# Full wwPDB X-ray Structure Validation Report (i)

May 26, 2020 – 08:05 am BST

| | | |
|---|---|---|
| PDB ID | : | 5D6S |
| Title | : | Structure of epoxyqueuosine reductase from Streptococcus thermophilus. |
| Authors | : | Payne, K.A.P.; Fisher, K.; Dunstan, M.S.; Sjuts, H.; Leys, D. |
| Deposited on | : | 2015-08-12 |
| Resolution | : | 2.65 Å(reported) |

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

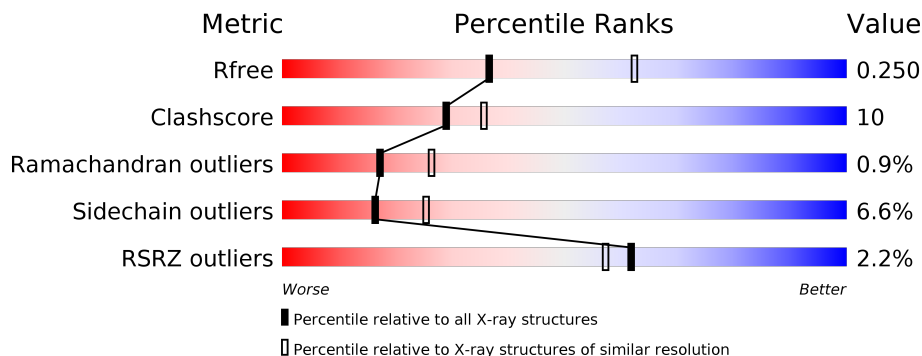| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 2.11 |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac | : | 5.8.0158 |
| CCP4 | : | 7.0.044 (Gargrove) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.11 |

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.65 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 | Percentile Ranks | Value |
|---|---|---|
| Rfree | | 0.250 |
| Clashscore | | 10 |
| Ramachandran outliers | | 0.9% |
| Sidechain outliers | | 6.6% |
| RSRZ outliers | | 2.2% |

*Worse* ← → *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|---|---|---|
| R$_{free}$ | 130704 | 1332 (2.68-2.64) |
| Clashscore | 141614 | 1374 (2.68-2.64) |
| Ramachandran outliers | 138981 | 1349 (2.68-2.64) |
| Sidechain outliers | 138945 | 1349 (2.68-2.64) |
| RSRZ outliers | 127900 | 1318 (2.68-2.64) |

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 >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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 | 399 | %  75% 14% • 7% |
| 1 | B | 399 | %  77% 12% • • 7% |
| 1 | C | 399 | 2%  77% 12% • 8% |
| 1 | D | 399 | 3%  76% 13% • • 7% |
| 1 | E | 399 | 4%  75% 14% • 7% |

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 |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 2 | SF4 | D | 402 | - | - | X | - |
| 3 | B12 | A | 403 | - | - | X | - |
| 3 | B12 | B | 403 | - | - | X | - |
| 3 | B12 | E | 403 | - | - | X | - |

# 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 15145 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 Epoxyqueuosine reductase.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---------|---------|-------|
| 1 | A | 370 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2912 | 1849 | 496 | 544 | 23 | | | |
| 1 | B | 370 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2912 | 1849 | 496 | 544 | 23 | | | |
| 1 | C | 367 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2888 | 1834 | 492 | 540 | 22 | | | |
| 1 | D | 370 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2912 | 1849 | 496 | 544 | 23 | | | |
| 1 | E | 370 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2912 | 1849 | 496 | 544 | 23 | | | |

There are 145 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------|-----------|
| A | -26 | MET | - | initiating methionine | UNP A0A0F7K4Z9 |
| A | -25 | VAL | - | expression tag | UNP A0A0F7K4Z9 |
| A | -24 | GLN | - | expression tag | UNP A0A0F7K4Z9 |
| A | -23 | THR | - | expression tag | UNP A0A0F7K4Z9 |
| A | -22 | SER | - | expression tag | UNP A0A0F7K4Z9 |
| A | -21 | PHE | - | expression tag | UNP A0A0F7K4Z9 |
| A | -20 | GLU | - | expression tag | UNP A0A0F7K4Z9 |
| A | -19 | HIS | - | expression tag | UNP A0A0F7K4Z9 |
| A | -18 | HIS | - | expression tag | UNP A0A0F7K4Z9 |
| A | -17 | HIS | - | expression tag | UNP A0A0F7K4Z9 |
| A | -16 | HIS | - | expression tag | UNP A0A0F7K4Z9 |
| A | -15 | HIS | - | expression tag | UNP A0A0F7K4Z9 |
| A | -14 | HIS | - | expression tag | UNP A0A0F7K4Z9 |
| A | -13 | SER | - | expression tag | UNP A0A0F7K4Z9 |
| A | -12 | ALA | - | expression tag | UNP A0A0F7K4Z9 |
| A | -11 | GLY | - | expression tag | UNP A0A0F7K4Z9 |
| A | -10 | GLU | - | expression tag | UNP A0A0F7K4Z9 |
| A | -9 | ASN | - | expression tag | UNP A0A0F7K4Z9 |
| A | -8 | LEU | - | expression tag | UNP A0A0F7K4Z9 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|:-----:|:-------:|:--------:|:------:|:-------:|:---------:|
| A | -7 | TYR | - | expression tag | UNP A0A0F7K4Z9 |
| A | -6 | PHE | - | expression tag | UNP A0A0F7K4Z9 |
| A | -5 | GLN | - | expression tag | UNP A0A0F7K4Z9 |
| A | -4 | GLY | - | expression tag | UNP A0A0F7K4Z9 |
| A | -3 | ALA | - | expression tag | UNP A0A0F7K4Z9 |
| A | -2 | GLN | - | expression tag | UNP A0A0F7K4Z9 |
| A | -1 | ILE | - | expression tag | UNP A0A0F7K4Z9 |
| A | 0 | SER | - | expression tag | UNP A0A0F7K4Z9 |
| A | 258 | ASP | GLU | conflict | UNP A0A0F7K4Z9 |
| A | 342 | GLY | ALA | conflict | UNP A0A0F7K4Z9 |
| B | -26 | MET | - | initiating methionine | UNP A0A0F7K4Z9 |
| B | -25 | VAL | - | expression tag | UNP A0A0F7K4Z9 |
| B | -24 | GLN | - | expression tag | UNP A0A0F7K4Z9 |
| B | -23 | THR | - | expression tag | UNP A0A0F7K4Z9 |
| B | -22 | SER | - | expression tag | UNP A0A0F7K4Z9 |
| B | -21 | PHE | - | expression tag | UNP A0A0F7K4Z9 |
| B | -20 | GLU | - | expression tag | UNP A0A0F7K4Z9 |
| B | -19 | HIS | - | expression tag | UNP A0A0F7K4Z9 |
| B | -18 | HIS | - | expression tag | UNP A0A0F7K4Z9 |
| B | -17 | HIS | - | expression tag | UNP A0A0F7K4Z9 |
| B | -16 | HIS | - | expression tag | UNP A0A0F7K4Z9 |
| B | -15 | HIS | - | expression tag | UNP A0A0F7K4Z9 |
| B | -14 | HIS | - | expression tag | UNP A0A0F7K4Z9 |
| B | -13 | SER | - | expression tag | UNP A0A0F7K4Z9 |
| B | -12 | ALA | - | expression tag | UNP A0A0F7K4Z9 |
| B | -11 | GLY | - | expression tag | UNP A0A0F7K4Z9 |
| B | -10 | GLU | - | expression tag | UNP A0A0F7K4Z9 |
| B | -9 | ASN | - | expression tag | UNP A0A0F7K4Z9 |
| B | -8 | LEU | - | expression tag | UNP A0A0F7K4Z9 |
| B | -7 | TYR | - | expression tag | UNP A0A0F7K4Z9 |
| B | -6 | PHE | - | expression tag | UNP A0A0F7K4Z9 |
| B | -5 | GLN | - | expression tag | UNP A0A0F7K4Z9 |
| B | -4 | GLY | - | expression tag | UNP A0A0F7K4Z9 |
| B | -3 | ALA | - | expression tag | UNP A0A0F7K4Z9 |
| B | -2 | GLN | - | expression tag | UNP A0A0F7K4Z9 |
| B | -1 | ILE | - | expression tag | UNP A0A0F7K4Z9 |
| B | 0 | SER | - | expression tag | UNP A0A0F7K4Z9 |
| B | 258 | ASP | GLU | conflict | UNP A0A0F7K4Z9 |
| B | 342 | GLY | ALA | conflict | UNP A0A0F7K4Z9 |
| C | -26 | MET | - | initiating methionine | UNP A0A0F7K4Z9 |
| C | -25 | VAL | - | expression tag | UNP A0A0F7K4Z9 |
| C | -24 | GLN | - | expression tag | UNP A0A0F7K4Z9 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|:-----:|:-------:|:--------:|:------:|:-------:|:---------:|
| C | -23 | THR | - | expression tag | UNP A0A0F7K4Z9 |
| C | -22 | SER | - | expression tag | UNP A0A0F7K4Z9 |
| C | -21 | PHE | - | expression tag | UNP A0A0F7K4Z9 |
| C | -20 | GLU | - | expression tag | UNP A0A0F7K4Z9 |
| C | -19 | HIS | - | expression tag | UNP A0A0F7K4Z9 |
| C | -18 | HIS | - | expression tag | UNP A0A0F7K4Z9 |
| C | -17 | HIS | - | expression tag | UNP A0A0F7K4Z9 |
| C | -16 | HIS | - | expression tag | UNP A0A0F7K4Z9 |
| C | -15 | HIS | - | expression tag | UNP A0A0F7K4Z9 |
| C | -14 | HIS | - | expression tag | UNP A0A0F7K4Z9 |
| C | -13 | SER | - | expression tag | UNP A0A0F7K4Z9 |
| C | -12 | ALA | - | expression tag | UNP A0A0F7K4Z9 |
| C | -11 | GLY | - | expression tag | UNP A0A0F7K4Z9 |
| C | -10 | GLU | - | expression tag | UNP A0A0F7K4Z9 |
| C | -9 | ASN | - | expression tag | UNP A0A0F7K4Z9 |
| C | -8 | LEU | - | expression tag | UNP A0A0F7K4Z9 |
| C | -7 | TYR | - | expression tag | UNP A0A0F7K4Z9 |
| C | -6 | PHE | - | expression tag | UNP A0A0F7K4Z9 |
| C | -5 | GLN | - | expression tag | UNP A0A0F7K4Z9 |
| C | -4 | GLY | - | expression tag | UNP A0A0F7K4Z9 |
| C | -3 | ALA | - | expression tag | UNP A0A0F7K4Z9 |
| C | -2 | GLN | - | expression tag | UNP A0A0F7K4Z9 |
| C | -1 | ILE | - | expression tag | UNP A0A0F7K4Z9 |
| C | 0 | SER | - | expression tag | UNP A0A0F7K4Z9 |
| C | 260 | ASP | GLU | conflict | UNP A0A0F7K4Z9 |
| C | 344 | GLY | ALA | conflict | UNP A0A0F7K4Z9 |
| D | -26 | MET | - | initiating methionine | UNP A0A0F7K4Z9 |
| D | -25 | VAL | - | expression tag | UNP A0A0F7K4Z9 |
| D | -24 | GLN | - | expression tag | UNP A0A0F7K4Z9 |
| D | -23 | THR | - | expression tag | UNP A0A0F7K4Z9 |
| D | -22 | SER | - | expression tag | UNP A0A0F7K4Z9 |
| D | -21 | PHE | - | expression tag | UNP A0A0F7K4Z9 |
| D | -20 | GLU | - | expression tag | UNP A0A0F7K4Z9 |
| D | -19 | HIS | - | expression tag | UNP A0A0F7K4Z9 |
| D | -18 | HIS | - | expression tag | UNP A0A0F7K4Z9 |
| D | -17 | HIS | - | expression tag | UNP A0A0F7K4Z9 |
| D | -16 | HIS | - | expression tag | UNP A0A0F7K4Z9 |
| D | -15 | HIS | - | expression tag | UNP A0A0F7K4Z9 |
| D | -14 | HIS | - | expression tag | UNP A0A0F7K4Z9 |
| D | -13 | SER | - | expression tag | UNP A0A0F7K4Z9 |
| D | -12 | ALA | - | expression tag | UNP A0A0F7K4Z9 |
| D | -11 | GLY | - | expression tag | UNP A0A0F7K4Z9 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------|-----------|
| D | -10 | GLU | - | expression tag | UNP A0A0F7K4Z9 |
| D | -9 | ASN | - | expression tag | UNP A0A0F7K4Z9 |
| D | -8 | LEU | - | expression tag | UNP A0A0F7K4Z9 |
| D | -7 | TYR | - | expression tag | UNP A0A0F7K4Z9 |
| D | -6 | PHE | - | expression tag | UNP A0A0F7K4Z9 |
| D | -5 | GLN | - | expression tag | UNP A0A0F7K4Z9 |
| D | -4 | GLY | - | expression tag | UNP A0A0F7K4Z9 |
| D | -3 | ALA | - | expression tag | UNP A0A0F7K4Z9 |
| D | -2 | GLN | - | expression tag | UNP A0A0F7K4Z9 |
| D | -1 | ILE | - | expression tag | UNP A0A0F7K4Z9 |
| D | 0 | SER | - | expression tag | UNP A0A0F7K4Z9 |
| D | 258 | ASP | GLU | conflict | UNP A0A0F7K4Z9 |
| D | 342 | GLY | ALA | conflict | UNP A0A0F7K4Z9 |
| E | -26 | MET | - | initiating methionine | UNP A0A0F7K4Z9 |
| E | -25 | VAL | - | expression tag | UNP A0A0F7K4Z9 |
| E | -24 | GLN | - | expression tag | UNP A0A0F7K4Z9 |
| E | -23 | THR | - | expression tag | UNP A0A0F7K4Z9 |
| E | -22 | SER | - | expression tag | UNP A0A0F7K4Z9 |
| E | -21 | PHE | - | expression tag | UNP A0A0F7K4Z9 |
| E | -20 | GLU | - | expression tag | UNP A0A0F7K4Z9 |
| E | -19 | HIS | - | expression tag | UNP A0A0F7K4Z9 |
| E | -18 | HIS | - | expression tag | UNP A0A0F7K4Z9 |
| E | -17 | HIS | - | expression tag | UNP A0A0F7K4Z9 |
| E | -16 | HIS | - | expression tag | UNP A0A0F7K4Z9 |
| E | -15 | HIS | - | expression tag | UNP A0A0F7K4Z9 |
| E | -14 | HIS | - | expression tag | UNP A0A0F7K4Z9 |
| E | -13 | SER | - | expression tag | UNP A0A0F7K4Z9 |
| E | -12 | ALA | - | expression tag | UNP A0A0F7K4Z9 |
| E | -11 | GLY | - | expression tag | UNP A0A0F7K4Z9 |
| E | -10 | GLU | - | expression tag | UNP A0A0F7K4Z9 |
| E | -9 | ASN | - | expression tag | UNP A0A0F7K4Z9 |
| E | -8 | LEU | - | expression tag | UNP A0A0F7K4Z9 |
| E | -7 | TYR | - | expression tag | UNP A0A0F7K4Z9 |
| E | -6 | PHE | - | expression tag | UNP A0A0F7K4Z9 |
| E | -5 | GLN | - | expression tag | UNP A0A0F7K4Z9 |
| E | -4 | GLY | - | expression tag | UNP A0A0F7K4Z9 |
| E | -3 | ALA | - | expression tag | UNP A0A0F7K4Z9 |
| E | -2 | GLN | - | expression tag | UNP A0A0F7K4Z9 |
| E | -1 | ILE | - | expression tag | UNP A0A0F7K4Z9 |
| E | 0 | SER | - | expression tag | UNP A0A0F7K4Z9 |
| E | 258 | ASP | GLU | conflict | UNP A0A0F7K4Z9 |
| E | 342 | GLY | ALA | conflict | UNP A0A0F7K4Z9 |

- Molecule 2 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: $Fe_4S_4$).
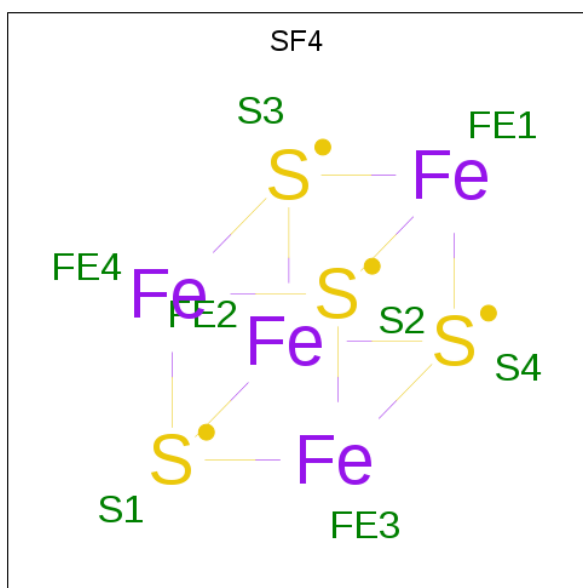


| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|
| 2 | A | 1 | Total 8 | Fe 4 | S 4 | 0 | 0 |
| 2 | A | 1 | Total 8 | Fe 4 | S 4 | 0 | 0 |
| 2 | B | 1 | Total 8 | Fe 4 | S 4 | 0 | 0 |
| 2 | B | 1 | Total 8 | Fe 4 | S 4 | 0 | 0 |
| 2 | C | 1 | Total 8 | Fe 4 | S 4 | 0 | 0 |
| 2 | C | 1 | Total 8 | Fe 4 | S 4 | 0 | 0 |
| 2 | D | 1 | Total 8 | Fe 4 | S 4 | 0 | 0 |
| 2 | D | 1 | Total 8 | Fe 4 | S 4 | 0 | 0 |
| 2 | E | 1 | Total 8 | Fe 4 | S 4 | 0 | 0 |
| 2 | E | 1 | Total 8 | Fe 4 | S 4 | 0 | 0 |

- Molecule 3 is COBALAMIN (three-letter code: B12) (formula: $C_{62}H_{89}CoN_{13}O_{14}P$).

B12

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|-----|-----|-----|-----|---------|---------|
| 3 | A | 1 | Total | C | Co | N | O | P | 0 | 0 |
| | | | 91 | 62 | 1 | 13 | 14 | 1 | | |
| 3 | B | 1 | Total | C | Co | N | O | P | 0 | 0 |
| | | | 91 | 62 | 1 | 13 | 14 | 1 | | |
| 3 | C | 1 | Total | C | Co | N | O | P | 0 | 0 |
| | | | 91 | 62 | 1 | 13 | 14 | 1 | | |
| 3 | D | 1 | Total | C | Co | N | O | P | 0 | 0 |
| | | | 91 | 62 | 1 | 13 | 14 | 1 | | |
| 3 | E | 1 | Total | C | Co | N | O | P | 0 | 0 |
| | | | 91 | 62 | 1 | 13 | 14 | 1 | | |

- Molecule 4 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 4 | A | 19 | Total | O | 0 | 0 |
| | | | 19 | 19 | | |
| 4 | B | 14 | Total | O | 0 | 0 |
| | | | 14 | 14 | | |
| 4 | C | 15 | Total | O | 0 | 0 |
| | | | 15 | 15 | | |
| 4 | D | 14 | Total | O | 0 | 0 |
| | | | 14 | 14 | | |
| 4 | E | 12 | Total | O | 0 | 0 |
| | | | 12 | 12 | | |

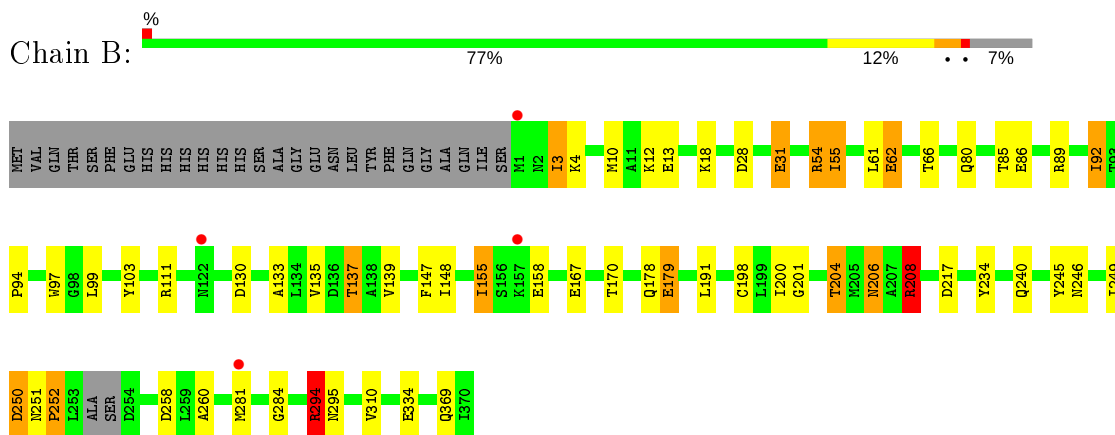# 3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.
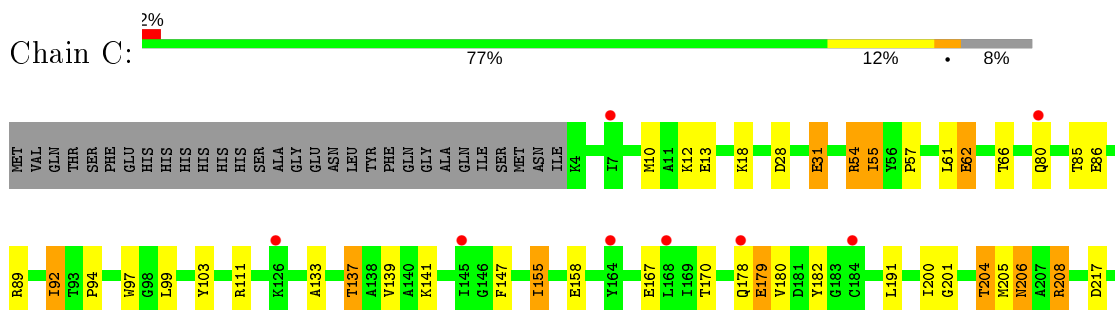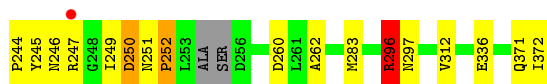
- Molecule 1: Epoxyqueuosine reductase
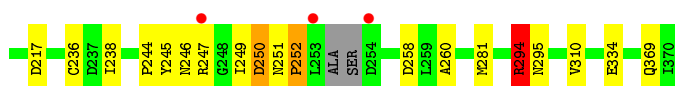


- Molecule 1: Epoxyqueuosine reductase
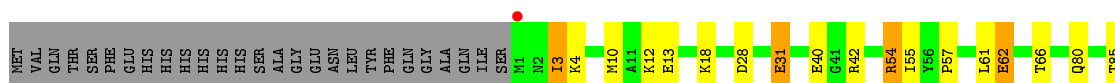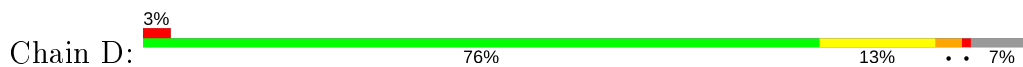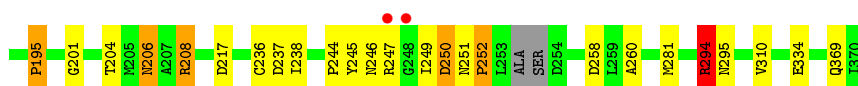


- Molecule 1: Epoxyqueuosine reductase

P244 Y245 N246 R247 G248 I249 D250 N251 P252 L253 ALA SER D256 D260 L261 A262 M283 R296 N297 V312 E336 Q371 I372

• Molecule 1: Epoxyqueuosine reductase

Chain D:

3%

76% 13% 7%

MET VAL GLN THR SER PHE GLU HIS HIS HIS HIS HIS HIS SER ALA GLY GLU ASN LEU TYR PHE GLN GLY ALA GLN ILE SER M1 N2 I3 K4 M10 A11 K12 E13 K18 D28 E31 E40 G41 R42 R54 I55 Y56 P57 L61 E62 T66 Q80 T85

E36 R89 I92 T93 P94 W97 G98 L99 Y103 R111 L119 Y125 A133 L134 V135 D136 T137 A138 V139 F147 I155 S156 K157 E158 E167 L168 I169 T170 Q178 E179 V180 D181 Y182 L191 P195 C198 L199 I200 G201 T204 M205 N206 A207 R208

D217 C236 D237 I238 P244 Y245 N246 R247 G248 I249 D250 N251 P252 L253 ALA SER D254 D258 L259 A260 M281 R294 N295 V310 E334 Q369 I370

• Molecule 1: Epoxyqueuosine reductase

Chain E:

4%

75% 14% 7%

MET VAL GLN THR SER PHE GLU HIS HIS HIS HIS HIS HIS SER ALA GLY GLU ASN LEU TYR PHE GLN GLY ALA GLN ILE SER M1 N2 I3 K4 L5 M10 A11 K12 E13 K18 T22 D28 E31 K32 S33 L34 E40 G41 R42 R54 I55 Y56 P57 L61 E62

T66 S69 I70 A71 Y74 Q80 T85 E86 R89 I92 T93 P94 W97 G98 L99 Y103 R111 L112 N122 D130 A133 L134 V135 D136 T137 A138 V139 F147 G152 I155 E158 E167 L168 I169 T170 E175 Q178 E179 L191

P195 G201 T204 M205 N206 A207 R208 D217 C236 D237 I238 P244 Y245 N246 R247 G248 I249 D250 N251 P252 L253 ALA SER D254 D258 L259 A260 M281 R294 N295 V310 E334 Q369 I370

# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 31 2 1 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 106.12Å　　106.12Å　　332.28Å<br>90.00°　　　90.00°　　　120.00° | Depositor |
| Resolution (Å) | 88.58　–　2.65<br>88.58　–　2.65 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 98.8 (88.58-2.65)<br>98.8 (88.58-2.65) | Depositor<br>EDS |
| $R_{merge}$ | 0.13 | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $<I/\sigma(I)>$ [1] | 2.57 (at 2.65Å) | Xtriage |
| Refinement program | REFMAC 5.7.0029 | Depositor |
| R, $R_{free}$ | 0.214　　,　　0.253<br>0.214　　,　　0.250 | Depositor<br>DCC |
| $R_{free}$ test set | 3163 reflections (4.99%) | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 65.9 | Xtriage |
| Anisotropy | 0.082 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.29 , 41.0 | EDS |
| L-test for twinning[2] | $<|L|>$ = 0.51, $<L^2>$ = 0.34 | Xtriage |
| Estimated twinning fraction | 0.000 for -h,-k,l | Xtriage |
| $F_o,F_c$ correlation | 0.95 | EDS |
| Total number of atoms | 15145 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 76.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.56% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

# 5 Model quality (i)

## 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, B12

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 | 0.52 | 0/2965 | 0.75 | 1/3993 (0.0%) |
| 1 | B | 0.54 | 0/2965 | 0.75 | 1/3993 (0.0%) |
| 1 | C | 0.53 | 0/2941 | 0.73 | 1/3961 (0.0%) |
| 1 | D | 0.51 | 0/2965 | 0.73 | 1/3993 (0.0%) |
| 1 | E | 0.49 | 0/2965 | 0.73 | 1/3993 (0.0%) |
| All | All | 0.52 | 0/14801 | 0.74 | 5/19933 (0.0%) |

There are no bond length outliers.

All (5) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|-----|-------|-----|------|-------|---|-----------|---------|
| 1 | A | 294 | ARG | NE-CZ-NH1 | 7.26 | 123.93 | 120.30 |
| 1 | B | 294 | ARG | NE-CZ-NH1 | 7.17 | 123.89 | 120.30 |
| 1 | C | 296 | ARG | NE-CZ-NH1 | 6.76 | 123.68 | 120.30 |
| 1 | D | 294 | ARG | NE-CZ-NH1 | 6.76 | 123.68 | 120.30 |
| 1 | E | 294 | ARG | NE-CZ-NH1 | 6.67 | 123.64 | 120.30 |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 2912 | 0 | 2929 | 50 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | B | 2912 | 0 | 2929 | 43 | 0 |
| 1 | C | 2888 | 0 | 2900 | 40 | 0 |
| 1 | D | 2912 | 0 | 2929 | 43 | 0 |
| 1 | E | 2912 | 0 | 2929 | 51 | 0 |
| 2 | A | 16 | 0 | 0 | 1 | 0 |
| 2 | B | 16 | 0 | 0 | 1 | 0 |
| 2 | C | 16 | 0 | 0 | 0 | 0 |
| 2 | D | 16 | 0 | 0 | 2 | 0 |
| 2 | E | 16 | 0 | 0 | 1 | 0 |
| 3 | A | 91 | 0 | 88 | 23 | 0 |
| 3 | B | 91 | 0 | 88 | 21 | 0 |
| 3 | C | 91 | 0 | 88 | 15 | 0 |
| 3 | D | 91 | 0 | 88 | 16 | 0 |
| 3 | E | 91 | 0 | 88 | 22 | 0 |
| 4 | A | 19 | 0 | 0 | 0 | 0 |
| 4 | B | 14 | 0 | 0 | 1 | 0 |
| 4 | C | 15 | 0 | 0 | 0 | 0 |
| 4 | D | 14 | 0 | 0 | 0 | 0 |
| 4 | E | 12 | 0 | 0 | 3 | 0 |
| All | All | 15145 | 0 | 15056 | 288 | 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 10.

All (288) 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:B:148:ILE:CD1 | 3:B:403:B12:H2B | 1.78 | 1.13 |
| 1:B:148:ILE:HD13 | 3:B:403:B12:H2B | 1.31 | 1.12 |
| 1:A:148:ILE:HD12 | 3:A:403:B12:N3B | 1.79 | 0.96 |
| 3:C:403:B12:H362 | 3:C:403:B12:H351 | 1.52 | 0.92 |
| 1:E:34:LEU:HD23 | 3:E:403:B12:H3P1 | 1.52 | 0.89 |
| 1:D:54:ARG:NH1 | 3:D:403:B12:O58 | 2.05 | 0.87 |
| 1:C:137:THR:HG21 | 3:C:403:B12:O8R | 1.74 | 0.87 |
| 1:B:54:ARG:NH1 | 3:B:403:B12:O58 | 2.08 | 0.85 |
| 3:D:403:B12:H362 | 3:D:403:B12:H351 | 1.58 | 0.83 |
| 3:D:403:B12:H531 | 3:D:403:B12:H552 | 1.60 | 0.82 |
| 1:E:34:LEU:CD2 | 3:E:403:B12:C3P | 2.56 | 0.82 |
| 1:B:148:ILE:HD12 | 3:B:403:B12:H2B | 1.60 | 0.81 |
| 1:E:34:LEU:CD2 | 3:E:403:B12:H3P1 | 2.11 | 0.80 |
| 1:E:54:ARG:NH1 | 3:E:403:B12:O58 | 2.11 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:141:LYS:NZ | 3:C:403:B12:H4B | 1.96 | 0.80 |
| 1:C:205:MET:SD | 3:C:403:B12:N52 | 2.54 | 0.79 |
| 1:A:148:ILE:CD1 | 3:A:403:B12:N3B | 2.46 | 0.79 |
| 3:B:403:B12:H362 | 3:B:403:B12:H351 | 1.62 | 0.79 |
| 1:E:74:TYR:OH | 4:E:501:HOH:O | 1.99 | 0.79 |
| 1:A:148:ILE:HD13 | 3:A:403:B12:C2B | 2.12 | 0.78 |
| 3:A:403:B12:H362 | 3:A:403:B12:H351 | 1.66 | 0.77 |
| 1:A:148:ILE:CD1 | 3:A:403:B12:C2B | 2.63 | 0.77 |
| 3:E:403:B12:H351 | 3:E:403:B12:H362 | 1.67 | 0.76 |
| 1:A:137:THR:HG21 | 3:A:403:B12:O8R | 1.87 | 0.74 |
| 1:B:294:ARG:NH1 | 1:B:295:ASN:OD1 | 2.20 | 0.73 |
| 1:D:294:ARG:NH1 | 1:D:295:ASN:OD1 | 2.21 | 0.73 |
| 3:C:403:B12:H551 | 3:C:403:B12:O63 | 1.89 | 0.73 |
| 1:A:141:LYS:NZ | 3:A:403:B12:H4B | 2.04 | 0.72 |
| 1:E:294:ARG:NH1 | 1:E:295:ASN:OD1 | 2.22 | 0.72 |
| 1:A:294:ARG:NH1 | 1:A:295:ASN:OD1 | 2.23 | 0.72 |
| 1:C:141:LYS:HZ3 | 3:C:403:B12:H4B | 1.54 | 0.72 |
| 1:E:34:LEU:HD21 | 3:E:403:B12:H3P3 | 1.72 | 0.71 |
| 1:C:296:ARG:NH1 | 1:C:297:ASN:OD1 | 2.24 | 0.71 |
| 3:E:403:B12:O2 | 3:E:403:B12:H3P2 | 1.92 | 0.70 |
| 3:C:403:B12:H421 | 3:C:403:B12:C10 | 2.21 | 0.70 |
| 1:B:137:THR:HG21 | 3:B:403:B12:O8R | 1.91 | 0.69 |
| 1:E:34:LEU:CD2 | 3:E:403:B12:H3P3 | 2.20 | 0.69 |
| 1:E:130:ASP:O | 3:E:403:B12:N62 | 2.26 | 0.68 |
| 3:C:403:B12:H491 | 3:C:403:B12:H473 | 1.74 | 0.68 |
| 3:B:403:B12:C10 | 3:B:403:B12:H421 | 2.23 | 0.68 |
| 1:E:294:ARG:HG2 | 1:E:294:ARG:HH11 | 1.57 | 0.67 |
| 1:A:294:ARG:HH11 | 1:A:294:ARG:HG2 | 1.58 | 0.67 |
| 3:D:403:B12:C55 | 3:D:403:B12:H531 | 2.22 | 0.66 |
| 1:A:130:ASP:OD1 | 3:A:403:B12:H542 | 1.96 | 0.66 |
| 1:D:294:ARG:HH11 | 1:D:294:ARG:HG2 | 1.59 | 0.66 |
| 1:C:296:ARG:HH11 | 1:C:296:ARG:HG2 | 1.60 | 0.65 |
| 1:B:294:ARG:HG2 | 1:B:294:ARG:HH11 | 1.62 | 0.64 |
| 1:E:33:SER:OG | 4:E:502:HOH:O | 2.15 | 0.64 |
| 1:A:141:LYS:HZ2 | 3:A:403:B12:H4B | 1.61 | 0.64 |
| 1:E:34:LEU:HD21 | 3:E:403:B12:C3P | 2.29 | 0.63 |
| 3:C:403:B12:H362 | 3:C:403:B12:C35 | 2.26 | 0.63 |
| 1:C:372:ILE:O | 1:C:372:ILE:HG22 | 1.97 | 0.62 |
| 3:A:403:B12:H421 | 3:A:403:B12:C10 | 2.30 | 0.61 |
| 1:B:85:THR:HG22 | 1:B:86:GLU:H | 1.69 | 0.58 |
| 1:B:246:ASN:HA | 1:B:249:ILE:CD1 | 2.33 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:246:ASN:HA | 1:A:249:ILE:CD1 | 2.34 | 0.57 |
| 1:D:246:ASN:HA | 1:D:249:ILE:CD1 | 2.33 | 0.57 |
| 1:C:246:ASN:HA | 1:C:249:ILE:CD1 | 2.35 | 0.57 |
| 1:C:85:THR:HG22 | 1:C:86:GLU:H | 1.69 | 0.57 |
| 3:A:403:B12:H311 | 3:A:403:B12:H353 | 1.87 | 0.57 |
| 1:B:198:CYS:SG | 2:B:402:SF4:S2 | 3.02 | 0.57 |
| 3:E:403:B12:C35 | 3:E:403:B12:H362 | 2.34 | 0.57 |
| 1:C:61:LEU:O | 1:C:62:GLU:CB | 2.52 | 0.57 |
| 1:A:206:ASN:HD22 | 1:A:206:ASN:C | 2.07 | 0.56 |
| 3:B:403:B12:H533 | 3:B:403:B12:H481 | 1.87 | 0.56 |
| 3:D:403:B12:H421 | 3:D:403:B12:C10 | 2.34 | 0.56 |
| 1:E:85:THR:HG22 | 1:E:86:GLU:H | 1.70 | 0.56 |
| 1:E:246:ASN:HA | 1:E:249:ILE:CD1 | 2.34 | 0.56 |
| 1:D:85:THR:HG22 | 1:D:86:GLU:H | 1.69 | 0.56 |
| 3:C:403:B12:H551 | 3:C:403:B12:C61 | 2.36 | 0.56 |
| 1:C:147:PHE:CE1 | 1:C:155:ILE:HB | 2.41 | 0.55 |
| 3:C:403:B12:H492 | 3:C:403:B12:N23 | 2.21 | 0.55 |
| 3:A:403:B12:H362 | 3:A:403:B12:C35 | 2.36 | 0.55 |
| 1:C:217:ASP:O | 1:C:296:ARG:NH2 | 2.39 | 0.55 |
| 3:D:403:B12:H533 | 3:D:403:B12:H481 | 1.87 | 0.55 |
| 3:D:403:B12:H473 | 3:D:403:B12:H491 | 1.87 | 0.55 |
| 1:E:152:GLY:O | 3:E:403:B12:O8R | 2.25 | 0.55 |
| 1:A:85:THR:HG22 | 1:A:86:GLU:H | 1.72 | 0.55 |
| 3:A:403:B12:H552 | 3:A:403:B12:H531 | 1.89 | 0.54 |
| 1:A:217:ASP:O | 1:A:294:ARG:NH2 | 2.41 | 0.54 |
| 3:A:403:B12:C55 | 3:A:403:B12:H531 | 2.36 | 0.54 |
| 1:E:217:ASP:O | 1:E:294:ARG:NH2 | 2.39 | 0.54 |
| 1:B:217:ASP:O | 1:B:294:ARG:NH2 | 2.40 | 0.54 |
| 1:D:206:ASN:C | 1:D:206:ASN:HD22 | 2.12 | 0.53 |
| 1:B:130:ASP:OD1 | 3:B:403:B12:H542 | 2.08 | 0.53 |
| 1:B:206:ASN:C | 1:B:206:ASN:HD22 | 2.11 | 0.53 |
| 3:B:403:B12:H252 | 3:B:403:B12:H601 | 1.90 | 0.53 |
| 3:B:403:B12:H491 | 3:B:403:B12:H473 | 1.90 | 0.53 |
| 1:A:147:PHE:CE1 | 1:A:155:ILE:HB | 2.43 | 0.53 |
| 3:A:403:B12:O28 | 3:A:403:B12:H3 | 2.08 | 0.53 |
| 1:B:147:PHE:CE1 | 1:B:155:ILE:HB | 2.43 | 0.53 |
| 3:E:403:B12:N62 | 3:E:403:B12:H541 | 2.23 | 0.53 |
| 1:D:147:PHE:CE1 | 1:D:155:ILE:HB | 2.45 | 0.53 |
| 1:E:147:PHE:CE1 | 1:E:155:ILE:HB | 2.44 | 0.53 |
| 1:B:139:VAL:HG11 | 1:B:167:GLU:HG2 | 1.91 | 0.52 |
| 1:D:206:ASN:HD21 | 1:D:208:ARG:HB2 | 1.74 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:A:403:B12:H491 | 3:A:403:B12:H473 | 1.92 | 0.52 |
| 3:A:403:B12:C53 | 3:A:403:B12:H561 | 2.39 | 0.52 |
| 1:C:139:VAL:HG11 | 1:C:167:GLU:HG2 | 1.92 | 0.52 |
| 1:D:137:THR:HG21 | 3:D:403:B12:O8R | 2.09 | 0.52 |
| 1:D:217:ASP:O | 1:D:294:ARG:NH2 | 2.42 | 0.52 |
| 1:D:206:ASN:ND2 | 1:D:208:ARG:HB2 | 2.24 | 0.52 |
| 1:A:139:VAL:HG11 | 1:A:167:GLU:HG2 | 1.92 | 0.51 |
| 1:D:139:VAL:HG11 | 1:D:167:GLU:HG2 | 1.92 | 0.51 |
| 1:E:61:LEU:O | 1:E:62:GLU:CB | 2.59 | 0.51 |
| 1:E:10:MET:HA | 1:E:13:GLU:HB3 | 1.93 | 0.51 |
| 1:E:139:VAL:HG11 | 1:E:167:GLU:HG2 | 1.93 | 0.51 |
| 1:D:10:MET:HA | 1:D:13:GLU:HB3 | 1.93 | 0.51 |
| 1:C:10:MET:HA | 1:C:13:GLU:HB3 | 1.93 | 0.50 |
| 3:B:403:B12:H2R | 3:B:403:B12:H7B | 1.91 | 0.50 |
| 3:D:403:B12:H362 | 3:D:403:B12:C35 | 2.35 | 0.50 |
| 3:E:403:B12:O2 | 3:E:403:B12:C3P | 2.59 | 0.50 |
| 1:A:158:GLU:N | 1:A:158:GLU:OE1 | 2.43 | 0.50 |
| 1:E:31:GLU:CG | 1:E:55:ILE:HD13 | 2.41 | 0.50 |
| 1:A:61:LEU:O | 1:A:62:GLU:CB | 2.59 | 0.50 |
| 1:A:206:ASN:ND2 | 1:A:208:ARG:HB2 | 2.26 | 0.50 |
| 1:B:206:ASN:ND2 | 1:B:208:ARG:HB2 | 2.26 | 0.50 |
| 1:B:31:GLU:CG | 1:B:55:ILE:HD13 | 2.42 | 0.49 |
| 1:C:206:ASN:ND2 | 1:C:208:ARG:HB2 | 2.27 | 0.49 |
| 1:E:206:ASN:C | 1:E:206:ASN:HD22 | 2.16 | 0.49 |
| 1:B:245:TYR:O | 1:B:249:ILE:HD11 | 2.12 | 0.49 |
| 1:C:245:TYR:O | 1:C:249:ILE:HD11 | 2.12 | 0.49 |
| 1:C:89:ARG:NH1 | 1:C:260:ASP:OD1 | 2.45 | 0.49 |
| 1:D:31:GLU:CG | 1:D:55:ILE:HD13 | 2.43 | 0.49 |
| 1:E:245:TYR:O | 1:E:249:ILE:HD11 | 2.13 | 0.49 |
| 1:D:89:ARG:NH1 | 1:D:258:ASP:OD1 | 2.46 | 0.49 |
| 1:E:236:CYS:HB3 | 2:E:402:SF4:S4 | 2.52 | 0.49 |
| 1:C:206:ASN:HD21 | 1:C:208:ARG:HB2 | 1.77 | 0.49 |
| 1:D:245:TYR:O | 1:D:249:ILE:HD11 | 2.13 | 0.49 |
| 1:A:245:TYR:O | 1:A:249:ILE:HD11 | 2.12 | 0.49 |
| 1:B:10:MET:HA | 1:B:13:GLU:HB3 | 1.94 | 0.49 |
| 1:C:31:GLU:CG | 1:C:55:ILE:HD13 | 2.42 | 0.48 |
| 1:A:206:ASN:HD21 | 1:A:208:ARG:HB2 | 1.78 | 0.48 |
| 1:A:31:GLU:CG | 1:A:55:ILE:HD13 | 2.43 | 0.48 |
| 3:B:403:B12:H362 | 3:B:403:B12:C35 | 2.37 | 0.48 |
| 1:C:85:THR:HG22 | 1:C:86:GLU:N | 2.28 | 0.48 |
| 1:A:3:ILE:HD12 | 1:A:4:LYS:H | 1.78 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:66:THR:HG23 | 1:B:170:THR:HG23 | 1.95 | 0.48 |
| 1:B:85:THR:HG22 | 1:B:86:GLU:N | 2.28 | 0.48 |
| 1:A:10:MET:HA | 1:A:13:GLU:HB3 | 1.95 | 0.48 |
| 1:E:206:ASN:HD21 | 1:E:208:ARG:HB2 | 1.78 | 0.48 |
| 1:A:66:THR:HG23 | 1:A:170:THR:HG23 | 1.96 | 0.48 |
| 1:A:85:THR:HG22 | 1:A:86:GLU:N | 2.28 | 0.48 |
| 3:A:403:B12:H481 | 3:A:403:B12:H533 | 1.96 | 0.47 |
| 1:D:250:ASP:C | 1:D:250:ASP:OD1 | 2.52 | 0.47 |
| 1:E:158:GLU:N | 1:E:158:GLU:OE1 | 2.43 | 0.47 |
| 1:E:85:THR:HG22 | 1:E:86:GLU:N | 2.29 | 0.47 |
| 1:B:250:ASP:OD1 | 1:B:250:ASP:C | 2.52 | 0.47 |
| 1:D:236:CYS:HB3 | 2:D:402:SF4:S4 | 2.53 | 0.47 |
| 1:D:85:THR:HG22 | 1:D:86:GLU:N | 2.29 | 0.47 |
| 1:A:54:ARG:HH12 | 3:A:403:B12:C57 | 2.25 | 0.47 |
| 1:E:206:ASN:ND2 | 1:E:208:ARG:HB2 | 2.28 | 0.47 |
| 1:E:66:THR:HG23 | 1:E:170:THR:HG23 | 1.95 | 0.47 |
| 1:A:89:ARG:NH1 | 1:A:258:ASP:OD1 | 2.48 | 0.47 |
| 1:E:294:ARG:CG | 1:E:294:ARG:HH11 | 2.26 | 0.47 |
| 3:E:403:B12:H421 | 3:E:403:B12:C10 | 2.45 | 0.47 |
| 1:A:94:PRO:HA | 1:A:97:TRP:CD2 | 2.50 | 0.47 |
| 1:C:296:ARG:HH11 | 1:C:296:ARG:CG | 2.27 | 0.47 |
| 1:E:250:ASP:C | 1:E:250:ASP:OD1 | 2.52 | 0.47 |
| 1:B:206:ASN:HD21 | 1:B:208:ARG:HB2 | 1.79 | 0.47 |
| 1:C:158:GLU:N | 1:C:158:GLU:OE1 | 2.42 | 0.47 |
| 1:E:89:ARG:NH1 | 1:E:258:ASP:OD1 | 2.48 | 0.47 |
| 1:A:250:ASP:C | 1:A:250:ASP:OD1 | 2.53 | 0.47 |
| 3:E:403:B12:H91 | 3:E:403:B12:H262 | 1.77 | 0.47 |
| 1:B:89:ARG:NH1 | 1:B:258:ASP:OD1 | 2.49 | 0.46 |
| 1:B:31:GLU:HG2 | 1:B:55:ILE:HD13 | 1.98 | 0.46 |
| 1:D:66:THR:HG23 | 1:D:170:THR:HG23 | 1.96 | 0.46 |
| 1:A:198:CYS:SG | 2:A:402:SF4:S2 | 3.13 | 0.46 |
| 1:B:158:GLU:OE1 | 1:B:158:GLU:N | 2.45 | 0.46 |
| 3:C:403:B12:H552 | 3:C:403:B12:H531 | 1.98 | 0.46 |
| 1:C:66:THR:HG23 | 1:C:170:THR:HG23 | 1.96 | 0.46 |
| 3:E:403:B12:C25 | 3:E:403:B12:H312 | 2.46 | 0.46 |
| 1:E:3:ILE:HD12 | 1:E:4:LYS:H | 1.79 | 0.46 |
| 1:B:61:LEU:O | 1:B:62:GLU:CB | 2.64 | 0.46 |
| 1:D:3:ILE:HD12 | 1:D:4:LYS:H | 1.79 | 0.46 |
| 1:D:158:GLU:N | 1:D:158:GLU:OE1 | 2.43 | 0.46 |
| 1:E:237:ASP:HA | 4:E:510:HOH:O | 2.16 | 0.46 |
| 3:D:403:B12:H8 | 3:D:403:B12:O39 | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------|--------|--------------------------|-------------------|
| 1:E:31:GLU:HG2 | 1:E:55:ILE:HD13 | 1.98 | 0.46 |
| 1:C:206:ASN:C | 1:C:206:ASN:HD22 | 2.18 | 0.46 |
| 1:D:178:GLN:O | 1:D:179:GLU:HB2 | 2.16 | 0.46 |
| 1:B:3:ILE:HD12 | 1:B:4:LYS:H | 1.81 | 0.46 |
| 1:D:94:PRO:HA | 1:D:97:TRP:CD2 | 2.51 | 0.46 |
| 1:C:250:ASP:C | 1:C:250:ASP:OD1 | 2.54 | 0.45 |
| 1:C:141:LYS:HZ2 | 3:C:403:B12:H4B | 1.75 | 0.45 |
| 3:C:403:B12:O28 | 3:C:403:B12:H3 | 2.16 | 0.45 |
| 3:B:403:B12:C2R | 3:B:403:B12:H7B | 2.47 | 0.45 |
| 1:B:148:ILE:HD12 | 3:B:403:B12:C2B | 2.38 | 0.45 |
| 1:C:251:ASN:HB3 | 1:C:252:PRO:CD | 2.47 | 0.45 |
| 1:C:31:GLU:HG2 | 1:C:55:ILE:HD13 | 1.99 | 0.45 |
| 1:B:240:GLN:NE2 | 4:B:503:HOH:O | 2.41 | 0.45 |
| 3:E:403:B12:H251 | 3:E:403:B12:H312 | 1.98 | 0.45 |
| 1:D:294:ARG:HH11 | 1:D:294:ARG:CG | 2.28 | 0.45 |
| 1:E:94:PRO:HA | 1:E:97:TRP:CD2 | 2.52 | 0.45 |
| 1:D:251:ASN:HB3 | 1:D:252:PRO:CD | 2.47 | 0.45 |
| 1:A:99:LEU:HD23 | 1:A:103:TYR:HD2 | 1.82 | 0.45 |
| 1:E:99:LEU:HD23 | 1:E:103:TYR:HD2 | 1.82 | 0.44 |
| 1:E:178:GLN:O | 1:E:179:GLU:HB2 | 2.18 | 0.44 |
| 3:A:403:B12:H301 | 3:A:403:B12:H253 | 1.84 | 0.44 |
| 3:A:403:B12:N23 | 3:A:403:B12:H492 | 2.33 | 0.44 |
| 1:D:31:GLU:HG2 | 1:D:55:ILE:HD13 | 2.00 | 0.44 |
| 1:E:251:ASN:HB3 | 1:E:252:PRO:CD | 2.48 | 0.44 |
| 1:A:31:GLU:HG2 | 1:A:55:ILE:HD13 | 2.00 | 0.44 |
| 3:B:403:B12:H301 | 3:B:403:B12:H253 | 1.76 | 0.44 |
| 1:C:178:GLN:O | 1:C:179:GLU:HB2 | 2.18 | 0.44 |
| 1:C:92:ILE:CG2 | 1:C:262:ALA:O | 2.66 | 0.44 |
| 1:A:234:TYR:CZ | 1:A:284:GLY:HA2 | 2.53 | 0.44 |
| 1:B:99:LEU:HD23 | 1:B:103:TYR:HD2 | 1.83 | 0.44 |
| 1:C:200:ILE:HB | 1:C:204:THR:HG22 | 2.00 | 0.43 |
| 3:C:403:B12:H531 | 3:C:403:B12:C55 | 2.48 | 0.43 |
| 1:B:94:PRO:HA | 1:B:97:TRP:CD2 | 2.53 | 0.43 |
| 1:C:191:LEU:HD21 | 1:C:201:GLY:HA2 | 2.00 | 0.43 |
| 1:B:130:ASP:HA | 3:B:403:B12:H602 | 2.01 | 0.43 |
| 1:B:178:GLN:O | 1:B:179:GLU:HB2 | 2.18 | 0.43 |
| 1:B:92:ILE:CG2 | 1:B:260:ALA:O | 2.66 | 0.43 |
| 1:A:206:ASN:ND2 | 1:A:206:ASN:C | 2.71 | 0.43 |
| 1:C:94:PRO:HA | 1:C:97:TRP:CD2 | 2.54 | 0.43 |
| 1:D:61:LEU:O | 1:D:62:GLU:CB | 2.67 | 0.43 |
| 1:A:54:ARG:HD2 | 1:A:133:ALA:O | 2.19 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:178:GLN:O | 1:A:179:GLU:HB2 | 2.18 | 0.43 |
| 1:C:92:ILE:HD13 | 1:C:92:ILE:HG21 | 1.75 | 0.43 |
| 3:E:403:B12:H541 | 3:E:403:B12:C61 | 2.49 | 0.43 |
| 1:A:200:ILE:HB | 1:A:204:THR:HG22 | 2.00 | 0.42 |
| 1:A:251:ASN:HB3 | 1:A:252:PRO:CD | 2.49 | 0.42 |
| 1:B:251:ASN:HB3 | 1:B:252:PRO:CD | 2.49 | 0.42 |
| 3:D:403:B12:C55 | 3:D:403:B12:C53 | 2.95 | 0.42 |
| 1:E:191:LEU:HD21 | 1:E:201:GLY:HA2 | 2.00 | 0.42 |
| 3:E:403:B12:H543 | 3:E:403:B12:H531 | 2.01 | 0.42 |
| 3:B:403:B12:H552 | 3:B:403:B12:H531 | 2.01 | 0.42 |
| 1:E:130:ASP:OD1 | 3:E:403:B12:H542 | 2.20 | 0.42 |
| 1:B:234:TYR:CZ | 1:B:284:GLY:HA2 | 2.54 | 0.42 |
| 1:D:92:ILE:CG2 | 1:D:260:ALA:O | 2.67 | 0.42 |
| 1:D:191:LEU:HD21 | 1:D:201:GLY:HA2 | 2.01 | 0.42 |
| 1:A:191:LEU:HD21 | 1:A:201:GLY:HA2 | 2.02 | 0.42 |
| 1:B:294:ARG:CG | 1:B:294:ARG:HH11 | 2.30 | 0.42 |
| 3:D:403:B12:H91 | 3:D:403:B12:H262 | 1.83 | 0.42 |
| 1:C:244:PRO:O | 1:C:247:ARG:HB2 | 2.20 | 0.42 |
| 1:E:92:ILE:CG2 | 1:E:260:ALA:O | 2.68 | 0.42 |
| 1:A:294:ARG:CG | 1:A:294:ARG:HH11 | 2.27 | 0.42 |
| 1:A:40:GLU:OE1 | 1:A:42:ARG:NH1 | 2.53 | 0.42 |
| 1:E:195:PRO:HG3 | 1:E:238:ILE:HD13 | 2.02 | 0.42 |
| 1:C:54:ARG:HD2 | 1:C:133:ALA:O | 2.20 | 0.42 |
| 1:B:200:ILE:HB | 1:B:204:THR:HG22 | 2.01 | 0.41 |
| 1:C:99:LEU:HD23 | 1:C:103:TYR:HD2 | 1.84 | 0.41 |
| 1:E:40:GLU:OE1 | 1:E:42:ARG:NH1 | 2.50 | 0.41 |
| 3:A:403:B12:H551 | 3:A:403:B12:C61 | 2.51 | 0.41 |
| 1:A:55:ILE:O | 1:A:57:PRO:HD3 | 2.20 | 0.41 |
| 1:A:92:ILE:HD11 | 1:A:96:SER:HB3 | 2.02 | 0.41 |
| 3:B:403:B12:C61 | 3:B:403:B12:H551 | 2.50 | 0.41 |
| 1:D:99:LEU:HD23 | 1:D:103:TYR:HD2 | 1.83 | 0.41 |
| 1:D:180:VAL:HG13 | 1:D:182:TYR:CD1 | 2.55 | 0.41 |
| 1:D:200:ILE:HB | 1:D:204:THR:HG22 | 2.02 | 0.41 |
| 3:D:403:B12:O63 | 3:D:403:B12:H551 | 2.20 | 0.41 |
| 1:E:31:GLU:HG3 | 1:E:55:ILE:HD13 | 2.02 | 0.41 |
| 1:B:54:ARG:HD2 | 1:B:133:ALA:O | 2.19 | 0.41 |
| 3:D:403:B12:H351 | 3:D:403:B12:C36 | 2.37 | 0.41 |
| 3:B:403:B12:H91 | 3:B:403:B12:H262 | 1.72 | 0.41 |
| 1:C:180:VAL:HG13 | 1:C:182:TYR:CD1 | 2.55 | 0.41 |
| 3:D:403:B12:H301 | 3:D:403:B12:H253 | 1.93 | 0.41 |
| 1:E:54:ARG:HD2 | 1:E:133:ALA:O | 2.19 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:55:ILE:O | 1:C:57:PRO:HD3 | 2.21 | 0.41 |
| 1:E:244:PRO:O | 1:E:247:ARG:HB2 | 2.20 | 0.41 |
| 1:B:135:VAL:HG12 | 1:B:137:THR:HG22 | 2.03 | 0.41 |
| 1:B:191:LEU:HD21 | 1:B:201:GLY:HA2 | 2.03 | 0.41 |
| 1:A:92:ILE:HG23 | 1:A:260:ALA:O | 2.21 | 0.41 |
| 1:E:236:CYS:O | 3:E:403:B12:O39 | 2.39 | 0.41 |
| 1:A:30:LEU:O | 1:A:31:GLU:C | 2.59 | 0.41 |
| 1:D:198:CYS:SG | 2:D:402:SF4:S2 | 3.18 | 0.41 |
| 1:E:55:ILE:O | 1:E:57:PRO:HD3 | 2.21 | 0.41 |
| 1:A:141:LYS:HZ3 | 3:A:403:B12:H4B | 1.81 | 0.41 |
| 1:A:97:TRP:HB3 | 1:A:255:ILE:HD12 | 2.03 | 0.41 |
| 1:D:135:VAL:HG12 | 1:D:137:THR:HG22 | 2.03 | 0.41 |
| 1:D:244:PRO:O | 1:D:247:ARG:HB2 | 2.21 | 0.41 |
| 1:D:40:GLU:OE1 | 1:D:42:ARG:NH1 | 2.51 | 0.41 |
| 1:D:54:ARG:HD2 | 1:D:133:ALA:O | 2.21 | 0.41 |
| 1:E:135:VAL:HG12 | 1:E:137:THR:HG22 | 2.03 | 0.40 |
| 1:A:135:VAL:HG12 | 1:A:137:THR:HG22 | 2.03 | 0.40 |
| 1:D:55:ILE:O | 1:D:57:PRO:HD3 | 2.21 | 0.40 |
| 1:D:92:ILE:HG21 | 1:D:92:ILE:HD13 | 1.75 | 0.40 |
| 1:E:99:LEU:HD23 | 1:E:103:TYR:CD2 | 2.56 | 0.40 |
| 1:A:195:PRO:HG3 | 1:A:238:ILE:HD13 | 2.04 | 0.40 |
| 1:C:31:GLU:HG3 | 1:C:55:ILE:HD13 | 2.03 | 0.40 |
| 3:B:403:B12:C7B | 3:B:403:B12:H2R | 2.51 | 0.40 |
| 1:D:178:GLN:O | 1:D:179:GLU:CB | 2.69 | 0.40 |
| 1:D:195:PRO:HG3 | 1:D:238:ILE:HD13 | 2.04 | 0.40 |
| 3:D:403:B12:C2B | 3:D:403:B12:O7R | 2.69 | 0.40 |
| 1:D:31:GLU:HG3 | 1:D:55:ILE:HD13 | 2.03 | 0.40 |
| 1:B:31:GLU:HG3 | 1:B:55:ILE:HD13 | 2.03 | 0.40 |

There are no symmetry-related clashes.

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|----------|----------|---------|----------|------|------|
| 1 | A | 366/399 (92%) | 339 (93%) | 24 (7%) | 3 (1%) | 19 | 29 |
| 1 | B | 366/399 (92%) | 341 (93%) | 21 (6%) | 4 (1%) | 14 | 21 |
| 1 | C | 363/399 (91%) | 335 (92%) | 25 (7%) | 3 (1%) | 19 | 29 |
| 1 | D | 366/399 (92%) | 340 (93%) | 22 (6%) | 4 (1%) | 14 | 21 |
| 1 | E | 366/399 (92%) | 339 (93%) | 24 (7%) | 3 (1%) | 19 | 29 |
| All | All | 1827/1995 (92%) | 1694 (93%) | 116 (6%) | 17 (1%) | 17 | 26 |

All (17) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 62 | GLU |
| 1 | A | 179 | GLU |
| 1 | B | 62 | GLU |
| 1 | B | 179 | GLU |
| 1 | B | 252 | PRO |
| 1 | C | 62 | GLU |
| 1 | C | 179 | GLU |
| 1 | C | 252 | PRO |
| 1 | D | 62 | GLU |
| 1 | D | 179 | GLU |
| 1 | D | 252 | PRO |
| 1 | E | 62 | GLU |
| 1 | E | 179 | GLU |
| 1 | E | 252 | PRO |
| 1 | A | 252 | PRO |
| 1 | D | 208 | ARG |
| 1 | B | 208 | ARG |

### 5.3.2 Protein sidechains (i)

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 | 314/342 (92%) | 294 (94%) | 20 (6%) | 17 | 27 |
| 1 | B | 314/342 (92%) | 293 (93%) | 21 (7%) | 16 | 25 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------|-----------|----------|-------------|---|
| 1 | C | 311/342 (91%) | 291 (94%) | 20 (6%) | 17 | 27 |
| 1 | D | 314/342 (92%) | 294 (94%) | 20 (6%) | 17 | 27 |
| 1 | E | 314/342 (92%) | 291 (93%) | 23 (7%) | 14 | 21 |
| All | All | 1567/1710 (92%) | 1463 (93%) | 104 (7%) | 16 | 25 |

All (104) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 3 | ILE |
| 1 | A | 12 | LYS |
| 1 | A | 18 | LYS |
| 1 | A | 28 | ASP |
| 1 | A | 31 | GLU |
| 1 | A | 54 | ARG |
| 1 | A | 55 | ILE |
| 1 | A | 80 | GLN |
| 1 | A | 92 | ILE |
| 1 | A | 111 | ARG |
| 1 | A | 137 | THR |
| 1 | A | 204 | THR |
| 1 | A | 206 | ASN |
| 1 | A | 208 | ARG |
| 1 | A | 250 | ASP |
| 1 | A | 281 | MET |
| 1 | A | 294 | ARG |
| 1 | A | 310 | VAL |
| 1 | A | 334 | GLU |
| 1 | A | 369 | GLN |
| 1 | B | 3 | ILE |
| 1 | B | 12 | LYS |
| 1 | B | 18 | LYS |
| 1 | B | 28 | ASP |
| 1 | B | 31 | GLU |
| 1 | B | 54 | ARG |
| 1 | B | 55 | ILE |
| 1 | B | 80 | GLN |
| 1 | B | 92 | ILE |
| 1 | B | 111 | ARG |
| 1 | B | 137 | THR |
| 1 | B | 155 | ILE |
| 1 | B | 204 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 206 | ASN |
| 1 | B | 208 | ARG |
| 1 | B | 250 | ASP |
| 1 | B | 281 | MET |
| 1 | B | 294 | ARG |
| 1 | B | 310 | VAL |
| 1 | B | 334 | GLU |
| 1 | B | 369 | GLN |
| 1 | C | 12 | LYS |
| 1 | C | 18 | LYS |
| 1 | C | 28 | ASP |
| 1 | C | 31 | GLU |
| 1 | C | 54 | ARG |
| 1 | C | 55 | ILE |
| 1 | C | 80 | GLN |
| 1 | C | 92 | ILE |
| 1 | C | 111 | ARG |
| 1 | C | 137 | THR |
| 1 | C | 155 | ILE |
| 1 | C | 204 | THR |
| 1 | C | 206 | ASN |
| 1 | C | 208 | ARG |
| 1 | C | 250 | ASP |
| 1 | C | 283 | MET |
| 1 | C | 296 | ARG |
| 1 | C | 312 | VAL |
| 1 | C | 336 | GLU |
| 1 | C | 371 | GLN |
| 1 | D | 3 | ILE |
| 1 | D | 12 | LYS |
| 1 | D | 18 | LYS |
| 1 | D | 28 | ASP |
| 1 | D | 31 | GLU |
| 1 | D | 54 | ARG |
| 1 | D | 80 | GLN |
| 1 | D | 92 | ILE |
| 1 | D | 111 | ARG |
| 1 | D | 137 | THR |
| 1 | D | 155 | ILE |
| 1 | D | 204 | THR |
| 1 | D | 206 | ASN |
| 1 | D | 208 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 250 | ASP |
| 1 | D | 281 | MET |
| 1 | D | 294 | ARG |
| 1 | D | 310 | VAL |
| 1 | D | 334 | GLU |
| 1 | D | 369 | GLN |
| 1 | E | 3 | ILE |
| 1 | E | 12 | LYS |
| 1 | E | 18 | LYS |
| 1 | E | 22 | THR |
| 1 | E | 28 | ASP |
| 1 | E | 31 | GLU |
| 1 | E | 54 | ARG |
| 1 | E | 55 | ILE |
| 1 | E | 80 | GLN |
| 1 | E | 92 | ILE |
| 1 | E | 111 | ARG |
| 1 | E | 137 | THR |
| 1 | E | 155 | ILE |
| 1 | E | 195 | PRO |
| 1 | E | 204 | THR |
| 1 | E | 206 | ASN |
| 1 | E | 208 | ARG |
| 1 | E | 250 | ASP |
| 1 | E | 281 | MET |
| 1 | E | 294 | ARG |
| 1 | E | 310 | VAL |
| 1 | E | 334 | GLU |
| 1 | E | 369 | GLN |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 48 | HIS |
| 1 | A | 80 | GLN |
| 1 | A | 178 | GLN |
| 1 | A | 206 | ASN |
| 1 | B | 48 | HIS |
| 1 | B | 80 | GLN |
| 1 | B | 178 | GLN |
| 1 | B | 206 | ASN |
| 1 | C | 48 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 80 | GLN |
| 1 | C | 178 | GLN |
| 1 | C | 206 | ASN |
| 1 | D | 48 | HIS |
| 1 | D | 80 | GLN |
| 1 | D | 178 | GLN |
| 1 | D | 206 | ASN |
| 1 | E | 80 | GLN |
| 1 | E | 178 | GLN |
| 1 | E | 206 | ASN |

### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry (i)

15 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------|------|-----------|--------|------|-----------|
| | | | | | Counts | RMSZ | #$|Z| > 2$ | Counts | RMSZ | #$|Z| > 2$ |
| 3 | B12 | C | 403 | - | 80,101,101 | 1.00 | 3 (3%) | 101,166,166 | 1.19 | 12 (11%) |
| 2 | SF4 | B | 402 | 1 | 0,12,12 | 0.00 | - | - | - | |
| 2 | SF4 | D | 402 | 1 | 0,12,12 | 0.00 | - | - | - | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------|------|-----------|--------|------|-----------|
| | | | | | Counts | RMSZ | #\|Z\| > 2 | Counts | RMSZ | #\|Z\| > 2 |
| 3 | B12 | A | 403 | 4 | 80,101,101 | 0.96 | 5 (6%) | 101,166,166 | 1.35 | 19 (18%) |
| 2 | SF4 | E | 402 | 1 | 0,12,12 | 0.00 | - | - | | |
| 2 | SF4 | C | 401 | 1 | 0,12,12 | 0.00 | - | - | | |
| 2 | SF4 | A | 402 | 1 | 0,12,12 | 0.00 | - | - | | |
| 2 | SF4 | C | 402 | 1 | 0,12,12 | 0.00 | - | - | | |
| 2 | SF4 | E | 401 | 1 | 0,12,12 | 0.00 | - | - | | |
| 2 | SF4 | D | 401 | 1 | 0,12,12 | 0.00 | - | - | | |
| 2 | SF4 | A | 401 | 1 | 0,12,12 | 0.00 | - | - | | |
| 2 | SF4 | B | 401 | 1 | 0,12,12 | 0.00 | - | - | | |
| 3 | B12 | B | 403 | - | 80,101,101 | 1.30 | 3 (3%) | 101,166,166 | 1.31 | 16 (15%) |
| 3 | B12 | E | 403 | 4 | 80,101,101 | 0.72 | 2 (2%) | 101,166,166 | 1.31 | 13 (12%) |
| 3 | B12 | D | 403 | - | 80,101,101 | 1.02 | 3 (3%) | 101,166,166 | 1.36 | 13 (12%) |

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 |
|-----|------|-------|-----|------|---------|----------|-------|
| 3 | B12 | C | 403 | - | - | 13/51/223/223 | 0/3/11/11 |
| 2 | SF4 | B | 402 | 1 | - | - | 0/6/5/5 |
| 2 | SF4 | B | 401 | 1 | - | - | 0/6/5/5 |
| 2 | SF4 | D | 402 | 1 | - | - | 0/6/5/5 |
| 3 | B12 | A | 403 | 4 | - | 19/51/223/223 | 0/3/11/11 |
| 3 | B12 | B | 403 | - | - | 16/51/223/223 | 0/3/11/11 |
| 2 | SF4 | C | 401 | 1 | - | - | 0/6/5/5 |
| 2 | SF4 | A | 402 | 1 | - | - | 0/6/5/5 |
| 3 | B12 | D | 403 | - | - | 17/51/223/223 | 0/3/11/11 |
| 2 | SF4 | E | 401 | 1 | - | - | 0/6/5/5 |
| 2 | SF4 | D | 401 | 1 | - | - | 0/6/5/5 |
| 2 | SF4 | A | 401 | 1 | - | - | 0/6/5/5 |
| 2 | SF4 | E | 402 | 1 | - | - | 0/6/5/5 |
| 3 | B12 | E | 403 | 4 | - | 11/51/223/223 | 0/3/11/11 |
| 2 | SF4 | C | 402 | 1 | - | - | 0/6/5/5 |

All (16) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 3 | B | 403 | B12 | C2B-N3B | -8.73 | 1.19 | 1.34 |
| 3 | C | 403 | B12 | C2B-N3B | -6.84 | 1.22 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|---|-------------|----------|
| 3 | D | 403 | B12 | C2B-N3B | -5.89 | 1.24 | 1.34 |
| 3 | D | 403 | B12 | O3-C2P | -4.33 | 1.34 | 1.45 |
| 3 | A | 403 | B12 | C11-C10 | -4.30 | 1.33 | 1.40 |
| 3 | B | 403 | B12 | P-O3 | -4.24 | 1.49 | 1.60 |
| 3 | B | 403 | B12 | O3-C2P | -3.93 | 1.35 | 1.45 |
| 3 | E | 403 | B12 | C2B-N3B | -3.75 | 1.28 | 1.34 |
| 3 | A | 403 | B12 | P-O3 | -3.16 | 1.52 | 1.60 |
| 3 | A | 403 | B12 | O3-C2P | -3.14 | 1.37 | 1.45 |
| 3 | D | 403 | B12 | P-O3 | -3.01 | 1.52 | 1.60 |
| 3 | A | 403 | B12 | C2B-N3B | -2.98 | 1.29 | 1.34 |
| 3 | A | 403 | B12 | P-O2 | -2.73 | 1.53 | 1.60 |
| 3 | C | 403 | B12 | O3-C2P | -2.51 | 1.39 | 1.45 |
| 3 | E | 403 | B12 | O3-C2P | -2.16 | 1.39 | 1.45 |
| 3 | C | 403 | B12 | C4B-C9B | -2.02 | 1.38 | 1.41 |

All (73) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|-----|-------|-----|------|-------|---|----------------|-------------|
| 3 | D | 403 | B12 | C2P-C1P-N59 | -7.66 | 101.64 | 112.93 |
| 3 | E | 403 | B12 | C3P-C2P-C1P | -4.64 | 102.38 | 111.39 |
| 3 | E | 403 | B12 | C2P-C1P-N59 | -4.56 | 106.22 | 112.93 |
| 3 | B | 403 | B12 | C36-C7-C37 | 4.00 | 117.66 | 110.83 |
| 3 | B | 403 | B12 | C2P-C1P-N59 | -3.70 | 107.48 | 112.93 |
| 3 | C | 403 | B12 | C6-C5-C4 | -3.48 | 118.85 | 124.27 |
| 3 | B | 403 | B12 | C30-C3-C2 | -3.36 | 112.02 | 119.13 |
| 3 | B | 403 | B12 | C13-C14-C15 | -3.32 | 119.63 | 131.68 |
| 3 | D | 403 | B12 | P-O2-C3R | 3.23 | 131.15 | 119.41 |
| 3 | A | 403 | B12 | O2-P-O4 | 3.22 | 121.53 | 109.47 |
| 3 | E | 403 | B12 | C55-C56-C57 | -3.21 | 104.22 | 111.23 |
| 3 | E | 403 | B12 | C16-C15-C14 | -3.18 | 119.30 | 124.27 |
| 3 | A | 403 | B12 | C30-C3-C2 | -3.17 | 112.41 | 119.13 |
| 3 | B | 403 | B12 | P-O2-C3R | 3.07 | 130.58 | 119.41 |
| 3 | D | 403 | B12 | C13-C14-C15 | -3.03 | 120.71 | 131.68 |
| 3 | A | 403 | B12 | C15-C14-N23 | 3.01 | 129.73 | 124.64 |
| 3 | E | 403 | B12 | C6-C5-C4 | -3.00 | 119.59 | 124.27 |
| 3 | A | 403 | B12 | C56-C55-C17 | -2.98 | 109.74 | 115.50 |
| 3 | A | 403 | B12 | C13-C14-C15 | -2.96 | 120.94 | 131.68 |
| 3 | D | 403 | B12 | C55-C56-C57 | -2.92 | 104.87 | 111.23 |
| 3 | B | 403 | B12 | C15-C14-N23 | 2.90 | 129.54 | 124.64 |
| 3 | A | 403 | B12 | C19-C1-N21 | -2.87 | 99.23 | 102.16 |
| 3 | C | 403 | B12 | C36-C7-C37 | 2.82 | 115.64 | 110.83 |
| 3 | C | 403 | B12 | C55-C56-C57 | -2.79 | 105.14 | 111.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------|---|-------------|----------|
| 3 | A | 403 | B12 | C2P-C1P-N59 | -2.78 | 108.84 | 112.93 |
| 3 | A | 403 | B12 | O3-C2P-C1P | -2.74 | 101.44 | 106.92 |
| 3 | C | 403 | B12 | C13-C14-C15 | -2.73 | 121.76 | 131.68 |
| 3 | D | 403 | B12 | C54-C17-C55 | -2.72 | 104.77 | 109.26 |
| 3 | D | 403 | B12 | C56-C55-C17 | -2.71 | 110.27 | 115.50 |
| 3 | E | 403 | B12 | C15-C14-N23 | 2.65 | 129.12 | 124.64 |
| 3 | A | 403 | B12 | C26-C2-C3 | -2.62 | 102.66 | 107.47 |
| 3 | C | 403 | B12 | C1-C19-N24 | -2.58 | 103.34 | 106.24 |
| 3 | E | 403 | B12 | C30-C3-C2 | -2.56 | 113.71 | 119.13 |
| 3 | A | 403 | B12 | C55-C17-C18 | -2.55 | 106.21 | 111.14 |
| 3 | B | 403 | B12 | C55-C56-C57 | -2.52 | 105.72 | 111.23 |
| 3 | A | 403 | B12 | C20-C1-C2 | 2.50 | 117.46 | 113.32 |
| 3 | D | 403 | B12 | C26-C2-C3 | -2.49 | 102.89 | 107.47 |
| 3 | D | 403 | B12 | O5-P-O3 | 2.47 | 116.53 | 106.78 |
| 3 | A | 403 | B12 | C55-C17-C16 | 2.47 | 118.14 | 109.92 |
| 3 | A | 403 | B12 | C20-C1-C19 | -2.46 | 106.98 | 109.36 |
| 3 | C | 403 | B12 | O3-P-O4 | 2.44 | 118.61 | 109.47 |
| 3 | B | 403 | B12 | O2-C3R-C2R | -2.44 | 102.85 | 111.68 |
| 3 | C | 403 | B12 | O2-P-O4 | 2.43 | 118.58 | 109.47 |
| 3 | B | 403 | B12 | C55-C17-C18 | -2.43 | 106.45 | 111.14 |
| 3 | E | 403 | B12 | C13-C14-C15 | -2.40 | 122.96 | 131.68 |
| 3 | E | 403 | B12 | P-O2-C3R | 2.39 | 128.11 | 119.41 |
| 3 | C | 403 | B12 | C1-C19-C18 | -2.39 | 117.98 | 121.93 |
| 3 | A | 403 | B12 | C26-C2-C1 | 2.39 | 113.73 | 110.02 |
| 3 | D | 403 | B12 | O2-P-O4 | 2.38 | 118.38 | 109.47 |
| 3 | A | 403 | B12 | C6-C5-C4 | -2.36 | 120.59 | 124.27 |
| 3 | A | 403 | B12 | C16-C15-C14 | -2.34 | 120.61 | 124.27 |
| 3 | E | 403 | B12 | O3-P-O4 | 2.33 | 118.21 | 109.47 |
| 3 | B | 403 | B12 | C1-C19-C18 | -2.32 | 118.09 | 121.93 |
| 3 | A | 403 | B12 | C3-C4-C5 | -2.31 | 123.29 | 131.68 |
| 3 | C | 403 | B12 | C2P-C1P-N59 | -2.28 | 109.58 | 112.93 |
| 3 | E | 403 | B12 | C20-C1-C2 | 2.27 | 117.07 | 113.32 |
| 3 | C | 403 | B12 | C16-C15-C14 | -2.26 | 120.75 | 124.27 |
| 3 | D | 403 | B12 | C9-C10-C11 | -2.25 | 123.07 | 130.91 |
| 3 | A | 403 | B12 | C36-C7-C37 | 2.24 | 114.65 | 110.83 |
| 3 | B | 403 | B12 | C55-C17-C16 | 2.22 | 117.33 | 109.92 |
| 3 | B | 403 | B12 | O3-C2P-C1P | -2.17 | 102.58 | 106.92 |
| 3 | B | 403 | B12 | O5-P-O3 | 2.15 | 115.27 | 106.78 |
| 3 | C | 403 | B12 | C19-C1-N21 | -2.14 | 99.97 | 102.16 |
| 3 | E | 403 | B12 | O5-P-O2 | 2.13 | 115.18 | 106.78 |
| 3 | B | 403 | B12 | C60-C18-C17 | 2.13 | 120.88 | 115.74 |
| 3 | D | 403 | B12 | C5-C6-N22 | -2.07 | 121.04 | 124.81 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|-----|-------|-----|------|-------|---|----------------|-------------|
| 3 | B | 403 | B12 | C54-C17-C55 | -2.07 | 105.85 | 109.26 |
| 3 | C | 403 | B12 | C3-C4-C5 | -2.06 | 124.21 | 131.68 |
| 3 | E | 403 | B12 | C26-C2-C3 | -2.05 | 103.70 | 107.47 |
| 3 | B | 403 | B12 | O7R-C2R-C3R | -2.05 | 105.35 | 111.17 |
| 3 | D | 403 | B12 | C3-C4-C5 | -2.05 | 124.26 | 131.68 |
| 3 | A | 403 | B12 | C4B-C9B-C8B | -2.04 | 119.01 | 121.10 |
| 3 | D | 403 | B12 | C30-C3-C2 | -2.04 | 114.81 | 119.13 |

There are no chirality outliers.

All (76) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------|
| 3 | C | 403 | B12 | N59-C1P-C2P-C3P |
| 3 | C | 403 | B12 | N59-C1P-C2P-O3 |
| 3 | A | 403 | B12 | C2-C3-C30-C31 |
| 3 | A | 403 | B12 | C56-C57-N59-C1P |
| 3 | A | 403 | B12 | N59-C1P-C2P-C3P |
| 3 | A | 403 | B12 | N59-C1P-C2P-O3 |
| 3 | A | 403 | B12 | C3R-O2-P-O4 |
| 3 | A | 403 | B12 | C3R-O2-P-O5 |
| 3 | B | 403 | B12 | N59-C1P-C2P-C3P |
| 3 | B | 403 | B12 | N59-C1P-C2P-O3 |
| 3 | B | 403 | B12 | C1P-C2P-O3-P |
| 3 | B | 403 | B12 | C3P-C2P-O3-P |
| 3 | B | 403 | B12 | C3R-O2-P-O5 |
| 3 | E | 403 | B12 | C56-C57-N59-C1P |
| 3 | E | 403 | B12 | N59-C1P-C2P-C3P |
| 3 | E | 403 | B12 | N59-C1P-C2P-O3 |
| 3 | E | 403 | B12 | C3P-C2P-O3-P |
| 3 | E | 403 | B12 | C3R-O2-P-O5 |
| 3 | D | 403 | B12 | C56-C57-N59-C1P |
| 3 | D | 403 | B12 | N59-C1P-C2P-O3 |
| 3 | D | 403 | B12 | C2P-O3-P-O5 |
| 3 | A | 403 | B12 | O58-C57-N59-C1P |
| 3 | E | 403 | B12 | O58-C57-N59-C1P |
| 3 | D | 403 | B12 | O58-C57-N59-C1P |
| 3 | E | 403 | B12 | C3R-C4R-C5R-O8R |
| 3 | E | 403 | B12 | O6R-C4R-C5R-O8R |
| 3 | C | 403 | B12 | C2P-O3-P-O2 |
| 3 | D | 403 | B12 | C3R-O2-P-O3 |
| 3 | B | 403 | B12 | C56-C57-N59-C1P |
| 3 | A | 403 | B12 | C3R-C4R-C5R-O8R |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------|
| 3 | A | 403 | B12 | C42-C41-C8-C7 |
| 3 | B | 403 | B12 | C2-C3-C30-C31 |
| 3 | D | 403 | B12 | C2-C3-C30-C31 |
| 3 | C | 403 | B12 | C3R-O2-P-O3 |
| 3 | A | 403 | B12 | C3R-O2-P-O3 |
| 3 | E | 403 | B12 | C3R-O2-P-O3 |
| 3 | D | 403 | B12 | C2P-O3-P-O2 |
| 3 | B | 403 | B12 | C3-C2-C26-C27 |
| 3 | E | 403 | B12 | C17-C18-C60-C61 |
| 3 | D | 403 | B12 | C3R-C4R-C5R-O8R |
| 3 | B | 403 | B12 | O58-C57-N59-C1P |
| 3 | A | 403 | B12 | O6R-C4R-C5R-O8R |
| 3 | D | 403 | B12 | O6R-C4R-C5R-O8R |
| 3 | C | 403 | B12 | C12-C13-C48-C49 |
| 3 | B | 403 | B12 | C3R-O2-P-O3 |
| 3 | C | 403 | B12 | C56-C57-N59-C1P |
| 3 | A | 403 | B12 | C8-C41-C42-C43 |
| 3 | C | 403 | B12 | O58-C57-N59-C1P |
| 3 | A | 403 | B12 | C12-C13-C48-C49 |
| 3 | C | 403 | B12 | C2P-O3-P-O4 |
| 3 | C | 403 | B12 | C3R-O2-P-O4 |
| 3 | C | 403 | B12 | C3R-O2-P-O5 |
| 3 | B | 403 | B12 | C3R-O2-P-O4 |
| 3 | E | 403 | B12 | C3R-O2-P-O4 |
| 3 | D | 403 | B12 | C2P-O3-P-O4 |
| 3 | D | 403 | B12 | C3R-O2-P-O4 |
| 3 | C | 403 | B12 | C1P-C2P-O3-P |
| 3 | B | 403 | B12 | C25-C2-C26-C27 |
| 3 | B | 403 | B12 | C7-C37-C38-N40 |
| 3 | A | 403 | B12 | C42-C41-C8-C9 |
| 3 | A | 403 | B12 | C2P-O3-P-O2 |
| 3 | A | 403 | B12 | C2P-C1P-N59-C57 |
| 3 | D | 403 | B12 | N59-C1P-C2P-C3P |
| 3 | A | 403 | B12 | C3-C30-C31-C32 |
| 3 | B | 403 | B12 | C7-C37-C38-O39 |
| 3 | D | 403 | B12 | C3R-O2-P-O5 |
| 3 | C | 403 | B12 | C2P-C1P-N59-C57 |
| 3 | C | 403 | B12 | C3P-C2P-O3-P |
| 3 | D | 403 | B12 | C1P-C2P-O3-P |
| 3 | B | 403 | B12 | C12-C13-C48-C49 |
| 3 | D | 403 | B12 | C12-C13-C48-C49 |
| 3 | D | 403 | B12 | C8-C41-C42-C43 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------|
| 3 | A | 403 | B12 | C4-C3-C30-C31 |
| 3 | B | 403 | B12 | C4-C3-C30-C31 |
| 3 | D | 403 | B12 | C4-C3-C30-C31 |
| 3 | A | 403 | B12 | C1P-C2P-O3-P |

There are no ring outliers.

9 monomers are involved in 102 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3 | C | 403 | B12 | 15 | 0 |
| 2 | B | 402 | SF4 | 1 | 0 |
| 2 | D | 402 | SF4 | 2 | 0 |
| 3 | A | 403 | B12 | 23 | 0 |
| 2 | E | 402 | SF4 | 1 | 0 |
| 2 | A | 402 | SF4 | 1 | 0 |
| 3 | B | 403 | B12 | 21 | 0 |
| 3 | E | 403 | B12 | 22 | 0 |
| 3 | D | 403 | B12 | 16 | 0 |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

## Ligand B12 C 403


Bond lengths


Bond angles


Torsions


Rings

## Ligand B12 A 403


Bond lengths


Bond angles


Torsions


Rings

## Ligand B12 B 403



Bond lengths



Bond angles



Torsions



Rings

## Ligand B12 E 403



Bond lengths



Bond angles



Torsions



Rings

**Ligand B12 D 403**


Bond lengths


Bond angles


Torsions


Rings
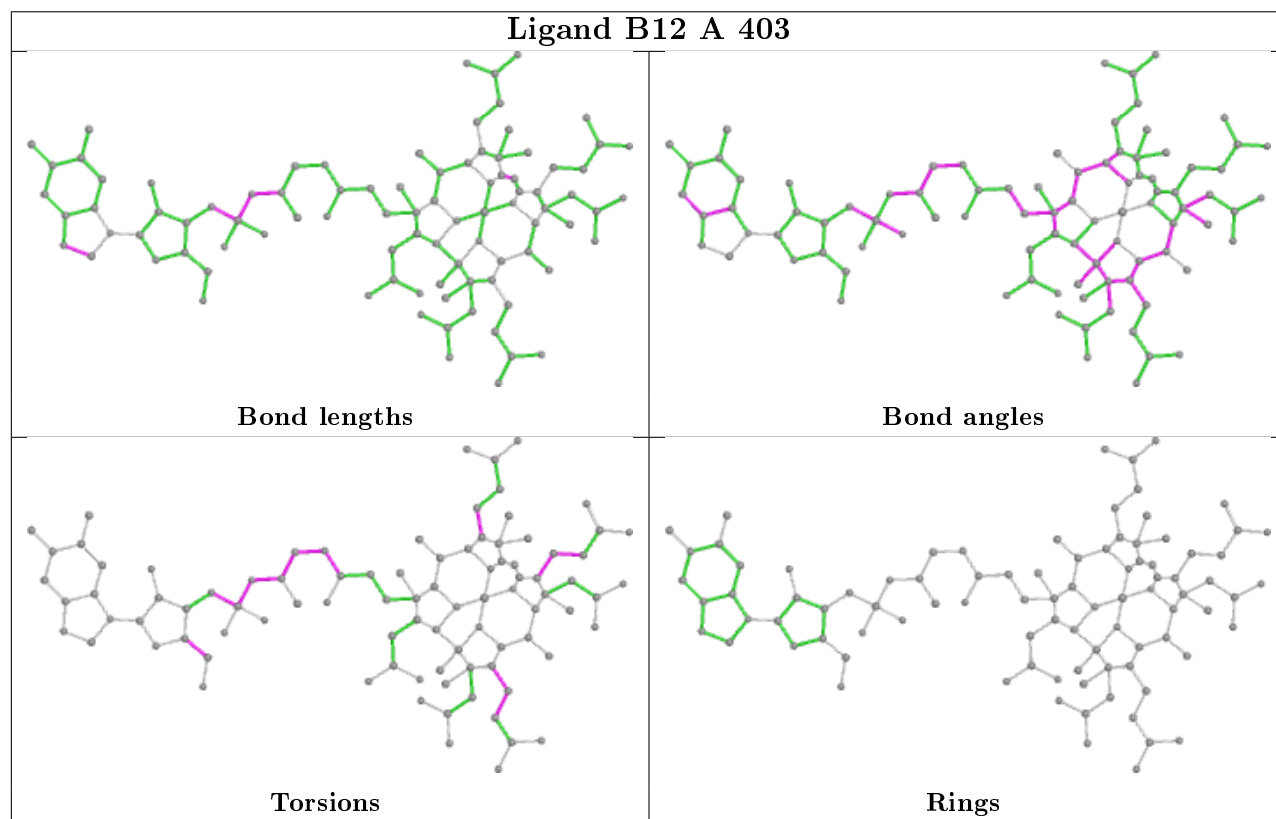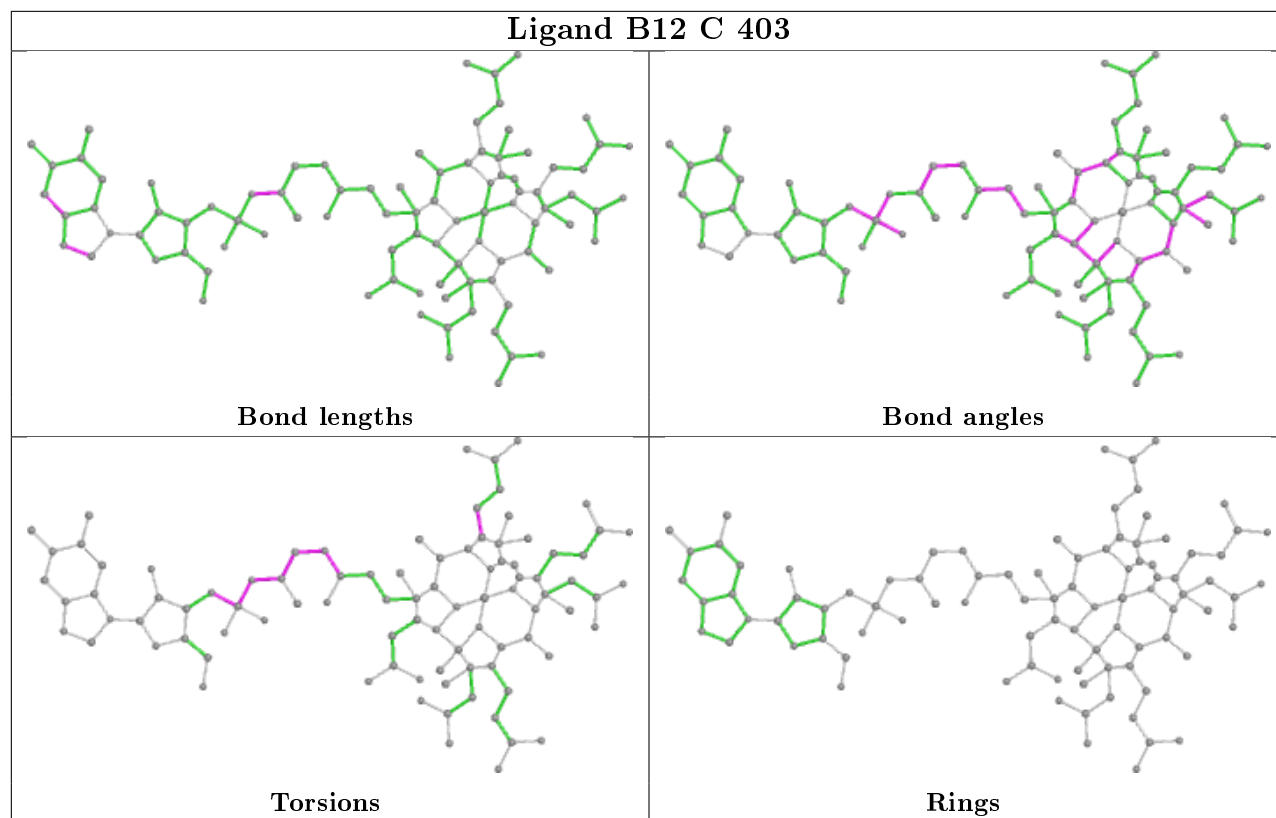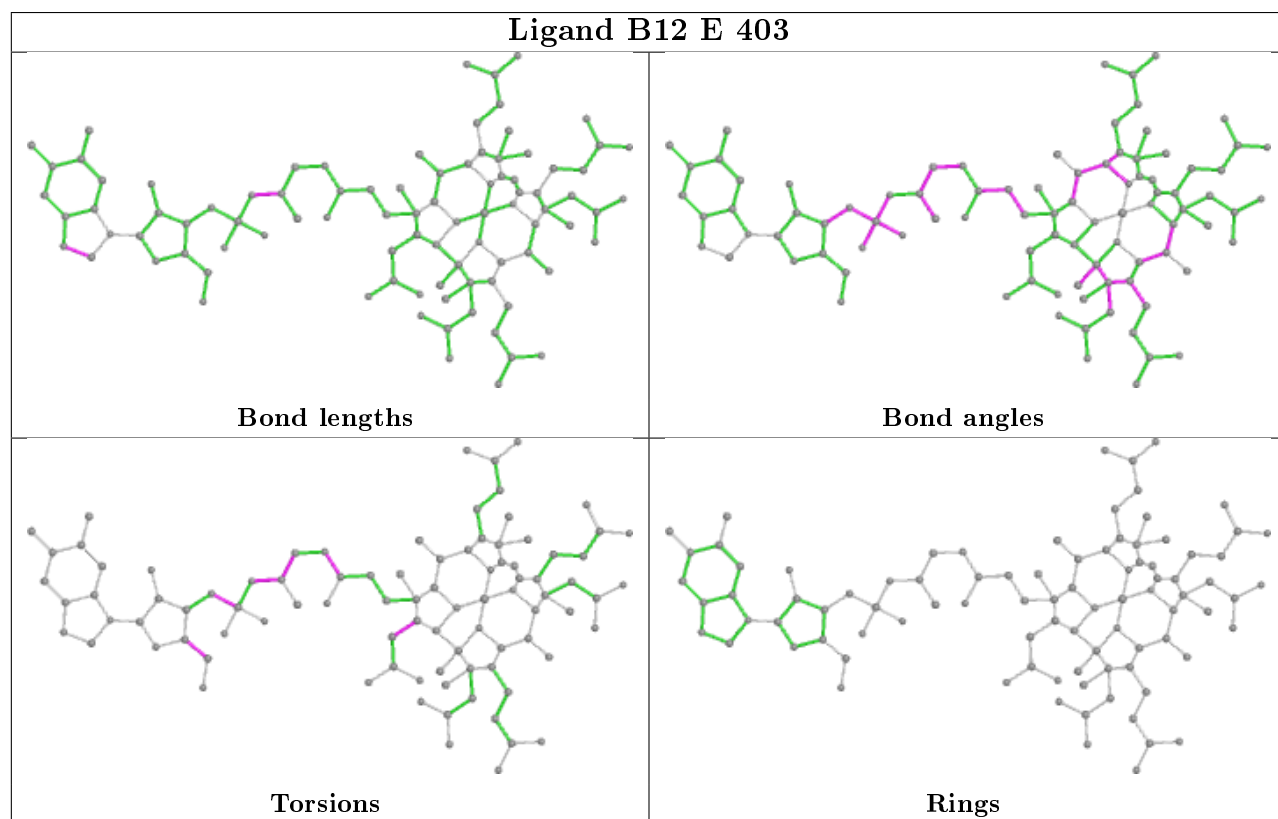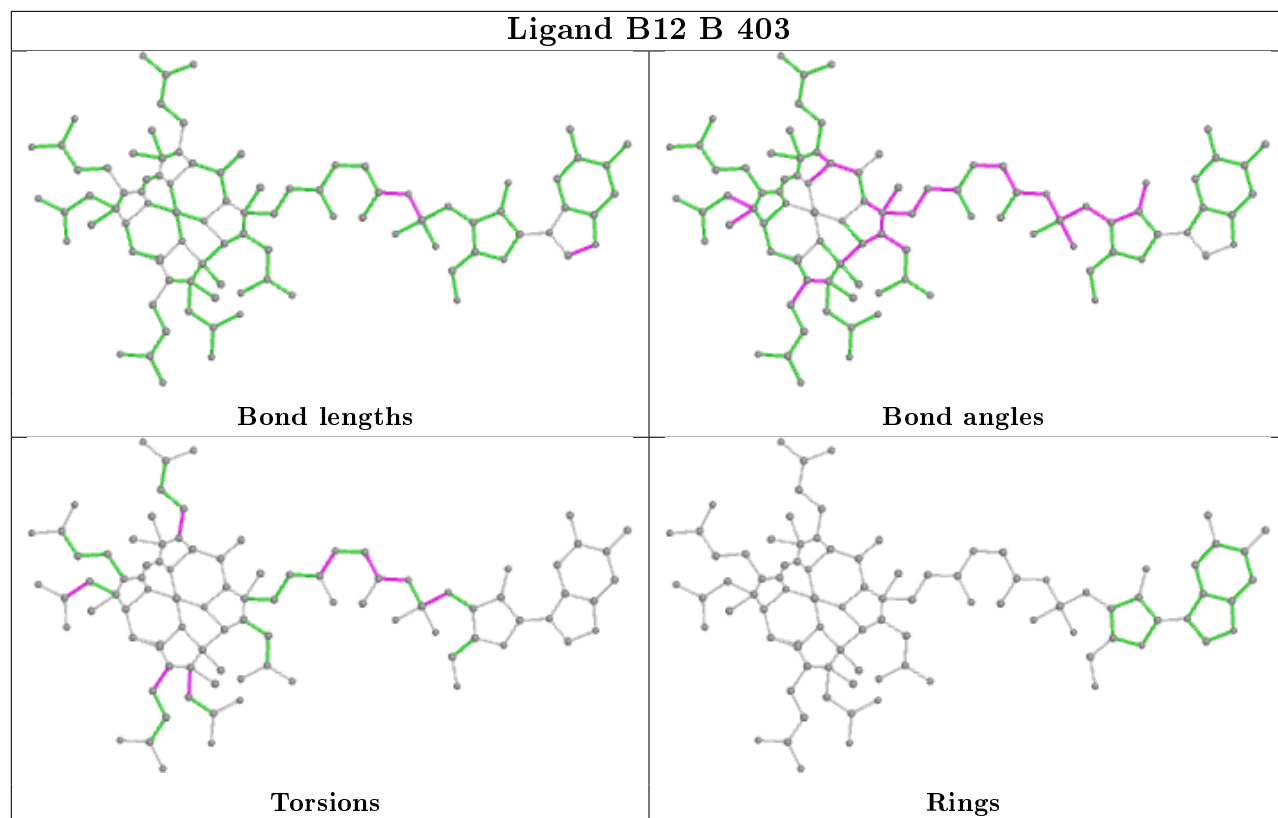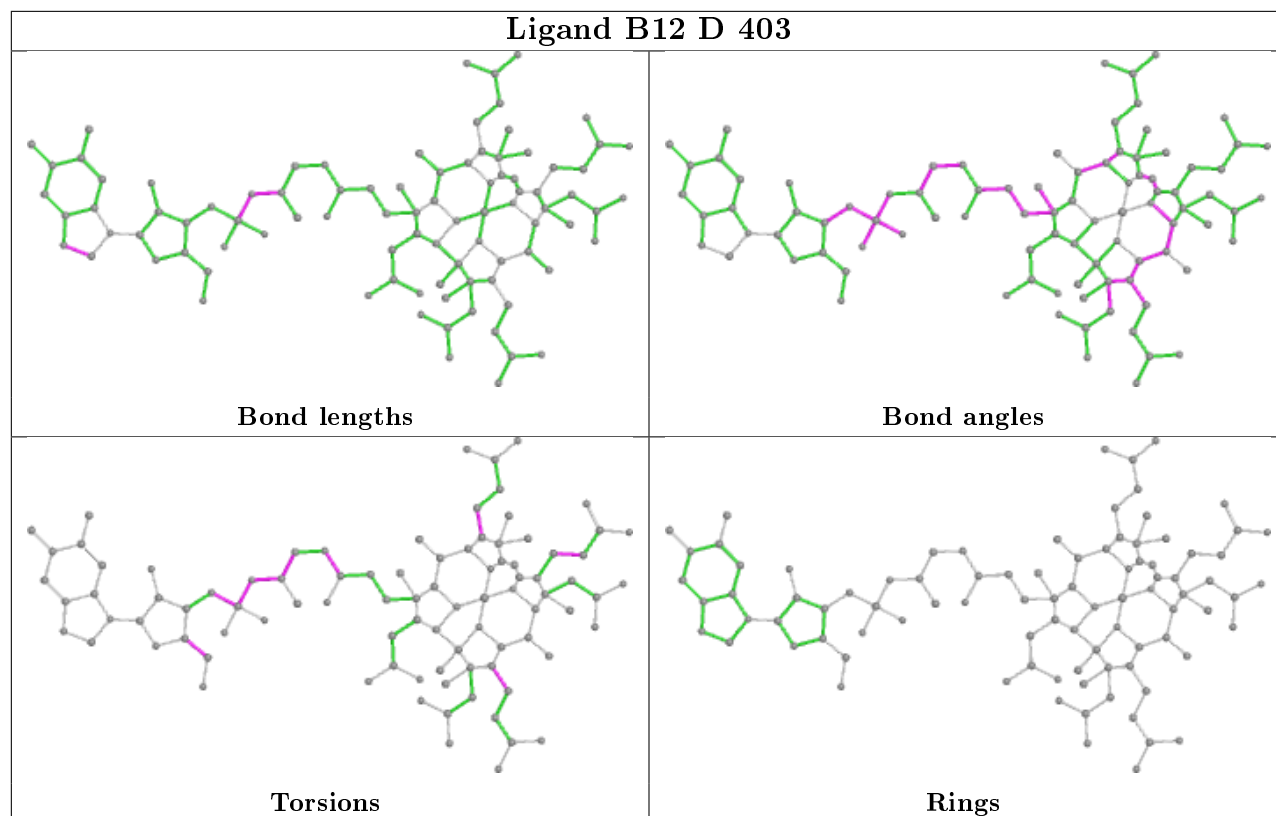
## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

# 6 Fit of model and data (i)

## 6.1 Protein, DNA and RNA chains (i)

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, $95^{th}$ 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$^2$) | Q<0.9 |
|-----|-------|----------|--------|---------|----|----|-------------|-------|
| 1 | A | 370/399 (92%) | -0.20 | 4 (1%) | 80 | 79 | 36, 67, 103, 130 | 0 |
| 1 | B | 370/399 (92%) | -0.22 | 4 (1%) | 80 | 79 | 39, 66, 108, 169 | 0 |
| 1 | C | 367/399 (91%) | 0.02 | 9 (2%) | 57 | 53 | 41, 78, 122, 148 | 0 |
| 1 | D | 370/399 (92%) | -0.03 | 10 (2%) | 54 | 50 | 46, 75, 116, 158 | 0 |
| 1 | E | 370/399 (92%) | 0.06 | 14 (3%) | 40 | 36 | 45, 82, 131, 181 | 0 |
| All | All | 1847/1995 (92%) | -0.07 | 41 (2%) | 62 | 57 | 36, 73, 119, 181 | 0 |

All (41) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | B | 1 | MET | 5.5 |
| 1 | D | 1 | MET | 4.9 |
| 1 | C | 145 | ILE | 4.9 |
| 1 | E | 1 | MET | 4.3 |
| 1 | D | 247 | ARG | 4.1 |
| 1 | C | 247 | ARG | 4.0 |
| 1 | E | 178 | GLN | 3.6 |
| 1 | E | 112 | LEU | 3.3 |
| 1 | A | 80 | GLN | 3.3 |
| 1 | E | 247 | ARG | 3.2 |
| 1 | E | 248 | GLY | 3.1 |
| 1 | C | 80 | GLN | 2.9 |
| 1 | D | 125 | TYR | 2.9 |
| 1 | C | 168 | LEU | 2.7 |
| 1 | D | 170 | THR | 2.7 |
| 1 | E | 169 | ILE | 2.7 |
| 1 | B | 157 | LYS | 2.5 |
| 1 | A | 103 | TYR | 2.5 |
| 1 | A | 1 | MET | 2.5 |
| 1 | D | 119 | LEU | 2.5 |

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Full wwPDB X-ray Structure Validation Report

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | E | 2 | ASN | 2.5 |
| 1 | D | 254 | ASP | 2.5 |
| 1 | E | 147 | PHE | 2.4 |
| 1 | A | 168 | LEU | 2.3 |
| 1 | E | 61 | LEU | 2.3 |
| 1 | C | 126 | LYS | 2.3 |
| 1 | D | 178 | GLN | 2.3 |
| 1 | E | 122 | ASN | 2.3 |
| 1 | E | 175 | GLU | 2.2 |
| 1 | C | 164 | TYR | 2.2 |
| 1 | E | 69 | SER | 2.1 |
| 1 | C | 7 | ILE | 2.1 |
| 1 | B | 122 | ASN | 2.1 |
| 1 | E | 5 | LEU | 2.1 |
| 1 | E | 71 | ALA | 2.1 |
| 1 | D | 253 | LEU | 2.0 |
| 1 | C | 178 | GLN | 2.0 |
| 1 | D | 168 | LEU | 2.0 |
| 1 | B | 281 | MET | 2.0 |
| 1 | C | 184 | CYS | 2.0 |
| 1 | D | 157 | LYS | 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. The B-factors column lists the minimum, median, $95^{th}$ 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 | B-factors(Å$^2$) | Q<0.9 |
|-----|------|-------|-----|-------|------|-----|------------------|-------|
| 3 | B12 | C | 403 | 91/91 | 0.96 | 0.15 | 52,71,102,110 | 0 |
| 3 | B12 | A | 403 | 91/91 | 0.97 | 0.15 | 42,55,108,118 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors($Å^2$) | Q<0.9 |
|-----|------|-------|-----|-------|------|-----|-------------------|-------|
| 2 | SF4 | C | 402 | 8/8 | 0.97 | 0.12 | 62,72,75,76 | 0 |
| 3 | B12 | B | 403 | 91/91 | 0.97 | 0.15 | 37,52,118,135 | 0 |
| 3 | B12 | E | 403 | 91/91 | 0.97 | 0.15 | 54,74,103,124 | 0 |
| 3 | B12 | D | 403 | 91/91 | 0.97 | 0.16 | 41,59,106,122 | 0 |
| 2 | SF4 | A | 401 | 8/8 | 0.98 | 0.12 | 65,73,76,78 | 0 |
| 2 | SF4 | C | 401 | 8/8 | 0.98 | 0.12 | 82,101,105,107 | 0 |
| 2 | SF4 | E | 401 | 8/8 | 0.98 | 0.10 | 89,102,106,110 | 0 |
| 2 | SF4 | D | 401 | 8/8 | 0.98 | 0.10 | 70,85,91,92 | 0 |
| 2 | SF4 | A | 402 | 8/8 | 0.99 | 0.14 | 53,57,60,64 | 0 |
| 2 | SF4 | B | 401 | 8/8 | 0.99 | 0.11 | 63,69,75,76 | 0 |
| 2 | SF4 | B | 402 | 8/8 | 0.99 | 0.14 | 46,51,55,55 | 0 |
| 2 | SF4 | E | 402 | 8/8 | 0.99 | 0.13 | 69,74,77,82 | 0 |
| 2 | SF4 | D | 402 | 8/8 | 0.99 | 0.14 | 51,58,62,66 | 0 |

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.
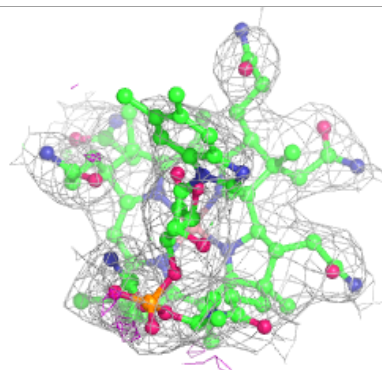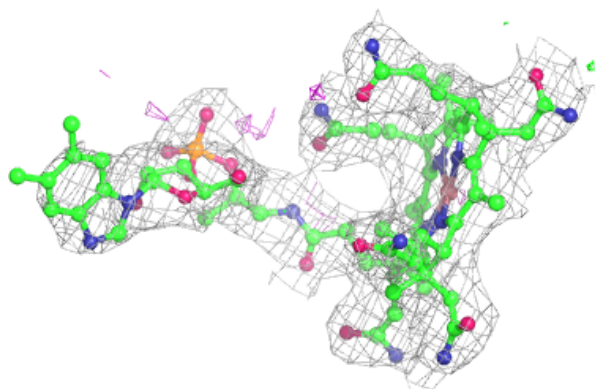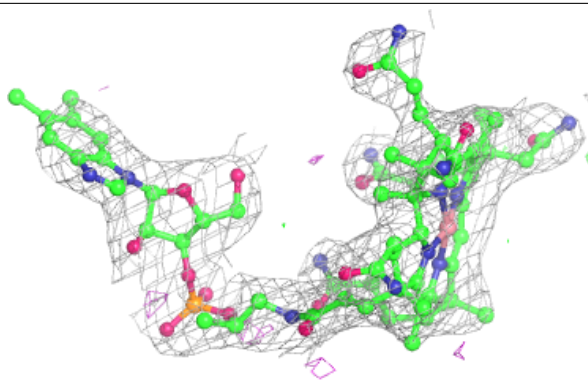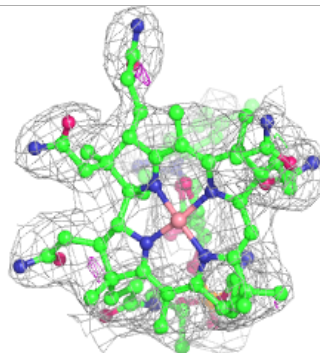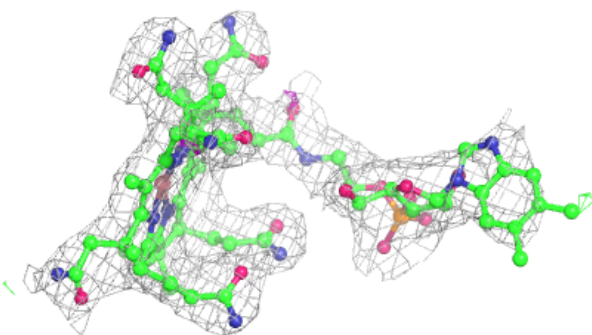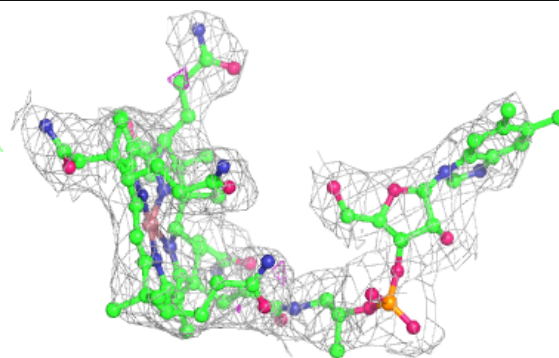
**Electron density around B12 C 403:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
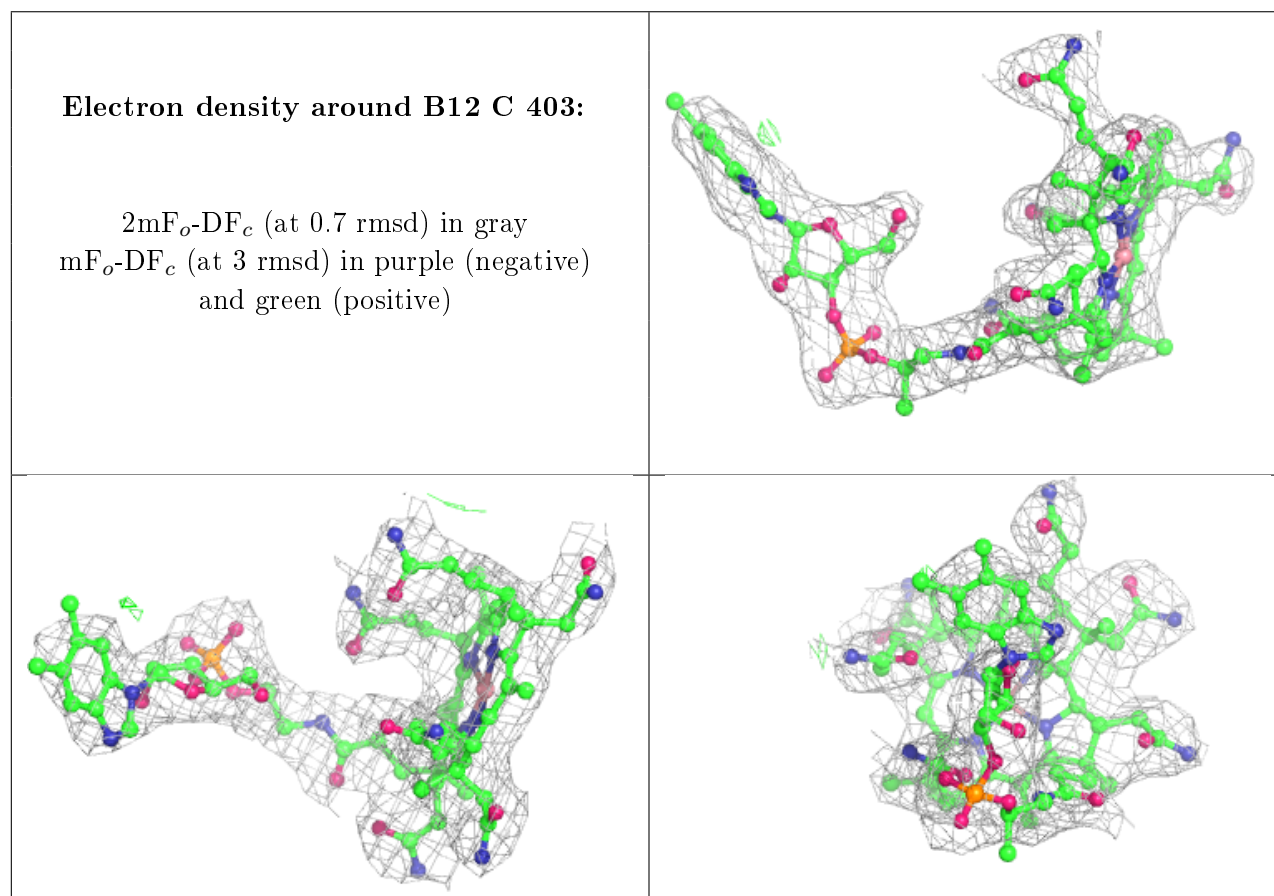
**Electron density around B12 A 403:**

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
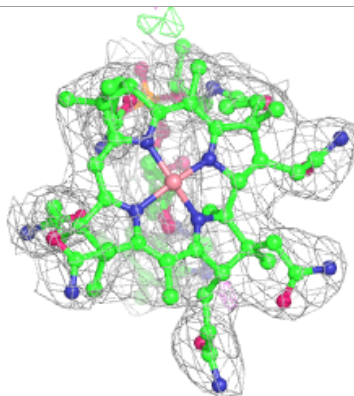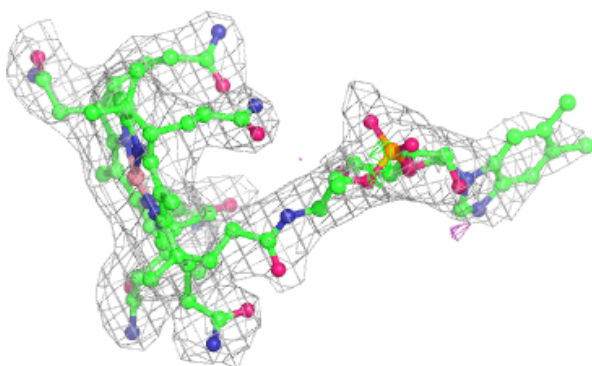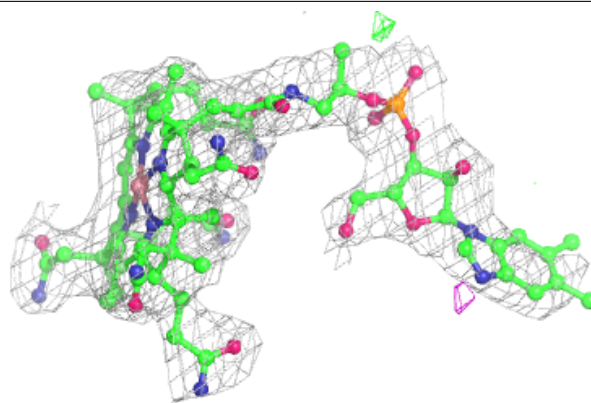


**Electron density around B12 B 403:**

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
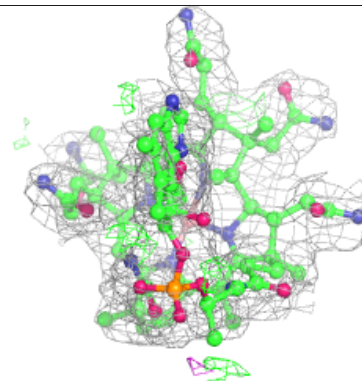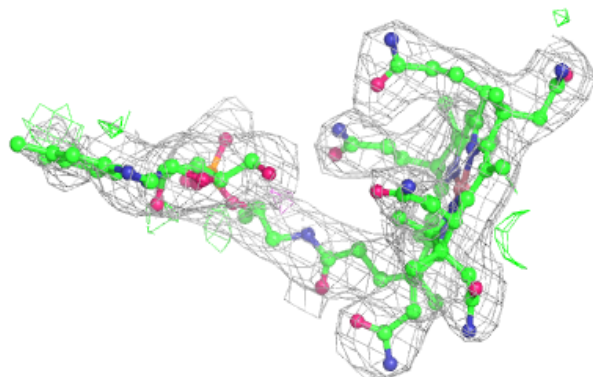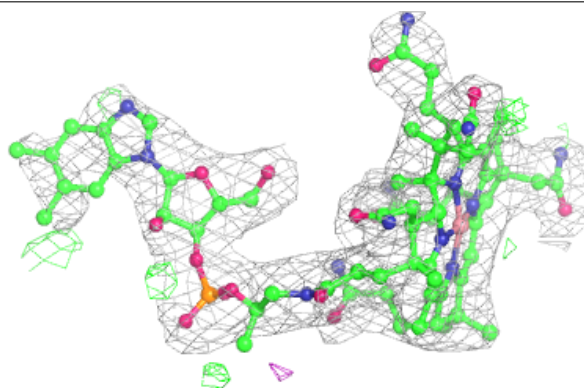
**Electron density around B12 E 403:**

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



**Electron density around B12 D 403:**

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

# 6.5 Other polymers (i)

There are no such residues in this entry.