



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 04:47 am GMT

PDB ID : 5D0F  
Title : Crystal Structure of the Candida Glabrata Glycogen Debranching Enzyme (E564Q) in complex with maltopentaose  
Authors : Zhai, L.; Xiang, S.  
Deposited on : 2015-08-03  
Resolution : 3.30 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                            | : | trunk28620   |
| 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) | : | recalc28949  |

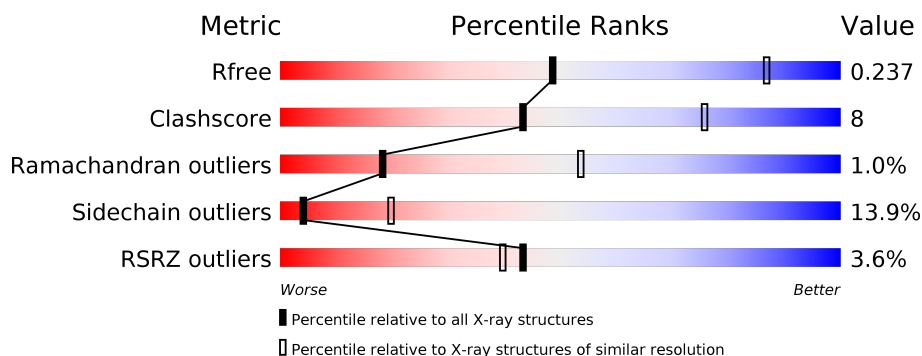
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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                      | 1034 (3.36-3.24)                                      |
| Clashscore            | 112137                      | 1100 (3.36-3.24)                                      |
| Ramachandran outliers | 110173                      | 1081 (3.36-3.24)                                      |
| Sidechain outliers    | 110143                      | 1080 (3.36-3.24)                                      |
| RSRZ outliers         | 101464                      | 1039 (3.36-3.24)                                      |

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     | 1528   | <div> <div>3%</div> <div> <div></div> <div>72%</div> <div>25%</div> <div>.</div> </div> </div> |
| 1   | B     | 1528   | <div> <div>4%</div> <div> <div></div> <div>71%</div> <div>25%</div> <div>.</div> </div> </div> |

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   | MTT  | A     | 2001 | -         | -        | -       | X                |
| 3   | CEX  | B     | 2002 | -         | -        | -       | X                |
| 3   | CEX  | B     | 2005 | -         | -        | -       | X                |

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 25070 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.

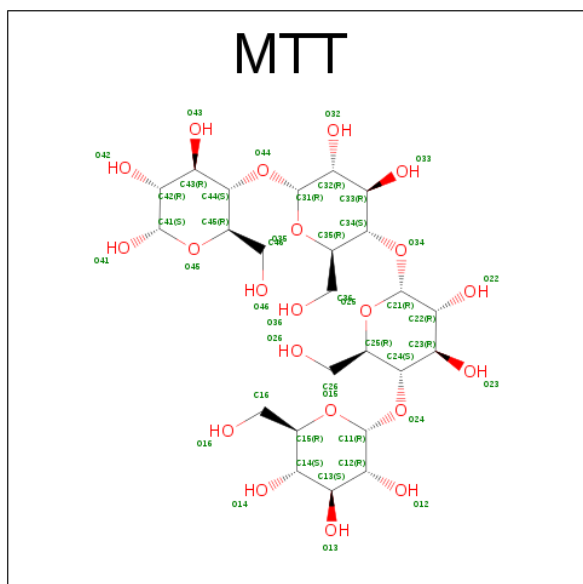
- Molecule 1 is a protein called Uncharacterized protein.

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 1   | A     | 1526     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 12278 | 7830 | 2066 | 2330 | 52 |         |         |       |
| 1   | B     | 1526     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 12278 | 7830 | 2066 | 2330 | 52 |         |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| A     | 564     | GLN      | GLU    | engineered mutation | UNP Q6FSK0 |
| B     | 564     | GLN      | GLU    | engineered mutation | UNP Q6FSK0 |

- Molecule 2 is MALTOTETRAOSE (three-letter code: MTT) (formula:  $C_{24}H_{42}O_{21}$ ).



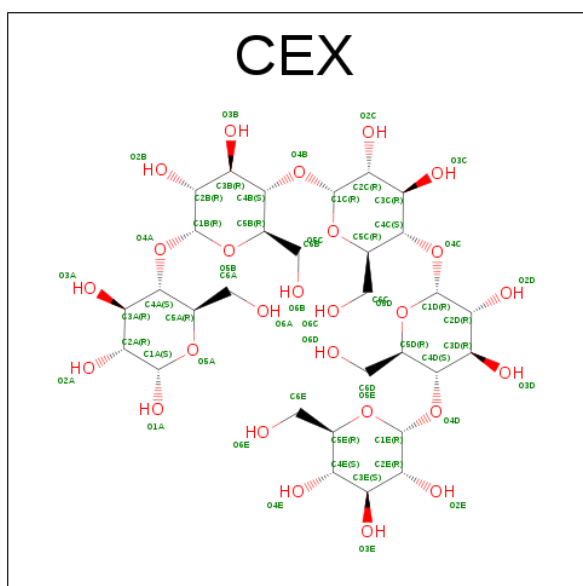
| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 2   | A     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 45    | 24 | 21 |         |         |

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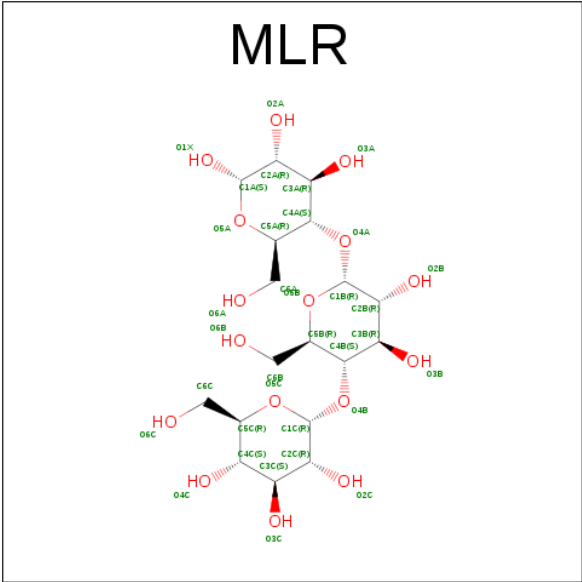
| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 2   | A     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 44    | 24 | 20 |         |         |
| 2   | A     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 44    | 24 | 20 |         |         |
| 2   | B     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 45    | 24 | 21 |         |         |
| 2   | B     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 44    | 24 | 20 |         |         |

- Molecule 3 is alpha-D-glucopyranosyl-(1->4)-alpha-D-glucopyranosyl-(1->4)-alpha-D-glucopyranosyl-(1->4)-alpha-D-glucopyranosyl-(1->4)-alpha-D-glucopyranose (three-letter code: CEX) (formula:  $C_{30}H_{52}O_{26}$ ).



| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 3   | A     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 56    | 30 | 26 |         |         |
| 3   | A     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 56    | 30 | 26 |         |         |
| 3   | B     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 56    | 30 | 26 |         |         |
| 3   | B     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 56    | 30 | 26 |         |         |

- Molecule 4 is MALTOTRIOSE (three-letter code: MLR) (formula:  $C_{18}H_{32}O_{16}$ ).

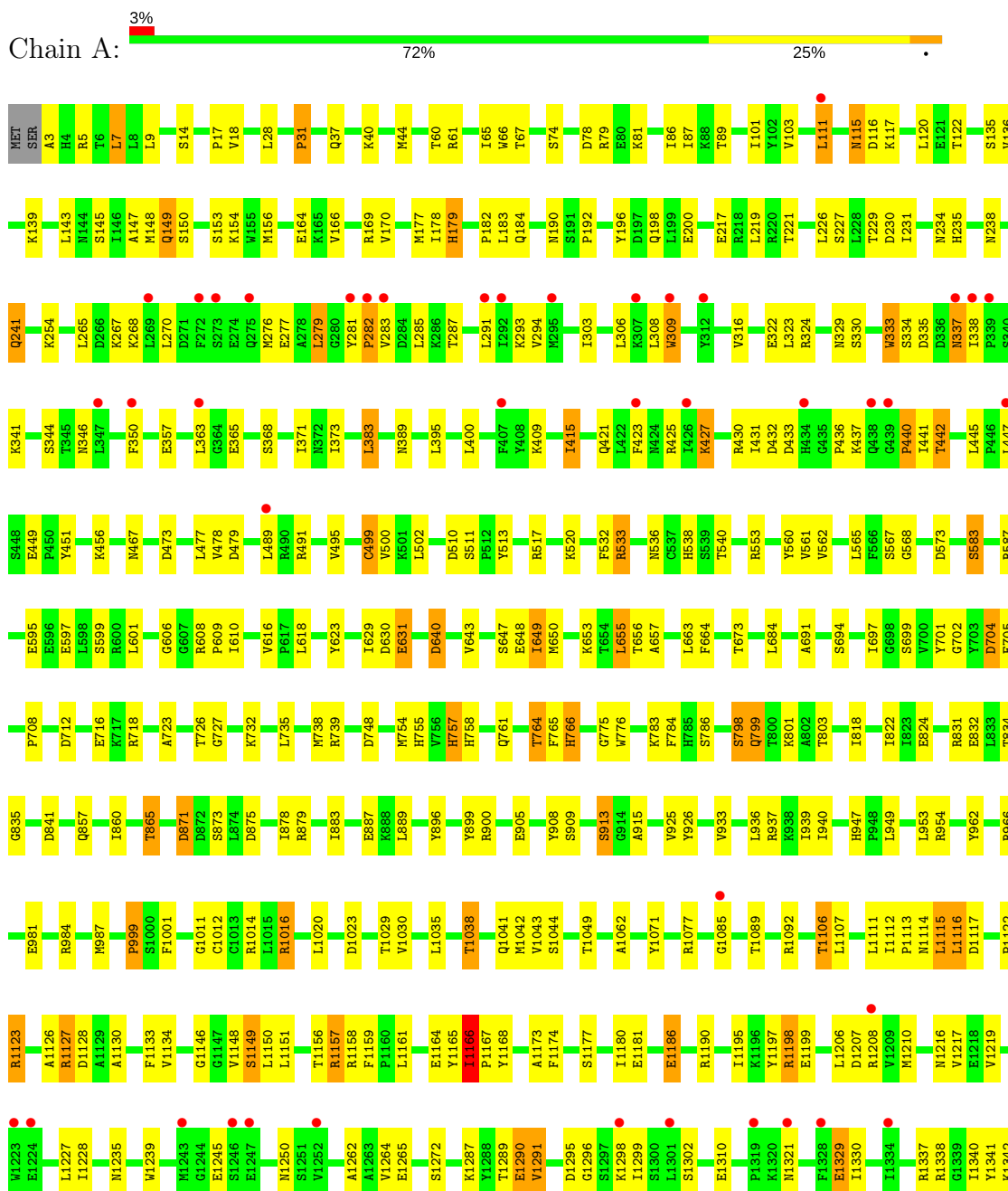


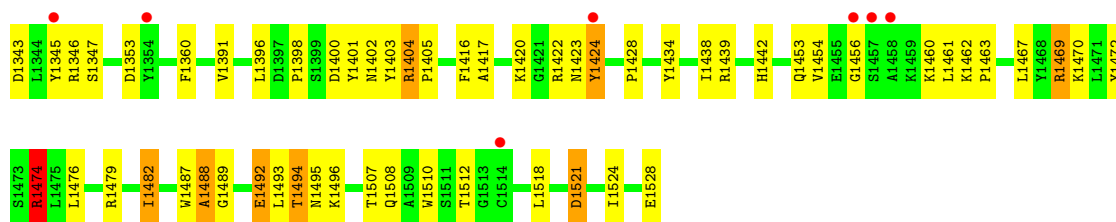
| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 4   | A     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 34    | 18 | 16 |         |         |
| 4   | B     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 34    | 18 | 16 |         |         |

### 3 Residue-property plots

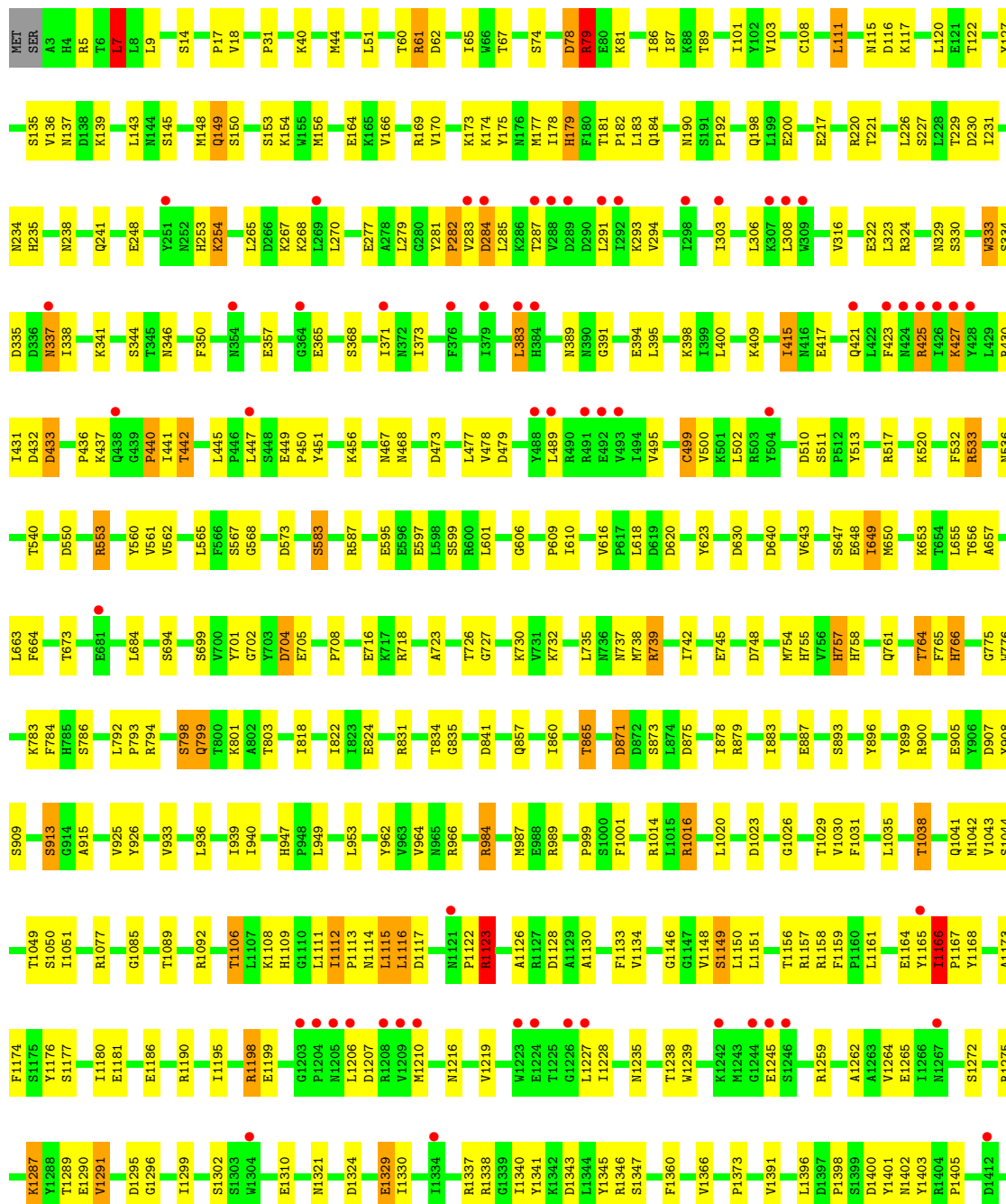
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Uncharacterized protein

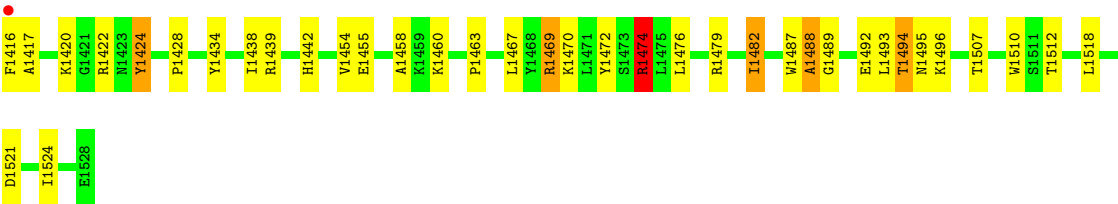




• Molecule 1: Uncharacterized protein







## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | C 1 2 1   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 158.07Å 202.01Å 135.24Å<br>90.00° 101.32° 90.00°            | Depositor        |
| Resolution (Å)  | 49.05 – 3.30<br>49.05 – 3.30                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 95.8 (49.05-3.30)<br>95.9 (49.05-3.30)                      | Depositor<br>EDS |
| $R_{merge}$   | (Not available)   | Depositor        |
| $R_{sym}$   | 0.09  | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.18 (at 3.33Å)   | Xtriage          |
| Refinement program  | PHENIX (phenix.refine: 1.9_1692)                            | Depositor        |
| R, $R_{free}$   | 0.192 , 0.228<br>0.201 , 0.237                              | Depositor<br>DCC |
| $R_{free}$ test set   | 3072 reflections (5.41%)                                    | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 85.3  | Xtriage          |
| Anisotropy  | 0.512   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.28 , 32.5   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$ | Xtriage          |
| Estimated twinning fraction   | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation  | 0.93  | EDS              |
| Total number of atoms   | 25070   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 93.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 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: MLR, MTT, CEX

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     | 0.81         | 2/12589 (0.0%) | 1.00        | 20/17071 (0.1%) |
| 1   | B     | 0.81         | 0/12589        | 1.00        | 26/17071 (0.2%) |
| All | All   | 0.81         | 2/25178 (0.0%) | 1.00        | 46/34142 (0.1%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 3                   |
| 1   | B     | 0                   | 4                   |
| All | All   | 0                   | 7                   |

All (2) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|------|-------------|----------|
| 1   | A     | 1071 | TYR  | CB-CG  | 5.10 | 1.59        | 1.51     |
| 1   | A     | 832  | GLU  | CD-OE2 | 5.09 | 1.31        | 1.25     |

All (46) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1   | B     | 1474 | ARG  | NE-CZ-NH1 | 8.80  | 124.70      | 120.30   |
| 1   | B     | 1469 | ARG  | NE-CZ-NH1 | 8.47  | 124.54      | 120.30   |
| 1   | B     | 61   | ARG  | NE-CZ-NH1 | 7.97  | 124.29      | 120.30   |
| 1   | B     | 1014 | ARG  | NE-CZ-NH2 | -7.81 | 116.40      | 120.30   |
| 1   | A     | 1469 | ARG  | NE-CZ-NH1 | 7.79  | 124.19      | 120.30   |
| 1   | A     | 1474 | ARG  | NE-CZ-NH1 | 7.31  | 123.96      | 120.30   |
| 1   | A     | 1014 | ARG  | NE-CZ-NH2 | -7.18 | 116.71      | 120.30   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1   | B     | 640  | ASP  | CB-CG-OD2 | -6.93 | 112.06      | 118.30   |
| 1   | A     | 533  | ARG  | NE-CZ-NH2 | -6.92 | 116.84      | 120.30   |
| 1   | B     | 533  | ARG  | NE-CZ-NH2 | -6.91 | 116.85      | 120.30   |
| 1   | B     | 79   | ARG  | NE-CZ-NH1 | 6.65  | 123.63      | 120.30   |
| 1   | A     | 61   | ARG  | NE-CZ-NH1 | 6.47  | 123.53      | 120.30   |
| 1   | B     | 1014 | ARG  | NE-CZ-NH1 | 6.43  | 123.52      | 120.30   |
| 1   | A     | 1488 | ALA  | N-CA-CB   | 6.30  | 118.91      | 110.10   |
| 1   | B     | 984  | ARG  | N-CA-CB   | 6.25  | 121.86      | 110.60   |
| 1   | B     | 1469 | ARG  | NE-CZ-NH2 | -6.25 | 117.17      | 120.30   |
| 1   | A     | 1014 | ARG  | NE-CZ-NH1 | 6.24  | 123.42      | 120.30   |
| 1   | B     | 553  | ARG  | NE-CZ-NH2 | -6.09 | 117.26      | 120.30   |
| 1   | A     | 954  | ARG  | NE-CZ-NH2 | -5.98 | 117.31      | 120.30   |
| 1   | B     | 1488 | ALA  | N-CA-CB   | 5.98  | 118.47      | 110.10   |
| 1   | A     | 739  | ARG  | NE-CZ-NH2 | -5.96 | 117.32      | 120.30   |
| 1   | A     | 1127 | ARG  | NE-CZ-NH1 | 5.95  | 123.28      | 120.30   |
| 1   | A     | 640  | ASP  | CB-CG-OD1 | 5.92  | 123.63      | 118.30   |
| 1   | A     | 5    | ARG  | NE-CZ-NH2 | -5.62 | 117.49      | 120.30   |
| 1   | B     | 1115 | LEU  | CA-CB-CG  | 5.59  | 128.15      | 115.30   |
| 1   | B     | 841  | ASP  | CB-CG-OD2 | 5.57  | 123.31      | 118.30   |
| 1   | B     | 1123 | ARG  | NE-CZ-NH1 | 5.52  | 123.06      | 120.30   |
| 1   | B     | 5    | ARG  | NE-CZ-NH2 | -5.51 | 117.55      | 120.30   |
| 1   | B     | 739  | ARG  | NE-CZ-NH2 | -5.50 | 117.55      | 120.30   |
| 1   | B     | 553  | ARG  | NE-CZ-NH1 | 5.46  | 123.03      | 120.30   |
| 1   | B     | 989  | ARG  | CG-CD-NE  | -5.46 | 100.33      | 111.80   |
| 1   | A     | 1115 | LEU  | CA-CB-CG  | 5.46  | 127.85      | 115.30   |
| 1   | A     | 533  | ARG  | NE-CZ-NH1 | 5.43  | 123.02      | 120.30   |
| 1   | B     | 51   | LEU  | CA-CB-CG  | -5.33 | 103.03      | 115.30   |
| 1   | A     | 1127 | ARG  | NE-CZ-NH2 | -5.33 | 117.64      | 120.30   |
| 1   | A     | 1469 | ARG  | NE-CZ-NH2 | -5.31 | 117.65      | 120.30   |
| 1   | B     | 78   | ASP  | CB-CG-OD1 | 5.25  | 123.03      | 118.30   |
| 1   | A     | 1127 | ARG  | CG-CD-NE  | 5.22  | 122.76      | 111.80   |
| 1   | B     | 1489 | GLY  | N-CA-C    | 5.15  | 125.98      | 113.10   |
| 1   | B     | 989  | ARG  | NE-CZ-NH2 | -5.13 | 117.73      | 120.30   |
| 1   | A     | 1489 | GLY  | N-CA-C    | 5.10  | 125.84      | 113.10   |
| 1   | B     | 79   | ARG  | NE-CZ-NH2 | -5.08 | 117.76      | 120.30   |
| 1   | B     | 640  | ASP  | CB-CG-OD1 | 5.06  | 122.86      | 118.30   |
| 1   | A     | 608  | ARG  | NE-CZ-NH1 | 5.06  | 122.83      | 120.30   |
| 1   | A     | 309  | TRP  | CA-CB-CG  | -5.04 | 104.13      | 113.70   |
| 1   | B     | 7    | LEU  | CA-CB-CG  | 5.03  | 126.87      | 115.30   |

There are no chirality outliers.

All (7) planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group   |
|-----|-------|------|------|---------|
| 1   | A     | 1492 | GLU  | Peptide |
| 1   | A     | 306  | LEU  | Peptide |
| 1   | A     | 442  | THR  | Peptide |
| 1   | B     | 1492 | GLU  | Peptide |
| 1   | B     | 241  | GLN  | Peptide |
| 1   | B     | 306  | LEU  | Peptide |
| 1   | B     | 442  | THR  | Peptide |

## 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     | 12278 | 0        | 11962    | 192     | 0            |
| 1   | B     | 12278 | 0        | 11962    | 192     | 0            |
| 2   | A     | 133   | 0        | 122      | 0       | 0            |
| 2   | B     | 89    | 0        | 82       | 0       | 0            |
| 3   | A     | 112   | 0        | 104      | 0       | 0            |
| 3   | B     | 112   | 0        | 104      | 1       | 0            |
| 4   | A     | 34    | 0        | 32       | 0       | 0            |
| 4   | B     | 34    | 0        | 32       | 1       | 0            |
| All | All   | 25070 | 0        | 24400    | 383     | 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 8.

All (383) 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:1158:ARG:O    | 1:B:1159:PHE:HD2 | 1.38                     | 1.04              |
| 1:B:1158:ARG:O    | 1:B:1159:PHE:CD2 | 2.17                     | 0.97              |
| 1:A:1062:ALA:O    | 1:A:1508:GLN:OE1 | 1.92                     | 0.86              |
| 1:A:230:ASP:OD1   | 1:A:533:ARG:HD3  | 1.77                     | 0.84              |
| 1:B:230:ASP:OD1   | 1:B:533:ARG:HD3  | 1.79                     | 0.83              |
| 1:B:757:HIS:HB3   | 1:B:764:THR:HG22 | 1.62                     | 0.82              |
| 1:B:1482:ILE:HG12 | 1:B:1488:ALA:O   | 1.82                     | 0.80              |
| 1:A:1482:ILE:HG12 | 1:A:1488:ALA:O   | 1.82                     | 0.79              |
| 1:A:757:HIS:HB3   | 1:A:764:THR:HG22 | 1.66                     | 0.78              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:B:871:ASP:N     | 1:B:871:ASP:OD1  | 2.20                     | 0.75              |
| 1:B:1041:GLN:NE2  | 1:B:1488:ALA:HB3 | 2.07                     | 0.70              |
| 1:A:1439:ARG:HD2  | 1:A:1521:ASP:OD2 | 1.91                     | 0.69              |
| 1:A:282:PRO:HB3   | 1:A:294:VAL:HG22 | 1.74                     | 0.69              |
| 1:B:1439:ARG:HD2  | 1:B:1521:ASP:OD2 | 1.94                     | 0.68              |
| 1:B:282:PRO:HB3   | 1:B:294:VAL:HG22 | 1.75                     | 0.68              |
| 1:B:964:VAL:HG11  | 1:B:984:ARG:HB3  | 1.75                     | 0.68              |
| 1:A:1041:GLN:NE2  | 1:A:1488:ALA:HB3 | 2.09                     | 0.67              |
| 1:A:1470:LYS:O    | 1:A:1474:ARG:HG3 | 1.94                     | 0.67              |
| 1:A:629:ILE:HD13  | 1:A:631:GLU:HG2  | 1.76                     | 0.67              |
| 1:A:871:ASP:N     | 1:A:871:ASP:OD1  | 2.28                     | 0.66              |
| 1:B:1470:LYS:O    | 1:B:1474:ARG:HG3 | 1.97                     | 0.65              |
| 1:A:3:ALA:HB3     | 1:A:640:ASP:HB3  | 1.77                     | 0.65              |
| 1:B:783:LYS:HG2   | 1:B:857:GLN:HB3  | 1.80                     | 0.64              |
| 1:A:1165:TYR:O    | 1:A:1167:PRO:CD  | 2.46                     | 0.64              |
| 1:A:783:LYS:HG2   | 1:A:857:GLN:HB3  | 1.78                     | 0.64              |
| 1:A:66:TRP:CZ3    | 1:B:1458:ALA:HB2 | 2.32                     | 0.64              |
| 1:A:148:MET:HA    | 1:A:177:MET:O    | 1.98                     | 0.63              |
| 1:A:705:GLU:N     | 1:A:705:GLU:OE1  | 2.31                     | 0.63              |
| 1:B:1165:TYR:O    | 1:B:1167:PRO:CD  | 2.46                     | 0.63              |
| 1:B:148:MET:HA    | 1:B:177:MET:O    | 1.98                     | 0.63              |
| 1:A:704:ASP:OD2   | 1:A:732:LYS:HG3  | 1.99                     | 0.63              |
| 1:B:1041:GLN:HE22 | 1:B:1488:ALA:HB3 | 1.64                     | 0.63              |
| 1:B:115:ASN:HB3   | 1:B:117:LYS:H    | 1.64                     | 0.63              |
| 1:B:656:THR:HG22  | 1:B:657:ALA:N    | 2.15                     | 0.62              |
| 1:A:115:ASN:HB3   | 1:A:117:LYS:H    | 1.64                     | 0.62              |
| 1:A:365:GLU:HB2   | 1:A:368:SER:HB3  | 1.82                     | 0.61              |
| 1:B:704:ASP:OD2   | 1:B:732:LYS:HG3  | 2.01                     | 0.61              |
| 1:A:915:ALA:HA    | 1:A:962:TYR:OH   | 2.00                     | 0.61              |
| 1:B:365:GLU:HB2   | 1:B:368:SER:HB3  | 1.83                     | 0.61              |
| 1:B:1085:GLY:O    | 1:B:1089:THR:HB  | 2.01                     | 0.61              |
| 1:A:1041:GLN:HE22 | 1:A:1488:ALA:HB3 | 1.65                     | 0.60              |
| 1:B:169:ARG:NH1   | 1:B:701:TYR:OH   | 2.34                     | 0.60              |
| 1:B:1146:GLY:O    | 1:B:1149:SER:OG  | 2.20                     | 0.60              |
| 1:B:684:LEU:HD11  | 1:B:860:ILE:HD12 | 1.83                     | 0.60              |
| 1:B:1472:TYR:OH   | 1:B:1479:ARG:NH1 | 2.34                     | 0.60              |
| 1:A:283:VAL:HA    | 1:A:441:ILE:HD11 | 1.85                     | 0.59              |
| 1:A:9:LEU:HD11    | 1:A:17:PRO:HB3   | 1.83                     | 0.59              |
| 1:B:757:HIS:HB3   | 1:B:764:THR:CG2  | 2.31                     | 0.59              |
| 1:A:1085:GLY:O    | 1:A:1089:THR:HB  | 2.02                     | 0.59              |
| 1:B:705:GLU:N     | 1:B:705:GLU:OE1  | 2.35                     | 0.59              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:1165:TYR:O    | 1:A:1167:PRO:HD3 | 2.03                     | 0.59              |
| 1:B:915:ALA:HA    | 1:B:962:TYR:OH   | 2.03                     | 0.59              |
| 1:A:1157:ARG:NH2  | 1:A:1186:GLU:OE2 | 2.36                     | 0.58              |
| 1:A:182:PRO:HG2   | 1:A:192:PRO:O    | 2.03                     | 0.58              |
| 1:A:467:ASN:HB2   | 1:A:499:CYS:O    | 2.03                     | 0.58              |
| 1:A:647:SER:OG    | 1:A:648:GLU:N    | 2.36                     | 0.58              |
| 1:B:1038:THR:HG21 | 1:B:1512:THR:OG1 | 2.03                     | 0.58              |
| 1:A:1038:THR:HG21 | 1:A:1512:THR:OG1 | 2.03                     | 0.57              |
| 1:B:1396:LEU:HD21 | 1:B:1400:ASP:HB3 | 1.86                     | 0.57              |
| 1:B:182:PRO:HG2   | 1:B:192:PRO:O    | 2.05                     | 0.57              |
| 1:A:169:ARG:NH1   | 1:A:701:TYR:OH   | 2.34                     | 0.57              |
| 1:B:432:ASP:HB2   | 1:B:436:PRO:HB3  | 1.86                     | 0.57              |
| 1:B:1165:TYR:O    | 1:B:1167:PRO:HD3 | 2.04                     | 0.57              |
| 1:B:283:VAL:HA    | 1:B:441:ILE:HD11 | 1.86                     | 0.57              |
| 1:B:430:ARG:NH1   | 1:B:440:PRO:O    | 2.38                     | 0.56              |
| 1:A:1158:ARG:O    | 1:A:1159:PHE:CD2 | 2.58                     | 0.56              |
| 1:A:432:ASP:HB2   | 1:A:436:PRO:HB3  | 1.87                     | 0.56              |
| 1:A:684:LEU:HD11  | 1:A:860:ILE:HD12 | 1.88                     | 0.56              |
| 1:B:467:ASN:HB2   | 1:B:499:CYS:O    | 2.05                     | 0.56              |
| 1:A:1146:GLY:O    | 1:A:1149:SER:OG  | 2.23                     | 0.56              |
| 1:A:1493:LEU:HD23 | 1:A:1494:THR:N   | 2.21                     | 0.56              |
| 1:A:1396:LEU:HD21 | 1:A:1400:ASP:HB3 | 1.88                     | 0.56              |
| 1:A:1492:GLU:HG3  | 1:A:1508:GLN:HG3 | 1.88                     | 0.56              |
| 1:B:1396:LEU:HD21 | 1:B:1400:ASP:CB  | 2.36                     | 0.56              |
| 1:A:1472:TYR:OH   | 1:A:1479:ARG:NH1 | 2.39                     | 0.55              |
| 1:A:1038:THR:HG21 | 1:A:1512:THR:CB  | 2.37                     | 0.55              |
| 1:A:1456:GLY:HA3  | 1:A:1462:LYS:HG3 | 1.88                     | 0.55              |
| 1:A:65:ILE:HG12   | 1:A:111:LEU:HD22 | 1.89                     | 0.55              |
| 1:A:430:ARG:NH1   | 1:A:440:PRO:O    | 2.39                     | 0.55              |
| 1:A:656:THR:HG22  | 1:A:657:ALA:N    | 2.22                     | 0.55              |
| 1:B:925:VAL:CG1   | 1:B:1487:TRP:CE2 | 2.90                     | 0.55              |
| 1:A:738:MET:HE2   | 1:A:776:TRP:CZ2  | 2.42                     | 0.55              |
| 1:B:630:ASP:O     | 1:B:648:GLU:HG2  | 2.07                     | 0.54              |
| 1:B:738:MET:HE3   | 1:B:776:TRP:CZ3  | 2.43                     | 0.54              |
| 1:B:79:ARG:HH21   | 1:B:550:ASP:CG   | 2.10                     | 0.54              |
| 1:A:1106:THR:HG21 | 1:A:1113:PRO:HG3 | 1.90                     | 0.54              |
| 1:A:1123:ARG:NH2  | 1:A:1207:ASP:OD2 | 2.41                     | 0.54              |
| 1:B:1493:LEU:HD23 | 1:B:1494:THR:N   | 2.22                     | 0.54              |
| 1:A:630:ASP:O     | 1:A:648:GLU:HG2  | 2.06                     | 0.54              |
| 1:B:65:ILE:HG12   | 1:B:111:LEU:HD22 | 1.90                     | 0.54              |
| 1:B:1405:PRO:HA   | 1:B:1428:PRO:HD3 | 1.89                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:606:GLY:O     | 1:A:694:SER:HB3   | 2.08                     | 0.54              |
| 1:A:303:ILE:HG13  | 1:A:415:ILE:HD11  | 1.90                     | 0.54              |
| 1:B:647:SER:OG    | 1:B:648:GLU:N     | 2.41                     | 0.53              |
| 1:A:1396:LEU:HD21 | 1:A:1400:ASP:CB   | 2.38                     | 0.53              |
| 1:A:196:TYR:OH    | 1:A:241:GLN:NE2   | 2.42                     | 0.53              |
| 1:B:303:ILE:HG13  | 1:B:415:ILE:HD11  | 1.91                     | 0.53              |
| 1:B:1029:THR:HG22 | 1:B:1030:VAL:N    | 2.23                     | 0.53              |
| 1:A:757:HIS:HB3   | 1:A:764:THR:CG2   | 2.37                     | 0.53              |
| 1:B:1340:ILE:HG22 | 1:B:1341:TYR:C    | 2.29                     | 0.53              |
| 1:B:1106:THR:HG21 | 1:B:1113:PRO:HG3  | 1.90                     | 0.53              |
| 1:A:1156:THR:CG2  | 1:A:1174:PHE:HA   | 2.39                     | 0.53              |
| 1:B:1123:ARG:NH2  | 1:B:1207:ASP:OD2  | 2.42                     | 0.52              |
| 1:B:1108:LYS:HE2  | 1:B:1159:PHE:CD1  | 2.45                     | 0.52              |
| 1:B:60:THR:HG22   | 1:B:87:ILE:HG21   | 1.91                     | 0.52              |
| 1:A:1340:ILE:HG22 | 1:A:1341:TYR:C    | 2.30                     | 0.52              |
| 1:A:738:MET:HB3   | 1:A:776:TRP:CH2   | 2.45                     | 0.52              |
| 1:B:1038:THR:HG21 | 1:B:1512:THR:CB   | 2.40                     | 0.52              |
| 1:B:606:GLY:O     | 1:B:694:SER:HB3   | 2.10                     | 0.52              |
| 1:A:148:MET:HE3   | 1:A:663:LEU:HD21  | 1.92                     | 0.52              |
| 1:B:560:TYR:CE2   | 1:B:562:VAL:CG2   | 2.93                     | 0.52              |
| 1:A:60:THR:HG22   | 1:A:87:ILE:HG21   | 1.92                     | 0.52              |
| 1:B:905:GLU:OE1   | 1:B:966:ARG:NH1   | 2.43                     | 0.52              |
| 1:B:1128:ASP:OD2  | 1:B:1239:TRP:N    | 2.43                     | 0.52              |
| 1:A:1114:ASN:HB2  | 1:A:1126:ALA:HB2  | 1.92                     | 0.51              |
| 1:A:1029:THR:HG22 | 1:A:1030:VAL:N    | 2.26                     | 0.51              |
| 1:B:925:VAL:CG1   | 1:B:1487:TRP:CD2  | 2.93                     | 0.51              |
| 1:A:798:SER:O     | 1:A:799:GLN:C     | 2.47                     | 0.51              |
| 1:A:281:TYR:N     | 1:A:282:PRO:HD3   | 2.25                     | 0.51              |
| 1:B:798:SER:O     | 1:B:799:GLN:C     | 2.49                     | 0.51              |
| 1:A:905:GLU:OE1   | 1:A:966:ARG:NH1   | 2.43                     | 0.51              |
| 1:B:1156:THR:CG2  | 1:B:1174:PHE:HA   | 2.39                     | 0.51              |
| 1:B:1262:ALA:HB3  | 1:B:1345:TYR:HB3  | 1.93                     | 0.51              |
| 1:A:1041:GLN:OE1  | 1:A:1507:THR:HG21 | 2.11                     | 0.51              |
| 1:A:287:THR:O     | 1:A:291:LEU:HG    | 2.11                     | 0.51              |
| 1:B:1114:ASN:HB2  | 1:B:1126:ALA:HB2  | 1.92                     | 0.51              |
| 1:B:9:LEU:HD11    | 1:B:17:PRO:HB3    | 1.92                     | 0.51              |
| 1:A:1404:ARG:O    | 1:A:1423:ASN:OD1  | 2.29                     | 0.51              |
| 1:A:909:SER:CB    | 1:A:913:SER:HB2   | 2.41                     | 0.51              |
| 1:A:1195:ILE:HG12 | 1:A:1219:VAL:HB   | 1.93                     | 0.50              |
| 1:B:1035:LEU:O    | 1:B:1038:THR:HG22 | 2.12                     | 0.50              |
| 1:A:1405:PRO:HA   | 1:A:1428:PRO:HD3  | 1.92                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1463:PRO:HB3  | 1:B:1467:LEU:HD23 | 1.94                     | 0.50              |
| 1:B:177:MET:HA    | 1:B:226:LEU:O     | 2.12                     | 0.50              |
| 1:B:925:VAL:HG11  | 1:B:1487:TRP:CD2  | 2.46                     | 0.50              |
| 1:A:1264:VAL:HG11 | 1:A:1360:PHE:HA   | 1.93                     | 0.50              |
| 1:A:231:ILE:HD12  | 1:A:532:PHE:CD1   | 2.47                     | 0.50              |
| 1:A:282:PRO:CB    | 1:A:294:VAL:HG22  | 2.40                     | 0.50              |
| 1:A:925:VAL:CG1   | 1:A:1487:TRP:CD2  | 2.95                     | 0.50              |
| 1:A:1156:THR:HG21 | 1:A:1174:PHE:HA   | 1.94                     | 0.50              |
| 1:A:1181:GLU:OE1  | 1:A:1287:LYS:HG3  | 2.12                     | 0.50              |
| 1:A:1291:VAL:CG2  | 1:A:1299:ILE:O    | 2.60                     | 0.50              |
| 1:B:1166:ILE:HD11 | 1:B:1168:TYR:HB2  | 1.94                     | 0.50              |
| 1:A:1128:ASP:OD2  | 1:A:1239:TRP:N    | 2.44                     | 0.50              |
| 1:B:834:THR:HG22  | 1:B:835:GLY:N     | 2.27                     | 0.49              |
| 1:A:834:THR:HG22  | 1:A:835:GLY:N     | 2.28                     | 0.49              |
| 1:B:775:GLY:O     | 1:B:776:TRP:HD1   | 1.94                     | 0.49              |
| 1:A:1166:ILE:HD11 | 1:A:1168:TYR:HB2  | 1.94                     | 0.49              |
| 1:A:925:VAL:HG11  | 1:A:1487:TRP:CD2  | 2.48                     | 0.49              |
| 1:A:761:GLN:NE2   | 1:A:857:GLN:OE1   | 2.44                     | 0.49              |
| 1:A:896:TYR:O     | 1:A:966:ARG:NH2   | 2.40                     | 0.49              |
| 1:B:1195:ILE:HG12 | 1:B:1219:VAL:HB   | 1.93                     | 0.49              |
| 1:A:1035:LEU:O    | 1:A:1038:THR:HG22 | 2.11                     | 0.49              |
| 1:A:1463:PRO:HB3  | 1:A:1467:LEU:HD23 | 1.95                     | 0.49              |
| 1:B:287:THR:O     | 1:B:291:LEU:HG    | 2.12                     | 0.49              |
| 1:B:1041:GLN:OE1  | 1:B:1507:THR:HG21 | 2.13                     | 0.49              |
| 1:B:282:PRO:CB    | 1:B:294:VAL:HG22  | 2.41                     | 0.49              |
| 1:A:925:VAL:CG1   | 1:A:1487:TRP:CE2  | 2.95                     | 0.49              |
| 1:B:148:MET:HE3   | 1:B:663:LEU:HD21  | 1.94                     | 0.49              |
| 1:B:766:HIS:CE1   | 1:B:865:THR:HG21  | 2.48                     | 0.49              |
| 1:A:441:ILE:HG22  | 1:A:442:THR:N     | 2.27                     | 0.49              |
| 1:B:896:TYR:O     | 1:B:966:ARG:NH2   | 2.43                     | 0.49              |
| 1:B:1198:ARG:HA   | 1:B:1216:ASN:HA   | 1.94                     | 0.48              |
| 1:B:1434:TYR:OH   | 1:B:1474:ARG:HB3  | 2.13                     | 0.48              |
| 1:B:909:SER:CB    | 1:B:913:SER:HB2   | 2.43                     | 0.48              |
| 1:B:567:SER:OG    | 1:B:568:GLY:N     | 2.46                     | 0.48              |
| 1:A:136:VAL:HG12  | 1:A:139:LYS:HB2   | 1.94                     | 0.48              |
| 1:A:595:GLU:HG3   | 1:A:784:PHE:CD2   | 2.48                     | 0.48              |
| 1:B:656:THR:CG2   | 1:B:657:ALA:N     | 2.77                     | 0.48              |
| 1:A:467:ASN:HA    | 1:A:500:VAL:HA    | 1.95                     | 0.48              |
| 1:A:513:TYR:CE2   | 1:A:517:ARG:HD2   | 2.48                     | 0.48              |
| 1:B:101:ILE:HD12  | 1:B:101:ILE:N     | 2.29                     | 0.48              |
| 1:B:253:HIS:CD2   | 1:B:254:LYS:N     | 2.82                     | 0.48              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:177:MET:HA    | 1:A:226:LEU:O    | 2.13                     | 0.48              |
| 1:B:1108:LYS:CE   | 1:B:1159:PHE:CD1 | 2.96                     | 0.48              |
| 1:B:441:ILE:HG22  | 1:B:442:THR:N    | 2.29                     | 0.48              |
| 1:A:1168:TYR:C    | 1:A:1168:TYR:CD1 | 2.86                     | 0.48              |
| 1:A:1262:ALA:HB3  | 1:A:1345:TYR:HB3 | 1.96                     | 0.48              |
| 1:B:1156:THR:HG21 | 1:B:1174:PHE:HA  | 1.95                     | 0.48              |
| 1:B:899:TYR:CD1   | 1:B:1041:GLN:HG2 | 2.49                     | 0.48              |
| 1:B:595:GLU:HG3   | 1:B:784:PHE:CD2  | 2.49                     | 0.48              |
| 1:A:560:TYR:CE2   | 1:A:562:VAL:CG2  | 2.96                     | 0.47              |
| 1:A:775:GLY:O     | 1:A:776:TRP:HD1  | 1.97                     | 0.47              |
| 1:B:1108:LYS:HE2  | 1:B:1159:PHE:HD1 | 1.78                     | 0.47              |
| 1:B:1291:VAL:CG2  | 1:B:1299:ILE:O   | 2.61                     | 0.47              |
| 1:B:1416:PHE:CE2  | 1:B:1422:ARG:NH2 | 2.81                     | 0.47              |
| 1:A:1398:PRO:HA   | 1:A:1403:TYR:CG  | 2.49                     | 0.47              |
| 1:A:899:TYR:CD1   | 1:A:1041:GLN:HG2 | 2.49                     | 0.47              |
| 1:B:1168:TYR:CD1  | 1:B:1168:TYR:O   | 2.67                     | 0.47              |
| 1:B:1417:ALA:O    | 1:B:1422:ARG:HB2 | 2.15                     | 0.47              |
| 1:A:427:LYS:HE2   | 1:A:433:ASP:OD2  | 2.14                     | 0.47              |
| 1:A:610:ILE:HD12  | 1:A:755:HIS:HB2  | 1.95                     | 0.47              |
| 1:B:7:LEU:HD22    | 1:B:643:VAL:HG21 | 1.96                     | 0.47              |
| 1:A:28:LEU:HB3    | 1:A:655:LEU:HD11 | 1.96                     | 0.47              |
| 1:A:567:SER:OG    | 1:A:568:GLY:N    | 2.48                     | 0.47              |
| 1:A:766:HIS:CE1   | 1:A:865:THR:HG21 | 2.50                     | 0.47              |
| 1:B:1165:TYR:O    | 1:B:1167:PRO:HD2 | 2.14                     | 0.47              |
| 1:A:1295:ASP:OD1  | 1:A:1296:GLY:N   | 2.47                     | 0.47              |
| 1:B:1198:ARG:O    | 1:B:1199:GLU:C   | 2.53                     | 0.47              |
| 1:B:766:HIS:HE1   | 1:B:865:THR:HG21 | 1.79                     | 0.47              |
| 1:A:101:ILE:N     | 1:A:101:ILE:HD12 | 2.29                     | 0.47              |
| 1:B:150:SER:OG    | 1:B:179:HIS:HD2  | 1.98                     | 0.47              |
| 1:B:757:HIS:CB    | 1:B:764:THR:HG22 | 2.39                     | 0.47              |
| 1:B:136:VAL:HG12  | 1:B:139:LYS:HG3  | 1.97                     | 0.47              |
| 1:B:234:ASN:OD1   | 1:B:540:THR:OG1  | 2.33                     | 0.47              |
| 1:A:766:HIS:HE1   | 1:A:865:THR:HG21 | 1.79                     | 0.47              |
| 1:A:1168:TYR:O    | 1:A:1168:TYR:CD1 | 2.67                     | 0.46              |
| 1:B:1038:THR:O    | 1:B:1042:MET:HG2 | 2.15                     | 0.46              |
| 1:B:1295:ASP:OD1  | 1:B:1296:GLY:N   | 2.48                     | 0.46              |
| 1:B:1398:PRO:HA   | 1:B:1403:TYR:CG  | 2.50                     | 0.46              |
| 1:B:648:GLU:HB3   | 1:B:883:ILE:HD12 | 1.98                     | 0.46              |
| 1:A:1198:ARG:HA   | 1:A:1216:ASN:HA  | 1.97                     | 0.46              |
| 1:B:1168:TYR:CD1  | 1:B:1168:TYR:C   | 2.87                     | 0.46              |
| 1:A:1016:ARG:O    | 1:A:1020:LEU:HG  | 2.16                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1165:TYR:O    | 1:A:1167:PRO:HD2  | 2.14                     | 0.46              |
| 1:A:623:TYR:CD2   | 1:A:649:ILE:HD11  | 2.50                     | 0.46              |
| 1:A:1038:THR:O    | 1:A:1042:MET:HG2  | 2.15                     | 0.46              |
| 1:A:277:GLU:OE2   | 1:A:283:VAL:HG22  | 2.15                     | 0.46              |
| 1:B:925:VAL:HG13  | 1:B:1487:TRP:CZ2  | 2.50                     | 0.46              |
| 1:A:1077:ARG:NH1  | 1:A:1114:ASN:OD1  | 2.49                     | 0.46              |
| 1:B:925:VAL:HG11  | 1:B:1487:TRP:CE2  | 2.50                     | 0.46              |
| 1:B:281:TYR:N     | 1:B:282:PRO:HD3   | 2.31                     | 0.46              |
| 1:B:775:GLY:O     | 1:B:776:TRP:CD1   | 2.69                     | 0.46              |
| 1:A:154:LYS:NZ    | 1:A:190:ASN:O     | 2.49                     | 0.46              |
| 1:B:1016:ARG:O    | 1:B:1020:LEU:HG   | 2.16                     | 0.46              |
| 1:A:1106:THR:CG2  | 1:A:1113:PRO:HG3  | 2.46                     | 0.46              |
| 1:A:1434:TYR:OH   | 1:A:1474:ARG:HB3  | 2.16                     | 0.46              |
| 1:A:947:HIS:HD2   | 1:A:949:LEU:H     | 1.64                     | 0.46              |
| 1:B:623:TYR:CD2   | 1:B:649:ILE:HD11  | 2.50                     | 0.46              |
| 1:A:567:SER:HB3   | 1:A:573:ASP:OD1   | 2.16                     | 0.46              |
| 1:B:1264:VAL:HG11 | 1:B:1360:PHE:HA   | 1.98                     | 0.46              |
| 1:B:1077:ARG:NH1  | 1:B:1114:ASN:OD1  | 2.49                     | 0.46              |
| 1:B:1438:ILE:HG23 | 1:B:1518:LEU:HD22 | 1.98                     | 0.46              |
| 1:A:235:HIS:HA    | 1:A:502:LEU:HG    | 1.97                     | 0.46              |
| 1:B:149:GLN:HA    | 1:B:699:SER:O     | 2.16                     | 0.46              |
| 1:B:235:HIS:HA    | 1:B:502:LEU:HG    | 1.97                     | 0.46              |
| 1:A:1417:ALA:O    | 1:A:1422:ARG:HB2  | 2.15                     | 0.45              |
| 1:B:154:LYS:NZ    | 1:B:190:ASN:O     | 2.49                     | 0.45              |
| 1:B:1405:PRO:HA   | 1:B:1428:PRO:CD   | 2.46                     | 0.45              |
| 1:B:513:TYR:CE2   | 1:B:517:ARG:HD2   | 2.51                     | 0.45              |
| 1:B:567:SER:HB3   | 1:B:573:ASP:OD1   | 2.17                     | 0.45              |
| 1:A:648:GLU:HB3   | 1:A:883:ILE:HD12  | 1.98                     | 0.45              |
| 1:A:936:LEU:O     | 1:A:940:ILE:HG13  | 2.16                     | 0.45              |
| 1:B:427:LYS:HE2   | 1:B:433:ASP:OD2   | 2.16                     | 0.45              |
| 1:A:1151:LEU:HA   | 1:A:1180:ILE:HG22 | 1.97                     | 0.45              |
| 1:A:702:GLY:HA2   | 1:A:705:GLU:HB2   | 1.98                     | 0.45              |
| 1:A:834:THR:HG22  | 1:A:835:GLY:H     | 1.81                     | 0.45              |
| 1:B:1158:ARG:HD3  | 1:B:1173:ALA:HB1  | 1.99                     | 0.45              |
| 1:B:561:VAL:H     | 1:B:583:SER:HG    | 1.65                     | 0.45              |
| 1:A:1416:PHE:CE2  | 1:A:1422:ARG:NH2  | 2.85                     | 0.45              |
| 1:A:1495:ASN:O    | 1:A:1496:LYS:C    | 2.53                     | 0.45              |
| 1:A:231:ILE:HD12  | 1:A:532:PHE:CG    | 2.51                     | 0.45              |
| 1:B:1106:THR:CG2  | 1:B:1113:PRO:HG3  | 2.47                     | 0.45              |
| 1:A:1438:ILE:HG23 | 1:A:1518:LEU:HD22 | 1.98                     | 0.45              |
| 1:A:7:LEU:HD22    | 1:A:643:VAL:HG21  | 1.99                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1107:LEU:O    | 1:A:1157:ARG:NH1  | 2.50                     | 0.44              |
| 1:A:309:TRP:N     | 1:A:309:TRP:CD1   | 2.85                     | 0.44              |
| 1:B:742:ILE:HD12  | 1:B:776:TRP:CH2   | 2.51                     | 0.44              |
| 1:B:702:GLY:HA2   | 1:B:705:GLU:HB2   | 1.99                     | 0.44              |
| 1:A:149:GLN:HA    | 1:A:699:SER:O     | 2.18                     | 0.44              |
| 1:B:277:GLU:OE2   | 1:B:283:VAL:HG22  | 2.16                     | 0.44              |
| 1:A:234:ASN:OD1   | 1:A:540:THR:OG1   | 2.33                     | 0.44              |
| 1:B:1151:LEU:HA   | 1:B:1180:ILE:HG22 | 1.99                     | 0.44              |
| 1:A:618:LEU:HD22  | 1:A:933:VAL:HG13  | 1.99                     | 0.44              |
| 1:A:1043:VAL:HB   | 1:A:1092:ARG:HH22 | 1.82                     | 0.44              |
| 1:A:1508:GLN:HA   | 1:A:1508:GLN:OE1  | 2.17                     | 0.44              |
| 1:A:1116:LEU:HA   | 1:A:1122:PRO:HB3  | 1.99                     | 0.44              |
| 1:A:1290:GLU:HG2  | 1:A:1298:LYS:NZ   | 2.33                     | 0.44              |
| 1:B:231:ILE:HD12  | 1:B:532:PHE:CD1   | 2.53                     | 0.44              |
| 1:B:338:ILE:HG21  | 1:B:383:LEU:HG    | 2.00                     | 0.44              |
| 1:B:761:GLN:NE2   | 1:B:857:GLN:OE1   | 2.51                     | 0.44              |
| 1:B:322:GLU:HB3   | 1:B:373:ILE:HD13  | 1.99                     | 0.44              |
| 1:B:478:VAL:O     | 1:B:479:ASP:C     | 2.56                     | 0.44              |
| 1:B:467:ASN:HA    | 1:B:500:VAL:HA    | 2.00                     | 0.44              |
| 1:B:1219:VAL:HG13 | 1:B:1228:ILE:HG23 | 2.01                     | 0.43              |
| 1:B:156:MET:HG2   | 1:B:166:VAL:HG21  | 2.00                     | 0.43              |
| 1:B:738:MET:HB3   | 1:B:776:TRP:CH2   | 2.53                     | 0.43              |
| 1:A:322:GLU:HB3   | 1:A:373:ILE:HD13  | 1.99                     | 0.43              |
| 1:B:149:GLN:HG2   | 1:B:170:VAL:HG11  | 1.98                     | 0.43              |
| 1:A:1492:GLU:HA   | 1:A:1508:GLN:CG   | 2.49                     | 0.43              |
| 1:A:281:TYR:N     | 1:A:282:PRO:CD    | 2.82                     | 0.43              |
| 1:A:738:MET:HE1   | 1:A:776:TRP:CE2   | 2.53                     | 0.43              |
| 1:B:173:LYS:HE3   | 1:B:175:TYR:HE1   | 1.84                     | 0.43              |
| 1:B:231:ILE:HD12  | 1:B:532:PHE:CG    | 2.53                     | 0.43              |
| 1:B:716:GLU:OE2   | 1:B:718:ARG:NH1   | 2.51                     | 0.43              |
| 1:B:899:TYR:O     | 1:B:926:TYR:HB3   | 2.18                     | 0.43              |
| 1:A:656:THR:CG2   | 1:A:657:ALA:N     | 2.82                     | 0.43              |
| 1:A:716:GLU:OE2   | 1:A:718:ARG:NH1   | 2.52                     | 0.43              |
| 1:A:899:TYR:O     | 1:A:926:TYR:HB3   | 2.19                     | 0.43              |
| 1:B:1043:VAL:HB   | 1:B:1092:ARG:HH22 | 1.83                     | 0.43              |
| 1:A:338:ILE:HG21  | 1:A:383:LEU:HG    | 2.00                     | 0.43              |
| 1:A:436:PRO:O     | 1:A:437:LYS:HG2   | 2.19                     | 0.43              |
| 1:A:478:VAL:O     | 1:A:479:ASP:C     | 2.57                     | 0.43              |
| 1:A:1405:PRO:HA   | 1:A:1428:PRO:CD   | 2.48                     | 0.43              |
| 1:A:981:GLU:OE1   | 1:A:984:ARG:NH1   | 2.52                     | 0.43              |
| 1:B:953:LEU:HD13  | 1:B:999:PRO:HA    | 2.00                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:111:LEU:N    | 1:A:111:LEU:HD23  | 2.33                     | 0.43              |
| 1:A:561:VAL:H    | 1:A:583:SER:HG    | 1.65                     | 0.43              |
| 1:B:1108:LYS:CE  | 1:B:1159:PHE:HD1  | 2.31                     | 0.43              |
| 1:B:174:LYS:HG3  | 1:B:737:ASN:OD1   | 2.18                     | 0.43              |
| 1:B:170:VAL:HG21 | 1:B:178:ILE:HD11  | 2.01                     | 0.43              |
| 1:B:610:ILE:HD12 | 1:B:755:HIS:HB2   | 2.01                     | 0.43              |
| 1:A:1011:GLY:O   | 1:A:1012:CYS:C    | 2.55                     | 0.43              |
| 1:A:1198:ARG:O   | 1:A:1199:GLU:C    | 2.58                     | 0.43              |
| 1:B:1116:LEU:HA  | 1:B:1122:PRO:HB3  | 1.99                     | 0.43              |
| 1:B:1130:ALA:O   | 1:B:1133:PHE:HB3  | 2.19                     | 0.43              |
| 1:A:1042:MET:CE  | 1:A:1507:THR:HG22 | 2.48                     | 0.43              |
| 1:A:170:VAL:HG21 | 1:A:178:ILE:HD11  | 2.00                     | 0.43              |
| 1:A:775:GLY:HA3  | 1:A:865:THR:CG2   | 2.49                     | 0.43              |
| 1:B:618:LEU:HD22 | 1:B:933:VAL:HG13  | 2.00                     | 0.42              |
| 1:B:1181:GLU:OE1 | 1:B:1287:LYS:HG3  | 2.19                     | 0.42              |
| 1:B:893:SER:HA   | 1:B:896:TYR:CD2   | 2.54                     | 0.42              |
| 1:A:939:ILE:HD11 | 1:A:947:HIS:CD2   | 2.54                     | 0.42              |
| 1:B:1329:GLU:O   | 1:B:1330:ILE:HG23 | 2.20                     | 0.42              |
| 1:A:451:TYR:CE1  | 1:A:495:VAL:HG21  | 2.55                     | 0.42              |
| 1:A:925:VAL:HG11 | 1:A:1487:TRP:CE2  | 2.54                     | 0.42              |
| 1:A:1158:ARG:HD3 | 1:A:1173:ALA:HB1  | 2.01                     | 0.42              |
| 1:A:1329:GLU:O   | 1:A:1330:ILE:HG23 | 2.20                     | 0.42              |
| 1:B:1157:ARG:HG2 | 1:B:1176:TYR:OH   | 2.19                     | 0.42              |
| 1:B:391:GLY:HA2  | 1:B:394:GLU:OE1   | 2.18                     | 0.42              |
| 1:B:878:ILE:HD13 | 1:B:1001:PHE:HD1  | 1.85                     | 0.42              |
| 1:A:1130:ALA:O   | 1:A:1133:PHE:HB3  | 2.19                     | 0.42              |
| 1:A:775:GLY:O    | 1:A:776:TRP:CD1   | 2.72                     | 0.42              |
| 1:B:436:PRO:O    | 1:B:437:LYS:HG2   | 2.20                     | 0.42              |
| 1:B:775:GLY:HA3  | 1:B:865:THR:CG2   | 2.50                     | 0.42              |
| 1:A:149:GLN:HG2  | 1:A:170:VAL:HG11  | 2.02                     | 0.42              |
| 1:A:436:PRO:O    | 1:A:437:LYS:CG    | 2.67                     | 0.42              |
| 1:A:841:ASP:C    | 1:A:841:ASP:OD1   | 2.58                     | 0.42              |
| 1:B:1495:ASN:O   | 1:B:1496:LYS:C    | 2.58                     | 0.42              |
| 1:B:217:GLU:O    | 1:B:221:THR:HG23  | 2.19                     | 0.42              |
| 1:B:834:THR:HG22 | 1:B:835:GLY:H     | 1.84                     | 0.42              |
| 1:A:217:GLU:O    | 1:A:221:THR:HG23  | 2.19                     | 0.42              |
| 1:B:875:ASP:OD2  | 1:B:879:ARG:HD2   | 2.19                     | 0.42              |
| 1:B:1108:LYS:HD2 | 1:B:1109:HIS:CD2  | 2.55                     | 0.42              |
| 1:A:147:ALA:HA   | 1:A:697:ILE:O     | 2.19                     | 0.42              |
| 1:A:783:LYS:HG2  | 1:A:857:GLN:CB    | 2.46                     | 0.42              |
| 1:B:148:MET:HG3  | 1:B:177:MET:HG2   | 2.01                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:939:ILE:HD11  | 1:B:947:HIS:CD2   | 2.55                     | 0.42              |
| 1:A:1219:VAL:HG13 | 1:A:1228:ILE:HG23 | 2.01                     | 0.41              |
| 1:B:1050:SER:OG   | 1:B:1051:ILE:N    | 2.52                     | 0.41              |
| 1:B:1238:THR:HG21 | 1:B:1259:ARG:NH1  | 2.35                     | 0.41              |
| 1:B:1275:ARG:NH2  | 1:B:1366:VAL:O    | 2.53                     | 0.41              |
| 1:B:108:CYS:HB3   | 1:B:127:TYR:CD2   | 2.55                     | 0.41              |
| 1:B:1112:ILE:HD13 | 1:B:1133:PHE:CG   | 2.55                     | 0.41              |
| 1:A:618:LEU:HD12  | 1:A:937:ARG:HG3   | 2.03                     | 0.41              |
| 1:B:1042:MET:CE   | 1:B:1507:THR:HG22 | 2.50                     | 0.41              |
| 1:B:284:ASP:OD1   | 1:B:284:ASP:N     | 2.54                     | 0.41              |
| 1:A:276:MET:O     | 1:A:279:LEU:O     | 2.38                     | 0.41              |
| 1:A:1264:VAL:HG23 | 1:A:1343:ASP:O    | 2.20                     | 0.41              |
| 1:A:937:ARG:HG2   | 1:A:937:ARG:NH1   | 2.36                     | 0.41              |
| 1:A:691:ALA:HA    | 1:A:697:ILE:HD13  | 2.03                     | 0.41              |
| 1:B:792:LEU:HA    | 1:B:793:PRO:HD3   | 1.91                     | 0.41              |
| 1:A:150:SER:OG    | 1:A:179:HIS:HD2   | 2.04                     | 0.41              |
| 1:A:230:ASP:OD1   | 1:A:533:ARG:CD    | 2.60                     | 0.41              |
| 1:B:337:ASN:OD1   | 1:B:337:ASN:N     | 2.54                     | 0.41              |
| 1:B:436:PRO:O     | 1:B:437:LYS:CG    | 2.69                     | 0.41              |
| 1:A:1492:GLU:HB2  | 1:A:1508:GLN:HG2  | 2.03                     | 0.41              |
| 1:A:337:ASN:OD1   | 1:A:337:ASN:N     | 2.54                     | 0.41              |
| 1:A:149:GLN:OE1   | 1:A:701:TYR:HA    | 2.21                     | 0.41              |
| 1:A:878:ILE:HD13  | 1:A:1001:PHE:HD1  | 1.85                     | 0.41              |
| 1:B:1400:ASP:HA   | 4:B:2004:MLR:O6A  | 2.21                     | 0.41              |
| 1:B:620:ASP:OD1   | 1:B:620:ASP:N     | 2.53                     | 0.41              |
| 1:B:793:PRO:O     | 1:B:794:ARG:C     | 2.59                     | 0.41              |
| 1:A:1453:GLN:NE2  | 1:A:1461:LEU:HD21 | 2.36                     | 0.41              |
| 1:A:875:ASP:OD2   | 1:A:879:ARG:HD2   | 2.21                     | 0.41              |
| 1:B:425:ARG:NE    | 3:B:2005:CEX:O6D  | 2.54                     | 0.41              |
| 1:A:156:MET:HG2   | 1:A:166:VAL:HG21  | 2.03                     | 0.40              |
| 1:A:333:TRP:CH2   | 1:A:350:PHE:HZ    | 2.38                     | 0.40              |
| 1:B:1264:VAL:HG23 | 1:B:1343:ASP:O    | 2.21                     | 0.40              |
| 1:B:451:TYR:CE1   | 1:B:495:VAL:HG21  | 2.55                     | 0.40              |
| 1:A:1197:TYR:CE1  | 1:A:1217:VAL:HG23 | 2.56                     | 0.40              |
| 1:A:1342:LYS:HB2  | 1:A:1353:ASP:O    | 2.21                     | 0.40              |
| 1:B:1030:VAL:O    | 1:B:1031:PHE:C    | 2.60                     | 0.40              |
| 1:B:136:VAL:HG13  | 1:B:137:ASN:N     | 2.35                     | 0.40              |
| 1:B:230:ASP:OD1   | 1:B:533:ARG:CD    | 2.61                     | 0.40              |
| 1:B:936:LEU:O     | 1:B:940:ILE:HG13  | 2.21                     | 0.40              |
| 1:B:947:HIS:HD2   | 1:B:949:LEU:H     | 1.68                     | 0.40              |
| 1:A:738:MET:CE    | 1:A:776:TRP:CE2   | 3.04                     | 0.40              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:A:947:HIS:CD2  | 1:A:949:LEU:H   | 2.39                     | 0.40              |
| 1:A:953:LEU:HD13 | 1:A:999:PRO:HA  | 2.03                     | 0.40              |
| 1:B:181:THR:HB   | 1:B:182:PRO:HD2 | 2.03                     | 0.40              |
| 1:B:333:TRP:CH2  | 1:B:350:PHE:HZ  | 2.39                     | 0.40              |
| 1:B:111:LEU:HD23 | 1:B:111:LEU:N   | 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     | 1524/1528 (100%) | 1314 (86%) | 195 (13%) | 15 (1%)  | 18          | 53 |
| 1   | B     | 1524/1528 (100%) | 1321 (87%) | 188 (12%) | 15 (1%)  | 18          | 53 |
| All | All   | 3048/3056 (100%) | 2635 (86%) | 383 (13%) | 30 (1%)  | 18          | 53 |

All (30) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 887  | GLU  |
| 1   | B     | 887  | GLU  |
| 1   | A     | 440  | PRO  |
| 1   | A     | 723  | ALA  |
| 1   | A     | 1424 | TYR  |
| 1   | B     | 440  | PRO  |
| 1   | B     | 1424 | TYR  |
| 1   | A     | 219  | LEU  |
| 1   | A     | 282  | PRO  |
| 1   | A     | 308  | LEU  |
| 1   | B     | 308  | LEU  |
| 1   | B     | 723  | ALA  |
| 1   | B     | 727  | GLY  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 745  | GLU  |
| 1   | B     | 1026 | GLY  |
| 1   | B     | 1166 | ILE  |
| 1   | A     | 31   | PRO  |
| 1   | A     | 538  | HIS  |
| 1   | A     | 708  | PRO  |
| 1   | A     | 1166 | ILE  |
| 1   | A     | 1521 | ASP  |
| 1   | B     | 31   | PRO  |
| 1   | B     | 282  | PRO  |
| 1   | A     | 115  | ASN  |
| 1   | A     | 727  | GLY  |
| 1   | B     | 708  | PRO  |
| 1   | A     | 511  | SER  |
| 1   | B     | 511  | SER  |
| 1   | B     | 450  | PRO  |
| 1   | B     | 1373 | PRO  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed         | Rotameric  | Outliers  | Percentiles |    |
|-----|-------|------------------|------------|-----------|-------------|----|
| 1   | A     | 1344/1346 (100%) | 1157 (86%) | 187 (14%) | 4           | 20 |
| 1   | B     | 1344/1346 (100%) | 1157 (86%) | 187 (14%) | 4           | 20 |
| All | All   | 2688/2692 (100%) | 2314 (86%) | 374 (14%) | 4           | 20 |

All (374) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 7   | LEU  |
| 1   | A     | 14  | SER  |
| 1   | A     | 18  | VAL  |
| 1   | A     | 31  | PRO  |
| 1   | A     | 37  | GLN  |
| 1   | A     | 40  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 44  | MET  |
| 1   | A     | 67  | THR  |
| 1   | A     | 74  | SER  |
| 1   | A     | 78  | ASP  |
| 1   | A     | 79  | ARG  |
| 1   | A     | 81  | LYS  |
| 1   | A     | 86  | ILE  |
| 1   | A     | 89  | THR  |
| 1   | A     | 103 | VAL  |
| 1   | A     | 111 | LEU  |
| 1   | A     | 116 | ASP  |
| 1   | A     | 120 | LEU  |
| 1   | A     | 122 | THR  |
| 1   | A     | 135 | SER  |
| 1   | A     | 143 | LEU  |
| 1   | A     | 145 | SER  |
| 1   | A     | 149 | GLN  |
| 1   | A     | 153 | SER  |
| 1   | A     | 164 | GLU  |
| 1   | A     | 179 | HIS  |
| 1   | A     | 183 | LEU  |
| 1   | A     | 184 | GLN  |
| 1   | A     | 198 | GLN  |
| 1   | A     | 200 | GLU  |
| 1   | A     | 227 | SER  |
| 1   | A     | 229 | THR  |
| 1   | A     | 238 | ASN  |
| 1   | A     | 241 | GLN  |
| 1   | A     | 254 | LYS  |
| 1   | A     | 265 | LEU  |
| 1   | A     | 267 | LYS  |
| 1   | A     | 268 | LYS  |
| 1   | A     | 270 | LEU  |
| 1   | A     | 279 | LEU  |
| 1   | A     | 285 | LEU  |
| 1   | A     | 293 | LYS  |
| 1   | A     | 316 | VAL  |
| 1   | A     | 323 | LEU  |
| 1   | A     | 324 | ARG  |
| 1   | A     | 329 | ASN  |
| 1   | A     | 330 | SER  |
| 1   | A     | 333 | TRP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 334 | SER  |
| 1   | A     | 335 | ASP  |
| 1   | A     | 337 | ASN  |
| 1   | A     | 341 | LYS  |
| 1   | A     | 344 | SER  |
| 1   | A     | 346 | ASN  |
| 1   | A     | 357 | GLU  |
| 1   | A     | 363 | LEU  |
| 1   | A     | 371 | ILE  |
| 1   | A     | 383 | LEU  |
| 1   | A     | 389 | ASN  |
| 1   | A     | 395 | LEU  |
| 1   | A     | 400 | LEU  |
| 1   | A     | 409 | LYS  |
| 1   | A     | 415 | ILE  |
| 1   | A     | 421 | GLN  |
| 1   | A     | 423 | PHE  |
| 1   | A     | 425 | ARG  |
| 1   | A     | 427 | LYS  |
| 1   | A     | 431 | ILE  |
| 1   | A     | 445 | LEU  |
| 1   | A     | 447 | LEU  |
| 1   | A     | 449 | GLU  |
| 1   | A     | 456 | LYS  |
| 1   | A     | 473 | ASP  |
| 1   | A     | 477 | LEU  |
| 1   | A     | 489 | LEU  |
| 1   | A     | 491 | ARG  |
| 1   | A     | 499 | CYS  |
| 1   | A     | 510 | ASP  |
| 1   | A     | 520 | LYS  |
| 1   | A     | 536 | ASN  |
| 1   | A     | 553 | ARG  |
| 1   | A     | 565 | LEU  |
| 1   | A     | 583 | SER  |
| 1   | A     | 587 | ARG  |
| 1   | A     | 597 | GLU  |
| 1   | A     | 599 | SER  |
| 1   | A     | 601 | LEU  |
| 1   | A     | 609 | PRO  |
| 1   | A     | 616 | VAL  |
| 1   | A     | 631 | GLU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 649  | ILE  |
| 1   | A     | 650  | MET  |
| 1   | A     | 653  | LYS  |
| 1   | A     | 655  | LEU  |
| 1   | A     | 664  | PHE  |
| 1   | A     | 673  | THR  |
| 1   | A     | 704  | ASP  |
| 1   | A     | 712  | ASP  |
| 1   | A     | 726  | THR  |
| 1   | A     | 735  | LEU  |
| 1   | A     | 748  | ASP  |
| 1   | A     | 754  | MET  |
| 1   | A     | 757  | HIS  |
| 1   | A     | 758  | HIS  |
| 1   | A     | 764  | THR  |
| 1   | A     | 765  | PHE  |
| 1   | A     | 766  | HIS  |
| 1   | A     | 786  | SER  |
| 1   | A     | 798  | SER  |
| 1   | A     | 799  | GLN  |
| 1   | A     | 801  | LYS  |
| 1   | A     | 803  | THR  |
| 1   | A     | 818  | ILE  |
| 1   | A     | 822  | ILE  |
| 1   | A     | 824  | GLU  |
| 1   | A     | 831  | ARG  |
| 1   | A     | 865  | THR  |
| 1   | A     | 871  | ASP  |
| 1   | A     | 873  | SER  |
| 1   | A     | 889  | LEU  |
| 1   | A     | 900  | ARG  |
| 1   | A     | 908  | TYR  |
| 1   | A     | 913  | SER  |
| 1   | A     | 987  | MET  |
| 1   | A     | 999  | PRO  |
| 1   | A     | 1016 | ARG  |
| 1   | A     | 1023 | ASP  |
| 1   | A     | 1038 | THR  |
| 1   | A     | 1044 | SER  |
| 1   | A     | 1049 | THR  |
| 1   | A     | 1106 | THR  |
| 1   | A     | 1111 | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1112 | ILE  |
| 1   | A     | 1115 | LEU  |
| 1   | A     | 1116 | LEU  |
| 1   | A     | 1117 | ASP  |
| 1   | A     | 1123 | ARG  |
| 1   | A     | 1127 | ARG  |
| 1   | A     | 1134 | VAL  |
| 1   | A     | 1148 | VAL  |
| 1   | A     | 1149 | SER  |
| 1   | A     | 1150 | LEU  |
| 1   | A     | 1157 | ARG  |
| 1   | A     | 1161 | LEU  |
| 1   | A     | 1164 | GLU  |
| 1   | A     | 1166 | ILE  |
| 1   | A     | 1177 | SER  |
| 1   | A     | 1186 | GLU  |
| 1   | A     | 1190 | ARG  |
| 1   | A     | 1198 | ARG  |
| 1   | A     | 1206 | LEU  |
| 1   | A     | 1208 | ARG  |
| 1   | A     | 1210 | MET  |
| 1   | A     | 1227 | LEU  |
| 1   | A     | 1235 | ASN  |
| 1   | A     | 1245 | GLU  |
| 1   | A     | 1250 | ASN  |
| 1   | A     | 1265 | GLU  |
| 1   | A     | 1272 | SER  |
| 1   | A     | 1289 | THR  |
| 1   | A     | 1290 | GLU  |
| 1   | A     | 1291 | VAL  |
| 1   | A     | 1302 | SER  |
| 1   | A     | 1310 | GLU  |
| 1   | A     | 1321 | ASN  |
| 1   | A     | 1329 | GLU  |
| 1   | A     | 1337 | ARG  |
| 1   | A     | 1338 | ARG  |
| 1   | A     | 1346 | ARG  |
| 1   | A     | 1347 | SER  |
| 1   | A     | 1391 | VAL  |
| 1   | A     | 1401 | TYR  |
| 1   | A     | 1402 | ASN  |
| 1   | A     | 1404 | ARG  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1420 | LYS  |
| 1   | A     | 1424 | TYR  |
| 1   | A     | 1442 | HIS  |
| 1   | A     | 1454 | VAL  |
| 1   | A     | 1460 | LYS  |
| 1   | A     | 1469 | ARG  |
| 1   | A     | 1474 | ARG  |
| 1   | A     | 1476 | LEU  |
| 1   | A     | 1482 | ILE  |
| 1   | A     | 1494 | THR  |
| 1   | A     | 1510 | TRP  |
| 1   | A     | 1524 | ILE  |
| 1   | A     | 1528 | GLU  |
| 1   | B     | 7    | LEU  |
| 1   | B     | 14   | SER  |
| 1   | B     | 18   | VAL  |
| 1   | B     | 40   | LYS  |
| 1   | B     | 44   | MET  |
| 1   | B     | 61   | ARG  |
| 1   | B     | 62   | ASP  |
| 1   | B     | 67   | THR  |
| 1   | B     | 74   | SER  |
| 1   | B     | 78   | ASP  |
| 1   | B     | 79   | ARG  |
| 1   | B     | 81   | LYS  |
| 1   | B     | 86   | ILE  |
| 1   | B     | 89   | THR  |
| 1   | B     | 103  | VAL  |
| 1   | B     | 111  | LEU  |
| 1   | B     | 116  | ASP  |
| 1   | B     | 120  | LEU  |
| 1   | B     | 122  | THR  |
| 1   | B     | 135  | SER  |
| 1   | B     | 143  | LEU  |
| 1   | B     | 145  | SER  |
| 1   | B     | 149  | GLN  |
| 1   | B     | 153  | SER  |
| 1   | B     | 164  | GLU  |
| 1   | B     | 179  | HIS  |
| 1   | B     | 183  | LEU  |
| 1   | B     | 184  | GLN  |
| 1   | B     | 198  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 200 | GLU  |
| 1   | B     | 220 | ARG  |
| 1   | B     | 227 | SER  |
| 1   | B     | 229 | THR  |
| 1   | B     | 238 | ASN  |
| 1   | B     | 248 | GLU  |
| 1   | B     | 254 | LYS  |
| 1   | B     | 265 | LEU  |
| 1   | B     | 267 | LYS  |
| 1   | B     | 268 | LYS  |
| 1   | B     | 270 | LEU  |
| 1   | B     | 279 | LEU  |
| 1   | B     | 284 | ASP  |
| 1   | B     | 285 | LEU  |
| 1   | B     | 293 | LYS  |
| 1   | B     | 316 | VAL  |
| 1   | B     | 323 | LEU  |
| 1   | B     | 324 | ARG  |
| 1   | B     | 329 | ASN  |
| 1   | B     | 330 | SER  |
| 1   | B     | 333 | TRP  |
| 1   | B     | 334 | SER  |
| 1   | B     | 335 | ASP  |
| 1   | B     | 337 | ASN  |
| 1   | B     | 341 | LYS  |
| 1   | B     | 344 | SER  |
| 1   | B     | 346 | ASN  |
| 1   | B     | 357 | GLU  |
| 1   | B     | 371 | ILE  |
| 1   | B     | 383 | LEU  |
| 1   | B     | 389 | ASN  |
| 1   | B     | 395 | LEU  |
| 1   | B     | 398 | LYS  |
| 1   | B     | 400 | LEU  |
| 1   | B     | 409 | LYS  |
| 1   | B     | 415 | ILE  |
| 1   | B     | 417 | GLU  |
| 1   | B     | 421 | GLN  |
| 1   | B     | 423 | PHE  |
| 1   | B     | 425 | ARG  |
| 1   | B     | 427 | LYS  |
| 1   | B     | 431 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 433 | ASP  |
| 1   | B     | 445 | LEU  |
| 1   | B     | 447 | LEU  |
| 1   | B     | 449 | GLU  |
| 1   | B     | 456 | LYS  |
| 1   | B     | 468 | ASN  |
| 1   | B     | 473 | ASP  |
| 1   | B     | 477 | LEU  |
| 1   | B     | 489 | LEU  |
| 1   | B     | 499 | CYS  |
| 1   | B     | 510 | ASP  |
| 1   | B     | 520 | LYS  |
| 1   | B     | 536 | ASN  |
| 1   | B     | 553 | ARG  |
| 1   | B     | 565 | LEU  |
| 1   | B     | 583 | SER  |
| 1   | B     | 587 | ARG  |
| 1   | B     | 597 | GLU  |
| 1   | B     | 599 | SER  |
| 1   | B     | 601 | LEU  |
| 1   | B     | 609 | PRO  |
| 1   | B     | 616 | VAL  |
| 1   | B     | 649 | ILE  |
| 1   | B     | 650 | MET  |
| 1   | B     | 653 | LYS  |
| 1   | B     | 655 | LEU  |
| 1   | B     | 664 | PHE  |
| 1   | B     | 673 | THR  |
| 1   | B     | 704 | ASP  |
| 1   | B     | 726 | THR  |
| 1   | B     | 730 | LYS  |
| 1   | B     | 735 | LEU  |
| 1   | B     | 739 | ARG  |
| 1   | B     | 748 | ASP  |
| 1   | B     | 754 | MET  |
| 1   | B     | 757 | HIS  |
| 1   | B     | 758 | HIS  |
| 1   | B     | 764 | THR  |
| 1   | B     | 765 | PHE  |
| 1   | B     | 766 | HIS  |
| 1   | B     | 786 | SER  |
| 1   | B     | 798 | SER  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 799  | GLN  |
| 1   | B     | 801  | LYS  |
| 1   | B     | 803  | THR  |
| 1   | B     | 818  | ILE  |
| 1   | B     | 822  | ILE  |
| 1   | B     | 824  | GLU  |
| 1   | B     | 831  | ARG  |
| 1   | B     | 865  | THR  |
| 1   | B     | 871  | ASP  |
| 1   | B     | 873  | SER  |
| 1   | B     | 900  | ARG  |
| 1   | B     | 907  | ASP  |
| 1   | B     | 908  | TYR  |
| 1   | B     | 913  | SER  |
| 1   | B     | 987  | MET  |
| 1   | B     | 1016 | ARG  |
| 1   | B     | 1023 | ASP  |
| 1   | B     | 1038 | THR  |
| 1   | B     | 1044 | SER  |
| 1   | B     | 1049 | THR  |
| 1   | B     | 1106 | THR  |
| 1   | B     | 1111 | LEU  |
| 1   | B     | 1112 | ILE  |
| 1   | B     | 1115 | LEU  |
| 1   | B     | 1116 | LEU  |
| 1   | B     | 1117 | ASP  |
| 1   | B     | 1123 | ARG  |
| 1   | B     | 1134 | VAL  |
| 1   | B     | 1148 | VAL  |
| 1   | B     | 1149 | SER  |
| 1   | B     | 1150 | LEU  |
| 1   | B     | 1161 | LEU  |
| 1   | B     | 1164 | GLU  |
| 1   | B     | 1166 | ILE  |
| 1   | B     | 1177 | SER  |
| 1   | B     | 1186 | GLU  |
| 1   | B     | 1190 | ARG  |
| 1   | B     | 1198 | ARG  |
| 1   | B     | 1206 | LEU  |
| 1   | B     | 1210 | MET  |
| 1   | B     | 1227 | LEU  |
| 1   | B     | 1235 | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 1245 | GLU  |
| 1   | B     | 1265 | GLU  |
| 1   | B     | 1272 | SER  |
| 1   | B     | 1287 | LYS  |
| 1   | B     | 1289 | THR  |
| 1   | B     | 1290 | GLU  |
| 1   | B     | 1291 | VAL  |
| 1   | B     | 1302 | SER  |
| 1   | B     | 1310 | GLU  |
| 1   | B     | 1321 | ASN  |
| 1   | B     | 1324 | ASP  |
| 1   | B     | 1329 | GLU  |
| 1   | B     | 1337 | ARG  |
| 1   | B     | 1338 | ARG  |
| 1   | B     | 1346 | ARG  |
| 1   | B     | 1347 | SER  |
| 1   | B     | 1391 | VAL  |
| 1   | B     | 1401 | TYR  |
| 1   | B     | 1402 | ASN  |
| 1   | B     | 1420 | LYS  |
| 1   | B     | 1424 | TYR  |
| 1   | B     | 1442 | HIS  |
| 1   | B     | 1454 | VAL  |
| 1   | B     | 1455 | GLU  |
| 1   | B     | 1460 | LYS  |
| 1   | B     | 1469 | ARG  |
| 1   | B     | 1474 | ARG  |
| 1   | B     | 1476 | LEU  |
| 1   | B     | 1482 | ILE  |
| 1   | B     | 1494 | THR  |
| 1   | B     | 1510 | TRP  |
| 1   | B     | 1524 | ILE  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 37  | GLN  |
| 1   | A     | 92  | HIS  |
| 1   | A     | 179 | HIS  |
| 1   | A     | 238 | ASN  |
| 1   | A     | 354 | ASN  |
| 1   | A     | 605 | HIS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 766  | HIS  |
| 1   | A     | 790  | GLN  |
| 1   | A     | 866  | GLN  |
| 1   | A     | 876  | HIS  |
| 1   | A     | 947  | HIS  |
| 1   | A     | 1309 | GLN  |
| 1   | A     | 1355 | GLN  |
| 1   | A     | 1409 | ASN  |
| 1   | A     | 1442 | HIS  |
| 1   | A     | 1453 | GLN  |
| 1   | B     | 92   | HIS  |
| 1   | B     | 179  | HIS  |
| 1   | B     | 238  | ASN  |
| 1   | B     | 241  | GLN  |
| 1   | B     | 253  | HIS  |
| 1   | B     | 354  | ASN  |
| 1   | B     | 766  | HIS  |
| 1   | B     | 790  | GLN  |
| 1   | B     | 866  | GLN  |
| 1   | B     | 876  | HIS  |
| 1   | B     | 947  | HIS  |
| 1   | B     | 1250 | ASN  |
| 1   | B     | 1355 | GLN  |
| 1   | B     | 1409 | ASN  |
| 1   | B     | 1442 | HIS  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

11 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$ |
| 2   | MTT  | A     | 2001 | -    | 48,48,48     | 1.15 | 4 (8%)      | 71,71,71    | 1.19 | 7 (9%)      |
| 3   | CEX  | A     | 2002 | -    | 60,60,60     | 0.98 | 4 (6%)      | 89,89,89    | 1.11 | 8 (8%)      |
| 2   | MTT  | A     | 2003 | -    | 47,47,48     | 0.98 | 3 (6%)      | 68,69,71    | 1.25 | 7 (10%)     |
| 4   | MLR  | A     | 2004 | -    | 36,36,36     | 1.11 | 5 (13%)     | 53,53,53    | 1.43 | 8 (15%)     |
| 3   | CEX  | A     | 2005 | -    | 60,60,60     | 1.00 | 5 (8%)      | 89,89,89    | 1.12 | 6 (6%)      |
| 2   | MTT  | A     | 2006 | -    | 47,47,48     | 1.14 | 3 (6%)      | 68,69,71    | 1.24 | 6 (8%)      |
| 2   | MTT  | B     | 2001 | -    | 48,48,48     | 1.13 | 2 (4%)      | 71,71,71    | 1.38 | 12 (16%)    |
| 3   | CEX  | B     | 2002 | -    | 60,60,60     | 1.14 | 7 (11%)     | 89,89,89    | 1.26 | 11 (12%)    |
| 2   | MTT  | B     | 2003 | -    | 47,47,48     | 1.16 | 7 (14%)     | 68,69,71    | 1.68 | 11 (16%)    |
| 4   | MLR  | B     | 2004 | -    | 36,36,36     | 0.78 | 0           | 53,53,53    | 1.13 | 4 (7%)      |
| 3   | CEX  | B     | 2005 | -    | 60,60,60     | 0.84 | 0           | 89,89,89    | 1.00 | 5 (5%)      |

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

| Mol | Type | Chain | Res  | Link | Chirals | Torsions     | Rings   |
|-----|------|-------|------|------|---------|--------------|---------|
| 2   | MTT  | A     | 2001 | -    | -       | 0/20/100/100 | 0/4/4/4 |
| 3   | CEX  | A     | 2002 | -    | -       | 0/26/126/126 | 0/5/5/5 |
| 2   | MTT  | A     | 2003 | -    | -       | 0/20/97/100  | 0/4/4/4 |
| 4   | MLR  | A     | 2004 | -    | -       | 0/14/74/74   | 0/3/3/3 |
| 3   | CEX  | A     | 2005 | -    | -       | 0/26/126/126 | 0/5/5/5 |
| 2   | MTT  | A     | 2006 | -    | -       | 0/20/97/100  | 0/4/4/4 |
| 2   | MTT  | B     | 2001 | -    | -       | 0/20/100/100 | 0/4/4/4 |
| 3   | CEX  | B     | 2002 | -    | -       | 0/26/126/126 | 0/5/5/5 |
| 2   | MTT  | B     | 2003 | -    | -       | 0/20/97/100  | 0/4/4/4 |
| 4   | MLR  | B     | 2004 | -    | -       | 0/14/74/74   | 0/3/3/3 |
| 3   | CEX  | B     | 2005 | -    | -       | 0/26/126/126 | 0/5/5/5 |

All (40) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2   | A     | 2003 | MTT  | O24-C24 | -2.02 | 1.39        | 1.43     |
| 3   | B     | 2002 | CEX  | O4A-C4A | 2.01  | 1.48        | 1.43     |
| 2   | A     | 2001 | MTT  | O34-C21 | 2.09  | 1.47        | 1.41     |
| 2   | A     | 2006 | MTT  | O15-C11 | 2.10  | 1.47        | 1.41     |
| 2   | B     | 2003 | MTT  | C43-C44 | 2.10  | 1.58        | 1.52     |
| 2   | A     | 2003 | MTT  | O44-C31 | 2.10  | 1.47        | 1.41     |
| 3   | A     | 2005 | CEX  | C3E-C4E | 2.13  | 1.57        | 1.52     |
| 3   | A     | 2002 | CEX  | O4D-C1E | 2.13  | 1.47        | 1.41     |
| 3   | B     | 2002 | CEX  | C4B-C5B | 2.15  | 1.58        | 1.52     |
| 4   | A     | 2004 | MLR  | O4A-C1B | 2.15  | 1.47        | 1.41     |
| 3   | A     | 2002 | CEX  | O4B-C1C | 2.16  | 1.47        | 1.41     |
| 3   | B     | 2002 | CEX  | O5E-C1E | 2.20  | 1.47        | 1.41     |
| 4   | A     | 2004 | MLR  | O5C-C1C | 2.20  | 1.47        | 1.41     |
| 3   | A     | 2005 | CEX  | O5A-C1A | 2.23  | 1.47        | 1.43     |
| 2   | B     | 2003 | MTT  | C42-C43 | 2.25  | 1.55        | 1.52     |
| 3   | A     | 2002 | CEX  | O4A-C1B | 2.26  | 1.47        | 1.41     |
| 3   | B     | 2002 | CEX  | O5D-C1D | 2.28  | 1.47        | 1.41     |
| 3   | A     | 2005 | CEX  | O5B-C1B | 2.32  | 1.47        | 1.41     |
| 4   | A     | 2004 | MLR  | O4B-C1C | 2.32  | 1.47        | 1.41     |
| 2   | B     | 2003 | MTT  | O44-C44 | 2.34  | 1.49        | 1.43     |
| 4   | A     | 2004 | MLR  | O5B-C1B | 2.36  | 1.47        | 1.41     |
| 2   | B     | 2003 | MTT  | O25-C21 | 2.37  | 1.47        | 1.41     |
| 2   | B     | 2003 | MTT  | O15-C11 | 2.42  | 1.47        | 1.41     |
| 3   | A     | 2005 | CEX  | O4A-C1B | 2.43  | 1.48        | 1.41     |
| 2   | B     | 2001 | MTT  | O24-C11 | 2.46  | 1.48        | 1.41     |
| 2   | A     | 2001 | MTT  | O15-C15 | 2.56  | 1.50        | 1.44     |
| 2   | A     | 2006 | MTT  | O35-C31 | 2.56  | 1.48        | 1.41     |
| 4   | A     | 2004 | MLR  | O5B-C5B | 2.60  | 1.50        | 1.44     |
| 2   | A     | 2006 | MTT  | O25-C21 | 2.60  | 1.48        | 1.41     |
| 2   | A     | 2003 | MTT  | O15-C11 | 2.66  | 1.48        | 1.41     |
| 3   | A     | 2005 | CEX  | C4E-C5E | 2.74  | 1.58        | 1.53     |
| 3   | B     | 2002 | CEX  | O4A-C1B | 2.78  | 1.49        | 1.41     |
| 3   | B     | 2002 | CEX  | O5B-C5B | 2.85  | 1.51        | 1.44     |
| 2   | A     | 2001 | MTT  | O24-C11 | 2.85  | 1.49        | 1.41     |
| 2   | B     | 2003 | MTT  | O44-C31 | 2.87  | 1.49        | 1.41     |
| 2   | B     | 2003 | MTT  | O34-C21 | 2.97  | 1.49        | 1.41     |
| 2   | A     | 2001 | MTT  | O15-C11 | 3.06  | 1.49        | 1.41     |
| 3   | A     | 2002 | CEX  | O5B-C1B | 3.14  | 1.49        | 1.41     |
| 2   | B     | 2001 | MTT  | O15-C11 | 3.36  | 1.50        | 1.41     |
| 3   | B     | 2002 | CEX  | O5B-C1B | 3.49  | 1.50        | 1.41     |

All (85) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | A     | 2001 | MTT  | C33-C34-C35 | -3.24 | 104.00      | 110.88   |
| 3   | B     | 2005 | CEX  | O4C-C1D-O5D | -3.03 | 103.35      | 110.70   |
| 2   | A     | 2001 | MTT  | C23-C24-C25 | -2.75 | 105.04      | 110.88   |
| 2   | B     | 2003 | MTT  | C23-C24-C25 | -2.60 | 105.36      | 110.88   |
| 2   | B     | 2003 | MTT  | O43-C43-C42 | -2.53 | 105.42      | 110.02   |
| 2   | B     | 2003 | MTT  | C33-C34-C35 | -2.51 | 105.54      | 110.88   |
| 3   | A     | 2002 | CEX  | C3D-C4D-C5D | -2.49 | 105.59      | 110.88   |
| 4   | B     | 2004 | MLR  | O6A-C6A-C5A | -2.41 | 103.23      | 111.34   |
| 2   | B     | 2001 | MTT  | C33-C34-C35 | -2.29 | 106.01      | 110.88   |
| 4   | A     | 2004 | MLR  | C6B-C5B-C4B | -2.25 | 107.11      | 113.24   |
| 3   | A     | 2005 | CEX  | O4C-C1D-O5D | -2.25 | 105.25      | 110.70   |
| 3   | A     | 2005 | CEX  | C6A-C5A-C4A | -2.19 | 107.27      | 113.24   |
| 2   | A     | 2003 | MTT  | C46-C45-C44 | -2.13 | 107.43      | 113.24   |
| 3   | B     | 2002 | CEX  | C3E-C4E-C5E | -2.12 | 106.47      | 110.22   |
| 3   | B     | 2002 | CEX  | C3A-C4A-C5A | -2.12 | 106.38      | 110.88   |
| 4   | A     | 2004 | MLR  | C3A-C4A-C5A | -2.11 | 106.40      | 110.88   |
| 3   | A     | 2005 | CEX  | O6E-C6E-C5E | -2.11 | 104.25      | 111.34   |
| 3   | B     | 2002 | CEX  | C6C-C5C-C4C | -2.11 | 107.49      | 113.24   |
| 3   | A     | 2002 | CEX  | C6A-C5A-C4A | -2.09 | 107.54      | 113.24   |
| 3   | A     | 2002 | CEX  | C4E-C3E-C2E | -2.07 | 107.18      | 110.84   |
| 2   | B     | 2001 | MTT  | O16-C16-C15 | -2.06 | 104.41      | 111.34   |
| 2   | A     | 2003 | MTT  | O16-C16-C15 | -2.02 | 104.56      | 111.34   |
| 4   | A     | 2004 | MLR  | O6C-C6C-C5C | -2.01 | 104.59      | 111.34   |
| 2   | B     | 2001 | MTT  | O46-C46-C45 | -2.00 | 104.61      | 111.34   |
| 3   | A     | 2002 | CEX  | O5A-C5A-C4A | 2.00  | 113.85      | 109.75   |
| 2   | B     | 2001 | MTT  | O45-C45-C44 | 2.01  | 113.87      | 109.75   |
| 3   | A     | 2005 | CEX  | C3C-C4C-C5C | 2.02  | 115.17      | 110.88   |
| 3   | B     | 2002 | CEX  | O5B-C5B-C6B | 2.05  | 111.33      | 106.41   |
| 2   | B     | 2003 | MTT  | O23-C23-C24 | 2.06  | 114.55      | 109.87   |
| 2   | B     | 2001 | MTT  | O25-C25-C26 | 2.07  | 111.38      | 106.41   |
| 2   | B     | 2001 | MTT  | O15-C15-C16 | 2.08  | 111.38      | 106.41   |
| 2   | A     | 2003 | MTT  | O35-C35-C36 | 2.09  | 111.41      | 106.41   |
| 3   | B     | 2002 | CEX  | O5B-C5B-C4B | 2.09  | 114.03      | 109.75   |
| 3   | A     | 2002 | CEX  | O5C-C5C-C6C | 2.12  | 111.49      | 106.41   |
| 3   | B     | 2002 | CEX  | O5E-C5E-C6E | 2.15  | 111.55      | 106.41   |
| 3   | B     | 2005 | CEX  | C3E-C4E-C5E | 2.15  | 114.00      | 110.22   |
| 2   | A     | 2006 | MTT  | O34-C34-C35 | 2.16  | 114.67      | 109.34   |
| 4   | A     | 2004 | MLR  | O4A-C1B-C2B | 2.18  | 113.03      | 108.11   |
| 3   | B     | 2002 | CEX  | O5D-C5D-C6D | 2.21  | 111.69      | 106.41   |
| 2   | A     | 2003 | MTT  | C42-C43-C44 | 2.22  | 114.96      | 110.47   |
| 3   | B     | 2005 | CEX  | O5E-C5E-C4E | 2.23  | 113.78      | 109.66   |
| 2   | B     | 2001 | MTT  | C42-C43-C44 | 2.23  | 114.24      | 109.61   |
| 2   | B     | 2001 | MTT  | O25-C25-C24 | 2.26  | 114.38      | 109.75   |

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| Mol | Chain | Res  | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 2   | A     | 2001 | MTT  | C21-C22-C23 | 2.27 | 114.20      | 109.98   |
| 3   | B     | 2002 | CEX  | O4A-C1B-O5B | 2.30 | 116.28      | 110.70   |
| 2   | B     | 2001 | MTT  | C31-O35-C35 | 2.33 | 118.10      | 113.72   |
| 2   | B     | 2001 | MTT  | O24-C11-O15 | 2.38 | 116.46      | 110.70   |
| 2   | A     | 2006 | MTT  | O35-C31-C32 | 2.46 | 115.03      | 110.30   |
| 2   | A     | 2003 | MTT  | O25-C25-C26 | 2.46 | 112.31      | 106.41   |
| 2   | A     | 2001 | MTT  | O34-C21-C22 | 2.51 | 113.77      | 108.11   |
| 3   | B     | 2005 | CEX  | O5A-C5A-C6A | 2.55 | 112.53      | 106.41   |
| 2   | A     | 2006 | MTT  | C21-O34-C34 | 2.59 | 124.31      | 118.00   |
| 2   | B     | 2003 | MTT  | O34-C21-O25 | 2.65 | 117.14      | 110.70   |
| 3   | A     | 2002 | CEX  | O4A-C1B-O5B | 2.71 | 117.28      | 110.70   |
| 4   | A     | 2004 | MLR  | O5B-C5B-C4B | 2.73 | 115.33      | 109.75   |
| 3   | A     | 2002 | CEX  | C1A-O5A-C5A | 2.76 | 118.36      | 113.39   |
| 3   | B     | 2002 | CEX  | O4A-C4A-C3A | 2.77 | 113.85      | 107.19   |
| 2   | B     | 2003 | MTT  | O45-C41-C42 | 2.82 | 115.21      | 110.79   |
| 2   | A     | 2001 | MTT  | O24-C11-O15 | 2.84 | 117.58      | 110.70   |
| 4   | B     | 2004 | MLR  | O5B-C5B-C4B | 2.87 | 115.63      | 109.75   |
| 4   | A     | 2004 | MLR  | C1C-O5C-C5C | 2.90 | 119.18      | 113.72   |
| 2   | B     | 2001 | MTT  | C11-O15-C15 | 2.99 | 119.34      | 113.72   |
| 3   | A     | 2002 | CEX  | O5B-C5B-C6B | 2.99 | 113.58      | 106.41   |
| 2   | A     | 2006 | MTT  | C31-O35-C35 | 3.00 | 119.37      | 113.72   |
| 2   | A     | 2001 | MTT  | O45-C45-C44 | 3.07 | 116.04      | 109.75   |
| 2   | A     | 2001 | MTT  | O15-C15-C16 | 3.09 | 113.81      | 106.41   |
| 3   | B     | 2005 | CEX  | C1D-O5D-C5D | 3.15 | 119.65      | 113.72   |
| 4   | A     | 2004 | MLR  | O5B-C5B-C6B | 3.17 | 114.00      | 106.41   |
| 4   | B     | 2004 | MLR  | C1C-O5C-C5C | 3.28 | 119.90      | 113.72   |
| 3   | A     | 2005 | CEX  | O5E-C5E-C4E | 3.41 | 115.94      | 109.66   |
| 3   | B     | 2002 | CEX  | O5C-C5C-C6C | 3.43 | 114.62      | 106.41   |
| 2   | A     | 2003 | MTT  | C41-O45-C45 | 3.46 | 116.94      | 112.17   |
| 2   | B     | 2003 | MTT  | C11-O15-C15 | 3.50 | 120.31      | 113.72   |
| 4   | B     | 2004 | MLR  | C1B-O5B-C5B | 3.60 | 120.50      | 113.72   |
| 2   | A     | 2006 | MTT  | O15-C15-C16 | 3.76 | 115.41      | 106.41   |
| 3   | A     | 2005 | CEX  | C3E-C4E-C5E | 3.78 | 116.88      | 110.22   |
| 2   | A     | 2006 | MTT  | C21-O25-C25 | 3.81 | 120.89      | 113.72   |
| 2   | B     | 2003 | MTT  | C41-C42-C43 | 3.98 | 114.69      | 109.65   |
| 2   | B     | 2003 | MTT  | C42-C43-C44 | 3.98 | 118.53      | 110.47   |
| 2   | B     | 2003 | MTT  | O25-C25-C26 | 4.04 | 116.08      | 106.41   |
| 2   | A     | 2003 | MTT  | C11-O15-C15 | 4.22 | 121.67      | 113.72   |
| 2   | B     | 2001 | MTT  | C21-O25-C25 | 5.34 | 123.77      | 113.72   |
| 4   | A     | 2004 | MLR  | C1B-O5B-C5B | 5.61 | 124.28      | 113.72   |
| 3   | B     | 2002 | CEX  | C1B-O5B-C5B | 6.10 | 125.20      | 113.72   |
| 2   | B     | 2003 | MTT  | C41-O45-C45 | 6.55 | 121.20      | 112.17   |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 4   | B     | 2004 | MLR  | 1       | 0            |
| 3   | B     | 2005 | CEX  | 1       | 0            |

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ > 2 |    |    | OWAB(Å <sup>2</sup> ) | Q < 0.9 |
|-----|-------|-----------------|--------|-----------|----|----|-----------------------|---------|
| 1   | A     | 1526/1528 (99%) | 0.06   | 49 (3%)   | 48 | 46 | 50, 86, 144, 176      | 0       |
| 1   | B     | 1526/1528 (99%) | 0.07   | 60 (3%)   | 40 | 37 | 50, 83, 146, 191      | 0       |
| All | All   | 3052/3056 (99%) | 0.07   | 109 (3%)  | 43 | 40 | 50, 85, 145, 191      | 0       |

All (109) RSRZ outliers are listed below:

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | A     | 281  | TYR  | 5.7  |
| 1   | B     | 1245 | GLU  | 5.7  |
| 1   | A     | 1457 | SER  | 5.5  |
| 1   | A     | 1458 | ALA  | 4.7  |
| 1   | B     | 289  | ASP  | 4.1  |
| 1   | B     | 1244 | GLY  | 4.1  |
| 1   | B     | 427  | LYS  | 4.1  |
| 1   | B     | 288  | VAL  | 4.0  |
| 1   | B     | 488  | TYR  | 3.8  |
| 1   | B     | 1242 | LYS  | 3.7  |
| 1   | B     | 308  | LEU  | 3.6  |
| 1   | B     | 1206 | LEU  | 3.5  |
| 1   | A     | 363  | LEU  | 3.5  |
| 1   | B     | 1165 | TYR  | 3.4  |
| 1   | B     | 489  | LEU  | 3.3  |
| 1   | A     | 1334 | ILE  | 3.3  |
| 1   | B     | 379  | ILE  | 3.3  |
| 1   | B     | 364  | GLY  | 3.2  |
| 1   | B     | 1224 | GLU  | 3.2  |
| 1   | B     | 423  | PHE  | 3.1  |
| 1   | A     | 282  | PRO  | 3.1  |
| 1   | B     | 425  | ARG  | 3.1  |
| 1   | B     | 1210 | MET  | 3.1  |
| 1   | A     | 1246 | SER  | 3.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | A     | 338  | ILE  | 3.1  |
| 1   | A     | 1328 | PHE  | 3.1  |
| 1   | B     | 426  | ILE  | 3.0  |
| 1   | B     | 371  | ILE  | 3.0  |
| 1   | B     | 1208 | ARG  | 3.0  |
| 1   | B     | 291  | LEU  | 3.0  |
| 1   | A     | 1301 | LEU  | 3.0  |
| 1   | B     | 1226 | GLY  | 2.9  |
| 1   | B     | 1412 | ASP  | 2.9  |
| 1   | B     | 283  | VAL  | 2.9  |
| 1   | A     | 438  | GLN  | 2.9  |
| 1   | B     | 447  | LEU  | 2.9  |
| 1   | A     | 273  | SER  | 2.8  |
| 1   | B     | 1416 | PHE  | 2.8  |
| 1   | A     | 337  | ASN  | 2.8  |
| 1   | A     | 309  | TRP  | 2.8  |
| 1   | B     | 298  | ILE  | 2.7  |
| 1   | B     | 421  | GLN  | 2.7  |
| 1   | A     | 275  | GLN  | 2.7  |
| 1   | B     | 1205 | ASN  | 2.7  |
| 1   | A     | 307  | LYS  | 2.7  |
| 1   | B     | 491  | ARG  | 2.7  |
| 1   | B     | 1246 | SER  | 2.7  |
| 1   | A     | 1298 | LYS  | 2.6  |
| 1   | A     | 1224 | GLU  | 2.6  |
| 1   | B     | 1223 | TRP  | 2.6  |
| 1   | B     | 493  | VAL  | 2.6  |
| 1   | B     | 424  | ASN  | 2.6  |
| 1   | B     | 1209 | VAL  | 2.6  |
| 1   | B     | 309  | TRP  | 2.6  |
| 1   | B     | 1204 | PRO  | 2.6  |
| 1   | B     | 303  | ILE  | 2.6  |
| 1   | B     | 384  | HIS  | 2.6  |
| 1   | A     | 1424 | TYR  | 2.5  |
| 1   | B     | 438  | GLN  | 2.5  |
| 1   | A     | 1247 | GLU  | 2.5  |
| 1   | A     | 283  | VAL  | 2.5  |
| 1   | A     | 312  | TYR  | 2.5  |
| 1   | B     | 251  | TYR  | 2.4  |
| 1   | B     | 307  | LYS  | 2.4  |
| 1   | A     | 339  | PRO  | 2.4  |
| 1   | B     | 269  | LEU  | 2.4  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | B     | 337  | ASN  | 2.4  |
| 1   | B     | 383  | LEU  | 2.3  |
| 1   | B     | 284  | ASP  | 2.3  |
| 1   | A     | 1243 | MET  | 2.3  |
| 1   | A     | 489  | LEU  | 2.3  |
| 1   | B     | 428  | TYR  | 2.3  |
| 1   | A     | 1223 | TRP  | 2.3  |
| 1   | A     | 423  | PHE  | 2.3  |
| 1   | B     | 1304 | TRP  | 2.3  |
| 1   | A     | 1514 | CYS  | 2.3  |
| 1   | A     | 1085 | GLY  | 2.3  |
| 1   | A     | 1456 | GLY  | 2.3  |
| 1   | A     | 447  | LEU  | 2.2  |
| 1   | B     | 292  | ILE  | 2.2  |
| 1   | A     | 1321 | ASN  | 2.2  |
| 1   | A     | 291  | LEU  | 2.2  |
| 1   | B     | 1267 | ASN  | 2.2  |
| 1   | B     | 681  | GLU  | 2.2  |
| 1   | A     | 350  | PHE  | 2.2  |
| 1   | A     | 1252 | VAL  | 2.2  |
| 1   | B     | 354  | ASN  | 2.2  |
| 1   | A     | 1345 | TYR  | 2.2  |
| 1   | B     | 504  | TYR  | 2.2  |
| 1   | A     | 407  | PHE  | 2.2  |
| 1   | A     | 439  | GLY  | 2.2  |
| 1   | A     | 426  | ILE  | 2.2  |
| 1   | A     | 434  | HIS  | 2.2  |
| 1   | A     | 1319 | PRO  | 2.1  |
| 1   | B     | 1334 | ILE  | 2.1  |
| 1   | B     | 376  | PHE  | 2.1  |
| 1   | A     | 1354 | TYR  | 2.1  |
| 1   | A     | 111  | LEU  | 2.1  |
| 1   | A     | 295  | MET  | 2.1  |
| 1   | B     | 1121 | ASN  | 2.1  |
| 1   | A     | 272  | PHE  | 2.1  |
| 1   | B     | 1227 | LEU  | 2.1  |
| 1   | A     | 292  | ILE  | 2.0  |
| 1   | B     | 287  | THR  | 2.0  |
| 1   | A     | 1208 | ARG  | 2.0  |
| 1   | B     | 1203 | GLY  | 2.0  |
| 1   | B     | 492  | GLU  | 2.0  |
| 1   | A     | 347  | LEU  | 2.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 269 | LEU  | 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(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|----------------------------|-------|
| 2   | MTT  | A     | 2001 | 45/45 | 0.82 | 0.38 | 3.67  | 98,123,149,171             | 0     |
| 3   | CEX  | A     | 2005 | 56/56 | 0.69 | 0.38 | 1.66  | 131,176,203,208            | 0     |
| 3   | CEX  | A     | 2002 | 56/56 | 0.86 | 0.39 | 0.71  | 112,136,159,173            | 0     |
| 2   | MTT  | B     | 2001 | 45/45 | 0.82 | 0.27 | 0.69  | 102,127,153,162            | 0     |
| 3   | CEX  | B     | 2002 | 56/56 | 0.88 | 0.48 | 0.68  | 105,128,144,145            | 0     |
| 3   | CEX  | B     | 2005 | 56/56 | 0.48 | 0.43 | 0.53  | 137,177,205,211            | 0     |
| 4   | MLR  | A     | 2004 | 34/34 | 0.85 | 0.26 | -0.08 | 129,164,179,185            | 0     |
| 2   | MTT  | A     | 2006 | 44/45 | 0.62 | 0.29 | -0.13 | 113,158,188,196            | 0     |
| 4   | MLR  | B     | 2004 | 34/34 | 0.85 | 0.19 | -0.36 | 114,134,162,190            | 0     |
| 2   | MTT  | A     | 2003 | 44/45 | 0.89 | 0.18 | -0.52 | 71,114,131,135             | 0     |
| 2   | MTT  | B     | 2003 | 44/45 | 0.87 | 0.23 | -0.71 | 91,116,130,136             | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.