



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:40 PM UTC

PDB ID : 1IPK / pdb\_00001ipk  
Title : CRYSTAL STRUCTURES OF RECOMBINANT AND NATIVE SOYBEAN BETA-CONGLYCININ BETA HOMOTRIMERS  
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Deposited on : 2001-05-16  
Resolution : 2.70 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                                             |
| 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                                                             |

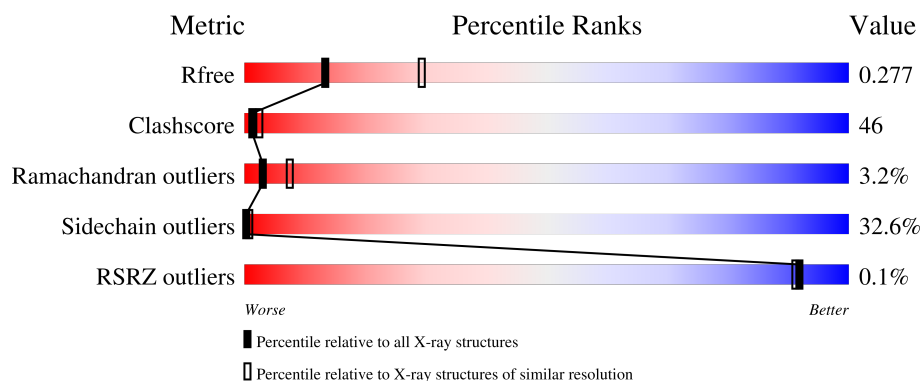
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

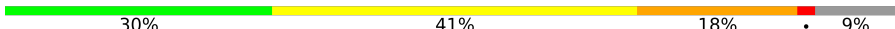
The reported resolution of this entry is 2.70 Å.

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                      | 3538 (2.70-2.70)                                      |
| Clashscore            | 190562                      | 3843 (2.70-2.70)                                      |
| Ramachandran outliers | 187476                      | 3778 (2.70-2.70)                                      |
| Sidechain outliers    | 187428                      | 3778 (2.70-2.70)                                      |
| RSRZ outliers         | 180081                      | 3538 (2.70-2.70)                                      |

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     | 416    |  |
| 1   | B     | 416    |  |
| 1   | C     | 416    |  |

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 9074 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 BETA-CONGLYCININ, BETA CHAIN.

| Mol | Chain | Residues | Atoms |      |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---------|---------|-------|
| 1   | A     | 368      | Total | C    | N   | O   | 0       | 0       | 0     |
|     |       |          | 3001  | 1900 | 534 | 567 |         |         |       |
| 1   | B     | 365      | Total | C    | N   | O   | 0       | 0       | 0     |
|     |       |          | 2977  | 1886 | 529 | 562 |         |         |       |
| 1   | C     | 379      | Total | C    | N   | O   | 0       | 0       | 0     |
|     |       |          | 3096  | 1953 | 552 | 591 |         |         |       |

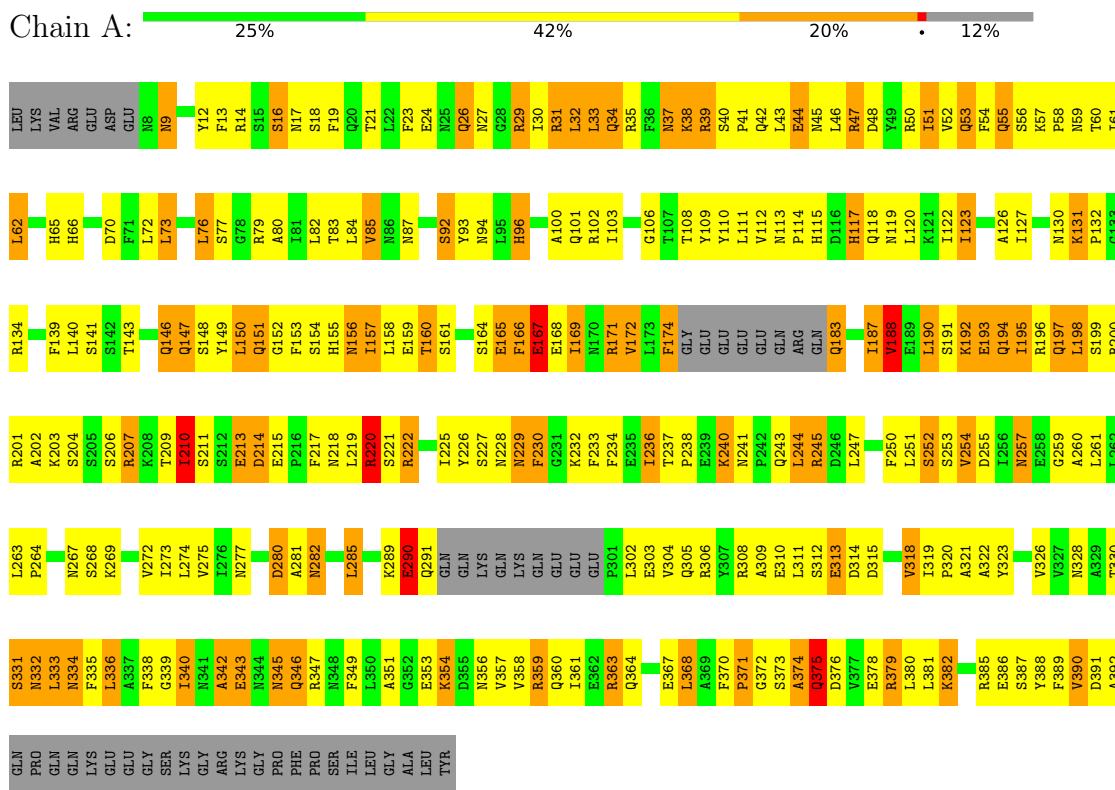
There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| A     | 28      | GLY      | VAL    | conflict | UNP P25974 |
| B     | 28      | GLY      | VAL    | conflict | UNP P25974 |
| C     | 28      | GLY      | VAL    | conflict | UNP P25974 |

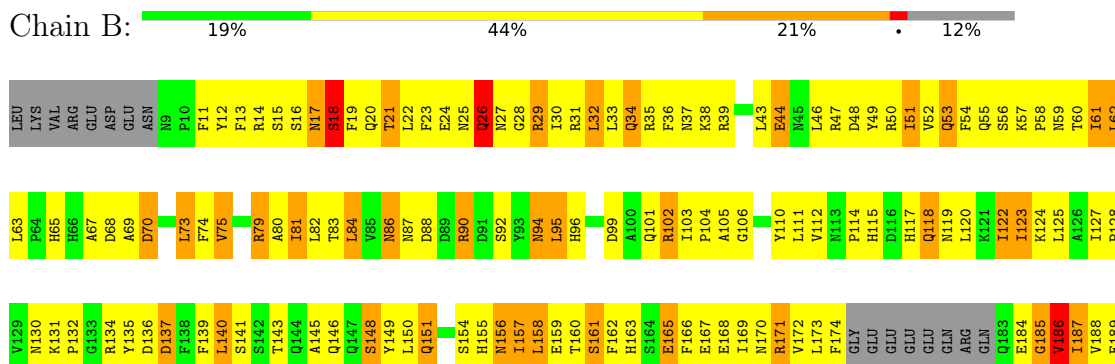
### 3 Residue-property plots

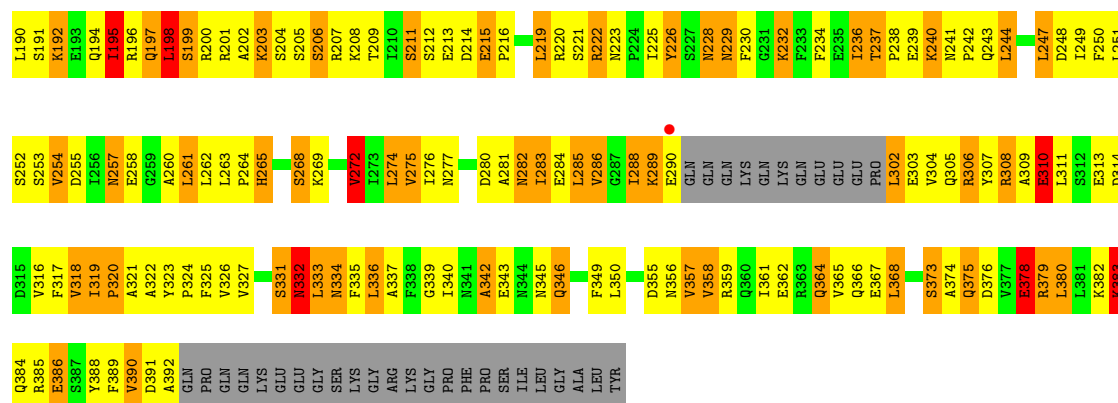
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: BETA-CONGLYCININ, BETA CHAIN

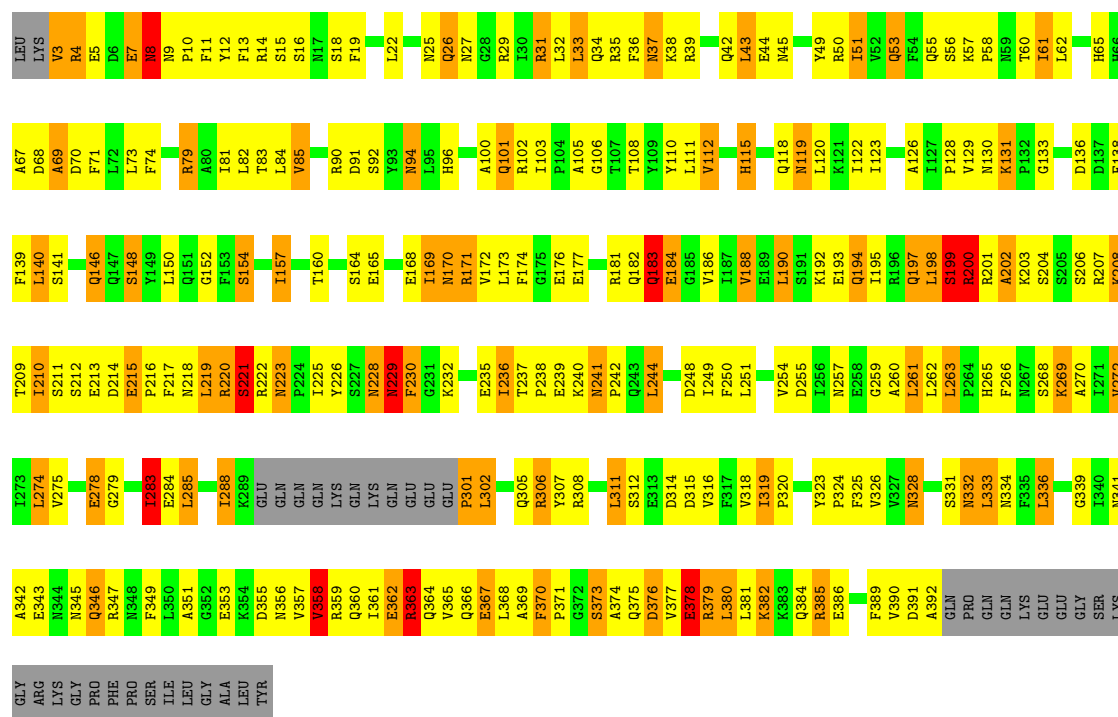


#### • Molecule 1: BETA-CONGLYCININ, BETA CHAIN





● Molecule 1: BETA-CONGLYCININ, BETA CHAIN



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 1 21 1                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 80.51Å 63.48Å 131.43Å<br>90.00° 90.01° 90.00°               | Depositor        |
| Resolution (Å)                                                          | 7.00 – 2.70<br>7.00 – 2.70                                  | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | (Not available) (7.00-2.70)<br>78.2 (7.00-2.70)             | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | 0.06                                                        | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 3.48 (at 2.70Å)                                             | Xtriage          |
| Refinement program                                                      |                                                             | Depositor        |
| R, $R_{free}$                                                           | 0.205 , 0.275<br>0.205 , 0.277                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 3003 reflections (10.16%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 45.1                                                        | Xtriage          |
| Anisotropy                                                              | 0.612                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.32 , 89.4                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$ | Xtriage          |
| Estimated twinning fraction                                             | 0.024 for h,-k,-l                                           | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.93                                                        | EDS              |
| Total number of atoms                                                   | 9074                                                        | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 25.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.71% 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     | 0.49         | 0/3062      | 1.00        | 14/4141 (0.3%)  |
| 1   | B     | 0.46         | 0/3037      | 0.97        | 16/4107 (0.4%)  |
| 1   | C     | 0.48         | 0/3158      | 1.05        | 20/4270 (0.5%)  |
| All | All   | 0.48         | 0/9257      | 1.01        | 50/12518 (0.4%) |

There are no bond length outliers.

All (50) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 1   | C     | 201 | ARG  | N-CA-C | -12.70 | 94.40       | 114.09   |
| 1   | C     | 7   | GLU  | N-CA-C | -9.57  | 102.41      | 114.56   |
| 1   | C     | 200 | ARG  | N-CA-C | 8.12   | 128.09      | 110.80   |
| 1   | A     | 342 | ALA  | N-CA-C | 7.49   | 122.54      | 112.88   |
| 1   | B     | 366 | GLN  | N-CA-C | -7.30  | 103.32      | 111.71   |
| 1   | B     | 272 | VAL  | N-CA-C | 7.06   | 119.23      | 108.71   |
| 1   | B     | 342 | ALA  | N-CA-C | 6.93   | 121.91      | 113.38   |
| 1   | C     | 378 | GLU  | N-CA-C | -6.92  | 104.09      | 112.54   |
| 1   | C     | 27  | ASN  | N-CA-C | 6.79   | 118.76      | 111.36   |
| 1   | C     | 202 | ALA  | N-CA-C | 6.75   | 119.27      | 110.43   |
| 1   | A     | 272 | VAL  | N-CA-C | 6.74   | 117.61      | 108.17   |
| 1   | C     | 8   | ASN  | N-CA-C | -6.72  | 105.06      | 112.72   |
| 1   | C     | 69  | ALA  | N-CA-C | 6.71   | 118.72      | 108.52   |
| 1   | A     | 9   | ASN  | CA-C-N | 6.67   | 128.18      | 119.84   |
| 1   | A     | 9   | ASN  | C-N-CA | 6.67   | 128.18      | 119.84   |
| 1   | B     | 254 | VAL  | N-CA-C | 6.58   | 117.35      | 107.80   |
| 1   | A     | 150 | LEU  | N-CA-C | -6.55  | 104.93      | 113.12   |
| 1   | B     | 241 | ASN  | CA-C-N | 6.54   | 126.47      | 119.28   |
| 1   | B     | 241 | ASN  | C-N-CA | 6.54   | 126.47      | 119.28   |
| 1   | C     | 283 | ILE  | N-CA-C | 6.46   | 117.79      | 108.48   |
| 1   | A     | 33  | LEU  | N-CA-C | -6.44  | 100.08      | 110.32   |
| 1   | A     | 375 | GLN  | N-CA-C | -6.42  | 106.07      | 114.04   |
| 1   | B     | 383 | LYS  | N-CA-C | -6.31  | 101.43      | 111.02   |
| 1   | B     | 199 | SER  | N-CA-C | 6.16   | 121.12      | 112.93   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | C     | 223 | ASN  | N-CA-C  | 6.10  | 118.85      | 110.01   |
| 1   | A     | 193 | GLU  | N-CA-C  | -6.09 | 104.27      | 111.03   |
| 1   | C     | 272 | VAL  | N-CA-C  | 6.01  | 116.59      | 108.17   |
| 1   | C     | 199 | SER  | N-CA-C  | 5.95  | 123.47      | 110.80   |
| 1   | B     | 18  | SER  | N-CA-C  | 5.87  | 119.69      | 111.30   |
| 1   | B     | 310 | GLU  | N-CA-C  | -5.85 | 100.95      | 110.20   |
| 1   | C     | 241 | ASN  | CA-C-N  | 5.78  | 125.25      | 119.24   |
| 1   | C     | 241 | ASN  | C-N-CA  | 5.78  | 125.25      | 119.24   |
| 1   | B     | 62  | LEU  | N-CA-C  | -5.75 | 101.11      | 110.20   |
| 1   | B     | 118 | GLN  | N-CA-C  | 5.73  | 117.87      | 108.52   |
| 1   | B     | 206 | SER  | N-CA-C  | 5.62  | 115.66      | 108.24   |
| 1   | A     | 207 | ARG  | N-CA-C  | -5.61 | 106.47      | 113.38   |
| 1   | B     | 248 | ASP  | N-CA-C  | -5.58 | 104.38      | 110.91   |
| 1   | A     | 247 | LEU  | N-CA-C  | -5.51 | 106.41      | 114.39   |
| 1   | B     | 237 | THR  | N-CA-C  | 5.47  | 119.01      | 109.82   |
| 1   | C     | 215 | GLU  | N-CA-C  | 5.46  | 118.58      | 110.39   |
| 1   | C     | 183 | GLN  | N-CA-C  | -5.46 | 101.68      | 110.14   |
| 1   | A     | 345 | ASN  | N-CA-C  | -5.35 | 103.83      | 110.41   |
| 1   | A     | 151 | GLN  | N-CA-C  | -5.30 | 104.97      | 111.75   |
| 1   | A     | 290 | GLU  | N-CA-C  | 5.25  | 117.99      | 108.69   |
| 1   | C     | 194 | GLN  | N-CA-C  | -5.25 | 105.25      | 110.97   |
| 1   | C     | 301 | PRO  | N-CA-CB | 5.24  | 108.76      | 103.00   |
| 1   | C     | 279 | GLY  | N-CA-C  | 5.19  | 118.32      | 111.52   |
| 1   | B     | 186 | VAL  | N-CA-C  | 5.11  | 119.50      | 113.22   |
| 1   | A     | 188 | VAL  | N-CA-C  | 5.06  | 116.58      | 108.89   |
| 1   | C     | 131 | LYS  | N-CA-C  | -5.02 | 103.36      | 110.29   |

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     | 3001  | 0        | 2945     | 275     | 0            |
| 1   | B     | 2977  | 0        | 2923     | 347     | 0            |
| 1   | C     | 3096  | 0        | 3026     | 270     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| All | All   | 9074  | 0        | 8894     | 833     | 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 46.

All (833) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:14:ARG:HB3   | 1:B:17:ASN:HB2   | 1.30                     | 1.09              |
| 1:A:379:ARG:HH11 | 1:A:379:ARG:HB3  | 1.20                     | 1.06              |
| 1:B:22:LEU:HD12  | 1:B:30:ILE:HG22  | 1.37                     | 1.06              |
| 1:C:359:ARG:HH22 | 1:C:382:LYS:HE3  | 1.20                     | 1.04              |
| 1:B:222:ARG:HH21 | 1:B:240:LYS:HD3  | 1.26                     | 0.99              |
| 1:C:220:ARG:HG2  | 1:C:220:ARG:HH11 | 1.24                     | 0.99              |
| 1:A:367:GLU:HB2  | 1:A:374:ALA:HB2  | 1.44                     | 0.99              |
| 1:B:24:GLU:HG3   | 1:B:29:ARG:HB3   | 1.45                     | 0.98              |
| 1:C:284:GLU:HG2  | 1:C:308:ARG:HG3  | 1.45                     | 0.98              |
| 1:A:29:ARG:HH11  | 1:A:55:GLN:HE22  | 1.10                     | 0.97              |
| 1:B:61:ILE:HG13  | 1:B:112:VAL:HG22 | 1.46                     | 0.94              |
| 1:C:270:ALA:H    | 1:C:345:ASN:ND2  | 1.68                     | 0.90              |
| 1:A:115:HIS:HD2  | 1:A:117:HIS:H    | 1.19                     | 0.89              |
| 1:C:184:GLU:O    | 1:C:184:GLU:HG2  | 1.71                     | 0.89              |
| 1:C:79:ARG:HH21  | 1:C:94:ASN:HD21  | 1.13                     | 0.88              |
| 1:C:29:ARG:HH21  | 1:C:55:GLN:HE22  | 1.21                     | 0.88              |
| 1:B:275:VAL:HG12 | 1:B:316:VAL:HG22 | 1.55                     | 0.88              |
| 1:B:158:LEU:HD23 | 1:B:162:PHE:HE2  | 1.38                     | 0.88              |
| 1:C:79:ARG:NH2   | 1:C:94:ASN:HD21  | 1.70                     | 0.88              |
| 1:B:22:LEU:HD21  | 1:B:32:LEU:HB2   | 1.56                     | 0.88              |
| 1:B:284:GLU:HB2  | 1:B:326:VAL:HG12 | 1.56                     | 0.87              |
| 1:C:261:LEU:HB2  | 1:C:328:ASN:ND2  | 1.90                     | 0.86              |
| 1:C:268:SER:HB3  | 1:C:346:GLN:H    | 1.41                     | 0.85              |
| 1:B:94:ASN:HB2   | 1:B:203:LYS:O    | 1.78                     | 0.84              |
| 1:C:197:GLN:HE21 | 1:C:197:GLN:HA   | 1.42                     | 0.84              |
| 1:B:115:HIS:CD2  | 1:B:118:GLN:H    | 1.95                     | 0.84              |
| 1:B:79:ARG:HG2   | 1:B:79:ARG:HH11  | 1.40                     | 0.84              |
| 1:B:140:LEU:O    | 1:B:148:SER:HB2  | 1.77                     | 0.84              |
| 1:C:379:ARG:HG3  | 1:C:380:LEU:N    | 1.93                     | 0.83              |
| 1:B:281:ALA:HB2  | 1:B:333:LEU:HD13 | 1.60                     | 0.83              |
| 1:C:261:LEU:HB2  | 1:C:328:ASN:HD22 | 1.38                     | 0.83              |
| 1:A:85:VAL:HG22  | 1:A:108:THR:HB   | 1.60                     | 0.83              |
| 1:C:207:ARG:NH1  | 1:C:222:ARG:HD3  | 1.92                     | 0.83              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:33:LEU:HD12  | 1:C:34:GLN:H     | 1.42                     | 0.83              |
| 1:C:33:LEU:HD12  | 1:C:34:GLN:N     | 1.94                     | 0.83              |
| 1:B:25:ASN:HD21  | 1:B:187:ILE:HB   | 1.42                     | 0.82              |
| 1:C:359:ARG:NH2  | 1:C:382:LYS:HE3  | 1.93                     | 0.82              |
| 1:A:306:ARG:HD3  | 1:C:152:GLY:O    | 1.80                     | 0.82              |
| 1:A:29:ARG:HH11  | 1:A:55:GLN:NE2   | 1.78                     | 0.82              |
| 1:C:288:ILE:HG21 | 1:C:302:LEU:HD22 | 1.62                     | 0.81              |
| 1:A:29:ARG:HD3   | 1:A:55:GLN:HE21  | 1.43                     | 0.81              |
| 1:B:75:VAL:HG12  | 1:B:122:ILE:HD11 | 1.62                     | 0.81              |
| 1:B:230:PHE:CE1  | 1:B:391:ASP:HB2  | 2.15                     | 0.81              |
| 1:C:33:LEU:HD22  | 1:C:316:VAL:HG21 | 1.61                     | 0.81              |
| 1:C:123:ILE:HG21 | 1:C:336:LEU:CD2  | 2.10                     | 0.81              |
| 1:A:47:ARG:HG3   | 1:A:48:ASP:OD1   | 1.82                     | 0.80              |
| 1:B:285:LEU:HD23 | 1:B:325:PHE:HB3  | 1.62                     | 0.79              |
| 1:C:220:ARG:HG2  | 1:C:220:ARG:NH1  | 1.96                     | 0.79              |
| 1:B:258:GLU:HB2  | 1:B:332:ASN:H    | 1.45                     | 0.79              |
| 1:C:123:ILE:HG21 | 1:C:336:LEU:HD21 | 1.64                     | 0.79              |
| 1:A:43:LEU:HD22  | 1:A:318:VAL:HG21 | 1.64                     | 0.79              |
| 1:C:250:PHE:CE1  | 1:C:339:GLY:HA3  | 2.18                     | 0.79              |
| 1:B:92:SER:O     | 1:B:202:ALA:HA   | 1.83                     | 0.79              |
| 1:B:220:ARG:HH22 | 1:B:255:ASP:CG   | 1.90                     | 0.79              |
| 1:B:115:HIS:HD2  | 1:B:118:GLN:H    | 1.30                     | 0.78              |
| 1:C:380:LEU:HD12 | 1:C:381:LEU:HG   | 1.63                     | 0.78              |
| 1:A:115:HIS:CD2  | 1:A:118:GLN:H    | 2.00                     | 0.78              |
| 1:A:225:ILE:HG13 | 1:A:226:TYR:H    | 1.49                     | 0.78              |
| 1:C:61:ILE:HG22  | 1:C:188:VAL:HG22 | 1.65                     | 0.78              |
| 1:B:219:LEU:HD11 | 1:B:234:PHE:HB3  | 1.66                     | 0.78              |
| 1:B:115:HIS:CD2  | 1:B:117:HIS:H    | 2.02                     | 0.78              |
| 1:A:321:ALA:HB3  | 1:C:130:ASN:HD21 | 1.47                     | 0.78              |
| 1:A:166:PHE:O    | 1:A:169:ILE:HG12 | 1.84                     | 0.78              |
| 1:C:380:LEU:CD1  | 1:C:381:LEU:HG   | 2.14                     | 0.77              |
| 1:A:373:SER:C    | 1:A:375:GLN:H    | 1.89                     | 0.77              |
| 1:B:14:ARG:HB3   | 1:B:17:ASN:CB    | 2.11                     | 0.77              |
| 1:B:61:ILE:HB    | 1:B:190:LEU:HD13 | 1.65                     | 0.77              |
| 1:A:61:ILE:HG13  | 1:A:112:VAL:HG22 | 1.67                     | 0.77              |
| 1:B:222:ARG:HH21 | 1:B:240:LYS:CD   | 1.98                     | 0.77              |
| 1:A:222:ARG:HH22 | 1:A:240:LYS:HG2  | 1.49                     | 0.76              |
| 1:B:166:PHE:O    | 1:B:169:ILE:HG12 | 1.85                     | 0.76              |
| 1:A:379:ARG:HB3  | 1:A:379:ARG:NH1  | 1.98                     | 0.76              |
| 1:A:26:GLN:HG2   | 1:A:27:ASN:ND2   | 2.01                     | 0.76              |
| 1:B:60:THR:HA    | 1:B:189:GLU:HA   | 1.65                     | 0.76              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:74:PHE:CE1   | 1:B:336:LEU:HD13 | 2.20                     | 0.76              |
| 1:C:250:PHE:CD1  | 1:C:339:GLY:HA3  | 2.21                     | 0.76              |
| 1:B:236:ILE:HD13 | 1:B:240:LYS:HB3  | 1.69                     | 0.75              |
| 1:B:228:ASN:OD1  | 1:B:389:PHE:HB2  | 1.86                     | 0.75              |
| 1:B:382:LYS:HE2  | 1:B:385:ARG:HH21 | 1.51                     | 0.75              |
| 1:B:21:THR:HA    | 1:B:31:ARG:HG2   | 1.67                     | 0.75              |
| 1:C:79:ARG:HH21  | 1:C:94:ASN:ND2   | 1.85                     | 0.75              |
| 1:C:226:TYR:OH   | 1:C:347:ARG:HD2  | 1.87                     | 0.74              |
| 1:B:169:ILE:HG22 | 1:C:380:LEU:HD21 | 1.68                     | 0.74              |
| 1:A:237:THR:HB   | 1:A:238:PRO:CD   | 2.18                     | 0.74              |
| 1:C:74:PHE:CD1   | 1:C:336:LEU:HD13 | 2.23                     | 0.74              |
| 1:C:176:GLU:O    | 1:C:177:GLU:HB2  | 1.87                     | 0.74              |
| 1:A:32:LEU:HD23  | 1:A:52:VAL:HG22  | 1.68                     | 0.74              |
| 1:A:115:HIS:CD2  | 1:A:117:HIS:H    | 2.06                     | 0.73              |
| 1:B:373:SER:HB3  | 1:B:376:ASP:OD2  | 1.88                     | 0.73              |
| 1:A:33:LEU:O     | 1:A:50:ARG:NH2   | 2.21                     | 0.73              |
| 1:B:115:HIS:HD2  | 1:B:117:HIS:H    | 1.36                     | 0.73              |
| 1:A:222:ARG:HH21 | 1:A:236:ILE:HG12 | 1.53                     | 0.73              |
| 1:A:282:ASN:ND2  | 1:A:328:ASN:HB3  | 2.03                     | 0.72              |
| 1:B:222:ARG:NH2  | 1:B:240:LYS:HD3  | 2.02                     | 0.72              |
| 1:A:225:ILE:HD11 | 1:A:233:PHE:CD1  | 2.25                     | 0.72              |
| 1:A:361:ILE:HG23 | 1:C:110:TYR:HE1  | 1.53                     | 0.72              |
| 1:B:32:LEU:HD11  | 1:B:135:TYR:HE1  | 1.54                     | 0.72              |
| 1:B:155:HIS:O    | 1:B:159:GLU:HB2  | 1.88                     | 0.72              |
| 1:A:193:GLU:HG3  | 1:A:197:GLN:HE22 | 1.54                     | 0.72              |
| 1:A:149:TYR:HE1  | 1:B:350:LEU:HD11 | 1.55                     | 0.72              |
| 1:B:33:LEU:HD23  | 1:B:34:GLN:O     | 1.89                     | 0.72              |
| 1:C:141:SER:OG   | 1:C:146:GLN:NE2  | 2.23                     | 0.72              |
| 1:C:270:ALA:N    | 1:C:345:ASN:ND2  | 2.38                     | 0.72              |
| 1:A:259:GLY:O    | 1:A:392:ALA:HB3  | 1.90                     | 0.71              |
| 1:A:160:THR:CG2  | 1:B:392:ALA:HA   | 2.19                     | 0.71              |
| 1:B:25:ASN:OD1   | 1:B:27:ASN:N     | 2.23                     | 0.71              |
| 1:B:65:HIS:HB3   | 1:B:139:PHE:CD2  | 2.25                     | 0.71              |
| 1:B:228:ASN:HD21 | 1:B:230:PHE:HD2  | 1.37                     | 0.71              |
| 1:C:218:ASN:HB3  | 1:C:221:SER:HB2  | 1.72                     | 0.71              |
| 1:B:156:ASN:ND2  | 1:B:156:ASN:H    | 1.85                     | 0.71              |
| 1:B:170:ASN:HD22 | 1:B:174:PHE:HD1  | 1.39                     | 0.71              |
| 1:C:382:LYS:HE2  | 1:C:385:ARG:NE   | 2.05                     | 0.71              |
| 1:B:258:GLU:HB2  | 1:B:332:ASN:N    | 2.05                     | 0.70              |
| 1:B:197:GLN:HE21 | 1:B:197:GLN:N    | 1.89                     | 0.70              |
| 1:C:207:ARG:HH11 | 1:C:222:ARG:HD3  | 1.56                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:367:GLU:OE1  | 1:C:373:SER:HA   | 1.91                     | 0.70              |
| 1:C:193:GLU:O    | 1:C:197:GLN:HG2  | 1.91                     | 0.70              |
| 1:C:207:ARG:HH11 | 1:C:222:ARG:CD   | 2.05                     | 0.70              |
| 1:A:156:ASN:HD22 | 1:A:156:ASN:H    | 1.40                     | 0.70              |
| 1:C:29:ARG:HH21  | 1:C:55:GLN:NE2   | 1.89                     | 0.70              |
| 1:C:220:ARG:HH22 | 1:C:255:ASP:CG   | 2.00                     | 0.70              |
| 1:A:29:ARG:NH1   | 1:A:55:GLN:HE22  | 1.86                     | 0.70              |
| 1:A:263:LEU:HD21 | 1:A:390:VAL:HG11 | 1.73                     | 0.70              |
| 1:B:32:LEU:CD2   | 1:B:52:VAL:HG22  | 2.22                     | 0.70              |
| 1:C:269:LYS:H    | 1:C:345:ASN:ND2  | 1.89                     | 0.70              |
| 1:A:263:LEU:HD13 | 1:A:351:ALA:HB3  | 1.73                     | 0.69              |
| 1:B:222:ARG:CB   | 1:B:222:ARG:HH11 | 2.05                     | 0.69              |
| 1:C:357:VAL:HG13 | 1:C:358:VAL:H    | 1.57                     | 0.69              |
| 1:B:367:GLU:OE2  | 1:B:374:ALA:HB2  | 1.92                     | 0.69              |
| 1:A:238:PRO:O    | 1:A:245:ARG:HB2  | 1.93                     | 0.69              |
| 1:B:158:LEU:HD23 | 1:B:162:PHE:CE2  | 2.24                     | 0.69              |
| 1:B:59:ASN:HA    | 1:B:195:ILE:HD11 | 1.73                     | 0.69              |
| 1:B:166:PHE:CE2  | 1:B:170:ASN:HB2  | 2.28                     | 0.69              |
| 1:C:363:ARG:HD3  | 1:C:374:ALA:HB1  | 1.75                     | 0.68              |
| 1:A:168:GLU:O    | 1:A:172:VAL:HG23 | 1.92                     | 0.68              |
| 1:B:143:THR:HG21 | 1:B:185:GLY:O    | 1.93                     | 0.68              |
| 1:B:75:VAL:CG1   | 1:B:122:ILE:HD11 | 2.23                     | 0.68              |
| 1:B:265:HIS:HB3  | 1:B:349:PHE:CD1  | 2.28                     | 0.68              |
| 1:A:220:ARG:NH2  | 1:A:255:ASP:OD1  | 2.27                     | 0.68              |
| 1:A:285:LEU:HD21 | 1:A:323:TYR:HB3  | 1.75                     | 0.68              |
| 1:A:263:LEU:HD22 | 1:A:264:PRO:HD2  | 1.74                     | 0.68              |
| 1:C:208:LYS:O    | 1:C:208:LYS:HG3  | 1.94                     | 0.68              |
| 1:C:384:GLN:HE21 | 1:C:386:GLU:H    | 1.42                     | 0.68              |
| 1:C:119:ASN:HD22 | 1:C:119:ASN:H    | 1.42                     | 0.68              |
| 1:B:79:ARG:HH11  | 1:B:79:ARG:CG    | 2.07                     | 0.67              |
| 1:A:160:THR:HG21 | 1:B:392:ALA:CB   | 2.25                     | 0.67              |
| 1:A:358:VAL:HG12 | 1:A:381:LEU:HD11 | 1.77                     | 0.67              |
| 1:B:234:PHE:HB2  | 1:B:253:SER:O    | 1.95                     | 0.67              |
| 1:C:380:LEU:HD13 | 1:C:380:LEU:C    | 2.20                     | 0.66              |
| 1:B:222:ARG:HH11 | 1:B:222:ARG:HB2  | 1.59                     | 0.66              |
| 1:A:390:VAL:CG2  | 1:A:391:ASP:N    | 2.58                     | 0.66              |
| 1:C:190:LEU:HB3  | 1:C:194:GLN:NE2  | 2.11                     | 0.66              |
| 1:A:13:PHE:CE1   | 1:A:39:ARG:HG3   | 2.30                     | 0.66              |
| 1:C:13:PHE:HB2   | 1:C:316:VAL:HB   | 1.78                     | 0.66              |
| 1:B:55:GLN:HA    | 1:B:120:LEU:O    | 1.96                     | 0.66              |
| 1:A:359:ARG:O    | 1:A:359:ARG:HG2  | 1.95                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:313:GLU:O    | 1:A:314:ASP:HB2  | 1.95                     | 0.65              |
| 1:B:203:LYS:HZ1  | 1:B:215:GLU:CD   | 2.04                     | 0.65              |
| 1:B:274:LEU:HD21 | 1:B:317:PHE:HB3  | 1.78                     | 0.65              |
| 1:A:191:SER:H    | 1:A:194:GLN:HG3  | 1.61                     | 0.65              |
| 1:C:284:GLU:CG   | 1:C:308:ARG:HG3  | 2.24                     | 0.65              |
| 1:A:160:THR:HG21 | 1:B:392:ALA:HA   | 1.78                     | 0.65              |
| 1:C:270:ALA:N    | 1:C:345:ASN:HD22 | 1.94                     | 0.65              |
| 1:B:25:ASN:O     | 1:B:27:ASN:N     | 2.29                     | 0.65              |
| 1:C:115:HIS:HD2  | 1:C:118:GLN:HB3  | 1.62                     | 0.65              |
| 1:B:228:ASN:O    | 1:B:230:PHE:N    | 2.30                     | 0.65              |
| 1:C:230:PHE:CE1  | 1:C:391:ASP:HB2  | 2.32                     | 0.65              |
| 1:C:101:GLN:HG3  | 1:C:102:ARG:N    | 2.12                     | 0.64              |
| 1:A:390:VAL:HG23 | 1:A:391:ASP:N    | 2.13                     | 0.64              |
| 1:B:283:ILE:HG21 | 1:B:317:PHE:CE1  | 2.32                     | 0.64              |
| 1:A:306:ARG:HH12 | 1:C:154:SER:HA   | 1.61                     | 0.64              |
| 1:B:333:LEU:HG   | 1:B:334:ASN:N    | 2.12                     | 0.64              |
| 1:B:243:GLN:O    | 1:B:247:LEU:HD12 | 1.97                     | 0.64              |
| 1:A:85:VAL:CG2   | 1:A:108:THR:HB   | 2.28                     | 0.64              |
| 1:C:12:TYR:CE2   | 1:C:311:LEU:HD23 | 2.32                     | 0.64              |
| 1:C:349:PHE:O    | 1:C:356:ASN:HA   | 1.98                     | 0.64              |
| 1:B:82:LEU:HD21  | 1:B:103:ILE:HD11 | 1.78                     | 0.64              |
| 1:B:75:VAL:HA    | 1:B:122:ILE:HG12 | 1.79                     | 0.64              |
| 1:B:284:GLU:O    | 1:B:325:PHE:HA   | 1.98                     | 0.64              |
| 1:B:21:THR:HA    | 1:B:31:ARG:CG    | 2.28                     | 0.64              |
| 1:B:96:HIS:O     | 1:B:99:ASP:HB2   | 1.98                     | 0.63              |
| 1:A:115:HIS:HD2  | 1:A:118:GLN:H    | 1.44                     | 0.63              |
| 1:B:250:PHE:CE1  | 1:B:339:GLY:HA3  | 2.34                     | 0.63              |
| 1:A:46:LEU:HD21  | 1:A:340:ILE:HG13 | 1.80                     | 0.63              |
| 1:C:33:LEU:HD23  | 1:C:51:ILE:HB    | 1.81                     | 0.62              |
| 1:C:190:LEU:HB3  | 1:C:194:GLN:HE21 | 1.62                     | 0.62              |
| 1:B:236:ILE:CD1  | 1:B:240:LYS:HB3  | 2.29                     | 0.62              |
| 1:B:254:VAL:O    | 1:B:334:ASN:HA   | 1.99                     | 0.62              |
| 1:B:275:VAL:CG1  | 1:B:316:VAL:HG22 | 2.27                     | 0.62              |
| 1:B:25:ASN:C     | 1:B:27:ASN:H     | 2.08                     | 0.62              |
| 1:A:281:ALA:HB2  | 1:A:333:LEU:HD13 | 1.81                     | 0.62              |
| 1:A:392:ALA:HA   | 1:C:160:THR:CG2  | 2.29                     | 0.62              |
| 1:C:363:ARG:HH11 | 1:C:374:ALA:HB1  | 1.64                     | 0.62              |
| 1:B:25:ASN:ND2   | 1:B:187:ILE:HB   | 2.14                     | 0.62              |
| 1:B:283:ILE:O    | 1:B:308:ARG:HG3  | 1.99                     | 0.62              |
| 1:B:220:ARG:NH2  | 1:B:255:ASP:OD2  | 2.30                     | 0.62              |
| 1:C:37:ASN:N     | 1:C:37:ASN:HD22  | 1.96                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:382:LYS:HE2  | 1:B:385:ARG:NH2  | 2.14                     | 0.61              |
| 1:A:390:VAL:HG23 | 1:A:391:ASP:H    | 1.64                     | 0.61              |
| 1:C:356:ASN:HD22 | 1:C:359:ARG:HB2  | 1.65                     | 0.61              |
| 1:C:85:VAL:HG22  | 1:C:108:THR:HB   | 1.83                     | 0.61              |
| 1:A:12:TYR:HE2   | 1:A:311:LEU:HD23 | 1.66                     | 0.61              |
| 1:C:217:PHE:CD2  | 1:C:236:ILE:HD12 | 2.36                     | 0.61              |
| 1:A:26:GLN:HG2   | 1:A:27:ASN:HD22  | 1.64                     | 0.61              |
| 1:A:37:ASN:HD22  | 1:A:37:ASN:H     | 1.48                     | 0.61              |
| 1:A:32:LEU:HD13  | 1:A:50:ARG:CZ    | 2.29                     | 0.61              |
| 1:A:361:ILE:HG23 | 1:C:110:TYR:CE1  | 2.35                     | 0.61              |
| 1:A:29:ARG:CD    | 1:A:55:GLN:HE21  | 2.13                     | 0.61              |
| 1:A:222:ARG:NH2  | 1:A:240:LYS:HG2  | 2.15                     | 0.61              |
| 1:B:331:SER:O    | 1:B:332:ASN:C    | 2.44                     | 0.61              |
| 1:C:274:LEU:HD12 | 1:C:274:LEU:C    | 2.26                     | 0.61              |
| 1:A:387:SER:O    | 1:A:389:PHE:N    | 2.34                     | 0.60              |
| 1:A:35:ARG:NH1   | 1:A:134:ARG:HD3  | 2.16                     | 0.60              |
| 1:B:74:PHE:CD1   | 1:B:336:LEU:HD13 | 2.36                     | 0.60              |
| 1:B:274:LEU:CD2  | 1:B:317:PHE:HB3  | 2.31                     | 0.60              |
| 1:B:285:LEU:O    | 1:B:306:ARG:HA   | 2.01                     | 0.60              |
| 1:A:169:ILE:HG22 | 1:B:380:LEU:HD11 | 1.81                     | 0.60              |
| 1:B:319:ILE:HG21 | 1:B:325:PHE:CD1  | 2.37                     | 0.60              |
| 1:A:225:ILE:HD12 | 1:A:226:TYR:CE1  | 2.36                     | 0.60              |
| 1:A:230:PHE:HB3  | 1:A:260:ALA:HB2  | 1.82                     | 0.60              |
| 1:A:237:THR:HB   | 1:A:238:PRO:HD2  | 1.82                     | 0.60              |
| 1:A:289:LYS:HD3  | 1:A:303:GLU:OE1  | 2.02                     | 0.59              |
| 1:B:191:SER:HB2  | 1:B:194:GLN:HE21 | 1.67                     | 0.59              |
| 1:A:311:LEU:HD22 | 1:A:315:ASP:HB3  | 1.84                     | 0.59              |
| 1:B:65:HIS:HD2   | 1:B:137:ASP:OD1  | 1.85                     | 0.59              |
| 1:B:258:GLU:H    | 1:B:332:ASN:ND2  | 2.00                     | 0.59              |
| 1:C:215:GLU:HB3  | 1:C:216:PRO:HD2  | 1.85                     | 0.59              |
| 1:C:229:ASN:HB3  | 1:C:230:PHE:CE2  | 2.38                     | 0.59              |
| 1:A:359:ARG:O    | 1:A:359:ARG:CG   | 2.50                     | 0.59              |
| 1:B:237:THR:HB   | 1:B:238:PRO:HD2  | 1.83                     | 0.59              |
| 1:A:289:LYS:HB2  | 1:A:303:GLU:HB3  | 1.83                     | 0.59              |
| 1:B:80:ALA:HB2   | 1:B:120:LEU:HD22 | 1.84                     | 0.59              |
| 1:A:127:ILE:O    | 1:A:127:ILE:HG22 | 2.03                     | 0.59              |
| 1:C:225:ILE:HD13 | 1:C:235:GLU:HB3  | 1.84                     | 0.59              |
| 1:A:130:ASN:HD21 | 1:B:321:ALA:H    | 1.49                     | 0.59              |
| 1:A:225:ILE:HG13 | 1:A:226:TYR:N    | 2.17                     | 0.59              |
| 1:A:373:SER:C    | 1:A:375:GLN:N    | 2.57                     | 0.59              |
| 1:B:225:ILE:HG13 | 1:B:226:TYR:H    | 1.68                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:228:ASN:ND2  | 1:B:230:PHE:HD2  | 2.01                     | 0.59              |
| 1:B:262:LEU:O    | 1:B:326:VAL:HG23 | 2.02                     | 0.59              |
| 1:C:74:PHE:HB3   | 1:C:123:ILE:HG22 | 1.84                     | 0.59              |
| 1:A:32:LEU:CD2   | 1:A:52:VAL:HG22  | 2.32                     | 0.59              |
| 1:C:50:ARG:HD3   | 1:C:133:GLY:O    | 2.02                     | 0.59              |
| 1:C:71:PHE:HE2   | 1:C:126:ALA:HB2  | 1.68                     | 0.59              |
| 1:C:379:ARG:HG3  | 1:C:380:LEU:H    | 1.64                     | 0.59              |
| 1:C:57:LYS:HE2   | 1:C:58:PRO:HD2   | 1.83                     | 0.59              |
| 1:B:32:LEU:HD23  | 1:B:52:VAL:HG22  | 1.84                     | 0.59              |
| 1:B:51:ILE:CG2   | 1:B:123:ILE:HD11 | 2.33                     | 0.58              |
| 1:B:163:HIS:HB2  | 1:C:384:GLN:HB2  | 1.85                     | 0.58              |
| 1:B:84:LEU:HD21  | 1:B:103:ILE:HG12 | 1.85                     | 0.58              |
| 1:C:57:LYS:CE    | 1:C:58:PRO:HD2   | 2.34                     | 0.58              |
| 1:B:59:ASN:ND2   | 1:B:115:HIS:O    | 2.35                     | 0.58              |
| 1:B:101:GLN:OE1  | 1:B:216:PRO:HB3  | 2.04                     | 0.58              |
| 1:C:139:PHE:CZ   | 1:C:186:VAL:HG11 | 2.38                     | 0.58              |
| 1:A:254:VAL:O    | 1:A:334:ASN:HA   | 2.02                     | 0.58              |
| 1:B:169:ILE:HG13 | 1:B:170:ASN:N    | 2.18                     | 0.58              |
| 1:A:161:SER:O    | 1:B:384:GLN:HG2  | 2.03                     | 0.58              |
| 1:A:281:ALA:CB   | 1:A:333:LEU:HD13 | 2.34                     | 0.58              |
| 1:B:170:ASN:HA   | 1:B:174:PHE:CD1  | 2.38                     | 0.58              |
| 1:B:304:VAL:CG1  | 1:B:305:GLN:N    | 2.66                     | 0.58              |
| 1:A:281:ALA:HA   | 1:A:330:THR:HG23 | 1.84                     | 0.58              |
| 1:B:173:LEU:C    | 1:C:371:PRO:HD2  | 2.29                     | 0.58              |
| 1:B:306:ARG:HG2  | 1:B:307:TYR:N    | 2.19                     | 0.58              |
| 1:B:115:HIS:CD2  | 1:B:118:GLN:N    | 2.69                     | 0.57              |
| 1:C:230:PHE:N    | 1:C:230:PHE:CD2  | 2.71                     | 0.57              |
| 1:A:23:PHE:CZ    | 1:A:139:PHE:HE1  | 2.22                     | 0.57              |
| 1:A:35:ARG:NH2   | 1:A:132:PRO:O    | 2.37                     | 0.57              |
| 1:B:283:ILE:CD1  | 1:B:327:VAL:HG22 | 2.33                     | 0.57              |
| 1:C:283:ILE:HG21 | 1:C:311:LEU:HD11 | 1.85                     | 0.57              |
| 1:C:349:PHE:HB2  | 1:C:355:ASP:O    | 2.03                     | 0.57              |
| 1:A:250:PHE:C    | 1:A:250:PHE:CD2  | 2.82                     | 0.57              |
| 1:A:331:SER:O    | 1:A:332:ASN:C    | 2.45                     | 0.57              |
| 1:B:22:LEU:N     | 1:B:30:ILE:O     | 2.35                     | 0.57              |
| 1:B:257:ASN:HD22 | 1:B:257:ASN:N    | 2.02                     | 0.57              |
| 1:C:301:PRO:O    | 1:C:302:LEU:HD23 | 2.04                     | 0.57              |
| 1:A:41:PRO:O     | 1:A:43:LEU:N     | 2.37                     | 0.57              |
| 1:B:219:LEU:HD21 | 1:B:253:SER:N    | 2.18                     | 0.57              |
| 1:C:115:HIS:CD2  | 1:C:118:GLN:HB3  | 2.40                     | 0.57              |
| 1:C:123:ILE:HG21 | 1:C:336:LEU:HD22 | 1.84                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:197:GLN:HG2  | 1:C:364:GLN:NE2  | 2.20                     | 0.57              |
| 1:C:25:ASN:OD1   | 1:C:25:ASN:C     | 2.48                     | 0.57              |
| 1:B:25:ASN:OD1   | 1:B:25:ASN:C     | 2.47                     | 0.57              |
| 1:B:115:HIS:HD2  | 1:B:117:HIS:N    | 2.03                     | 0.57              |
| 1:A:241:ASN:OD1  | 1:A:243:GLN:HB2  | 2.05                     | 0.56              |
| 1:B:73:LEU:HD23  | 1:B:103:ILE:HD12 | 1.87                     | 0.56              |
| 1:B:357:VAL:CG1  | 1:B:358:VAL:N    | 2.68                     | 0.56              |
| 1:C:270:ALA:H    | 1:C:345:ASN:HD21 | 1.52                     | 0.56              |
| 1:A:263:LEU:HD13 | 1:A:351:ALA:CB   | 2.35                     | 0.56              |
| 1:A:263:LEU:CD2  | 1:A:390:VAL:HG11 | 2.34                     | 0.56              |
| 1:A:373:SER:O    | 1:A:375:GLN:N    | 2.38                     | 0.56              |
| 1:B:23:PHE:O     | 1:B:29:ARG:HA    | 2.06                     | 0.56              |
| 1:B:24:GLU:HA    | 1:B:28:GLY:O     | 2.04                     | 0.56              |
| 1:B:198:LEU:HD23 | 1:B:198:LEU:N    | 2.20                     | 0.56              |
| 1:A:51:ILE:HD11  | 1:A:273:ILE:HG21 | 1.87                     | 0.56              |
| 1:B:306:ARG:HG2  | 1:B:307:TYR:H    | 1.70                     | 0.56              |
| 1:B:313:GLU:O    | 1:B:314:ASP:HB2  | 2.04                     | 0.56              |
| 1:B:32:LEU:HD21  | 1:B:52:VAL:HG22  | 1.86                     | 0.56              |
| 1:B:57:LYS:HB3   | 1:B:58:PRO:HD2   | 1.87                     | 0.56              |
| 1:C:15:SER:HB3   | 1:C:314:ASP:O    | 2.05                     | 0.56              |
| 1:C:380:LEU:HD13 | 1:C:381:LEU:N    | 2.20                     | 0.56              |
| 1:B:272:VAL:CG1  | 1:B:319:ILE:HD12 | 2.35                     | 0.56              |
| 1:A:80:ALA:HB2   | 1:A:120:LEU:CD1  | 2.34                     | 0.56              |
| 1:B:211:SER:O    | 1:B:212:SER:C    | 2.48                     | 0.56              |
| 1:B:359:ARG:HH22 | 1:B:382:LYS:HE3  | 1.70                     | 0.56              |
| 1:C:250:PHE:HB3  | 1:C:342:ALA:HB1  | 1.88                     | 0.56              |
| 1:C:265:HIS:HB3  | 1:C:349:PHE:CD1  | 2.41                     | 0.56              |
| 1:A:92:SER:HB3   | 1:A:202:ALA:HA   | 1.88                     | 0.56              |
| 1:B:44:GLU:O     | 1:B:47:ARG:HG2   | 2.06                     | 0.56              |
| 1:B:174:PHE:O    | 1:C:371:PRO:HG3  | 2.06                     | 0.56              |
| 1:B:190:LEU:HD21 | 1:B:198:LEU:HD11 | 1.87                     | 0.56              |
| 1:A:167:GLU:O    | 1:A:171:ARG:NH1  | 2.39                     | 0.56              |
| 1:C:250:PHE:HB3  | 1:C:342:ALA:CB   | 2.36                     | 0.56              |
| 1:C:220:ARG:NH1  | 1:C:220:ARG:CG   | 2.69                     | 0.55              |
| 1:A:160:THR:HG21 | 1:B:392:ALA:CA   | 2.36                     | 0.55              |
| 1:B:283:ILE:O    | 1:B:308:ARG:HA   | 2.06                     | 0.55              |
| 1:B:283:ILE:HA   | 1:B:326:VAL:O    | 2.07                     | 0.55              |
| 1:B:364:GLN:O    | 1:B:367:GLU:HB3  | 2.06                     | 0.55              |
| 1:C:363:ARG:O    | 1:C:366:GLN:HB2  | 2.07                     | 0.55              |
| 1:A:190:LEU:HD21 | 1:A:198:LEU:HD11 | 1.89                     | 0.55              |
| 1:C:248:ASP:OD2  | 1:C:343:GLU:HB2  | 2.06                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:191:SER:O    | 1:B:192:LYS:C    | 2.50                     | 0.55              |
| 1:C:283:ILE:HD11 | 1:C:325:PHE:HD2  | 1.72                     | 0.55              |
| 1:B:166:PHE:CZ   | 1:B:170:ASN:HB2  | 2.41                     | 0.55              |
| 1:A:21:THR:HA    | 1:A:31:ARG:HB3   | 1.88                     | 0.55              |
| 1:A:379:ARG:HH11 | 1:A:379:ARG:CB   | 2.07                     | 0.55              |
| 1:B:191:SER:CB   | 1:B:194:GLN:HE21 | 2.19                     | 0.55              |
| 1:A:80:ALA:HB2   | 1:A:120:LEU:HD13 | 1.89                     | 0.54              |
| 1:B:47:ARG:HH11  | 1:B:132:PRO:HG3  | 1.72                     | 0.54              |
| 1:C:228:ASN:OD1  | 1:C:389:PHE:HB2  | 2.08                     | 0.54              |
| 1:B:75:VAL:HG22  | 1:B:99:ASP:O     | 2.08                     | 0.54              |
| 1:A:191:SER:O    | 1:A:194:GLN:N    | 2.41                     | 0.54              |
| 1:A:194:GLN:O    | 1:A:197:GLN:HB2  | 2.07                     | 0.54              |
| 1:B:27:ASN:HD22  | 1:B:60:THR:HG22  | 1.72                     | 0.54              |
| 1:B:375:GLN:O    | 1:B:376:ASP:C    | 2.49                     | 0.54              |
| 1:A:50:ARG:HB2   | 1:A:126:ALA:HB3  | 1.89                     | 0.54              |
| 1:A:164:SER:OG   | 1:A:168:GLU:OE2  | 2.26                     | 0.54              |
| 1:A:392:ALA:HA   | 1:C:160:THR:HG21 | 1.89                     | 0.54              |
| 1:B:18:SER:O     | 1:B:33:LEU:HA    | 2.08                     | 0.54              |
| 1:B:73:LEU:HD23  | 1:B:103:ILE:CD1  | 2.37                     | 0.54              |
| 1:B:197:GLN:HE21 | 1:B:197:GLN:CA   | 2.20                     | 0.54              |
| 1:B:275:VAL:CG2  | 1:B:336:LEU:HD23 | 2.37                     | 0.54              |
| 1:C:386:GLU:HB3  | 1:C:390:VAL:HG12 | 1.90                     | 0.54              |
| 1:A:311:LEU:HD22 | 1:A:315:ASP:CB   | 2.37                     | 0.54              |
| 1:B:214:ASP:OD2  | 1:B:215:GLU:N    | 2.41                     | 0.54              |
| 1:C:29:ARG:NH2   | 1:C:55:GLN:HE22  | 2.00                     | 0.54              |
| 1:A:321:ALA:O    | 1:A:322:ALA:HB3  | 2.08                     | 0.54              |
| 1:A:166:PHE:C    | 1:A:168:GLU:H    | 2.16                     | 0.53              |
| 1:A:363:ARG:HG2  | 1:A:374:ALA:HB1  | 1.89                     | 0.53              |
| 1:B:281:ALA:CB   | 1:B:333:LEU:HD13 | 2.35                     | 0.53              |
| 1:A:24:GLU:CD    | 1:A:29:ARG:HB2   | 2.32                     | 0.53              |
| 1:A:172:VAL:HG13 | 1:B:376:ASP:HB3  | 1.90                     | 0.53              |
| 1:B:357:VAL:HG13 | 1:B:358:VAL:N    | 2.22                     | 0.53              |
| 1:C:130:ASN:N    | 1:C:130:ASN:HD22 | 2.05                     | 0.53              |
| 1:B:203:LYS:NZ   | 1:B:215:GLU:CD   | 2.67                     | 0.53              |
| 1:C:139:PHE:HB3  | 1:C:146:GLN:NE2  | 2.23                     | 0.53              |
| 1:C:237:THR:HB   | 1:C:238:PRO:HD2  | 1.90                     | 0.53              |
| 1:A:83:THR:HG21  | 1:A:110:TYR:OH   | 2.07                     | 0.53              |
| 1:C:331:SER:O    | 1:C:332:ASN:C    | 2.52                     | 0.53              |
| 1:A:360:GLN:O    | 1:C:90:ARG:HD3   | 2.08                     | 0.53              |
| 1:A:364:GLN:HB2  | 1:C:198:LEU:HD21 | 1.91                     | 0.53              |
| 1:A:30:ILE:HG12  | 1:A:54:PHE:HD1   | 1.72                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:371:PRO:HG3  | 1:C:174:PHE:C    | 2.34                     | 0.53              |
| 1:B:189:GLU:HG2  | 1:B:190:LEU:O    | 2.08                     | 0.53              |
| 1:C:197:GLN:HA   | 1:C:197:GLN:NE2  | 2.20                     | 0.53              |
| 1:B:49:TYR:CD1   | 1:B:125:LEU:HD11 | 2.44                     | 0.53              |
| 1:B:205:SER:N    | 1:B:216:PRO:HG2  | 2.24                     | 0.53              |
| 1:A:149:TYR:CE1  | 1:B:350:LEU:HD11 | 2.41                     | 0.52              |
| 1:A:61:ILE:HG12  | 1:A:62:LEU:H     | 1.74                     | 0.52              |
| 1:B:29:ARG:HD3   | 1:B:55:GLN:HE21  | 1.73                     | 0.52              |
| 1:A:269:LYS:H    | 1:A:345:ASN:HD22 | 1.58                     | 0.52              |
| 1:A:367:GLU:CB   | 1:A:374:ALA:HB2  | 2.30                     | 0.52              |
| 1:C:12:TYR:HE2   | 1:C:311:LEU:HD23 | 1.71                     | 0.52              |
| 1:C:364:GLN:O    | 1:C:368:LEU:HD12 | 2.10                     | 0.52              |
| 1:A:269:LYS:HD3  | 1:A:343:GLU:O    | 2.09                     | 0.52              |
| 1:C:61:ILE:HG13  | 1:C:112:VAL:HG22 | 1.91                     | 0.52              |
| 1:A:371:PRO:HG3  | 1:C:174:PHE:O    | 2.09                     | 0.52              |
| 1:C:129:VAL:C    | 1:C:130:ASN:HD22 | 2.17                     | 0.52              |
| 1:A:122:ILE:CG2  | 1:A:123:ILE:N    | 2.73                     | 0.52              |
| 1:B:58:PRO:HB2   | 1:B:115:HIS:O    | 2.09                     | 0.52              |
| 1:B:203:LYS:O    | 1:B:204:SER:HB3  | 2.09                     | 0.52              |
| 1:C:257:ASN:N    | 1:C:257:ASN:HD22 | 2.07                     | 0.52              |
| 1:B:59:ASN:O     | 1:B:189:GLU:HG3  | 2.09                     | 0.52              |
| 1:A:147:GLN:O    | 1:A:148:SER:C    | 2.53                     | 0.52              |
| 1:B:70:ASP:HB2   | 1:B:127:ILE:HB   | 1.92                     | 0.52              |
| 1:B:190:LEU:HD21 | 1:B:198:LEU:CD1  | 2.40                     | 0.52              |
| 1:C:230:PHE:HB3  | 1:C:260:ALA:HB2  | 1.92                     | 0.52              |
| 1:A:61:ILE:O     | 1:A:187:ILE:HA   | 2.10                     | 0.52              |
| 1:A:23:PHE:O     | 1:A:24:GLU:HB2   | 2.09                     | 0.51              |
| 1:B:25:ASN:OD1   | 1:B:27:ASN:HB2   | 2.10                     | 0.51              |
| 1:C:9:ASN:C      | 1:C:9:ASN:HD22   | 2.17                     | 0.51              |
| 1:C:262:LEU:HD13 | 1:C:389:PHE:CE1  | 2.45                     | 0.51              |
| 1:A:18:SER:O     | 1:A:34:GLN:HG3   | 2.10                     | 0.51              |
| 1:A:236:ILE:HG22 | 1:A:251:LEU:HB2  | 1.92                     | 0.51              |
| 1:B:73:LEU:HD21  | 1:B:82:LEU:HD22  | 1.92                     | 0.51              |
| 1:B:272:VAL:HG12 | 1:B:319:ILE:HD12 | 1.91                     | 0.51              |
| 1:A:59:ASN:HD22  | 1:A:195:ILE:CD1  | 2.23                     | 0.51              |
| 1:A:174:PHE:N    | 1:A:174:PHE:CD2  | 2.78                     | 0.51              |
| 1:B:88:ASP:OD2   | 1:B:88:ASP:N     | 2.43                     | 0.51              |
| 1:B:191:SER:O    | 1:B:194:GLN:N    | 2.43                     | 0.51              |
| 1:B:280:ASP:HA   | 1:B:311:LEU:O    | 2.10                     | 0.51              |
| 1:C:81:ILE:O     | 1:C:111:LEU:HD12 | 2.10                     | 0.51              |
| 1:B:261:LEU:CD2  | 1:B:390:VAL:HG22 | 2.41                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:92:SER:O     | 1:C:202:ALA:HA   | 2.10                     | 0.51              |
| 1:A:280:ASP:HB2  | 1:A:330:THR:OG1  | 2.11                     | 0.51              |
| 1:A:363:ARG:CG   | 1:A:374:ALA:HB1  | 2.41                     | 0.51              |
| 1:B:24:GLU:CG    | 1:B:29:ARG:HB3   | 2.31                     | 0.51              |
| 1:B:68:ASP:OD2   | 1:B:68:ASP:N     | 2.44                     | 0.51              |
| 1:A:166:PHE:O    | 1:A:168:GLU:N    | 2.43                     | 0.51              |
| 1:B:21:THR:CA    | 1:B:31:ARG:HG2   | 2.38                     | 0.51              |
| 1:B:67:ALA:HB1   | 1:B:136:ASP:O    | 2.10                     | 0.51              |
| 1:B:170:ASN:ND2  | 1:B:174:PHE:HD1  | 2.08                     | 0.51              |
| 1:B:228:ASN:ND2  | 1:B:228:ASN:C    | 2.67                     | 0.51              |
| 1:B:359:ARG:HH22 | 1:B:382:LYS:HG3  | 1.75                     | 0.51              |
| 1:C:139:PHE:CE1  | 1:C:186:VAL:HG11 | 2.46                     | 0.51              |
| 1:A:359:ARG:HH22 | 1:A:382:LYS:HD3  | 1.75                     | 0.51              |
| 1:A:274:LEU:HD23 | 1:A:319:ILE:HD11 | 1.93                     | 0.51              |
| 1:B:101:GLN:HG3  | 1:B:102:ARG:N    | 2.25                     | 0.51              |
| 1:B:265:HIS:HE1  | 1:B:325:PHE:CZ   | 2.29                     | 0.51              |
| 1:C:229:ASN:HB3  | 1:C:230:PHE:CD2  | 2.46                     | 0.51              |
| 1:A:225:ILE:HD12 | 1:A:226:TYR:CD1  | 2.46                     | 0.51              |
| 1:A:277:ASN:HB3  | 1:A:334:ASN:ND2  | 2.26                     | 0.50              |
| 1:B:161:SER:O    | 1:C:384:GLN:HG2  | 2.11                     | 0.50              |
| 1:B:173:LEU:O    | 1:C:370:PHE:HB3  | 2.11                     | 0.50              |
| 1:C:81:ILE:CD1   | 1:C:199:SER:HA   | 2.41                     | 0.50              |
| 1:C:210:ILE:HG22 | 1:C:211:SER:OG   | 2.10                     | 0.50              |
| 1:B:13:PHE:HE1   | 1:B:39:ARG:HD3   | 1.75                     | 0.50              |
| 1:B:244:LEU:HD11 | 1:B:251:LEU:HD11 | 1.93                     | 0.50              |
| 1:B:159:GLU:HG3  | 1:B:166:PHE:N    | 2.26                     | 0.50              |
| 1:B:197:GLN:HB3  | 1:B:198:LEU:HD23 | 1.93                     | 0.50              |
| 1:B:257:ASN:N    | 1:B:257:ASN:ND2  | 2.59                     | 0.50              |
| 1:C:8:ASN:O      | 1:C:10:PRO:HD3   | 2.12                     | 0.50              |
| 1:A:61:ILE:HG12  | 1:A:62:LEU:N     | 2.26                     | 0.50              |
| 1:A:213:GLU:HG3  | 1:A:214:ASP:OD1  | 2.11                     | 0.50              |
| 1:B:80:ALA:HB2   | 1:B:120:LEU:CD2  | 2.40                     | 0.50              |
| 1:B:250:PHE:C    | 1:B:250:PHE:CD2  | 2.90                     | 0.50              |
| 1:B:373:SER:O    | 1:B:376:ASP:HB2  | 2.12                     | 0.50              |
| 1:A:370:PHE:O    | 1:A:372:GLY:N    | 2.39                     | 0.50              |
| 1:B:168:GLU:O    | 1:B:172:VAL:HG23 | 2.12                     | 0.50              |
| 1:A:59:ASN:HD22  | 1:A:195:ILE:HD11 | 1.77                     | 0.50              |
| 1:A:79:ARG:NH1   | 1:A:94:ASN:OD1   | 2.45                     | 0.50              |
| 1:A:222:ARG:NH2  | 1:A:240:LYS:HD3  | 2.27                     | 0.50              |
| 1:A:371:PRO:HD2  | 1:C:173:LEU:O    | 2.12                     | 0.50              |
| 1:B:69:ALA:CB    | 1:B:128:PRO:HA   | 2.42                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:288:ILE:CG2  | 1:C:302:LEU:HD22 | 2.39                     | 0.50              |
| 1:A:111:LEU:HD21 | 1:A:122:ILE:HD12 | 1.94                     | 0.49              |
| 1:C:359:ARG:HH22 | 1:C:382:LYS:CE   | 2.08                     | 0.49              |
| 1:A:54:PHE:CE2   | 1:A:111:LEU:HD23 | 2.47                     | 0.49              |
| 1:C:206:SER:OG   | 1:C:209:THR:HG23 | 2.12                     | 0.49              |
| 1:B:75:VAL:HG12  | 1:B:122:ILE:CD1  | 2.40                     | 0.49              |
| 1:B:286:VAL:O    | 1:B:324:PRO:HD2  | 2.12                     | 0.49              |
| 1:C:119:ASN:N    | 1:C:119:ASN:ND2  | 2.60                     | 0.49              |
| 1:A:79:ARG:NH1   | 1:A:94:ASN:HD21  | 2.09                     | 0.49              |
| 1:A:225:ILE:HG13 | 1:A:233:PHE:O    | 2.12                     | 0.49              |
| 1:B:130:ASN:O    | 1:C:45:ASN:HB2   | 2.11                     | 0.49              |
| 1:A:289:LYS:C    | 1:A:290:GLU:HG3  | 2.37                     | 0.49              |
| 1:B:254:VAL:HG21 | 1:B:335:PHE:CZ   | 2.47                     | 0.49              |
| 1:C:19:PHE:HD2   | 1:C:31:ARG:HB2   | 1.78                     | 0.49              |
| 1:A:267:ASN:HB3  | 1:A:345:ASN:HD21 | 1.78                     | 0.49              |
| 1:B:25:ASN:C     | 1:B:27:ASN:N     | 2.69                     | 0.49              |
| 1:B:209:THR:HB   | 1:B:215:GLU:HB3  | 1.93                     | 0.49              |
| 1:A:183:GLN:NE2  | 1:B:368:LEU:O    | 2.45                     | 0.49              |
| 1:A:274:LEU:HD23 | 1:A:319:ILE:CD1  | 2.41                     | 0.49              |
| 1:C:37:ASN:HD22  | 1:C:37:ASN:H     | 1.58                     | 0.49              |
| 1:A:165:GLU:O    | 1:A:166:PHE:C    | 2.56                     | 0.49              |
| 1:B:13:PHE:CE1   | 1:B:39:ARG:HD3   | 2.47                     | 0.49              |
| 1:B:166:PHE:HD2  | 1:B:169:ILE:HD11 | 1.78                     | 0.49              |
| 1:C:359:ARG:HH12 | 1:C:382:LYS:HE3  | 1.77                     | 0.49              |
| 1:A:159:GLU:HG2  | 1:A:166:PHE:H    | 1.78                     | 0.49              |
| 1:B:87:ASN:O     | 1:C:355:ASP:HA   | 2.13                     | 0.49              |
| 1:B:174:PHE:C    | 1:C:371:PRO:HG3  | 2.38                     | 0.49              |
| 1:C:278:GLU:O    | 1:C:333:LEU:HA   | 2.12                     | 0.49              |
| 1:A:66:HIS:CD2   | 1:B:322:ALA:HB1  | 2.48                     | 0.49              |
| 1:A:154:SER:OG   | 1:A:157:ILE:HB   | 2.13                     | 0.49              |
| 1:C:228:ASN:O    | 1:C:230:PHE:N    | 2.45                     | 0.49              |
| 1:A:26:GLN:H     | 1:A:26:GLN:NE2   | 2.11                     | 0.48              |
| 1:B:161:SER:HB3  | 1:C:263:LEU:HD22 | 1.95                     | 0.48              |
| 1:A:55:GLN:HA    | 1:A:120:LEU:O    | 2.12                     | 0.48              |
| 1:A:153:PHE:CZ   | 1:B:264:PRO:HB3  | 2.49                     | 0.48              |
| 1:B:157:ILE:O    | 1:B:161:SER:OG   | 2.31                     | 0.48              |
| 1:C:65:HIS:HB2   | 1:C:138:PHE:O    | 2.13                     | 0.48              |
| 1:C:119:ASN:HD22 | 1:C:119:ASN:N    | 2.08                     | 0.48              |
| 1:A:29:ARG:HD3   | 1:A:55:GLN:NE2   | 2.21                     | 0.48              |
| 1:B:79:ARG:O     | 1:B:120:LEU:HD13 | 2.12                     | 0.48              |
| 1:B:265:HIS:CE1  | 1:B:325:PHE:CZ   | 3.02                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:356:ASN:ND2  | 1:C:359:ARG:HB2  | 2.28                     | 0.48              |
| 1:A:263:LEU:HG   | 1:A:390:VAL:HG12 | 1.94                     | 0.48              |
| 1:C:83:THR:HA    | 1:C:91:ASP:O     | 2.12                     | 0.48              |
| 1:A:41:PRO:C     | 1:A:43:LEU:N     | 2.72                     | 0.48              |
| 1:A:376:ASP:CG   | 1:C:171:ARG:HH21 | 2.20                     | 0.48              |
| 1:A:392:ALA:HA   | 1:C:160:THR:HG23 | 1.94                     | 0.48              |
| 1:C:57:LYS:O     | 1:C:60:THR:HG23  | 2.13                     | 0.48              |
| 1:C:69:ALA:HB2   | 1:C:128:PRO:HA   | 1.95                     | 0.48              |
| 1:C:319:ILE:HD13 | 1:C:325:PHE:CD1  | 2.49                     | 0.48              |
| 1:C:382:LYS:HE2  | 1:C:385:ARG:HE   | 1.76                     | 0.48              |
| 1:B:159:GLU:HG3  | 1:B:166:PHE:H    | 1.79                     | 0.48              |
| 1:C:164:SER:OG   | 1:C:168:GLU:HB3  | 2.13                     | 0.48              |
| 1:C:263:LEU:HD13 | 1:C:351:ALA:O    | 2.13                     | 0.48              |
| 1:B:61:ILE:HA    | 1:B:111:LEU:O    | 2.13                     | 0.48              |
| 1:B:172:VAL:HG11 | 1:C:376:ASP:O    | 2.14                     | 0.48              |
| 1:C:269:LYS:HE2  | 1:C:341:ASN:OD1  | 2.14                     | 0.48              |
| 1:A:123:ILE:HG21 | 1:A:336:LEU:CD2  | 2.43                     | 0.48              |
| 1:A:236:ILE:HD11 | 1:A:240:LYS:HB3  | 1.94                     | 0.48              |
| 1:A:368:LEU:HD12 | 1:C:183:GLN:OE1  | 2.13                     | 0.48              |
| 1:B:141:SER:HB2  | 1:C:369:ALA:O    | 2.13                     | 0.48              |
| 1:C:312:SER:O    | 1:C:315:ASP:HB2  | 2.14                     | 0.48              |
| 1:A:112:VAL:O    | 1:A:114:PRO:HD3  | 2.12                     | 0.48              |
| 1:A:225:ILE:HD12 | 1:A:226:TYR:CZ   | 2.49                     | 0.48              |
| 1:A:349:PHE:O    | 1:A:356:ASN:HA   | 2.14                     | 0.48              |
| 1:B:12:TYR:HB2   | 1:B:317:PHE:HE2  | 1.79                     | 0.48              |
| 1:A:217:PHE:CD1  | 1:A:241:ASN:ND2  | 2.82                     | 0.48              |
| 1:B:49:TYR:CZ    | 1:B:340:ILE:HD12 | 2.49                     | 0.48              |
| 1:C:71:PHE:CE2   | 1:C:126:ALA:HB2  | 2.49                     | 0.48              |
| 1:A:29:ARG:CD    | 1:A:55:GLN:NE2   | 2.77                     | 0.47              |
| 1:B:65:HIS:CD2   | 1:B:137:ASP:OD1  | 2.67                     | 0.47              |
| 1:B:269:LYS:H    | 1:B:345:ASN:HD22 | 1.61                     | 0.47              |
| 1:B:310:GLU:O    | 1:B:311:LEU:HD23 | 2.13                     | 0.47              |
| 1:A:23:PHE:CE1   | 1:B:302:LEU:HD13 | 2.49                     | 0.47              |
| 1:C:120:LEU:HD11 | 1:C:122:ILE:HD11 | 1.96                     | 0.47              |
| 1:C:197:GLN:HE21 | 1:C:197:GLN:CA   | 2.13                     | 0.47              |
| 1:C:3:VAL:HG13   | 1:C:4:ARG:N      | 2.29                     | 0.47              |
| 1:C:244:LEU:HG   | 1:C:249:ILE:O    | 2.14                     | 0.47              |
| 1:A:210:ILE:HD11 | 1:A:221:SER:OG   | 2.15                     | 0.47              |
| 1:C:36:PHE:HB3   | 1:C:43:LEU:CD1   | 2.45                     | 0.47              |
| 1:A:166:PHE:HA   | 1:A:169:ILE:HD11 | 1.95                     | 0.47              |
| 1:B:75:VAL:HG21  | 1:B:96:HIS:O     | 2.14                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:95:LEU:N     | 1:B:95:LEU:HD23  | 2.29                     | 0.47              |
| 1:C:213:GLU:HG2  | 1:C:242:PRO:CB   | 2.44                     | 0.47              |
| 1:A:228:ASN:O    | 1:A:230:PHE:N    | 2.46                     | 0.47              |
| 1:A:273:ILE:HB   | 1:A:338:PHE:HB2  | 1.96                     | 0.47              |
| 1:B:34:GLN:NE2   | 1:B:39:ARG:HD3   | 2.30                     | 0.47              |
| 1:B:165:GLU:O    | 1:B:166:PHE:C    | 2.58                     | 0.47              |
| 1:A:268:SER:HB3  | 1:A:346:GLN:H    | 1.79                     | 0.47              |
| 1:A:305:GLN:HE21 | 1:A:306:ARG:H    | 1.62                     | 0.47              |
| 1:A:373:SER:HB3  | 1:A:376:ASP:CG   | 2.39                     | 0.47              |
| 1:B:23:PHE:HZ    | 1:B:145:ALA:CB   | 2.28                     | 0.47              |
| 1:B:140:LEU:HG   | 1:B:149:TYR:OH   | 2.15                     | 0.47              |
| 1:B:284:GLU:HB2  | 1:B:326:VAL:CG1  | 2.39                     | 0.47              |
| 1:C:55:GLN:HA    | 1:C:120:LEU:O    | 2.15                     | 0.47              |
| 1:C:359:ARG:CZ   | 1:C:382:LYS:HE3  | 2.45                     | 0.47              |
| 1:A:57:LYS:HA    | 1:A:119:ASN:OD1  | 2.14                     | 0.47              |
| 1:A:333:LEU:HG   | 1:A:334:ASN:N    | 2.30                     | 0.47              |
| 1:A:14:ARG:HG2   | 1:A:16:SER:H     | 1.79                     | 0.47              |
| 1:B:150:LEU:HD22 | 1:B:162:PHE:HZ   | 1.79                     | 0.47              |
| 1:C:154:SER:OG   | 1:C:157:ILE:HD13 | 2.15                     | 0.47              |
| 1:A:84:LEU:HD21  | 1:A:103:ILE:HG12 | 1.96                     | 0.47              |
| 1:B:86:ASN:N     | 1:B:86:ASN:HD22  | 2.11                     | 0.46              |
| 1:A:228:ASN:OD1  | 1:A:389:PHE:HB2  | 2.15                     | 0.46              |
| 1:A:370:PHE:C    | 1:A:372:GLY:H    | 2.23                     | 0.46              |
| 1:B:51:ILE:HG23  | 1:B:123:ILE:HD11 | 1.97                     | 0.46              |
| 1:B:69:ALA:HB2   | 1:B:128:PRO:HA   | 1.98                     | 0.46              |
| 1:B:283:ILE:HD11 | 1:B:327:VAL:HG22 | 1.97                     | 0.46              |
| 1:B:319:ILE:O    | 1:B:320:PRO:O    | 2.33                     | 0.46              |
| 1:C:218:ASN:O    | 1:C:221:SER:HB2  | 2.15                     | 0.46              |
| 1:C:384:GLN:HE21 | 1:C:386:GLU:N    | 2.09                     | 0.46              |
| 1:A:150:LEU:C    | 1:A:152:GLY:N    | 2.69                     | 0.46              |
| 1:A:157:ILE:HG22 | 1:A:158:LEU:N    | 2.30                     | 0.46              |
| 1:A:219:LEU:HD23 | 1:A:253:SER:HB2  | 1.97                     | 0.46              |
| 1:B:79:ARG:CG    | 1:B:79:ARG:NH1   | 2.71                     | 0.46              |
| 1:B:230:PHE:HB3  | 1:B:260:ALA:HB2  | 1.96                     | 0.46              |
| 1:B:375:GLN:O    | 1:B:378:GLU:N    | 2.48                     | 0.46              |
| 1:C:319:ILE:CD1  | 1:C:325:PHE:CD1  | 2.98                     | 0.46              |
| 1:C:366:GLN:O    | 1:C:369:ALA:N    | 2.48                     | 0.46              |
| 1:A:191:SER:O    | 1:A:193:GLU:N    | 2.48                     | 0.46              |
| 1:B:73:LEU:HD11  | 1:B:95:LEU:HD12  | 1.98                     | 0.46              |
| 1:B:225:ILE:HG13 | 1:B:226:TYR:N    | 2.31                     | 0.46              |
| 1:B:258:GLU:H    | 1:B:332:ASN:HD22 | 1.63                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:230:PHE:HE1  | 1:C:391:ASP:OD1  | 1.98                     | 0.46              |
| 1:C:236:ILE:O    | 1:C:236:ILE:HG23 | 2.15                     | 0.46              |
| 1:A:37:ASN:H     | 1:A:37:ASN:ND2   | 2.12                     | 0.46              |
| 1:A:257:ASN:N    | 1:A:257:ASN:ND2  | 2.62                     | 0.46              |
| 1:B:47:ARG:HH11  | 1:B:132:PRO:CG   | 2.29                     | 0.46              |
| 1:B:184:GLU:O    | 1:B:185:GLY:O    | 2.34                     | 0.46              |
| 1:B:282:ASN:O    | 1:B:327:VAL:HA   | 2.13                     | 0.46              |
| 1:C:68:ASP:O     | 1:C:68:ASP:OD2   | 2.34                     | 0.46              |
| 1:C:366:GLN:O    | 1:C:367:GLU:C    | 2.58                     | 0.46              |
| 1:A:12:TYR:CE2   | 1:A:311:LEU:HD23 | 2.50                     | 0.46              |
| 1:A:65:HIS:HB3   | 1:A:139:PHE:CD2  | 2.50                     | 0.46              |
| 1:A:376:ASP:CG   | 1:C:171:ARG:NH2  | 2.74                     | 0.46              |
| 1:B:197:GLN:HE21 | 1:B:197:GLN:H    | 1.62                     | 0.46              |
| 1:B:349:PHE:O    | 1:B:356:ASN:HA   | 2.16                     | 0.46              |
| 1:B:25:ASN:HD21  | 1:B:187:ILE:CB   | 2.19                     | 0.46              |
| 1:B:54:PHE:CE2   | 1:B:111:LEU:HD23 | 2.50                     | 0.46              |
| 1:B:250:PHE:HD1  | 1:B:342:ALA:CB   | 2.29                     | 0.46              |
| 1:B:308:ARG:CG   | 1:B:309:ALA:N    | 2.78                     | 0.46              |
| 1:B:349:PHE:CE2  | 1:B:388:TYR:HD2  | 2.34                     | 0.46              |
| 1:C:236:ILE:O    | 1:C:236:ILE:CG2  | 2.63                     | 0.46              |
| 1:B:173:LEU:O    | 1:C:371:PRO:HD2  | 2.14                     | 0.46              |
| 1:A:183:GLN:HG2  | 1:A:188:VAL:HG11 | 1.97                     | 0.46              |
| 1:B:244:LEU:HD21 | 1:B:251:LEU:HD12 | 1.98                     | 0.46              |
| 1:A:234:PHE:HB2  | 1:A:253:SER:O    | 2.16                     | 0.45              |
| 1:B:36:PHE:CD2   | 1:B:46:LEU:HB3   | 2.51                     | 0.45              |
| 1:C:83:THR:HB    | 1:C:110:TYR:CE2  | 2.51                     | 0.45              |
| 1:C:146:GLN:OE1  | 1:C:186:VAL:HG12 | 2.16                     | 0.45              |
| 1:C:210:ILE:HG22 | 1:C:211:SER:N    | 2.30                     | 0.45              |
| 1:C:374:ALA:O    | 1:C:378:GLU:N    | 2.49                     | 0.45              |
| 1:C:219:LEU:HD13 | 1:C:236:ILE:HB   | 1.98                     | 0.45              |
| 1:C:384:GLN:NE2  | 1:C:386:GLU:H    | 2.11                     | 0.45              |
| 1:A:61:ILE:HG22  | 1:A:188:VAL:HG22 | 1.98                     | 0.45              |
| 1:A:156:ASN:N    | 1:A:156:ASN:ND2  | 2.63                     | 0.45              |
| 1:C:140:LEU:O    | 1:C:148:SER:OG   | 2.29                     | 0.45              |
| 1:A:76:LEU:HD13  | 1:A:277:ASN:CG   | 2.41                     | 0.45              |
| 1:A:58:PRO:HA    | 1:A:113:ASN:ND2  | 2.32                     | 0.45              |
| 1:B:261:LEU:HD23 | 1:B:390:VAL:HG22 | 1.98                     | 0.45              |
| 1:B:283:ILE:HG13 | 1:B:327:VAL:HG22 | 1.99                     | 0.45              |
| 1:C:37:ASN:N     | 1:C:37:ASN:ND2   | 2.64                     | 0.45              |
| 1:B:63:LEU:HD12  | 1:B:186:VAL:HA   | 1.99                     | 0.45              |
| 1:B:112:VAL:O    | 1:B:114:PRO:HD3  | 2.16                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:226:TYR:HB3  | 1:B:388:TYR:CD1  | 2.52                     | 0.45              |
| 1:C:171:ARG:O    | 1:C:181:ARG:NH2  | 2.50                     | 0.45              |
| 1:C:195:ILE:O    | 1:C:199:SER:CB   | 2.64                     | 0.45              |
| 1:C:241:ASN:HA   | 1:C:242:PRO:HD2  | 1.83                     | 0.45              |
| 1:A:156:ASN:H    | 1:A:156:ASN:ND2  | 2.08                     | 0.45              |
| 1:B:63:LEU:HD23  | 1:B:63:LEU:HA    | 1.78                     | 0.45              |
| 1:B:140:LEU:HD13 | 1:C:358:VAL:HG13 | 1.99                     | 0.45              |
| 1:B:197:GLN:CA   | 1:B:197:GLN:NE2  | 2.78                     | 0.45              |
| 1:B:283:ILE:HG13 | 1:B:326:VAL:O    | 2.17                     | 0.45              |
| 1:B:289:LYS:HB2  | 1:B:303:GLU:O    | 2.17                     | 0.45              |
| 1:C:81:ILE:HD13  | 1:C:199:SER:HA   | 1.98                     | 0.45              |
| 1:C:306:ARG:H    | 1:C:306:ARG:HG2  | 1.56                     | 0.45              |
| 1:A:12:TYR:HE2   | 1:A:311:LEU:CD2  | 2.28                     | 0.45              |
| 1:A:87:ASN:O     | 1:B:355:ASP:HA   | 2.17                     | 0.45              |
| 1:A:183:GLN:OE1  | 1:B:368:LEU:HD12 | 2.17                     | 0.45              |
| 1:A:236:ILE:O    | 1:A:236:ILE:CG2  | 2.63                     | 0.45              |
| 1:B:356:ASN:HB3  | 1:B:359:ARG:HB3  | 1.98                     | 0.45              |
| 1:C:12:TYR:CD2   | 1:C:311:LEU:HD23 | 2.51                     | 0.45              |
| 1:C:65:HIS:HB3   | 1:C:139:PHE:CD2  | 2.51                     | 0.45              |
| 1:C:11:PHE:HB3   | 1:C:318:VAL:O    | 2.17                     | 0.44              |
| 1:C:25:ASN:O     | 1:C:26:GLN:C     | 2.58                     | 0.44              |
| 1:A:148:SER:C    | 1:A:150:LEU:H    | 2.25                     | 0.44              |
| 1:A:166:PHE:C    | 1:A:168:GLU:N    | 2.75                     | 0.44              |
| 1:B:84:LEU:O     | 1:B:90:ARG:HA    | 2.18                     | 0.44              |
| 1:B:304:VAL:HG12 | 1:B:305:GLN:N    | 2.32                     | 0.44              |
| 1:C:146:GLN:OE1  | 1:C:186:VAL:CG1  | 2.65                     | 0.44              |
| 1:A:166:PHE:HA   | 1:A:169:ILE:CD1  | 2.48                     | 0.44              |
| 1:A:308:ARG:HG2  | 1:A:309:ALA:N    | 2.32                     | 0.44              |
| 1:B:11:PHE:HB3   | 1:B:318:VAL:O    | 2.17                     | 0.44              |
| 1:B:232:LYS:HE3  | 1:B:232:LYS:HB2  | 1.72                     | 0.44              |
| 1:A:73:LEU:O     | 1:A:100:ALA:HA   | 2.17                     | 0.44              |
| 1:C:172:VAL:O    | 1:C:172:VAL:HG12 | 2.17                     | 0.44              |
| 1:C:362:GLU:O    | 1:C:363:ARG:C    | 2.61                     | 0.44              |
| 1:B:234:PHE:O    | 1:B:252:SER:HA   | 2.17                     | 0.44              |
| 1:A:193:GLU:CG   | 1:A:197:GLN:HE22 | 2.26                     | 0.44              |
| 1:A:379:ARG:O    | 1:A:379:ARG:HG2  | 2.16                     | 0.44              |
| 1:B:268:SER:HB3  | 1:B:346:GLN:H    | 1.82                     | 0.44              |
| 1:B:356:ASN:HB3  | 1:B:359:ARG:HD2  | 2.00                     | 0.44              |
| 1:B:263:LEU:HG   | 1:B:390:VAL:HG13 | 2.00                     | 0.44              |
| 1:C:84:LEU:HD21  | 1:C:103:ILE:HG12 | 1.99                     | 0.44              |
| 1:C:357:VAL:O    | 1:C:358:VAL:C    | 2.61                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:359:ARG:NH1  | 1:C:382:LYS:HE3  | 2.33                     | 0.44              |
| 1:A:357:VAL:HG13 | 1:A:358:VAL:N    | 2.33                     | 0.44              |
| 1:B:81:ILE:HG13  | 1:B:114:PRO:HD3  | 2.00                     | 0.44              |
| 1:B:254:VAL:O    | 1:B:254:VAL:HG23 | 2.18                     | 0.44              |
| 1:A:35:ARG:HB2   | 1:A:38:LYS:HB3   | 2.00                     | 0.44              |
| 1:A:43:LEU:CD2   | 1:A:318:VAL:HG21 | 2.40                     | 0.44              |
| 1:A:45:ASN:HB2   | 1:C:130:ASN:O    | 2.18                     | 0.44              |
| 1:A:209:THR:C    | 1:A:211:SER:N    | 2.76                     | 0.44              |
| 1:B:12:TYR:HB2   | 1:B:317:PHE:CE2  | 2.53                     | 0.44              |
| 1:B:166:PHE:O    | 1:B:169:ILE:CG1  | 2.62                     | 0.44              |
| 1:B:288:ILE:HG22 | 1:B:289:LYS:O    | 2.17                     | 0.44              |
| 1:A:47:ARG:HG3   | 1:A:48:ASP:N     | 2.33                     | 0.43              |
| 1:A:79:ARG:O     | 1:A:120:LEU:HD13 | 2.17                     | 0.43              |
| 1:A:289:LYS:HD3  | 1:A:303:GLU:CD   | 2.43                     | 0.43              |
| 1:B:236:ILE:HD13 | 1:B:240:LYS:CB   | 2.43                     | 0.43              |
| 1:B:263:LEU:HD23 | 1:B:263:LEU:HA   | 1.68                     | 0.43              |
| 1:C:74:PHE:CE2   | 1:C:219:LEU:HD23 | 2.53                     | 0.43              |
| 1:A:66:HIS:HD2   | 1:A:106:GLY:HA2  | 1.83                     | 0.43              |
| 1:A:93:TYR:HA    | 1:A:203:LYS:O    | 2.17                     | 0.43              |
| 1:A:115:HIS:CD2  | 1:A:118:GLN:N    | 2.78                     | 0.43              |
| 1:A:149:TYR:O    | 1:B:286:VAL:HG21 | 2.19                     | 0.43              |
| 1:A:220:ARG:HA   | 1:A:234:PHE:CD2  | 2.53                     | 0.43              |
| 1:A:230:PHE:N    | 1:A:230:PHE:CD2  | 2.85                     | 0.43              |
| 1:A:236:ILE:CD1  | 1:A:240:LYS:HB3  | 2.48                     | 0.43              |
| 1:B:284:GLU:OE1  | 1:B:306:ARG:HD3  | 2.19                     | 0.43              |
| 1:C:12:TYR:HD2   | 1:C:311:LEU:HD21 | 1.83                     | 0.43              |
| 1:C:285:LEU:HD21 | 1:C:323:TYR:HB3  | 2.00                     | 0.43              |
| 1:A:250:PHE:HD1  | 1:A:342:ALA:CB   | 2.32                     | 0.43              |
| 1:A:277:ASN:HB3  | 1:A:334:ASN:O    | 2.18                     | 0.43              |
| 1:A:376:ASP:C    | 1:C:172:VAL:HG11 | 2.43                     | 0.43              |
| 1:B:258:GLU:HG3  | 1:B:331:SER:HA   | 2.00                     | 0.43              |
| 1:C:220:ARG:NH2  | 1:C:255:ASP:CG   | 2.74                     | 0.43              |
| 1:C:379:ARG:O    | 1:C:380:LEU:C    | 2.61                     | 0.43              |
| 1:A:156:ASN:HD22 | 1:A:156:ASN:N    | 2.12                     | 0.43              |
| 1:A:191:SER:C    | 1:A:193:GLU:N    | 2.75                     | 0.43              |
| 1:A:358:VAL:CG1  | 1:A:381:LEU:HD11 | 2.45                     | 0.43              |
| 1:B:190:LEU:HB3  | 1:B:191:SER:H    | 1.64                     | 0.43              |
| 1:C:3:VAL:CG1    | 1:C:4:ARG:N      | 2.79                     | 0.43              |
| 1:C:67:ALA:C     | 1:C:69:ALA:H     | 2.26                     | 0.43              |
| 1:C:220:ARG:NH2  | 1:C:255:ASP:OD2  | 2.51                     | 0.43              |
| 1:B:19:PHE:HD2   | 1:B:31:ARG:CZ    | 2.32                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:105:ALA:O    | 1:B:106:GLY:C    | 2.62                     | 0.43              |
| 1:B:336:LEU:HG   | 1:B:337:ALA:N    | 2.33                     | 0.43              |
| 1:C:170:ASN:HD22 | 1:C:170:ASN:HA   | 1.63                     | 0.43              |
| 1:C:357:VAL:HG13 | 1:C:358:VAL:N    | 2.27                     | 0.43              |
| 1:A:143:THR:HB   | 1:A:183:GLN:O    | 2.18                     | 0.43              |
| 1:A:218:ASN:HB3  | 1:A:221:SER:HB3  | 2.00                     | 0.43              |
| 1:B:286:VAL:O    | 1:B:286:VAL:HG22 | 2.19                     | 0.43              |
| 1:C:197:GLN:NE2  | 1:C:197:GLN:CA   | 2.80                     | 0.43              |
| 1:C:266:PHE:HB3  | 1:C:324:PRO:HA   | 1.99                     | 0.43              |
| 1:A:41:PRO:C     | 1:A:43:LEU:H     | 2.27                     | 0.43              |
| 1:B:14:ARG:C     | 1:B:16:SER:H     | 2.27                     | 0.43              |
| 1:B:244:LEU:HG   | 1:B:249:ILE:O    | 2.19                     | 0.43              |
| 1:C:49:TYR:O     | 1:C:50:ARG:HD2   | 2.19                     | 0.43              |
| 1:C:218:ASN:HB3  | 1:C:221:SER:CB   | 2.45                     | 0.43              |
| 1:A:250:PHE:CE1  | 1:A:339:GLY:HA3  | 2.53                     | 0.43              |
| 1:C:169:ILE:CG2  | 1:C:173:LEU:HD12 | 2.49                     | 0.43              |
| 1:C:359:ARG:HH12 | 1:C:382:LYS:CE   | 2.32                     | 0.43              |
| 1:A:19:PHE:HA    | 1:A:32:LEU:O     | 2.18                     | 0.43              |
| 1:B:73:LEU:HB2   | 1:B:124:LYS:HG2  | 2.01                     | 0.43              |
| 1:B:219:LEU:HD21 | 1:B:253:SER:HB2  | 2.01                     | 0.43              |
| 1:B:285:LEU:HD23 | 1:B:325:PHE:CB   | 2.42                     | 0.43              |
| 1:B:320:PRO:HB2  | 1:B:323:TYR:CG   | 2.54                     | 0.43              |
| 1:B:359:ARG:HH22 | 1:B:382:LYS:CG   | 2.32                     | 0.43              |
| 1:A:209:THR:O    | 1:A:211:SER:N    | 2.52                     | 0.43              |
| 1:A:306:ARG:HH12 | 1:C:154:SER:CA   | 2.31                     | 0.43              |
| 1:A:330:THR:O    | 1:A:331:SER:HB3  | 2.17                     | 0.43              |
| 1:B:19:PHE:HE2   | 1:B:53:GLN:HE21  | 1.65                     | 0.43              |
| 1:B:349:PHE:CE2  | 1:B:388:TYR:CD2  | 3.07                     | 0.43              |
| 1:A:60:THR:O     | 1:A:112:VAL:HG13 | 2.19                     | 0.42              |
| 1:A:96:HIS:CD2   | 1:A:96:HIS:N     | 2.86                     | 0.42              |
| 1:A:146:GLN:HA   | 1:B:302:LEU:HB3  | 2.01                     | 0.42              |
| 1:A:192:LYS:HA   | 1:A:195:ILE:HG13 | 2.01                     | 0.42              |
| 1:A:220:ARG:H    | 1:A:220:ARG:HG3  | 1.53                     | 0.42              |
| 1:B:151:GLN:OE1  | 1:B:174:PHE:CD1  | 2.72                     | 0.42              |
| 1:B:151:GLN:HE21 | 1:B:151:GLN:HB3  | 1.59                     | 0.42              |
| 1:B:275:VAL:HG21 | 1:B:336:LEU:HD23 | 2.01                     | 0.42              |
| 1:B:285:LEU:HD21 | 1:B:319:ILE:HG23 | 2.01                     | 0.42              |
| 1:C:36:PHE:HB3   | 1:C:43:LEU:HD12  | 2.01                     | 0.42              |
| 1:C:248:ASP:OD1  | 1:C:341:ASN:HA   | 2.19                     | 0.42              |
| 1:A:161:SER:HB3  | 1:B:263:LEU:HD22 | 2.01                     | 0.42              |
| 1:A:263:LEU:HD23 | 1:A:263:LEU:HA   | 1.80                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:358:VAL:HG12 | 1:A:358:VAL:O    | 2.18                     | 0.42              |
| 1:B:219:LEU:HD11 | 1:B:234:PHE:C    | 2.44                     | 0.42              |
| 1:C:130:ASN:N    | 1:C:130:ASN:ND2  | 2.65                     | 0.42              |
| 1:C:225:ILE:CD1  | 1:C:235:GLU:HB3  | 2.48                     | 0.42              |
| 1:C:265:HIS:HB3  | 1:C:349:PHE:CE1  | 2.54                     | 0.42              |
| 1:B:141:SER:HB2  | 1:C:369:ALA:HA   | 2.00                     | 0.42              |
| 1:B:335:PHE:C    | 1:B:335:PHE:CD2  | 2.97                     | 0.42              |
| 1:B:361:ILE:O    | 1:B:362:GLU:C    | 2.62                     | 0.42              |
| 1:C:259:GLY:O    | 1:C:392:ALA:N    | 2.49                     | 0.42              |
| 1:C:269:LYS:HE2  | 1:C:269:LYS:HB2  | 1.84                     | 0.42              |
| 1:A:53:GLN:HG3   | 1:A:123:ILE:HD12 | 2.02                     | 0.42              |
| 1:C:68:ASP:HB3   | 1:C:136:ASP:H    | 1.84                     | 0.42              |
| 1:A:159:GLU:CG   | 1:A:166:PHE:H    | 2.32                     | 0.42              |
| 1:B:25:ASN:ND2   | 1:B:187:ILE:HG13 | 2.35                     | 0.42              |
| 1:C:357:VAL:O    | 1:C:359:ARG:N    | 2.52                     | 0.42              |
| 1:B:226:TYR:N    | 1:B:226:TYR:CD1  | 2.87                     | 0.42              |
| 1:C:73:LEU:O     | 1:C:100:ALA:HA   | 2.20                     | 0.42              |
| 1:C:154:SER:OG   | 1:C:157:ILE:CD1  | 2.68                     | 0.42              |
| 1:C:230:PHE:HB3  | 1:C:260:ALA:CB   | 2.50                     | 0.42              |
| 1:A:150:LEU:O    | 1:A:151:GLN:C    | 2.61                     | 0.42              |
| 1:A:244:LEU:HD11 | 1:A:251:LEU:CD1  | 2.50                     | 0.42              |
| 1:A:333:LEU:HD21 | 1:A:335:PHE:HD1  | 1.85                     | 0.42              |
| 1:B:80:ALA:HA    | 1:B:112:VAL:O    | 2.19                     | 0.42              |
| 1:B:365:VAL:C    | 1:B:367:GLU:N    | 2.75                     | 0.42              |
| 1:A:154:SER:O    | 1:A:155:HIS:C    | 2.63                     | 0.42              |
| 1:B:27:ASN:HD22  | 1:B:60:THR:CG2   | 2.32                     | 0.42              |
| 1:B:140:LEU:CD1  | 1:C:358:VAL:HG13 | 2.50                     | 0.42              |
| 1:C:37:ASN:H     | 1:C:37:ASN:ND2   | 2.16                     | 0.42              |
| 1:C:164:SER:HB2  | 1:C:168:GLU:OE2  | 2.20                     | 0.42              |
| 1:A:250:PHE:HE2  | 1:A:252:SER:OG   | 2.03                     | 0.42              |
| 1:B:54:PHE:CZ    | 1:B:56:SER:HB3   | 2.55                     | 0.42              |
| 1:B:195:ILE:O    | 1:B:196:ARG:C    | 2.62                     | 0.42              |
| 1:B:211:SER:O    | 1:B:242:PRO:HG3  | 2.20                     | 0.42              |
| 1:B:219:LEU:CD2  | 1:B:253:SER:HB2  | 2.50                     | 0.42              |
| 1:B:269:LYS:H    | 1:B:345:ASN:ND2  | 2.18                     | 0.42              |
| 1:B:276:ILE:HD12 | 1:B:333:LEU:HD11 | 2.01                     | 0.42              |
| 1:B:284:GLU:OE1  | 1:B:306:ARG:NH1  | 2.51                     | 0.42              |
| 1:B:286:VAL:HG13 | 1:B:324:PRO:HD2  | 2.01                     | 0.42              |
| 1:C:285:LEU:HD11 | 1:C:320:PRO:HD2  | 2.00                     | 0.42              |
| 1:C:384:GLN:O    | 1:C:384:GLN:HG3  | 2.19                     | 0.42              |
| 1:A:122:ILE:HG22 | 1:A:123:ILE:N    | 2.34                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:376:ASP:OD1  | 1:C:171:ARG:NH2  | 2.48                     | 0.42              |
| 1:B:35:ARG:O     | 1:B:38:LYS:HB3   | 2.20                     | 0.42              |
| 1:B:86:ASN:N     | 1:B:86:ASN:ND2   | 2.68                     | 0.42              |
| 1:A:101:GLN:HG3  | 1:A:102:ARG:H    | 1.85                     | 0.41              |
| 1:A:371:PRO:O    | 1:C:181:ARG:NH2  | 2.53                     | 0.41              |
| 1:B:378:GLU:O    | 1:B:379:ARG:C    | 2.63                     | 0.41              |
| 1:B:391:ASP:OD2  | 1:B:392:ALA:N    | 2.53                     | 0.41              |
| 1:C:12:TYR:CD2   | 1:C:311:LEU:CD2  | 3.03                     | 0.41              |
| 1:A:191:SER:O    | 1:A:192:LYS:C    | 2.63                     | 0.41              |
| 1:B:305:GLN:HG3  | 1:B:306:ARG:N    | 2.34                     | 0.41              |
| 1:B:359:ARG:NH2  | 1:B:382:LYS:HE3  | 2.34                     | 0.41              |
| 1:C:31:ARG:HH11  | 1:C:53:GLN:HE22  | 1.68                     | 0.41              |
| 1:A:191:SER:N    | 1:A:194:GLN:HG3  | 2.31                     | 0.41              |
| 1:B:191:SER:H    | 1:B:194:GLN:HB2  | 1.85                     | 0.41              |
| 1:C:56:SER:HB2   | 1:C:60:THR:OG1   | 2.21                     | 0.41              |
| 1:C:199:SER:O    | 1:C:200:ARG:HG2  | 2.20                     | 0.41              |
| 1:C:342:ALA:O    | 1:C:343:GLU:C    | 2.63                     | 0.41              |
| 1:A:373:SER:O    | 1:A:376:ASP:N    | 2.52                     | 0.41              |
| 1:C:31:ARG:HH11  | 1:C:53:GLN:NE2   | 2.18                     | 0.41              |
| 1:C:35:ARG:HG3   | 1:C:50:ARG:CZ    | 2.51                     | 0.41              |
| 1:A:34:GLN:HG3   | 1:A:34:GLN:H     | 1.57                     | 0.41              |
| 1:A:198:LEU:H    | 1:A:198:LEU:HG   | 1.58                     | 0.41              |
| 1:B:29:ARG:NH1   | 1:B:31:ARG:CZ    | 2.83                     | 0.41              |
| 1:B:94:ASN:C     | 1:B:95:LEU:HD23  | 2.45                     | 0.41              |
| 1:B:222:ARG:O    | 1:B:223:ASN:C    | 2.64                     | 0.41              |
| 1:A:44:GLU:C     | 1:A:46:LEU:H     | 2.29                     | 0.41              |
| 1:A:277:ASN:C    | 1:A:277:ASN:ND2  | 2.78                     | 0.41              |
| 1:B:14:ARG:CB    | 1:B:17:ASN:HB2   | 2.22                     | 0.41              |
| 1:B:35:ARG:O     | 1:B:36:PHE:C     | 2.63                     | 0.41              |
| 1:B:205:SER:CA   | 1:B:216:PRO:HG2  | 2.51                     | 0.41              |
| 1:C:210:ILE:O    | 1:C:241:ASN:HB2  | 2.21                     | 0.41              |
| 1:C:236:ILE:HG22 | 1:C:251:LEU:HB2  | 2.03                     | 0.41              |
| 1:C:169:ILE:HG22 | 1:C:173:LEU:HD12 | 2.03                     | 0.41              |
| 1:A:244:LEU:HD21 | 1:A:251:LEU:HD12 | 2.03                     | 0.41              |
| 1:B:25:ASN:HB2   | 1:B:26:GLN:NE2   | 2.36                     | 0.41              |
| 1:B:128:PRO:HB3  | 1:B:135:TYR:HB3  | 2.03                     | 0.41              |
| 1:C:53:GLN:HE21  | 1:C:55:GLN:HE21  | 1.69                     | 0.41              |
| 1:C:359:ARG:HH12 | 1:C:382:LYS:NZ   | 2.18                     | 0.41              |
| 1:B:83:THR:HG23  | 1:B:92:SER:OG    | 2.20                     | 0.41              |
| 1:B:169:ILE:C    | 1:B:171:ARG:H    | 2.29                     | 0.41              |
| 1:B:173:LEU:HA   | 1:C:370:PHE:HB3  | 2.03                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:12:TYR:OH    | 1:C:14:ARG:HG3   | 2.21                     | 0.41              |
| 1:C:119:ASN:H    | 1:C:119:ASN:ND2  | 2.12                     | 0.41              |
| 1:C:380:LEU:HD13 | 1:C:381:LEU:HG   | 1.97                     | 0.41              |
| 1:A:340:ILE:H    | 1:A:340:ILE:HG12 | 1.76                     | 0.41              |
| 1:B:386:GLU:OE1  | 1:B:386:GLU:HA   | 2.20                     | 0.41              |
| 1:A:83:THR:O     | 1:A:109:TYR:HB2  | 2.21                     | 0.40              |
| 1:B:25:ASN:ND2   | 1:B:187:ILE:O    | 2.54                     | 0.40              |
| 1:B:110:TYR:CZ   | 1:C:365:VAL:HG21 | 2.56                     | 0.40              |
| 1:B:237:THR:HB   | 1:B:238:PRO:CD   | 2.51                     | 0.40              |
| 1:A:263:LEU:CD2  | 1:A:390:VAL:CG1  | 2.97                     | 0.40              |
| 1:C:84:LEU:HD11  | 1:C:101:GLN:HE21 | 1.86                     | 0.40              |
| 1:C:269:LYS:H    | 1:C:345:ASN:HD22 | 1.64                     | 0.40              |
| 1:C:283:ILE:HG12 | 1:C:284:GLU:N    | 2.36                     | 0.40              |
| 1:C:377:VAL:C    | 1:C:379:ARG:N    | 2.77                     | 0.40              |
| 1:A:354:LYS:HB2  | 1:A:387:SER:HB3  | 2.02                     | 0.40              |
| 1:B:49:TYR:O     | 1:B:50:ARG:HD2   | 2.20                     | 0.40              |
| 1:C:285:LEU:HB3  | 1:C:307:TYR:HB2  | 2.03                     | 0.40              |
| 1:B:380:LEU:HD23 | 1:B:383:LYS:HD2  | 2.03                     | 0.40              |
| 1:A:131:LYS:HD2  | 1:A:134:ARG:O    | 2.22                     | 0.40              |
| 1:A:353:GLU:O    | 1:A:353:GLU:HG2  | 2.21                     | 0.40              |
| 1:B:14:ARG:C     | 1:B:16:SER:N     | 2.79                     | 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     | 362/416 (87%)   | 307 (85%) | 39 (11%)  | 16 (4%)  | 2           | 4  |
| 1   | B     | 359/416 (86%)   | 293 (82%) | 55 (15%)  | 11 (3%)  | 3           | 8  |
| 1   | C     | 375/416 (90%)   | 325 (87%) | 42 (11%)  | 8 (2%)   | 5           | 15 |
| All | All   | 1096/1248 (88%) | 925 (84%) | 136 (12%) | 35 (3%)  | 3           | 7  |

All (35) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 166 | PHE  |
| 1   | A     | 229 | ASN  |
| 1   | A     | 388 | TYR  |
| 1   | B     | 26  | GLN  |
| 1   | B     | 185 | GLY  |
| 1   | B     | 229 | ASN  |
| 1   | B     | 320 | PRO  |
| 1   | C     | 199 | SER  |
| 1   | C     | 221 | SER  |
| 1   | C     | 229 | ASN  |
| 1   | A     | 42  | GLN  |
| 1   | A     | 141 | SER  |
| 1   | A     | 167 | GLU  |
| 1   | A     | 374 | ALA  |
| 1   | A     | 192 | LYS  |
| 1   | A     | 220 | ARG  |
| 1   | A     | 320 | PRO  |
| 1   | A     | 331 | SER  |
| 1   | B     | 34  | GLN  |
| 1   | A     | 206 | SER  |
| 1   | A     | 332 | ASN  |
| 1   | B     | 198 | LEU  |
| 1   | B     | 332 | ASN  |
| 1   | B     | 378 | GLU  |
| 1   | C     | 105 | ALA  |
| 1   | A     | 199 | SER  |
| 1   | B     | 331 | SER  |
| 1   | C     | 263 | LEU  |
| 1   | C     | 363 | ARG  |
| 1   | A     | 371 | PRO  |
| 1   | C     | 106 | GLY  |
| 1   | C     | 358 | VAL  |
| 1   | B     | 104 | PRO  |
| 1   | A     | 210 | ILE  |
| 1   | B     | 195 | 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     | 333/375 (89%)   | 227 (68%) | 106 (32%) | 0           | 1 |
| 1   | B     | 330/375 (88%)   | 216 (66%) | 114 (34%) | 0           | 0 |
| 1   | C     | 343/375 (92%)   | 235 (68%) | 108 (32%) | 0           | 1 |
| All | All   | 1006/1125 (89%) | 678 (67%) | 328 (33%) | 0           | 1 |

All (328) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 9   | ASN  |
| 1   | A     | 16  | SER  |
| 1   | A     | 17  | ASN  |
| 1   | A     | 26  | GLN  |
| 1   | A     | 29  | ARG  |
| 1   | A     | 31  | ARG  |
| 1   | A     | 32  | LEU  |
| 1   | A     | 34  | GLN  |
| 1   | A     | 37  | ASN  |
| 1   | A     | 38  | LYS  |
| 1   | A     | 39  | ARG  |
| 1   | A     | 40  | SER  |
| 1   | A     | 44  | GLU  |
| 1   | A     | 47  | ARG  |
| 1   | A     | 51  | ILE  |
| 1   | A     | 53  | GLN  |
| 1   | A     | 55  | GLN  |
| 1   | A     | 56  | SER  |
| 1   | A     | 62  | LEU  |
| 1   | A     | 70  | ASP  |
| 1   | A     | 72  | LEU  |
| 1   | A     | 73  | LEU  |
| 1   | A     | 76  | LEU  |
| 1   | A     | 77  | SER  |
| 1   | A     | 82  | LEU  |
| 1   | A     | 85  | VAL  |
| 1   | A     | 92  | SER  |
| 1   | A     | 96  | HIS  |
| 1   | A     | 117 | HIS  |
| 1   | A     | 123 | ILE  |
| 1   | A     | 131 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 140 | LEU  |
| 1   | A     | 146 | GLN  |
| 1   | A     | 147 | GLN  |
| 1   | A     | 156 | ASN  |
| 1   | A     | 157 | ILE  |
| 1   | A     | 160 | THR  |
| 1   | A     | 165 | GLU  |
| 1   | A     | 167 | GLU  |
| 1   | A     | 169 | ILE  |
| 1   | A     | 171 | ARG  |
| 1   | A     | 172 | VAL  |
| 1   | A     | 174 | PHE  |
| 1   | A     | 183 | GLN  |
| 1   | A     | 187 | ILE  |
| 1   | A     | 188 | VAL  |
| 1   | A     | 190 | LEU  |
| 1   | A     | 194 | GLN  |
| 1   | A     | 195 | ILE  |
| 1   | A     | 196 | ARG  |
| 1   | A     | 197 | GLN  |
| 1   | A     | 198 | LEU  |
| 1   | A     | 200 | ARG  |
| 1   | A     | 201 | ARG  |
| 1   | A     | 204 | SER  |
| 1   | A     | 207 | ARG  |
| 1   | A     | 210 | ILE  |
| 1   | A     | 213 | GLU  |
| 1   | A     | 214 | ASP  |
| 1   | A     | 215 | GLU  |
| 1   | A     | 220 | ARG  |
| 1   | A     | 222 | ARG  |
| 1   | A     | 227 | SER  |
| 1   | A     | 229 | ASN  |
| 1   | A     | 230 | PHE  |
| 1   | A     | 232 | LYS  |
| 1   | A     | 236 | ILE  |
| 1   | A     | 240 | LYS  |
| 1   | A     | 244 | LEU  |
| 1   | A     | 245 | ARG  |
| 1   | A     | 252 | SER  |
| 1   | A     | 254 | VAL  |
| 1   | A     | 257 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 261 | LEU  |
| 1   | A     | 275 | VAL  |
| 1   | A     | 280 | ASP  |
| 1   | A     | 282 | ASN  |
| 1   | A     | 285 | LEU  |
| 1   | A     | 290 | GLU  |
| 1   | A     | 291 | GLN  |
| 1   | A     | 302 | LEU  |
| 1   | A     | 304 | VAL  |
| 1   | A     | 310 | GLU  |
| 1   | A     | 312 | SER  |
| 1   | A     | 313 | GLU  |
| 1   | A     | 318 | VAL  |
| 1   | A     | 326 | VAL  |
| 1   | A     | 333 | LEU  |
| 1   | A     | 334 | ASN  |
| 1   | A     | 336 | LEU  |
| 1   | A     | 340 | ILE  |
| 1   | A     | 343 | GLU  |
| 1   | A     | 346 | GLN  |
| 1   | A     | 347 | ARG  |
| 1   | A     | 354 | LYS  |
| 1   | A     | 359 | ARG  |
| 1   | A     | 363 | ARG  |
| 1   | A     | 368 | LEU  |
| 1   | A     | 375 | GLN  |
| 1   | A     | 378 | GLU  |
| 1   | A     | 379 | ARG  |
| 1   | A     | 380 | LEU  |
| 1   | A     | 382 | LYS  |
| 1   | A     | 385 | ARG  |
| 1   | A     | 386 | GLU  |
| 1   | A     | 390 | VAL  |
| 1   | B     | 15  | SER  |
| 1   | B     | 17  | ASN  |
| 1   | B     | 18  | SER  |
| 1   | B     | 20  | GLN  |
| 1   | B     | 21  | THR  |
| 1   | B     | 26  | GLN  |
| 1   | B     | 29  | ARG  |
| 1   | B     | 32  | LEU  |
| 1   | B     | 37  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 43  | LEU  |
| 1   | B     | 44  | GLU  |
| 1   | B     | 48  | ASP  |
| 1   | B     | 51  | ILE  |
| 1   | B     | 53  | GLN  |
| 1   | B     | 61  | ILE  |
| 1   | B     | 62  | LEU  |
| 1   | B     | 70  | ASP  |
| 1   | B     | 73  | LEU  |
| 1   | B     | 75  | VAL  |
| 1   | B     | 79  | ARG  |
| 1   | B     | 81  | ILE  |
| 1   | B     | 84  | LEU  |
| 1   | B     | 86  | ASN  |
| 1   | B     | 90  | ARG  |
| 1   | B     | 94  | ASN  |
| 1   | B     | 95  | LEU  |
| 1   | B     | 102 | ARG  |
| 1   | B     | 119 | ASN  |
| 1   | B     | 122 | ILE  |
| 1   | B     | 123 | ILE  |
| 1   | B     | 131 | LYS  |
| 1   | B     | 134 | ARG  |
| 1   | B     | 137 | ASP  |
| 1   | B     | 140 | LEU  |
| 1   | B     | 146 | GLN  |
| 1   | B     | 148 | SER  |
| 1   | B     | 151 | GLN  |
| 1   | B     | 154 | SER  |
| 1   | B     | 156 | ASN  |
| 1   | B     | 157 | ILE  |
| 1   | B     | 158 | LEU  |
| 1   | B     | 160 | THR  |
| 1   | B     | 161 | SER  |
| 1   | B     | 165 | GLU  |
| 1   | B     | 167 | GLU  |
| 1   | B     | 171 | ARG  |
| 1   | B     | 186 | VAL  |
| 1   | B     | 187 | ILE  |
| 1   | B     | 188 | VAL  |
| 1   | B     | 192 | LYS  |
| 1   | B     | 195 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 197 | GLN  |
| 1   | B     | 198 | LEU  |
| 1   | B     | 199 | SER  |
| 1   | B     | 200 | ARG  |
| 1   | B     | 201 | ARG  |
| 1   | B     | 203 | LYS  |
| 1   | B     | 206 | SER  |
| 1   | B     | 207 | ARG  |
| 1   | B     | 208 | LYS  |
| 1   | B     | 211 | SER  |
| 1   | B     | 213 | GLU  |
| 1   | B     | 215 | GLU  |
| 1   | B     | 219 | LEU  |
| 1   | B     | 221 | SER  |
| 1   | B     | 222 | ARG  |
| 1   | B     | 226 | TYR  |
| 1   | B     | 228 | ASN  |
| 1   | B     | 229 | ASN  |
| 1   | B     | 232 | LYS  |
| 1   | B     | 236 | ILE  |
| 1   | B     | 239 | GLU  |
| 1   | B     | 240 | LYS  |
| 1   | B     | 244 | LEU  |
| 1   | B     | 247 | LEU  |
| 1   | B     | 257 | ASN  |
| 1   | B     | 261 | LEU  |
| 1   | B     | 265 | HIS  |
| 1   | B     | 268 | SER  |
| 1   | B     | 272 | VAL  |
| 1   | B     | 274 | LEU  |
| 1   | B     | 275 | VAL  |
| 1   | B     | 277 | ASN  |
| 1   | B     | 282 | ASN  |
| 1   | B     | 283 | ILE  |
| 1   | B     | 285 | LEU  |
| 1   | B     | 286 | VAL  |
| 1   | B     | 288 | ILE  |
| 1   | B     | 289 | LYS  |
| 1   | B     | 290 | GLU  |
| 1   | B     | 302 | LEU  |
| 1   | B     | 306 | ARG  |
| 1   | B     | 308 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 310 | GLU  |
| 1   | B     | 318 | VAL  |
| 1   | B     | 319 | ILE  |
| 1   | B     | 332 | ASN  |
| 1   | B     | 333 | LEU  |
| 1   | B     | 334 | ASN  |
| 1   | B     | 336 | LEU  |
| 1   | B     | 343 | GLU  |
| 1   | B     | 346 | GLN  |
| 1   | B     | 357 | VAL  |
| 1   | B     | 358 | VAL  |
| 1   | B     | 364 | GLN  |
| 1   | B     | 368 | LEU  |
| 1   | B     | 373 | SER  |
| 1   | B     | 375 | GLN  |
| 1   | B     | 378 | GLU  |
| 1   | B     | 379 | ARG  |
| 1   | B     | 380 | LEU  |
| 1   | B     | 383 | LYS  |
| 1   | B     | 386 | GLU  |
| 1   | B     | 390 | VAL  |
| 1   | C     | 3   | VAL  |
| 1   | C     | 4   | ARG  |
| 1   | C     | 5   | GLU  |
| 1   | C     | 7   | GLU  |
| 1   | C     | 8   | ASN  |
| 1   | C     | 16  | SER  |
| 1   | C     | 18  | SER  |
| 1   | C     | 22  | LEU  |
| 1   | C     | 26  | GLN  |
| 1   | C     | 31  | ARG  |
| 1   | C     | 32  | LEU  |
| 1   | C     | 33  | LEU  |
| 1   | C     | 37  | ASN  |
| 1   | C     | 38  | LYS  |
| 1   | C     | 39  | ARG  |
| 1   | C     | 42  | GLN  |
| 1   | C     | 43  | LEU  |
| 1   | C     | 44  | GLU  |
| 1   | C     | 51  | ILE  |
| 1   | C     | 53  | GLN  |
| 1   | C     | 61  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 62  | LEU  |
| 1   | C     | 70  | ASP  |
| 1   | C     | 79  | ARG  |
| 1   | C     | 82  | LEU  |
| 1   | C     | 85  | VAL  |
| 1   | C     | 94  | ASN  |
| 1   | C     | 96  | HIS  |
| 1   | C     | 101 | GLN  |
| 1   | C     | 112 | VAL  |
| 1   | C     | 115 | HIS  |
| 1   | C     | 119 | ASN  |
| 1   | C     | 131 | LYS  |
| 1   | C     | 140 | LEU  |
| 1   | C     | 146 | GLN  |
| 1   | C     | 148 | SER  |
| 1   | C     | 150 | LEU  |
| 1   | C     | 154 | SER  |
| 1   | C     | 157 | ILE  |
| 1   | C     | 165 | GLU  |
| 1   | C     | 169 | ILE  |
| 1   | C     | 170 | ASN  |
| 1   | C     | 171 | ARG  |
| 1   | C     | 182 | GLN  |
| 1   | C     | 183 | GLN  |
| 1   | C     | 184 | GLU  |
| 1   | C     | 188 | VAL  |
| 1   | C     | 190 | LEU  |
| 1   | C     | 192 | LYS  |
| 1   | C     | 197 | GLN  |
| 1   | C     | 198 | LEU  |
| 1   | C     | 200 | ARG  |
| 1   | C     | 203 | LYS  |
| 1   | C     | 204 | SER  |
| 1   | C     | 208 | LYS  |
| 1   | C     | 210 | ILE  |
| 1   | C     | 212 | SER  |
| 1   | C     | 214 | ASP  |
| 1   | C     | 219 | LEU  |
| 1   | C     | 220 | ARG  |
| 1   | C     | 221 | SER  |
| 1   | C     | 223 | ASN  |
| 1   | C     | 228 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 229 | ASN  |
| 1   | C     | 230 | PHE  |
| 1   | C     | 232 | LYS  |
| 1   | C     | 236 | ILE  |
| 1   | C     | 239 | GLU  |
| 1   | C     | 240 | LYS  |
| 1   | C     | 244 | LEU  |
| 1   | C     | 254 | VAL  |
| 1   | C     | 261 | LEU  |
| 1   | C     | 269 | LYS  |
| 1   | C     | 272 | VAL  |
| 1   | C     | 274 | LEU  |
| 1   | C     | 275 | VAL  |
| 1   | C     | 278 | GLU  |
| 1   | C     | 283 | ILE  |
| 1   | C     | 285 | LEU  |
| 1   | C     | 288 | ILE  |
| 1   | C     | 302 | LEU  |
| 1   | C     | 305 | GLN  |
| 1   | C     | 306 | ARG  |
| 1   | C     | 311 | LEU  |
| 1   | C     | 319 | ILE  |
| 1   | C     | 326 | VAL  |
| 1   | C     | 328 | ASN  |
| 1   | C     | 332 | ASN  |
| 1   | C     | 333 | LEU  |
| 1   | C     | 334 | ASN  |
| 1   | C     | 336 | LEU  |
| 1   | C     | 346 | GLN  |
| 1   | C     | 353 | GLU  |
| 1   | C     | 358 | VAL  |
| 1   | C     | 360 | GLN  |
| 1   | C     | 361 | ILE  |
| 1   | C     | 362 | GLU  |
| 1   | C     | 363 | ARG  |
| 1   | C     | 367 | GLU  |
| 1   | C     | 370 | PHE  |
| 1   | C     | 373 | SER  |
| 1   | C     | 375 | GLN  |
| 1   | C     | 376 | ASP  |
| 1   | C     | 378 | GLU  |
| 1   | C     | 379 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 380 | LEU  |
| 1   | C     | 382 | LYS  |
| 1   | C     | 385 | ARG  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (83) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 9   | ASN  |
| 1   | A     | 17  | ASN  |
| 1   | A     | 26  | GLN  |
| 1   | A     | 27  | ASN  |
| 1   | A     | 37  | ASN  |
| 1   | A     | 53  | GLN  |
| 1   | A     | 55  | GLN  |
| 1   | A     | 59  | ASN  |
| 1   | A     | 65  | HIS  |
| 1   | A     | 66  | HIS  |
| 1   | A     | 96  | HIS  |
| 1   | A     | 113 | ASN  |
| 1   | A     | 115 | HIS  |
| 1   | A     | 118 | GLN  |
| 1   | A     | 130 | ASN  |
| 1   | A     | 156 | ASN  |
| 1   | A     | 197 | GLN  |
| 1   | A     | 277 | ASN  |
| 1   | A     | 282 | ASN  |
| 1   | A     | 305 | GLN  |
| 1   | A     | 328 | ASN  |
| 1   | A     | 334 | ASN  |
| 1   | A     | 341 | ASN  |
| 1   | A     | 344 | ASN  |
| 1   | A     | 345 | ASN  |
| 1   | A     | 348 | ASN  |
| 1   | A     | 356 | ASN  |
| 1   | A     | 366 | GLN  |
| 1   | B     | 20  | GLN  |
| 1   | B     | 27  | ASN  |
| 1   | B     | 34  | GLN  |
| 1   | B     | 53  | GLN  |
| 1   | B     | 55  | GLN  |
| 1   | B     | 59  | ASN  |
| 1   | B     | 65  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 86  | ASN  |
| 1   | B     | 115 | HIS  |
| 1   | B     | 118 | GLN  |
| 1   | B     | 151 | GLN  |
| 1   | B     | 156 | ASN  |
| 1   | B     | 163 | HIS  |
| 1   | B     | 170 | ASN  |
| 1   | B     | 183 | GLN  |
| 1   | B     | 194 | GLN  |
| 1   | B     | 197 | GLN  |
| 1   | B     | 228 | ASN  |
| 1   | B     | 257 | ASN  |
| 1   | B     | 265 | HIS  |
| 1   | B     | 267 | ASN  |
| 1   | B     | 282 | ASN  |
| 1   | B     | 305 | GLN  |
| 1   | B     | 328 | ASN  |
| 1   | B     | 332 | ASN  |
| 1   | B     | 334 | ASN  |
| 1   | B     | 344 | ASN  |
| 1   | B     | 345 | ASN  |
| 1   | B     | 346 | GLN  |
| 1   | C     | 26  | GLN  |
| 1   | C     | 27  | ASN  |
| 1   | C     | 37  | ASN  |
| 1   | C     | 42  | GLN  |
| 1   | C     | 53  | GLN  |
| 1   | C     | 55  | GLN  |
| 1   | C     | 94  | ASN  |
| 1   | C     | 115 | HIS  |
| 1   | C     | 119 | ASN  |
| 1   | C     | 130 | ASN  |
| 1   | C     | 146 | GLN  |
| 1   | C     | 170 | ASN  |
| 1   | C     | 194 | GLN  |
| 1   | C     | 197 | GLN  |
| 1   | C     | 218 | ASN  |
| 1   | C     | 257 | ASN  |
| 1   | C     | 277 | ASN  |
| 1   | C     | 328 | ASN  |
| 1   | C     | 334 | ASN  |
| 1   | C     | 341 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 344 | ASN  |
| 1   | C     | 345 | ASN  |
| 1   | C     | 356 | ASN  |
| 1   | C     | 360 | GLN  |
| 1   | C     | 375 | GLN  |
| 1   | C     | 384 | GLN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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     | 368/416 (88%)   | -0.64  | 0 <b>100</b> <b>100</b>    | 5, 20, 41, 55         | 0     |
| 1   | B     | 365/416 (87%)   | -0.45  | 1 (0%) <b>90</b> <b>89</b> | 9, 31, 49, 59         | 0     |
| 1   | C     | 379/416 (91%)   | -0.61  | 0 <b>100</b> <b>100</b>    | 5, 21, 43, 55         | 0     |
| All | All   | 1112/1248 (89%) | -0.57  | 1 (0%) <b>92</b> <b>91</b> | 5, 24, 45, 59         | 0     |

All (1) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 290 | GLU  | 2.1  |

### 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.