



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:30 PM UTC

PDB ID : 3F8U / pdb\_00003f8u  
Title : Tapasin/ERp57 heterodimer  
Authors : Dong, G.; Reinisch, K.M.  
Deposited on : 2008-11-13  
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

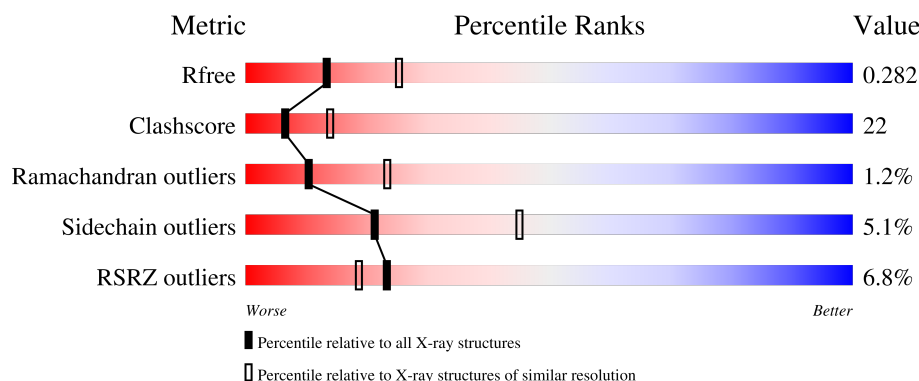
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 4008 (2.60-2.60)                                      |
| Clashscore            | 190562                      | 4347 (2.60-2.60)                                      |
| Ramachandran outliers | 187476                      | 4277 (2.60-2.60)                                      |
| Sidechain outliers    | 187428                      | 4277 (2.60-2.60)                                      |
| RSRZ outliers         | 180081                      | 4008 (2.60-2.60)                                      |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 481    |                  |
| 1   | C     | 481    |                  |
| 2   | B     | 401    |                  |
| 2   | D     | 401    |                  |

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13051 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 Protein disulfide-isomerase A3ERp57.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 469      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3724  | 2362 | 625 | 724 | 13 |         |         |       |
| 1   | C     | 462      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3675  | 2335 | 617 | 710 | 13 |         |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| A     | 60      | ALA      | CYS    | engineered mutation | UNP P30101 |
| C     | 60      | ALA      | CYS    | engineered mutation | UNP P30101 |

- Molecule 2 is a protein called Tapasin.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 2   | B     | 361      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2755  | 1766 | 486 | 492 | 11 |         |         |       |
| 2   | D     | 361      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2757  | 1769 | 486 | 491 | 11 |         |         |       |

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



| Mol | Chain | Residues | Atoms |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 3   | B     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 3   | D     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |

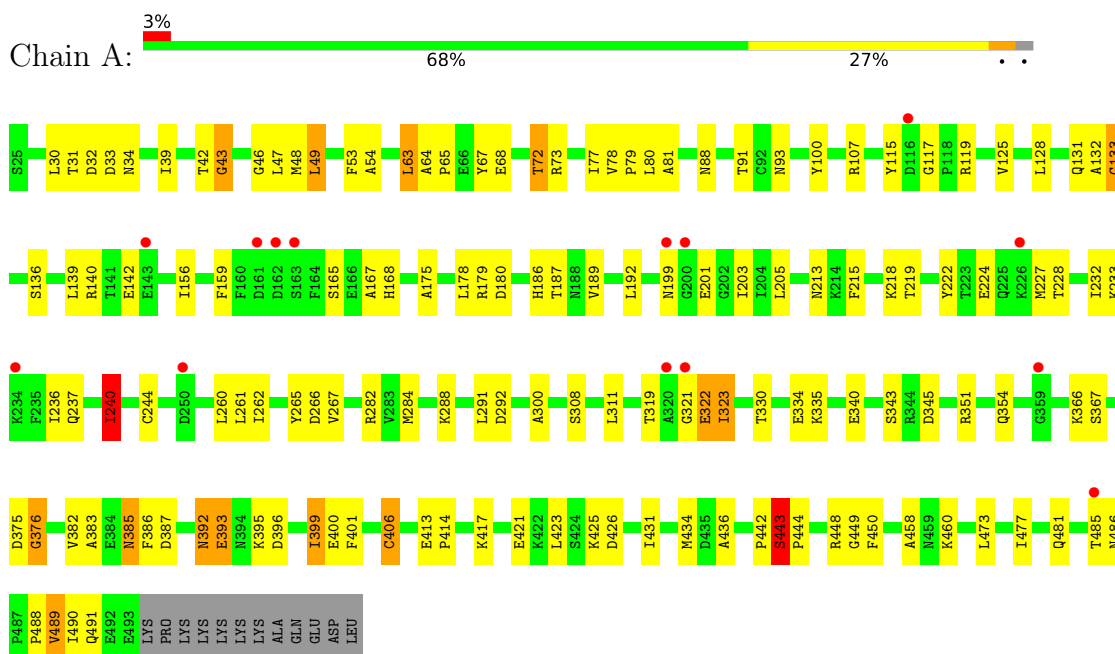
- Molecule 4 is water.

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 4   | A     | 36       | Total | O  | 0       | 0       |
|     |       |          | 36    | 36 |         |         |
| 4   | B     | 49       | Total | O  | 0       | 0       |
|     |       |          | 49    | 49 |         |         |
| 4   | C     | 7        | Total | O  | 0       | 0       |
|     |       |          | 7     | 7  |         |         |
| 4   | D     | 20       | Total | O  | 0       | 0       |
|     |       |          | 20    | 20 |         |         |

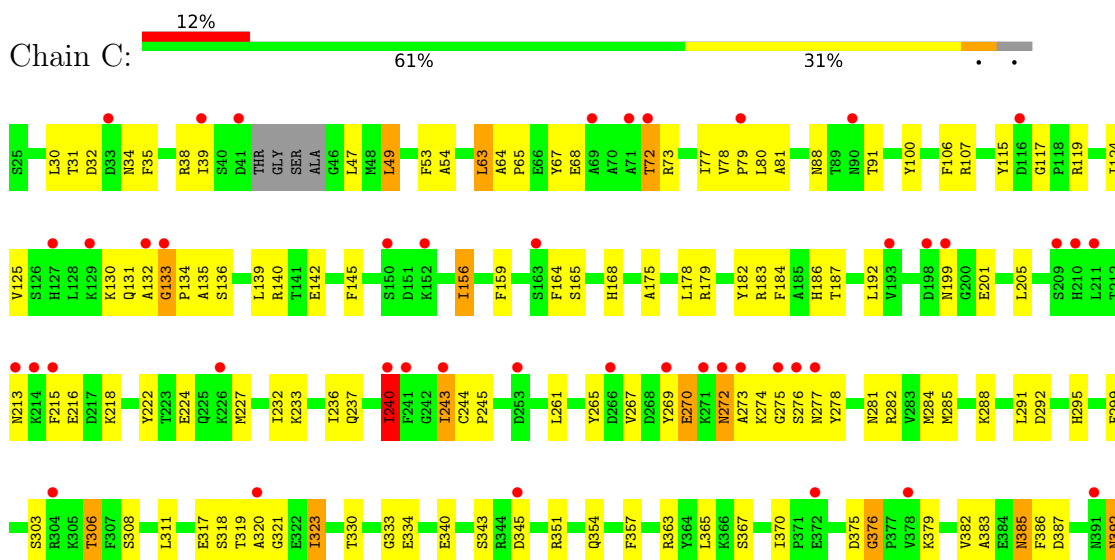
### 3 Residue-property plots

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

#### • Molecule 1: Protein disulfide-isomerase A3Erp57



#### • Molecule 1: Protein disulfide-isomerase A3Erp57





## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 1 21 1                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 74.10Å 72.30Å 200.19Å<br>90.00° 94.61° 90.00°               | Depositor        |
| Resolution (Å)                                                          | 20.00 – 2.60<br>20.00 – 2.60                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 97.4 (20.00-2.60)<br>97.2 (20.00-2.60)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.07                                                        | Depositor        |
| $R_{sym}$                                                               | 0.07                                                        | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 3.89 (at 2.51Å)                                             | Xtriage          |
| Refinement program                                                      | CNS 1.2                                                     | Depositor        |
| R, $R_{free}$                                                           | 0.245 , 0.285<br>0.247 , 0.282                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 3296 reflections (4.66%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 57.4                                                        | Xtriage          |
| Anisotropy                                                              | 0.151                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.33 , 41.2                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.92                                                        | EDS              |
| Total number of atoms                                                   | 13051                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 62.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths |             | Bond angles |                 |
|-----|-------|--------------|-------------|-------------|-----------------|
|     |       | RMSZ         | # $ Z  > 5$ | RMSZ        | # $ Z  > 5$     |
| 1   | A     | 0.48         | 0/3808      | 0.93        | 6/5142 (0.1%)   |
| 1   | C     | 0.41         | 0/3758      | 0.92        | 6/5073 (0.1%)   |
| 2   | B     | 0.50         | 0/2849      | 1.04        | 15/3906 (0.4%)  |
| 2   | D     | 0.47         | 0/2849      | 1.04        | 15/3905 (0.4%)  |
| All | All   | 0.46         | 0/13264     | 0.98        | 42/18026 (0.2%) |

There are no bond length outliers.

All (42) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | D     | 321 | GLN  | OE1-CD-NE2 | -9.79 | 112.81      | 122.60   |
| 2   | B     | 321 | GLN  | OE1-CD-NE2 | -9.76 | 112.84      | 122.60   |
| 2   | B     | 48  | VAL  | N-CA-C     | 8.72  | 121.15      | 107.98   |
| 2   | D     | 48  | VAL  | N-CA-C     | 8.24  | 120.74      | 108.54   |
| 2   | B     | 298 | SER  | N-CA-C     | 8.04  | 123.11      | 110.17   |
| 2   | D     | 41  | ASP  | N-CA-C     | 7.64  | 126.70      | 109.81   |
| 2   | B     | 41  | ASP  | N-CA-C     | 7.42  | 126.21      | 109.81   |
| 2   | D     | 298 | SER  | N-CA-C     | 7.40  | 122.09      | 110.17   |
| 2   | B     | 43  | GLU  | N-CA-C     | -7.33 | 104.31      | 113.18   |
| 2   | D     | 43  | GLU  | N-CA-C     | -7.12 | 104.56      | 113.18   |
| 2   | B     | 247 | GLY  | N-CA-C     | 7.01  | 120.83      | 110.60   |
| 2   | B     | 46  | LEU  | N-CA-C     | 6.76  | 120.26      | 109.24   |
| 2   | B     | 321 | GLN  | CG-CD-NE2  | 6.64  | 126.36      | 116.40   |
| 2   | D     | 321 | GLN  | CG-CD-NE2  | 6.64  | 126.35      | 116.40   |
| 2   | D     | 247 | GLY  | N-CA-C     | 6.52  | 119.23      | 110.43   |
| 2   | D     | 46  | LEU  | N-CA-C     | 6.35  | 119.58      | 109.24   |
| 2   | D     | 227 | TRP  | N-CA-C     | 6.32  | 121.93      | 113.72   |
| 2   | D     | 331 | ALA  | N-CA-C     | -6.27 | 102.44      | 110.53   |
| 2   | B     | 225 | GLU  | CA-C-N     | 6.26  | 127.66      | 119.84   |
| 2   | B     | 225 | GLU  | C-N-CA     | 6.26  | 127.66      | 119.84   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 395 | LYS  | N-CA-C  | 6.08  | 118.42      | 109.24   |
| 2   | B     | 331 | ALA  | N-CA-C  | -6.06 | 102.72      | 110.53   |
| 2   | B     | 227 | TRP  | N-CA-C  | 5.85  | 121.46      | 113.97   |
| 1   | A     | 240 | ILE  | N-CA-C  | 5.83  | 117.27      | 110.62   |
| 2   | D     | 225 | GLU  | CA-C-N  | 5.77  | 127.06      | 119.84   |
| 2   | D     | 225 | GLU  | C-N-CA  | 5.77  | 127.06      | 119.84   |
| 1   | A     | 34  | ASN  | N-CA-C  | 5.67  | 119.90      | 112.92   |
| 1   | A     | 443 | SER  | N-CA-C  | 5.50  | 121.97      | 109.81   |
| 1   | A     | 406 | CYS  | N-CA-C  | 5.46  | 117.62      | 109.59   |
| 1   | C     | 395 | LYS  | N-CA-C  | 5.44  | 117.45      | 109.24   |
| 2   | D     | 238 | LEU  | CA-C-N  | 5.42  | 125.18      | 119.76   |
| 2   | D     | 238 | LEU  | C-N-CA  | 5.42  | 125.18      | 119.76   |
| 1   | C     | 240 | ILE  | N-CA-C  | 5.39  | 116.77      | 110.62   |
| 1   | C     | 34  | ASN  | N-CA-C  | 5.31  | 119.45      | 112.92   |
| 1   | C     | 243 | ILE  | CB-CA-C | -5.19 | 105.29      | 112.24   |
| 2   | B     | 1   | GLY  | CA-C-N  | 5.17  | 125.17      | 119.90   |
| 2   | B     | 1   | GLY  | C-N-CA  | 5.17  | 125.17      | 119.90   |
| 1   | C     | 406 | CYS  | N-CA-C  | 5.15  | 117.13      | 109.25   |
| 1   | A     | 396 | ASP  | N-CA-C  | -5.14 | 100.85      | 109.24   |
| 1   | C     | 443 | SER  | N-CA-C  | 5.07  | 121.02      | 109.81   |
| 2   | D     | 355 | GLN  | N-CA-C  | -5.04 | 107.81      | 114.31   |
| 2   | B     | 68  | ALA  | N-CA-C  | -5.03 | 103.69      | 109.93   |

There are no chirality outliers.

There are no planarity outliers.

## 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     | 3724  | 0        | 3619     | 143     | 0            |
| 1   | C     | 3675  | 0        | 3578     | 191     | 0            |
| 2   | B     | 2755  | 0        | 2713     | 122     | 0            |
| 2   | D     | 2757  | 0        | 2720     | 112     | 0            |
| 3   | B     | 14    | 0        | 13       | 0       | 0            |
| 3   | D     | 14    | 0        | 13       | 1       | 0            |
| 4   | A     | 36    | 0        | 0        | 1       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4   | B     | 49    | 0        | 0        | 2       | 0            |
| 4   | C     | 7     | 0        | 0        | 0       | 0            |
| 4   | D     | 20    | 0        | 0        | 1       | 0            |
| All | All   | 13051 | 0        | 12656    | 558     | 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 22.

All (558) 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:A:42:THR:HG21  | 1:A:47:LEU:N     | 1.70                     | 1.06              |
| 1:C:215:PHE:CE1  | 1:C:285:MET:HA   | 1.92                     | 1.05              |
| 2:B:317:GLY:O    | 2:B:321:GLN:CG   | 2.08                     | 1.01              |
| 2:D:283:ARG:HA   | 2:D:381:GLU:HB3  | 1.43                     | 1.00              |
| 1:A:448:ARG:HG3  | 1:A:449:GLY:H    | 1.26                     | 0.98              |
| 1:C:448:ARG:HG3  | 1:C:449:GLY:H    | 1.27                     | 0.97              |
| 2:D:42:PRO:HG3   | 2:D:131:LEU:HG   | 1.47                     | 0.96              |
| 2:B:317:GLY:O    | 2:B:321:GLN:HG3  | 1.65                     | 0.96              |
| 2:B:132:ILE:HD13 | 2:B:133:THR:N    | 1.81                     | 0.95              |
| 2:B:42:PRO:HG3   | 2:B:131:LEU:HG   | 1.44                     | 0.95              |
| 1:A:308:SER:HA   | 1:A:311:LEU:HD23 | 1.46                     | 0.95              |
| 2:B:283:ARG:HA   | 2:B:381:GLU:HB3  | 1.46                     | 0.95              |
| 1:A:32:ASP:H     | 1:A:88:ASN:HD22  | 1.07                     | 0.94              |
| 1:C:32:ASP:H     | 1:C:88:ASN:HD22  | 1.01                     | 0.93              |
| 1:C:308:SER:HA   | 1:C:311:LEU:HD23 | 1.51                     | 0.93              |
| 1:C:130:LYS:HZ1  | 1:C:184:PHE:H    | 1.15                     | 0.92              |
| 2:D:160:LEU:H    | 2:D:235:THR:HG22 | 1.34                     | 0.91              |
| 2:B:160:LEU:H    | 2:B:235:THR:HG22 | 1.36                     | 0.90              |
| 1:C:142:GLU:HG2  | 1:C:192:LEU:HD21 | 1.56                     | 0.88              |
| 1:A:142:GLU:HG2  | 1:A:192:LEU:HD21 | 1.56                     | 0.87              |
| 1:C:100:TYR:OH   | 2:D:97:ARG:HG3   | 1.74                     | 0.87              |
| 2:B:233:ASN:OD1  | 2:B:235:THR:HG23 | 1.75                     | 0.87              |
| 2:D:233:ASN:OD1  | 2:D:235:THR:HG23 | 1.75                     | 0.87              |
| 1:C:323:ILE:HD12 | 1:C:323:ILE:H    | 1.41                     | 0.86              |
| 1:C:243:ILE:HG13 | 1:C:244:CYS:N    | 1.91                     | 0.84              |
| 1:C:32:ASP:H     | 1:C:88:ASN:ND2   | 1.73                     | 0.84              |
| 1:A:32:ASP:H     | 1:A:88:ASN:ND2   | 1.76                     | 0.84              |
| 2:B:60:ARG:HA    | 2:B:60:ARG:HH11  | 1.43                     | 0.84              |
| 1:A:203:ILE:HD12 | 1:A:232:ILE:HD12 | 1.59                     | 0.84              |
| 2:D:34:PRO:O     | 2:D:130:VAL:HG21 | 1.78                     | 0.83              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:60:ARG:HA    | 2:D:60:ARG:HH11  | 1.44                     | 0.81              |
| 1:C:426:ASP:OD1  | 1:C:429:ILE:HD13 | 1.80                     | 0.81              |
| 2:B:317:GLY:O    | 2:B:321:GLN:HG2  | 1.81                     | 0.80              |
| 2:B:90:THR:HG22  | 2:B:90:THR:O     | 1.81                     | 0.79              |
| 1:C:130:LYS:NZ   | 1:C:184:PHE:H    | 1.80                     | 0.79              |
| 1:C:119:ARG:HH11 | 1:C:119:ARG:HG2  | 1.50                     | 0.77              |
| 1:A:323:ILE:HD12 | 1:A:323:ILE:H    | 1.49                     | 0.76              |
| 1:A:222:TYR:CE2  | 1:A:232:ILE:HD13 | 2.21                     | 0.76              |
| 2:B:59:PHE:HZ    | 2:B:108:ILE:HG21 | 1.49                     | 0.76              |
| 1:A:119:ARG:HG2  | 1:A:119:ARG:HH11 | 1.51                     | 0.75              |
| 1:C:477:ILE:HG23 | 1:C:490:ILE:HD13 | 1.68                     | 0.75              |
| 2:B:47:SER:N     | 2:B:132:ILE:HD11 | 2.02                     | 0.74              |
| 1:A:367:SER:HB2  | 1:A:383:ALA:HB3  | 1.68                     | 0.74              |
| 2:D:90:THR:HG22  | 2:D:90:THR:O     | 1.87                     | 0.74              |
| 2:B:79:LEU:HD12  | 2:B:80:PRO:HD2   | 1.68                     | 0.74              |
| 1:C:215:PHE:HE1  | 1:C:285:MET:HA   | 1.51                     | 0.74              |
| 2:D:160:LEU:HD21 | 2:D:253:ILE:HD11 | 1.69                     | 0.74              |
| 2:B:47:SER:HB2   | 2:B:132:ILE:HD12 | 1.71                     | 0.73              |
| 2:D:34:PRO:HG2   | 2:D:130:VAL:CG2  | 2.19                     | 0.72              |
| 1:C:367:SER:HB2  | 1:C:383:ALA:HB3  | 1.70                     | 0.72              |
| 1:A:42:THR:HG21  | 1:A:46:GLY:C     | 2.15                     | 0.72              |
| 1:C:64:ALA:HB3   | 1:C:65:PRO:HD3   | 1.71                     | 0.72              |
| 1:A:93:ASN:ND2   | 2:B:97:ARG:HH12  | 1.88                     | 0.71              |
| 1:A:77:ILE:HG22  | 1:A:78:VAL:HG23  | 1.72                     | 0.71              |
| 1:A:382:VAL:H    | 1:A:385:ASN:HD21 | 1.37                     | 0.71              |
| 1:C:133:GLY:N    | 1:C:179:ARG:HH12 | 1.88                     | 0.71              |
| 1:C:31:THR:HB    | 1:C:88:ASN:HD21  | 1.55                     | 0.70              |
| 1:A:42:THR:HG22  | 1:A:43:GLY:N     | 2.05                     | 0.70              |
| 2:D:52:ALA:HB1   | 2:D:163:ALA:HB1  | 1.73                     | 0.70              |
| 1:C:399:ILE:HD13 | 1:C:400:GLU:N    | 2.06                     | 0.69              |
| 1:C:130:LYS:HE2  | 1:C:182:TYR:O    | 1.91                     | 0.69              |
| 1:A:260:LEU:HD21 | 1:A:262:ILE:HD11 | 1.73                     | 0.69              |
| 1:A:93:ASN:HD22  | 2:B:97:ARG:HH12  | 1.40                     | 0.69              |
| 1:A:425:LYS:HE3  | 1:A:491:GLN:HE21 | 1.56                     | 0.69              |
| 1:C:448:ARG:HG3  | 1:C:449:GLY:N    | 2.07                     | 0.68              |
| 2:D:59:PHE:HZ    | 2:D:108:ILE:HG21 | 1.58                     | 0.68              |
| 1:A:262:ILE:HD13 | 1:A:300:ALA:HB3  | 1.76                     | 0.68              |
| 2:B:52:ALA:HB1   | 2:B:163:ALA:HB1  | 1.76                     | 0.68              |
| 1:A:262:ILE:CD1  | 1:A:300:ALA:HB3  | 2.24                     | 0.68              |
| 1:A:392:ASN:C    | 1:A:392:ASN:HD22 | 2.01                     | 0.68              |
| 1:C:370:ILE:HD13 | 1:C:382:VAL:CG2  | 2.24                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:385:ASN:C    | 1:C:385:ASN:HD22 | 2.00                     | 0.67              |
| 1:C:485:THR:HG23 | 1:C:486:ASN:N    | 2.09                     | 0.67              |
| 1:A:399:ILE:HD13 | 1:A:399:ILE:C    | 2.20                     | 0.67              |
| 1:C:426:ASP:CB   | 1:C:489:VAL:HG13 | 2.25                     | 0.67              |
| 1:C:269:TYR:O    | 1:C:273:ALA:HB2  | 1.93                     | 0.67              |
| 1:C:428:ASN:HB2  | 1:C:429:ILE:HD12 | 1.77                     | 0.67              |
| 1:C:77:ILE:H     | 1:C:77:ILE:HD12  | 1.59                     | 0.67              |
| 1:C:35:PHE:CZ    | 1:C:39:ILE:HD12  | 2.31                     | 0.66              |
| 1:C:399:ILE:HD13 | 1:C:399:ILE:C    | 2.21                     | 0.66              |
| 2:D:283:ARG:HG2  | 2:D:381:GLU:CG   | 2.26                     | 0.66              |
| 1:A:485:THR:HG23 | 1:A:486:ASN:N    | 2.10                     | 0.65              |
| 1:A:203:ILE:HD12 | 1:A:232:ILE:CD1  | 2.25                     | 0.65              |
| 2:B:361:ALA:HB2  | 2:B:377:GLU:HB3  | 1.78                     | 0.65              |
| 1:C:215:PHE:CE1  | 1:C:285:MET:CA   | 2.77                     | 0.65              |
| 1:A:448:ARG:HG3  | 1:A:449:GLY:N    | 2.06                     | 0.65              |
| 2:D:361:ALA:HB2  | 2:D:377:GLU:HB3  | 1.79                     | 0.65              |
| 1:A:266:ASP:OD1  | 1:A:322:GLU:HA   | 1.96                     | 0.65              |
| 2:D:79:LEU:HD12  | 2:D:80:PRO:HD2   | 1.78                     | 0.65              |
| 1:A:64:ALA:HB3   | 1:A:65:PRO:HD3   | 1.77                     | 0.65              |
| 1:C:426:ASP:CG   | 1:C:429:ILE:HD13 | 2.20                     | 0.65              |
| 2:D:127:GLN:HB3  | 2:D:130:VAL:O    | 1.96                     | 0.65              |
| 2:B:274:VAL:HG11 | 2:B:364:ILE:HD13 | 1.79                     | 0.64              |
| 2:B:364:ILE:N    | 2:B:364:ILE:HD12 | 2.12                     | 0.64              |
| 2:D:113:LEU:C    | 2:D:113:LEU:HD12 | 2.21                     | 0.64              |
| 1:C:485:THR:HG23 | 1:C:486:ASN:H    | 1.63                     | 0.64              |
| 2:D:4:VAL:HG12   | 2:D:26:LEU:HD12  | 1.80                     | 0.64              |
| 1:C:130:LYS:HE2  | 1:C:183:ARG:HA   | 1.79                     | 0.64              |
| 1:C:261:LEU:C    | 1:C:261:LEU:HD23 | 2.23                     | 0.64              |
| 2:B:115:LEU:C    | 2:B:115:LEU:HD23 | 2.22                     | 0.64              |
| 1:C:133:GLY:CA   | 1:C:179:ARG:HH12 | 2.11                     | 0.64              |
| 1:C:429:ILE:HD12 | 1:C:429:ILE:N    | 2.13                     | 0.64              |
| 1:A:319:THR:C    | 1:A:321:GLY:H    | 2.05                     | 0.64              |
| 1:C:159:PHE:O    | 1:C:201:GLU:HA   | 1.98                     | 0.64              |
| 2:D:115:LEU:HD23 | 2:D:115:LEU:C    | 2.23                     | 0.64              |
| 1:C:222:TYR:CE1  | 1:C:224:GLU:HB2  | 2.33                     | 0.64              |
| 1:A:385:ASN:C    | 1:A:385:ASN:HD22 | 2.06                     | 0.64              |
| 2:B:127:GLN:HG3  | 2:B:129:PRO:HD2  | 1.80                     | 0.64              |
| 1:A:399:ILE:HD13 | 1:A:400:GLU:N    | 2.13                     | 0.63              |
| 1:C:130:LYS:CE   | 1:C:183:ARG:HA   | 2.28                     | 0.63              |
| 1:A:42:THR:HB    | 1:A:46:GLY:HA2   | 1.80                     | 0.63              |
| 1:C:39:ILE:HD11  | 1:C:106:PHE:CD2  | 2.32                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:308:SER:CA   | 1:A:311:LEU:HD23 | 2.26                     | 0.63              |
| 1:C:35:PHE:CE2   | 1:C:39:ILE:HD12  | 2.33                     | 0.63              |
| 1:C:426:ASP:HB2  | 1:C:489:VAL:HG13 | 1.79                     | 0.63              |
| 2:B:79:LEU:HD12  | 2:B:80:PRO:CD    | 2.29                     | 0.63              |
| 1:C:47:LEU:HD21  | 1:C:107:ARG:CZ   | 2.29                     | 0.62              |
| 2:D:75:ARG:HG3   | 2:D:75:ARG:HH11  | 1.64                     | 0.62              |
| 2:D:141:VAL:CG1  | 2:D:253:ILE:HD13 | 2.29                     | 0.62              |
| 1:C:370:ILE:HD12 | 1:C:385:ASN:HB3  | 1.79                     | 0.62              |
| 1:A:31:THR:HB    | 1:A:88:ASN:HD21  | 1.62                     | 0.62              |
| 2:B:290:PRO:HD3  | 2:B:351:VAL:HG13 | 1.82                     | 0.62              |
| 1:C:282:ARG:HG2  | 1:C:282:ARG:HH11 | 1.64                     | 0.62              |
| 2:B:4:VAL:HG12   | 2:B:26:LEU:HD12  | 1.80                     | 0.62              |
| 1:C:178:LEU:CD1  | 1:C:236:ILE:HD12 | 2.30                     | 0.62              |
| 2:D:290:PRO:HD3  | 2:D:351:VAL:HG13 | 1.82                     | 0.62              |
| 1:A:485:THR:HG23 | 1:A:486:ASN:H    | 1.65                     | 0.61              |
| 2:B:127:GLN:HB3  | 2:B:130:VAL:O    | 2.00                     | 0.61              |
| 2:B:314:GLY:H    | 2:B:319:ARG:HA   | 1.64                     | 0.61              |
| 2:B:34:PRO:O     | 2:B:130:VAL:HG21 | 2.00                     | 0.61              |
| 1:A:232:ILE:O    | 1:A:236:ILE:HG12 | 2.01                     | 0.61              |
| 2:D:34:PRO:HG2   | 2:D:130:VAL:HB   | 1.83                     | 0.61              |
| 1:A:282:ARG:HG2  | 1:A:282:ARG:HH11 | 1.65                     | 0.61              |
| 1:C:130:LYS:NZ   | 1:C:183:ARG:HA   | 2.15                     | 0.61              |
| 2:B:113:LEU:C    | 2:B:113:LEU:HD12 | 2.26                     | 0.60              |
| 1:C:232:ILE:O    | 1:C:236:ILE:HG13 | 2.01                     | 0.60              |
| 2:D:125:PRO:O    | 2:D:126:GLN:O    | 2.18                     | 0.60              |
| 1:A:386:PHE:CE2  | 1:A:442:PRO:HG3  | 2.36                     | 0.60              |
| 2:B:283:ARG:HG2  | 2:B:381:GLU:CG   | 2.31                     | 0.60              |
| 1:C:49:LEU:HB3   | 1:C:80:LEU:HD22  | 1.83                     | 0.60              |
| 1:A:142:GLU:HG2  | 1:A:192:LEU:CD2  | 2.31                     | 0.60              |
| 1:A:261:LEU:C    | 1:A:261:LEU:HD23 | 2.27                     | 0.60              |
| 2:B:34:PRO:HG2   | 2:B:130:VAL:HB   | 1.84                     | 0.60              |
| 2:B:272:PRO:HB3  | 2:B:300:PHE:HB3  | 1.83                     | 0.59              |
| 1:C:410:LYS:HD3  | 2:D:237:TRP:CZ3  | 2.37                     | 0.59              |
| 1:C:375:ASP:O    | 1:C:376:GLY:O    | 2.20                     | 0.59              |
| 1:C:77:ILE:HG22  | 1:C:78:VAL:HG23  | 1.84                     | 0.59              |
| 1:C:156:ILE:HD11 | 1:C:182:TYR:HB3  | 1.84                     | 0.59              |
| 1:A:375:ASP:O    | 1:A:376:GLY:O    | 2.19                     | 0.59              |
| 1:C:308:SER:CA   | 1:C:311:LEU:HD23 | 2.30                     | 0.59              |
| 2:D:342:LEU:C    | 2:D:342:LEU:HD23 | 2.27                     | 0.59              |
| 2:B:190:HIS:ND1  | 2:B:191:LEU:HG   | 2.18                     | 0.59              |
| 1:C:133:GLY:H    | 1:C:179:ARG:HH12 | 1.50                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:85:TRP:CD1   | 2:B:85:TRP:C     | 2.81                     | 0.59              |
| 1:C:133:GLY:CA   | 1:C:134:PRO:C    | 2.76                     | 0.59              |
| 1:C:343:SER:C    | 1:C:345:ASP:H    | 2.10                     | 0.59              |
| 1:A:159:PHE:O    | 1:A:201:GLU:HA   | 2.03                     | 0.58              |
| 1:C:382:VAL:H    | 1:C:385:ASN:HD21 | 1.50                     | 0.58              |
| 1:A:68:GLU:O     | 1:A:72:THR:HG22  | 2.03                     | 0.58              |
| 1:C:413:GLU:HB3  | 1:C:414:PRO:HD3  | 1.85                     | 0.58              |
| 1:C:428:ASN:C    | 1:C:429:ILE:HD12 | 2.28                     | 0.58              |
| 1:C:386:PHE:CE2  | 1:C:442:PRO:HG3  | 2.39                     | 0.58              |
| 1:C:32:ASP:OD2   | 1:C:88:ASN:HB3   | 2.04                     | 0.58              |
| 1:C:370:ILE:HD13 | 1:C:382:VAL:HG21 | 1.85                     | 0.58              |
| 1:A:132:ALA:O    | 1:A:133:GLY:O    | 2.22                     | 0.57              |
| 1:A:165:SER:OG   | 1:A:168:HIS:HB2  | 2.04                     | 0.57              |
| 2:B:75:ARG:HG3   | 2:B:75:ARG:HH11  | 1.68                     | 0.57              |
| 2:B:352:THR:CG2  | 2:B:354:GLU:HG2  | 2.34                     | 0.57              |
| 2:D:141:VAL:HG13 | 2:D:253:ILE:HD13 | 1.85                     | 0.57              |
| 1:A:340:GLU:OE2  | 1:A:351:ARG:NH1  | 2.37                     | 0.57              |
| 1:A:42:THR:CG2   | 1:A:43:GLY:N     | 2.68                     | 0.57              |
| 1:C:68:GLU:O     | 1:C:72:THR:HG22  | 2.04                     | 0.57              |
| 1:C:192:LEU:HD22 | 1:C:192:LEU:H    | 1.69                     | 0.57              |
| 1:A:426:ASP:CB   | 1:A:489:VAL:HG13 | 2.34                     | 0.57              |
| 2:B:186:TRP:CE2  | 2:B:236:PHE:HB2  | 2.39                     | 0.57              |
| 1:C:392:ASN:HD22 | 1:C:392:ASN:C    | 2.10                     | 0.57              |
| 2:D:60:ARG:HA    | 2:D:60:ARG:NH1   | 2.18                     | 0.57              |
| 1:A:222:TYR:CE1  | 1:A:224:GLU:HB2  | 2.40                     | 0.57              |
| 2:B:125:PRO:O    | 2:B:126:GLN:O    | 2.22                     | 0.57              |
| 1:C:131:GLN:C    | 1:C:133:GLY:H    | 2.13                     | 0.57              |
| 2:D:283:ARG:HG2  | 2:D:381:GLU:HG2  | 1.87                     | 0.57              |
| 2:D:84:LYS:O     | 2:D:84:LYS:HD3   | 2.04                     | 0.57              |
| 1:C:136:SER:OG   | 1:C:186:HIS:HD2  | 1.88                     | 0.56              |
| 1:A:39:ILE:HG13  | 1:A:39:ILE:O     | 2.04                     | 0.56              |
| 1:C:178:LEU:HD13 | 1:C:236:ILE:HD12 | 1.85                     | 0.56              |
| 2:D:186:TRP:CE2  | 2:D:236:PHE:HB2  | 2.40                     | 0.56              |
| 2:D:190:HIS:ND1  | 2:D:191:LEU:HG   | 2.19                     | 0.56              |
| 2:D:85:TRP:CD1   | 2:D:85:TRP:C     | 2.84                     | 0.56              |
| 1:A:431:ILE:N    | 1:A:431:ILE:HD12 | 2.21                     | 0.56              |
| 1:A:49:LEU:HB3   | 1:A:80:LEU:HD22  | 1.87                     | 0.56              |
| 1:A:343:SER:C    | 1:A:345:ASP:H    | 2.12                     | 0.56              |
| 2:D:272:PRO:HB3  | 2:D:300:PHE:HB3  | 1.87                     | 0.56              |
| 1:C:489:VAL:HG22 | 1:C:489:VAL:O    | 2.05                     | 0.56              |
| 1:C:205:LEU:HD11 | 1:C:240:ILE:HG22 | 1.88                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:41:ASP:OD2   | 2:B:43:GLU:HB2   | 2.07                     | 0.55              |
| 1:A:392:ASN:C    | 1:A:392:ASN:ND2  | 2.63                     | 0.55              |
| 1:A:366:LYS:NZ   | 2:B:207:GLN:HE22 | 2.04                     | 0.55              |
| 2:B:41:ASP:HB3   | 2:B:43:GLU:H     | 1.71                     | 0.55              |
| 1:C:39:ILE:HD11  | 1:C:106:PHE:CG   | 2.42                     | 0.55              |
| 1:C:133:GLY:HA3  | 1:C:134:PRO:C    | 2.32                     | 0.55              |
| 2:D:160:LEU:N    | 2:D:235:THR:HG22 | 2.13                     | 0.55              |
| 1:A:42:THR:HG21  | 1:A:47:LEU:H     | 1.61                     | 0.55              |
| 2:D:50:ASP:HB3   | 2:D:56:GLN:HG3   | 1.87                     | 0.55              |
| 2:D:151:ARG:HH12 | 2:D:271:PRO:HG3  | 1.72                     | 0.55              |
| 1:C:139:LEU:HB2  | 1:C:187:THR:HB   | 1.88                     | 0.55              |
| 1:A:131:GLN:C    | 1:A:133:GLY:H    | 2.13                     | 0.55              |
| 1:C:32:ASP:N     | 1:C:88:ASN:HD22  | 1.86                     | 0.55              |
| 1:C:63:LEU:HD22  | 1:C:67:TYR:HB2   | 1.90                     | 0.55              |
| 1:C:47:LEU:HD21  | 1:C:107:ARG:NH1  | 2.22                     | 0.54              |
| 1:A:93:ASN:ND2   | 2:B:97:ARG:NH1   | 2.54                     | 0.54              |
| 1:C:156:ILE:N    | 1:C:156:ILE:HD12 | 2.23                     | 0.54              |
| 1:C:481:GLN:HA   | 1:C:488:PRO:HG3  | 1.89                     | 0.54              |
| 2:B:168:THR:HG21 | 1:C:168:HIS:HB3  | 1.87                     | 0.54              |
| 2:D:28:ARG:NH2   | 2:D:34:PRO:HB3   | 2.22                     | 0.54              |
| 2:B:315:GLY:C    | 2:B:317:GLY:H    | 2.16                     | 0.54              |
| 2:B:60:ARG:HA    | 2:B:60:ARG:NH1   | 2.19                     | 0.54              |
| 2:B:50:ASP:HB3   | 2:B:56:GLN:HG3   | 1.90                     | 0.54              |
| 2:B:235:THR:HG21 | 4:B:2027:HOH:O   | 2.07                     | 0.54              |
| 1:C:399:ILE:HD13 | 1:C:400:GLU:C    | 2.33                     | 0.54              |
| 1:A:32:ASP:OD2   | 1:A:88:ASN:HB3   | 2.07                     | 0.53              |
| 1:A:139:LEU:HB2  | 1:A:187:THR:HB   | 1.89                     | 0.53              |
| 2:B:352:THR:HG22 | 2:B:354:GLU:HG2  | 1.90                     | 0.53              |
| 1:C:142:GLU:HG2  | 1:C:192:LEU:CD2  | 2.32                     | 0.53              |
| 2:D:34:PRO:HG2   | 2:D:130:VAL:CB   | 2.38                     | 0.53              |
| 1:C:100:TYR:CZ   | 2:D:97:ARG:HG3   | 2.43                     | 0.53              |
| 1:A:136:SER:OG   | 1:A:186:HIS:HD2  | 1.90                     | 0.53              |
| 2:B:198:LEU:HD23 | 2:B:199:ALA:N    | 2.23                     | 0.53              |
| 2:D:352:THR:CG2  | 2:D:354:GLU:HG2  | 2.39                     | 0.53              |
| 2:B:41:ASP:HB3   | 2:B:43:GLU:N     | 2.23                     | 0.53              |
| 1:C:288:LYS:HG2  | 1:C:292:ASP:OD2  | 2.09                     | 0.53              |
| 1:C:385:ASN:HD22 | 1:C:386:PHE:N    | 2.05                     | 0.53              |
| 2:D:79:LEU:HD12  | 2:D:80:PRO:CD    | 2.39                     | 0.53              |
| 2:B:167:PRO:HG3  | 1:C:164:PHE:CZ   | 2.43                     | 0.53              |
| 2:D:218:PHE:CG   | 3:D:1233:NAG:H62 | 2.44                     | 0.53              |
| 2:B:274:VAL:HG11 | 2:B:364:ILE:CD1  | 2.38                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:243:PRO:O    | 2:B:246:GLU:HB2  | 2.09                     | 0.53              |
| 1:A:63:LEU:HD22  | 1:A:67:TYR:HB2   | 1.90                     | 0.53              |
| 1:A:399:ILE:HD13 | 1:A:400:GLU:C    | 2.34                     | 0.52              |
| 1:A:413:GLU:HB3  | 1:A:414:PRO:HD3  | 1.90                     | 0.52              |
| 1:A:425:LYS:HE3  | 1:A:491:GLN:NE2  | 2.24                     | 0.52              |
| 1:A:426:ASP:HB2  | 1:A:489:VAL:HG13 | 1.90                     | 0.52              |
| 2:B:79:LEU:CD1   | 2:B:80:PRO:HD2   | 2.36                     | 0.52              |
| 1:A:42:THR:HG23  | 1:A:47:LEU:O     | 2.09                     | 0.52              |
| 1:A:140:ARG:HG2  | 1:A:140:ARG:HH11 | 1.73                     | 0.52              |
| 2:B:342:LEU:C    | 2:B:342:LEU:HD23 | 2.35                     | 0.52              |
| 1:A:485:THR:HG23 | 1:A:486:ASN:ND2  | 2.24                     | 0.52              |
| 1:A:448:ARG:CG   | 1:A:449:GLY:H    | 2.08                     | 0.52              |
| 2:B:283:ARG:HG2  | 2:B:381:GLU:HG2  | 1.92                     | 0.52              |
| 2:B:287:GLY:C    | 2:B:350:PRO:HB3  | 2.34                     | 0.52              |
| 1:C:473:LEU:O    | 1:C:477:ILE:HG12 | 2.09                     | 0.52              |
| 1:C:77:ILE:HD12  | 1:C:77:ILE:N     | 2.24                     | 0.52              |
| 1:A:288:LYS:HG2  | 1:A:292:ASP:OD2  | 2.10                     | 0.51              |
| 1:A:473:LEU:O    | 1:A:477:ILE:HG12 | 2.09                     | 0.51              |
| 1:C:119:ARG:HG2  | 1:C:119:ARG:NH1  | 2.22                     | 0.51              |
| 1:A:192:LEU:H    | 1:A:192:LEU:HD22 | 1.76                     | 0.51              |
| 1:A:489:VAL:O    | 1:A:489:VAL:HG22 | 2.09                     | 0.51              |
| 1:C:401:PHE:CE1  | 1:C:434:MET:HE2  | 2.45                     | 0.51              |
| 1:A:201:GLU:O    | 1:A:201:GLU:HG3  | 2.09                     | 0.51              |
| 2:B:170:GLU:HA   | 4:B:2047:HOH:O   | 2.11                     | 0.51              |
| 1:C:131:GLN:O    | 1:C:179:ARG:NH1  | 2.43                     | 0.51              |
| 2:D:287:GLY:C    | 2:D:350:PRO:HB3  | 2.35                     | 0.51              |
| 2:D:127:GLN:HG3  | 2:D:129:PRO:HD2  | 1.93                     | 0.51              |
| 1:A:488:PRO:HB2  | 1:A:490:ILE:HD11 | 1.92                     | 0.51              |
| 1:C:215:PHE:CD2  | 1:C:284:MET:HB2  | 2.46                     | 0.51              |
| 1:C:130:LYS:HZ3  | 1:C:183:ARG:HA   | 1.75                     | 0.51              |
| 1:C:192:LEU:HD22 | 1:C:192:LEU:N    | 2.26                     | 0.51              |
| 1:A:321:GLY:O    | 1:A:322:GLU:HB3  | 2.11                     | 0.51              |
| 1:A:401:PHE:CE1  | 1:A:434:MET:HE2  | 2.46                     | 0.51              |
| 1:C:140:ARG:HG2  | 1:C:140:ARG:HH11 | 1.75                     | 0.51              |
| 1:C:453:ILE:N    | 1:C:453:ILE:HD12 | 2.25                     | 0.51              |
| 1:C:49:LEU:CB    | 1:C:80:LEU:HD22  | 2.41                     | 0.51              |
| 2:D:164:TYR:OH   | 2:D:167:PRO:HD3  | 2.11                     | 0.51              |
| 1:A:393:GLU:O    | 1:A:458:ALA:O    | 2.29                     | 0.50              |
| 1:C:201:GLU:O    | 1:C:201:GLU:HG3  | 2.10                     | 0.50              |
| 2:D:249:TYR:C    | 2:D:250:LEU:HD12 | 2.36                     | 0.50              |
| 1:C:165:SER:OG   | 1:C:168:HIS:HB2  | 2.11                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:96:PRO:HD3   | 2:D:257:TYR:CE1  | 2.45                     | 0.50              |
| 1:C:278:TYR:CE2  | 1:C:282:ARG:NH2  | 2.73                     | 0.50              |
| 1:C:485:THR:HG23 | 1:C:486:ASN:ND2  | 2.26                     | 0.50              |
| 1:C:53:PHE:HA    | 1:C:100:TYR:CD1  | 2.46                     | 0.50              |
| 1:A:319:THR:C    | 1:A:321:GLY:N    | 2.69                     | 0.50              |
| 2:B:190:HIS:CE1  | 2:B:191:LEU:HG   | 2.46                     | 0.50              |
| 2:B:223:ASP:OD2  | 2:B:225:GLU:HG2  | 2.11                     | 0.50              |
| 1:C:132:ALA:O    | 1:C:133:GLY:C    | 2.54                     | 0.50              |
| 2:D:151:ARG:HH12 | 2:D:271:PRO:CG   | 2.24                     | 0.50              |
| 2:D:90:THR:O     | 2:D:90:THR:CG2   | 2.58                     | 0.50              |
| 1:A:49:LEU:CB    | 1:A:80:LEU:HD22  | 2.42                     | 0.50              |
| 1:A:322:GLU:HG2  | 4:A:2032:HOH:O   | 2.12                     | 0.50              |
| 1:C:115:TYR:CZ   | 1:C:124:ILE:HD13 | 2.47                     | 0.50              |
| 1:C:319:THR:C    | 1:C:321:GLY:H    | 2.19                     | 0.50              |
| 1:C:436:ALA:HB3  | 1:C:450:PHE:HE2  | 1.76                     | 0.50              |
| 1:C:222:TYR:CZ   | 1:C:224:GLU:HB2  | 2.46                     | 0.49              |
| 2:D:243:PRO:O    | 2:D:246:GLU:HB2  | 2.13                     | 0.49              |
| 1:C:31:THR:HB    | 1:C:88:ASN:ND2   | 2.25                     | 0.49              |
| 2:B:55:LEU:CD1   | 2:B:115:LEU:HD11 | 2.42                     | 0.49              |
| 2:B:132:ILE:HD13 | 2:B:133:THR:H    | 1.73                     | 0.49              |
| 1:C:429:ILE:N    | 1:C:429:ILE:CD1  | 2.75                     | 0.49              |
| 1:C:485:THR:CG2  | 1:C:486:ASN:N    | 2.75                     | 0.49              |
| 2:B:34:PRO:HG2   | 2:B:130:VAL:CG2  | 2.43                     | 0.49              |
| 2:B:167:PRO:C    | 2:B:169:SER:H    | 2.19                     | 0.49              |
| 1:C:370:ILE:CD1  | 1:C:385:ASN:HB3  | 2.42                     | 0.49              |
| 2:D:6:GLU:CD     | 2:D:37:ARG:HH22  | 2.21                     | 0.49              |
| 1:C:233:LYS:O    | 1:C:237:GLN:HG3  | 2.13                     | 0.49              |
| 1:A:178:LEU:HD21 | 1:A:233:LYS:HD2  | 1.95                     | 0.49              |
| 2:B:49:HIS:CE1   | 2:B:51:PRO:HG3   | 2.47                     | 0.49              |
| 1:C:133:GLY:CA   | 1:C:134:PRO:O    | 2.61                     | 0.49              |
| 2:D:4:VAL:HG12   | 2:D:26:LEU:CD1   | 2.42                     | 0.49              |
| 1:A:47:LEU:HD21  | 1:A:107:ARG:CZ   | 2.43                     | 0.49              |
| 2:B:4:VAL:HG12   | 2:B:26:LEU:CD1   | 2.43                     | 0.49              |
| 1:C:243:ILE:CG1  | 1:C:244:CYS:N    | 2.71                     | 0.49              |
| 1:C:426:ASP:CA   | 1:C:489:VAL:HG13 | 2.43                     | 0.49              |
| 2:D:42:PRO:HG2   | 2:D:125:PRO:HB3  | 1.95                     | 0.49              |
| 1:A:39:ILE:HD12  | 1:A:48:MET:SD    | 2.53                     | 0.49              |
| 2:B:90:THR:O     | 2:B:90:THR:CG2   | 2.53                     | 0.49              |
| 2:B:288:GLU:O    | 2:B:351:VAL:HG22 | 2.13                     | 0.49              |
| 1:C:100:TYR:O    | 2:D:94:ASN:HB2   | 2.13                     | 0.49              |
| 2:D:182:PHE:O    | 2:D:201:THR:HA   | 2.12                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:119:ARG:HG2  | 1:A:119:ARG:NH1  | 2.23                     | 0.48              |
| 2:B:316:PRO:HD3  | 2:B:354:GLU:O    | 2.13                     | 0.48              |
| 1:C:485:THR:CG2  | 1:C:486:ASN:H    | 2.26                     | 0.48              |
| 1:C:393:GLU:O    | 1:C:458:ALA:O    | 2.30                     | 0.48              |
| 2:D:352:THR:HG22 | 2:D:354:GLU:HG2  | 1.94                     | 0.48              |
| 1:C:319:THR:O    | 1:C:321:GLY:N    | 2.46                     | 0.48              |
| 2:B:283:ARG:HG3  | 2:B:283:ARG:HH11 | 1.78                     | 0.48              |
| 1:C:133:GLY:H    | 1:C:179:ARG:NH1  | 2.10                     | 0.48              |
| 2:D:110:SER:HB2  | 2:D:111:PRO:HD2  | 1.96                     | 0.48              |
| 1:C:192:LEU:H    | 1:C:192:LEU:CD2  | 2.26                     | 0.48              |
| 1:C:343:SER:C    | 1:C:345:ASP:N    | 2.70                     | 0.48              |
| 1:A:382:VAL:H    | 1:A:385:ASN:ND2  | 2.06                     | 0.48              |
| 1:A:385:ASN:C    | 1:A:385:ASN:ND2  | 2.69                     | 0.48              |
| 2:D:250:LEU:HD23 | 2:D:261:GLN:OE1  | 2.14                     | 0.48              |
| 1:A:481:GLN:HA   | 1:A:488:PRO:HG3  | 1.95                     | 0.48              |
| 1:C:156:ILE:CD1  | 1:C:182:TYR:HB3  | 2.43                     | 0.48              |
| 2:D:182:PHE:CE1  | 2:D:202:PRO:HG2  | 2.49                     | 0.48              |
| 2:B:96:PRO:HD3   | 2:B:257:TYR:CE1  | 2.49                     | 0.48              |
| 1:C:319:THR:C    | 1:C:321:GLY:N    | 2.72                     | 0.48              |
| 2:D:190:HIS:CE1  | 2:D:191:LEU:HG   | 2.49                     | 0.48              |
| 2:D:223:ASP:OD2  | 2:D:225:GLU:HG2  | 2.14                     | 0.48              |
| 1:A:485:THR:CG2  | 1:A:486:ASN:H    | 2.27                     | 0.47              |
| 1:A:485:THR:CG2  | 1:A:486:ASN:N    | 2.77                     | 0.47              |
| 2:B:8:TRP:CG     | 2:B:20:LYS:HZ1   | 2.32                     | 0.47              |
| 2:B:182:PHE:CE1  | 2:B:202:PRO:HG2  | 2.49                     | 0.47              |
| 2:D:151:ARG:O    | 2:D:154:GLN:HB2  | 2.13                     | 0.47              |
| 2:B:47:SER:CB    | 2:B:132:ILE:HD12 | 2.42                     | 0.47              |
| 2:D:171:ALA:O    | 2:D:172:ALA:HB2  | 2.14                     | 0.47              |
| 1:C:243:ILE:HG13 | 1:C:244:CYS:H    | 1.73                     | 0.47              |
| 1:C:443:SER:HB3  | 1:C:444:PRO:HD3  | 1.95                     | 0.47              |
| 2:B:182:PHE:O    | 2:B:201:THR:HA   | 2.15                     | 0.47              |
| 1:A:30:LEU:HG    | 1:A:81:ALA:HB1   | 1.96                     | 0.47              |
| 2:B:132:ILE:HD13 | 2:B:132:ILE:C    | 2.39                     | 0.47              |
| 2:B:160:LEU:N    | 2:B:235:THR:HG22 | 2.18                     | 0.47              |
| 2:B:250:LEU:HD23 | 2:B:261:GLN:OE1  | 2.14                     | 0.47              |
| 1:C:385:ASN:C    | 1:C:385:ASN:ND2  | 2.66                     | 0.47              |
| 2:D:41:ASP:HB3   | 2:D:43:GLU:N     | 2.30                     | 0.47              |
| 1:A:133:GLY:HA2  | 1:A:179:ARG:HH12 | 1.80                     | 0.47              |
| 1:C:215:PHE:CD2  | 1:C:284:MET:CB   | 2.98                     | 0.47              |
| 2:D:113:LEU:HD12 | 2:D:113:LEU:O    | 2.14                     | 0.47              |
| 1:A:426:ASP:HA   | 1:A:489:VAL:HG13 | 1.97                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:364:ILE:N    | 2:B:364:ILE:CD1  | 2.77                     | 0.46              |
| 1:C:455:PHE:O    | 1:C:457:PRO:HD3  | 2.15                     | 0.46              |
| 2:D:113:LEU:C    | 2:D:113:LEU:CD1  | 2.88                     | 0.46              |
| 1:A:343:SER:C    | 1:A:345:ASP:N    | 2.72                     | 0.46              |
| 1:C:132:ALA:O    | 1:C:133:GLY:O    | 2.32                     | 0.46              |
| 1:C:275:GLY:O    | 1:C:278:TYR:HB3  | 2.16                     | 0.46              |
| 1:A:321:GLY:O    | 1:A:323:ILE:HD12 | 2.15                     | 0.46              |
| 1:A:436:ALA:HB3  | 1:A:450:PHE:HE2  | 1.81                     | 0.46              |
| 1:A:490:ILE:N    | 1:A:490:ILE:HD12 | 2.31                     | 0.46              |
| 2:B:255:LEU:O    | 2:B:256:PRO:C    | 2.55                     | 0.46              |
| 1:A:385:ASN:HD22 | 1:A:386:PHE:N    | 2.12                     | 0.46              |
| 2:B:55:LEU:HD12  | 2:B:115:LEU:HD11 | 1.97                     | 0.46              |
| 1:C:30:LEU:HG    | 1:C:81:ALA:HB1   | 1.97                     | 0.46              |
| 1:C:213:ASN:HD22 | 1:C:215:PHE:H    | 1.62                     | 0.46              |
| 1:A:227:MET:HG3  | 1:A:232:ILE:HD11 | 1.97                     | 0.46              |
| 1:C:215:PHE:O    | 1:C:288:LYS:HE2  | 2.16                     | 0.46              |
| 1:A:386:PHE:CD2  | 1:A:442:PRO:HG3  | 2.50                     | 0.46              |
| 1:C:240:ILE:HD13 | 1:C:240:ILE:N    | 2.31                     | 0.46              |
| 1:A:53:PHE:HA    | 1:A:100:TYR:CD1  | 2.51                     | 0.46              |
| 2:B:277:MET:HA   | 2:B:278:PRO:C    | 2.39                     | 0.46              |
| 2:B:281:LEU:HD12 | 2:B:380:LEU:HD23 | 1.98                     | 0.46              |
| 2:D:198:LEU:HD23 | 2:D:199:ALA:N    | 2.31                     | 0.46              |
| 1:C:363:ARG:CZ   | 1:C:365:LEU:HD11 | 2.46                     | 0.46              |
| 2:D:41:ASP:HB3   | 2:D:43:GLU:H     | 1.80                     | 0.46              |
| 1:A:222:TYR:CZ   | 1:A:224:GLU:HB2  | 2.51                     | 0.46              |
| 2:B:42:PRO:HG2   | 2:B:125:PRO:HB3  | 1.97                     | 0.46              |
| 2:D:277:MET:HA   | 2:D:278:PRO:C    | 2.40                     | 0.46              |
| 1:A:218:LYS:HG3  | 1:A:219:THR:HG23 | 1.97                     | 0.45              |
| 1:C:139:LEU:HD13 | 1:C:145:PHE:HA   | 1.98                     | 0.45              |
| 1:C:340:GLU:OE2  | 1:C:351:ARG:NH1  | 2.49                     | 0.45              |
| 2:D:8:TRP:CG     | 2:D:20:LYS:HZ1   | 2.33                     | 0.45              |
| 2:B:59:PHE:CZ    | 2:B:108:ILE:HG21 | 2.38                     | 0.45              |
| 2:B:6:GLU:CD     | 2:B:37:ARG:HH22  | 2.23                     | 0.45              |
| 2:D:281:LEU:HG   | 2:D:378:VAL:HG21 | 1.97                     | 0.45              |
| 2:D:288:GLU:O    | 2:D:351:VAL:HG22 | 2.16                     | 0.45              |
| 1:A:42:THR:O     | 1:A:43:GLY:O     | 2.34                     | 0.45              |
| 1:A:156:ILE:HD12 | 1:A:236:ILE:HD12 | 1.98                     | 0.45              |
| 1:A:213:ASN:HD22 | 1:A:215:PHE:H    | 1.62                     | 0.45              |
| 1:C:386:PHE:CD2  | 1:C:442:PRO:HG3  | 2.51                     | 0.45              |
| 1:A:31:THR:HB    | 1:A:88:ASN:ND2   | 2.31                     | 0.45              |
| 2:B:84:LYS:HD3   | 2:B:84:LYS:O     | 2.17                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:273:ALA:O    | 1:C:274:LYS:C    | 2.59                     | 0.45              |
| 1:C:477:ILE:CG2  | 1:C:490:ILE:HD13 | 2.40                     | 0.45              |
| 1:A:426:ASP:CA   | 1:A:489:VAL:HG13 | 2.46                     | 0.45              |
| 2:B:91:PRO:HG2   | 2:B:92:ALA:H     | 1.82                     | 0.45              |
| 2:B:191:LEU:C    | 2:B:193:LYS:H    | 2.23                     | 0.45              |
| 2:D:91:PRO:HG2   | 2:D:92:ALA:H     | 1.80                     | 0.45              |
| 2:B:110:SER:HB2  | 2:B:111:PRO:HD2  | 1.99                     | 0.45              |
| 1:C:156:ILE:CD1  | 1:C:183:ARG:O    | 2.65                     | 0.45              |
| 1:A:156:ILE:HD13 | 1:A:205:LEU:HG   | 1.99                     | 0.45              |
| 2:B:100:ASP:O    | 2:B:120:ARG:NH2  | 2.50                     | 0.45              |
| 1:C:133:GLY:HA2  | 1:C:134:PRO:O    | 2.16                     | 0.45              |
| 2:D:141:VAL:HG11 | 2:D:253:ILE:HD13 | 1.98                     | 0.45              |
| 2:D:322:LYS:HE2  | 2:D:327:ARG:NH1  | 2.32                     | 0.45              |
| 2:B:139:LEU:HD13 | 2:B:255:LEU:HD12 | 1.98                     | 0.45              |
| 1:C:399:ILE:C    | 1:C:399:ILE:CD1  | 2.87                     | 0.45              |
| 1:C:426:ASP:HA   | 1:C:489:VAL:HG13 | 1.99                     | 0.45              |
| 2:D:128:GLU:HB2  | 2:D:129:PRO:CD   | 2.47                     | 0.45              |
| 2:D:186:TRP:CZ3  | 2:D:251:ALA:HB2  | 2.52                     | 0.45              |
| 1:A:192:LEU:HD22 | 1:A:192:LEU:N    | 2.32                     | 0.45              |
| 2:D:276:LEU:HD23 | 2:D:295:CYS:HA   | 1.98                     | 0.45              |
| 1:A:119:ARG:HH11 | 1:A:119:ARG:CG   | 2.26                     | 0.44              |
| 1:C:134:PRO:O    | 1:C:135:ALA:C    | 2.61                     | 0.44              |
| 2:D:242:GLN:HB3  | 2:D:244:PHE:CD1  | 2.52                     | 0.44              |
| 1:A:240:ILE:N    | 1:A:240:ILE:HD13 | 2.33                     | 0.44              |
| 2:B:83:ALA:HB1   | 2:B:85:TRP:CE3   | 2.52                     | 0.44              |
| 1:C:73:ARG:HD2   | 1:C:125:VAL:HG11 | 1.99                     | 0.44              |
| 1:C:213:ASN:HD21 | 1:C:216:GLU:HG2  | 1.82                     | 0.44              |
| 1:C:319:THR:O    | 1:C:319:THR:HG22 | 2.17                     | 0.44              |
| 2:D:88:GLY:O     | 2:D:204:LEU:HD21 | 2.17                     | 0.44              |
| 2:D:100:ASP:O    | 2:D:120:ARG:NH2  | 2.50                     | 0.44              |
| 2:D:191:LEU:C    | 2:D:193:LYS:H    | 2.26                     | 0.44              |
| 2:D:255:LEU:O    | 2:D:256:PRO:C    | 2.59                     | 0.44              |
| 2:B:306:LEU:HD13 | 2:B:307:GLU:N    | 2.31                     | 0.44              |
| 1:A:93:ASN:HD22  | 1:A:93:ASN:HA    | 1.63                     | 0.44              |
| 1:A:205:LEU:HD11 | 1:A:240:ILE:HG22 | 2.00                     | 0.44              |
| 2:D:55:LEU:CD1   | 2:D:115:LEU:HD11 | 2.48                     | 0.44              |
| 2:D:349:PRO:HB3  | 4:D:2088:HOH:O   | 2.17                     | 0.44              |
| 1:A:399:ILE:C    | 1:A:399:ILE:CD1  | 2.86                     | 0.44              |
| 1:C:382:VAL:H    | 1:C:385:ASN:ND2  | 2.15                     | 0.44              |
| 2:D:199:ALA:HB3  | 2:D:209:PRO:HD2  | 1.99                     | 0.44              |
| 2:D:120:ARG:HD2  | 2:D:138:VAL:HG21 | 1.99                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:281:LEU:HD12 | 2:D:380:LEU:HD23 | 2.00                     | 0.44              |
| 2:D:294:LEU:C    | 2:D:294:LEU:HD23 | 2.43                     | 0.44              |
| 1:C:417:LYS:O    | 1:C:421:GLU:HG3  | 2.18                     | 0.44              |
| 1:A:228:THR:O    | 1:A:232:ILE:HG12 | 2.17                     | 0.44              |
| 2:B:130:VAL:HG12 | 2:B:131:LEU:N    | 2.33                     | 0.44              |
| 1:C:282:ARG:HG2  | 1:C:282:ARG:NH1  | 2.31                     | 0.44              |
| 1:C:275:GLY:O    | 1:C:276:SER:C    | 2.61                     | 0.44              |
| 1:A:49:LEU:HD12  | 1:A:128:LEU:HD11 | 2.00                     | 0.43              |
| 1:A:32:ASP:HA    | 1:A:91:THR:HG23  | 2.00                     | 0.43              |
| 1:A:73:ARG:HD2   | 1:A:125:VAL:HG11 | 2.00                     | 0.43              |
| 2:D:80:PRO:HD3   | 2:D:257:TYR:CE2  | 2.53                     | 0.43              |
| 2:D:283:ARG:HG3  | 2:D:283:ARG:HH11 | 1.81                     | 0.43              |
| 1:A:54:ALA:HB2   | 1:A:100:TYR:CE2  | 2.53                     | 0.43              |
| 2:D:83:ALA:HB1   | 2:D:85:TRP:CE3   | 2.53                     | 0.43              |
| 2:D:290:PRO:CG   | 2:D:348:PRO:HB2  | 2.48                     | 0.43              |
| 1:C:130:LYS:NZ   | 1:C:184:PHE:N    | 2.59                     | 0.43              |
| 1:C:330:THR:CG2  | 1:C:334:GLU:HB2  | 2.48                     | 0.43              |
| 1:A:187:THR:OG1  | 1:A:189:VAL:HG23 | 2.18                     | 0.43              |
| 2:B:168:THR:O    | 2:B:168:THR:HG22 | 2.18                     | 0.43              |
| 2:B:34:PRO:HG2   | 2:B:130:VAL:CB   | 2.49                     | 0.43              |
| 1:A:321:GLY:C    | 1:A:323:ILE:HD12 | 2.44                     | 0.43              |
| 1:C:32:ASP:N     | 1:C:88:ASN:ND2   | 2.53                     | 0.43              |
| 1:C:303:SER:HB3  | 1:C:306:THR:OG1  | 2.19                     | 0.43              |
| 2:B:120:ARG:HD2  | 2:B:138:VAL:HG21 | 1.99                     | 0.43              |
| 2:B:249:TYR:C    | 2:B:250:LEU:HD12 | 2.43                     | 0.43              |
| 1:C:295:HIS:HB3  | 1:C:357:PHE:CE1  | 2.54                     | 0.43              |
| 2:D:115:LEU:HD23 | 2:D:116:SER:N    | 2.34                     | 0.43              |
| 2:B:322:LYS:HE2  | 2:B:327:ARG:NH1  | 2.34                     | 0.43              |
| 1:C:265:TYR:CE1  | 1:C:267:VAL:HG22 | 2.54                     | 0.43              |
| 1:C:428:ASN:HB2  | 1:C:429:ILE:CD1  | 2.44                     | 0.43              |
| 1:C:218:LYS:HB2  | 1:C:218:LYS:HE3  | 1.86                     | 0.42              |
| 1:C:392:ASN:C    | 1:C:392:ASN:ND2  | 2.71                     | 0.42              |
| 2:D:52:ALA:CB    | 2:D:163:ALA:HB1  | 2.47                     | 0.42              |
| 1:C:38:ARG:O     | 1:C:38:ARG:HG3   | 2.18                     | 0.42              |
| 1:C:205:LEU:HD11 | 1:C:240:ILE:CG2  | 2.48                     | 0.42              |
| 2:D:303:SER:HB2  | 2:D:332:LEU:HD21 | 2.01                     | 0.42              |
| 2:D:306:LEU:HD13 | 2:D:307:GLU:N    | 2.34                     | 0.42              |
| 1:C:399:ILE:HD12 | 1:C:401:PHE:CE1  | 2.53                     | 0.42              |
| 1:C:450:PHE:HA   | 1:C:451:PRO:HA   | 1.81                     | 0.42              |
| 2:D:55:LEU:HD12  | 2:D:115:LEU:HD11 | 2.01                     | 0.42              |
| 2:B:199:ALA:HB3  | 2:B:209:PRO:HD2  | 2.02                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:281:LEU:HG   | 2:B:378:VAL:HG21 | 2.02                     | 0.42              |
| 1:C:270:GLU:C    | 1:C:272:ASN:H    | 2.28                     | 0.42              |
| 1:C:461:LYS:HA   | 1:C:461:LYS:HD3  | 1.83                     | 0.42              |
| 1:A:175:ALA:O    | 1:A:179:ARG:N    | 2.52                     | 0.42              |
| 2:B:25:LEU:HD21  | 2:B:73:MET:HE2   | 2.02                     | 0.42              |
| 1:A:203:ILE:CD1  | 1:A:232:ILE:HD12 | 2.41                     | 0.42              |
| 2:B:47:SER:N     | 2:B:132:ILE:CD1  | 2.79                     | 0.42              |
| 1:C:275:GLY:O    | 1:C:278:TYR:N    | 2.52                     | 0.42              |
| 2:B:46:LEU:C     | 2:B:132:ILE:HD11 | 2.44                     | 0.42              |
| 2:B:124:GLU:HA   | 2:B:125:PRO:HD3  | 1.86                     | 0.42              |
| 1:C:32:ASP:HA    | 1:C:91:THR:HG23  | 2.02                     | 0.42              |
| 1:C:156:ILE:HD13 | 1:C:183:ARG:O    | 2.19                     | 0.42              |
| 1:C:278:TYR:CE1  | 1:C:282:ARG:NE   | 2.80                     | 0.42              |
| 2:B:363:ARG:C    | 2:B:364:ILE:HD12 | 2.45                     | 0.42              |
| 2:B:165:MET:SD   | 2:B:229:PRO:HB3  | 2.60                     | 0.42              |
| 1:C:419:LEU:O    | 1:C:423:LEU:HD23 | 2.20                     | 0.42              |
| 1:A:115:TYR:CZ   | 1:A:117:GLY:HA3  | 2.55                     | 0.41              |
| 1:A:244:CYS:HB3  | 1:A:284:MET:HG2  | 2.02                     | 0.41              |
| 2:B:115:LEU:C    | 2:B:115:LEU:CD2  | 2.92                     | 0.41              |
| 1:C:47:LEU:O     | 1:C:79:PRO:HD2   | 2.20                     | 0.41              |
| 1:C:115:TYR:CZ   | 1:C:117:GLY:HA3  | 2.55                     | 0.41              |
| 2:D:190:HIS:HD1  | 2:D:191:LEU:HG   | 1.83                     | 0.41              |
| 1:A:31:THR:OG1   | 1:A:33:ASP:HB3   | 2.20                     | 0.41              |
| 1:A:32:ASP:N     | 1:A:88:ASN:ND2   | 2.57                     | 0.41              |
| 1:A:423:LEU:CB   | 1:A:431:ILE:HD11 | 2.50                     | 0.41              |
| 2:B:151:ARG:O    | 2:B:154:GLN:HB2  | 2.20                     | 0.41              |
| 1:C:379:LYS:HB3  | 1:C:432:ALA:HB2  | 2.02                     | 0.41              |
| 2:D:59:PHE:CZ    | 2:D:108:ILE:HG21 | 2.45                     | 0.41              |
| 2:D:79:LEU:CD1   | 2:D:80:PRO:HD2   | 2.46                     | 0.41              |
| 2:B:290:PRO:CG   | 2:B:348:PRO:HB2  | 2.49                     | 0.41              |
| 1:C:54:ALA:HB2   | 1:C:100:TYR:CE2  | 2.56                     | 0.41              |
| 2:B:1:GLY:HA3    | 2:B:59:PHE:O     | 2.20                     | 0.41              |
| 2:B:198:LEU:HD23 | 2:B:198:LEU:C    | 2.45                     | 0.41              |
| 2:D:327:ARG:HA   | 2:D:345:HIS:O    | 2.20                     | 0.41              |
| 2:B:186:TRP:CZ3  | 2:B:251:ALA:HB2  | 2.56                     | 0.41              |
| 1:C:175:ALA:O    | 1:C:179:ARG:HB3  | 2.20                     | 0.41              |
| 1:C:213:ASN:ND2  | 1:C:215:PHE:HB2  | 2.35                     | 0.41              |
| 2:B:113:LEU:C    | 2:B:113:LEU:CD1  | 2.92                     | 0.41              |
| 2:D:98:ALA:HB1   | 2:D:167:PRO:HB3  | 2.02                     | 0.41              |
| 2:D:177:PRO:O    | 2:D:226:PRO:O    | 2.38                     | 0.41              |
| 1:A:156:ILE:CD1  | 1:A:205:LEU:HG   | 2.50                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:43:GLU:HG2   | 2:B:125:PRO:HG3  | 2.03                     | 0.41              |
| 2:B:61:ARG:O     | 2:B:62:TYR:C     | 2.63                     | 0.41              |
| 1:C:426:ASP:HA   | 1:C:489:VAL:CG1  | 2.51                     | 0.41              |
| 2:D:114:SER:HB3  | 2:D:143:THR:CG2  | 2.51                     | 0.41              |
| 1:A:417:LYS:O    | 1:A:421:GLU:HG3  | 2.21                     | 0.41              |
| 1:A:443:SER:HB3  | 1:A:444:PRO:HD3  | 2.03                     | 0.41              |
| 1:C:277:ASN:O    | 1:C:281:ASN:ND2  | 2.54                     | 0.41              |
| 1:A:131:GLN:C    | 1:A:133:GLY:N    | 2.79                     | 0.41              |
| 1:A:167:ALA:HB1  | 1:A:227:MET:SD   | 2.60                     | 0.41              |
| 1:A:213:ASN:ND2  | 1:A:215:PHE:HB2  | 2.36                     | 0.41              |
| 1:A:330:THR:CG2  | 1:A:334:GLU:HB2  | 2.51                     | 0.41              |
| 2:B:115:LEU:HD23 | 2:B:116:SER:N    | 2.35                     | 0.41              |
| 2:B:276:LEU:HD23 | 2:B:295:CYS:HA   | 2.02                     | 0.41              |
| 2:D:62:TYR:HA    | 2:D:63:PRO:HD3   | 1.88                     | 0.41              |
| 1:A:321:GLY:O    | 1:A:322:GLU:CB   | 2.68                     | 0.41              |
| 2:B:62:TYR:HA    | 2:B:63:PRO:HD3   | 1.92                     | 0.41              |
| 1:C:77:ILE:H     | 1:C:77:ILE:CD1   | 2.32                     | 0.41              |
| 1:C:265:TYR:CZ   | 1:C:267:VAL:HG22 | 2.56                     | 0.41              |
| 1:C:317:GLU:O    | 1:C:319:THR:N    | 2.53                     | 0.41              |
| 2:D:26:LEU:HD21  | 2:D:28:ARG:HE    | 1.85                     | 0.41              |
| 1:A:47:LEU:O     | 1:A:79:PRO:HD2   | 2.21                     | 0.40              |
| 1:A:178:LEU:C    | 1:A:180:ASP:N    | 2.77                     | 0.40              |
| 1:C:245:PRO:HD2  | 1:C:299:PHE:O    | 2.21                     | 0.40              |
| 2:D:281:LEU:HG   | 2:D:378:VAL:CG2  | 2.51                     | 0.40              |
| 2:B:190:HIS:HD1  | 2:B:191:LEU:HG   | 1.85                     | 0.40              |
| 1:C:39:ILE:O     | 1:C:39:ILE:HG12  | 2.20                     | 0.40              |
| 2:D:43:GLU:HG2   | 2:D:125:PRO:HG3  | 2.03                     | 0.40              |
| 2:D:75:ARG:HH11  | 2:D:75:ARG:CG    | 2.31                     | 0.40              |
| 1:C:107:ARG:NH2  | 1:C:131:GLN:HE21 | 2.20                     | 0.40              |
| 1:C:227:MET:HE3  | 1:C:227:MET:HB2  | 2.01                     | 0.40              |
| 1:C:240:ILE:HD13 | 1:C:240:ILE:H    | 1.87                     | 0.40              |
| 1:A:178:LEU:C    | 1:A:180:ASP:H    | 2.30                     | 0.40              |
| 1:A:233:LYS:O    | 1:A:237:GLN:HG3  | 2.22                     | 0.40              |
| 1:A:265:TYR:CZ   | 1:A:267:VAL:HG22 | 2.56                     | 0.40              |
| 2:B:242:GLN:HB3  | 2:B:244:PHE:CD1  | 2.56                     | 0.40              |
| 2:D:28:ARG:HH21  | 2:D:34:PRO:HB3   | 1.86                     | 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     | 467/481 (97%)   | 432 (92%)  | 30 (6%) | 5 (1%)   | 11          | 25 |
| 1   | C     | 458/481 (95%)   | 418 (91%)  | 31 (7%) | 9 (2%)   | 6           | 12 |
| 2   | B     | 353/401 (88%)   | 329 (93%)  | 21 (6%) | 3 (1%)   | 16          | 34 |
| 2   | D     | 351/401 (88%)   | 331 (94%)  | 17 (5%) | 3 (1%)   | 14          | 30 |
| All | All   | 1629/1764 (92%) | 1510 (93%) | 99 (6%) | 20 (1%)  | 10          | 23 |

All (20) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 376 | GLY  |
| 2   | B     | 126 | GLN  |
| 1   | C     | 376 | GLY  |
| 2   | D     | 126 | GLN  |
| 1   | A     | 43  | GLY  |
| 1   | A     | 133 | GLY  |
| 1   | A     | 393 | GLU  |
| 1   | C     | 133 | GLY  |
| 1   | C     | 318 | SER  |
| 1   | C     | 320 | ALA  |
| 1   | C     | 393 | GLU  |
| 2   | D     | 129 | PRO  |
| 2   | B     | 129 | PRO  |
| 1   | C     | 270 | GLU  |
| 1   | C     | 272 | ASN  |
| 2   | D     | 299 | HIS  |
| 2   | B     | 316 | PRO  |
| 1   | C     | 443 | SER  |
| 1   | A     | 443 | SER  |
| 1   | C     | 333 | GLY  |

### 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     | 402/413 (97%)   | 385 (96%)  | 17 (4%)  | 26          | 52 |
| 1   | C     | 397/413 (96%)   | 380 (96%)  | 17 (4%)  | 26          | 51 |
| 2   | B     | 291/316 (92%)   | 272 (94%)  | 19 (6%)  | 15          | 35 |
| 2   | D     | 290/316 (92%)   | 272 (94%)  | 18 (6%)  | 16          | 36 |
| All | All   | 1380/1458 (95%) | 1309 (95%) | 71 (5%)  | 21          | 45 |

All (71) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 49  | LEU  |
| 1   | A     | 63  | LEU  |
| 1   | A     | 72  | THR  |
| 1   | A     | 199 | ASN  |
| 1   | A     | 240 | ILE  |
| 1   | A     | 291 | LEU  |
| 1   | A     | 322 | GLU  |
| 1   | A     | 323 | ILE  |
| 1   | A     | 335 | LYS  |
| 1   | A     | 354 | GLN  |
| 1   | A     | 385 | ASN  |
| 1   | A     | 387 | ASP  |
| 1   | A     | 392 | ASN  |
| 1   | A     | 399 | ILE  |
| 1   | A     | 406 | CYS  |
| 1   | A     | 460 | LYS  |
| 1   | A     | 489 | VAL  |
| 2   | B     | 6   | GLU  |
| 2   | B     | 20  | LYS  |
| 2   | B     | 42  | PRO  |
| 2   | B     | 44  | LEU  |
| 2   | B     | 60  | ARG  |
| 2   | B     | 85  | TRP  |
| 2   | B     | 115 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 124 | GLU  |
| 2   | B     | 132 | ILE  |
| 2   | B     | 134 | MET  |
| 2   | B     | 154 | GLN  |
| 2   | B     | 196 | LEU  |
| 2   | B     | 226 | PRO  |
| 2   | B     | 242 | GLN  |
| 2   | B     | 259 | GLN  |
| 2   | B     | 306 | LEU  |
| 2   | B     | 342 | LEU  |
| 2   | B     | 364 | ILE  |
| 2   | B     | 374 | ARG  |
| 1   | C     | 49  | LEU  |
| 1   | C     | 63  | LEU  |
| 1   | C     | 72  | THR  |
| 1   | C     | 156 | ILE  |
| 1   | C     | 199 | ASN  |
| 1   | C     | 240 | ILE  |
| 1   | C     | 291 | LEU  |
| 1   | C     | 306 | THR  |
| 1   | C     | 323 | ILE  |
| 1   | C     | 354 | GLN  |
| 1   | C     | 385 | ASN  |
| 1   | C     | 387 | ASP  |
| 1   | C     | 392 | ASN  |
| 1   | C     | 399 | ILE  |
| 1   | C     | 406 | CYS  |
| 1   | C     | 429 | ILE  |
| 1   | C     | 489 | VAL  |
| 2   | D     | 6   | GLU  |
| 2   | D     | 20  | LYS  |
| 2   | D     | 42  | PRO  |
| 2   | D     | 44  | LEU  |
| 2   | D     | 60  | ARG  |
| 2   | D     | 85  | TRP  |
| 2   | D     | 115 | LEU  |
| 2   | D     | 124 | GLU  |
| 2   | D     | 134 | MET  |
| 2   | D     | 154 | GLN  |
| 2   | D     | 196 | LEU  |
| 2   | D     | 226 | PRO  |
| 2   | D     | 242 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | D     | 255 | LEU  |
| 2   | D     | 259 | GLN  |
| 2   | D     | 306 | LEU  |
| 2   | D     | 342 | LEU  |
| 2   | D     | 374 | ARG  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 59  | HIS  |
| 1   | A     | 88  | ASN  |
| 1   | A     | 93  | ASN  |
| 1   | A     | 131 | GLN  |
| 1   | A     | 177 | ASN  |
| 1   | A     | 181 | ASN  |
| 1   | A     | 186 | HIS  |
| 1   | A     | 194 | ASN  |
| 1   | A     | 213 | ASN  |
| 1   | A     | 239 | ASN  |
| 1   | A     | 339 | GLN  |
| 1   | A     | 354 | GLN  |
| 1   | A     | 360 | ASN  |
| 1   | A     | 385 | ASN  |
| 1   | A     | 392 | ASN  |
| 1   | A     | 394 | ASN  |
| 1   | A     | 411 | ASN  |
| 1   | A     | 491 | GLN  |
| 2   | B     | 49  | HIS  |
| 2   | B     | 127 | GLN  |
| 2   | B     | 154 | GLN  |
| 2   | B     | 207 | GLN  |
| 2   | B     | 212 | GLN  |
| 2   | B     | 254 | HIS  |
| 2   | B     | 259 | GLN  |
| 2   | B     | 299 | HIS  |
| 2   | B     | 345 | HIS  |
| 2   | B     | 347 | GLN  |
| 2   | B     | 355 | GLN  |
| 1   | C     | 88  | ASN  |
| 1   | C     | 93  | ASN  |
| 1   | C     | 131 | GLN  |
| 1   | C     | 177 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 186 | HIS  |
| 1   | C     | 194 | ASN  |
| 1   | C     | 213 | ASN  |
| 1   | C     | 237 | GLN  |
| 1   | C     | 239 | ASN  |
| 1   | C     | 246 | HIS  |
| 1   | C     | 281 | ASN  |
| 1   | C     | 295 | HIS  |
| 1   | C     | 339 | GLN  |
| 1   | C     | 354 | GLN  |
| 1   | C     | 360 | ASN  |
| 1   | C     | 385 | ASN  |
| 1   | C     | 392 | ASN  |
| 1   | C     | 394 | ASN  |
| 1   | C     | 411 | ASN  |
| 2   | D     | 154 | GLN  |
| 2   | D     | 207 | GLN  |
| 2   | D     | 212 | GLN  |
| 2   | D     | 259 | GLN  |
| 2   | D     | 299 | HIS  |
| 2   | D     | 345 | HIS  |
| 2   | D     | 347 | GLN  |
| 2   | D     | 355 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry ⓘ

2 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 | $\# Z  > 2$ |
| 3   | NAG  | D     | 1233 | 2    | 14,14,15     | 0.55 | 0           | 17,19,21    | 1.08 | 2 (11%)     |
| 3   | NAG  | B     | 1233 | 2    | 14,14,15     | 0.77 | 0           | 17,19,21    | 0.98 | 1 (5%)      |

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

| Mol | Type | Chain | Res  | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|------|------|---------|-----------|---------|
| 3   | NAG  | D     | 1233 | 2    | -       | 2/6/23/26 | 0/1/1/1 |
| 3   | NAG  | B     | 1233 | 2    | -       | 2/6/23/26 | 0/1/1/1 |

There are no bond length outliers.

All (3) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 3   | D     | 1233 | NAG  | C2-N2-C7 | -3.04 | 118.82      | 122.90   |
| 3   | B     | 1233 | NAG  | C2-N2-C7 | -2.24 | 119.90      | 122.90   |
| 3   | D     | 1233 | NAG  | C4-C3-C2 | -2.06 | 108.00      | 111.02   |

There are no chirality outliers.

All (4) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       |
|-----|-------|------|------|-------------|
| 3   | B     | 1233 | NAG  | O7-C7-N2-C2 |
| 3   | D     | 1233 | NAG  | C8-C7-N2-C2 |
| 3   | D     | 1233 | NAG  | O7-C7-N2-C2 |
| 3   | B     | 1233 | NAG  | C8-C7-N2-C2 |

There are no ring outliers.

1 monomer is involved in 1 short contact:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 3   | D     | 1233 | NAG  | 1       | 0            |

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 1   | A     | 469/481 (97%)   | 0.15   | 14 (2%) 52 47  | 29, 54, 75, 94        | 0     |
| 1   | C     | 462/481 (96%)   | 0.93   | 60 (12%) 7 5   | 43, 78, 107, 119      | 0     |
| 2   | B     | 361/401 (90%)   | 0.23   | 26 (7%) 21 17  | 29, 50, 100, 130      | 0     |
| 2   | D     | 361/401 (90%)   | 0.21   | 12 (3%) 49 43  | 30, 52, 98, 125       | 0     |
| All | All   | 1653/1764 (93%) | 0.40   | 112 (6%) 23 19 | 29, 58, 100, 130      | 0     |

All (112) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | B     | 168 | THR  | 4.8  |
| 1   | C     | 215 | PHE  | 4.5  |
| 1   | C     | 214 | LYS  | 4.4  |
| 1   | C     | 116 | ASP  | 4.4  |
| 2   | B     | 40  | LEU  | 4.2  |
| 2   | D     | 128 | GLU  | 4.0  |
| 2   | B     | 227 | TRP  | 3.9  |
| 1   | C     | 213 | ASN  | 3.9  |
| 2   | B     | 126 | GLN  | 3.9  |
| 2   | B     | 127 | GLN  | 3.7  |
| 2   | D     | 127 | GLN  | 3.5  |
| 2   | B     | 177 | PRO  | 3.5  |
| 1   | C     | 273 | ALA  | 3.4  |
| 2   | B     | 131 | LEU  | 3.4  |
| 1   | C     | 266 | ASP  | 3.4  |
| 2   | D     | 357 | GLY  | 3.3  |
| 1   | C     | 33  | ASP  | 3.2  |
| 1   | C     | 133 | GLY  | 3.2  |
| 1   | C     | 193 | VAL  | 3.2  |
| 2   | B     | 41  | ASP  | 3.2  |
| 1   | A     | 359 | GLY  | 3.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 79  | PRO  | 3.1  |
| 2   | B     | 169 | SER  | 3.1  |
| 1   | C     | 272 | ASN  | 3.1  |
| 1   | C     | 427 | PRO  | 3.0  |
| 2   | B     | 132 | ILE  | 3.0  |
| 1   | C     | 391 | ASN  | 3.0  |
| 1   | A     | 161 | ASP  | 3.0  |
| 1   | C     | 152 | LYS  | 3.0  |
| 1   | C     | 276 | SER  | 3.0  |
| 2   | D     | 350 | PRO  | 3.0  |
| 2   | D     | 282 | ALA  | 3.0  |
| 1   | C     | 129 | LYS  | 2.9  |
| 2   | D     | 321 | GLN  | 2.9  |
| 1   | C     | 132 | ALA  | 2.9  |
| 2   | B     | 42  | PRO  | 2.9  |
| 1   | C     | 163 | SER  | 2.9  |
| 1   | C     | 41  | ASP  | 2.9  |
| 1   | C     | 275 | GLY  | 2.9  |
| 2   | B     | 318 | GLY  | 2.9  |
| 1   | C     | 424 | SER  | 2.9  |
| 1   | C     | 443 | SER  | 2.9  |
| 1   | C     | 199 | ASN  | 2.9  |
| 1   | C     | 210 | HIS  | 2.9  |
| 2   | B     | 133 | THR  | 2.8  |
| 1   | C     | 304 | ARG  | 2.8  |
| 1   | C     | 198 | ASP  | 2.8  |
| 1   | C     | 269 | TYR  | 2.8  |
| 2   | B     | 94  | ASN  | 2.8  |
| 1   | C     | 485 | THR  | 2.8  |
| 2   | D     | 177 | PRO  | 2.7  |
| 1   | C     | 490 | ILE  | 2.7  |
| 1   | C     | 69  | ALA  | 2.7  |
| 2   | B     | 381 | GLU  | 2.7  |
| 1   | C     | 487 | PRO  | 2.7  |
| 1   | C     | 396 | ASP  | 2.7  |
| 1   | C     | 39  | ILE  | 2.7  |
| 1   | C     | 209 | SER  | 2.7  |
| 2   | D     | 358 | ALA  | 2.7  |
| 2   | B     | 226 | PRO  | 2.6  |
| 1   | C     | 486 | ASN  | 2.6  |
| 1   | C     | 150 | SER  | 2.5  |
| 1   | A     | 250 | ASP  | 2.5  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 241 | PHE  | 2.5  |
| 2   | D     | 191 | LEU  | 2.5  |
| 1   | A     | 116 | ASP  | 2.5  |
| 2   | B     | 130 | VAL  | 2.5  |
| 1   | A     | 162 | ASP  | 2.4  |
| 1   | A     | 320 | ALA  | 2.4  |
| 1   | C     | 71  | ALA  | 2.4  |
| 1   | C     | 72  | THR  | 2.4  |
| 1   | C     | 394 | ASN  | 2.4  |
| 1   | C     | 488 | PRO  | 2.4  |
| 1   | A     | 199 | ASN  | 2.4  |
| 1   | A     | 226 | LYS  | 2.4  |
| 1   | C     | 90  | ASN  | 2.4  |
| 2   | B     | 20  | LYS  | 2.4  |
| 1   | A     | 321 | GLY  | 2.4  |
| 2   | B     | 64  | ARG  | 2.4  |
| 1   | C     | 320 | ALA  | 2.4  |
| 1   | C     | 127 | HIS  | 2.3  |
| 1   | C     | 395 | LYS  | 2.3  |
| 2   | B     | 129 | PRO  | 2.3  |
| 1   | A     | 200 | GLY  | 2.3  |
| 1   | C     | 372 | GLU  | 2.3  |
| 1   | C     | 240 | ILE  | 2.2  |
| 1   | C     | 243 | ILE  | 2.2  |
| 1   | C     | 226 | LYS  | 2.2  |
| 1   | A     | 143 | GLU  | 2.2  |
| 2   | B     | 56  | GLN  | 2.2  |
| 1   | C     | 345 | ASP  | 2.2  |
| 1   | C     | 211 | LEU  | 2.2  |
| 1   | C     | 458 | ALA  | 2.2  |
| 2   | B     | 45  | TYR  | 2.2  |
| 1   | A     | 234 | LYS  | 2.2  |
| 1   | C     | 271 | LYS  | 2.2  |
| 2   | B     | 128 | GLU  | 2.2  |
| 2   | D     | 41  | ASP  | 2.2  |
| 1   | C     | 378 | VAL  | 2.1  |
| 1   | C     | 489 | VAL  | 2.1  |
| 1   | A     | 485 | THR  | 2.1  |
| 1   | C     | 444 | PRO  | 2.1  |
| 2   | B     | 7   | CYS  | 2.1  |
| 2   | D     | 65  | GLY  | 2.1  |
| 1   | C     | 253 | ASP  | 2.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 163 | SER  | 2.1  |
| 2   | B     | 352 | THR  | 2.1  |
| 1   | C     | 277 | ASN  | 2.1  |
| 2   | D     | 373 | GLY  | 2.1  |
| 1   | C     | 397 | VAL  | 2.1  |
| 1   | C     | 448 | ARG  | 2.0  |
| 2   | B     | 125 | PRO  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 3   | NAG  | D     | 1233 | 14/15 | 0.83 | 0.11 | 59,61,65,67                 | 0     |
| 3   | NAG  | B     | 1233 | 14/15 | 0.86 | 0.11 | 53,56,61,62                 | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.