



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 08:15 PM UTC

PDB ID : 4RCN / pdb\_00004rcn  
Title : Structure and function of a single-chain, multi-domain long-chain acyl-coa carboxylase  
Authors : Tran, T.H.; Tong, L.  
Deposited on : 2014-09-16  
Resolution : 3.01 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                                                             |

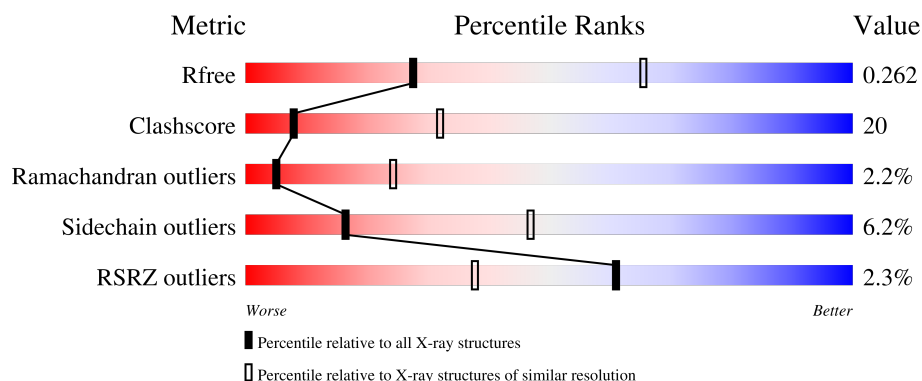
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.01 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                      | 3131 (3.04-3.00)                                      |
| Clashscore            | 190562                      | 3444 (3.04-3.00)                                      |
| Ramachandran outliers | 187476                      | 3319 (3.04-3.00)                                      |
| Sidechain outliers    | 187428                      | 3322 (3.04-3.00)                                      |
| RSRZ outliers         | 180081                      | 3130 (3.04-3.00)                                      |

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     | 1093   | <div> <div>2%</div> <div> <div></div> <div>54%</div> <div>31%</div> <div>•</div> <div>11%</div> </div> </div> |
| 1   | B     | 1093   | <div> <div>3%</div> <div> <div></div> <div>56%</div> <div>32%</div> <div>•</div> <div>9%</div> </div> </div>  |

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 14630 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 long-chain acyl-CoA carboxylase.

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 1   | A     | 972      | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 7211  | 4528 | 1319 | 1340 | 24 |         |         |       |
| 1   | B     | 1000     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 7419  | 4661 | 1354 | 1377 | 27 |         |         |       |

There are 36 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 1076    | GLU      | -      | expression tag | UNP Q73VY8 |
| A     | 1077    | LEU      | -      | expression tag | UNP Q73VY8 |
| A     | 1078    | LEU      | -      | expression tag | UNP Q73VY8 |
| A     | 1079    | VAL      | -      | expression tag | UNP Q73VY8 |
| A     | 1080    | ASP      | -      | expression tag | UNP Q73VY8 |
| A     | 1081    | LYS      | -      | expression tag | UNP Q73VY8 |
| A     | 1082    | LEU      | -      | expression tag | UNP Q73VY8 |
| A     | 1083    | ALA      | -      | expression tag | UNP Q73VY8 |
| A     | 1084    | ALA      | -      | expression tag | UNP Q73VY8 |
| A     | 1085    | ALA      | -      | expression tag | UNP Q73VY8 |
| A     | 1086    | LEU      | -      | expression tag | UNP Q73VY8 |
| A     | 1087    | GLU      | -      | expression tag | UNP Q73VY8 |
| A     | 1088    | HIS      | -      | expression tag | UNP Q73VY8 |
| A     | 1089    | HIS      | -      | expression tag | UNP Q73VY8 |
| A     | 1090    | HIS      | -      | expression tag | UNP Q73VY8 |
| A     | 1091    | HIS      | -      | expression tag | UNP Q73VY8 |
| A     | 1092    | HIS      | -      | expression tag | UNP Q73VY8 |
| A     | 1093    | HIS      | -      | expression tag | UNP Q73VY8 |
| B     | 1076    | GLU      | -      | expression tag | UNP Q73VY8 |
| B     | 1077    | LEU      | -      | expression tag | UNP Q73VY8 |
| B     | 1078    | LEU      | -      | expression tag | UNP Q73VY8 |
| B     | 1079    | VAL      | -      | expression tag | UNP Q73VY8 |
| B     | 1080    | ASP      | -      | expression tag | UNP Q73VY8 |
| B     | 1081    | LYS      | -      | expression tag | UNP Q73VY8 |
| B     | 1082    | LEU      | -      | expression tag | UNP Q73VY8 |

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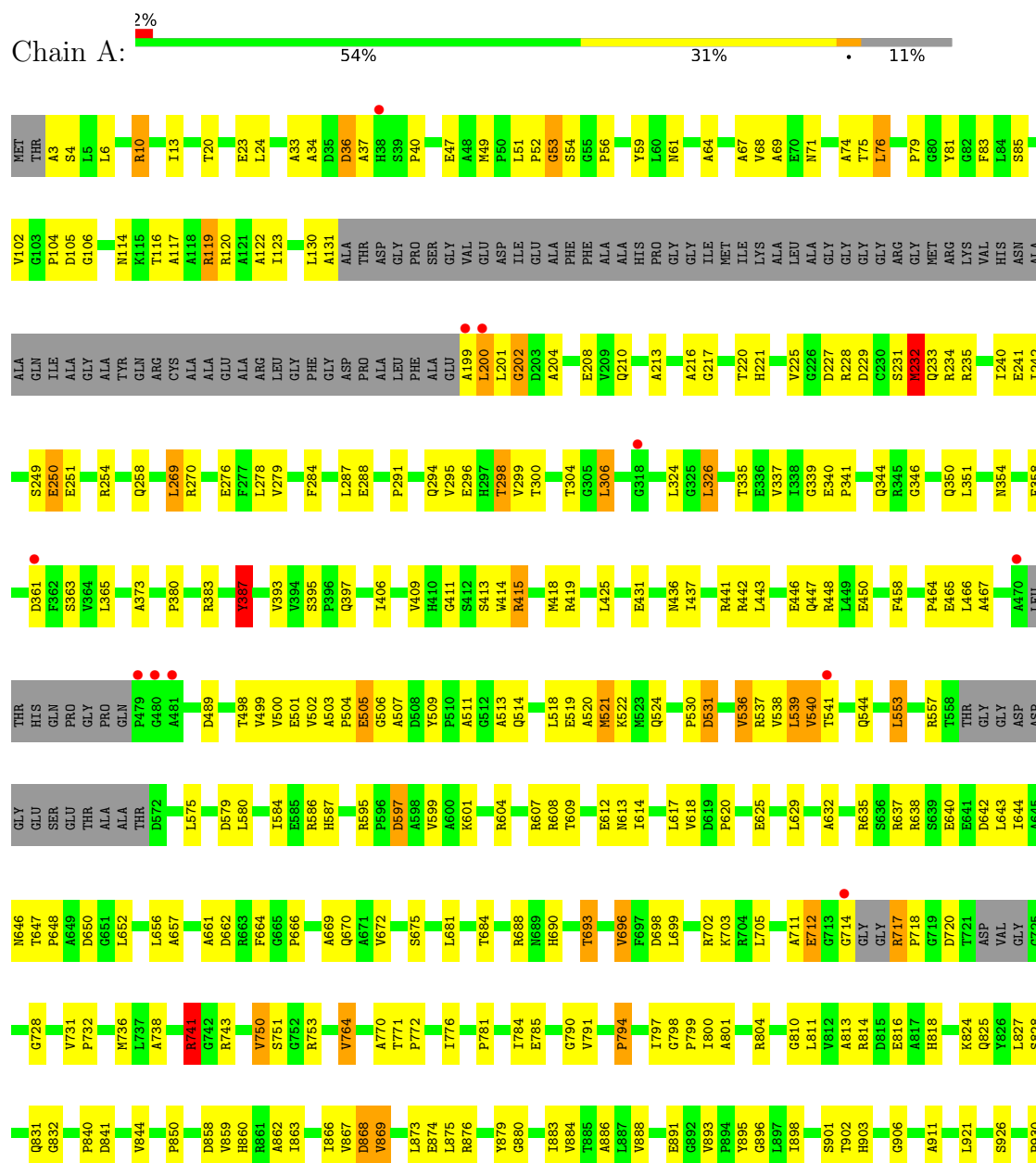
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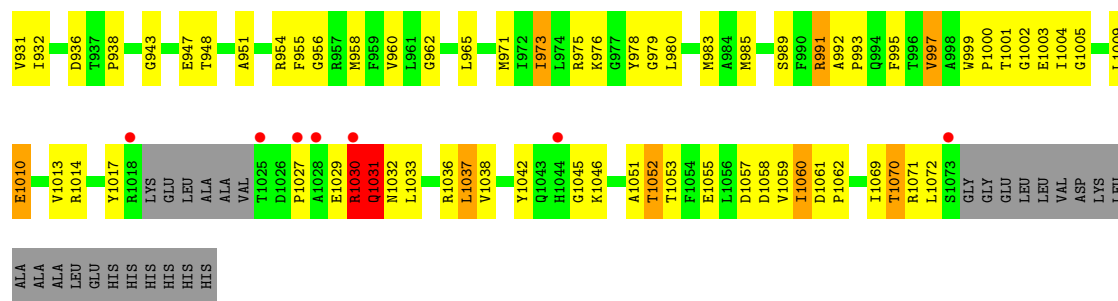
| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| B     | 1083    | ALA      | -      | expression tag | UNP Q73VY8 |
| B     | 1084    | ALA      | -      | expression tag | UNP Q73VY8 |
| B     | 1085    | ALA      | -      | expression tag | UNP Q73VY8 |
| B     | 1086    | LEU      | -      | expression tag | UNP Q73VY8 |
| B     | 1087    | GLU      | -      | expression tag | UNP Q73VY8 |
| B     | 1088    | HIS      | -      | expression tag | UNP Q73VY8 |
| B     | 1089    | HIS      | -      | expression tag | UNP Q73VY8 |
| B     | 1090    | HIS      | -      | expression tag | UNP Q73VY8 |
| B     | 1091    | HIS      | -      | expression tag | UNP Q73VY8 |
| B     | 1092    | HIS      | -      | expression tag | UNP Q73VY8 |
| B     | 1093    | HIS      | -      | expression tag | UNP Q73VY8 |

### 3 Residue-property plots

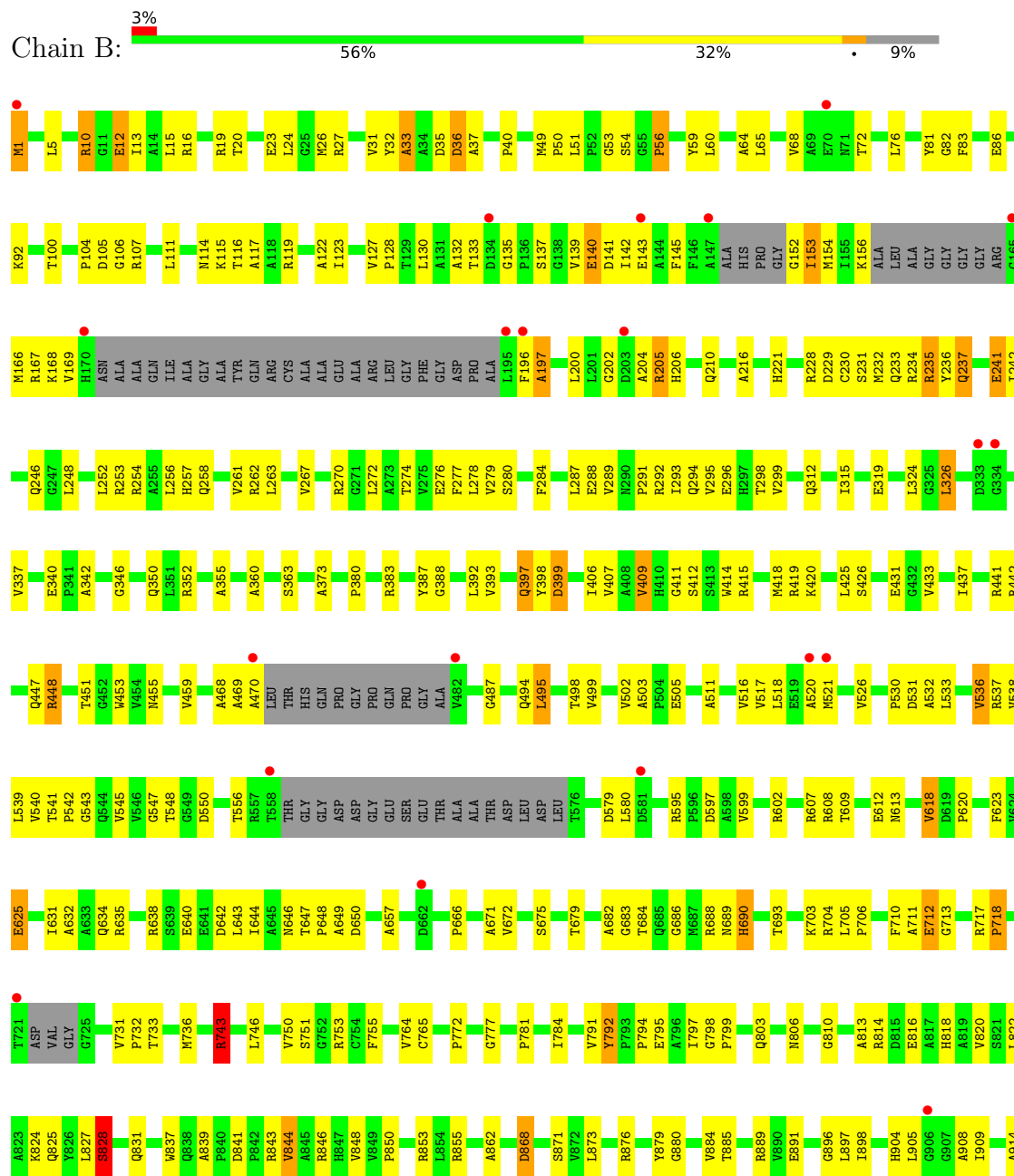
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

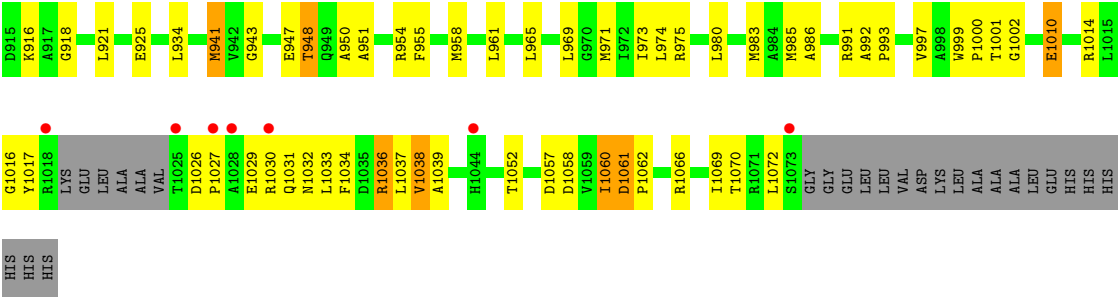
- Molecule 1: long-chain acyl-CoA carboxylase





- Molecule 1: long-chain acyl-CoA carboxylase





## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 3                                                      | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 220.88Å 220.88Å 220.88Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 49.39 – 3.01<br>49.39 – 3.01                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 91.0 (49.39-3.01)<br>91.1 (49.39-3.01)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.10                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.10 (at 3.01Å)                                             | Xtriage          |
| Refinement program                                                      | CNS 1.3                                                     | Depositor        |
| R, $R_{free}$                                                           | 0.209 , 0.262<br>0.209 , 0.262                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 3516 reflections (5.09%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 63.4                                                        | Xtriage          |
| Anisotropy                                                              | 0.000                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.32 , 52.3                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$ | Xtriage          |
| Estimated twinning fraction                                             | 0.026 for l,-k,h                                            | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.93                                                        | EDS              |
| Total number of atoms                                                   | 14630                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 66.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.77% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality

### 5.1 Standard geometry

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

| Mol | Chain | Bond lengths |             | Bond angles |                 |
|-----|-------|--------------|-------------|-------------|-----------------|
|     |       | RMSZ         | $\# Z  > 5$ | RMSZ        | $\# Z  > 5$     |
| 1   | A     | 0.48         | 0/7339      | 1.02        | 30/9980 (0.3%)  |
| 1   | B     | 0.51         | 0/7550      | 1.00        | 21/10259 (0.2%) |
| All | All   | 0.50         | 0/14889     | 1.01        | 51/20239 (0.3%) |

There are no bond length outliers.

All (51) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | A     | 764  | VAL  | N-CA-C  | -9.28 | 103.99      | 112.90   |
| 1   | B     | 1061 | ASP  | N-CA-C  | -7.26 | 98.67       | 109.42   |
| 1   | A     | 37   | ALA  | N-CA-C  | 7.03  | 118.95      | 111.28   |
| 1   | A     | 1060 | ILE  | N-CA-C  | 6.99  | 119.93      | 109.17   |
| 1   | A     | 387  | TYR  | N-CA-C  | -6.79 | 106.19      | 114.75   |
| 1   | A     | 717  | ARG  | CA-C-N  | 6.78  | 128.31      | 119.84   |
| 1   | A     | 717  | ARG  | C-N-CA  | 6.78  | 128.31      | 119.84   |
| 1   | B     | 397  | GLN  | N-CA-C  | 6.74  | 119.64      | 111.82   |
| 1   | A     | 1061 | ASP  | N-CA-C  | -6.58 | 99.69       | 109.42   |
| 1   | A     | 1030 | ARG  | N-CA-C  | -6.44 | 103.77      | 111.69   |
| 1   | B     | 1060 | ILE  | N-CA-C  | 6.42  | 119.06      | 109.17   |
| 1   | A     | 637  | ARG  | N-CA-C  | -6.25 | 105.43      | 114.12   |
| 1   | A     | 751  | SER  | N-CA-C  | -6.25 | 99.81       | 109.24   |
| 1   | A     | 83   | PHE  | CB-CA-C | -6.23 | 109.37      | 116.54   |
| 1   | B     | 750  | VAL  | N-CA-C  | 6.07  | 116.75      | 107.77   |
| 1   | B     | 56   | PRO  | N-CA-C  | 6.03  | 118.06      | 110.70   |
| 1   | B     | 33   | ALA  | N-CA-C  | -5.98 | 102.63      | 110.53   |
| 1   | B     | 743  | ARG  | N-CA-C  | 5.95  | 118.66      | 111.40   |
| 1   | A     | 869  | VAL  | N-CA-C  | 5.95  | 121.72      | 109.34   |
| 1   | A     | 298  | THR  | N-CA-C  | 5.79  | 117.59      | 111.28   |
| 1   | A     | 339  | GLY  | N-CA-C  | 5.76  | 117.91      | 112.04   |
| 1   | B     | 896  | GLY  | N-CA-C  | -5.72 | 100.47      | 112.04   |
| 1   | A     | 625  | GLU  | N-CA-C  | 5.71  | 118.52      | 110.23   |
| 1   | A     | 666  | PRO  | N-CA-C  | -5.70 | 106.58      | 114.27   |
| 1   | A     | 750  | VAL  | N-CA-C  | 5.69  | 116.48      | 108.17   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 1   | B     | 690  | HIS  | N-CA-C | -5.68 | 105.23      | 111.82   |
| 1   | B     | 132  | ALA  | N-CA-C | 5.67  | 115.88      | 107.88   |
| 1   | B     | 37   | ALA  | N-CA-C | 5.66  | 118.99      | 111.75   |
| 1   | A     | 690  | HIS  | N-CA-C | -5.62 | 105.07      | 111.14   |
| 1   | B     | 1036 | ARG  | N-CA-C | -5.62 | 106.10      | 113.12   |
| 1   | B     | 412  | SER  | N-CA-C | 5.61  | 118.52      | 109.83   |
| 1   | A     | 306  | LEU  | N-CA-C | 5.60  | 117.76      | 110.43   |
| 1   | A     | 938  | PRO  | N-CA-C | -5.57 | 106.75      | 114.27   |
| 1   | B     | 625  | GLU  | N-CA-C | 5.57  | 118.31      | 110.23   |
| 1   | B     | 954  | ARG  | N-CA-C | 5.56  | 117.42      | 111.36   |
| 1   | B     | 666  | PRO  | N-CA-C | -5.55 | 107.42      | 114.35   |
| 1   | A     | 893  | VAL  | CA-C-N | 5.50  | 126.35      | 120.13   |
| 1   | A     | 893  | VAL  | C-N-CA | 5.50  | 126.35      | 120.13   |
| 1   | B     | 236  | TYR  | N-CA-C | 5.38  | 119.79      | 113.23   |
| 1   | A     | 522  | LYS  | N-CA-C | -5.35 | 107.76      | 114.56   |
| 1   | B     | 27   | ARG  | N-CA-C | -5.32 | 101.02      | 109.96   |
| 1   | B     | 298  | THR  | N-CA-C | 5.29  | 117.05      | 111.28   |
| 1   | A     | 896  | GLY  | N-CA-C | -5.24 | 101.45      | 112.04   |
| 1   | A     | 832  | GLY  | N-CA-C | 5.18  | 117.73      | 110.38   |
| 1   | A     | 906  | GLY  | N-CA-C | -5.17 | 108.49      | 115.36   |
| 1   | B     | 828  | SER  | N-CA-C | 5.16  | 117.57      | 111.33   |
| 1   | B     | 618  | VAL  | N-CA-C | 5.10  | 116.98      | 109.63   |
| 1   | A     | 931  | VAL  | N-CA-C | 5.05  | 115.85      | 108.53   |
| 1   | A     | 217  | GLY  | N-CA-C | -5.04 | 101.23      | 113.18   |
| 1   | A     | 868  | ASP  | N-CA-C | 5.04  | 117.54      | 110.23   |
| 1   | A     | 962  | GLY  | N-CA-C | -5.03 | 106.32      | 113.86   |

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     | 7211  | 0        | 7244     | 285     | 0            |
| 1   | B     | 7419  | 0        | 7452     | 300     | 0            |
| All | All   | 14630 | 0        | 14696    | 577     | 0            |

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

All (577) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:632:ALA:H    | 1:A:647:THR:HG21  | 1.27                     | 1.00              |
| 1:A:504:PRO:HD2  | 1:A:509:TYR:OH    | 1.65                     | 0.96              |
| 1:A:210:GLN:HE21 | 1:A:228:ARG:HH12  | 1.03                     | 0.94              |
| 1:B:753:ARG:HG2  | 1:B:753:ARG:HH11  | 1.34                     | 0.92              |
| 1:B:92:LYS:HE2   | 1:B:107:ARG:NH1   | 1.84                     | 0.92              |
| 1:B:231:SER:O    | 1:B:233:GLN:HG2   | 1.71                     | 0.91              |
| 1:B:156:LYS:HE2  | 1:B:166:MET:HE3   | 1.52                     | 0.91              |
| 1:B:326:LEU:HD12 | 1:B:326:LEU:H     | 1.36                     | 0.91              |
| 1:B:608:ARG:HH11 | 1:B:613:ASN:HD22  | 1.18                     | 0.91              |
| 1:B:499:VAL:HG21 | 1:B:540:VAL:HG11  | 1.54                     | 0.90              |
| 1:B:92:LYS:HE2   | 1:B:107:ARG:HH11  | 1.36                     | 0.88              |
| 1:A:632:ALA:N    | 1:A:647:THR:HG21  | 1.90                     | 0.87              |
| 1:B:1033:LEU:O   | 1:B:1037:LEU:HD13 | 1.74                     | 0.86              |
| 1:A:500:VAL:HG21 | 1:A:519:GLU:HG3   | 1.60                     | 0.84              |
| 1:B:850:PRO:HG2  | 1:B:975:ARG:HH22  | 1.43                     | 0.84              |
| 1:A:859:VAL:HG11 | 1:A:901:SER:HA    | 1.60                     | 0.84              |
| 1:B:632:ALA:H    | 1:B:647:THR:HG21  | 1.44                     | 0.83              |
| 1:B:373:ALA:HB3  | 1:B:431:GLU:HB3   | 1.61                     | 0.83              |
| 1:B:914:ALA:HA   | 1:B:958:MET:HE2   | 1.61                     | 0.82              |
| 1:B:814:ARG:H    | 1:B:818:HIS:HD2   | 1.25                     | 0.82              |
| 1:A:210:GLN:NE2  | 1:A:228:ARG:HH12  | 1.78                     | 0.82              |
| 1:B:425:LEU:HD22 | 1:B:437:ILE:HG23  | 1.63                     | 0.81              |
| 1:B:711:ALA:O    | 1:B:712:GLU:HB2   | 1.80                     | 0.81              |
| 1:B:426:SER:HB3  | 1:B:441:ARG:NH2   | 1.96                     | 0.80              |
| 1:A:49:MET:HE1   | 1:B:494:GLN:HB3   | 1.63                     | 0.80              |
| 1:A:642:ASP:HB2  | 1:A:646:ASN:ND2   | 1.96                     | 0.80              |
| 1:B:941:MET:HE3  | 1:B:941:MET:HA    | 1.62                     | 0.79              |
| 1:A:800:ILE:O    | 1:A:804:ARG:HB2   | 1.83                     | 0.77              |
| 1:A:781:PRO:HG2  | 1:A:794:PRO:HG3   | 1.66                     | 0.77              |
| 1:A:580:LEU:O    | 1:A:584:ILE:HG12  | 1.83                     | 0.77              |
| 1:A:199:ALA:O    | 1:A:200:LEU:HG    | 1.84                     | 0.77              |
| 1:B:278:LEU:HG   | 1:B:287:LEU:HD22  | 1.67                     | 0.76              |
| 1:A:601:LYS:HD3  | 1:A:604:ARG:HE    | 1.50                     | 0.75              |
| 1:B:499:VAL:HG21 | 1:B:540:VAL:CG1   | 2.15                     | 0.75              |
| 1:A:298:THR:HB   | 1:A:406:ILE:HD13  | 1.69                     | 0.75              |
| 1:B:234:ARG:NH2  | 1:B:235:ARG:HE    | 1.85                     | 0.75              |
| 1:B:772:PRO:HD3  | 1:B:813:ALA:O     | 1.85                     | 0.75              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:231:SER:O    | 1:A:233:GLN:HG2  | 1.87                     | 0.75              |
| 1:A:841:ASP:HB3  | 1:A:844:VAL:HG23 | 1.67                     | 0.75              |
| 1:B:152:GLY:O    | 1:B:153:ILE:HD12 | 1.87                     | 0.74              |
| 1:B:608:ARG:HH11 | 1:B:613:ASN:ND2  | 1.86                     | 0.74              |
| 1:A:201:LEU:HD12 | 1:A:202:GLY:H    | 1.52                     | 0.74              |
| 1:A:958:MET:HE1  | 1:A:985:MET:HE2  | 1.71                     | 0.73              |
| 1:A:304:THR:CG2  | 1:A:306:LEU:HG   | 2.19                     | 0.72              |
| 1:A:772:PRO:HD3  | 1:A:813:ALA:O    | 1.88                     | 0.72              |
| 1:B:254:ARG:HH11 | 1:B:258:GLN:HE21 | 1.37                     | 0.72              |
| 1:A:119:ARG:HH21 | 1:A:130:LEU:H    | 1.36                     | 0.72              |
| 1:A:49:MET:HG3   | 1:A:68:VAL:HG13  | 1.71                     | 0.71              |
| 1:A:640:GLU:O    | 1:A:644:ILE:HG13 | 1.91                     | 0.71              |
| 1:A:632:ALA:H    | 1:A:647:THR:CG2  | 2.03                     | 0.71              |
| 1:A:521:MET:HE2  | 1:A:521:MET:HA   | 1.73                     | 0.71              |
| 1:B:35:ASP:HB2   | 1:B:54:SER:OG    | 1.90                     | 0.71              |
| 1:B:234:ARG:HH22 | 1:B:235:ARG:HE   | 1.35                     | 0.71              |
| 1:A:350:GLN:HG3  | 1:A:406:ILE:HG12 | 1.72                     | 0.70              |
| 1:A:608:ARG:HH11 | 1:A:613:ASN:HD22 | 1.38                     | 0.70              |
| 1:B:753:ARG:HG2  | 1:B:753:ARG:NH1  | 2.07                     | 0.70              |
| 1:B:609:THR:OG1  | 1:B:612:GLU:HG3  | 1.92                     | 0.69              |
| 1:A:409:VAL:HG23 | 1:B:23:GLU:OE1   | 1.91                     | 0.69              |
| 1:A:672:VAL:HG11 | 1:A:696:VAL:HG13 | 1.73                     | 0.69              |
| 1:B:254:ARG:HH11 | 1:B:258:GLN:NE2  | 1.90                     | 0.69              |
| 1:B:814:ARG:H    | 1:B:818:HIS:CD2  | 2.09                     | 0.69              |
| 1:A:503:ALA:HB1  | 1:A:509:TYR:OH   | 1.92                     | 0.69              |
| 1:A:119:ARG:HH21 | 1:A:130:LEU:HB2  | 1.57                     | 0.69              |
| 1:A:119:ARG:NH2  | 1:A:130:LEU:H    | 1.90                     | 0.69              |
| 1:A:304:THR:HG22 | 1:A:306:LEU:HG   | 1.75                     | 0.69              |
| 1:A:642:ASP:HB2  | 1:A:646:ASN:HD22 | 1.56                     | 0.69              |
| 1:A:753:ARG:HG2  | 1:A:753:ARG:HH11 | 1.59                     | 0.68              |
| 1:B:992:ALA:HB3  | 1:B:993:PRO:HD3  | 1.75                     | 0.68              |
| 1:B:632:ALA:HB2  | 1:B:647:THR:HG21 | 1.75                     | 0.68              |
| 1:A:448:ARG:HD2  | 1:A:458:PHE:HE2  | 1.58                     | 0.68              |
| 1:A:632:ALA:HB2  | 1:A:647:THR:HG21 | 1.74                     | 0.68              |
| 1:A:859:VAL:CG1  | 1:A:901:SER:HA   | 2.23                     | 0.68              |
| 1:B:15:LEU:O     | 1:B:19:ARG:HG3   | 1.93                     | 0.68              |
| 1:B:205:ARG:NH2  | 1:B:246:GLN:O    | 2.26                     | 0.68              |
| 1:B:632:ALA:N    | 1:B:647:THR:HG21 | 2.08                     | 0.68              |
| 1:A:326:LEU:HD12 | 1:A:326:LEU:H    | 1.59                     | 0.68              |
| 1:B:642:ASP:HB2  | 1:B:646:ASN:ND2  | 2.09                     | 0.68              |
| 1:A:743:ARG:HG3  | 1:A:743:ARG:HH11 | 1.58                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:64:ALA:O     | 1:B:68:VAL:HG23  | 1.94                     | 0.67              |
| 1:B:632:ALA:CB   | 1:B:647:THR:HG21 | 2.25                     | 0.67              |
| 1:B:1033:LEU:HA  | 1:B:1036:ARG:HD2 | 1.77                     | 0.67              |
| 1:B:683:GLY:O    | 1:B:713:GLY:HA3  | 1.95                     | 0.66              |
| 1:A:980:LEU:HD23 | 1:A:983:MET:HE3  | 1.77                     | 0.66              |
| 1:B:1:MET:N      | 1:B:24:LEU:HB3   | 2.10                     | 0.66              |
| 1:A:541:THR:O    | 1:A:544:GLN:HG2  | 1.94                     | 0.66              |
| 1:A:1017:TYR:CE2 | 1:A:1037:LEU:HG  | 2.30                     | 0.66              |
| 1:B:607:ARG:NH1  | 1:B:607:ARG:HB3  | 2.11                     | 0.66              |
| 1:A:539:LEU:N    | 1:A:539:LEU:HD23 | 2.11                     | 0.66              |
| 1:A:500:VAL:CG2  | 1:A:519:GLU:HG3  | 2.27                     | 0.65              |
| 1:B:517:VAL:HG22 | 1:B:526:VAL:HG22 | 1.79                     | 0.64              |
| 1:A:607:ARG:NH2  | 1:A:712:GLU:OE2  | 2.30                     | 0.64              |
| 1:A:850:PRO:HG2  | 1:A:975:ARG:HH22 | 1.62                     | 0.64              |
| 1:A:104:PRO:HG3  | 1:A:291:PRO:HB2  | 1.77                     | 0.64              |
| 1:A:776:ILE:O    | 1:A:798:GLY:HA3  | 1.98                     | 0.64              |
| 1:B:315:ILE:HG13 | 1:B:324:LEU:HD21 | 1.80                     | 0.64              |
| 1:A:351:LEU:HD13 | 1:A:425:LEU:HD11 | 1.79                     | 0.64              |
| 1:A:79:PRO:HB2   | 1:A:85:SER:HA    | 1.81                     | 0.63              |
| 1:A:540:VAL:HA   | 1:A:544:GLN:OE1  | 1.98                     | 0.63              |
| 1:A:951:ALA:HB1  | 1:A:955:PHE:CE2  | 2.33                     | 0.63              |
| 1:B:909:ILE:HG21 | 1:B:958:MET:HE1  | 1.80                     | 0.63              |
| 1:B:743:ARG:HG3  | 1:B:743:ARG:HH11 | 1.63                     | 0.63              |
| 1:A:448:ARG:HG3  | 1:A:448:ARG:HH11 | 1.64                     | 0.63              |
| 1:A:464:PRO:HG2  | 1:A:465:GLU:OE2  | 1.98                     | 0.63              |
| 1:A:609:THR:HG23 | 1:A:612:GLU:OE1  | 1.98                     | 0.63              |
| 1:B:51:LEU:HD21  | 1:B:65:LEU:HD23  | 1.80                     | 0.63              |
| 1:A:114:ASN:HB3  | 1:A:117:ALA:HB3  | 1.81                     | 0.63              |
| 1:B:1:MET:H3     | 1:B:24:LEU:HB3   | 1.63                     | 0.63              |
| 1:A:415:ARG:HD2  | 1:A:419:ARG:HH12 | 1.64                     | 0.63              |
| 1:A:232:MET:HE2  | 1:A:240:ILE:HD12 | 1.79                     | 0.63              |
| 1:A:1032:ASN:HB3 | 1:A:1036:ARG:NH1 | 2.13                     | 0.62              |
| 1:B:272:LEU:HG   | 1:B:312:GLN:HG3  | 1.79                     | 0.62              |
| 1:A:604:ARG:HG3  | 1:A:604:ARG:HH11 | 1.64                     | 0.62              |
| 1:A:632:ALA:CB   | 1:A:647:THR:HG21 | 2.28                     | 0.62              |
| 1:B:59:TYR:HB2   | 1:B:83:PHE:CE1   | 2.35                     | 0.62              |
| 1:B:839:ALA:HB2  | 1:B:1066:ARG:NH1 | 2.15                     | 0.61              |
| 1:B:607:ARG:NH2  | 1:B:712:GLU:OE2  | 2.33                     | 0.61              |
| 1:B:934:LEU:HB3  | 1:B:974:LEU:HD11 | 1.82                     | 0.61              |
| 1:A:672:VAL:CG1  | 1:A:696:VAL:HG13 | 2.31                     | 0.61              |
| 1:A:1053:THR:OG1 | 1:A:1055:GLU:HG3 | 2.00                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:650:ASP:OD2  | 1:B:688:ARG:HB2  | 2.00                     | 0.61              |
| 1:B:635:ARG:HG2  | 1:B:635:ARG:HH11 | 1.65                     | 0.60              |
| 1:B:951:ALA:HB1  | 1:B:955:PHE:CE2  | 2.36                     | 0.60              |
| 1:A:304:THR:HG22 | 1:A:306:LEU:H    | 1.67                     | 0.60              |
| 1:B:753:ARG:HD3  | 1:B:794:PRO:HB3  | 1.84                     | 0.60              |
| 1:A:373:ALA:HB3  | 1:A:431:GLU:HB2  | 1.84                     | 0.60              |
| 1:B:618:VAL:HG13 | 1:B:657:ALA:HB1  | 1.83                     | 0.60              |
| 1:A:1032:ASN:O   | 1:A:1036:ARG:HD3 | 2.01                     | 0.60              |
| 1:B:119:ARG:O    | 1:B:123:ILE:HG13 | 2.02                     | 0.60              |
| 1:B:969:LEU:HD23 | 1:B:969:LEU:C    | 2.27                     | 0.59              |
| 1:B:205:ARG:HD2  | 1:B:453:TRP:CE3  | 2.37                     | 0.59              |
| 1:B:258:GLN:HG2  | 1:B:337:VAL:HG11 | 1.83                     | 0.59              |
| 1:A:703:LYS:HB2  | 1:A:705:LEU:HG   | 1.84                     | 0.59              |
| 1:B:86:GLU:OE2   | 1:B:292:ARG:HD3  | 2.03                     | 0.59              |
| 1:B:350:GLN:HG3  | 1:B:406:ILE:HG13 | 1.83                     | 0.59              |
| 1:B:885:THR:HG23 | 1:B:916:LYS:HE2  | 1.84                     | 0.59              |
| 1:A:618:VAL:HG13 | 1:A:657:ALA:HB1  | 1.84                     | 0.59              |
| 1:B:743:ARG:HG3  | 1:B:743:ARG:NH1  | 2.16                     | 0.58              |
| 1:A:216:ALA:HB3  | 1:A:221:HIS:CE1  | 2.39                     | 0.58              |
| 1:A:213:ALA:HB3  | 1:A:269:LEU:HD23 | 1.85                     | 0.58              |
| 1:B:1029:GLU:HB3 | 1:B:1032:ASN:ND2 | 2.17                     | 0.58              |
| 1:A:119:ARG:NH2  | 1:A:130:LEU:HB2  | 2.19                     | 0.58              |
| 1:A:131:ALA:HB3  | 1:A:199:ALA:N    | 2.19                     | 0.58              |
| 1:A:119:ARG:HH21 | 1:A:130:LEU:N    | 2.02                     | 0.58              |
| 1:A:647:THR:HG22 | 1:A:647:THR:O    | 2.04                     | 0.58              |
| 1:B:114:ASN:HB3  | 1:B:117:ALA:HB3  | 1.85                     | 0.58              |
| 1:A:688:ARG:HG3  | 1:A:688:ARG:HH11 | 1.69                     | 0.58              |
| 1:B:595:ARG:O    | 1:B:599:VAL:HG23 | 2.03                     | 0.58              |
| 1:A:991:ARG:HG3  | 1:A:991:ARG:HH11 | 1.68                     | 0.58              |
| 1:B:288:GLU:HG2  | 1:B:289:VAL:N    | 2.18                     | 0.58              |
| 1:B:373:ALA:HB3  | 1:B:431:GLU:CB   | 2.33                     | 0.58              |
| 1:A:717:ARG:HB2  | 1:A:720:ASP:OD2  | 2.04                     | 0.57              |
| 1:B:216:ALA:HB3  | 1:B:221:HIS:CE1  | 2.39                     | 0.57              |
| 1:B:712:GLU:HG3  | 1:B:751:SER:O    | 2.04                     | 0.57              |
| 1:B:5:LEU:HB2    | 1:B:26:MET:CE    | 2.34                     | 0.57              |
| 1:B:703:LYS:HB2  | 1:B:705:LEU:HG   | 1.86                     | 0.57              |
| 1:B:230:CYS:SG   | 1:B:241:GLU:HG3  | 2.45                     | 0.57              |
| 1:B:505:GLU:HG2  | 1:B:538:VAL:HG23 | 1.86                     | 0.57              |
| 1:B:784:ILE:HD11 | 1:B:797:ILE:HD12 | 1.86                     | 0.57              |
| 1:B:904:HIS:CD2  | 1:B:905:LEU:HG   | 2.40                     | 0.57              |
| 1:A:586:ARG:HH21 | 1:A:644:ILE:HD13 | 1.69                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:553:LEU:C     | 1:A:553:LEU:HD12  | 2.30                     | 0.57              |
| 1:B:415:ARG:NH1   | 1:B:419:ARG:HH22  | 2.02                     | 0.57              |
| 1:A:64:ALA:O      | 1:A:68:VAL:HG23   | 2.05                     | 0.57              |
| 1:A:511:ALA:HB2   | 1:A:531:ASP:HA    | 1.86                     | 0.57              |
| 1:B:139:VAL:HG12  | 1:B:143:GLU:OE2   | 2.05                     | 0.56              |
| 1:B:638:ARG:HD3   | 1:B:642:ASP:OD2   | 2.05                     | 0.56              |
| 1:A:595:ARG:O     | 1:A:599:VAL:HG23  | 2.05                     | 0.56              |
| 1:A:1013:VAL:HG21 | 1:A:1038:VAL:HG22 | 1.86                     | 0.56              |
| 1:A:530:PRO:O     | 1:A:531:ASP:HB3   | 2.05                     | 0.56              |
| 1:A:656:LEU:HD21  | 1:A:699:LEU:HD13  | 1.88                     | 0.56              |
| 1:B:274:THR:HG21  | 1:B:294:GLN:OE1   | 2.06                     | 0.56              |
| 1:B:632:ALA:H     | 1:B:647:THR:CG2   | 2.15                     | 0.56              |
| 1:B:643:LEU:O     | 1:B:647:THR:HB    | 2.06                     | 0.56              |
| 1:A:448:ARG:HG3   | 1:A:448:ARG:NH1   | 2.20                     | 0.56              |
| 1:A:1029:GLU:HB3  | 1:A:1032:ASN:HD22 | 1.70                     | 0.56              |
| 1:A:1010:GLU:O    | 1:A:1014:ARG:HG3  | 2.05                     | 0.56              |
| 1:B:871:SER:HB2   | 1:B:889:ARG:HB2   | 1.87                     | 0.56              |
| 1:B:32:TYR:CE1    | 1:B:50:PRO:HB3    | 2.41                     | 0.56              |
| 1:A:502:VAL:HG12  | 1:A:503:ALA:N     | 2.21                     | 0.56              |
| 1:A:354:ASN:N     | 1:A:436:ASN:OD1   | 2.36                     | 0.56              |
| 1:A:799:PRO:C     | 1:A:801:ALA:H     | 2.14                     | 0.56              |
| 1:B:153:ILE:CG2   | 1:B:154:MET:N     | 2.69                     | 0.55              |
| 1:B:234:ARG:O     | 1:B:237:GLN:HG2   | 2.06                     | 0.55              |
| 1:A:447:GLN:HA    | 1:A:450:GLU:OE2   | 2.07                     | 0.55              |
| 1:B:905:LEU:HB2   | 1:B:908:ALA:HB3   | 1.88                     | 0.55              |
| 1:A:249:SER:C     | 1:A:251:GLU:H     | 2.12                     | 0.55              |
| 1:A:874:GLU:HA    | 1:A:886:ALA:HB2   | 1.88                     | 0.55              |
| 1:B:234:ARG:O     | 1:B:235:ARG:C     | 2.49                     | 0.55              |
| 1:A:797:ILE:C     | 1:A:799:PRO:HD3   | 2.30                     | 0.55              |
| 1:A:1030:ARG:HG3  | 1:A:1031:GLN:N    | 2.21                     | 0.55              |
| 1:B:688:ARG:HG3   | 1:B:688:ARG:HH11  | 1.72                     | 0.55              |
| 1:B:986:ALA:HB1   | 1:B:993:PRO:CG    | 2.36                     | 0.55              |
| 1:A:81:TYR:CZ     | 1:A:295:VAL:HG22  | 2.42                     | 0.55              |
| 1:B:415:ARG:HG2   | 1:B:419:ARG:HH12  | 1.71                     | 0.55              |
| 1:B:635:ARG:HG2   | 1:B:635:ARG:NH1   | 2.21                     | 0.55              |
| 1:B:640:GLU:O     | 1:B:644:ILE:HG13  | 2.06                     | 0.55              |
| 1:B:848:VAL:HG11  | 1:B:862:ALA:HA    | 1.87                     | 0.55              |
| 1:B:986:ALA:HB1   | 1:B:993:PRO:HG2   | 1.88                     | 0.55              |
| 1:A:20:THR:O      | 1:A:24:LEU:HG     | 2.07                     | 0.55              |
| 1:A:635:ARG:HE    | 1:A:640:GLU:HB2   | 1.72                     | 0.55              |
| 1:B:843:ARG:HG2   | 1:B:846:ARG:NH1   | 2.21                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:499:VAL:HG23  | 1:A:544:GLN:O     | 2.07                     | 0.55              |
| 1:A:728:GLY:O     | 1:A:731:VAL:HG23  | 2.07                     | 0.55              |
| 1:B:40:PRO:HG2    | 1:B:387:TYR:O     | 2.06                     | 0.55              |
| 1:A:324:LEU:HB2   | 1:A:326:LEU:HD11  | 1.89                     | 0.55              |
| 1:A:502:VAL:HG21  | 1:A:540:VAL:HG12  | 1.89                     | 0.55              |
| 1:B:499:VAL:HA    | 1:B:518:LEU:HD23  | 1.89                     | 0.55              |
| 1:B:248:LEU:HD22  | 1:B:252:LEU:HD23  | 1.89                     | 0.54              |
| 1:B:1029:GLU:HB3  | 1:B:1032:ASN:HD21 | 1.72                     | 0.54              |
| 1:A:511:ALA:CB    | 1:A:531:ASP:HA    | 2.38                     | 0.54              |
| 1:A:1000:PRO:HD3  | 1:A:1060:ILE:O    | 2.07                     | 0.54              |
| 1:B:154:MET:SD    | 1:B:166:MET:HE2   | 2.48                     | 0.54              |
| 1:B:536:VAL:HG12  | 1:B:537:ARG:HD3   | 1.89                     | 0.54              |
| 1:A:743:ARG:HG3   | 1:A:743:ARG:NH1   | 2.23                     | 0.54              |
| 1:B:241:GLU:HG2   | 1:B:296:GLU:CB    | 2.37                     | 0.54              |
| 1:B:647:THR:HG22  | 1:B:647:THR:O     | 2.07                     | 0.54              |
| 1:A:1032:ASN:HB3  | 1:A:1036:ARG:HH11 | 1.72                     | 0.54              |
| 1:B:216:ALA:HB3   | 1:B:221:HIS:ND1   | 2.23                     | 0.54              |
| 1:A:437:ILE:O     | 1:A:441:ARG:HB2   | 2.07                     | 0.54              |
| 1:A:652:LEU:HD12  | 1:A:675:SER:O     | 2.07                     | 0.54              |
| 1:A:711:ALA:O     | 1:A:712:GLU:HB2   | 2.07                     | 0.54              |
| 1:A:1052:THR:HG22 | 1:A:1053:THR:HG23 | 1.89                     | 0.54              |
| 1:B:1069:ILE:O    | 1:B:1072:LEU:HB2  | 2.08                     | 0.54              |
| 1:A:992:ALA:HB3   | 1:A:993:PRO:HD3   | 1.90                     | 0.54              |
| 1:B:487:GLY:O     | 1:B:556:THR:HG23  | 2.09                     | 0.53              |
| 1:B:210:GLN:HE21  | 1:B:228:ARG:HH12  | 1.56                     | 0.53              |
| 1:B:631:ILE:O     | 1:B:688:ARG:HG3   | 2.09                     | 0.53              |
| 1:A:608:ARG:HD2   | 1:A:613:ASN:ND2   | 2.23                     | 0.53              |
| 1:A:647:THR:HG22  | 1:A:650:ASP:HA    | 1.89                     | 0.53              |
| 1:B:547:GLY:H     | 1:B:550:ASP:CG    | 2.17                     | 0.53              |
| 1:A:507:ALA:HB3   | 1:A:509:TYR:HE1   | 1.73                     | 0.53              |
| 1:B:897:LEU:C     | 1:B:897:LEU:HD23  | 2.34                     | 0.53              |
| 1:A:936:ASP:HA    | 1:A:976:LYS:O     | 2.09                     | 0.53              |
| 1:B:257:HIS:O     | 1:B:261:VAL:HG22  | 2.09                     | 0.53              |
| 1:A:507:ALA:HB3   | 1:A:509:TYR:CE1   | 2.43                     | 0.53              |
| 1:A:49:MET:SD     | 1:B:494:GLN:OE1   | 2.67                     | 0.52              |
| 1:B:684:THR:OG1   | 1:B:717:ARG:HD3   | 2.09                     | 0.52              |
| 1:A:414:TRP:NE1   | 1:A:418:MET:HE2   | 2.25                     | 0.52              |
| 1:A:536:VAL:HG12  | 1:A:537:ARG:HG3   | 1.91                     | 0.52              |
| 1:A:738:ALA:O     | 1:A:741:ARG:HB2   | 2.10                     | 0.52              |
| 1:B:153:ILE:HG23  | 1:B:154:MET:N     | 2.24                     | 0.52              |
| 1:A:116:THR:HG22  | 1:A:120:ARG:NH2   | 2.25                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:504:PRO:HD2   | 1:A:509:TYR:HH    | 1.72                     | 0.52              |
| 1:B:119:ARG:NH2   | 1:B:130:LEU:O     | 2.41                     | 0.52              |
| 1:B:234:ARG:HH22  | 1:B:235:ARG:NE    | 2.03                     | 0.52              |
| 1:B:843:ARG:NE    | 1:B:846:ARG:HH12  | 2.06                     | 0.52              |
| 1:A:711:ALA:O     | 1:A:712:GLU:CB    | 2.57                     | 0.52              |
| 1:A:249:SER:C     | 1:A:251:GLU:N     | 2.67                     | 0.52              |
| 1:A:489:ASP:OD2   | 1:A:557:ARG:NH1   | 2.43                     | 0.52              |
| 1:A:505:GLU:HG2   | 1:A:538:VAL:HB    | 1.92                     | 0.52              |
| 1:B:407:VAL:HB    | 1:B:420:LYS:HG2   | 1.92                     | 0.52              |
| 1:B:879:TYR:O     | 1:B:880:GLY:C     | 2.53                     | 0.52              |
| 1:B:607:ARG:NH1   | 1:B:816:GLU:CD    | 2.68                     | 0.52              |
| 1:B:850:PRO:HG3   | 1:B:855:ARG:O     | 2.10                     | 0.52              |
| 1:A:418:MET:HE1   | 1:A:450:GLU:HA    | 1.91                     | 0.51              |
| 1:B:167:ARG:O     | 1:B:169:VAL:HG23  | 2.10                     | 0.51              |
| 1:B:1038:VAL:HG12 | 1:B:1039:ALA:N    | 2.25                     | 0.51              |
| 1:B:12:GLU:HG3    | 1:B:13:ILE:N      | 2.25                     | 0.51              |
| 1:A:300:THR:O     | 1:A:304:THR:HB    | 2.10                     | 0.51              |
| 1:B:204:ALA:O     | 1:B:455:ASN:HB2   | 2.09                     | 0.51              |
| 1:A:632:ALA:CA    | 1:A:647:THR:HG21  | 2.40                     | 0.51              |
| 1:A:874:GLU:HA    | 1:A:886:ALA:CB    | 2.40                     | 0.51              |
| 1:B:732:PRO:O     | 1:B:736:MET:HG3   | 2.10                     | 0.51              |
| 1:B:975:ARG:O     | 1:B:1002:GLY:HA2  | 2.09                     | 0.51              |
| 1:A:810:GLY:HA2   | 1:A:876:ARG:HG2   | 1.93                     | 0.51              |
| 1:A:326:LEU:HD12  | 1:A:326:LEU:N     | 2.25                     | 0.51              |
| 1:A:443:LEU:O     | 1:A:443:LEU:HD23  | 2.10                     | 0.51              |
| 1:A:503:ALA:HB1   | 1:A:504:PRO:HD2   | 1.93                     | 0.51              |
| 1:A:932:ILE:HD11  | 1:A:1069:ILE:HG21 | 1.91                     | 0.51              |
| 1:B:753:ARG:NH1   | 1:B:753:ARG:CG    | 2.74                     | 0.51              |
| 1:A:201:LEU:HD12  | 1:A:202:GLY:N     | 2.22                     | 0.51              |
| 1:A:799:PRO:C     | 1:A:801:ALA:N     | 2.65                     | 0.51              |
| 1:A:884:VAL:O     | 1:A:898:ILE:HA    | 2.11                     | 0.51              |
| 1:B:105:ASP:OD1   | 1:B:106:GLY:N     | 2.44                     | 0.51              |
| 1:B:791:VAL:HG13  | 1:B:791:VAL:O     | 2.10                     | 0.51              |
| 1:A:858:ASP:OD2   | 1:A:860:HIS:HB2   | 2.11                     | 0.51              |
| 1:A:210:GLN:HE21  | 1:A:228:ARG:NH1   | 1.88                     | 0.50              |
| 1:B:498:THR:OG1   | 1:B:545:VAL:HG22  | 2.11                     | 0.50              |
| 1:B:607:ARG:NH1   | 1:B:816:GLU:OE2   | 2.43                     | 0.50              |
| 1:A:540:VAL:HG22  | 1:A:544:GLN:OE1   | 2.12                     | 0.50              |
| 1:A:867:VAL:HG11  | 1:A:888:VAL:HG21  | 1.93                     | 0.50              |
| 1:A:995:PHE:O     | 1:A:995:PHE:CD1   | 2.64                     | 0.50              |
| 1:B:971:MET:CE    | 1:B:986:ALA:HB2   | 2.42                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:269:LEU:HG   | 1:A:270:ARG:N    | 2.26                     | 0.50              |
| 1:A:883:ILE:HD13 | 1:A:985:MET:HE1  | 1.94                     | 0.50              |
| 1:B:671:ALA:HB2  | 1:B:706:PRO:HG2  | 1.93                     | 0.50              |
| 1:A:298:THR:CB   | 1:A:406:ILE:HD13 | 2.39                     | 0.50              |
| 1:A:380:PRO:HB3  | 1:B:383:ARG:CZ   | 2.41                     | 0.50              |
| 1:A:741:ARG:HD2  | 1:A:741:ARG:C    | 2.36                     | 0.50              |
| 1:B:495:LEU:HD23 | 1:B:495:LEU:O    | 2.11                     | 0.50              |
| 1:B:841:ASP:O    | 1:B:844:VAL:HB   | 2.11                     | 0.50              |
| 1:B:111:LEU:HD21 | 1:B:267:VAL:HG12 | 1.94                     | 0.50              |
| 1:A:501:GLU:OE2  | 1:A:514:GLN:NE2  | 2.44                     | 0.50              |
| 1:A:652:LEU:CD2  | 1:A:693:THR:HG23 | 2.41                     | 0.50              |
| 1:B:810:GLY:HA2  | 1:B:876:ARG:HG2  | 1.94                     | 0.50              |
| 1:B:1026:ASP:HB2 | 1:B:1030:ARG:HB3 | 1.94                     | 0.50              |
| 1:A:614:ILE:HD11 | 1:A:675:SER:HB3  | 1.94                     | 0.49              |
| 1:A:980:LEU:HA   | 1:A:983:MET:HE3  | 1.94                     | 0.49              |
| 1:A:1010:GLU:CD  | 1:A:1010:GLU:H   | 2.19                     | 0.49              |
| 1:B:60:LEU:CD2   | 1:B:83:PHE:HD1   | 2.25                     | 0.49              |
| 1:B:154:MET:HB2  | 1:B:200:LEU:HD13 | 1.94                     | 0.49              |
| 1:B:541:THR:OG1  | 1:B:542:PRO:HD2  | 2.12                     | 0.49              |
| 1:A:52:PRO:HG2   | 1:A:53:GLY:H     | 1.76                     | 0.49              |
| 1:A:976:LYS:HG2  | 1:A:978:TYR:HE2  | 1.77                     | 0.49              |
| 1:B:10:ARG:HG2   | 1:B:59:TYR:CZ    | 2.47                     | 0.49              |
| 1:B:415:ARG:HH11 | 1:B:419:ARG:HH12 | 1.60                     | 0.49              |
| 1:A:784:ILE:HD11 | 1:A:797:ILE:HD12 | 1.92                     | 0.49              |
| 1:A:956:GLY:O    | 1:A:960:VAL:HG23 | 2.13                     | 0.49              |
| 1:B:12:GLU:HG3   | 1:B:13:ILE:H     | 1.78                     | 0.49              |
| 1:B:116:THR:O    | 1:B:119:ARG:HG2  | 2.13                     | 0.49              |
| 1:B:871:SER:CB   | 1:B:889:ARG:HB2  | 2.42                     | 0.49              |
| 1:B:825:GLN:HG2  | 1:B:873:LEU:HD22 | 1.94                     | 0.49              |
| 1:A:661:ALA:O    | 1:A:664:PHE:O    | 2.29                     | 0.49              |
| 1:B:35:ASP:HB2   | 1:B:54:SER:HG    | 1.77                     | 0.49              |
| 1:B:104:PRO:HG3  | 1:B:291:PRO:HB2  | 1.94                     | 0.49              |
| 1:A:681:LEU:O    | 1:A:684:THR:HG23 | 2.13                     | 0.49              |
| 1:A:750:VAL:O    | 1:A:770:ALA:HA   | 2.13                     | 0.49              |
| 1:B:296:GLU:OE1  | 1:B:352:ARG:NH2  | 2.46                     | 0.49              |
| 1:B:299:VAL:CG1  | 1:B:350:GLN:HB2  | 2.43                     | 0.49              |
| 1:A:10:ARG:HG2   | 1:A:59:TYR:CE2   | 2.48                     | 0.48              |
| 1:B:279:VAL:HG12 | 1:B:280:SER:N    | 2.28                     | 0.48              |
| 1:B:602:ARG:HD3  | 1:B:679:THR:CG2  | 2.43                     | 0.48              |
| 1:A:234:ARG:HH12 | 1:A:235:ARG:HE   | 1.59                     | 0.48              |
| 1:A:632:ALA:HB3  | 1:A:643:LEU:HD22 | 1.95                     | 0.48              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:980:LEU:HD23  | 1:A:983:MET:CE   | 2.43                     | 0.48              |
| 1:B:533:LEU:HD12  | 1:B:533:LEU:O    | 2.14                     | 0.48              |
| 1:B:791:VAL:O     | 1:B:791:VAL:CG1  | 2.61                     | 0.48              |
| 1:B:884:VAL:O     | 1:B:898:ILE:HA   | 2.13                     | 0.48              |
| 1:A:1057:ASP:O    | 1:A:1058:ASP:HB2 | 2.12                     | 0.48              |
| 1:B:210:GLN:NE2   | 1:B:228:ARG:HH12 | 2.10                     | 0.48              |
| 1:B:355:ALA:HB1   | 1:B:433:VAL:HG11 | 1.95                     | 0.48              |
| 1:B:448:ARG:O     | 1:B:451:THR:HG23 | 2.12                     | 0.48              |
| 1:A:519:GLU:HG2   | 1:A:524:GLN:HG2  | 1.95                     | 0.48              |
| 1:B:447:GLN:O     | 1:B:448:ARG:C    | 2.56                     | 0.48              |
| 1:A:669:ALA:HA    | 1:A:831:GLN:NE2  | 2.29                     | 0.48              |
| 1:B:426:SER:HB3   | 1:B:441:ARG:CZ   | 2.41                     | 0.48              |
| 1:A:607:ARG:NH1   | 1:A:816:GLU:OE2  | 2.47                     | 0.48              |
| 1:A:971:MET:HE3   | 1:A:973:ILE:CD1  | 2.43                     | 0.48              |
| 1:B:797:ILE:C     | 1:B:799:PRO:HD3  | 2.39                     | 0.48              |
| 1:A:6:LEU:HD22    | 1:A:69:ALA:HB2   | 1.96                     | 0.47              |
| 1:B:843:ARG:HA    | 1:B:846:ARG:HD2  | 1.96                     | 0.47              |
| 1:A:1004:ILE:HG22 | 1:A:1005:GLY:N   | 2.29                     | 0.47              |
| 1:A:643:LEU:O     | 1:A:647:THR:HB   | 2.15                     | 0.47              |
| 1:B:792:TYR:N     | 1:B:792:TYR:CD1  | 2.82                     | 0.47              |
| 1:B:607:ARG:HB3   | 1:B:607:ARG:HH11 | 1.78                     | 0.47              |
| 1:B:975:ARG:HH11  | 1:B:975:ARG:HG3  | 1.78                     | 0.47              |
| 1:A:608:ARG:HD2   | 1:A:613:ASN:HD21 | 1.79                     | 0.47              |
| 1:A:652:LEU:HD21  | 1:A:693:THR:HG23 | 1.96                     | 0.47              |
| 1:A:814:ARG:H     | 1:A:818:HIS:HD2  | 1.63                     | 0.47              |
| 1:A:879:TYR:O     | 1:A:880:GLY:C    | 2.57                     | 0.47              |
| 1:B:49:MET:HE2    | 1:B:72:THR:CG2   | 2.45                     | 0.47              |
| 1:B:511:ALA:HA    | 1:B:531:ASP:HA   | 1.97                     | 0.47              |
| 1:B:820:VAL:HG12  | 1:B:824:LYS:HE3  | 1.97                     | 0.47              |
| 1:A:383:ARG:CZ    | 1:B:380:PRO:HB3  | 2.45                     | 0.47              |
| 1:A:446:GLU:OE1   | 1:A:466:LEU:HD21 | 2.15                     | 0.47              |
| 1:A:989:SER:C     | 1:A:991:ARG:H    | 2.22                     | 0.47              |
| 1:B:81:TYR:CZ     | 1:B:295:VAL:HG22 | 2.50                     | 0.47              |
| 1:B:498:THR:HG23  | 1:B:543:GLY:O    | 2.15                     | 0.47              |
| 1:B:985:MET:HE2   | 1:B:985:MET:HA   | 1.96                     | 0.47              |
| 1:A:361:ASP:C     | 1:A:363:SER:N    | 2.70                     | 0.47              |
| 1:B:608:ARG:HD2   | 1:B:613:ASN:HD21 | 1.80                     | 0.47              |
| 1:B:868:ASP:OD2   | 1:B:891:GLU:N    | 2.45                     | 0.47              |
| 1:A:119:ARG:HH21  | 1:A:130:LEU:CB   | 2.25                     | 0.47              |
| 1:A:287:LEU:O     | 1:A:288:GLU:HB2  | 2.15                     | 0.47              |
| 1:B:388:GLY:HA2   | 1:B:392:LEU:HD22 | 1.97                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:579:ASP:OD1  | 1:B:580:LEU:N    | 2.47                     | 0.47              |
| 1:A:698:ASP:O    | 1:A:702:ARG:HG2  | 2.15                     | 0.46              |
| 1:A:975:ARG:O    | 1:A:1002:GLY:HA2 | 2.15                     | 0.46              |
| 1:B:414:TRP:CD1  | 1:B:418:MET:HE2  | 2.51                     | 0.46              |
| 1:A:4:SER:HB3    | 1:A:75:THR:H     | 1.79                     | 0.46              |
| 1:A:895:TYR:CD2  | 1:A:930:PRO:HG2  | 2.50                     | 0.46              |
| 1:B:818:HIS:O    | 1:B:822:LEU:HG   | 2.14                     | 0.46              |
| 1:A:40:PRO:HG2   | 1:A:387:TYR:O    | 2.15                     | 0.46              |
| 1:A:921:LEU:HD22 | 1:A:965:LEU:HD11 | 1.97                     | 0.46              |
| 1:B:205:ARG:NH1  | 1:B:229:ASP:OD2  | 2.49                     | 0.46              |
| 1:B:468:ALA:C    | 1:B:470:ALA:H    | 2.23                     | 0.46              |
| 1:B:675:SER:HB2  | 1:B:710:PHE:HB2  | 1.97                     | 0.46              |
| 1:A:753:ARG:HH11 | 1:A:753:ARG:CG   | 2.24                     | 0.46              |
| 1:A:814:ARG:H    | 1:A:818:HIS:CD2  | 2.34                     | 0.46              |
| 1:B:703:LYS:O    | 1:B:704:ARG:C    | 2.59                     | 0.46              |
| 1:A:227:ASP:H    | 1:A:344:GLN:HE22 | 1.63                     | 0.46              |
| 1:B:441:ARG:HG2  | 1:B:441:ARG:NH1  | 2.31                     | 0.46              |
| 1:A:340:GLU:O    | 1:A:341:PRO:C    | 2.57                     | 0.46              |
| 1:B:49:MET:HG3   | 1:B:68:VAL:HG13  | 1.98                     | 0.46              |
| 1:B:76:LEU:HD23  | 1:B:100:THR:HB   | 1.98                     | 0.46              |
| 1:B:196:PHE:O    | 1:B:197:ALA:HB2  | 2.15                     | 0.46              |
| 1:B:254:ARG:NH1  | 1:B:258:GLN:HE21 | 2.11                     | 0.46              |
| 1:B:346:GLY:HA2  | 1:B:411:GLY:O    | 2.16                     | 0.46              |
| 1:B:634:GLN:O    | 1:B:634:GLN:HG3  | 2.16                     | 0.45              |
| 1:B:784:ILE:CD1  | 1:B:797:ILE:HD12 | 2.45                     | 0.45              |
| 1:B:254:ARG:O    | 1:B:258:GLN:HG3  | 2.17                     | 0.45              |
| 1:B:288:GLU:HG2  | 1:B:289:VAL:H    | 1.81                     | 0.45              |
| 1:A:863:ILE:O    | 1:A:867:VAL:HG22 | 2.17                     | 0.45              |
| 1:B:31:VAL:HA    | 1:B:49:MET:O     | 2.16                     | 0.45              |
| 1:B:803:GLN:HA   | 1:B:806:ASN:OD1  | 2.16                     | 0.45              |
| 1:A:358:PHE:CE2  | 1:A:467:ALA:HA   | 2.50                     | 0.45              |
| 1:A:608:ARG:HH11 | 1:A:613:ASN:ND2  | 2.11                     | 0.45              |
| 1:B:803:GLN:HA   | 1:B:803:GLN:OE1  | 2.16                     | 0.45              |
| 1:A:943:GLY:O    | 1:A:947:GLU:HG2  | 2.16                     | 0.45              |
| 1:A:1029:GLU:OE2 | 1:A:1031:GLN:HB2 | 2.16                     | 0.45              |
| 1:A:498:THR:O    | 1:A:518:LEU:HA   | 2.17                     | 0.45              |
| 1:B:13:ILE:O     | 1:B:16:ARG:HB3   | 2.17                     | 0.45              |
| 1:B:254:ARG:NH2  | 1:B:340:GLU:OE2  | 2.49                     | 0.45              |
| 1:A:395:SER:OG   | 1:A:397:GLN:HG3  | 2.16                     | 0.45              |
| 1:A:504:PRO:O    | 1:A:506:GLY:N    | 2.50                     | 0.45              |
| 1:A:586:ARG:HG2  | 1:A:586:ARG:HH11 | 1.82                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:647:THR:N    | 1:A:648:PRO:CD   | 2.80                     | 0.45              |
| 1:A:811:LEU:HD21 | 1:A:875:LEU:HD23 | 1.99                     | 0.45              |
| 1:B:122:ALA:HA   | 1:B:263:LEU:HD13 | 1.99                     | 0.45              |
| 1:B:795:GLU:OE1  | 1:B:795:GLU:N    | 2.49                     | 0.45              |
| 1:B:820:VAL:CG1  | 1:B:824:LYS:HE3  | 2.47                     | 0.45              |
| 1:B:1010:GLU:HB2 | 1:B:1014:ARG:NH1 | 2.31                     | 0.45              |
| 1:A:119:ARG:O    | 1:A:122:ALA:HB3  | 2.17                     | 0.45              |
| 1:A:798:GLY:N    | 1:A:799:PRO:HD3  | 2.33                     | 0.45              |
| 1:A:638:ARG:HD3  | 1:A:642:ASP:OD2  | 2.16                     | 0.44              |
| 1:B:426:SER:CB   | 1:B:441:ARG:NH2  | 2.75                     | 0.44              |
| 1:B:133:THR:CG2  | 1:B:137:SER:OG   | 2.64                     | 0.44              |
| 1:B:206:HIS:CD2  | 1:B:206:HIS:C    | 2.95                     | 0.44              |
| 1:A:840:PRO:HD3  | 1:A:868:ASP:HA   | 1.99                     | 0.44              |
| 1:B:10:ARG:NE    | 1:B:36:ASP:OD2   | 2.42                     | 0.44              |
| 1:B:152:GLY:C    | 1:B:153:ILE:HD12 | 2.43                     | 0.44              |
| 1:B:237:GLN:HE21 | 1:B:237:GLN:HA   | 1.83                     | 0.44              |
| 1:A:67:ALA:O     | 1:A:71:ASN:ND2   | 2.51                     | 0.44              |
| 1:A:597:ASP:OD1  | 1:A:597:ASP:N    | 2.47                     | 0.44              |
| 1:B:142:ILE:O    | 1:B:145:PHE:HB3  | 2.17                     | 0.44              |
| 1:B:459:VAL:O    | 1:B:459:VAL:HG12 | 2.18                     | 0.44              |
| 1:B:647:THR:N    | 1:B:648:PRO:CD   | 2.80                     | 0.44              |
| 1:A:10:ARG:NE    | 1:A:36:ASP:OD2   | 2.49                     | 0.44              |
| 1:A:229:ASP:HB3  | 1:A:242:ILE:HB   | 1.99                     | 0.44              |
| 1:A:999:TRP:CD2  | 1:A:1062:PRO:HB3 | 2.53                     | 0.44              |
| 1:B:60:LEU:HD21  | 1:B:83:PHE:HD1   | 1.83                     | 0.44              |
| 1:B:168:LYS:HE2  | 1:B:200:LEU:HD11 | 2.00                     | 0.44              |
| 1:B:1000:PRO:HD3 | 1:B:1060:ILE:O   | 2.17                     | 0.44              |
| 1:A:785:GLU:HA   | 1:A:790:GLY:O    | 2.18                     | 0.44              |
| 1:B:848:VAL:HG11 | 1:B:862:ALA:CA   | 2.48                     | 0.44              |
| 1:A:204:ALA:HA   | 1:A:279:VAL:O    | 2.18                     | 0.43              |
| 1:A:681:LEU:HD23 | 1:A:681:LEU:H    | 1.83                     | 0.43              |
| 1:B:533:LEU:HD12 | 1:B:533:LEU:C    | 2.43                     | 0.43              |
| 1:B:703:LYS:HD3  | 1:B:705:LEU:HD11 | 2.00                     | 0.43              |
| 1:B:755:PHE:HA   | 1:B:777:GLY:O    | 2.18                     | 0.43              |
| 1:A:299:VAL:HG13 | 1:A:350:GLN:HB2  | 1.99                     | 0.43              |
| 1:A:617:LEU:HA   | 1:A:824:LYS:HE3  | 1.98                     | 0.43              |
| 1:B:502:VAL:HG12 | 1:B:503:ALA:N    | 2.33                     | 0.43              |
| 1:B:798:GLY:O    | 1:B:799:PRO:C    | 2.60                     | 0.43              |
| 1:A:632:ALA:HB2  | 1:A:647:THR:CG2  | 2.44                     | 0.43              |
| 1:B:241:GLU:HG2  | 1:B:296:GLU:HB3  | 1.99                     | 0.43              |
| 1:A:3:ALA:HB1    | 1:A:76:LEU:HD11  | 2.00                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:4:SER:HB3     | 1:A:74:ALA:HA     | 2.01                     | 0.43              |
| 1:A:33:ALA:O      | 1:A:34:ALA:C      | 2.61                     | 0.43              |
| 1:B:276:GLU:O     | 1:B:287:LEU:HB3   | 2.19                     | 0.43              |
| 1:B:618:VAL:CG1   | 1:B:657:ALA:HB1   | 2.49                     | 0.43              |
| 1:A:242:ILE:HD13  | 1:A:414:TRP:CH2   | 2.54                     | 0.43              |
| 1:A:346:GLY:HA2   | 1:A:411:GLY:O     | 2.19                     | 0.43              |
| 1:B:229:ASP:HB3   | 1:B:242:ILE:HB    | 2.01                     | 0.43              |
| 1:B:272:LEU:CG    | 1:B:312:GLN:HG3   | 2.47                     | 0.43              |
| 1:B:284:PHE:CD1   | 1:B:284:PHE:C     | 2.96                     | 0.43              |
| 1:B:441:ARG:HG2   | 1:B:441:ARG:HH11  | 1.83                     | 0.43              |
| 1:A:105:ASP:OD1   | 1:A:106:GLY:N     | 2.49                     | 0.43              |
| 1:A:791:VAL:HG13  | 1:A:791:VAL:O     | 2.18                     | 0.43              |
| 1:A:1033:LEU:HD12 | 1:A:1033:LEU:O    | 2.19                     | 0.43              |
| 1:B:92:LYS:HG2    | 1:B:107:ARG:HH12  | 1.84                     | 0.43              |
| 1:B:261:VAL:HG23  | 1:B:262:ARG:N     | 2.32                     | 0.43              |
| 1:A:732:PRO:O     | 1:A:736:MET:HG3   | 2.18                     | 0.43              |
| 1:B:261:VAL:HG23  | 1:B:262:ARG:H     | 1.83                     | 0.43              |
| 1:B:648:PRO:O     | 1:B:649:ALA:HB3   | 2.19                     | 0.43              |
| 1:B:921:LEU:HD22  | 1:B:965:LEU:HD11  | 2.00                     | 0.43              |
| 1:B:1016:GLY:C    | 1:B:1017:TYR:CD1  | 2.96                     | 0.43              |
| 1:A:13:ILE:HB     | 1:A:81:TYR:CE2    | 2.54                     | 0.43              |
| 1:A:784:ILE:CD1   | 1:A:797:ILE:CD1   | 2.96                     | 0.43              |
| 1:A:1009:LEU:CD1  | 1:A:1042:TYR:HA   | 2.49                     | 0.43              |
| 1:B:850:PRO:CG    | 1:B:975:ARG:HH22  | 2.22                     | 0.43              |
| 1:B:991:ARG:HD3   | 1:B:991:ARG:HA    | 1.73                     | 0.43              |
| 1:A:586:ARG:HG2   | 1:A:586:ARG:NH1   | 2.34                     | 0.43              |
| 1:B:127:VAL:HA    | 1:B:128:PRO:HD2   | 1.81                     | 0.43              |
| 1:B:415:ARG:NH1   | 1:B:419:ARG:NH2   | 2.66                     | 0.43              |
| 1:B:33:ALA:HB1    | 1:B:54:SER:HA     | 1.99                     | 0.43              |
| 1:B:547:GLY:O     | 1:B:548:THR:C     | 2.62                     | 0.43              |
| 1:B:690:HIS:CE1   | 1:B:731:VAL:HG11  | 2.54                     | 0.43              |
| 1:A:409:VAL:HG23  | 1:B:23:GLU:CD     | 2.43                     | 0.42              |
| 1:B:437:ILE:O     | 1:B:441:ARG:HB2   | 2.19                     | 0.42              |
| 1:B:495:LEU:HD23  | 1:B:495:LEU:C     | 2.44                     | 0.42              |
| 1:B:531:ASP:O     | 1:B:532:ALA:C     | 2.61                     | 0.42              |
| 1:B:682:ALA:O     | 1:B:713:GLY:HA2   | 2.19                     | 0.42              |
| 1:B:925:GLU:HB2   | 1:B:965:LEU:HD23  | 2.01                     | 0.42              |
| 1:B:948:THR:C     | 1:B:950:ALA:H     | 2.27                     | 0.42              |
| 1:A:825:GLN:O     | 1:A:828:SER:OG    | 2.37                     | 0.42              |
| 1:A:973:ILE:HG21  | 1:A:1004:ILE:HD11 | 2.02                     | 0.42              |
| 1:B:999:TRP:CD2   | 1:B:1062:PRO:HB3  | 2.54                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:511:ALA:CB    | 1:B:531:ASP:HA    | 2.49                     | 0.42              |
| 1:B:746:LEU:O     | 1:B:765:CYS:HB3   | 2.19                     | 0.42              |
| 1:B:914:ALA:CA    | 1:B:958:MET:HE2   | 2.40                     | 0.42              |
| 1:A:208:GLU:HG2   | 1:A:276:GLU:HG2   | 2.02                     | 0.42              |
| 1:A:753:ARG:CG    | 1:A:753:ARG:NH1   | 2.81                     | 0.42              |
| 1:A:753:ARG:HD3   | 1:A:794:PRO:HB3   | 2.01                     | 0.42              |
| 1:A:587:HIS:CE1   | 1:A:629:LEU:HD11  | 2.55                     | 0.42              |
| 1:A:1033:LEU:O    | 1:A:1037:LEU:HB2  | 2.20                     | 0.42              |
| 1:A:284:PHE:CD1   | 1:A:284:PHE:C     | 2.97                     | 0.42              |
| 1:B:941:MET:HA    | 1:B:941:MET:CE    | 2.41                     | 0.42              |
| 1:A:827:LEU:O     | 1:A:831:GLN:HG3   | 2.20                     | 0.42              |
| 1:B:248:LEU:HB2   | 1:B:253:ARG:HH12  | 1.84                     | 0.42              |
| 1:A:978:TYR:OH    | 1:A:1003:GLU:HG3  | 2.20                     | 0.42              |
| 1:A:995:PHE:CD1   | 1:A:995:PHE:C     | 2.98                     | 0.42              |
| 1:B:827:LEU:O     | 1:B:831:GLN:HG3   | 2.19                     | 0.42              |
| 1:A:254:ARG:O     | 1:A:258:GLN:HG3   | 2.20                     | 0.42              |
| 1:A:632:ALA:HA    | 1:A:650:ASP:OD1   | 2.20                     | 0.42              |
| 1:A:997:VAL:CG2   | 1:A:1060:ILE:HG23 | 2.50                     | 0.42              |
| 1:B:154:MET:CE    | 1:B:168:LYS:HB2   | 2.50                     | 0.42              |
| 1:A:47:GLU:HG2    | 1:B:495:LEU:HB3   | 2.01                     | 0.42              |
| 1:A:351:LEU:HD13  | 1:A:425:LEU:CD1   | 2.46                     | 0.42              |
| 1:A:638:ARG:NH2   | 1:A:681:LEU:HD21  | 2.35                     | 0.42              |
| 1:B:1034:PHE:C    | 1:B:1036:ARG:H    | 2.26                     | 0.42              |
| 1:B:1061:ASP:C    | 1:B:1061:ASP:OD1  | 2.63                     | 0.42              |
| 1:B:837:TRP:HZ3   | 1:B:839:ALA:HB2   | 1.85                     | 0.41              |
| 1:A:23:GLU:OE1    | 1:B:409:VAL:HG22  | 2.20                     | 0.41              |
| 1:A:241:GLU:HG2   | 1:A:296:GLU:HB3   | 2.02                     | 0.41              |
| 1:B:686:GLY:H     | 1:B:689:ASN:ND2   | 2.18                     | 0.41              |
| 1:A:119:ARG:O     | 1:A:123:ILE:HG13  | 2.20                     | 0.41              |
| 1:A:276:GLU:HB3   | 1:A:287:LEU:HD23  | 2.02                     | 0.41              |
| 1:A:298:THR:OG1   | 1:A:350:GLN:NE2   | 2.53                     | 0.41              |
| 1:A:811:LEU:CD1   | 1:A:873:LEU:HD11  | 2.50                     | 0.41              |
| 1:A:862:ALA:O     | 1:A:866:ILE:HG13  | 2.21                     | 0.41              |
| 1:A:911:ALA:HB1   | 1:A:954:ARG:CZ    | 2.50                     | 0.41              |
| 1:B:154:MET:HE1   | 1:B:168:LYS:HB2   | 2.02                     | 0.41              |
| 1:B:918:GLY:O     | 1:B:961:LEU:HD13  | 2.20                     | 0.41              |
| 1:A:210:GLN:HG3   | 1:A:225:VAL:CG2   | 2.50                     | 0.41              |
| 1:A:250:GLU:O     | 1:A:250:GLU:HG2   | 2.20                     | 0.41              |
| 1:A:1013:VAL:HG13 | 1:A:1017:TYR:HD2  | 1.86                     | 0.41              |
| 1:B:31:VAL:HB     | 1:B:51:LEU:HG     | 2.01                     | 0.41              |
| 1:B:256:LEU:HD22  | 1:B:277:PHE:CD2   | 2.56                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:608:ARG:CD   | 1:B:613:ASN:ND2   | 2.83                     | 0.41              |
| 1:B:753:ARG:HD3  | 1:B:794:PRO:CB    | 2.50                     | 0.41              |
| 1:B:828:SER:HG   | 1:B:889:ARG:HH12  | 1.66                     | 0.41              |
| 1:A:4:SER:CB     | 1:A:74:ALA:HA     | 2.51                     | 0.41              |
| 1:A:199:ALA:O    | 1:A:200:LEU:CG    | 2.60                     | 0.41              |
| 1:B:1017:TYR:CG  | 1:B:1037:LEU:HD23 | 2.56                     | 0.41              |
| 1:A:642:ASP:O    | 1:A:646:ASN:N     | 2.54                     | 0.41              |
| 1:A:799:PRO:O    | 1:A:801:ALA:N     | 2.54                     | 0.41              |
| 1:A:4:SER:OG     | 1:A:74:ALA:HA     | 2.21                     | 0.41              |
| 1:A:502:VAL:CG1  | 1:A:503:ALA:N     | 2.84                     | 0.41              |
| 1:B:82:GLY:O     | 1:B:83:PHE:C      | 2.64                     | 0.41              |
| 1:B:140:GLU:O    | 1:B:141:ASP:C     | 2.63                     | 0.41              |
| 1:B:516:VAL:HG12 | 1:B:517:VAL:N     | 2.36                     | 0.41              |
| 1:B:642:ASP:HB2  | 1:B:646:ASN:HD22  | 1.85                     | 0.41              |
| 1:B:975:ARG:HG3  | 1:B:975:ARG:NH1   | 2.36                     | 0.41              |
| 1:A:258:GLN:HG2  | 1:A:337:VAL:HG11  | 2.03                     | 0.41              |
| 1:A:736:MET:HE2  | 1:A:736:MET:HB3   | 1.88                     | 0.41              |
| 1:A:868:ASP:OD2  | 1:A:891:GLU:N     | 2.54                     | 0.41              |
| 1:B:530:PRO:HD2  | 1:B:533:LEU:CD2   | 2.50                     | 0.41              |
| 1:B:154:MET:HB2  | 1:B:200:LEU:CD1   | 2.51                     | 0.40              |
| 1:B:270:ARG:HB3  | 1:B:270:ARG:NH1   | 2.36                     | 0.40              |
| 1:A:79:PRO:CB    | 1:A:85:SER:HA     | 2.49                     | 0.40              |
| 1:A:201:LEU:HD23 | 1:A:278:LEU:HB3   | 2.02                     | 0.40              |
| 1:A:448:ARG:HD2  | 1:A:458:PHE:CE2   | 2.48                     | 0.40              |
| 1:A:509:TYR:HB3  | 1:A:513:ALA:HB3   | 2.03                     | 0.40              |
| 1:A:638:ARG:HD2  | 1:A:643:LEU:CD2   | 2.51                     | 0.40              |
| 1:A:681:LEU:HD23 | 1:A:681:LEU:N     | 2.35                     | 0.40              |
| 1:A:684:THR:HG22 | 1:A:714:GLY:C     | 2.46                     | 0.40              |
| 1:B:640:GLU:HG2  | 1:B:644:ILE:HD11  | 2.03                     | 0.40              |
| 1:B:1030:ARG:C   | 1:B:1032:ASN:N    | 2.79                     | 0.40              |
| 1:B:398:TYR:O    | 1:B:399:ASP:C     | 2.64                     | 0.40              |
| 1:B:943:GLY:O    | 1:B:947:GLU:HG2   | 2.21                     | 0.40              |
| 1:B:1057:ASP:O   | 1:B:1058:ASP:HB2  | 2.21                     | 0.40              |
| 1:A:703:LYS:HD3  | 1:A:705:LEU:HD11  | 2.04                     | 0.40              |
| 1:A:1070:THR:C   | 1:A:1072:LEU:H    | 2.29                     | 0.40              |
| 1:B:133:THR:O    | 1:B:196:PHE:CE1   | 2.74                     | 0.40              |
| 1:B:499:VAL:HG11 | 1:B:540:VAL:CG1   | 2.52                     | 0.40              |
| 1:B:499:VAL:CG2  | 1:B:540:VAL:HG11  | 2.37                     | 0.40              |
| 1:B:635:ARG:HE   | 1:B:640:GLU:H     | 1.69                     | 0.40              |
| 1:B:743:ARG:H    | 1:B:743:ARG:HG2   | 1.63                     | 0.40              |
| 1:A:604:ARG:HH11 | 1:A:604:ARG:CG    | 2.32                     | 0.40              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:975:ARG:HG3  | 1:A:975:ARG:HH11  | 1.86                     | 0.40              |
| 1:A:1029:GLU:HB3 | 1:A:1032:ASN:ND2  | 2.37                     | 0.40              |
| 1:A:1051:ALA:HB2 | 1:A:1059:VAL:HG23 | 2.02                     | 0.40              |
| 1:B:258:GLN:O    | 1:B:262:ARG:HB2   | 2.22                     | 0.40              |
| 1:B:623:PHE:CE2  | 1:B:625:GLU:HB2   | 2.57                     | 0.40              |
| 1:B:731:VAL:HG12 | 1:B:733:THR:H     | 1.86                     | 0.40              |
| 1:B:980:LEU:HA   | 1:B:983:MET:HE2   | 2.03                     | 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     | 958/1093 (88%)  | 870 (91%)  | 64 (7%)  | 24 (2%)  | 4           | 21 |
| 1   | B     | 984/1093 (90%)  | 893 (91%)  | 73 (7%)  | 18 (2%)  | 6           | 29 |
| All | All   | 1942/2186 (89%) | 1763 (91%) | 137 (7%) | 42 (2%)  | 5           | 24 |

All (42) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 200 | LEU  |
| 1   | A     | 520 | ALA  |
| 1   | A     | 712 | GLU  |
| 1   | B     | 360 | ALA  |
| 1   | B     | 520 | ALA  |
| 1   | B     | 712 | GLU  |
| 1   | A     | 53  | GLY  |
| 1   | A     | 202 | GLY  |
| 1   | A     | 232 | MET  |
| 1   | A     | 505 | GLU  |
| 1   | A     | 579 | ASP  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 979  | GLY  |
| 1   | A     | 1046 | LYS  |
| 1   | B     | 202  | GLY  |
| 1   | B     | 232  | MET  |
| 1   | B     | 853  | ARG  |
| 1   | A     | 61   | ASN  |
| 1   | A     | 335  | THR  |
| 1   | A     | 521  | MET  |
| 1   | A     | 575  | LEU  |
| 1   | A     | 869  | VAL  |
| 1   | A     | 1031 | GLN  |
| 1   | B     | 197  | ALA  |
| 1   | B     | 342  | ALA  |
| 1   | B     | 1031 | GLN  |
| 1   | A     | 413  | SER  |
| 1   | A     | 620  | PRO  |
| 1   | A     | 741  | ARG  |
| 1   | B     | 235  | ARG  |
| 1   | B     | 399  | ASP  |
| 1   | B     | 718  | PRO  |
| 1   | A     | 102  | VAL  |
| 1   | A     | 531  | ASP  |
| 1   | B     | 135  | GLY  |
| 1   | B     | 1027 | PRO  |
| 1   | B     | 469  | ALA  |
| 1   | B     | 620  | PRO  |
| 1   | A     | 1027 | PRO  |
| 1   | B     | 53   | GLY  |
| 1   | B     | 536  | VAL  |
| 1   | A     | 1045 | GLY  |
| 1   | A     | 536  | VAL  |

### 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.

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1   | A     | 718/796 (90%)   | 672 (94%)  | 46 (6%)  | 16          | 46 |
| 1   | B     | 738/796 (93%)   | 694 (94%)  | 44 (6%)  | 17          | 48 |
| All | All   | 1456/1592 (92%) | 1366 (94%) | 90 (6%)  | 16          | 47 |

All (90) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 10  | ARG  |
| 1   | A     | 36  | ASP  |
| 1   | A     | 51  | LEU  |
| 1   | A     | 54  | SER  |
| 1   | A     | 56  | PRO  |
| 1   | A     | 76  | LEU  |
| 1   | A     | 119 | ARG  |
| 1   | A     | 220 | THR  |
| 1   | A     | 232 | MET  |
| 1   | A     | 250 | GLU  |
| 1   | A     | 269 | LEU  |
| 1   | A     | 294 | GLN  |
| 1   | A     | 326 | LEU  |
| 1   | A     | 365 | LEU  |
| 1   | A     | 387 | TYR  |
| 1   | A     | 393 | VAL  |
| 1   | A     | 415 | ARG  |
| 1   | A     | 442 | ARG  |
| 1   | A     | 539 | LEU  |
| 1   | A     | 540 | VAL  |
| 1   | A     | 553 | LEU  |
| 1   | A     | 597 | ASP  |
| 1   | A     | 662 | ASP  |
| 1   | A     | 670 | GLN  |
| 1   | A     | 693 | THR  |
| 1   | A     | 696 | VAL  |
| 1   | A     | 718 | PRO  |
| 1   | A     | 741 | ARG  |
| 1   | A     | 764 | VAL  |
| 1   | A     | 771 | THR  |
| 1   | A     | 794 | PRO  |
| 1   | A     | 902 | THR  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 903  | HIS  |
| 1   | A     | 926  | SER  |
| 1   | A     | 948  | THR  |
| 1   | A     | 973  | ILE  |
| 1   | A     | 991  | ARG  |
| 1   | A     | 997  | VAL  |
| 1   | A     | 1001 | THR  |
| 1   | A     | 1010 | GLU  |
| 1   | A     | 1030 | ARG  |
| 1   | A     | 1031 | GLN  |
| 1   | A     | 1037 | LEU  |
| 1   | A     | 1052 | THR  |
| 1   | A     | 1070 | THR  |
| 1   | A     | 1071 | ARG  |
| 1   | B     | 1    | MET  |
| 1   | B     | 10   | ARG  |
| 1   | B     | 12   | GLU  |
| 1   | B     | 20   | THR  |
| 1   | B     | 36   | ASP  |
| 1   | B     | 56   | PRO  |
| 1   | B     | 115  | LYS  |
| 1   | B     | 140  | GLU  |
| 1   | B     | 153  | ILE  |
| 1   | B     | 205  | ARG  |
| 1   | B     | 237  | GLN  |
| 1   | B     | 241  | GLU  |
| 1   | B     | 293  | ILE  |
| 1   | B     | 319  | GLU  |
| 1   | B     | 326  | LEU  |
| 1   | B     | 363  | SER  |
| 1   | B     | 393  | VAL  |
| 1   | B     | 397  | GLN  |
| 1   | B     | 409  | VAL  |
| 1   | B     | 442  | ARG  |
| 1   | B     | 448  | ARG  |
| 1   | B     | 495  | LEU  |
| 1   | B     | 521  | MET  |
| 1   | B     | 539  | LEU  |
| 1   | B     | 597  | ASP  |
| 1   | B     | 672  | VAL  |
| 1   | B     | 693  | THR  |
| 1   | B     | 718  | PRO  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 743  | ARG  |
| 1   | B     | 764  | VAL  |
| 1   | B     | 781  | PRO  |
| 1   | B     | 792  | TYR  |
| 1   | B     | 828  | SER  |
| 1   | B     | 844  | VAL  |
| 1   | B     | 868  | ASP  |
| 1   | B     | 941  | MET  |
| 1   | B     | 948  | THR  |
| 1   | B     | 973  | ILE  |
| 1   | B     | 997  | VAL  |
| 1   | B     | 1001 | THR  |
| 1   | B     | 1010 | GLU  |
| 1   | B     | 1038 | VAL  |
| 1   | B     | 1052 | THR  |
| 1   | B     | 1070 | THR  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 71   | ASN  |
| 1   | A     | 99   | HIS  |
| 1   | A     | 210  | GLN  |
| 1   | A     | 219  | GLN  |
| 1   | A     | 237  | GLN  |
| 1   | A     | 290  | ASN  |
| 1   | A     | 344  | GLN  |
| 1   | A     | 350  | GLN  |
| 1   | A     | 397  | GLN  |
| 1   | A     | 605  | GLN  |
| 1   | A     | 613  | ASN  |
| 1   | A     | 646  | ASN  |
| 1   | A     | 689  | ASN  |
| 1   | A     | 775  | ASN  |
| 1   | A     | 818  | HIS  |
| 1   | A     | 831  | GLN  |
| 1   | A     | 851  | GLN  |
| 1   | A     | 994  | GLN  |
| 1   | A     | 1032 | ASN  |
| 1   | B     | 43   | HIS  |
| 1   | B     | 206  | HIS  |
| 1   | B     | 210  | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 219  | GLN  |
| 1   | B     | 233  | GLN  |
| 1   | B     | 237  | GLN  |
| 1   | B     | 258  | GLN  |
| 1   | B     | 344  | GLN  |
| 1   | B     | 350  | GLN  |
| 1   | B     | 397  | GLN  |
| 1   | B     | 514  | GLN  |
| 1   | B     | 613  | ASN  |
| 1   | B     | 646  | ASN  |
| 1   | B     | 670  | GLN  |
| 1   | B     | 818  | HIS  |
| 1   | B     | 838  | GLN  |
| 1   | B     | 904  | HIS  |
| 1   | B     | 994  | GLN  |
| 1   | B     | 1032 | ASN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ > 2 |       | OWAB(Å <sup>2</sup> ) | Q < 0.9 |
|-----|-------|-----------------|--------|-----------|-------|-----------------------|---------|
| 1   | A     | 972/1093 (88%)  | -0.11  | 18 (1%)   | 66 43 | 35, 63, 96, 139       | 0       |
| 1   | B     | 1000/1093 (91%) | -0.10  | 28 (2%)   | 55 32 | 34, 61, 101, 138      | 0       |
| All | All   | 1972/2186 (90%) | -0.10  | 46 (2%)   | 61 38 | 34, 62, 99, 139       | 0       |

All (46) RSRZ outliers are listed below:

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | A     | 479  | PRO  | 4.7  |
| 1   | B     | 195  | LEU  | 4.4  |
| 1   | B     | 470  | ALA  | 4.0  |
| 1   | B     | 482  | VAL  | 3.8  |
| 1   | A     | 1025 | THR  | 3.4  |
| 1   | A     | 199  | ALA  | 3.4  |
| 1   | A     | 1028 | ALA  | 3.3  |
| 1   | B     | 334  | GLY  | 3.3  |
| 1   | B     | 1025 | THR  | 3.2  |
| 1   | A     | 470  | ALA  | 3.2  |
| 1   | B     | 520  | ALA  | 3.1  |
| 1   | A     | 200  | LEU  | 3.1  |
| 1   | B     | 170  | HIS  | 2.9  |
| 1   | A     | 481  | ALA  | 2.9  |
| 1   | A     | 1027 | PRO  | 2.9  |
| 1   | B     | 1073 | SER  | 2.8  |
| 1   | A     | 1073 | SER  | 2.7  |
| 1   | A     | 714  | GLY  | 2.7  |
| 1   | B     | 1028 | ALA  | 2.7  |
| 1   | B     | 906  | GLY  | 2.7  |
| 1   | B     | 1018 | ARG  | 2.7  |
| 1   | B     | 1    | MET  | 2.7  |
| 1   | B     | 333  | ASP  | 2.6  |
| 1   | B     | 662  | ASP  | 2.6  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | A     | 1030 | ARG  | 2.6  |
| 1   | A     | 480  | GLY  | 2.5  |
| 1   | B     | 70   | GLU  | 2.5  |
| 1   | A     | 361  | ASP  | 2.4  |
| 1   | A     | 38   | HIS  | 2.4  |
| 1   | B     | 721  | THR  | 2.4  |
| 1   | B     | 165  | GLY  | 2.4  |
| 1   | B     | 1030 | ARG  | 2.3  |
| 1   | B     | 143  | GLU  | 2.3  |
| 1   | B     | 521  | MET  | 2.3  |
| 1   | B     | 203  | ASP  | 2.3  |
| 1   | A     | 1044 | HIS  | 2.3  |
| 1   | B     | 558  | THR  | 2.2  |
| 1   | A     | 541  | THR  | 2.1  |
| 1   | B     | 147  | ALA  | 2.1  |
| 1   | A     | 1018 | ARG  | 2.1  |
| 1   | B     | 134  | ASP  | 2.1  |
| 1   | B     | 1027 | PRO  | 2.1  |
| 1   | B     | 1044 | HIS  | 2.1  |
| 1   | B     | 581  | ASP  | 2.1  |
| 1   | B     | 196  | PHE  | 2.1  |
| 1   | A     | 318  | GLY  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.