



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 11:05 AM UTC

PDB ID : 6DQG / pdb\_00006dqq  
Title : Human glutamate dehydrogenase, H454Y mutant  
Authors : Smith, T.J.  
Deposited on : 2018-06-10  
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                     |
| Xtriage (Phenix)               | : | 2.0                                                              |
| EDS                            | : | 3.0                                                              |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4                           | : | 9.0.010 (Gargrove)                                               |
| Density-Fitness                | : | 1.0.12                                                           |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

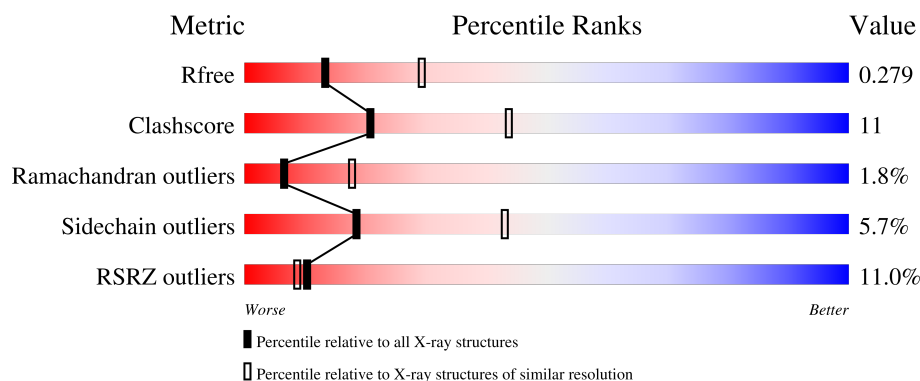
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 3538 (2.70-2.70)                                      |
| Clashscore            | 190562                      | 3843 (2.70-2.70)                                      |
| Ramachandran outliers | 187476                      | 3778 (2.70-2.70)                                      |
| Sidechain outliers    | 187428                      | 3778 (2.70-2.70)                                      |
| RSRZ outliers         | 180081                      | 3538 (2.70-2.70)                                      |

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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     | 496    | <div> <div>8%</div> <div>77%</div> <div>20%</div> <div>.</div> </div>   |
| 1   | B     | 496    | <div> <div>13%</div> <div>72%</div> <div>24%</div> <div>.</div> </div>  |
| 1   | C     | 496    | <div> <div>23%</div> <div>74%</div> <div>23%</div> <div>..</div> </div> |
| 1   | D     | 496    | <div> <div>10%</div> <div>72%</div> <div>24%</div> <div>.</div> </div>  |
| 1   | E     | 496    | <div> <div>3%</div> <div>73%</div> <div>23%</div> <div>.</div> </div>   |

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| Mol | Chain | Length | Quality of chain                                                                   |
|-----|-------|--------|------------------------------------------------------------------------------------|
| 1   | F     | 496    |  |

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   | PO4  | A     | 1001 | -         | -        | X       | -                |
| 2   | PO4  | D     | 603  | -         | -        | X       | -                |

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 23591 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 Glutamate dehydrogenase 1, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 496      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3876  | 2453 | 677 | 727 | 19 |         |         |       |
| 1   | B     | 496      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3876  | 2453 | 677 | 727 | 19 |         |         |       |
| 1   | C     | 496      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3876  | 2453 | 677 | 727 | 19 |         |         |       |
| 1   | D     | 496      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3876  | 2453 | 677 | 727 | 19 |         |         |       |
| 1   | E     | 496      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3876  | 2453 | 677 | 727 | 19 |         |         |       |
| 1   | F     | 496      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3876  | 2453 | 677 | 727 | 19 |         |         |       |

There are 6 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| A     | 454     | TYR      | HIS    | engineered mutation | UNP P00367 |
| B     | 454     | TYR      | HIS    | engineered mutation | UNP P00367 |
| C     | 454     | TYR      | HIS    | engineered mutation | UNP P00367 |
| D     | 454     | TYR      | HIS    | engineered mutation | UNP P00367 |
| E     | 454     | TYR      | HIS    | engineered mutation | UNP P00367 |
| F     | 454     | TYR      | HIS    | engineered mutation | UNP P00367 |

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O<sub>4</sub>P).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 2   | A     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | B     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | B     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | C     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | C     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | D     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | D     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | D     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | E     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | E     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | E     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | F     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | F     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | F     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

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| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 2   | F     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

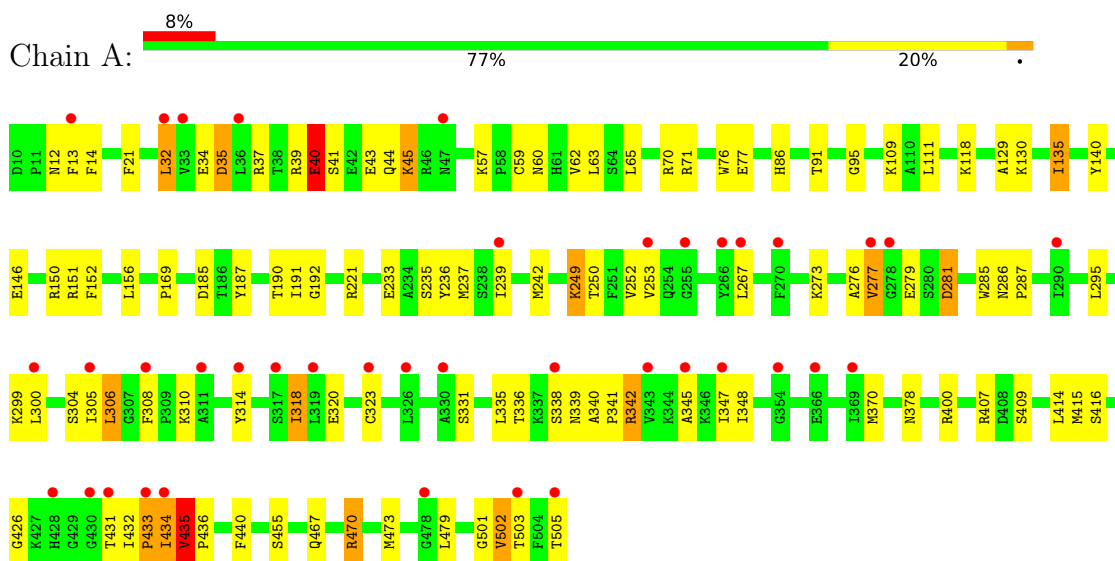
- Molecule 3 is water.

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 3   | A     | 31       | Total | O  | 0       | 0       |
|     |       |          | 31    | 31 |         |         |
| 3   | B     | 51       | Total | O  | 0       | 0       |
|     |       |          | 51    | 51 |         |         |
| 3   | C     | 46       | Total | O  | 0       | 0       |
|     |       |          | 46    | 46 |         |         |
| 3   | D     | 49       | Total | O  | 0       | 0       |
|     |       |          | 49    | 49 |         |         |
| 3   | E     | 47       | Total | O  | 0       | 0       |
|     |       |          | 47    | 47 |         |         |
| 3   | F     | 36       | Total | O  | 0       | 0       |
|     |       |          | 36    | 36 |         |         |

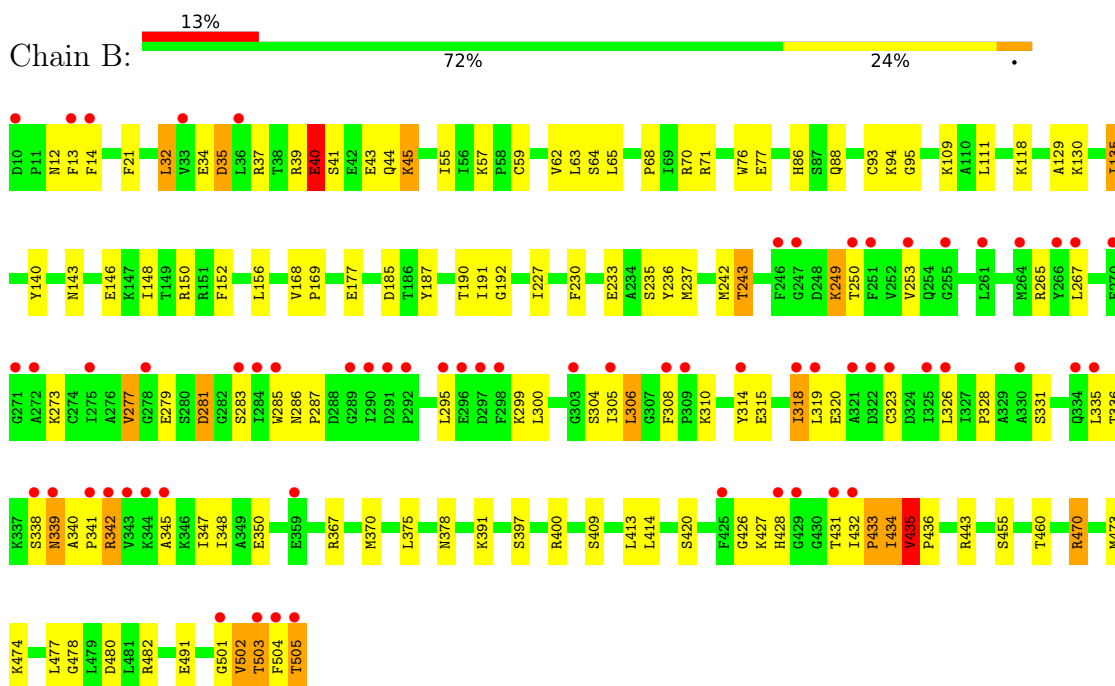
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

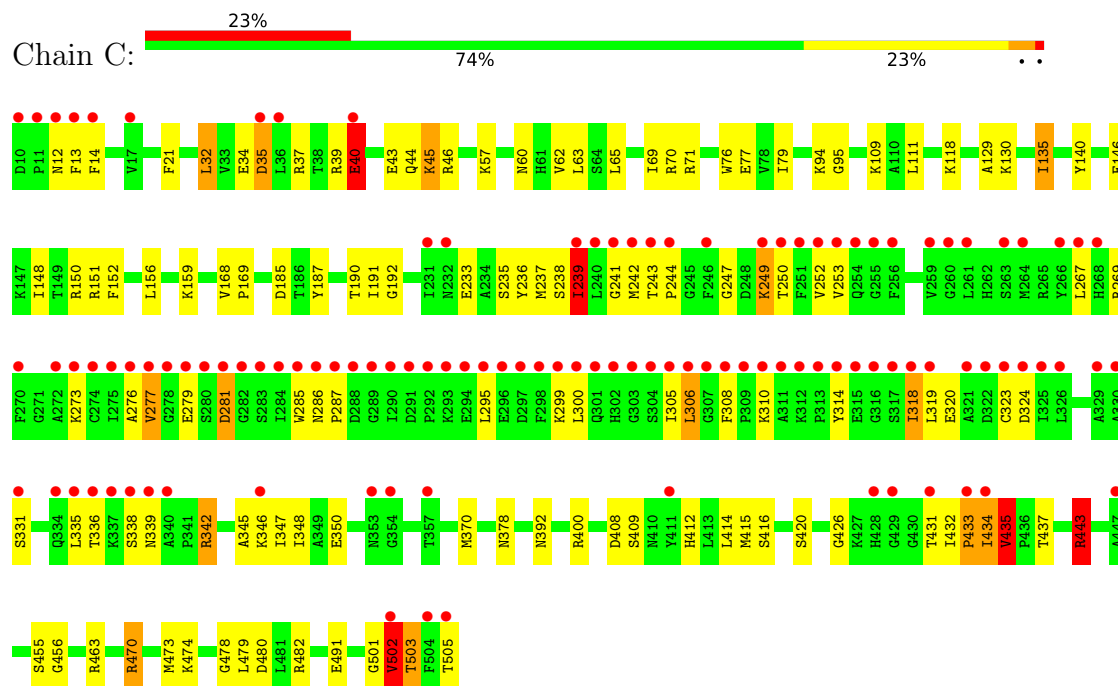
- Molecule 1: Glutamate dehydrogenase 1, mitochondrial



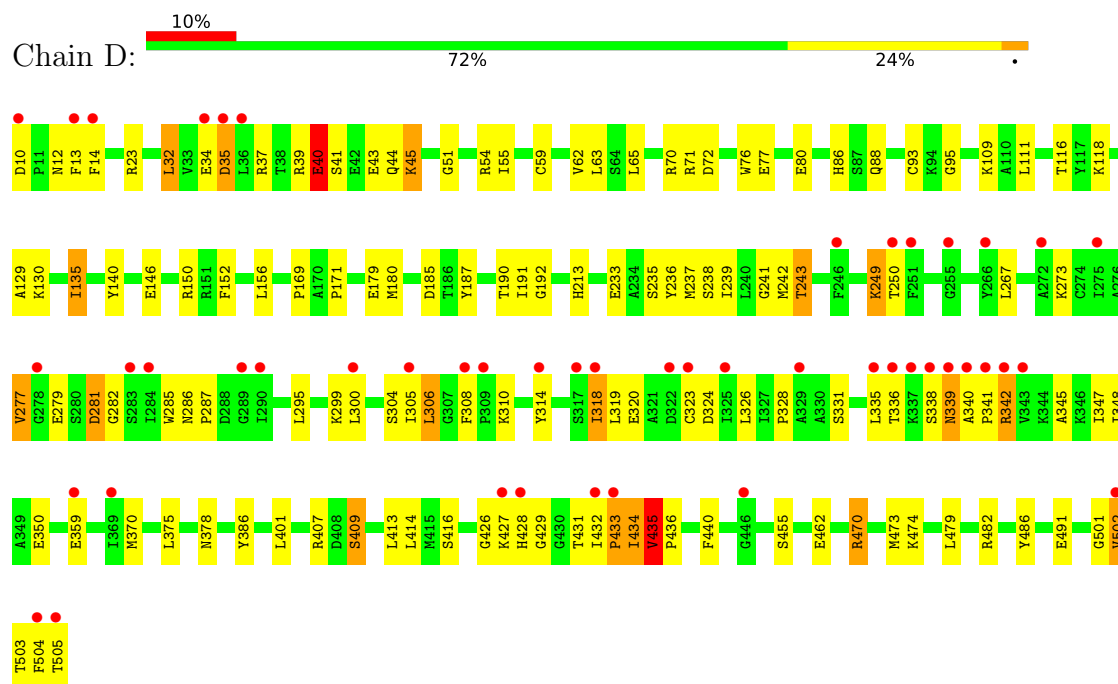
- Molecule 1: Glutamate dehydrogenase 1, mitochondrial



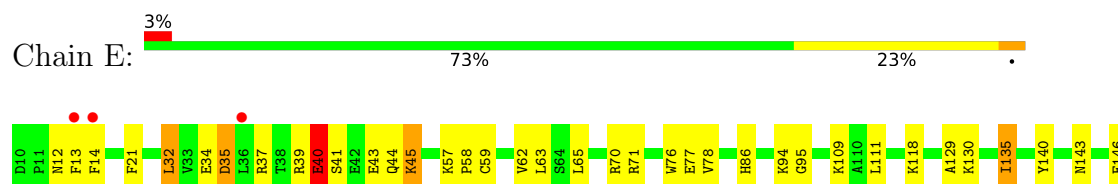
• Molecule 1: Glutamate dehydrogenase 1, mitochondrial

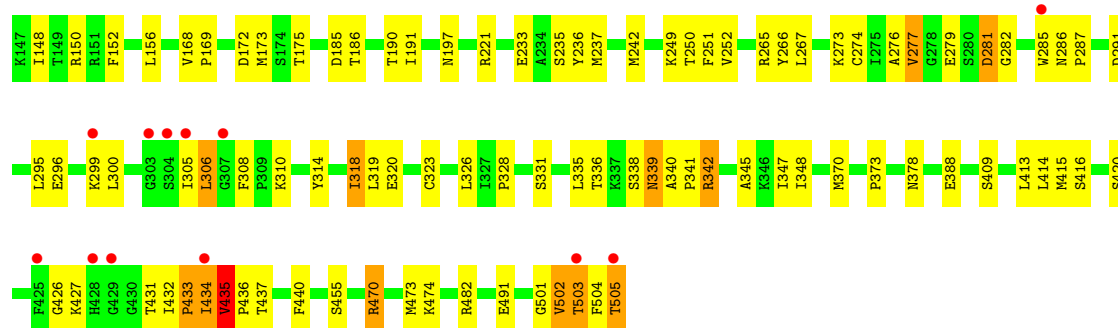


• Molecule 1: Glutamate dehydrogenase 1, mitochondrial

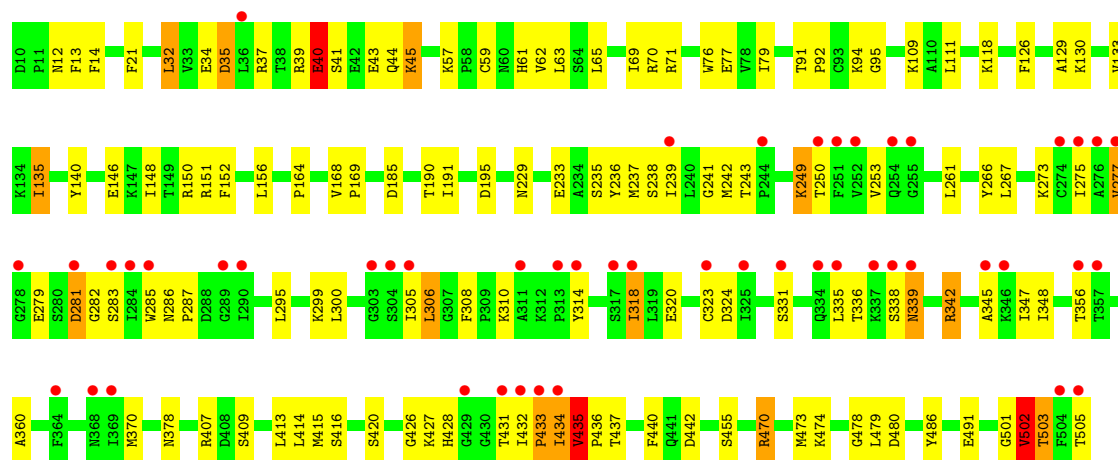


• Molecule 1: Glutamate dehydrogenase 1, mitochondrial





• Molecule 1: Glutamate dehydrogenase 1, mitochondrial



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 1                                                         | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 96.80Å 98.38Å 124.30Å<br>85.94° 69.35° 61.00°               | Depositor        |
| Resolution (Å)                                                          | 29.77 – 2.70<br>29.77 – 2.70                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 88.9 (29.77-2.70)<br>88.8 (29.77-2.70)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 0.63 (at 2.68Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX 1.12_2829                                            | Depositor        |
| R, $R_{free}$                                                           | 0.241 , 0.279<br>0.243 , 0.279                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 4609 reflections (4.50%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 45.7                                                        | Xtriage          |
| Anisotropy                                                              | 0.455                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.33 , 47.5                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$ | Xtriage          |
| Estimated twinning fraction                                             | 0.008 for h,h-k,h-l                                         | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.91                                                        | EDS              |
| Total number of atoms                                                   | 23591                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 61.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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     | 0.34         | 0/3960      | 0.59        | 3/5343 (0.1%)   |
| 1   | B     | 0.39         | 0/3960      | 0.60        | 3/5343 (0.1%)   |
| 1   | C     | 0.41         | 0/3960      | 0.67        | 6/5343 (0.1%)   |
| 1   | D     | 0.39         | 0/3960      | 0.54        | 0/5343          |
| 1   | E     | 0.38         | 0/3960      | 0.54        | 0/5343          |
| 1   | F     | 0.37         | 0/3960      | 0.54        | 0/5343          |
| All | All   | 0.38         | 0/23760     | 0.58        | 12/32058 (0.0%) |

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                   | 1                   |
| 1   | C     | 0                   | 1                   |
| 1   | D     | 0                   | 1                   |
| 1   | E     | 0                   | 1                   |
| 1   | F     | 0                   | 3                   |
| All | All   | 0                   | 10                  |

There are no bond length outliers.

All (12) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1   | C     | 46  | ARG  | NE-CZ-NH2 | 12.18  | 130.16      | 119.20   |
| 1   | C     | 443 | ARG  | NE-CZ-NH2 | 12.10  | 130.09      | 119.20   |
| 1   | A     | 221 | ARG  | NE-CZ-NH2 | 11.72  | 129.75      | 119.20   |
| 1   | C     | 46  | ARG  | NE-CZ-NH1 | -11.70 | 109.80      | 121.50   |

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| Mol | Chain | Res | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1   | A     | 221 | ARG  | NE-CZ-NH1 | -11.65 | 109.85      | 121.50   |
| 1   | C     | 443 | ARG  | NE-CZ-NH1 | -11.33 | 110.17      | 121.50   |
| 1   | B     | 367 | ARG  | NE-CZ-NH1 | -10.95 | 110.55      | 121.50   |
| 1   | B     | 367 | ARG  | NE-CZ-NH2 | 10.81  | 128.93      | 119.20   |
| 1   | C     | 46  | ARG  | CD-NE-CZ  | 9.33   | 137.47      | 124.40   |
| 1   | A     | 221 | ARG  | CD-NE-CZ  | 9.09   | 137.12      | 124.40   |
| 1   | C     | 443 | ARG  | CD-NE-CZ  | 8.96   | 136.95      | 124.40   |
| 1   | B     | 367 | ARG  | CD-NE-CZ  | 7.33   | 134.66      | 124.40   |

There are no chirality outliers.

All (10) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group             |
|-----|-------|-----|------|-------------------|
| 1   | A     | 433 | PRO  | Peptide           |
| 1   | A     | 91  | THR  | Mainchain,Peptide |
| 1   | B     | 433 | PRO  | Peptide           |
| 1   | C     | 433 | PRO  | Peptide           |
| 1   | D     | 433 | PRO  | Peptide           |
| 1   | E     | 433 | PRO  | Peptide           |
| 1   | F     | 433 | PRO  | Peptide           |
| 1   | F     | 91  | THR  | Mainchain,Peptide |

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 3876  | 0        | 3843     | 67      | 0            |
| 1   | B     | 3876  | 0        | 3843     | 101     | 0            |
| 1   | C     | 3876  | 0        | 3843     | 90      | 0            |
| 1   | D     | 3876  | 0        | 3843     | 102     | 0            |
| 1   | E     | 3876  | 0        | 3843     | 97      | 0            |
| 1   | F     | 3876  | 0        | 3843     | 91      | 0            |
| 2   | A     | 5     | 0        | 0        | 2       | 0            |
| 2   | B     | 10    | 0        | 0        | 1       | 0            |
| 2   | C     | 10    | 0        | 0        | 0       | 0            |
| 2   | D     | 15    | 0        | 0        | 3       | 0            |
| 2   | E     | 15    | 0        | 0        | 1       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | F     | 20    | 0        | 0        | 2       | 0            |
| 3   | A     | 31    | 0        | 0        | 7       | 0            |
| 3   | B     | 51    | 0        | 0        | 15      | 0            |
| 3   | C     | 46    | 0        | 0        | 13      | 0            |
| 3   | D     | 49    | 0        | 0        | 18      | 0            |
| 3   | E     | 47    | 0        | 0        | 15      | 0            |
| 3   | F     | 36    | 0        | 0        | 12      | 0            |
| All | All   | 23591 | 0        | 23058    | 513     | 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 11.

All (513) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:C:370:MET:SD  | 3:C:746:HOH:O    | 2.01                     | 1.18              |
| 1:B:227:ILE:O   | 3:B:702:HOH:O    | 1.85                     | 0.94              |
| 1:E:58:PRO:O    | 3:E:701:HOH:O    | 1.85                     | 0.94              |
| 1:B:315:GLU:OE2 | 3:B:701:HOH:O    | 1.84                     | 0.93              |
| 1:F:478:GLY:N   | 3:F:2101:HOH:O   | 2.00                     | 0.92              |
| 1:D:433:PRO:HA  | 1:E:420:SER:HB3  | 1.51                     | 0.92              |
| 1:B:88:GLN:OE1  | 3:B:703:HOH:O    | 1.88                     | 0.91              |
| 1:F:59:CYS:SG   | 3:F:2130:HOH:O   | 2.14                     | 0.90              |
| 1:B:177:GLU:OE1 | 3:B:704:HOH:O    | 1.91                     | 0.89              |
| 1:D:88:GLN:OE1  | 3:D:702:HOH:O    | 1.92                     | 0.88              |
| 1:D:72:ASP:OD2  | 3:D:701:HOH:O    | 1.92                     | 0.88              |
| 1:B:433:PRO:HA  | 1:F:420:SER:HB3  | 1.54                     | 0.88              |
| 1:F:59:CYS:SG   | 3:F:2120:HOH:O   | 2.28                     | 0.86              |
| 1:D:462:GLU:OE2 | 3:D:703:HOH:O    | 1.95                     | 0.84              |
| 1:D:10:ASP:N    | 3:D:706:HOH:O    | 2.12                     | 0.83              |
| 1:D:43:GLU:HG2  | 1:D:44:GLN:HG2   | 1.60                     | 0.82              |
| 1:E:43:GLU:HG2  | 1:E:44:GLN:HG2   | 1.60                     | 0.81              |
| 1:B:230:PHE:HB2 | 3:B:702:HOH:O    | 1.81                     | 0.81              |
| 1:A:43:GLU:HG2  | 1:A:44:GLN:HG2   | 1.62                     | 0.81              |
| 1:C:43:GLU:HG2  | 1:C:44:GLN:HG2   | 1.62                     | 0.81              |
| 1:A:467:GLN:O   | 3:A:1101:HOH:O   | 1.99                     | 0.80              |
| 1:B:177:GLU:HG2 | 3:B:727:HOH:O    | 1.82                     | 0.79              |
| 1:D:433:PRO:HA  | 1:E:420:SER:CB   | 2.12                     | 0.78              |
| 1:F:281:ASP:HB2 | 1:F:306:LEU:HD11 | 1.65                     | 0.78              |
| 1:B:43:GLU:HG2  | 1:B:44:GLN:HG2   | 1.63                     | 0.78              |
| 2:F:2003:PO4:O4 | 3:F:2102:HOH:O   | 2.01                     | 0.77              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:433:PRO:HA   | 1:F:420:SER:CB   | 2.14                     | 0.77              |
| 1:C:281:ASP:HB2  | 1:C:306:LEU:HD11 | 1.68                     | 0.76              |
| 1:A:281:ASP:HB2  | 1:A:306:LEU:HD11 | 1.67                     | 0.76              |
| 1:C:320:GLU:OE1  | 1:C:342:ARG:NH2  | 2.18                     | 0.76              |
| 1:C:408:ASP:OD2  | 3:C:702:HOH:O    | 2.04                     | 0.76              |
| 1:F:43:GLU:HG2   | 1:F:44:GLN:HG2   | 1.65                     | 0.76              |
| 1:E:281:ASP:HB2  | 1:E:306:LEU:HD11 | 1.69                     | 0.73              |
| 1:D:281:ASP:HB2  | 1:D:306:LEU:HD11 | 1.70                     | 0.73              |
| 1:C:286:ASN:ND2  | 3:C:701:HOH:O    | 2.02                     | 0.72              |
| 1:D:80:GLU:OE1   | 3:D:705:HOH:O    | 2.06                     | 0.72              |
| 1:B:320:GLU:OE1  | 1:B:342:ARG:NH2  | 2.23                     | 0.72              |
| 1:B:281:ASP:HB2  | 1:B:306:LEU:HD11 | 1.71                     | 0.72              |
| 1:E:265:ARG:HD3  | 3:E:706:HOH:O    | 1.90                     | 0.72              |
| 1:A:233:GLU:HG2  | 1:A:236:TYR:HD2  | 1.55                     | 0.71              |
| 1:B:478:GLY:N    | 3:B:708:HOH:O    | 2.23                     | 0.71              |
| 1:E:77:GLU:OE1   | 3:E:703:HOH:O    | 2.08                     | 0.71              |
| 1:C:233:GLU:HG2  | 1:C:236:TYR:HD2  | 1.54                     | 0.71              |
| 1:E:291:ASP:OD2  | 3:E:704:HOH:O    | 2.09                     | 0.71              |
| 1:F:229:ASN:O    | 3:F:2103:HOH:O   | 2.09                     | 0.71              |
| 1:E:71:ARG:NH1   | 3:E:708:HOH:O    | 2.23                     | 0.70              |
| 1:A:59:CYS:SG    | 3:A:1126:HOH:O   | 2.17                     | 0.70              |
| 1:C:118:LYS:NZ   | 1:C:378:ASN:OD1  | 2.25                     | 0.70              |
| 1:E:250:THR:HG22 | 1:E:273:LYS:HB3  | 1.72                     | 0.70              |
| 1:C:392:ASN:O    | 3:C:706:HOH:O    | 2.09                     | 0.70              |
| 1:B:150:ARG:NH2  | 1:B:185:ASP:OD2  | 2.25                     | 0.70              |
| 1:C:269:ARG:O    | 3:C:705:HOH:O    | 2.09                     | 0.70              |
| 1:E:150:ARG:NH2  | 1:E:185:ASP:OD2  | 2.25                     | 0.70              |
| 1:F:250:THR:HG22 | 1:F:273:LYS:HB3  | 1.73                     | 0.70              |
| 1:B:391:LYS:NZ   | 3:B:709:HOH:O    | 2.23                     | 0.70              |
| 1:A:407:ARG:NH1  | 3:A:1106:HOH:O   | 2.25                     | 0.69              |
| 2:A:1001:PO4:O2  | 3:A:1102:HOH:O   | 2.10                     | 0.69              |
| 1:D:250:THR:HG22 | 1:D:273:LYS:HB3  | 1.75                     | 0.69              |
| 1:F:150:ARG:NH2  | 1:F:185:ASP:OD2  | 2.25                     | 0.69              |
| 1:A:250:THR:HG22 | 1:A:273:LYS:HB3  | 1.73                     | 0.69              |
| 1:A:320:GLU:OE1  | 1:A:342:ARG:NH2  | 2.26                     | 0.68              |
| 1:E:233:GLU:HG2  | 1:E:236:TYR:HD2  | 1.58                     | 0.68              |
| 1:F:233:GLU:HG2  | 1:F:236:TYR:HD2  | 1.56                     | 0.68              |
| 1:F:320:GLU:OE1  | 1:F:342:ARG:NH2  | 2.26                     | 0.68              |
| 2:A:1001:PO4:O3  | 3:A:1103:HOH:O   | 2.11                     | 0.68              |
| 1:D:233:GLU:HG2  | 1:D:236:TYR:HD2  | 1.58                     | 0.68              |
| 1:D:320:GLU:OE1  | 1:D:342:ARG:NH2  | 2.27                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:407:ARG:NH1  | 3:F:2108:HOH:O   | 2.26                     | 0.68              |
| 1:D:23:ARG:NH2   | 3:D:709:HOH:O    | 2.17                     | 0.68              |
| 1:F:146:GLU:OE2  | 1:F:150:ARG:NH1  | 2.27                     | 0.67              |
| 1:E:320:GLU:OE1  | 1:E:342:ARG:NH2  | 2.28                     | 0.67              |
| 1:C:250:THR:HG22 | 1:C:273:LYS:HB3  | 1.77                     | 0.67              |
| 1:C:269:ARG:HG2  | 3:C:705:HOH:O    | 1.93                     | 0.67              |
| 1:E:175:THR:O    | 3:E:705:HOH:O    | 2.11                     | 0.67              |
| 1:B:233:GLU:HG2  | 1:B:236:TYR:HD2  | 1.58                     | 0.67              |
| 1:B:146:GLU:OE2  | 1:B:150:ARG:NH1  | 2.29                     | 0.66              |
| 1:B:55:ILE:O     | 3:B:705:HOH:O    | 2.13                     | 0.66              |
| 1:B:443:ARG:NH1  | 3:B:707:HOH:O    | 2.21                     | 0.65              |
| 1:A:150:ARG:NH2  | 1:A:185:ASP:OD2  | 2.29                     | 0.65              |
| 2:D:603:PO4:O2   | 3:D:708:HOH:O    | 2.14                     | 0.64              |
| 1:B:68:PRO:HB3   | 1:D:55:ILE:HG12  | 1.80                     | 0.64              |
| 1:B:243:THR:O    | 1:B:249:LYS:NZ   | 2.19                     | 0.64              |
| 1:B:250:THR:HG22 | 1:B:273:LYS:HB3  | 1.78                     | 0.64              |
| 1:C:150:ARG:NH2  | 1:C:185:ASP:OD2  | 2.31                     | 0.64              |
| 1:E:146:GLU:OE2  | 1:E:150:ARG:NH1  | 2.30                     | 0.63              |
| 1:B:491:GLU:OE1  | 3:B:706:HOH:O    | 2.15                     | 0.63              |
| 1:E:221:ARG:NE   | 3:E:702:HOH:O    | 2.02                     | 0.63              |
| 1:B:431:THR:HG22 | 1:B:433:PRO:HD3  | 1.80                     | 0.63              |
| 1:D:146:GLU:OE2  | 1:D:150:ARG:NH1  | 2.31                     | 0.63              |
| 1:A:146:GLU:OE2  | 1:A:150:ARG:NH1  | 2.32                     | 0.62              |
| 1:F:442:ASP:OD1  | 3:F:2104:HOH:O   | 2.16                     | 0.62              |
| 1:E:431:THR:HG22 | 1:E:433:PRO:HD3  | 1.82                     | 0.61              |
| 1:C:416:SER:OG   | 1:E:436:PRO:HA   | 2.00                     | 0.61              |
| 1:C:146:GLU:OE2  | 1:C:150:ARG:NH1  | 2.34                     | 0.61              |
| 1:D:150:ARG:NH2  | 1:D:185:ASP:OD2  | 2.32                     | 0.61              |
| 1:F:480:ASP:HB3  | 3:F:2101:HOH:O   | 2.00                     | 0.61              |
| 1:C:286:ASN:ND2  | 1:C:310:LYS:O    | 2.27                     | 0.61              |
| 1:A:277:VAL:HG21 | 1:A:295:LEU:HD21 | 1.83                     | 0.60              |
| 1:A:502:VAL:HB   | 1:E:76:TRP:CH2   | 2.36                     | 0.60              |
| 1:A:416:SER:HA   | 1:F:437:THR:HG23 | 1.84                     | 0.60              |
| 1:C:277:VAL:HG21 | 1:C:295:LEU:HD21 | 1.83                     | 0.60              |
| 1:D:277:VAL:HG21 | 1:D:295:LEU:HD21 | 1.82                     | 0.60              |
| 1:C:247:GLY:N    | 3:C:712:HOH:O    | 2.33                     | 0.60              |
| 1:D:431:THR:HG22 | 1:D:433:PRO:HD3  | 1.83                     | 0.60              |
| 1:E:296:GLU:OE1  | 3:E:706:HOH:O    | 2.16                     | 0.60              |
| 1:B:277:VAL:HG21 | 1:B:295:LEU:HD21 | 1.83                     | 0.59              |
| 1:E:427:LYS:NZ   | 3:E:712:HOH:O    | 2.29                     | 0.59              |
| 1:C:323:CYS:O    | 1:C:345:ALA:HA   | 2.02                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:277:VAL:HG21 | 1:F:295:LEU:HD21 | 1.83                     | 0.59              |
| 1:D:12:ASN:C     | 1:D:14:PHE:H     | 2.11                     | 0.59              |
| 1:E:277:VAL:HG21 | 1:E:295:LEU:HD21 | 1.84                     | 0.59              |
| 1:D:190:THR:OG1  | 1:D:191:ILE:N    | 2.36                     | 0.59              |
| 1:F:12:ASN:C     | 1:F:14:PHE:H     | 2.11                     | 0.59              |
| 1:B:12:ASN:C     | 1:B:14:PHE:H     | 2.11                     | 0.58              |
| 1:E:266:TYR:OH   | 2:E:602:PO4:O4   | 2.15                     | 0.58              |
| 1:A:12:ASN:C     | 1:A:14:PHE:H     | 2.12                     | 0.58              |
| 1:D:470:ARG:HA   | 1:D:473:MET:HE2  | 1.85                     | 0.58              |
| 1:D:95:GLY:HA3   | 1:D:129:ALA:O    | 2.03                     | 0.58              |
| 1:E:12:ASN:C     | 1:E:14:PHE:H     | 2.11                     | 0.57              |
| 1:E:197:ASN:ND2  | 3:E:720:HOH:O    | 2.37                     | 0.57              |
| 1:B:414:LEU:HB3  | 1:B:434:ILE:HA   | 1.86                     | 0.57              |
| 1:E:414:LEU:HB3  | 1:E:434:ILE:HA   | 1.85                     | 0.57              |
| 1:F:109:LYS:HB3  | 3:F:2130:HOH:O   | 2.03                     | 0.57              |
| 1:C:12:ASN:C     | 1:C:14:PHE:H     | 2.12                     | 0.57              |
| 1:B:434:ILE:HG23 | 1:B:435:VAL:H    | 1.69                     | 0.57              |
| 1:C:243:THR:O    | 1:C:249:LYS:NZ   | 2.23                     | 0.57              |
| 1:A:431:THR:HG22 | 1:A:433:PRO:HD3  | 1.86                     | 0.57              |
| 1:C:414:LEU:HB3  | 1:C:434:ILE:HA   | 1.87                     | 0.57              |
| 1:D:243:THR:O    | 1:D:249:LYS:NZ   | 2.27                     | 0.57              |
| 1:E:470:ARG:HA   | 1:E:473:MET:HE2  | 1.87                     | 0.57              |
| 1:F:190:THR:OG1  | 1:F:191:ILE:N    | 2.38                     | 0.57              |
| 1:A:286:ASN:ND2  | 1:A:310:LYS:O    | 2.28                     | 0.57              |
| 1:A:135:ILE:HG13 | 1:A:140:TYR:CE1  | 2.40                     | 0.57              |
| 1:E:135:ILE:HG13 | 1:E:140:TYR:CE1  | 2.40                     | 0.56              |
| 1:D:54:ARG:NH2   | 3:D:707:HOH:O    | 2.14                     | 0.56              |
| 1:D:414:LEU:HB3  | 1:D:434:ILE:HA   | 1.87                     | 0.56              |
| 1:E:434:ILE:HG23 | 1:E:435:VAL:H    | 1.69                     | 0.56              |
| 1:A:414:LEU:HB3  | 1:A:434:ILE:HA   | 1.88                     | 0.56              |
| 1:C:135:ILE:HG13 | 1:C:140:TYR:CE1  | 2.40                     | 0.56              |
| 1:D:118:LYS:NZ   | 1:D:378:ASN:OD1  | 2.39                     | 0.56              |
| 1:F:12:ASN:O     | 1:F:14:PHE:N     | 2.39                     | 0.56              |
| 1:F:434:ILE:HG23 | 1:F:435:VAL:H    | 1.71                     | 0.56              |
| 1:B:95:GLY:HA3   | 1:B:129:ALA:O    | 2.05                     | 0.56              |
| 1:C:151:ARG:NH1  | 1:F:503:THR:HG23 | 2.21                     | 0.56              |
| 1:A:470:ARG:HA   | 1:A:473:MET:HE2  | 1.88                     | 0.55              |
| 1:E:34:GLU:HA    | 1:E:37:ARG:O     | 2.06                     | 0.55              |
| 1:C:470:ARG:HA   | 1:C:473:MET:HE2  | 1.88                     | 0.55              |
| 1:F:135:ILE:HG13 | 1:F:140:TYR:CE1  | 2.41                     | 0.55              |
| 1:F:118:LYS:NZ   | 1:F:378:ASN:OD1  | 2.39                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:503:THR:HG23 | 1:F:151:ARG:HH11 | 1.72                     | 0.55              |
| 1:C:34:GLU:HA    | 1:C:37:ARG:O     | 2.07                     | 0.55              |
| 1:E:190:THR:OG1  | 1:E:191:ILE:N    | 2.40                     | 0.55              |
| 1:E:62:VAL:HG21  | 1:E:109:LYS:HD3  | 1.89                     | 0.54              |
| 1:F:431:THR:HG22 | 1:F:433:PRO:HD3  | 1.88                     | 0.54              |
| 1:A:95:GLY:HA3   | 1:A:129:ALA:O    | 2.07                     | 0.54              |
| 1:C:416:SER:HA   | 1:E:437:THR:HG23 | 1.89                     | 0.54              |
| 1:D:63:LEU:HD21  | 1:D:65:LEU:HD21  | 1.90                     | 0.54              |
| 1:F:146:GLU:O    | 1:F:150:ARG:HG3  | 2.07                     | 0.54              |
| 1:B:34:GLU:HA    | 1:B:37:ARG:O     | 2.07                     | 0.54              |
| 1:B:59:CYS:SG    | 3:B:744:HOH:O    | 2.15                     | 0.54              |
| 1:B:339:ASN:OD1  | 1:B:339:ASN:N    | 2.35                     | 0.54              |
| 1:D:179:GLU:OE1  | 3:D:710:HOH:O    | 2.18                     | 0.54              |
| 1:B:319:LEU:HD12 | 1:B:319:LEU:H    | 1.73                     | 0.54              |
| 1:B:76:TRP:O     | 3:D:707:HOH:O    | 2.19                     | 0.54              |
| 1:B:470:ARG:HA   | 1:B:473:MET:HE2  | 1.90                     | 0.54              |
| 1:D:323:CYS:O    | 1:D:345:ALA:HA   | 2.08                     | 0.54              |
| 1:B:12:ASN:O     | 1:B:14:PHE:N     | 2.41                     | 0.54              |
| 1:D:51:GLY:HA2   | 3:D:707:HOH:O    | 2.07                     | 0.54              |
| 1:F:323:CYS:O    | 1:F:345:ALA:HA   | 2.08                     | 0.54              |
| 1:E:323:CYS:O    | 1:E:345:ALA:HA   | 2.08                     | 0.54              |
| 1:F:486:TYR:OH   | 3:F:2105:HOH:O   | 2.18                     | 0.54              |
| 1:B:76:TRP:CH2   | 1:D:502:VAL:HB   | 2.44                     | 0.53              |
| 1:C:95:GLY:HA3   | 1:C:129:ALA:O    | 2.08                     | 0.53              |
| 1:D:146:GLU:O    | 1:D:150:ARG:HG3  | 2.08                     | 0.53              |
| 1:A:152:PHE:CE2  | 1:A:156:LEU:HD11 | 2.43                     | 0.53              |
| 1:C:71:ARG:HD2   | 1:C:77:GLU:OE2   | 2.09                     | 0.53              |
| 1:D:135:ILE:HG13 | 1:D:140:TYR:CE1  | 2.44                     | 0.53              |
| 1:F:470:ARG:HA   | 1:F:473:MET:HE2  | 1.90                     | 0.53              |
| 1:A:118:LYS:NZ   | 1:A:378:ASN:OD1  | 2.41                     | 0.53              |
| 1:C:233:GLU:HG2  | 1:C:236:TYR:CD2  | 2.41                     | 0.53              |
| 1:C:420:SER:HB3  | 1:E:433:PRO:HA   | 1.91                     | 0.53              |
| 1:C:478:GLY:N    | 3:C:703:HOH:O    | 2.07                     | 0.53              |
| 1:D:116:THR:O    | 3:D:711:HOH:O    | 2.19                     | 0.53              |
| 1:F:34:GLU:HA    | 1:F:37:ARG:O     | 2.08                     | 0.53              |
| 1:E:95:GLY:HA3   | 1:E:129:ALA:O    | 2.09                     | 0.53              |
| 1:E:118:LYS:NZ   | 1:E:378:ASN:OD1  | 2.41                     | 0.53              |
| 1:C:190:THR:OG1  | 1:C:191:ILE:N    | 2.35                     | 0.53              |
| 1:D:501:GLY:O    | 1:D:502:VAL:HG23 | 2.09                     | 0.53              |
| 1:B:323:CYS:O    | 1:B:345:ALA:HA   | 2.09                     | 0.52              |
| 1:D:407:ARG:NH1  | 3:D:718:HOH:O    | 2.41                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:414:LEU:HB3  | 1:F:434:ILE:HA   | 1.91                     | 0.52              |
| 1:D:213:HIS:HD1  | 2:D:601:PO4:P    | 2.31                     | 0.52              |
| 1:E:63:LEU:HD21  | 1:E:65:LEU:HD21  | 1.91                     | 0.52              |
| 1:E:70:ARG:HD3   | 1:E:76:TRP:CZ2   | 2.45                     | 0.52              |
| 1:E:173:MET:N    | 3:E:705:HOH:O    | 2.28                     | 0.52              |
| 1:F:95:GLY:HA3   | 1:F:129:ALA:O    | 2.09                     | 0.52              |
| 1:F:70:ARG:HD3   | 1:F:76:TRP:CZ2   | 2.44                     | 0.52              |
| 1:B:39:ARG:HG3   | 1:B:40:GLU:HB3   | 1.90                     | 0.52              |
| 1:A:190:THR:OG1  | 1:A:191:ILE:N    | 2.39                     | 0.52              |
| 1:A:323:CYS:O    | 1:A:345:ALA:HA   | 2.10                     | 0.52              |
| 1:C:62:VAL:HG21  | 1:C:109:LYS:HD3  | 1.91                     | 0.52              |
| 1:D:434:ILE:HG23 | 1:D:435:VAL:H    | 1.74                     | 0.52              |
| 1:A:34:GLU:HA    | 1:A:37:ARG:O     | 2.09                     | 0.52              |
| 1:C:431:THR:HG22 | 1:C:433:PRO:HD3  | 1.92                     | 0.52              |
| 1:D:286:ASN:ND2  | 1:D:310:LYS:O    | 2.31                     | 0.52              |
| 1:E:501:GLY:O    | 1:E:502:VAL:HG23 | 2.10                     | 0.52              |
| 1:B:63:LEU:HD21  | 1:B:65:LEU:HD21  | 1.92                     | 0.52              |
| 1:D:39:ARG:HG3   | 1:D:40:GLU:HB3   | 1.92                     | 0.52              |
| 1:B:70:ARG:HD3   | 1:B:76:TRP:CZ2   | 2.45                     | 0.52              |
| 1:B:135:ILE:HG13 | 1:B:140:TYR:CE1  | 2.45                     | 0.52              |
| 1:B:501:GLY:O    | 1:B:502:VAL:HG23 | 2.10                     | 0.52              |
| 1:E:39:ARG:HG3   | 1:E:40:GLU:HB3   | 1.92                     | 0.52              |
| 1:C:135:ILE:HD12 | 1:C:148:ILE:HD13 | 1.92                     | 0.51              |
| 1:C:437:THR:HG23 | 1:D:416:SER:HA   | 1.92                     | 0.51              |
| 1:D:12:ASN:O     | 1:D:14:PHE:N     | 2.42                     | 0.51              |
| 1:D:34:GLU:HA    | 1:D:37:ARG:O     | 2.09                     | 0.51              |
| 1:D:152:PHE:CE2  | 1:D:156:LEU:HD11 | 2.45                     | 0.51              |
| 1:E:152:PHE:CE2  | 1:E:156:LEU:HD11 | 2.45                     | 0.51              |
| 1:E:12:ASN:O     | 1:E:14:PHE:N     | 2.43                     | 0.51              |
| 1:C:279:GLU:OE2  | 1:C:299:LYS:NZ   | 2.43                     | 0.51              |
| 1:D:71:ARG:HD2   | 1:D:77:GLU:OE2   | 2.10                     | 0.51              |
| 1:B:436:PRO:HA   | 1:F:416:SER:OG   | 2.09                     | 0.51              |
| 1:B:64:SER:HB2   | 1:D:62:VAL:HB    | 1.93                     | 0.51              |
| 1:B:76:TRP:HB2   | 1:D:51:GLY:HA3   | 1.93                     | 0.51              |
| 1:B:335:LEU:HD13 | 1:B:348:ILE:HD13 | 1.91                     | 0.51              |
| 1:F:233:GLU:HG2  | 1:F:236:TYR:CD2  | 2.43                     | 0.51              |
| 1:A:12:ASN:O     | 1:A:14:PHE:N     | 2.44                     | 0.51              |
| 1:A:151:ARG:NH1  | 1:E:503:THR:HG23 | 2.26                     | 0.51              |
| 1:D:339:ASN:OD1  | 1:D:339:ASN:N    | 2.38                     | 0.51              |
| 1:D:462:GLU:CD   | 3:D:703:HOH:O    | 2.49                     | 0.51              |
| 1:F:71:ARG:HD2   | 1:F:77:GLU:OE2   | 2.11                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:152:PHE:CE2  | 1:F:156:LEU:HD11 | 2.46                     | 0.51              |
| 1:B:118:LYS:NZ   | 1:B:378:ASN:OD1  | 2.42                     | 0.51              |
| 1:B:190:THR:OG1  | 1:B:191:ILE:N    | 2.44                     | 0.51              |
| 1:C:12:ASN:O     | 1:C:14:PHE:N     | 2.44                     | 0.51              |
| 1:C:434:ILE:HG23 | 1:C:435:VAL:H    | 1.76                     | 0.50              |
| 1:E:146:GLU:O    | 1:E:150:ARG:HG3  | 2.12                     | 0.50              |
| 1:F:62:VAL:HG21  | 1:F:109:LYS:HD3  | 1.94                     | 0.50              |
| 1:F:501:GLY:O    | 1:F:502:VAL:HG23 | 2.12                     | 0.50              |
| 1:A:39:ARG:HG3   | 1:A:40:GLU:HB3   | 1.93                     | 0.50              |
| 1:C:39:ARG:HG3   | 1:C:40:GLU:HB3   | 1.93                     | 0.50              |
| 1:A:279:GLU:OE2  | 1:A:299:LYS:NZ   | 2.44                     | 0.50              |
| 1:F:286:ASN:ND2  | 1:F:310:LYS:O    | 2.30                     | 0.50              |
| 1:C:480:ASP:HB3  | 3:C:703:HOH:O    | 2.12                     | 0.50              |
| 1:D:335:LEU:HD13 | 1:D:348:ILE:HD13 | 1.94                     | 0.50              |
| 1:C:347:ILE:HG12 | 1:C:370:MET:HE2  | 1.93                     | 0.50              |
| 1:C:503:THR:HG23 | 1:F:151:ARG:NH1  | 2.25                     | 0.50              |
| 1:D:59:CYS:HA    | 1:D:86:HIS:HA    | 1.94                     | 0.50              |
| 1:A:70:ARG:CZ    | 1:E:505:THR:HB   | 2.41                     | 0.50              |
| 1:C:146:GLU:O    | 1:C:150:ARG:HG3  | 2.12                     | 0.49              |
| 1:E:319:LEU:HD12 | 1:E:319:LEU:H    | 1.77                     | 0.49              |
| 1:B:146:GLU:O    | 1:B:150:ARG:HG3  | 2.12                     | 0.49              |
| 1:A:501:GLY:O    | 1:A:502:VAL:HG23 | 2.12                     | 0.49              |
| 1:C:152:PHE:CE2  | 1:C:156:LEU:HD11 | 2.47                     | 0.49              |
| 1:F:239:ILE:HG21 | 1:F:479:LEU:HD21 | 1.94                     | 0.49              |
| 1:A:63:LEU:HD21  | 1:A:65:LEU:HD21  | 1.93                     | 0.49              |
| 1:B:285:TRP:HE1  | 1:B:287:PRO:HG3  | 1.77                     | 0.49              |
| 1:B:480:ASP:N    | 3:B:708:HOH:O    | 2.45                     | 0.49              |
| 1:A:335:LEU:HD13 | 1:A:348:ILE:HD13 | 1.95                     | 0.49              |
| 1:C:151:ARG:HH11 | 1:F:503:THR:HG23 | 1.77                     | 0.49              |
| 1:F:238:SER:O    | 1:F:241:GLY:N    | 2.40                     | 0.49              |
| 1:A:285:TRP:HE1  | 1:A:287:PRO:HG3  | 1.77                     | 0.49              |
| 1:E:335:LEU:HD13 | 1:E:348:ILE:HD13 | 1.94                     | 0.49              |
| 1:A:233:GLU:HG2  | 1:A:236:TYR:CD2  | 2.41                     | 0.49              |
| 1:F:339:ASN:OD1  | 1:F:339:ASN:N    | 2.41                     | 0.49              |
| 1:C:70:ARG:HD3   | 1:C:76:TRP:CZ2   | 2.48                     | 0.48              |
| 1:A:62:VAL:HG21  | 1:A:109:LYS:HD3  | 1.94                     | 0.48              |
| 1:D:70:ARG:HD3   | 1:D:76:TRP:CZ2   | 2.48                     | 0.48              |
| 1:B:62:VAL:HG21  | 1:B:109:LYS:HD3  | 1.96                     | 0.48              |
| 1:C:249:LYS:HD3  | 1:C:249:LYS:N    | 2.28                     | 0.48              |
| 1:A:434:ILE:HG23 | 1:A:435:VAL:H    | 1.78                     | 0.48              |
| 1:B:265:ARG:NH2  | 2:B:602:PO4:O2   | 2.45                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:279:GLU:OE2  | 1:B:299:LYS:NZ   | 2.45                     | 0.48              |
| 1:E:286:ASN:ND2  | 1:E:310:LYS:O    | 2.32                     | 0.48              |
| 1:F:285:TRP:HE1  | 1:F:287:PRO:HG3  | 1.79                     | 0.48              |
| 1:B:336:THR:HG23 | 1:B:338:SER:H    | 1.78                     | 0.48              |
| 1:B:59:CYS:HA    | 1:B:86:HIS:HA    | 1.95                     | 0.48              |
| 1:B:70:ARG:NH2   | 1:E:143:ASN:OD1  | 2.48                     | 0.47              |
| 1:B:400:ARG:O    | 1:B:400:ARG:HG3  | 2.14                     | 0.47              |
| 1:E:78:VAL:HG23  | 3:E:721:HOH:O    | 2.12                     | 0.47              |
| 1:F:266:TYR:OH   | 2:F:2002:PO4:O4  | 2.31                     | 0.47              |
| 1:A:400:ARG:O    | 1:A:400:ARG:HG3  | 2.13                     | 0.47              |
| 1:C:501:GLY:O    | 1:C:502:VAL:HG23 | 2.14                     | 0.47              |
| 1:D:62:VAL:HG21  | 1:D:109:LYS:HD3  | 1.96                     | 0.47              |
| 1:F:39:ARG:HG3   | 1:F:40:GLU:HB3   | 1.96                     | 0.47              |
| 1:A:71:ARG:HD2   | 1:A:77:GLU:OE2   | 2.15                     | 0.47              |
| 1:D:378:ASN:HA   | 3:D:724:HOH:O    | 2.14                     | 0.47              |
| 1:C:456:GLY:HA3  | 1:D:401:LEU:HD23 | 1.95                     | 0.47              |
| 1:F:32:LEU:O     | 1:F:37:ARG:HB3   | 2.15                     | 0.47              |
| 1:F:335:LEU:HD13 | 1:F:348:ILE:HD13 | 1.96                     | 0.47              |
| 1:B:71:ARG:HD2   | 1:B:77:GLU:OE2   | 2.15                     | 0.47              |
| 1:C:45:LYS:HD2   | 1:C:45:LYS:HA    | 1.68                     | 0.47              |
| 1:D:95:GLY:O     | 1:D:169:PRO:HA   | 2.15                     | 0.47              |
| 1:D:279:GLU:OE2  | 1:D:299:LYS:NZ   | 2.48                     | 0.47              |
| 1:E:339:ASN:OD1  | 1:E:339:ASN:N    | 2.39                     | 0.47              |
| 1:B:326:LEU:O    | 1:B:328:PRO:HD3  | 2.15                     | 0.47              |
| 1:E:95:GLY:O     | 1:E:169:PRO:HA   | 2.15                     | 0.47              |
| 1:B:95:GLY:O     | 1:B:169:PRO:HA   | 2.14                     | 0.47              |
| 1:C:420:SER:CB   | 1:E:433:PRO:HA   | 2.44                     | 0.47              |
| 1:A:347:ILE:HG12 | 1:A:370:MET:HE2  | 1.96                     | 0.46              |
| 1:C:463:ARG:NH2  | 2:D:603:PO4:O4   | 2.47                     | 0.46              |
| 1:D:386:TYR:OH   | 3:D:704:HOH:O    | 2.03                     | 0.46              |
| 1:F:347:ILE:HG12 | 1:F:370:MET:HE2  | 1.97                     | 0.46              |
| 1:B:233:GLU:HG2  | 1:B:236:TYR:CD2  | 2.45                     | 0.46              |
| 1:A:95:GLY:O     | 1:A:169:PRO:HA   | 2.15                     | 0.46              |
| 1:B:340:ALA:HB3  | 1:B:341:PRO:HD3  | 1.97                     | 0.46              |
| 1:C:60:ASN:OD1   | 3:C:707:HOH:O    | 2.20                     | 0.46              |
| 1:C:111:LEU:HD13 | 1:C:130:LYS:HE3  | 1.98                     | 0.46              |
| 1:B:286:ASN:ND2  | 1:B:310:LYS:O    | 2.33                     | 0.46              |
| 1:B:350:GLU:OE2  | 1:B:482:ARG:NH2  | 2.49                     | 0.46              |
| 1:D:233:GLU:HG2  | 1:D:236:TYR:CD2  | 2.45                     | 0.46              |
| 1:D:413:LEU:HD13 | 1:E:413:LEU:HD13 | 1.97                     | 0.46              |
| 1:E:347:ILE:HG12 | 1:E:370:MET:HE2  | 1.97                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:285:TRP:HE1  | 1:C:287:PRO:HG3  | 1.80                     | 0.46              |
| 1:D:434:ILE:O    | 1:E:420:SER:OG   | 2.33                     | 0.46              |
| 1:E:41:SER:HB2   | 1:E:45:LYS:NZ    | 2.31                     | 0.46              |
| 1:A:436:PRO:HB3  | 1:A:440:PHE:CD2  | 2.51                     | 0.46              |
| 1:C:400:ARG:O    | 1:C:400:ARG:HG3  | 2.16                     | 0.46              |
| 1:C:95:GLY:O     | 1:C:169:PRO:HA   | 2.16                     | 0.45              |
| 1:D:32:LEU:O     | 1:D:37:ARG:HB3   | 2.15                     | 0.45              |
| 1:A:70:ARG:HD3   | 1:A:76:TRP:CZ2   | 2.51                     | 0.45              |
| 1:E:71:ARG:HD2   | 1:E:77:GLU:OE2   | 2.17                     | 0.45              |
| 1:D:45:LYS:HD2   | 1:D:45:LYS:HA    | 1.67                     | 0.45              |
| 1:D:340:ALA:HB3  | 1:D:341:PRO:HD3  | 1.99                     | 0.45              |
| 1:B:460:THR:HA   | 3:B:730:HOH:O    | 2.16                     | 0.45              |
| 1:C:252:VAL:HG13 | 1:C:276:ALA:HB3  | 1.99                     | 0.45              |
| 1:C:336:THR:HG23 | 1:C:338:SER:H    | 1.81                     | 0.45              |
| 1:D:285:TRP:HE1  | 1:D:287:PRO:HG3  | 1.80                     | 0.45              |
| 1:E:279:GLU:OE2  | 1:E:299:LYS:NZ   | 2.46                     | 0.45              |
| 1:B:319:LEU:HD12 | 1:B:319:LEU:N    | 2.32                     | 0.45              |
| 1:E:59:CYS:HA    | 1:E:86:HIS:HA    | 1.98                     | 0.45              |
| 1:F:428:HIS:HD2  | 3:F:2112:HOH:O   | 1.99                     | 0.45              |
| 1:C:21:PHE:CE2   | 1:C:57:LYS:HB2   | 2.52                     | 0.45              |
| 1:E:277:VAL:HG23 | 1:E:305:ILE:HD12 | 1.97                     | 0.45              |
| 1:C:443:ARG:NH2  | 1:D:409:SER:OG   | 2.50                     | 0.45              |
| 1:D:281:ASP:HB2  | 1:D:282:GLY:H    | 1.61                     | 0.45              |
| 1:C:273:LYS:HD2  | 3:C:722:HOH:O    | 2.17                     | 0.45              |
| 1:A:336:THR:HG23 | 1:A:338:SER:H    | 1.81                     | 0.44              |
| 1:D:239:ILE:HG21 | 1:D:479:LEU:HD21 | 1.98                     | 0.44              |
| 1:F:95:GLY:O     | 1:F:169:PRO:HA   | 2.16                     | 0.44              |
| 1:B:505:THR:HB   | 1:D:70:ARG:NH2   | 2.32                     | 0.44              |
| 1:C:32:LEU:O     | 1:C:37:ARG:HB3   | 2.17                     | 0.44              |
| 1:D:347:ILE:HG12 | 1:D:370:MET:HE2  | 1.99                     | 0.44              |
| 1:E:326:LEU:O    | 1:E:328:PRO:HD3  | 2.18                     | 0.44              |
| 1:F:308:PHE:C    | 1:F:310:LYS:H    | 2.26                     | 0.44              |
| 1:A:433:PRO:HA   | 1:B:420:SER:HB3  | 2.00                     | 0.44              |
| 1:E:265:ARG:CD   | 3:E:706:HOH:O    | 2.58                     | 0.44              |
| 1:F:21:PHE:CE2   | 1:F:57:LYS:HB2   | 2.53                     | 0.44              |
| 1:A:32:LEU:O     | 1:A:37:ARG:HB3   | 2.17                     | 0.44              |
| 1:B:45:LYS:HD2   | 1:B:45:LYS:HA    | 1.68                     | 0.44              |
| 1:C:319:LEU:HD12 | 1:C:319:LEU:H    | 1.83                     | 0.44              |
| 1:B:187:TYR:CE2  | 1:B:192:GLY:HA3  | 2.53                     | 0.44              |
| 1:D:242:MET:HE2  | 1:D:249:LYS:HE3  | 1.99                     | 0.44              |
| 1:B:477:LEU:HB3  | 3:B:708:HOH:O    | 2.17                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:63:LEU:HD21  | 1:F:65:LEU:HD21  | 2.00                     | 0.44              |
| 1:E:265:ARG:HG2  | 3:E:716:HOH:O    | 2.18                     | 0.43              |
| 1:D:504:PHE:CZ   | 1:E:186:THR:HG23 | 2.53                     | 0.43              |
| 1:E:340:ALA:HB3  | 1:E:341:PRO:HD3  | 1.98                     | 0.43              |
| 1:F:71:ARG:HE    | 1:F:71:ARG:HB3   | 1.68                     | 0.43              |
| 1:A:249:LYS:HD3  | 1:A:249:LYS:N    | 2.32                     | 0.43              |
| 1:B:434:ILE:O    | 1:F:420:SER:OG   | 2.30                     | 0.43              |
| 1:D:429:GLY:HA3  | 3:D:719:HOH:O    | 2.17                     | 0.43              |
| 1:A:60:ASN:OD1   | 3:A:1104:HOH:O   | 2.21                     | 0.43              |
| 1:B:375:LEU:HD12 | 1:B:375:LEU:HA   | 1.84                     | 0.43              |
| 1:F:314:TYR:CE2  | 1:F:318:ILE:HA   | 2.53                     | 0.43              |
| 1:A:237:MET:HE3  | 1:A:242:MET:HB2  | 2.01                     | 0.43              |
| 1:B:143:ASN:OD1  | 1:E:70:ARG:NH2   | 2.52                     | 0.43              |
| 1:D:350:GLU:OE1  | 1:D:482:ARG:NH2  | 2.50                     | 0.43              |
| 1:E:32:LEU:O     | 1:E:37:ARG:HB3   | 2.19                     | 0.43              |
| 1:F:261:LEU:HD11 | 3:F:2111:HOH:O   | 2.17                     | 0.43              |
| 1:F:281:ASP:HB2  | 1:F:282:GLY:H    | 1.58                     | 0.43              |
| 1:B:152:PHE:CE2  | 1:B:156:LEU:HD11 | 2.54                     | 0.43              |
| 1:C:63:LEU:HD21  | 1:C:65:LEU:HD21  | 1.99                     | 0.43              |
| 1:C:310:LYS:HG2  | 3:C:701:HOH:O    | 2.19                     | 0.43              |
| 1:D:111:LEU:HD13 | 1:D:130:LYS:HE3  | 2.01                     | 0.43              |
| 1:D:187:TYR:CE2  | 1:D:192:GLY:HA3  | 2.53                     | 0.43              |
| 1:D:308:PHE:C    | 1:D:310:LYS:H    | 2.26                     | 0.43              |
| 1:E:41:SER:HB2   | 1:E:45:LYS:HZ1   | 1.83                     | 0.43              |
| 1:F:277:VAL:HG23 | 1:F:305:ILE:HD12 | 2.01                     | 0.43              |
| 1:A:146:GLU:O    | 1:A:150:ARG:HG3  | 2.18                     | 0.43              |
| 1:A:314:TYR:CE2  | 1:A:318:ILE:HA   | 2.54                     | 0.43              |
| 1:B:347:ILE:HG12 | 1:B:370:MET:HE2  | 2.01                     | 0.43              |
| 1:D:436:PRO:HA   | 1:E:416:SER:OG   | 2.19                     | 0.43              |
| 1:F:164:PRO:HG2  | 1:F:195:ASP:OD2  | 2.19                     | 0.43              |
| 1:A:416:SER:OG   | 1:F:436:PRO:HA   | 2.18                     | 0.43              |
| 1:B:41:SER:HB2   | 1:B:45:LYS:NZ    | 2.34                     | 0.43              |
| 1:C:314:TYR:CE2  | 1:C:318:ILE:HA   | 2.53                     | 0.43              |
| 1:C:474:LYS:NZ   | 1:C:491:GLU:OE2  | 2.52                     | 0.43              |
| 1:F:253:VAL:O    | 1:F:277:VAL:HA   | 2.19                     | 0.43              |
| 1:B:32:LEU:O     | 1:B:37:ARG:HB3   | 2.19                     | 0.43              |
| 1:C:159:LYS:HE3  | 1:F:61:HIS:CD2   | 2.54                     | 0.43              |
| 1:C:335:LEU:HD13 | 1:C:348:ILE:HD13 | 2.00                     | 0.43              |
| 1:E:308:PHE:C    | 1:E:310:LYS:H    | 2.27                     | 0.43              |
| 1:B:304:SER:OG   | 1:B:305:ILE:N    | 2.52                     | 0.42              |
| 1:B:413:LEU:HD13 | 1:F:413:LEU:HD13 | 2.01                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:285:TRP:HE1  | 1:E:287:PRO:HG3  | 1.84                     | 0.42              |
| 1:E:319:LEU:HD12 | 1:E:319:LEU:N    | 2.34                     | 0.42              |
| 1:C:285:TRP:CD1  | 1:C:285:TRP:C    | 2.97                     | 0.42              |
| 1:C:470:ARG:HE   | 1:C:470:ARG:HB2  | 1.70                     | 0.42              |
| 1:F:336:THR:HG23 | 1:F:338:SER:H    | 1.85                     | 0.42              |
| 1:A:187:TYR:CE2  | 1:A:192:GLY:HA3  | 2.54                     | 0.42              |
| 1:E:111:LEU:HD13 | 1:E:130:LYS:HE3  | 2.00                     | 0.42              |
| 1:F:12:ASN:C     | 1:F:14:PHE:N     | 2.77                     | 0.42              |
| 1:F:436:PRO:HB3  | 1:F:440:PHE:CD2  | 2.55                     | 0.42              |
| 1:A:59:CYS:HA    | 1:A:86:HIS:HA    | 2.00                     | 0.42              |
| 1:A:277:VAL:HG23 | 1:A:305:ILE:HD12 | 2.01                     | 0.42              |
| 1:B:21:PHE:CE2   | 1:B:57:LYS:HB2   | 2.54                     | 0.42              |
| 1:B:94:LYS:HD2   | 1:B:168:VAL:HB   | 2.01                     | 0.42              |
| 1:B:308:PHE:C    | 1:B:310:LYS:H    | 2.26                     | 0.42              |
| 1:B:470:ARG:HE   | 1:B:470:ARG:HB2  | 1.69                     | 0.42              |
| 1:C:308:PHE:C    | 1:C:310:LYS:H    | 2.27                     | 0.42              |
| 1:C:412:HIS:HB3  | 1:E:440:PHE:CG   | 2.54                     | 0.42              |
| 1:D:171:PRO:HG3  | 1:D:180:MET:HG3  | 2.02                     | 0.42              |
| 1:D:237:MET:HE3  | 1:D:242:MET:HB2  | 2.01                     | 0.42              |
| 1:E:21:PHE:CE2   | 1:E:57:LYS:HB2   | 2.55                     | 0.42              |
| 1:F:279:GLU:OE2  | 1:F:299:LYS:NZ   | 2.49                     | 0.42              |
| 1:D:77:GLU:OE1   | 1:D:140:TYR:OH   | 2.32                     | 0.42              |
| 1:D:249:LYS:N    | 1:D:249:LYS:HD3  | 2.34                     | 0.42              |
| 1:F:41:SER:HB2   | 1:F:45:LYS:NZ    | 2.35                     | 0.42              |
| 1:F:133:VAL:O    | 1:F:135:ILE:HG22 | 2.20                     | 0.42              |
| 1:A:304:SER:OG   | 1:A:305:ILE:N    | 2.53                     | 0.42              |
| 1:D:326:LEU:O    | 1:D:328:PRO:HD3  | 2.20                     | 0.42              |
| 1:B:135:ILE:HD12 | 1:B:148:ILE:HD13 | 2.00                     | 0.42              |
| 1:B:253:VAL:O    | 1:B:277:VAL:HA   | 2.20                     | 0.42              |
| 1:C:43:GLU:N     | 1:C:43:GLU:OE1   | 2.53                     | 0.42              |
| 1:C:350:GLU:OE1  | 1:C:482:ARG:NH2  | 2.52                     | 0.42              |
| 1:F:135:ILE:HD12 | 1:F:148:ILE:HD13 | 2.01                     | 0.42              |
| 1:A:70:ARG:NH2   | 1:E:505:THR:HB   | 2.35                     | 0.42              |
| 1:F:111:LEU:HD13 | 1:F:130:LYS:HE3  | 2.02                     | 0.42              |
| 1:F:249:LYS:HD3  | 1:F:249:LYS:N    | 2.35                     | 0.42              |
| 1:A:43:GLU:OE1   | 1:A:43:GLU:N     | 2.53                     | 0.41              |
| 1:E:336:THR:HG23 | 1:E:338:SER:H    | 1.83                     | 0.41              |
| 1:F:69:ILE:HG12  | 1:F:79:ILE:HD11  | 2.02                     | 0.41              |
| 1:F:237:MET:HE3  | 1:F:242:MET:HB2  | 2.01                     | 0.41              |
| 1:A:253:VAL:O    | 1:A:277:VAL:HA   | 2.20                     | 0.41              |
| 1:B:93:CYS:HB3   | 1:B:129:ALA:HB2  | 2.02                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:239:ILE:HG21 | 1:C:479:LEU:HD21 | 2.02                     | 0.41              |
| 1:D:427:LYS:HB2  | 1:D:428:HIS:H    | 1.72                     | 0.41              |
| 1:E:12:ASN:C     | 1:E:14:PHE:N     | 2.77                     | 0.41              |
| 1:E:77:GLU:OE1   | 1:E:140:TYR:OH   | 2.30                     | 0.41              |
| 1:E:94:LYS:HD2   | 1:E:168:VAL:HB   | 2.02                     | 0.41              |
| 1:E:388:GLU:CD   | 3:E:707:HOH:O    | 2.62                     | 0.41              |
| 1:E:503:THR:HB   | 1:E:504:PHE:H    | 1.66                     | 0.41              |
| 1:D:12:ASN:C     | 1:D:14:PHE:N     | 2.77                     | 0.41              |
| 1:D:93:CYS:HB3   | 1:D:129:ALA:HB2  | 2.03                     | 0.41              |
| 1:B:427:LYS:HB2  | 1:B:428:HIS:H    | 1.65                     | 0.41              |
| 1:C:412:HIS:HB3  | 1:E:440:PHE:CD1  | 2.56                     | 0.41              |
| 1:F:243:THR:O    | 1:F:249:LYS:NZ   | 2.26                     | 0.41              |
| 1:D:285:TRP:CD1  | 1:D:285:TRP:C    | 2.98                     | 0.41              |
| 1:D:436:PRO:HB3  | 1:D:440:PHE:CD2  | 2.55                     | 0.41              |
| 1:E:314:TYR:CE2  | 1:E:318:ILE:HA   | 2.55                     | 0.41              |
| 1:A:252:VAL:HG13 | 1:A:276:ALA:HB3  | 2.03                     | 0.41              |
| 1:A:340:ALA:HB3  | 1:A:341:PRO:HD3  | 2.03                     | 0.41              |
| 1:B:12:ASN:C     | 1:B:14:PHE:N     | 2.78                     | 0.41              |
| 1:B:277:VAL:HG23 | 1:B:305:ILE:HD12 | 2.03                     | 0.41              |
| 1:D:238:SER:O    | 1:D:241:GLY:N    | 2.41                     | 0.41              |
| 1:D:304:SER:OG   | 1:D:305:ILE:N    | 2.53                     | 0.41              |
| 1:D:336:THR:HG23 | 1:D:338:SER:H    | 1.85                     | 0.41              |
| 1:D:375:LEU:HD22 | 1:D:486:TYR:CE1  | 2.55                     | 0.41              |
| 1:E:474:LYS:NZ   | 1:E:491:GLU:OE2  | 2.54                     | 0.41              |
| 1:F:94:LYS:HD3   | 1:F:126:PHE:CE2  | 2.55                     | 0.41              |
| 1:F:356:THR:HG23 | 1:F:360:ALA:HB3  | 2.02                     | 0.41              |
| 1:F:474:LYS:NZ   | 1:F:491:GLU:OE2  | 2.53                     | 0.41              |
| 1:A:308:PHE:C    | 1:A:310:LYS:H    | 2.28                     | 0.41              |
| 1:E:237:MET:HE3  | 1:E:242:MET:HB2  | 2.02                     | 0.41              |
| 1:A:21:PHE:CE2   | 1:A:57:LYS:HB2   | 2.55                     | 0.41              |
| 1:B:237:MET:HE3  | 1:B:242:MET:HB2  | 2.01                     | 0.41              |
| 1:C:69:ILE:HG12  | 1:C:79:ILE:HD11  | 2.02                     | 0.41              |
| 1:E:281:ASP:HB2  | 1:E:282:GLY:H    | 1.58                     | 0.41              |
| 1:B:111:LEU:HD13 | 1:B:130:LYS:HE3  | 2.03                     | 0.41              |
| 1:B:314:TYR:CE2  | 1:B:318:ILE:HA   | 2.56                     | 0.41              |
| 1:B:503:THR:HB   | 1:B:504:PHE:H    | 1.68                     | 0.41              |
| 1:C:237:MET:HE3  | 1:C:242:MET:HB2  | 2.02                     | 0.41              |
| 1:D:249:LYS:HG3  | 1:D:324:ASP:CB   | 2.51                     | 0.41              |
| 1:D:359:GLU:HG3  | 3:D:706:HOH:O    | 2.20                     | 0.41              |
| 1:E:32:LEU:HD12  | 1:E:32:LEU:HA    | 1.82                     | 0.41              |
| 1:E:135:ILE:HD12 | 1:E:148:ILE:HD13 | 2.02                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:94:LYS:HD2   | 1:F:168:VAL:HB   | 2.03                     | 0.41              |
| 1:F:249:LYS:HG3  | 1:F:324:ASP:CB   | 2.51                     | 0.41              |
| 1:A:71:ARG:HE    | 1:A:71:ARG:HB3   | 1.68                     | 0.41              |
| 1:C:94:LYS:HD2   | 1:C:168:VAL:HB   | 2.03                     | 0.41              |
| 1:D:314:TYR:CE2  | 1:D:318:ILE:HA   | 2.56                     | 0.41              |
| 1:D:470:ARG:HE   | 1:D:470:ARG:HB2  | 1.68                     | 0.41              |
| 1:F:275:ILE:HD11 | 1:F:323:CYS:HB3  | 2.03                     | 0.41              |
| 1:B:71:ARG:HE    | 1:B:71:ARG:HB3   | 1.65                     | 0.40              |
| 1:C:249:LYS:HG3  | 1:C:324:ASP:CB   | 2.51                     | 0.40              |
| 1:D:71:ARG:HE    | 1:D:71:ARG:HB3   | 1.66                     | 0.40              |
| 1:D:375:LEU:HD12 | 1:D:375:LEU:HA   | 1.86                     | 0.40              |
| 1:E:251:PHE:CZ   | 1:E:274:CYS:HB2  | 2.56                     | 0.40              |
| 1:B:283:SER:OG   | 1:B:314:TYR:HB3  | 2.21                     | 0.40              |
| 1:B:474:LYS:NZ   | 1:B:491:GLU:OE2  | 2.54                     | 0.40              |
| 1:D:37:ARG:NH1   | 1:D:39:ARG:HB2   | 2.36                     | 0.40              |
| 1:E:71:ARG:HE    | 1:E:71:ARG:HB3   | 1.63                     | 0.40              |
| 1:F:283:SER:OG   | 1:F:314:TYR:HB3  | 2.22                     | 0.40              |
| 1:A:111:LEU:HD13 | 1:A:130:LYS:HE3  | 2.04                     | 0.40              |
| 3:A:1103:HOH:O   | 1:B:397:SER:OG   | 2.22                     | 0.40              |
| 1:B:310:LYS:HE3  | 1:B:310:LYS:HB2  | 1.91                     | 0.40              |
| 1:B:319:LEU:H    | 1:B:319:LEU:CD1  | 2.33                     | 0.40              |
| 1:C:187:TYR:CE2  | 1:C:192:GLY:HA3  | 2.57                     | 0.40              |
| 1:D:41:SER:HB2   | 1:D:45:LYS:NZ    | 2.35                     | 0.40              |
| 1:E:45:LYS:HA    | 1:E:45:LYS:HD2   | 1.66                     | 0.40              |
| 1:A:41:SER:HB2   | 1:A:45:LYS:NZ    | 2.36                     | 0.40              |
| 1:C:238:SER:O    | 1:C:241:GLY:N    | 2.40                     | 0.40              |
| 1:C:277:VAL:HG23 | 1:C:305:ILE:HD12 | 2.02                     | 0.40              |
| 1:D:319:LEU:H    | 1:D:319:LEU:HD12 | 1.86                     | 0.40              |
| 1:F:41:SER:HB2   | 1:F:45:LYS:HZ1   | 1.85                     | 0.40              |
| 1:F:427:LYS:HB2  | 1:F:428:HIS:H    | 1.66                     | 0.40              |
| 1:A:239:ILE:HG21 | 1:A:479:LEU:HD21 | 2.02                     | 0.40              |
| 1:C:253:VAL:O    | 1:C:277:VAL:HA   | 2.22                     | 0.40              |
| 1:C:346:LYS:CE   | 3:C:708:HOH:O    | 2.69                     | 0.40              |
| 1:D:474:LYS:NZ   | 1:D:491:GLU:OE2  | 2.55                     | 0.40              |
| 1:E:252:VAL:HG13 | 1:E:276:ALA:HB3  | 2.03                     | 0.40              |
| 1:E:373:PRO:HG3  | 1:E:482:ARG:HA   | 2.04                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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     | 494/496 (100%)   | 452 (92%)  | 34 (7%)  | 8 (2%)   | 7           | 20 |
| 1   | B     | 494/496 (100%)   | 453 (92%)  | 33 (7%)  | 8 (2%)   | 7           | 20 |
| 1   | C     | 494/496 (100%)   | 448 (91%)  | 36 (7%)  | 10 (2%)  | 6           | 16 |
| 1   | D     | 494/496 (100%)   | 452 (92%)  | 34 (7%)  | 8 (2%)   | 7           | 20 |
| 1   | E     | 494/496 (100%)   | 455 (92%)  | 30 (6%)  | 9 (2%)   | 6           | 18 |
| 1   | F     | 494/496 (100%)   | 448 (91%)  | 37 (8%)  | 9 (2%)   | 6           | 18 |
| All | All   | 2964/2976 (100%) | 2708 (91%) | 204 (7%) | 52 (2%)  | 6           | 18 |

All (52) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 35  | ASP  |
| 1   | A     | 40  | GLU  |
| 1   | A     | 434 | ILE  |
| 1   | B     | 35  | ASP  |
| 1   | B     | 40  | GLU  |
| 1   | B     | 434 | ILE  |
| 1   | C     | 35  | ASP  |
| 1   | C     | 40  | GLU  |
| 1   | C     | 434 | ILE  |
| 1   | D     | 35  | ASP  |
| 1   | D     | 40  | GLU  |
| 1   | D     | 434 | ILE  |
| 1   | E     | 35  | ASP  |
| 1   | E     | 40  | GLU  |
| 1   | E     | 434 | ILE  |
| 1   | F     | 35  | ASP  |
| 1   | F     | 40  | GLU  |
| 1   | F     | 434 | ILE  |
| 1   | A     | 13  | PHE  |
| 1   | A     | 426 | GLY  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 502 | VAL  |
| 1   | B     | 13  | PHE  |
| 1   | B     | 426 | GLY  |
| 1   | B     | 502 | VAL  |
| 1   | C     | 13  | PHE  |
| 1   | C     | 426 | GLY  |
| 1   | C     | 502 | VAL  |
| 1   | D     | 13  | PHE  |
| 1   | D     | 426 | GLY  |
| 1   | D     | 502 | VAL  |
| 1   | E     | 13  | PHE  |
| 1   | E     | 426 | GLY  |
| 1   | E     | 502 | VAL  |
| 1   | F     | 13  | PHE  |
| 1   | F     | 92  | PRO  |
| 1   | F     | 426 | GLY  |
| 1   | F     | 502 | VAL  |
| 1   | A     | 331 | SER  |
| 1   | B     | 331 | SER  |
| 1   | C     | 331 | SER  |
| 1   | C     | 435 | VAL  |
| 1   | D     | 331 | SER  |
| 1   | E     | 331 | SER  |
| 1   | F     | 331 | SER  |
| 1   | F     | 435 | VAL  |
| 1   | A     | 435 | VAL  |
| 1   | B     | 435 | VAL  |
| 1   | D     | 435 | VAL  |
| 1   | E     | 172 | ASP  |
| 1   | E     | 435 | VAL  |
| 1   | C     | 244 | PRO  |
| 1   | C     | 239 | ILE  |

### 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     | 413/413 (100%)   | 390 (94%)  | 23 (6%)  | 19          | 44 |
| 1   | B     | 413/413 (100%)   | 390 (94%)  | 23 (6%)  | 19          | 44 |
| 1   | C     | 413/413 (100%)   | 387 (94%)  | 26 (6%)  | 16          | 39 |
| 1   | D     | 413/413 (100%)   | 390 (94%)  | 23 (6%)  | 19          | 44 |
| 1   | E     | 413/413 (100%)   | 390 (94%)  | 23 (6%)  | 19          | 44 |
| 1   | F     | 413/413 (100%)   | 389 (94%)  | 24 (6%)  | 18          | 42 |
| All | All   | 2478/2478 (100%) | 2336 (94%) | 142 (6%) | 18          | 43 |

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

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 32  | LEU  |
| 1   | A     | 35  | ASP  |
| 1   | A     | 40  | GLU  |
| 1   | A     | 45  | LYS  |
| 1   | A     | 135 | ILE  |
| 1   | A     | 235 | SER  |
| 1   | A     | 249 | LYS  |
| 1   | A     | 267 | LEU  |
| 1   | A     | 277 | VAL  |
| 1   | A     | 281 | ASP  |
| 1   | A     | 300 | LEU  |
| 1   | A     | 306 | LEU  |
| 1   | A     | 318 | ILE  |
| 1   | A     | 339 | ASN  |
| 1   | A     | 342 | ARG  |
| 1   | A     | 409 | SER  |
| 1   | A     | 415 | MET  |
| 1   | A     | 432 | ILE  |
| 1   | A     | 435 | VAL  |
| 1   | A     | 455 | SER  |
| 1   | A     | 470 | ARG  |
| 1   | A     | 503 | THR  |
| 1   | A     | 505 | THR  |
| 1   | B     | 32  | LEU  |
| 1   | B     | 35  | ASP  |
| 1   | B     | 40  | GLU  |
| 1   | B     | 45  | LYS  |
| 1   | B     | 135 | ILE  |
| 1   | B     | 235 | SER  |
| 1   | B     | 243 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 249 | LYS  |
| 1   | B     | 267 | LEU  |
| 1   | B     | 277 | VAL  |
| 1   | B     | 281 | ASP  |
| 1   | B     | 300 | LEU  |
| 1   | B     | 306 | LEU  |
| 1   | B     | 318 | ILE  |
| 1   | B     | 339 | ASN  |
| 1   | B     | 342 | ARG  |
| 1   | B     | 409 | SER  |
| 1   | B     | 432 | ILE  |
| 1   | B     | 435 | VAL  |
| 1   | B     | 455 | SER  |
| 1   | B     | 470 | ARG  |
| 1   | B     | 503 | THR  |
| 1   | B     | 505 | THR  |
| 1   | C     | 32  | LEU  |
| 1   | C     | 35  | ASP  |
| 1   | C     | 40  | GLU  |
| 1   | C     | 45  | LYS  |
| 1   | C     | 135 | ILE  |
| 1   | C     | 235 | SER  |
| 1   | C     | 239 | ILE  |
| 1   | C     | 249 | LYS  |
| 1   | C     | 267 | LEU  |
| 1   | C     | 277 | VAL  |
| 1   | C     | 281 | ASP  |
| 1   | C     | 300 | LEU  |
| 1   | C     | 306 | LEU  |
| 1   | C     | 318 | ILE  |
| 1   | C     | 339 | ASN  |
| 1   | C     | 342 | ARG  |
| 1   | C     | 409 | SER  |
| 1   | C     | 415 | MET  |
| 1   | C     | 432 | ILE  |
| 1   | C     | 435 | VAL  |
| 1   | C     | 443 | ARG  |
| 1   | C     | 455 | SER  |
| 1   | C     | 470 | ARG  |
| 1   | C     | 502 | VAL  |
| 1   | C     | 503 | THR  |
| 1   | C     | 505 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 32  | LEU  |
| 1   | D     | 35  | ASP  |
| 1   | D     | 40  | GLU  |
| 1   | D     | 45  | LYS  |
| 1   | D     | 135 | ILE  |
| 1   | D     | 235 | SER  |
| 1   | D     | 243 | THR  |
| 1   | D     | 249 | LYS  |
| 1   | D     | 267 | LEU  |
| 1   | D     | 277 | VAL  |
| 1   | D     | 281 | ASP  |
| 1   | D     | 300 | LEU  |
| 1   | D     | 306 | LEU  |
| 1   | D     | 318 | ILE  |
| 1   | D     | 339 | ASN  |
| 1   | D     | 342 | ARG  |
| 1   | D     | 409 | SER  |
| 1   | D     | 432 | ILE  |
| 1   | D     | 435 | VAL  |
| 1   | D     | 455 | SER  |
| 1   | D     | 470 | ARG  |
| 1   | D     | 503 | THR  |
| 1   | D     | 505 | THR  |
| 1   | E     | 32  | LEU  |
| 1   | E     | 35  | ASP  |
| 1   | E     | 40  | GLU  |
| 1   | E     | 45  | LYS  |
| 1   | E     | 135 | ILE  |
| 1   | E     | 235 | SER  |
| 1   | E     | 249 | LYS  |
| 1   | E     | 267 | LEU  |
| 1   | E     | 277 | VAL  |
| 1   | E     | 281 | ASP  |
| 1   | E     | 300 | LEU  |
| 1   | E     | 306 | LEU  |
| 1   | E     | 318 | ILE  |
| 1   | E     | 339 | ASN  |
| 1   | E     | 342 | ARG  |
| 1   | E     | 409 | SER  |
| 1   | E     | 415 | MET  |
| 1   | E     | 432 | ILE  |
| 1   | E     | 435 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 455 | SER  |
| 1   | E     | 470 | ARG  |
| 1   | E     | 503 | THR  |
| 1   | E     | 505 | THR  |
| 1   | F     | 32  | LEU  |
| 1   | F     | 35  | ASP  |
| 1   | F     | 40  | GLU  |
| 1   | F     | 45  | LYS  |
| 1   | F     | 135 | ILE  |
| 1   | F     | 235 | SER  |
| 1   | F     | 249 | LYS  |
| 1   | F     | 267 | LEU  |
| 1   | F     | 277 | VAL  |
| 1   | F     | 281 | ASP  |
| 1   | F     | 300 | LEU  |
| 1   | F     | 306 | LEU  |
| 1   | F     | 318 | ILE  |
| 1   | F     | 339 | ASN  |
| 1   | F     | 342 | ARG  |
| 1   | F     | 409 | SER  |
| 1   | F     | 415 | MET  |
| 1   | F     | 432 | ILE  |
| 1   | F     | 435 | VAL  |
| 1   | F     | 455 | SER  |
| 1   | F     | 470 | ARG  |
| 1   | F     | 502 | VAL  |
| 1   | F     | 503 | THR  |
| 1   | F     | 505 | THR  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 225 | HIS  |
| 1   | A     | 412 | HIS  |
| 1   | A     | 488 | ASN  |
| 1   | B     | 139 | ASN  |
| 1   | B     | 232 | ASN  |
| 1   | C     | 232 | ASN  |
| 1   | D     | 139 | ASN  |
| 1   | D     | 232 | ASN  |
| 1   | D     | 488 | ASN  |
| 1   | E     | 232 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 302 | HIS  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

15 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 2   | PO4  | E     | 601  | -    | 4,4,4        | 0.92 | 0           | 6,6,6       | 0.39 | 0           |
| 2   | PO4  | E     | 603  | -    | 4,4,4        | 0.80 | 0           | 6,6,6       | 0.51 | 0           |
| 2   | PO4  | F     | 2001 | -    | 4,4,4        | 0.74 | 0           | 6,6,6       | 0.61 | 0           |
| 2   | PO4  | B     | 602  | -    | 4,4,4        | 0.76 | 0           | 6,6,6       | 0.55 | 0           |
| 2   | PO4  | C     | 601  | -    | 4,4,4        | 0.68 | 0           | 6,6,6       | 0.74 | 0           |
| 2   | PO4  | F     | 2002 | -    | 4,4,4        | 0.89 | 0           | 6,6,6       | 0.50 | 0           |
| 2   | PO4  | F     | 2003 | -    | 4,4,4        | 0.85 | 0           | 6,6,6       | 0.45 | 0           |
| 2   | PO4  | B     | 601  | -    | 4,4,4        | 0.72 | 0           | 6,6,6       | 0.73 | 0           |
| 2   | PO4  | A     | 1001 | -    | 4,4,4        | 0.86 | 0           | 6,6,6       | 0.64 | 0           |
| 2   | PO4  | E     | 602  | -    | 4,4,4        | 0.96 | 0           | 6,6,6       | 0.44 | 0           |
| 2   | PO4  | D     | 601  | -    | 4,4,4        | 0.89 | 0           | 6,6,6       | 0.33 | 0           |
| 2   | PO4  | F     | 2004 | -    | 4,4,4        | 0.89 | 0           | 6,6,6       | 0.88 | 0           |
| 2   | PO4  | D     | 602  | -    | 4,4,4        | 0.74 | 0           | 6,6,6       | 0.52 | 0           |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 2   | PO4  | C     | 602 | -    | 4,4,4        | 0.94 | 0        | 6,6,6       | 1.33 | 1 (16%)  |
| 2   | PO4  | D     | 603 | -    | 4,4,4        | 1.04 | 0        | 6,6,6       | 0.76 | 0        |

There are no bond length outliers.

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | C     | 602 | PO4  | O2-P-O1 | -2.35 | 102.63      | 110.95   |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 9 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 2   | B     | 602  | PO4  | 1       | 0            |
| 2   | F     | 2002 | PO4  | 1       | 0            |
| 2   | F     | 2003 | PO4  | 1       | 0            |
| 2   | A     | 1001 | PO4  | 2       | 0            |
| 2   | E     | 602  | PO4  | 1       | 0            |
| 2   | D     | 601  | PO4  | 1       | 0            |
| 2   | D     | 603  | PO4  | 2       | 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     | 496/496 (100%)   | 0.51   | 39 (7%) 18 16  | 30, 65, 131, 142      | 0     |
| 1   | B     | 496/496 (100%)   | 0.63   | 63 (12%) 8 7   | 28, 54, 103, 122      | 0     |
| 1   | C     | 496/496 (100%)   | 1.07   | 113 (22%) 2 2  | 26, 50, 128, 153      | 0     |
| 1   | D     | 496/496 (100%)   | 0.46   | 48 (9%) 13 11  | 25, 52, 109, 126      | 0     |
| 1   | E     | 496/496 (100%)   | 0.15   | 15 (3%) 52 49  | 27, 49, 84, 116       | 0     |
| 1   | F     | 496/496 (100%)   | 0.49   | 49 (9%) 13 10  | 29, 54, 113, 133      | 0     |
| All | All   | 2976/2976 (100%) | 0.55   | 327 (10%) 10 9 | 25, 54, 116, 153      | 0     |

All (327) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 255 | GLY  | 11.3 |
| 1   | C     | 285 | TRP  | 8.4  |
| 1   | C     | 274 | CYS  | 8.3  |
| 1   | C     | 290 | ILE  | 7.6  |
| 1   | C     | 284 | ILE  | 7.6  |
| 1   | C     | 318 | ILE  | 7.5  |
| 1   | C     | 305 | ILE  | 7.1  |
| 1   | C     | 317 | SER  | 7.0  |
| 1   | C     | 296 | GLU  | 6.9  |
| 1   | C     | 268 | HIS  | 6.7  |
| 1   | C     | 295 | LEU  | 6.7  |
| 1   | C     | 308 | PHE  | 6.5  |
| 1   | C     | 311 | ALA  | 6.2  |
| 1   | D     | 338 | SER  | 6.1  |
| 1   | C     | 292 | PRO  | 6.0  |
| 1   | C     | 272 | ALA  | 5.9  |
| 1   | C     | 326 | LEU  | 5.7  |
| 1   | A     | 36  | LEU  | 5.7  |
| 1   | C     | 313 | PRO  | 5.6  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 275 | ILE  | 5.3  |
| 1   | D     | 305 | ILE  | 5.3  |
| 1   | C     | 300 | LEU  | 5.2  |
| 1   | C     | 323 | CYS  | 5.2  |
| 1   | C     | 264 | MET  | 5.1  |
| 1   | C     | 286 | ASN  | 5.1  |
| 1   | C     | 267 | LEU  | 5.1  |
| 1   | B     | 13  | PHE  | 5.1  |
| 1   | F     | 505 | THR  | 5.0  |
| 1   | C     | 261 | LEU  | 5.0  |
| 1   | C     | 256 | PHE  | 5.0  |
| 1   | C     | 433 | PRO  | 5.0  |
| 1   | C     | 319 | LEU  | 4.9  |
| 1   | D     | 36  | LEU  | 4.9  |
| 1   | B     | 309 | PRO  | 4.9  |
| 1   | C     | 254 | GLN  | 4.9  |
| 1   | F     | 36  | LEU  | 4.8  |
| 1   | C     | 298 | PHE  | 4.8  |
| 1   | C     | 314 | TYR  | 4.5  |
| 1   | D     | 309 | PRO  | 4.5  |
| 1   | C     | 250 | THR  | 4.4  |
| 1   | C     | 291 | ASP  | 4.4  |
| 1   | C     | 252 | VAL  | 4.4  |
| 1   | C     | 263 | SER  | 4.3  |
| 1   | D     | 13  | PHE  | 4.3  |
| 1   | F     | 318 | ILE  | 4.3  |
| 1   | C     | 276 | ALA  | 4.2  |
| 1   | C     | 339 | ASN  | 4.2  |
| 1   | C     | 434 | ILE  | 4.2  |
| 1   | B     | 255 | GLY  | 4.2  |
| 1   | E     | 428 | HIS  | 4.1  |
| 1   | C     | 306 | LEU  | 4.1  |
| 1   | C     | 354 | GLY  | 4.0  |
| 1   | E     | 503 | THR  | 4.0  |
| 1   | C     | 277 | VAL  | 4.0  |
| 1   | B     | 330 | ALA  | 3.9  |
| 1   | C     | 251 | PHE  | 3.9  |
| 1   | C     | 36  | LEU  | 3.9  |
| 1   | C     | 316 | GLY  | 3.9  |
| 1   | C     | 13  | PHE  | 3.9  |
| 1   | A     | 433 | PRO  | 3.8  |
| 1   | C     | 309 | PRO  | 3.8  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 312 | LYS  | 3.8  |
| 1   | F     | 277 | VAL  | 3.8  |
| 1   | B     | 341 | PRO  | 3.8  |
| 1   | C     | 246 | PHE  | 3.7  |
| 1   | A     | 369 | ILE  | 3.7  |
| 1   | C     | 336 | THR  | 3.7  |
| 1   | D     | 505 | THR  | 3.7  |
| 1   | E     | 13  | PHE  | 3.7  |
| 1   | B     | 343 | VAL  | 3.7  |
| 1   | C     | 253 | VAL  | 3.7  |
| 1   | D     | 337 | LYS  | 3.6  |
| 1   | B     | 318 | ILE  | 3.6  |
| 1   | C     | 278 | GLY  | 3.6  |
| 1   | B     | 308 | PHE  | 3.6  |
| 1   | D     | 369 | ILE  | 3.6  |
| 1   | A     | 308 | PHE  | 3.6  |
| 1   | C     | 270 | PHE  | 3.6  |
| 1   | A     | 32  | LEU  | 3.6  |
| 1   | C     | 302 | HIS  | 3.5  |
| 1   | C     | 231 | ILE  | 3.5  |
| 1   | B     | 278 | GLY  | 3.4  |
| 1   | C     | 289 | GLY  | 3.4  |
| 1   | C     | 279 | GLU  | 3.4  |
| 1   | C     | 283 | SER  | 3.4  |
| 1   | C     | 260 | GLY  | 3.4  |
| 1   | D     | 35  | ASP  | 3.4  |
| 1   | B     | 335 | LEU  | 3.4  |
| 1   | F     | 335 | LEU  | 3.4  |
| 1   | B     | 290 | ILE  | 3.3  |
| 1   | F     | 369 | ILE  | 3.3  |
| 1   | A     | 505 | THR  | 3.3  |
| 1   | F     | 284 | ILE  | 3.3  |
| 1   | C     | 280 | SER  | 3.3  |
| 1   | B     | 267 | LEU  | 3.3  |
| 1   | B     | 253 | VAL  | 3.3  |
| 1   | C     | 287 | PRO  | 3.3  |
| 1   | C     | 282 | GLY  | 3.3  |
| 1   | C     | 307 | GLY  | 3.3  |
| 1   | E     | 505 | THR  | 3.2  |
| 1   | A     | 270 | PHE  | 3.2  |
| 1   | B     | 431 | THR  | 3.2  |
| 1   | D     | 308 | PHE  | 3.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | E     | 425 | PHE  | 3.2  |
| 1   | C     | 240 | LEU  | 3.2  |
| 1   | C     | 11  | PRO  | 3.2  |
| 1   | B     | 251 | PHE  | 3.2  |
| 1   | F     | 281 | ASP  | 3.1  |
| 1   | F     | 433 | PRO  | 3.1  |
| 1   | F     | 254 | GLN  | 3.1  |
| 1   | C     | 429 | GLY  | 3.1  |
| 1   | B     | 246 | PHE  | 3.1  |
| 1   | B     | 359 | GLU  | 3.1  |
| 1   | A     | 278 | GLY  | 3.1  |
| 1   | B     | 291 | ASP  | 3.1  |
| 1   | C     | 288 | ASP  | 3.1  |
| 1   | B     | 271 | GLY  | 3.1  |
| 1   | D     | 272 | ALA  | 3.1  |
| 1   | C     | 324 | ASP  | 3.0  |
| 1   | A     | 478 | GLY  | 3.0  |
| 1   | F     | 345 | ALA  | 3.0  |
| 1   | C     | 259 | VAL  | 3.0  |
| 1   | F     | 251 | PHE  | 3.0  |
| 1   | C     | 266 | TYR  | 3.0  |
| 1   | C     | 241 | GLY  | 3.0  |
| 1   | C     | 340 | ALA  | 3.0  |
| 1   | A     | 253 | VAL  | 3.0  |
| 1   | B     | 342 | ARG  | 3.0  |
| 1   | D     | 329 | ALA  | 3.0  |
| 1   | D     | 502 | VAL  | 2.9  |
| 1   | A     | 430 | GLY  | 2.9  |
| 1   | F     | 252 | VAL  | 2.9  |
| 1   | F     | 285 | TRP  | 2.9  |
| 1   | F     | 283 | SER  | 2.9  |
| 1   | A     | 305 | ILE  | 2.9  |
| 1   | C     | 303 | GLY  | 2.9  |
| 1   | C     | 504 | PHE  | 2.9  |
| 1   | D     | 335 | LEU  | 2.8  |
| 1   | F     | 334 | GLN  | 2.8  |
| 1   | B     | 283 | SER  | 2.8  |
| 1   | F     | 339 | ASN  | 2.8  |
| 1   | F     | 364 | PHE  | 2.8  |
| 1   | A     | 317 | SER  | 2.8  |
| 1   | C     | 304 | SER  | 2.8  |
| 1   | C     | 281 | ASP  | 2.8  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | E     | 36  | LEU  | 2.8  |
| 1   | A     | 311 | ALA  | 2.8  |
| 1   | C     | 242 | MET  | 2.8  |
| 1   | C     | 14  | PHE  | 2.8  |
| 1   | F     | 255 | GLY  | 2.7  |
| 1   | D     | 428 | HIS  | 2.7  |
| 1   | A     | 345 | ALA  | 2.7  |
| 1   | C     | 329 | ALA  | 2.7  |
| 1   | B     | 270 | PHE  | 2.7  |
| 1   | C     | 431 | THR  | 2.7  |
| 1   | C     | 293 | LYS  | 2.7  |
| 1   | F     | 303 | GLY  | 2.7  |
| 1   | A     | 330 | ALA  | 2.7  |
| 1   | A     | 13  | PHE  | 2.7  |
| 1   | D     | 433 | PRO  | 2.7  |
| 1   | D     | 14  | PHE  | 2.7  |
| 1   | D     | 340 | ALA  | 2.7  |
| 1   | D     | 266 | TYR  | 2.7  |
| 1   | C     | 239 | ILE  | 2.7  |
| 1   | A     | 277 | VAL  | 2.7  |
| 1   | C     | 310 | LYS  | 2.7  |
| 1   | D     | 251 | PHE  | 2.7  |
| 1   | A     | 347 | ILE  | 2.6  |
| 1   | A     | 300 | LEU  | 2.6  |
| 1   | B     | 289 | GLY  | 2.6  |
| 1   | C     | 294 | GLU  | 2.6  |
| 1   | F     | 368 | ASN  | 2.6  |
| 1   | D     | 250 | THR  | 2.6  |
| 1   | D     | 336 | THR  | 2.6  |
| 1   | D     | 341 | PRO  | 2.6  |
| 1   | B     | 305 | ILE  | 2.6  |
| 1   | B     | 325 | ILE  | 2.6  |
| 1   | D     | 284 | ILE  | 2.6  |
| 1   | F     | 275 | ILE  | 2.6  |
| 1   | F     | 314 | TYR  | 2.6  |
| 1   | B     | 319 | LEU  | 2.6  |
| 1   | C     | 357 | THR  | 2.6  |
| 1   | F     | 357 | THR  | 2.6  |
| 1   | B     | 334 | GLN  | 2.6  |
| 1   | B     | 266 | TYR  | 2.6  |
| 1   | B     | 247 | GLY  | 2.6  |
| 1   | B     | 303 | GLY  | 2.6  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | E     | 303 | GLY  | 2.6  |
| 1   | A     | 47  | ASN  | 2.6  |
| 1   | C     | 12  | ASN  | 2.6  |
| 1   | C     | 353 | ASN  | 2.6  |
| 1   | F     | 244 | PRO  | 2.6  |
| 1   | A     | 431 | THR  | 2.6  |
| 1   | C     | 331 | SER  | 2.6  |
| 1   | B     | 295 | LEU  | 2.6  |
| 1   | A     | 266 | TYR  | 2.6  |
| 1   | B     | 314 | TYR  | 2.6  |
| 1   | A     | 354 | GLY  | 2.6  |
| 1   | D     | 289 | GLY  | 2.6  |
| 1   | C     | 244 | PRO  | 2.6  |
| 1   | D     | 427 | LYS  | 2.5  |
| 1   | A     | 33  | VAL  | 2.5  |
| 1   | F     | 313 | PRO  | 2.5  |
| 1   | B     | 14  | PHE  | 2.5  |
| 1   | B     | 504 | PHE  | 2.5  |
| 1   | C     | 321 | ALA  | 2.5  |
| 1   | D     | 290 | ILE  | 2.5  |
| 1   | C     | 299 | LYS  | 2.5  |
| 1   | D     | 359 | GLU  | 2.5  |
| 1   | D     | 246 | PHE  | 2.5  |
| 1   | C     | 243 | THR  | 2.5  |
| 1   | F     | 274 | CYS  | 2.5  |
| 1   | A     | 434 | ILE  | 2.5  |
| 1   | C     | 297 | ASP  | 2.5  |
| 1   | B     | 429 | GLY  | 2.5  |
| 1   | D     | 278 | GLY  | 2.5  |
| 1   | A     | 326 | LEU  | 2.5  |
| 1   | D     | 322 | ASP  | 2.5  |
| 1   | D     | 342 | ARG  | 2.4  |
| 1   | D     | 34  | GLU  | 2.4  |
| 1   | F     | 278 | GLY  | 2.4  |
| 1   | D     | 343 | VAL  | 2.4  |
| 1   | D     | 318 | ILE  | 2.4  |
| 1   | D     | 339 | ASN  | 2.4  |
| 1   | B     | 275 | ILE  | 2.4  |
| 1   | F     | 250 | THR  | 2.4  |
| 1   | B     | 33  | VAL  | 2.4  |
| 1   | B     | 284 | ILE  | 2.4  |
| 1   | B     | 432 | ILE  | 2.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | E     | 434 | ILE  | 2.4  |
| 1   | A     | 338 | SER  | 2.4  |
| 1   | B     | 338 | SER  | 2.4  |
| 1   | B     | 297 | ASP  | 2.4  |
| 1   | B     | 323 | CYS  | 2.4  |
| 1   | A     | 343 | VAL  | 2.4  |
| 1   | F     | 239 | ILE  | 2.3  |
| 1   | B     | 264 | MET  | 2.3  |
| 1   | F     | 331 | SER  | 2.3  |
| 1   | B     | 425 | PHE  | 2.3  |
| 1   | B     | 326 | LEU  | 2.3  |
| 1   | B     | 503 | THR  | 2.3  |
| 1   | C     | 322 | ASP  | 2.3  |
| 1   | A     | 267 | LEU  | 2.3  |
| 1   | F     | 504 | PHE  | 2.3  |
| 1   | A     | 290 | ILE  | 2.3  |
| 1   | F     | 325 | ILE  | 2.3  |
| 1   | B     | 428 | HIS  | 2.3  |
| 1   | B     | 250 | THR  | 2.3  |
| 1   | E     | 299 | LYS  | 2.3  |
| 1   | B     | 292 | PRO  | 2.3  |
| 1   | E     | 429 | GLY  | 2.3  |
| 1   | F     | 338 | SER  | 2.3  |
| 1   | D     | 255 | GLY  | 2.3  |
| 1   | E     | 307 | GLY  | 2.3  |
| 1   | B     | 321 | ALA  | 2.2  |
| 1   | C     | 330 | ALA  | 2.2  |
| 1   | D     | 325 | ILE  | 2.2  |
| 1   | F     | 276 | ALA  | 2.2  |
| 1   | C     | 273 | LYS  | 2.2  |
| 1   | D     | 314 | TYR  | 2.2  |
| 1   | C     | 17  | VAL  | 2.2  |
| 1   | D     | 300 | LEU  | 2.2  |
| 1   | D     | 275 | ILE  | 2.2  |
| 1   | E     | 14  | PHE  | 2.2  |
| 1   | F     | 311 | ALA  | 2.2  |
| 1   | A     | 503 | THR  | 2.2  |
| 1   | F     | 431 | THR  | 2.2  |
| 1   | F     | 429 | GLY  | 2.2  |
| 1   | B     | 261 | LEU  | 2.2  |
| 1   | F     | 434 | ILE  | 2.2  |
| 1   | D     | 323 | CYS  | 2.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 411 | TYR  | 2.2  |
| 1   | C     | 334 | GLN  | 2.2  |
| 1   | B     | 344 | LYS  | 2.2  |
| 1   | C     | 10  | ASP  | 2.2  |
| 1   | C     | 35  | ASP  | 2.2  |
| 1   | F     | 289 | GLY  | 2.2  |
| 1   | C     | 338 | SER  | 2.2  |
| 1   | D     | 10  | ASP  | 2.2  |
| 1   | E     | 304 | SER  | 2.2  |
| 1   | D     | 432 | ILE  | 2.2  |
| 1   | E     | 305 | ILE  | 2.2  |
| 1   | F     | 432 | ILE  | 2.2  |
| 1   | B     | 296 | GLU  | 2.2  |
| 1   | F     | 356 | THR  | 2.2  |
| 1   | A     | 323 | CYS  | 2.2  |
| 1   | B     | 339 | ASN  | 2.2  |
| 1   | C     | 502 | VAL  | 2.2  |
| 1   | C     | 40  | GLU  | 2.1  |
| 1   | C     | 232 | ASN  | 2.1  |
| 1   | C     | 335 | LEU  | 2.1  |
| 1   | A     | 255 | GLY  | 2.1  |
| 1   | A     | 428 | HIS  | 2.1  |
| 1   | C     | 428 | HIS  | 2.1  |
| 1   | D     | 317 | SER  | 2.1  |
| 1   | F     | 304 | SER  | 2.1  |
| 1   | F     | 305 | ILE  | 2.1  |
| 1   | D     | 504 | PHE  | 2.1  |
| 1   | B     | 505 | THR  | 2.1  |
| 1   | A     | 319 | LEU  | 2.1  |
| 1   | B     | 36  | LEU  | 2.1  |
| 1   | B     | 298 | PHE  | 2.1  |
| 1   | C     | 447 | ALA  | 2.1  |
| 1   | B     | 285 | TRP  | 2.1  |
| 1   | E     | 285 | TRP  | 2.1  |
| 1   | C     | 249 | LYS  | 2.1  |
| 1   | F     | 337 | LYS  | 2.1  |
| 1   | F     | 346 | LYS  | 2.1  |
| 1   | F     | 323 | CYS  | 2.1  |
| 1   | B     | 501 | GLY  | 2.1  |
| 1   | C     | 325 | ILE  | 2.1  |
| 1   | B     | 10  | ASP  | 2.1  |
| 1   | B     | 272 | ALA  | 2.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 345 | ALA  | 2.1  |
| 1   | C     | 337 | LYS  | 2.1  |
| 1   | C     | 301 | GLN  | 2.1  |
| 1   | A     | 239 | ILE  | 2.1  |
| 1   | F     | 290 | ILE  | 2.1  |
| 1   | B     | 322 | ASP  | 2.0  |
| 1   | C     | 315 | GLU  | 2.0  |
| 1   | D     | 283 | SER  | 2.0  |
| 1   | C     | 346 | LYS  | 2.0  |
| 1   | A     | 366 | GLU  | 2.0  |
| 1   | F     | 317 | SER  | 2.0  |
| 1   | C     | 505 | THR  | 2.0  |
| 1   | D     | 446 | GLY  | 2.0  |
| 1   | A     | 314 | TYR  | 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 oligosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<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  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 2   | PO4  | B     | 601  | 5/5   | 0.78 | 0.14 | 75,87,101,103               | 0     |
| 2   | PO4  | C     | 602  | 5/5   | 0.78 | 0.13 | 39,41,54,80                 | 0     |
| 2   | PO4  | F     | 2003 | 5/5   | 0.78 | 0.14 | 49,60,69,91                 | 0     |
| 2   | PO4  | D     | 602  | 5/5   | 0.83 | 0.11 | 68,69,74,91                 | 0     |
| 2   | PO4  | D     | 601  | 5/5   | 0.83 | 0.18 | 58,60,88,89                 | 0     |
| 2   | PO4  | A     | 1001 | 5/5   | 0.85 | 0.12 | 49,65,83,100                | 0     |
| 2   | PO4  | E     | 603  | 5/5   | 0.86 | 0.16 | 50,62,64,78                 | 0     |
| 2   | PO4  | C     | 601  | 5/5   | 0.91 | 0.08 | 61,65,79,81                 | 0     |
| 2   | PO4  | F     | 2001 | 5/5   | 0.91 | 0.13 | 55,68,72,83                 | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 2   | PO4  | E     | 601  | 5/5   | 0.91 | 0.19 | 52,55,68,87                 | 0     |
| 2   | PO4  | B     | 602  | 5/5   | 0.92 | 0.06 | 71,74,81,94                 | 0     |
| 2   | PO4  | F     | 2002 | 5/5   | 0.94 | 0.07 | 55,64,70,76                 | 0     |
| 2   | PO4  | E     | 602  | 5/5   | 0.94 | 0.09 | 53,55,63,75                 | 0     |
| 2   | PO4  | F     | 2004 | 5/5   | 0.96 | 0.07 | 39,43,46,53                 | 0     |
| 2   | PO4  | D     | 603  | 5/5   | 0.98 | 0.04 | 34,38,43,44                 | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.