



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 07:14 pm BST

PDB ID : 1NGM  
Title : Crystal structure of a yeast Brf1-TBP-DNA ternary complex  
Authors : Juo, Z.S.; Kassavetis, G.A.; Wang, J.; Geiduschek, E.P.; Sigler, P.B.  
Deposited on : 2002-12-17  
Resolution : 2.95 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

<https://www.wwpdb.org/validation/2017/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  |
| Xtriage (Phenix)               | : | 1.13   |
| EDS                            | : | 2.11   |
| Percentile statistics          | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac                         | : | 5.8.0158   |
| CCP4                           | : | 7.0.044 (Gargrove)   |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)  |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)  |
| Validation Pipeline (wwPDB-VP) | : | 2.11   |

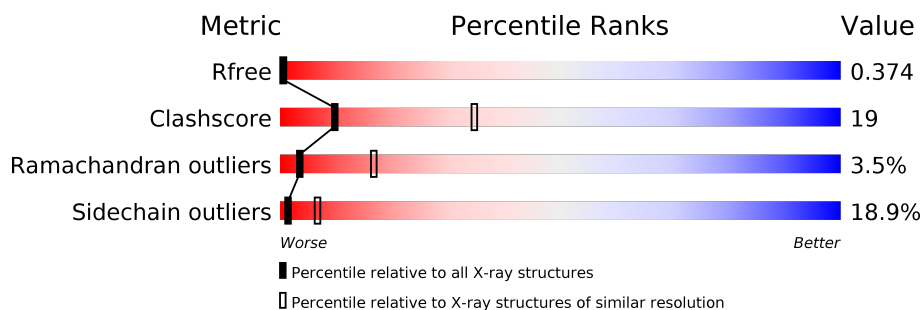
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.95 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.






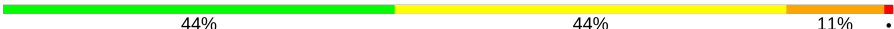
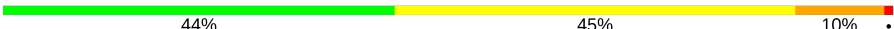


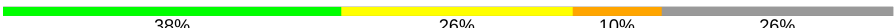

| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 130704                      | 3104 (3.00-2.92)                                      |
| Clashscore            | 141614                      | 3462 (3.00-2.92)                                      |
| Ramachandran outliers | 138981                      | 3340 (3.00-2.92)                                      |
| Sidechain outliers    | 138945                      | 3343 (3.00-2.92)                                      |

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 respectively. 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  $\leq 5\%$ .

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | C     | 19     | 16% 74% 11%      |
| 1   | G     | 19     | 37% 37% 26%      |
| 1   | K     | 19     | 37% 42% 21%      |
| 1   | O     | 19     | 16% 53% 32%      |
| 2   | D     | 19     | 42% 47% 11%      |
| 2   | H     | 19     | 26% 58% 16%      |
| 2   | L     | 19     | 32% 47% 21%      |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 2   | P     | 19     |  |
| 3   | A     | 180    |  |
| 3   | E     | 180    |  |
| 3   | I     | 180    |  |
| 3   | M     | 180    |  |
| 4   | B     | 72     |  |
| 4   | F     | 72     |  |
| 4   | J     | 72     |  |
| 4   | N     | 72     |  |

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 10800 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 5'-D(\*CP\*TP\*AP\*TP\*AP\*AP\*AP\*AP\*AP\*AP\*T  
P\*GP\*TP\*TP\*TP\*TP\*TP\*T)-3'.

| Mol | Chain | Residues | Atoms |     |    |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|---------|-------|
| 1   | C     | 19       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 386   | 189 | 66 | 113 | 18 |         |         |       |
| 1   | G     | 19       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 386   | 189 | 66 | 113 | 18 |         |         |       |
| 1   | K     | 19       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 386   | 189 | 66 | 113 | 18 |         |         |       |
| 1   | O     | 19       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 386   | 189 | 66 | 113 | 18 |         |         |       |

- Molecule 2 is a DNA chain called 5'-D(\*AP\*AP\*AP\*AP\*AP\*AP\*CP\*AP\*TP\*TP\*TP\*TP  
\*TP\*TP\*TP\*AP\*TP\*AP\*G)-3'.

| Mol | Chain | Residues | Atoms |     |    |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|---------|-------|
| 2   | D     | 19       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 387   | 189 | 69 | 111 | 18 |         |         |       |
| 2   | H     | 19       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 387   | 189 | 69 | 111 | 18 |         |         |       |
| 2   | L     | 19       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 387   | 189 | 69 | 111 | 18 |         |         |       |
| 2   | P     | 19       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 387   | 189 | 69 | 111 | 18 |         |         |       |

- Molecule 3 is a protein called Transcription initiation factor TFIIID.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 3   | A     | 180      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1416  | 921 | 242 | 247 | 6 |         |         |       |
| 3   | E     | 180      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1416  | 921 | 242 | 247 | 6 |         |         |       |
| 3   | I     | 180      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1416  | 921 | 242 | 247 | 6 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 3   | M     | 180      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1416  | 921 | 242 | 247 | 6 |         |         |       |

- Molecule 4 is a protein called Transcription factor IIIB BRF1 subunit.

| Mol | Chain | Residues | Atoms |     |    |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---|---------|---------|-------|
| 4   | B     | 72       | Total | C   | N  | O   | S | 0       | 0       | 0     |
|     |       |          | 586   | 363 | 98 | 124 | 1 |         |         |       |
| 4   | F     | 72       | Total | C   | N  | O   | S | 0       | 0       | 0     |
|     |       |          | 586   | 363 | 98 | 124 | 1 |         |         |       |
| 4   | J     | 53       | Total | C   | N  | O   |   | 0       | 0       | 0     |
|     |       |          | 436   | 268 | 73 | 95  |   |         |         |       |
| 4   | N     | 53       | Total | C   | N  | O   |   | 0       | 0       | 0     |
|     |       |          | 436   | 268 | 73 | 95  |   |         |         |       |

There are 8 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment          | Reference  |
|-------|---------|----------|--------|------------------|------------|
| B     | 435     | GLY      | -      | CLONING ARTIFACT | UNP P29056 |
| B     | 436     | SER      | -      | CLONING ARTIFACT | UNP P29056 |
| F     | 435     | GLY      | -      | CLONING ARTIFACT | UNP P29056 |
| F     | 436     | SER      | -      | CLONING ARTIFACT | UNP P29056 |
| J     | 435     | GLY      | -      | CLONING ARTIFACT | UNP P29056 |
| J     | 436     | SER      | -      | CLONING ARTIFACT | UNP P29056 |
| N     | 435     | GLY      | -      | CLONING ARTIFACT | UNP P29056 |
| N     | 436     | SER      | -      | CLONING ARTIFACT | UNP P29056 |

### 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 the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

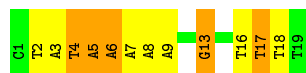
- Molecule 1: 5'-D(\*CP\*TP\*AP\*TP\*AP\*AP\*AP\*AP\*AP\*AP\*TP\*GP\*TP\*TP\*TP\*TP\*TP\*TP\*TP)-3'

Chain C: 



- Molecule 1: 5'-D(\*CP\*TP\*AP\*TP\*AP\*AP\*AP\*AP\*AP\*AP\*TP\*GP\*TP\*TP\*TP\*TP\*TP\*TP\*TP)-3'

Chain G: 




- Molecule 1: 5'-D(\*CP\*TP\*AP\*TP\*AP\*AP\*AP\*AP\*AP\*AP\*TP\*GP\*TP\*TP\*TP\*TP\*TP\*TP\*TP)-3'

Chain K: 



- Molecule 1: 5'-D(\*CP\*TP\*AP\*TP\*AP\*AP\*AP\*AP\*AP\*AP\*TP\*GP\*TP\*TP\*TP\*TP\*TP\*TP\*TP)-3'

Chain O: 



- Molecule 2: 5'-D(\*AP\*AP\*AP\*AP\*AP\*AP\*CP\*AP\*TP\*TP\*TP\*TP\*TP\*TP\*TP\*TP\*AP\*TP\*A P\*G)-3'

Chain D: 



- Molecule 2: 5'-D(\*AP\*AP\*AP\*AP\*AP\*AP\*CP\*AP\*TP\*TP\*TP\*TP\*TP\*TP\*TP\*AP\*TP\*AP\*G)-3'

Chain H: 



- Molecule 2: 5'-D(\*AP\*AP\*AP\*AP\*AP\*AP\*CP\*AP\*TP\*TP\*TP\*TP\*TP\*TP\*TP\*AP\*TP\*AP\*G)-3'

Chain L: 



- Molecule 2: 5'-D(\*AP\*AP\*AP\*AP\*AP\*AP\*CP\*AP\*TP\*TP\*TP\*TP\*TP\*TP\*TP\*AP\*TP\*AP\*G)-3'

Chain P: 



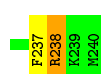
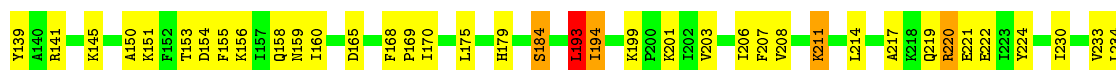
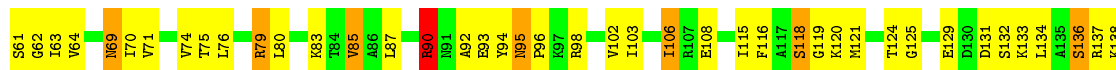
- Molecule 3: Transcription initiation factor TFIID

Chain A: 

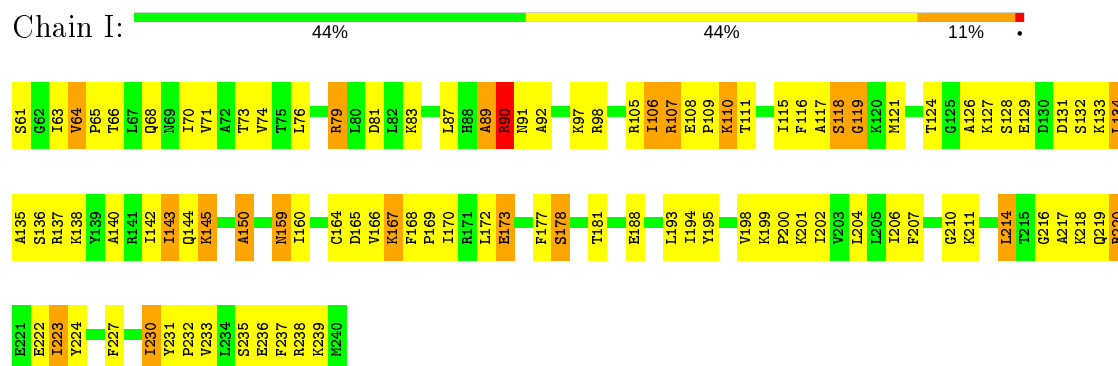


- Molecule 3: Transcription initiation factor TFIID

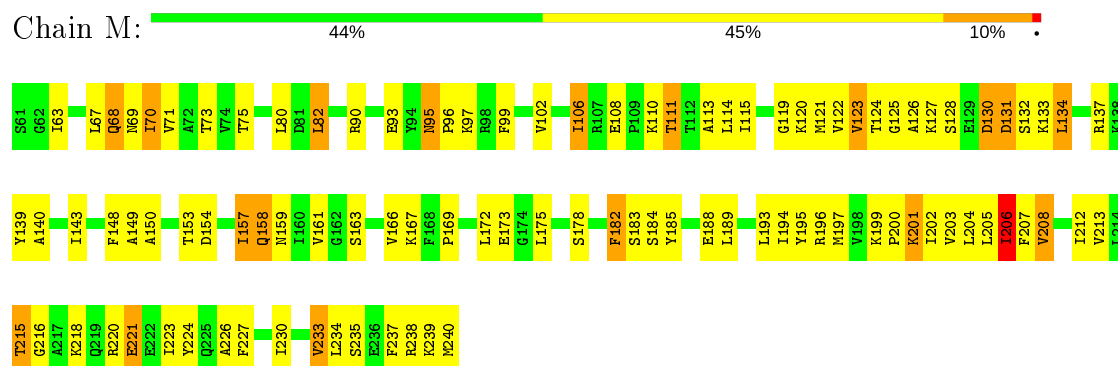
Chain E: 



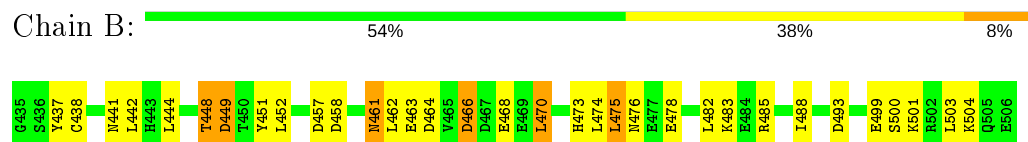
- Molecule 3: Transcription initiation factor TFIID



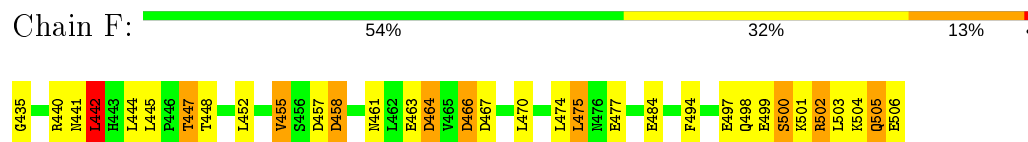
- Molecule 3: Transcription initiation factor TFIID



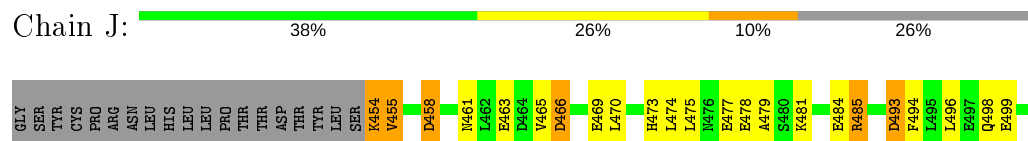
- Molecule 4: Transcription factor IIIB BRF1 subunit



- Molecule 4: Transcription factor IIIB BRF1 subunit



- Molecule 4: Transcription factor IIIB BRF1 subunit



- Molecule 4: Transcription factor IIIB BRF1 subunit





|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |      |      |      |      |      |      |      |  |      |  |      |      |      |  |      |  |      |  |      |      |      |  |      |  |      |  |      |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|--|------|--|------|------|------|--|------|--|------|--|------|------|------|--|------|--|------|--|------|
| GLY | SER | TYR | CYS | PRO | ARG | ASN | LEU | HIS | LEU | LEU | PRO | THR | THR | ASP | THR | TYR | LEU | SER | K454 | V455 | S456 | D457 | D458 | E459 | D460 |  | D464 |  | D467 | E468 | E469 |  | L474 |  | I486 |  | D493 | F494 | L495 |  | Q498 |  | K501 |  | E506 |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|--|------|--|------|------|------|--|------|--|------|--|------|------|------|--|------|--|------|--|------|

## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 21 21 2   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 93.61Å 152.60Å 256.64Å<br>90.00° 90.00° 90.00°              | Depositor        |
| Resolution (Å)  | 50.00 – 2.95<br>47.29 – 2.95                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | (Not available) (50.00-2.95)<br>95.2 (47.29-2.95)           | Depositor<br>EDS |
| $R_{merge}$   | 0.06  | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 4.18 (at 2.96Å)   | Xtriage          |
| Refinement program  | REFMAC  | Depositor        |
| R, $R_{free}$   | 0.276 , 0.308<br>0.365 , 0.374                              | Depositor<br>DCC |
| $R_{free}$ test set   | 7532 reflections (10.09%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 38.3  | Xtriage          |
| Anisotropy  | 0.759   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.28 , 18.5   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.31$ , $\langle L^2 \rangle = 0.14$ | Xtriage          |
| Estimated twinning fraction   | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation  | 0.71  | EDS              |
| Total number of atoms   | 10800   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 28.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.23 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.9524e-03.*

<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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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     | 0.79         | 0/432          | 1.52        | 2/665 (0.3%)     |
| 1   | G     | 1.03         | 2/432 (0.5%)   | 1.80        | 12/665 (1.8%)    |
| 1   | K     | 0.98         | 0/432          | 1.80        | 15/665 (2.3%)    |
| 1   | O     | 0.83         | 0/432          | 1.72        | 10/665 (1.5%)    |
| 2   | D     | 0.77         | 0/434          | 1.59        | 9/668 (1.3%)     |
| 2   | H     | 0.86         | 0/434          | 1.62        | 9/668 (1.3%)     |
| 2   | L     | 1.01         | 0/434          | 1.81        | 14/668 (2.1%)    |
| 2   | P     | 0.82         | 0/434          | 1.47        | 6/668 (0.9%)     |
| 3   | A     | 0.41         | 0/1443         | 0.68        | 1/1942 (0.1%)    |
| 3   | E     | 0.59         | 0/1443         | 0.82        | 2/1942 (0.1%)    |
| 3   | I     | 0.59         | 0/1443         | 0.83        | 2/1942 (0.1%)    |
| 3   | M     | 0.43         | 0/1443         | 0.70        | 2/1942 (0.1%)    |
| 4   | B     | 0.35         | 0/595          | 0.82        | 5/804 (0.6%)     |
| 4   | F     | 0.54         | 0/595          | 0.91        | 4/804 (0.5%)     |
| 4   | J     | 0.48         | 0/440          | 0.85        | 2/590 (0.3%)     |
| 4   | N     | 0.31         | 0/440          | 0.80        | 5/590 (0.8%)     |
| All | All   | 0.64         | 2/11306 (0.0%) | 1.16        | 100/15888 (0.6%) |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | G     | 5   | DA   | C3'-O3' | -5.62 | 1.36        | 1.44     |
| 1   | G     | 9   | DA   | C3'-O3' | -5.05 | 1.37        | 1.44     |

All (100) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 2   | L     | 16  | DA   | O4'-C1'-N9  | 12.42  | 116.69      | 108.00   |
| 1   | K     | 6   | DA   | O4'-C1'-N9  | 11.14  | 115.80      | 108.00   |
| 1   | O     | 1   | DC   | O4'-C1'-N1  | 10.36  | 115.25      | 108.00   |
| 1   | G     | 2   | DT   | O4'-C4'-C3' | -10.09 | 99.94       | 106.00   |
| 2   | D     | 5   | DA   | O4'-C1'-N9  | 9.88   | 114.91      | 108.00   |
| 1   | C     | 10  | DA   | O4'-C1'-N9  | 9.18   | 114.42      | 108.00   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | H     | 7   | DC   | O4'-C1'-N1  | 9.14  | 114.40      | 108.00   |
| 1   | G     | 7   | DA   | O4'-C1'-N9  | 9.09  | 114.36      | 108.00   |
| 1   | O     | 15  | DT   | O4'-C1'-N1  | 8.27  | 113.79      | 108.00   |
| 1   | O     | 8   | DA   | O4'-C4'-C3' | -8.06 | 101.16      | 106.00   |
| 1   | O     | 11  | DA   | O4'-C1'-N9  | 7.76  | 113.43      | 108.00   |
| 1   | G     | 5   | DA   | O4'-C4'-C3' | 7.69  | 110.61      | 106.00   |
| 2   | L     | 15  | DT   | O4'-C1'-N1  | -7.29 | 102.90      | 108.00   |
| 2   | P     | 13  | DT   | O4'-C4'-C3' | -7.16 | 101.64      | 104.50   |
| 3   | E     | 193 | LEU  | CA-CB-CG    | 7.08  | 131.59      | 115.30   |
| 1   | O     | 15  | DT   | C1'-O4'-C4' | -7.06 | 103.04      | 110.10   |
| 1   | K     | 16  | DT   | O4'-C1'-N1  | 6.97  | 112.88      | 108.00   |
| 2   | L     | 17  | DT   | C5-C4-O4    | -6.96 | 120.03      | 124.90   |
| 1   | G     | 4   | DT   | C4-C5-C7    | 6.92  | 123.15      | 119.00   |
| 2   | P     | 15  | DT   | O4'-C1'-N1  | 6.77  | 112.74      | 108.00   |
| 4   | N     | 467 | ASP  | CB-CG-OD2   | 6.76  | 124.38      | 118.30   |
| 1   | G     | 4   | DT   | C6-C5-C7    | -6.75 | 118.85      | 122.90   |
| 2   | H     | 19  | DG   | O4'-C4'-C3' | -6.71 | 101.81      | 104.50   |
| 1   | G     | 5   | DA   | O4'-C1'-N9  | 6.61  | 112.62      | 108.00   |
| 3   | M     | 130 | ASP  | CB-CG-OD2   | 6.60  | 124.24      | 118.30   |
| 1   | K     | 4   | DT   | C6-C5-C7    | -6.56 | 118.96      | 122.90   |
| 2   | H     | 14  | DT   | C5-C4-O4    | -6.50 | 120.35      | 124.90   |
| 2   | L     | 12  | DT   | C6-C5-C7    | -6.50 | 119.00      | 122.90   |
| 2   | D     | 5   | DA   | C1'-O4'-C4' | -6.44 | 103.66      | 110.10   |
| 1   | O     | 15  | DT   | O4'-C1'-C2' | -6.39 | 100.79      | 105.90   |
| 1   | O     | 5   | DA   | O4'-C1'-N9  | 6.34  | 112.44      | 108.00   |
| 2   | L     | 12  | DT   | C4-C5-C7    | 6.32  | 122.79      | 119.00   |
| 2   | L     | 17  | DT   | N3-C4-O4    | 6.30  | 123.68      | 119.90   |
| 2   | H     | 14  | DT   | N3-C4-O4    | 6.25  | 123.65      | 119.90   |
| 3   | I     | 131 | ASP  | CB-CG-OD2   | 6.17  | 123.86      | 118.30   |
| 1   | K     | 1   | DC   | O4'-C1'-N1  | -6.17 | 103.68      | 108.00   |
| 2   | L     | 9   | DT   | P-O3'-C3'   | 6.15  | 127.08      | 119.70   |
| 2   | P     | 12  | DT   | O4'-C1'-N1  | 6.12  | 112.28      | 108.00   |
| 2   | P     | 8   | DA   | P-O3'-C3'   | 6.10  | 127.03      | 119.70   |
| 2   | D     | 1   | DA   | O4'-C1'-N9  | 6.10  | 112.27      | 108.00   |
| 1   | K     | 6   | DA   | O4'-C4'-C3' | 6.09  | 109.66      | 106.00   |
| 1   | G     | 2   | DT   | C5-C4-O4    | -6.06 | 120.66      | 124.90   |
| 2   | L     | 19  | DG   | O4'-C1'-N9  | -6.06 | 103.76      | 108.00   |
| 1   | O     | 13  | DG   | O4'-C1'-N9  | 6.05  | 112.24      | 108.00   |
| 1   | K     | 2   | DT   | O4'-C4'-C3' | -6.01 | 102.09      | 104.50   |
| 1   | O     | 7   | DA   | O4'-C1'-N9  | 6.00  | 112.20      | 108.00   |
| 2   | D     | 12  | DT   | C4-C5-C7    | 5.99  | 122.60      | 119.00   |
| 4   | B     | 449 | ASP  | CB-CG-OD2   | 5.97  | 123.67      | 118.30   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | C     | 8   | DA   | O4'-C1'-N9  | 5.96  | 112.17      | 108.00   |
| 1   | K     | 4   | DT   | C4-C5-C7    | 5.96  | 122.58      | 119.00   |
| 2   | L     | 18  | DA   | O5'-P-OP1   | -5.93 | 100.36      | 105.70   |
| 1   | K     | 3   | DA   | C2-N3-C4    | 5.91  | 113.55      | 110.60   |
| 3   | I     | 81  | ASP  | CB-CG-OD2   | 5.91  | 123.62      | 118.30   |
| 2   | D     | 18  | DA   | C1'-O4'-C4' | -5.90 | 104.20      | 110.10   |
| 2   | L     | 9   | DT   | O4'-C1'-N1  | -5.88 | 103.88      | 108.00   |
| 4   | F     | 464 | ASP  | CB-CG-OD2   | 5.87  | 123.58      | 118.30   |
| 2   | D     | 11  | DT   | O4'-C1'-N1  | 5.77  | 112.04      | 108.00   |
| 1   | G     | 2   | DT   | N3-C4-O4    | 5.77  | 123.36      | 119.90   |
| 1   | O     | 9   | DA   | O4'-C1'-N9  | 5.69  | 111.98      | 108.00   |
| 1   | G     | 17  | DT   | O4'-C1'-N1  | 5.66  | 111.96      | 108.00   |
| 4   | F     | 458 | ASP  | CB-CG-OD2   | 5.64  | 123.37      | 118.30   |
| 2   | D     | 7   | DC   | O4'-C1'-N1  | 5.63  | 111.94      | 108.00   |
| 4   | F     | 457 | ASP  | CB-CG-OD2   | 5.62  | 123.36      | 118.30   |
| 2   | P     | 14  | DT   | N3-C4-O4    | 5.58  | 123.25      | 119.90   |
| 4   | N     | 460 | ASP  | CB-CG-OD2   | 5.54  | 123.29      | 118.30   |
| 2   | L     | 18  | DA   | O4'-C1'-N9  | 5.53  | 111.87      | 108.00   |
| 1   | K     | 9   | DA   | O4'-C1'-N9  | 5.50  | 111.85      | 108.00   |
| 2   | D     | 12  | DT   | C6-C5-C7    | -5.41 | 119.65      | 122.90   |
| 4   | J     | 458 | ASP  | CB-CG-OD2   | 5.36  | 123.13      | 118.30   |
| 2   | H     | 17  | DT   | O4'-C4'-C3' | -5.35 | 102.36      | 104.50   |
| 2   | H     | 9   | DT   | N3-C4-O4    | 5.35  | 123.11      | 119.90   |
| 3   | A     | 80  | LEU  | CA-CB-CG    | 5.35  | 127.59      | 115.30   |
| 1   | K     | 16  | DT   | O4'-C1'-C2' | -5.34 | 101.63      | 105.90   |
| 4   | N     | 493 | ASP  | CB-CG-OD2   | 5.32  | 123.08      | 118.30   |
| 2   | P     | 17  | DT   | N3-C4-O4    | 5.31  | 123.08      | 119.90   |
| 1   | G     | 5   | DA   | O4'-C1'-C2' | 5.27  | 110.11      | 105.90   |
| 4   | B     | 493 | ASP  | CB-CG-OD2   | 5.25  | 123.03      | 118.30   |
| 2   | H     | 16  | DA   | OP2-P-O3'   | 5.23  | 116.70      | 105.20   |
| 4   | J     | 493 | ASP  | CB-CG-OD2   | 5.22  | 123.00      | 118.30   |
| 2   | H     | 14  | DT   | O4'-C1'-C2' | 5.19  | 110.05      | 105.90   |
| 1   | K     | 2   | DT   | N3-C2-O2    | -5.17 | 119.20      | 122.30   |
| 1   | K     | 15  | DT   | O4'-C1'-C2' | -5.14 | 101.79      | 105.90   |
| 1   | K     | 14  | DT   | C3'-C2'-C1' | -5.13 | 96.34       | 102.50   |
| 3   | M     | 154 | ASP  | CB-CG-OD2   | 5.12  | 122.91      | 118.30   |
| 1   | G     | 6   | DA   | N1-C6-N6    | 5.11  | 121.67      | 118.60   |
| 1   | G     | 13  | DG   | O4'-C1'-N9  | 5.09  | 111.56      | 108.00   |
| 2   | L     | 14  | DT   | P-O5'-C5'   | -5.08 | 112.77      | 120.90   |
| 4   | B     | 466 | ASP  | CB-CG-OD2   | 5.07  | 122.86      | 118.30   |
| 4   | N     | 458 | ASP  | CB-CG-OD2   | 5.07  | 122.86      | 118.30   |
| 2   | D     | 18  | DA   | C3'-C2'-C1' | -5.05 | 96.44       | 102.50   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 4   | B     | 458 | ASP  | CB-CG-OD2   | 5.05  | 122.84      | 118.30   |
| 4   | B     | 457 | ASP  | CB-CG-OD2   | 5.05  | 122.84      | 118.30   |
| 4   | N     | 464 | ASP  | CB-CG-OD2   | 5.04  | 122.84      | 118.30   |
| 1   | K     | 17  | DT   | O4'-C1'-N1  | 5.04  | 111.53      | 108.00   |
| 2   | L     | 17  | DT   | P-O5'-C5'   | -5.04 | 112.84      | 120.90   |
| 1   | K     | 18  | DT   | O4'-C1'-N1  | 5.03  | 111.52      | 108.00   |
| 3   | E     | 131 | ASP  | CB-CG-OD2   | 5.02  | 122.82      | 118.30   |
| 2   | L     | 16  | DA   | O4'-C4'-C3' | 5.02  | 109.01      | 106.00   |
| 4   | F     | 466 | ASP  | CB-CG-OD2   | 5.02  | 122.82      | 118.30   |
| 2   | H     | 17  | DT   | C1'-O4'-C4' | -5.01 | 105.09      | 110.10   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of 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     | 386   | 0        | 220      | 14      | 0            |
| 1   | G     | 386   | 0        | 220      | 9       | 0            |
| 1   | K     | 386   | 0        | 220      | 5       | 0            |
| 1   | O     | 386   | 0        | 220      | 20      | 0            |
| 2   | D     | 387   | 0        | 219      | 9       | 0            |
| 2   | H     | 387   | 0        | 219      | 15      | 0            |
| 2   | L     | 387   | 0        | 219      | 12      | 0            |
| 2   | P     | 387   | 0        | 219      | 17      | 0            |
| 3   | A     | 1416  | 0        | 1493     | 86      | 0            |
| 3   | E     | 1416  | 0        | 1493     | 64      | 0            |
| 3   | I     | 1416  | 0        | 1493     | 79      | 0            |
| 3   | M     | 1416  | 0        | 1493     | 74      | 0            |
| 4   | B     | 586   | 0        | 562      | 23      | 0            |
| 4   | F     | 586   | 0        | 562      | 30      | 0            |
| 4   | J     | 436   | 0        | 417      | 17      | 0            |
| 4   | N     | 436   | 0        | 417      | 5       | 0            |
| All | All   | 10800 | 0        | 9686     | 394     | 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 19.

All (394) 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) |
|------------------|------------------|--------------------------|-------------------|
| 3:A:111:THR:HG21 | 3:A:135:ALA:HB1  | 1.25                     | 1.19              |
| 2:L:13:DT:H2''   | 2:L:14:DT:H5''   | 1.23                     | 1.12              |
| 3:A:111:THR:HG21 | 3:A:135:ALA:CB   | 1.82                     | 1.08              |
| 3:I:89:ALA:O     | 4:J:475:LEU:HG   | 1.62                     | 0.99              |
| 3:I:145:LYS:HG2  | 4:J:474:LEU:HD11 | 1.45                     | 0.98              |
| 1:G:5:DA:H5''    | 3:E:203:VAL:HG21 | 1.42                     | 0.98              |
| 3:E:129:GLU:HG2  | 4:F:448:THR:HG23 | 1.47                     | 0.95              |
| 3:E:90:ARG:HH11  | 3:E:90:ARG:HG2   | 1.32                     | 0.93              |
| 3:A:129:GLU:HB2  | 4:B:451:TYR:HB3  | 1.50                     | 0.90              |
| 3:E:79:ARG:HA    | 3:E:118:SER:O    | 1.73                     | 0.88              |
| 3:E:156:LYS:HE3  | 3:E:158:GLN:HE22 | 1.41                     | 0.85              |
| 4:F:435:GLY:HA2  | 3:I:128:SER:HB3  | 1.58                     | 0.84              |
| 3:A:71:VAL:HG22  | 3:A:124:THR:HG22 | 1.64                     | 0.79              |
| 3:M:169:PRO:HB2  | 3:M:239:LYS:HB3  | 1.65                     | 0.79              |
| 3:A:214:LEU:HD21 | 3:A:226:ALA:HB3  | 1.64                     | 0.78              |
| 3:A:89:ALA:HA    | 4:B:473:HIS:O    | 1.82                     | 0.78              |
| 2:L:14:DT:OP1    | 3:I:105:ARG:NH1  | 2.16                     | 0.78              |
| 2:L:13:DT:H2''   | 2:L:14:DT:C5'    | 2.08                     | 0.78              |
| 3:A:115:ILE:HD12 | 3:A:121:MET:HB3  | 1.67                     | 0.76              |
| 3:E:237:PHE:O    | 3:E:238:ARG:CB   | 2.33                     | 0.76              |
| 3:E:90:ARG:HG2   | 3:E:90:ARG:NH1   | 1.98                     | 0.76              |
| 3:M:82:LEU:HG    | 3:M:102:VAL:HG23 | 1.66                     | 0.75              |
| 3:A:106:ILE:HG13 | 3:A:107:ARG:N    | 2.00                     | 0.75              |
| 3:I:168:PHE:CD1  | 3:I:238:ARG:HG3  | 2.22                     | 0.74              |
| 1:C:9:DA:H1'     | 1:C:10:DA:C8     | 2.23                     | 0.73              |
| 3:A:102:VAL:HB   | 3:A:115:ILE:HG22 | 1.71                     | 0.73              |
| 3:A:202:ILE:HG12 | 3:A:217:ALA:HB2  | 1.72                     | 0.71              |
| 3:E:64:VAL:HG11  | 3:I:64:VAL:HG22  | 1.73                     | 0.71              |
| 3:I:204:LEU:HD21 | 3:I:230:ILE:HG21 | 1.72                     | 0.71              |
| 3:I:74:VAL:HG11  | 3:I:121:MET:HE3  | 1.73                     | 0.70              |
| 3:M:182:PHE:N    | 3:M:182:PHE:HD1  | 1.89                     | 0.70              |
| 3:M:184:SER:HB2  | 3:M:194:ILE:HB   | 1.72                     | 0.70              |
| 3:E:156:LYS:HE3  | 3:E:158:GLN:NE2  | 2.07                     | 0.70              |
| 3:I:79:ARG:HA    | 3:I:118:SER:O    | 1.91                     | 0.70              |
| 4:J:485:ARG:HG3  | 4:J:485:ARG:HH11 | 1.57                     | 0.70              |
| 2:P:16:DA:C2     | 3:M:213:VAL:HG11 | 2.28                     | 0.69              |
| 3:M:206:ILE:HD13 | 3:M:212:ILE:HD12 | 1.73                     | 0.69              |
| 3:A:111:THR:CG2  | 3:A:135:ALA:HB1  | 2.15                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:E:237:PHE:O    | 3:E:238:ARG:HB3  | 1.92                     | 0.69              |
| 3:M:182:PHE:CD1  | 3:M:182:PHE:N    | 2.60                     | 0.68              |
| 3:M:71:VAL:HB    | 3:M:159:ASN:HB3  | 1.76                     | 0.68              |
| 4:B:466:ASP:HA   | 4:B:470:LEU:HD22 | 1.76                     | 0.68              |
| 3:M:68:GLN:HG3   | 3:M:163:SER:HB3  | 1.75                     | 0.67              |
| 3:M:133:LYS:HD2  | 4:N:455:VAL:CG1  | 2.24                     | 0.67              |
| 3:M:99:PHE:HE2   | 3:M:114:LEU:HD22 | 1.59                     | 0.67              |
| 3:M:183:SER:HB3  | 3:M:193:LEU:HD21 | 1.77                     | 0.67              |
| 3:A:111:THR:CG2  | 3:A:135:ALA:CB   | 2.69                     | 0.66              |
| 2:D:1:DA:H2''    | 2:D:2:DA:H5'     | 1.78                     | 0.66              |
| 3:A:82:LEU:HG    | 3:A:117:ALA:HB2  | 1.78                     | 0.66              |
| 1:O:4:DT:H3      | 2:P:16:DA:H61    | 1.43                     | 0.66              |
| 3:A:113:ALA:HA   | 3:A:123:VAL:HA   | 1.78                     | 0.65              |
| 3:E:95:ASN:C     | 3:E:95:ASN:HD22  | 2.00                     | 0.65              |
| 3:M:195:TYR:HB3  | 3:M:204:LEU:HB2  | 1.77                     | 0.65              |
| 3:M:69:ASN:HD21  | 3:M:125:GLY:H    | 1.41                     | 0.65              |
| 3:M:207:PHE:HE2  | 3:M:213:VAL:HG23 | 1.62                     | 0.65              |
| 3:M:128:SER:HB3  | 3:M:131:ASP:HB2  | 1.80                     | 0.64              |
| 3:I:173:GLU:CD   | 3:I:173:GLU:H    | 2.00                     | 0.64              |
| 1:C:19:DT:H2'    | 2:H:1:DA:C2      | 2.33                     | 0.64              |
| 2:H:1:DA:H2'     | 2:H:2:DA:C8      | 2.32                     | 0.64              |
| 3:E:90:ARG:CG    | 3:E:90:ARG:HH11  | 2.10                     | 0.63              |
| 2:P:16:DA:H2     | 3:M:213:VAL:HG11 | 1.63                     | 0.63              |
| 3:A:214:LEU:HD21 | 3:A:226:ALA:CB   | 2.27                     | 0.63              |
| 1:O:6:DA:H2      | 3:M:71:VAL:HG21  | 1.63                     | 0.63              |
| 1:G:5:DA:C5'     | 3:E:203:VAL:HG21 | 2.25                     | 0.63              |
| 3:E:90:ARG:HA    | 4:F:475:LEU:HD21 | 1.81                     | 0.63              |
| 1:G:17:DT:H2'    | 1:G:18:DT:C6     | 2.33                     | 0.62              |
| 2:H:17:DT:H5''   | 3:E:211:LYS:HZ2  | 1.64                     | 0.62              |
| 3:M:172:LEU:HG   | 3:M:208:VAL:HG13 | 1.79                     | 0.62              |
| 3:A:142:ILE:O    | 3:A:146:ILE:HG13 | 2.00                     | 0.62              |
| 4:F:435:GLY:HA2  | 3:I:128:SER:CB   | 2.28                     | 0.62              |
| 3:I:76:LEU:HB2   | 3:I:119:GLY:O    | 2.00                     | 0.61              |
| 3:A:111:THR:HG21 | 3:A:135:ALA:HB2  | 1.77                     | 0.61              |
| 1:O:4:DT:H2''    | 1:O:5:DA:H5'     | 1.82                     | 0.61              |
| 3:I:164:CYS:SG   | 3:I:227:PHE:CE1  | 2.95                     | 0.60              |
| 3:A:91:ASN:HB2   | 3:A:104:MET:HA   | 1.83                     | 0.60              |
| 4:F:440:ARG:HH11 | 4:F:440:ARG:HG3  | 1.65                     | 0.60              |
| 3:A:129:GLU:HB2  | 4:B:451:TYR:CB   | 2.27                     | 0.60              |
| 4:F:448:THR:HG22 | 4:F:452:LEU:CD1  | 2.30                     | 0.60              |
| 3:E:76:LEU:HA    | 3:E:151:LYS:O    | 2.02                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:J:485:ARG:HG3  | 4:J:485:ARG:NH1  | 2.16                     | 0.60              |
| 3:I:74:VAL:HG11  | 3:I:121:MET:CE   | 2.32                     | 0.60              |
| 3:E:83:LYS:O     | 3:E:87:LEU:HG    | 2.02                     | 0.59              |
| 1:O:3:DA:H2''    | 1:O:4:DT:H5'     | 1.83                     | 0.59              |
| 3:E:137:ARG:NH1  | 4:F:464:ASP:OD1  | 2.36                     | 0.59              |
| 3:I:71:VAL:HG22  | 3:I:124:THR:HG22 | 1.84                     | 0.59              |
| 2:D:12:DT:H5''   | 3:A:98:ARG:HD3   | 1.84                     | 0.59              |
| 4:F:440:ARG:HD3  | 4:F:445:LEU:HD11 | 1.85                     | 0.59              |
| 1:O:7:DA:H2''    | 1:O:8:DA:O4'     | 2.03                     | 0.59              |
| 2:H:17:DT:H5''   | 3:E:211:LYS:NZ   | 2.18                     | 0.59              |
| 1:C:7:DA:H2''    | 1:C:8:DA:H5'     | 1.84                     | 0.58              |
| 1:C:4:DT:O2      | 3:A:215:THR:HG21 | 2.03                     | 0.58              |
| 3:M:133:LYS:HD2  | 4:N:455:VAL:HG11 | 1.85                     | 0.58              |
| 3:M:73:THR:HG22  | 3:M:158:GLN:NE2  | 2.18                     | 0.58              |
| 1:O:11:DA:H61    | 2:P:9:DT:H3      | 1.52                     | 0.58              |
| 3:I:111:THR:HB   | 3:I:124:THR:O    | 2.03                     | 0.58              |
| 2:P:11:DT:H2'    | 2:P:12:DT:C6     | 2.38                     | 0.57              |
| 3:E:153:THR:O    | 3:E:154:ASP:HB2  | 2.02                     | 0.57              |
| 3:E:106:ILE:HG22 | 3:E:139:TYR:CZ   | 2.39                     | 0.57              |
| 3:E:61:SER:O     | 3:E:63:ILE:N     | 2.35                     | 0.57              |
| 1:K:8:DA:H1'     | 3:I:116:PHE:CE1  | 2.39                     | 0.57              |
| 3:E:133:LYS:HD3  | 4:F:455:VAL:HG22 | 1.86                     | 0.57              |
| 1:O:13:DG:H1'    | 1:O:14:DT:H5''   | 1.87                     | 0.57              |
| 3:A:205:LEU:HB2  | 3:A:213:VAL:HB   | 1.86                     | 0.57              |
| 3:I:118:SER:OG   | 3:I:119:GLY:N    | 2.37                     | 0.57              |
| 3:I:129:GLU:OE1  | 3:I:220:ARG:NH2  | 2.32                     | 0.56              |
| 3:A:171:ARG:NH1  | 3:A:174:GLY:HA3  | 2.21                     | 0.56              |
| 3:A:116:PHE:HE1  | 3:A:122:VAL:HG23 | 1.70                     | 0.56              |
| 3:A:106:ILE:HD12 | 4:B:473:HIS:NE2  | 2.20                     | 0.56              |
| 3:A:214:LEU:HD22 | 3:A:223:ILE:HG23 | 1.88                     | 0.56              |
| 3:E:206:ILE:HD12 | 3:E:234:LEU:HD21 | 1.88                     | 0.56              |
| 3:A:141:ARG:HH21 | 3:A:145:LYS:HG3  | 1.69                     | 0.56              |
| 3:M:67:LEU:HD21  | 3:M:220:ARG:HG3  | 1.87                     | 0.55              |
| 2:L:14:DT:H2''   | 2:L:15:DT:H5'    | 1.87                     | 0.55              |
| 1:O:6:DA:C2      | 3:M:71:VAL:HG21  | 2.41                     | 0.55              |
| 2:P:14:DT:H2''   | 2:P:15:DT:H5'    | 1.88                     | 0.55              |
| 3:A:206:ILE:HD13 | 3:A:212:ILE:HG23 | 1.87                     | 0.55              |
| 2:P:8:DA:H2''    | 2:P:9:DT:O5'     | 2.06                     | 0.55              |
| 4:J:503:LEU:O    | 4:J:506:GLU:HB2  | 2.07                     | 0.55              |
| 3:I:90:ARG:HA    | 4:J:475:LEU:HD21 | 1.89                     | 0.55              |
| 4:J:461:ASN:ND2  | 4:J:463:GLU:HG3  | 2.21                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:E:145:LYS:HD2  | 4:F:474:LEU:HD11 | 1.88                     | 0.54              |
| 3:E:64:VAL:HG12  | 3:I:66:THR:HG22  | 1.89                     | 0.54              |
| 3:I:202:ILE:HD11 | 3:I:217:ALA:HB2  | 1.89                     | 0.54              |
| 3:M:207:PHE:CE2  | 3:M:213:VAL:HG23 | 2.41                     | 0.54              |
| 3:M:206:ILE:HD12 | 3:M:234:LEU:HD21 | 1.89                     | 0.54              |
| 1:K:6:DA:C2      | 3:I:71:VAL:HG21  | 2.42                     | 0.54              |
| 2:D:14:DT:H2''   | 2:D:15:DT:H5'    | 1.89                     | 0.54              |
| 3:A:70:ILE:HG12  | 3:A:126:ALA:O    | 2.07                     | 0.54              |
| 1:O:2:DT:H2''    | 1:O:3:DA:H8      | 1.72                     | 0.54              |
| 3:E:175:LEU:HD22 | 3:E:193:LEU:HD21 | 1.89                     | 0.54              |
| 3:A:134:LEU:HA   | 3:A:137:ARG:HB2  | 1.89                     | 0.54              |
| 3:A:70:ILE:HG23  | 3:A:160:ILE:HG12 | 1.90                     | 0.54              |
| 3:A:163:SER:HA   | 3:A:212:ILE:O    | 2.07                     | 0.54              |
| 2:H:2:DA:H2''    | 2:H:3:DA:C8      | 2.43                     | 0.54              |
| 3:E:74:VAL:HG21  | 3:E:136:SER:HB3  | 1.90                     | 0.54              |
| 3:E:85:VAL:HG22  | 3:E:102:VAL:HG11 | 1.89                     | 0.54              |
| 3:A:185:TYR:HB2  | 3:A:193:LEU:HD12 | 1.90                     | 0.54              |
| 3:A:106:ILE:HG13 | 3:A:107:ARG:H    | 1.71                     | 0.53              |
| 3:A:195:TYR:HD2  | 3:A:204:LEU:HD13 | 1.73                     | 0.53              |
| 2:L:16:DA:H4'    | 3:I:68:GLN:HG3   | 1.90                     | 0.53              |
| 1:C:17:DT:N3     | 2:D:4:DA:H2      | 2.06                     | 0.53              |
| 3:I:231:TYR:HB3  | 3:I:232:PRO:HD3  | 1.90                     | 0.53              |
| 2:H:1:DA:H2'     | 2:H:2:DA:H8      | 1.72                     | 0.53              |
| 4:F:448:THR:HG22 | 4:F:452:LEU:HD12 | 1.90                     | 0.53              |
| 3:M:71:VAL:HG22  | 3:M:124:THR:HG22 | 1.90                     | 0.53              |
| 2:L:13:DT:C2'    | 2:L:14:DT:H5''   | 2.17                     | 0.53              |
| 3:A:137:ARG:HG3  | 3:A:152:PHE:CE1  | 2.44                     | 0.52              |
| 3:M:178:SER:CB   | 3:M:237:PHE:HZ   | 2.22                     | 0.52              |
| 3:M:178:SER:HB2  | 3:M:237:PHE:HZ   | 1.74                     | 0.52              |
| 4:J:470:LEU:O    | 4:J:473:HIS:HB2  | 2.10                     | 0.52              |
| 3:A:206:ILE:HG23 | 3:A:212:ILE:HD12 | 1.92                     | 0.52              |
| 1:K:16:DT:H2''   | 1:K:17:DT:O5'    | 2.09                     | 0.52              |
| 3:M:99:PHE:CE2   | 3:M:114:LEU:HD22 | 2.44                     | 0.52              |
| 3:M:130:ASP:O    | 3:M:134:LEU:HB2  | 2.09                     | 0.52              |
| 3:A:166:VAL:HG21 | 3:A:170:ILE:HD11 | 1.92                     | 0.52              |
| 3:I:109:PRO:O    | 3:I:111:THR:HG23 | 2.10                     | 0.52              |
| 3:A:106:ILE:HG22 | 3:A:139:TYR:OH   | 2.10                     | 0.52              |
| 3:A:95:ASN:HD22  | 3:A:98:ARG:HB2   | 1.75                     | 0.52              |
| 2:L:15:DT:H2''   | 2:L:16:DA:C8     | 2.45                     | 0.52              |
| 3:I:129:GLU:O    | 3:I:132:SER:HB3  | 2.10                     | 0.51              |
| 1:C:14:DT:H3     | 2:D:6:DA:H2      | 1.58                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:E:220:ARG:HG2  | 3:E:224:TYR:CE2  | 2.45                     | 0.51              |
| 1:G:8:DA:H1'     | 3:E:116:PHE:CE1  | 2.45                     | 0.51              |
| 2:L:17:DT:H1'    | 3:I:207:PHE:CZ   | 2.45                     | 0.51              |
| 3:I:74:VAL:CG1   | 3:I:121:MET:CE   | 2.88                     | 0.51              |
| 3:M:73:THR:HG22  | 3:M:158:GLN:HE21 | 1.75                     | 0.51              |
| 3:M:215:THR:OG1  | 3:M:216:GLY:N    | 2.44                     | 0.51              |
| 3:A:155:PHE:HE2  | 4:B:452:LEU:HD21 | 1.76                     | 0.51              |
| 3:M:137:ARG:NH2  | 4:N:458:ASP:O    | 2.43                     | 0.51              |
| 3:A:99:PHE:CD2   | 3:A:101:ALA:HB3  | 2.45                     | 0.51              |
| 3:A:88:HIS:O     | 3:A:89:ALA:HB2   | 2.11                     | 0.51              |
| 3:I:97:LYS:HG3   | 4:J:494:PHE:HB2  | 1.92                     | 0.51              |
| 3:E:106:ILE:HG13 | 3:E:108:GLU:H    | 1.77                     | 0.50              |
| 3:I:87:LEU:HD13  | 4:J:484:GLU:HB2  | 1.92                     | 0.50              |
| 3:I:204:LEU:HD23 | 3:I:206:ILE:HD11 | 1.93                     | 0.50              |
| 3:A:140:ALA:HB3  | 4:B:462:LEU:HD22 | 1.92                     | 0.50              |
| 3:A:105:ARG:HD3  | 3:A:112:THR:HG23 | 1.92                     | 0.50              |
| 3:E:75:THR:HG23  | 3:E:120:LYS:HD3  | 1.93                     | 0.50              |
| 4:B:441:ASN:HB3  | 4:B:444:LEU:HD12 | 1.93                     | 0.50              |
| 4:F:440:ARG:NH1  | 4:F:440:ARG:HG3  | 2.27                     | 0.50              |
| 3:M:221:GLU:O    | 3:M:224:TYR:N    | 2.44                     | 0.50              |
| 3:A:129:GLU:OE2  | 4:B:448:THR:HA   | 2.12                     | 0.50              |
| 2:P:16:DA:H2     | 3:M:213:VAL:CG1  | 2.24                     | 0.50              |
| 3:E:71:VAL:HG13  | 3:E:124:THR:HG22 | 1.92                     | 0.50              |
| 1:C:17:DT:H2'    | 1:C:18:DT:C6     | 2.47                     | 0.50              |
| 3:A:111:THR:CG2  | 3:A:135:ALA:HB2  | 2.40                     | 0.50              |
| 1:K:6:DA:H2      | 3:I:71:VAL:HG21  | 1.77                     | 0.50              |
| 3:A:137:ARG:HG2  | 4:B:462:LEU:HD23 | 1.94                     | 0.49              |
| 3:E:133:LYS:HG3  | 3:E:155:PHE:CE2  | 2.47                     | 0.49              |
| 1:C:5:DA:C6      | 1:C:6:DA:N6      | 2.81                     | 0.49              |
| 3:I:143:ILE:HG22 | 3:I:150:ALA:HB2  | 1.93                     | 0.49              |
| 3:M:133:LYS:HD2  | 4:N:455:VAL:HG13 | 1.93                     | 0.49              |
| 3:A:180:GLY:HA2  | 3:A:183:SER:HB2  | 1.94                     | 0.49              |
| 3:A:129:GLU:HG2  | 4:B:448:THR:HG23 | 1.94                     | 0.49              |
| 3:I:129:GLU:CD   | 3:I:220:ARG:HH21 | 2.15                     | 0.49              |
| 2:H:6:DA:C2      | 2:H:7:DC:C2      | 3.00                     | 0.49              |
| 3:I:223:ILE:HG22 | 3:I:224:TYR:N    | 2.27                     | 0.49              |
| 3:I:76:LEU:HD21  | 3:I:140:ALA:HA   | 1.94                     | 0.49              |
| 2:D:14:DT:C7     | 2:D:15:DT:H73    | 2.43                     | 0.49              |
| 3:E:133:LYS:HD2  | 4:F:452:LEU:HD23 | 1.95                     | 0.49              |
| 4:F:458:ASP:OD1  | 4:F:461:ASN:N    | 2.41                     | 0.49              |
| 3:A:139:TYR:N    | 3:A:139:TYR:CD1  | 2.80                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:E:165:ASP:HB2  | 3:E:211:LYS:HD2  | 1.94                     | 0.49              |
| 3:E:159:ASN:HA   | 3:E:217:ALA:O    | 2.13                     | 0.49              |
| 3:A:137:ARG:HH12 | 4:B:462:LEU:HA   | 1.78                     | 0.48              |
| 4:F:448:THR:HG22 | 4:F:452:LEU:HD11 | 1.95                     | 0.48              |
| 4:B:470:LEU:HA   | 4:B:473:HIS:HD2  | 1.78                     | 0.48              |
| 2:L:16:DA:C4'    | 3:I:68:GLN:HG3   | 2.43                     | 0.48              |
| 1:O:5:DA:H2''    | 1:O:6:DA:H5'     | 1.95                     | 0.48              |
| 3:E:94:TYR:CZ    | 3:E:96:PRO:HG3   | 2.48                     | 0.48              |
| 3:M:223:ILE:O    | 3:M:226:ALA:HB3  | 2.13                     | 0.48              |
| 3:A:121:MET:HG3  | 3:A:123:VAL:HG23 | 1.96                     | 0.48              |
| 4:F:435:GLY:CA   | 3:I:128:SER:HB3  | 2.38                     | 0.48              |
| 3:I:219:GLN:N    | 3:I:222:GLU:OE1  | 2.46                     | 0.48              |
| 4:J:454:LYS:HD3  | 4:J:455:VAL:H    | 1.78                     | 0.48              |
| 3:A:102:VAL:HB   | 3:A:115:ILE:CG2  | 2.42                     | 0.48              |
| 3:E:219:GLN:HG2  | 3:E:222:GLU:OE2  | 2.14                     | 0.48              |
| 2:H:7:DC:H2''    | 2:H:8:DA:C8      | 2.49                     | 0.48              |
| 1:O:10:DA:C2     | 1:O:11:DA:C6     | 3.01                     | 0.48              |
| 2:D:14:DT:H5''   | 3:A:112:THR:OG1  | 2.13                     | 0.48              |
| 3:E:93:GLU:HG3   | 3:E:103:ILE:HB   | 1.95                     | 0.48              |
| 3:E:184:SER:HB2  | 3:E:194:ILE:HD12 | 1.95                     | 0.48              |
| 3:M:203:VAL:O    | 3:M:204:LEU:HD23 | 2.14                     | 0.48              |
| 3:E:133:LYS:HG3  | 3:E:155:PHE:CD2  | 2.48                     | 0.48              |
| 3:E:221:GLU:CG   | 4:F:447:THR:HG22 | 2.44                     | 0.48              |
| 2:L:6:DA:C2      | 2:L:7:DC:C2      | 3.02                     | 0.48              |
| 3:M:75:THR:HG23  | 3:M:120:LYS:HD3  | 1.95                     | 0.47              |
| 3:A:195:TYR:CD2  | 3:A:204:LEU:HD13 | 2.49                     | 0.47              |
| 3:E:69:ASN:HD21  | 3:E:125:GLY:H    | 1.62                     | 0.47              |
| 3:E:90:ARG:HD3   | 3:E:90:ARG:HA    | 1.62                     | 0.47              |
| 3:I:107:ARG:O    | 3:I:108:GLU:CG   | 2.61                     | 0.47              |
| 3:I:74:VAL:CG1   | 3:I:121:MET:HE3  | 2.42                     | 0.47              |
| 3:M:110:LYS:O    | 3:M:111:THR:HG23 | 2.14                     | 0.47              |
| 3:A:186:GLU:HB2  | 3:A:189:LEU:HB3  | 1.95                     | 0.47              |
| 3:M:161:VAL:HG22 | 3:M:215:THR:HB   | 1.97                     | 0.47              |
| 3:M:206:ILE:HG23 | 3:M:212:ILE:CD1  | 2.44                     | 0.47              |
| 3:I:116:PHE:O    | 3:I:117:ALA:C    | 2.52                     | 0.47              |
| 3:A:205:LEU:O    | 3:A:212:ILE:HA   | 2.15                     | 0.47              |
| 3:A:88:HIS:HA    | 4:B:475:LEU:CD1  | 2.44                     | 0.47              |
| 4:F:502:ARG:HA   | 4:F:505:GLN:HB2  | 1.97                     | 0.47              |
| 3:A:88:HIS:HA    | 4:B:475:LEU:HD11 | 1.96                     | 0.47              |
| 3:M:197:MET:HB3  | 3:M:202:ILE:H    | 1.79                     | 0.46              |
| 3:A:159:ASN:HD21 | 3:A:216:GLY:H    | 1.63                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:A:217:ALA:HB3  | 3:A:223:ILE:HG13 | 1.97                     | 0.46              |
| 1:O:6:DA:H2''    | 1:O:7:DA:O5'     | 2.15                     | 0.46              |
| 1:C:7:DA:C2'     | 1:C:8:DA:H5'     | 2.45                     | 0.46              |
| 3:I:106:ILE:HG12 | 3:I:108:GLU:H    | 1.80                     | 0.46              |
| 3:I:74:VAL:HG13  | 3:I:121:MET:HE2  | 1.98                     | 0.46              |
| 3:I:217:ALA:HB3  | 3:I:223:ILE:HD12 | 1.98                     | 0.46              |
| 3:I:70:ILE:HG23  | 3:I:160:ILE:HG12 | 1.97                     | 0.46              |
| 3:I:195:TYR:HB3  | 3:I:204:LEU:HB2  | 1.97                     | 0.46              |
| 4:B:437:TYR:CD2  | 4:B:438:CYS:N    | 2.84                     | 0.46              |
| 2:H:14:DT:H1'    | 3:E:69:ASN:OD1   | 2.16                     | 0.46              |
| 3:E:169:PRO:HA   | 3:E:208:VAL:O    | 2.15                     | 0.46              |
| 3:E:87:LEU:HD13  | 4:F:484:GLU:HB2  | 1.97                     | 0.46              |
| 3:M:63:ILE:HD13  | 3:M:166:VAL:HG12 | 1.97                     | 0.46              |
| 3:E:138:LYS:HG2  | 4:F:470:LEU:HD12 | 1.98                     | 0.46              |
| 2:H:13:DT:OP1    | 3:E:98:ARG:NH2   | 2.42                     | 0.46              |
| 3:I:145:LYS:HB3  | 4:J:474:LEU:HD21 | 1.97                     | 0.46              |
| 3:A:70:ILE:HG13  | 3:A:128:SER:O    | 2.16                     | 0.46              |
| 1:C:2:DT:O4      | 1:C:3:DA:N6      | 2.49                     | 0.46              |
| 3:I:199:LYS:HA   | 3:I:200:PRO:HA   | 1.79                     | 0.46              |
| 3:I:235:SER:O    | 3:I:236:GLU:C    | 2.52                     | 0.46              |
| 3:I:90:ARG:HG2   | 3:I:91:ASN:ND2   | 2.31                     | 0.46              |
| 3:M:140:ALA:HA   | 3:M:143:ILE:HD12 | 1.97                     | 0.46              |
| 3:I:115:ILE:HD13 | 3:I:143:ILE:HD11 | 1.98                     | 0.45              |
| 3:M:182:PHE:CD2  | 3:M:196:ARG:O    | 2.69                     | 0.45              |
| 3:A:206:ILE:HG23 | 3:A:212:ILE:CD1  | 2.46                     | 0.45              |
| 3:I:230:ILE:HG13 | 3:I:230:ILE:O    | 2.15                     | 0.45              |
| 3:M:185:TYR:HB2  | 3:M:193:LEU:HD23 | 1.97                     | 0.45              |
| 2:P:16:DA:C2     | 3:M:213:VAL:CG1  | 2.98                     | 0.45              |
| 4:F:441:ASN:OD1  | 4:F:441:ASN:O    | 2.33                     | 0.45              |
| 3:M:69:ASN:HD21  | 3:M:125:GLY:N    | 2.13                     | 0.45              |
| 3:A:104:MET:O    | 3:A:112:THR:O    | 2.34                     | 0.45              |
| 3:A:141:ARG:O    | 3:A:145:LYS:HB2  | 2.17                     | 0.45              |
| 4:B:500:SER:HA   | 4:B:503:LEU:HD12 | 1.99                     | 0.45              |
| 3:E:115:ILE:HG13 | 3:E:121:MET:HG3  | 1.99                     | 0.45              |
| 1:O:6:DA:N3      | 3:M:71:VAL:HG11  | 2.32                     | 0.45              |
| 1:O:8:DA:H61     | 2:P:12:DT:H3     | 1.65                     | 0.45              |
| 1:O:8:DA:N6      | 2:P:12:DT:H3     | 2.14                     | 0.45              |
| 3:I:90:ARG:HB3   | 4:J:473:HIS:O    | 2.17                     | 0.45              |
| 1:O:2:DT:H2''    | 1:O:3:DA:O5'     | 2.17                     | 0.45              |
| 2:P:11:DT:C2'    | 2:P:12:DT:C6     | 3.00                     | 0.45              |
| 1:C:17:DT:N3     | 2:D:4:DA:C2      | 2.85                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:I:231:TYR:HB3  | 3:I:232:PRO:CD   | 2.47                     | 0.44              |
| 4:J:463:GLU:O    | 4:J:466:ASP:HB2  | 2.17                     | 0.44              |
| 1:K:4:DT:H5''    | 3:I:194:ILE:HG12 | 1.99                     | 0.44              |
| 3:A:166:VAL:HG22 | 3:A:210:GLY:O    | 2.17                     | 0.44              |
| 3:A:199:LYS:HA   | 3:A:200:PRO:HA   | 1.75                     | 0.44              |
| 3:I:134:LEU:O    | 3:I:138:LYS:HG3  | 2.16                     | 0.44              |
| 3:I:61:SER:C     | 3:I:63:ILE:H     | 2.20                     | 0.44              |
| 3:A:141:ARG:HB3  | 4:B:470:LEU:HD11 | 1.98                     | 0.44              |
| 3:E:214:LEU:HD12 | 3:E:214:LEU:N    | 2.33                     | 0.44              |
| 1:G:13:DG:C2     | 2:H:8:DA:C2      | 3.05                     | 0.44              |
| 2:H:6:DA:H2''    | 2:H:7:DC:O5'     | 2.18                     | 0.44              |
| 3:M:80:LEU:HD12  | 3:M:119:GLY:HA2  | 1.99                     | 0.44              |
| 1:O:1:DC:H42     | 2:P:19:DG:H1     | 1.66                     | 0.44              |
| 3:M:197:MET:O    | 3:M:201:LYS:HA   | 2.18                     | 0.44              |
| 3:I:74:VAL:CG1   | 3:I:121:MET:HE2  | 2.48                     | 0.44              |
| 3:I:159:ASN:HD21 | 3:I:216:GLY:CA   | 2.30                     | 0.44              |
| 3:A:152:PHE:HB2  | 4:B:462:LEU:HD21 | 2.00                     | 0.44              |
| 3:E:133:LYS:HB3  | 4:F:455:VAL:HG21 | 2.00                     | 0.44              |
| 3:E:141:ARG:NH2  | 3:E:145:LYS:HE3  | 2.33                     | 0.44              |
| 2:H:11:DT:C5     | 2:H:12:DT:H73    | 2.53                     | 0.44              |
| 3:M:106:ILE:HB   | 3:M:139:TYR:CE1  | 2.53                     | 0.43              |
| 3:A:196:ARG:HD3  | 3:A:203:VAL:HG22 | 2.00                     | 0.43              |
| 3:E:168:PHE:CE1  | 3:E:238:ARG:HB2  | 2.53                     | 0.43              |
| 3:M:206:ILE:HD12 | 3:M:234:LEU:CD2  | 2.48                     | 0.43              |
| 3:I:159:ASN:HD21 | 3:I:216:GLY:H    | 1.64                     | 0.43              |
| 3:I:172:LEU:HD22 | 3:I:193:LEU:HB2  | 1.98                     | 0.43              |
| 3:E:237:PHE:O    | 3:E:238:ARG:HB2  | 2.16                     | 0.43              |
| 4:F:441:ASN:C    | 4:F:441:ASN:OD1  | 2.56                     | 0.43              |
| 3:I:165:ASP:OD2  | 3:I:211:LYS:HE2  | 2.19                     | 0.43              |
| 3:I:70:ILE:HA    | 3:I:159:ASN:O    | 2.18                     | 0.43              |
| 3:M:143:ILE:HG22 | 3:M:148:PHE:HB2  | 2.00                     | 0.43              |
| 3:M:70:ILE:N     | 3:M:126:ALA:O    | 2.51                     | 0.43              |
| 3:A:139:TYR:HD1  | 3:A:139:TYR:N    | 2.17                     | 0.43              |
| 3:I:138:LYS:HE2  | 4:J:465:VAL:HB   | 2.00                     | 0.43              |
| 4:F:463:GLU:HA   | 4:F:466:ASP:OD2  | 2.18                     | 0.43              |
| 2:P:17:DT:H4'    | 3:M:207:PHE:CE2  | 2.54                     | 0.43              |
| 4:F:504:LYS:C    | 4:F:506:GLU:H    | 2.21                     | 0.43              |
| 3:A:86:ALA:C     | 3:A:88:HIS:H     | 2.21                     | 0.43              |
| 4:F:466:ASP:O    | 4:F:467:ASP:HB3  | 2.18                     | 0.43              |
| 1:C:7:DA:O4'     | 3:A:158:GLN:HG3  | 2.19                     | 0.43              |
| 3:A:94:TYR:CZ    | 3:A:96:PRO:HG3   | 2.54                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:6:DA:C2      | 3:E:71:VAL:HG21  | 2.54                     | 0.43              |
| 2:P:17:DT:H2''   | 2:P:18:DA:C8     | 2.54                     | 0.43              |
| 3:A:113:ALA:HA   | 3:A:122:VAL:O    | 2.19                     | 0.42              |
| 3:A:219:GLN:O    | 3:A:222:GLU:HB2  | 2.19                     | 0.42              |
| 3:M:230:ILE:O    | 3:M:230:ILE:HG12 | 2.18                     | 0.42              |
| 3:M:63:ILE:HB    | 3:M:227:PHE:CE2  | 2.54                     | 0.42              |
| 3:I:165:ASP:OD1  | 3:I:167:LYS:HD2  | 2.18                     | 0.42              |
| 1:O:17:DT:H2''   | 1:O:18:DT:O5'    | 2.18                     | 0.42              |
| 3:A:116:PHE:CE1  | 3:A:122:VAL:HG23 | 2.53                     | 0.42              |
| 4:F:470:LEU:C    | 4:F:470:LEU:HD23 | 2.40                     | 0.42              |
| 3:E:70:ILE:HG23  | 3:E:160:ILE:HG12 | 2.00                     | 0.42              |
| 2:H:13:DT:H2''   | 2:H:14:DT:H5'    | 2.02                     | 0.42              |
| 3:I:64:VAL:HA    | 3:I:65:PRO:HD3   | 1.89                     | 0.42              |
| 2:L:15:DT:H6     | 2:L:15:DT:H2'    | 1.64                     | 0.42              |
| 3:A:105:ARG:HA   | 3:A:112:THR:HA   | 2.01                     | 0.42              |
| 4:B:461:ASN:C    | 4:B:463:GLU:H    | 2.22                     | 0.42              |
| 1:G:16:DT:H2''   | 1:G:17:DT:H6     | 1.84                     | 0.42              |
| 1:C:11:DA:H2''   | 1:C:12:DT:C6     | 2.55                     | 0.42              |
| 4:F:441:ASN:O    | 4:F:442:LEU:C    | 2.57                     | 0.42              |
| 3:I:89:ALA:HB3   | 3:I:92:ALA:HB2   | 2.00                     | 0.42              |
| 1:O:5:DA:OP1     | 3:M:196:ARG:NH1  | 2.51                     | 0.42              |
| 1:G:3:DA:H2''    | 1:G:4:DT:H5'     | 2.01                     | 0.42              |
| 3:I:166:VAL:HG22 | 3:I:210:GLY:O    | 2.20                     | 0.42              |
| 3:A:186:GLU:HA   | 3:A:187:PRO:HD3  | 1.91                     | 0.41              |
| 3:A:82:LEU:O     | 3:A:83:LYS:C     | 2.58                     | 0.41              |
| 4:F:444:LEU:HD23 | 4:F:444:LEU:HA   | 1.85                     | 0.41              |
| 3:M:70:ILE:HG23  | 3:M:157:ILE:CG2  | 2.50                     | 0.41              |
| 3:M:133:LYS:HB3  | 4:N:455:VAL:HG21 | 2.02                     | 0.41              |
| 3:E:220:ARG:CG   | 3:E:224:TYR:CE2  | 3.03                     | 0.41              |
| 1:O:4:DT:H3      | 2:P:16:DA:N6     | 2.14                     | 0.41              |
| 3:I:111:THR:HG22 | 3:I:126:ALA:N    | 2.35                     | 0.41              |
| 3:M:102:VAL:O    | 3:M:115:ILE:HD12 | 2.20                     | 0.41              |
| 3:M:161:VAL:HG22 | 3:M:215:THR:CB   | 2.51                     | 0.41              |
| 4:J:475:LEU:HB3  | 4:J:479:ALA:HB3  | 2.03                     | 0.41              |
| 3:A:76:LEU:HB3   | 3:A:150:ALA:HB1  | 2.03                     | 0.41              |
| 3:A:197:MET:O    | 3:A:201:LYS:HA   | 2.20                     | 0.41              |
| 4:F:500:SER:O    | 4:F:503:LEU:HB2  | 2.20                     | 0.41              |
| 3:I:230:ILE:O    | 3:I:233:VAL:HB   | 2.20                     | 0.41              |
| 3:M:199:LYS:HA   | 3:M:200:PRO:HA   | 1.84                     | 0.41              |
| 3:M:95:ASN:HA    | 3:M:96:PRO:HD3   | 1.88                     | 0.41              |
| 3:A:99:PHE:HD2   | 3:A:101:ALA:HB3  | 1.84                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:M:113:ALA:HA   | 3:M:122:VAL:O    | 2.21                     | 0.41              |
| 4:B:437:TYR:HD2  | 4:B:438:CYS:H    | 1.68                     | 0.41              |
| 3:I:109:PRO:HD2  | 3:I:135:ALA:HB2  | 2.03                     | 0.41              |
| 3:M:159:ASN:ND2  | 3:M:216:GLY:H    | 2.19                     | 0.41              |
| 3:A:155:PHE:CE2  | 4:B:452:LEU:HD21 | 2.56                     | 0.41              |
| 3:E:211:LYS:HG2  | 3:E:211:LYS:H    | 1.70                     | 0.41              |
| 1:G:5:DA:H8      | 1:G:5:DA:H2'     | 1.81                     | 0.41              |
| 3:M:123:VAL:HG12 | 3:M:123:VAL:O    | 2.21                     | 0.41              |
| 3:M:182:PHE:H    | 3:M:182:PHE:HD1  | 1.66                     | 0.41              |
| 2:L:3:DA:C2      | 2:L:4:DA:C4      | 3.09                     | 0.40              |
| 3:M:205:LEU:HB2  | 3:M:213:VAL:HB   | 2.03                     | 0.40              |
| 3:M:233:VAL:HG13 | 3:M:233:VAL:O    | 2.20                     | 0.40              |
| 2:P:11:DT:C6     | 2:P:12:DT:H72    | 2.56                     | 0.40              |
| 4:B:470:LEU:HA   | 4:B:473:HIS:CD2  | 2.56                     | 0.40              |
| 3:E:230:ILE:O    | 3:E:233:VAL:HB   | 2.22                     | 0.40              |
| 3:I:137:ARG:HH22 | 4:J:458:ASP:HB3  | 1.86                     | 0.40              |
| 3:I:178:SER:HG   | 3:I:237:PHE:HZ   | 1.68                     | 0.40              |
| 3:I:214:LEU:HD21 | 3:I:227:PHE:HB2  | 2.02                     | 0.40              |
| 1:C:1:DC:H2'     | 1:C:2:DT:C6      | 2.57                     | 0.40              |
| 3:I:169:PRO:HG2  | 3:I:239:LYS:HB3  | 2.02                     | 0.40              |
| 3:M:106:ILE:HD13 | 3:M:108:GLU:H    | 1.87                     | 0.40              |
| 3:M:178:SER:CB   | 3:M:237:PHE:CZ   | 3.03                     | 0.40              |
| 3:E:95:ASN:C     | 3:E:95:ASN:ND2   | 2.70                     | 0.40              |
| 2:H:17:DT:H1'    | 3:E:207:PHE:CE2  | 2.56                     | 0.40              |
| 3:A:161:VAL:HA   | 3:A:215:THR:HA   | 2.03                     | 0.40              |
| 2:D:1:DA:H2''    | 2:D:2:DA:C5'     | 2.50                     | 0.40              |
| 3:I:117:ALA:O    | 3:I:118:SER:C    | 2.59                     | 0.40              |
| 3:I:230:ILE:HG13 | 3:I:233:VAL:HB   | 2.03                     | 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 |     |
|-----|-------|----------------|-----------|-----------|----------|-------------|-----|
| 3   | A     | 178/180 (99%)  | 140 (79%) | 29 (16%)  | 9 (5%)   | 2           | 9   |
| 3   | E     | 178/180 (99%)  | 154 (86%) | 15 (8%)   | 9 (5%)   | 2           | 9   |
| 3   | I     | 178/180 (99%)  | 159 (89%) | 12 (7%)   | 7 (4%)   | 3           | 14  |
| 3   | M     | 178/180 (99%)  | 154 (86%) | 20 (11%)  | 4 (2%)   | 6           | 28  |
| 4   | B     | 70/72 (97%)    | 58 (83%)  | 11 (16%)  | 1 (1%)   | 11          | 39  |
| 4   | F     | 70/72 (97%)    | 56 (80%)  | 12 (17%)  | 2 (3%)   | 4           | 21  |
| 4   | J     | 51/72 (71%)    | 46 (90%)  | 4 (8%)    | 1 (2%)   | 7           | 30  |
| 4   | N     | 51/72 (71%)    | 47 (92%)  | 4 (8%)    | 0        | 100         | 100 |
| All | All   | 954/1008 (95%) | 814 (85%) | 107 (11%) | 33 (4%)  | 3           | 17  |

All (33) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | A     | 106 | ILE  |
| 3   | E     | 90  | ARG  |
| 3   | E     | 118 | SER  |
| 3   | E     | 150 | ALA  |
| 3   | E     | 238 | ARG  |
| 4   | F     | 442 | LEU  |
| 3   | I     | 89  | ALA  |
| 3   | I     | 118 | SER  |
| 3   | I     | 150 | ALA  |
| 3   | M     | 206 | ILE  |
| 3   | A     | 149 | ALA  |
| 3   | E     | 62  | GLY  |
| 3   | E     | 220 | ARG  |
| 3   | I     | 110 | LYS  |
| 3   | I     | 201 | LYS  |
| 4   | J     | 493 | ASP  |
| 3   | M     | 93  | GLU  |
| 3   | M     | 150 | ALA  |
| 3   | A     | 89  | ALA  |
| 3   | A     | 98  | ARG  |
| 3   | A     | 110 | LYS  |
| 3   | A     | 114 | LEU  |
| 3   | A     | 146 | ILE  |
| 3   | A     | 150 | ALA  |
| 3   | E     | 92  | ALA  |
| 3   | M     | 149 | ALA  |
| 4   | B     | 476 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | E     | 119 | GLY  |
| 3   | I     | 119 | GLY  |
| 3   | A     | 87  | LEU  |
| 3   | E     | 179 | HIS  |
| 4   | F     | 505 | GLN  |
| 3   | I     | 90  | ARG  |

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed       | Rotameric | Outliers  | Percentiles |    |
|-----|-------|----------------|-----------|-----------|-------------|----|
| 3   | A     | 152/152 (100%) | 124 (82%) | 28 (18%)  | 1           | 7  |
| 3   | E     | 152/152 (100%) | 135 (89%) | 17 (11%)  | 6           | 22 |
| 3   | I     | 152/152 (100%) | 121 (80%) | 31 (20%)  | 1           | 5  |
| 3   | M     | 152/152 (100%) | 119 (78%) | 33 (22%)  | 1           | 4  |
| 4   | B     | 67/67 (100%)   | 50 (75%)  | 17 (25%)  | 0           | 2  |
| 4   | F     | 67/67 (100%)   | 55 (82%)  | 12 (18%)  | 2           | 7  |
| 4   | J     | 49/67 (73%)    | 36 (74%)  | 13 (26%)  | 0           | 2  |
| 4   | N     | 49/67 (73%)    | 41 (84%)  | 8 (16%)   | 2           | 9  |
| All | All   | 840/876 (96%)  | 681 (81%) | 159 (19%) | 1           | 7  |

All (159) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | A     | 61  | SER  |
| 3   | A     | 63  | ILE  |
| 3   | A     | 70  | ILE  |
| 3   | A     | 78  | CYS  |
| 3   | A     | 80  | LEU  |
| 3   | A     | 91  | ASN  |
| 3   | A     | 98  | ARG  |
| 3   | A     | 107 | ARG  |
| 3   | A     | 108 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | A     | 110 | LYS  |
| 3   | A     | 120 | LYS  |
| 3   | A     | 130 | ASP  |
| 3   | A     | 132 | SER  |
| 3   | A     | 134 | LEU  |
| 3   | A     | 136 | SER  |
| 3   | A     | 139 | TYR  |
| 3   | A     | 145 | LYS  |
| 3   | A     | 154 | ASP  |
| 3   | A     | 175 | LEU  |
| 3   | A     | 181 | THR  |
| 3   | A     | 184 | SER  |
| 3   | A     | 186 | GLU  |
| 3   | A     | 189 | LEU  |
| 3   | A     | 193 | LEU  |
| 3   | A     | 198 | VAL  |
| 3   | A     | 214 | LEU  |
| 3   | A     | 215 | THR  |
| 3   | A     | 218 | LYS  |
| 4   | B     | 442 | LEU  |
| 4   | B     | 448 | THR  |
| 4   | B     | 449 | ASP  |
| 4   | B     | 461 | ASN  |
| 4   | B     | 464 | ASP  |
| 4   | B     | 468 | GLU  |
| 4   | B     | 470 | LEU  |
| 4   | B     | 474 | LEU  |
| 4   | B     | 475 | LEU  |
| 4   | B     | 478 | GLU  |
| 4   | B     | 482 | LEU  |
| 4   | B     | 483 | LYS  |
| 4   | B     | 485 | ARG  |
| 4   | B     | 488 | ILE  |
| 4   | B     | 499 | GLU  |
| 4   | B     | 501 | LYS  |
| 4   | B     | 504 | LYS  |
| 3   | E     | 69  | ASN  |
| 3   | E     | 79  | ARG  |
| 3   | E     | 80  | LEU  |
| 3   | E     | 85  | VAL  |
| 3   | E     | 90  | ARG  |
| 3   | E     | 95  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | E     | 106 | ILE  |
| 3   | E     | 132 | SER  |
| 3   | E     | 134 | LEU  |
| 3   | E     | 136 | SER  |
| 3   | E     | 170 | ILE  |
| 3   | E     | 184 | SER  |
| 3   | E     | 193 | LEU  |
| 3   | E     | 194 | ILE  |
| 3   | E     | 199 | LYS  |
| 3   | E     | 201 | LYS  |
| 3   | E     | 211 | LYS  |
| 4   | F     | 442 | LEU  |
| 4   | F     | 447 | THR  |
| 4   | F     | 455 | VAL  |
| 4   | F     | 475 | LEU  |
| 4   | F     | 477 | GLU  |
| 4   | F     | 494 | PHE  |
| 4   | F     | 497 | GLU  |
| 4   | F     | 498 | GLN  |
| 4   | F     | 499 | GLU  |
| 4   | F     | 500 | SER  |
| 4   | F     | 501 | LYS  |
| 4   | F     | 502 | ARG  |
| 3   | I     | 64  | VAL  |
| 3   | I     | 73  | THR  |
| 3   | I     | 79  | ARG  |
| 3   | I     | 83  | LYS  |
| 3   | I     | 90  | ARG  |
| 3   | I     | 98  | ARG  |
| 3   | I     | 106 | ILE  |
| 3   | I     | 107 | ARG  |
| 3   | I     | 110 | LYS  |
| 3   | I     | 127 | LYS  |
| 3   | I     | 133 | LYS  |
| 3   | I     | 134 | LEU  |
| 3   | I     | 136 | SER  |
| 3   | I     | 142 | ILE  |
| 3   | I     | 143 | ILE  |
| 3   | I     | 144 | GLN  |
| 3   | I     | 145 | LYS  |
| 3   | I     | 159 | ASN  |
| 3   | I     | 167 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | I     | 170 | ILE  |
| 3   | I     | 173 | GLU  |
| 3   | I     | 177 | PHE  |
| 3   | I     | 178 | SER  |
| 3   | I     | 181 | THR  |
| 3   | I     | 188 | GLU  |
| 3   | I     | 198 | VAL  |
| 3   | I     | 214 | LEU  |
| 3   | I     | 218 | LYS  |
| 3   | I     | 220 | ARG  |
| 3   | I     | 223 | ILE  |
| 3   | I     | 230 | ILE  |
| 4   | J     | 454 | LYS  |
| 4   | J     | 455 | VAL  |
| 4   | J     | 466 | ASP  |
| 4   | J     | 469 | GLU  |
| 4   | J     | 477 | GLU  |
| 4   | J     | 478 | GLU  |
| 4   | J     | 481 | LYS  |
| 4   | J     | 485 | ARG  |
| 4   | J     | 496 | LEU  |
| 4   | J     | 498 | GLN  |
| 4   | J     | 499 | GLU  |
| 4   | J     | 502 | ARG  |
| 4   | J     | 503 | LEU  |
| 3   | M     | 68  | GLN  |
| 3   | M     | 70  | ILE  |
| 3   | M     | 82  | LEU  |
| 3   | M     | 90  | ARG  |
| 3   | M     | 95  | ASN  |
| 3   | M     | 97  | LYS  |
| 3   | M     | 106 | ILE  |
| 3   | M     | 111 | THR  |
| 3   | M     | 121 | MET  |
| 3   | M     | 123 | VAL  |
| 3   | M     | 127 | LYS  |
| 3   | M     | 131 | ASP  |
| 3   | M     | 132 | SER  |
| 3   | M     | 134 | LEU  |
| 3   | M     | 153 | THR  |
| 3   | M     | 157 | ILE  |
| 3   | M     | 158 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | M     | 167 | LYS  |
| 3   | M     | 173 | GLU  |
| 3   | M     | 175 | LEU  |
| 3   | M     | 182 | PHE  |
| 3   | M     | 188 | GLU  |
| 3   | M     | 189 | LEU  |
| 3   | M     | 201 | LYS  |
| 3   | M     | 206 | ILE  |
| 3   | M     | 208 | VAL  |
| 3   | M     | 215 | THR  |
| 3   | M     | 218 | LYS  |
| 3   | M     | 221 | GLU  |
| 3   | M     | 233 | VAL  |
| 3   | M     | 235 | SER  |
| 3   | M     | 238 | ARG  |
| 3   | M     | 240 | MET  |
| 4   | N     | 457 | ASP  |
| 4   | N     | 468 | GLU  |
| 4   | N     | 469 | GLU  |
| 4   | N     | 474 | LEU  |
| 4   | N     | 486 | ILE  |
| 4   | N     | 495 | LEU  |
| 4   | N     | 498 | GLN  |
| 4   | N     | 501 | LYS  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | A     | 95  | ASN  |
| 3   | A     | 159 | ASN  |
| 3   | E     | 69  | ASN  |
| 3   | E     | 95  | ASN  |
| 3   | E     | 158 | GLN  |
| 4   | F     | 498 | GLN  |
| 4   | F     | 505 | GLN  |
| 3   | I     | 68  | GLN  |
| 3   | I     | 88  | HIS  |
| 3   | I     | 91  | ASN  |
| 3   | I     | 159 | ASN  |
| 3   | I     | 225 | GLN  |
| 4   | J     | 461 | ASN  |
| 4   | J     | 473 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | J     | 498 | GLN  |
| 3   | M     | 69  | ASN  |
| 3   | M     | 88  | HIS  |
| 3   | M     | 158 | GLN  |
| 3   | M     | 159 | ASN  |
| 4   | N     | 498 | GLN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.