



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 31, 2017 – 03:46 PM EDT

PDB ID : 3OL8  
Title : Poliovirus polymerase elongation complex with CTP-Mn  
Authors : Gong, P.; Peersen, O.B.  
Deposited on : unknown  
Resolution : 2.75 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : rb-20030345

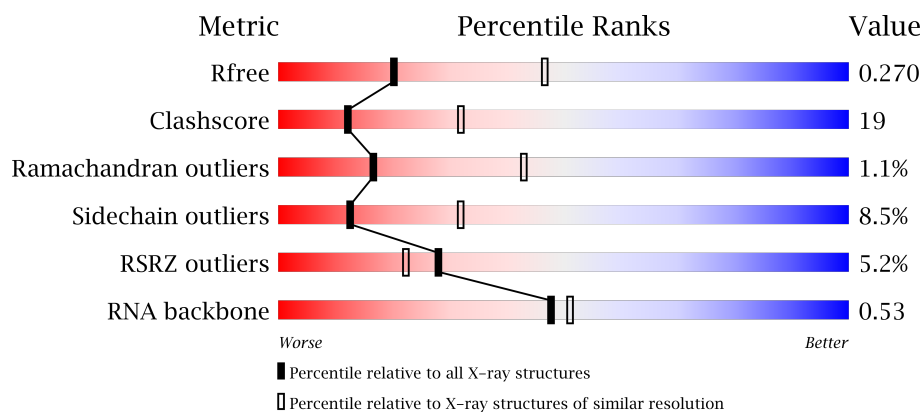
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 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)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 100719                      | 3666 (2.80-2.72)                                      |
| Clashscore            | 112137                      | 4174 (2.80-2.72)                                      |
| Ramachandran outliers | 110173                      | 4103 (2.80-2.72)                                      |
| Sidechain outliers    | 110143                      | 4106 (2.80-2.72)                                      |
| RSRZ outliers         | 101464                      | 3697 (2.80-2.72)                                      |
| RNA backbone          | 2435                        | 1024 (3.10-2.42)                                      |

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   | A     | 471    | <div> <div>3%</div> <div>64%</div> <div>29%</div> <div>5%</div> <div>.</div> </div> |
| 1   | E     | 471    | <div> <div>3%</div> <div>64%</div> <div>30%</div> <div>5%</div> <div>.</div> </div> |
| 1   | I     | 471    | <div> <div>5%</div> <div>60%</div> <div>34%</div> <div>.</div> <div>.</div> </div>  |
| 1   | M     | 471    | <div> <div>7%</div> <div>58%</div> <div>35%</div> <div>.</div> <div>.</div> </div>  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 2   | B     | 26     |                  |
| 2   | F     | 26     |                  |
| 2   | J     | 26     |                  |
| 2   | N     | 26     |                  |
| 3   | C     | 15     |                  |
| 3   | G     | 15     |                  |
| 3   | K     | 15     |                  |
| 3   | O     | 15     |                  |
| 4   | D     | 9      |                  |
| 4   | H     | 9      |                  |
| 4   | L     | 9      |                  |
| 4   | P     | 9      |                  |

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 |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 7   | POP  | I     | 5002 | -         | -        | -       | X                |
| 8   | IPA  | A     | 6011 | -         | -        | X       | -                |
| 8   | IPA  | A     | 6028 | -         | -        | -       | X                |
| 8   | IPA  | A     | 6030 | -         | -        | -       | X                |
| 8   | IPA  | E     | 6014 | -         | -        | X       | -                |
| 8   | IPA  | E     | 6029 | -         | -        | -       | X                |
| 8   | IPA  | M     | 6019 | -         | -        | X       | X                |
| 9   | GOL  | J     | 8005 | -         | -        | -       | X                |
| 9   | GOL  | N     | 8010 | -         | -        | -       | X                |

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 18318 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 protein called Polymerase.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 461      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3697  | 2370 | 610 | 695 | 22 |         |         |       |
| 1   | E     | 461      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3697  | 2370 | 610 | 695 | 22 |         |         |       |
| 1   | I     | 461      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3697  | 2370 | 610 | 695 | 22 |         |         |       |
| 1   | M     | 461      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3697  | 2370 | 610 | 695 | 22 |         |         |       |

There are 44 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| A     | 446     | ASP      | LEU    | ENGINEERED MUTATION | UNP B3VQP5 |
| A     | 462     | GLY      | -      | EXPRESSION TAG      | UNP B3VQP5 |
| A     | 463     | SER      | -      | EXPRESSION TAG      | UNP B3VQP5 |
| A     | 464     | SER      | -      | EXPRESSION TAG      | UNP B3VQP5 |
| A     | 465     | SER      | -      | EXPRESSION TAG      | UNP B3VQP5 |
| A     | 466     | HIS      | -      | EXPRESSION TAG      | UNP B3VQP5 |
| A     | 467     | HIS      | -      | EXPRESSION TAG      | UNP B3VQP5 |
| A     | 468     | HIS      | -      | EXPRESSION TAG      | UNP B3VQP5 |
| A     | 469     | HIS      | -      | EXPRESSION TAG      | UNP B3VQP5 |
| A     | 470     | HIS      | -      | EXPRESSION TAG      | UNP B3VQP5 |
| A     | 471     | HIS      | -      | EXPRESSION TAG      | UNP B3VQP5 |
| E     | 446     | ASP      | LEU    | ENGINEERED MUTATION | UNP B3VQP5 |
| E     | 462     | GLY      | -      | EXPRESSION TAG      | UNP B3VQP5 |
| E     | 463     | SER      | -      | EXPRESSION TAG      | UNP B3VQP5 |
| E     | 464     | SER      | -      | EXPRESSION TAG      | UNP B3VQP5 |
| E     | 465     | SER      | -      | EXPRESSION TAG      | UNP B3VQP5 |
| E     | 466     | HIS      | -      | EXPRESSION TAG      | UNP B3VQP5 |
| E     | 467     | HIS      | -      | EXPRESSION TAG      | UNP B3VQP5 |
| E     | 468     | HIS      | -      | EXPRESSION TAG      | UNP B3VQP5 |
| E     | 469     | HIS      | -      | EXPRESSION TAG      | UNP B3VQP5 |
| E     | 470     | HIS      | -      | EXPRESSION TAG      | UNP B3VQP5 |

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| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| E     | 471     | HIS      | -      | EXPRESSION TAG      | UNP B3VQP5 |
| I     | 446     | ASP      | LEU    | ENGINEERED MUTATION | UNP B3VQP5 |
| I     | 462     | GLY      | -      | EXPRESSION TAG      | UNP B3VQP5 |
| I     | 463     | SER      | -      | EXPRESSION TAG      | UNP B3VQP5 |
| I     | 464     | SER      | -      | EXPRESSION TAG      | UNP B3VQP5 |
| I     | 465     | SER      | -      | EXPRESSION TAG      | UNP B3VQP5 |
| I     | 466     | HIS      | -      | EXPRESSION TAG      | UNP B3VQP5 |
| I     | 467     | HIS      | -      | EXPRESSION TAG      | UNP B3VQP5 |
| I     | 468     | HIS      | -      | EXPRESSION TAG      | UNP B3VQP5 |
| I     | 469     | HIS      | -      | EXPRESSION TAG      | UNP B3VQP5 |
| I     | 470     | HIS      | -      | EXPRESSION TAG      | UNP B3VQP5 |
| I     | 471     | HIS      | -      | EXPRESSION TAG      | UNP B3VQP5 |
| M     | 446     | ASP      | LEU    | ENGINEERED MUTATION | UNP B3VQP5 |
| M     | 462     | GLY      | -      | EXPRESSION TAG      | UNP B3VQP5 |
| M     | 463     | SER      | -      | EXPRESSION TAG      | UNP B3VQP5 |
| M     | 464     | SER      | -      | EXPRESSION TAG      | UNP B3VQP5 |
| M     | 465     | SER      | -      | EXPRESSION TAG      | UNP B3VQP5 |
| M     | 466     | HIS      | -      | EXPRESSION TAG      | UNP B3VQP5 |
| M     | 467     | HIS      | -      | EXPRESSION TAG      | UNP B3VQP5 |
| M     | 468     | HIS      | -      | EXPRESSION TAG      | UNP B3VQP5 |
| M     | 469     | HIS      | -      | EXPRESSION TAG      | UNP B3VQP5 |
| M     | 470     | HIS      | -      | EXPRESSION TAG      | UNP B3VQP5 |
| M     | 471     | HIS      | -      | EXPRESSION TAG      | UNP B3VQP5 |

- Molecule 2 is a RNA chain called RNA (5'-R(\*AP\*AP\*GP\*UP\*CP\*UP\*CP\*CP\*AP\*GP\*GP\*UP\*CP\*UP\*CP\*UP\*CP\*GP\*UP\*CP\*CP\*GP\*GP\*AP\*AP\*A)-3').

| Mol | Chain | Residues | Atoms |     |    |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|---------|-------|
| 2   | B     | 17       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 341   | 150 | 56 | 118 | 17 |         |         |       |
| 2   | F     | 17       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 341   | 150 | 56 | 118 | 17 |         |         |       |
| 2   | J     | 17       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 341   | 150 | 56 | 118 | 17 |         |         |       |
| 2   | N     | 17       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 341   | 150 | 56 | 118 | 17 |         |         |       |

- Molecule 3 is a RNA chain called RNA (5'-R(\*GP\*CP\*CP\*CP\*GP\*GP\*AP\*CP\*GP\*AP\*GP\*AP\*GP\*AP\*C)-3').

| Mol | Chain | Residues | Atoms |     |    |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|----|---------|---------|-------|
| 3   | C     | 15       | Total | C   | N  | O  | P  | 0       | 0       | 0     |
|     |       |          | 323   | 145 | 65 | 99 | 14 |         |         |       |
| 3   | G     | 15       | Total | C   | N  | O  | P  | 0       | 0       | 0     |
|     |       |          | 323   | 145 | 65 | 99 | 14 |         |         |       |
| 3   | K     | 15       | Total | C   | N  | O  | P  | 0       | 0       | 0     |
|     |       |          | 323   | 145 | 65 | 99 | 14 |         |         |       |
| 3   | O     | 15       | Total | C   | N  | O  | P  | 0       | 0       | 0     |
|     |       |          | 323   | 145 | 65 | 99 | 14 |         |         |       |

- Molecule 4 is a RNA chain called RNA (5'-R(\*GP\*GP\*GP\*AP\*GP\*AP\*UP\*GP\*A)-3').

| Mol | Chain | Residues | Atoms |    |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|---------|-------|
| 4   | D     | 3        | Total | C  | N  | O  | P | 0       | 0       | 0     |
|     |       |          | 68    | 30 | 15 | 20 | 3 |         |         |       |
| 4   | H     | 3        | Total | C  | N  | O  | P | 0       | 0       | 0     |
|     |       |          | 68    | 30 | 15 | 20 | 3 |         |         |       |
| 4   | L     | 4        | Total | C  | N  | O  | P | 0       | 0       | 0     |
|     |       |          | 91    | 40 | 20 | 27 | 4 |         |         |       |
| 4   | P     | 4        | Total | C  | N  | O  | P | 0       | 0       | 0     |
|     |       |          | 91    | 40 | 20 | 27 | 4 |         |         |       |

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 5   | I     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 5   | A     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 5   | M     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 5   | E     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 6 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

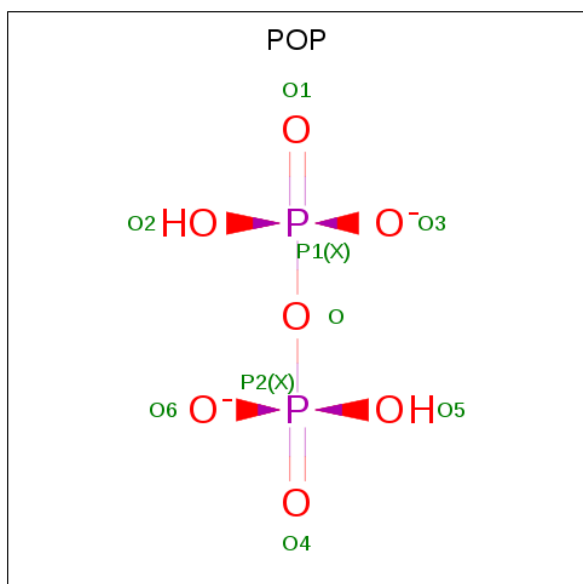
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 6   | I     | 2        | Total | Mn | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 6   | A     | 2        | Total | Mn | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 6   | M     | 2        | Total | Mn | 0       | 0       |
|     |       |          | 2     | 2  |         |         |

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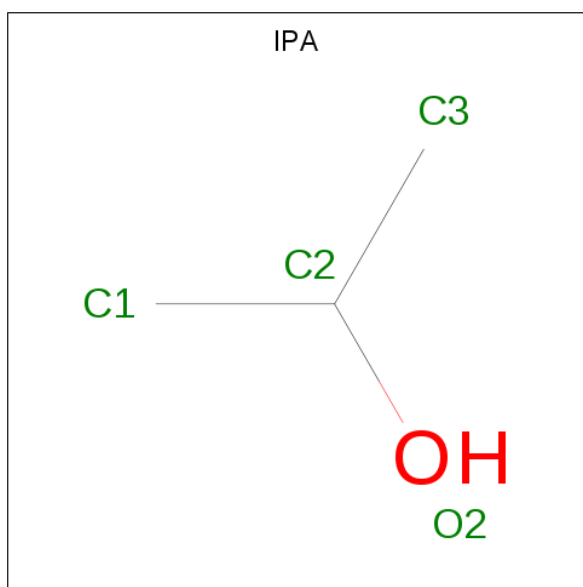
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 6   | E     | 2        | Total | Mn | 0       | 0       |
|     |       |          | 2     | 2  |         |         |

- Molecule 7 is PYROPHOSPHATE 2- (three-letter code: POP) (formula:  $\text{H}_2\text{O}_7\text{P}_2$ ).



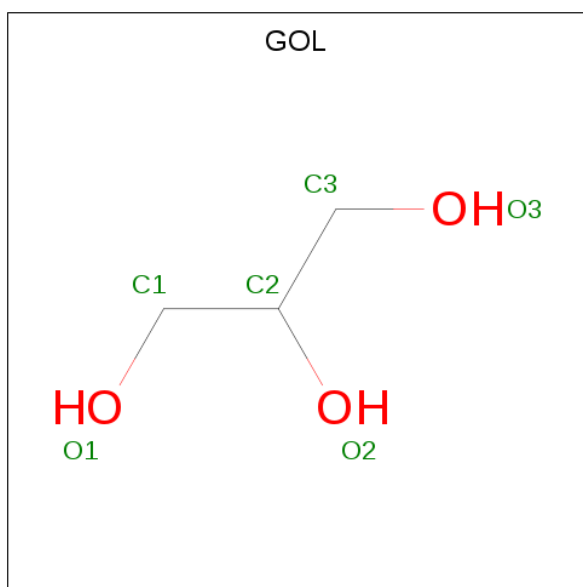
| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 7   | A     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 9     | 7 | 2 |         |         |
| 7   | G     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 9     | 7 | 2 |         |         |
| 7   | I     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 9     | 7 | 2 |         |         |
| 7   | O     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 9     | 7 | 2 |         |         |

- Molecule 8 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula:  $\text{C}_3\text{H}_8\text{O}$ ).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 8   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 3 | 1 |         |         |
| 8   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 3 | 1 |         |         |
| 8   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 3 | 1 |         |         |
| 8   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 3 | 1 |         |         |
| 8   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 3 | 1 |         |         |
| 8   | E     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 3 | 1 |         |         |
| 8   | E     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 3 | 1 |         |         |
| 8   | M     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 3 | 1 |         |         |
| 8   | M     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 3 | 1 |         |         |

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 9   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 9   | E     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 9   | J     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 9   | N     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |

- Molecule 10 is water.

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 10  | A     | 106      | Total | O   | 0       | 0       |
|     |       |          | 106   | 106 |         |         |
| 10  | B     | 12       | Total | O   | 0       | 0       |
|     |       |          | 12    | 12  |         |         |
| 10  | C     | 7        | Total | O   | 0       | 0       |
|     |       |          | 7     | 7   |         |         |
| 10  | E     | 111      | Total | O   | 0       | 0       |
|     |       |          | 111   | 111 |         |         |
| 10  | F     | 13       | Total | O   | 0       | 0       |
|     |       |          | 13    | 13  |         |         |
| 10  | G     | 8        | Total | O   | 0       | 0       |
|     |       |          | 8     | 8   |         |         |
| 10  | I     | 76       | Total | O   | 0       | 0       |
|     |       |          | 76    | 76  |         |         |
| 10  | J     | 14       | Total | O   | 0       | 0       |
|     |       |          | 14    | 14  |         |         |

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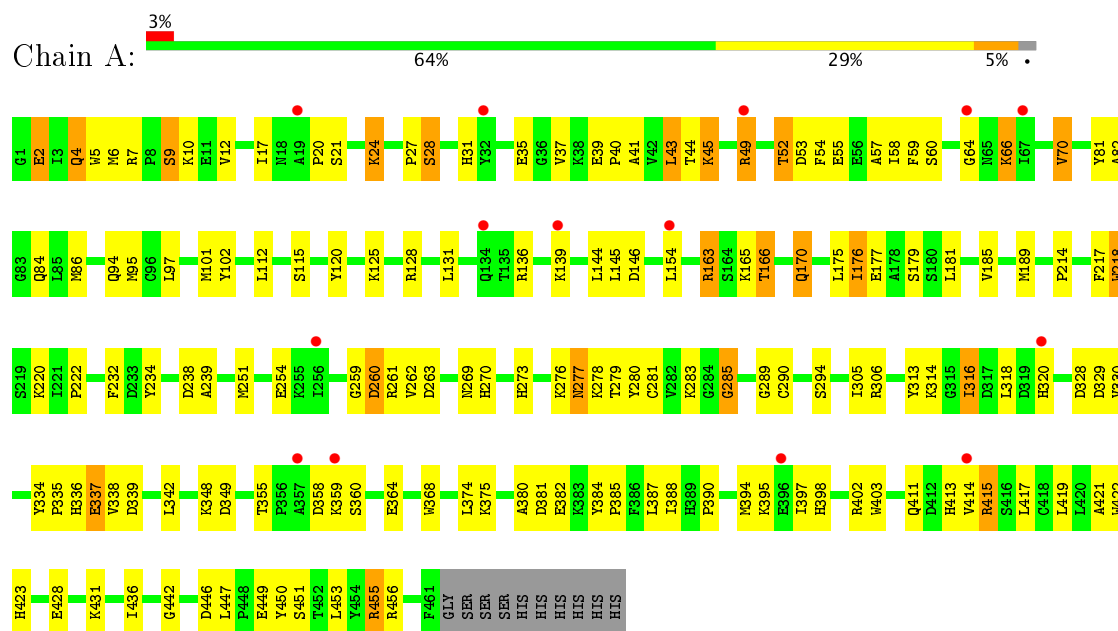
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| Mol | Chain | Residues | Atoms       |         | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 10  | K     | 5        | Total<br>5  | O<br>5  | 0       | 0       |
| 10  | M     | 74       | Total<br>74 | O<br>74 | 0       | 0       |
| 10  | N     | 16       | Total<br>16 | O<br>16 | 0       | 0       |
| 10  | O     | 4        | Total<br>4  | O<br>4  | 0       | 0       |
| 10  | P     | 2        | Total<br>2  | O<br>2  | 0       | 0       |

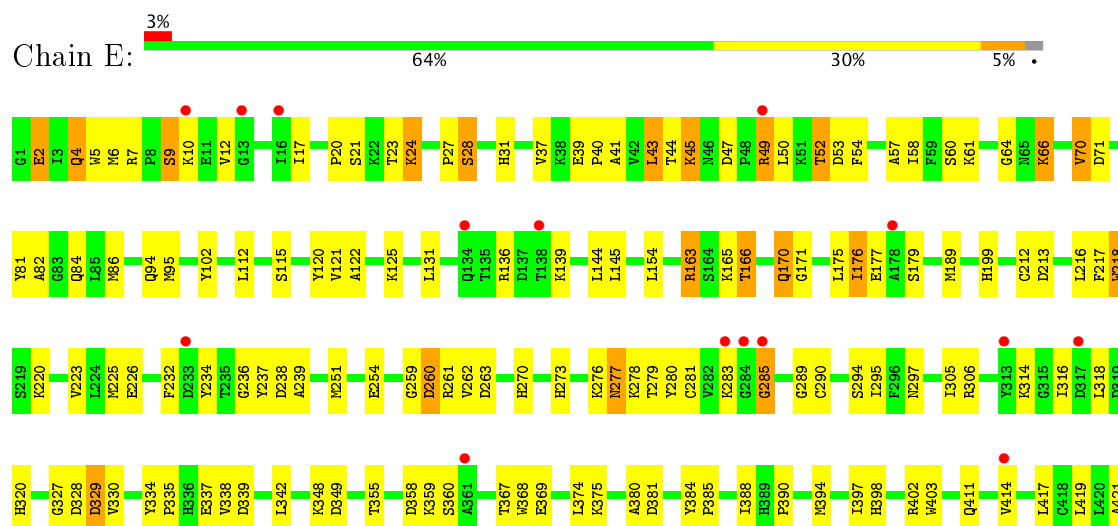
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: Polymerase

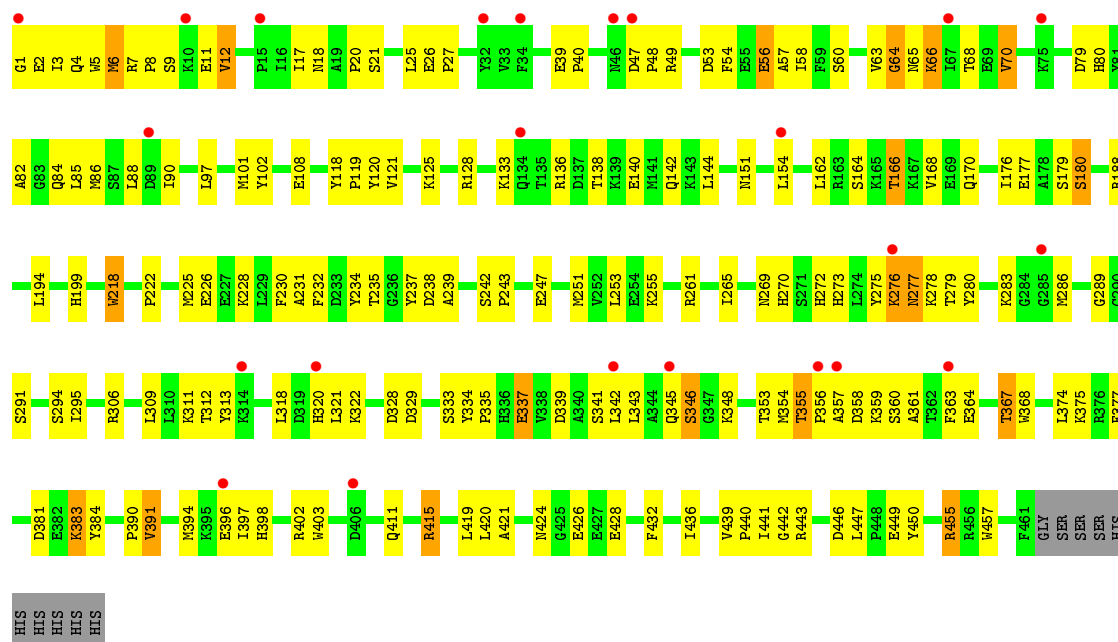


#### • Molecule 1: Polymerase

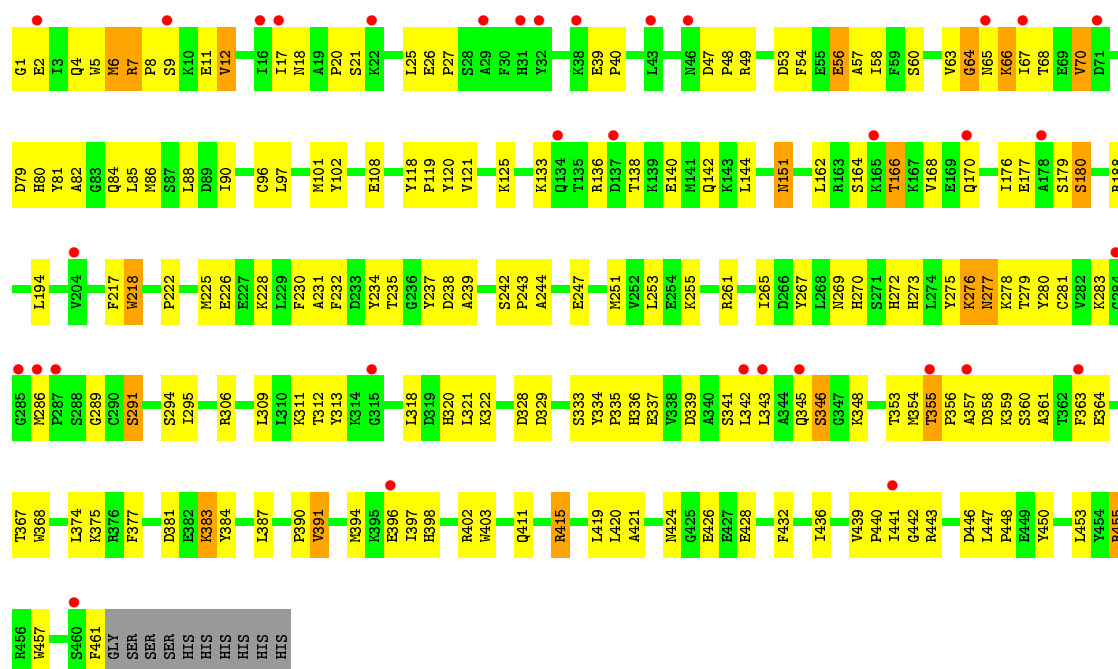




### • Molecule 1: Polymerase



### • Molecule 1: Polymerase



- Molecule 2: RNA (5'-R(\*AP\*AP\*GP\*UP\*CP\*UP\*CP\*CP\*AP\*GP\*GP\*UP\*CP\*UP\*CP\*UP\*CP\*GP\*UP\*CP\*CP\*GP\*GP\*AP\*AP\*A)-3')

Chain B: 



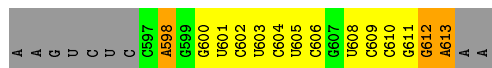
- Molecule 2: RNA (5'-R(\*AP\*AP\*GP\*UP\*CP\*UP\*CP\*CP\*AP\*GP\*GP\*UP\*CP\*UP\*CP\*UP\*CP\*GP\*UP\*CP\*CP\*GP\*GP\*AP\*AP\*A)-3')

Chain F: 




- Molecule 2: RNA (5'-R(\*AP\*AP\*GP\*UP\*CP\*UP\*CP\*CP\*AP\*GP\*GP\*UP\*CP\*UP\*CP\*UP\*CP\*GP\*UP\*CP\*CP\*GP\*GP\*AP\*AP\*A)-3')

Chain J: 



- Molecule 2: RNA (5'-R(\*AP\*AP\*GP\*UP\*CP\*UP\*CP\*CP\*AP\*GP\*GP\*UP\*CP\*UP\*CP\*UP\*CP\*GP\*UP\*CP\*CP\*GP\*GP\*AP\*AP\*A)-3')

Chain N: 



- Molecule 3: RNA (5'-R(\*GP\*CP\*CP\*CP\*GP\*GP\*AP\*CP\*GP\*AP\*GP\*AP\*GP\*AP\*C)-3')

Chain C: 

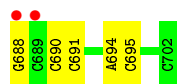


- Molecule 3: RNA (5'-R(\*GP\*CP\*CP\*CP\*GP\*GP\*AP\*CP\*GP\*AP\*GP\*AP\*GP\*AP\*C)-3')

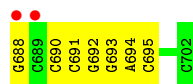
Chain G: 



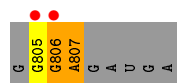
- Molecule 3: RNA (5'-R(\*GP\*CP\*CP\*CP\*GP\*GP\*AP\*CP\*GP\*AP\*GP\*AP\*GP\*AP\*C)-3')



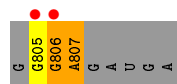
- Molecule 3: RNA (5'-R(\*GP\*CP\*CP\*CP\*GP\*GP\*AP\*CP\*GP\*AP\*GP\*AP\*GP\*AP\*C)-3')



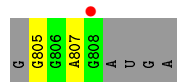
- Molecule 4: RNA (5'-R(\*GP\*GP\*GP\*AP\*GP\*AP\*UP\*GP\*A)-3')



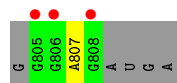
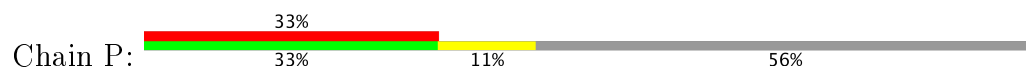
- Molecule 4: RNA (5'-R(\*GP\*GP\*GP\*AP\*GP\*AP\*UP\*GP\*A)-3')



- Molecule 4: RNA (5'-R(\*GP\*GP\*GP\*AP\*GP\*AP\*UP\*GP\*A)-3')



- Molecule 4: RNA (5'-R(\*GP\*GP\*GP\*AP\*GP\*AP\*UP\*GP\*A)-3')



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 1   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 60.78 Å 60.86 Å 193.08 Å<br>83.06° 83.04° 76.81°            | Depositor        |
| Resolution (Å)  | 44.16 – 2.75<br>44.16 – 2.40                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 97.0 (44.16-2.75)<br>94.0 (44.16-2.40)                      | Depositor<br>EDS |
| $R_{merge}$   | 0.08  | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.16 (at 2.39 Å)  | Xtriage          |
| Refinement program  | PHENIX (phenix.refine: 1.6.4_486)                           | Depositor        |
| R, $R_{free}$   | 0.224 , 0.277<br>0.212 , 0.270                              | Depositor<br>DCC |
| $R_{free}$ test set   | 3397 reflections (5.07%)                                    | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 67.0  | Xtriage          |
| Anisotropy  | 0.337   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.32 , 50.1   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.63$ , $\langle L^2 \rangle = 0.49$ | Xtriage          |
| Estimated twinning fraction   | 0.398 for -k,-h,-l  | Xtriage          |
| $F_o, F_c$ correlation  | 0.95  | EDS              |
| Total number of atoms   | 18318   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 72.0  | 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 45.86 % 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 1.2443e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZN, IPA, POP, MN

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   | A     | 0.46         | 0/3787         | 0.60        | 0/5122         |
| 1   | E     | 0.47         | 0/3787         | 0.59        | 0/5122         |
| 1   | I     | 0.46         | 0/3787         | 0.60        | 0/5122         |
| 1   | M     | 0.45         | 0/3787         | 0.60        | 0/5122         |
| 2   | B     | 0.83         | 2/378 (0.5%)   | 1.19        | 1/587 (0.2%)   |
| 2   | F     | 0.81         | 2/378 (0.5%)   | 1.13        | 0/587          |
| 2   | J     | 0.80         | 2/378 (0.5%)   | 1.06        | 0/587          |
| 2   | N     | 0.82         | 2/378 (0.5%)   | 1.06        | 0/587          |
| 3   | C     | 0.76         | 0/362          | 1.16        | 0/564          |
| 3   | G     | 0.68         | 0/362          | 1.13        | 1/564 (0.2%)   |
| 3   | K     | 0.70         | 0/362          | 1.08        | 0/564          |
| 3   | O     | 0.68         | 0/362          | 1.03        | 0/564          |
| 4   | D     | 0.36         | 0/76           | 0.63        | 0/117          |
| 4   | H     | 0.33         | 0/76           | 0.61        | 0/117          |
| 4   | L     | 0.38         | 0/102          | 0.69        | 0/158          |
| 4   | P     | 0.36         | 0/102          | 0.68        | 0/158          |
| All | All   | 0.52         | 8/18464 (0.0%) | 0.72        | 2/25642 (0.0%) |

All (8) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 2   | N     | 613 | A    | P-OP1 | 7.56 | 1.61        | 1.49     |
| 2   | J     | 613 | A    | P-OP1 | 7.12 | 1.61        | 1.49     |
| 2   | B     | 613 | A    | P-OP1 | 6.94 | 1.60        | 1.49     |
| 2   | F     | 613 | A    | P-OP1 | 6.77 | 1.60        | 1.49     |
| 2   | B     | 613 | A    | P-OP2 | 6.57 | 1.60        | 1.49     |
| 2   | F     | 613 | A    | P-OP2 | 6.43 | 1.59        | 1.49     |
| 2   | J     | 613 | A    | P-OP2 | 6.24 | 1.59        | 1.49     |
| 2   | N     | 613 | A    | P-OP2 | 5.79 | 1.58        | 1.49     |

All (2) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 3   | G     | 690 | C    | C5-C6-N1 | 5.51 | 123.76      | 121.00   |
| 2   | B     | 602 | C    | C6-N1-C2 | 5.26 | 122.40      | 120.30   |

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   | A     | 3697  | 0        | 3658     | 121     | 0            |
| 1   | E     | 3697  | 0        | 3658     | 122     | 0            |
| 1   | I     | 3697  | 0        | 3658     | 151     | 0            |
| 1   | M     | 3697  | 0        | 3658     | 167     | 0            |
| 2   | B     | 341   | 0        | 172      | 23      | 0            |
| 2   | F     | 341   | 0        | 172      | 17      | 0            |
| 2   | J     | 341   | 0        | 172      | 15      | 0            |
| 2   | N     | 341   | 0        | 172      | 13      | 0            |
| 3   | C     | 323   | 0        | 167      | 12      | 0            |
| 3   | G     | 323   | 0        | 167      | 14      | 0            |
| 3   | K     | 323   | 0        | 167      | 3       | 0            |
| 3   | O     | 323   | 0        | 167      | 5       | 0            |
| 4   | D     | 68    | 0        | 34       | 6       | 0            |
| 4   | H     | 68    | 0        | 34       | 4       | 0            |
| 4   | L     | 91    | 0        | 45       | 1       | 0            |
| 4   | P     | 91    | 0        | 45       | 0       | 0            |
| 5   | A     | 1     | 0        | 0        | 0       | 0            |
| 5   | E     | 1     | 0        | 0        | 0       | 0            |
| 5   | I     | 1     | 0        | 0        | 0       | 0            |
| 5   | M     | 1     | 0        | 0        | 0       | 0            |
| 6   | A     | 2     | 0        | 0        | 0       | 0            |
| 6   | E     | 2     | 0        | 0        | 0       | 0            |
| 6   | I     | 2     | 0        | 0        | 0       | 0            |
| 6   | M     | 2     | 0        | 0        | 0       | 0            |
| 7   | A     | 9     | 0        | 0        | 0       | 0            |
| 7   | G     | 9     | 0        | 0        | 1       | 0            |
| 7   | I     | 9     | 0        | 0        | 1       | 0            |
| 7   | O     | 9     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 8   | A     | 20    | 0        | 40       | 12      | 0            |
| 8   | E     | 8     | 0        | 16       | 14      | 0            |
| 8   | M     | 8     | 0        | 16       | 6       | 0            |
| 9   | A     | 6     | 0        | 8        | 0       | 0            |
| 9   | E     | 6     | 0        | 8        | 0       | 0            |
| 9   | J     | 6     | 0        | 8        | 0       | 0            |
| 9   | N     | 6     | 0        | 8        | 0       | 0            |
| 10  | A     | 106   | 0        | 0        | 7       | 0            |
| 10  | B     | 12    | 0        | 0        | 1       | 0            |
| 10  | C     | 7     | 0        | 0        | 2       | 0            |
| 10  | E     | 111   | 0        | 0        | 9       | 0            |
| 10  | F     | 13    | 0        | 0        | 0       | 0            |
| 10  | G     | 8     | 0        | 0        | 1       | 0            |
| 10  | I     | 76    | 0        | 0        | 6       | 0            |
| 10  | J     | 14    | 0        | 0        | 0       | 0            |
| 10  | K     | 5     | 0        | 0        | 0       | 0            |
| 10  | M     | 74    | 0        | 0        | 5       | 0            |
| 10  | N     | 16    | 0        | 0        | 1       | 0            |
| 10  | O     | 4     | 0        | 0        | 0       | 0            |
| 10  | P     | 2     | 0        | 0        | 0       | 0            |
| All | All   | 18318 | 0        | 16250    | 647     | 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 (647) 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:M:247:GLU:O    | 1:M:251:MET:HG3  | 1.64                     | 0.97              |
| 1:I:247:GLU:O    | 1:I:251:MET:HG3  | 1.65                     | 0.96              |
| 1:E:368:TRP:HB3  | 8:E:6029:IPA:H2  | 1.49                     | 0.94              |
| 1:A:128:ARG:HG3  | 10:A:564:HOH:O   | 1.66                     | 0.93              |
| 2:B:613:A:O5'    | 3:G:688:G:H5'    | 1.68                     | 0.93              |
| 1:E:217:PHE:HB2  | 8:E:6014:IPA:H32 | 1.53                     | 0.89              |
| 1:I:311:LYS:HD3  | 1:I:346:SER:HB3  | 1.55                     | 0.88              |
| 1:M:311:LYS:HD3  | 1:M:346:SER:HB3  | 1.55                     | 0.87              |
| 1:M:309:LEU:HD23 | 1:M:343:LEU:HD21 | 1.57                     | 0.85              |
| 3:C:688:G:H5'    | 2:F:613:A:O5'    | 1.75                     | 0.84              |
| 1:I:309:LEU:HD23 | 1:I:343:LEU:HD21 | 1.57                     | 0.84              |
| 1:M:243:PRO:HB3  | 10:M:492:HOH:O   | 1.77                     | 0.83              |
| 1:I:270:HIS:HD2  | 1:I:283:LYS:HG2  | 1.42                     | 0.83              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:E:6:MET:HG2   | 1:E:280:TYR:HB3  | 1.60                     | 0.82              |
| 1:M:377:PHE:HB2 | 1:M:391:VAL:HG22 | 1.61                     | 0.82              |
| 2:B:598:A:H1'   | 4:D:805:G:N2     | 1.94                     | 0.82              |
| 1:E:254:GLU:HG3 | 1:E:262:VAL:HG11 | 1.61                     | 0.82              |
| 1:E:9:SER:HB3   | 1:E:277:ASN:O    | 1.79                     | 0.82              |
| 1:A:9:SER:HB3   | 1:A:277:ASN:O    | 1.78                     | 0.82              |
| 1:A:6:MET:HG2   | 1:A:280:TYR:HB3  | 1.60                     | 0.82              |
| 1:M:7:ARG:HD2   | 1:M:12:VAL:HG23  | 1.63                     | 0.80              |
| 1:M:270:HIS:HD2 | 1:M:283:LYS:HG2  | 1.44                     | 0.80              |
| 1:A:254:GLU:HG3 | 1:A:262:VAL:HG11 | 1.63                     | 0.80              |
| 1:I:7:ARG:HD2   | 1:I:12:VAL:HG23  | 1.64                     | 0.79              |
| 1:A:9:SER:HB2   | 1:A:279:THR:OG1  | 1.83                     | 0.79              |
| 1:A:270:HIS:HD2 | 1:A:283:LYS:HG2  | 1.47                     | 0.79              |
| 1:E:270:HIS:HD2 | 1:E:283:LYS:HG2  | 1.47                     | 0.78              |
| 1:M:12:VAL:HG12 | 1:M:12:VAL:O     | 1.83                     | 0.78              |
| 1:E:212:CYS:HA  | 8:E:6014:IPA:H33 | 1.66                     | 0.77              |
| 1:I:377:PHE:HB2 | 1:I:391:VAL:HG22 | 1.65                     | 0.77              |
| 1:E:213:ASP:H   | 8:E:6014:IPA:H33 | 1.49                     | 0.77              |
| 1:M:291:SER:HB2 | 10:N:299:HOH:O   | 1.86                     | 0.76              |
| 1:A:27:PRO:HB3  | 1:A:31:HIS:ND1   | 2.00                     | 0.76              |
| 1:I:253:LEU:CD1 | 1:I:265:ILE:HD11 | 2.15                     | 0.76              |
| 1:I:12:VAL:HG12 | 1:I:12:VAL:O     | 1.86                     | 0.76              |
| 1:M:253:LEU:CD1 | 1:M:265:ILE:HD11 | 2.16                     | 0.76              |
| 1:M:49:ARG:HE   | 1:M:168:VAL:HG11 | 1.50                     | 0.76              |
| 1:I:4:GLN:HG3   | 1:I:283:LYS:HE3  | 1.68                     | 0.75              |
| 1:E:9:SER:HB2   | 1:E:279:THR:OG1  | 1.87                     | 0.75              |
| 1:E:70:VAL:HG21 | 1:E:251:MET:CE   | 2.18                     | 0.74              |
| 2:N:600:G:O2'   | 2:N:601:U:H5'    | 1.87                     | 0.73              |
| 1:I:49:ARG:HE   | 1:I:168:VAL:HG11 | 1.51                     | 0.72              |
| 2:J:600:G:O2'   | 2:J:601:U:H5'    | 1.89                     | 0.72              |
| 1:A:70:VAL:HG21 | 1:A:251:MET:CE   | 2.20                     | 0.72              |
| 1:M:1:GLY:HA2   | 1:M:65:ASN:OD1   | 1.88                     | 0.72              |
| 1:A:115:SER:HB2 | 10:A:545:HOH:O   | 1.89                     | 0.71              |
| 1:M:336:HIS:HB2 | 8:M:6019:IPA:H31 | 1.72                     | 0.71              |
| 2:F:600:G:O2'   | 2:F:601:U:H5'    | 1.90                     | 0.71              |
| 1:I:80:HIS:CE1  | 1:I:318:LEU:HB3  | 2.25                     | 0.71              |
| 1:M:18:ASN:OD1  | 1:M:276:LYS:HG3  | 1.91                     | 0.71              |
| 1:E:27:PRO:HB3  | 1:E:31:HIS:ND1   | 2.04                     | 0.71              |
| 1:I:18:ASN:OD1  | 1:I:276:LYS:HG3  | 1.90                     | 0.71              |
| 1:M:80:HIS:CE1  | 1:M:318:LEU:HB3  | 2.24                     | 0.71              |
| 1:M:4:GLN:HG3   | 1:M:283:LYS:HE3  | 1.71                     | 0.71              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:41:ALA:HB2   | 1:A:163:ARG:HD3  | 1.73                     | 0.71              |
| 1:I:7:ARG:HD2    | 1:I:12:VAL:CG2   | 2.21                     | 0.70              |
| 1:I:1:GLY:HA2    | 1:I:65:ASN:OD1   | 1.91                     | 0.70              |
| 1:M:232:PHE:HE1  | 1:M:354:MET:HE2  | 1.55                     | 0.70              |
| 1:A:270:HIS:CD2  | 1:A:283:LYS:HG2  | 2.27                     | 0.69              |
| 1:I:232:PHE:HE1  | 1:I:354:MET:HE2  | 1.56                     | 0.69              |
| 1:I:20:PRO:HG3   | 2:J:598:A:C4     | 2.27                     | 0.69              |
| 1:M:313:TYR:HD2  | 8:M:6019:IPA:H11 | 1.57                     | 0.69              |
| 1:M:7:ARG:HD2    | 1:M:12:VAL:CG2   | 2.22                     | 0.69              |
| 1:M:217:PHE:HD1  | 8:M:6018:IPA:H32 | 1.56                     | 0.69              |
| 1:A:37:VAL:HG13  | 1:A:165:LYS:HD2  | 1.75                     | 0.69              |
| 1:E:41:ALA:HB2   | 1:E:163:ARG:HD3  | 1.75                     | 0.69              |
| 2:F:598:A:H3'    | 2:F:599:G:H5'    | 1.74                     | 0.69              |
| 1:E:381:ASP:HB3  | 1:E:384:TYR:O    | 1.92                     | 0.69              |
| 2:B:602:C:H2'    | 2:B:603:U:C6     | 2.28                     | 0.68              |
| 2:B:600:G:O2'    | 2:B:601:U:H5'    | 1.92                     | 0.68              |
| 1:A:337:GLU:HB2  | 10:A:571:HOH:O   | 1.93                     | 0.68              |
| 1:E:37:VAL:HG13  | 1:E:165:LYS:HD2  | 1.76                     | 0.68              |
| 1:I:415:ARG:HG2  | 1:I:415:ARG:HH11 | 1.58                     | 0.68              |
| 3:C:694:A:N7     | 10:C:243:HOH:O   | 2.26                     | 0.68              |
| 1:I:253:LEU:HD12 | 1:I:265:ILE:CD1  | 2.24                     | 0.68              |
| 1:M:311:LYS:O    | 1:M:311:LYS:HG2  | 1.93                     | 0.68              |
| 2:N:609:C:C4     | 2:N:610:C:C5     | 2.82                     | 0.68              |
| 1:A:381:ASP:HB3  | 1:A:384:TYR:O    | 1.94                     | 0.68              |
| 1:M:232:PHE:CE1  | 1:M:354:MET:HE2  | 2.29                     | 0.68              |
| 1:M:7:ARG:HH11   | 1:M:11:GLU:HG2   | 1.58                     | 0.67              |
| 2:B:598:A:H3'    | 2:B:599:G:H5'    | 1.75                     | 0.67              |
| 1:E:374:LEU:O    | 1:E:375:LYS:HB2  | 1.94                     | 0.67              |
| 1:E:380:ALA:HA   | 1:E:388:ILE:HD13 | 1.78                     | 0.66              |
| 2:J:609:C:C4     | 2:J:610:C:C5     | 2.84                     | 0.66              |
| 1:E:270:HIS:CD2  | 1:E:283:LYS:HG2  | 2.27                     | 0.66              |
| 1:I:311:LYS:O    | 1:I:311:LYS:HG2  | 1.95                     | 0.66              |
| 1:E:213:ASP:H    | 8:E:6014:IPA:C3  | 2.08                     | 0.66              |
| 2:F:602:C:H2'    | 2:F:603:U:C6     | 2.30                     | 0.66              |
| 1:M:235:THR:HG22 | 1:M:353:THR:HB   | 1.78                     | 0.66              |
| 1:E:57:ALA:O     | 1:E:60:SER:HB3   | 1.96                     | 0.66              |
| 1:M:96:CYS:HB3   | 10:M:536:HOH:O   | 1.94                     | 0.66              |
| 1:A:374:LEU:O    | 1:A:375:LYS:HB2  | 1.94                     | 0.65              |
| 1:E:199:HIS:NE2  | 10:E:497:HOH:O   | 2.28                     | 0.65              |
| 1:M:20:PRO:HG3   | 2:N:598:A:C4     | 2.30                     | 0.65              |
| 1:A:380:ALA:HA   | 1:A:388:ILE:HD13 | 1.78                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:232:PHE:CE1  | 1:I:354:MET:HE2  | 2.32                     | 0.65              |
| 1:A:336:HIS:HB2  | 8:A:6011:IPA:H11 | 1.78                     | 0.65              |
| 1:A:388:ILE:HD12 | 8:A:6030:IPA:H32 | 1.78                     | 0.65              |
| 1:M:253:LEU:HD12 | 1:M:265:ILE:CD1  | 2.26                     | 0.65              |
| 1:M:419:LEU:HD11 | 2:N:606:C:H4'    | 1.77                     | 0.64              |
| 10:E:560:HOH:O   | 3:G:697:A:H2     | 1.80                     | 0.64              |
| 1:I:140:GLU:O    | 1:I:144:LEU:HG   | 1.97                     | 0.64              |
| 1:E:212:CYS:CA   | 8:E:6014:IPA:H33 | 2.28                     | 0.64              |
| 1:I:7:ARG:HH11   | 1:I:11:GLU:HG2   | 1.60                     | 0.64              |
| 1:E:213:ASP:N    | 8:E:6014:IPA:H33 | 2.13                     | 0.63              |
| 1:A:20:PRO:HG3   | 2:B:598:A:C4     | 2.34                     | 0.63              |
| 1:A:57:ALA:O     | 1:A:60:SER:HB3   | 1.98                     | 0.63              |
| 1:I:419:LEU:HD11 | 2:J:606:C:H4'    | 1.79                     | 0.63              |
| 1:M:49:ARG:HH21  | 1:M:168:VAL:HG13 | 1.62                     | 0.63              |
| 3:C:688:G:HO5'   | 3:C:688:G:H8     | 1.45                     | 0.63              |
| 1:E:306:ARG:HG2  | 1:E:318:LEU:HD13 | 1.79                     | 0.63              |
| 1:I:235:THR:HG22 | 1:I:353:THR:HB   | 1.80                     | 0.63              |
| 1:A:259:GLY:O    | 1:A:262:VAL:HG22 | 1.98                     | 0.63              |
| 1:E:21:SER:HB2   | 1:E:44:THR:HG21  | 1.81                     | 0.63              |
| 1:I:309:LEU:HD12 | 1:I:321:LEU:HD22 | 1.81                     | 0.63              |
| 1:I:397:ILE:HD13 | 1:I:421:ALA:HB2  | 1.80                     | 0.63              |
| 1:E:20:PRO:HG3   | 2:F:598:A:C4     | 2.33                     | 0.62              |
| 1:M:238:ASP:OD1  | 1:M:239:ALA:N    | 2.33                     | 0.62              |
| 1:M:270:HIS:NE2  | 1:M:281:CYS:SG   | 2.73                     | 0.62              |
| 1:E:70:VAL:HG21  | 1:E:251:MET:HE3  | 1.81                     | 0.62              |
| 1:E:71:ASP:HB3   | 10:E:482:HOH:O   | 1.99                     | 0.62              |
| 1:M:397:ILE:HD13 | 1:M:421:ALA:HB2  | 1.82                     | 0.62              |
| 1:A:21:SER:HB2   | 1:A:44:THR:HG21  | 1.80                     | 0.61              |
| 1:E:47:ASP:OD1   | 1:E:49:ARG:HD3   | 1.99                     | 0.61              |
| 1:I:356:PRO:HG2  | 1:I:361:ALA:H    | 1.66                     | 0.61              |
| 1:I:49:ARG:HH21  | 1:I:168:VAL:HG13 | 1.64                     | 0.61              |
| 1:E:289:GLY:HA2  | 2:F:600:G:N3     | 2.16                     | 0.61              |
| 1:I:118:TYR:CD1  | 1:I:119:PRO:HA   | 2.36                     | 0.61              |
| 1:E:259:GLY:O    | 1:E:262:VAL:HG22 | 2.00                     | 0.61              |
| 1:I:199:HIS:NE2  | 10:I:493:HOH:O   | 2.31                     | 0.61              |
| 1:I:367:THR:HB   | 10:I:515:HOH:O   | 2.00                     | 0.61              |
| 2:B:598:A:H1'    | 4:D:805:G:C2     | 2.36                     | 0.61              |
| 1:M:277:ASN:ND2  | 1:M:278:LYS:HG2  | 2.15                     | 0.61              |
| 1:I:334:TYR:CG   | 1:I:335:PRO:HD2  | 2.35                     | 0.60              |
| 1:M:356:PRO:HG2  | 1:M:361:ALA:H    | 1.66                     | 0.60              |
| 1:E:234:TYR:CD1  | 1:E:328:ASP:HB2  | 2.36                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:415:ARG:HD3  | 2:B:606:C:O2'    | 2.01                     | 0.60              |
| 1:M:56:GLU:HG2   | 10:M:522:HOH:O   | 2.00                     | 0.60              |
| 1:M:140:GLU:O    | 1:M:144:LEU:HG   | 2.00                     | 0.60              |
| 1:M:309:LEU:HD12 | 1:M:321:LEU:HD22 | 1.83                     | 0.60              |
| 1:M:234:TYR:CD1  | 1:M:328:ASP:HB2  | 2.36                     | 0.60              |
| 1:I:270:HIS:CD2  | 1:I:283:LYS:HE2  | 2.37                     | 0.60              |
| 1:M:270:HIS:CD2  | 1:M:283:LYS:HE2  | 2.36                     | 0.60              |
| 1:A:58:ILE:HD12  | 1:A:175:LEU:HD21 | 1.83                     | 0.60              |
| 1:E:37:VAL:O     | 1:E:37:VAL:HG12  | 2.02                     | 0.60              |
| 1:M:118:TYR:CD1  | 1:M:119:PRO:HA   | 2.36                     | 0.60              |
| 1:I:238:ASP:OD1  | 1:I:239:ALA:N    | 2.35                     | 0.59              |
| 1:E:115:SER:HB2  | 10:E:567:HOH:O   | 2.02                     | 0.59              |
| 3:G:688:G:H8     | 3:G:688:G:HO5'   | 1.48                     | 0.59              |
| 1:M:415:ARG:HG2  | 1:M:415:ARG:HH11 | 1.65                     | 0.59              |
| 1:I:277:ASN:ND2  | 1:I:278:LYS:HG2  | 2.18                     | 0.59              |
| 1:M:334:TYR:CG   | 1:M:335:PRO:HD2  | 2.37                     | 0.59              |
| 1:A:375:LYS:HD2  | 3:C:700:G:H5''   | 1.84                     | 0.59              |
| 1:M:446:ASP:C    | 1:M:447:LEU:HD23 | 2.23                     | 0.59              |
| 1:M:166:THR:HG22 | 1:M:170:GLN:NE2  | 2.18                     | 0.59              |
| 1:M:6:MET:HG2    | 1:M:280:TYR:HB3  | 1.84                     | 0.59              |
| 1:A:368:TRP:HB3  | 8:A:6030:IPA:H2  | 1.84                     | 0.59              |
| 1:I:65:ASN:O     | 1:I:242:SER:HB3  | 2.02                     | 0.59              |
| 1:M:341:SER:HA   | 1:M:363:PHE:CD2  | 2.38                     | 0.59              |
| 1:I:166:THR:HG22 | 1:I:170:GLN:NE2  | 2.17                     | 0.59              |
| 1:I:355:THR:HB   | 1:I:356:PRO:CD   | 2.32                     | 0.59              |
| 1:M:455:ARG:O    | 1:M:455:ARG:HD3  | 2.03                     | 0.59              |
| 1:E:177:GLU:O    | 1:E:289:GLY:HA3  | 2.03                     | 0.59              |
| 1:I:341:SER:HA   | 1:I:363:PHE:CD2  | 2.38                     | 0.59              |
| 1:A:95:MET:O     | 1:A:189:MET:HG2  | 2.03                     | 0.58              |
| 1:M:235:THR:CG2  | 1:M:353:THR:HB   | 2.33                     | 0.58              |
| 1:I:426:GLU:N    | 1:I:450:TYR:CE1  | 2.71                     | 0.58              |
| 1:M:269:ASN:O    | 1:M:283:LYS:HA   | 2.04                     | 0.58              |
| 1:M:398:HIS:O    | 1:M:402:ARG:HG3  | 2.03                     | 0.58              |
| 1:M:65:ASN:O     | 1:M:66:LYS:HB2   | 2.02                     | 0.58              |
| 1:I:6:MET:HG2    | 1:I:280:TYR:HB3  | 1.84                     | 0.58              |
| 1:A:37:VAL:HG12  | 1:A:37:VAL:O     | 2.03                     | 0.58              |
| 1:I:446:ASP:C    | 1:I:447:LEU:HD23 | 2.24                     | 0.58              |
| 1:I:235:THR:CG2  | 1:I:353:THR:HB   | 2.34                     | 0.58              |
| 1:M:355:THR:HB   | 1:M:356:PRO:CD   | 2.34                     | 0.58              |
| 1:A:306:ARG:HG2  | 1:A:318:LEU:HD13 | 1.85                     | 0.58              |
| 1:M:313:TYR:CD2  | 8:M:6019:IPA:H11 | 2.38                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:234:TYR:CD1  | 1:A:328:ASP:HB2  | 2.38                     | 0.58              |
| 1:I:8:PRO:HB2    | 1:I:11:GLU:HB2   | 1.85                     | 0.58              |
| 1:I:234:TYR:CD1  | 1:I:328:ASP:HB2  | 2.39                     | 0.58              |
| 1:A:397:ILE:HD13 | 1:A:421:ALA:HB2  | 1.85                     | 0.57              |
| 1:I:232:PHE:HA   | 1:I:357:ALA:HB2  | 1.86                     | 0.57              |
| 1:I:398:HIS:O    | 1:I:402:ARG:HG3  | 2.04                     | 0.57              |
| 2:J:605:U:H2'    | 2:J:606:C:C6     | 2.38                     | 0.57              |
| 1:A:289:GLY:HA2  | 2:B:600:G:N3     | 2.19                     | 0.57              |
| 1:E:213:ASP:HB3  | 8:E:6014:IPA:H12 | 1.86                     | 0.57              |
| 1:I:269:ASN:O    | 1:I:283:LYS:HA   | 2.04                     | 0.57              |
| 1:A:177:GLU:O    | 1:A:289:GLY:HA3  | 2.04                     | 0.57              |
| 1:I:342:LEU:O    | 1:I:345:GLN:HB3  | 2.05                     | 0.57              |
| 1:E:425:GLY:HA2  | 10:E:505:HOH:O   | 2.03                     | 0.57              |
| 2:N:605:U:H2'    | 2:N:606:C:C6     | 2.39                     | 0.57              |
| 1:E:58:ILE:HD12  | 1:E:175:LEU:HD21 | 1.86                     | 0.57              |
| 1:E:82:ALA:O     | 1:E:86:MET:HG2   | 2.04                     | 0.57              |
| 1:I:439:VAL:HG23 | 1:I:442:GLY:H    | 1.70                     | 0.57              |
| 1:M:11:GLU:O     | 1:M:12:VAL:HG23  | 2.05                     | 0.57              |
| 1:I:11:GLU:O     | 1:I:12:VAL:HG23  | 2.04                     | 0.57              |
| 1:M:439:VAL:HG23 | 1:M:442:GLY:H    | 1.68                     | 0.57              |
| 1:A:82:ALA:O     | 1:A:86:MET:HG2   | 2.05                     | 0.57              |
| 1:I:133:LYS:HD3  | 10:I:512:HOH:O   | 2.04                     | 0.56              |
| 1:E:2:GLU:HG3    | 1:E:64:GLY:HA2   | 1.87                     | 0.56              |
| 1:M:426:GLU:N    | 1:M:450:TYR:CE1  | 2.74                     | 0.56              |
| 1:A:270:HIS:CD2  | 1:A:283:LYS:HE2  | 2.40                     | 0.56              |
| 1:E:375:LYS:HD2  | 3:G:700:G:H5''   | 1.87                     | 0.56              |
| 1:M:49:ARG:HH21  | 1:M:168:VAL:CG1  | 2.16                     | 0.56              |
| 1:A:2:GLU:HG3    | 1:A:64:GLY:HA2   | 1.87                     | 0.56              |
| 1:A:419:LEU:HD11 | 2:B:606:C:H4'    | 1.87                     | 0.56              |
| 1:M:8:PRO:HB2    | 1:M:11:GLU:HB2   | 1.86                     | 0.56              |
| 1:M:289:GLY:HA2  | 2:N:600:G:N3     | 2.20                     | 0.56              |
| 1:M:65:ASN:O     | 1:M:242:SER:HB3  | 2.05                     | 0.56              |
| 1:M:342:LEU:O    | 1:M:345:GLN:HB3  | 2.06                     | 0.56              |
| 1:E:419:LEU:HD11 | 2:F:606:C:H4'    | 1.87                     | 0.56              |
| 1:I:270:HIS:CE1  | 1:I:272:HIS:HE1  | 2.24                     | 0.56              |
| 1:M:356:PRO:HG2  | 1:M:361:ALA:N    | 2.21                     | 0.56              |
| 1:A:260:ASP:N    | 1:A:260:ASP:OD1  | 2.34                     | 0.56              |
| 1:E:260:ASP:OD1  | 1:E:260:ASP:N    | 2.36                     | 0.56              |
| 1:A:52:THR:CG2   | 1:A:53:ASP:N     | 2.69                     | 0.55              |
| 1:E:397:ILE:HD13 | 1:E:421:ALA:HB2  | 1.88                     | 0.55              |
| 1:I:426:GLU:HA   | 1:I:450:TYR:CD1  | 2.42                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:7:ARG:HD3    | 1:A:12:VAL:CG2   | 2.37                     | 0.55              |
| 1:E:270:HIS:CD2  | 1:E:283:LYS:HE2  | 2.41                     | 0.55              |
| 1:I:356:PRO:HG2  | 1:I:361:ALA:N    | 2.21                     | 0.55              |
| 3:K:688:G:HO5'   | 3:K:688:G:H8     | 1.54                     | 0.55              |
| 1:A:112:LEU:HD21 | 1:A:131:LEU:HB2  | 1.88                     | 0.55              |
| 1:I:455:ARG:HD2  | 1:I:455:ARG:O    | 2.05                     | 0.55              |
| 1:M:232:PHE:HB3  | 1:M:355:THR:O    | 2.07                     | 0.55              |
| 1:A:451:SER:O    | 1:A:455:ARG:HD2  | 2.07                     | 0.55              |
| 1:M:49:ARG:HE    | 1:M:168:VAL:CG1  | 2.19                     | 0.55              |
| 1:I:397:ILE:HD11 | 1:I:420:LEU:HB3  | 1.88                     | 0.54              |
| 1:A:120:TYR:CE1  | 1:A:144:LEU:HD13 | 2.42                     | 0.54              |
| 1:I:120:TYR:HB3  | 1:I:125:LYS:HB3  | 1.89                     | 0.54              |
| 1:I:49:ARG:HH21  | 1:I:168:VAL:CG1  | 2.19                     | 0.54              |
| 1:E:218:TRP:CD1  | 1:E:390:PRO:HA   | 2.43                     | 0.54              |
| 1:E:428:GLU:HB2  | 10:E:579:HOH:O   | 2.08                     | 0.54              |
| 1:I:232:PHE:HB3  | 1:I:355:THR:O    | 2.08                     | 0.54              |
| 1:M:426:GLU:HA   | 1:M:450:TYR:CD1  | 2.43                     | 0.54              |
| 1:M:12:VAL:O     | 1:M:12:VAL:CG1   | 2.55                     | 0.54              |
| 1:E:23:THR:HG22  | 10:E:547:HOH:O   | 2.08                     | 0.54              |
| 2:F:605:U:H2'    | 2:F:606:C:C6     | 2.43                     | 0.54              |
| 1:E:112:LEU:HD21 | 1:E:131:LEU:HB2  | 1.89                     | 0.53              |
| 1:M:120:TYR:HB3  | 1:M:125:LYS:HB3  | 1.89                     | 0.53              |
| 1:M:133:LYS:HD3  | 10:M:511:HOH:O   | 2.08                     | 0.53              |
| 1:A:66:LYS:HG2   | 1:A:349:ASP:O    | 2.08                     | 0.53              |
| 1:I:118:TYR:O    | 1:I:180:SER:HB2  | 2.08                     | 0.53              |
| 1:E:451:SER:O    | 1:E:455:ARG:HD2  | 2.09                     | 0.53              |
| 2:J:598:A:H1'    | 4:L:805:G:N2     | 2.24                     | 0.53              |
| 2:B:602:C:H2'    | 2:B:603:U:H6     | 1.73                     | 0.53              |
| 2:B:605:U:H2'    | 2:B:606:C:C6     | 2.43                     | 0.53              |
| 1:I:289:GLY:HA2  | 2:J:600:G:N3     | 2.23                     | 0.53              |
| 1:M:232:PHE:HA   | 1:M:357:ALA:HB2  | 1.89                     | 0.53              |
| 3:O:688:G:H8     | 3:O:688:G:HO5'   | 1.56                     | 0.53              |
| 1:I:232:PHE:CE1  | 1:I:354:MET:CE   | 2.92                     | 0.53              |
| 1:E:95:MET:O     | 1:E:189:MET:HG2  | 2.08                     | 0.53              |
| 1:I:374:LEU:O    | 1:I:375:LYS:HB2  | 2.08                     | 0.53              |
| 1:I:65:ASN:O     | 1:I:66:LYS:HB2   | 2.07                     | 0.53              |
| 1:M:84:GLN:OE1   | 1:M:306:ARG:NH2  | 2.41                     | 0.53              |
| 1:E:52:THR:CG2   | 1:E:53:ASP:N     | 2.72                     | 0.53              |
| 1:M:270:HIS:CE1  | 1:M:272:HIS:HE1  | 2.27                     | 0.53              |
| 1:I:230:PHE:O    | 1:I:231:ALA:HB2  | 2.08                     | 0.53              |
| 1:I:270:HIS:CE1  | 1:I:272:HIS:CE1  | 2.96                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:381:ASP:HB3  | 1:M:384:TYR:O    | 2.08                     | 0.53              |
| 1:I:84:GLN:OE1   | 1:I:306:ARG:NH2  | 2.42                     | 0.53              |
| 7:I:5002:POP:O4  | 7:I:5002:POP:O1  | 2.25                     | 0.53              |
| 1:M:232:PHE:CE1  | 1:M:354:MET:CE   | 2.92                     | 0.52              |
| 1:E:238:ASP:OD1  | 1:E:239:ALA:N    | 2.42                     | 0.52              |
| 1:M:277:ASN:HD22 | 1:M:278:LYS:HG2  | 1.74                     | 0.52              |
| 1:M:234:TYR:HD1  | 1:M:328:ASP:HB2  | 1.74                     | 0.52              |
| 1:I:277:ASN:HD22 | 1:I:278:LYS:N    | 2.08                     | 0.52              |
| 1:I:436:ILE:O    | 1:I:442:GLY:HA3  | 2.10                     | 0.52              |
| 1:E:37:VAL:O     | 1:E:37:VAL:CG1   | 2.57                     | 0.52              |
| 1:I:381:ASP:HB3  | 1:I:384:TYR:O    | 2.11                     | 0.51              |
| 1:I:320:HIS:HB2  | 1:I:334:TYR:CE1  | 2.46                     | 0.51              |
| 1:M:230:PHE:O    | 1:M:231:ALA:HB2  | 2.10                     | 0.51              |
| 1:M:277:ASN:HD22 | 1:M:278:LYS:N    | 2.08                     | 0.51              |
| 2:B:597:C:O2     | 2:B:597:C:H2'    | 2.09                     | 0.51              |
| 1:E:414:VAL:CG1  | 1:E:436:ILE:HD13 | 2.40                     | 0.51              |
| 1:E:176:ILE:HG13 | 2:F:600:G:C8     | 2.45                     | 0.51              |
| 1:I:449:GLU:HB2  | 10:I:513:HOH:O   | 2.11                     | 0.51              |
| 1:A:238:ASP:OD1  | 1:A:239:ALA:N    | 2.43                     | 0.51              |
| 2:F:597:C:O2     | 2:F:597:C:H2'    | 2.09                     | 0.51              |
| 1:I:177:GLU:O    | 1:I:289:GLY:HA3  | 2.10                     | 0.51              |
| 1:M:177:GLU:O    | 1:M:289:GLY:HA3  | 2.11                     | 0.51              |
| 1:E:66:LYS:HG2   | 1:E:349:ASP:O    | 2.11                     | 0.51              |
| 1:M:320:HIS:HB2  | 1:M:334:TYR:CE1  | 2.46                     | 0.51              |
| 1:I:334:TYR:CD1  | 1:I:335:PRO:HD2  | 2.46                     | 0.51              |
| 1:M:85:LEU:HA    | 1:M:88:LEU:HD12  | 1.93                     | 0.51              |
| 1:A:374:LEU:N    | 10:A:540:HOH:O   | 2.44                     | 0.50              |
| 1:A:37:VAL:CG1   | 1:A:37:VAL:O     | 2.60                     | 0.50              |
| 1:E:24:LYS:HE3   | 10:E:524:HOH:O   | 2.12                     | 0.50              |
| 1:I:251:MET:O    | 1:I:255:LYS:HG3  | 2.10                     | 0.50              |
| 1:M:334:TYR:CD2  | 1:M:335:PRO:HD2  | 2.46                     | 0.50              |
| 1:M:270:HIS:CE1  | 1:M:272:HIS:CE1  | 2.99                     | 0.50              |
| 1:M:358:ASP:O    | 1:M:359:LYS:HB2  | 2.11                     | 0.50              |
| 1:E:120:TYR:CE1  | 1:E:144:LEU:HD13 | 2.46                     | 0.50              |
| 1:I:234:TYR:HD1  | 1:I:328:ASP:HB2  | 1.77                     | 0.50              |
| 1:I:334:TYR:CD2  | 1:I:335:PRO:HD2  | 2.47                     | 0.50              |
| 1:M:336:HIS:CB   | 8:M:6019:IPA:H31 | 2.40                     | 0.50              |
| 1:E:39:GLU:OE2   | 1:E:165:LYS:HG3  | 2.11                     | 0.50              |
| 1:I:334:TYR:CG   | 1:I:335:PRO:CD   | 2.94                     | 0.50              |
| 1:M:238:ASP:HB2  | 1:M:286:MET:HB3  | 1.94                     | 0.50              |
| 1:A:70:VAL:HG11  | 1:A:251:MET:CE   | 2.42                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:70:VAL:HG21  | 1:A:251:MET:HE3  | 1.91                     | 0.50              |
| 1:E:236:GLY:HA2  | 7:G:5003:POP:O6  | 2.12                     | 0.50              |
| 2:N:612:G:H5''   | 2:N:613:A:OP1    | 2.12                     | 0.50              |
| 1:A:313:TYR:CD1  | 8:A:6011:IPA:H32 | 2.47                     | 0.50              |
| 1:A:316:ILE:HD12 | 8:A:6011:IPA:H33 | 1.93                     | 0.50              |
| 1:E:414:VAL:HG11 | 1:E:436:ILE:HD13 | 1.93                     | 0.50              |
| 1:M:374:LEU:O    | 1:M:375:LYS:HB2  | 2.11                     | 0.50              |
| 1:I:421:ALA:O    | 1:I:424:ASN:HB2  | 2.12                     | 0.49              |
| 2:N:609:C:C4     | 2:N:610:C:H5     | 2.30                     | 0.49              |
| 1:A:40:PRO:HD3   | 1:A:403:TRP:CH2  | 2.47                     | 0.49              |
| 1:I:79:ASP:OD1   | 1:I:255:LYS:HE2  | 2.12                     | 0.49              |
| 1:M:218:TRP:CD1  | 1:M:390:PRO:HA   | 2.47                     | 0.49              |
| 1:E:217:PHE:CD1  | 8:E:6014:IPA:H31 | 2.47                     | 0.49              |
| 1:M:118:TYR:O    | 1:M:180:SER:HB2  | 2.12                     | 0.49              |
| 1:M:312:THR:HG22 | 1:M:313:TYR:CD1  | 2.48                     | 0.49              |
| 1:M:334:TYR:CG   | 1:M:335:PRO:CD   | 2.95                     | 0.49              |
| 1:M:54:PHE:CE1   | 1:M:58:ILE:CG2   | 2.95                     | 0.49              |
| 1:E:154:LEU:HD22 | 1:E:177:GLU:HB3  | 1.95                     | 0.49              |
| 2:J:612:G:H5''   | 2:J:613:A:OP1    | 2.13                     | 0.49              |
| 1:M:251:MET:O    | 1:M:255:LYS:HG3  | 2.11                     | 0.49              |
| 1:M:336:HIS:CD2  | 8:M:6019:IPA:H31 | 2.48                     | 0.49              |
| 1:M:397:ILE:HD11 | 1:M:420:LEU:HB3  | 1.94                     | 0.49              |
| 1:A:176:ILE:HG13 | 2:B:600:G:C8     | 2.47                     | 0.49              |
| 1:A:336:HIS:HB2  | 8:A:6011:IPA:C1  | 2.42                     | 0.49              |
| 2:B:598:A:C1'    | 4:D:805:G:N2     | 2.73                     | 0.49              |
| 1:I:277:ASN:HD22 | 1:I:278:LYS:HG2  | 1.77                     | 0.49              |
| 2:F:602:C:H2'    | 2:F:603:U:H6     | 1.73                     | 0.49              |
| 1:M:334:TYR:CD1  | 1:M:335:PRO:HD2  | 2.48                     | 0.49              |
| 1:E:7:ARG:HD3    | 1:E:12:VAL:CG2   | 2.43                     | 0.49              |
| 1:I:238:ASP:HB2  | 1:I:286:MET:HB3  | 1.95                     | 0.49              |
| 2:B:604:C:H2'    | 2:B:605:U:C6     | 2.48                     | 0.48              |
| 3:K:690:C:H2'    | 3:K:691:C:O4'    | 2.13                     | 0.48              |
| 2:N:608:U:H2'    | 2:N:609:C:O4'    | 2.12                     | 0.48              |
| 1:A:81:TYR:O     | 1:A:84:GLN:HB2   | 2.13                     | 0.48              |
| 1:E:339:ASP:HB3  | 1:E:342:LEU:HD12 | 1.95                     | 0.48              |
| 2:B:613:A:O5'    | 3:G:688:G:C5'    | 2.53                     | 0.48              |
| 1:I:358:ASP:O    | 1:I:359:LYS:HB2  | 2.13                     | 0.48              |
| 1:A:154:LEU:HD22 | 1:A:177:GLU:HB3  | 1.94                     | 0.48              |
| 1:A:384:TYR:CE2  | 8:A:6028:IPA:H2  | 2.48                     | 0.48              |
| 1:I:53:ASP:HB3   | 1:I:56:GLU:HB3   | 1.95                     | 0.48              |
| 2:J:609:C:C4     | 2:J:610:C:H5     | 2.31                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:97:LEU:O     | 1:M:101:MET:HG3  | 2.13                     | 0.48              |
| 1:E:216:LEU:HB2  | 8:E:6014:IPA:H13 | 1.94                     | 0.48              |
| 1:M:225:MET:HE2  | 1:M:225:MET:HA   | 1.95                     | 0.48              |
| 1:E:28:SER:HB2   | 1:E:402:ARG:C    | 2.33                     | 0.48              |
| 1:I:128:ARG:HG3  | 10:I:527:HOH:O   | 2.14                     | 0.48              |
| 1:I:54:PHE:CE1   | 1:I:58:ILE:CG2   | 2.97                     | 0.48              |
| 1:I:9:SER:HA     | 1:I:279:THR:OG1  | 2.13                     | 0.48              |
| 1:M:237:TYR:CG   | 1:M:328:ASP:HB3  | 2.48                     | 0.48              |
| 1:A:146:ASP:HA   | 10:A:534:HOH:O   | 2.12                     | 0.48              |
| 1:A:358:ASP:OD1  | 1:A:360:SER:HB3  | 2.13                     | 0.48              |
| 1:I:49:ARG:HE    | 1:I:168:VAL:CG1  | 2.21                     | 0.48              |
| 1:M:218:TRP:O    | 1:M:222:PRO:HD3  | 2.14                     | 0.48              |
| 1:I:12:VAL:CG1   | 1:I:12:VAL:O     | 2.58                     | 0.48              |
| 1:I:97:LEU:O     | 1:I:101:MET:HG3  | 2.12                     | 0.48              |
| 1:A:232:PHE:HA   | 1:A:355:THR:O    | 2.14                     | 0.48              |
| 1:I:237:TYR:CG   | 1:I:328:ASP:HB3  | 2.49                     | 0.48              |
| 1:I:339:ASP:CG   | 1:I:341:SER:HG   | 2.17                     | 0.48              |
| 1:M:411:GLN:HB3  | 10:M:496:HOH:O   | 2.14                     | 0.48              |
| 1:I:312:THR:HG22 | 1:I:313:TYR:CD1  | 2.49                     | 0.47              |
| 1:I:40:PRO:HD3   | 1:I:403:TRP:CH2  | 2.49                     | 0.47              |
| 2:J:608:U:H2'    | 2:J:609:C:O4'    | 2.14                     | 0.47              |
| 1:A:154:LEU:O    | 1:A:273:HIS:HA   | 2.14                     | 0.47              |
| 1:A:166:THR:O    | 1:A:170:GLN:HB2  | 2.13                     | 0.47              |
| 1:A:45:LYS:H     | 1:A:45:LYS:HG3   | 1.39                     | 0.47              |
| 1:E:166:THR:O    | 1:E:170:GLN:HB2  | 2.15                     | 0.47              |
| 2:F:604:C:H2'    | 2:F:605:U:C6     | 2.49                     | 0.47              |
| 1:I:85:LEU:HA    | 1:I:88:LEU:HD12  | 1.95                     | 0.47              |
| 1:M:11:GLU:O     | 1:M:12:VAL:CG2   | 2.62                     | 0.47              |
| 3:O:690:C:H2'    | 3:O:691:C:O4'    | 2.14                     | 0.47              |
| 1:A:5:TRP:O      | 1:A:280:TYR:HA   | 2.14                     | 0.47              |
| 1:A:339:ASP:HB3  | 1:A:342:LEU:HD12 | 1.95                     | 0.47              |
| 1:M:108:GLU:O    | 1:M:188:ARG:NH2  | 2.39                     | 0.47              |
| 1:M:70:VAL:HG21  | 1:M:251:MET:SD   | 2.53                     | 0.47              |
| 1:A:39:GLU:OE2   | 1:A:165:LYS:HG3  | 2.13                     | 0.47              |
| 3:C:690:C:H5''   | 3:C:690:C:H6     | 1.80                     | 0.47              |
| 1:E:45:LYS:HG3   | 1:E:45:LYS:H     | 1.39                     | 0.47              |
| 1:I:97:LEU:HD23  | 1:I:138:THR:HB   | 1.95                     | 0.47              |
| 1:A:398:HIS:O    | 1:A:402:ARG:HG3  | 2.14                     | 0.47              |
| 1:A:387:LEU:HD11 | 8:A:6028:IPA:H33 | 1.96                     | 0.47              |
| 4:H:805:G:H2'    | 4:H:806:G:O5'    | 2.15                     | 0.47              |
| 1:M:436:ILE:O    | 1:M:442:GLY:HA3  | 2.14                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:154:LEU:O    | 1:E:273:HIS:HA   | 2.13                     | 0.47              |
| 1:M:226:GLU:HG2  | 1:M:322:LYS:HG3  | 1.95                     | 0.47              |
| 3:C:700:G:H3'    | 10:C:165:HOH:O   | 2.14                     | 0.47              |
| 3:G:690:C:H5''   | 3:G:690:C:H6     | 1.79                     | 0.47              |
| 1:I:54:PHE:O     | 1:I:57:ALA:N     | 2.45                     | 0.47              |
| 1:E:422:TRP:CD1  | 1:E:453:LEU:HD13 | 2.50                     | 0.47              |
| 1:A:270:HIS:NE2  | 1:A:283:LYS:HE2  | 2.29                     | 0.47              |
| 1:A:414:VAL:CG1  | 1:A:436:ILE:HD13 | 2.45                     | 0.47              |
| 3:G:688:G:O5'    | 3:G:688:G:H8     | 1.98                     | 0.47              |
| 1:E:70:VAL:HG11  | 1:E:251:MET:CE   | 2.45                     | 0.47              |
| 1:I:11:GLU:O     | 1:I:12:VAL:CG2   | 2.62                     | 0.47              |
| 1:M:53:ASP:HB3   | 1:M:56:GLU:HB3   | 1.97                     | 0.47              |
| 1:A:411:GLN:HE22 | 1:A:446:ASP:N    | 2.12                     | 0.47              |
| 1:E:277:ASN:ND2  | 1:E:278:LYS:HG3  | 2.30                     | 0.47              |
| 1:E:81:TYR:O     | 1:E:84:GLN:HB2   | 2.14                     | 0.47              |
| 1:E:225:MET:HA   | 1:E:225:MET:HE2  | 1.97                     | 0.46              |
| 1:E:5:TRP:O      | 1:E:280:TYR:HA   | 2.15                     | 0.46              |
| 1:E:270:HIS:NE2  | 1:E:283:LYS:HE2  | 2.30                     | 0.46              |
| 1:I:142:GLN:OE1  | 1:I:142:GLN:HA   | 2.15                     | 0.46              |
| 1:M:40:PRO:HD3   | 1:M:403:TRP:CH2  | 2.51                     | 0.46              |
| 3:G:692:G:O2'    | 3:G:693:G:H5'    | 2.16                     | 0.46              |
| 4:H:806:G:O2'    | 4:H:807:A:H5'    | 2.15                     | 0.46              |
| 1:I:218:TRP:O    | 1:I:222:PRO:HD3  | 2.15                     | 0.46              |
| 1:I:65:ASN:HB3   | 1:I:243:PRO:HD2  | 1.97                     | 0.46              |
| 1:A:54:PHE:O     | 1:A:57:ALA:N     | 2.45                     | 0.46              |
| 1:M:421:ALA:O    | 1:M:424:ASN:HB2  | 2.15                     | 0.46              |
| 1:M:253:LEU:CD1  | 1:M:265:ILE:CD1  | 2.85                     | 0.46              |
| 1:M:339:ASP:OD2  | 1:M:342:LEU:HG   | 2.15                     | 0.46              |
| 1:M:9:SER:HA     | 1:M:279:THR:OG1  | 2.15                     | 0.46              |
| 4:D:805:G:H2'    | 4:D:806:G:O5'    | 2.15                     | 0.46              |
| 1:I:226:GLU:HG2  | 1:I:322:LYS:HG3  | 1.97                     | 0.46              |
| 1:I:432:PHE:CZ   | 1:I:436:ILE:HD11 | 2.50                     | 0.46              |
| 4:H:806:G:C2'    | 4:H:807:A:H5'    | 2.46                     | 0.46              |
| 1:I:102:TYR:CE1  | 1:I:136:ARG:HA   | 2.51                     | 0.46              |
| 1:M:54:PHE:CE1   | 1:M:58:ILE:HG21  | 2.51                     | 0.46              |
| 1:E:232:PHE:HA   | 1:E:355:THR:O    | 2.16                     | 0.46              |
| 1:I:108:GLU:O    | 1:I:188:ARG:NH2  | 2.38                     | 0.46              |
| 1:I:231:ALA:C    | 1:I:232:PHE:CD2  | 2.90                     | 0.46              |
| 1:M:79:ASP:OD1   | 1:M:255:LYS:HE2  | 2.16                     | 0.46              |
| 1:A:277:ASN:ND2  | 1:A:278:LYS:HG3  | 2.30                     | 0.45              |
| 1:E:238:ASP:O    | 1:E:285:GLY:HA2  | 2.16                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:28:SER:HB2   | 1:A:402:ARG:C    | 2.37                     | 0.45              |
| 1:A:334:TYR:CG   | 1:A:335:PRO:HD2  | 2.51                     | 0.45              |
| 1:I:70:VAL:HG21  | 1:I:251:MET:SD   | 2.56                     | 0.45              |
| 1:M:25:LEU:HB2   | 1:M:40:PRO:HG3   | 1.98                     | 0.45              |
| 1:A:338:VAL:HG23 | 1:A:339:ASP:N    | 2.31                     | 0.45              |
| 1:I:27:PRO:HD3   | 1:I:403:TRP:CZ3  | 2.50                     | 0.45              |
| 1:I:394:MET:SD   | 1:I:421:ALA:HB1  | 2.57                     | 0.45              |
| 1:M:231:ALA:C    | 1:M:232:PHE:CD2  | 2.89                     | 0.45              |
| 1:E:436:ILE:O    | 1:E:442:GLY:HA3  | 2.16                     | 0.45              |
| 2:N:609:C:H2'    | 2:N:610:C:H5'    | 1.98                     | 0.45              |
| 1:A:238:ASP:O    | 1:A:285:GLY:HA2  | 2.16                     | 0.45              |
| 1:A:431:LYS:HE2  | 1:A:431:LYS:HB2  | 1.76                     | 0.45              |
| 1:E:446:ASP:C    | 1:E:447:LEU:HD23 | 2.37                     | 0.45              |
| 1:M:97:LEU:HD23  | 1:M:138:THR:HB   | 1.99                     | 0.45              |
| 1:A:218:TRP:CD1  | 1:A:390:PRO:HA   | 2.51                     | 0.45              |
| 4:D:806:G:C2'    | 4:D:807:A:H5'    | 2.47                     | 0.45              |
| 1:E:17:ILE:O     | 1:E:276:LYS:HA   | 2.16                     | 0.45              |
| 1:A:411:GLN:HE22 | 1:A:446:ASP:H    | 1.63                     | 0.45              |
| 1:M:339:ASP:CG   | 1:M:341:SER:HG   | 2.19                     | 0.45              |
| 1:A:102:TYR:CE1  | 1:A:136:ARG:HA   | 2.51                     | 0.45              |
| 1:I:275:TYR:O    | 1:I:275:TYR:HD2  | 1.99                     | 0.45              |
| 1:E:334:TYR:CG   | 1:E:335:PRO:HD2  | 2.52                     | 0.45              |
| 1:M:151:ASN:ND2  | 1:M:267:TYR:CD2  | 2.79                     | 0.45              |
| 1:A:52:THR:HG23  | 1:A:53:ASP:N     | 2.32                     | 0.44              |
| 1:I:225:MET:HA   | 1:I:225:MET:HE2  | 1.99                     | 0.44              |
| 1:E:54:PHE:O     | 1:E:57:ALA:N     | 2.46                     | 0.44              |
| 1:E:329:ASP:OD2  | 3:G:701:A:H5''   | 2.18                     | 0.44              |
| 1:I:277:ASN:HD22 | 1:I:277:ASN:C    | 2.21                     | 0.44              |
| 2:J:602:C:H2'    | 2:J:603:U:C6     | 2.53                     | 0.44              |
| 1:M:102:TYR:CE1  | 1:M:136:ARG:HA   | 2.52                     | 0.44              |
| 1:M:339:ASP:OD2  | 1:M:341:SER:OG   | 2.35                     | 0.44              |
| 1:E:40:PRO:HD3   | 1:E:403:TRP:CH2  | 2.52                     | 0.44              |
| 1:I:218:TRP:CD1  | 1:I:390:PRO:HA   | 2.52                     | 0.44              |
| 1:A:436:ILE:O    | 1:A:442:GLY:HA3  | 2.17                     | 0.44              |
| 1:E:358:ASP:OD1  | 1:E:360:SER:HB3  | 2.18                     | 0.44              |
| 1:E:398:HIS:O    | 1:E:402:ARG:HG3  | 2.17                     | 0.44              |
| 2:F:598:A:C3'    | 2:F:599:G:H5'    | 2.44                     | 0.44              |
| 2:F:600:G:C2'    | 2:F:601:U:H5'    | 2.48                     | 0.44              |
| 1:M:375:LYS:HD3  | 1:M:396:GLU:OE1  | 2.18                     | 0.44              |
| 1:A:181:LEU:O    | 1:A:185:VAL:HG23 | 2.18                     | 0.44              |
| 1:M:277:ASN:HD22 | 1:M:277:ASN:C    | 2.21                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:395:LYS:HB3  | 1:A:395:LYS:HE2  | 1.70                     | 0.44              |
| 1:A:446:ASP:C    | 1:A:447:LEU:HD23 | 2.38                     | 0.44              |
| 1:E:394:MET:SD   | 1:E:421:ALA:HB1  | 2.57                     | 0.44              |
| 1:M:275:TYR:HD2  | 1:M:275:TYR:O    | 2.00                     | 0.44              |
| 1:M:397:ILE:CD1  | 1:M:421:ALA:HB2  | 2.46                     | 0.44              |
| 1:E:305:ILE:HD11 | 1:E:330:VAL:HG11 | 1.99                     | 0.44              |
| 1:I:339:ASP:OD2  | 1:I:342:LEU:HG   | 2.18                     | 0.44              |
| 1:M:8:PRO:HB2    | 1:M:11:GLU:CB    | 2.48                     | 0.44              |
| 1:A:364:GLU:HG2  | 10:A:555:HOH:O   | 2.18                     | 0.44              |
| 1:A:422:TRP:CD1  | 1:A:453:LEU:HD13 | 2.52                     | 0.44              |
| 1:E:102:TYR:CE1  | 1:E:136:ARG:HA   | 2.53                     | 0.44              |
| 1:I:440:PRO:HA   | 1:I:443:ARG:NH1  | 2.33                     | 0.44              |
| 1:M:7:ARG:NH1    | 1:M:11:GLU:HG2   | 2.30                     | 0.44              |
| 1:M:276:LYS:HB3  | 1:M:277:ASN:H    | 1.60                     | 0.44              |
| 1:A:17:ILE:O     | 1:A:276:LYS:HA   | 2.17                     | 0.44              |
| 3:C:692:G:O2'    | 3:C:693:G:H5'    | 2.17                     | 0.44              |
| 1:I:339:ASP:OD2  | 1:I:341:SER:OG   | 2.35                     | 0.44              |
| 3:G:688:G:H1'    | 10:G:281:HOH:O   | 2.18                     | 0.43              |
| 1:I:358:ASP:HB2  | 1:I:360:SER:OG   | 2.18                     | 0.43              |
| 1:I:8:PRO:HB2    | 1:I:11:GLU:CB    | 2.47                     | 0.43              |
| 1:A:414:VAL:HG11 | 1:A:436:ILE:HD13 | 2.00                     | 0.43              |
| 1:E:338:VAL:HG23 | 1:E:339:ASP:N    | 2.33                     | 0.43              |
| 1:I:17:ILE:O     | 1:I:276:LYS:HA   | 2.18                     | 0.43              |
| 1:I:355:THR:CB   | 1:I:356:PRO:CD   | 2.96                     | 0.43              |
| 1:A:43:LEU:HA    | 1:A:43:LEU:HD12  | 1.75                     | 0.43              |
| 2:B:600:G:C2'    | 2:B:601:U:H5'    | 2.49                     | 0.43              |
| 4:D:806:G:O2'    | 4:D:807:A:H5'    | 2.18                     | 0.43              |
| 1:E:411:GLN:HE22 | 1:E:446:ASP:N    | 2.17                     | 0.43              |
| 1:I:222:PRO:HA   | 1:I:368:TRP:CZ2  | 2.54                     | 0.43              |
| 1:I:54:PHE:CE1   | 1:I:58:ILE:HG21  | 2.53                     | 0.43              |
| 1:M:2:GLU:HB3    | 1:M:64:GLY:HA2   | 2.00                     | 0.43              |
| 1:M:228:LYS:O    | 1:M:333:SER:HB2  | 2.19                     | 0.43              |
| 2:F:609:C:C2'    | 2:F:610:C:H5'    | 2.49                     | 0.43              |
| 1:I:80:HIS:CE1   | 1:I:318:LEU:CB   | 3.01                     | 0.43              |
| 1:A:397:ILE:HG23 | 1:A:417:LEU:HD13 | 1.99                     | 0.43              |
| 1:A:49:ARG:HE    | 1:A:49:ARG:HB2   | 1.63                     | 0.43              |
| 1:I:2:GLU:HB3    | 1:I:64:GLY:HA2   | 2.00                     | 0.43              |
| 2:J:612:G:C5'    | 2:J:613:A:OP1    | 2.67                     | 0.43              |
| 1:M:320:HIS:HB3  | 1:M:335:PRO:CG   | 2.49                     | 0.43              |
| 3:C:688:G:O5'    | 3:C:688:G:H8     | 1.98                     | 0.43              |
| 3:G:690:C:C5'    | 3:G:690:C:H6     | 2.31                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:J:609:C:H2'    | 2:J:610:C:H5'    | 2.00                     | 0.43              |
| 1:M:222:PRO:HA   | 1:M:368:TRP:CZ2  | 2.54                     | 0.43              |
| 1:M:276:LYS:HE2  | 1:M:276:LYS:HB2  | 1.79                     | 0.43              |
| 1:M:54:PHE:O     | 1:M:57:ALA:N     | 2.45                     | 0.43              |
| 1:A:27:PRO:HB3   | 1:A:31:HIS:CE1   | 2.54                     | 0.42              |
| 1:E:4:GLN:HG2    | 1:E:283:LYS:HE3  | 2.01                     | 0.42              |
| 1:M:17:ILE:O     | 1:M:276:LYS:HA   | 2.19                     | 0.42              |
| 1:E:43:LEU:HA    | 1:E:43:LEU:HD12  | 1.79                     | 0.42              |
| 1:M:65:ASN:HB3   | 1:M:243:PRO:HD2  | 2.00                     | 0.42              |
| 1:M:275:TYR:CE2  | 1:M:276:LYS:HE2  | 2.54                     | 0.42              |
| 1:M:394:MET:SD   | 1:M:421:ALA:HB1  | 2.60                     | 0.42              |
| 3:O:694:A:H2'    | 3:O:695:C:C6     | 2.54                     | 0.42              |
| 3:O:694:A:H2'    | 3:O:695:C:H6     | 1.85                     | 0.42              |
| 1:I:90:ILE:HD13  | 1:I:194:LEU:HD12 | 2.00                     | 0.42              |
| 1:I:273:HIS:HB2  | 1:I:280:TYR:CZ   | 2.54                     | 0.42              |
| 1:A:394:MET:SD   | 1:A:421:ALA:HB1  | 2.59                     | 0.42              |
| 1:E:297:ASN:HB3  | 1:E:327:GLY:HA2  | 2.00                     | 0.42              |
| 1:E:384:TYR:HA   | 1:E:385:PRO:HD3  | 1.83                     | 0.42              |
| 1:M:142:GLN:OE1  | 1:M:142:GLN:HA   | 2.19                     | 0.42              |
| 1:M:162:LEU:HD11 | 1:M:403:TRP:CD1  | 2.54                     | 0.42              |
| 1:M:7:ARG:O      | 1:M:7:ARG:HG3    | 2.19                     | 0.42              |
| 2:N:612:G:C5'    | 2:N:613:A:OP1    | 2.67                     | 0.42              |
| 1:A:422:TRP:CZ2  | 1:A:423:HIS:CE1  | 3.07                     | 0.42              |
| 1:E:179:SER:HB2  | 1:E:290:CYS:HA   | 2.00                     | 0.42              |
| 1:E:422:TRP:CZ2  | 1:E:423:HIS:CE1  | 3.08                     | 0.42              |
| 3:G:701:A:H2'    | 3:G:702:C:O4'    | 2.18                     | 0.42              |
| 1:I:154:LEU:HD22 | 1:I:177:GLU:HB3  | 2.00                     | 0.42              |
| 1:M:81:TYR:O     | 1:M:84:GLN:HB2   | 2.20                     | 0.42              |
| 3:C:693:G:H2'    | 3:C:694:A:H8     | 1.85                     | 0.42              |
| 3:C:701:A:H2'    | 3:C:702:C:O4'    | 2.19                     | 0.42              |
| 1:E:120:TYR:HB3  | 1:E:125:LYS:HB3  | 2.01                     | 0.42              |
| 1:E:306:ARG:CG   | 1:E:318:LEU:HD13 | 2.46                     | 0.42              |
| 1:E:397:ILE:HG23 | 1:E:417:LEU:HD13 | 2.02                     | 0.42              |
| 1:I:25:LEU:HB2   | 1:I:40:PRO:HG3   | 2.01                     | 0.42              |
| 1:M:90:ILE:HD13  | 1:M:194:LEU:HD12 | 2.01                     | 0.42              |
| 1:A:320:HIS:O    | 1:A:335:PRO:HD3  | 2.20                     | 0.42              |
| 1:I:275:TYR:CE2  | 1:I:276:LYS:HE2  | 2.53                     | 0.42              |
| 1:A:145:LEU:HD23 | 1:A:145:LEU:HA   | 1.87                     | 0.42              |
| 1:A:269:ASN:ND2  | 10:A:552:HOH:O   | 2.49                     | 0.42              |
| 1:A:413:HIS:CD2  | 3:C:698:G:H4'    | 2.55                     | 0.42              |
| 2:J:604:C:H2'    | 2:J:605:U:O4'    | 2.19                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:7:ARG:HD3    | 1:M:11:GLU:HG2   | 2.02                     | 0.42              |
| 2:B:609:C:C2'    | 2:B:610:C:H5'    | 2.49                     | 0.41              |
| 3:C:690:C:H6     | 3:C:690:C:C5'    | 2.32                     | 0.41              |
| 1:E:388:ILE:HD12 | 8:E:6029:IPA:H13 | 2.03                     | 0.41              |
| 1:I:320:HIS:HB3  | 1:I:335:PRO:CG   | 2.50                     | 0.41              |
| 1:M:118:TYR:CG   | 1:M:119:PRO:HA   | 2.55                     | 0.41              |
| 1:M:273:HIS:HB2  | 1:M:280:TYR:CZ   | 2.55                     | 0.41              |
| 1:M:387:LEU:HD22 | 1:M:461:PHE:CZ   | 2.55                     | 0.41              |
| 1:A:449:GLU:O    | 1:A:450:TYR:C    | 2.57                     | 0.41              |
| 1:A:368:TRP:CB   | 8:A:6030:IPA:H2  | 2.49                     | 0.41              |
| 1:I:397:ILE:CD1  | 1:I:421:ALA:HB2  | 2.46                     | 0.41              |
| 1:A:35:GLU:O     | 1:A:402:ARG:HD2  | 2.20                     | 0.41              |
| 2:B:605:U:H5     | 10:B:492:HOH:O   | 2.03                     | 0.41              |
| 1:I:82:ALA:O     | 1:I:86:MET:HG2   | 2.20                     | 0.41              |
| 1:M:237:TYR:O    | 1:M:238:ASP:C    | 2.59                     | 0.41              |
| 1:M:232:PHE:CB   | 1:M:355:THR:O    | 2.69                     | 0.41              |
| 1:M:383:LYS:HB3  | 1:M:384:TYR:CD1  | 2.56                     | 0.41              |
| 1:A:4:GLN:HG2    | 1:A:283:LYS:HE3  | 2.02                     | 0.41              |
| 1:M:140:GLU:O    | 1:M:140:GLU:HG3  | 2.18                     | 0.41              |
| 1:M:318:LEU:HA   | 1:M:318:LEU:HD23 | 1.74                     | 0.41              |
| 1:M:27:PRO:HD3   | 1:M:403:TRP:CZ3  | 2.55                     | 0.41              |
| 1:M:47:ASP:HA    | 1:M:48:PRO:HD3   | 1.89                     | 0.41              |
| 1:E:368:TRP:CB   | 8:E:6029:IPA:H2  | 2.34                     | 0.41              |
| 1:M:355:THR:CB   | 1:M:356:PRO:CD   | 2.99                     | 0.41              |
| 1:A:218:TRP:O    | 1:A:222:PRO:HD3  | 2.21                     | 0.41              |
| 1:A:97:LEU:O     | 1:A:101:MET:HG3  | 2.21                     | 0.41              |
| 3:G:693:G:H2'    | 3:G:694:A:H8     | 1.85                     | 0.41              |
| 1:M:447:LEU:HD23 | 1:M:447:LEU:N    | 2.34                     | 0.41              |
| 1:A:306:ARG:CG   | 1:A:318:LEU:HD13 | 2.51                     | 0.41              |
| 1:A:384:TYR:HA   | 1:A:385:PRO:HD3  | 1.82                     | 0.41              |
| 2:B:598:A:C3'    | 2:B:599:G:H5'    | 2.46                     | 0.41              |
| 1:E:50:LEU:HD21  | 1:E:171:GLY:HA3  | 2.03                     | 0.41              |
| 1:I:118:TYR:CG   | 1:I:119:PRO:HA   | 2.55                     | 0.41              |
| 1:I:11:GLU:C     | 1:I:12:VAL:HG23  | 2.41                     | 0.41              |
| 1:I:7:ARG:HD3    | 1:I:11:GLU:HG2   | 2.02                     | 0.41              |
| 1:A:55:GLU:O     | 1:A:59:PHE:HD2   | 2.03                     | 0.41              |
| 1:A:381:ASP:OD1  | 8:A:6027:IPA:H2  | 2.21                     | 0.41              |
| 1:M:321:LEU:HD12 | 1:M:322:LYS:N    | 2.35                     | 0.41              |
| 1:A:305:ILE:HD11 | 1:A:330:VAL:HG11 | 2.03                     | 0.41              |
| 2:J:604:C:H2'    | 2:J:605:U:C6     | 2.56                     | 0.41              |
| 3:K:694:A:H2'    | 3:K:695:C:C6     | 2.56                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:O:692:G:O2'    | 3:O:693:G:H5'    | 2.21                     | 0.41              |
| 1:A:24:LYS:HB2   | 1:A:24:LYS:HE3   | 1.76                     | 0.41              |
| 1:A:217:PHE:HD1  | 8:A:6009:IPA:H12 | 1.85                     | 0.41              |
| 1:E:27:PRO:HB3   | 1:E:31:HIS:CE1   | 2.55                     | 0.41              |
| 1:E:295:ILE:HG12 | 10:E:507:HOH:O   | 2.21                     | 0.41              |
| 1:E:226:GLU:HG3  | 1:E:320:HIS:O    | 2.21                     | 0.41              |
| 1:E:411:GLN:HE22 | 1:E:446:ASP:H    | 1.69                     | 0.41              |
| 1:E:52:THR:HG23  | 1:E:53:ASP:N     | 2.35                     | 0.41              |
| 1:I:228:LYS:O    | 1:I:333:SER:HB2  | 2.21                     | 0.41              |
| 1:I:275:TYR:CD2  | 1:I:275:TYR:O    | 2.74                     | 0.41              |
| 1:M:275:TYR:O    | 1:M:276:LYS:CB   | 2.69                     | 0.41              |
| 1:M:82:ALA:O     | 1:M:86:MET:HG2   | 2.21                     | 0.41              |
| 2:N:604:C:H2'    | 2:N:605:U:C6     | 2.55                     | 0.41              |
| 1:A:120:TYR:HB3  | 1:A:125:LYS:HB3  | 2.03                     | 0.41              |
| 2:B:610:C:C2'    | 2:B:611:G:O5'    | 2.69                     | 0.41              |
| 1:E:213:ASP:HB3  | 8:E:6014:IPA:C1  | 2.50                     | 0.41              |
| 1:E:223:VAL:HG23 | 1:E:223:VAL:O    | 2.21                     | 0.41              |
| 1:E:254:GLU:HG2  | 1:E:259:GLY:HA2  | 2.01                     | 0.41              |
| 1:I:275:TYR:O    | 1:I:276:LYS:CB   | 2.69                     | 0.41              |
| 1:M:432:PHE:CZ   | 1:M:436:ILE:HD11 | 2.55                     | 0.41              |
| 2:N:604:C:H2'    | 2:N:605:U:O4'    | 2.21                     | 0.41              |
| 2:F:598:A:H1'    | 4:H:805:G:C2     | 2.57                     | 0.40              |
| 1:I:270:HIS:NE2  | 1:I:283:LYS:HE2  | 2.36                     | 0.40              |
| 1:I:47:ASP:HA    | 1:I:48:PRO:HD3   | 1.87                     | 0.40              |
| 1:M:226:GLU:HG3  | 1:M:320:HIS:O    | 2.20                     | 0.40              |
| 1:A:179:SER:HB2  | 1:A:290:CYS:HA   | 2.02                     | 0.40              |
| 1:A:254:GLU:HG2  | 1:A:259:GLY:HA2  | 2.02                     | 0.40              |
| 1:A:382:GLU:HB2  | 8:A:6027:IPA:H33 | 2.03                     | 0.40              |
| 1:A:95:MET:HE3   | 1:A:95:MET:HB2   | 1.94                     | 0.40              |
| 1:E:237:TYR:CG   | 1:E:328:ASP:HB3  | 2.56                     | 0.40              |
| 1:E:212:CYS:HB2  | 8:E:6014:IPA:C3  | 2.51                     | 0.40              |
| 2:F:610:C:C2'    | 2:F:611:G:O5'    | 2.69                     | 0.40              |
| 1:I:162:LEU:HD11 | 1:I:403:TRP:CD1  | 2.56                     | 0.40              |
| 1:I:318:LEU:HD23 | 1:I:318:LEU:HA   | 1.75                     | 0.40              |
| 1:M:11:GLU:C     | 1:M:12:VAL:HG23  | 2.42                     | 0.40              |
| 1:M:448:PRO:HG2  | 1:M:453:LEU:HD21 | 2.02                     | 0.40              |
| 1:A:20:PRO:HA    | 2:B:598:A:N1     | 2.36                     | 0.40              |
| 1:E:334:TYR:CD2  | 1:E:335:PRO:HD2  | 2.55                     | 0.40              |
| 1:I:375:LYS:HD3  | 1:I:396:GLU:OE1  | 2.21                     | 0.40              |
| 1:M:67:ILE:HG23  | 1:M:244:ALA:HB3  | 2.04                     | 0.40              |
| 1:A:214:PRO:O    | 1:A:390:PRO:HG3  | 2.22                     | 0.40              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:A:58:ILE:HD11  | 1:A:59:PHE:CE2  | 2.57                     | 0.40              |
| 1:E:121:VAL:CG1  | 1:E:122:ALA:N   | 2.85                     | 0.40              |
| 1:E:367:THR:C    | 1:E:369:GLU:H   | 2.25                     | 0.40              |
| 1:E:449:GLU:O    | 1:E:450:TYR:C   | 2.59                     | 0.40              |
| 1:E:61:LYS:HD2   | 1:E:239:ALA:CB  | 2.51                     | 0.40              |
| 1:E:70:VAL:HG11  | 1:E:251:MET:HE3 | 2.03                     | 0.40              |
| 3:G:693:G:H2'    | 3:G:694:A:C8    | 2.57                     | 0.40              |
| 1:M:270:HIS:NE2  | 1:M:283:LYS:HE2 | 2.36                     | 0.40              |
| 1:E:145:LEU:HD23 | 1:E:145:LEU:HA  | 1.90                     | 0.40              |
| 1:I:275:TYR:O    | 1:I:276:LYS:HB3 | 2.22                     | 0.40              |
| 1:I:321:LEU:HD12 | 1:I:322:LYS:N   | 2.36                     | 0.40              |
| 1:I:334:TYR:CD1  | 1:I:335:PRO:CD  | 3.05                     | 0.40              |
| 1:I:337:GLU:C    | 1:I:337:GLU:OE2 | 2.60                     | 0.40              |
| 1:I:355:THR:HB   | 1:I:356:PRO:HD3 | 2.03                     | 0.40              |
| 1:I:383:LYS:HB3  | 1:I:384:TYR:CD1 | 2.57                     | 0.40              |
| 1:I:411:GLN:HB3  | 10:I:546:HOH:O  | 2.22                     | 0.40              |
| 1:M:334:TYR:CD1  | 1:M:335:PRO:CD  | 3.04                     | 0.40              |
| 1:M:358:ASP:HB2  | 1:M:360:SER:OG  | 2.22                     | 0.40              |
| 1:M:440:PRO:HA   | 1:M:443:ARG:NH1 | 2.36                     | 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 |    |
|-----|-------|-----------------|------------|----------|----------|-------------|----|
| 1   | A     | 459/471 (98%)   | 434 (95%)  | 23 (5%)  | 2 (0%)   | 38          | 69 |
| 1   | E     | 459/471 (98%)   | 432 (94%)  | 25 (5%)  | 2 (0%)   | 38          | 69 |
| 1   | I     | 459/471 (98%)   | 406 (88%)  | 45 (10%) | 8 (2%)   | 11          | 30 |
| 1   | M     | 459/471 (98%)   | 407 (89%)  | 44 (10%) | 8 (2%)   | 11          | 30 |
| All | All   | 1836/1884 (98%) | 1679 (91%) | 137 (8%) | 20 (1%)  | 17          | 43 |

All (20) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 285 | GLY  |
| 1   | E     | 285 | GLY  |
| 1   | I     | 12  | VAL  |
| 1   | I     | 64  | GLY  |
| 1   | I     | 70  | VAL  |
| 1   | I     | 164 | SER  |
| 1   | M     | 64  | GLY  |
| 1   | M     | 70  | VAL  |
| 1   | M     | 164 | SER  |
| 1   | I     | 66  | LYS  |
| 1   | M     | 12  | VAL  |
| 1   | M     | 66  | LYS  |
| 1   | I     | 276 | LYS  |
| 1   | I     | 355 | THR  |
| 1   | I     | 457 | TRP  |
| 1   | M     | 276 | LYS  |
| 1   | M     | 355 | THR  |
| 1   | M     | 457 | TRP  |
| 1   | E     | 70  | VAL  |
| 1   | A     | 70  | 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.

| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1   | A     | 403/412 (98%)   | 368 (91%)  | 35 (9%)  | 12          | 30 |
| 1   | E     | 403/412 (98%)   | 369 (92%)  | 34 (8%)  | 13          | 32 |
| 1   | I     | 403/412 (98%)   | 369 (92%)  | 34 (8%)  | 13          | 32 |
| 1   | M     | 403/412 (98%)   | 369 (92%)  | 34 (8%)  | 13          | 32 |
| All | All   | 1612/1648 (98%) | 1475 (92%) | 137 (8%) | 12          | 32 |

All (137) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 2   | GLU  |
| 1   | A     | 4   | GLN  |
| 1   | A     | 9   | SER  |
| 1   | A     | 10  | LYS  |
| 1   | A     | 24  | LYS  |
| 1   | A     | 28  | SER  |
| 1   | A     | 43  | LEU  |
| 1   | A     | 45  | LYS  |
| 1   | A     | 49  | ARG  |
| 1   | A     | 52  | THR  |
| 1   | A     | 66  | LYS  |
| 1   | A     | 94  | GLN  |
| 1   | A     | 139 | LYS  |
| 1   | A     | 163 | ARG  |
| 1   | A     | 166 | THR  |
| 1   | A     | 170 | GLN  |
| 1   | A     | 176 | ILE  |
| 1   | A     | 218 | TRP  |
| 1   | A     | 220 | LYS  |
| 1   | A     | 260 | ASP  |
| 1   | A     | 261 | ARG  |
| 1   | A     | 263 | ASP  |
| 1   | A     | 277 | ASN  |
| 1   | A     | 281 | CYS  |
| 1   | A     | 294 | SER  |
| 1   | A     | 314 | LYS  |
| 1   | A     | 316 | ILE  |
| 1   | A     | 329 | ASP  |
| 1   | A     | 337 | GLU  |
| 1   | A     | 348 | LYS  |
| 1   | A     | 359 | LYS  |
| 1   | A     | 415 | ARG  |
| 1   | A     | 428 | GLU  |
| 1   | A     | 455 | ARG  |
| 1   | A     | 456 | ARG  |
| 1   | E     | 2   | GLU  |
| 1   | E     | 4   | GLN  |
| 1   | E     | 9   | SER  |
| 1   | E     | 10  | LYS  |
| 1   | E     | 24  | LYS  |
| 1   | E     | 28  | SER  |
| 1   | E     | 43  | LEU  |
| 1   | E     | 45  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 49  | ARG  |
| 1   | E     | 52  | THR  |
| 1   | E     | 66  | LYS  |
| 1   | E     | 94  | GLN  |
| 1   | E     | 139 | LYS  |
| 1   | E     | 163 | ARG  |
| 1   | E     | 166 | THR  |
| 1   | E     | 170 | GLN  |
| 1   | E     | 176 | ILE  |
| 1   | E     | 218 | TRP  |
| 1   | E     | 220 | LYS  |
| 1   | E     | 260 | ASP  |
| 1   | E     | 261 | ARG  |
| 1   | E     | 263 | ASP  |
| 1   | E     | 277 | ASN  |
| 1   | E     | 281 | CYS  |
| 1   | E     | 294 | SER  |
| 1   | E     | 314 | LYS  |
| 1   | E     | 316 | ILE  |
| 1   | E     | 329 | ASP  |
| 1   | E     | 337 | GLU  |
| 1   | E     | 348 | LYS  |
| 1   | E     | 359 | LYS  |
| 1   | E     | 428 | GLU  |
| 1   | E     | 455 | ARG  |
| 1   | E     | 456 | ARG  |
| 1   | I     | 3   | ILE  |
| 1   | I     | 5   | TRP  |
| 1   | I     | 6   | MET  |
| 1   | I     | 21  | SER  |
| 1   | I     | 26  | GLU  |
| 1   | I     | 39  | GLU  |
| 1   | I     | 56  | GLU  |
| 1   | I     | 60  | SER  |
| 1   | I     | 63  | VAL  |
| 1   | I     | 68  | THR  |
| 1   | I     | 121 | VAL  |
| 1   | I     | 151 | ASN  |
| 1   | I     | 166 | THR  |
| 1   | I     | 176 | ILE  |
| 1   | I     | 179 | SER  |
| 1   | I     | 180 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | I     | 218 | TRP  |
| 1   | I     | 261 | ARG  |
| 1   | I     | 277 | ASN  |
| 1   | I     | 291 | SER  |
| 1   | I     | 294 | SER  |
| 1   | I     | 295 | ILE  |
| 1   | I     | 329 | ASP  |
| 1   | I     | 337 | GLU  |
| 1   | I     | 346 | SER  |
| 1   | I     | 348 | LYS  |
| 1   | I     | 364 | GLU  |
| 1   | I     | 367 | THR  |
| 1   | I     | 383 | LYS  |
| 1   | I     | 391 | VAL  |
| 1   | I     | 415 | ARG  |
| 1   | I     | 428 | GLU  |
| 1   | I     | 441 | ILE  |
| 1   | I     | 455 | ARG  |
| 1   | M     | 5   | TRP  |
| 1   | M     | 6   | MET  |
| 1   | M     | 7   | ARG  |
| 1   | M     | 21  | SER  |
| 1   | M     | 26  | GLU  |
| 1   | M     | 39  | GLU  |
| 1   | M     | 56  | GLU  |
| 1   | M     | 60  | SER  |
| 1   | M     | 63  | VAL  |
| 1   | M     | 68  | THR  |
| 1   | M     | 121 | VAL  |
| 1   | M     | 151 | ASN  |
| 1   | M     | 166 | THR  |
| 1   | M     | 176 | ILE  |
| 1   | M     | 179 | SER  |
| 1   | M     | 180 | SER  |
| 1   | M     | 218 | TRP  |
| 1   | M     | 261 | ARG  |
| 1   | M     | 277 | ASN  |
| 1   | M     | 291 | SER  |
| 1   | M     | 294 | SER  |
| 1   | M     | 295 | ILE  |
| 1   | M     | 329 | ASP  |
| 1   | M     | 337 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | M     | 346 | SER  |
| 1   | M     | 348 | LYS  |
| 1   | M     | 364 | GLU  |
| 1   | M     | 367 | THR  |
| 1   | M     | 383 | LYS  |
| 1   | M     | 391 | VAL  |
| 1   | M     | 415 | ARG  |
| 1   | M     | 428 | GLU  |
| 1   | M     | 441 | ILE  |
| 1   | M     | 455 | ARG  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 277 | ASN  |
| 1   | A     | 411 | GLN  |
| 1   | E     | 277 | ASN  |
| 1   | E     | 411 | GLN  |
| 1   | I     | 170 | GLN  |
| 1   | I     | 270 | HIS  |
| 1   | I     | 272 | HIS  |
| 1   | I     | 277 | ASN  |
| 1   | I     | 398 | HIS  |
| 1   | I     | 424 | ASN  |
| 1   | M     | 170 | GLN  |
| 1   | M     | 269 | ASN  |
| 1   | M     | 270 | HIS  |
| 1   | M     | 272 | HIS  |
| 1   | M     | 277 | ASN  |
| 1   | M     | 336 | HIS  |
| 1   | M     | 398 | HIS  |

### 5.3.3 RNA [i](#)

| Mol | Chain | Analysed    | Backbone Outliers | Pucker Outliers |
|-----|-------|-------------|-------------------|-----------------|
| 2   | B     | 15/26 (57%) | 2 (13%)           | 2 (13%)         |
| 2   | F     | 15/26 (57%) | 2 (13%)           | 2 (13%)         |
| 2   | J     | 15/26 (57%) | 2 (13%)           | 1 (6%)          |
| 2   | N     | 15/26 (57%) | 2 (13%)           | 1 (6%)          |
| 3   | C     | 14/15 (93%) | 1 (7%)            | 0               |

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| Mol | Chain | Analysed      | Backbone Outliers | Pucker Outliers |
|-----|-------|---------------|-------------------|-----------------|
| 3   | G     | 14/15 (93%)   | 1 (7%)            | 0               |
| 3   | K     | 14/15 (93%)   | 0                 | 0               |
| 3   | O     | 14/15 (93%)   | 0                 | 0               |
| 4   | D     | 2/9 (22%)     | 2 (100%)          | 0               |
| 4   | H     | 2/9 (22%)     | 2 (100%)          | 0               |
| 4   | L     | 3/9 (33%)     | 1 (33%)           | 0               |
| 4   | P     | 3/9 (33%)     | 1 (33%)           | 0               |
| All | All   | 126/200 (63%) | 16 (12%)          | 6 (4%)          |

All (16) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 599 | G    |
| 2   | B     | 600 | G    |
| 3   | C     | 690 | C    |
| 4   | D     | 806 | G    |
| 4   | D     | 807 | A    |
| 2   | F     | 599 | G    |
| 2   | F     | 600 | G    |
| 3   | G     | 690 | C    |
| 4   | H     | 806 | G    |
| 4   | H     | 807 | A    |
| 2   | J     | 611 | G    |
| 2   | J     | 612 | G    |
| 4   | L     | 807 | A    |
| 2   | N     | 611 | G    |
| 2   | N     | 612 | G    |
| 4   | P     | 807 | A    |

All (6) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 598 | A    |
| 2   | B     | 599 | G    |
| 2   | F     | 598 | A    |
| 2   | F     | 599 | G    |
| 2   | J     | 598 | A    |
| 2   | N     | 598 | A    |

## 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](#)

Of 29 ligands modelled in this entry, 12 are monoatomic - leaving 17 for Mogul analysis.

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 | $\# Z  > 2$ |
| 7   | POP  | A     | 5004 | 6    | 8,8,8        | 1.03 | 0           | 8,13,13     | 0.66 | 0           |
| 8   | IPA  | A     | 6009 | -    | 3,3,3        | 0.65 | 0           | 3,3,3       | 0.22 | 0           |
| 8   | IPA  | A     | 6011 | -    | 3,3,3        | 0.52 | 0           | 3,3,3       | 0.38 | 0           |
| 8   | IPA  | A     | 6027 | -    | 3,3,3        | 0.62 | 0           | 3,3,3       | 0.16 | 0           |
| 8   | IPA  | A     | 6028 | -    | 3,3,3        | 0.65 | 0           | 3,3,3       | 0.27 | 0           |
| 8   | IPA  | A     | 6030 | -    | 3,3,3        | 0.51 | 0           | 3,3,3       | 0.51 | 0           |
| 9   | GOL  | A     | 8012 | -    | 5,5,5        | 0.35 | 0           | 5,5,5       | 0.43 | 0           |
| 8   | IPA  | E     | 6014 | -    | 3,3,3        | 0.42 | 0           | 3,3,3       | 0.65 | 0           |
| 8   | IPA  | E     | 6029 | -    | 3,3,3        | 0.55 | 0           | 3,3,3       | 0.24 | 0           |
| 9   | GOL  | E     | 8011 | 5    | 5,5,5        | 0.28 | 0           | 5,5,5       | 0.39 | 0           |
| 7   | POP  | G     | 5003 | 6    | 8,8,8        | 0.75 | 0           | 8,13,13     | 0.60 | 0           |
| 7   | POP  | I     | 5002 | 6    | 8,8,8        | 0.57 | 0           | 8,13,13     | 0.57 | 0           |
| 9   | GOL  | J     | 8005 | -    | 5,5,5        | 0.40 | 0           | 5,5,5       | 0.82 | 0           |
| 8   | IPA  | M     | 6018 | -    | 3,3,3        | 0.62 | 0           | 3,3,3       | 0.26 | 0           |
| 8   | IPA  | M     | 6019 | -    | 3,3,3        | 0.53 | 0           | 3,3,3       | 0.40 | 0           |
| 9   | GOL  | N     | 8010 | -    | 5,5,5        | 0.36 | 0           | 5,5,5       | 0.85 | 0           |
| 7   | POP  | O     | 5001 | 6    | 8,8,8        | 0.91 | 0           | 8,13,13     | 0.39 | 0           |

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   |
|-----|------|-------|------|------|---------|----------|---------|
| 7   | POP  | A     | 5004 | 6    | -       | 0/6/6/6  | 0/0/0/0 |
| 8   | IPA  | A     | 6009 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 8   | IPA  | A     | 6011 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 8   | IPA  | A     | 6027 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 8   | IPA  | A     | 6028 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 8   | IPA  | A     | 6030 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 9   | GOL  | A     | 8012 | -    | -       | 0/4/4/4  | 0/0/0/0 |
| 8   | IPA  | E     | 6014 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 8   | IPA  | E     | 6029 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 9   | GOL  | E     | 8011 | 5    | -       | 0/4/4/4  | 0/0/0/0 |
| 7   | POP  | G     | 5003 | 6    | -       | 0/6/6/6  | 0/0/0/0 |
| 7   | POP  | I     | 5002 | 6    | -       | 0/6/6/6  | 0/0/0/0 |
| 9   | GOL  | J     | 8005 | -    | -       | 0/4/4/4  | 0/0/0/0 |
| 8   | IPA  | M     | 6018 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 8   | IPA  | M     | 6019 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 9   | GOL  | N     | 8010 | -    | -       | 0/4/4/4  | 0/0/0/0 |
| 7   | POP  | O     | 5001 | 6    | -       | 0/6/6/6  | 0/0/0/0 |

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.

11 monomers are involved in 34 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 8   | A     | 6009 | IPA  | 1       | 0            |
| 8   | A     | 6011 | IPA  | 4       | 0            |
| 8   | A     | 6027 | IPA  | 2       | 0            |
| 8   | A     | 6028 | IPA  | 2       | 0            |
| 8   | A     | 6030 | IPA  | 3       | 0            |
| 8   | E     | 6014 | IPA  | 11      | 0            |
| 8   | E     | 6029 | IPA  | 3       | 0            |
| 7   | G     | 5003 | POP  | 1       | 0            |
| 7   | I     | 5002 | POP  | 1       | 0            |
| 8   | M     | 6018 | IPA  | 1       | 0            |
| 8   | M     | 6019 | IPA  | 5       | 0            |

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2  |     |     | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|----------|-----|-----|-----------------------|-------|
| 1   | A     | 461/471 (97%)   | -0.06  | 14 (3%)  | 51  | 45  | 37, 61, 92, 111       | 0     |
| 1   | E     | 461/471 (97%)   | -0.05  | 15 (3%)  | 47  | 41  | 39, 60, 93, 110       | 0     |
| 1   | I     | 461/471 (97%)   | 0.05   | 23 (4%)  | 30  | 24  | 40, 68, 115, 143      | 0     |
| 1   | M     | 461/471 (97%)   | 0.13   | 34 (7%)  | 15  | 11  | 38, 68, 115, 143      | 0     |
| 2   | B     | 17/26 (65%)     | -0.66  | 0        | 100 | 100 | 47, 62, 135, 164      | 0     |
| 2   | F     | 17/26 (65%)     | -0.49  | 0        | 100 | 100 | 47, 62, 134, 164      | 0     |
| 2   | J     | 17/26 (65%)     | -0.22  | 0        | 100 | 100 | 53, 75, 166, 182      | 0     |
| 2   | N     | 17/26 (65%)     | -0.16  | 1 (5%)   | 23  | 18  | 51, 76, 166, 182      | 0     |
| 3   | C     | 15/15 (100%)    | -0.24  | 2 (13%)  | 4   | 3   | 49, 65, 124, 141      | 0     |
| 3   | G     | 15/15 (100%)    | -0.04  | 2 (13%)  | 4   | 3   | 49, 65, 124, 141      | 0     |
| 3   | K     | 15/15 (100%)    | 0.02   | 2 (13%)  | 4   | 3   | 52, 83, 145, 149      | 0     |
| 3   | O     | 15/15 (100%)    | 0.10   | 2 (13%)  | 4   | 3   | 52, 84, 145, 149      | 0     |
| 4   | D     | 3/9 (33%)       | 1.77   | 2 (66%)  | 0   | 0   | 168, 168, 172, 173    | 0     |
| 4   | H     | 3/9 (33%)       | 4.60   | 2 (66%)  | 0   | 0   | 168, 168, 172, 173    | 0     |
| 4   | L     | 4/9 (44%)       | 1.66   | 1 (25%)  | 1   | 0   | 146, 152, 157, 173    | 0     |
| 4   | P     | 4/9 (44%)       | 2.64   | 3 (75%)  | 0   | 0   | 146, 152, 158, 173    | 0     |
| All | All   | 1986/2084 (95%) | 0.02   | 103 (5%) | 28  | 22  | 37, 64, 114, 182      | 0     |

All (103) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 4   | H     | 805 | G    | 7.0  |
| 1   | E     | 284 | GLY  | 6.8  |
| 1   | I     | 357 | ALA  | 5.6  |
| 1   | I     | 342 | LEU  | 5.2  |
| 4   | H     | 806 | G    | 5.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | E     | 285 | GLY  | 4.9  |
| 1   | M     | 134 | GLN  | 4.8  |
| 4   | P     | 805 | G    | 4.7  |
| 1   | M     | 285 | GLY  | 4.6  |
| 1   | M     | 284 | GLY  | 4.1  |
| 1   | A     | 19  | ALA  | 4.0  |
| 1   | M     | 32  | TYR  | 3.9  |
| 3   | G     | 689 | C    | 3.8  |
| 1   | I     | 134 | GLN  | 3.8  |
| 1   | E     | 283 | LYS  | 3.7  |
| 1   | M     | 65  | ASN  | 3.6  |
| 1   | A     | 67  | ILE  | 3.6  |
| 1   | M     | 38  | LYS  | 3.6  |
| 1   | E     | 134 | GLN  | 3.5  |
| 1   | E     | 49  | ARG  | 3.5  |
| 3   | C     | 688 | G    | 3.5  |
| 3   | K     | 689 | C    | 3.4  |
| 1   | A     | 64  | GLY  | 3.3  |
| 1   | M     | 363 | PHE  | 3.3  |
| 3   | K     | 688 | G    | 3.3  |
| 1   | A     | 32  | TYR  | 3.3  |
| 1   | M     | 342 | LEU  | 3.3  |
| 3   | O     | 689 | C    | 3.2  |
| 1   | I     | 46  | ASN  | 3.2  |
| 3   | O     | 688 | G    | 3.2  |
| 4   | L     | 808 | G    | 3.2  |
| 1   | M     | 396 | GLU  | 3.1  |
| 1   | I     | 32  | TYR  | 3.1  |
| 1   | M     | 165 | LYS  | 3.1  |
| 1   | M     | 17  | ILE  | 3.0  |
| 1   | E     | 16  | ILE  | 2.9  |
| 1   | M     | 204 | VAL  | 2.9  |
| 1   | M     | 345 | GLN  | 2.9  |
| 1   | A     | 134 | GLN  | 2.8  |
| 4   | P     | 806 | G    | 2.8  |
| 3   | C     | 689 | C    | 2.8  |
| 1   | A     | 139 | LYS  | 2.8  |
| 1   | M     | 22  | LYS  | 2.8  |
| 1   | A     | 357 | ALA  | 2.8  |
| 1   | I     | 406 | ASP  | 2.7  |
| 1   | I     | 363 | PHE  | 2.7  |
| 1   | E     | 138 | THR  | 2.7  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | I     | 89  | ASP  | 2.7  |
| 1   | A     | 320 | HIS  | 2.7  |
| 1   | M     | 16  | ILE  | 2.6  |
| 1   | M     | 357 | ALA  | 2.6  |
| 1   | A     | 154 | LEU  | 2.6  |
| 1   | M     | 460 | SER  | 2.5  |
| 1   | E     | 178 | ALA  | 2.5  |
| 1   | I     | 47  | ASP  | 2.5  |
| 1   | I     | 356 | PRO  | 2.4  |
| 1   | E     | 233 | ASP  | 2.4  |
| 1   | M     | 46  | ASN  | 2.4  |
| 1   | I     | 15  | PRO  | 2.4  |
| 1   | A     | 256 | ILE  | 2.4  |
| 4   | D     | 806 | G    | 2.4  |
| 1   | I     | 396 | GLU  | 2.4  |
| 1   | M     | 29  | ALA  | 2.4  |
| 1   | A     | 396 | GLU  | 2.4  |
| 3   | G     | 688 | G    | 2.4  |
| 1   | M     | 343 | LEU  | 2.3  |
| 2   | N     | 597 | C    | 2.3  |
| 1   | I     | 276 | LYS  | 2.3  |
| 1   | I     | 345 | GLN  | 2.3  |
| 1   | I     | 67  | ILE  | 2.3  |
| 1   | E     | 361 | ALA  | 2.3  |
| 1   | M     | 2   | GLU  | 2.3  |
| 1   | I     | 75  | LYS  | 2.3  |
| 1   | I     | 154 | LEU  | 2.3  |
| 1   | I     | 1   | GLY  | 2.2  |
| 1   | M     | 286 | MET  | 2.2  |
| 1   | M     | 31  | HIS  | 2.2  |
| 1   | M     | 43  | LEU  | 2.2  |
| 1   | M     | 355 | THR  | 2.2  |
| 1   | A     | 359 | LYS  | 2.2  |
| 1   | I     | 10  | LYS  | 2.2  |
| 1   | I     | 314 | LYS  | 2.2  |
| 1   | M     | 441 | ILE  | 2.2  |
| 1   | I     | 285 | GLY  | 2.2  |
| 1   | M     | 71  | ASP  | 2.2  |
| 1   | E     | 13  | GLY  | 2.2  |
| 1   | A     | 49  | ARG  | 2.2  |
| 4   | P     | 808 | G    | 2.2  |
| 1   | M     | 9   | SER  | 2.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | M     | 315 | GLY  | 2.2  |
| 4   | D     | 805 | G    | 2.1  |
| 1   | M     | 178 | ALA  | 2.1  |
| 1   | E     | 10  | LYS  | 2.1  |
| 1   | A     | 414 | VAL  | 2.1  |
| 1   | E     | 317 | ASP  | 2.1  |
| 1   | M     | 137 | ASP  | 2.1  |
| 1   | M     | 67  | ILE  | 2.1  |
| 1   | E     | 313 | TYR  | 2.1  |
| 1   | E     | 414 | VAL  | 2.0  |
| 1   | M     | 287 | PRO  | 2.0  |
| 1   | I     | 320 | HIS  | 2.0  |
| 1   | M     | 170 | GLN  | 2.0  |
| 1   | I     | 34  | PHE  | 2.0  |

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

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

## 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( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 9   | GOL  | N     | 8010 | 6/6   | 0.88 | 0.34 | 7.36 | 55,71,72,86                 | 0     |
| 8   | IPA  | E     | 6029 | 4/4   | 0.90 | 0.57 | 5.99 | 67,75,80,84                 | 0     |
| 7   | POP  | I     | 5002 | 9/9   | 0.69 | 0.27 | 4.96 | 97,119,129,136              | 9     |
| 8   | IPA  | A     | 6030 | 4/4   | 0.96 | 0.36 | 4.87 | 68,73,76,78                 | 0     |
| 8   | IPA  | A     | 6028 | 4/4   | 0.91 | 0.28 | 3.24 | 60,80,87,112                | 0     |
| 8   | IPA  | M     | 6019 | 4/4   | 0.73 | 0.41 | 3.12 | 80,96,100,105               | 0     |
| 9   | GOL  | J     | 8005 | 6/6   | 0.91 | 0.21 | 2.31 | 47,55,64,73                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 7   | POP  | O     | 5001 | 9/9   | 0.80 | 0.24 | 1.52  | 41,73,93,98                 | 9     |
| 8   | IPA  | A     | 6027 | 4/4   | 0.74 | 0.23 | 1.37  | 84,91,95,98                 | 0     |
| 8   | IPA  | E     | 6014 | 4/4   | 0.91 | 0.24 | 1.19  | 53,58,75,75                 | 0     |
| 7   | POP  | A     | 5004 | 9/9   | 0.78 | 0.24 | 1.03  | 45,77,111,115               | 9     |
| 8   | IPA  | M     | 6018 | 4/4   | 0.96 | 0.17 | 0.43  | 47,52,58,72                 | 0     |
| 7   | POP  | G     | 5003 | 9/9   | 0.79 | 0.19 | -0.06 | 47,60,88,89                 | 9     |
| 5   | ZN   | E     | 2003 | 1/1   | 0.96 | 0.17 | -0.34 | 88,88,88,88                 | 1     |
| 8   | IPA  | A     | 6009 | 4/4   | 0.93 | 0.14 | -0.86 | 64,72,75,78                 | 0     |
| 6   | MN   | A     | 3007 | 1/1   | 0.93 | 0.07 | -1.12 | 91,91,91,91                 | 0     |
| 6   | MN   | E     | 3005 | 1/1   | 0.94 | 0.05 | -1.80 | 87,87,87,87                 | 0     |
| 6   | MN   | M     | 3001 | 1/1   | 0.94 | 0.06 | -2.44 | 127,127,127,127             | 0     |
| 6   | MN   | M     | 3002 | 1/1   | 0.98 | 0.08 | -2.48 | 86,86,86,86                 | 0     |
| 6   | MN   | I     | 3003 | 1/1   | 0.94 | 0.05 | -4.99 | 120,120,120,120             | 0     |
| 9   | GOL  | A     | 8012 | 6/6   | 0.87 | 0.20 | -     | 71,86,94,98                 | 0     |
| 8   | IPA  | A     | 6011 | 4/4   | 0.78 | 0.77 | -     | 65,88,92,106                | 0     |
| 6   | MN   | I     | 3004 | 1/1   | 0.98 | 0.09 | -     | 90,90,90,90                 | 0     |
| 5   | ZN   | M     | 2001 | 1/1   | 0.95 | 0.15 | -     | 70,70,70,70                 | 1     |
| 6   | MN   | A     | 3008 | 1/1   | 0.99 | 0.08 | -     | 74,74,74,74                 | 0     |
| 5   | ZN   | A     | 2004 | 1/1   | 0.98 | 0.10 | -     | 81,81,81,81                 | 1     |
| 9   | GOL  | E     | 8011 | 6/6   | 0.88 | 0.16 | -     | 69,82,89,94                 | 0     |
| 6   | MN   | E     | 3006 | 1/1   | 0.98 | 0.09 | -     | 74,74,74,74                 | 0     |
| 5   | ZN   | I     | 2002 | 1/1   | 0.98 | 0.14 | -     | 70,70,70,70                 | 1     |

## 6.5 Other polymers

There are no such residues in this entry.