



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2020 – 05:16 PM BST

PDB ID : 4LNO  
Title : B. subtilis glutamine synthetase structures reveal large active site conformational changes and basis for isoenzyme specific regulation: form two of GS-1  
Authors : Schumacher, M.A.; Chinnam, N.; Tonthat, N.; Fisher, S.; Wray, L.  
Deposited on : 2013-07-11  
Resolution : 2.90 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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.14.4.dev1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.14.4.dev1

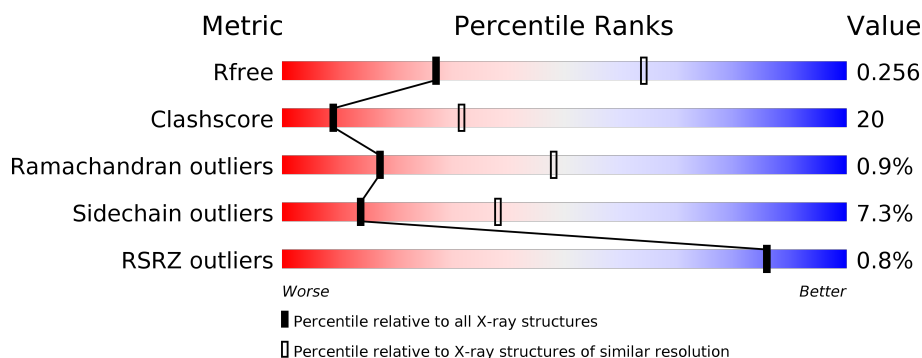
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 130704                      | 1957 (2.90-2.90)                                      |
| Clashscore            | 141614                      | 2172 (2.90-2.90)                                      |
| Ramachandran outliers | 138981                      | 2115 (2.90-2.90)                                      |
| Sidechain outliers    | 138945                      | 2117 (2.90-2.90)                                      |
| RSRZ outliers         | 127900                      | 1906 (2.90-2.90)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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     | 443    | <div> <div>%</div> <div> <div></div> <div>65%</div> <div>30%</div> <div>•</div> </div> </div>  |
| 1   | B     | 443    | <div> <div></div> <div>58%</div> <div>37%</div> <div>•</div> </div>                            |
| 1   | C     | 443    | <div> <div>%</div> <div> <div></div> <div>61%</div> <div>35%</div> <div>•</div> </div> </div>  |
| 1   | D     | 443    | <div> <div>%</div> <div> <div></div> <div>62%</div> <div>33%</div> <div>5%</div> </div> </div> |
| 1   | E     | 443    | <div> <div>%</div> <div> <div></div> <div>59%</div> <div>37%</div> <div>•</div> </div> </div>  |
| 1   | F     | 443    | <div> <div>%</div> <div> <div></div> <div>58%</div> <div>36%</div> <div>5%</div> </div> </div> |

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 21993 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.

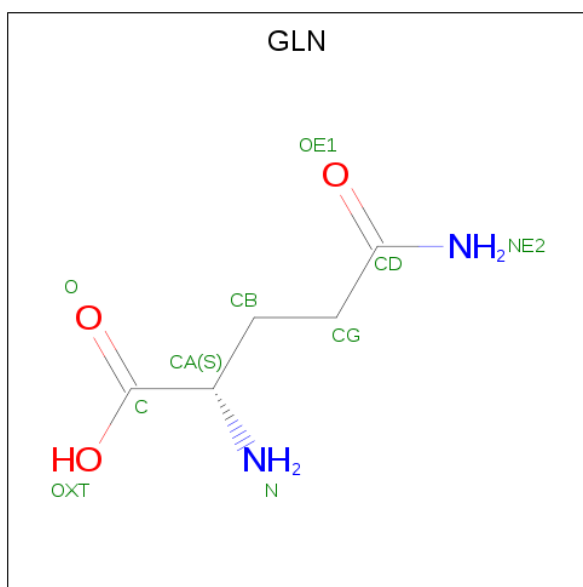
- Molecule 1 is a protein called Glutamine synthetase.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 443      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3535  | 2259 | 590 | 670 | 16 |         |         |       |
| 1   | B     | 443      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3535  | 2259 | 590 | 670 | 16 |         |         |       |
| 1   | C     | 443      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3535  | 2259 | 590 | 670 | 16 |         |         |       |
| 1   | D     | 443      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3535  | 2259 | 590 | 670 | 16 |         |         |       |
| 1   | E     | 443      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3535  | 2259 | 590 | 670 | 16 |         |         |       |
| 1   | F     | 443      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3535  | 2259 | 590 | 670 | 16 |         |         |       |

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 2   | D     | 2        | Total | Mg | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 2   | E     | 2        | Total | Mg | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 2   | B     | 2        | Total | Mg | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 2   | C     | 2        | Total | Mg | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 2   | A     | 2        | Total | Mg | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 2   | F     | 2        | Total | Mg | 0       | 0       |
|     |       |          | 2     | 2  |         |         |

- Molecule 3 is GLUTAMINE (three-letter code: GLN) (formula: C<sub>5</sub>H<sub>10</sub>N<sub>2</sub>O<sub>3</sub>).



| Mol | Chain | Residues | Atoms |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 3   | A     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 9     | 5 | 2 | 2 |         |         |
| 3   | B     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 9     | 5 | 2 | 2 |         |         |
| 3   | C     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 10    | 5 | 2 | 3 |         |         |
| 3   | D     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 10    | 5 | 2 | 3 |         |         |
| 3   | E     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 10    | 5 | 2 | 3 |         |         |
| 3   | F     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 10    | 5 | 2 | 3 |         |         |

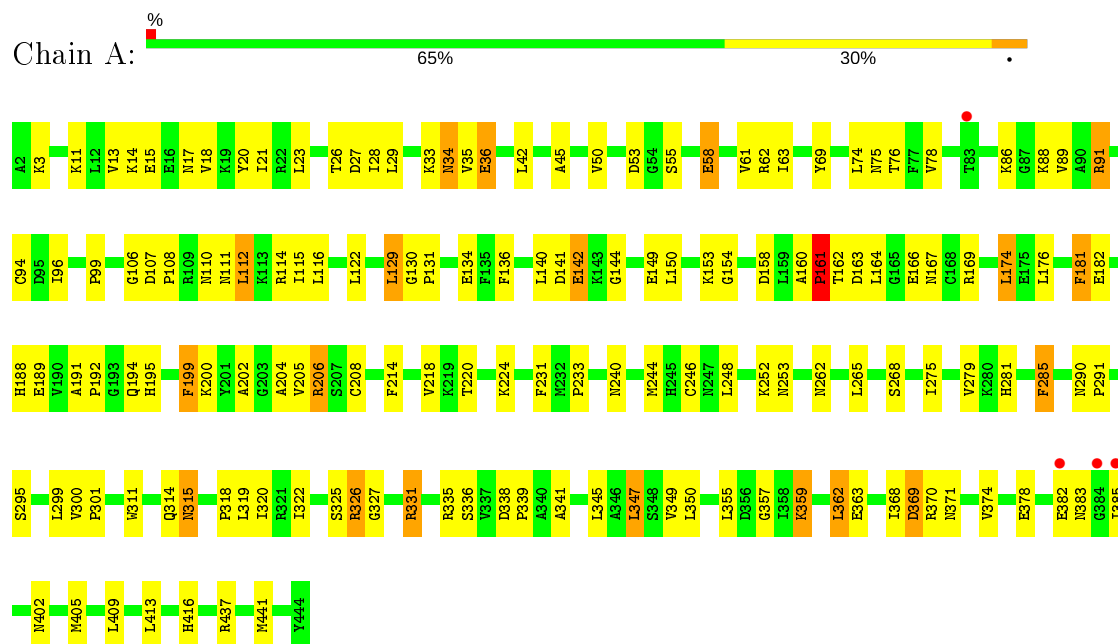
- Molecule 4 is water.

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 4   | A     | 122      | Total | O   | 0       | 0       |
|     |       |          | 122   | 122 |         |         |
| 4   | B     | 117      | Total | O   | 0       | 0       |
|     |       |          | 117   | 117 |         |         |
| 4   | C     | 123      | Total | O   | 0       | 0       |
|     |       |          | 123   | 123 |         |         |
| 4   | D     | 114      | Total | O   | 0       | 0       |
|     |       |          | 114   | 114 |         |         |
| 4   | E     | 134      | Total | O   | 0       | 0       |
|     |       |          | 134   | 134 |         |         |
| 4   | F     | 103      | Total | O   | 0       | 0       |
|     |       |          | 103   | 103 |         |         |

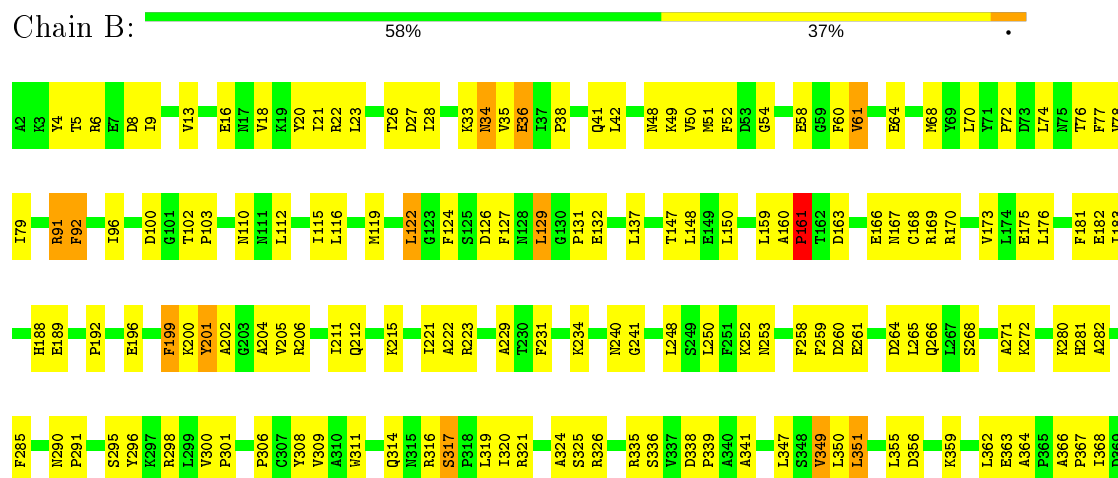
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Glutamine synthetase

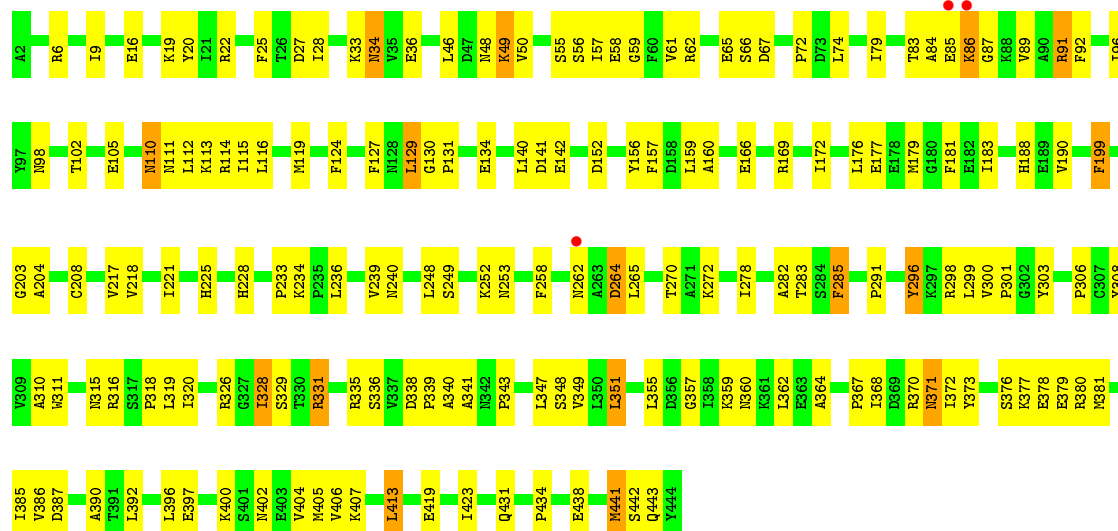


#### • Molecule 1: Glutamine synthetase

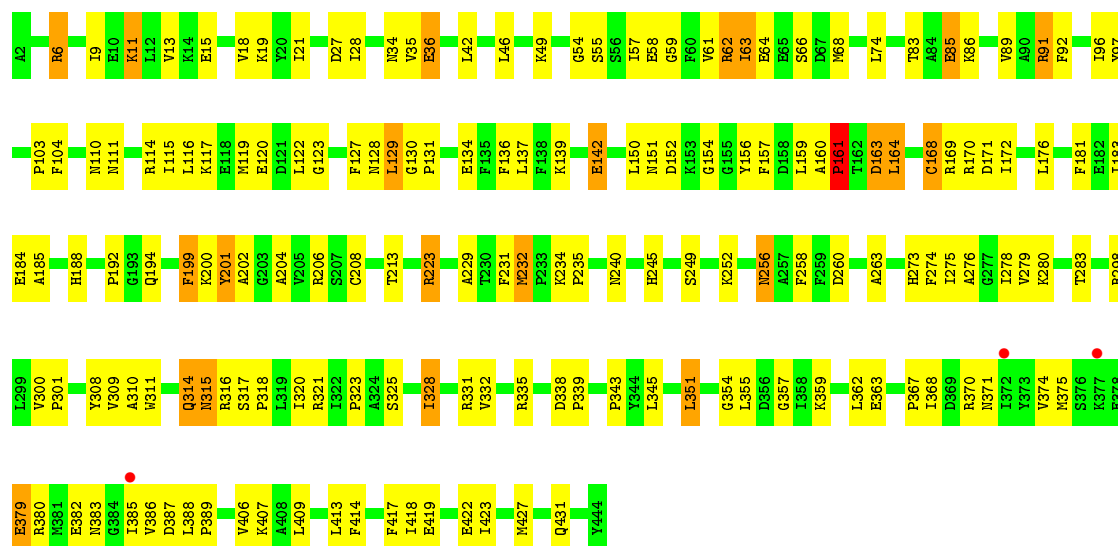




• Molecule 1: Glutamine synthetase

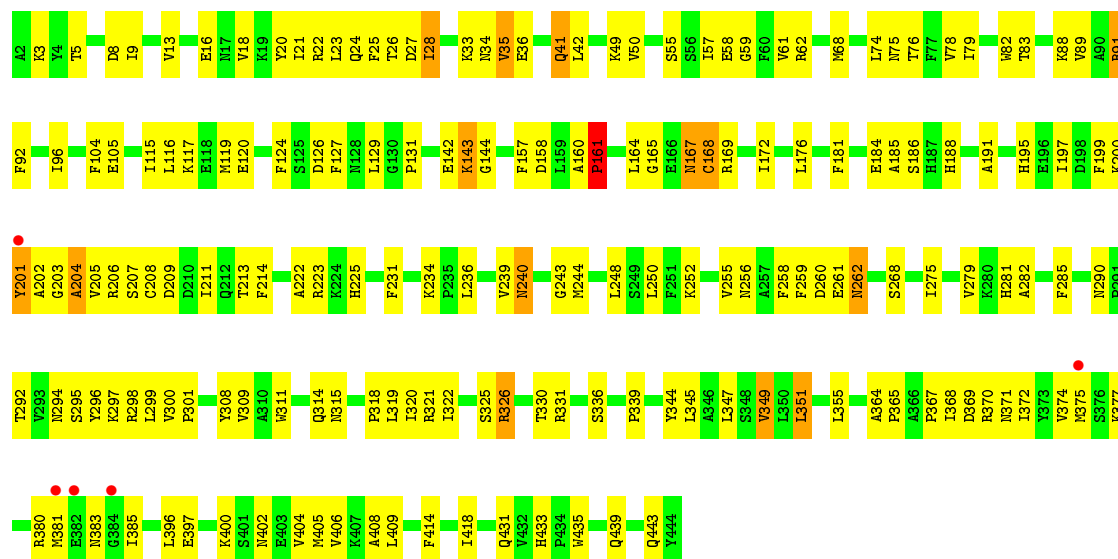


• Molecule 1: Glutamine synthetase

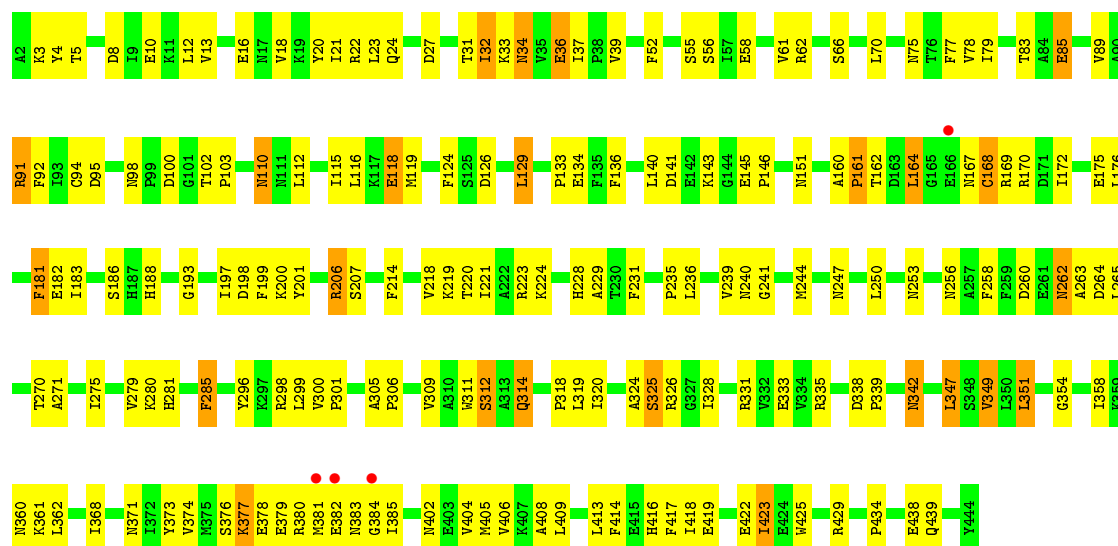


• Molecule 1: Glutamine synthetase





• Molecule 1: Glutamine synthetase



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | C 1 2 1   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 209.86Å 138.94Å 144.73Å<br>90.00° 125.17° 90.00°            | Depositor        |
| Resolution (Å)  | 71.68 – 2.90<br>71.68 – 2.90                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.7 (71.68-2.90)<br>99.8 (71.68-2.90)                      | Depositor<br>EDS |
| $R_{merge}$   | (Not available)   | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 3.88 (at 2.91Å)   | Xtriage          |
| Refinement program  | CNS 1.2   | Depositor        |
| R, $R_{free}$   | 0.196 , 0.256<br>0.195 , 0.256                              | Depositor<br>DCC |
| $R_{free}$ test set   | 4572 reflections (6.08%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 40.7  | Xtriage          |
| Anisotropy  | 0.429   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.34 , 52.1   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$ | Xtriage          |
| Estimated twinning fraction   | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation  | 0.93  | EDS              |
| Total number of atoms   | 21993   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 38.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% 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: MG

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     | 0.44         | 0/3618      | 0.61        | 0/4895      |
| 1   | B     | 0.44         | 0/3618      | 0.61        | 0/4895      |
| 1   | C     | 0.46         | 0/3618      | 0.62        | 0/4895      |
| 1   | D     | 0.44         | 0/3618      | 0.61        | 0/4895      |
| 1   | E     | 0.43         | 0/3618      | 0.62        | 0/4895      |
| 1   | F     | 0.44         | 0/3618      | 0.61        | 0/4895      |
| All | All   | 0.44         | 0/21708     | 0.61        | 0/29370     |

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   | B     | 0                   | 1                   |
| 1   | C     | 0                   | 1                   |
| 1   | E     | 0                   | 1                   |
| 1   | F     | 0                   | 1                   |
| All | All   | 0                   | 4                   |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | B     | 296 | TYR  | Sidechain |
| 1   | C     | 296 | TYR  | Sidechain |
| 1   | E     | 296 | TYR  | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | F     | 296 | TYR  | Sidechain |

## 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     | 3535  | 0        | 3466     | 130     | 0            |
| 1   | B     | 3535  | 0        | 3466     | 146     | 0            |
| 1   | C     | 3535  | 0        | 3466     | 138     | 0            |
| 1   | D     | 3535  | 0        | 3466     | 147     | 0            |
| 1   | E     | 3535  | 0        | 3466     | 153     | 0            |
| 1   | F     | 3535  | 0        | 3466     | 166     | 0            |
| 2   | A     | 2     | 0        | 0        | 0       | 0            |
| 2   | B     | 2     | 0        | 0        | 0       | 0            |
| 2   | C     | 2     | 0        | 0        | 0       | 0            |
| 2   | D     | 2     | 0        | 0        | 0       | 0            |
| 2   | E     | 2     | 0        | 0        | 0       | 0            |
| 2   | F     | 2     | 0        | 0        | 0       | 0            |
| 3   | A     | 9     | 0        | 7        | 2       | 0            |
| 3   | B     | 9     | 0        | 7        | 1       | 0            |
| 3   | C     | 10    | 0        | 7        | 2       | 0            |
| 3   | D     | 10    | 0        | 7        | 1       | 0            |
| 3   | E     | 10    | 0        | 7        | 0       | 0            |
| 3   | F     | 10    | 0        | 7        | 2       | 0            |
| 4   | A     | 122   | 0        | 0        | 6       | 0            |
| 4   | B     | 117   | 0        | 0        | 6       | 0            |
| 4   | C     | 123   | 0        | 0        | 10      | 0            |
| 4   | D     | 114   | 0        | 0        | 7       | 0            |
| 4   | E     | 134   | 0        | 0        | 8       | 0            |
| 4   | F     | 103   | 0        | 0        | 4       | 0            |
| All | All   | 21993 | 0        | 20838    | 847     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

All (847) 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:E:160:ALA:HB1  | 1:E:161:PRO:HD2  | 1.29                     | 1.10              |
| 1:C:328:ILE:HD13 | 1:C:328:ILE:H    | 1.11                     | 1.09              |
| 1:D:160:ALA:HB1  | 1:D:161:PRO:HD2  | 1.38                     | 1.05              |
| 1:D:160:ALA:HB3  | 1:D:169:ARG:HH22 | 1.22                     | 1.03              |
| 1:D:63:ILE:HG22  | 1:D:64:GLU:HG3   | 1.43                     | 0.95              |
| 1:A:160:ALA:HB3  | 1:A:169:ARG:HH12 | 1.28                     | 0.95              |
| 1:D:160:ALA:HB3  | 1:D:169:ARG:NH2  | 1.80                     | 0.95              |
| 1:A:160:ALA:HB1  | 1:A:161:PRO:HD2  | 1.48                     | 0.95              |
| 1:A:370:ARG:HG2  | 1:A:371:ASN:H    | 1.33                     | 0.93              |
| 1:D:357:GLY:HA2  | 1:D:362:LEU:HD13 | 1.50                     | 0.93              |
| 1:B:160:ALA:HB1  | 1:B:161:PRO:HD2  | 1.52                     | 0.91              |
| 1:A:74:LEU:HD22  | 1:A:74:LEU:H     | 1.37                     | 0.90              |
| 1:C:16:GLU:HG2   | 1:C:79:ILE:HD13  | 1.52                     | 0.90              |
| 1:F:27:ASP:HB3   | 1:F:33:LYS:HD2   | 1.52                     | 0.88              |
| 1:D:129:LEU:HD13 | 1:D:131:PRO:HD3  | 1.56                     | 0.87              |
| 1:C:368:ILE:HG21 | 1:C:372:ILE:HD11 | 1.56                     | 0.86              |
| 1:F:160:ALA:HB1  | 1:F:161:PRO:HD2  | 1.57                     | 0.85              |
| 1:C:129:LEU:HD13 | 1:C:131:PRO:HD3  | 1.58                     | 0.84              |
| 1:B:20:TYR:OH    | 1:B:36:GLU:HG3   | 1.77                     | 0.84              |
| 1:E:57:ILE:HD11  | 1:E:96:ILE:HG12  | 1.60                     | 0.83              |
| 1:D:256:ASN:HD22 | 1:D:258:PHE:H    | 1.26                     | 0.83              |
| 1:C:328:ILE:CD1  | 1:C:328:ILE:H    | 1.91                     | 0.83              |
| 1:F:338:ASP:HB2  | 1:F:339:PRO:HD2  | 1.61                     | 0.82              |
| 1:B:5:THR:HG22   | 1:B:8:ASP:CG     | 2.00                     | 0.81              |
| 1:B:380:ARG:HG3  | 1:B:385:ILE:HB   | 1.63                     | 0.81              |
| 1:D:328:ILE:HD13 | 1:D:328:ILE:H    | 1.44                     | 0.81              |
| 1:B:311:TRP:CZ2  | 1:B:367:PRO:HG3  | 2.17                     | 0.80              |
| 1:D:164:LEU:HD21 | 1:E:223:ARG:HD3  | 1.65                     | 0.79              |
| 1:B:160:ALA:HB2  | 1:B:188:HIS:HB2  | 1.66                     | 0.77              |
| 1:B:22:ARG:HB3   | 1:B:34:ASN:HD22  | 1.49                     | 0.77              |
| 1:F:13:VAL:HG13  | 1:F:18:VAL:HB    | 1.66                     | 0.77              |
| 1:D:13:VAL:HG13  | 1:D:18:VAL:HB    | 1.67                     | 0.77              |
| 1:C:20:TYR:OH    | 1:C:36:GLU:HG3   | 1.84                     | 0.77              |
| 1:E:349:VAL:HG22 | 1:E:405:MET:SD   | 2.25                     | 0.76              |
| 1:D:321:ARG:HD2  | 4:E:663:HOH:O    | 1.84                     | 0.76              |
| 1:B:13:VAL:HG13  | 1:B:18:VAL:HB    | 1.66                     | 0.76              |
| 1:C:57:ILE:HD11  | 1:C:96:ILE:HG12  | 1.68                     | 0.76              |
| 1:B:58:GLU:HG2   | 4:B:627:HOH:O    | 1.87                     | 0.75              |
| 1:C:58:GLU:HG2   | 4:C:615:HOH:O    | 1.87                     | 0.74              |
| 1:F:244:MET:H    | 1:F:338:ASP:HA   | 1.52                     | 0.74              |
| 1:A:338:ASP:HB2  | 1:A:339:PRO:HD2  | 1.68                     | 0.74              |
| 1:E:281:HIS:CD2  | 1:E:402:ASN:HD21 | 2.05                     | 0.74              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:349:VAL:HG22 | 1:B:405:MET:SD   | 2.28                     | 0.74              |
| 1:C:328:ILE:HD13 | 1:C:328:ILE:N    | 1.96                     | 0.74              |
| 1:F:182:GLU:HB3  | 1:F:200:LYS:HD3  | 1.70                     | 0.74              |
| 1:D:351:LEU:HD22 | 1:D:355:LEU:HG   | 1.71                     | 0.73              |
| 1:D:338:ASP:HB2  | 1:D:339:PRO:HD2  | 1.72                     | 0.71              |
| 1:D:375:MET:HB3  | 1:D:379:GLU:HB3  | 1.73                     | 0.71              |
| 1:A:220:THR:HG23 | 1:F:162:THR:HB   | 1.73                     | 0.70              |
| 1:D:311:TRP:CZ2  | 1:D:367:PRO:HG3  | 2.26                     | 0.70              |
| 1:A:142:GLU:CD   | 1:A:142:GLU:H    | 1.94                     | 0.70              |
| 1:E:13:VAL:HG13  | 1:E:18:VAL:HB    | 1.72                     | 0.70              |
| 1:C:172:ILE:HD13 | 1:C:218:VAL:HG22 | 1.73                     | 0.70              |
| 1:D:142:GLU:CD   | 1:D:142:GLU:H    | 1.95                     | 0.70              |
| 1:F:100:ASP:OD2  | 1:F:102:THR:HG22 | 1.91                     | 0.69              |
| 1:A:129:LEU:HD13 | 1:A:131:PRO:HG3  | 1.74                     | 0.69              |
| 1:E:176:LEU:O    | 1:E:181:PHE:HB2  | 1.92                     | 0.69              |
| 1:D:283:THR:HG23 | 4:D:616:HOH:O    | 1.92                     | 0.69              |
| 1:E:9:ILE:HG13   | 1:E:74:LEU:HD12  | 1.75                     | 0.69              |
| 1:F:376:SER:HB3  | 1:F:379:GLU:OE1  | 1.91                     | 0.69              |
| 1:B:176:LEU:O    | 1:B:181:PHE:HB2  | 1.92                     | 0.68              |
| 1:C:338:ASP:HB2  | 1:C:339:PRO:HD2  | 1.74                     | 0.68              |
| 1:C:208:CYS:SG   | 1:C:343:PRO:HB2  | 2.33                     | 0.68              |
| 1:B:22:ARG:HB3   | 1:B:34:ASN:ND2   | 2.08                     | 0.68              |
| 1:E:281:HIS:HD2  | 1:E:402:ASN:HD21 | 1.40                     | 0.68              |
| 1:F:377:LYS:O    | 1:F:381:MET:HG2  | 1.94                     | 0.68              |
| 1:E:160:ALA:HB1  | 1:E:161:PRO:CD   | 2.16                     | 0.67              |
| 1:E:160:ALA:CB   | 1:E:161:PRO:HD2  | 2.14                     | 0.67              |
| 1:B:131:PRO:HG2  | 1:B:199:PHE:CD1  | 2.30                     | 0.67              |
| 1:F:349:VAL:HG22 | 1:F:405:MET:SD   | 2.35                     | 0.67              |
| 1:A:114:ARG:HH21 | 1:A:115:ILE:HD11 | 1.60                     | 0.66              |
| 1:B:252:LYS:HG2  | 1:B:253:ASN:ND2  | 2.10                     | 0.66              |
| 1:E:259:PHE:CZ   | 1:E:261:GLU:HB2  | 2.31                     | 0.66              |
| 1:F:402:ASN:O    | 1:F:406:VAL:HG23 | 1.95                     | 0.66              |
| 1:D:328:ILE:HD13 | 1:D:328:ILE:N    | 2.12                     | 0.65              |
| 1:A:76:THR:O     | 1:A:91:ARG:NH1   | 2.29                     | 0.65              |
| 1:C:265:LEU:O    | 1:C:326:ARG:NH1  | 2.28                     | 0.65              |
| 1:E:168:CYS:SG   | 1:E:225:HIS:HD2  | 2.19                     | 0.65              |
| 1:A:345:LEU:HD22 | 1:A:409:LEU:HD22 | 1.78                     | 0.65              |
| 1:C:402:ASN:OD1  | 1:C:404:VAL:HG12 | 1.95                     | 0.65              |
| 1:C:349:VAL:HG22 | 1:C:405:MET:SD   | 2.37                     | 0.65              |
| 1:D:11:LYS:HA    | 1:D:11:LYS:HE3   | 1.78                     | 0.65              |
| 1:C:371:ASN:HD21 | 1:C:373:TYR:HB2  | 1.61                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:16:GLU:HG2   | 1:C:79:ILE:CD1   | 2.27                     | 0.65              |
| 1:F:300:VAL:HG13 | 1:F:301:PRO:HD2  | 1.77                     | 0.65              |
| 1:E:185:ALA:HB2  | 1:F:37:ILE:HG22  | 1.79                     | 0.64              |
| 1:D:275:ILE:O    | 1:D:279:VAL:HG23 | 1.96                     | 0.64              |
| 1:E:371:ASN:ND2  | 1:E:374:VAL:HG23 | 2.12                     | 0.64              |
| 1:F:311:TRP:HB3  | 1:F:320:ILE:HB   | 1.79                     | 0.63              |
| 1:D:116:LEU:HD23 | 1:D:351:LEU:HD11 | 1.80                     | 0.63              |
| 1:A:129:LEU:HD21 | 1:A:246:CYS:HB3  | 1.80                     | 0.63              |
| 1:D:11:LYS:O     | 1:D:15:GLU:HG3   | 1.99                     | 0.63              |
| 1:E:28:ILE:O     | 1:E:28:ILE:HD13  | 1.98                     | 0.63              |
| 1:A:160:ALA:HB3  | 1:A:169:ARG:NH1  | 2.07                     | 0.63              |
| 1:D:117:LYS:HD2  | 4:D:655:HOH:O    | 1.97                     | 0.63              |
| 1:A:176:LEU:O    | 1:A:181:PHE:HB2  | 1.98                     | 0.63              |
| 1:A:74:LEU:CD2   | 1:A:74:LEU:H     | 2.12                     | 0.63              |
| 1:C:141:ASP:HB2  | 1:C:142:GLU:OE1  | 1.99                     | 0.63              |
| 1:D:328:ILE:H    | 1:D:328:ILE:CD1  | 2.11                     | 0.63              |
| 1:D:55:SER:O     | 1:D:62:ARG:HG2   | 1.98                     | 0.63              |
| 1:E:314:GLN:HE22 | 1:F:66:SER:HB3   | 1.62                     | 0.63              |
| 1:B:300:VAL:HG13 | 1:B:301:PRO:HD2  | 1.81                     | 0.63              |
| 1:E:129:LEU:HD23 | 1:E:248:LEU:HD23 | 1.81                     | 0.63              |
| 1:F:281:HIS:CD2  | 1:F:402:ASN:HD21 | 2.16                     | 0.63              |
| 1:D:131:PRO:HG2  | 1:D:199:PHE:CD1  | 2.34                     | 0.62              |
| 1:D:129:LEU:HD22 | 1:D:130:GLY:N    | 2.14                     | 0.62              |
| 1:D:315:ASN:ND2  | 1:D:316:ARG:H    | 1.96                     | 0.62              |
| 1:E:74:LEU:H     | 1:E:74:LEU:HD22  | 1.63                     | 0.62              |
| 1:A:314:GLN:NE2  | 1:B:64:GLU:HB2   | 2.14                     | 0.62              |
| 1:B:372:ILE:HD11 | 1:B:385:ILE:HG21 | 1.81                     | 0.62              |
| 1:D:114:ARG:HH21 | 1:D:115:ILE:HD11 | 1.65                     | 0.62              |
| 1:D:116:LEU:HD11 | 1:D:204:ALA:HB3  | 1.80                     | 0.62              |
| 1:E:127:PHE:CE2  | 1:E:351:LEU:HG   | 2.35                     | 0.62              |
| 1:B:338:ASP:HB2  | 1:B:339:PRO:HD2  | 1.82                     | 0.62              |
| 1:E:311:TRP:CZ2  | 1:E:367:PRO:HG3  | 2.35                     | 0.62              |
| 1:F:83:THR:HG21  | 1:F:89:VAL:HB    | 1.81                     | 0.62              |
| 1:D:68:MET:CE    | 1:D:104:PHE:HB2  | 2.30                     | 0.62              |
| 1:F:236:LEU:HB2  | 1:F:239:VAL:CG2  | 2.30                     | 0.62              |
| 1:A:314:GLN:HE21 | 1:B:64:GLU:HB2   | 1.66                     | 0.61              |
| 1:A:160:ALA:HB2  | 1:A:188:HIS:CD2  | 2.35                     | 0.61              |
| 1:F:342:ASN:HD22 | 1:F:342:ASN:C    | 2.03                     | 0.61              |
| 1:E:115:ILE:HG22 | 1:E:351:LEU:HD13 | 1.82                     | 0.61              |
| 1:F:175:GLU:HG3  | 1:F:221:ILE:CD1  | 2.31                     | 0.61              |
| 1:A:300:VAL:HG13 | 1:A:301:PRO:HD2  | 1.82                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:127:PHE:HE2  | 1:B:347:LEU:HD12 | 1.66                     | 0.60              |
| 1:D:231:PHE:HB3  | 1:D:339:PRO:HB2  | 1.82                     | 0.60              |
| 1:E:311:TRP:CB   | 1:E:320:ILE:HB   | 2.31                     | 0.60              |
| 1:F:58:GLU:O     | 1:F:61:VAL:HG22  | 2.00                     | 0.60              |
| 1:D:383:ASN:HB2  | 1:D:385:ILE:HG13 | 1.83                     | 0.60              |
| 1:A:281:HIS:CD2  | 1:A:402:ASN:HD21 | 2.18                     | 0.60              |
| 1:E:234:LYS:HD3  | 1:E:298:ARG:HA   | 1.82                     | 0.60              |
| 1:D:58:GLU:O     | 1:D:61:VAL:HG22  | 2.00                     | 0.60              |
| 1:D:160:ALA:HB2  | 1:D:188:HIS:CD2  | 2.36                     | 0.60              |
| 1:F:201:TYR:CE2  | 1:F:331:ARG:HD2  | 2.35                     | 0.60              |
| 1:A:208:CYS:SG   | 1:A:347:LEU:HD23 | 2.42                     | 0.60              |
| 1:A:11:LYS:O     | 1:A:15:GLU:HB2   | 2.02                     | 0.60              |
| 1:A:281:HIS:HD2  | 1:A:402:ASN:HD21 | 1.50                     | 0.60              |
| 1:E:205:VAL:HG12 | 4:E:618:HOH:O    | 2.00                     | 0.60              |
| 1:E:59:GLY:O     | 1:E:62:ARG:HG3   | 2.02                     | 0.59              |
| 1:A:182:GLU:HB3  | 1:A:200:LYS:HD2  | 1.84                     | 0.59              |
| 1:B:129:LEU:HD13 | 1:B:131:PRO:HD3  | 1.84                     | 0.59              |
| 1:E:96:ILE:N     | 1:E:96:ILE:HD12  | 2.17                     | 0.59              |
| 1:D:370:ARG:HG2  | 1:D:371:ASN:N    | 2.18                     | 0.59              |
| 1:E:200:LYS:HE2  | 1:E:201:TYR:HD2  | 1.65                     | 0.59              |
| 1:A:252:LYS:O    | 1:A:253:ASN:HB2  | 2.02                     | 0.59              |
| 1:C:402:ASN:O    | 1:C:406:VAL:HG23 | 2.01                     | 0.59              |
| 1:D:423:ILE:HD13 | 4:D:662:HOH:O    | 2.01                     | 0.59              |
| 1:E:57:ILE:CD1   | 1:E:96:ILE:HG12  | 2.31                     | 0.59              |
| 1:F:176:LEU:O    | 1:F:181:PHE:HB2  | 2.03                     | 0.59              |
| 1:D:260:ASP:OD1  | 1:D:263:ALA:HB2  | 2.03                     | 0.59              |
| 1:C:56:SER:HA    | 1:C:62:ARG:HD2   | 1.85                     | 0.59              |
| 1:D:256:ASN:HD21 | 1:D:258:PHE:HB2  | 1.68                     | 0.59              |
| 1:E:129:LEU:HD13 | 1:E:131:PRO:HD3  | 1.85                     | 0.59              |
| 1:E:200:LYS:HG2  | 1:E:201:TYR:H    | 1.67                     | 0.59              |
| 1:A:160:ALA:HB2  | 1:A:188:HIS:HB2  | 1.85                     | 0.58              |
| 1:D:308:TYR:HA   | 1:D:387:ASP:HA   | 1.85                     | 0.58              |
| 1:C:248:LEU:O    | 1:C:331:ARG:HB2  | 2.03                     | 0.58              |
| 1:D:116:LEU:HD23 | 1:D:351:LEU:CD1  | 2.33                     | 0.58              |
| 1:F:206:ARG:HG3  | 1:F:206:ARG:HH11 | 1.67                     | 0.58              |
| 1:C:291:PRO:HG3  | 1:C:341:ALA:HA   | 1.84                     | 0.58              |
| 1:D:256:ASN:ND2  | 1:D:258:PHE:H    | 1.98                     | 0.58              |
| 1:F:311:TRP:CB   | 1:F:320:ILE:HB   | 2.33                     | 0.58              |
| 1:E:160:ALA:HB2  | 1:E:188:HIS:HD2  | 1.68                     | 0.58              |
| 1:A:74:LEU:N     | 1:A:74:LEU:HD22  | 2.13                     | 0.58              |
| 1:C:152:ASP:HB2  | 4:C:649:HOH:O    | 2.02                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:175:GLU:HG3  | 1:F:221:ILE:HD13 | 1.86                     | 0.58              |
| 1:F:22:ARG:HH11  | 1:F:22:ARG:HG2   | 1.67                     | 0.58              |
| 1:F:265:LEU:O    | 1:F:326:ARG:NH1  | 2.36                     | 0.58              |
| 1:C:176:LEU:O    | 1:C:181:PHE:HB2  | 2.03                     | 0.58              |
| 1:A:129:LEU:HD23 | 1:A:248:LEU:HD23 | 1.85                     | 0.58              |
| 1:A:169:ARG:NH2  | 1:A:195:HIS:ND1  | 2.50                     | 0.57              |
| 1:B:261:GLU:HG3  | 1:B:266:GLN:HE21 | 1.69                     | 0.57              |
| 1:C:308:TYR:HD2  | 1:C:387:ASP:HB3  | 1.69                     | 0.57              |
| 1:F:182:GLU:CB   | 1:F:200:LYS:HD3  | 2.34                     | 0.57              |
| 1:B:223:ARG:NH1  | 1:B:223:ARG:HG3  | 2.19                     | 0.57              |
| 1:A:129:LEU:CD1  | 1:A:131:PRO:HG3  | 2.34                     | 0.57              |
| 1:E:55:SER:O     | 1:E:62:ARG:HG2   | 2.04                     | 0.57              |
| 1:F:56:SER:HA    | 1:F:62:ARG:HD2   | 1.86                     | 0.57              |
| 1:A:13:VAL:HG13  | 1:A:18:VAL:HB    | 1.86                     | 0.57              |
| 1:B:371:ASN:HD22 | 1:B:372:ILE:N    | 2.03                     | 0.57              |
| 1:A:205:VAL:HG23 | 4:A:603:HOH:O    | 2.05                     | 0.57              |
| 1:E:3:LYS:H      | 1:E:75:ASN:ND2   | 2.02                     | 0.57              |
| 1:F:78:VAL:HG12  | 1:F:79:ILE:N     | 2.20                     | 0.57              |
| 1:E:311:TRP:HB3  | 1:E:320:ILE:HB   | 1.86                     | 0.57              |
| 1:E:68:MET:HE1   | 1:E:104:PHE:HB2  | 1.87                     | 0.57              |
| 1:F:160:ALA:HB2  | 1:F:188:HIS:CD2  | 2.40                     | 0.57              |
| 1:B:280:LYS:HD2  | 1:B:362:LEU:HD21 | 1.87                     | 0.57              |
| 1:A:58:GLU:O     | 1:A:61:VAL:HG22  | 2.05                     | 0.56              |
| 1:B:115:ILE:HG22 | 1:B:351:LEU:HD13 | 1.87                     | 0.56              |
| 1:B:50:VAL:HB    | 4:B:633:HOH:O    | 2.05                     | 0.56              |
| 1:D:311:TRP:HB3  | 1:D:320:ILE:HB   | 1.87                     | 0.56              |
| 1:E:345:LEU:HD22 | 1:E:409:LEU:HD22 | 1.87                     | 0.56              |
| 1:C:310:ALA:HB1  | 1:C:368:ILE:HD13 | 1.86                     | 0.56              |
| 1:D:163:ASP:HB2  | 1:E:82:TRP:HE1   | 1.70                     | 0.56              |
| 1:F:380:ARG:O    | 1:F:385:ILE:HB   | 2.05                     | 0.56              |
| 1:F:58:GLU:HG2   | 1:F:416:HIS:CD2  | 2.41                     | 0.56              |
| 1:D:176:LEU:O    | 1:D:181:PHE:HB2  | 2.05                     | 0.56              |
| 1:D:256:ASN:HB2  | 1:D:328:ILE:HA   | 1.88                     | 0.56              |
| 1:C:127:PHE:HE2  | 1:C:347:LEU:HD12 | 1.70                     | 0.56              |
| 1:C:129:LEU:HG   | 1:C:347:LEU:HD21 | 1.85                     | 0.56              |
| 1:C:419:GLU:O    | 1:C:423:ILE:HG12 | 2.06                     | 0.56              |
| 1:C:55:SER:O     | 1:C:62:ARG:HG2   | 2.06                     | 0.56              |
| 1:B:319:LEU:CD1  | 1:B:336:SER:HB3  | 2.36                     | 0.56              |
| 1:B:35:VAL:O     | 1:B:35:VAL:HG13  | 2.06                     | 0.56              |
| 1:C:28:ILE:HD12  | 1:C:413:LEU:HD23 | 1.88                     | 0.56              |
| 1:E:74:LEU:N     | 1:E:74:LEU:HD22  | 2.21                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:371:ASN:ND2  | 1:B:373:TYR:H    | 2.03                     | 0.56              |
| 1:E:142:GLU:H    | 1:E:142:GLU:CD   | 2.10                     | 0.56              |
| 1:D:160:ALA:CB   | 1:D:188:HIS:CD2  | 2.89                     | 0.56              |
| 1:C:111:ASN:O    | 1:C:115:ILE:HG12 | 2.06                     | 0.56              |
| 1:C:252:LYS:HG2  | 1:C:253:ASN:ND2  | 2.20                     | 0.56              |
| 1:C:329:SER:O    | 1:C:331:ARG:HD3  | 2.06                     | 0.56              |
| 1:D:170:ARG:NH1  | 1:D:171:ASP:OD2  | 2.39                     | 0.56              |
| 1:C:156:TYR:HB2  | 1:C:190:VAL:HA   | 1.88                     | 0.55              |
| 1:E:160:ALA:HB3  | 1:E:169:ARG:NH1  | 2.22                     | 0.55              |
| 1:F:20:TYR:HB3   | 1:F:89:VAL:HG22  | 1.88                     | 0.55              |
| 1:A:265:LEU:O    | 1:A:326:ARG:NH1  | 2.39                     | 0.55              |
| 1:B:116:LEU:HD11 | 1:B:204:ALA:HB3  | 1.87                     | 0.55              |
| 1:B:76:THR:O     | 1:B:78:VAL:HG23  | 2.05                     | 0.55              |
| 1:E:205:VAL:HG13 | 1:E:206:ARG:N    | 2.22                     | 0.55              |
| 1:E:311:TRP:CH2  | 1:E:367:PRO:HG3  | 2.41                     | 0.55              |
| 1:E:58:GLU:O     | 1:E:61:VAL:HG22  | 2.07                     | 0.55              |
| 1:D:6:ARG:HG2    | 1:D:46:LEU:HD13  | 1.88                     | 0.55              |
| 1:F:419:GLU:O    | 1:F:423:ILE:HG23 | 2.06                     | 0.55              |
| 1:B:314:GLN:HE22 | 1:C:66:SER:HB2   | 1.71                     | 0.55              |
| 1:D:160:ALA:CB   | 1:D:161:PRO:HD2  | 2.19                     | 0.55              |
| 1:E:402:ASN:OD1  | 1:E:404:VAL:HG12 | 2.07                     | 0.55              |
| 1:F:160:ALA:HB3  | 1:F:169:ARG:NH2  | 2.22                     | 0.55              |
| 1:B:4:TYR:HB3    | 1:B:9:ILE:CD1    | 2.37                     | 0.55              |
| 1:C:91:ARG:C     | 1:C:91:ARG:HD2   | 2.27                     | 0.55              |
| 1:B:147:THR:HG22 | 1:B:148:LEU:N    | 2.21                     | 0.55              |
| 1:C:115:ILE:HG13 | 1:C:348:SER:HB3  | 1.88                     | 0.55              |
| 1:C:311:TRP:CB   | 1:C:320:ILE:HB   | 2.37                     | 0.55              |
| 1:E:252:LYS:O    | 1:E:255:VAL:HG22 | 2.07                     | 0.55              |
| 1:F:172:ILE:HD12 | 1:F:218:VAL:HA   | 1.87                     | 0.55              |
| 1:F:270:THR:HG23 | 1:F:358:ILE:HD12 | 1.88                     | 0.55              |
| 1:A:202:ALA:HB1  | 1:A:206:ARG:HG2  | 1.89                     | 0.55              |
| 1:A:370:ARG:HG2  | 1:A:371:ASN:N    | 2.14                     | 0.55              |
| 1:C:300:VAL:HG13 | 1:C:301:PRO:HD2  | 1.88                     | 0.55              |
| 1:B:434:PRO:O    | 1:B:438:GLU:HG3  | 2.07                     | 0.55              |
| 1:D:150:LEU:HD13 | 1:D:192:PRO:HB2  | 1.89                     | 0.55              |
| 1:C:318:PRO:O    | 1:C:335:ARG:HD3  | 2.07                     | 0.55              |
| 1:F:167:ASN:HD22 | 1:F:170:ARG:H    | 1.53                     | 0.55              |
| 1:B:169:ARG:NH1  | 1:C:36:GLU:OE1   | 2.40                     | 0.54              |
| 1:C:431:GLN:HG3  | 4:C:646:HOH:O    | 2.06                     | 0.54              |
| 1:E:5:THR:H      | 1:E:8:ASP:HB2    | 1.71                     | 0.54              |
| 1:E:68:MET:HE2   | 1:E:96:ILE:HG22  | 1.89                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:401:SER:HB2  | 4:B:687:HOH:O    | 2.07                     | 0.54              |
| 1:E:116:LEU:O    | 1:E:119:MET:HB3  | 2.07                     | 0.54              |
| 1:E:164:LEU:HD13 | 1:F:224:LYS:HB2  | 1.89                     | 0.54              |
| 1:F:91:ARG:HD2   | 1:F:92:PHE:N     | 2.22                     | 0.54              |
| 1:B:282:ALA:HA   | 1:B:285:PHE:CZ   | 2.42                     | 0.54              |
| 1:D:68:MET:HE1   | 1:D:104:PHE:HB2  | 1.88                     | 0.54              |
| 1:F:140:LEU:HD21 | 1:F:228:HIS:HB2  | 1.89                     | 0.54              |
| 1:F:236:LEU:HB2  | 1:F:239:VAL:HG21 | 1.89                     | 0.54              |
| 1:B:119:MET:HB2  | 1:B:355:LEU:HD11 | 1.90                     | 0.54              |
| 1:E:160:ALA:HB2  | 1:E:188:HIS:CD2  | 2.43                     | 0.54              |
| 1:F:371:ASN:ND2  | 1:F:374:VAL:HG13 | 2.23                     | 0.54              |
| 1:F:91:ARG:HD2   | 1:F:91:ARG:C     | 2.27                     | 0.54              |
| 1:E:319:LEU:CD1  | 1:E:336:SER:HB3  | 2.37                     | 0.54              |
| 1:D:163:ASP:HB3  | 1:E:83:THR:HG22  | 1.90                     | 0.54              |
| 1:E:16:GLU:O     | 1:E:88:LYS:HD2   | 2.07                     | 0.54              |
| 1:F:264:ASP:O    | 1:F:265:LEU:HB2  | 2.06                     | 0.54              |
| 1:A:69:TYR:CE1   | 1:A:99:PRO:HA    | 2.43                     | 0.54              |
| 1:B:285:PHE:HB2  | 1:B:349:VAL:HG11 | 1.89                     | 0.54              |
| 1:B:96:ILE:HD12  | 1:B:96:ILE:N     | 2.22                     | 0.54              |
| 1:C:376:SER:HB3  | 1:C:379:GLU:HG3  | 1.90                     | 0.54              |
| 1:E:383:ASN:HB2  | 1:E:385:ILE:HG12 | 1.90                     | 0.54              |
| 1:C:377:LYS:HD2  | 1:C:380:ARG:HH12 | 1.73                     | 0.54              |
| 1:B:122:LEU:HD11 | 1:B:359:LYS:HG3  | 1.89                     | 0.53              |
| 1:F:32:ILE:HD13  | 4:F:652:HOH:O    | 2.07                     | 0.53              |
| 1:A:136:PHE:CE2  | 1:A:194:GLN:HB2  | 2.43                     | 0.53              |
| 1:C:298:ARG:NH1  | 3:C:501:GLN:O    | 2.40                     | 0.53              |
| 1:E:300:VAL:HG13 | 1:E:301:PRO:HD2  | 1.90                     | 0.53              |
| 1:A:166:GLU:HB3  | 4:A:670:HOH:O    | 2.08                     | 0.53              |
| 1:D:300:VAL:HG13 | 1:D:301:PRO:HD2  | 1.91                     | 0.53              |
| 1:D:278:ILE:CG2  | 1:D:320:ILE:HD11 | 2.38                     | 0.53              |
| 1:F:281:HIS:HD2  | 1:F:402:ASN:HD21 | 1.56                     | 0.53              |
| 1:E:68:MET:CE    | 1:E:104:PHE:HB2  | 2.39                     | 0.53              |
| 1:F:262:ASN:ND2  | 1:F:262:ASN:H    | 2.06                     | 0.53              |
| 1:A:189:GLU:HB3  | 1:A:194:GLN:NE2  | 2.23                     | 0.53              |
| 1:D:61:VAL:O     | 1:D:63:ILE:HD12  | 2.08                     | 0.53              |
| 1:E:294:ASN:HA   | 1:E:297:LYS:HG2  | 1.89                     | 0.53              |
| 1:F:256:ASN:HB2  | 1:F:328:ILE:HA   | 1.89                     | 0.53              |
| 1:A:26:THR:HG22  | 1:A:27:ASP:O     | 2.09                     | 0.53              |
| 1:F:20:TYR:OH    | 1:F:36:GLU:HG3   | 2.08                     | 0.53              |
| 1:B:23:LEU:HD13  | 1:B:70:LEU:HD23  | 1.91                     | 0.53              |
| 1:E:160:ALA:O    | 1:E:161:PRO:C    | 2.46                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:357:GLY:HA2  | 1:A:362:LEU:HD22 | 1.91                     | 0.53              |
| 1:A:378:GLU:O    | 1:A:382:GLU:HG2  | 2.09                     | 0.53              |
| 1:F:16:GLU:HG2   | 1:F:79:ILE:HD12  | 1.91                     | 0.53              |
| 1:D:223:ARG:HG2  | 1:D:223:ARG:HH11 | 1.74                     | 0.52              |
| 1:B:160:ALA:HB3  | 1:B:169:ARG:HH22 | 1.73                     | 0.52              |
| 1:B:281:HIS:CD2  | 1:B:402:ASN:HD21 | 2.27                     | 0.52              |
| 1:B:402:ASN:O    | 1:B:406:VAL:HG23 | 2.09                     | 0.52              |
| 1:E:74:LEU:H     | 1:E:74:LEU:CD2   | 2.23                     | 0.52              |
| 1:B:223:ARG:HH11 | 1:B:223:ARG:HG3  | 1.73                     | 0.52              |
| 1:A:160:ALA:CB   | 1:A:161:PRO:HD2  | 2.28                     | 0.52              |
| 1:C:282:ALA:HA   | 1:C:285:PHE:CZ   | 2.45                     | 0.52              |
| 1:A:319:LEU:CD1  | 1:A:336:SER:HB3  | 2.40                     | 0.52              |
| 1:B:129:LEU:HD23 | 1:B:248:LEU:HD23 | 1.91                     | 0.52              |
| 1:E:119:MET:HG2  | 1:E:124:PHE:HB2  | 1.92                     | 0.52              |
| 1:F:231:PHE:O    | 1:F:339:PRO:HG2  | 2.08                     | 0.52              |
| 1:B:122:LEU:HD21 | 1:B:359:LYS:HG2  | 1.91                     | 0.52              |
| 1:D:176:LEU:HD13 | 1:D:183:ILE:HD11 | 1.90                     | 0.52              |
| 1:E:169:ARG:HE   | 1:E:195:HIS:HD2  | 1.57                     | 0.52              |
| 1:B:380:ARG:HG2  | 1:B:380:ARG:HH11 | 1.73                     | 0.52              |
| 1:D:170:ARG:HH11 | 1:D:170:ARG:HG2  | 1.75                     | 0.52              |
| 1:E:321:ARG:HD2  | 4:E:630:HOH:O    | 2.09                     | 0.52              |
| 1:B:28:ILE:HD12  | 1:B:413:LEU:HD23 | 1.90                     | 0.52              |
| 1:B:419:GLU:O    | 1:B:423:ILE:HD12 | 2.09                     | 0.52              |
| 1:F:168:CYS:O    | 1:F:172:ILE:HG12 | 2.10                     | 0.52              |
| 1:F:183:ILE:HG23 | 1:F:198:ASP:O    | 2.10                     | 0.52              |
| 1:A:86:LYS:HD3   | 4:A:669:HOH:O    | 2.10                     | 0.52              |
| 1:B:9:ILE:HD11   | 1:B:74:LEU:HB3   | 1.91                     | 0.52              |
| 1:C:59:GLY:O     | 1:C:62:ARG:HG3   | 2.09                     | 0.52              |
| 1:C:351:LEU:HD22 | 1:C:355:LEU:HG   | 1.92                     | 0.51              |
| 1:D:19:LYS:HG3   | 1:D:86:LYS:O     | 2.10                     | 0.51              |
| 1:A:322:ILE:N    | 1:A:322:ILE:HD12 | 2.25                     | 0.51              |
| 1:C:169:ARG:HH11 | 1:D:36:GLU:CD    | 2.14                     | 0.51              |
| 1:F:77:PHE:HB2   | 1:F:92:PHE:CE2   | 2.46                     | 0.51              |
| 1:A:69:TYR:HE1   | 1:A:99:PRO:HA    | 1.74                     | 0.51              |
| 1:B:9:ILE:CD1    | 1:B:74:LEU:HB3   | 2.40                     | 0.51              |
| 1:D:159:LEU:HD11 | 1:E:22:ARG:HD3   | 1.92                     | 0.51              |
| 1:D:278:ILE:HG22 | 1:D:320:ILE:HD11 | 1.91                     | 0.51              |
| 1:F:136:PHE:CD1  | 1:F:235:PRO:HG2  | 2.45                     | 0.51              |
| 1:C:199:PHE:CD2  | 1:C:199:PHE:N    | 2.77                     | 0.51              |
| 1:C:28:ILE:HG12  | 1:C:57:ILE:O     | 2.09                     | 0.51              |
| 1:D:202:ALA:HB1  | 1:D:206:ARG:HD3  | 1.93                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:345:LEU:HD22 | 1:D:409:LEU:HD22 | 1.92                     | 0.51              |
| 1:F:167:ASN:ND2  | 1:F:170:ARG:H    | 2.08                     | 0.51              |
| 1:F:360:ASN:HB2  | 1:F:362:LEU:CD1  | 2.41                     | 0.51              |
| 1:A:58:GLU:HG2   | 1:A:416:HIS:CD2  | 2.45                     | 0.51              |
| 3:A:503:GLN:N    | 4:A:609:HOH:O    | 2.42                     | 0.51              |
| 1:C:22:ARG:HH11  | 1:C:34:ASN:HD21  | 1.57                     | 0.51              |
| 1:E:91:ARG:HD2   | 1:E:92:PHE:N     | 2.25                     | 0.51              |
| 1:F:231:PHE:HB3  | 1:F:339:PRO:HB2  | 1.92                     | 0.51              |
| 1:B:119:MET:HG2  | 1:B:124:PHE:HB2  | 1.92                     | 0.51              |
| 1:E:200:LYS:HG2  | 1:E:201:TYR:N    | 2.26                     | 0.51              |
| 1:E:24:GLN:OE1   | 1:E:91:ARG:HD3   | 2.11                     | 0.51              |
| 1:A:111:ASN:O    | 1:A:115:ILE:HG12 | 2.10                     | 0.51              |
| 1:D:9:ILE:HG21   | 1:D:92:PHE:HZ    | 1.76                     | 0.51              |
| 1:E:208:CYS:SG   | 1:E:347:LEU:HD12 | 2.50                     | 0.51              |
| 1:E:282:ALA:HA   | 1:E:285:PHE:CZ   | 2.45                     | 0.51              |
| 1:F:21:ILE:HD12  | 1:F:39:VAL:HA    | 1.93                     | 0.51              |
| 1:F:285:PHE:HB3  | 1:F:405:MET:SD   | 2.51                     | 0.51              |
| 1:F:418:ILE:O    | 1:F:422:GLU:HB2  | 2.11                     | 0.51              |
| 1:B:231:PHE:HB3  | 1:B:339:PRO:HB2  | 1.92                     | 0.51              |
| 1:A:36:GLU:HG2   | 1:F:186:SER:O    | 2.11                     | 0.51              |
| 1:C:166:GLU:HG3  | 1:C:225:HIS:HD1  | 1.75                     | 0.50              |
| 1:C:134:GLU:OE1  | 3:C:501:GLN:N    | 2.43                     | 0.50              |
| 1:D:137:LEU:HD23 | 1:D:229:ALA:HA   | 1.93                     | 0.50              |
| 1:D:91:ARG:C     | 1:D:91:ARG:HD2   | 2.32                     | 0.50              |
| 1:A:3:LYS:HG2    | 1:A:3:LYS:O      | 2.10                     | 0.50              |
| 1:C:208:CYS:SG   | 1:C:343:PRO:C    | 2.90                     | 0.50              |
| 1:C:65:GLU:O     | 1:C:65:GLU:HG3   | 2.10                     | 0.50              |
| 1:D:232:MET:HB3  | 1:D:235:PRO:HG3  | 1.92                     | 0.50              |
| 1:F:133:PRO:HD2  | 1:F:197:ILE:O    | 2.10                     | 0.50              |
| 1:D:200:LYS:HE3  | 1:E:41:GLN:OE1   | 2.11                     | 0.50              |
| 1:E:351:LEU:HD22 | 1:E:355:LEU:HG   | 1.93                     | 0.50              |
| 1:F:384:GLY:O    | 1:F:385:ILE:HD13 | 2.11                     | 0.50              |
| 1:F:425:TRP:HE1  | 1:F:429:ARG:HD3  | 1.77                     | 0.50              |
| 1:C:380:ARG:HB3  | 1:C:385:ILE:HB   | 1.93                     | 0.50              |
| 1:D:59:GLY:O     | 1:D:62:ARG:HG3   | 2.12                     | 0.50              |
| 1:E:375:MET:HG3  | 1:E:375:MET:O    | 2.12                     | 0.50              |
| 1:C:22:ARG:HB3   | 1:C:34:ASN:HD22  | 1.77                     | 0.50              |
| 1:E:372:ILE:HD13 | 1:E:375:MET:HE3  | 1.94                     | 0.50              |
| 1:F:409:LEU:O    | 1:F:413:LEU:HB2  | 2.11                     | 0.50              |
| 1:F:85:GLU:N     | 1:F:85:GLU:CD    | 2.65                     | 0.50              |
| 1:B:290:ASN:HB3  | 1:B:295:SER:HB3  | 1.94                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:58:GLU:O     | 1:C:61:VAL:HG22  | 2.10                     | 0.50              |
| 1:F:31:THR:HG23  | 4:F:630:HOH:O    | 2.12                     | 0.50              |
| 1:A:275:ILE:O    | 1:A:279:VAL:HG23 | 2.12                     | 0.50              |
| 1:B:182:GLU:HB3  | 1:B:200:LYS:CD   | 2.42                     | 0.50              |
| 1:C:278:ILE:O    | 1:C:282:ALA:HB2  | 2.11                     | 0.50              |
| 1:D:260:ASP:CG   | 1:D:263:ALA:HB2  | 2.32                     | 0.50              |
| 1:B:100:ASP:OD1  | 1:B:102:THR:HG23 | 2.11                     | 0.49              |
| 1:B:77:PHE:HB2   | 1:B:92:PHE:CE2   | 2.47                     | 0.49              |
| 1:C:156:TYR:O    | 1:C:157:PHE:HB2  | 2.12                     | 0.49              |
| 1:C:217:VAL:O    | 1:C:221:ILE:HG12 | 2.11                     | 0.49              |
| 1:D:380:ARG:O    | 1:D:385:ILE:HB   | 2.12                     | 0.49              |
| 1:B:21:ILE:HD13  | 1:B:42:LEU:HD13  | 1.94                     | 0.49              |
| 1:C:306:PRO:HG2  | 1:C:335:ARG:C    | 2.33                     | 0.49              |
| 1:E:285:PHE:HB3  | 1:E:405:MET:SD   | 2.51                     | 0.49              |
| 1:D:152:ASP:HB2  | 4:D:701:HOH:O    | 2.11                     | 0.49              |
| 1:F:318:PRO:O    | 1:F:335:ARG:HD3  | 2.11                     | 0.49              |
| 1:A:248:LEU:O    | 1:A:331:ARG:HB2  | 2.12                     | 0.49              |
| 1:A:53:ASP:CG    | 1:A:55:SER:HG    | 2.16                     | 0.49              |
| 1:B:168:CYS:SG   | 1:B:222:ALA:HA   | 2.52                     | 0.49              |
| 1:B:429:ARG:HD3  | 1:B:430:THR:HG23 | 1.93                     | 0.49              |
| 1:C:169:ARG:HH22 | 1:C:188:HIS:HB2  | 1.76                     | 0.49              |
| 1:A:21:ILE:HD13  | 1:A:42:LEU:HD13  | 1.94                     | 0.49              |
| 1:B:351:LEU:HD22 | 1:B:355:LEU:HG   | 1.94                     | 0.49              |
| 1:D:383:ASN:C    | 1:D:385:ILE:H    | 2.14                     | 0.49              |
| 1:E:158:ASP:OD1  | 1:F:33:LYS:HE3   | 2.13                     | 0.49              |
| 1:A:27:ASP:HB3   | 1:A:33:LYS:HE3   | 1.93                     | 0.49              |
| 1:C:311:TRP:HB3  | 1:C:320:ILE:HB   | 1.94                     | 0.49              |
| 1:D:331:ARG:HH21 | 1:D:331:ARG:HG2  | 1.76                     | 0.49              |
| 1:F:206:ARG:NH1  | 1:F:206:ARG:HG3  | 2.28                     | 0.49              |
| 1:F:24:GLN:HB2   | 1:F:32:ILE:HD11  | 1.94                     | 0.49              |
| 1:B:160:ALA:O    | 1:B:161:PRO:C    | 2.51                     | 0.49              |
| 1:D:131:PRO:HG2  | 1:D:199:PHE:HD1  | 1.77                     | 0.49              |
| 1:F:116:LEU:HD23 | 1:F:351:LEU:HD11 | 1.94                     | 0.49              |
| 1:B:160:ALA:HB3  | 1:B:169:ARG:HH12 | 1.77                     | 0.49              |
| 1:E:433:HIS:HB3  | 4:E:640:HOH:O    | 2.12                     | 0.49              |
| 1:D:249:SER:HA   | 1:D:258:PHE:CE1  | 2.47                     | 0.49              |
| 1:F:22:ARG:NH1   | 1:F:22:ARG:HG2   | 2.28                     | 0.49              |
| 1:F:423:ILE:C    | 1:F:423:ILE:HD12 | 2.33                     | 0.49              |
| 1:A:231:PHE:HB3  | 1:A:339:PRO:HB2  | 1.94                     | 0.49              |
| 1:C:264:ASP:O    | 1:C:265:LEU:HB2  | 2.13                     | 0.49              |
| 1:C:234:LYS:HD3  | 1:C:298:ARG:HA   | 1.95                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:260:ASP:O    | 1:B:266:GLN:HA   | 2.13                     | 0.48              |
| 1:C:357:GLY:HA2  | 1:C:362:LEU:HD12 | 1.95                     | 0.48              |
| 1:C:441:MET:O    | 1:C:441:MET:HG3  | 2.12                     | 0.48              |
| 1:E:21:ILE:HD13  | 1:E:42:LEU:HD13  | 1.94                     | 0.48              |
| 1:B:260:ASP:HB2  | 1:B:268:SER:HB3  | 1.95                     | 0.48              |
| 1:E:405:MET:O    | 1:E:408:ALA:HB3  | 2.13                     | 0.48              |
| 1:F:236:LEU:HB2  | 1:F:239:VAL:HG22 | 1.94                     | 0.48              |
| 1:F:3:LYS:HB3    | 1:F:75:ASN:OD1   | 2.13                     | 0.48              |
| 1:D:314:GLN:O    | 1:D:314:GLN:HG3  | 2.11                     | 0.48              |
| 4:E:704:HOH:O    | 1:F:223:ARG:HD3  | 2.14                     | 0.48              |
| 1:A:27:ASP:HB3   | 1:A:33:LYS:CE    | 2.43                     | 0.48              |
| 1:B:272:LYS:O    | 1:B:364:ALA:HB2  | 2.13                     | 0.48              |
| 1:C:377:LYS:HD2  | 1:C:380:ARG:NH1  | 2.28                     | 0.48              |
| 1:F:169:ARG:NH2  | 1:F:188:HIS:HB2  | 2.29                     | 0.48              |
| 1:A:122:LEU:CD1  | 1:A:355:LEU:HD22 | 2.44                     | 0.48              |
| 1:D:116:LEU:O    | 1:D:119:MET:HB3  | 2.13                     | 0.48              |
| 1:E:23:LEU:HB2   | 1:E:35:VAL:HG13  | 1.94                     | 0.48              |
| 1:F:279:VAL:HG13 | 1:F:309:VAL:HG12 | 1.96                     | 0.48              |
| 1:D:27:ASP:C     | 1:D:27:ASP:OD2   | 2.50                     | 0.48              |
| 1:B:264:ASP:OD2  | 1:B:265:LEU:HD13 | 2.13                     | 0.48              |
| 1:A:114:ARG:NH2  | 1:A:115:ILE:HD11 | 2.28                     | 0.48              |
| 1:A:14:LYS:HE2   | 4:A:676:HOH:O    | 2.14                     | 0.48              |
| 1:B:137:LEU:HD23 | 1:B:229:ALA:HA   | 1.95                     | 0.48              |
| 1:B:16:GLU:HG2   | 1:B:79:ILE:HD13  | 1.96                     | 0.48              |
| 1:C:392:LEU:O    | 1:C:396:LEU:HG   | 2.13                     | 0.48              |
| 1:D:317:SER:HB2  | 1:D:335:ARG:HH22 | 1.79                     | 0.48              |
| 1:E:223:ARG:HG3  | 1:E:223:ARG:NH1  | 2.28                     | 0.48              |
| 1:E:396:LEU:O    | 1:E:400:LYS:HG3  | 2.14                     | 0.48              |
| 1:E:76:THR:O     | 1:E:78:VAL:HG23  | 2.13                     | 0.48              |
| 1:F:58:GLU:HB3   | 1:F:61:VAL:HG23  | 1.96                     | 0.48              |
| 1:F:20:TYR:CZ    | 1:F:36:GLU:HB2   | 2.49                     | 0.48              |
| 1:D:379:GLU:HA   | 1:D:382:GLU:OE1  | 2.14                     | 0.48              |
| 1:A:359:LYS:NZ   | 1:A:359:LYS:HB2  | 2.28                     | 0.47              |
| 1:B:202:ALA:HB1  | 1:B:206:ARG:HD3  | 1.96                     | 0.47              |
| 1:B:259:PHE:CD1  | 1:B:326:ARG:HG3  | 2.49                     | 0.47              |
| 1:C:129:LEU:HD23 | 1:C:248:LEU:HD23 | 1.95                     | 0.47              |
| 1:C:169:ARG:NH2  | 1:C:188:HIS:HB2  | 2.29                     | 0.47              |
| 1:C:96:ILE:N     | 1:C:96:ILE:HD12  | 2.29                     | 0.47              |
| 1:E:157:PHE:O    | 1:F:33:LYS:HB3   | 2.14                     | 0.47              |
| 1:C:49:LYS:HE3   | 4:C:610:HOH:O    | 2.13                     | 0.47              |
| 1:D:274:PHE:CD2  | 1:D:332:VAL:HG11 | 2.49                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:164:LEU:HB2  | 1:F:220:THR:CG2  | 2.44                     | 0.47              |
| 1:E:435:TRP:O    | 1:E:439:GLN:HG2  | 2.14                     | 0.47              |
| 1:E:91:ARG:HH12  | 1:E:213:THR:CG2  | 2.27                     | 0.47              |
| 1:F:85:GLU:H     | 1:F:85:GLU:CD    | 2.18                     | 0.47              |
| 1:C:434:PRO:O    | 1:C:438:GLU:HG3  | 2.14                     | 0.47              |
| 1:E:370:ARG:HD3  | 1:E:375:MET:HE1  | 1.95                     | 0.47              |
| 1:A:23:LEU:HB3   | 1:A:94:CYS:SG    | 2.54                     | 0.47              |
| 1:B:321:ARG:HH22 | 1:C:67:ASP:CG    | 2.17                     | 0.47              |
| 1:D:160:ALA:HB2  | 1:D:188:HIS:CG   | 2.50                     | 0.47              |
| 1:D:223:ARG:HG2  | 1:D:223:ARG:NH1  | 2.29                     | 0.47              |
| 1:D:68:MET:HE2   | 1:D:104:PHE:HB2  | 1.95                     | 0.47              |
| 1:A:164:LEU:C    | 1:A:166:GLU:H    | 2.16                     | 0.47              |
| 1:C:377:LYS:O    | 1:C:381:MET:HG2  | 2.15                     | 0.47              |
| 1:C:83:THR:HG21  | 1:C:89:VAL:HG23  | 1.97                     | 0.47              |
| 1:E:116:LEU:HD11 | 1:E:204:ALA:HB3  | 1.95                     | 0.47              |
| 1:F:241:GLY:HA3  | 1:F:298:ARG:HG2  | 1.96                     | 0.47              |
| 1:F:3:LYS:HE2    | 1:F:4:TYR:CE2    | 2.49                     | 0.47              |
| 1:A:162:THR:O    | 1:A:164:LEU:N    | 2.47                     | 0.47              |
| 1:A:160:ALA:CB   | 1:A:188:HIS:HD2  | 2.28                     | 0.47              |
| 1:B:38:PRO:HD2   | 1:B:41:GLN:HG3   | 1.95                     | 0.47              |
| 1:C:27:ASP:HB2   | 1:C:57:ILE:O     | 2.15                     | 0.47              |
| 1:E:418:ILE:HD12 | 1:E:418:ILE:N    | 2.30                     | 0.47              |
| 1:F:55:SER:O     | 1:F:62:ARG:HG2   | 2.15                     | 0.47              |
| 1:A:164:LEU:HD21 | 1:B:223:ARG:HG2  | 1.95                     | 0.47              |
| 1:B:309:VAL:HA   | 1:B:319:LEU:HD22 | 1.96                     | 0.47              |
| 1:A:140:LEU:HD22 | 1:A:144:GLY:O    | 2.14                     | 0.47              |
| 1:B:311:TRP:HB3  | 1:B:320:ILE:HB   | 1.95                     | 0.47              |
| 1:C:308:TYR:CD2  | 1:C:387:ASP:HB3  | 2.48                     | 0.47              |
| 1:F:32:ILE:HD12  | 1:F:33:LYS:N     | 2.30                     | 0.47              |
| 1:A:20:TYR:HB3   | 1:A:89:VAL:HG22  | 1.97                     | 0.47              |
| 1:B:429:ARG:CD   | 1:B:430:THR:HG23 | 2.45                     | 0.47              |
| 1:C:110:ASN:O    | 1:C:113:LYS:HB2  | 2.14                     | 0.47              |
| 1:C:177:GLU:C    | 1:C:179:MET:H    | 2.18                     | 0.47              |
| 1:D:120:GLU:C    | 1:D:122:LEU:H    | 2.17                     | 0.47              |
| 1:E:184:GLU:O    | 1:E:185:ALA:HB2  | 2.15                     | 0.47              |
| 1:E:290:ASN:HB3  | 1:E:295:SER:HB3  | 1.96                     | 0.47              |
| 1:F:160:ALA:O    | 1:F:161:PRO:O    | 2.33                     | 0.47              |
| 1:A:160:ALA:HB2  | 1:A:188:HIS:HD2  | 1.78                     | 0.46              |
| 1:A:169:ARG:HD3  | 1:A:195:HIS:HB3  | 1.97                     | 0.46              |
| 1:B:4:TYR:HB3    | 1:B:9:ILE:HD12   | 1.97                     | 0.46              |
| 1:F:285:PHE:CD1  | 1:F:285:PHE:C    | 2.87                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:233:PRO:HG2  | 1:A:295:SER:OG   | 2.15                     | 0.46              |
| 1:B:205:VAL:HG22 | 4:B:631:HOH:O    | 2.15                     | 0.46              |
| 1:C:33:LYS:O     | 1:C:34:ASN:HB3   | 2.15                     | 0.46              |
| 1:F:160:ALA:CB   | 1:F:188:HIS:CD2  | 2.98                     | 0.46              |
| 1:F:378:GLU:O    | 1:F:381:MET:HB2  | 2.15                     | 0.46              |
| 1:A:182:GLU:CB   | 1:A:200:LYS:HD2  | 2.45                     | 0.46              |
| 1:B:78:VAL:HG12  | 1:B:79:ILE:N     | 2.31                     | 0.46              |
| 1:C:6:ARG:HD2    | 1:C:46:LEU:HD13  | 1.97                     | 0.46              |
| 1:F:170:ARG:HG2  | 1:F:170:ARG:HH11 | 1.80                     | 0.46              |
| 1:B:52:PHE:CE2   | 1:B:54:GLY:HA2   | 2.51                     | 0.46              |
| 1:C:49:LYS:HE2   | 1:C:49:LYS:HA    | 1.97                     | 0.46              |
| 1:D:273:HIS:O    | 1:D:276:ALA:HB3  | 2.15                     | 0.46              |
| 1:E:377:LYS:HB2  | 4:E:682:HOH:O    | 2.15                     | 0.46              |
| 1:E:185:ALA:CB   | 1:F:37:ILE:HG22  | 2.44                     | 0.46              |
| 1:C:234:LYS:HE3  | 1:C:239:VAL:O    | 2.16                     | 0.46              |
| 1:A:96:ILE:N     | 1:A:96:ILE:HD12  | 2.30                     | 0.46              |
| 1:B:5:THR:HG23   | 1:B:8:ASP:H      | 1.80                     | 0.46              |
| 1:C:20:TYR:CZ    | 1:C:36:GLU:HG3   | 2.50                     | 0.46              |
| 1:E:322:ILE:HG22 | 1:E:326:ARG:HH21 | 1.80                     | 0.46              |
| 1:A:116:LEU:HD11 | 1:A:204:ALA:HB3  | 1.97                     | 0.46              |
| 1:B:116:LEU:HD23 | 1:B:351:LEU:HD11 | 1.98                     | 0.46              |
| 1:E:279:VAL:HG13 | 1:E:309:VAL:HG12 | 1.97                     | 0.46              |
| 1:E:370:ARG:HG2  | 1:E:370:ARG:HH11 | 1.81                     | 0.46              |
| 1:E:368:ILE:HD13 | 1:E:385:ILE:HD11 | 1.98                     | 0.46              |
| 1:F:379:GLU:HA   | 1:F:382:GLU:OE1  | 2.16                     | 0.46              |
| 1:A:318:PRO:O    | 1:A:335:ARG:HD3  | 2.15                     | 0.46              |
| 1:B:258:PHE:HA   | 1:B:271:ALA:HB2  | 1.96                     | 0.46              |
| 1:C:48:ASN:OD1   | 1:C:72:PRO:HD2   | 2.16                     | 0.46              |
| 1:D:91:ARG:HH12  | 1:D:213:THR:HG23 | 1.81                     | 0.46              |
| 1:E:78:VAL:HG12  | 1:E:79:ILE:N     | 2.31                     | 0.46              |
| 1:F:219:LYS:HA   | 1:F:229:ALA:HB3  | 1.98                     | 0.46              |
| 1:F:134:GLU:OE2  | 3:F:503:GLN:HG3  | 2.15                     | 0.46              |
| 1:A:291:PRO:HG3  | 1:A:341:ALA:HA   | 1.98                     | 0.46              |
| 1:B:170:ARG:HG3  | 1:C:20:TYR:CD2   | 2.51                     | 0.46              |
| 1:C:372:ILE:CG2  | 1:C:380:ARG:HD3  | 2.45                     | 0.46              |
| 1:D:97:TYR:HA    | 1:D:103:PRO:HA   | 1.97                     | 0.46              |
| 1:E:25:PHE:HE2   | 1:E:35:VAL:HG12  | 1.79                     | 0.46              |
| 1:E:371:ASN:HD21 | 1:E:374:VAL:HG23 | 1.80                     | 0.46              |
| 1:D:279:VAL:HG13 | 1:D:309:VAL:HG12 | 1.98                     | 0.46              |
| 1:D:139:LYS:HE2  | 1:E:143:LYS:HE3  | 1.97                     | 0.46              |
| 1:A:106:GLY:O    | 1:A:413:LEU:HD21 | 2.15                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:183:ILE:HD12 | 1:C:183:ILE:N    | 2.30                     | 0.45              |
| 1:E:20:TYR:HB3   | 1:E:89:VAL:HG22  | 1.98                     | 0.45              |
| 1:A:199:PHE:N    | 1:A:199:PHE:CD2  | 2.83                     | 0.45              |
| 1:B:150:LEU:HD13 | 1:B:192:PRO:HB2  | 1.98                     | 0.45              |
| 1:D:418:ILE:HD12 | 1:D:418:ILE:N    | 2.31                     | 0.45              |
| 1:E:260:ASP:HB2  | 1:E:268:SER:HB3  | 1.99                     | 0.45              |
| 1:A:378:GLU:H    | 1:A:378:GLU:CD   | 2.19                     | 0.45              |
| 1:C:116:LEU:HD23 | 1:C:351:LEU:CD1  | 2.46                     | 0.45              |
| 1:B:170:ARG:HG3  | 1:C:20:TYR:CE2   | 2.51                     | 0.45              |
| 1:D:311:TRP:CB   | 1:D:320:ILE:HB   | 2.45                     | 0.45              |
| 1:E:164:LEU:HD23 | 1:E:165:GLY:N    | 2.30                     | 0.45              |
| 1:E:168:CYS:SG   | 1:E:225:HIS:CD2  | 3.06                     | 0.45              |
| 1:F:16:GLU:HG2   | 1:F:79:ILE:CD1   | 2.46                     | 0.45              |
| 1:A:129:LEU:HD22 | 1:A:130:GLY:N    | 2.31                     | 0.45              |
| 1:A:191:ALA:H    | 1:A:194:GLN:NE2  | 2.15                     | 0.45              |
| 1:B:58:GLU:O     | 1:B:61:VAL:HG23  | 2.15                     | 0.45              |
| 1:E:186:SER:O    | 1:F:36:GLU:HG2   | 2.16                     | 0.45              |
| 1:A:220:THR:HG23 | 1:F:162:THR:CB   | 2.45                     | 0.45              |
| 1:B:234:LYS:HD3  | 1:B:298:ARG:HA   | 1.99                     | 0.45              |
| 1:D:123:GLY:O    | 1:D:252:LYS:HG3  | 2.17                     | 0.45              |
| 1:E:27:ASP:HB3   | 1:E:33:LYS:HD3   | 1.98                     | 0.45              |
| 1:A:325:SER:HB3  | 1:B:51:MET:CE    | 2.47                     | 0.45              |
| 1:F:103:PRO:HB3  | 1:F:110:ASN:HD21 | 1.81                     | 0.45              |
| 1:D:418:ILE:HG23 | 1:D:422:GLU:HG3  | 1.98                     | 0.45              |
| 1:F:260:ASP:OD1  | 1:F:263:ALA:HB2  | 2.17                     | 0.45              |
| 1:A:17:ASN:O     | 1:A:88:LYS:HB2   | 2.17                     | 0.45              |
| 1:A:28:ILE:HG13  | 1:A:29:LEU:N     | 2.30                     | 0.45              |
| 1:B:173:VAL:HG13 | 1:B:183:ILE:CD1  | 2.47                     | 0.45              |
| 1:F:118:GLU:HG2  | 1:F:118:GLU:H    | 1.53                     | 0.45              |
| 1:C:270:THR:HG21 | 4:C:631:HOH:O    | 2.16                     | 0.45              |
| 1:C:378:GLU:H    | 1:C:378:GLU:CD   | 2.20                     | 0.45              |
| 1:E:191:ALA:HB2  | 1:E:240:ASN:HB2  | 1.99                     | 0.45              |
| 1:F:281:HIS:CE1  | 1:F:404:VAL:HG11 | 2.52                     | 0.45              |
| 1:F:417:PHE:HD2  | 1:F:418:ILE:HD12 | 1.82                     | 0.45              |
| 1:F:78:VAL:CG1   | 1:F:79:ILE:N     | 2.80                     | 0.45              |
| 1:D:256:ASN:ND2  | 1:D:258:PHE:HB2  | 2.32                     | 0.45              |
| 1:E:275:ILE:O    | 1:E:279:VAL:HG23 | 2.15                     | 0.45              |
| 1:E:431:GLN:HG3  | 4:E:639:HOH:O    | 2.16                     | 0.45              |
| 1:C:22:ARG:HH11  | 1:C:22:ARG:HG2   | 1.82                     | 0.44              |
| 1:C:19:LYS:HB2   | 1:C:87:GLY:HA3   | 1.99                     | 0.44              |
| 1:B:131:PRO:HG2  | 1:B:199:PHE:HD1  | 1.79                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:74:LEU:HA    | 1:B:92:PHE:HE2   | 1.81                     | 0.44              |
| 1:F:116:LEU:HD23 | 1:F:351:LEU:CD1  | 2.46                     | 0.44              |
| 1:B:173:VAL:HG13 | 1:B:183:ILE:HD12 | 1.99                     | 0.44              |
| 1:B:392:LEU:O    | 1:B:396:LEU:HG   | 2.17                     | 0.44              |
| 1:B:319:LEU:HD12 | 1:B:336:SER:HB3  | 1.99                     | 0.44              |
| 1:B:4:TYR:HB3    | 1:B:9:ILE:HD11   | 1.98                     | 0.44              |
| 1:C:308:TYR:HA   | 1:C:387:ASP:HA   | 2.00                     | 0.44              |
| 1:D:156:TYR:CZ   | 1:D:157:PHE:HE1  | 2.35                     | 0.44              |
| 1:E:199:PHE:HZ   | 1:E:214:PHE:CG   | 2.36                     | 0.44              |
| 1:F:175:GLU:HG3  | 1:F:221:ILE:HD11 | 1.99                     | 0.44              |
| 1:A:150:LEU:HD13 | 1:A:192:PRO:HB2  | 1.99                     | 0.44              |
| 1:A:311:TRP:CB   | 1:A:320:ILE:HB   | 2.47                     | 0.44              |
| 1:A:134:GLU:OE2  | 3:A:503:GLN:HB3  | 2.17                     | 0.44              |
| 1:B:124:PHE:CE2  | 1:B:250:LEU:HD13 | 2.53                     | 0.44              |
| 1:B:241:GLY:HA3  | 1:B:298:ARG:HG3  | 2.00                     | 0.44              |
| 1:C:203:GLY:O    | 1:C:204:ALA:C    | 2.56                     | 0.44              |
| 1:D:131:PRO:HG2  | 1:D:199:PHE:CE1  | 2.51                     | 0.44              |
| 1:E:169:ARG:HE   | 1:E:195:HIS:CD2  | 2.34                     | 0.44              |
| 1:A:154:GLY:O    | 1:A:188:HIS:CE1  | 2.70                     | 0.44              |
| 1:A:285:PHE:C    | 1:A:285:PHE:CD1  | 2.91                     | 0.44              |
| 1:C:160:ALA:O    | 1:C:169:ARG:NH2  | 2.50                     | 0.44              |
| 1:F:129:LEU:HD13 | 1:F:207:SER:OG   | 2.18                     | 0.44              |
| 1:A:370:ARG:CG   | 1:A:371:ASN:H    | 2.11                     | 0.44              |
| 1:B:285:PHE:HB2  | 1:B:349:VAL:CG1  | 2.48                     | 0.44              |
| 1:C:233:PRO:HD3  | 1:C:340:ALA:HB2  | 1.99                     | 0.44              |
| 1:C:85:GLU:O     | 1:C:86:LYS:C     | 2.55                     | 0.44              |
| 1:D:127:PHE:CD2  | 1:D:351:LEU:HG   | 2.53                     | 0.44              |
| 1:B:160:ALA:HB2  | 1:B:188:HIS:CD2  | 2.53                     | 0.44              |
| 1:C:119:MET:HG2  | 1:C:124:PHE:HB2  | 1.99                     | 0.44              |
| 1:C:272:LYS:O    | 1:C:364:ALA:HB2  | 2.18                     | 0.44              |
| 1:E:168:CYS:SG   | 1:E:222:ALA:HA   | 2.58                     | 0.44              |
| 1:F:260:ASP:HB3  | 1:F:263:ALA:HB3  | 1.99                     | 0.44              |
| 1:F:434:PRO:O    | 1:F:438:GLU:HG3  | 2.18                     | 0.44              |
| 1:B:122:LEU:HD13 | 1:B:355:LEU:HD22 | 1.99                     | 0.44              |
| 1:D:111:ASN:O    | 1:D:115:ILE:HG12 | 2.18                     | 0.44              |
| 1:D:274:PHE:CE1  | 1:D:354:GLY:HA3  | 2.53                     | 0.44              |
| 1:E:169:ARG:HH12 | 1:E:188:HIS:HB2  | 1.83                     | 0.44              |
| 1:E:197:ILE:HB   | 1:E:214:PHE:CZ   | 2.53                     | 0.44              |
| 1:D:159:LEU:HD13 | 1:E:34:ASN:CG    | 2.37                     | 0.44              |
| 1:F:418:ILE:N    | 1:F:418:ILE:HD12 | 2.33                     | 0.44              |
| 1:A:368:ILE:HG21 | 1:A:385:ILE:HD11 | 1.99                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:114:ARG:NH2  | 1:D:407:LYS:O    | 2.49                     | 0.43              |
| 1:E:209:ASP:OD2  | 1:E:344:TYR:OH   | 2.25                     | 0.43              |
| 1:E:236:LEU:HB2  | 1:E:239:VAL:HG22 | 2.00                     | 0.43              |
| 1:F:312:SER:HB2  | 1:F:368:ILE:O    | 2.18                     | 0.43              |
| 1:F:314:GLN:HE21 | 1:F:314:GLN:HB3  | 1.58                     | 0.43              |
| 1:A:244:MET:HE2  | 1:A:339:PRO:HA   | 1.98                     | 0.43              |
| 1:F:402:ASN:OD1  | 1:F:404:VAL:HG12 | 2.18                     | 0.43              |
| 1:B:91:ARG:HD2   | 1:B:92:PHE:N     | 2.32                     | 0.43              |
| 1:D:28:ILE:HD11  | 1:D:417:PHE:HA   | 2.00                     | 0.43              |
| 1:D:28:ILE:HD11  | 1:D:417:PHE:CA   | 2.48                     | 0.43              |
| 1:E:27:ASP:C     | 1:E:27:ASP:OD2   | 2.55                     | 0.43              |
| 1:E:368:ILE:CD1  | 1:E:385:ILE:HD11 | 2.49                     | 0.43              |
| 1:A:33:LYS:O     | 1:A:34:ASN:HB3   | 2.18                     | 0.43              |
| 1:B:26:THR:HG22  | 1:B:27:ASP:O     | 2.18                     | 0.43              |
| 1:B:291:PRO:HG3  | 1:B:341:ALA:HA   | 2.00                     | 0.43              |
| 1:B:425:TRP:O    | 1:B:429:ARG:HG3  | 2.18                     | 0.43              |
| 1:F:201:TYR:OH   | 1:F:331:ARG:NE   | 2.46                     | 0.43              |
| 1:A:220:THR:O    | 1:A:224:LYS:HG3  | 2.19                     | 0.43              |
| 1:B:212:GLN:OE1  | 1:B:215:LYS:NZ   | 2.52                     | 0.43              |
| 1:C:91:ARG:HD2   | 1:C:92:PHE:N     | 2.33                     | 0.43              |
| 1:D:21:ILE:HD13  | 1:D:42:LEU:HD13  | 2.01                     | 0.43              |
| 1:F:285:PHE:HD1  | 1:F:285:PHE:C    | 2.22                     | 0.43              |
| 1:F:5:THR:H      | 1:F:8:ASP:HB2    | 1.83                     | 0.43              |
| 1:B:211:ILE:O    | 1:B:215:LYS:HG3  | 2.19                     | 0.43              |
| 1:B:393:ALA:HB2  | 1:B:425:TRP:CE2  | 2.54                     | 0.43              |
| 1:C:160:ALA:HB3  | 1:C:188:HIS:CD2  | 2.53                     | 0.43              |
| 1:D:159:LEU:HD13 | 1:E:34:ASN:CB    | 2.49                     | 0.43              |
| 1:D:274:PHE:O    | 1:D:278:ILE:HD13 | 2.19                     | 0.43              |
| 1:E:167:ASN:C    | 1:E:167:ASN:HD22 | 2.21                     | 0.43              |
| 1:A:402:ASN:HB3  | 1:A:405:MET:HB2  | 2.00                     | 0.43              |
| 1:A:62:ARG:O     | 1:A:63:ILE:HD13  | 2.18                     | 0.43              |
| 1:C:396:LEU:O    | 1:C:400:LYS:HG3  | 2.17                     | 0.43              |
| 1:D:85:GLU:H     | 1:D:85:GLU:CD    | 2.20                     | 0.43              |
| 1:E:9:ILE:HG21   | 1:E:92:PHE:HZ    | 1.84                     | 0.43              |
| 1:F:119:MET:HG2  | 1:F:124:PHE:HB2  | 2.00                     | 0.43              |
| 1:F:201:TYR:CD1  | 1:F:201:TYR:N    | 2.86                     | 0.43              |
| 1:A:437:ARG:O    | 1:A:441:MET:HB3  | 2.18                     | 0.43              |
| 1:D:117:LYS:HG2  | 4:D:706:HOH:O    | 2.19                     | 0.43              |
| 1:D:136:PHE:CE2  | 1:D:194:GLN:HB2  | 2.54                     | 0.43              |
| 1:D:28:ILE:HD11  | 1:D:417:PHE:N    | 2.34                     | 0.43              |
| 1:B:367:PRO:C    | 1:B:368:ILE:HD12 | 2.39                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:249:SER:HA   | 1:C:258:PHE:CE1  | 2.54                     | 0.43              |
| 1:E:124:PHE:CE2  | 1:E:250:LEU:HD13 | 2.54                     | 0.43              |
| 1:E:300:VAL:CG1  | 1:E:301:PRO:HD2  | 2.49                     | 0.43              |
| 1:E:326:ARG:HD3  | 1:E:330:THR:OG1  | 2.18                     | 0.43              |
| 1:E:20:TYR:OH    | 1:E:36:GLU:HG3   | 2.19                     | 0.43              |
| 1:E:377:LYS:HA   | 1:E:380:ARG:HB2  | 2.01                     | 0.43              |
| 1:F:342:ASN:ND2  | 1:F:342:ASN:C    | 2.69                     | 0.43              |
| 1:B:182:GLU:HB3  | 1:B:200:LYS:HD3  | 2.01                     | 0.43              |
| 1:C:300:VAL:CG1  | 1:C:301:PRO:HD2  | 2.49                     | 0.43              |
| 1:E:203:GLY:O    | 1:E:204:ALA:C    | 2.57                     | 0.43              |
| 1:F:197:ILE:HB   | 1:F:214:PHE:CZ   | 2.54                     | 0.43              |
| 1:A:141:ASP:HB2  | 1:A:142:GLU:OE2  | 2.19                     | 0.42              |
| 1:A:383:ASN:O    | 1:A:385:ILE:N    | 2.48                     | 0.42              |
| 1:C:84:ALA:O     | 1:C:85:GLU:HG3   | 2.20                     | 0.42              |
| 1:D:9:ILE:HD13   | 1:D:92:PHE:CZ    | 2.54                     | 0.42              |
| 1:A:174:LEU:HD12 | 1:A:174:LEU:HA   | 1.84                     | 0.42              |
| 1:B:112:LEU:HD23 | 1:B:205:VAL:HG12 | 2.00                     | 0.42              |
| 1:B:306:PRO:HG2  | 1:B:335:ARG:C    | 2.40                     | 0.42              |
| 1:C:351:LEU:CD2  | 1:C:355:LEU:HG   | 2.49                     | 0.42              |
| 1:D:280:LYS:HD2  | 1:D:362:LEU:CD2  | 2.49                     | 0.42              |
| 1:E:223:ARG:HG3  | 1:E:223:ARG:HH11 | 1.84                     | 0.42              |
| 1:E:211:ILE:HD13 | 1:E:244:MET:HE3  | 2.01                     | 0.42              |
| 1:F:324:ALA:O    | 1:F:325:SER:C    | 2.57                     | 0.42              |
| 1:F:331:ARG:HG2  | 1:F:331:ARG:HH21 | 1.84                     | 0.42              |
| 1:F:354:GLY:O    | 1:F:358:ILE:HG12 | 2.19                     | 0.42              |
| 1:C:283:THR:HG23 | 4:C:619:HOH:O    | 2.20                     | 0.42              |
| 1:D:156:TYR:O    | 1:D:157:PHE:HB2  | 2.19                     | 0.42              |
| 1:C:116:LEU:HD11 | 1:C:204:ALA:HB3  | 2.01                     | 0.42              |
| 1:D:184:GLU:O    | 1:D:185:ALA:HB2  | 2.20                     | 0.42              |
| 1:E:211:ILE:HD13 | 1:E:244:MET:CE   | 2.49                     | 0.42              |
| 1:F:280:LYS:HE3  | 1:F:280:LYS:HB2  | 1.85                     | 0.42              |
| 1:F:309:VAL:HA   | 1:F:319:LEU:HD23 | 2.01                     | 0.42              |
| 1:F:405:MET:O    | 1:F:408:ALA:HB3  | 2.18                     | 0.42              |
| 1:B:316:ARG:HD2  | 1:B:371:ASN:ND2  | 2.34                     | 0.42              |
| 1:B:6:ARG:HD3    | 4:B:697:HOH:O    | 2.19                     | 0.42              |
| 1:C:127:PHE:CE2  | 1:C:347:LEU:HD12 | 2.52                     | 0.42              |
| 1:C:114:ARG:NH2  | 1:C:407:LYS:O    | 2.51                     | 0.42              |
| 1:D:370:ARG:HG2  | 1:D:371:ASN:H    | 1.85                     | 0.42              |
| 1:D:388:LEU:HB3  | 1:D:389:PRO:HD2  | 2.01                     | 0.42              |
| 1:D:427:MET:O    | 1:D:431:GLN:HG2  | 2.19                     | 0.42              |
| 1:F:311:TRP:HA   | 1:F:320:ILE:O    | 2.19                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:201:TYR:CZ   | 1:F:331:ARG:HD2  | 2.53                     | 0.42              |
| 1:A:164:LEU:HD22 | 1:B:223:ARG:HD3  | 2.02                     | 0.42              |
| 3:B:503:GLN:HG2  | 4:C:607:HOH:O    | 2.20                     | 0.42              |
| 1:D:91:ARG:HG2   | 1:D:91:ARG:HH11  | 1.84                     | 0.42              |
| 1:F:258:PHE:HA   | 1:F:271:ALA:HB2  | 2.02                     | 0.42              |
| 1:B:27:ASP:OD1   | 1:B:33:LYS:HE3   | 2.19                     | 0.42              |
| 1:C:22:ARG:HG2   | 1:C:22:ARG:NH1   | 2.34                     | 0.42              |
| 1:D:122:LEU:HD12 | 1:D:355:LEU:HD22 | 2.00                     | 0.42              |
| 1:E:282:ALA:HA   | 1:E:285:PHE:CE2  | 2.55                     | 0.42              |
| 1:F:383:ASN:O    | 1:F:385:ILE:N    | 2.52                     | 0.42              |
| 1:F:145:GLU:HA   | 1:F:146:PRO:HD3  | 1.95                     | 0.42              |
| 1:F:129:LEU:HG   | 1:F:347:LEU:HD21 | 2.02                     | 0.42              |
| 1:B:201:TYR:HD2  | 1:B:201:TYR:H    | 1.68                     | 0.42              |
| 1:E:202:ALA:HB3  | 1:E:207:SER:HB2  | 2.02                     | 0.42              |
| 1:F:275:ILE:O    | 1:F:279:VAL:HG23 | 2.19                     | 0.42              |
| 1:A:281:HIS:HD2  | 1:A:402:ASN:ND2  | 2.15                     | 0.42              |
| 1:A:3:LYS:HB3    | 1:A:75:ASN:ND2   | 2.35                     | 0.42              |
| 1:B:391:THR:OG1  | 1:B:394:GLU:HG3  | 2.20                     | 0.42              |
| 1:C:140:LEU:HD21 | 1:C:228:HIS:HB2  | 2.00                     | 0.42              |
| 1:D:318:PRO:O    | 1:D:335:ARG:HD3  | 2.20                     | 0.42              |
| 1:D:309:VAL:HG23 | 1:D:386:VAL:O    | 2.18                     | 0.42              |
| 1:E:117:LYS:HA   | 1:E:120:GLU:OE1  | 2.20                     | 0.42              |
| 1:F:406:VAL:HG13 | 1:F:414:PHE:CD1  | 2.55                     | 0.42              |
| 1:A:370:ARG:CG   | 1:A:371:ASN:N    | 2.80                     | 0.41              |
| 1:B:176:LEU:HD12 | 1:B:183:ILE:HD11 | 2.01                     | 0.41              |
| 1:B:366:ALA:O    | 1:B:368:ILE:HD12 | 2.20                     | 0.41              |
| 1:C:65:GLU:HG2   | 4:C:623:HOH:O    | 2.20                     | 0.41              |
| 1:C:98:ASN:HD22  | 1:C:102:THR:HG23 | 1.84                     | 0.41              |
| 1:D:323:PRO:HG2  | 4:D:626:HOH:O    | 2.20                     | 0.41              |
| 1:D:371:ASN:ND2  | 1:D:374:VAL:HG13 | 2.34                     | 0.41              |
| 1:F:183:ILE:N    | 1:F:183:ILE:HD12 | 2.35                     | 0.41              |
| 1:B:359:LYS:CB   | 1:B:359:LYS:NZ   | 2.82                     | 0.41              |
| 1:D:154:GLY:O    | 1:D:188:HIS:CE1  | 2.73                     | 0.41              |
| 1:E:26:THR:HG22  | 1:E:27:ASP:O     | 2.20                     | 0.41              |
| 1:F:161:PRO:HB2  | 1:F:167:ASN:OD1  | 2.20                     | 0.41              |
| 1:F:33:LYS:O     | 1:F:34:ASN:HB3   | 2.20                     | 0.41              |
| 1:A:129:LEU:HD22 | 1:A:130:GLY:H    | 1.86                     | 0.41              |
| 1:B:349:VAL:CG1  | 1:B:350:LEU:N    | 2.82                     | 0.41              |
| 1:B:377:LYS:O    | 1:B:381:MET:HG2  | 2.20                     | 0.41              |
| 1:C:9:ILE:CD1    | 1:C:74:LEU:HD22  | 2.50                     | 0.41              |
| 1:D:315:ASN:ND2  | 1:D:316:ARG:N    | 2.66                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:351:LEU:HD22 | 1:D:355:LEU:CG   | 2.44                     | 0.41              |
| 1:E:164:LEU:HD11 | 1:F:224:LYS:HD3  | 2.02                     | 0.41              |
| 1:A:231:PHE:O    | 1:A:339:PRO:HG2  | 2.20                     | 0.41              |
| 1:A:290:ASN:HB3  | 1:A:295:SER:HB3  | 2.02                     | 0.41              |
| 1:A:311:TRP:HE3  | 1:A:322:ILE:HD13 | 1.85                     | 0.41              |
| 1:A:34:ASN:C     | 1:A:34:ASN:ND2   | 2.73                     | 0.41              |
| 1:B:166:GLU:O    | 1:B:167:ASN:C    | 2.59                     | 0.41              |
| 1:C:129:LEU:HD22 | 1:C:130:GLY:N    | 2.36                     | 0.41              |
| 1:C:303:TYR:HB2  | 4:C:613:HOH:O    | 2.19                     | 0.41              |
| 1:C:33:LYS:O     | 1:C:34:ASN:CB    | 2.68                     | 0.41              |
| 1:D:201:TYR:H    | 1:D:201:TYR:HD2  | 1.67                     | 0.41              |
| 1:D:310:ALA:HB1  | 1:D:368:ILE:HD13 | 2.02                     | 0.41              |
| 1:E:315:ASN:HB3  | 1:E:318:PRO:HD3  | 2.02                     | 0.41              |
| 1:A:220:THR:CG2  | 1:F:162:THR:HB   | 2.48                     | 0.41              |
| 1:F:373:TYR:HE2  | 4:F:610:HOH:O    | 2.03                     | 0.41              |
| 1:A:154:GLY:C    | 1:A:188:HIS:CE1  | 2.94                     | 0.41              |
| 1:A:160:ALA:O    | 1:A:161:PRO:C    | 2.59                     | 0.41              |
| 1:B:175:GLU:HG2  | 1:B:221:ILE:HD11 | 2.02                     | 0.41              |
| 1:C:296:TYR:HB3  | 1:C:390:ALA:O    | 2.20                     | 0.41              |
| 1:D:54:GLY:HA3   | 1:D:68:MET:SD    | 2.60                     | 0.41              |
| 1:E:292:THR:O    | 1:E:295:SER:HB2  | 2.20                     | 0.41              |
| 1:F:115:ILE:HG22 | 1:F:351:LEU:HD13 | 2.02                     | 0.41              |
| 1:F:24:GLN:NE2   | 1:F:91:ARG:HH11  | 2.19                     | 0.41              |
| 1:B:282:ALA:HA   | 1:B:285:PHE:CE2  | 2.56                     | 0.41              |
| 1:C:142:GLU:H    | 1:C:142:GLU:CD   | 2.17                     | 0.41              |
| 1:D:134:GLU:OE2  | 3:D:503:GLN:OE1  | 2.39                     | 0.41              |
| 1:F:305:ALA:HA   | 1:F:306:PRO:HD3  | 1.97                     | 0.41              |
| 1:F:134:GLU:OE1  | 3:F:503:GLN:N    | 2.53                     | 0.41              |
| 1:A:112:LEU:HD11 | 1:A:204:ALA:HB1  | 2.03                     | 0.41              |
| 1:A:149:GLU:HG2  | 4:A:713:HOH:O    | 2.20                     | 0.41              |
| 1:E:169:ARG:NH1  | 1:E:188:HIS:HB2  | 2.34                     | 0.41              |
| 1:E:199:PHE:HZ   | 1:E:214:PHE:HB2  | 1.85                     | 0.41              |
| 1:E:256:ASN:OD1  | 1:E:258:PHE:HB2  | 2.20                     | 0.41              |
| 1:A:107:ASP:HA   | 1:A:108:PRO:HD3  | 1.91                     | 0.41              |
| 1:A:78:VAL:HG12  | 1:A:91:ARG:NH1   | 2.36                     | 0.41              |
| 1:B:102:THR:HA   | 1:B:103:PRO:HD3  | 1.95                     | 0.41              |
| 1:C:208:CYS:SG   | 1:C:343:PRO:O    | 2.78                     | 0.41              |
| 1:D:54:GLY:HA3   | 1:D:68:MET:HG3   | 2.03                     | 0.41              |
| 1:F:116:LEU:O    | 1:F:119:MET:HB3  | 2.21                     | 0.41              |
| 1:F:23:LEU:HB3   | 1:F:94:CYS:SG    | 2.60                     | 0.41              |
| 1:B:176:LEU:CD1  | 1:B:183:ILE:HD11 | 2.51                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:25:PHE:CD2   | 1:C:25:PHE:N     | 2.88                     | 0.41              |
| 1:D:245:HIS:CE1  | 1:D:335:ARG:HE   | 2.39                     | 0.41              |
| 1:D:74:LEU:HG    | 4:D:639:HOH:O    | 2.21                     | 0.41              |
| 1:F:247:ASN:ND2  | 1:F:333:GLU:HB2  | 2.35                     | 0.41              |
| 1:F:8:ASP:O      | 1:F:12:LEU:HG    | 2.21                     | 0.41              |
| 1:A:347:LEU:HD13 | 1:A:347:LEU:HA   | 1.87                     | 0.41              |
| 1:A:36:GLU:OE2   | 1:F:169:ARG:NH1  | 2.54                     | 0.41              |
| 1:C:236:LEU:HB2  | 1:C:239:VAL:CG2  | 2.51                     | 0.41              |
| 1:C:319:LEU:HD12 | 1:C:336:SER:HB3  | 2.03                     | 0.41              |
| 1:C:315:ASN:ND2  | 1:C:370:ARG:O    | 2.54                     | 0.41              |
| 1:E:315:ASN:HD22 | 1:E:369:ASP:HA   | 1.85                     | 0.41              |
| 1:E:91:ARG:HH12  | 1:E:213:THR:HG23 | 1.86                     | 0.41              |
| 1:A:45:ALA:HA    | 1:A:50:VAL:HG23  | 2.03                     | 0.41              |
| 1:B:160:ALA:HB2  | 1:B:188:HIS:CB   | 2.43                     | 0.41              |
| 1:C:386:VAL:HG12 | 1:C:387:ASP:N    | 2.35                     | 0.41              |
| 1:E:325:SER:HB2  | 1:E:331:ARG:HH22 | 1.86                     | 0.41              |
| 1:F:98:ASN:HB2   | 1:F:102:THR:HG22 | 2.02                     | 0.41              |
| 1:F:151:ASN:OD1  | 1:F:193:GLY:HA2  | 2.21                     | 0.41              |
| 1:F:27:ASP:HB3   | 1:F:33:LYS:CD    | 2.37                     | 0.41              |
| 1:B:206:ARG:HB2  | 4:B:612:HOH:O    | 2.21                     | 0.40              |
| 1:A:158:ASP:OD2  | 1:B:33:LYS:HE2   | 2.22                     | 0.40              |
| 1:C:50:VAL:HB    | 4:C:606:HOH:O    | 2.21                     | 0.40              |
| 1:C:316:ARG:CZ   | 1:D:63:ILE:HG23  | 2.50                     | 0.40              |
| 1:E:231:PHE:HB3  | 1:E:339:PRO:HB2  | 2.03                     | 0.40              |
| 1:E:309:VAL:HA   | 1:E:319:LEU:HD22 | 2.03                     | 0.40              |
| 1:E:406:VAL:HG22 | 1:E:414:PHE:CE1  | 2.56                     | 0.40              |
| 1:F:52:PHE:CD1   | 1:F:70:LEU:HD13  | 2.56                     | 0.40              |
| 1:F:70:LEU:HG    | 1:F:94:CYS:HB2   | 2.03                     | 0.40              |
| 1:A:326:ARG:HB3  | 1:A:327:GLY:H    | 1.60                     | 0.40              |
| 1:B:176:LEU:HB3  | 1:B:181:PHE:CB   | 2.51                     | 0.40              |
| 1:B:311:TRP:CH2  | 1:B:367:PRO:HG3  | 2.54                     | 0.40              |
| 1:C:319:LEU:CD1  | 1:C:336:SER:HB3  | 2.51                     | 0.40              |
| 1:D:128:ASN:HA   | 1:D:202:ALA:O    | 2.21                     | 0.40              |
| 1:D:234:LYS:HD2  | 1:D:298:ARG:HA   | 2.04                     | 0.40              |
| 1:F:201:TYR:H    | 1:F:201:TYR:HD1  | 1.69                     | 0.40              |
| 1:A:214:PHE:O    | 1:A:218:VAL:HG23 | 2.21                     | 0.40              |
| 1:A:326:ARG:HD3  | 1:A:326:ARG:HA   | 1.78                     | 0.40              |
| 1:B:324:ALA:O    | 1:B:325:SER:C    | 2.59                     | 0.40              |
| 1:B:48:ASN:OD1   | 1:B:72:PRO:HD2   | 2.21                     | 0.40              |
| 1:C:355:LEU:O    | 1:C:359:LYS:HG2  | 2.22                     | 0.40              |
| 1:D:208:CYS:SG   | 1:D:343:PRO:C    | 3.00                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:406:VAL:HG22 | 1:D:414:PHE:CE1  | 2.56                     | 0.40              |
| 1:D:83:THR:HG21  | 1:D:89:VAL:HB    | 2.02                     | 0.40              |
| 1:E:50:VAL:HB    | 4:E:612:HOH:O    | 2.21                     | 0.40              |
| 1:A:349:VAL:HG23 | 1:A:350:LEU:N    | 2.37                     | 0.40              |
| 1:A:359:LYS:HB2  | 1:A:359:LYS:HZ2  | 1.87                     | 0.40              |
| 1:A:315:ASN:ND2  | 1:A:369:ASP:HA   | 2.36                     | 0.40              |
| 1:B:132:GLU:HB3  | 1:B:196:GLU:OE1  | 2.22                     | 0.40              |
| 1:B:189:GLU:OE1  | 1:B:196:GLU:OE2  | 2.38                     | 0.40              |
| 1:B:316:ARG:O    | 1:B:317:SER:HB3  | 2.22                     | 0.40              |
| 1:B:281:HIS:CE1  | 1:B:356:ASP:OD2  | 2.74                     | 0.40              |
| 1:B:52:PHE:CZ    | 1:B:54:GLY:HA2   | 2.56                     | 0.40              |
| 1:C:311:TRP:CZ2  | 1:C:367:PRO:HD3  | 2.55                     | 0.40              |
| 1:D:208:CYS:SG   | 1:D:343:PRO:O    | 2.80                     | 0.40              |
| 1:D:419:GLU:O    | 1:D:423:ILE:HG12 | 2.21                     | 0.40              |
| 1:D:57:ILE:CD1   | 1:D:96:ILE:HG13  | 2.52                     | 0.40              |
| 1:E:351:LEU:CD2  | 1:E:355:LEU:HG   | 2.50                     | 0.40              |
| 1:E:370:ARG:HG2  | 1:E:371:ASN:H    | 1.86                     | 0.40              |
| 1:F:199:PHE:N    | 1:F:199:PHE:CD2  | 2.86                     | 0.40              |
| 1:F:52:PHE:CE1   | 1:F:70:LEU:HD13  | 2.55                     | 0.40              |
| 1:A:150:LEU:HD13 | 1:A:192:PRO:O    | 2.21                     | 0.40              |
| 1:B:231:PHE:O    | 1:B:339:PRO:HG2  | 2.21                     | 0.40              |
| 1:D:168:CYS:O    | 1:D:172:ILE:HG13 | 2.22                     | 0.40              |
| 1:E:243:GLY:C    | 1:E:339:PRO:HD3  | 2.42                     | 0.40              |
| 1:E:364:ALA:HA   | 1:E:365:PRO:HD3  | 1.99                     | 0.40              |
| 1:F:162:THR:C    | 1:F:164:LEU:H    | 2.25                     | 0.40              |
| 1:F:206:ARG:HB2  | 4:F:624:HOH:O    | 2.21                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed         | Favoured   | Allowed  | Outliers | Percentiles |    |
|-----|-------|------------------|------------|----------|----------|-------------|----|
| 1   | A     | 441/443 (100%)   | 397 (90%)  | 39 (9%)  | 5 (1%)   | 14          | 42 |
| 1   | B     | 441/443 (100%)   | 412 (93%)  | 25 (6%)  | 4 (1%)   | 17          | 48 |
| 1   | C     | 441/443 (100%)   | 404 (92%)  | 36 (8%)  | 1 (0%)   | 47          | 78 |
| 1   | D     | 441/443 (100%)   | 403 (91%)  | 33 (8%)  | 5 (1%)   | 14          | 42 |
| 1   | E     | 441/443 (100%)   | 401 (91%)  | 35 (8%)  | 5 (1%)   | 14          | 42 |
| 1   | F     | 441/443 (100%)   | 418 (95%)  | 20 (4%)  | 3 (1%)   | 22          | 54 |
| All | All   | 2646/2658 (100%) | 2435 (92%) | 188 (7%) | 23 (1%)  | 17          | 48 |

All (23) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 161 | PRO  |
| 1   | B     | 161 | PRO  |
| 1   | D     | 161 | PRO  |
| 1   | E     | 143 | LYS  |
| 1   | E     | 161 | PRO  |
| 1   | F     | 161 | PRO  |
| 1   | A     | 163 | ASP  |
| 1   | A     | 369 | ASP  |
| 1   | B     | 163 | ASP  |
| 1   | D     | 325 | SER  |
| 1   | E     | 262 | ASN  |
| 1   | F     | 325 | SER  |
| 1   | B     | 60  | PHE  |
| 1   | D     | 62  | ARG  |
| 1   | D     | 163 | ASP  |
| 1   | E     | 204 | ALA  |
| 1   | F     | 141 | ASP  |
| 1   | A     | 268 | SER  |
| 1   | C     | 86  | LYS  |
| 1   | A     | 374 | VAL  |
| 1   | E     | 144 | GLY  |
| 1   | B     | 317 | SER  |
| 1   | D     | 63  | ILE  |

### 5.3.2 Protein sidechains ⓘ

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



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

| Mol | Chain | Analysed         | Rotameric  | Outliers | Percentiles |    |
|-----|-------|------------------|------------|----------|-------------|----|
| 1   | A     | 382/382 (100%)   | 355 (93%)  | 27 (7%)  | 14          | 40 |
| 1   | B     | 382/382 (100%)   | 352 (92%)  | 30 (8%)  | 12          | 34 |
| 1   | C     | 382/382 (100%)   | 358 (94%)  | 24 (6%)  | 18          | 46 |
| 1   | D     | 382/382 (100%)   | 352 (92%)  | 30 (8%)  | 12          | 34 |
| 1   | E     | 382/382 (100%)   | 360 (94%)  | 22 (6%)  | 20          | 50 |
| 1   | F     | 382/382 (100%)   | 349 (91%)  | 33 (9%)  | 10          | 30 |
| All | All   | 2292/2292 (100%) | 2126 (93%) | 166 (7%) | 14          | 39 |

All (166) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 34  | ASN  |
| 1   | A     | 35  | VAL  |
| 1   | A     | 36  | GLU  |
| 1   | A     | 58  | GLU  |
| 1   | A     | 91  | ARG  |
| 1   | A     | 110 | ASN  |
| 1   | A     | 112 | LEU  |
| 1   | A     | 129 | LEU  |
| 1   | A     | 142 | GLU  |
| 1   | A     | 153 | LYS  |
| 1   | A     | 161 | PRO  |
| 1   | A     | 167 | ASN  |
| 1   | A     | 174 | LEU  |
| 1   | A     | 181 | PHE  |
| 1   | A     | 199 | PHE  |
| 1   | A     | 206 | ARG  |
| 1   | A     | 240 | ASN  |
| 1   | A     | 262 | ASN  |
| 1   | A     | 285 | PHE  |
| 1   | A     | 299 | LEU  |
| 1   | A     | 315 | ASN  |
| 1   | A     | 326 | ARG  |
| 1   | A     | 331 | ARG  |
| 1   | A     | 347 | LEU  |
| 1   | A     | 359 | LYS  |
| 1   | A     | 362 | LEU  |
| 1   | A     | 363 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 34  | ASN  |
| 1   | B     | 36  | GLU  |
| 1   | B     | 49  | LYS  |
| 1   | B     | 61  | VAL  |
| 1   | B     | 68  | MET  |
| 1   | B     | 91  | ARG  |
| 1   | B     | 92  | PHE  |
| 1   | B     | 110 | ASN  |
| 1   | B     | 122 | LEU  |
| 1   | B     | 126 | ASP  |
| 1   | B     | 129 | LEU  |
| 1   | B     | 159 | LEU  |
| 1   | B     | 161 | PRO  |
| 1   | B     | 199 | PHE  |
| 1   | B     | 201 | TYR  |
| 1   | B     | 240 | ASN  |
| 1   | B     | 308 | TYR  |
| 1   | B     | 349 | VAL  |
| 1   | B     | 351 | LEU  |
| 1   | B     | 363 | GLU  |
| 1   | B     | 370 | ARG  |
| 1   | B     | 371 | ASN  |
| 1   | B     | 377 | LYS  |
| 1   | B     | 380 | ARG  |
| 1   | B     | 415 | GLU  |
| 1   | B     | 423 | ILE  |
| 1   | B     | 426 | ASP  |
| 1   | B     | 429 | ARG  |
| 1   | B     | 441 | MET  |
| 1   | B     | 443 | GLN  |
| 1   | C     | 34  | ASN  |
| 1   | C     | 49  | LYS  |
| 1   | C     | 91  | ARG  |
| 1   | C     | 105 | GLU  |
| 1   | C     | 110 | ASN  |
| 1   | C     | 112 | LEU  |
| 1   | C     | 129 | LEU  |
| 1   | C     | 159 | LEU  |
| 1   | C     | 199 | PHE  |
| 1   | C     | 240 | ASN  |
| 1   | C     | 262 | ASN  |
| 1   | C     | 264 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 285 | PHE  |
| 1   | C     | 299 | LEU  |
| 1   | C     | 328 | ILE  |
| 1   | C     | 331 | ARG  |
| 1   | C     | 351 | LEU  |
| 1   | C     | 360 | ASN  |
| 1   | C     | 371 | ASN  |
| 1   | C     | 397 | GLU  |
| 1   | C     | 413 | LEU  |
| 1   | C     | 441 | MET  |
| 1   | C     | 442 | SER  |
| 1   | C     | 443 | GLN  |
| 1   | D     | 6   | ARG  |
| 1   | D     | 11  | LYS  |
| 1   | D     | 34  | ASN  |
| 1   | D     | 35  | VAL  |
| 1   | D     | 36  | GLU  |
| 1   | D     | 49  | LYS  |
| 1   | D     | 66  | SER  |
| 1   | D     | 85  | GLU  |
| 1   | D     | 91  | ARG  |
| 1   | D     | 110 | ASN  |
| 1   | D     | 129 | LEU  |
| 1   | D     | 142 | GLU  |
| 1   | D     | 151 | ASN  |
| 1   | D     | 161 | PRO  |
| 1   | D     | 164 | LEU  |
| 1   | D     | 168 | CYS  |
| 1   | D     | 199 | PHE  |
| 1   | D     | 201 | TYR  |
| 1   | D     | 223 | ARG  |
| 1   | D     | 232 | MET  |
| 1   | D     | 240 | ASN  |
| 1   | D     | 256 | ASN  |
| 1   | D     | 314 | GLN  |
| 1   | D     | 315 | ASN  |
| 1   | D     | 328 | ILE  |
| 1   | D     | 351 | LEU  |
| 1   | D     | 359 | LYS  |
| 1   | D     | 363 | GLU  |
| 1   | D     | 379 | GLU  |
| 1   | D     | 413 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 28  | ILE  |
| 1   | E     | 35  | VAL  |
| 1   | E     | 41  | GLN  |
| 1   | E     | 49  | LYS  |
| 1   | E     | 91  | ARG  |
| 1   | E     | 105 | GLU  |
| 1   | E     | 126 | ASP  |
| 1   | E     | 161 | PRO  |
| 1   | E     | 167 | ASN  |
| 1   | E     | 168 | CYS  |
| 1   | E     | 172 | ILE  |
| 1   | E     | 201 | TYR  |
| 1   | E     | 240 | ASN  |
| 1   | E     | 262 | ASN  |
| 1   | E     | 299 | LEU  |
| 1   | E     | 308 | TYR  |
| 1   | E     | 326 | ARG  |
| 1   | E     | 349 | VAL  |
| 1   | E     | 351 | LEU  |
| 1   | E     | 381 | MET  |
| 1   | E     | 397 | GLU  |
| 1   | E     | 443 | GLN  |
| 1   | F     | 10  | GLU  |
| 1   | F     | 32  | ILE  |
| 1   | F     | 34  | ASN  |
| 1   | F     | 36  | GLU  |
| 1   | F     | 85  | GLU  |
| 1   | F     | 91  | ARG  |
| 1   | F     | 95  | ASP  |
| 1   | F     | 110 | ASN  |
| 1   | F     | 112 | LEU  |
| 1   | F     | 118 | GLU  |
| 1   | F     | 126 | ASP  |
| 1   | F     | 129 | LEU  |
| 1   | F     | 143 | LYS  |
| 1   | F     | 164 | LEU  |
| 1   | F     | 168 | CYS  |
| 1   | F     | 181 | PHE  |
| 1   | F     | 206 | ARG  |
| 1   | F     | 240 | ASN  |
| 1   | F     | 250 | LEU  |
| 1   | F     | 253 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 262 | ASN  |
| 1   | F     | 285 | PHE  |
| 1   | F     | 299 | LEU  |
| 1   | F     | 312 | SER  |
| 1   | F     | 314 | GLN  |
| 1   | F     | 342 | ASN  |
| 1   | F     | 347 | LEU  |
| 1   | F     | 349 | VAL  |
| 1   | F     | 351 | LEU  |
| 1   | F     | 361 | LYS  |
| 1   | F     | 377 | LYS  |
| 1   | F     | 423 | ILE  |
| 1   | F     | 439 | GLN  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 17  | ASN  |
| 1   | A     | 75  | ASN  |
| 1   | A     | 110 | ASN  |
| 1   | A     | 128 | ASN  |
| 1   | A     | 167 | ASN  |
| 1   | A     | 194 | GLN  |
| 1   | A     | 240 | ASN  |
| 1   | A     | 253 | ASN  |
| 1   | A     | 281 | HIS  |
| 1   | A     | 290 | ASN  |
| 1   | A     | 315 | ASN  |
| 1   | A     | 360 | ASN  |
| 1   | A     | 431 | GLN  |
| 1   | A     | 443 | GLN  |
| 1   | B     | 17  | ASN  |
| 1   | B     | 34  | ASN  |
| 1   | B     | 128 | ASN  |
| 1   | B     | 194 | GLN  |
| 1   | B     | 225 | HIS  |
| 1   | B     | 240 | ASN  |
| 1   | B     | 253 | ASN  |
| 1   | B     | 262 | ASN  |
| 1   | B     | 266 | GLN  |
| 1   | B     | 281 | HIS  |
| 1   | B     | 290 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 314 | GLN  |
| 1   | B     | 371 | ASN  |
| 1   | B     | 383 | ASN  |
| 1   | C     | 24  | GLN  |
| 1   | C     | 34  | ASN  |
| 1   | C     | 98  | ASN  |
| 1   | C     | 128 | ASN  |
| 1   | C     | 194 | GLN  |
| 1   | C     | 240 | ASN  |
| 1   | C     | 253 | ASN  |
| 1   | C     | 281 | HIS  |
| 1   | C     | 290 | ASN  |
| 1   | C     | 360 | ASN  |
| 1   | C     | 371 | ASN  |
| 1   | C     | 383 | ASN  |
| 1   | C     | 443 | GLN  |
| 1   | D     | 128 | ASN  |
| 1   | D     | 194 | GLN  |
| 1   | D     | 240 | ASN  |
| 1   | D     | 245 | HIS  |
| 1   | D     | 253 | ASN  |
| 1   | D     | 256 | ASN  |
| 1   | D     | 281 | HIS  |
| 1   | D     | 290 | ASN  |
| 1   | D     | 314 | GLN  |
| 1   | D     | 315 | ASN  |
| 1   | E     | 17  | ASN  |
| 1   | E     | 34  | ASN  |
| 1   | E     | 75  | ASN  |
| 1   | E     | 110 | ASN  |
| 1   | E     | 167 | ASN  |
| 1   | E     | 195 | HIS  |
| 1   | E     | 225 | HIS  |
| 1   | E     | 262 | ASN  |
| 1   | E     | 281 | HIS  |
| 1   | E     | 290 | ASN  |
| 1   | E     | 314 | GLN  |
| 1   | F     | 24  | GLN  |
| 1   | F     | 110 | ASN  |
| 1   | F     | 128 | ASN  |
| 1   | F     | 167 | ASN  |
| 1   | F     | 194 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 225 | HIS  |
| 1   | F     | 247 | ASN  |
| 1   | F     | 253 | ASN  |
| 1   | F     | 262 | ASN  |
| 1   | F     | 281 | HIS  |
| 1   | F     | 290 | ASN  |
| 1   | F     | 314 | GLN  |
| 1   | F     | 342 | ASN  |
| 1   | F     | 439 | 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 12 are monoatomic - leaving 6 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 3   | GLN  | E     | 503 | 2    | 5,9,9        | 0.72 | 0           | 5,11,11     | 0.38 | 0           |
| 3   | GLN  | A     | 503 | -    | 7,8,9        | 0.94 | 0           | 4,9,11      | 0.34 | 0           |
| 3   | GLN  | F     | 503 | -    | 5,9,9        | 0.57 | 0           | 5,11,11     | 0.26 | 0           |
| 3   | GLN  | D     | 503 | 2    | 5,9,9        | 0.48 | 0           | 5,11,11     | 0.17 | 0           |
| 3   | GLN  | C     | 501 | -    | 5,9,9        | 0.38 | 0           | 5,11,11     | 0.20 | 0           |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | GLN  | B     | 503 | 2    | 7,8,9        | 0.49 | 0        | 4,9,11      | 0.13 | 0        |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|-------|
| 3   | GLN  | E     | 503 | 2    | -       | 0/5/9/9  | -     |
| 3   | GLN  | A     | 503 | -    | -       | 1/6/7/9  | -     |
| 3   | GLN  | F     | 503 | -    | -       | 2/5/9/9  | -     |
| 3   | GLN  | D     | 503 | 2    | -       | 1/5/9/9  | -     |
| 3   | GLN  | C     | 501 | -    | -       | 2/5/9/9  | -     |
| 3   | GLN  | B     | 503 | 2    | -       | 1/6/7/9  | -     |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms        |
|-----|-------|-----|------|--------------|
| 3   | A     | 503 | GLN  | O-C-CA-CB    |
| 3   | F     | 503 | GLN  | N-CA-CB-CG   |
| 3   | F     | 503 | GLN  | C-CA-CB-CG   |
| 3   | D     | 503 | GLN  | CA-CB-CG-CD  |
| 3   | B     | 503 | GLN  | CA-CB-CG-CD  |
| 3   | C     | 501 | GLN  | OE1-CD-CG-CB |
| 3   | C     | 501 | GLN  | NE2-CD-CG-CB |

There are no ring outliers.

5 monomers are involved in 8 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | A     | 503 | GLN  | 2       | 0            |
| 3   | F     | 503 | GLN  | 2       | 0            |
| 3   | D     | 503 | GLN  | 1       | 0            |
| 3   | C     | 501 | GLN  | 2       | 0            |
| 3   | B     | 503 | GLN  | 1       | 0            |



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed         | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|------------------|--------|---------------|-----------------------|-------|
| 1   | A     | 443/443 (100%)   | -0.05  | 4 (0%) 84 84  | 19, 37, 66, 98        | 0     |
| 1   | B     | 443/443 (100%)   | -0.11  | 2 (0%) 91 91  | 18, 36, 61, 93        | 0     |
| 1   | C     | 443/443 (100%)   | -0.14  | 3 (0%) 87 87  | 19, 35, 62, 91        | 0     |
| 1   | D     | 443/443 (100%)   | -0.10  | 3 (0%) 87 87  | 19, 36, 62, 96        | 0     |
| 1   | E     | 443/443 (100%)   | -0.10  | 5 (1%) 80 80  | 14, 35, 63, 94        | 0     |
| 1   | F     | 443/443 (100%)   | -0.06  | 4 (0%) 84 84  | 19, 37, 66, 101       | 0     |
| All | All   | 2658/2658 (100%) | -0.09  | 21 (0%) 86 86 | 14, 36, 64, 101       | 0     |

All (21) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | F     | 384 | GLY  | 4.0  |
| 1   | C     | 86  | LYS  | 3.9  |
| 1   | A     | 384 | GLY  | 3.1  |
| 1   | D     | 385 | ILE  | 2.9  |
| 1   | B     | 377 | LYS  | 2.9  |
| 1   | E     | 201 | TYR  | 2.8  |
| 1   | F     | 381 | MET  | 2.8  |
| 1   | D     | 377 | LYS  | 2.8  |
| 1   | A     | 83  | THR  | 2.6  |
| 1   | F     | 382 | GLU  | 2.6  |
| 1   | A     | 385 | ILE  | 2.6  |
| 1   | B     | 382 | GLU  | 2.6  |
| 1   | C     | 85  | GLU  | 2.5  |
| 1   | E     | 381 | MET  | 2.4  |
| 1   | E     | 382 | GLU  | 2.3  |
| 1   | C     | 262 | ASN  | 2.2  |
| 1   | F     | 166 | GLU  | 2.1  |
| 1   | A     | 382 | GLU  | 2.0  |
| 1   | D     | 372 | ILE  | 2.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | E     | 384 | GLY  | 2.0  |
| 1   | E     | 375 | MET  | 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 monosaccharides 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(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 2   | MG   | E     | 502 | 1/1   | 0.90 | 0.19 | 27,27,27,27                | 0     |
| 3   | GLN  | B     | 503 | 9/10  | 0.91 | 0.22 | 27,29,31,32                | 0     |
| 2   | MG   | A     | 501 | 1/1   | 0.92 | 0.17 | 12,12,12,12                | 0     |
| 3   | GLN  | E     | 503 | 10/10 | 0.93 | 0.25 | 38,41,42,43                | 0     |
| 3   | GLN  | A     | 503 | 9/10  | 0.93 | 0.26 | 28,32,33,35                | 0     |
| 2   | MG   | C     | 502 | 1/1   | 0.93 | 0.26 | 31,31,31,31                | 0     |
| 2   | MG   | A     | 502 | 1/1   | 0.94 | 0.18 | 17,17,17,17                | 0     |
| 3   | GLN  | F     | 503 | 10/10 | 0.95 | 0.17 | 28,32,34,36                | 0     |
| 3   | GLN  | C     | 501 | 10/10 | 0.96 | 0.19 | 25,27,29,34                | 0     |
| 2   | MG   | B     | 501 | 1/1   | 0.97 | 0.14 | 18,18,18,18                | 0     |
| 2   | MG   | E     | 501 | 1/1   | 0.97 | 0.14 | 20,20,20,20                | 0     |
| 3   | GLN  | D     | 503 | 10/10 | 0.97 | 0.21 | 34,36,39,42                | 0     |
| 2   | MG   | D     | 501 | 1/1   | 0.98 | 0.20 | 16,16,16,16                | 0     |
| 2   | MG   | F     | 502 | 1/1   | 0.98 | 0.12 | 18,18,18,18                | 0     |
| 2   | MG   | C     | 503 | 1/1   | 0.98 | 0.18 | 13,13,13,13                | 0     |
| 2   | MG   | D     | 502 | 1/1   | 0.98 | 0.17 | 14,14,14,14                | 0     |
| 2   | MG   | B     | 502 | 1/1   | 0.98 | 0.24 | 32,32,32,32                | 0     |
| 2   | MG   | F     | 501 | 1/1   | 0.98 | 0.17 | 24,24,24,24                | 0     |

## 6.5 Other polymers

There are no such residues in this entry.