO:O    | 4:A:108:SER:C    | 2.49                     | 0.49              |
| 3:D:122:DT:C5'   | 4:B:97:MET:HE2   | 2.34                     | 0.49              |
| 4:E:57:LYS:O     | 4:E:58:LEU:HB2   | 2.13                     | 0.49              |
| 4:F:273:TYR:CD1  | 4:F:273:TYR:N    | 2.80                     | 0.49              |
| 4:E:287:SER:N    | 4:E:290:SER:OG   | 2.44                     | 0.49              |
| 4:F:227:VAL:O    | 4:F:227:VAL:CG1  | 2.61                     | 0.49              |
| 4:E:185:ILE:HG21 | 4:E:193:MET:CE   | 2.43                     | 0.48              |
| 3:H:134:DA:C2'   | 3:H:135:DT:H5"   | 2.38                     | 0.48              |
| 4:E:238:LEU:HD23 | 4:E:238:LEU:O    | 2.13                     | 0.48              |
| 4:A:245:ASN:OD1  | 4:A:247:VAL:HB   | 2.13                     | 0.48              |
| 4:B:326:ARG:NH1  | 4:B:326:ARG:HG3  | 2.28                     | 0.48              |
| 4:F:180:ILE:HD13 | 4:F:195:ILE:HD13 | 1.95                     | 0.48              |
| 4:E:68:PRO:O     | 4:E:69:GLU:C     | 2.52                     | 0.48              |
| 4:E:235:ASN:HD22 | 4:E:235:ASN:N    | 2.09                     | 0.48              |
| 4:B:221:VAL:O    | 4:B:225:ILE:HG13 | 2.13                     | 0.48              |
| 4:A:80:ALA:C     | 4:A:82:GLY:N     | 2.65                     | 0.48              |
| 4:B:217:VAL:O    | 4:B:221:VAL:HG23 | 2.14                     | 0.48              |
| 4:A:200:THR:HG21 | 4:A:205:SER:OG   | 2.13                     | 0.48              |
| 4:F:169:ASN:C    | 4:F:169:ASN:HD22 | 2.14                     | 0.48              |
| 3:D:103:DT:O2    | 4:A:244:LYS:HE3  | 2.12                     | 0.48              |
| 4:E:221:VAL:O    | 4:E:225:ILE:HG13 | 2.13                     | 0.48              |
| 3:H:114:DA:H5"   | 4:E:132:LYS:O    | 2.13                     | 0.48              |
| 4:F:72:ARG:NH1   | 4:F:72:ARG:CG    | 2.77                     | 0.48              |
| 4:E:187:ARG:HH22 | 4:E:222:GLU:HG2  | 1.78                     | 0.48              |
| 4:E:78:LEU:HD12  | 4:E:78:LEU:H     | 1.77                     | 0.48              |
| 4:F:333:GLY:O    | 4:F:334:ALA:CB   | 2.61                     | 0.48              |
| 4:E:248:ALA:O    | 4:E:250:PRO:HD3  | 2.13                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:A:321:VAL:HG23 | 4:A:321:VAL:O    | 2.14                     | 0.48              |
| 4:B:145:VAL:HG11 | 4:B:164:LEU:HD12 | 1.94                     | 0.48              |
| 2:X:118:DT:H2"   | 2:X:119:DA:C8    | 2.49                     | 0.48              |
| 4:B:78:LEU:HD22  | 4:B:83:LEU:HD12  | 1.96                     | 0.48              |
| 1:G:106:DC:H2"   | 1:G:107:UMP:O5'  | 2.14                     | 0.48              |
| 4:E:171:LEU:HD22 | 4:E:295:ALA:CB   | 2.43                     | 0.48              |
| 4:F:146:ARG:O    | 4:F:150:GLU:N    | 2.47                     | 0.48              |
| 4:A:14:LEU:HD12  | 4:A:19:THR:CG2   | 2.42                     | 0.48              |
| 4:E:163:PHE:CD2  | 4:E:261:LEU:HD22 | 2.48                     | 0.48              |
| 2:Y:117:DG:H2'   | 2:Y:118:DT:C7    | 2.44                     | 0.47              |
| 4:E:74:TYR:O     | 4:E:78:LEU:HD13  | 2.14                     | 0.47              |
| 4:A:134:ALA:HA   | 4:A:283:TYR:CE2  | 2.49                     | 0.47              |
| 4:B:90:GLN:HE21  | 4:B:94:GLN:CG    | 2.27                     | 0.47              |
| 4:E:256:LEU:HD22 | 4:E:260:ALA:HB3  | 1.96                     | 0.47              |
| 3:H:108:DT:H2"   | 3:H:109:DC:H5"   | 1.96                     | 0.47              |
| 4:B:258:THR:CA   | 4:B:261:LEU:HD12 | 2.40                     | 0.47              |
| 4:A:317:ASN:O    | 4:A:318:VAL:C    | 2.52                     | 0.47              |
| 4:F:107:PRO:C    | 4:F:109:ASP:H    | 2.17                     | 0.47              |
| 4:E:187:ARG:HH12 | 4:E:222:GLU:CD   | 2.18                     | 0.47              |
| 4:F:329:ASP:O    | 4:F:330:SER:C    | 2.53                     | 0.47              |
| 4:F:339:LEU:HD23 | 4:F:339:LEU:HA   | 1.57                     | 0.47              |
| 4:E:163:PHE:HB2  | 4:E:239:PHE:CE2  | 2.50                     | 0.47              |
| 4:E:23:VAL:HA    | 4:E:26:ASN:HD22  | 1.79                     | 0.47              |
| 4:A:92:LEU:HD21  | 4:A:108:SER:HB2  | 1.96                     | 0.47              |
| 4:A:256:LEU:HD23 | 4:A:256:LEU:HA   | 1.50                     | 0.47              |
| 4:F:121:ARG:CG   | 4:F:121:ARG:NH1  | 2.75                     | 0.47              |
| 4:F:272:ILE:CG2  | 4:F:273:TYR:HE1  | 2.27                     | 0.47              |
| 4:E:26:ASN:CB    | 4:E:102:SER:HA   | 2.45                     | 0.47              |
| 4:E:256:LEU:O    | 4:E:257:SER:O    | 2.33                     | 0.47              |
| 4:A:177:ILE:HG23 | 4:A:180:ILE:HD12 | 1.96                     | 0.47              |
| 4:E:49:CYS:SG    | 4:E:98:LEU:HD22  | 2.55                     | 0.47              |
| 4:E:243:ARG:NH1  | 4:E:243:ARG:CG   | 2.75                     | 0.47              |
| 4:F:161:LEU:O    | 4:F:161:LEU:HG   | 2.15                     | 0.47              |
| 4:E:102:SER:C    | 4:E:104:LEU:H    | 2.17                     | 0.47              |
| 1:C:106:DC:H2"   | 1:C:107:UMP:H6   | 1.80                     | 0.47              |
| 4:A:310:MET:HE3  | 4:A:318:VAL:N    | 2.30                     | 0.47              |
| 4:E:154:ARG:CB   | 4:E:154:ARG:NH1  | 2.79                     | 0.46              |
| 4:F:320:ILE:HD12 | 4:F:320:ILE:H    | 1.78                     | 0.46              |
| 4:E:156:GLN:C    | 4:E:158:ILE:N    | 2.68                     | 0.46              |
| 4:F:185:ILE:HD11 | 4:F:238:LEU:HD22 | 1.95                     | 0.46              |
| 4:F:60:ASN:C     | 4:F:61:ARG:HD3   | 2.35                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:F:64:PHE:HA    | 4:F:65:PRO:C     | 2.34                     | 0.46              |
| 3:H:124:DA:H2'   | 3:H:125:DT:H72   | 1.97                     | 0.46              |
| 4:F:269:HIS:C    | 4:F:271:LEU:H    | 2.19                     | 0.46              |
| 4:B:319:ASN:O    | 4:B:319:ASN:ND2  | 2.48                     | 0.46              |
| 4:E:142:PHE:CE1  | 4:E:165:GLY:HA2  | 2.50                     | 0.46              |
| 4:B:139:ARG:HG2  | 4:B:139:ARG:NH1  | 2.30                     | 0.46              |
| 4:E:86:LYS:O     | 4:E:86:LYS:HD3   | 2.16                     | 0.46              |
| 4:E:195:ILE:CD1  | 4:E:213:LEU:HD21 | 2.45                     | 0.46              |
| 4:F:236:ASN:OD1  | 4:F:251:SER:O    | 2.34                     | 0.46              |
| 4:B:148:LEU:HD11 | 4:B:271:LEU:HD12 | 1.98                     | 0.46              |
| 4:F:38:SER:O     | 4:F:41:THR:N     | 2.45                     | 0.46              |
| 4:B:57:LYS:O     | 4:B:59:ASN:N     | 2.48                     | 0.46              |
| 1:G:106:DC:H2''  | 1:G:107:UMP:H6   | 1.81                     | 0.46              |
| 4:F:230:VAL:C    | 4:F:232:ASP:H    | 2.19                     | 0.46              |
| 3:D:105:DA:H2''  | 3:D:106:DC:O5'   | 2.14                     | 0.46              |
| 4:F:166:ILE:HG12 | 4:F:213:LEU:HD21 | 1.97                     | 0.46              |
| 2:Y:116:DT:O5'   | 4:F:201:LYS:HE3  | 2.15                     | 0.46              |
| 4:F:329:ASP:CA   | 4:F:332:THR:HG23 | 2.45                     | 0.46              |
| 3:D:107:DT:H2''  | 3:D:108:DT:H5'   | 1.96                     | 0.46              |
| 4:A:204:VAL:HG22 | 4:A:204:VAL:O    | 2.16                     | 0.46              |
| 4:E:173:ARG:O    | 4:E:177:ILE:HG13 | 2.15                     | 0.46              |
| 4:E:44:MET:HA    | 4:E:47:SER:HB3   | 1.98                     | 0.46              |
| 4:A:318:VAL:CG2  | 4:A:319:ASN:N    | 2.79                     | 0.46              |
| 3:D:118:DT:H2''  | 3:D:119:DA:N7    | 2.31                     | 0.46              |
| 4:E:74:TYR:O     | 4:E:78:LEU:CD1   | 2.65                     | 0.45              |
| 4:E:165:GLY:O    | 4:E:169:ASN:HB2  | 2.16                     | 0.45              |
| 3:H:122:DT:OP2   | 4:F:101:ARG:NH1  | 2.49                     | 0.45              |
| 3:D:123:DT:H2''  | 3:D:124:DA:H5''  | 1.98                     | 0.45              |
| 4:B:245:ASN:OD1  | 4:B:247:VAL:CG2  | 2.63                     | 0.45              |
| 4:E:248:ALA:C    | 4:E:250:PRO:HD3  | 2.36                     | 0.45              |
| 4:F:276:LYS:O    | 4:F:277:ASP:O    | 2.35                     | 0.45              |
| 2:Y:118:DT:H1'   | 2:Y:119:DA:C5    | 2.50                     | 0.45              |
| 4:E:94:GLN:HA    | 4:E:94:GLN:NE2   | 2.31                     | 0.45              |
| 4:B:61:ARG:NH1   | 4:B:61:ARG:HG2   | 2.32                     | 0.45              |
| 4:B:270:ARG:HG2  | 4:B:274:GLY:O    | 2.17                     | 0.45              |
| 4:A:224:TRP:CZ3  | 4:A:228:SER:HB3  | 2.51                     | 0.45              |
| 4:A:181:ARG:O    | 4:A:184:ASP:HB2  | 2.15                     | 0.45              |
| 4:E:306:ILE:N    | 4:E:307:PRO:HD2  | 2.32                     | 0.45              |
| 4:F:25:LYS:O     | 4:F:25:LYS:HD3   | 2.17                     | 0.45              |
| 3:D:104:DA:H2''  | 3:D:105:DA:O5'   | 2.16                     | 0.45              |
| 3:D:115:DG:O6    | 4:A:86:LYS:HE2   | 2.16                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:A:80:ALA:C     | 4:A:82:GLY:H     | 2.19                     | 0.45              |
| 4:A:182:VAL:C    | 4:A:184:ASP:H    | 2.19                     | 0.45              |
| 4:F:329:ASP:O    | 4:F:332:THR:N    | 2.50                     | 0.45              |
| 4:E:167:ALA:O    | 4:E:291:ALA:HB1  | 2.17                     | 0.45              |
| 4:A:340:GLU:OE2  | 4:F:192:ARG:NH1  | 2.50                     | 0.45              |
| 4:E:316:THR:HG23 | 4:E:317:ASN:ND2  | 2.31                     | 0.45              |
| 4:E:209:VAL:HG12 | 4:E:209:VAL:O    | 2.16                     | 0.45              |
| 4:F:238:LEU:HD12 | 4:F:238:LEU:O    | 2.17                     | 0.45              |
| 2:X:116:DT:H4'   | 4:B:202:THR:CG2  | 2.46                     | 0.45              |
| 4:F:72:ARG:HH11  | 4:F:72:ARG:HG3   | 1.81                     | 0.45              |
| 4:B:293:VAL:CG2  | 4:B:294:GLY:N    | 2.78                     | 0.45              |
| 4:B:237:TYR:CE1  | 4:B:255:GLN:HG2  | 2.52                     | 0.45              |
| 4:F:223:ARG:HH11 | 4:F:223:ARG:HG2  | 1.82                     | 0.45              |
| 4:A:15:PRO:CB    | 4:A:18:ALA:CB    | 2.81                     | 0.45              |
| 3:D:128:DG:H2''  | 3:D:129:DA:H5'   | 1.98                     | 0.45              |
| 4:B:142:PHE:CZ   | 4:B:165:GLY:HA2  | 2.52                     | 0.45              |
| 4:A:97:MET:O     | 4:A:98:LEU:C     | 2.55                     | 0.45              |
| 4:A:64:PHE:HA    | 4:A:65:PRO:C     | 2.36                     | 0.45              |
| 4:F:67:GLU:HG3   | 4:F:68:PRO:HD2   | 1.99                     | 0.45              |
| 4:B:319:ASN:ND2  | 4:B:323:ASN:OD1  | 2.50                     | 0.44              |
| 4:F:54:ALA:O     | 4:F:55:TRP:C     | 2.55                     | 0.44              |
| 4:E:32:ARG:HD2   | 4:F:72:ARG:NH2   | 2.28                     | 0.44              |
| 4:B:327:ASN:OD1  | 4:B:328:LEU:HD12 | 2.17                     | 0.44              |
| 4:F:305:SER:OG   | 4:F:307:PRO:HG2  | 2.17                     | 0.44              |
| 4:E:23:VAL:CG2   | 4:E:24:ARG:N     | 2.80                     | 0.44              |
| 4:B:181:ARG:O    | 4:B:184:ASP:HB2  | 2.17                     | 0.44              |
| 2:X:116:DT:O5'   | 4:B:173:ARG:NH2  | 2.50                     | 0.44              |
| 1:C:108:DT:C2'   | 1:C:109:DC:H5'   | 2.47                     | 0.44              |
| 4:A:20:SER:O     | 4:A:21:ASP:CB    | 2.65                     | 0.44              |
| 4:B:25:LYS:O     | 4:B:28:MET:N     | 2.51                     | 0.44              |
| 4:B:52:TRP:O     | 4:B:56:CYS:HB2   | 2.17                     | 0.44              |
| 2:Y:135:DT:O2    | 4:E:244:LYS:HD3  | 2.18                     | 0.44              |
| 4:F:219:LYS:HD3  | 4:F:222:GLU:OE1  | 2.17                     | 0.44              |
| 4:E:72:ARG:HE    | 4:E:116:VAL:CG1  | 2.31                     | 0.44              |
| 4:E:311:GLN:CG   | 4:E:312:ALA:N    | 2.80                     | 0.44              |
| 4:E:163:PHE:HD1  | 4:E:164:LEU:HD23 | 1.81                     | 0.44              |
| 4:B:42:TRP:O     | 4:B:43:LYS:C     | 2.56                     | 0.44              |
| 4:F:245:ASN:CG   | 4:F:247:VAL:HG23 | 2.35                     | 0.44              |
| 4:E:243:ARG:HG2  | 4:E:243:ARG:NH1  | 2.19                     | 0.44              |
| 3:D:133:DT:C2'   | 3:D:134:DA:C8    | 3.01                     | 0.44              |
| 4:A:13:ALA:O     | 4:A:15:PRO:CD    | 2.66                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:A:72:ARG:HD2   | 4:A:116:VAL:CG2  | 2.47                     | 0.44              |
| 2:Y:131:DG:C2'   | 2:Y:132:DT:H5''  | 2.45                     | 0.44              |
| 4:B:319:ASN:HD22 | 4:B:319:ASN:C    | 2.21                     | 0.44              |
| 4:E:295:ALA:O    | 4:E:296:ALA:C    | 2.55                     | 0.44              |
| 4:A:145:VAL:HG12 | 4:A:145:VAL:O    | 2.17                     | 0.44              |
| 4:B:31:PHE:O     | 4:B:34:ARG:HB3   | 2.18                     | 0.44              |
| 4:E:177:ILE:O    | 4:E:177:ILE:HG22 | 2.18                     | 0.44              |
| 4:F:269:HIS:HB2  | 4:F:286:TRP:CE3  | 2.53                     | 0.44              |
| 4:E:111:ASN:O    | 4:E:115:LEU:HB2  | 2.17                     | 0.44              |
| 4:A:68:PRO:O     | 4:A:69:GLU:C     | 2.54                     | 0.44              |
| 4:B:158:ILE:HA   | 4:B:158:ILE:HD13 | 1.82                     | 0.44              |
| 4:E:310:MET:CE   | 4:E:317:ASN:O    | 2.66                     | 0.43              |
| 4:B:92:LEU:HD23  | 4:B:117:MET:HG2  | 1.99                     | 0.43              |
| 4:A:187:ARG:CB   | 4:A:187:ARG:HH11 | 2.29                     | 0.43              |
| 4:A:59:ASN:HB3   | 4:A:61:ARG:HH11  | 1.83                     | 0.43              |
| 4:F:335:MET:CE   | 4:F:335:MET:HA   | 2.47                     | 0.43              |
| 4:F:322:MET:HA   | 4:F:322:MET:HE3  | 2.00                     | 0.43              |
| 4:A:320:ILE:C    | 4:A:322:MET:N    | 2.71                     | 0.43              |
| 3:D:134:DA:C8    | 3:D:135:DT:H72   | 2.53                     | 0.43              |
| 4:A:101:ARG:NH2  | 4:B:115:LEU:HD21 | 2.33                     | 0.43              |
| 4:B:31:PHE:CD1   | 4:B:42:TRP:CH2   | 3.05                     | 0.43              |
| 3:H:133:DT:H2''  | 3:H:134:DA:C8    | 2.53                     | 0.43              |
| 4:B:185:ILE:HG21 | 4:B:193:MET:CE   | 2.48                     | 0.43              |
| 4:A:14:LEU:HG    | 4:A:27:LEU:CD2   | 2.48                     | 0.43              |
| 4:A:192:ARG:HH21 | 4:A:215:LEU:HD21 | 1.83                     | 0.43              |
| 4:E:306:ILE:HG22 | 4:F:306:ILE:HD11 | 2.01                     | 0.43              |
| 4:A:126:ASP:C    | 4:A:128:GLY:N    | 2.70                     | 0.43              |
| 4:F:325:ILE:HG21 | 4:F:327:ASN:ND2  | 2.34                     | 0.43              |
| 4:E:339:LEU:HD23 | 4:E:339:LEU:HA   | 1.79                     | 0.43              |
| 4:E:106:ARG:HG3  | 4:E:106:ARG:HH11 | 1.83                     | 0.43              |
| 4:B:171:LEU:O    | 4:B:292:ARG:HG3  | 2.18                     | 0.43              |
| 4:E:323:ASN:HD22 | 4:E:323:ASN:HA   | 1.56                     | 0.43              |
| 4:A:84:ALA:O     | 4:A:88:ILE:HG13  | 2.19                     | 0.43              |
| 2:Y:118:DT:H2'   | 2:Y:118:DT:H6    | 1.55                     | 0.43              |
| 4:E:78:LEU:CD1   | 4:E:78:LEU:H     | 2.31                     | 0.43              |
| 3:D:119:DA:OP1   | 4:B:121:ARG:NH2  | 2.37                     | 0.43              |
| 4:E:289:HIS:O    | 4:E:291:ALA:N    | 2.52                     | 0.43              |
| 4:F:289:HIS:O    | 4:F:293:VAL:HG12 | 2.17                     | 0.43              |
| 1:G:115:A3P:O3'  | 2:Y:116:DT:C5'   | 2.67                     | 0.43              |
| 4:F:159:ARG:O    | 4:F:162:ALA:N    | 2.39                     | 0.43              |
| 4:B:170:THR:OG1  | 4:B:172:LEU:HD12 | 2.19                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:B:209:VAL:CG2  | 4:B:210:GLU:N    | 2.81                     | 0.43              |
| 4:F:89:GLN:O     | 4:F:90:GLN:C     | 2.57                     | 0.43              |
| 4:F:99:HIS:O     | 4:F:102:SER:N    | 2.52                     | 0.43              |
| 4:F:124:ASN:O    | 4:F:129:GLU:HB3  | 2.19                     | 0.43              |
| 4:B:309:ILE:HG21 | 4:B:321:VAL:HG13 | 2.00                     | 0.43              |
| 4:A:182:VAL:C    | 4:A:184:ASP:N    | 2.72                     | 0.43              |
| 4:B:193:MET:HG3  | 4:B:218:THR:OG1  | 2.19                     | 0.43              |
| 3:D:126:DA:OP2   | 4:B:262:GLU:OE1  | 2.36                     | 0.43              |
| 4:A:95:LEU:HA    | 4:A:95:LEU:HD12  | 1.83                     | 0.43              |
| 4:E:35:GLN:HB2   | 4:F:119:ARG:HD2  | 2.01                     | 0.43              |
| 4:F:93:GLY:O     | 4:F:96:ASN:HB2   | 2.19                     | 0.43              |
| 4:A:306:ILE:N    | 4:A:307:PRO:CD   | 2.82                     | 0.43              |
| 4:B:163:PHE:CE1  | 4:B:261:LEU:HD22 | 2.54                     | 0.43              |
| 4:A:63:TRP:O     | 4:A:64:PHE:HB2   | 2.19                     | 0.43              |
| 4:A:310:MET:SD   | 4:A:318:VAL:HG12 | 2.58                     | 0.43              |
| 4:A:169:ASN:C    | 4:A:169:ASN:ND2  | 2.70                     | 0.43              |
| 4:B:332:THR:HG22 | 4:B:333:GLY:N    | 2.33                     | 0.43              |
| 4:E:230:VAL:CG1  | 4:E:236:ASN:HB3  | 2.49                     | 0.43              |
| 4:B:24:ARG:O     | 4:B:28:MET:HG2   | 2.19                     | 0.43              |
| 4:A:260:ALA:O    | 4:A:264:ILE:HG13 | 2.19                     | 0.43              |
| 4:B:96:ASN:OD1   | 4:B:107:PRO:HG2  | 2.19                     | 0.42              |
| 4:F:116:VAL:O    | 4:F:120:ILE:HG13 | 2.19                     | 0.42              |
| 3:H:126:DA:OP1   | 4:F:289:HIS:N    | 2.45                     | 0.42              |
| 4:E:161:LEU:HD23 | 4:E:220:LEU:HD21 | 2.01                     | 0.42              |
| 4:B:139:ARG:HD2  | 4:B:139:ARG:O    | 2.19                     | 0.42              |
| 4:F:145:VAL:HG11 | 4:F:268:THR:HG21 | 2.01                     | 0.42              |
| 1:G:101:DG:H2''  | 1:G:102:DA:O5'   | 2.19                     | 0.42              |
| 4:B:68:PRO:O     | 4:B:69:GLU:C     | 2.57                     | 0.42              |
| 4:B:221:VAL:C    | 4:B:223:ARG:N    | 2.71                     | 0.42              |
| 4:A:12:PRO:HG2   | 4:A:63:TRP:CZ3   | 2.54                     | 0.42              |
| 4:E:26:ASN:HB3   | 4:E:102:SER:HA   | 2.00                     | 0.42              |
| 4:F:271:LEU:HD13 | 4:F:271:LEU:C    | 2.40                     | 0.42              |
| 2:Y:126:DA:OP2   | 4:E:262:GLU:OE1  | 2.36                     | 0.42              |
| 4:E:41:THR:O     | 4:E:42:TRP:C     | 2.57                     | 0.42              |
| 2:Y:117:DG:O6    | 3:H:120:DC:N3    | 2.52                     | 0.42              |
| 4:E:48:VAL:HG11  | 4:E:94:GLN:HB2   | 2.01                     | 0.42              |
| 4:E:126:ASP:C    | 4:E:128:GLY:N    | 2.72                     | 0.42              |
| 4:A:192:ARG:HB3  | 4:A:215:LEU:CD2  | 2.45                     | 0.42              |
| 4:F:328:LEU:H    | 4:F:328:LEU:HD12 | 1.84                     | 0.42              |
| 4:B:185:ILE:HG21 | 4:B:193:MET:HE3  | 2.01                     | 0.42              |
| 4:B:107:PRO:C    | 4:B:109:ASP:H    | 2.23                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:B:328:LEU:H    | 4:B:328:LEU:HD12 | 1.84                     | 0.42              |
| 4:E:213:LEU:HD22 | 4:E:213:LEU:H    | 1.83                     | 0.42              |
| 4:B:115:LEU:N    | 4:B:115:LEU:HD23 | 2.34                     | 0.42              |
| 4:F:272:ILE:HG22 | 4:F:273:TYR:HD1  | 1.83                     | 0.42              |
| 3:D:118:DT:OP1   | 4:A:202:THR:HG23 | 2.18                     | 0.42              |
| 4:E:194:LEU:HD11 | 4:F:329:ASP:OD1  | 2.20                     | 0.42              |
| 4:E:304:VAL:CG1  | 4:E:309:ILE:HG13 | 2.49                     | 0.42              |
| 4:F:139:ARG:O    | 4:F:140:THR:C    | 2.58                     | 0.42              |
| 4:A:215:LEU:O    | 4:A:218:THR:HB   | 2.18                     | 0.42              |
| 4:F:112:ALA:O    | 4:F:116:VAL:HG12 | 2.20                     | 0.42              |
| 4:B:67:GLU:O     | 4:B:68:PRO:C     | 2.58                     | 0.42              |
| 4:F:75:LEU:O     | 4:F:78:LEU:HB2   | 2.19                     | 0.42              |
| 4:B:116:VAL:HG13 | 4:B:117:MET:N    | 2.34                     | 0.42              |
| 4:E:236:ASN:OD1  | 4:E:252:ALA:HB2  | 2.19                     | 0.42              |
| 4:A:164:LEU:CD1  | 4:A:268:THR:HG21 | 2.49                     | 0.42              |
| 4:B:334:ALA:O    | 4:B:337:ARG:N    | 2.52                     | 0.42              |
| 4:F:304:VAL:HG12 | 4:F:308:GLU:HB2  | 2.02                     | 0.42              |
| 4:A:78:LEU:O     | 4:A:79:GLN:C     | 2.55                     | 0.42              |
| 4:E:57:LYS:O     | 4:E:58:LEU:CB    | 2.68                     | 0.42              |
| 4:A:158:ILE:HD11 | 4:A:223:ARG:NH2  | 2.34                     | 0.42              |
| 1:C:106:DC:H2''  | 1:C:107:UMP:C6   | 2.54                     | 0.42              |
| 4:B:226:SER:O    | 4:B:227:VAL:C    | 2.56                     | 0.42              |
| 4:E:181:ARG:O    | 4:E:184:ASP:N    | 2.53                     | 0.42              |
| 4:B:159:ARG:HB2  | 4:B:224:TRP:CE3  | 2.55                     | 0.42              |
| 4:F:35:GLN:HB2   | 4:F:35:GLN:HE21  | 1.64                     | 0.42              |
| 4:E:313:GLY:HA3  | 4:E:315:TRP:CE3  | 2.56                     | 0.41              |
| 4:F:161:LEU:HG   | 4:F:220:LEU:HD22 | 2.02                     | 0.41              |
| 4:E:112:ALA:O    | 4:E:116:VAL:HG22 | 2.20                     | 0.41              |
| 4:A:121:ARG:NH1  | 4:F:204:VAL:HG13 | 2.35                     | 0.41              |
| 4:E:106:ARG:NH1  | 4:E:106:ARG:HG3  | 2.36                     | 0.41              |
| 3:D:112:DA:H2''  | 3:D:113:DT:H5'   | 2.01                     | 0.41              |
| 4:A:177:ILE:HG21 | 4:A:177:ILE:HD13 | 1.83                     | 0.41              |
| 4:B:76:LEU:HA    | 4:B:76:LEU:HD23  | 1.65                     | 0.41              |
| 4:A:172:LEU:HA   | 4:A:172:LEU:HD23 | 1.88                     | 0.41              |
| 4:A:106:ARG:O    | 4:A:109:ASP:HB3  | 2.20                     | 0.41              |
| 4:F:44:MET:HB3   | 4:F:90:GLN:OE1   | 2.20                     | 0.41              |
| 4:A:85:VAL:HG23  | 4:A:129:GLU:OE1  | 2.21                     | 0.41              |
| 4:B:336:VAL:O    | 4:B:340:GLU:HG3  | 2.20                     | 0.41              |
| 4:E:66:ALA:HB3   | 4:E:99:HIS:NE2   | 2.36                     | 0.41              |
| 4:E:75:LEU:HD23  | 4:E:75:LEU:HA    | 1.85                     | 0.41              |
| 4:B:168:TYR:CD2  | 4:B:168:TYR:O    | 2.72                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:F:31:PHE:CD1   | 4:F:31:PHE:N     | 2.87                     | 0.41              |
| 4:B:58:LEU:O     | 4:B:58:LEU:CD1   | 2.55                     | 0.41              |
| 4:B:223:ARG:O    | 4:B:226:SER:N    | 2.53                     | 0.41              |
| 4:F:89:GLN:O     | 4:F:91:HIS:N     | 2.53                     | 0.41              |
| 4:F:27:LEU:HD12  | 4:F:30:MET:CE    | 2.50                     | 0.41              |
| 1:C:107:UMP:OP2  | 4:B:257:SER:HB3  | 2.20                     | 0.41              |
| 4:A:182:VAL:O    | 4:A:184:ASP:N    | 2.53                     | 0.41              |
| 4:B:193:MET:SD   | 4:B:221:VAL:HB   | 2.60                     | 0.41              |
| 2:Y:117:DG:OP2   | 4:F:320:ILE:HD13 | 2.20                     | 0.41              |
| 4:B:139:ARG:HB2  | 4:B:168:TYR:OH   | 2.20                     | 0.41              |
| 4:F:318:VAL:O    | 4:F:322:MET:HB2  | 2.20                     | 0.41              |
| 4:B:75:LEU:HD23  | 4:B:75:LEU:HA    | 1.84                     | 0.41              |
| 4:A:307:PRO:HG3  | 4:B:306:ILE:HD11 | 1.99                     | 0.41              |
| 4:E:147:SER:OG   | 4:E:148:LEU:N    | 2.53                     | 0.41              |
| 4:F:62:LYS:HB2   | 4:F:62:LYS:HZ2   | 1.82                     | 0.41              |
| 4:E:230:VAL:HG12 | 4:E:236:ASN:HB3  | 2.03                     | 0.41              |
| 4:B:270:ARG:O    | 4:B:272:ILE:N    | 2.54                     | 0.41              |
| 4:A:74:TYR:O     | 4:A:77:TYR:HB3   | 2.20                     | 0.41              |
| 4:E:200:THR:HG21 | 4:E:205:SER:HB2  | 2.02                     | 0.41              |
| 4:A:325:ILE:HG13 | 4:A:325:ILE:O    | 2.21                     | 0.41              |
| 4:A:328:LEU:HD23 | 4:A:328:LEU:HA   | 1.87                     | 0.41              |
| 4:B:195:ILE:CG2  | 4:B:196:HIS:N    | 2.84                     | 0.41              |
| 4:A:34:ARG:C     | 4:A:36:ALA:N     | 2.74                     | 0.41              |
| 4:A:157:ASP:O    | 4:A:158:ILE:C    | 2.55                     | 0.41              |
| 3:D:105:DA:C2    | 3:D:106:DC:C2    | 3.09                     | 0.41              |
| 4:A:277:ASP:HB3  | 4:A:284:LEU:HD13 | 2.03                     | 0.41              |
| 4:E:214:SER:OG   | 4:E:215:LEU:N    | 2.52                     | 0.41              |
| 3:H:106:DC:H4'   | 4:E:241:ARG:HG3  | 2.03                     | 0.41              |
| 4:F:163:PHE:C    | 4:F:163:PHE:CD2  | 2.94                     | 0.41              |
| 4:B:71:VAL:O     | 4:B:74:TYR:HB3   | 2.21                     | 0.41              |
| 4:A:201:LYS:HE3  | 4:A:201:LYS:HB2  | 1.81                     | 0.41              |
| 4:A:320:ILE:C    | 4:A:322:MET:H    | 2.24                     | 0.41              |
| 4:E:64:PHE:C     | 4:E:64:PHE:CD1   | 2.94                     | 0.41              |
| 4:B:320:ILE:O    | 4:B:323:ASN:N    | 2.54                     | 0.40              |
| 3:D:108:DT:H1'   | 3:D:109:DC:H5''  | 2.03                     | 0.40              |
| 4:B:83:LEU:HD23  | 4:B:83:LEU:HA    | 1.87                     | 0.40              |
| 4:B:269:HIS:CG   | 4:B:285:ALA:HB1  | 2.56                     | 0.40              |
| 4:B:116:VAL:CG1  | 4:B:117:MET:N    | 2.85                     | 0.40              |
| 4:A:164:LEU:HD23 | 4:A:164:LEU:HA   | 1.86                     | 0.40              |
| 4:F:106:ARG:HD3  | 4:F:109:ASP:OD1  | 2.22                     | 0.40              |
| 4:B:104:LEU:HB3  | 4:B:105:PRO:HD2  | 2.03                     | 0.40              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 4:E:185:ILE:HG21 | 4:E:193:MET:HE1 | 2.02                     | 0.40              |
| 4:F:297:ARG:O    | 4:F:299:MET:N   | 2.54                     | 0.40              |
| 4:E:78:LEU:CD1   | 4:E:78:LEU:N    | 2.83                     | 0.40              |
| 4:B:74:TYR:O     | 4:B:77:TYR:N    | 2.55                     | 0.40              |
| 4:F:233:ASP:HB3  | 4:F:236:ASN:ND2 | 2.37                     | 0.40              |
| 4:A:58:LEU:HG    | 4:A:58:LEU:O    | 2.22                     | 0.40              |
| 4:E:188:THR:C    | 4:E:190:GLY:H   | 2.24                     | 0.40              |
| 4:B:330:SER:O    | 4:B:332:THR:OG1 | 2.37                     | 0.40              |
| 4:E:119:ARG:O    | 4:E:123:GLU:HB2 | 2.21                     | 0.40              |
| 4:A:163:PHE:O    | 4:A:164:LEU:C   | 2.60                     | 0.40              |
| 4:B:171:LEU:HD13 | 4:B:312:ALA:O   | 2.20                     | 0.40              |
| 4:A:11:LEU:HD13  | 4:A:14:LEU:CD2  | 2.49                     | 0.40              |
| 4:E:171:LEU:HD12 | 4:E:313:GLY:HA2 | 2.03                     | 0.40              |
| 4:F:48:VAL:HG22  | 4:F:91:HIS:CG   | 2.57                     | 0.40              |
| 4:F:85:VAL:HG23  | 4:F:129:GLU:OE2 | 2.22                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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 |    |
|-----|-------|-----------------|------------|-----------|----------|-------------|----|
| 4   | A     | 330/343 (96%)   | 274 (83%)  | 42 (13%)  | 14 (4%)  | 3           | 26 |
| 4   | B     | 320/343 (93%)   | 232 (72%)  | 64 (20%)  | 24 (8%)  | 1           | 9  |
| 4   | E     | 319/343 (93%)   | 239 (75%)  | 63 (20%)  | 17 (5%)  | 2           | 19 |
| 4   | F     | 320/343 (93%)   | 259 (81%)  | 42 (13%)  | 19 (6%)  | 2           | 16 |
| All | All   | 1289/1372 (94%) | 1004 (78%) | 211 (16%) | 74 (6%)  | 2           | 17 |

All (74) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | A     | 21  | ASP  |
| 4   | A     | 200 | THR  |
| 4   | B     | 148 | LEU  |
| 4   | B     | 248 | ALA  |
| 4   | B     | 327 | ASN  |
| 4   | E     | 58  | LEU  |
| 4   | E     | 149 | MET  |
| 4   | E     | 182 | VAL  |
| 4   | E     | 232 | ASP  |
| 4   | E     | 257 | SER  |
| 4   | E     | 277 | ASP  |
| 4   | F     | 134 | ALA  |
| 4   | F     | 275 | ALA  |
| 4   | F     | 277 | ASP  |
| 4   | F     | 324 | TYR  |
| 4   | F     | 327 | ASN  |
| 4   | F     | 328 | LEU  |
| 4   | F     | 330 | SER  |
| 4   | A     | 12  | PRO  |
| 4   | A     | 35  | GLN  |
| 4   | A     | 111 | ASN  |
| 4   | A     | 205 | SER  |
| 4   | A     | 277 | ASP  |
| 4   | A     | 318 | VAL  |
| 4   | B     | 54  | ALA  |
| 4   | B     | 58  | LEU  |
| 4   | B     | 111 | ASN  |
| 4   | B     | 147 | SER  |
| 4   | B     | 227 | VAL  |
| 4   | B     | 235 | ASN  |
| 4   | B     | 249 | ALA  |
| 4   | B     | 271 | LEU  |
| 4   | B     | 286 | TRP  |
| 4   | B     | 331 | GLU  |
| 4   | E     | 200 | THR  |
| 4   | E     | 208 | GLY  |
| 4   | E     | 214 | SER  |
| 4   | F     | 90  | GLN  |
| 4   | F     | 227 | VAL  |
| 4   | F     | 274 | GLY  |
| 4   | F     | 334 | ALA  |
| 4   | A     | 182 | VAL  |
| 4   | B     | 68  | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | B     | 81  | ARG  |
| 4   | B     | 250 | PRO  |
| 4   | E     | 147 | SER  |
| 4   | E     | 157 | ASP  |
| 4   | E     | 198 | GLY  |
| 4   | E     | 286 | TRP  |
| 4   | F     | 59  | ASN  |
| 4   | F     | 89  | GLN  |
| 4   | F     | 332 | THR  |
| 4   | A     | 183 | LYS  |
| 4   | A     | 244 | LYS  |
| 4   | A     | 279 | SER  |
| 4   | B     | 55  | TRP  |
| 4   | B     | 160 | ASN  |
| 4   | B     | 302 | ALA  |
| 4   | B     | 335 | MET  |
| 4   | E     | 102 | SER  |
| 4   | E     | 244 | LYS  |
| 4   | F     | 108 | SER  |
| 4   | F     | 127 | ALA  |
| 4   | F     | 298 | ASP  |
| 4   | A     | 193 | MET  |
| 4   | B     | 128 | GLY  |
| 4   | B     | 328 | LEU  |
| 4   | E     | 279 | SER  |
| 4   | F     | 54  | ALA  |
| 4   | F     | 323 | ASN  |
| 4   | A     | 25  | LYS  |
| 4   | B     | 226 | SER  |
| 4   | E     | 246 | GLY  |
| 4   | B     | 23  | VAL  |

### 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.

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| Mol | Chain | Analysed        | Rotameric | Outliers  | Percentiles |
|-----|-------|-----------------|-----------|-----------|-------------|
| 4   | A     | 277/287 (96%)   | 240 (87%) | 37 (13%)  | 5 22        |
| 4   | B     | 269/287 (94%)   | 242 (90%) | 27 (10%)  | 9 37        |
| 4   | E     | 268/287 (93%)   | 230 (86%) | 38 (14%)  | 4 19        |
| 4   | F     | 269/287 (94%)   | 229 (85%) | 40 (15%)  | 4 17        |
| All | All   | 1083/1148 (94%) | 941 (87%) | 142 (13%) | 5 24        |

All (142) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | A     | 19  | THR  |
| 4   | A     | 24  | ARG  |
| 4   | A     | 34  | ARG  |
| 4   | A     | 39  | GLU  |
| 4   | A     | 61  | ARG  |
| 4   | A     | 63  | TRP  |
| 4   | A     | 67  | GLU  |
| 4   | A     | 68  | PRO  |
| 4   | A     | 69  | GLU  |
| 4   | A     | 87  | THR  |
| 4   | A     | 90  | GLN  |
| 4   | A     | 92  | LEU  |
| 4   | A     | 95  | LEU  |
| 4   | A     | 98  | LEU  |
| 4   | A     | 101 | ARG  |
| 4   | A     | 108 | SER  |
| 4   | A     | 140 | THR  |
| 4   | A     | 144 | GLN  |
| 4   | A     | 161 | LEU  |
| 4   | A     | 169 | ASN  |
| 4   | A     | 170 | THR  |
| 4   | A     | 187 | ARG  |
| 4   | A     | 203 | LEU  |
| 4   | A     | 214 | SER  |
| 4   | A     | 220 | LEU  |
| 4   | A     | 225 | ILE  |
| 4   | A     | 232 | ASP  |
| 4   | A     | 238 | LEU  |
| 4   | A     | 242 | VAL  |
| 4   | A     | 247 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | A     | 256 | LEU  |
| 4   | A     | 258 | THR  |
| 4   | A     | 278 | ASP  |
| 4   | A     | 289 | HIS  |
| 4   | A     | 311 | GLN  |
| 4   | A     | 316 | THR  |
| 4   | A     | 317 | ASN  |
| 4   | B     | 21  | ASP  |
| 4   | B     | 27  | LEU  |
| 4   | B     | 30  | MET  |
| 4   | B     | 35  | GLN  |
| 4   | B     | 56  | CYS  |
| 4   | B     | 58  | LEU  |
| 4   | B     | 60  | ASN  |
| 4   | B     | 63  | TRP  |
| 4   | B     | 95  | LEU  |
| 4   | B     | 101 | ARG  |
| 4   | B     | 106 | ARG  |
| 4   | B     | 108 | SER  |
| 4   | B     | 118 | ARG  |
| 4   | B     | 133 | GLN  |
| 4   | B     | 140 | THR  |
| 4   | B     | 144 | GLN  |
| 4   | B     | 156 | GLN  |
| 4   | B     | 171 | LEU  |
| 4   | B     | 176 | GLU  |
| 4   | B     | 206 | THR  |
| 4   | B     | 242 | VAL  |
| 4   | B     | 261 | LEU  |
| 4   | B     | 271 | LEU  |
| 4   | B     | 304 | VAL  |
| 4   | B     | 311 | GLN  |
| 4   | B     | 318 | VAL  |
| 4   | B     | 319 | ASN  |
| 4   | E     | 27  | LEU  |
| 4   | E     | 30  | MET  |
| 4   | E     | 38  | SER  |
| 4   | E     | 48  | VAL  |
| 4   | E     | 57  | LYS  |
| 4   | E     | 58  | LEU  |
| 4   | E     | 60  | ASN  |
| 4   | E     | 89  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | E     | 92  | LEU  |
| 4   | E     | 95  | LEU  |
| 4   | E     | 104 | LEU  |
| 4   | E     | 106 | ARG  |
| 4   | E     | 115 | LEU  |
| 4   | E     | 116 | VAL  |
| 4   | E     | 117 | MET  |
| 4   | E     | 132 | LYS  |
| 4   | E     | 140 | THR  |
| 4   | E     | 147 | SER  |
| 4   | E     | 148 | LEU  |
| 4   | E     | 151 | ASN  |
| 4   | E     | 153 | ASP  |
| 4   | E     | 154 | ARG  |
| 4   | E     | 157 | ASP  |
| 4   | E     | 158 | ILE  |
| 4   | E     | 171 | LEU  |
| 4   | E     | 173 | ARG  |
| 4   | E     | 182 | VAL  |
| 4   | E     | 189 | ASP  |
| 4   | E     | 194 | LEU  |
| 4   | E     | 206 | THR  |
| 4   | E     | 220 | LEU  |
| 4   | E     | 243 | ARG  |
| 4   | E     | 256 | LEU  |
| 4   | E     | 289 | HIS  |
| 4   | E     | 311 | GLN  |
| 4   | E     | 316 | THR  |
| 4   | E     | 317 | ASN  |
| 4   | E     | 323 | ASN  |
| 4   | F     | 27  | LEU  |
| 4   | F     | 29  | ASP  |
| 4   | F     | 35  | GLN  |
| 4   | F     | 45  | LEU  |
| 4   | F     | 55  | TRP  |
| 4   | F     | 56  | CYS  |
| 4   | F     | 61  | ARG  |
| 4   | F     | 72  | ARG  |
| 4   | F     | 76  | LEU  |
| 4   | F     | 77  | TYR  |
| 4   | F     | 81  | ARG  |
| 4   | F     | 90  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | F     | 95  | LEU  |
| 4   | F     | 101 | ARG  |
| 4   | F     | 106 | ARG  |
| 4   | F     | 121 | ARG  |
| 4   | F     | 130 | ARG  |
| 4   | F     | 133 | GLN  |
| 4   | F     | 135 | LEU  |
| 4   | F     | 153 | ASP  |
| 4   | F     | 155 | CYS  |
| 4   | F     | 169 | ASN  |
| 4   | F     | 171 | LEU  |
| 4   | F     | 193 | MET  |
| 4   | F     | 205 | SER  |
| 4   | F     | 206 | THR  |
| 4   | F     | 223 | ARG  |
| 4   | F     | 243 | ARG  |
| 4   | F     | 253 | THR  |
| 4   | F     | 273 | TYR  |
| 4   | F     | 278 | ASP  |
| 4   | F     | 284 | LEU  |
| 4   | F     | 289 | HIS  |
| 4   | F     | 297 | ARG  |
| 4   | F     | 318 | VAL  |
| 4   | F     | 322 | MET  |
| 4   | F     | 323 | ASN  |
| 4   | F     | 325 | ILE  |
| 4   | F     | 329 | ASP  |
| 4   | F     | 332 | THR  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | A     | 89  | GLN  |
| 4   | A     | 90  | GLN  |
| 4   | A     | 133 | GLN  |
| 4   | A     | 196 | HIS  |
| 4   | A     | 311 | GLN  |
| 4   | B     | 35  | GLN  |
| 4   | B     | 40  | HIS  |
| 4   | B     | 60  | ASN  |
| 4   | B     | 90  | GLN  |
| 4   | B     | 156 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | B     | 235 | ASN  |
| 4   | B     | 236 | ASN  |
| 4   | B     | 255 | GLN  |
| 4   | B     | 319 | ASN  |
| 4   | E     | 26  | ASN  |
| 4   | E     | 35  | GLN  |
| 4   | E     | 79  | GLN  |
| 4   | E     | 89  | GLN  |
| 4   | E     | 90  | GLN  |
| 4   | E     | 94  | GLN  |
| 4   | E     | 144 | GLN  |
| 4   | E     | 235 | ASN  |
| 4   | E     | 317 | ASN  |
| 4   | E     | 323 | ASN  |
| 4   | F     | 35  | GLN  |
| 4   | F     | 59  | ASN  |
| 4   | F     | 94  | GLN  |
| 4   | F     | 96  | ASN  |
| 4   | F     | 111 | ASN  |
| 4   | F     | 133 | GLN  |
| 4   | F     | 144 | GLN  |
| 4   | F     | 236 | ASN  |
| 4   | F     | 281 | GLN  |
| 4   | F     | 317 | ASN  |
| 4   | F     | 319 | ASN  |
| 4   | F     | 327 | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 1   | UMP  | C     | 107 | 1,3   | 11,20,21     | 1.16 | 1 (9%)   | 17,28,31    | 3.30 | 2 (11%)  |
| 1   | A3P  | C     | 115 | 1,4   | 15,26,29     | 2.05 | 2 (13%)  | 17,37,45    | 1.59 | 5 (29%)  |
| 1   | UMP  | G     | 107 | 1,3   | 11,20,21     | 1.09 | 1 (9%)   | 17,28,31    | 3.27 | 2 (11%)  |
| 1   | A3P  | G     | 115 | 1,3,4 | 15,26,29     | 1.13 | 1 (6%)   | 17,37,45    | 1.52 | 1 (5%)   |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link  | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|-------|---------|-----------|---------|
| 1   | UMP  | C     | 107 | 1,3   | -       | 0/3/21/22 | 0/2/2/2 |
| 1   | A3P  | C     | 115 | 1,4   | -       | 0/5/25/31 | 0/3/3/3 |
| 1   | UMP  | G     | 107 | 1,3   | -       | 0/3/21/22 | 0/2/2/2 |
| 1   | A3P  | G     | 115 | 1,3,4 | -       | 0/5/25/31 | 0/3/3/3 |

All (5) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | C     | 115 | A3P  | O4'-C4' | -6.50 | 1.30        | 1.45     |
| 1   | C     | 115 | A3P  | O3'-C3' | -3.72 | 1.41        | 1.46     |
| 1   | G     | 115 | A3P  | O3'-C3' | -3.33 | 1.41        | 1.46     |
| 1   | G     | 107 | UMP  | C4-N3   | 2.76  | 1.38        | 1.33     |
| 1   | C     | 107 | UMP  | C4-N3   | 2.86  | 1.38        | 1.33     |

All (10) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | C     | 107 | UMP  | C5-C4-N3    | -3.33 | 114.58      | 123.12   |
| 1   | G     | 107 | UMP  | C5-C4-N3    | -3.31 | 114.64      | 123.12   |
| 1   | C     | 115 | A3P  | O4'-C4'-C5' | -3.03 | 98.47       | 109.32   |
| 1   | C     | 115 | A3P  | O3'-C3'-C4' | -2.57 | 100.96      | 108.64   |
| 1   | C     | 115 | A3P  | C4'-O4'-C1' | -2.03 | 104.34      | 109.47   |
| 1   | C     | 115 | A3P  | C5'-C4'-C3' | 2.02  | 119.34      | 114.46   |
| 1   | C     | 115 | A3P  | C2'-C1'-N9  | 2.81  | 121.00      | 114.16   |
| 1   | G     | 115 | A3P  | C2'-C1'-N9  | 4.18  | 124.33      | 114.16   |
| 1   | G     | 107 | UMP  | C4-N3-C2    | 12.86 | 126.87      | 114.14   |
| 1   | C     | 107 | UMP  | C4-N3-C2    | 12.86 | 126.88      | 114.14   |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 7 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 1   | C     | 107 | UMP  | 3       | 0            |
| 1   | G     | 107 | UMP  | 2       | 0            |
| 1   | G     | 115 | A3P  | 2       | 0            |

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 9 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.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)























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   | C     | 14/16 (87%)     | -0.30  | 0             | 26, 58, 80, 81        | 0       |
| 1   | G     | 14/16 (87%)     | -0.17  | 0             | 31, 58, 109, 136      | 0       |
| 2   | X     | 21/21 (100%)    | 0.68   | 4 (19%)      | 22, 43, 86, 97        | 4 (19%) |
| 2   | Y     | 21/21 (100%)    | 0.67   | 3 (14%)      | 39, 72, 93, 99        | 3 (14%) |
| 3   | D     | 37/37 (100%)    | -0.37  | 0             | 21, 44, 79, 89        | 0       |
| 3   | H     | 37/37 (100%)    | -0.20  | 0             | 31, 61, 91, 108       | 0       |
| 4   | A     | 332/343 (96%)   | -0.29  | 1 (0%)        | 15, 40, 80, 121       | 0       |
| 4   | B     | 322/343 (93%)   | 0.00   | 5 (1%)    | 28, 59, 91, 126       | 0       |
| 4   | E     | 321/343 (93%)   | 0.10   | 4 (1%)    | 35, 69, 101, 137      | 0       |
| 4   | F     | 322/343 (93%)   | -0.23  | 3 (0%)    | 23, 52, 86, 126       | 0       |
| All | All   | 1441/1520 (94%) | -0.10  | 20 (1%)   | 15, 56, 93, 137       | 7 (0%)  |

All (20) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | X     | 117 | DG   | 7.6  |
| 2   | Y     | 118 | DT   | 7.1  |
| 2   | Y     | 117 | DG   | 7.1  |
| 2   | X     | 118 | DT   | 5.8  |
| 2   | X     | 119 | DA   | 5.7  |
| 2   | Y     | 119 | DA   | 5.7  |
| 4   | E     | 155 | CYS  | 3.8  |
| 4   | F     | 331 | GLU  | 3.7  |
| 4   | E     | 240 | CYS  | 3.7  |
| 4   | A     | 19  | THR  | 3.4  |
| 4   | F     | 330 | SER  | 3.3  |
| 2   | X     | 120 | DT   | 3.1  |
| 4   | E     | 49  | CYS  | 3.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 4   | B     | 155 | CYS  | 2.8  |
| 4   | E     | 63  | TRP  | 2.4  |
| 4   | B     | 330 | SER  | 2.2  |
| 4   | B     | 244 | LYS  | 2.1  |
| 4   | F     | 270 | ARG  | 2.1  |
| 4   | B     | 49  | CYS  | 2.1  |
| 4   | B     | 228 | SER  | 2.0  |

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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 | RSCC | RSR  | LLDF | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|------|----------------------------|-------|
| 1   | UMP  | C     | 107 | 19/20 | 0.95 | 0.15 | -    | 48,56,62,65                | 0     |
| 1   | A3P  | C     | 115 | 24/27 | 0.93 | 0.22 | -    | 29,42,50,56                | 0     |
| 1   | UMP  | G     | 107 | 19/20 | 0.96 | 0.18 | -    | 51,56,60,63                | 0     |
| 1   | A3P  | G     | 115 | 24/27 | 0.96 | 0.18 | -    | 23,27,36,44                | 0     |

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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 | RSCC | RSR  | LLDF | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|------|----------------------------|-------|
| 5   | MG   | A     | 347 | 1/1   | 0.90 | 0.29 | 5.12 | 42,42,42,42                | 0     |
| 5   | MG   | A     | 344 | 1/1   | 0.87 | 0.32 | 3.94 | 43,43,43,43                | 0     |
| 5   | MG   | A     | 345 | 1/1   | 0.88 | 0.41 | -    | 48,48,48,48                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 5   | MG   | F     | 344  | 1/1   | 0.86 | 1.08 | -    | 25,25,25,25                 | 1     |
| 5   | MG   | A     | 346  | 1/1   | 0.96 | 0.57 | -    | 36,36,36,36                 | 0     |
| 5   | MG   | H     | 307  | 1/1   | 0.70 | 0.55 | -    | 70,70,70,70                 | 1     |
| 6   | IOD  | C     | 1107 | 1/1   | 0.97 | 0.11 | -    | 53,53,53,53                 | 1     |
| 6   | IOD  | F     | 2107 | 1/1   | 0.97 | 0.15 | -    | 54,54,54,54                 | 1     |
| 5   | MG   | D     | 310  | 1/1   | 0.64 | 0.31 | -    | 46,46,46,46                 | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.