



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:57 AM GMT

PDB ID : 3K92  
Title : Crystal structure of a E93K mutant of the major Bacillus subtilis glutamate dehydrogenase RocG  
Authors : Gunka, K.; Newman, J.A.; Commichau, F.M.; Herzberg, C.; Rodrigues, C.; Hewitt, L.; Lewis, R.J.; Stulke, J.  
Deposited on : 2009-10-15  
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

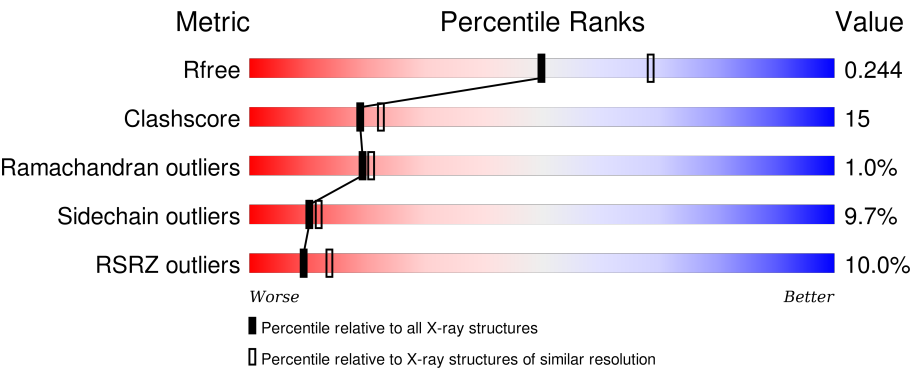
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R <sub>free</sub>     | 91344                       | 3852 (2.30-2.30)                                      |
| Clashscore            | 102246                      | 4452 (2.30-2.30)                                      |
| Ramachandran outliers | 100387                      | 4410 (2.30-2.30)                                      |
| Sidechain outliers    | 100360                      | 4409 (2.30-2.30)                                      |
| RSRZ outliers         | 91569                       | 3857 (2.30-2.30)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain                               |
|-----|-------|--------|--|
| 1   | A     | 424    | <div><div>3%</div><div>73%20%6%..</div></div>  |
| 1   | B     | 424    | <div><div>4%</div><div>71%19%6%.</div></div>   |
| 1   | C     | 424    | <div><div>14%</div><div>69%21%6%.</div></div>  |
| 1   | D     | 424    | <div><div>7%</div><div>71%20%5%.</div></div>   |
| 1   | E     | 424    | <div><div>15%</div><div>62%25%6%7%</div></div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | F     | 424    |                  |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 2   | PEG  | D     | 425 | -         | -        | X       | -                |
| 2   | PEG  | E     | 425 | -         | -        | X       | -                |

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19628 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.

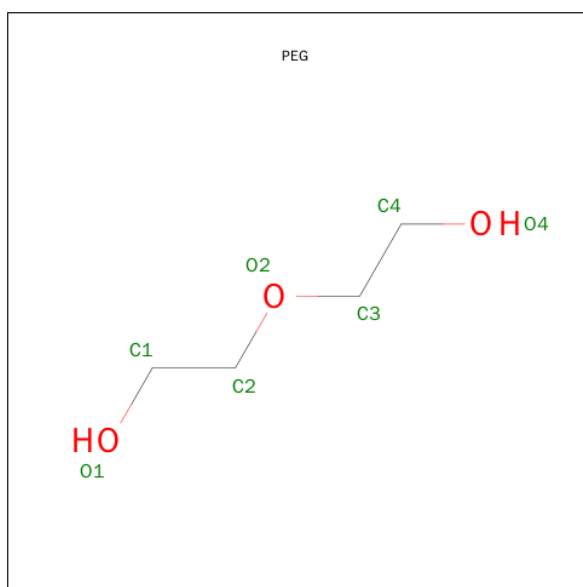
- Molecule 1 is a protein called NAD-specific glutamate dehydrogenase.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 418      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3230  | 2042 | 556 | 614 | 18 |         |         |       |
| 1   | B     | 409      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3158  | 1999 | 545 | 596 | 18 |         |         |       |
| 1   | C     | 409      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3158  | 1999 | 545 | 596 | 18 |         |         |       |
| 1   | D     | 406      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3129  | 1980 | 542 | 590 | 17 |         |         |       |
| 1   | E     | 396      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3051  | 1932 | 528 | 574 | 17 |         |         |       |
| 1   | F     | 395      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3043  | 1928 | 526 | 572 | 17 |         |         |       |

There are 12 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| A     | 93      | LYS      | GLU    | ENGINEERED MUTATION | UNP P39633 |
| A     | 324     | ARG      | ALA    | SEE REMARK 999      | UNP P39633 |
| B     | 93      | LYS      | GLU    | ENGINEERED MUTATION | UNP P39633 |
| B     | 324     | ARG      | ALA    | SEE REMARK 999      | UNP P39633 |
| C     | 93      | LYS      | GLU    | ENGINEERED MUTATION | UNP P39633 |
| C     | 324     | ARG      | ALA    | SEE REMARK 999      | UNP P39633 |
| D     | 93      | LYS      | GLU    | ENGINEERED MUTATION | UNP P39633 |
| D     | 324     | ARG      | ALA    | SEE REMARK 999      | UNP P39633 |
| E     | 93      | LYS      | GLU    | ENGINEERED MUTATION | UNP P39633 |
| E     | 324     | ARG      | ALA    | SEE REMARK 999      | UNP P39633 |
| F     | 93      | LYS      | GLU    | ENGINEERED MUTATION | UNP P39633 |
| F     | 324     | ARG      | ALA    | SEE REMARK 999      | UNP P39633 |

- Molecule 2 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 2   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 7     | 4 | 3 |         |         |
| 2   | C     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 7     | 4 | 3 |         |         |
| 2   | D     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 7     | 4 | 3 |         |         |
| 2   | E     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 7     | 4 | 3 |         |         |
| 2   | F     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 7     | 4 | 3 |         |         |

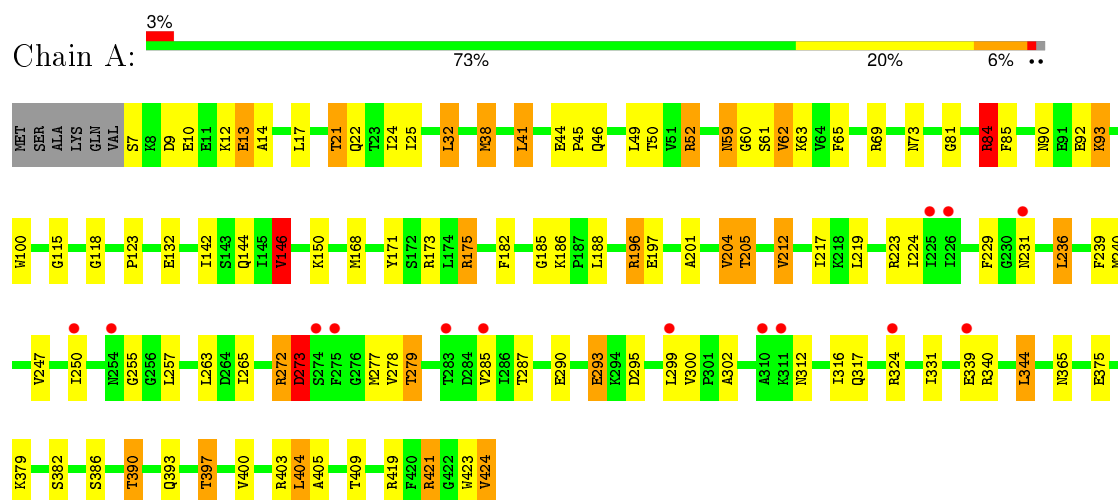
- Molecule 3 is water.

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 3   | A     | 187      | Total | O   | 0       | 0       |
|     |       |          | 187   | 187 |         |         |
| 3   | B     | 161      | Total | O   | 0       | 0       |
|     |       |          | 161   | 161 |         |         |
| 3   | C     | 133      | Total | O   | 0       | 0       |
|     |       |          | 133   | 133 |         |         |
| 3   | D     | 112      | Total | O   | 0       | 0       |
|     |       |          | 112   | 112 |         |         |
| 3   | E     | 108      | Total | O   | 0       | 0       |
|     |       |          | 108   | 108 |         |         |
| 3   | F     | 123      | Total | O   | 0       | 0       |
|     |       |          | 123   | 123 |         |         |

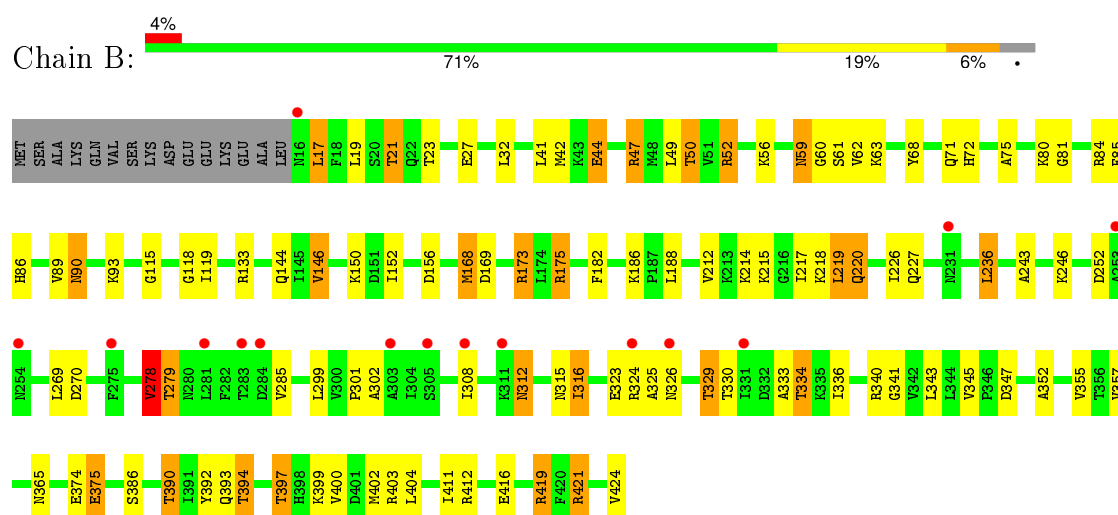
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: NAD-specific glutamate dehydrogenase



- Molecule 1: NAD-specific glutamate dehydrogenase

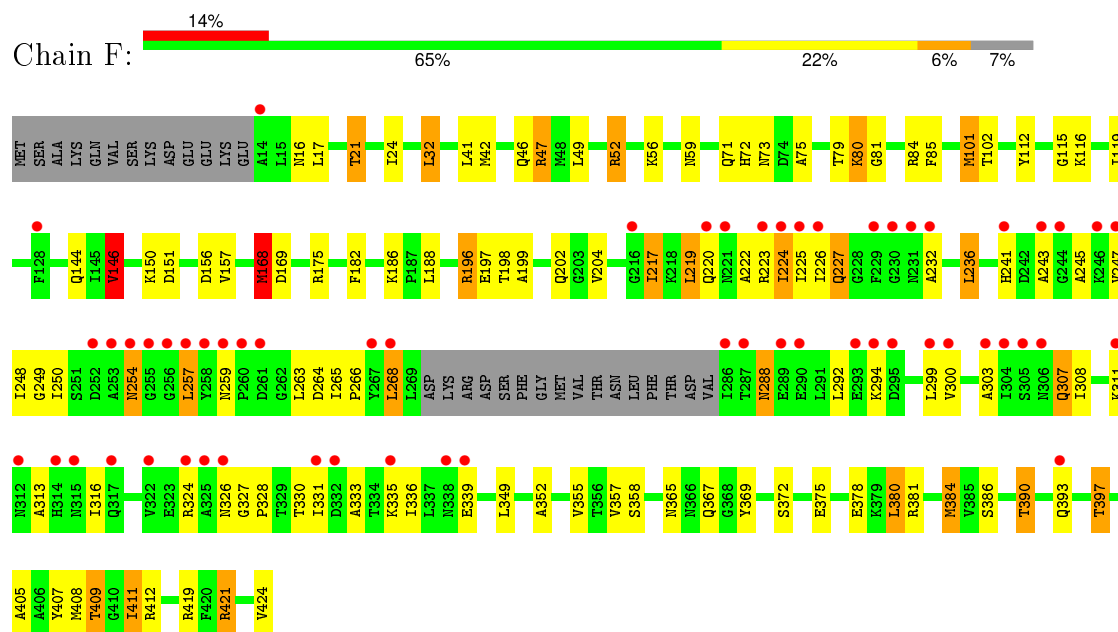


- Molecule 1: NAD-specific glutamate dehydrogenase





Chain F:





## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 21 21 21  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 137.61Å 143.07Å 162.61Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)  | 18.67 – 2.30<br>18.64 – 2.30                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.8 (18.67-2.30)<br>99.8 (18.64-2.30)                      | Depositor<br>EDS |
| $R_{merge}$   | (Not available)   | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.55 (at 2.30Å)   | Xtriage          |
| Refinement program  | REFMAC 5.5.0072   | Depositor        |
| R, $R_{free}$   | 0.182 , 0.238<br>0.189 , 0.244                              | Depositor<br>DCC |
| $R_{free}$ test set   | 7159 reflections (5.31%)                                    | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 36.9  | Xtriage          |
| Anisotropy  | 0.118   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.36 , 53.5   | EDS              |
| Estimated twinning fraction   | 0.011 for k,h,-l  | Xtriage          |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$ | Xtriage          |
| Outliers  | 0 of 141978 reflections                                     | Xtriage          |
| $F_o, F_c$ correlation  | 0.95  | EDS              |
| Total number of atoms   | 19628   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 52.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.35% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: PEG

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     | 1.12         | 5/3289 (0.2%)   | 1.10        | 20/4443 (0.5%)  |
| 1   | B     | 1.09         | 5/3217 (0.2%)   | 1.12        | 14/4348 (0.3%)  |
| 1   | C     | 1.00         | 1/3217 (0.0%)   | 0.97        | 11/4348 (0.3%)  |
| 1   | D     | 0.96         | 1/3186 (0.0%)   | 0.93        | 9/4306 (0.2%)   |
| 1   | E     | 1.01         | 0/3107          | 1.05        | 17/4197 (0.4%)  |
| 1   | F     | 1.00         | 2/3099 (0.1%)   | 0.97        | 14/4188 (0.3%)  |
| All | All   | 1.03         | 14/19115 (0.1%) | 1.03        | 85/25830 (0.3%) |

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   | D     | 0                   | 1                   |

All (14) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | B     | 63  | LYS  | CE-NZ  | 6.78  | 1.66        | 1.49     |
| 1   | B     | 374 | GLU  | CG-CD  | 5.97  | 1.60        | 1.51     |
| 1   | B     | 27  | GLU  | CG-CD  | 5.81  | 1.60        | 1.51     |
| 1   | B     | 375 | GLU  | CB-CG  | 5.66  | 1.62        | 1.52     |
| 1   | C     | 40  | GLU  | CB-CG  | 5.65  | 1.62        | 1.52     |
| 1   | B     | 75  | ALA  | CA-CB  | 5.61  | 1.64        | 1.52     |
| 1   | A     | 421 | ARG  | CD-NE  | -5.59 | 1.36        | 1.46     |
| 1   | F     | 75  | ALA  | CA-CB  | 5.46  | 1.64        | 1.52     |
| 1   | A     | 13  | GLU  | CG-CD  | 5.43  | 1.60        | 1.51     |
| 1   | A     | 375 | GLU  | CG-CD  | 5.19  | 1.59        | 1.51     |
| 1   | F     | 196 | ARG  | CZ-NH1 | 5.16  | 1.39        | 1.33     |
| 1   | D     | 378 | GLU  | CG-CD  | 5.16  | 1.59        | 1.51     |

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| Mol | Chain | Res | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1   | A     | 204 | VAL  | CB-CG2 | 5.11 | 1.63        | 1.52     |
| 1   | A     | 339 | GLU  | CG-CD  | 5.03 | 1.59        | 1.51     |

All (85) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 1   | B     | 133 | ARG  | NE-CZ-NH2  | -18.35 | 111.12      | 120.30   |
| 1   | B     | 175 | ARG  | NE-CZ-NH1  | 15.37  | 127.98      | 120.30   |
| 1   | E     | 47  | ARG  | NE-CZ-NH2  | -14.57 | 113.01      | 120.30   |
| 1   | E     | 133 | ARG  | NE-CZ-NH2  | -14.01 | 113.30      | 120.30   |
| 1   | C     | 133 | ARG  | NE-CZ-NH2  | -13.97 | 113.32      | 120.30   |
| 1   | A     | 52  | ARG  | NE-CZ-NH2  | -13.81 | 113.39      | 120.30   |
| 1   | B     | 175 | ARG  | NE-CZ-NH2  | -13.61 | 113.50      | 120.30   |
| 1   | E     | 175 | ARG  | NE-CZ-NH1  | 12.39  | 126.50      | 120.30   |
| 1   | B     | 133 | ARG  | NE-CZ-NH1  | 12.22  | 126.41      | 120.30   |
| 1   | E     | 175 | ARG  | NE-CZ-NH2  | -11.87 | 114.37      | 120.30   |
| 1   | C     | 175 | ARG  | NE-CZ-NH1  | 11.76  | 126.18      | 120.30   |
| 1   | E     | 47  | ARG  | NE-CZ-NH1  | 11.52  | 126.06      | 120.30   |
| 1   | C     | 133 | ARG  | NE-CZ-NH1  | 10.05  | 125.33      | 120.30   |
| 1   | A     | 175 | ARG  | NE-CZ-NH1  | 9.86   | 125.23      | 120.30   |
| 1   | C     | 175 | ARG  | NE-CZ-NH2  | -9.81  | 115.40      | 120.30   |
| 1   | B     | 47  | ARG  | NE-CZ-NH2  | -9.75  | 115.43      | 120.30   |
| 1   | F     | 47  | ARG  | NE-CZ-NH1  | 9.45   | 125.02      | 120.30   |
| 1   | E     | 133 | ARG  | NE-CZ-NH1  | 9.27   | 124.94      | 120.30   |
| 1   | B     | 52  | ARG  | NE-CZ-NH2  | -9.14  | 115.73      | 120.30   |
| 1   | F     | 196 | ARG  | NE-CZ-NH2  | -9.12  | 115.74      | 120.30   |
| 1   | D     | 52  | ARG  | NE-CZ-NH2  | -9.10  | 115.75      | 120.30   |
| 1   | A     | 52  | ARG  | NE-CZ-NH1  | 8.97   | 124.79      | 120.30   |
| 1   | F     | 52  | ARG  | NE-CZ-NH2  | -8.79  | 115.91      | 120.30   |
| 1   | A     | 421 | ARG  | NE-CZ-NH2  | -8.68  | 115.96      | 120.30   |
| 1   | D     | 52  | ARG  | NE-CZ-NH1  | 8.60   | 124.60      | 120.30   |
| 1   | A     | 175 | ARG  | NE-CZ-NH2  | -8.47  | 116.07      | 120.30   |
| 1   | B     | 47  | ARG  | NE-CZ-NH1  | 8.30   | 124.45      | 120.30   |
| 1   | A     | 196 | ARG  | NE-CZ-NH2  | -8.27  | 116.17      | 120.30   |
| 1   | A     | 146 | VAL  | CG1-CB-CG2 | 8.12   | 123.89      | 110.90   |
| 1   | B     | 421 | ARG  | NE-CZ-NH2  | -8.11  | 116.25      | 120.30   |
| 1   | F     | 47  | ARG  | NE-CZ-NH2  | -8.09  | 116.26      | 120.30   |
| 1   | C     | 101 | MET  | CG-SD-CE   | -8.00  | 87.39       | 100.20   |
| 1   | F     | 168 | MET  | CG-SD-CE   | 7.84   | 112.75      | 100.20   |
| 1   | B     | 52  | ARG  | NE-CZ-NH1  | 7.80   | 124.20      | 120.30   |
| 1   | A     | 421 | ARG  | NE-CZ-NH1  | 6.99   | 123.80      | 120.30   |
| 1   | E     | 52  | ARG  | NE-CZ-NH1  | 6.93   | 123.76      | 120.30   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | F     | 101 | MET  | CG-SD-CE   | -6.84 | 89.26       | 100.20   |
| 1   | A     | 403 | ARG  | NE-CZ-NH1  | 6.83  | 123.71      | 120.30   |
| 1   | F     | 196 | ARG  | NE-CZ-NH1  | 6.74  | 123.67      | 120.30   |
| 1   | F     | 52  | ARG  | NE-CZ-NH1  | 6.74  | 123.67      | 120.30   |
| 1   | D     | 175 | ARG  | NE-CZ-NH2  | 6.65  | 123.62      | 120.30   |
| 1   | C     | 52  | ARG  | NE-CZ-NH1  | 6.62  | 123.61      | 120.30   |
| 1   | A     | 340 | ARG  | NE-CZ-NH2  | -6.59 | 117.00      | 120.30   |
| 1   | B     | 133 | ARG  | CG-CD-NE   | -6.53 | 98.09       | 111.80   |
| 1   | B     | 175 | ARG  | CD-NE-CZ   | 6.52  | 132.72      | 123.60   |
| 1   | A     | 69  | ARG  | NE-CZ-NH1  | 6.34  | 123.47      | 120.30   |
| 1   | C     | 32  | LEU  | CA-CB-CG   | 6.24  | 129.66      | 115.30   |
| 1   | A     | 340 | ARG  | NE-CZ-NH1  | 6.12  | 123.36      | 120.30   |
| 1   | A     | 32  | LEU  | CA-CB-CG   | 6.07  | 129.27      | 115.30   |
| 1   | E     | 133 | ARG  | CG-CD-NE   | -6.05 | 99.09       | 111.80   |
| 1   | E     | 175 | ARG  | CD-NE-CZ   | 6.00  | 132.00      | 123.60   |
| 1   | A     | 295 | ASP  | CB-CG-OD1  | 5.98  | 123.68      | 118.30   |
| 1   | F     | 411 | ILE  | CB-CA-C    | -5.88 | 99.83       | 111.60   |
| 1   | A     | 84  | ARG  | NE-CZ-NH2  | -5.77 | 117.42      | 120.30   |
| 1   | B     | 44  | GLU  | CA-CB-CG   | 5.74  | 126.02      | 113.40   |
| 1   | A     | 196 | ARG  | NE-CZ-NH1  | 5.67  | 123.14      | 120.30   |
| 1   | E     | 324 | ARG  | NE-CZ-NH2  | -5.67 | 117.46      | 120.30   |
| 1   | F     | 421 | ARG  | NE-CZ-NH2  | -5.65 | 117.47      | 120.30   |
| 1   | E     | 421 | ARG  | NE-CZ-NH2  | -5.59 | 117.50      | 120.30   |
| 1   | D     | 146 | VAL  | CG1-CB-CG2 | 5.59  | 119.84      | 110.90   |
| 1   | B     | 421 | ARG  | NE-CZ-NH1  | 5.58  | 123.09      | 120.30   |
| 1   | D     | 196 | ARG  | NE-CZ-NH1  | 5.58  | 123.09      | 120.30   |
| 1   | A     | 403 | ARG  | NE-CZ-NH2  | -5.45 | 117.58      | 120.30   |
| 1   | D     | 196 | ARG  | NE-CZ-NH2  | -5.44 | 117.58      | 120.30   |
| 1   | E     | 69  | ARG  | NE-CZ-NH2  | -5.41 | 117.60      | 120.30   |
| 1   | E     | 424 | VAL  | CB-CA-C    | -5.40 | 101.13      | 111.40   |
| 1   | E     | 101 | MET  | CG-SD-CE   | -5.37 | 91.61       | 100.20   |
| 1   | F     | 175 | ARG  | NE-CZ-NH2  | 5.37  | 122.98      | 120.30   |
| 1   | F     | 424 | VAL  | CB-CA-C    | -5.35 | 101.24      | 111.40   |
| 1   | C     | 69  | ARG  | NE-CZ-NH1  | 5.34  | 122.97      | 120.30   |
| 1   | A     | 273 | ASP  | CB-CA-C    | -5.34 | 99.73       | 110.40   |
| 1   | C     | 412 | ARG  | CG-CD-NE   | -5.32 | 100.64      | 111.80   |
| 1   | F     | 412 | ARG  | NE-CZ-NH1  | 5.31  | 122.96      | 120.30   |
| 1   | A     | 344 | LEU  | CA-CB-CG   | 5.30  | 127.50      | 115.30   |
| 1   | D     | 69  | ARG  | NE-CZ-NH2  | -5.29 | 117.66      | 120.30   |
| 1   | D     | 412 | ARG  | NE-CZ-NH2  | -5.28 | 117.66      | 120.30   |
| 1   | E     | 52  | ARG  | NE-CZ-NH2  | -5.25 | 117.67      | 120.30   |
| 1   | F     | 146 | VAL  | CG1-CB-CG2 | 5.15  | 119.13      | 110.90   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | A     | 223 | ARG  | NE-CZ-NH2 | -5.12 | 117.74      | 120.30   |
| 1   | C     | 48  | MET  | CG-SD-CE  | -5.12 | 92.01       | 100.20   |
| 1   | E     | 412 | ARG  | NE-CZ-NH1 | 5.12  | 122.86      | 120.30   |
| 1   | B     | 44  | GLU  | N-CA-CB   | -5.11 | 101.41      | 110.60   |
| 1   | C     | 133 | ARG  | CG-CD-NE  | -5.03 | 101.24      | 111.80   |
| 1   | E     | 48  | MET  | CG-SD-CE  | -5.01 | 92.19       | 100.20   |
| 1   | D     | 421 | ARG  | NE-CZ-NH2 | -5.00 | 117.80      | 120.30   |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | D     | 325 | ALA  | Peptide |

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 3230  | 0        | 3248     | 101     | 0            |
| 1   | B     | 3158  | 0        | 3179     | 91      | 0            |
| 1   | C     | 3158  | 0        | 3179     | 107     | 0            |
| 1   | D     | 3129  | 0        | 3145     | 95      | 0            |
| 1   | E     | 3051  | 0        | 3075     | 113     | 0            |
| 1   | F     | 3043  | 0        | 3072     | 105     | 0            |
| 2   | A     | 7     | 0        | 10       | 0       | 0            |
| 2   | C     | 7     | 0        | 10       | 3       | 0            |
| 2   | D     | 7     | 0        | 10       | 4       | 0            |
| 2   | E     | 7     | 0        | 10       | 4       | 0            |
| 2   | F     | 7     | 0        | 10       | 0       | 0            |
| 3   | A     | 187   | 0        | 0        | 6       | 0            |
| 3   | B     | 161   | 0        | 0        | 11      | 0            |
| 3   | C     | 133   | 0        | 0        | 7       | 0            |
| 3   | D     | 112   | 0        | 0        | 4       | 0            |
| 3   | E     | 108   | 0        | 0        | 5       | 0            |
| 3   | F     | 123   | 0        | 0        | 7       | 0            |
| All | All   | 19628 | 0        | 18948    | 579     | 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 15.

All (579) 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:295:ASP:HA   | 1:E:317:GLN:HE21 | 1.07                     | 1.16              |
| 1:B:17:LEU:O     | 1:B:21:THR:HG23  | 1.59                     | 1.02              |
| 1:A:38:MET:HA    | 1:A:38:MET:HE3   | 1.43                     | 0.98              |
| 1:E:14:ALA:HB2   | 1:E:93:LYS:HE3   | 1.45                     | 0.96              |
| 1:E:295:ASP:CA   | 1:E:317:GLN:HE21 | 1.79                     | 0.95              |
| 1:A:205:THR:HG22 | 1:A:236:LEU:CD2  | 1.96                     | 0.95              |
| 1:C:16:ASN:N     | 1:C:19:LEU:HD23  | 1.81                     | 0.95              |
| 1:C:90:ASN:HD21  | 1:C:93:LYS:HE3   | 1.32                     | 0.95              |
| 1:A:205:THR:HG22 | 1:A:236:LEU:HD21 | 1.50                     | 0.93              |
| 1:A:405:ALA:O    | 1:A:409:THR:HG23 | 1.68                     | 0.92              |
| 1:E:310:ALA:HB3  | 1:E:311:LYS:CE   | 2.01                     | 0.91              |
| 1:D:325:ALA:HB1  | 1:D:326:ASN:HB2  | 1.52                     | 0.90              |
| 1:F:386:SER:O    | 1:F:390:THR:HG23 | 1.71                     | 0.90              |
| 1:F:250:ILE:HD13 | 1:F:263:LEU:HD22 | 1.51                     | 0.90              |
| 1:E:333:ALA:O    | 1:E:337:LEU:HD13 | 1.72                     | 0.89              |
| 1:E:312:ASN:O    | 1:E:316:ILE:HD12 | 1.72                     | 0.89              |
| 1:E:295:ASP:HA   | 1:E:317:GLN:NE2  | 1.87                     | 0.89              |
| 1:A:236:LEU:HD22 | 1:A:324:ARG:NH2  | 1.86                     | 0.89              |
| 1:E:295:ASP:CA   | 1:E:317:GLN:NE2  | 2.36                     | 0.88              |
| 1:C:215:LYS:O    | 1:C:217:ILE:HD12 | 1.73                     | 0.87              |
| 1:E:90:ASN:ND2   | 1:E:93:LYS:HD2   | 1.89                     | 0.87              |
| 1:C:16:ASN:N     | 1:C:19:LEU:CD2   | 2.39                     | 0.86              |
| 1:A:150:LYS:NZ   | 1:B:144:GLN:HE21 | 1.73                     | 0.86              |
| 1:C:268:LEU:HD23 | 1:C:278:VAL:HG11 | 1.57                     | 0.85              |
| 1:F:219:LEU:HD13 | 1:F:243:ALA:HB1  | 1.57                     | 0.85              |
| 1:A:300:VAL:HG11 | 1:A:324:ARG:NE   | 1.93                     | 0.83              |
| 1:E:310:ALA:HB3  | 1:E:311:LYS:HE3  | 1.61                     | 0.83              |
| 1:A:201:ALA:O    | 1:A:205:THR:HG23 | 1.78                     | 0.82              |
| 1:D:160:ASN:HD21 | 2:D:425:PEG:C2   | 1.93                     | 0.82              |
| 1:F:42:MET:CE    | 1:F:72:HIS:CE1   | 2.62                     | 0.82              |
| 1:A:279:THR:HG22 | 1:A:285:VAL:HG22 | 1.61                     | 0.81              |
| 1:B:390:THR:O    | 1:B:394:THR:HG23 | 1.80                     | 0.81              |
| 1:C:247:VAL:HG12 | 1:C:250:ILE:HD11 | 1.61                     | 0.81              |
| 1:E:225:ILE:HD13 | 1:E:291:LEU:HD22 | 1.60                     | 0.81              |
| 1:D:330:THR:O    | 1:D:334:THR:HG23 | 1.81                     | 0.81              |
| 1:E:90:ASN:HD21  | 1:E:93:LYS:CD    | 1.94                     | 0.81              |
| 1:F:393:GLN:O    | 1:F:397:THR:HG23 | 1.82                     | 0.79              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:50:THR:HG21  | 3:B:639:HOH:O    | 1.82                     | 0.79              |
| 1:C:90:ASN:HD21  | 1:C:93:LYS:CE    | 1.94                     | 0.79              |
| 1:E:393:GLN:O    | 1:E:397:THR:HG23 | 1.82                     | 0.79              |
| 1:D:304:ILE:CG2  | 1:D:307:GLN:NE2  | 2.45                     | 0.79              |
| 1:A:52:ARG:HD2   | 1:B:44:GLU:HB3   | 1.62                     | 0.79              |
| 1:B:17:LEU:O     | 1:B:21:THR:CG2   | 2.31                     | 0.78              |
| 1:F:308:ILE:HG22 | 1:F:333:ALA:HB1  | 1.64                     | 0.78              |
| 1:D:52:ARG:HD3   | 3:E:445:HOH:O    | 1.82                     | 0.78              |
| 1:A:44:GLU:HB3   | 1:B:52:ARG:HD2   | 1.66                     | 0.78              |
| 1:E:212:VAL:CG1  | 1:E:217:ILE:O    | 2.32                     | 0.77              |
| 1:E:321:VAL:HG12 | 1:E:344:LEU:HD23 | 1.65                     | 0.77              |
| 1:B:323:GLU:OE1  | 1:B:329:THR:HG23 | 1.84                     | 0.77              |
| 1:A:247:VAL:HB   | 1:A:265:ILE:HD11 | 1.65                     | 0.77              |
| 1:F:247:VAL:HB   | 1:F:265:ILE:HD11 | 1.66                     | 0.76              |
| 1:A:52:ARG:HD3   | 3:B:428:HOH:O    | 1.85                     | 0.76              |
| 1:A:142:ILE:HD12 | 1:A:146:VAL:HG21 | 1.68                     | 0.76              |
| 1:F:227:GLN:NE2  | 1:F:292:LEU:HD21 | 2.02                     | 0.75              |
| 1:B:386:SER:O    | 1:B:390:THR:HG23 | 1.86                     | 0.74              |
| 1:A:62:VAL:HG21  | 1:B:424:VAL:HG12 | 1.67                     | 0.74              |
| 1:B:59:ASN:HD22  | 1:B:59:ASN:C     | 1.91                     | 0.74              |
| 1:F:219:LEU:CD1  | 1:F:243:ALA:HB1  | 2.15                     | 0.74              |
| 1:F:224:ILE:HD11 | 1:F:300:VAL:HG23 | 1.68                     | 0.74              |
| 1:D:304:ILE:HG22 | 1:D:307:GLN:HE21 | 1.52                     | 0.74              |
| 1:F:17:LEU:O     | 1:F:21:THR:HG23  | 1.88                     | 0.74              |
| 1:C:173:ARG:HG3  | 3:C:819:HOH:O    | 1.88                     | 0.73              |
| 1:D:302:ALA:HB2  | 1:D:324:ARG:NH1  | 2.02                     | 0.73              |
| 1:B:227:GLN:NE2  | 1:B:302:ALA:H    | 1.85                     | 0.73              |
| 1:F:331:ILE:H    | 1:F:331:ILE:HD12 | 1.54                     | 0.73              |
| 1:F:236:LEU:HD21 | 1:F:324:ARG:HD3  | 1.69                     | 0.73              |
| 1:D:160:ASN:HD21 | 2:D:425:PEG:H21  | 1.54                     | 0.72              |
| 1:E:110:LEU:HD11 | 1:E:355:VAL:HG12 | 1.70                     | 0.72              |
| 1:F:225:ILE:HD11 | 3:F:635:HOH:O    | 1.87                     | 0.72              |
| 1:A:393:GLN:O    | 1:A:397:THR:HG23 | 1.89                     | 0.72              |
| 1:C:390:THR:O    | 1:C:394:THR:CG2  | 2.38                     | 0.71              |
| 1:A:17:LEU:O     | 1:A:21:THR:HG23  | 1.90                     | 0.71              |
| 1:E:146:VAL:HG13 | 1:E:182:PHE:CE1  | 2.25                     | 0.71              |
| 1:F:204:VAL:HG21 | 1:F:324:ARG:HD2  | 1.72                     | 0.71              |
| 1:C:278:VAL:HG12 | 1:C:279:THR:H    | 1.56                     | 0.71              |
| 1:A:236:LEU:HD13 | 1:A:324:ARG:HD3  | 1.71                     | 0.70              |
| 1:A:44:GLU:HG3   | 1:A:45:PRO:HD2   | 1.72                     | 0.70              |
| 1:B:42:MET:HE2   | 1:B:72:HIS:CE1   | 2.27                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:175:ARG:HD2  | 3:A:441:HOH:O    | 1.90                     | 0.70              |
| 1:A:293:GLU:O    | 1:A:317:GLN:NE2  | 2.21                     | 0.70              |
| 1:E:32:LEU:HD13  | 1:E:408:MET:HE2  | 1.73                     | 0.70              |
| 1:B:330:THR:O    | 1:B:334:THR:CG2  | 2.40                     | 0.69              |
| 1:B:227:GLN:HE21 | 1:B:302:ALA:H    | 1.38                     | 0.69              |
| 1:B:42:MET:CE    | 1:B:72:HIS:CE1   | 2.75                     | 0.69              |
| 1:B:90:ASN:ND2   | 1:B:93:LYS:H     | 1.90                     | 0.69              |
| 1:B:146:VAL:HG13 | 1:B:182:PHE:CE1  | 2.27                     | 0.69              |
| 1:F:116:LYS:NZ   | 1:F:156:ASP:OD2  | 2.25                     | 0.69              |
| 1:D:304:ILE:HG22 | 1:D:307:GLN:NE2  | 2.06                     | 0.69              |
| 1:D:144:GLN:HE21 | 1:E:150:LYS:NZ   | 1.91                     | 0.69              |
| 1:D:32:LEU:HD13  | 1:D:408:MET:HE3  | 1.75                     | 0.69              |
| 1:E:212:VAL:HG12 | 1:E:217:ILE:O    | 1.90                     | 0.69              |
| 1:E:14:ALA:CB    | 1:E:93:LYS:HE3   | 2.20                     | 0.69              |
| 1:E:310:ALA:HB3  | 1:E:311:LYS:HE2  | 1.75                     | 0.68              |
| 1:F:101:MET:HE1  | 3:F:503:HOH:O    | 1.94                     | 0.68              |
| 1:D:150:LYS:NZ   | 1:E:144:GLN:HE21 | 1.91                     | 0.68              |
| 1:C:337:LEU:O    | 1:C:342:VAL:HG13 | 1.93                     | 0.68              |
| 1:D:205:THR:CG2  | 1:D:236:LEU:HD13 | 2.23                     | 0.68              |
| 1:C:206:ILE:HD13 | 1:C:381:ARG:HA   | 1.76                     | 0.68              |
| 1:D:160:ASN:HD21 | 2:D:425:PEG:H22  | 1.59                     | 0.68              |
| 1:A:285:VAL:HG12 | 1:A:285:VAL:O    | 1.94                     | 0.68              |
| 1:A:236:LEU:HD13 | 1:A:324:ARG:CD   | 2.24                     | 0.68              |
| 1:E:206:ILE:HD13 | 1:E:381:ARG:HA   | 1.76                     | 0.68              |
| 1:E:298:ILE:HG23 | 1:E:320:ILE:HG22 | 1.76                     | 0.67              |
| 1:E:90:ASN:HD21  | 1:E:93:LYS:CG    | 2.07                     | 0.67              |
| 1:D:304:ILE:HG21 | 1:D:307:GLN:NE2  | 2.09                     | 0.67              |
| 1:F:380:LEU:O    | 1:F:380:LEU:HD22 | 1.93                     | 0.67              |
| 1:F:24:ILE:HG23  | 1:F:407:TYR:CD1  | 2.29                     | 0.67              |
| 1:A:132:GLU:OE2  | 3:A:517:HOH:O    | 2.13                     | 0.66              |
| 1:B:212:VAL:HG13 | 1:B:217:ILE:O    | 1.95                     | 0.66              |
| 1:C:225:ILE:HD11 | 1:C:291:LEU:HG   | 1.76                     | 0.66              |
| 1:A:236:LEU:HD13 | 1:A:324:ARG:NE   | 2.10                     | 0.66              |
| 1:C:44:GLU:HB2   | 1:F:52:ARG:HD2   | 1.77                     | 0.66              |
| 1:E:337:LEU:HB3  | 1:E:342:VAL:HG13 | 1.76                     | 0.66              |
| 1:F:101:MET:CE   | 3:F:503:HOH:O    | 2.44                     | 0.66              |
| 1:E:90:ASN:ND2   | 1:E:93:LYS:CD    | 2.52                     | 0.65              |
| 1:C:251:SER:HB2  | 1:C:291:LEU:HD23 | 1.78                     | 0.65              |
| 1:D:47:ARG:NH1   | 1:D:71:GLN:OE1   | 2.29                     | 0.65              |
| 1:A:17:LEU:O     | 1:A:21:THR:CG2   | 2.45                     | 0.65              |
| 1:D:205:THR:HG22 | 1:D:236:LEU:HD13 | 1.79                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:332:ASP:O    | 1:C:336:ILE:HD12 | 1.96                     | 0.65              |
| 1:A:150:LYS:HZ3  | 1:B:144:GLN:HE21 | 1.45                     | 0.64              |
| 1:D:32:LEU:HD13  | 1:D:408:MET:CE   | 2.26                     | 0.64              |
| 1:F:32:LEU:HD13  | 1:F:408:MET:HE3  | 1.79                     | 0.64              |
| 1:A:204:VAL:HG11 | 1:A:324:ARG:HE   | 1.62                     | 0.64              |
| 1:A:236:LEU:HB3  | 1:A:324:ARG:NH1  | 2.12                     | 0.64              |
| 1:F:419:ARG:HG3  | 1:F:419:ARG:HH11 | 1.63                     | 0.64              |
| 1:C:390:THR:O    | 1:C:394:THR:HG22 | 1.98                     | 0.64              |
| 1:F:254:ASN:N    | 1:F:254:ASN:HD22 | 1.96                     | 0.64              |
| 1:A:204:VAL:HB   | 1:A:236:LEU:HD11 | 1.79                     | 0.64              |
| 1:B:330:THR:O    | 1:B:334:THR:HG23 | 1.96                     | 0.64              |
| 1:A:279:THR:HG22 | 1:A:285:VAL:CG2  | 2.27                     | 0.64              |
| 1:C:321:VAL:HB   | 1:C:344:LEU:HD12 | 1.80                     | 0.64              |
| 1:E:90:ASN:HD21  | 1:E:93:LYS:HG3   | 1.62                     | 0.63              |
| 1:A:236:LEU:CB   | 1:A:324:ARG:NH1  | 2.61                     | 0.63              |
| 1:A:146:VAL:HG13 | 1:A:182:PHE:HE1  | 1.64                     | 0.63              |
| 1:E:258:TYR:CE1  | 1:E:294:LYS:HB3  | 2.34                     | 0.62              |
| 1:D:229:PHE:CE1  | 1:D:250:ILE:HD11 | 2.34                     | 0.62              |
| 1:D:44:GLU:HB2   | 1:E:52:ARG:HD2   | 1.81                     | 0.62              |
| 1:B:175:ARG:HD2  | 3:B:463:HOH:O    | 1.99                     | 0.62              |
| 1:C:160:ASN:HD21 | 2:C:425:PEG:C2   | 2.11                     | 0.62              |
| 1:A:287:THR:OG1  | 1:A:290:GLU:HG3  | 1.99                     | 0.62              |
| 1:B:393:GLN:O    | 1:B:397:THR:HG23 | 1.99                     | 0.62              |
| 1:C:393:GLN:NE2  | 1:C:393:GLN:HA   | 2.15                     | 0.62              |
| 1:A:279:THR:CG2  | 1:A:285:VAL:HG22 | 2.30                     | 0.62              |
| 1:C:81:GLY:HA3   | 1:C:115:GLY:O    | 1.99                     | 0.62              |
| 1:B:59:ASN:ND2   | 1:B:61:SER:H     | 1.98                     | 0.61              |
| 1:F:405:ALA:O    | 1:F:409:THR:HG23 | 2.00                     | 0.61              |
| 1:F:247:VAL:HG12 | 1:F:250:ILE:HD11 | 1.81                     | 0.61              |
| 1:F:331:ILE:N    | 1:F:331:ILE:HD12 | 2.16                     | 0.61              |
| 1:C:16:ASN:CA    | 1:C:19:LEU:HD23  | 2.30                     | 0.61              |
| 3:A:438:HOH:O    | 1:B:52:ARG:HD3   | 2.01                     | 0.61              |
| 1:F:32:LEU:HD13  | 1:F:408:MET:CE   | 2.31                     | 0.61              |
| 1:F:247:VAL:CG1  | 1:F:250:ILE:HD11 | 2.31                     | 0.61              |
| 1:A:400:VAL:HG11 | 1:A:404:LEU:HD13 | 1.83                     | 0.60              |
| 1:D:334:THR:HG22 | 1:D:403:ARG:HH21 | 1.66                     | 0.60              |
| 1:F:313:ALA:HB3  | 1:F:336:ILE:HD13 | 1.83                     | 0.60              |
| 1:B:85:PHE:CE2   | 1:B:119:ILE:HD12 | 2.36                     | 0.60              |
| 1:A:46:GLN:OE1   | 1:A:73:ASN:HA    | 2.00                     | 0.60              |
| 1:D:250:ILE:HG23 | 1:D:251:SER:N    | 2.15                     | 0.60              |
| 1:A:204:VAL:HG21 | 1:A:324:ARG:HG2  | 1.84                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:224:ILE:HG21 | 1:D:240:MET:HG2  | 1.84                     | 0.60              |
| 1:A:205:THR:HG22 | 1:A:236:LEU:HD23 | 1.80                     | 0.60              |
| 1:B:146:VAL:HG13 | 1:B:182:PHE:HE1  | 1.65                     | 0.60              |
| 1:C:48:MET:HE1   | 1:C:50:THR:HG22  | 1.84                     | 0.60              |
| 1:E:321:VAL:CG1  | 1:E:344:LEU:HD23 | 2.31                     | 0.59              |
| 1:A:24:ILE:HD11  | 1:A:331:ILE:HD11 | 1.84                     | 0.59              |
| 1:A:52:ARG:CD    | 3:B:428:HOH:O    | 2.46                     | 0.59              |
| 1:A:81:GLY:HA3   | 1:A:115:GLY:O    | 2.03                     | 0.59              |
| 1:B:301:PRO:O    | 1:B:324:ARG:HD2  | 2.03                     | 0.59              |
| 1:A:255:GLY:HA3  | 1:A:285:VAL:CG1  | 2.33                     | 0.59              |
| 1:A:146:VAL:HG13 | 1:A:182:PHE:CE1  | 2.36                     | 0.59              |
| 1:E:319:SER:C    | 1:E:342:VAL:HG23 | 2.23                     | 0.59              |
| 1:D:229:PHE:CZ   | 1:D:250:ILE:HD11 | 2.37                     | 0.59              |
| 1:D:219:LEU:CD2  | 1:D:240:MET:CE   | 2.81                     | 0.59              |
| 1:A:255:GLY:HA3  | 1:A:285:VAL:HG13 | 1.84                     | 0.59              |
| 1:C:309:THR:HG22 | 1:C:310:ALA:N    | 2.18                     | 0.59              |
| 1:F:46:GLN:OE1   | 1:F:73:ASN:HA    | 2.03                     | 0.59              |
| 1:C:280:ASN:OD1  | 1:C:281:LEU:HD23 | 2.03                     | 0.59              |
| 1:E:393:GLN:O    | 1:E:397:THR:CG2  | 2.51                     | 0.58              |
| 1:C:337:LEU:O    | 1:C:342:VAL:CG1  | 2.51                     | 0.58              |
| 1:E:227:GLN:C    | 1:E:302:ALA:HB2  | 2.23                     | 0.58              |
| 1:E:160:ASN:HD21 | 2:E:425:PEG:C2   | 2.15                     | 0.58              |
| 1:A:224:ILE:HD13 | 1:A:240:MET:HG3  | 1.85                     | 0.58              |
| 1:B:59:ASN:HD22  | 1:B:60:GLY:N     | 2.01                     | 0.58              |
| 1:C:393:GLN:HE21 | 1:C:393:GLN:HA   | 1.67                     | 0.58              |
| 1:C:16:ASN:HA    | 1:C:19:LEU:HD23  | 1.84                     | 0.58              |
| 1:C:247:VAL:CG1  | 1:C:250:ILE:HD11 | 2.34                     | 0.58              |
| 1:C:309:THR:CG2  | 1:C:310:ALA:N    | 2.66                     | 0.58              |
| 1:C:44:GLU:CB    | 1:F:52:ARG:HD2   | 2.33                     | 0.58              |
| 1:D:337:LEU:HB3  | 1:D:342:VAL:HG22 | 1.86                     | 0.58              |
| 1:D:219:LEU:HD21 | 1:D:240:MET:CE   | 2.34                     | 0.58              |
| 1:E:201:ALA:O    | 1:E:205:THR:HG23 | 2.04                     | 0.58              |
| 1:D:334:THR:CG2  | 1:D:403:ARG:HH21 | 2.17                     | 0.58              |
| 1:F:352:ALA:O    | 1:F:355:VAL:HG12 | 2.03                     | 0.58              |
| 1:A:38:MET:HA    | 1:A:38:MET:CE    | 2.28                     | 0.58              |
| 1:D:194:GLN:NE2  | 3:D:441:HOH:O    | 2.37                     | 0.58              |
| 1:E:47:ARG:HD2   | 1:E:71:GLN:OE1   | 2.04                     | 0.58              |
| 1:F:219:LEU:HD13 | 1:F:243:ALA:CB   | 2.34                     | 0.57              |
| 1:E:224:ILE:HG21 | 1:E:240:MET:HG3  | 1.85                     | 0.57              |
| 1:B:186:LYS:NZ   | 1:B:365:ASN:HD21 | 2.02                     | 0.57              |
| 1:C:257:LEU:CD2  | 1:C:279:THR:HG22 | 2.35                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:205:THR:HG22 | 1:D:236:LEU:CD1  | 2.34                     | 0.57              |
| 1:E:405:ALA:O    | 1:E:409:THR:HG23 | 2.05                     | 0.57              |
| 1:E:268:LEU:C    | 1:E:269:LEU:HD22 | 2.24                     | 0.57              |
| 1:A:236:LEU:HD22 | 1:A:324:ARG:HH21 | 1.68                     | 0.57              |
| 1:A:386:SER:O    | 1:A:390:THR:HG23 | 2.04                     | 0.57              |
| 1:E:295:ASP:N    | 1:E:317:GLN:NE2  | 2.52                     | 0.56              |
| 1:E:122:ASP:OD1  | 1:E:124:ARG:HD2  | 2.05                     | 0.56              |
| 1:E:295:ASP:CB   | 1:E:317:GLN:NE2  | 2.68                     | 0.56              |
| 1:E:48:MET:HE1   | 1:E:50:THR:HG22  | 1.87                     | 0.56              |
| 1:F:294:LYS:HB3  | 3:F:635:HOH:O    | 2.06                     | 0.56              |
| 1:B:390:THR:O    | 1:B:394:THR:CG2  | 2.52                     | 0.56              |
| 1:F:247:VAL:O    | 1:F:263:LEU:HD13 | 2.06                     | 0.56              |
| 1:C:250:ILE:HD13 | 1:C:263:LEU:HD22 | 1.88                     | 0.56              |
| 1:F:42:MET:HE2   | 1:F:72:HIS:CE1   | 2.41                     | 0.56              |
| 1:D:219:LEU:CD2  | 1:D:240:MET:HE3  | 2.36                     | 0.56              |
| 1:A:300:VAL:HG11 | 1:A:324:ARG:CD   | 2.36                     | 0.56              |
| 1:E:404:LEU:HD22 | 1:E:404:LEU:O    | 2.05                     | 0.56              |
| 1:C:249:GLY:HA3  | 1:C:291:LEU:HD11 | 1.86                     | 0.56              |
| 1:B:47:ARG:HD2   | 1:B:71:GLN:OE1   | 2.05                     | 0.56              |
| 1:C:390:THR:O    | 1:C:394:THR:HG23 | 2.06                     | 0.56              |
| 1:A:263:LEU:O    | 1:A:265:ILE:HD12 | 2.05                     | 0.55              |
| 1:C:48:MET:CE    | 1:C:50:THR:HG22  | 2.36                     | 0.55              |
| 1:D:349:LEU:HD22 | 1:D:391:ILE:HD12 | 1.86                     | 0.55              |
| 1:C:309:THR:HG22 | 1:C:311:LYS:H    | 1.70                     | 0.55              |
| 1:D:212:VAL:HG21 | 1:D:298:ILE:HD11 | 1.88                     | 0.55              |
| 1:D:217:ILE:HG22 | 1:D:218:LYS:O    | 2.06                     | 0.55              |
| 1:D:86:HIS:CE1   | 1:D:88:GLU:HG2   | 2.40                     | 0.55              |
| 1:B:90:ASN:HD22  | 1:B:90:ASN:C     | 2.08                     | 0.55              |
| 1:F:247:VAL:HG21 | 1:F:265:ILE:HG13 | 1.89                     | 0.55              |
| 1:A:424:VAL:HG12 | 1:B:62:VAL:HG11  | 1.88                     | 0.55              |
| 1:C:333:ALA:O    | 1:C:337:LEU:HD13 | 2.07                     | 0.55              |
| 1:A:300:VAL:HG11 | 1:A:324:ARG:CZ   | 2.36                     | 0.55              |
| 1:F:386:SER:O    | 1:F:390:THR:CG2  | 2.51                     | 0.55              |
| 1:E:16:ASN:O     | 1:E:20:SER:HB3   | 2.06                     | 0.55              |
| 1:B:315:ASN:N    | 1:B:315:ASN:HD22 | 2.05                     | 0.55              |
| 1:B:400:VAL:HG11 | 1:B:404:LEU:HD23 | 1.89                     | 0.55              |
| 1:C:259:ASN:HB3  | 1:C:263:LEU:HD12 | 1.89                     | 0.54              |
| 1:D:256:GLY:HA3  | 1:D:291:LEU:HD22 | 1.88                     | 0.54              |
| 1:E:212:VAL:HG13 | 1:E:217:ILE:HB   | 1.89                     | 0.54              |
| 1:A:186:LYS:NZ   | 1:A:365:ASN:HD21 | 2.05                     | 0.54              |
| 1:B:329:THR:OG1  | 1:B:334:THR:HG22 | 2.06                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:59:ASN:C     | 1:B:59:ASN:ND2   | 2.61                     | 0.54              |
| 1:E:169:ASP:HB2  | 1:F:421:ARG:HD3  | 1.90                     | 0.54              |
| 1:E:335:LYS:NZ   | 1:E:339:GLU:OE2  | 2.40                     | 0.54              |
| 1:C:150:LYS:NZ   | 1:F:144:GLN:HE21 | 2.06                     | 0.54              |
| 1:F:146:VAL:HG13 | 1:F:182:PHE:CE1  | 2.41                     | 0.54              |
| 1:C:90:ASN:HD21  | 1:C:93:LYS:CD    | 2.19                     | 0.54              |
| 1:B:330:THR:O    | 1:B:334:THR:HG22 | 2.08                     | 0.54              |
| 1:E:389:GLU:OE2  | 1:E:393:GLN:OE1  | 2.26                     | 0.54              |
| 1:D:150:LYS:HZ2  | 1:E:144:GLN:HE21 | 1.54                     | 0.54              |
| 1:D:160:ASN:ND2  | 2:D:425:PEG:H21  | 2.21                     | 0.53              |
| 1:D:144:GLN:HE21 | 1:E:150:LYS:HZ3  | 1.55                     | 0.53              |
| 3:C:437:HOH:O    | 1:F:52:ARG:HD3   | 2.08                     | 0.53              |
| 1:E:160:ASN:HD21 | 2:E:425:PEG:H22  | 1.72                     | 0.53              |
| 1:F:331:ILE:H    | 1:F:331:ILE:CD1  | 2.21                     | 0.53              |
| 1:D:110:LEU:HD11 | 1:D:355:VAL:HG12 | 1.90                     | 0.53              |
| 1:F:17:LEU:O     | 1:F:21:THR:CG2   | 2.55                     | 0.53              |
| 1:E:186:LYS:NZ   | 1:E:365:ASN:HD21 | 2.07                     | 0.53              |
| 1:F:247:VAL:HG12 | 1:F:250:ILE:CD1  | 2.39                     | 0.53              |
| 1:F:156:ASP:OD1  | 1:F:157:VAL:N    | 2.41                     | 0.53              |
| 1:D:405:ALA:O    | 1:D:409:THR:HG23 | 2.09                     | 0.53              |
| 1:E:337:LEU:HB3  | 1:E:342:VAL:CG1  | 2.39                     | 0.53              |
| 1:E:21:THR:O     | 1:E:25:ILE:HD13  | 2.08                     | 0.53              |
| 1:D:63:LYS:HE2   | 3:D:591:HOH:O    | 2.09                     | 0.53              |
| 1:E:48:MET:CE    | 1:E:50:THR:HG22  | 2.38                     | 0.53              |
| 1:B:214:LYS:HG2  | 1:B:392:TYR:CZ   | 2.44                     | 0.53              |
| 1:A:59:ASN:C     | 1:A:59:ASN:HD22  | 2.10                     | 0.53              |
| 1:A:236:LEU:HB3  | 1:A:324:ARG:CZ   | 2.38                     | 0.53              |
| 1:B:386:SER:O    | 1:B:390:THR:CG2  | 2.57                     | 0.53              |
| 1:C:84:ARG:NH1   | 1:C:156:ASP:OD1  | 2.42                     | 0.53              |
| 1:A:38:MET:CE    | 1:A:424:VAL:HG21 | 2.39                     | 0.53              |
| 1:E:311:LYS:O    | 1:E:312:ASN:CG   | 2.47                     | 0.53              |
| 1:B:334:THR:HG21 | 1:B:403:ARG:HH21 | 1.73                     | 0.53              |
| 1:B:219:LEU:HD13 | 1:B:243:ALA:HB1  | 1.90                     | 0.53              |
| 1:C:303:ALA:C    | 1:C:304:ILE:HD13 | 2.30                     | 0.53              |
| 1:B:345:VAL:HA   | 1:B:402:MET:HE3  | 1.90                     | 0.52              |
| 1:D:186:LYS:NZ   | 1:D:365:ASN:HD21 | 2.06                     | 0.52              |
| 1:B:42:MET:HA    | 1:B:42:MET:HE3   | 1.90                     | 0.52              |
| 1:F:80:LYS:HG3   | 1:F:112:TYR:CD2  | 2.44                     | 0.52              |
| 1:E:367:GLN:HE21 | 1:F:367:GLN:HE21 | 1.58                     | 0.52              |
| 1:E:212:VAL:HG13 | 1:E:217:ILE:O    | 2.08                     | 0.52              |
| 1:A:38:MET:HE1   | 1:A:41:LEU:HD12  | 1.90                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:52:ARG:HD2   | 1:E:44:GLU:HB3   | 1.91                     | 0.52              |
| 1:C:390:THR:HG22 | 3:C:745:HOH:O    | 2.07                     | 0.52              |
| 1:E:367:GLN:NE2  | 1:F:367:GLN:HE21 | 2.06                     | 0.52              |
| 1:B:218:LYS:NZ   | 3:B:586:HOH:O    | 2.43                     | 0.52              |
| 1:A:379:LYS:HE2  | 1:F:369:TYR:OH   | 2.10                     | 0.52              |
| 1:B:226:ILE:HD13 | 1:B:236:LEU:HB3  | 1.91                     | 0.52              |
| 1:F:204:VAL:HG21 | 1:F:324:ARG:CD   | 2.40                     | 0.52              |
| 1:E:146:VAL:HG13 | 1:E:182:PHE:HE1  | 1.70                     | 0.52              |
| 1:A:150:LYS:NZ   | 1:B:144:GLN:NE2  | 2.51                     | 0.52              |
| 1:A:273:ASP:HB2  | 1:A:277:MET:H    | 1.74                     | 0.52              |
| 1:C:160:ASN:HD21 | 2:C:425:PEG:H21  | 1.74                     | 0.51              |
| 1:A:144:GLN:HE21 | 1:B:150:LYS:NZ   | 2.08                     | 0.51              |
| 1:D:17:LEU:HD12  | 1:D:93:LYS:HE3   | 1.91                     | 0.51              |
| 1:B:419:ARG:C    | 1:B:419:ARG:HD2  | 2.30                     | 0.51              |
| 1:C:81:GLY:O     | 1:C:153:PRO:HA   | 2.11                     | 0.51              |
| 1:E:265:ILE:HA   | 1:E:268:LEU:HD12 | 1.92                     | 0.51              |
| 1:D:101:MET:SD   | 3:D:801:HOH:O    | 2.60                     | 0.51              |
| 1:A:229:PHE:CD1  | 1:A:250:ILE:HD12 | 2.44                     | 0.51              |
| 1:B:186:LYS:HZ1  | 1:B:365:ASN:HD21 | 1.56                     | 0.51              |
| 1:C:100:TRP:CZ3  | 1:C:348:ILE:HD12 | 2.45                     | 0.51              |
| 1:A:393:GLN:NE2  | 1:A:393:GLN:HA   | 2.25                     | 0.51              |
| 1:D:205:THR:CG2  | 1:D:236:LEU:CD1  | 2.89                     | 0.51              |
| 1:C:160:ASN:HD21 | 2:C:425:PEG:H22  | 1.76                     | 0.51              |
| 1:D:227:GLN:HB2  | 1:D:302:ALA:H    | 1.76                     | 0.51              |
| 1:E:146:VAL:CG1  | 1:E:182:PHE:CE1  | 2.94                     | 0.51              |
| 1:E:404:LEU:O    | 1:E:404:LEU:CD2  | 2.59                     | 0.51              |
| 1:F:349:LEU:HD11 | 1:F:384:MET:HE1  | 1.93                     | 0.51              |
| 1:C:394:THR:HG21 | 3:C:482:HOH:O    | 2.09                     | 0.51              |
| 1:E:330:THR:HG23 | 3:E:655:HOH:O    | 2.11                     | 0.51              |
| 1:E:290:GLU:O    | 1:E:294:LYS:HG2  | 2.11                     | 0.50              |
| 1:C:327:GLY:N    | 1:C:328:PRO:CD   | 2.75                     | 0.50              |
| 3:D:470:HOH:O    | 1:E:52:ARG:HD3   | 2.10                     | 0.50              |
| 1:C:186:LYS:NZ   | 1:C:365:ASN:HD21 | 2.10                     | 0.50              |
| 1:C:302:ALA:O    | 1:C:303:ALA:HB3  | 2.11                     | 0.50              |
| 1:F:81:GLY:HA3   | 1:F:115:GLY:O    | 2.12                     | 0.50              |
| 1:A:204:VAL:HG11 | 1:A:324:ARG:NE   | 2.25                     | 0.50              |
| 1:B:315:ASN:N    | 1:B:315:ASN:ND2  | 2.56                     | 0.50              |
| 1:C:90:ASN:ND2   | 1:C:93:LYS:HD2   | 2.26                     | 0.50              |
| 1:E:131:LEU:HD13 | 2:E:425:PEG:H42  | 1.92                     | 0.50              |
| 1:E:404:LEU:HD22 | 1:E:408:MET:HG3  | 1.94                     | 0.49              |
| 1:A:24:ILE:HD11  | 1:A:331:ILE:CD1  | 2.42                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:306:ASN:OD1  | 1:C:306:ASN:N    | 2.45                     | 0.49              |
| 1:A:236:LEU:CB   | 1:A:324:ARG:CZ   | 2.90                     | 0.49              |
| 1:F:224:ILE:HD12 | 1:F:226:ILE:HG13 | 1.94                     | 0.49              |
| 1:F:308:ILE:HG22 | 1:F:333:ALA:CB   | 2.40                     | 0.49              |
| 1:C:405:ALA:O    | 1:C:409:THR:HG23 | 2.12                     | 0.49              |
| 1:D:345:VAL:HA   | 1:D:402:MET:CE   | 2.43                     | 0.49              |
| 1:C:90:ASN:ND2   | 1:C:93:LYS:CD    | 2.76                     | 0.49              |
| 1:D:304:ILE:N    | 1:D:304:ILE:HD13 | 2.28                     | 0.49              |
| 1:C:386:SER:O    | 1:C:390:THR:HG23 | 2.11                     | 0.49              |
| 1:B:84:ARG:NH1   | 1:B:156:ASP:OD1  | 2.46                     | 0.49              |
| 1:A:386:SER:O    | 1:A:390:THR:CG2  | 2.61                     | 0.49              |
| 1:B:316:ILE:O    | 1:B:340:ARG:NH1  | 2.44                     | 0.49              |
| 1:C:257:LEU:HB2  | 1:C:263:LEU:HD21 | 1.95                     | 0.49              |
| 1:B:375:GLU:HB3  | 3:B:482:HOH:O    | 2.13                     | 0.49              |
| 1:C:340:ARG:HD3  | 3:C:625:HOH:O    | 2.13                     | 0.48              |
| 1:C:40:GLU:OE1   | 1:C:43:LYS:NZ    | 2.26                     | 0.48              |
| 1:C:201:ALA:HB2  | 1:C:324:ARG:HH22 | 1.76                     | 0.48              |
| 1:C:304:ILE:HG22 | 1:C:305:SER:H    | 1.78                     | 0.48              |
| 1:E:330:THR:CG2  | 3:E:655:HOH:O    | 2.61                     | 0.48              |
| 1:D:220:GLN:O    | 1:D:244:GLY:O    | 2.32                     | 0.48              |
| 1:D:393:GLN:O    | 1:D:397:THR:HG23 | 2.13                     | 0.48              |
| 1:F:247:VAL:CB   | 1:F:265:ILE:HD11 | 2.40                     | 0.48              |
| 1:B:90:ASN:HD21  | 1:B:93:LYS:H     | 1.61                     | 0.48              |
| 1:C:19:LEU:H     | 1:C:19:LEU:HD22  | 1.77                     | 0.48              |
| 1:D:304:ILE:H    | 1:D:304:ILE:HD13 | 1.77                     | 0.48              |
| 1:B:308:ILE:HB   | 1:B:329:THR:HB   | 1.96                     | 0.48              |
| 1:D:232:ALA:O    | 1:D:236:LEU:HD23 | 2.14                     | 0.48              |
| 1:A:38:MET:CE    | 1:A:41:LEU:HD12  | 2.43                     | 0.48              |
| 1:A:14:ALA:HB1   | 1:A:90:ASN:HD21  | 1.79                     | 0.48              |
| 1:A:302:ALA:HB2  | 1:A:324:ARG:HD2  | 1.95                     | 0.48              |
| 1:D:227:GLN:HE21 | 1:D:288:ASN:HD22 | 1.60                     | 0.48              |
| 1:D:404:LEU:HD22 | 1:D:404:LEU:O    | 2.14                     | 0.48              |
| 1:A:257:LEU:HG   | 1:A:279:THR:HG23 | 1.94                     | 0.47              |
| 1:D:44:GLU:CB    | 1:E:52:ARG:HD2   | 2.44                     | 0.47              |
| 1:E:313:ALA:HB1  | 1:E:336:ILE:HG21 | 1.95                     | 0.47              |
| 1:A:38:MET:CA    | 1:A:38:MET:HE3   | 2.31                     | 0.47              |
| 1:A:38:MET:HE3   | 1:A:424:VAL:HG21 | 1.96                     | 0.47              |
| 1:B:252:ASP:OD2  | 1:B:278:VAL:O    | 2.32                     | 0.47              |
| 1:C:175:ARG:NH2  | 1:E:176:GLU:OE2  | 2.36                     | 0.47              |
| 1:D:302:ALA:HB2  | 1:D:324:ARG:HH12 | 1.75                     | 0.47              |
| 1:F:219:LEU:CD1  | 1:F:243:ALA:CB   | 2.88                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:393:GLN:HE21 | 1:A:393:GLN:HA   | 1.78                     | 0.47              |
| 1:F:24:ILE:HD13  | 1:F:407:TYR:CE1  | 2.49                     | 0.47              |
| 1:E:265:ILE:N    | 1:E:266:PRO:CD   | 2.78                     | 0.47              |
| 1:D:85:PHE:CE2   | 1:D:119:ILE:HD12 | 2.49                     | 0.47              |
| 1:B:279:THR:O    | 1:B:285:VAL:HG21 | 2.14                     | 0.47              |
| 1:E:232:ALA:HB1  | 1:E:324:ARG:HD3  | 1.97                     | 0.47              |
| 1:E:302:ALA:O    | 1:E:304:ILE:N    | 2.47                     | 0.47              |
| 1:D:257:LEU:N    | 1:D:257:LEU:HD22 | 2.29                     | 0.47              |
| 1:C:169:ASP:OD1  | 1:D:421:ARG:HD2  | 2.15                     | 0.47              |
| 1:D:48:MET:HE2   | 1:D:91:GLU:HG3   | 1.97                     | 0.47              |
| 1:C:284:ASP:O    | 1:C:285:VAL:HG23 | 2.15                     | 0.47              |
| 1:A:205:THR:HG21 | 1:A:239:PHE:CG   | 2.49                     | 0.47              |
| 1:F:59:ASN:OD1   | 1:F:59:ASN:C     | 2.52                     | 0.47              |
| 1:B:220:GLN:HG2  | 3:B:811:HOH:O    | 2.14                     | 0.47              |
| 1:E:194:GLN:NE2  | 3:E:838:HOH:O    | 2.48                     | 0.47              |
| 1:B:50:THR:HB    | 1:B:68:TYR:CD1   | 2.49                     | 0.47              |
| 1:D:219:LEU:HD23 | 1:D:240:MET:HE3  | 1.96                     | 0.47              |
| 1:E:81:GLY:O     | 1:E:153:PRO:HA   | 2.14                     | 0.47              |
| 1:E:175:ARG:HD2  | 3:E:448:HOH:O    | 2.15                     | 0.46              |
| 1:F:405:ALA:O    | 1:F:409:THR:CG2  | 2.63                     | 0.46              |
| 1:D:219:LEU:HD23 | 1:D:240:MET:CE   | 2.45                     | 0.46              |
| 1:E:73:ASN:O     | 1:E:113:GLY:HA3  | 2.15                     | 0.46              |
| 1:E:296:CYS:SG   | 1:E:318:ALA:HB2  | 2.56                     | 0.46              |
| 1:E:226:ILE:HA   | 1:E:300:VAL:HG13 | 1.96                     | 0.46              |
| 1:D:248:ILE:CG2  | 1:D:258:TYR:CE1  | 2.98                     | 0.46              |
| 1:F:335:LYS:O    | 1:F:339:GLU:HG2  | 2.15                     | 0.46              |
| 1:A:421:ARG:HD2  | 1:F:169:ASP:OD1  | 2.15                     | 0.46              |
| 1:C:201:ALA:HB1  | 1:C:235:PHE:CD1  | 2.50                     | 0.46              |
| 1:F:42:MET:HE3   | 1:F:72:HIS:CE1   | 2.50                     | 0.46              |
| 1:F:24:ILE:CG2   | 1:F:407:TYR:CD1  | 2.97                     | 0.46              |
| 1:E:81:GLY:HA3   | 1:E:115:GLY:O    | 2.15                     | 0.46              |
| 1:C:86:HIS:CG    | 1:C:87:PRO:HD2   | 2.51                     | 0.46              |
| 1:C:278:VAL:HG12 | 1:C:279:THR:N    | 2.28                     | 0.46              |
| 1:C:90:ASN:ND2   | 1:C:93:LYS:CE    | 2.72                     | 0.46              |
| 1:C:225:ILE:HD12 | 1:C:291:LEU:CD1  | 2.45                     | 0.46              |
| 1:D:229:PHE:CD1  | 1:D:250:ILE:HD11 | 2.51                     | 0.46              |
| 1:F:232:ALA:O    | 1:F:236:LEU:HD22 | 2.16                     | 0.46              |
| 1:C:227:GLN:HA   | 1:C:251:SER:HB3  | 1.98                     | 0.46              |
| 1:A:185:GLY:HA2  | 1:A:196:ARG:HD3  | 1.98                     | 0.46              |
| 1:F:264:ASP:O    | 1:F:268:LEU:HD13 | 2.15                     | 0.46              |
| 1:A:196:ARG:HG2  | 1:A:197:GLU:N    | 2.30                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:224:ILE:HD13 | 1:C:240:MET:HG3  | 1.98                     | 0.46              |
| 1:E:90:ASN:HD22  | 1:E:93:LYS:HD2   | 1.74                     | 0.46              |
| 1:F:224:ILE:HD11 | 1:F:300:VAL:CG2  | 2.41                     | 0.46              |
| 1:E:337:LEU:O    | 1:E:342:VAL:HG12 | 2.16                     | 0.46              |
| 1:E:292:LEU:HD13 | 1:E:307:GLN:O    | 2.16                     | 0.46              |
| 1:B:80:LYS:HD2   | 1:B:152:ILE:HB   | 1.98                     | 0.46              |
| 1:F:47:ARG:HD2   | 1:F:71:GLN:OE1   | 2.16                     | 0.46              |
| 1:A:236:LEU:HD22 | 1:A:324:ARG:CZ   | 2.44                     | 0.45              |
| 1:D:325:ALA:O    | 1:D:328:PRO:HD3  | 2.16                     | 0.45              |
| 1:D:344:LEU:C    | 1:D:344:LEU:HD23 | 2.36                     | 0.45              |
| 1:E:311:LYS:O    | 1:E:312:ASN:CB   | 2.64                     | 0.45              |
| 1:D:408:MET:O    | 1:D:412:ARG:HB2  | 2.16                     | 0.45              |
| 1:B:215:LYS:NZ   | 1:B:341:GLY:O    | 2.49                     | 0.45              |
| 1:A:59:ASN:C     | 1:A:59:ASN:ND2   | 2.69                     | 0.45              |
| 1:C:100:TRP:HZ3  | 1:C:348:ILE:HD12 | 1.80                     | 0.45              |
| 1:D:279:THR:HG23 | 1:D:285:VAL:CG2  | 2.46                     | 0.45              |
| 1:F:196:ARG:HD2  | 3:F:634:HOH:O    | 2.16                     | 0.45              |
| 1:F:219:LEU:O    | 1:F:245:ALA:HB2  | 2.16                     | 0.45              |
| 1:F:372:SER:OG   | 1:F:375:GLU:HG3  | 2.17                     | 0.45              |
| 1:C:250:ILE:HG22 | 1:C:250:ILE:O    | 2.17                     | 0.45              |
| 1:F:307:GLN:OE1  | 1:F:307:GLN:CA   | 2.64                     | 0.45              |
| 1:D:214:LYS:HD2  | 1:D:392:TYR:CE2  | 2.52                     | 0.45              |
| 1:A:59:ASN:ND2   | 1:A:61:SER:H     | 2.15                     | 0.45              |
| 1:F:217:ILE:HD11 | 1:F:222:ALA:HB2  | 1.99                     | 0.45              |
| 1:E:327:GLY:N    | 1:E:328:PRO:CD   | 2.79                     | 0.45              |
| 1:D:205:THR:HG23 | 1:D:236:LEU:HD13 | 1.97                     | 0.45              |
| 1:A:212:VAL:HG13 | 1:A:217:ILE:O    | 2.17                     | 0.45              |
| 1:A:7:SER:HB3    | 1:A:10:GLU:OE1   | 2.17                     | 0.45              |
| 1:C:255:GLY:O    | 1:C:279:THR:HG21 | 2.17                     | 0.45              |
| 1:A:22:GLN:O     | 1:A:25:ILE:HG22  | 2.17                     | 0.45              |
| 1:E:160:ASN:HD21 | 2:E:425:PEG:H21  | 1.81                     | 0.45              |
| 1:A:150:LYS:HZ2  | 1:B:144:GLN:HE21 | 1.57                     | 0.44              |
| 3:A:428:HOH:O    | 1:B:50:THR:HG23  | 2.16                     | 0.44              |
| 1:C:268:LEU:O    | 1:C:272:ARG:HG3  | 2.16                     | 0.44              |
| 1:D:73:ASN:O     | 1:D:113:GLY:HA3  | 2.17                     | 0.44              |
| 1:B:352:ALA:O    | 1:B:355:VAL:HG22 | 2.18                     | 0.44              |
| 1:E:408:MET:O    | 1:E:411:ILE:HD12 | 2.17                     | 0.44              |
| 1:B:86:HIS:HB3   | 1:B:89:VAL:HG23  | 1.98                     | 0.44              |
| 1:D:333:ALA:O    | 1:D:337:LEU:HD12 | 2.18                     | 0.44              |
| 1:C:82:GLY:O     | 1:C:116:LYS:HD3  | 2.18                     | 0.44              |
| 1:C:247:VAL:HB   | 1:C:265:ILE:HD11 | 1.99                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:333:ALA:O    | 1:C:337:LEU:CD1  | 2.66                     | 0.44              |
| 1:E:305:SER:O    | 1:E:307:GLN:HG3  | 2.18                     | 0.44              |
| 1:B:19:LEU:O     | 1:B:23:THR:HG23  | 2.17                     | 0.44              |
| 1:D:62:VAL:HG11  | 1:E:424:VAL:HG12 | 1.97                     | 0.44              |
| 1:F:241:HIS:CE1  | 1:F:266:PRO:HD3  | 2.53                     | 0.44              |
| 1:F:384:MET:HA   | 1:F:384:MET:HE3  | 2.00                     | 0.44              |
| 1:F:85:PHE:CE2   | 1:F:119:ILE:HD12 | 2.53                     | 0.44              |
| 1:E:303:ALA:HA   | 1:E:325:ALA:HB2  | 1.99                     | 0.44              |
| 1:C:248:ILE:HG22 | 1:C:249:GLY:N    | 2.32                     | 0.44              |
| 1:E:405:ALA:O    | 1:E:409:THR:CG2  | 2.65                     | 0.44              |
| 1:E:250:ILE:HG22 | 1:E:251:SER:N    | 2.32                     | 0.44              |
| 1:A:85:PHE:HB3   | 1:A:123:PRO:HG3  | 1.99                     | 0.44              |
| 1:F:80:LYS:CG    | 1:F:112:TYR:CD2  | 3.01                     | 0.44              |
| 1:C:144:GLN:HE21 | 1:F:150:LYS:NZ   | 2.16                     | 0.44              |
| 1:F:186:LYS:NZ   | 1:F:365:ASN:HD21 | 2.15                     | 0.44              |
| 1:C:257:LEU:HD23 | 1:C:257:LEU:N    | 2.33                     | 0.43              |
| 1:F:224:ILE:HG22 | 1:F:247:VAL:HA   | 1.99                     | 0.43              |
| 1:C:201:ALA:O    | 1:C:205:THR:HG23 | 2.18                     | 0.43              |
| 1:A:236:LEU:HB2  | 1:A:324:ARG:NH1  | 2.33                     | 0.43              |
| 1:A:229:PHE:CE1  | 1:A:250:ILE:HD12 | 2.53                     | 0.43              |
| 1:B:312:ASN:H    | 1:B:312:ASN:HD22 | 1.66                     | 0.43              |
| 1:D:286:ILE:HD12 | 1:D:290:GLU:HG3  | 2.01                     | 0.43              |
| 1:F:308:ILE:O    | 1:F:330:THR:HG23 | 2.19                     | 0.43              |
| 1:E:215:LYS:HB3  | 1:E:217:ILE:HD12 | 1.99                     | 0.43              |
| 1:D:212:VAL:CG2  | 1:D:298:ILE:HD11 | 2.48                     | 0.43              |
| 1:A:273:ASP:OD2  | 1:A:277:MET:HB2  | 2.18                     | 0.43              |
| 1:E:198:THR:O    | 1:E:198:THR:HG22 | 2.19                     | 0.43              |
| 1:A:63:LYS:HG3   | 1:A:65:PHE:CE1   | 2.53                     | 0.43              |
| 1:F:42:MET:HE1   | 1:F:72:HIS:CE1   | 2.52                     | 0.43              |
| 1:E:110:LEU:HD11 | 1:E:355:VAL:CG1  | 2.45                     | 0.43              |
| 1:D:324:ARG:HG2  | 1:D:324:ARG:O    | 2.19                     | 0.43              |
| 1:C:250:ILE:CD1  | 1:C:263:LEU:HD22 | 2.47                     | 0.43              |
| 1:B:400:VAL:CG1  | 1:B:404:LEU:HD23 | 2.48                     | 0.43              |
| 1:D:345:VAL:HG22 | 1:D:402:MET:HE1  | 2.00                     | 0.43              |
| 1:C:175:ARG:HD2  | 3:C:444:HOH:O    | 2.18                     | 0.43              |
| 1:D:325:ALA:CB   | 1:D:326:ASN:HB2  | 2.35                     | 0.43              |
| 1:C:173:ARG:CG   | 3:C:819:HOH:O    | 2.58                     | 0.43              |
| 1:B:343:LEU:HD11 | 1:B:402:MET:CE   | 2.48                     | 0.43              |
| 1:B:84:ARG:CG    | 1:B:156:ASP:OD1  | 2.67                     | 0.43              |
| 1:C:90:ASN:ND2   | 1:C:93:LYS:HE3   | 2.14                     | 0.43              |
| 1:F:259:ASN:HB3  | 1:F:263:LEU:HD12 | 2.01                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:16:ASN:N     | 1:C:19:LEU:HD22  | 2.29                     | 0.42              |
| 1:F:224:ILE:HD13 | 1:F:225:ILE:N    | 2.34                     | 0.42              |
| 1:C:408:MET:O    | 1:C:412:ARG:HB2  | 2.19                     | 0.42              |
| 1:F:42:MET:HE3   | 1:F:72:HIS:NE2   | 2.35                     | 0.42              |
| 1:B:90:ASN:HD21  | 1:B:93:LYS:HG3   | 1.84                     | 0.42              |
| 1:C:144:GLN:HE21 | 1:F:150:LYS:HZ3  | 1.68                     | 0.42              |
| 1:E:289:GLU:N    | 1:E:289:GLU:OE2  | 2.50                     | 0.42              |
| 1:B:412:ARG:CG   | 1:B:416:GLU:OE2  | 2.67                     | 0.42              |
| 1:C:264:ASP:O    | 1:C:268:LEU:HD12 | 2.19                     | 0.42              |
| 1:B:227:GLN:HE21 | 1:B:302:ALA:N    | 2.12                     | 0.42              |
| 1:D:32:LEU:CD1   | 1:D:408:MET:HE2  | 2.50                     | 0.42              |
| 1:E:268:LEU:O    | 1:E:269:LEU:HD13 | 2.19                     | 0.42              |
| 1:E:48:MET:HE2   | 1:E:48:MET:HB3   | 1.80                     | 0.42              |
| 1:D:186:LYS:HZ1  | 1:D:365:ASN:HD21 | 1.67                     | 0.42              |
| 1:B:375:GLU:OE2  | 3:B:482:HOH:O    | 2.21                     | 0.42              |
| 1:A:90:ASN:ND2   | 1:A:93:LYS:HB3   | 2.34                     | 0.42              |
| 1:F:168:MET:HE3  | 1:F:169:ASP:HA   | 2.00                     | 0.42              |
| 1:F:198:THR:OG1  | 1:F:202:GLN:NE2  | 2.51                     | 0.42              |
| 1:A:150:LYS:HD3  | 1:B:144:GLN:HE22 | 1.85                     | 0.42              |
| 1:C:265:ILE:HG22 | 1:C:269:LEU:HD22 | 2.00                     | 0.42              |
| 1:C:257:LEU:HD21 | 1:C:279:THR:HG22 | 2.02                     | 0.42              |
| 3:A:428:HOH:O    | 1:B:50:THR:CG2   | 2.67                     | 0.42              |
| 1:E:268:LEU:O    | 1:E:269:LEU:HD22 | 2.19                     | 0.42              |
| 1:E:206:ILE:HG21 | 1:E:384:MET:HB2  | 2.01                     | 0.42              |
| 1:D:47:ARG:NH2   | 1:D:74:ASP:OD2   | 2.52                     | 0.42              |
| 1:A:144:GLN:HE21 | 1:B:150:LYS:HZ2  | 1.66                     | 0.42              |
| 1:B:325:ALA:HA   | 1:B:347:ASP:OD1  | 2.19                     | 0.42              |
| 1:D:316:ILE:O    | 1:D:340:ARG:NH2  | 2.52                     | 0.42              |
| 1:E:173:ARG:HH11 | 1:E:173:ARG:HA   | 1.85                     | 0.42              |
| 1:B:168:MET:HE3  | 1:B:169:ASP:HA   | 2.01                     | 0.42              |
| 1:F:199:ALA:HB2  | 1:F:357:VAL:HG21 | 2.01                     | 0.42              |
| 1:D:79:THR:HA    | 1:D:113:GLY:O    | 2.20                     | 0.42              |
| 1:B:246:LYS:NZ   | 3:B:437:HOH:O    | 2.52                     | 0.42              |
| 1:C:44:GLU:HB2   | 1:F:52:ARG:CD    | 2.46                     | 0.42              |
| 1:D:86:HIS:ND1   | 1:D:88:GLU:HG2   | 2.35                     | 0.42              |
| 1:A:59:ASN:HD22  | 1:A:60:GLY:N     | 2.17                     | 0.42              |
| 1:F:327:GLY:N    | 1:F:328:PRO:CD   | 2.83                     | 0.42              |
| 1:C:19:LEU:N     | 1:C:19:LEU:HD22  | 2.34                     | 0.41              |
| 1:F:217:ILE:HD11 | 1:F:222:ALA:CB   | 2.50                     | 0.41              |
| 1:A:21:THR:HG21  | 1:A:100:TRP:HE1  | 1.85                     | 0.41              |
| 1:F:80:LYS:HG3   | 1:F:112:TYR:CE2  | 2.55                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:307:GLN:OE1  | 1:F:307:GLN:HA   | 2.20                     | 0.41              |
| 1:B:81:GLY:HA3   | 1:B:115:GLY:O    | 2.20                     | 0.41              |
| 1:D:324:ARG:O    | 1:D:325:ALA:HB2  | 2.21                     | 0.41              |
| 1:C:268:LEU:HD23 | 1:C:278:VAL:CG1  | 2.41                     | 0.41              |
| 1:F:409:THR:HB   | 3:F:843:HOH:O    | 2.20                     | 0.41              |
| 1:A:186:LYS:HZ2  | 1:A:365:ASN:HD21 | 1.67                     | 0.41              |
| 1:E:299:LEU:HD22 | 1:E:300:VAL:N    | 2.35                     | 0.41              |
| 1:E:372:SER:O    | 1:E:376:VAL:HG23 | 2.20                     | 0.41              |
| 1:F:249:GLY:C    | 1:F:250:ILE:HD12 | 2.41                     | 0.41              |
| 1:C:309:THR:CG2  | 1:C:310:ALA:H    | 2.32                     | 0.41              |
| 1:B:336:ILE:O    | 1:B:340:ARG:HG3  | 2.20                     | 0.41              |
| 1:B:345:VAL:HG22 | 1:B:402:MET:CE   | 2.51                     | 0.41              |
| 1:C:186:LYS:HZ2  | 1:C:365:ASN:HD21 | 1.67                     | 0.41              |
| 1:E:28:ALA:HB1   | 1:E:411:ILE:HD11 | 2.03                     | 0.41              |
| 1:E:298:ILE:HA   | 1:E:320:ILE:O    | 2.21                     | 0.41              |
| 1:C:323:GLU:OE2  | 1:C:344:LEU:HD21 | 2.19                     | 0.41              |
| 1:D:48:MET:CE    | 1:D:91:GLU:HG3   | 2.51                     | 0.41              |
| 1:C:273:ASP:HB3  | 1:C:277:MET:H    | 1.85                     | 0.41              |
| 1:E:90:ASN:ND2   | 1:E:93:LYS:CG    | 2.79                     | 0.41              |
| 1:B:421:ARG:HD2  | 1:D:169:ASP:OD1  | 2.21                     | 0.41              |
| 1:C:214:LYS:HD3  | 1:C:392:TYR:CZ   | 2.56                     | 0.41              |
| 1:D:300:VAL:HG12 | 1:D:324:ARG:HH21 | 1.86                     | 0.41              |
| 1:A:423:TRP:CD1  | 1:A:423:TRP:N    | 2.87                     | 0.41              |
| 1:F:79:THR:O     | 1:F:151:ASP:HA   | 2.21                     | 0.41              |
| 1:F:257:LEU:N    | 1:F:257:LEU:HD23 | 2.36                     | 0.41              |
| 1:B:390:THR:HG21 | 3:B:729:HOH:O    | 2.21                     | 0.41              |
| 1:A:171:TYR:OH   | 1:A:175:ARG:NH1  | 2.54                     | 0.41              |
| 1:F:288:ASN:HD22 | 1:F:288:ASN:N    | 2.19                     | 0.41              |
| 1:B:308:ILE:HG22 | 1:B:333:ALA:HB1  | 2.02                     | 0.41              |
| 1:F:101:MET:O    | 1:F:102:THR:C    | 2.60                     | 0.41              |
| 1:D:256:GLY:C    | 1:D:257:LEU:HD22 | 2.42                     | 0.41              |
| 1:F:80:LYS:CG    | 1:F:112:TYR:CE2  | 3.04                     | 0.41              |
| 1:D:49:LEU:HD13  | 1:D:142:ILE:HG22 | 2.03                     | 0.41              |
| 1:C:50:THR:HG23  | 3:F:430:HOH:O    | 2.21                     | 0.40              |
| 1:C:186:LYS:HZ2  | 1:C:365:ASN:ND2  | 2.19                     | 0.40              |
| 1:E:84:ARG:O     | 1:E:118:GLY:HA2  | 2.21                     | 0.40              |
| 1:F:257:LEU:O    | 1:F:263:LEU:HD21 | 2.22                     | 0.40              |
| 1:F:254:ASN:N    | 1:F:254:ASN:ND2  | 2.66                     | 0.40              |
| 1:C:303:ALA:HB1  | 1:C:304:ILE:HG12 | 2.03                     | 0.40              |
| 1:A:272:ARG:HD2  | 3:A:536:HOH:O    | 2.20                     | 0.40              |
| 1:A:84:ARG:O     | 1:A:118:GLY:HA2  | 2.21                     | 0.40              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:D:26:LYS:O     | 1:D:30:ARG:HB2  | 2.21                     | 0.40              |
| 1:D:226:ILE:HG23 | 1:D:324:ARG:NH2 | 2.37                     | 0.40              |
| 1:C:259:ASN:HB3  | 1:C:263:LEU:CD1 | 2.50                     | 0.40              |
| 1:C:230:GLY:O    | 1:C:234:SER:OG  | 2.34                     | 0.40              |
| 1:B:17:LEU:HD22  | 1:B:21:THR:CG2  | 2.51                     | 0.40              |
| 1:F:42:MET:CE    | 1:F:72:HIS:HE1  | 2.30                     | 0.40              |
| 1:B:84:ARG:O     | 1:B:118:GLY:HA2 | 2.22                     | 0.40              |
| 1:B:173:ARG:NH2  | 3:B:549:HOH:O   | 2.53                     | 0.40              |
| 1:D:380:LEU:HD22 | 1:D:384:MET:HG2 | 2.03                     | 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     | 416/424 (98%)   | 400 (96%)  | 13 (3%)  | 3 (1%)   | 26          | 31 |
| 1   | B     | 407/424 (96%)   | 396 (97%)  | 10 (2%)  | 1 (0%)   | 52          | 64 |
| 1   | C     | 407/424 (96%)   | 376 (92%)  | 19 (5%)  | 12 (3%)  | 6           | 3  |
| 1   | D     | 402/424 (95%)   | 383 (95%)  | 17 (4%)  | 2 (0%)   | 34          | 41 |
| 1   | E     | 392/424 (92%)   | 360 (92%)  | 27 (7%)  | 5 (1%)   | 15          | 15 |
| 1   | F     | 391/424 (92%)   | 367 (94%)  | 22 (6%)  | 2 (0%)   | 34          | 41 |
| All | All   | 2415/2544 (95%) | 2282 (94%) | 108 (4%) | 25 (1%)  | 19          | 21 |

All (25) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 273 | ASP  |
| 1   | C     | 248 | ILE  |
| 1   | C     | 283 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 303 | ALA  |
| 1   | E     | 306 | ASN  |
| 1   | F     | 303 | ALA  |
| 1   | A     | 312 | ASN  |
| 1   | B     | 278 | VAL  |
| 1   | C     | 302 | ALA  |
| 1   | C     | 311 | LYS  |
| 1   | C     | 312 | ASN  |
| 1   | D     | 303 | ALA  |
| 1   | D     | 304 | ILE  |
| 1   | E     | 312 | ASN  |
| 1   | C     | 280 | ASN  |
| 1   | C     | 303 | ALA  |
| 1   | E     | 232 | ALA  |
| 1   | F     | 268 | LEU  |
| 1   | C     | 216 | GLY  |
| 1   | C     | 279 | THR  |
| 1   | C     | 285 | VAL  |
| 1   | E     | 259 | ASN  |
| 1   | A     | 278 | VAL  |
| 1   | C     | 278 | VAL  |
| 1   | C     | 259 | ASN  |

### 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     | 346/351 (99%)   | 311 (90%)  | 35 (10%)  | 9           | 11 |
| 1   | B     | 338/351 (96%)   | 305 (90%)  | 33 (10%)  | 10          | 11 |
| 1   | C     | 338/351 (96%)   | 306 (90%)  | 32 (10%)  | 11          | 12 |
| 1   | D     | 333/351 (95%)   | 311 (93%)  | 22 (7%)   | 21          | 27 |
| 1   | E     | 324/351 (92%)   | 288 (89%)  | 36 (11%)  | 8           | 8  |
| 1   | F     | 324/351 (92%)   | 287 (89%)  | 37 (11%)  | 7           | 7  |
| All | All   | 2003/2106 (95%) | 1808 (90%) | 195 (10%) | 10          | 12 |

All (195) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 9   | ASP  |
| 1   | A     | 12  | LYS  |
| 1   | A     | 13  | GLU  |
| 1   | A     | 21  | THR  |
| 1   | A     | 32  | LEU  |
| 1   | A     | 38  | MET  |
| 1   | A     | 41  | LEU  |
| 1   | A     | 49  | LEU  |
| 1   | A     | 50  | THR  |
| 1   | A     | 59  | ASN  |
| 1   | A     | 62  | VAL  |
| 1   | A     | 84  | ARG  |
| 1   | A     | 92  | GLU  |
| 1   | A     | 93  | LYS  |
| 1   | A     | 146 | VAL  |
| 1   | A     | 168 | MET  |
| 1   | A     | 173 | ARG  |
| 1   | A     | 188 | LEU  |
| 1   | A     | 205 | THR  |
| 1   | A     | 212 | VAL  |
| 1   | A     | 219 | LEU  |
| 1   | A     | 231 | ASN  |
| 1   | A     | 236 | LEU  |
| 1   | A     | 272 | ARG  |
| 1   | A     | 279 | THR  |
| 1   | A     | 293 | GLU  |
| 1   | A     | 299 | LEU  |
| 1   | A     | 316 | ILE  |
| 1   | A     | 344 | LEU  |
| 1   | A     | 382 | SER  |
| 1   | A     | 390 | THR  |
| 1   | A     | 397 | THR  |
| 1   | A     | 404 | LEU  |
| 1   | A     | 419 | ARG  |
| 1   | A     | 424 | VAL  |
| 1   | B     | 17  | LEU  |
| 1   | B     | 21  | THR  |
| 1   | B     | 32  | LEU  |
| 1   | B     | 41  | LEU  |
| 1   | B     | 49  | LEU  |
| 1   | B     | 50  | THR  |
| 1   | B     | 56  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 59  | ASN  |
| 1   | B     | 90  | ASN  |
| 1   | B     | 146 | VAL  |
| 1   | B     | 168 | MET  |
| 1   | B     | 173 | ARG  |
| 1   | B     | 188 | LEU  |
| 1   | B     | 219 | LEU  |
| 1   | B     | 220 | GLN  |
| 1   | B     | 236 | LEU  |
| 1   | B     | 269 | LEU  |
| 1   | B     | 270 | ASP  |
| 1   | B     | 278 | VAL  |
| 1   | B     | 279 | THR  |
| 1   | B     | 299 | LEU  |
| 1   | B     | 312 | ASN  |
| 1   | B     | 316 | ILE  |
| 1   | B     | 326 | ASN  |
| 1   | B     | 329 | THR  |
| 1   | B     | 334 | THR  |
| 1   | B     | 357 | VAL  |
| 1   | B     | 390 | THR  |
| 1   | B     | 394 | THR  |
| 1   | B     | 397 | THR  |
| 1   | B     | 399 | LYS  |
| 1   | B     | 411 | ILE  |
| 1   | B     | 419 | ARG  |
| 1   | C     | 17  | LEU  |
| 1   | C     | 19  | LEU  |
| 1   | C     | 32  | LEU  |
| 1   | C     | 41  | LEU  |
| 1   | C     | 48  | MET  |
| 1   | C     | 49  | LEU  |
| 1   | C     | 50  | THR  |
| 1   | C     | 52  | ARG  |
| 1   | C     | 188 | LEU  |
| 1   | C     | 214 | LYS  |
| 1   | C     | 219 | LEU  |
| 1   | C     | 220 | GLN  |
| 1   | C     | 225 | ILE  |
| 1   | C     | 229 | PHE  |
| 1   | C     | 234 | SER  |
| 1   | C     | 236 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 267 | TYR  |
| 1   | C     | 281 | LEU  |
| 1   | C     | 282 | PHE  |
| 1   | C     | 286 | ILE  |
| 1   | C     | 299 | LEU  |
| 1   | C     | 304 | ILE  |
| 1   | C     | 305 | SER  |
| 1   | C     | 306 | ASN  |
| 1   | C     | 342 | VAL  |
| 1   | C     | 367 | GLN  |
| 1   | C     | 380 | LEU  |
| 1   | C     | 389 | GLU  |
| 1   | C     | 390 | THR  |
| 1   | C     | 394 | THR  |
| 1   | C     | 404 | LEU  |
| 1   | C     | 409 | THR  |
| 1   | D     | 17  | LEU  |
| 1   | D     | 30  | ARG  |
| 1   | D     | 32  | LEU  |
| 1   | D     | 41  | LEU  |
| 1   | D     | 49  | LEU  |
| 1   | D     | 88  | GLU  |
| 1   | D     | 93  | LYS  |
| 1   | D     | 146 | VAL  |
| 1   | D     | 188 | LEU  |
| 1   | D     | 215 | LYS  |
| 1   | D     | 219 | LEU  |
| 1   | D     | 250 | ILE  |
| 1   | D     | 251 | SER  |
| 1   | D     | 271 | LYS  |
| 1   | D     | 299 | LEU  |
| 1   | D     | 317 | GLN  |
| 1   | D     | 326 | ASN  |
| 1   | D     | 342 | VAL  |
| 1   | D     | 358 | SER  |
| 1   | D     | 380 | LEU  |
| 1   | D     | 404 | LEU  |
| 1   | D     | 409 | THR  |
| 1   | E     | 12  | LYS  |
| 1   | E     | 13  | GLU  |
| 1   | E     | 15  | LEU  |
| 1   | E     | 30  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 32  | LEU  |
| 1   | E     | 41  | LEU  |
| 1   | E     | 48  | MET  |
| 1   | E     | 49  | LEU  |
| 1   | E     | 50  | THR  |
| 1   | E     | 84  | ARG  |
| 1   | E     | 100 | TRP  |
| 1   | E     | 146 | VAL  |
| 1   | E     | 173 | ARG  |
| 1   | E     | 188 | LEU  |
| 1   | E     | 219 | LEU  |
| 1   | E     | 231 | ASN  |
| 1   | E     | 251 | SER  |
| 1   | E     | 254 | ASN  |
| 1   | E     | 267 | TYR  |
| 1   | E     | 291 | LEU  |
| 1   | E     | 294 | LYS  |
| 1   | E     | 299 | LEU  |
| 1   | E     | 311 | LYS  |
| 1   | E     | 317 | GLN  |
| 1   | E     | 326 | ASN  |
| 1   | E     | 344 | LEU  |
| 1   | E     | 374 | GLU  |
| 1   | E     | 380 | LEU  |
| 1   | E     | 393 | GLN  |
| 1   | E     | 397 | THR  |
| 1   | E     | 404 | LEU  |
| 1   | E     | 409 | THR  |
| 1   | E     | 411 | ILE  |
| 1   | E     | 412 | ARG  |
| 1   | E     | 419 | ARG  |
| 1   | E     | 424 | VAL  |
| 1   | F     | 16  | ASN  |
| 1   | F     | 21  | THR  |
| 1   | F     | 32  | LEU  |
| 1   | F     | 41  | LEU  |
| 1   | F     | 49  | LEU  |
| 1   | F     | 56  | LYS  |
| 1   | F     | 80  | LYS  |
| 1   | F     | 84  | ARG  |
| 1   | F     | 146 | VAL  |
| 1   | F     | 168 | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 188 | LEU  |
| 1   | F     | 197 | GLU  |
| 1   | F     | 217 | ILE  |
| 1   | F     | 219 | LEU  |
| 1   | F     | 220 | GLN  |
| 1   | F     | 223 | ARG  |
| 1   | F     | 224 | ILE  |
| 1   | F     | 227 | GLN  |
| 1   | F     | 236 | LEU  |
| 1   | F     | 248 | ILE  |
| 1   | F     | 254 | ASN  |
| 1   | F     | 257 | LEU  |
| 1   | F     | 288 | ASN  |
| 1   | F     | 299 | LEU  |
| 1   | F     | 307 | GLN  |
| 1   | F     | 311 | LYS  |
| 1   | F     | 316 | ILE  |
| 1   | F     | 326 | ASN  |
| 1   | F     | 358 | SER  |
| 1   | F     | 378 | GLU  |
| 1   | F     | 380 | LEU  |
| 1   | F     | 381 | ARG  |
| 1   | F     | 384 | MET  |
| 1   | F     | 390 | THR  |
| 1   | F     | 397 | THR  |
| 1   | F     | 409 | THR  |
| 1   | F     | 411 | ILE  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 16  | ASN  |
| 1   | A     | 59  | ASN  |
| 1   | A     | 90  | ASN  |
| 1   | A     | 144 | GLN  |
| 1   | A     | 194 | GLN  |
| 1   | A     | 312 | ASN  |
| 1   | A     | 365 | ASN  |
| 1   | A     | 367 | GLN  |
| 1   | A     | 393 | GLN  |
| 1   | B     | 59  | ASN  |
| 1   | B     | 90  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 144 | GLN  |
| 1   | B     | 194 | GLN  |
| 1   | B     | 202 | GLN  |
| 1   | B     | 227 | GLN  |
| 1   | B     | 231 | ASN  |
| 1   | B     | 254 | ASN  |
| 1   | B     | 288 | ASN  |
| 1   | B     | 312 | ASN  |
| 1   | B     | 315 | ASN  |
| 1   | B     | 365 | ASN  |
| 1   | B     | 367 | GLN  |
| 1   | B     | 393 | GLN  |
| 1   | C     | 90  | ASN  |
| 1   | C     | 144 | GLN  |
| 1   | C     | 162 | GLN  |
| 1   | C     | 194 | GLN  |
| 1   | C     | 202 | GLN  |
| 1   | C     | 288 | ASN  |
| 1   | C     | 312 | ASN  |
| 1   | C     | 365 | ASN  |
| 1   | C     | 367 | GLN  |
| 1   | C     | 393 | GLN  |
| 1   | D     | 144 | GLN  |
| 1   | D     | 160 | ASN  |
| 1   | D     | 194 | GLN  |
| 1   | D     | 202 | GLN  |
| 1   | D     | 220 | GLN  |
| 1   | D     | 221 | ASN  |
| 1   | D     | 227 | GLN  |
| 1   | D     | 231 | ASN  |
| 1   | D     | 288 | ASN  |
| 1   | D     | 307 | GLN  |
| 1   | D     | 312 | ASN  |
| 1   | D     | 365 | ASN  |
| 1   | E     | 90  | ASN  |
| 1   | E     | 144 | GLN  |
| 1   | E     | 194 | GLN  |
| 1   | E     | 254 | ASN  |
| 1   | E     | 259 | ASN  |
| 1   | E     | 312 | ASN  |
| 1   | E     | 317 | GLN  |
| 1   | E     | 365 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 367 | GLN  |
| 1   | F     | 144 | GLN  |
| 1   | F     | 202 | GLN  |
| 1   | F     | 220 | GLN  |
| 1   | F     | 221 | ASN  |
| 1   | F     | 227 | GLN  |
| 1   | F     | 241 | HIS  |
| 1   | F     | 254 | ASN  |
| 1   | F     | 288 | ASN  |
| 1   | F     | 326 | ASN  |
| 1   | F     | 365 | ASN  |
| 1   | F     | 393 | 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

5 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 2   | PEG  | A     | 425 | -    | 6,6,6        | 0.51 | 0           | 5,5,5       | 0.64 | 0           |
| 2   | PEG  | C     | 425 | -    | 6,6,6        | 0.38 | 0           | 5,5,5       | 0.75 | 0           |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 2   | PEG  | D     | 425 | -    | 6,6,6        | 0.52 | 0        | 5,5,5       | 0.48 | 0        |
| 2   | PEG  | E     | 425 | -    | 6,6,6        | 0.67 | 0        | 5,5,5       | 0.42 | 0        |
| 2   | PEG  | F     | 425 | -    | 6,6,6        | 0.41 | 0        | 5,5,5       | 0.31 | 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   |
|-----|------|-------|-----|------|---------|----------|---------|
| 2   | PEG  | A     | 425 | -    | -       | 0/4/4/4  | 0/0/0/0 |
| 2   | PEG  | C     | 425 | -    | -       | 0/4/4/4  | 0/0/0/0 |
| 2   | PEG  | D     | 425 | -    | -       | 0/4/4/4  | 0/0/0/0 |
| 2   | PEG  | E     | 425 | -    | -       | 0/4/4/4  | 0/0/0/0 |
| 2   | PEG  | F     | 425 | -    | -       | 0/4/4/4  | 0/0/0/0 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 11 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2   | C     | 425 | PEG  | 3       | 0            |
| 2   | D     | 425 | PEG  | 4       | 0            |
| 2   | E     | 425 | PEG  | 4       | 0            |

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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     | 418/424 (98%)   | -0.06  | 14 (3%)  | 50 59 | 26, 40, 64, 80        | 0     |
| 1   | B     | 409/424 (96%)   | -0.00  | 15 (3%)  | 45 54 | 27, 44, 69, 82        | 0     |
| 1   | C     | 409/424 (96%)   | 0.47   | 61 (14%) | 3 5   | 30, 48, 104, 114      | 0     |
| 1   | D     | 406/424 (95%)   | 0.25   | 31 (7%)  | 17 24 | 29, 51, 83, 99        | 0     |
| 1   | E     | 396/424 (93%)   | 0.54   | 64 (16%) | 3 4   | 30, 50, 112, 125      | 0     |
| 1   | F     | 395/424 (93%)   | 0.47   | 58 (14%) | 3 5   | 29, 49, 107, 113      | 0     |
| All | All   | 2433/2544 (95%) | 0.27   | 243 (9%) | 9 14  | 26, 47, 99, 125       | 0     |

All (243) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | F     | 267 | TYR  | 9.1  |
| 1   | E     | 267 | TYR  | 8.1  |
| 1   | F     | 303 | ALA  | 8.0  |
| 1   | F     | 304 | ILE  | 6.9  |
| 1   | F     | 226 | ILE  | 6.0  |
| 1   | E     | 258 | TYR  | 5.8  |
| 1   | F     | 231 | ASN  | 5.7  |
| 1   | C     | 283 | THR  | 5.6  |
| 1   | C     | 275 | PHE  | 5.5  |
| 1   | F     | 261 | ASP  | 5.5  |
| 1   | F     | 254 | ASN  | 5.4  |
| 1   | F     | 253 | ALA  | 5.4  |
| 1   | C     | 250 | ILE  | 5.4  |
| 1   | F     | 268 | LEU  | 5.3  |
| 1   | D     | 303 | ALA  | 5.3  |
| 1   | E     | 231 | ASN  | 5.2  |
| 1   | D     | 285 | VAL  | 5.1  |
| 1   | F     | 324 | ARG  | 5.0  |
| 1   | E     | 254 | ASN  | 4.9  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | F     | 306 | ASN  | 4.9  |
| 1   | F     | 246 | LYS  | 4.9  |
| 1   | C     | 324 | ARG  | 4.8  |
| 1   | E     | 257 | LEU  | 4.8  |
| 1   | E     | 261 | ASP  | 4.7  |
| 1   | B     | 283 | THR  | 4.7  |
| 1   | C     | 284 | ASP  | 4.7  |
| 1   | A     | 275 | PHE  | 4.6  |
| 1   | F     | 335 | LYS  | 4.5  |
| 1   | E     | 295 | ASP  | 4.4  |
| 1   | D     | 308 | ILE  | 4.4  |
| 1   | E     | 299 | LEU  | 4.4  |
| 1   | E     | 263 | LEU  | 4.3  |
| 1   | E     | 287 | THR  | 4.3  |
| 1   | C     | 303 | ALA  | 4.2  |
| 1   | F     | 260 | PRO  | 4.2  |
| 1   | F     | 224 | ILE  | 4.2  |
| 1   | C     | 260 | PRO  | 4.2  |
| 1   | C     | 304 | ILE  | 4.2  |
| 1   | C     | 246 | LYS  | 4.2  |
| 1   | F     | 339 | GLU  | 4.2  |
| 1   | C     | 274 | SER  | 4.1  |
| 1   | D     | 324 | ARG  | 4.1  |
| 1   | E     | 324 | ARG  | 4.1  |
| 1   | E     | 303 | ALA  | 4.1  |
| 1   | D     | 231 | ASN  | 4.1  |
| 1   | F     | 287 | THR  | 4.1  |
| 1   | E     | 253 | ALA  | 4.0  |
| 1   | C     | 221 | ASN  | 4.0  |
| 1   | C     | 220 | GLN  | 4.0  |
| 1   | E     | 266 | PRO  | 3.9  |
| 1   | C     | 280 | ASN  | 3.9  |
| 1   | F     | 232 | ALA  | 3.9  |
| 1   | E     | 314 | HIS  | 3.9  |
| 1   | E     | 290 | GLU  | 3.9  |
| 1   | F     | 229 | PHE  | 3.8  |
| 1   | C     | 226 | ILE  | 3.8  |
| 1   | F     | 247 | VAL  | 3.8  |
| 1   | C     | 261 | ASP  | 3.8  |
| 1   | F     | 252 | ASP  | 3.8  |
| 1   | C     | 314 | HIS  | 3.7  |
| 1   | C     | 286 | ILE  | 3.7  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | F     | 225 | ILE  | 3.7  |
| 1   | C     | 267 | TYR  | 3.7  |
| 1   | D     | 226 | ILE  | 3.7  |
| 1   | A     | 274 | SER  | 3.7  |
| 1   | B     | 284 | ASP  | 3.6  |
| 1   | E     | 226 | ILE  | 3.6  |
| 1   | C     | 241 | HIS  | 3.6  |
| 1   | F     | 314 | HIS  | 3.6  |
| 1   | F     | 326 | ASN  | 3.6  |
| 1   | E     | 315 | ASN  | 3.5  |
| 1   | E     | 264 | ASP  | 3.5  |
| 1   | F     | 14  | ALA  | 3.5  |
| 1   | C     | 308 | ILE  | 3.5  |
| 1   | F     | 331 | ILE  | 3.5  |
| 1   | C     | 231 | ASN  | 3.5  |
| 1   | A     | 311 | LYS  | 3.5  |
| 1   | C     | 273 | ASP  | 3.5  |
| 1   | E     | 243 | ALA  | 3.4  |
| 1   | E     | 310 | ALA  | 3.4  |
| 1   | E     | 247 | VAL  | 3.4  |
| 1   | C     | 254 | ASN  | 3.4  |
| 1   | E     | 216 | GLY  | 3.4  |
| 1   | E     | 224 | ILE  | 3.4  |
| 1   | E     | 304 | ILE  | 3.4  |
| 1   | E     | 220 | GLN  | 3.4  |
| 1   | C     | 335 | LYS  | 3.4  |
| 1   | D     | 253 | ALA  | 3.3  |
| 1   | D     | 270 | ASP  | 3.3  |
| 1   | C     | 278 | VAL  | 3.3  |
| 1   | F     | 230 | GLY  | 3.3  |
| 1   | E     | 262 | GLY  | 3.2  |
| 1   | D     | 261 | ASP  | 3.2  |
| 1   | D     | 267 | TYR  | 3.2  |
| 1   | F     | 290 | GLU  | 3.2  |
| 1   | F     | 294 | LYS  | 3.2  |
| 1   | E     | 255 | GLY  | 3.2  |
| 1   | C     | 285 | VAL  | 3.2  |
| 1   | F     | 332 | ASP  | 3.2  |
| 1   | D     | 254 | ASN  | 3.2  |
| 1   | E     | 288 | ASN  | 3.2  |
| 1   | F     | 221 | ASN  | 3.2  |
| 1   | F     | 286 | ILE  | 3.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 324 | ARG  | 3.2  |
| 1   | C     | 315 | ASN  | 3.2  |
| 1   | E     | 265 | ILE  | 3.1  |
| 1   | C     | 277 | MET  | 3.1  |
| 1   | F     | 317 | GLN  | 3.1  |
| 1   | D     | 331 | ILE  | 3.1  |
| 1   | D     | 242 | ASP  | 3.1  |
| 1   | E     | 242 | ASP  | 3.1  |
| 1   | F     | 259 | ASN  | 3.1  |
| 1   | E     | 225 | ILE  | 3.1  |
| 1   | F     | 325 | ALA  | 3.1  |
| 1   | E     | 218 | LYS  | 3.1  |
| 1   | E     | 229 | PHE  | 3.1  |
| 1   | B     | 303 | ALA  | 3.1  |
| 1   | C     | 279 | THR  | 3.0  |
| 1   | C     | 339 | GLU  | 3.0  |
| 1   | D     | 339 | GLU  | 3.0  |
| 1   | A     | 283 | THR  | 3.0  |
| 1   | E     | 334 | THR  | 3.0  |
| 1   | F     | 257 | LEU  | 3.0  |
| 1   | F     | 258 | TYR  | 2.9  |
| 1   | C     | 93  | LYS  | 2.9  |
| 1   | C     | 262 | GLY  | 2.9  |
| 1   | C     | 319 | SER  | 2.9  |
| 1   | E     | 326 | ASN  | 2.9  |
| 1   | D     | 304 | ILE  | 2.9  |
| 1   | E     | 15  | LEU  | 2.9  |
| 1   | E     | 251 | SER  | 2.9  |
| 1   | D     | 334 | THR  | 2.9  |
| 1   | F     | 305 | SER  | 2.9  |
| 1   | E     | 223 | ARG  | 2.8  |
| 1   | D     | 326 | ASN  | 2.8  |
| 1   | D     | 221 | ASN  | 2.8  |
| 1   | E     | 93  | LYS  | 2.8  |
| 1   | C     | 247 | VAL  | 2.8  |
| 1   | E     | 250 | ILE  | 2.8  |
| 1   | C     | 290 | GLU  | 2.8  |
| 1   | E     | 246 | LYS  | 2.8  |
| 1   | F     | 256 | GLY  | 2.7  |
| 1   | F     | 311 | LYS  | 2.7  |
| 1   | E     | 244 | GLY  | 2.7  |
| 1   | E     | 248 | ILE  | 2.7  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | E     | 317 | GLN  | 2.7  |
| 1   | E     | 338 | ASN  | 2.7  |
| 1   | A     | 254 | ASN  | 2.7  |
| 1   | B     | 326 | ASN  | 2.7  |
| 1   | C     | 340 | ARG  | 2.7  |
| 1   | E     | 291 | LEU  | 2.7  |
| 1   | D     | 216 | GLY  | 2.7  |
| 1   | C     | 270 | ASP  | 2.7  |
| 1   | C     | 119 | ILE  | 2.6  |
| 1   | D     | 284 | ASP  | 2.6  |
| 1   | F     | 295 | ASP  | 2.6  |
| 1   | D     | 411 | ILE  | 2.6  |
| 1   | C     | 332 | ASP  | 2.6  |
| 1   | F     | 299 | LEU  | 2.6  |
| 1   | E     | 221 | ASN  | 2.6  |
| 1   | E     | 13  | GLU  | 2.6  |
| 1   | F     | 255 | GLY  | 2.6  |
| 1   | E     | 300 | VAL  | 2.6  |
| 1   | A     | 339 | GLU  | 2.5  |
| 1   | E     | 269 | LEU  | 2.5  |
| 1   | C     | 301 | PRO  | 2.5  |
| 1   | D     | 249 | GLY  | 2.5  |
| 1   | D     | 250 | ILE  | 2.5  |
| 1   | B     | 311 | LYS  | 2.5  |
| 1   | E     | 238 | LYS  | 2.5  |
| 1   | E     | 296 | CYS  | 2.5  |
| 1   | D     | 302 | ALA  | 2.5  |
| 1   | D     | 283 | THR  | 2.5  |
| 1   | B     | 308 | ILE  | 2.5  |
| 1   | C     | 325 | ALA  | 2.5  |
| 1   | C     | 341 | GLY  | 2.5  |
| 1   | C     | 258 | TYR  | 2.4  |
| 1   | C     | 282 | PHE  | 2.4  |
| 1   | D     | 244 | GLY  | 2.4  |
| 1   | E     | 239 | PHE  | 2.4  |
| 1   | C     | 271 | LYS  | 2.4  |
| 1   | A     | 250 | ILE  | 2.4  |
| 1   | E     | 322 | VAL  | 2.4  |
| 1   | C     | 251 | SER  | 2.4  |
| 1   | E     | 249 | GLY  | 2.4  |
| 1   | F     | 216 | GLY  | 2.4  |
| 1   | C     | 249 | GLY  | 2.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | F     | 300 | VAL  | 2.4  |
| 1   | A     | 324 | ARG  | 2.4  |
| 1   | F     | 338 | ASN  | 2.3  |
| 1   | C     | 326 | ASN  | 2.3  |
| 1   | C     | 230 | GLY  | 2.3  |
| 1   | F     | 244 | GLY  | 2.3  |
| 1   | E     | 292 | LEU  | 2.3  |
| 1   | C     | 223 | ARG  | 2.3  |
| 1   | B     | 16  | ASN  | 2.3  |
| 1   | E     | 345 | VAL  | 2.3  |
| 1   | C     | 197 | GLU  | 2.3  |
| 1   | F     | 289 | GLU  | 2.3  |
| 1   | A     | 225 | ILE  | 2.2  |
| 1   | B     | 231 | ASN  | 2.2  |
| 1   | F     | 220 | GLN  | 2.2  |
| 1   | C     | 300 | VAL  | 2.2  |
| 1   | F     | 241 | HIS  | 2.2  |
| 1   | E     | 235 | PHE  | 2.2  |
| 1   | E     | 230 | GLY  | 2.2  |
| 1   | D     | 335 | LYS  | 2.2  |
| 1   | E     | 259 | ASN  | 2.2  |
| 1   | A     | 226 | ILE  | 2.2  |
| 1   | C     | 224 | ILE  | 2.2  |
| 1   | F     | 322 | VAL  | 2.2  |
| 1   | E     | 301 | PRO  | 2.2  |
| 1   | B     | 331 | ILE  | 2.2  |
| 1   | F     | 128 | PHE  | 2.2  |
| 1   | E     | 234 | SER  | 2.2  |
| 1   | C     | 298 | ILE  | 2.1  |
| 1   | C     | 317 | GLN  | 2.1  |
| 1   | B     | 275 | PHE  | 2.1  |
| 1   | D     | 251 | SER  | 2.1  |
| 1   | C     | 253 | ALA  | 2.1  |
| 1   | C     | 265 | ILE  | 2.1  |
| 1   | F     | 223 | ARG  | 2.1  |
| 1   | C     | 310 | ALA  | 2.1  |
| 1   | D     | 16  | ASN  | 2.1  |
| 1   | B     | 281 | LEU  | 2.1  |
| 1   | F     | 315 | ASN  | 2.1  |
| 1   | B     | 305 | SER  | 2.1  |
| 1   | F     | 393 | GLN  | 2.1  |
| 1   | A     | 231 | ASN  | 2.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | F     | 293 | GLU  | 2.1  |
| 1   | B     | 253 | ALA  | 2.1  |
| 1   | E     | 100 | TRP  | 2.1  |
| 1   | D     | 332 | ASP  | 2.1  |
| 1   | A     | 285 | VAL  | 2.1  |
| 1   | A     | 299 | LEU  | 2.0  |
| 1   | A     | 310 | ALA  | 2.0  |
| 1   | C     | 227 | GLN  | 2.0  |
| 1   | D     | 305 | SER  | 2.0  |
| 1   | C     | 30  | ARG  | 2.0  |
| 1   | F     | 312 | ASN  | 2.0  |
| 1   | C     | 219 | LEU  | 2.0  |
| 1   | F     | 243 | ALA  | 2.0  |
| 1   | B     | 254 | ASN  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | LLDF  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-------|----------------------------|-------|
| 2   | PEG  | C     | 425 | 7/7   | 0.87 | 0.17 | 0.98  | 54,56,60,64                | 0     |
| 2   | PEG  | A     | 425 | 7/7   | 0.91 | 0.15 | 0.71  | 44,49,57,58                | 0     |
| 2   | PEG  | F     | 425 | 7/7   | 0.88 | 0.16 | 0.43  | 44,45,51,59                | 0     |
| 2   | PEG  | E     | 425 | 7/7   | 0.89 | 0.14 | -0.24 | 59,60,65,65                | 0     |
| 2   | PEG  | D     | 425 | 7/7   | 0.91 | 0.11 | -0.41 | 51,52,56,56                | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.