



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 07:31 PM UTC

PDB ID : 3VLF / pdb\_00003vlf  
Title : Crystal structure of yeast proteasome interacting protein  
Authors : Takagi, K.; Kim, S.; Kato, K.; Tanaka, K.; Saeki, Y.; Mizushima, T.  
Deposited on : 2011-12-01  
Resolution : 3.80 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

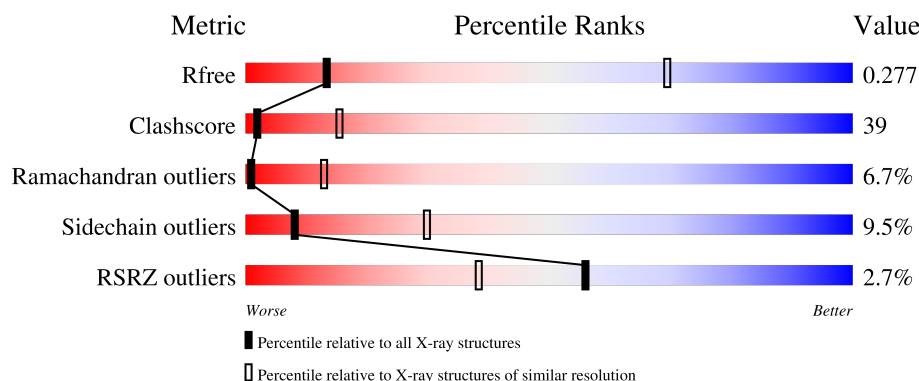
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

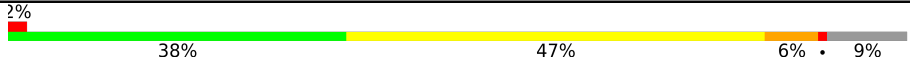
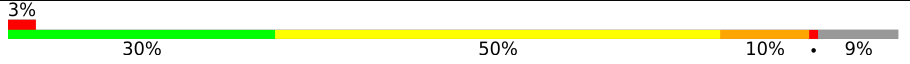
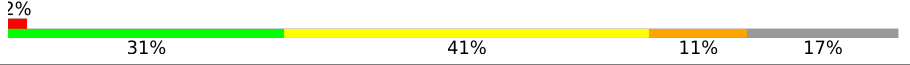
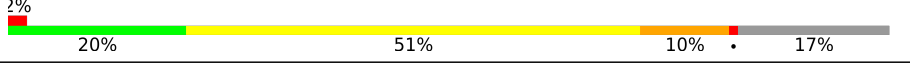
The reported resolution of this entry is 3.80 Å.

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                      | 1065 (3.96-3.64)                                      |
| Clashscore            | 190562                      | 1012 (3.94-3.66)                                      |
| Ramachandran outliers | 187476                      | 1048 (3.96-3.64)                                      |
| Sidechain outliers    | 187428                      | 1043 (3.96-3.64)                                      |
| RSRZ outliers         | 180081                      | 1064 (3.96-3.64)                                      |

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     | 500    |  |
| 1   | C     | 500    |  |
| 2   | B     | 88     |  |
| 2   | D     | 88     |  |

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8594 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 DNA mismatch repair protein HSM3.

| Mol | Chain | Residues | Atoms |      |     |     |   |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|----|---------|---------|-------|
| 1   | A     | 457      | Total | C    | N   | O   | S | Se | 0       | 0       | 0     |
|     |       |          | 3727  | 2403 | 596 | 715 | 5 | 8  |         |         |       |
| 1   | C     | 454      | Total | C    | N   | O   | S | Se | 0       | 0       | 0     |
|     |       |          | 3717  | 2396 | 594 | 714 | 5 | 8  |         |         |       |

There are 40 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | -19     | MSE      | -      | expression tag | UNP P38348 |
| A     | -18     | GLY      | -      | expression tag | UNP P38348 |
| A     | -17     | SER      | -      | expression tag | UNP P38348 |
| A     | -16     | SER      | -      | expression tag | UNP P38348 |
| A     | -15     | HIS      | -      | expression tag | UNP P38348 |
| A     | -14     | HIS      | -      | expression tag | UNP P38348 |
| A     | -13     | HIS      | -      | expression tag | UNP P38348 |
| A     | -12     | HIS      | -      | expression tag | UNP P38348 |
| A     | -11     | HIS      | -      | expression tag | UNP P38348 |
| A     | -10     | HIS      | -      | expression tag | UNP P38348 |
| A     | -9      | SER      | -      | expression tag | UNP P38348 |
| A     | -8      | SER      | -      | expression tag | UNP P38348 |
| A     | -7      | GLY      | -      | expression tag | UNP P38348 |
| A     | -6      | LEU      | -      | expression tag | UNP P38348 |
| A     | -5      | VAL      | -      | expression tag | UNP P38348 |
| A     | -4      | PRO      | -      | expression tag | UNP P38348 |
| A     | -3      | ARG      | -      | expression tag | UNP P38348 |
| A     | -2      | GLY      | -      | expression tag | UNP P38348 |
| A     | -1      | SER      | -      | expression tag | UNP P38348 |
| A     | 0       | HIS      | -      | expression tag | UNP P38348 |
| C     | -19     | MSE      | -      | expression tag | UNP P38348 |
| C     | -18     | GLY      | -      | expression tag | UNP P38348 |
| C     | -17     | SER      | -      | expression tag | UNP P38348 |
| C     | -16     | SER      | -      | expression tag | UNP P38348 |
| C     | -15     | HIS      | -      | expression tag | UNP P38348 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| C     | -14     | HIS      | -      | expression tag | UNP P38348 |
| C     | -13     | HIS      | -      | expression tag | UNP P38348 |
| C     | -12     | HIS      | -      | expression tag | UNP P38348 |
| C     | -11     | HIS      | -      | expression tag | UNP P38348 |
| C     | -10     | HIS      | -      | expression tag | UNP P38348 |
| C     | -9      | SER      | -      | expression tag | UNP P38348 |
| C     | -8      | SER      | -      | expression tag | UNP P38348 |
| C     | -7      | GLY      | -      | expression tag | UNP P38348 |
| C     | -6      | LEU      | -      | expression tag | UNP P38348 |
| C     | -5      | VAL      | -      | expression tag | UNP P38348 |
| C     | -4      | PRO      | -      | expression tag | UNP P38348 |
| C     | -3      | ARG      | -      | expression tag | UNP P38348 |
| C     | -2      | GLY      | -      | expression tag | UNP P38348 |
| C     | -1      | SER      | -      | expression tag | UNP P38348 |
| C     | 0       | HIS      | -      | expression tag | UNP P38348 |

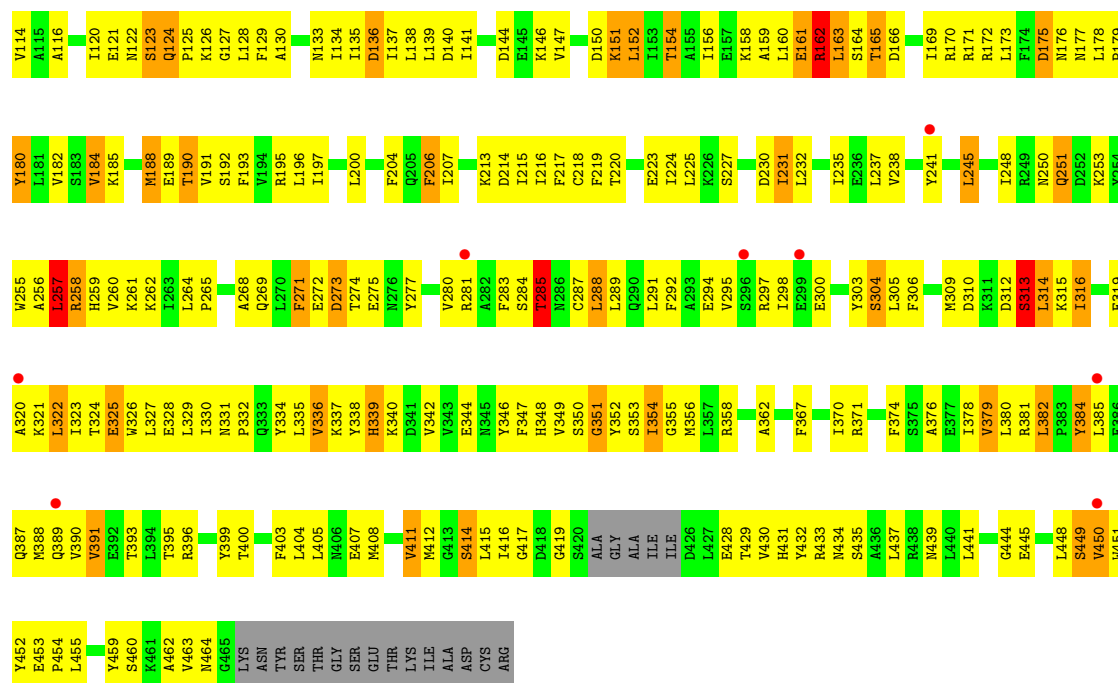
- Molecule 2 is a protein called 26S protease regulatory subunit 7 homolog.

| Mol | Chain | Residues | Atoms |     |     |     |   |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|----|---------|---------|-------|
| 2   | B     | 73       | Total | C   | N   | O   | S | Se | 0       | 0       | 0     |
|     |       |          | 575   | 357 | 110 | 103 | 2 | 3  |         |         |       |
| 2   | D     | 73       | Total | C   | N   | O   | S | Se | 0       | 0       | 0     |
|     |       |          | 575   | 357 | 110 | 103 | 2 | 3  |         |         |       |

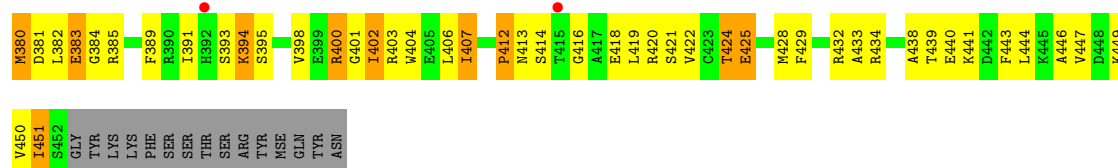
There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| B     | 380     | MSE      | -      | expression tag | UNP P33299 |
| D     | 380     | MSE      | -      | expression tag | UNP P33299 |

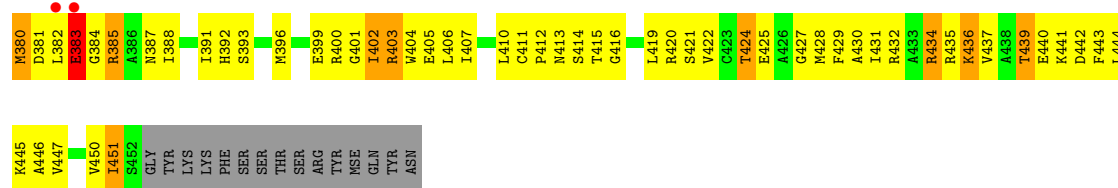
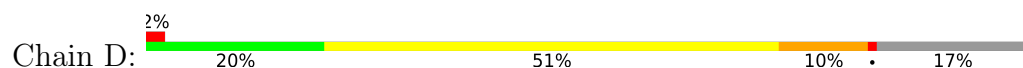




• Molecule 2: 26S protease regulatory subunit 7 homolog



• Molecule 2: 26S protease regulatory subunit 7 homolog



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 65 2 2                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 187.28Å 187.28Å 379.57Å<br>90.00° 90.00° 120.00°            | Depositor        |
| Resolution (Å)                                                          | 30.00 – 3.80<br>30.00 – 3.80                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | (Not available) (30.00-3.80)<br>99.3 (30.00-3.80)           | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.08                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 6.80 (at 3.77Å)                                             | Xtriage          |
| Refinement program                                                      | CNS 1.3                                                     | Depositor        |
| R, $R_{free}$                                                           | 0.251 , 0.278<br>0.251 , 0.277                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 1961 reflections (4.96%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 143.2                                                       | Xtriage          |
| Anisotropy                                                              | 0.147                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.34 , 135.7                                                | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.94                                                        | EDS              |
| Total number of atoms                                                   | 8594                                                        | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 163.0                                                       | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.48% 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 [i](#)

### 5.1 Standard geometry [i](#)

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     | 0.42         | 0/3785  | 0.73        | 2/5114 (0.0%)  |
| 1   | C     | 0.41         | 0/3775  | 0.77        | 1/5099 (0.0%)  |
| 2   | B     | 0.40         | 0/579   | 0.77        | 1/769 (0.1%)   |
| 2   | D     | 0.42         | 0/579   | 0.78        | 0/769          |
| All | All   | 0.41         | 0/8718  | 0.76        | 4/11751 (0.0%) |

There are no bond length outliers.

All (4) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | B     | 384 | GLY  | N-CA-C | -5.53 | 105.96      | 113.37   |
| 1   | A     | 124 | GLN  | CA-C-N | -5.38 | 113.61      | 120.23   |
| 1   | A     | 124 | GLN  | C-N-CA | -5.38 | 113.61      | 120.23   |
| 1   | C     | 271 | PHE  | N-CA-C | -5.04 | 106.64      | 112.89   |

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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     | 3727  | 0        | 3763     | 247     | 0            |
| 1   | C     | 3717  | 0        | 3742     | 327     | 0            |
| 2   | B     | 575   | 0        | 598      | 49      | 0            |
| 2   | D     | 575   | 0        | 598      | 69      | 0            |
| All | All   | 8594  | 0        | 8701     | 674     | 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 39.

All (674) 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:464:ASN:OD1  | 1:C:82:LYS:NZ    | 1.93                     | 1.01              |
| 1:C:88:ASP:HB3   | 1:C:91:ASP:HB2   | 1.42                     | 1.01              |
| 1:C:124:GLN:HB2  | 1:C:125:PRO:HD3  | 1.43                     | 0.98              |
| 1:A:320:ALA:HA   | 1:A:323:ILE:HG13 | 1.44                     | 0.98              |
| 1:A:321:LYS:H    | 1:A:321:LYS:HD2  | 1.34                     | 0.90              |
| 1:A:433:ARG:HH12 | 1:A:458:GLU:HG3  | 1.37                     | 0.89              |
| 1:C:441:LEU:HD11 | 1:C:455:LEU:HB3  | 1.54                     | 0.88              |
| 2:B:400:ARG:HG3  | 2:B:401:GLY:H    | 1.39                     | 0.87              |
| 1:A:124:GLN:HB3  | 1:A:125:PRO:HD3  | 1.57                     | 0.86              |
| 1:C:219:PHE:HE1  | 1:C:237:LEU:HD22 | 1.40                     | 0.86              |
| 2:D:441:LYS:HA   | 2:D:444:LEU:HD13 | 1.58                     | 0.85              |
| 1:A:393:THR:HA   | 1:A:396:ARG:HD3  | 1.59                     | 0.84              |
| 1:A:263:ILE:HD13 | 1:A:263:ILE:H    | 1.42                     | 0.84              |
| 2:B:391:ILE:HA   | 2:B:394:LYS:HE3  | 1.59                     | 0.83              |
| 1:A:213:LYS:HB3  | 1:A:215:ILE:HG22 | 1.59                     | 0.83              |
| 1:C:17:GLU:HG2   | 1:C:32:LEU:HD21  | 1.65                     | 0.79              |
| 1:A:218:CYS:SG   | 1:A:259:HIS:HB3  | 2.24                     | 0.77              |
| 1:C:16:LEU:O     | 1:C:20:LEU:HB2   | 1.83                     | 0.77              |
| 2:D:422:VAL:HA   | 2:D:450:VAL:HG21 | 1.67                     | 0.77              |
| 1:C:163:LEU:HD22 | 1:C:169:ILE:HD13 | 1.66                     | 0.77              |
| 2:D:402:ILE:HA   | 2:D:440:GLU:HG3  | 1.67                     | 0.77              |
| 1:A:453:GLU:HB2  | 1:A:454:PRO:HD3  | 1.66                     | 0.77              |
| 1:C:285:THR:O    | 1:C:289:LEU:HB2  | 1.84                     | 0.77              |
| 1:C:349:VAL:HG23 | 1:C:378:ILE:HG21 | 1.65                     | 0.77              |
| 2:D:385:ARG:CZ   | 2:D:412:PRO:HA   | 2.16                     | 0.75              |
| 1:C:265:PRO:HA   | 1:C:309:MSE:HE3  | 1.66                     | 0.75              |
| 1:C:387:GLN:O    | 1:C:390:VAL:HG22 | 1.86                     | 0.75              |
| 1:C:347:PHE:HD1  | 1:C:370:ILE:HG21 | 1.52                     | 0.74              |
| 2:B:381:ASP:HA   | 2:B:385:ARG:HH12 | 1.53                     | 0.74              |
| 1:C:40:LEU:HD11  | 1:C:46:LEU:HD21  | 1.69                     | 0.74              |
| 1:A:238:VAL:HG11 | 1:A:288:LEU:HD23 | 1.70                     | 0.73              |
| 1:C:382:LEU:H    | 1:C:382:LEU:HD12 | 1.53                     | 0.73              |
| 1:A:330:ILE:HG22 | 1:A:335:LEU:HG   | 1.69                     | 0.73              |
| 1:C:250:ASN:O    | 1:C:251:GLN:HG3  | 1.89                     | 0.73              |
| 1:C:139:LEU:HD11 | 1:C:173:LEU:HD23 | 1.70                     | 0.73              |
| 1:C:144:ASP:HB3  | 1:C:147:VAL:HG23 | 1.71                     | 0.73              |
| 1:C:219:PHE:CE1  | 1:C:237:LEU:HD22 | 2.24                     | 0.73              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:382:LEU:O    | 2:D:383:GLU:HG3  | 1.88                     | 0.72              |
| 1:C:268:ALA:HB2  | 1:C:309:MSE:HE2  | 1.71                     | 0.72              |
| 1:A:297:ARG:NH1  | 1:A:331:ASN:HA   | 2.03                     | 0.72              |
| 1:C:166:ASP:HB3  | 1:C:169:ILE:HG22 | 1.71                     | 0.72              |
| 1:C:178:LEU:O    | 1:C:182:VAL:HG23 | 1.89                     | 0.72              |
| 1:A:323:ILE:O    | 1:A:327:LEU:HD12 | 1.89                     | 0.71              |
| 1:C:459:TYR:O    | 1:C:463:VAL:HG22 | 1.89                     | 0.71              |
| 1:A:37:SER:HA    | 1:A:40:LEU:HD12  | 1.72                     | 0.71              |
| 2:B:419:LEU:HD22 | 2:B:419:LEU:H    | 1.56                     | 0.70              |
| 1:C:324:THR:HG21 | 1:C:352:TYR:OH   | 1.92                     | 0.70              |
| 1:C:25:LEU:HD11  | 1:C:66:VAL:HG12  | 1.73                     | 0.70              |
| 1:C:367:PHE:CE1  | 1:C:400:THR:HA   | 2.27                     | 0.69              |
| 1:C:389:GLN:O    | 1:C:393:THR:HG23 | 1.92                     | 0.69              |
| 1:C:162:ARG:NH1  | 1:C:162:ARG:HB2  | 2.07                     | 0.69              |
| 2:D:399:GLU:HB2  | 2:D:439:THR:HA   | 1.73                     | 0.69              |
| 1:C:184:VAL:HB   | 1:C:196:LEU:HD22 | 1.75                     | 0.69              |
| 1:A:257:LEU:HD22 | 1:A:298:ILE:HD11 | 1.74                     | 0.69              |
| 1:C:80:VAL:O     | 1:C:84:VAL:HG23  | 1.94                     | 0.68              |
| 1:C:238:VAL:HG11 | 1:C:288:LEU:HA   | 1.74                     | 0.68              |
| 1:C:218:CYS:SG   | 1:C:259:HIS:HB3  | 2.33                     | 0.68              |
| 2:D:385:ARG:NH1  | 2:D:412:PRO:HA   | 2.09                     | 0.68              |
| 2:B:450:VAL:HG12 | 2:B:451:ILE:HD13 | 1.76                     | 0.67              |
| 1:C:11:ASN:HB3   | 1:C:47:PRO:HG2   | 1.75                     | 0.67              |
| 2:D:399:GLU:HG2  | 2:D:400:ARG:H    | 1.60                     | 0.67              |
| 1:A:260:VAL:HA   | 1:A:263:ILE:HD11 | 1.77                     | 0.67              |
| 1:C:156:ILE:O    | 1:C:160:LEU:HD12 | 1.94                     | 0.67              |
| 1:C:378:ILE:C    | 1:C:380:LEU:H    | 2.01                     | 0.67              |
| 1:C:135:ILE:HD12 | 1:C:172:ARG:HG2  | 1.76                     | 0.67              |
| 1:C:367:PHE:HE1  | 1:C:400:THR:HA   | 1.60                     | 0.67              |
| 1:C:388:MSE:HE3  | 1:C:433:ARG:HB2  | 1.75                     | 0.67              |
| 1:C:245:LEU:O    | 1:C:248:ILE:HG22 | 1.96                     | 0.66              |
| 1:A:325:GLU:O    | 1:A:329:LEU:HD12 | 1.96                     | 0.66              |
| 1:C:109:ILE:HG23 | 1:C:111:PRO:HD2  | 1.77                     | 0.66              |
| 1:C:416:ILE:HG12 | 1:C:454:PRO:HB2  | 1.77                     | 0.66              |
| 1:C:33:LEU:HD13  | 1:C:76:LEU:HA    | 1.78                     | 0.66              |
| 1:C:347:PHE:CD1  | 1:C:370:ILE:HG21 | 2.31                     | 0.66              |
| 1:C:388:MSE:HE3  | 1:C:433:ARG:HG3  | 1.78                     | 0.66              |
| 1:A:254:TYR:CE1  | 1:A:299:GLU:HG3  | 2.32                     | 0.65              |
| 1:C:144:ASP:OD2  | 1:C:146:LYS:HB2  | 1.96                     | 0.65              |
| 1:A:457:ARG:HG3  | 1:A:458:GLU:N    | 2.09                     | 0.65              |
| 2:D:388:ILE:HD12 | 2:D:419:LEU:HD12 | 1.77                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:9:VAL:HG21   | 1:C:47:PRO:HG3   | 1.77                     | 0.65              |
| 1:C:327:LEU:HB2  | 1:C:356:MSE:HG2  | 1.76                     | 0.65              |
| 2:D:403:ARG:HG3  | 2:D:406:LEU:HD12 | 1.78                     | 0.65              |
| 2:D:380:MSE:SE   | 2:D:388:ILE:HD11 | 2.47                     | 0.64              |
| 2:D:450:VAL:HG12 | 2:D:451:ILE:HD13 | 1.79                     | 0.64              |
| 1:C:220:THR:OG1  | 1:C:223:GLU:HG3  | 1.98                     | 0.64              |
| 1:C:58:ILE:HG23  | 1:C:76:LEU:HD21  | 1.78                     | 0.64              |
| 1:C:126:LYS:HG3  | 1:C:166:ASP:HB2  | 1.79                     | 0.64              |
| 1:C:178:LEU:N    | 1:C:179:PRO:HD2  | 2.12                     | 0.64              |
| 1:A:276:ASN:O    | 1:A:277:TYR:HB2  | 1.98                     | 0.64              |
| 1:C:52:LYS:N     | 1:C:53:PRO:HD2   | 2.13                     | 0.64              |
| 1:C:110:ASP:HA   | 1:C:113:LYS:HD3  | 1.78                     | 0.63              |
| 1:C:358:ARG:HE   | 1:C:396:ARG:HH21 | 1.44                     | 0.63              |
| 1:A:327:LEU:HD23 | 1:A:343:VAL:HG22 | 1.79                     | 0.63              |
| 1:C:64:SER:O     | 1:C:65:ASN:HB2   | 1.97                     | 0.63              |
| 2:D:436:LYS:HD2  | 2:D:437:VAL:HG23 | 1.80                     | 0.63              |
| 1:C:441:LEU:CD1  | 1:C:455:LEU:HB3  | 2.28                     | 0.63              |
| 2:D:382:LEU:C    | 2:D:384:GLY:H    | 2.07                     | 0.63              |
| 1:C:29:ILE:HG22  | 1:C:71:LEU:HD23  | 1.81                     | 0.62              |
| 1:C:384:TYR:CD2  | 1:C:388:MSE:HG2  | 2.34                     | 0.62              |
| 1:C:391:VAL:O    | 1:C:395:THR:HG23 | 1.99                     | 0.62              |
| 1:A:235:ILE:HD11 | 1:A:283:PHE:O    | 1.98                     | 0.62              |
| 1:C:264:LEU:HD23 | 1:C:305:LEU:HD21 | 1.82                     | 0.62              |
| 1:A:433:ARG:HH12 | 1:A:458:GLU:CG   | 2.11                     | 0.62              |
| 1:C:391:VAL:HG12 | 1:C:404:LEU:HD11 | 1.81                     | 0.62              |
| 1:C:358:ARG:HE   | 1:C:396:ARG:NH2  | 1.97                     | 0.62              |
| 1:A:158:LYS:HZ2  | 2:B:382:LEU:HG   | 1.65                     | 0.62              |
| 1:A:316:ILE:HD11 | 1:A:330:ILE:HG12 | 1.82                     | 0.62              |
| 1:A:436:ALA:O    | 1:A:440:LEU:HB2  | 2.00                     | 0.62              |
| 1:C:170:ARG:HH21 | 1:C:207:ILE:HA   | 1.65                     | 0.62              |
| 1:A:124:GLN:CB   | 1:A:125:PRO:HD3  | 2.28                     | 0.61              |
| 1:A:324:THR:O    | 1:A:328:GLU:HG3  | 2.00                     | 0.61              |
| 1:C:297:ARG:HG2  | 1:C:331:ASN:HB2  | 1.82                     | 0.61              |
| 1:C:332:PRO:HG3  | 1:C:362:ALA:HB3  | 1.81                     | 0.61              |
| 1:C:193:PHE:HE1  | 1:C:237:LEU:HD21 | 1.64                     | 0.61              |
| 1:C:109:ILE:CG2  | 1:C:111:PRO:HD2  | 2.30                     | 0.61              |
| 2:B:400:ARG:HG3  | 2:B:401:GLY:N    | 2.15                     | 0.61              |
| 2:D:422:VAL:HG22 | 2:D:450:VAL:HG11 | 1.82                     | 0.61              |
| 1:A:13:LEU:HD23  | 1:A:16:LEU:HD23  | 1.81                     | 0.61              |
| 1:C:351:GLY:O    | 1:C:354:ILE:HD13 | 2.00                     | 0.61              |
| 1:A:264:LEU:HD13 | 1:A:295:VAL:HG22 | 1.81                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:444:LEU:H    | 2:D:444:LEU:HD12 | 1.65                     | 0.61              |
| 1:A:149:ASN:ND2  | 1:A:152:LEU:HB2  | 2.16                     | 0.61              |
| 1:C:172:ARG:HD3  | 1:C:176:ASN:HB2  | 1.83                     | 0.61              |
| 1:A:268:ALA:HB2  | 1:A:309:MSE:HE3  | 1.83                     | 0.60              |
| 1:A:321:LYS:HD2  | 1:A:321:LYS:N    | 2.10                     | 0.60              |
| 1:A:434:ASN:ND2  | 1:A:462:ALA:HB1  | 2.16                     | 0.60              |
| 1:C:40:LEU:HD12  | 1:C:86:MSE:SE    | 2.51                     | 0.60              |
| 1:C:289:LEU:HD22 | 1:C:329:LEU:HD22 | 1.83                     | 0.60              |
| 2:D:382:LEU:O    | 2:D:384:GLY:N    | 2.34                     | 0.60              |
| 2:D:434:ARG:HH11 | 2:D:434:ARG:HG2  | 1.66                     | 0.60              |
| 1:C:388:MSE:HE3  | 1:C:433:ARG:CG   | 2.31                     | 0.60              |
| 1:A:84:VAL:N     | 1:A:85:PRO:HD2   | 2.16                     | 0.60              |
| 1:C:47:PRO:C     | 1:C:49:MSE:H     | 2.09                     | 0.60              |
| 1:C:52:LYS:HB2   | 1:C:91:ASP:OD1   | 2.01                     | 0.60              |
| 1:A:178:LEU:N    | 1:A:179:PRO:HD2  | 2.17                     | 0.60              |
| 1:A:388:MSE:HG3  | 1:A:433:ARG:HB2  | 1.83                     | 0.60              |
| 2:B:412:PRO:HG2  | 2:B:413:ASN:H    | 1.66                     | 0.60              |
| 1:C:30:ASN:HA    | 1:C:71:LEU:HD22  | 1.84                     | 0.60              |
| 1:A:354:ILE:HD13 | 1:A:354:ILE:O    | 2.01                     | 0.60              |
| 1:C:83:LEU:C     | 1:C:85:PRO:HD2   | 2.27                     | 0.60              |
| 1:C:204:PHE:O    | 1:C:207:ILE:HG22 | 2.02                     | 0.60              |
| 1:C:336:VAL:C    | 1:C:338:TYR:H    | 2.10                     | 0.60              |
| 1:A:434:ASN:HD21 | 1:A:462:ALA:HB1  | 1.67                     | 0.60              |
| 1:A:264:LEU:N    | 1:A:265:PRO:HD2  | 2.17                     | 0.59              |
| 2:D:425:GLU:O    | 2:D:428:MSE:HB2  | 2.02                     | 0.59              |
| 1:C:303:TYR:HD1  | 1:C:334:TYR:HD1  | 1.50                     | 0.59              |
| 1:A:321:LYS:H    | 1:A:321:LYS:CD   | 2.05                     | 0.59              |
| 1:A:440:LEU:O    | 1:A:448:LEU:HD11 | 2.03                     | 0.59              |
| 1:C:280:VAL:O    | 1:C:284:SER:HB2  | 2.03                     | 0.59              |
| 1:C:30:ASN:HA    | 1:C:71:LEU:HD13  | 1.84                     | 0.59              |
| 1:C:224:ILE:HD12 | 1:C:224:ILE:H    | 1.68                     | 0.59              |
| 1:A:138:LEU:HD22 | 1:A:156:ILE:HG23 | 1.84                     | 0.59              |
| 1:C:388:MSE:HE3  | 1:C:433:ARG:CB   | 2.33                     | 0.59              |
| 1:C:388:MSE:O    | 1:C:391:VAL:HG23 | 2.03                     | 0.58              |
| 2:B:381:ASP:C    | 2:B:383:GLU:H    | 2.10                     | 0.58              |
| 1:C:151:LYS:HB2  | 1:C:151:LYS:NZ   | 2.18                     | 0.58              |
| 1:A:180:TYR:O    | 1:A:183:SER:HB3  | 2.02                     | 0.58              |
| 1:C:292:PHE:CD2  | 1:C:314:LEU:HD21 | 2.38                     | 0.58              |
| 1:A:153:ILE:HD12 | 1:A:195:ARG:NH1  | 2.18                     | 0.58              |
| 1:A:257:LEU:O    | 1:A:261:LYS:HB2  | 2.03                     | 0.58              |
| 1:C:138:LEU:HD22 | 1:C:156:ILE:HG23 | 1.84                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:10:GLU:HB3   | 1:C:13:LEU:HG    | 1.84                     | 0.58              |
| 1:A:144:ASP:OD1  | 1:A:146:LYS:HB2  | 2.04                     | 0.58              |
| 1:C:29:ILE:HG22  | 1:C:71:LEU:CD2   | 2.34                     | 0.58              |
| 1:A:52:LYS:H     | 1:A:53:PRO:HD2   | 1.69                     | 0.58              |
| 1:A:125:PRO:C    | 1:A:127:GLY:H    | 2.11                     | 0.58              |
| 1:C:162:ARG:HB2  | 1:C:162:ARG:HH11 | 1.67                     | 0.58              |
| 1:A:178:LEU:O    | 1:A:182:VAL:HG23 | 2.03                     | 0.57              |
| 1:A:52:LYS:N     | 1:A:53:PRO:HD2   | 2.18                     | 0.57              |
| 1:C:367:PHE:HD1  | 1:C:399:TYR:HD1  | 1.52                     | 0.57              |
| 1:A:460:SER:HA   | 1:C:38:LEU:HD21  | 1.85                     | 0.57              |
| 1:A:327:LEU:HD21 | 1:A:342:VAL:HG12 | 1.86                     | 0.57              |
| 1:A:221:LYS:O    | 1:A:225:LEU:HD12 | 2.04                     | 0.57              |
| 1:C:156:ILE:O    | 1:C:159:ALA:HB3  | 2.04                     | 0.57              |
| 1:C:84:VAL:N     | 1:C:85:PRO:HD2   | 2.20                     | 0.57              |
| 1:C:163:LEU:C    | 1:C:165:THR:H    | 2.12                     | 0.57              |
| 1:A:249:ARG:HH11 | 1:A:297:ARG:HG2  | 1.68                     | 0.57              |
| 2:B:402:ILE:HG12 | 2:B:440:GLU:HB2  | 1.85                     | 0.57              |
| 1:C:309:MSE:O    | 1:C:314:LEU:HD12 | 2.04                     | 0.57              |
| 1:A:245:LEU:HD11 | 1:A:264:LEU:HD11 | 1.87                     | 0.57              |
| 1:A:297:ARG:HD3  | 1:A:331:ASN:HD22 | 1.70                     | 0.57              |
| 1:A:413:GLY:C    | 1:A:415:LEU:H    | 2.13                     | 0.57              |
| 2:B:420:ARG:HG2  | 2:B:420:ARG:HH11 | 1.69                     | 0.57              |
| 1:A:50:ASP:OD2   | 1:A:52:LYS:HG2   | 2.03                     | 0.56              |
| 1:A:249:ARG:NH1  | 1:A:297:ARG:HG2  | 2.20                     | 0.56              |
| 1:A:435:SER:HA   | 1:A:438:ARG:NH1  | 2.19                     | 0.56              |
| 1:C:124:GLN:CD   | 1:C:124:GLN:H    | 2.12                     | 0.56              |
| 1:A:249:ARG:HH11 | 1:A:297:ARG:HB3  | 1.70                     | 0.56              |
| 1:C:54:LEU:O     | 1:C:58:ILE:HG13  | 2.06                     | 0.56              |
| 1:C:93:LEU:C     | 1:C:95:VAL:H     | 2.12                     | 0.56              |
| 1:C:300:GLU:CD   | 1:C:305:LEU:H    | 2.12                     | 0.56              |
| 2:D:436:LYS:H    | 2:D:436:LYS:CE   | 2.19                     | 0.56              |
| 1:C:125:PRO:O    | 1:C:126:LYS:HG2  | 2.06                     | 0.56              |
| 1:A:115:ALA:O    | 1:A:119:VAL:HG23 | 2.04                     | 0.56              |
| 2:B:429:PHE:HZ   | 2:B:449:LYS:HD2  | 1.70                     | 0.56              |
| 1:C:124:GLN:CB   | 1:C:125:PRO:HD3  | 2.29                     | 0.56              |
| 1:A:145:GLU:HG2  | 1:A:189:GLU:OE1  | 2.05                     | 0.56              |
| 2:D:403:ARG:HD3  | 2:D:440:GLU:OE2  | 2.05                     | 0.56              |
| 1:A:354:ILE:HD11 | 1:A:389:GLN:HB3  | 1.88                     | 0.56              |
| 2:D:430:ALA:HB1  | 2:D:435:ARG:HG3  | 1.87                     | 0.56              |
| 1:A:25:LEU:HD21  | 1:A:61:PHE:HE1   | 1.71                     | 0.56              |
| 2:D:428:MSE:HA   | 2:D:431:ILE:HD13 | 1.88                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:180:TYR:C    | 1:C:180:TYR:HD1  | 2.14                     | 0.56              |
| 2:B:414:SER:HA   | 2:B:418:GLU:OE1  | 2.07                     | 0.55              |
| 1:A:135:ILE:HD12 | 1:A:172:ARG:HG2  | 1.86                     | 0.55              |
| 1:C:284:SER:O    | 1:C:285:THR:C    | 2.49                     | 0.55              |
| 1:C:450:VAL:HG22 | 1:C:450:VAL:O    | 2.05                     | 0.55              |
| 1:A:149:ASN:O    | 1:A:153:ILE:HG12 | 2.06                     | 0.55              |
| 1:C:65:ASN:C     | 1:C:67:SER:H     | 2.15                     | 0.55              |
| 2:B:450:VAL:HG12 | 2:B:451:ILE:N    | 2.21                     | 0.55              |
| 1:A:188:MSE:HE1  | 1:A:223:GLU:O    | 2.06                     | 0.55              |
| 1:A:374:PHE:CD1  | 1:A:408:MSE:HE1  | 2.42                     | 0.55              |
| 2:B:419:LEU:H    | 2:B:419:LEU:CD2  | 2.20                     | 0.55              |
| 1:A:391:VAL:O    | 1:A:395:THR:HG23 | 2.07                     | 0.55              |
| 1:A:333:GLN:HB3  | 1:A:337:LYS:NZ   | 2.21                     | 0.55              |
| 1:A:340:LYS:HE2  | 1:A:344:GLU:OE2  | 2.06                     | 0.55              |
| 1:C:79:VAL:O     | 1:C:83:LEU:HB2   | 2.06                     | 0.55              |
| 1:C:449:SER:C    | 1:C:451:TRP:H    | 2.15                     | 0.55              |
| 2:D:420:ARG:O    | 2:D:424:THR:HG22 | 2.07                     | 0.55              |
| 1:A:120:ILE:HG22 | 1:A:163:LEU:HD11 | 1.89                     | 0.54              |
| 1:A:238:VAL:CG1  | 1:A:288:LEU:HD23 | 2.36                     | 0.54              |
| 1:C:180:TYR:C    | 1:C:180:TYR:CD1  | 2.85                     | 0.54              |
| 1:A:81:ASP:HB2   | 1:A:118:ARG:HH11 | 1.71                     | 0.54              |
| 2:B:385:ARG:HH11 | 2:B:385:ARG:HG2  | 1.73                     | 0.54              |
| 1:C:154:THR:CG2  | 2:D:383:GLU:HB3  | 2.37                     | 0.54              |
| 1:C:206:PHE:CD1  | 1:C:206:PHE:N    | 2.75                     | 0.54              |
| 1:A:154:THR:HG23 | 2:B:383:GLU:HG2  | 1.90                     | 0.54              |
| 1:C:444:GLY:O    | 1:C:448:LEU:HD12 | 2.07                     | 0.54              |
| 1:A:380:LEU:HA   | 1:A:387:GLN:NE2  | 2.22                     | 0.54              |
| 2:B:393:SER:C    | 2:B:395:SER:H    | 2.15                     | 0.54              |
| 1:C:250:ASN:O    | 1:C:251:GLN:CG   | 2.55                     | 0.54              |
| 2:D:427:GLY:O    | 2:D:431:ILE:HD12 | 2.08                     | 0.54              |
| 1:C:245:LEU:C    | 1:C:248:ILE:HG22 | 2.32                     | 0.54              |
| 2:D:421:SER:HA   | 2:D:424:THR:CG2  | 2.38                     | 0.54              |
| 1:A:89:PHE:CZ    | 1:A:123:SER:HA   | 2.43                     | 0.54              |
| 1:A:219:PHE:HE1  | 1:A:237:LEU:HD22 | 1.73                     | 0.54              |
| 1:A:303:TYR:O    | 1:A:307:LYS:HB2  | 2.08                     | 0.54              |
| 1:A:33:LEU:HA    | 1:A:36:CYS:SG    | 2.49                     | 0.53              |
| 1:C:272:GLU:O    | 1:C:274:THR:N    | 2.42                     | 0.53              |
| 1:A:320:ALA:HA   | 1:A:323:ILE:CG1  | 2.27                     | 0.53              |
| 1:A:343:VAL:HG13 | 1:A:360:LEU:HD21 | 1.91                     | 0.53              |
| 1:A:332:PRO:HG3  | 1:A:362:ALA:HB3  | 1.89                     | 0.53              |
| 1:C:71:LEU:HD12  | 1:C:72:ASN:H     | 1.72                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:439:THR:HG23 | 2:D:442:ASP:OD1  | 2.08                     | 0.53              |
| 1:C:51:VAL:C     | 1:C:53:PRO:HD2   | 2.34                     | 0.53              |
| 1:C:303:TYR:CD1  | 1:C:334:TYR:HD1  | 2.27                     | 0.53              |
| 1:A:336:VAL:O    | 1:A:340:LYS:HB2  | 2.09                     | 0.53              |
| 1:C:122:ASN:O    | 1:C:123:SER:C    | 2.51                     | 0.52              |
| 1:C:216:ILE:HD12 | 1:C:217:PHE:N    | 2.23                     | 0.52              |
| 1:C:232:LEU:CD2  | 2:D:410:LEU:HD11 | 2.39                     | 0.52              |
| 1:C:323:ILE:HG21 | 1:C:346:TYR:CG   | 2.44                     | 0.52              |
| 1:C:17:GLU:O     | 1:C:19:GLU:N     | 2.41                     | 0.52              |
| 1:C:163:LEU:HD22 | 1:C:169:ILE:CD1  | 2.37                     | 0.52              |
| 1:A:88:ASP:O     | 1:A:92:VAL:HG23  | 2.09                     | 0.52              |
| 1:A:189:GLU:O    | 1:A:190:THR:C    | 2.51                     | 0.52              |
| 1:A:328:GLU:HG2  | 1:A:356:MSE:HG2  | 1.90                     | 0.52              |
| 1:C:251:GLN:OE1  | 1:C:253:LYS:HE3  | 2.09                     | 0.52              |
| 1:A:20:LEU:HD22  | 1:A:32:LEU:HD22  | 1.90                     | 0.52              |
| 1:C:144:ASP:HB3  | 1:C:147:VAL:CG2  | 2.40                     | 0.52              |
| 2:D:443:PHE:O    | 2:D:447:VAL:HG23 | 2.10                     | 0.52              |
| 1:A:16:LEU:O     | 1:A:20:LEU:HD13  | 2.10                     | 0.52              |
| 1:A:105:LEU:HD11 | 1:A:134:ILE:HG23 | 1.91                     | 0.52              |
| 2:B:404:TRP:HZ3  | 2:B:443:PHE:CE1  | 2.28                     | 0.52              |
| 1:C:19:GLU:C     | 1:C:21:ASN:H     | 2.18                     | 0.52              |
| 1:C:189:GLU:O    | 1:C:190:THR:C    | 2.53                     | 0.52              |
| 1:C:384:TYR:CE2  | 1:C:388:MSE:HE2  | 2.45                     | 0.52              |
| 1:A:72:ASN:C     | 1:A:72:ASN:HD22  | 2.16                     | 0.52              |
| 2:B:429:PHE:CZ   | 2:B:449:LYS:HD2  | 2.45                     | 0.52              |
| 1:A:166:ASP:OD2  | 1:A:168:LEU:HB2  | 2.10                     | 0.51              |
| 1:C:116:ALA:O    | 1:C:120:ILE:HG13 | 2.10                     | 0.51              |
| 1:C:379:VAL:HA   | 1:C:382:LEU:HD11 | 1.91                     | 0.51              |
| 1:A:145:GLU:HG3  | 1:A:192:SER:HB3  | 1.92                     | 0.51              |
| 1:C:154:THR:HG21 | 2:D:383:GLU:HB3  | 1.90                     | 0.51              |
| 1:A:422:GLY:C    | 1:A:424:ILE:H    | 2.17                     | 0.51              |
| 1:A:127:GLY:HA2  | 1:A:169:ILE:HD13 | 1.92                     | 0.51              |
| 1:A:283:PHE:HE2  | 2:B:444:LEU:HB2  | 1.75                     | 0.51              |
| 1:A:149:ASN:HD22 | 1:A:152:LEU:HB2  | 1.75                     | 0.51              |
| 1:A:300:GLU:OE1  | 1:A:305:LEU:N    | 2.44                     | 0.51              |
| 1:A:441:LEU:HA   | 1:A:448:LEU:HD11 | 1.91                     | 0.51              |
| 1:C:124:GLN:HB2  | 1:C:125:PRO:CD   | 2.27                     | 0.51              |
| 1:A:20:LEU:HG    | 1:A:26:PRO:HG2   | 1.92                     | 0.51              |
| 2:D:411:CYS:HB3  | 2:D:451:ILE:HG13 | 1.92                     | 0.51              |
| 1:A:125:PRO:C    | 1:A:127:GLY:N    | 2.69                     | 0.51              |
| 1:A:134:ILE:HA   | 1:A:137:ILE:HD12 | 1.91                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:367:PHE:C    | 1:A:369:ALA:H    | 2.19                     | 0.51              |
| 1:C:196:LEU:O    | 1:C:200:LEU:HG   | 2.10                     | 0.51              |
| 1:C:403:PHE:CE2  | 1:C:408:MSE:HE2  | 2.46                     | 0.51              |
| 1:A:116:ALA:O    | 1:A:120:ILE:HG13 | 2.11                     | 0.51              |
| 1:A:110:ASP:HB2  | 1:A:111:PRO:HD3  | 1.93                     | 0.51              |
| 1:A:398:GLU:HG3  | 1:A:399:TYR:N    | 2.26                     | 0.51              |
| 1:C:358:ARG:NE   | 1:C:396:ARG:HH21 | 2.08                     | 0.51              |
| 2:D:393:SER:HA   | 2:D:396:MSE:HG2  | 1.93                     | 0.51              |
| 1:A:213:LYS:C    | 1:A:215:ILE:H    | 2.20                     | 0.50              |
| 1:C:125:PRO:HD2  | 1:C:128:LEU:HB2  | 1.93                     | 0.50              |
| 2:B:419:LEU:HD22 | 2:B:419:LEU:N    | 2.26                     | 0.50              |
| 1:C:37:SER:O     | 1:C:41:VAL:HG23  | 2.11                     | 0.50              |
| 1:C:109:ILE:HG22 | 1:C:112:LEU:H    | 1.77                     | 0.50              |
| 1:A:163:LEU:C    | 1:A:165:THR:H    | 2.19                     | 0.50              |
| 1:C:121:GLU:CB   | 1:C:159:ALA:HA   | 2.41                     | 0.50              |
| 1:C:158:LYS:O    | 1:C:161:GLU:HB3  | 2.12                     | 0.50              |
| 1:C:284:SER:HB3  | 1:C:288:LEU:CB   | 2.42                     | 0.50              |
| 1:C:76:LEU:O     | 1:C:80:VAL:HG23  | 2.12                     | 0.50              |
| 1:C:161:GLU:C    | 1:C:163:LEU:H    | 2.19                     | 0.50              |
| 1:C:347:PHE:CD2  | 1:C:348:HIS:N    | 2.80                     | 0.50              |
| 1:C:390:VAL:HG23 | 1:C:391:VAL:N    | 2.26                     | 0.50              |
| 1:A:322:LEU:O    | 1:A:323:ILE:C    | 2.55                     | 0.50              |
| 1:C:445:GLU:HB2  | 1:C:452:TYR:CE2  | 2.47                     | 0.50              |
| 1:A:96:TYR:CD1   | 1:A:119:VAL:HG21 | 2.46                     | 0.50              |
| 1:A:263:ILE:HD13 | 1:A:263:ILE:N    | 2.19                     | 0.50              |
| 2:D:385:ARG:HH11 | 2:D:385:ARG:HG3  | 1.76                     | 0.50              |
| 1:C:54:LEU:HG    | 1:C:58:ILE:HD11  | 1.93                     | 0.50              |
| 1:C:230:ASP:O    | 1:C:232:LEU:N    | 2.45                     | 0.50              |
| 1:C:371:ARG:NH1  | 1:C:403:PHE:HD1  | 2.08                     | 0.50              |
| 1:C:10:GLU:O     | 1:C:13:LEU:HB2   | 2.11                     | 0.49              |
| 1:C:125:PRO:C    | 1:C:127:GLY:H    | 2.18                     | 0.49              |
| 1:C:136:ASP:OD1  | 1:C:172:ARG:HD2  | 2.12                     | 0.49              |
| 1:C:385:LEU:HD23 | 1:C:429:THR:OG1  | 2.12                     | 0.49              |
| 1:A:44:VAL:O     | 1:A:86:MSE:HE2   | 2.11                     | 0.49              |
| 2:B:425:GLU:O    | 2:B:428:MSE:HB2  | 2.12                     | 0.49              |
| 1:C:206:PHE:H    | 1:C:206:PHE:HD1  | 1.60                     | 0.49              |
| 1:A:178:LEU:HD21 | 1:A:213:LYS:HG2  | 1.94                     | 0.49              |
| 1:C:378:ILE:O    | 1:C:380:LEU:N    | 2.46                     | 0.49              |
| 1:A:209:GLY:N    | 1:A:210:PRO:HD2  | 2.27                     | 0.49              |
| 1:A:260:VAL:O    | 1:A:264:LEU:HG   | 2.13                     | 0.49              |
| 1:C:268:ALA:O    | 1:C:271:PHE:HB3  | 2.13                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:310:ASP:O    | 1:C:315:LYS:HA   | 2.12                     | 0.49              |
| 2:D:431:ILE:HD12 | 2:D:431:ILE:H    | 1.78                     | 0.49              |
| 1:A:249:ARG:HH11 | 1:A:297:ARG:CB   | 2.26                     | 0.49              |
| 1:A:367:PHE:CE1  | 1:A:400:THR:HG22 | 2.48                     | 0.49              |
| 1:C:283:PHE:HE1  | 2:D:445:LYS:HD2  | 1.78                     | 0.49              |
| 1:C:388:MSE:CE   | 1:C:433:ARG:HG3  | 2.43                     | 0.49              |
| 1:A:40:LEU:O     | 1:A:86:MSE:HE1   | 2.13                     | 0.49              |
| 1:A:124:GLN:HB3  | 1:A:125:PRO:CD   | 2.34                     | 0.49              |
| 1:A:459:TYR:O    | 1:A:463:VAL:HG23 | 2.12                     | 0.49              |
| 1:A:144:ASP:HB3  | 1:A:147:VAL:HG23 | 1.95                     | 0.49              |
| 1:C:12:LEU:O     | 1:C:15:GLN:HB2   | 2.13                     | 0.49              |
| 1:A:353:SER:HB2  | 1:A:356:MSE:HE3  | 1.95                     | 0.48              |
| 2:B:389:PHE:CE2  | 2:B:419:LEU:HD12 | 2.47                     | 0.48              |
| 1:C:322:LEU:HD13 | 1:C:325:GLU:HG3  | 1.95                     | 0.48              |
| 1:C:405:LEU:HD23 | 1:C:412:MSE:SE   | 2.62                     | 0.48              |
| 1:C:428:GLU:O    | 1:C:431:HIS:HB3  | 2.13                     | 0.48              |
| 1:C:460:SER:O    | 1:C:464:ASN:HB2  | 2.12                     | 0.48              |
| 1:C:50:ASP:OD2   | 1:C:53:PRO:HD3   | 2.13                     | 0.48              |
| 1:C:250:ASN:C    | 1:C:251:GLN:HG3  | 2.37                     | 0.48              |
| 1:C:295:VAL:O    | 1:C:298:ILE:HG13 | 2.12                     | 0.48              |
| 2:D:446:ALA:O    | 2:D:450:VAL:N    | 2.43                     | 0.48              |
| 1:A:407:GLU:C    | 1:A:409:PRO:HD3  | 2.38                     | 0.48              |
| 2:D:387:ASN:O    | 2:D:391:ILE:HD13 | 2.13                     | 0.48              |
| 2:D:404:TRP:HA   | 2:D:407:ILE:HG22 | 1.95                     | 0.48              |
| 1:A:194:VAL:HG11 | 2:B:406:LEU:HD22 | 1.95                     | 0.48              |
| 1:C:316:ILE:HG12 | 1:C:326:TRP:CG   | 2.49                     | 0.48              |
| 1:A:111:PRO:O    | 1:A:114:VAL:HG12 | 2.12                     | 0.48              |
| 1:C:121:GLU:HB3  | 1:C:159:ALA:HA   | 1.94                     | 0.48              |
| 1:C:416:ILE:CG1  | 1:C:454:PRO:HB2  | 2.43                     | 0.48              |
| 2:D:383:GLU:O    | 2:D:384:GLY:C    | 2.56                     | 0.48              |
| 1:C:261:LYS:HB2  | 1:C:305:LEU:HD22 | 1.95                     | 0.48              |
| 1:C:349:VAL:HG11 | 1:C:374:PHE:CD1  | 2.49                     | 0.48              |
| 1:A:185:LYS:HE2  | 1:A:215:ILE:O    | 2.14                     | 0.48              |
| 1:A:272:GLU:HG3  | 1:A:273:ASP:N    | 2.28                     | 0.48              |
| 1:C:133:ASN:HA   | 1:C:136:ASP:OD2  | 2.14                     | 0.48              |
| 1:C:260:VAL:HG12 | 1:C:264:LEU:HD13 | 1.96                     | 0.48              |
| 1:C:306:PHE:HZ   | 1:C:330:ILE:HD12 | 1.78                     | 0.48              |
| 1:C:353:SER:O    | 1:C:354:ILE:C    | 2.56                     | 0.48              |
| 2:D:412:PRO:O    | 2:D:414:SER:N    | 2.47                     | 0.48              |
| 1:A:139:LEU:HD11 | 1:A:173:LEU:CD2  | 2.44                     | 0.48              |
| 1:A:283:PHE:HZ   | 2:B:441:LYS:HB3  | 1.79                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:457:ARG:HG3  | 1:A:458:GLU:H    | 1.77                     | 0.48              |
| 2:B:428:MSE:HB3  | 2:B:432:ARG:HH21 | 1.79                     | 0.48              |
| 1:C:125:PRO:C    | 1:C:127:GLY:N    | 2.71                     | 0.48              |
| 1:C:281:ARG:O    | 1:C:285:THR:HG23 | 2.14                     | 0.48              |
| 1:C:336:VAL:C    | 1:C:338:TYR:N    | 2.71                     | 0.48              |
| 2:D:382:LEU:C    | 2:D:384:GLY:N    | 2.72                     | 0.48              |
| 1:A:130:ALA:HB2  | 1:A:169:ILE:HD12 | 1.96                     | 0.47              |
| 1:A:189:GLU:HB3  | 1:A:192:SER:OG   | 2.14                     | 0.47              |
| 1:A:253:LYS:C    | 1:A:255:TRP:H    | 2.22                     | 0.47              |
| 1:C:269:GLN:O    | 1:C:272:GLU:HB3  | 2.14                     | 0.47              |
| 1:A:79:VAL:O     | 1:A:83:LEU:HG    | 2.13                     | 0.47              |
| 2:D:385:ARG:HA   | 2:D:419:LEU:CD1  | 2.44                     | 0.47              |
| 1:A:276:ASN:O    | 1:A:277:TYR:CB   | 2.62                     | 0.47              |
| 2:B:414:SER:HB2  | 2:B:418:GLU:HB2  | 1.96                     | 0.47              |
| 2:B:443:PHE:O    | 2:B:447:VAL:HG23 | 2.15                     | 0.47              |
| 1:C:93:LEU:HD21  | 1:C:124:GLN:HE22 | 1.80                     | 0.47              |
| 1:C:232:LEU:HD22 | 2:D:410:LEU:HD11 | 1.95                     | 0.47              |
| 1:C:428:GLU:H    | 1:C:428:GLU:CD   | 2.23                     | 0.47              |
| 2:D:382:LEU:O    | 2:D:382:LEU:HD23 | 2.14                     | 0.47              |
| 1:A:232:LEU:HD13 | 1:A:232:LEU:O    | 2.14                     | 0.47              |
| 1:C:19:GLU:HA    | 1:C:22:GLU:OE1   | 2.14                     | 0.47              |
| 1:C:59:LYS:HB2   | 1:C:96:TYR:CE1   | 2.48                     | 0.47              |
| 1:C:135:ILE:CD1  | 1:C:169:ILE:HG13 | 2.43                     | 0.47              |
| 1:C:185:LYS:HE3  | 1:C:219:PHE:CD2  | 2.50                     | 0.47              |
| 1:A:84:VAL:HG13  | 1:A:92:VAL:HG11  | 1.96                     | 0.47              |
| 1:A:340:LYS:O    | 1:A:344:GLU:HB2  | 2.14                     | 0.47              |
| 1:A:357:LEU:HD13 | 1:A:393:THR:HG21 | 1.96                     | 0.47              |
| 1:A:392:GLU:OE2  | 1:A:396:ARG:HD2  | 2.13                     | 0.47              |
| 1:A:447:LYS:O    | 1:A:449:SER:N    | 2.47                     | 0.47              |
| 2:B:398:VAL:HG22 | 2:B:438:ALA:HB3  | 1.97                     | 0.47              |
| 1:C:272:GLU:O    | 1:C:274:THR:HG23 | 2.14                     | 0.47              |
| 1:C:291:LEU:O    | 1:C:295:VAL:HG23 | 2.14                     | 0.47              |
| 1:C:9:VAL:CG2    | 1:C:47:PRO:HG3   | 2.42                     | 0.47              |
| 1:C:123:SER:HB3  | 1:C:126:LYS:HA   | 1.97                     | 0.47              |
| 1:C:135:ILE:HD13 | 1:C:169:ILE:HG13 | 1.95                     | 0.47              |
| 1:A:20:LEU:HB3   | 1:A:29:ILE:HD13  | 1.97                     | 0.47              |
| 1:A:52:LYS:NZ    | 1:A:91:ASP:HB3   | 2.30                     | 0.47              |
| 1:C:271:PHE:CE2  | 1:C:281:ARG:NE   | 2.82                     | 0.47              |
| 1:C:289:LEU:HD22 | 1:C:329:LEU:CD2  | 2.43                     | 0.47              |
| 1:C:327:LEU:CB   | 1:C:356:MSE:HG2  | 2.41                     | 0.47              |
| 1:C:434:ASN:HD21 | 1:C:462:ALA:HB1  | 1.79                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:96:TYR:CE1   | 1:A:119:VAL:HG21 | 2.50                     | 0.47              |
| 1:A:313:SER:O    | 1:A:315:LYS:N    | 2.48                     | 0.47              |
| 1:C:257:LEU:O    | 1:C:258:ARG:C    | 2.58                     | 0.47              |
| 1:C:295:VAL:C    | 1:C:297:ARG:H    | 2.22                     | 0.47              |
| 2:D:407:ILE:HD11 | 2:D:443:PHE:HB3  | 1.97                     | 0.46              |
| 1:A:293:ALA:HB2  | 1:A:329:LEU:HB3  | 1.96                     | 0.46              |
| 1:C:110:ASP:O    | 1:C:114:VAL:HG23 | 2.15                     | 0.46              |
| 1:C:152:LEU:HD22 | 1:C:156:ILE:HD11 | 1.97                     | 0.46              |
| 2:D:382:LEU:C    | 2:D:383:GLU:HG3  | 2.41                     | 0.46              |
| 1:A:177:ASN:C    | 1:A:179:PRO:HD2  | 2.41                     | 0.46              |
| 2:B:381:ASP:C    | 2:B:383:GLU:N    | 2.73                     | 0.46              |
| 1:C:171:ARG:HB3  | 1:C:171:ARG:CZ   | 2.46                     | 0.46              |
| 1:C:260:VAL:C    | 1:C:262:LYS:H    | 2.23                     | 0.46              |
| 1:A:333:GLN:HB3  | 1:A:337:LYS:HZ3  | 1.81                     | 0.46              |
| 1:A:17:GLU:HA    | 1:A:32:LEU:HD21  | 1.97                     | 0.46              |
| 1:A:435:SER:HA   | 1:A:438:ARG:HH12 | 1.81                     | 0.46              |
| 2:B:389:PHE:O    | 2:B:393:SER:HB3  | 2.15                     | 0.46              |
| 2:B:404:TRP:CZ3  | 2:B:443:PHE:CE1  | 3.04                     | 0.46              |
| 2:B:422:VAL:HG11 | 2:B:447:VAL:HG22 | 1.98                     | 0.46              |
| 1:A:255:TRP:CD1  | 1:A:255:TRP:C    | 2.92                     | 0.46              |
| 1:A:219:PHE:O    | 1:A:263:ILE:HG21 | 2.15                     | 0.46              |
| 1:C:165:THR:HG22 | 1:C:206:PHE:CE2  | 2.50                     | 0.46              |
| 1:A:353:SER:C    | 1:A:355:GLY:N    | 2.74                     | 0.46              |
| 2:B:400:ARG:HA   | 2:B:400:ARG:NE   | 2.31                     | 0.46              |
| 1:C:326:TRP:CE3  | 1:C:330:ILE:HD11 | 2.50                     | 0.46              |
| 1:A:133:ASN:O    | 1:A:137:ILE:HG13 | 2.16                     | 0.46              |
| 1:A:185:LYS:HD2  | 1:A:219:PHE:HE2  | 1.81                     | 0.46              |
| 1:A:413:GLY:C    | 1:A:415:LEU:N    | 2.73                     | 0.46              |
| 1:A:416:ILE:HD11 | 1:A:451:TRP:HE3  | 1.81                     | 0.46              |
| 1:C:26:PRO:O     | 1:C:29:ILE:HG13  | 2.16                     | 0.46              |
| 1:C:378:ILE:C    | 1:C:380:LEU:N    | 2.68                     | 0.45              |
| 1:C:417:GLY:C    | 1:C:419:GLY:H    | 2.24                     | 0.45              |
| 1:A:142:LEU:O    | 1:A:195:ARG:HD2  | 2.17                     | 0.45              |
| 1:A:327:LEU:CD2  | 1:A:343:VAL:HA   | 2.46                     | 0.45              |
| 1:C:10:GLU:HB3   | 1:C:13:LEU:CD2   | 2.47                     | 0.45              |
| 1:C:25:LEU:HD11  | 1:C:66:VAL:CG1   | 2.41                     | 0.45              |
| 2:D:399:GLU:HG2  | 2:D:400:ARG:N    | 2.29                     | 0.45              |
| 1:A:219:PHE:HE1  | 1:A:237:LEU:CD2  | 2.30                     | 0.45              |
| 1:C:102:VAL:HG22 | 1:C:134:ILE:HG12 | 1.98                     | 0.45              |
| 1:A:324:THR:HG23 | 1:A:325:GLU:H    | 1.81                     | 0.45              |
| 1:C:324:THR:O    | 1:C:328:GLU:HG2  | 2.17                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:340:LYS:HE2  | 1:C:344:GLU:CD   | 2.41                     | 0.45              |
| 1:C:399:TYR:CE1  | 1:C:400:THR:HG23 | 2.52                     | 0.45              |
| 1:A:201:THR:HG21 | 1:A:243:LYS:HD2  | 1.99                     | 0.45              |
| 1:C:34:ARG:O     | 1:C:38:LEU:HD12  | 2.17                     | 0.45              |
| 1:C:213:LYS:C    | 1:C:215:ILE:H    | 2.24                     | 0.45              |
| 1:C:232:LEU:HD23 | 2:D:444:LEU:HD21 | 1.99                     | 0.45              |
| 1:C:367:PHE:O    | 1:C:370:ILE:HG13 | 2.17                     | 0.45              |
| 1:C:384:TYR:CZ   | 1:C:388:MSE:HE2  | 2.52                     | 0.45              |
| 1:C:10:GLU:HB3   | 1:C:13:LEU:CG    | 2.47                     | 0.45              |
| 1:C:295:VAL:HA   | 1:C:298:ILE:HG13 | 1.99                     | 0.45              |
| 1:A:249:ARG:HH11 | 1:A:297:ARG:CG   | 2.29                     | 0.45              |
| 1:C:55:LEU:C     | 1:C:95:VAL:HG11  | 2.41                     | 0.45              |
| 1:C:177:ASN:C    | 1:C:179:PRO:HD2  | 2.41                     | 0.45              |
| 1:C:235:ILE:HG23 | 1:C:287:CYS:SG   | 2.57                     | 0.45              |
| 1:C:313:SER:HB2  | 1:C:314:LEU:H    | 1.57                     | 0.45              |
| 1:A:23:ASP:HB3   | 1:A:24:ASN:H     | 1.54                     | 0.45              |
| 1:A:185:LYS:HD3  | 1:A:216:ILE:HD12 | 1.99                     | 0.45              |
| 2:B:398:VAL:CG1  | 2:B:402:ILE:HD12 | 2.47                     | 0.45              |
| 1:C:12:LEU:HA    | 1:C:15:GLN:HE21  | 1.81                     | 0.45              |
| 1:C:185:LYS:HE3  | 1:C:219:PHE:HD2  | 1.80                     | 0.45              |
| 1:C:325:GLU:O    | 1:C:329:LEU:HD13 | 2.17                     | 0.45              |
| 1:C:453:GLU:N    | 1:C:454:PRO:HD2  | 2.32                     | 0.45              |
| 1:A:60:ARG:O     | 1:A:64:SER:HB3   | 2.16                     | 0.45              |
| 1:A:137:ILE:O    | 1:A:141:ILE:HG13 | 2.17                     | 0.45              |
| 2:D:392:HIS:CE1  | 2:D:420:ARG:HH11 | 2.35                     | 0.45              |
| 1:A:425:ILE:N    | 1:A:425:ILE:HD12 | 2.31                     | 0.44              |
| 1:C:321:LYS:HD2  | 1:C:321:LYS:N    | 2.32                     | 0.44              |
| 2:D:400:ARG:HG3  | 2:D:400:ARG:HH11 | 1.82                     | 0.44              |
| 1:A:154:THR:CG2  | 2:B:383:GLU:HG2  | 2.47                     | 0.44              |
| 1:C:411:VAL:HA   | 1:C:414:SER:OG   | 2.17                     | 0.44              |
| 2:D:402:ILE:HG21 | 2:D:404:TRP:CH2  | 2.52                     | 0.44              |
| 1:A:230:ASP:O    | 1:A:231:ILE:C    | 2.59                     | 0.44              |
| 2:D:414:SER:O    | 2:D:415:THR:C    | 2.61                     | 0.44              |
| 1:A:140:ASP:O    | 1:A:144:ASP:HB2  | 2.18                     | 0.44              |
| 1:A:259:HIS:C    | 1:A:261:LYS:H    | 2.26                     | 0.44              |
| 2:B:383:GLU:OE1  | 2:B:383:GLU:HA   | 2.16                     | 0.44              |
| 2:B:429:PHE:HE2  | 2:B:446:ALA:HA   | 1.82                     | 0.44              |
| 1:A:106:ARG:HG2  | 1:A:106:ARG:HH11 | 1.82                     | 0.44              |
| 1:A:331:ASN:OD1  | 1:A:333:GLN:N    | 2.51                     | 0.44              |
| 1:A:397:TYR:HB2  | 1:A:400:THR:OG1  | 2.17                     | 0.44              |
| 1:C:52:LYS:N     | 1:C:53:PRO:CD    | 2.80                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:204:PHE:CD1  | 1:C:207:ILE:HG21 | 2.53                     | 0.44              |
| 1:C:260:VAL:C    | 1:C:262:LYS:N    | 2.76                     | 0.44              |
| 2:D:404:TRP:O    | 2:D:407:ILE:HG22 | 2.17                     | 0.44              |
| 1:A:347:PHE:CD2  | 1:A:370:ILE:HB   | 2.53                     | 0.44              |
| 1:C:195:ARG:HD3  | 2:D:405:GLU:OE1  | 2.18                     | 0.44              |
| 1:C:255:TRP:CZ3  | 1:C:256:ALA:HB2  | 2.53                     | 0.44              |
| 1:C:322:LEU:HB3  | 1:C:326:TRP:NE1  | 2.33                     | 0.44              |
| 1:A:368:ASN:HA   | 1:A:371:ARG:HG2  | 2.00                     | 0.44              |
| 1:A:451:TRP:O    | 1:A:455:LEU:HG   | 2.18                     | 0.44              |
| 1:C:11:ASN:HB3   | 1:C:47:PRO:CG    | 2.44                     | 0.44              |
| 1:C:264:LEU:HB3  | 1:C:265:PRO:HD3  | 2.00                     | 0.44              |
| 1:C:339:HIS:HB3  | 1:C:342:VAL:CG2  | 2.48                     | 0.44              |
| 1:A:11:ASN:HD22  | 1:A:14:THR:HB    | 1.82                     | 0.44              |
| 1:C:30:ASN:OD1   | 1:C:71:LEU:HD13  | 2.16                     | 0.44              |
| 1:C:135:ILE:HA   | 1:C:138:LEU:HD12 | 1.99                     | 0.44              |
| 1:C:272:GLU:HG3  | 1:C:273:ASP:N    | 2.33                     | 0.44              |
| 1:C:412:MSE:HE2  | 1:C:451:TRP:CD2  | 2.53                     | 0.44              |
| 1:C:124:GLN:N    | 1:C:124:GLN:OE1  | 2.51                     | 0.43              |
| 1:C:241:TYR:CE1  | 1:C:260:VAL:HG13 | 2.53                     | 0.43              |
| 1:C:245:LEU:CD2  | 1:C:295:VAL:HG22 | 2.48                     | 0.43              |
| 1:C:412:MSE:HE3  | 1:C:412:MSE:HB3  | 1.90                     | 0.43              |
| 2:D:383:GLU:C    | 2:D:383:GLU:OE1  | 2.61                     | 0.43              |
| 2:D:412:PRO:C    | 2:D:414:SER:N    | 2.75                     | 0.43              |
| 1:A:139:LEU:HD11 | 1:A:173:LEU:HD23 | 2.00                     | 0.43              |
| 1:C:10:GLU:OE1   | 1:C:13:LEU:HD21  | 2.18                     | 0.43              |
| 1:C:437:LEU:O    | 1:C:441:LEU:HD13 | 2.17                     | 0.43              |
| 1:A:316:ILE:HG12 | 1:A:326:TRP:CD2  | 2.53                     | 0.43              |
| 1:A:379:VAL:O    | 1:A:382:LEU:HG   | 2.17                     | 0.43              |
| 1:A:425:ILE:HD12 | 1:A:425:ILE:H    | 1.84                     | 0.43              |
| 1:C:20:LEU:HD23  | 1:C:26:PRO:HG2   | 2.00                     | 0.43              |
| 1:A:125:PRO:HD2  | 1:A:128:LEU:HB2  | 2.00                     | 0.43              |
| 1:A:180:TYR:O    | 1:A:184:VAL:HG23 | 2.17                     | 0.43              |
| 1:A:232:LEU:HD13 | 1:A:232:LEU:C    | 2.43                     | 0.43              |
| 1:C:97:SER:O     | 1:C:98:ALA:C     | 2.62                     | 0.43              |
| 1:C:188:MSE:HE2  | 1:C:188:MSE:HB3  | 1.71                     | 0.43              |
| 1:A:11:ASN:HA    | 1:A:14:THR:OG1   | 2.18                     | 0.43              |
| 1:A:24:ASN:O     | 1:A:25:LEU:HB2   | 2.19                     | 0.43              |
| 1:A:109:ILE:O    | 1:A:113:LYS:HG3  | 2.18                     | 0.43              |
| 1:C:380:LEU:HD21 | 1:C:411:VAL:HG23 | 2.00                     | 0.43              |
| 2:D:385:ARG:NH1  | 2:D:385:ARG:HG3  | 2.34                     | 0.43              |
| 1:A:105:LEU:O    | 1:A:113:LYS:HE2  | 2.19                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:407:ILE:HD11 | 2:B:443:PHE:HB3  | 2.00                     | 0.43              |
| 1:C:77:LEU:O     | 1:C:80:VAL:HB    | 2.19                     | 0.43              |
| 1:C:109:ILE:O    | 1:C:113:LYS:HG3  | 2.19                     | 0.43              |
| 1:C:159:ALA:O    | 1:C:163:LEU:HB2  | 2.19                     | 0.43              |
| 1:C:295:VAL:C    | 1:C:297:ARG:N    | 2.77                     | 0.43              |
| 1:C:432:TYR:O    | 1:C:433:ARG:C    | 2.61                     | 0.43              |
| 1:A:178:LEU:N    | 1:A:179:PRO:CD   | 2.82                     | 0.43              |
| 1:A:210:PRO:HG2  | 1:A:211:GLU:H    | 1.83                     | 0.43              |
| 1:C:93:LEU:C     | 1:C:95:VAL:N     | 2.76                     | 0.43              |
| 1:C:24:ASN:HD22  | 1:C:24:ASN:HA    | 1.62                     | 0.43              |
| 1:C:316:ILE:HD11 | 1:C:330:ILE:HG13 | 2.01                     | 0.43              |
| 1:A:109:ILE:HB   | 1:A:112:LEU:HB3  | 1.99                     | 0.43              |
| 1:C:268:ALA:HB2  | 1:C:309:MSE:CE   | 2.42                     | 0.43              |
| 1:C:314:LEU:HD12 | 1:C:314:LEU:N    | 2.33                     | 0.43              |
| 2:D:402:ILE:HG21 | 2:D:404:TRP:CZ2  | 2.53                     | 0.43              |
| 2:D:422:VAL:CG2  | 2:D:450:VAL:HG11 | 2.47                     | 0.43              |
| 2:D:436:LYS:NZ   | 2:D:437:VAL:HG23 | 2.33                     | 0.43              |
| 2:B:385:ARG:HG2  | 2:B:385:ARG:NH1  | 2.33                     | 0.43              |
| 1:C:47:PRO:C     | 1:C:49:MSE:N     | 2.74                     | 0.43              |
| 1:C:47:PRO:O     | 1:C:49:MSE:N     | 2.52                     | 0.43              |
| 1:C:166:ASP:HB3  | 1:C:169:ILE:CG2  | 2.46                     | 0.43              |
| 1:C:225:LEU:HD23 | 1:C:277:TYR:OH   | 2.19                     | 0.43              |
| 1:C:245:LEU:HD21 | 1:C:295:VAL:HG22 | 2.01                     | 0.43              |
| 1:C:320:ALA:HA   | 1:C:323:ILE:HG12 | 2.00                     | 0.43              |
| 1:C:327:LEU:HD23 | 1:C:335:LEU:HD13 | 2.01                     | 0.43              |
| 2:D:384:GLY:O    | 2:D:385:ARG:C    | 2.62                     | 0.43              |
| 2:D:392:HIS:NE2  | 2:D:420:ARG:HG2  | 2.33                     | 0.43              |
| 1:A:196:LEU:O    | 1:A:200:LEU:HG   | 2.18                     | 0.42              |
| 1:A:336:VAL:O    | 1:A:336:VAL:HG22 | 2.19                     | 0.42              |
| 1:A:367:PHE:C    | 1:A:369:ALA:N    | 2.77                     | 0.42              |
| 1:C:121:GLU:HA   | 1:C:163:LEU:CD1  | 2.49                     | 0.42              |
| 1:C:163:LEU:O    | 1:C:169:ILE:HG21 | 2.18                     | 0.42              |
| 1:C:193:PHE:O    | 1:C:197:ILE:HG13 | 2.19                     | 0.42              |
| 1:C:403:PHE:HE2  | 1:C:408:MSE:HE2  | 1.84                     | 0.42              |
| 1:A:72:ASN:HB3   | 1:A:75:TYR:HD2   | 1.84                     | 0.42              |
| 1:A:227:SER:HB2  | 1:A:233:VAL:HG12 | 1.99                     | 0.42              |
| 1:A:302:GLU:HG3  | 1:A:302:GLU:O    | 2.20                     | 0.42              |
| 1:C:85:PRO:HA    | 1:C:122:ASN:HD22 | 1.85                     | 0.42              |
| 1:C:93:LEU:HD21  | 1:C:124:GLN:NE2  | 2.34                     | 0.42              |
| 1:C:129:PHE:O    | 1:C:130:ALA:C    | 2.62                     | 0.42              |
| 1:C:178:LEU:N    | 1:C:179:PRO:CD   | 2.81                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:350:SER:O    | 1:C:351:GLY:C    | 2.63                     | 0.42              |
| 2:D:385:ARG:HA   | 2:D:419:LEU:HD13 | 2.01                     | 0.42              |
| 2:D:436:LYS:H    | 2:D:436:LYS:HE3  | 1.83                     | 0.42              |
| 1:C:110:ASP:N    | 1:C:111:PRO:CD   | 2.82                     | 0.42              |
| 1:A:133:ASN:ND2  | 1:A:137:ILE:HD11 | 2.35                     | 0.42              |
| 1:A:146:LYS:H    | 1:A:146:LYS:HD2  | 1.84                     | 0.42              |
| 1:A:187:ARG:HD2  | 1:A:192:SER:OG   | 2.20                     | 0.42              |
| 1:A:234:PHE:CE2  | 1:A:280:VAL:HG13 | 2.55                     | 0.42              |
| 1:A:277:TYR:N    | 1:A:278:PRO:CD   | 2.82                     | 0.42              |
| 1:A:353:SER:CB   | 1:A:356:MSE:HE3  | 2.49                     | 0.42              |
| 1:A:232:LEU:HD23 | 2:B:444:LEU:HD21 | 2.00                     | 0.42              |
| 1:A:320:ALA:C    | 1:A:322:LEU:N    | 2.76                     | 0.42              |
| 2:B:424:THR:HG21 | 1:C:459:TYR:HE2  | 1.85                     | 0.42              |
| 1:A:322:LEU:HA   | 1:A:325:GLU:OE1  | 2.19                     | 0.42              |
| 1:C:85:PRO:HG2   | 1:C:86:MSE:H     | 1.84                     | 0.42              |
| 1:C:231:ILE:HG23 | 1:C:232:LEU:N    | 2.35                     | 0.42              |
| 1:C:310:ASP:O    | 1:C:314:LEU:O    | 2.37                     | 0.42              |
| 1:C:340:LYS:HE2  | 1:C:344:GLU:OE1  | 2.19                     | 0.42              |
| 2:D:415:THR:O    | 2:D:416:GLY:C    | 2.62                     | 0.42              |
| 1:A:52:LYS:N     | 1:A:53:PRO:CD    | 2.83                     | 0.42              |
| 1:A:241:TYR:HE1  | 1:A:260:VAL:HG12 | 1.85                     | 0.42              |
| 1:C:152:LEU:O    | 1:C:156:ILE:HG13 | 2.20                     | 0.42              |
| 1:C:271:PHE:HE2  | 1:C:281:ARG:NE   | 2.17                     | 0.42              |
| 1:C:46:LEU:CD1   | 1:C:86:MSE:HB2   | 2.49                     | 0.42              |
| 1:C:273:ASP:C    | 1:C:275:GLU:H    | 2.25                     | 0.42              |
| 1:A:80:VAL:O     | 1:A:84:VAL:HG23  | 2.20                     | 0.42              |
| 1:A:261:LYS:HG2  | 1:A:305:LEU:HD22 | 2.00                     | 0.42              |
| 1:C:347:PHE:HE1  | 1:C:370:ILE:HD13 | 1.84                     | 0.42              |
| 1:C:433:ARG:HG2  | 1:C:437:LEU:HD13 | 2.02                     | 0.42              |
| 1:A:124:GLN:CB   | 1:A:125:PRO:CD   | 2.95                     | 0.42              |
| 1:A:187:ARG:O    | 1:A:188:MSE:C    | 2.62                     | 0.42              |
| 1:A:279:ASP:O    | 1:A:280:VAL:C    | 2.62                     | 0.42              |
| 1:A:81:ASP:OD1   | 1:A:118:ARG:HD3  | 2.20                     | 0.41              |
| 1:A:84:VAL:N     | 1:A:85:PRO:CD    | 2.81                     | 0.41              |
| 1:A:230:ASP:O    | 1:A:232:LEU:N    | 2.53                     | 0.41              |
| 1:C:319:GLU:HB3  | 1:C:321:LYS:HD2  | 2.02                     | 0.41              |
| 1:A:220:THR:HG23 | 1:A:223:GLU:OE1  | 2.19                     | 0.41              |
| 2:B:380:MSE:HE2  | 2:B:380:MSE:HB2  | 1.99                     | 0.41              |
| 1:C:306:PHE:CZ   | 1:C:330:ILE:HD12 | 2.55                     | 0.41              |
| 1:A:114:VAL:HG23 | 1:A:155:ALA:CB   | 2.50                     | 0.41              |
| 1:A:199:PHE:CD1  | 1:A:199:PHE:C    | 2.98                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:241:TYR:CZ   | 1:A:263:ILE:HG13 | 2.56                     | 0.41              |
| 1:A:335:LEU:O    | 1:A:339:HIS:C    | 2.63                     | 0.41              |
| 2:B:433:ALA:O    | 2:B:434:ARG:HG2  | 2.20                     | 0.41              |
| 1:C:101:LEU:HD21 | 1:C:120:ILE:HG12 | 2.02                     | 0.41              |
| 1:C:319:GLU:C    | 1:C:321:LYS:H    | 2.27                     | 0.41              |
| 1:C:324:THR:O    | 1:C:325:GLU:C    | 2.62                     | 0.41              |
| 1:C:54:LEU:HA    | 1:C:57:THR:OG1   | 2.20                     | 0.41              |
| 1:C:163:LEU:C    | 1:C:165:THR:N    | 2.78                     | 0.41              |
| 2:D:436:LYS:H    | 2:D:436:LYS:CD   | 2.33                     | 0.41              |
| 1:A:109:ILE:HG22 | 1:A:112:LEU:H    | 1.86                     | 0.41              |
| 1:A:220:THR:OG1  | 1:A:223:GLU:HG3  | 2.20                     | 0.41              |
| 1:A:324:THR:HG23 | 1:A:325:GLU:N    | 2.36                     | 0.41              |
| 1:A:388:MSE:N    | 1:A:388:MSE:HE2  | 2.35                     | 0.41              |
| 2:B:407:ILE:HD11 | 2:B:444:LEU:HD23 | 2.02                     | 0.41              |
| 2:B:416:GLY:O    | 2:B:419:LEU:HD23 | 2.20                     | 0.41              |
| 1:C:40:LEU:CD1   | 1:C:46:LEU:HD21  | 2.45                     | 0.41              |
| 1:C:128:LEU:C    | 1:C:130:ALA:H    | 2.28                     | 0.41              |
| 1:A:187:ARG:HG3  | 1:A:188:MSE:N    | 2.34                     | 0.41              |
| 1:A:234:PHE:O    | 1:A:238:VAL:HG23 | 2.21                     | 0.41              |
| 1:C:33:LEU:HA    | 1:C:36:CYS:SG    | 2.60                     | 0.41              |
| 1:C:190:THR:HG21 | 2:D:403:ARG:NH1  | 2.35                     | 0.41              |
| 1:C:300:GLU:OE1  | 1:C:305:LEU:N    | 2.54                     | 0.41              |
| 1:C:354:ILE:HG22 | 1:C:355:GLY:N    | 2.35                     | 0.41              |
| 1:C:435:SER:O    | 1:C:439:ASN:ND2  | 2.54                     | 0.41              |
| 2:D:429:PHE:HA   | 2:D:432:ARG:HH11 | 1.85                     | 0.41              |
| 1:A:13:LEU:HD13  | 1:A:36:CYS:HA    | 2.01                     | 0.41              |
| 1:A:433:ARG:O    | 1:A:437:LEU:HG   | 2.19                     | 0.41              |
| 1:C:128:LEU:HD22 | 1:C:129:PHE:CD1  | 2.56                     | 0.41              |
| 1:C:193:PHE:CE1  | 1:C:197:ILE:HD11 | 2.56                     | 0.41              |
| 1:A:374:PHE:HD1  | 1:A:408:MSE:HE1  | 1.83                     | 0.41              |
| 1:A:405:LEU:HD13 | 1:A:405:LEU:HA   | 1.83                     | 0.41              |
| 2:B:420:ARG:HG2  | 2:B:420:ARG:NH1  | 2.33                     | 0.41              |
| 1:C:30:ASN:CA    | 1:C:71:LEU:HD22  | 2.51                     | 0.41              |
| 1:C:83:LEU:C     | 1:C:83:LEU:HD23  | 2.46                     | 0.41              |
| 1:C:331:ASN:ND2  | 1:C:334:TYR:H    | 2.18                     | 0.41              |
| 1:C:347:PHE:CD2  | 1:C:347:PHE:C    | 2.98                     | 0.41              |
| 1:C:68:TYR:C     | 1:C:70:SER:H     | 2.29                     | 0.41              |
| 1:C:151:LYS:HB2  | 1:C:151:LYS:HZ3  | 1.84                     | 0.41              |
| 1:C:378:ILE:HA   | 1:C:381:ARG:HG2  | 2.02                     | 0.41              |
| 1:A:38:LEU:HD13  | 1:A:38:LEU:O     | 2.21                     | 0.41              |
| 1:A:163:LEU:C    | 1:A:165:THR:N    | 2.78                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:353:SER:O    | 1:C:355:GLY:N    | 2.54                     | 0.41              |
| 1:C:66:VAL:HG12  | 1:C:66:VAL:O     | 2.21                     | 0.40              |
| 1:C:300:GLU:OE2  | 1:C:304:SER:HB2  | 2.21                     | 0.40              |
| 1:A:327:LEU:HD21 | 1:A:343:VAL:HA   | 2.03                     | 0.40              |
| 1:C:102:VAL:HG13 | 1:C:137:ILE:CD1  | 2.51                     | 0.40              |
| 1:C:133:ASN:O    | 1:C:137:ILE:HG13 | 2.21                     | 0.40              |
| 1:A:264:LEU:N    | 1:A:265:PRO:CD   | 2.83                     | 0.40              |
| 1:A:272:GLU:CD   | 1:A:272:GLU:C    | 2.90                     | 0.40              |
| 1:A:366:CYS:O    | 1:A:369:ALA:HB3  | 2.21                     | 0.40              |
| 1:A:454:PRO:O    | 1:A:458:GLU:HB2  | 2.22                     | 0.40              |
| 1:C:11:ASN:C     | 1:C:13:LEU:H     | 2.30                     | 0.40              |
| 1:C:284:SER:HB3  | 1:C:288:LEU:HB3  | 2.04                     | 0.40              |
| 1:C:349:VAL:O    | 1:C:350:SER:HB3  | 2.22                     | 0.40              |
| 1:A:117:CYS:SG   | 1:A:156:ILE:HG12 | 2.61                     | 0.40              |
| 1:A:295:VAL:HG11 | 1:A:309:MSE:SE   | 2.71                     | 0.40              |
| 1:A:384:TYR:HE1  | 1:A:414:SER:O    | 2.05                     | 0.40              |
| 2:B:407:ILE:CD1  | 2:B:443:PHE:HB3  | 2.51                     | 0.40              |
| 1:C:156:ILE:HG22 | 1:C:160:LEU:HD11 | 2.02                     | 0.40              |
| 1:C:171:ARG:O    | 1:C:175:ASP:HB3  | 2.21                     | 0.40              |
| 1:C:224:ILE:O    | 1:C:227:SER:OG   | 2.34                     | 0.40              |
| 1:A:333:GLN:O    | 1:A:337:LYS:HG3  | 2.21                     | 0.40              |
| 1:C:269:GLN:O    | 1:C:272:GLU:N    | 2.52                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 1   | A     | 455/500 (91%) | 366 (80%) | 67 (15%) | 22 (5%)  | 2           | 17 |
| 1   | C     | 450/500 (90%) | 330 (73%) | 83 (18%) | 37 (8%)  | 0           | 10 |
| 2   | B     | 71/88 (81%)   | 55 (78%)  | 11 (16%) | 5 (7%)   | 1           | 12 |

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| Mol | Chain | Analysed        | Favoured  | Allowed   | Outliers | Percentiles |    |
|-----|-------|-----------------|-----------|-----------|----------|-------------|----|
| 2   | D     | 71/88 (81%)     | 50 (70%)  | 15 (21%)  | 6 (8%)   | 0           | 9  |
| All | All   | 1047/1176 (89%) | 801 (76%) | 176 (17%) | 70 (7%)  | 1           | 13 |

All (70) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 124 | GLN  |
| 1   | A     | 190 | THR  |
| 1   | A     | 231 | ILE  |
| 1   | A     | 281 | ARG  |
| 1   | A     | 449 | SER  |
| 1   | C     | 18  | ASN  |
| 1   | C     | 65  | ASN  |
| 1   | C     | 70  | SER  |
| 1   | C     | 161 | GLU  |
| 1   | C     | 190 | THR  |
| 1   | C     | 231 | ILE  |
| 1   | C     | 258 | ARG  |
| 1   | C     | 273 | ASP  |
| 1   | C     | 285 | THR  |
| 1   | C     | 313 | SER  |
| 1   | C     | 354 | ILE  |
| 2   | D     | 383 | GLU  |
| 1   | A     | 260 | VAL  |
| 1   | A     | 284 | SER  |
| 1   | A     | 314 | LEU  |
| 2   | B     | 400 | ARG  |
| 2   | B     | 402 | ILE  |
| 1   | C     | 48  | ASP  |
| 1   | C     | 66  | VAL  |
| 1   | C     | 191 | VAL  |
| 1   | C     | 214 | ASP  |
| 1   | C     | 304 | SER  |
| 1   | C     | 351 | GLY  |
| 1   | C     | 376 | ALA  |
| 1   | C     | 379 | VAL  |
| 1   | C     | 449 | SER  |
| 1   | C     | 450 | VAL  |
| 2   | D     | 381 | ASP  |
| 2   | D     | 401 | GLY  |
| 2   | D     | 413 | ASN  |
| 1   | A     | 47  | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 254 | TYR  |
| 1   | A     | 283 | PHE  |
| 1   | A     | 346 | TYR  |
| 1   | A     | 448 | LEU  |
| 1   | C     | 27  | GLU  |
| 1   | C     | 49  | MSE  |
| 1   | C     | 87  | ALA  |
| 1   | C     | 162 | ARG  |
| 1   | C     | 164 | SER  |
| 1   | C     | 257 | LEU  |
| 1   | C     | 312 | ASP  |
| 1   | C     | 407 | GLU  |
| 1   | A     | 280 | VAL  |
| 2   | B     | 394 | LYS  |
| 2   | B     | 412 | PRO  |
| 1   | C     | 175 | ASP  |
| 1   | C     | 251 | GLN  |
| 1   | C     | 337 | LYS  |
| 2   | D     | 434 | ARG  |
| 1   | A     | 23  | ASP  |
| 1   | A     | 277 | TYR  |
| 1   | A     | 304 | SER  |
| 1   | A     | 409 | PRO  |
| 1   | C     | 24  | ASN  |
| 1   | C     | 98  | ALA  |
| 1   | C     | 339 | HIS  |
| 2   | B     | 403 | ARG  |
| 1   | C     | 123 | SER  |
| 1   | A     | 416 | ILE  |
| 1   | A     | 349 | VAL  |
| 1   | A     | 323 | ILE  |
| 2   | D     | 402 | ILE  |
| 1   | A     | 147 | VAL  |
| 1   | C     | 316 | ILE  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 1   | A     | 424/452 (94%)  | 392 (92%) | 32 (8%)  | 12          | 38 |
| 1   | C     | 424/452 (94%)  | 380 (90%) | 44 (10%) | 7           | 26 |
| 2   | B     | 62/72 (86%)    | 54 (87%)  | 8 (13%)  | 4           | 20 |
| 2   | D     | 62/72 (86%)    | 54 (87%)  | 8 (13%)  | 4           | 20 |
| All | All   | 972/1048 (93%) | 880 (90%) | 92 (10%) | 8           | 30 |

All (92) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 22  | GLU  |
| 1   | A     | 65  | ASN  |
| 1   | A     | 136 | ASP  |
| 1   | A     | 147 | VAL  |
| 1   | A     | 151 | LYS  |
| 1   | A     | 154 | THR  |
| 1   | A     | 169 | ILE  |
| 1   | A     | 175 | ASP  |
| 1   | A     | 206 | PHE  |
| 1   | A     | 221 | LYS  |
| 1   | A     | 251 | GLN  |
| 1   | A     | 263 | ILE  |
| 1   | A     | 272 | GLU  |
| 1   | A     | 290 | GLN  |
| 1   | A     | 297 | ARG  |
| 1   | A     | 308 | THR  |
| 1   | A     | 311 | LYS  |
| 1   | A     | 314 | LEU  |
| 1   | A     | 321 | LYS  |
| 1   | A     | 322 | LEU  |
| 1   | A     | 329 | LEU  |
| 1   | A     | 354 | ILE  |
| 1   | A     | 360 | LEU  |
| 1   | A     | 371 | ARG  |
| 1   | A     | 372 | ASN  |
| 1   | A     | 381 | ARG  |
| 1   | A     | 382 | LEU  |
| 1   | A     | 386 | GLU  |
| 1   | A     | 405 | LEU  |
| 1   | A     | 408 | MSE  |
| 1   | A     | 416 | ILE  |
| 1   | A     | 457 | ARG  |
| 2   | B     | 380 | MSE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 383 | GLU  |
| 2   | B     | 407 | ILE  |
| 2   | B     | 421 | SER  |
| 2   | B     | 424 | THR  |
| 2   | B     | 425 | GLU  |
| 2   | B     | 439 | THR  |
| 2   | B     | 451 | ILE  |
| 1   | C     | 8   | TYR  |
| 1   | C     | 13  | LEU  |
| 1   | C     | 15  | GLN  |
| 1   | C     | 19  | GLU  |
| 1   | C     | 24  | ASN  |
| 1   | C     | 38  | LEU  |
| 1   | C     | 40  | LEU  |
| 1   | C     | 57  | THR  |
| 1   | C     | 89  | PHE  |
| 1   | C     | 91  | ASP  |
| 1   | C     | 99  | GLU  |
| 1   | C     | 124 | GLN  |
| 1   | C     | 136 | ASP  |
| 1   | C     | 140 | ASP  |
| 1   | C     | 141 | ILE  |
| 1   | C     | 150 | ASP  |
| 1   | C     | 151 | LYS  |
| 1   | C     | 152 | LEU  |
| 1   | C     | 154 | THR  |
| 1   | C     | 162 | ARG  |
| 1   | C     | 163 | LEU  |
| 1   | C     | 165 | THR  |
| 1   | C     | 180 | TYR  |
| 1   | C     | 184 | VAL  |
| 1   | C     | 188 | MSE  |
| 1   | C     | 192 | SER  |
| 1   | C     | 206 | PHE  |
| 1   | C     | 245 | LEU  |
| 1   | C     | 257 | LEU  |
| 1   | C     | 285 | THR  |
| 1   | C     | 288 | LEU  |
| 1   | C     | 294 | GLU  |
| 1   | C     | 313 | SER  |
| 1   | C     | 314 | LEU  |
| 1   | C     | 322 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 325 | GLU  |
| 1   | C     | 336 | VAL  |
| 1   | C     | 382 | LEU  |
| 1   | C     | 384 | TYR  |
| 1   | C     | 391 | VAL  |
| 1   | C     | 411 | VAL  |
| 1   | C     | 414 | SER  |
| 1   | C     | 415 | LEU  |
| 1   | C     | 430 | VAL  |
| 2   | D     | 380 | MSE  |
| 2   | D     | 383 | GLU  |
| 2   | D     | 385 | ARG  |
| 2   | D     | 403 | ARG  |
| 2   | D     | 424 | THR  |
| 2   | D     | 436 | LYS  |
| 2   | D     | 439 | THR  |
| 2   | D     | 451 | ILE  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 11  | ASN  |
| 1   | A     | 21  | ASN  |
| 1   | A     | 65  | ASN  |
| 1   | A     | 72  | ASN  |
| 1   | A     | 149 | ASN  |
| 1   | A     | 269 | GLN  |
| 1   | A     | 333 | GLN  |
| 1   | A     | 348 | HIS  |
| 1   | A     | 359 | ASN  |
| 1   | A     | 387 | GLN  |
| 1   | A     | 389 | GLN  |
| 1   | C     | 24  | ASN  |
| 1   | C     | 122 | ASN  |
| 1   | C     | 124 | GLN  |
| 1   | C     | 177 | ASN  |
| 1   | C     | 239 | ASN  |
| 1   | C     | 250 | ASN  |
| 1   | C     | 276 | ASN  |
| 1   | C     | 290 | GLN  |
| 1   | C     | 331 | ASN  |
| 1   | C     | 333 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 387 | GLN  |
| 1   | C     | 389 | GLN  |
| 1   | C     | 439 | ASN  |
| 1   | C     | 464 | ASN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 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     | 449/500 (89%)   | 0.02   | 11 (2%) 59 41 | 87, 158, 255, 289     | 0     |
| 1   | C     | 446/500 (89%)   | 0.31   | 13 (2%) 53 37 | 102, 156, 216, 274    | 0     |
| 2   | B     | 70/88 (79%)     | 0.12   | 2 (2%) 53 37  | 106, 154, 195, 221    | 0     |
| 2   | D     | 70/88 (79%)     | 0.27   | 2 (2%) 53 37  | 98, 144, 178, 202     | 0     |
| All | All   | 1035/1176 (88%) | 0.17   | 28 (2%) 56 38 | 87, 156, 236, 289     | 0     |

All (28) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 346 | TYR  | 5.0  |
| 1   | A     | 13  | LEU  | 4.1  |
| 1   | C     | 16  | LEU  | 3.4  |
| 1   | A     | 12  | LEU  | 3.1  |
| 1   | A     | 9   | VAL  | 3.0  |
| 1   | A     | 422 | GLY  | 3.0  |
| 1   | C     | 17  | GLU  | 2.9  |
| 1   | A     | 16  | LEU  | 2.9  |
| 1   | A     | 21  | ASN  | 2.9  |
| 1   | A     | 348 | HIS  | 2.9  |
| 2   | D     | 382 | LEU  | 2.5  |
| 1   | C     | 34  | ARG  | 2.5  |
| 1   | C     | 281 | ARG  | 2.3  |
| 1   | C     | 385 | LEU  | 2.3  |
| 1   | C     | 39  | ASN  | 2.3  |
| 1   | C     | 241 | TYR  | 2.3  |
| 2   | B     | 415 | THR  | 2.3  |
| 1   | A     | 10  | GLU  | 2.3  |
| 1   | C     | 296 | SER  | 2.2  |
| 2   | B     | 392 | HIS  | 2.2  |
| 1   | C     | 299 | GLU  | 2.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 389 | GLN  | 2.1  |
| 1   | C     | 31  | THR  | 2.1  |
| 1   | A     | 20  | LEU  | 2.1  |
| 2   | D     | 383 | GLU  | 2.1  |
| 1   | A     | 44  | VAL  | 2.1  |
| 1   | C     | 320 | ALA  | 2.0  |
| 1   | C     | 450 | VAL  | 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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.