



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:39 PM UTC

PDB ID : 4B7C / pdb\_00004b7c  
Title : Crystal structure of hypothetical protein PA1648 from *Pseudomonas aeruginosa*.  
Authors : Alpey, M.S.; McMahon, S.A.; Duthie, F.G.; Naismith, J.H.  
Deposited on : 2012-08-17  
Resolution : 2.10 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                                                             |

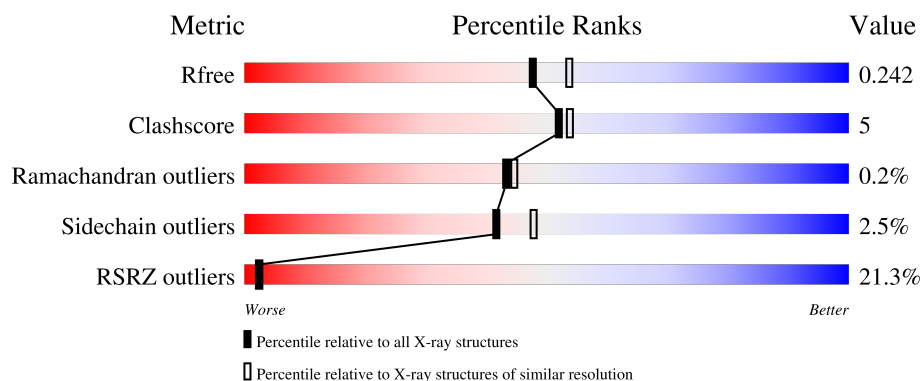
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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                      | 6658 (2.10-2.10)                                      |
| Clashscore            | 190562                      | 7164 (2.10-2.10)                                      |
| Ramachandran outliers | 187476                      | 7099 (2.10-2.10)                                      |
| Sidechain outliers    | 187428                      | 7100 (2.10-2.10)                                      |
| RSRZ outliers         | 180081                      | 6662 (2.10-2.10)                                      |

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     | 336    |                  |
| 1   | B     | 336    |                  |
| 1   | C     | 336    |                  |
| 1   | D     | 336    |                  |
| 1   | E     | 336    |                  |

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| Mol | Chain | Length | Quality of chain                                                                                                 |
|-----|-------|--------|------------------------------------------------------------------------------------------------------------------|
| 1   | F     | 336    | <div><div>22%</div><div><div></div><div>86%</div><div>10%</div><div></div><div></div></div><div>..</div></div>   |
| 1   | G     | 336    | <div><div>17%</div><div><div></div><div>85%</div><div>11%</div><div></div><div></div></div><div>..</div></div>   |
| 1   | H     | 336    | <div><div>20%</div><div><div></div><div>85%</div><div>10%</div><div></div><div>5%</div></div><div></div></div>   |
| 1   | I     | 336    | <div><div>22%</div><div><div></div><div>85%</div><div>9%</div><div></div><div></div></div><div>..</div></div>    |
| 1   | J     | 336    | <div><div>34%</div><div><div></div><div>78%</div><div>10%</div><div></div><div>10%</div></div><div>•</div></div> |
| 1   | K     | 336    | <div><div>54%</div><div><div></div><div>74%</div><div>10%</div><div></div><div>15%</div></div><div>•</div></div> |
| 1   | L     | 336    | <div><div>14%</div><div><div></div><div>83%</div><div>12%</div><div></div><div></div></div><div>..</div></div>   |

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 30125 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 PROBABLE OXIDOREDUCTASE.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 325      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2473  | 1579 | 423 | 458 | 13 |         |         |       |
| 1   | B     | 331      | Total | C    | N   | O   | S  | 0       | 1       | 0     |
|     |       |          | 2529  | 1613 | 437 | 466 | 13 |         |         |       |
| 1   | C     | 323      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2450  | 1567 | 421 | 449 | 13 |         |         |       |
| 1   | D     | 325      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2472  | 1579 | 423 | 457 | 13 |         |         |       |
| 1   | E     | 320      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2424  | 1548 | 416 | 447 | 13 |         |         |       |
| 1   | F     | 325      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2475  | 1581 | 425 | 456 | 13 |         |         |       |
| 1   | G     | 323      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2452  | 1566 | 420 | 453 | 13 |         |         |       |
| 1   | H     | 320      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2424  | 1548 | 415 | 448 | 13 |         |         |       |
| 1   | I     | 323      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2454  | 1567 | 422 | 452 | 13 |         |         |       |
| 1   | J     | 302      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2289  | 1463 | 392 | 422 | 12 |         |         |       |
| 1   | K     | 286      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2172  | 1394 | 367 | 399 | 12 |         |         |       |
| 1   | L     | 325      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2475  | 1581 | 425 | 456 | 13 |         |         |       |

There are 24 discrepancies between the modelled and reference sequences:

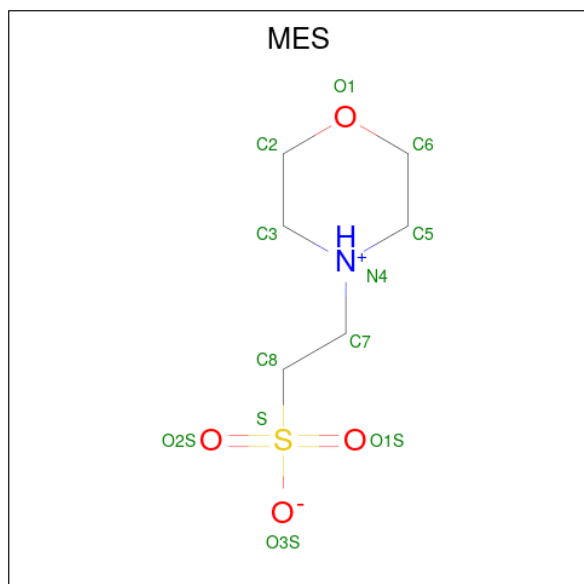
| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | -1      | GLY      | -      | expression tag | UNP B7UV73 |
| A     | 0       | ALA      | -      | expression tag | UNP B7UV73 |
| B     | -1      | GLY      | -      | expression tag | UNP B7UV73 |
| B     | 0       | ALA      | -      | expression tag | UNP B7UV73 |
| C     | -1      | GLY      | -      | expression tag | UNP B7UV73 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| C     | 0       | ALA      | -      | expression tag | UNP B7UV73 |
| D     | -1      | GLY      | -      | expression tag | UNP B7UV73 |
| D     | 0       | ALA      | -      | expression tag | UNP B7UV73 |
| E     | -1      | GLY      | -      | expression tag | UNP B7UV73 |
| E     | 0       | ALA      | -      | expression tag | UNP B7UV73 |
| F     | -1      | GLY      | -      | expression tag | UNP B7UV73 |
| F     | 0       | ALA      | -      | expression tag | UNP B7UV73 |
| G     | -1      | GLY      | -      | expression tag | UNP B7UV73 |
| G     | 0       | ALA      | -      | expression tag | UNP B7UV73 |
| H     | -1      | GLY      | -      | expression tag | UNP B7UV73 |
| H     | 0       | ALA      | -      | expression tag | UNP B7UV73 |
| I     | -1      | GLY      | -      | expression tag | UNP B7UV73 |
| I     | 0       | ALA      | -      | expression tag | UNP B7UV73 |
| J     | -1      | GLY      | -      | expression tag | UNP B7UV73 |
| J     | 0       | ALA      | -      | expression tag | UNP B7UV73 |
| K     | -1      | GLY      | -      | expression tag | UNP B7UV73 |
| K     | 0       | ALA      | -      | expression tag | UNP B7UV73 |
| L     | -1      | GLY      | -      | expression tag | UNP B7UV73 |
| L     | 0       | ALA      | -      | expression tag | UNP B7UV73 |

- Molecule 2 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula:  $C_6H_{13}NO_4S$ ).



| Mol | Chain | Residues | Atoms |   |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---|---------|---------|
| 2   | D     | 1        | Total | C | N | O | S | 0       | 0       |
|     |       |          | 12    | 6 | 1 | 4 | 1 |         |         |

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| Mol | Chain | Residues | Atoms |   |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---|---------|---------|
| 2   | F     | 1        | Total | C | N | O | S | 0       | 0       |
|     |       |          | 12    | 6 | 1 | 4 | 1 |         |         |
| 2   | G     | 1        | Total | C | N | O | S | 0       | 0       |
|     |       |          | 12    | 6 | 1 | 4 | 1 |         |         |
| 2   | H     | 1        | Total | C | N | O | S | 0       | 0       |
|     |       |          | 12    | 6 | 1 | 4 | 1 |         |         |
| 2   | I     | 1        | Total | C | N | O | S | 0       | 0       |
|     |       |          | 12    | 6 | 1 | 4 | 1 |         |         |

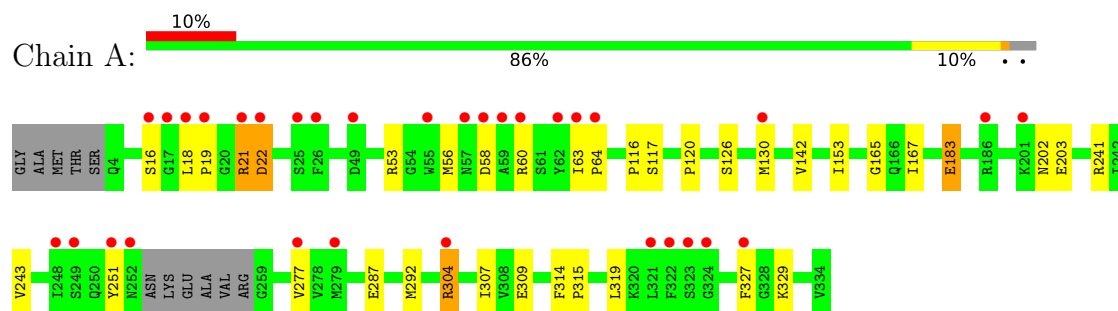
- Molecule 3 is water.

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 3   | A     | 146      | Total | O   | 0       | 0       |
|     |       |          | 146   | 146 |         |         |
| 3   | B     | 88       | Total | O   | 0       | 0       |
|     |       |          | 88    | 88  |         |         |
| 3   | C     | 77       | Total | O   | 0       | 0       |
|     |       |          | 77    | 77  |         |         |
| 3   | D     | 141      | Total | O   | 0       | 0       |
|     |       |          | 141   | 141 |         |         |
| 3   | E     | 132      | Total | O   | 0       | 0       |
|     |       |          | 132   | 132 |         |         |
| 3   | F     | 55       | Total | O   | 0       | 0       |
|     |       |          | 55    | 55  |         |         |
| 3   | G     | 87       | Total | O   | 0       | 0       |
|     |       |          | 87    | 87  |         |         |
| 3   | H     | 36       | Total | O   | 0       | 0       |
|     |       |          | 36    | 36  |         |         |
| 3   | I     | 48       | Total | O   | 0       | 0       |
|     |       |          | 48    | 48  |         |         |
| 3   | J     | 72       | Total | O   | 0       | 0       |
|     |       |          | 72    | 72  |         |         |
| 3   | K     | 24       | Total | O   | 0       | 0       |
|     |       |          | 24    | 24  |         |         |
| 3   | L     | 70       | Total | O   | 0       | 0       |
|     |       |          | 70    | 70  |         |         |

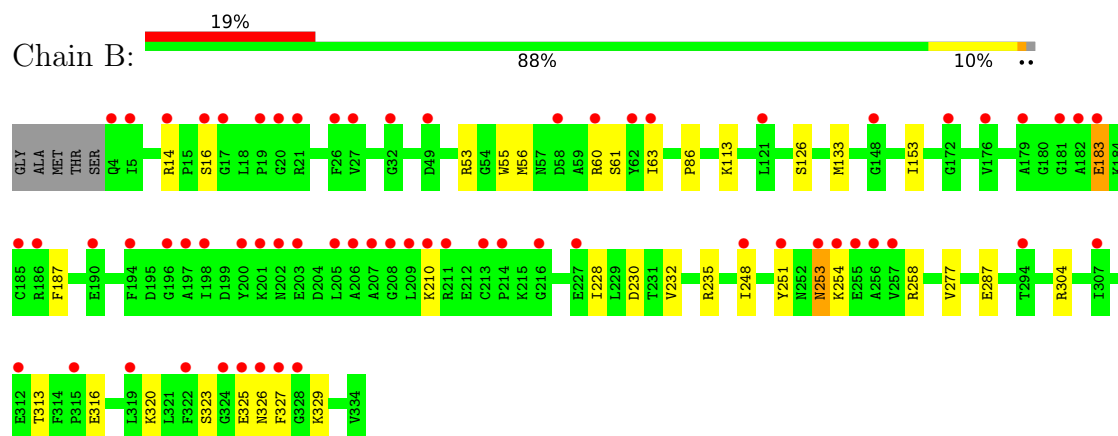
### 3 Residue-property plots [i](#)

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.

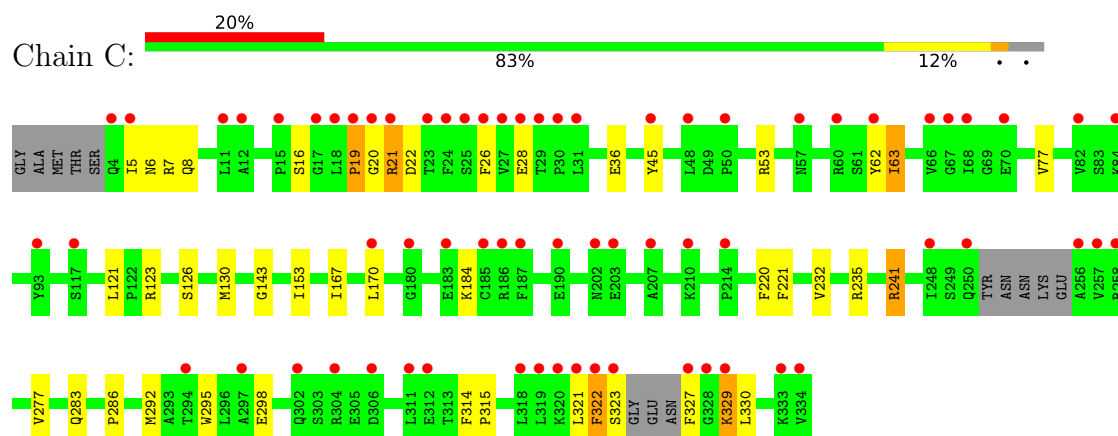
#### • Molecule 1: PROBABLE OXIDOREDUCTASE



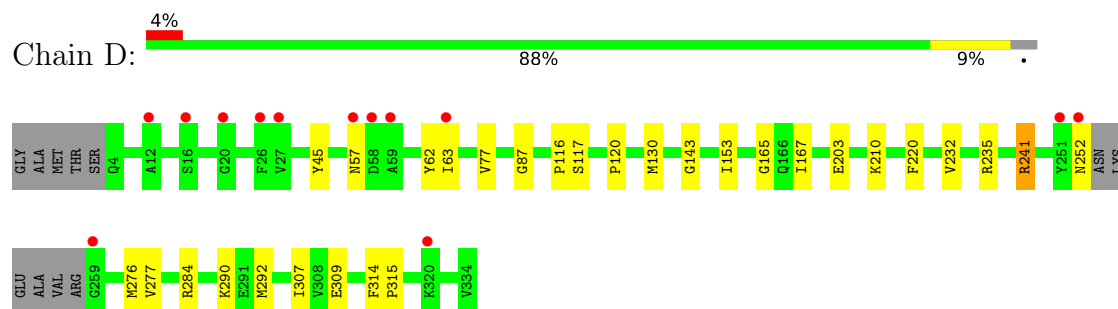
#### • Molecule 1: PROBABLE OXIDOREDUCTASE



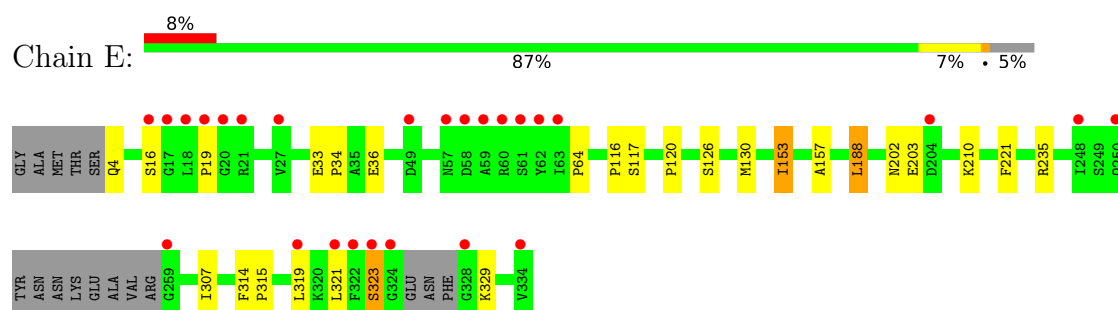
#### • Molecule 1: PROBABLE OXIDOREDUCTASE



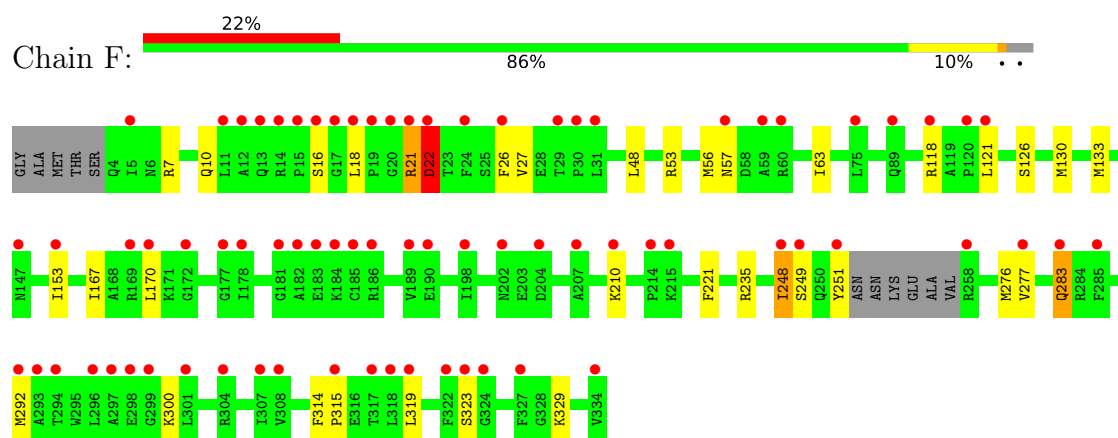
● Molecule 1: PROBABLE OXIDOREDUCTASE



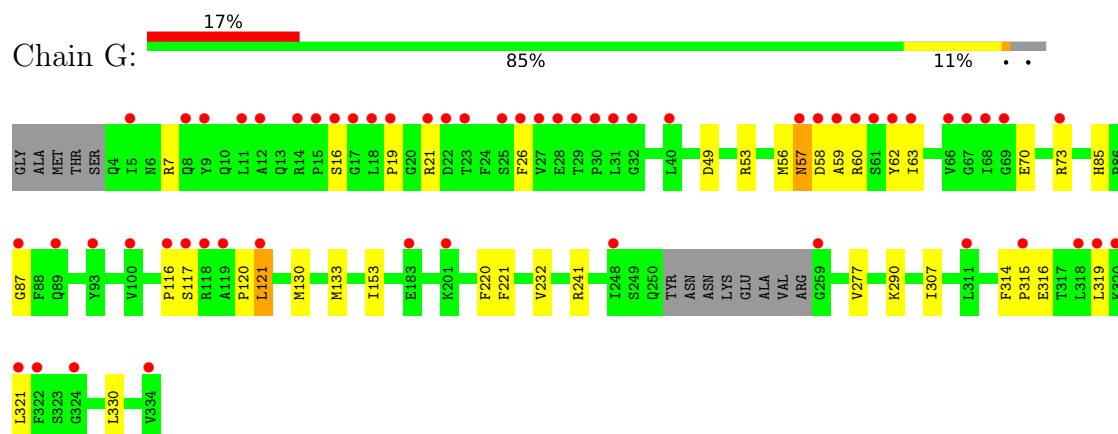
● Molecule 1: PROBABLE OXIDOREDUCTASE



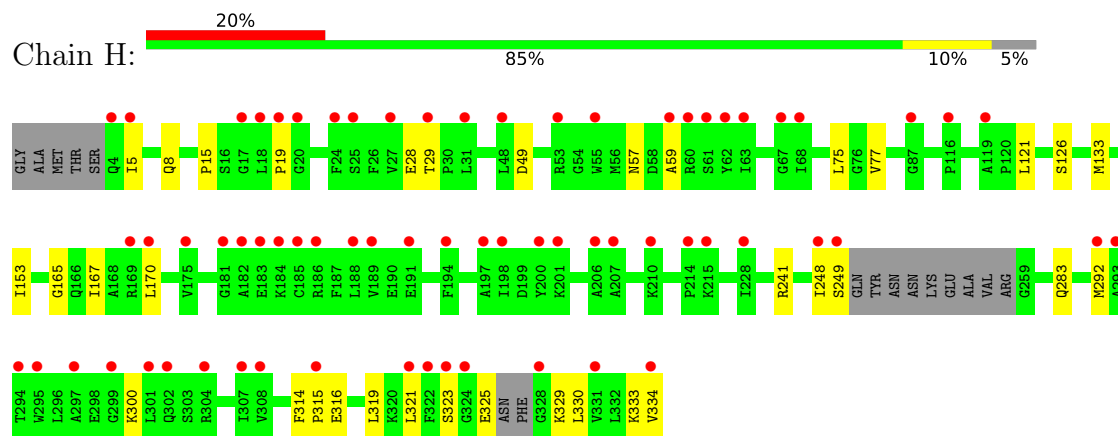
● Molecule 1: PROBABLE OXIDOREDUCTASE



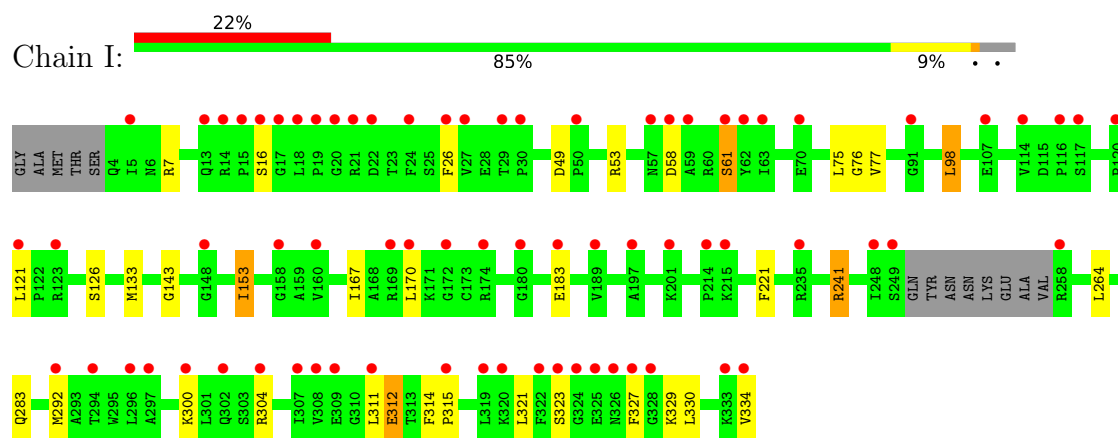
● Molecule 1: PROBABLE OXIDOREDUCTASE



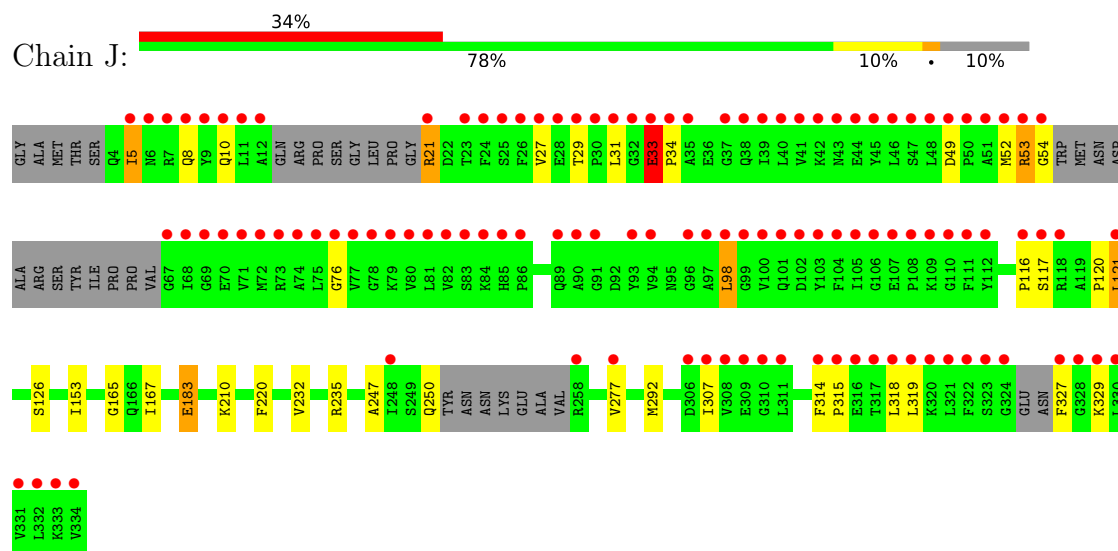
• Molecule 1: PROBABLE OXIDOREDUCTASE



• Molecule 1: PROBABLE OXIDOREDUCTASE

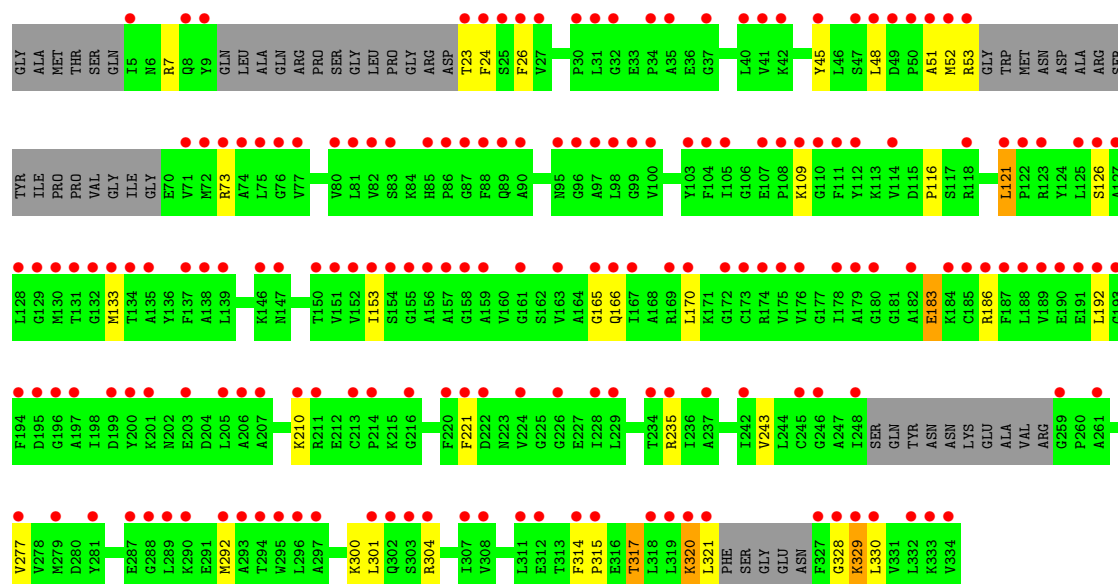


• Molecule 1: PROBABLE OXIDOREDUCTASE

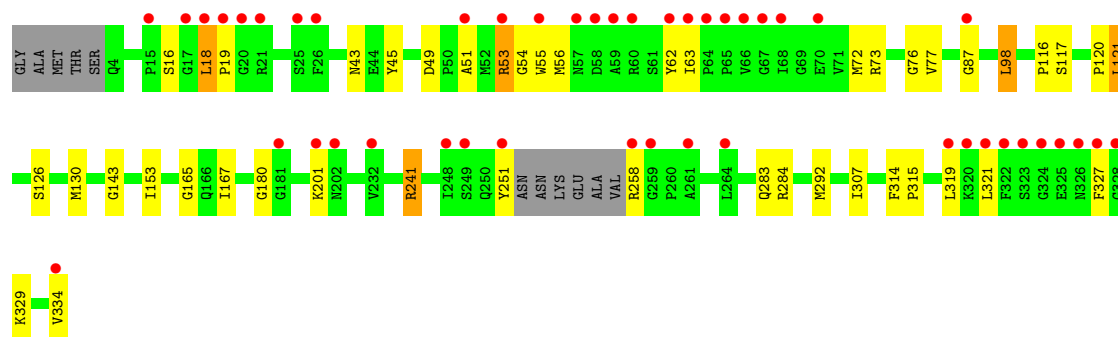
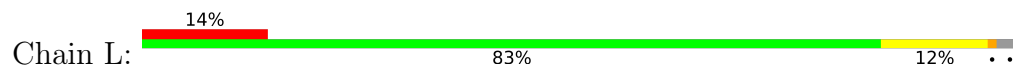


• Molecule 1: PROBABLE OXIDOREDUCTASE





• Molecule 1: PROBABLE OXIDOREDUCTASE



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 21 21                                                  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 170.93Å 177.09Å 181.66Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 73.06 – 2.10<br>73.06 – 2.10                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.1 (73.06-2.10)<br>99.1 (73.06-2.10)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.05                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.48 (at 2.10Å)                                             | Xtriage          |
| Refinement program                                                      | REFMAC 5.6.0117                                             | Depositor        |
| R, $R_{free}$                                                           | 0.223 , 0.243<br>0.224 , 0.242                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 16092 reflections (5.05%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 38.4                                                        | Xtriage          |
| Anisotropy                                                              | 0.180                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.36 , 37.0                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$ | Xtriage          |
| Estimated twinning fraction                                             | 0.015 for -h,l,k                                            | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.94                                                        | EDS              |
| Total number of atoms                                                   | 30125                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 47.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.93% 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: MES

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     | 0.71         | 1/2520 (0.0%)  | 0.91        | 8/3401 (0.2%)   |
| 1   | B     | 0.64         | 0/2580         | 0.82        | 1/3483 (0.0%)   |
| 1   | C     | 0.68         | 0/2495         | 0.87        | 4/3367 (0.1%)   |
| 1   | D     | 0.67         | 0/2519         | 0.85        | 7/3401 (0.2%)   |
| 1   | E     | 0.68         | 1/2468 (0.0%)  | 0.81        | 0/3330          |
| 1   | F     | 0.64         | 1/2522 (0.0%)  | 0.78        | 1/3404 (0.0%)   |
| 1   | G     | 0.62         | 0/2498         | 0.79        | 2/3372 (0.1%)   |
| 1   | H     | 0.62         | 0/2468         | 0.84        | 3/3330 (0.1%)   |
| 1   | I     | 0.64         | 0/2500         | 0.84        | 4/3374 (0.1%)   |
| 1   | J     | 0.64         | 0/2325         | 0.82        | 3/3128 (0.1%)   |
| 1   | K     | 0.65         | 2/2207 (0.1%)  | 0.86        | 4/2972 (0.1%)   |
| 1   | L     | 0.63         | 0/2522         | 0.86        | 5/3404 (0.1%)   |
| All | All   | 0.65         | 5/29624 (0.0%) | 0.84        | 42/39966 (0.1%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | C     | 0                   | 1                   |

All (5) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 1   | E     | 64  | PRO  | CA-C  | 6.06 | 1.55        | 1.51     |
| 1   | K     | 328 | GLY  | N-CA  | 5.97 | 1.54        | 1.45     |
| 1   | F     | 22  | ASP  | CA-CB | 5.52 | 1.61        | 1.53     |
| 1   | K     | 186 | ARG  | CA-CB | 5.35 | 1.61        | 1.53     |
| 1   | A     | 64  | PRO  | CA-C  | 5.34 | 1.54        | 1.51     |

All (42) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1   | C     | 241 | ARG  | NE-CZ-NH2 | -11.36 | 108.97      | 119.20   |
| 1   | C     | 241 | ARG  | NE-CZ-NH1 | 10.76  | 132.26      | 121.50   |
| 1   | J     | 31  | LEU  | N-CA-C    | 10.26  | 125.67      | 112.34   |
| 1   | L     | 284 | ARG  | NE-CZ-NH2 | 8.42   | 126.78      | 119.20   |
| 1   | D     | 284 | ARG  | NE-CZ-NH2 | 8.37   | 126.73      | 119.20   |
| 1   | A     | 241 | ARG  | NE-CZ-NH2 | -8.26  | 111.77      | 119.20   |
| 1   | H     | 241 | ARG  | NE-CZ-NH2 | -8.21  | 111.82      | 119.20   |
| 1   | G     | 241 | ARG  | NE-CZ-NH2 | -8.06  | 111.95      | 119.20   |
| 1   | L     | 284 | ARG  | CD-NE-CZ  | -7.72  | 113.59      | 124.40   |
| 1   | I     | 323 | SER  | N-CA-C    | -7.64  | 99.22       | 110.52   |
| 1   | D     | 284 | ARG  | CD-NE-CZ  | -7.42  | 114.01      | 124.40   |
| 1   | F     | 323 | SER  | N-CA-C    | -7.38  | 99.88       | 110.59   |
| 1   | A     | 63  | ILE  | CB-CA-C   | -7.29  | 103.05      | 110.13   |
| 1   | L     | 241 | ARG  | NE-CZ-NH1 | 7.23   | 128.73      | 121.50   |
| 1   | A     | 241 | ARG  | NE-CZ-NH1 | 7.11   | 128.61      | 121.50   |
| 1   | I     | 241 | ARG  | NE-CZ-NH1 | 7.03   | 128.53      | 121.50   |
| 1   | I     | 241 | ARG  | NE-CZ-NH2 | -6.99  | 112.91      | 119.20   |
| 1   | D     | 241 | ARG  | NE-CZ-NH1 | 6.96   | 128.46      | 121.50   |
| 1   | K     | 183 | GLU  | N-CA-CB   | -6.93  | 100.02      | 110.07   |
| 1   | D     | 284 | ARG  | NE-CZ-NH1 | -6.91  | 114.59      | 121.50   |
| 1   | H     | 241 | ARG  | NE-CZ-NH1 | 6.91   | 128.41      | 121.50   |
| 1   | G     | 241 | ARG  | NE-CZ-NH1 | 6.90   | 128.40      | 121.50   |
| 1   | L     | 241 | ARG  | NE-CZ-NH2 | -6.80  | 113.08      | 119.20   |
| 1   | D     | 241 | ARG  | NE-CZ-NH2 | -6.68  | 113.19      | 119.20   |
| 1   | L     | 284 | ARG  | NE-CZ-NH1 | -6.66  | 114.84      | 121.50   |
| 1   | K     | 317 | THR  | CB-CA-C   | -6.61  | 97.27       | 110.42   |
| 1   | H     | 59  | ALA  | N-CA-C    | 6.46   | 118.12      | 111.14   |
| 1   | B     | 287 | GLU  | CB-CG-CD  | -6.29  | 101.90      | 112.60   |
| 1   | K     | 329 | LYS  | N-CA-CB   | 6.18   | 119.39      | 110.37   |
| 1   | I     | 61  | SER  | N-CA-C    | 6.11   | 119.11      | 110.50   |
| 1   | C     | 298 | GLU  | CG-CD-OE2 | 5.90   | 131.98      | 118.40   |
| 1   | C     | 329 | LYS  | N-CA-C    | 5.70   | 118.03      | 108.96   |
| 1   | D     | 309 | GLU  | CG-CD-OE2 | 5.57   | 131.20      | 118.40   |
| 1   | A     | 309 | GLU  | CG-CD-OE2 | 5.50   | 131.05      | 118.40   |
| 1   | A     | 21  | ARG  | N-CA-C    | 5.49   | 118.18      | 111.82   |
| 1   | A     | 309 | GLU  | CG-CD-OE1 | -5.39  | 106.01      | 118.40   |
| 1   | D     | 309 | GLU  | CG-CD-OE1 | -5.35  | 106.09      | 118.40   |
| 1   | K     | 183 | GLU  | CA-CB-CG  | 5.30   | 124.71      | 114.10   |
| 1   | J     | 33  | GLU  | CA-C-N    | -5.24  | 114.52      | 119.76   |
| 1   | J     | 33  | GLU  | C-N-CA    | -5.24  | 114.52      | 119.76   |
| 1   | A     | 287 | GLU  | N-CA-CB   | -5.06  | 102.67      | 110.16   |
| 1   | A     | 287 | GLU  | CA-CB-CG  | 5.01   | 124.12      | 114.10   |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | C     | 19  | PRO  | 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     | 2473  | 0        | 2491     | 21      | 1            |
| 1   | B     | 2529  | 0        | 2557     | 24      | 0            |
| 1   | C     | 2450  | 0        | 2481     | 29      | 1            |
| 1   | D     | 2472  | 0        | 2491     | 24      | 0            |
| 1   | E     | 2424  | 0        | 2454     | 18      | 1            |
| 1   | F     | 2475  | 0        | 2498     | 25      | 0            |
| 1   | G     | 2452  | 0        | 2476     | 29      | 0            |
| 1   | H     | 2424  | 0        | 2452     | 24      | 0            |
| 1   | I     | 2454  | 0        | 2481     | 25      | 0            |
| 1   | J     | 2289  | 0        | 2322     | 41      | 0            |
| 1   | K     | 2172  | 0        | 2210     | 31      | 1            |
| 1   | L     | 2475  | 0        | 2498     | 38      | 0            |
| 2   | D     | 12    | 0        | 13       | 0       | 0            |
| 2   | F     | 12    | 0        | 13       | 0       | 0            |
| 2   | G     | 12    | 0        | 13       | 0       | 0            |
| 2   | H     | 12    | 0        | 13       | 2       | 0            |
| 2   | I     | 12    | 0        | 13       | 2       | 0            |
| 3   | A     | 146   | 0        | 0        | 0       | 0            |
| 3   | B     | 88    | 0        | 0        | 1       | 0            |
| 3   | C     | 77    | 0        | 0        | 1       | 0            |
| 3   | D     | 141   | 0        | 0        | 1       | 0            |
| 3   | E     | 132   | 0        | 0        | 2       | 0            |
| 3   | F     | 55    | 0        | 0        | 2       | 0            |
| 3   | G     | 87    | 0        | 0        | 2       | 0            |
| 3   | H     | 36    | 0        | 0        | 0       | 0            |
| 3   | I     | 48    | 0        | 0        | 0       | 0            |
| 3   | J     | 72    | 0        | 0        | 0       | 0            |
| 3   | K     | 24    | 0        | 0        | 0       | 0            |
| 3   | L     | 70    | 0        | 0        | 0       | 0            |
| All | All   | 30125 | 0        | 29476    | 297     | 2            |

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 5.

All (297) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:323:SER:OG   | 1:B:325:GLU:HB2  | 1.58                     | 1.01              |
| 1:J:52:MET:C     | 1:J:54:GLY:H     | 1.76                     | 0.89              |
| 1:E:130:MET:HE3  | 3:E:2040:HOH:O   | 1.80                     | 0.82              |
| 1:K:321:LEU:HD13 | 1:K:330:LEU:HD23 | 1.62                     | 0.82              |
| 1:C:36:GLU:CG    | 1:J:5:ILE:HD12   | 2.16                     | 0.76              |
| 1:G:120:PRO:HB3  | 1:J:116:PRO:O    | 1.86                     | 0.76              |
| 1:J:52:MET:HE1   | 1:J:318:LEU:CD1  | 2.17                     | 0.75              |
| 1:H:15:PRO:O     | 1:H:57:ASN:ND2   | 2.20                     | 0.75              |
| 1:D:120:PRO:HB3  | 1:E:116:PRO:O    | 1.87                     | 0.74              |
| 1:A:304:ARG:NH2  | 1:A:327:PHE:CE1  | 2.56                     | 0.74              |
| 1:F:283:GLN:HA   | 1:F:283:GLN:NE2  | 2.00                     | 0.74              |
| 1:I:312:GLU:H    | 1:I:312:GLU:CD   | 1.96                     | 0.73              |
| 1:I:76:GLY:C     | 1:I:98:LEU:HD22  | 2.15                     | 0.72              |
| 1:J:33:GLU:HG3   | 1:J:34:PRO:HD2   | 1.72                     | 0.72              |
| 1:L:18:LEU:CD2   | 1:L:319:LEU:HD22 | 2.20                     | 0.72              |
| 1:D:130:MET:HE2  | 1:D:130:MET:HA   | 1.73                     | 0.71              |
| 1:E:210:LYS:HA   | 1:E:235:ARG:HH12 | 1.55                     | 0.71              |
| 1:J:52:MET:C     | 1:J:54:GLY:N     | 2.48                     | 0.70              |
| 1:K:48:LEU:HD12  | 1:K:330:LEU:HG   | 1.72                     | 0.69              |
| 1:C:170:LEU:HD11 | 1:C:295:TRP:CD1  | 2.28                     | 0.69              |
| 1:J:76:GLY:C     | 1:J:98:LEU:HD22  | 2.18                     | 0.69              |
| 1:I:75:LEU:HD22  | 2:I:1335:MES:S   | 2.33                     | 0.68              |
| 1:A:116:PRO:O    | 1:L:120:PRO:HB3  | 1.93                     | 0.68              |
| 1:J:52:MET:O     | 1:J:54:GLY:N     | 2.28                     | 0.66              |
| 1:L:76:GLY:C     | 1:L:98:LEU:HD22  | 2.20                     | 0.66              |
| 1:A:53:ARG:NH1   | 1:A:251:TYR:O    | 2.29                     | 0.65              |
| 1:B:210:LYS:HA   | 1:B:235:ARG:HH12 | 1.61                     | 0.65              |
| 1:B:323:SER:OG   | 1:B:325:GLU:CB   | 2.41                     | 0.65              |
| 1:L:18:LEU:HD21  | 1:L:319:LEU:HD22 | 1.77                     | 0.65              |
| 1:K:166:GLN:CB   | 1:K:301:LEU:CD1  | 2.74                     | 0.64              |
| 1:A:22:ASP:OD1   | 1:A:22:ASP:N     | 2.24                     | 0.64              |
| 1:F:21:ARG:NH2   | 1:F:319:LEU:HD11 | 2.11                     | 0.64              |
| 1:F:130:MET:HE2  | 1:F:130:MET:HA   | 1.79                     | 0.64              |
| 1:I:321:LEU:HD13 | 1:I:330:LEU:HD23 | 1.80                     | 0.64              |
| 1:F:153:ILE:HD13 | 1:F:221:PHE:HB3  | 1.79                     | 0.63              |
| 1:C:36:GLU:HG2   | 1:J:5:ILE:HD12   | 1.81                     | 0.62              |
| 1:E:210:LYS:HA   | 1:E:235:ARG:NH1  | 2.14                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:153:ILE:HD13 | 1:G:221:PHE:HB3  | 1.79                     | 0.62              |
| 1:K:166:GLN:HB2  | 1:K:301:LEU:CD1  | 2.29                     | 0.62              |
| 1:J:52:MET:CE    | 1:J:318:LEU:HD11 | 2.29                     | 0.62              |
| 1:I:283:GLN:HA   | 1:L:87:GLY:HA3   | 1.82                     | 0.62              |
| 1:F:63:ILE:HD12  | 3:F:2012:HOH:O   | 1.98                     | 0.62              |
| 1:B:210:LYS:HB2  | 1:B:235:ARG:HH22 | 1.64                     | 0.62              |
| 1:K:317:THR:HG22 | 1:K:317:THR:O    | 2.00                     | 0.61              |
| 1:G:21:ARG:NH1   | 1:G:316:GLU:OE2  | 2.33                     | 0.61              |
| 1:H:133:MET:HE2  | 1:H:133:MET:HA   | 1.83                     | 0.61              |
| 1:F:57:ASN:HD21  | 1:F:251:TYR:C    | 2.09                     | 0.61              |
| 1:K:133:MET:HE2  | 1:K:133:MET:HA   | 1.83                     | 0.60              |
| 1:B:187:PHE:CZ   | 1:B:304:ARG:HD2  | 2.36                     | 0.60              |
| 1:G:57:ASN:HD21  | 1:G:59:ALA:HB2   | 1.66                     | 0.60              |
| 1:C:143:GLY:O    | 1:C:241:ARG:HD2  | 2.02                     | 0.59              |
| 1:J:10:GLN:NE2   | 1:J:27:VAL:HG21  | 2.18                     | 0.59              |
| 1:A:142:VAL:HG12 | 1:A:243:VAL:HG22 | 1.84                     | 0.59              |
| 1:K:153:ILE:HD11 | 1:K:165:GLY:HA2  | 1.84                     | 0.59              |
| 1:L:153:ILE:HD11 | 1:L:165:GLY:HA2  | 1.84                     | 0.59              |
| 1:C:153:ILE:HD13 | 1:C:221:PHE:HB3  | 1.85                     | 0.59              |
| 1:J:52:MET:CE    | 1:J:318:LEU:CD1  | 2.80                     | 0.58              |
| 1:G:57:ASN:HD21  | 1:G:59:ALA:CB    | 2.17                     | 0.58              |
| 1:D:167:ILE:HD11 | 1:D:292:MET:HE1  | 1.85                     | 0.58              |
| 1:F:283:GLN:HA   | 1:F:283:GLN:HE21 | 1.66                     | 0.58              |
| 1:K:170:LEU:HD21 | 1:K:300:LYS:HB3  | 1.85                     | 0.58              |
| 1:L:143:GLY:O    | 1:L:241:ARG:HD2  | 2.04                     | 0.58              |
| 1:C:321:LEU:C    | 1:C:323:SER:H    | 2.11                     | 0.58              |
| 1:J:52:MET:HE3   | 1:J:318:LEU:HD11 | 1.85                     | 0.57              |
| 1:G:117:SER:HB2  | 1:J:307:ILE:CD1  | 2.35                     | 0.57              |
| 1:I:143:GLY:O    | 1:I:241:ARG:HD2  | 2.05                     | 0.57              |
| 1:B:86:PRO:HG2   | 3:E:2035:HOH:O   | 2.03                     | 0.57              |
| 1:B:133:MET:HA   | 1:B:133:MET:HE2  | 1.86                     | 0.57              |
| 1:G:117:SER:CB   | 1:J:307:ILE:CD1  | 2.82                     | 0.57              |
| 1:D:143:GLY:O    | 1:D:241:ARG:HD2  | 2.04                     | 0.57              |
| 3:D:2067:HOH:O   | 1:G:290:LYS:HE2  | 2.03                     | 0.57              |
| 1:J:153:ILE:HD11 | 1:J:165:GLY:HA2  | 1.87                     | 0.57              |
| 1:I:133:MET:HE2  | 1:I:133:MET:HA   | 1.87                     | 0.57              |
| 1:F:248:ILE:C    | 1:F:248:ILE:HD12 | 2.29                     | 0.57              |
| 1:H:153:ILE:HD11 | 1:H:165:GLY:HA2  | 1.87                     | 0.57              |
| 1:J:33:GLU:HG3   | 1:J:34:PRO:CD    | 2.34                     | 0.56              |
| 1:J:210:LYS:HA   | 1:J:235:ARG:HH21 | 1.70                     | 0.56              |
| 1:D:57:ASN:HD21  | 1:D:252:ASN:HA   | 1.70                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:120:PRO:HB3  | 1:L:116:PRO:O    | 2.06                     | 0.56              |
| 1:L:18:LEU:CD2   | 1:L:319:LEU:CD2  | 2.83                     | 0.56              |
| 1:G:130:MET:HE2  | 1:G:130:MET:HA   | 1.87                     | 0.56              |
| 1:J:21:ARG:HH12  | 1:J:319:LEU:HD11 | 1.71                     | 0.55              |
| 1:H:321:LEU:HD13 | 1:H:330:LEU:HD23 | 1.88                     | 0.55              |
| 1:D:57:ASN:HD21  | 1:D:252:ASN:CA   | 2.20                     | 0.55              |
| 1:J:153:ILE:CD1  | 1:J:165:GLY:HA2  | 2.36                     | 0.55              |
| 1:F:22:ASP:OD1   | 1:F:22:ASP:N     | 2.39                     | 0.55              |
| 1:F:210:LYS:HA   | 1:F:235:ARG:HH21 | 1.70                     | 0.55              |
| 1:H:153:ILE:CD1  | 1:H:165:GLY:HA2  | 2.37                     | 0.54              |
| 1:K:321:LEU:HD13 | 1:K:330:LEU:CD2  | 2.35                     | 0.54              |
| 1:B:55:TRP:NE1   | 1:B:63:ILE:HD11  | 2.22                     | 0.54              |
| 1:B:53:ARG:HA    | 1:B:56:MET:HE3   | 1.89                     | 0.54              |
| 1:D:87:GLY:HA3   | 1:H:283:GLN:HA   | 1.89                     | 0.54              |
| 1:B:113:LYS:NZ   | 1:E:36:GLU:OE2   | 2.39                     | 0.54              |
| 1:D:210:LYS:HA   | 1:D:235:ARG:HH21 | 1.71                     | 0.54              |
| 1:G:153:ILE:HD13 | 1:G:221:PHE:CB   | 2.38                     | 0.54              |
| 1:E:19:PRO:O     | 1:E:319:LEU:HD21 | 2.06                     | 0.54              |
| 1:J:52:MET:HE1   | 1:J:318:LEU:HD13 | 1.90                     | 0.54              |
| 1:A:153:ILE:HD11 | 1:A:165:GLY:HA2  | 1.89                     | 0.54              |
| 1:K:166:GLN:NE2  | 1:K:192:LEU:HD22 | 2.23                     | 0.54              |
| 1:L:55:TRP:HE1   | 1:L:63:ILE:HD12  | 1.72                     | 0.54              |
| 1:C:283:GLN:HA   | 1:G:87:GLY:HA3   | 1.89                     | 0.54              |
| 1:E:33:GLU:HB3   | 1:E:34:PRO:HD2   | 1.89                     | 0.54              |
| 1:K:166:GLN:HB3  | 1:K:301:LEU:CD1  | 2.38                     | 0.54              |
| 1:G:277:VAL:HG13 | 3:G:2071:HOH:O   | 2.08                     | 0.53              |
| 1:L:180:GLY:HA3  | 1:L:201:LYS:HE3  | 1.90                     | 0.53              |
| 1:I:153:ILE:HD13 | 1:I:221:PHE:HB3  | 1.89                     | 0.53              |
| 1:F:21:ARG:HH22  | 1:F:319:LEU:HD11 | 1.73                     | 0.52              |
| 1:F:57:ASN:ND2   | 1:F:251:TYR:C    | 2.67                     | 0.52              |
| 1:F:153:ILE:HD13 | 1:F:221:PHE:CB   | 2.40                     | 0.52              |
| 1:C:6:ASN:ND2    | 1:C:8:GLN:HE21   | 2.07                     | 0.52              |
| 1:C:286:PRO:HG2  | 1:G:85:HIS:NE2   | 2.25                     | 0.52              |
| 1:J:49:ASP:H     | 1:J:52:MET:HE2   | 1.75                     | 0.52              |
| 1:K:23:THR:HG23  | 1:K:24:PHE:H     | 1.76                     | 0.51              |
| 1:F:21:ARG:HH22  | 1:F:319:LEU:CD1  | 2.23                     | 0.51              |
| 1:D:116:PRO:O    | 1:E:120:PRO:HB3  | 2.11                     | 0.51              |
| 1:F:170:LEU:HD21 | 1:F:300:LYS:HB3  | 1.92                     | 0.51              |
| 1:L:153:ILE:CD1  | 1:L:165:GLY:HA2  | 2.41                     | 0.51              |
| 1:C:184:LYS:HG2  | 1:C:327:PHE:CE1  | 2.45                     | 0.51              |
| 1:D:153:ILE:HD11 | 1:D:165:GLY:HA2  | 1.93                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:153:ILE:CD1  | 1:K:165:GLY:HA2  | 2.41                     | 0.50              |
| 1:A:117:SER:HB3  | 1:L:307:ILE:CD1  | 2.41                     | 0.50              |
| 1:C:62:TYR:CD2   | 1:C:63:ILE:HG13  | 2.46                     | 0.50              |
| 1:J:33:GLU:CG    | 1:J:34:PRO:HD2   | 2.40                     | 0.50              |
| 1:B:248:ILE:HA   | 1:B:251:TYR:CD2  | 2.47                     | 0.50              |
| 1:C:5:ILE:HD11   | 1:C:28:GLU:HB3   | 1.93                     | 0.50              |
| 1:E:130:MET:HE2  | 1:E:130:MET:HA   | 1.94                     | 0.50              |
| 1:H:170:LEU:HD21 | 1:H:300:LYS:HB3  | 1.94                     | 0.50              |
| 1:L:167:ILE:HD11 | 1:L:292:MET:HE1  | 1.94                     | 0.50              |
| 1:A:167:ILE:HD11 | 1:A:292:MET:HE1  | 1.93                     | 0.49              |
| 1:L:63:ILE:HG22  | 1:L:73:ARG:NH1   | 2.27                     | 0.49              |
| 1:C:36:GLU:HG3   | 1:J:5:ILE:HD12   | 1.91                     | 0.49              |
| 1:J:153:ILE:CD1  | 1:J:165:GLY:CA   | 2.90                     | 0.49              |
| 1:B:304:ARG:HH12 | 1:B:327:PHE:HD2  | 1.61                     | 0.49              |
| 1:C:153:ILE:HD13 | 1:C:221:PHE:CB   | 2.43                     | 0.49              |
| 1:A:153:ILE:CD1  | 1:A:165:GLY:HA2  | 2.43                     | 0.49              |
| 1:E:153:ILE:HD13 | 1:E:221:PHE:HB3  | 1.93                     | 0.49              |
| 1:K:166:GLN:CD   | 1:K:301:LEU:HD12 | 2.38                     | 0.49              |
| 1:L:56:MET:HG3   | 1:L:72:MET:HE1   | 1.95                     | 0.49              |
| 1:B:230:ASP:HB2  | 1:B:258:ARG:HH12 | 1.78                     | 0.49              |
| 1:A:130:MET:HA   | 1:A:130:MET:HE2  | 1.95                     | 0.49              |
| 1:D:117:SER:CB   | 1:E:307:ILE:CD1  | 2.91                     | 0.49              |
| 1:H:323:SER:OG   | 1:H:325:GLU:HG3  | 2.14                     | 0.48              |
| 1:L:116:PRO:HB3  | 1:L:121:LEU:HD11 | 1.96                     | 0.48              |
| 1:F:277:VAL:HG13 | 3:F:2047:HOH:O   | 2.14                     | 0.47              |
| 1:K:170:LEU:CD2  | 1:K:300:LYS:HB3  | 2.44                     | 0.47              |
| 1:G:321:LEU:HD13 | 1:G:330:LEU:HD23 | 1.97                     | 0.47              |
| 1:D:153:ILE:CD1  | 1:D:165:GLY:HA2  | 2.45                     | 0.47              |
| 1:F:167:ILE:HD11 | 1:F:292:MET:HE1  | 1.96                     | 0.47              |
| 1:A:117:SER:CB   | 1:L:307:ILE:CD1  | 2.92                     | 0.47              |
| 1:G:49:ASP:C     | 1:G:321:LEU:HD21 | 2.40                     | 0.47              |
| 1:H:75:LEU:HD12  | 2:H:1335:MES:S   | 2.54                     | 0.47              |
| 1:I:58:ASP:HB3   | 1:I:61:SER:OG    | 2.15                     | 0.47              |
| 1:K:210:LYS:HA   | 1:K:235:ARG:HH21 | 1.78                     | 0.47              |
| 1:H:167:ILE:HD11 | 1:H:292:MET:HE1  | 1.97                     | 0.47              |
| 1:I:321:LEU:HD13 | 1:I:330:LEU:CD2  | 2.43                     | 0.47              |
| 1:H:77:VAL:HG11  | 1:H:121:LEU:HD22 | 1.97                     | 0.47              |
| 1:H:49:ASP:C     | 1:H:321:LEU:HD21 | 2.41                     | 0.46              |
| 1:C:170:LEU:HD11 | 1:C:295:TRP:CG   | 2.50                     | 0.46              |
| 1:B:228:ILE:O    | 1:B:232:VAL:HG23 | 2.15                     | 0.46              |
| 1:H:153:ILE:CD1  | 1:H:165:GLY:CA   | 2.93                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:75:LEU:HD12  | 2:H:1335:MES:O2S | 2.16                     | 0.46              |
| 1:C:130:MET:HA   | 1:C:130:MET:HE2  | 1.97                     | 0.46              |
| 1:L:49:ASP:C     | 1:L:321:LEU:HD21 | 2.41                     | 0.46              |
| 1:B:183:GLU:HA   | 1:B:183:GLU:OE1  | 2.15                     | 0.46              |
| 1:B:210:LYS:CA   | 1:B:235:ARG:HH12 | 2.29                     | 0.46              |
| 1:A:116:PRO:HG2  | 1:L:45:TYR:OH    | 2.16                     | 0.45              |
| 1:D:220:PHE:CG   | 1:D:232:VAL:HG11 | 2.51                     | 0.45              |
| 1:L:45:TYR:HB2   | 1:L:77:VAL:CG2   | 2.47                     | 0.45              |
| 1:G:53:ARG:HA    | 1:G:56:MET:HE2   | 1.98                     | 0.45              |
| 1:I:170:LEU:HD21 | 1:I:300:LYS:HB3  | 1.98                     | 0.45              |
| 1:G:117:SER:HB3  | 1:J:307:ILE:CD1  | 2.47                     | 0.45              |
| 1:L:63:ILE:CG2   | 1:L:73:ARG:NH1   | 2.79                     | 0.45              |
| 1:I:76:GLY:CA    | 1:I:98:LEU:HD22  | 2.47                     | 0.45              |
| 1:K:153:ILE:CD1  | 1:K:165:GLY:CA   | 2.95                     | 0.45              |
| 1:L:153:ILE:CD1  | 1:L:165:GLY:CA   | 2.95                     | 0.45              |
| 1:I:264:LEU:HD11 | 1:J:247:ALA:HB3  | 1.99                     | 0.45              |
| 1:L:43:ASN:O     | 1:L:334:VAL:HG23 | 2.17                     | 0.45              |
| 1:C:77:VAL:HG11  | 1:C:121:LEU:HD22 | 1.99                     | 0.45              |
| 1:I:153:ILE:HD13 | 1:I:221:PHE:CB   | 2.46                     | 0.45              |
| 1:K:166:GLN:CB   | 1:K:301:LEU:HD13 | 2.47                     | 0.45              |
| 1:K:7:ARG:HD2    | 1:K:26:PHE:HZ    | 1.82                     | 0.45              |
| 1:L:18:LEU:HD23  | 1:L:19:PRO:HD2   | 1.98                     | 0.44              |
| 1:L:53:ARG:HA    | 1:L:56:MET:HE3   | 1.99                     | 0.44              |
| 1:A:19:PRO:O     | 1:A:319:LEU:HD21 | 2.18                     | 0.44              |
| 1:F:133:MET:HE2  | 1:F:133:MET:HA   | 1.99                     | 0.44              |
| 1:J:49:ASP:O     | 1:J:52:MET:HE2   | 2.16                     | 0.44              |
| 1:G:63:ILE:HG22  | 1:G:73:ARG:NH1   | 2.32                     | 0.44              |
| 1:I:75:LEU:HD22  | 2:I:1335:MES:O2S | 2.17                     | 0.44              |
| 1:G:314:PHE:HB3  | 1:G:315:PRO:HD3  | 1.99                     | 0.44              |
| 1:J:220:PHE:CG   | 1:J:232:VAL:HG11 | 2.52                     | 0.44              |
| 1:L:130:MET:HE2  | 1:L:130:MET:HA   | 2.00                     | 0.44              |
| 1:L:314:PHE:HB3  | 1:L:315:PRO:HD3  | 2.00                     | 0.44              |
| 1:G:7:ARG:HD2    | 1:G:26:PHE:HZ    | 1.83                     | 0.44              |
| 1:K:48:LEU:HD11  | 1:K:317:THR:O    | 2.18                     | 0.44              |
| 1:B:277:VAL:HG13 | 3:B:2073:HOH:O   | 2.17                     | 0.44              |
| 1:K:292:MET:SD   | 1:K:301:LEU:CD2  | 3.05                     | 0.44              |
| 1:K:320:LYS:HE3  | 1:K:320:LYS:HB2  | 1.72                     | 0.44              |
| 1:I:49:ASP:C     | 1:I:321:LEU:HD21 | 2.42                     | 0.44              |
| 1:A:183:GLU:OE1  | 1:A:183:GLU:HA   | 2.17                     | 0.43              |
| 1:B:320:LYS:HE2  | 1:B:326:ASN:HA   | 1.99                     | 0.43              |
| 1:C:19:PRO:HG3   | 1:C:322:PHE:HE2  | 1.84                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:117:SER:HB2  | 1:E:307:ILE:CD1  | 2.48                     | 0.43              |
| 1:G:220:PHE:CG   | 1:G:232:VAL:HG11 | 2.52                     | 0.43              |
| 1:I:7:ARG:HD2    | 1:I:26:PHE:HZ    | 1.82                     | 0.43              |
| 1:A:126:SER:HB3  | 1:A:329:LYS:HG2  | 2.00                     | 0.43              |
| 1:E:157:ALA:HA   | 1:E:188:LEU:HD11 | 2.00                     | 0.43              |
| 1:H:8:GLN:OE1    | 1:H:29:THR:HG21  | 2.19                     | 0.43              |
| 1:C:7:ARG:HD2    | 1:C:26:PHE:HZ    | 1.82                     | 0.43              |
| 1:C:321:LEU:C    | 1:C:323:SER:N    | 2.76                     | 0.43              |
| 1:G:19:PRO:O     | 1:G:319:LEU:HD21 | 2.19                     | 0.43              |
| 1:I:167:ILE:HD11 | 1:I:292:MET:HE1  | 1.99                     | 0.43              |
| 1:L:51:ALA:HA    | 1:L:251:TYR:CZ   | 2.53                     | 0.43              |
| 1:D:290:LYS:HE2  | 3:G:2030:HOH:O   | 2.18                     | 0.43              |
| 1:G:133:MET:HA   | 1:G:133:MET:HE2  | 2.00                     | 0.43              |
| 1:A:307:ILE:CD1  | 1:L:117:SER:HB2  | 2.48                     | 0.43              |
| 1:B:60:ARG:HD2   | 1:B:61:SER:N     | 2.34                     | 0.43              |
| 1:E:153:ILE:HD13 | 1:E:221:PHE:CB   | 2.49                     | 0.43              |
| 1:G:116:PRO:O    | 1:J:120:PRO:HB3  | 2.18                     | 0.43              |
| 1:J:49:ASP:N     | 1:J:52:MET:HE2   | 2.34                     | 0.43              |
| 1:C:170:LEU:HD11 | 1:C:295:TRP:CE2  | 2.54                     | 0.43              |
| 1:C:170:LEU:HD11 | 1:C:295:TRP:NE1  | 2.33                     | 0.43              |
| 1:D:130:MET:HA   | 1:D:130:MET:CE   | 2.47                     | 0.43              |
| 1:J:314:PHE:HB3  | 1:J:315:PRO:HD3  | 2.01                     | 0.43              |
| 1:H:19:PRO:O     | 1:H:319:LEU:HD21 | 2.18                     | 0.43              |
| 1:I:314:PHE:HB3  | 1:I:315:PRO:HD3  | 2.01                     | 0.43              |
| 1:G:63:ILE:CG2   | 1:G:73:ARG:NH1   | 2.81                     | 0.43              |
| 1:H:316:GLU:OE1  | 1:H:316:GLU:HA   | 2.18                     | 0.43              |
| 1:H:153:ILE:HD13 | 1:H:165:GLY:CA   | 2.49                     | 0.43              |
| 1:J:116:PRO:HB3  | 1:J:121:LEU:CD1  | 2.48                     | 0.43              |
| 1:J:183:GLU:HA   | 1:J:183:GLU:OE1  | 2.18                     | 0.42              |
| 1:H:126:SER:HB3  | 1:H:329:LYS:HG2  | 2.01                     | 0.42              |
| 1:H:314:PHE:HB3  | 1:H:315:PRO:HD3  | 2.01                     | 0.42              |
| 1:J:126:SER:HB3  | 1:J:329:LYS:HG2  | 2.01                     | 0.42              |
| 1:C:314:PHE:HB3  | 1:C:315:PRO:HD3  | 2.01                     | 0.42              |
| 1:D:314:PHE:HB3  | 1:D:315:PRO:HD3  | 2.00                     | 0.42              |
| 1:F:314:PHE:HB3  | 1:F:315:PRO:HD3  | 2.00                     | 0.42              |
| 1:H:5:ILE:HD13   | 1:H:28:GLU:OE2   | 2.20                     | 0.42              |
| 1:B:230:ASP:CB   | 1:B:258:ARG:HH12 | 2.31                     | 0.42              |
| 1:H:248:ILE:O    | 1:H:249:SER:C    | 2.61                     | 0.42              |
| 1:I:126:SER:HB3  | 1:I:329:LYS:HG2  | 2.01                     | 0.42              |
| 1:E:314:PHE:HB3  | 1:E:315:PRO:HD3  | 2.01                     | 0.42              |
| 1:K:126:SER:HB3  | 1:K:329:LYS:HG2  | 2.01                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:7:ARG:HD2    | 1:F:26:PHE:HZ    | 1.85                     | 0.42              |
| 1:H:333:LYS:O    | 1:H:334:VAL:HB   | 2.20                     | 0.42              |
| 1:F:276:MET:C    | 1:F:276:MET:SD   | 3.03                     | 0.42              |
| 1:C:167:ILE:HD11 | 1:C:292:MET:HE1  | 2.01                     | 0.42              |
| 1:G:116:PRO:HB3  | 1:G:121:LEU:HD11 | 2.02                     | 0.42              |
| 1:C:277:VAL:HG13 | 3:C:2066:HOH:O   | 2.18                     | 0.42              |
| 1:D:87:GLY:CA    | 1:H:283:GLN:HA   | 2.50                     | 0.42              |
| 1:F:126:SER:HB3  | 1:F:329:LYS:HG2  | 2.01                     | 0.42              |
| 1:K:116:PRO:HB3  | 1:K:121:LEU:HD13 | 2.01                     | 0.42              |
| 1:A:314:PHE:HB3  | 1:A:315:PRO:HD3  | 2.01                     | 0.41              |
| 1:B:53:ARG:HA    | 1:B:53:ARG:HD2   | 1.87                     | 0.41              |
| 1:I:264:LEU:HD11 | 1:J:247:ALA:CB   | 2.50                     | 0.41              |
| 1:I:283:GLN:HA   | 1:L:87:GLY:CA    | 2.48                     | 0.41              |
| 1:K:116:PRO:HB3  | 1:K:121:LEU:CD1  | 2.49                     | 0.41              |
| 1:A:53:ARG:HA    | 1:A:56:MET:HE3   | 2.03                     | 0.41              |
| 1:D:45:TYR:HB2   | 1:D:77:VAL:CG2   | 2.50                     | 0.41              |
| 1:K:221:PHE:HA   | 1:K:243:VAL:HG13 | 2.02                     | 0.41              |
| 1:K:314:PHE:HB3  | 1:K:315:PRO:HD3  | 2.02                     | 0.41              |
| 1:L:126:SER:HB3  | 1:L:329:LYS:HG2  | 2.02                     | 0.41              |
| 1:E:126:SER:HB3  | 1:E:329:LYS:HG2  | 2.01                     | 0.41              |
| 1:L:55:TRP:NE1   | 1:L:63:ILE:HD12  | 2.34                     | 0.41              |
| 1:A:153:ILE:CD1  | 1:A:165:GLY:CA   | 2.99                     | 0.41              |
| 1:K:292:MET:SD   | 1:K:301:LEU:HD23 | 2.60                     | 0.41              |
| 1:B:313:THR:O    | 1:B:316:GLU:HG2  | 2.21                     | 0.41              |
| 1:I:77:VAL:HG11  | 1:I:121:LEU:HD22 | 2.02                     | 0.41              |
| 1:I:311:LEU:HB2  | 1:I:334:VAL:HG13 | 2.03                     | 0.41              |
| 1:J:8:GLN:OE1    | 1:J:29:THR:HG21  | 2.21                     | 0.41              |
| 1:L:62:TYR:CD2   | 1:L:63:ILE:HG13  | 2.56                     | 0.41              |
| 1:D:62:TYR:CD2   | 1:D:63:ILE:HG13  | 2.56                     | 0.41              |
| 1:F:10:GLN:NE2   | 1:F:27:VAL:HG21  | 2.36                     | 0.41              |
| 1:L:54:GLY:HA3   | 1:L:251:TYR:CE1  | 2.55                     | 0.41              |
| 1:C:20:GLY:O     | 1:C:22:ASP:N     | 2.53                     | 0.41              |
| 1:C:126:SER:HB3  | 1:C:329:LYS:HG2  | 2.03                     | 0.41              |
| 1:D:117:SER:HB3  | 1:E:307:ILE:CD1  | 2.51                     | 0.41              |
| 1:G:62:TYR:CD2   | 1:G:63:ILE:HG13  | 2.56                     | 0.41              |
| 1:K:166:GLN:CB   | 1:K:301:LEU:HD12 | 2.49                     | 0.41              |
| 1:B:253:ASN:HD22 | 1:B:254:LYS:N    | 2.18                     | 0.41              |
| 1:D:276:MET:SD   | 1:D:276:MET:C    | 3.04                     | 0.41              |
| 1:F:53:ARG:HA    | 1:F:56:MET:HE3   | 2.01                     | 0.41              |
| 1:G:307:ILE:CD1  | 1:J:117:SER:CB   | 2.99                     | 0.41              |
| 1:I:312:GLU:CD   | 1:I:312:GLU:N    | 2.73                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:116:PRO:HB3  | 1:J:121:LEU:HD11 | 2.03                     | 0.41              |
| 1:K:51:ALA:O     | 1:K:53:ARG:N     | 2.54                     | 0.41              |
| 1:L:19:PRO:O     | 1:L:319:LEU:HD21 | 2.21                     | 0.41              |
| 1:G:117:SER:HB2  | 1:J:307:ILE:HD11 | 2.03                     | 0.41              |
| 1:L:180:GLY:CA   | 1:L:201:LYS:HE3  | 2.51                     | 0.41              |
| 1:A:307:ILE:CD1  | 1:L:117:SER:CB   | 2.99                     | 0.40              |
| 1:C:321:LEU:HD13 | 1:C:330:LEU:HD23 | 2.03                     | 0.40              |
| 1:D:153:ILE:CD1  | 1:D:165:GLY:CA   | 2.99                     | 0.40              |
| 1:J:167:ILE:HD11 | 1:J:292:MET:HE1  | 2.03                     | 0.40              |
| 1:C:220:PHE:CG   | 1:C:232:VAL:HG11 | 2.56                     | 0.40              |
| 1:B:126:SER:HB3  | 1:B:329:LYS:HG2  | 2.02                     | 0.40              |
| 1:D:307:ILE:CD1  | 1:E:117:SER:HB3  | 2.51                     | 0.40              |
| 1:K:51:ALA:HB1   | 1:K:73:ARG:HH22  | 1.86                     | 0.40              |
| 1:F:121:LEU:HD23 | 1:F:121:LEU:HA   | 1.93                     | 0.40              |

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:A:202:ASN:OD1 | 1:K:45:TYR:OH[2_554]   | 1.54                     | 0.66              |
| 1:C:45:TYR:OH   | 1:E:202:ASN:OD1[3_655] | 1.58                     | 0.62              |

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | A     | 321/336 (96%) | 317 (99%) | 4 (1%)  | 0        | 100         | 100 |
| 1   | B     | 330/336 (98%) | 324 (98%) | 6 (2%)  | 0        | 100         | 100 |
| 1   | C     | 317/336 (94%) | 311 (98%) | 4 (1%)  | 2 (1%)   | 21          | 18  |
| 1   | D     | 321/336 (96%) | 317 (99%) | 4 (1%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|---------|----------|-------------|-----|
| 1   | E     | 314/336 (94%)   | 309 (98%)  | 4 (1%)  | 1 (0%)   | 36          | 36  |
| 1   | F     | 321/336 (96%)   | 317 (99%)  | 4 (1%)  | 0        | 100         | 100 |
| 1   | G     | 319/336 (95%)   | 315 (99%)  | 4 (1%)  | 0        | 100         | 100 |
| 1   | H     | 314/336 (94%)   | 307 (98%)  | 7 (2%)  | 0        | 100         | 100 |
| 1   | I     | 319/336 (95%)   | 309 (97%)  | 9 (3%)  | 1 (0%)   | 36          | 36  |
| 1   | J     | 292/336 (87%)   | 286 (98%)  | 5 (2%)  | 1 (0%)   | 36          | 36  |
| 1   | K     | 276/336 (82%)   | 269 (98%)  | 6 (2%)  | 1 (0%)   | 30          | 28  |
| 1   | L     | 321/336 (96%)   | 316 (98%)  | 5 (2%)  | 0        | 100         | 100 |
| All | All   | 3765/4032 (93%) | 3697 (98%) | 62 (2%) | 6 (0%)   | 43          | 44  |

All (6) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | J     | 53  | ARG  |
| 1   | C     | 21  | ARG  |
| 1   | C     | 322 | PHE  |
| 1   | E     | 323 | SER  |
| 1   | I     | 327 | PHE  |
| 1   | K     | 52  | MET  |

### 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     | 255/263 (97%) | 245 (96%) | 10 (4%)  | 28          | 31 |
| 1   | B     | 261/263 (99%) | 256 (98%) | 5 (2%)   | 50          | 58 |
| 1   | C     | 252/263 (96%) | 246 (98%) | 6 (2%)   | 43          | 49 |
| 1   | D     | 255/263 (97%) | 253 (99%) | 2 (1%)   | 73          | 81 |
| 1   | E     | 250/263 (95%) | 243 (97%) | 7 (3%)   | 38          | 43 |
| 1   | F     | 255/263 (97%) | 246 (96%) | 9 (4%)   | 32          | 35 |
| 1   | G     | 253/263 (96%) | 247 (98%) | 6 (2%)   | 43          | 49 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 1   | H     | 250/263 (95%)   | 250 (100%) | 0        | 100         | 100 |
| 1   | I     | 253/263 (96%)   | 246 (97%)  | 7 (3%)   | 38          | 43  |
| 1   | J     | 235/263 (89%)   | 225 (96%)  | 10 (4%)  | 26          | 27  |
| 1   | K     | 224/263 (85%)   | 218 (97%)  | 6 (3%)   | 39          | 45  |
| 1   | L     | 255/263 (97%)   | 247 (97%)  | 8 (3%)   | 35          | 39  |
| All | All   | 2998/3156 (95%) | 2922 (98%) | 76 (2%)  | 42          | 48  |

All (76) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 16  | SER  |
| 1   | A     | 18  | LEU  |
| 1   | A     | 21  | ARG  |
| 1   | A     | 22  | ASP  |
| 1   | A     | 58  | ASP  |
| 1   | A     | 60  | ARG  |
| 1   | A     | 183 | GLU  |
| 1   | A     | 203 | GLU  |
| 1   | A     | 277 | VAL  |
| 1   | A     | 304 | ARG  |
| 1   | B     | 14  | ARG  |
| 1   | B     | 16  | SER  |
| 1   | B     | 153 | ILE  |
| 1   | B     | 183 | GLU  |
| 1   | B     | 253 | ASN  |
| 1   | C     | 16  | SER  |
| 1   | C     | 21  | ARG  |
| 1   | C     | 53  | ARG  |
| 1   | C     | 63  | ILE  |
| 1   | C     | 123 | ARG  |
| 1   | C     | 235 | ARG  |
| 1   | D     | 203 | GLU  |
| 1   | D     | 277 | VAL  |
| 1   | E     | 4   | GLN  |
| 1   | E     | 16  | SER  |
| 1   | E     | 153 | ILE  |
| 1   | E     | 188 | LEU  |
| 1   | E     | 203 | GLU  |
| 1   | E     | 321 | LEU  |
| 1   | E     | 323 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 16  | SER  |
| 1   | F     | 18  | LEU  |
| 1   | F     | 21  | ARG  |
| 1   | F     | 22  | ASP  |
| 1   | F     | 48  | LEU  |
| 1   | F     | 118 | ARG  |
| 1   | F     | 248 | ILE  |
| 1   | F     | 249 | SER  |
| 1   | F     | 283 | GLN  |
| 1   | G     | 16  | SER  |
| 1   | G     | 57  | ASN  |
| 1   | G     | 58  | ASP  |
| 1   | G     | 60  | ARG  |
| 1   | G     | 70  | GLU  |
| 1   | G     | 121 | LEU  |
| 1   | I     | 16  | SER  |
| 1   | I     | 53  | ARG  |
| 1   | I     | 98  | LEU  |
| 1   | I     | 153 | ILE  |
| 1   | I     | 183 | GLU  |
| 1   | I     | 304 | ARG  |
| 1   | I     | 312 | GLU  |
| 1   | J     | 5   | ILE  |
| 1   | J     | 21  | ARG  |
| 1   | J     | 33  | GLU  |
| 1   | J     | 53  | ARG  |
| 1   | J     | 98  | LEU  |
| 1   | J     | 121 | LEU  |
| 1   | J     | 183 | GLU  |
| 1   | J     | 250 | GLN  |
| 1   | J     | 277 | VAL  |
| 1   | J     | 327 | PHE  |
| 1   | K     | 109 | LYS  |
| 1   | K     | 121 | LEU  |
| 1   | K     | 183 | GLU  |
| 1   | K     | 277 | VAL  |
| 1   | K     | 304 | ARG  |
| 1   | K     | 320 | LYS  |
| 1   | L     | 16  | SER  |
| 1   | L     | 18  | LEU  |
| 1   | L     | 53  | ARG  |
| 1   | L     | 98  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | L     | 121 | LEU  |
| 1   | L     | 258 | ARG  |
| 1   | L     | 283 | GLN  |
| 1   | L     | 327 | PHE  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 89  | GLN  |
| 1   | A     | 223 | ASN  |
| 1   | A     | 302 | GLN  |
| 1   | B     | 8   | GLN  |
| 1   | B     | 253 | ASN  |
| 1   | B     | 302 | GLN  |
| 1   | C     | 8   | GLN  |
| 1   | C     | 223 | ASN  |
| 1   | D     | 8   | GLN  |
| 1   | D     | 57  | ASN  |
| 1   | D     | 223 | ASN  |
| 1   | D     | 302 | GLN  |
| 1   | E     | 283 | GLN  |
| 1   | F     | 57  | ASN  |
| 1   | F     | 283 | GLN  |
| 1   | F     | 326 | ASN  |
| 1   | G     | 4   | GLN  |
| 1   | G     | 57  | ASN  |
| 1   | G     | 89  | GLN  |
| 1   | G     | 223 | ASN  |
| 1   | G     | 302 | GLN  |
| 1   | H     | 223 | ASN  |
| 1   | H     | 302 | GLN  |
| 1   | I     | 4   | GLN  |
| 1   | I     | 89  | GLN  |
| 1   | I     | 302 | GLN  |
| 1   | I     | 326 | ASN  |
| 1   | J     | 8   | GLN  |
| 1   | J     | 302 | GLN  |
| 1   | K     | 223 | ASN  |
| 1   | K     | 302 | GLN  |
| 1   | L     | 89  | GLN  |
| 1   | L     | 223 | ASN  |
| 1   | L     | 302 | GLN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

5 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   | MES  | G     | 1335 | -    | 12,12,12     | 2.13 | 1 (8%)      | 15,16,16    | 1.73 | 3 (20%)     |
| 2   | MES  | H     | 1335 | -    | 12,12,12     | 2.15 | 1 (8%)      | 15,16,16    | 5.82 | 7 (46%)     |
| 2   | MES  | I     | 1335 | -    | 12,12,12     | 2.08 | 1 (8%)      | 15,16,16    | 5.73 | 6 (40%)     |
| 2   | MES  | D     | 1335 | -    | 12,12,12     | 1.64 | 1 (8%)      | 15,16,16    | 1.73 | 4 (26%)     |
| 2   | MES  | F     | 1335 | -    | 12,12,12     | 2.01 | 1 (8%)      | 15,16,16    | 5.59 | 9 (60%)     |

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

| Mol | Type | Chain | Res  | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|------|------|---------|-----------|---------|
| 2   | MES  | G     | 1335 | -    | -       | 1/6/14/14 | 0/1/1/1 |
| 2   | MES  | H     | 1335 | -    | -       | 3/6/14/14 | 0/1/1/1 |
| 2   | MES  | I     | 1335 | -    | -       | 2/6/14/14 | 0/1/1/1 |
| 2   | MES  | D     | 1335 | -    | -       | 1/6/14/14 | 0/1/1/1 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|------|------|---------|-----------|---------|
| 2   | MES  | F     | 1335 | -    | -       | 2/6/14/14 | 0/1/1/1 |

All (5) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 2   | H     | 1335 | MES  | C8-S  | -6.88 | 1.67        | 1.77     |
| 2   | G     | 1335 | MES  | C8-S  | -6.81 | 1.68        | 1.77     |
| 2   | I     | 1335 | MES  | C8-S  | -6.68 | 1.68        | 1.77     |
| 2   | F     | 1335 | MES  | C8-S  | -6.20 | 1.68        | 1.77     |
| 2   | D     | 1335 | MES  | C8-S  | -4.96 | 1.70        | 1.77     |

All (29) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 2   | H     | 1335 | MES  | O1S-S-C8  | -12.70 | 87.54       | 106.73   |
| 2   | I     | 1335 | MES  | O1S-S-C8  | -12.63 | 87.65       | 106.73   |
| 2   | H     | 1335 | MES  | O3S-S-O1S | -12.30 | 80.62       | 111.40   |
| 2   | F     | 1335 | MES  | O1S-S-C8  | -11.09 | 89.98       | 106.73   |
| 2   | I     | 1335 | MES  | O3S-S-O1S | -10.98 | 83.93       | 111.40   |
| 2   | F     | 1335 | MES  | O2S-S-O1S | -10.14 | 80.85       | 113.82   |
| 2   | I     | 1335 | MES  | O2S-S-O1S | -9.94  | 81.50       | 113.82   |
| 2   | F     | 1335 | MES  | O3S-S-O1S | -9.26  | 88.23       | 111.40   |
| 2   | H     | 1335 | MES  | O2S-S-O1S | -9.12  | 84.15       | 113.82   |
| 2   | F     | 1335 | MES  | O2S-S-C8  | 8.99   | 120.31      | 106.73   |
| 2   | H     | 1335 | MES  | O3S-S-C8  | 7.96   | 121.58      | 106.00   |
| 2   | I     | 1335 | MES  | O2S-S-C8  | 7.07   | 117.40      | 106.73   |
| 2   | I     | 1335 | MES  | O3S-S-C8  | 6.77   | 119.26      | 106.00   |
| 2   | F     | 1335 | MES  | O3S-S-C8  | 6.09   | 117.92      | 106.00   |
| 2   | H     | 1335 | MES  | O2S-S-C8  | 5.14   | 114.50      | 106.73   |
| 2   | H     | 1335 | MES  | O3S-S-O2S | 3.72   | 120.70      | 111.40   |
| 2   | F     | 1335 | MES  | O3S-S-O2S | 3.65   | 120.53      | 111.40   |
| 2   | I     | 1335 | MES  | O3S-S-O2S | 3.62   | 120.45      | 111.40   |
| 2   | D     | 1335 | MES  | C6-C5-N4  | 3.43   | 115.34      | 110.12   |
| 2   | G     | 1335 | MES  | C6-C5-N4  | 3.39   | 115.27      | 110.12   |
| 2   | G     | 1335 | MES  | C2-C3-N4  | 3.37   | 115.24      | 110.12   |
| 2   | F     | 1335 | MES  | C2-C3-N4  | 3.10   | 114.83      | 110.12   |
| 2   | F     | 1335 | MES  | C6-C5-N4  | 3.01   | 114.70      | 110.12   |
| 2   | D     | 1335 | MES  | C5-N4-C3  | 2.95   | 115.19      | 108.84   |
| 2   | G     | 1335 | MES  | C5-N4-C3  | 2.58   | 114.41      | 108.84   |
| 2   | D     | 1335 | MES  | C2-C3-N4  | 2.44   | 113.82      | 110.12   |
| 2   | H     | 1335 | MES  | C6-C5-N4  | 2.16   | 113.40      | 110.12   |
| 2   | F     | 1335 | MES  | C5-N4-C3  | 2.01   | 113.18      | 108.84   |

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| Mol | Chain | Res  | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|------|-------------|----------|
| 2   | D     | 1335 | MES  | O3S-S-C8 | 2.00 | 109.92      | 106.00   |

There are no chirality outliers.

All (9) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       |
|-----|-------|------|------|-------------|
| 2   | D     | 1335 | MES  | C8-C7-N4-C5 |
| 2   | G     | 1335 | MES  | C8-C7-N4-C5 |
| 2   | H     | 1335 | MES  | C7-C8-S-O3S |
| 2   | I     | 1335 | MES  | C7-C8-S-O2S |
| 2   | F     | 1335 | MES  | C7-C8-S-O3S |
| 2   | H     | 1335 | MES  | N4-C7-C8-S  |
| 2   | I     | 1335 | MES  | C7-C8-S-O3S |
| 2   | F     | 1335 | MES  | C7-C8-S-O2S |
| 2   | H     | 1335 | MES  | C7-C8-S-O2S |

There are no ring outliers.

2 monomers are involved in 4 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 2   | H     | 1335 | MES  | 2       | 0            |
| 2   | I     | 1335 | MES  | 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     | 325/336 (96%)   | 0.40   | 32 (9%) 13 13 | 20, 31, 66, 88        | 0      |
| 1   | B     | 331/336 (98%)   | 1.10   | 64 (19%) 3 3  | 19, 42, 70, 102       | 1 (0%) |
| 1   | C     | 323/336 (96%)   | 1.21   | 68 (21%) 2 2  | 26, 46, 77, 98        | 0      |
| 1   | D     | 325/336 (96%)   | 0.26   | 13 (4%) 42 44 | 21, 32, 53, 73        | 0      |
| 1   | E     | 320/336 (95%)   | 0.28   | 26 (8%) 18 19 | 20, 30, 61, 93        | 0      |
| 1   | F     | 325/336 (96%)   | 1.32   | 75 (23%) 2 2  | 30, 49, 80, 101       | 0      |
| 1   | G     | 323/336 (96%)   | 0.82   | 57 (17%) 4 4  | 23, 42, 77, 100       | 0      |
| 1   | H     | 320/336 (95%)   | 1.34   | 68 (21%) 2 2  | 31, 54, 82, 102       | 0      |
| 1   | I     | 323/336 (96%)   | 1.41   | 73 (22%) 2 2  | 33, 53, 83, 117       | 0      |
| 1   | J     | 302/336 (89%)   | 1.54   | 114 (37%) 1 1 | 27, 45, 83, 109       | 0      |
| 1   | K     | 286/336 (85%)   | 2.55   | 180 (62%) 0 0 | 39, 66, 99, 115       | 0      |
| 1   | L     | 325/336 (96%)   | 0.85   | 46 (14%) 6 6  | 25, 39, 80, 118       | 0      |
| All | All   | 3828/4032 (94%) | 1.07   | 816 (21%) 2 2 | 19, 44, 81, 118       | 1 (0%) |

All (816) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | J     | 68  | ILE  | 8.6  |
| 1   | B     | 327 | PHE  | 8.2  |
| 1   | J     | 324 | GLY  | 7.7  |
| 1   | J     | 24  | PHE  | 7.5  |
| 1   | K     | 327 | PHE  | 7.4  |
| 1   | J     | 327 | PHE  | 6.8  |
| 1   | J     | 11  | LEU  | 6.8  |
| 1   | J     | 71  | VAL  | 6.7  |
| 1   | J     | 12  | ALA  | 6.6  |
| 1   | L     | 18  | LEU  | 6.6  |
| 1   | K     | 187 | PHE  | 6.6  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | E     | 63  | ILE  | 6.3  |
| 1   | J     | 52  | MET  | 6.3  |
| 1   | H     | 248 | ILE  | 6.3  |
| 1   | C     | 327 | PHE  | 6.2  |
| 1   | J     | 67  | GLY  | 6.0  |
| 1   | L     | 327 | PHE  | 6.0  |
| 1   | K     | 321 | LEU  | 6.0  |
| 1   | C     | 328 | GLY  | 6.0  |
| 1   | K     | 26  | PHE  | 5.9  |
| 1   | J     | 26  | PHE  | 5.9  |
| 1   | K     | 328 | GLY  | 5.9  |
| 1   | K     | 193 | GLY  | 5.7  |
| 1   | J     | 99  | GLY  | 5.7  |
| 1   | K     | 112 | TYR  | 5.7  |
| 1   | K     | 192 | LEU  | 5.6  |
| 1   | G     | 12  | ALA  | 5.6  |
| 1   | J     | 27  | VAL  | 5.5  |
| 1   | J     | 78  | GLY  | 5.3  |
| 1   | C     | 322 | PHE  | 5.3  |
| 1   | I     | 248 | ILE  | 5.3  |
| 1   | C     | 5   | ILE  | 5.2  |
| 1   | K     | 23  | THR  | 5.2  |
| 1   | H     | 60  | ARG  | 5.1  |
| 1   | K     | 52  | MET  | 5.1  |
| 1   | F     | 248 | ILE  | 5.0  |
| 1   | G     | 116 | PRO  | 5.0  |
| 1   | J     | 74  | ALA  | 5.0  |
| 1   | K     | 297 | ALA  | 4.9  |
| 1   | J     | 25  | SER  | 4.9  |
| 1   | K     | 182 | ALA  | 4.9  |
| 1   | L     | 59  | ALA  | 4.9  |
| 1   | K     | 294 | THR  | 4.8  |
| 1   | C     | 26  | PHE  | 4.8  |
| 1   | A     | 251 | TYR  | 4.8  |
| 1   | H     | 334 | VAL  | 4.8  |
| 1   | J     | 105 | ILE  | 4.8  |
| 1   | K     | 97  | ALA  | 4.8  |
| 1   | H     | 197 | ALA  | 4.7  |
| 1   | C     | 170 | LEU  | 4.7  |
| 1   | E     | 324 | GLY  | 4.7  |
| 1   | G     | 26  | PHE  | 4.7  |
| 1   | K     | 319 | LEU  | 4.6  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | J     | 258 | ARG  | 4.6  |
| 1   | E     | 322 | PHE  | 4.6  |
| 1   | K     | 314 | PHE  | 4.6  |
| 1   | E     | 16  | SER  | 4.6  |
| 1   | J     | 29  | THR  | 4.5  |
| 1   | J     | 32  | GLY  | 4.5  |
| 1   | K     | 25  | SER  | 4.5  |
| 1   | I     | 327 | PHE  | 4.5  |
| 1   | K     | 27  | VAL  | 4.5  |
| 1   | J     | 72  | MET  | 4.4  |
| 1   | K     | 105 | ILE  | 4.4  |
| 1   | C     | 27  | VAL  | 4.4  |
| 1   | J     | 121 | LEU  | 4.4  |
| 1   | K     | 24  | PHE  | 4.4  |
| 1   | A     | 249 | SER  | 4.4  |
| 1   | J     | 40  | LEU  | 4.3  |
| 1   | K     | 170 | LEU  | 4.3  |
| 1   | C     | 25  | SER  | 4.3  |
| 1   | J     | 80  | VAL  | 4.3  |
| 1   | J     | 319 | LEU  | 4.3  |
| 1   | K     | 155 | GLY  | 4.3  |
| 1   | L     | 63  | ILE  | 4.3  |
| 1   | J     | 321 | LEU  | 4.2  |
| 1   | K     | 82  | VAL  | 4.2  |
| 1   | B     | 20  | GLY  | 4.2  |
| 1   | C     | 68  | ILE  | 4.2  |
| 1   | F     | 251 | TYR  | 4.2  |
| 1   | I     | 308 | VAL  | 4.2  |
| 1   | H     | 20  | GLY  | 4.2  |
| 1   | K     | 213 | CYS  | 4.2  |
| 1   | J     | 5   | ILE  | 4.2  |
| 1   | C     | 30  | PRO  | 4.2  |
| 1   | I     | 26  | PHE  | 4.2  |
| 1   | J     | 332 | LEU  | 4.2  |
| 1   | K     | 332 | LEU  | 4.2  |
| 1   | A     | 62  | TYR  | 4.2  |
| 1   | L     | 251 | TYR  | 4.2  |
| 1   | C     | 4   | GLN  | 4.1  |
| 1   | J     | 48  | LEU  | 4.1  |
| 1   | I     | 334 | VAL  | 4.1  |
| 1   | J     | 54  | GLY  | 4.1  |
| 1   | K     | 49  | ASP  | 4.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | K     | 185 | CYS  | 4.1  |
| 1   | K     | 156 | ALA  | 4.1  |
| 1   | J     | 75  | LEU  | 4.1  |
| 1   | J     | 104 | PHE  | 4.1  |
| 1   | K     | 189 | VAL  | 4.1  |
| 1   | H     | 5   | ILE  | 4.1  |
| 1   | F     | 258 | ARG  | 4.1  |
| 1   | K     | 51  | ALA  | 4.1  |
| 1   | C     | 319 | LEU  | 4.1  |
| 1   | F     | 26  | PHE  | 4.1  |
| 1   | E     | 61  | SER  | 4.1  |
| 1   | K     | 173 | CYS  | 4.0  |
| 1   | K     | 301 | LEU  | 4.0  |
| 1   | K     | 111 | PHE  | 4.0  |
| 1   | L     | 62  | TYR  | 4.0  |
| 1   | K     | 194 | PHE  | 4.0  |
| 1   | I     | 307 | ILE  | 4.0  |
| 1   | J     | 31  | LEU  | 4.0  |
| 1   | J     | 100 | VAL  | 4.0  |
| 1   | J     | 50  | PRO  | 4.0  |
| 1   | K     | 34  | PRO  | 4.0  |
| 1   | H     | 297 | ALA  | 3.9  |
| 1   | I     | 326 | ASN  | 3.9  |
| 1   | L     | 20  | GLY  | 3.9  |
| 1   | C     | 18  | LEU  | 3.9  |
| 1   | C     | 323 | SER  | 3.9  |
| 1   | H     | 301 | LEU  | 3.9  |
| 1   | G     | 27  | VAL  | 3.9  |
| 1   | J     | 322 | PHE  | 3.9  |
| 1   | K     | 50  | PRO  | 3.9  |
| 1   | J     | 117 | SER  | 3.9  |
| 1   | I     | 21  | ARG  | 3.9  |
| 1   | K     | 176 | VAL  | 3.9  |
| 1   | L     | 322 | PHE  | 3.9  |
| 1   | K     | 132 | GLY  | 3.9  |
| 1   | K     | 90  | ALA  | 3.9  |
| 1   | G     | 334 | VAL  | 3.8  |
| 1   | J     | 314 | PHE  | 3.8  |
| 1   | F     | 20  | GLY  | 3.8  |
| 1   | K     | 248 | ILE  | 3.8  |
| 1   | A     | 60  | ARG  | 3.8  |
| 1   | H     | 170 | LEU  | 3.8  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | K     | 311 | LEU  | 3.8  |
| 1   | L     | 26  | PHE  | 3.8  |
| 1   | L     | 324 | GLY  | 3.8  |
| 1   | E     | 62  | TYR  | 3.8  |
| 1   | K     | 9   | TYR  | 3.8  |
| 1   | F     | 57  | ASN  | 3.8  |
| 1   | B     | 294 | THR  | 3.8  |
| 1   | A     | 63  | ILE  | 3.7  |
| 1   | D     | 57  | ASN  | 3.7  |
| 1   | J     | 334 | VAL  | 3.7  |
| 1   | K     | 71  | VAL  | 3.7  |
| 1   | H     | 322 | PHE  | 3.7  |
| 1   | K     | 88  | PHE  | 3.7  |
| 1   | L     | 326 | ASN  | 3.7  |
| 1   | J     | 248 | ILE  | 3.7  |
| 1   | K     | 5   | ILE  | 3.7  |
| 1   | F     | 294 | THR  | 3.7  |
| 1   | J     | 317 | THR  | 3.7  |
| 1   | B     | 254 | LYS  | 3.7  |
| 1   | J     | 38  | GLN  | 3.7  |
| 1   | E     | 20  | GLY  | 3.7  |
| 1   | J     | 41  | VAL  | 3.7  |
| 1   | J     | 308 | VAL  | 3.7  |
| 1   | K     | 114 | VAL  | 3.7  |
| 1   | J     | 47  | SER  | 3.7  |
| 1   | K     | 45  | TYR  | 3.7  |
| 1   | K     | 75  | LEU  | 3.7  |
| 1   | K     | 121 | LEU  | 3.7  |
| 1   | J     | 30  | PRO  | 3.7  |
| 1   | G     | 117 | SER  | 3.7  |
| 1   | K     | 228 | ILE  | 3.7  |
| 1   | B     | 214 | PRO  | 3.6  |
| 1   | J     | 315 | PRO  | 3.6  |
| 1   | L     | 64  | PRO  | 3.6  |
| 1   | J     | 316 | GLU  | 3.6  |
| 1   | B     | 322 | PHE  | 3.6  |
| 1   | K     | 98  | LEU  | 3.6  |
| 1   | A     | 252 | ASN  | 3.6  |
| 1   | K     | 37  | GLY  | 3.6  |
| 1   | L     | 68  | ILE  | 3.6  |
| 1   | J     | 93  | TYR  | 3.6  |
| 1   | J     | 307 | ILE  | 3.6  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 29  | THR  | 3.6  |
| 1   | K     | 197 | ALA  | 3.6  |
| 1   | H     | 18  | LEU  | 3.6  |
| 1   | I     | 328 | GLY  | 3.6  |
| 1   | J     | 9   | TYR  | 3.6  |
| 1   | J     | 8   | GLN  | 3.6  |
| 1   | J     | 21  | ARG  | 3.5  |
| 1   | B     | 253 | ASN  | 3.5  |
| 1   | J     | 34  | PRO  | 3.5  |
| 1   | K     | 86  | PRO  | 3.5  |
| 1   | K     | 318 | LEU  | 3.5  |
| 1   | I     | 324 | GLY  | 3.5  |
| 1   | K     | 295 | TRP  | 3.5  |
| 1   | J     | 77  | VAL  | 3.5  |
| 1   | K     | 334 | VAL  | 3.5  |
| 1   | K     | 304 | ARG  | 3.5  |
| 1   | I     | 294 | THR  | 3.5  |
| 1   | L     | 248 | ILE  | 3.5  |
| 1   | B     | 256 | ALA  | 3.5  |
| 1   | I     | 297 | ALA  | 3.5  |
| 1   | F     | 301 | LEU  | 3.5  |
| 1   | J     | 81  | LEU  | 3.5  |
| 1   | J     | 318 | LEU  | 3.5  |
| 1   | J     | 53  | ARG  | 3.5  |
| 1   | L     | 21  | ARG  | 3.5  |
| 1   | J     | 82  | VAL  | 3.5  |
| 1   | J     | 331 | VAL  | 3.5  |
| 1   | K     | 77  | VAL  | 3.5  |
| 1   | B     | 326 | ASN  | 3.5  |
| 1   | C     | 248 | ILE  | 3.5  |
| 1   | B     | 179 | ALA  | 3.5  |
| 1   | F     | 214 | PRO  | 3.5  |
| 1   | J     | 108 | PRO  | 3.5  |
| 1   | K     | 159 | ALA  | 3.5  |
| 1   | K     | 206 | ALA  | 3.5  |
| 1   | J     | 110 | GLY  | 3.5  |
| 1   | K     | 205 | LEU  | 3.5  |
| 1   | B     | 183 | GLU  | 3.5  |
| 1   | B     | 32  | GLY  | 3.4  |
| 1   | G     | 322 | PHE  | 3.4  |
| 1   | D     | 58  | ASP  | 3.4  |
| 1   | F     | 292 | MET  | 3.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 250 | GLN  | 3.4  |
| 1   | E     | 334 | VAL  | 3.4  |
| 1   | G     | 29  | THR  | 3.4  |
| 1   | H     | 328 | GLY  | 3.4  |
| 1   | K     | 108 | PRO  | 3.4  |
| 1   | F     | 14  | ARG  | 3.4  |
| 1   | K     | 76  | GLY  | 3.4  |
| 1   | B     | 209 | LEU  | 3.4  |
| 1   | K     | 296 | LEU  | 3.4  |
| 1   | K     | 320 | LYS  | 3.4  |
| 1   | K     | 166 | GLN  | 3.4  |
| 1   | K     | 103 | TYR  | 3.4  |
| 1   | B     | 197 | ALA  | 3.4  |
| 1   | E     | 319 | LEU  | 3.4  |
| 1   | B     | 26  | PHE  | 3.4  |
| 1   | C     | 186 | ARG  | 3.3  |
| 1   | F     | 22  | ASP  | 3.3  |
| 1   | I     | 117 | SER  | 3.3  |
| 1   | J     | 86  | PRO  | 3.3  |
| 1   | J     | 116 | PRO  | 3.3  |
| 1   | H     | 63  | ILE  | 3.3  |
| 1   | K     | 315 | PRO  | 3.3  |
| 1   | B     | 176 | VAL  | 3.3  |
| 1   | J     | 112 | TYR  | 3.3  |
| 1   | G     | 18  | LEU  | 3.3  |
| 1   | J     | 98  | LEU  | 3.3  |
| 1   | K     | 53  | ARG  | 3.3  |
| 1   | K     | 312 | GLU  | 3.3  |
| 1   | I     | 214 | PRO  | 3.3  |
| 1   | H     | 189 | VAL  | 3.3  |
| 1   | K     | 153 | ILE  | 3.3  |
| 1   | A     | 18  | LEU  | 3.3  |
| 1   | C     | 321 | LEU  | 3.3  |
| 1   | F     | 319 | LEU  | 3.3  |
| 1   | J     | 46  | LEU  | 3.3  |
| 1   | G     | 57  | ASN  | 3.3  |
| 1   | H     | 4   | GLN  | 3.3  |
| 1   | F     | 323 | SER  | 3.2  |
| 1   | C     | 67  | GLY  | 3.2  |
| 1   | G     | 32  | GLY  | 3.2  |
| 1   | D     | 12  | ALA  | 3.2  |
| 1   | J     | 51  | ALA  | 3.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | K     | 48  | LEU  | 3.2  |
| 1   | K     | 289 | LEU  | 3.2  |
| 1   | F     | 249 | SER  | 3.2  |
| 1   | G     | 25  | SER  | 3.2  |
| 1   | F     | 17  | GLY  | 3.2  |
| 1   | L     | 15  | PRO  | 3.2  |
| 1   | J     | 70  | GLU  | 3.2  |
| 1   | K     | 191 | GLU  | 3.2  |
| 1   | H     | 27  | VAL  | 3.2  |
| 1   | K     | 152 | VAL  | 3.2  |
| 1   | J     | 97  | ALA  | 3.2  |
| 1   | B     | 248 | ILE  | 3.2  |
| 1   | K     | 81  | LEU  | 3.2  |
| 1   | A     | 25  | SER  | 3.2  |
| 1   | B     | 19  | PRO  | 3.2  |
| 1   | L     | 261 | ALA  | 3.2  |
| 1   | H     | 200 | TYR  | 3.2  |
| 1   | K     | 40  | LEU  | 3.2  |
| 1   | K     | 195 | ASP  | 3.2  |
| 1   | C     | 312 | GLU  | 3.2  |
| 1   | E     | 323 | SER  | 3.2  |
| 1   | C     | 20  | GLY  | 3.2  |
| 1   | J     | 69  | GLY  | 3.2  |
| 1   | L     | 17  | GLY  | 3.2  |
| 1   | C     | 214 | PRO  | 3.2  |
| 1   | L     | 19  | PRO  | 3.2  |
| 1   | L     | 65  | PRO  | 3.2  |
| 1   | F     | 12  | ALA  | 3.1  |
| 1   | J     | 35  | ALA  | 3.1  |
| 1   | B     | 319 | LEU  | 3.1  |
| 1   | I     | 5   | ILE  | 3.1  |
| 1   | G     | 9   | TYR  | 3.1  |
| 1   | F     | 21  | ARG  | 3.1  |
| 1   | J     | 94  | VAL  | 3.1  |
| 1   | K     | 72  | MET  | 3.1  |
| 1   | B     | 17  | GLY  | 3.1  |
| 1   | J     | 306 | ASP  | 3.1  |
| 1   | C     | 12  | ALA  | 3.1  |
| 1   | C     | 257 | VAL  | 3.1  |
| 1   | I     | 309 | GLU  | 3.1  |
| 1   | K     | 237 | ALA  | 3.1  |
| 1   | H     | 307 | ILE  | 3.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 323 | SER  | 3.1  |
| 1   | E     | 259 | GLY  | 3.1  |
| 1   | A     | 327 | PHE  | 3.1  |
| 1   | F     | 15  | PRO  | 3.1  |
| 1   | B     | 206 | ALA  | 3.1  |
| 1   | K     | 261 | ALA  | 3.1  |
| 1   | H     | 323 | SER  | 3.1  |
| 1   | I     | 249 | SER  | 3.1  |
| 1   | D     | 252 | ASN  | 3.0  |
| 1   | K     | 139 | LEU  | 3.0  |
| 1   | I     | 174 | ARG  | 3.0  |
| 1   | K     | 196 | GLY  | 3.0  |
| 1   | K     | 259 | GLY  | 3.0  |
| 1   | K     | 214 | PRO  | 3.0  |
| 1   | I     | 320 | LYS  | 3.0  |
| 1   | C     | 31  | LEU  | 3.0  |
| 1   | F     | 18  | LEU  | 3.0  |
| 1   | F     | 121 | LEU  | 3.0  |
| 1   | K     | 47  | SER  | 3.0  |
| 1   | L     | 319 | LEU  | 3.0  |
| 1   | G     | 118 | ARG  | 3.0  |
| 1   | L     | 60  | ARG  | 3.0  |
| 1   | I     | 57  | ASN  | 3.0  |
| 1   | K     | 87  | GLY  | 3.0  |
| 1   | I     | 50  | PRO  | 3.0  |
| 1   | E     | 204 | ASP  | 3.0  |
| 1   | F     | 327 | PHE  | 3.0  |
| 1   | C     | 82  | VAL  | 3.0  |
| 1   | K     | 100 | VAL  | 3.0  |
| 1   | K     | 188 | LEU  | 3.0  |
| 1   | K     | 287 | GLU  | 3.0  |
| 1   | K     | 216 | GLY  | 3.0  |
| 1   | L     | 320 | LYS  | 3.0  |
| 1   | C     | 258 | ARG  | 2.9  |
| 1   | A     | 59  | ALA  | 2.9  |
| 1   | H     | 59  | ALA  | 2.9  |
| 1   | I     | 197 | ALA  | 2.9  |
| 1   | J     | 6   | ASN  | 2.9  |
| 1   | K     | 242 | ILE  | 2.9  |
| 1   | H     | 214 | PRO  | 2.9  |
| 1   | B     | 60  | ARG  | 2.9  |
| 1   | C     | 45  | TYR  | 2.9  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | I     | 258 | ARG  | 2.9  |
| 1   | F     | 297 | ALA  | 2.9  |
| 1   | K     | 293 | ALA  | 2.9  |
| 1   | I     | 170 | LEU  | 2.9  |
| 1   | K     | 96  | GLY  | 2.9  |
| 1   | K     | 184 | LYS  | 2.9  |
| 1   | E     | 248 | ILE  | 2.9  |
| 1   | K     | 131 | THR  | 2.9  |
| 1   | H     | 315 | PRO  | 2.9  |
| 1   | F     | 298 | GLU  | 2.9  |
| 1   | D     | 26  | PHE  | 2.9  |
| 1   | K     | 42  | LYS  | 2.9  |
| 1   | D     | 59  | ALA  | 2.9  |
| 1   | F     | 31  | LEU  | 2.9  |
| 1   | I     | 18  | LEU  | 2.9  |
| 1   | J     | 106 | GLY  | 2.9  |
| 1   | K     | 158 | GLY  | 2.9  |
| 1   | K     | 85  | HIS  | 2.9  |
| 1   | A     | 21  | ARG  | 2.9  |
| 1   | H     | 198 | ILE  | 2.9  |
| 1   | A     | 19  | PRO  | 2.9  |
| 1   | K     | 203 | GLU  | 2.9  |
| 1   | G     | 62  | TYR  | 2.9  |
| 1   | I     | 16  | SER  | 2.9  |
| 1   | J     | 43  | ASN  | 2.9  |
| 1   | J     | 109 | LYS  | 2.9  |
| 1   | C     | 297 | ALA  | 2.9  |
| 1   | F     | 293 | ALA  | 2.9  |
| 1   | H     | 295 | TRP  | 2.9  |
| 1   | A     | 58  | ASP  | 2.8  |
| 1   | E     | 328 | GLY  | 2.9  |
| 1   | L     | 87  | GLY  | 2.9  |
| 1   | G     | 63  | ILE  | 2.8  |
| 1   | I     | 120 | PRO  | 2.8  |
| 1   | L     | 57  | ASN  | 2.8  |
| 1   | B     | 251 | TYR  | 2.8  |
| 1   | J     | 10  | GLN  | 2.8  |
| 1   | B     | 182 | ALA  | 2.8  |
| 1   | B     | 328 | GLY  | 2.8  |
| 1   | D     | 20  | GLY  | 2.8  |
| 1   | K     | 246 | GLY  | 2.8  |
| 1   | I     | 323 | SER  | 2.8  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | F     | 169 | ARG  | 2.8  |
| 1   | H     | 62  | TYR  | 2.8  |
| 1   | L     | 67  | GLY  | 2.8  |
| 1   | G     | 40  | LEU  | 2.8  |
| 1   | H     | 19  | PRO  | 2.8  |
| 1   | I     | 116 | PRO  | 2.8  |
| 1   | G     | 248 | ILE  | 2.8  |
| 1   | K     | 109 | LYS  | 2.8  |
| 1   | K     | 147 | ASN  | 2.8  |
| 1   | B     | 172 | GLY  | 2.8  |
| 1   | C     | 187 | PHE  | 2.8  |
| 1   | F     | 11  | LEU  | 2.8  |
| 1   | K     | 95  | ASN  | 2.7  |
| 1   | B     | 216 | GLY  | 2.7  |
| 1   | J     | 111 | PHE  | 2.7  |
| 1   | G     | 319 | LEU  | 2.7  |
| 1   | B     | 186 | ARG  | 2.7  |
| 1   | D     | 27  | VAL  | 2.7  |
| 1   | I     | 27  | VAL  | 2.7  |
| 1   | I     | 58  | ASP  | 2.7  |
| 1   | H     | 119 | ALA  | 2.7  |
| 1   | K     | 179 | ALA  | 2.7  |
| 1   | H     | 169 | ARG  | 2.7  |
| 1   | H     | 294 | THR  | 2.7  |
| 1   | L     | 321 | LEU  | 2.7  |
| 1   | B     | 200 | TYR  | 2.7  |
| 1   | D     | 251 | TYR  | 2.7  |
| 1   | G     | 8   | GLN  | 2.7  |
| 1   | C     | 70  | GLU  | 2.7  |
| 1   | H     | 308 | VAL  | 2.7  |
| 1   | J     | 107 | GLU  | 2.7  |
| 1   | B     | 5   | ILE  | 2.7  |
| 1   | K     | 178 | ILE  | 2.7  |
| 1   | A     | 201 | LYS  | 2.7  |
| 1   | K     | 329 | LYS  | 2.7  |
| 1   | G     | 67  | GLY  | 2.7  |
| 1   | G     | 259 | GLY  | 2.7  |
| 1   | K     | 32  | GLY  | 2.7  |
| 1   | K     | 172 | GLY  | 2.7  |
| 1   | J     | 73  | ARG  | 2.7  |
| 1   | F     | 182 | ALA  | 2.7  |
| 1   | H     | 207 | ALA  | 2.7  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | K     | 302 | GLN  | 2.7  |
| 1   | I     | 311 | LEU  | 2.7  |
| 1   | C     | 28  | GLU  | 2.7  |
| 1   | H     | 116 | PRO  | 2.7  |
| 1   | K     | 126 | SER  | 2.7  |
| 1   | G     | 5   | ILE  | 2.7  |
| 1   | I     | 63  | ILE  | 2.7  |
| 1   | J     | 39  | ILE  | 2.7  |
| 1   | H     | 201 | LYS  | 2.7  |
| 1   | F     | 324 | GLY  | 2.7  |
| 1   | I     | 17  | GLY  | 2.7  |
| 1   | J     | 328 | GLY  | 2.7  |
| 1   | F     | 183 | GLU  | 2.6  |
| 1   | F     | 30  | PRO  | 2.6  |
| 1   | K     | 30  | PRO  | 2.6  |
| 1   | K     | 83  | SER  | 2.6  |
| 1   | B     | 201 | LYS  | 2.6  |
| 1   | J     | 79  | LYS  | 2.6  |
| 1   | B     | 198 | ILE  | 2.6  |
| 1   | K     | 169 | ARG  | 2.6  |
| 1   | I     | 148 | GLY  | 2.6  |
| 1   | B     | 325 | GLU  | 2.6  |
| 1   | L     | 325 | GLU  | 2.6  |
| 1   | I     | 59  | ALA  | 2.6  |
| 1   | K     | 150 | THR  | 2.6  |
| 1   | J     | 311 | LEU  | 2.6  |
| 1   | K     | 122 | PRO  | 2.6  |
| 1   | K     | 125 | LEU  | 2.6  |
| 1   | I     | 300 | LYS  | 2.6  |
| 1   | K     | 303 | SER  | 2.6  |
| 1   | A     | 304 | ARG  | 2.6  |
| 1   | C     | 60  | ARG  | 2.6  |
| 1   | G     | 60  | ARG  | 2.6  |
| 1   | I     | 235 | ARG  | 2.6  |
| 1   | K     | 200 | TYR  | 2.6  |
| 1   | C     | 334 | VAL  | 2.6  |
| 1   | K     | 307 | ILE  | 2.6  |
| 1   | F     | 207 | ALA  | 2.6  |
| 1   | H     | 182 | ALA  | 2.6  |
| 1   | J     | 90  | ALA  | 2.6  |
| 1   | K     | 128 | LEU  | 2.6  |
| 1   | F     | 24  | PHE  | 2.6  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | K     | 151 | VAL  | 2.6  |
| 1   | K     | 308 | VAL  | 2.6  |
| 1   | B     | 185 | CYS  | 2.6  |
| 1   | H     | 87  | GLY  | 2.6  |
| 1   | J     | 76  | GLY  | 2.6  |
| 1   | H     | 292 | MET  | 2.6  |
| 1   | A     | 49  | ASP  | 2.6  |
| 1   | B     | 315 | PRO  | 2.6  |
| 1   | C     | 21  | ARG  | 2.6  |
| 1   | E     | 60  | ARG  | 2.6  |
| 1   | G     | 14  | ARG  | 2.6  |
| 1   | K     | 157 | ALA  | 2.6  |
| 1   | K     | 207 | ALA  | 2.6  |
| 1   | G     | 315 | PRO  | 2.6  |
| 1   | F     | 170 | LEU  | 2.6  |
| 1   | H     | 61  | SER  | 2.6  |
| 1   | A     | 322 | PHE  | 2.5  |
| 1   | A     | 248 | ILE  | 2.5  |
| 1   | D     | 63  | ILE  | 2.5  |
| 1   | I     | 91  | GLY  | 2.5  |
| 1   | K     | 281 | TYR  | 2.5  |
| 1   | A     | 130 | MET  | 2.5  |
| 1   | A     | 16  | SER  | 2.5  |
| 1   | F     | 315 | PRO  | 2.5  |
| 1   | G     | 59  | ALA  | 2.5  |
| 1   | I     | 61  | SER  | 2.5  |
| 1   | F     | 318 | LEU  | 2.5  |
| 1   | K     | 229 | LEU  | 2.5  |
| 1   | A     | 26  | PHE  | 2.5  |
| 1   | B     | 194 | PHE  | 2.5  |
| 1   | H     | 24  | PHE  | 2.5  |
| 1   | H     | 194 | PHE  | 2.5  |
| 1   | K     | 137 | PHE  | 2.5  |
| 1   | G     | 68  | ILE  | 2.5  |
| 1   | G     | 87  | GLY  | 2.5  |
| 1   | H     | 17  | GLY  | 2.5  |
| 1   | I     | 180 | GLY  | 2.5  |
| 1   | J     | 96  | GLY  | 2.5  |
| 1   | K     | 110 | GLY  | 2.5  |
| 1   | B     | 210 | LYS  | 2.5  |
| 1   | C     | 93  | TYR  | 2.5  |
| 1   | C     | 210 | LYS  | 2.5  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | J     | 84  | LYS  | 2.5  |
| 1   | K     | 186 | ARG  | 2.5  |
| 1   | B     | 255 | GLU  | 2.5  |
| 1   | G     | 30  | PRO  | 2.5  |
| 1   | G     | 119 | ALA  | 2.5  |
| 1   | H     | 249 | SER  | 2.5  |
| 1   | K     | 107 | GLU  | 2.5  |
| 1   | A     | 321 | LEU  | 2.5  |
| 1   | H     | 55  | TRP  | 2.5  |
| 1   | B     | 63  | ILE  | 2.5  |
| 1   | F     | 186 | ARG  | 2.5  |
| 1   | I     | 62  | TYR  | 2.5  |
| 1   | J     | 44  | GLU  | 2.5  |
| 1   | J     | 101 | GLN  | 2.5  |
| 1   | L     | 25  | SER  | 2.5  |
| 1   | B     | 207 | ALA  | 2.5  |
| 1   | B     | 205 | LEU  | 2.5  |
| 1   | E     | 321 | LEU  | 2.5  |
| 1   | I     | 121 | LEU  | 2.5  |
| 1   | K     | 130 | MET  | 2.5  |
| 1   | F     | 322 | PHE  | 2.5  |
| 1   | I     | 14  | ARG  | 2.5  |
| 1   | I     | 322 | PHE  | 2.5  |
| 1   | C     | 180 | GLY  | 2.5  |
| 1   | J     | 37  | GLY  | 2.5  |
| 1   | K     | 226 | GLY  | 2.5  |
| 1   | F     | 334 | VAL  | 2.4  |
| 1   | H     | 68  | ILE  | 2.5  |
| 1   | K     | 277 | VAL  | 2.4  |
| 1   | B     | 312 | GLU  | 2.4  |
| 1   | E     | 58  | ASP  | 2.4  |
| 1   | B     | 62  | TYR  | 2.4  |
| 1   | C     | 62  | TYR  | 2.4  |
| 1   | C     | 294 | THR  | 2.4  |
| 1   | H     | 29  | THR  | 2.4  |
| 1   | I     | 19  | PRO  | 2.4  |
| 1   | K     | 133 | MET  | 2.4  |
| 1   | K     | 31  | LEU  | 2.4  |
| 1   | K     | 330 | LEU  | 2.4  |
| 1   | K     | 333 | LYS  | 2.4  |
| 1   | L     | 264 | LEU  | 2.4  |
| 1   | K     | 123 | ARG  | 2.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | F     | 177 | GLY  | 2.4  |
| 1   | F     | 285 | PHE  | 2.4  |
| 1   | K     | 165 | GLY  | 2.4  |
| 1   | B     | 190 | GLU  | 2.4  |
| 1   | B     | 58  | ASP  | 2.4  |
| 1   | K     | 80  | VAL  | 2.4  |
| 1   | F     | 29  | THR  | 2.4  |
| 1   | B     | 211 | ARG  | 2.4  |
| 1   | F     | 304 | ARG  | 2.4  |
| 1   | G     | 320 | LYS  | 2.4  |
| 1   | H     | 215 | LYS  | 2.4  |
| 1   | C     | 48  | LEU  | 2.4  |
| 1   | I     | 296 | LEU  | 2.4  |
| 1   | F     | 172 | GLY  | 2.4  |
| 1   | I     | 172 | GLY  | 2.4  |
| 1   | B     | 202 | ASN  | 2.4  |
| 1   | F     | 147 | ASN  | 2.4  |
| 1   | F     | 202 | ASN  | 2.4  |
| 1   | K     | 175 | VAL  | 2.4  |
| 1   | F     | 16  | SER  | 2.4  |
| 1   | L     | 55  | TRP  | 2.4  |
| 1   | L     | 323 | SER  | 2.4  |
| 1   | C     | 185 | CYS  | 2.4  |
| 1   | C     | 333 | LYS  | 2.4  |
| 1   | F     | 60  | ARG  | 2.4  |
| 1   | F     | 185 | CYS  | 2.4  |
| 1   | H     | 185 | CYS  | 2.4  |
| 1   | K     | 245 | CYS  | 2.4  |
| 1   | G     | 93  | TYR  | 2.4  |
| 1   | J     | 103 | TYR  | 2.4  |
| 1   | H     | 31  | LEU  | 2.4  |
| 1   | A     | 324 | GLY  | 2.4  |
| 1   | B     | 196 | GLY  | 2.4  |
| 1   | C     | 17  | GLY  | 2.4  |
| 1   | F     | 13  | GLN  | 2.4  |
| 1   | H     | 181 | GLY  | 2.4  |
| 1   | J     | 102 | ASP  | 2.4  |
| 1   | B     | 257 | VAL  | 2.4  |
| 1   | E     | 21  | ARG  | 2.4  |
| 1   | J     | 277 | VAL  | 2.4  |
| 1   | G     | 16  | SER  | 2.4  |
| 1   | J     | 83  | SER  | 2.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | F     | 59  | ALA  | 2.3  |
| 1   | J     | 33  | GLU  | 2.3  |
| 1   | G     | 318 | LEU  | 2.3  |
| 1   | A     | 17  | GLY  | 2.3  |
| 1   | B     | 324 | GLY  | 2.3  |
| 1   | D     | 259 | GLY  | 2.3  |
| 1   | B     | 21  | ARG  | 2.3  |
| 1   | K     | 73  | ARG  | 2.3  |
| 1   | K     | 104 | PHE  | 2.3  |
| 1   | K     | 201 | LYS  | 2.3  |
| 1   | K     | 220 | PHE  | 2.3  |
| 1   | G     | 100 | VAL  | 2.3  |
| 1   | C     | 50  | PRO  | 2.3  |
| 1   | B     | 208 | GLY  | 2.3  |
| 1   | F     | 181 | GLY  | 2.3  |
| 1   | G     | 11  | LEU  | 2.3  |
| 1   | G     | 17  | GLY  | 2.3  |
| 1   | H     | 67  | GLY  | 2.3  |
| 1   | L     | 181 | GLY  | 2.3  |
| 1   | B     | 49  | ASP  | 2.3  |
| 1   | H     | 186 | ARG  | 2.3  |
| 1   | K     | 235 | ARG  | 2.3  |
| 1   | I     | 201 | LYS  | 2.3  |
| 1   | J     | 329 | LYS  | 2.3  |
| 1   | D     | 16  | SER  | 2.3  |
| 1   | F     | 153 | ILE  | 2.3  |
| 1   | F     | 198 | ILE  | 2.3  |
| 1   | J     | 28  | GLU  | 2.3  |
| 1   | J     | 309 | GLU  | 2.3  |
| 1   | L     | 66  | VAL  | 2.3  |
| 1   | I     | 15  | PRO  | 2.3  |
| 1   | I     | 302 | GLN  | 2.3  |
| 1   | E     | 59  | ALA  | 2.3  |
| 1   | K     | 74  | ALA  | 2.3  |
| 1   | B     | 14  | ARG  | 2.3  |
| 1   | J     | 91  | GLY  | 2.3  |
| 1   | L     | 58  | ASP  | 2.3  |
| 1   | C     | 320 | LYS  | 2.3  |
| 1   | I     | 215 | LYS  | 2.3  |
| 1   | K     | 292 | MET  | 2.3  |
| 1   | B     | 307 | ILE  | 2.3  |
| 1   | F     | 189 | VAL  | 2.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | I     | 169 | ARG  | 2.3  |
| 1   | J     | 7   | ARG  | 2.3  |
| 1   | K     | 211 | ARG  | 2.3  |
| 1   | H     | 184 | LYS  | 2.3  |
| 1   | J     | 42  | LYS  | 2.3  |
| 1   | K     | 135 | ALA  | 2.3  |
| 1   | H     | 299 | GLY  | 2.3  |
| 1   | K     | 161 | GLY  | 2.3  |
| 1   | K     | 210 | LYS  | 2.3  |
| 1   | K     | 279 | MET  | 2.3  |
| 1   | G     | 28  | GLU  | 2.2  |
| 1   | H     | 191 | GLU  | 2.2  |
| 1   | B     | 16  | SER  | 2.2  |
| 1   | C     | 302 | GLN  | 2.2  |
| 1   | F     | 283 | GLN  | 2.2  |
| 1   | L     | 249 | SER  | 2.2  |
| 1   | F     | 178 | ILE  | 2.2  |
| 1   | A     | 277 | VAL  | 2.2  |
| 1   | C     | 15  | PRO  | 2.2  |
| 1   | I     | 30  | PRO  | 2.2  |
| 1   | K     | 134 | THR  | 2.2  |
| 1   | L     | 334 | VAL  | 2.2  |
| 1   | K     | 174 | ARG  | 2.2  |
| 1   | G     | 22  | ASP  | 2.2  |
| 1   | G     | 69  | GLY  | 2.2  |
| 1   | C     | 318 | LEU  | 2.2  |
| 1   | G     | 121 | LEU  | 2.2  |
| 1   | J     | 330 | LEU  | 2.2  |
| 1   | G     | 183 | GLU  | 2.2  |
| 1   | H     | 183 | GLU  | 2.2  |
| 1   | I     | 70  | GLU  | 2.2  |
| 1   | G     | 73  | ARG  | 2.2  |
| 1   | L     | 53  | ARG  | 2.2  |
| 1   | A     | 57  | ASN  | 2.2  |
| 1   | B     | 27  | VAL  | 2.2  |
| 1   | C     | 19  | PRO  | 2.2  |
| 1   | F     | 120 | PRO  | 2.2  |
| 1   | H     | 175 | VAL  | 2.2  |
| 1   | H     | 331 | VAL  | 2.2  |
| 1   | I     | 22  | ASP  | 2.2  |
| 1   | I     | 292 | MET  | 2.2  |
| 1   | I     | 20  | GLY  | 2.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | K     | 129 | GLY  | 2.2  |
| 1   | B     | 203 | GLU  | 2.2  |
| 1   | C     | 190 | GLU  | 2.2  |
| 1   | C     | 11  | LEU  | 2.2  |
| 1   | E     | 250 | GLN  | 2.2  |
| 1   | F     | 89  | GLN  | 2.2  |
| 1   | J     | 323 | SER  | 2.2  |
| 1   | H     | 304 | ARG  | 2.2  |
| 1   | K     | 146 | LYS  | 2.2  |
| 1   | C     | 202 | ASN  | 2.2  |
| 1   | L     | 202 | ASN  | 2.2  |
| 1   | H     | 228 | ILE  | 2.2  |
| 1   | I     | 29  | THR  | 2.2  |
| 1   | J     | 23  | THR  | 2.2  |
| 1   | B     | 227 | GLU  | 2.2  |
| 1   | C     | 183 | GLU  | 2.2  |
| 1   | I     | 325 | GLU  | 2.2  |
| 1   | C     | 207 | ALA  | 2.2  |
| 1   | C     | 256 | ALA  | 2.2  |
| 1   | G     | 89  | GLN  | 2.2  |
| 1   | C     | 311 | LEU  | 2.2  |
| 1   | A     | 186 | ARG  | 2.2  |
| 1   | I     | 304 | ARG  | 2.2  |
| 1   | F     | 210 | LYS  | 2.2  |
| 1   | J     | 333 | LYS  | 2.2  |
| 1   | C     | 23  | THR  | 2.2  |
| 1   | J     | 49  | ASP  | 2.2  |
| 1   | C     | 24  | PHE  | 2.1  |
| 1   | F     | 190 | GLU  | 2.1  |
| 1   | I     | 183 | GLU  | 2.1  |
| 1   | K     | 190 | GLU  | 2.1  |
| 1   | C     | 66  | VAL  | 2.1  |
| 1   | F     | 308 | VAL  | 2.1  |
| 1   | K     | 41  | VAL  | 2.1  |
| 1   | K     | 163 | VAL  | 2.1  |
| 1   | H     | 302 | GLN  | 2.1  |
| 1   | K     | 180 | GLY  | 2.1  |
| 1   | K     | 35  | ALA  | 2.1  |
| 1   | G     | 21  | ARG  | 2.1  |
| 1   | I     | 319 | LEU  | 2.1  |
| 1   | F     | 184 | LYS  | 2.1  |
| 1   | F     | 215 | LYS  | 2.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | H     | 210 | LYS  | 2.1  |
| 1   | J     | 45  | TYR  | 2.1  |
| 1   | A     | 22  | ASP  | 2.1  |
| 1   | E     | 49  | ASP  | 2.1  |
| 1   | F     | 204 | ASP  | 2.1  |
| 1   | F     | 19  | PRO  | 2.1  |
| 1   | F     | 307 | ILE  | 2.1  |
| 1   | J     | 89  | GLN  | 2.1  |
| 1   | K     | 8   | GLN  | 2.1  |
| 1   | K     | 167 | ILE  | 2.1  |
| 1   | K     | 221 | PHE  | 2.1  |
| 1   | E     | 27  | VAL  | 2.1  |
| 1   | G     | 324 | GLY  | 2.1  |
| 1   | I     | 160 | VAL  | 2.1  |
| 1   | J     | 85  | HIS  | 2.1  |
| 1   | J     | 118 | ARG  | 2.1  |
| 1   | H     | 293 | ALA  | 2.1  |
| 1   | C     | 329 | LYS  | 2.1  |
| 1   | G     | 321 | LEU  | 2.1  |
| 1   | J     | 320 | LYS  | 2.1  |
| 1   | K     | 290 | LYS  | 2.1  |
| 1   | A     | 279 | MET  | 2.1  |
| 1   | E     | 57  | ASN  | 2.1  |
| 1   | C     | 306 | ASP  | 2.1  |
| 1   | A     | 64  | PRO  | 2.1  |
| 1   | B     | 4   | GLN  | 2.1  |
| 1   | G     | 15  | PRO  | 2.1  |
| 1   | I     | 315 | PRO  | 2.1  |
| 1   | B     | 181 | GLY  | 2.1  |
| 1   | H     | 324 | GLY  | 2.1  |
| 1   | K     | 118 | ARG  | 2.1  |
| 1   | L     | 258 | ARG  | 2.1  |
| 1   | F     | 277 | VAL  | 2.1  |
| 1   | I     | 114 | VAL  | 2.1  |
| 1   | L     | 232 | VAL  | 2.1  |
| 1   | H     | 206 | ALA  | 2.1  |
| 1   | K     | 127 | ALA  | 2.1  |
| 1   | F     | 75  | LEU  | 2.1  |
| 1   | G     | 61  | SER  | 2.1  |
| 1   | K     | 154 | SER  | 2.1  |
| 1   | I     | 107 | GLU  | 2.1  |
| 1   | G     | 58  | ASP  | 2.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | K     | 222 | ASP  | 2.1  |
| 1   | G     | 23  | THR  | 2.1  |
| 1   | H     | 53  | ARG  | 2.1  |
| 1   | I     | 158 | GLY  | 2.1  |
| 1   | K     | 99  | GLY  | 2.1  |
| 1   | D     | 320 | LYS  | 2.1  |
| 1   | F     | 5   | ILE  | 2.1  |
| 1   | G     | 201 | LYS  | 2.1  |
| 1   | I     | 333 | LYS  | 2.1  |
| 1   | K     | 224 | VAL  | 2.1  |
| 1   | C     | 203 | GLU  | 2.0  |
| 1   | K     | 138 | ALA  | 2.1  |
| 1   | L     | 51  | ALA  | 2.1  |
| 1   | E     | 18  | LEU  | 2.0  |
| 1   | G     | 311 | LEU  | 2.0  |
| 1   | H     | 188 | LEU  | 2.0  |
| 1   | H     | 321 | LEU  | 2.0  |
| 1   | B     | 213 | CYS  | 2.0  |
| 1   | F     | 118 | ARG  | 2.0  |
| 1   | E     | 17  | GLY  | 2.0  |
| 1   | F     | 299 | GLY  | 2.0  |
| 1   | J     | 310 | GLY  | 2.0  |
| 1   | G     | 66  | VAL  | 2.0  |
| 1   | I     | 24  | PHE  | 2.0  |
| 1   | I     | 189 | VAL  | 2.0  |
| 1   | L     | 70  | GLU  | 2.0  |
| 1   | C     | 117 | SER  | 2.0  |
| 1   | H     | 25  | SER  | 2.0  |
| 1   | A     | 55  | TRP  | 2.0  |
| 1   | C     | 57  | ASN  | 2.0  |
| 1   | B     | 121 | LEU  | 2.0  |
| 1   | F     | 296 | LEU  | 2.0  |
| 1   | G     | 31  | LEU  | 2.0  |
| 1   | H     | 48  | LEU  | 2.0  |
| 1   | I     | 13  | GLN  | 2.0  |
| 1   | K     | 89  | GLN  | 2.0  |
| 1   | K     | 199 | ASP  | 2.0  |
| 1   | C     | 304 | ARG  | 2.0  |
| 1   | I     | 123 | ARG  | 2.0  |
| 1   | C     | 84  | LYS  | 2.0  |
| 1   | L     | 201 | LYS  | 2.0  |
| 1   | E     | 19  | PRO  | 2.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | F     | 317 | THR  | 2.0  |
| 1   | G     | 19  | PRO  | 2.0  |
| 1   | K     | 234 | THR  | 2.0  |
| 1   | B     | 148 | GLY  | 2.0  |
| 1   | K     | 288 | GLY  | 2.0  |
| 1   | L     | 259 | GLY  | 2.0  |
| 1   | L     | 328 | GLY  | 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   | MES  | I     | 1335 | 12/12 | 0.86 | 0.17 | 61,65,73,73                 | 0     |
| 2   | MES  | H     | 1335 | 12/12 | 0.88 | 0.17 | 73,75,77,78                 | 0     |
| 2   | MES  | F     | 1335 | 12/12 | 0.92 | 0.15 | 41,51,52,53                 | 0     |
| 2   | MES  | G     | 1335 | 12/12 | 0.94 | 0.11 | 40,41,41,42                 | 0     |
| 2   | MES  | D     | 1335 | 12/12 | 0.97 | 0.08 | 28,32,33,34                 | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.