



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 03:14 PM UTC

PDB ID : 4Z6Y / pdb\_00004z6y  
Title : Structure of the TBC1D7-TSC1 complex  
Authors : Gai, Z.; Wu, G.  
Deposited on : 2015-04-06  
Resolution : 2.81 Å(reported)

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

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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                                                             |

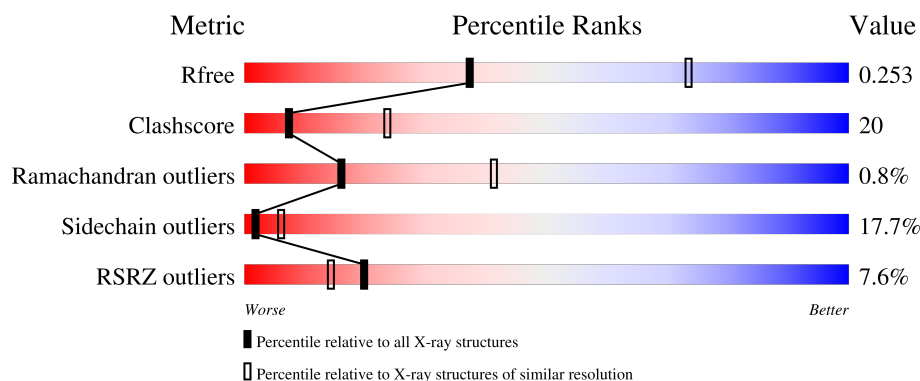
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.81 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                      | 4591 (2.84-2.80)                                      |
| Clashscore            | 190562                      | 5010 (2.84-2.80)                                      |
| Ramachandran outliers | 187476                      | 4916 (2.84-2.80)                                      |
| Sidechain outliers    | 187428                      | 4918 (2.84-2.80)                                      |
| RSRZ outliers         | 180081                      | 4594 (2.84-2.80)                                      |

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     | 273    |                  |
| 1   | B     | 273    |                  |
| 1   | E     | 273    |                  |
| 1   | G     | 273    |                  |
| 2   | C     | 56     |                  |

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| Mol | Chain | Length | Quality of chain                                                                                                                                    |
|-----|-------|--------|-----------------------------------------------------------------------------------------------------------------------------------------------------|
| 2   | D     | 56     | <div><div>48%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>59%</div><div>30%</div><div>5%</div><div>5%</div></div>   |
| 2   | F     | 56     | <div><div>43%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>61%</div><div>29%</div><div>7%</div><div>•</div></div>    |
| 2   | H     | 56     | <div><div>41%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>55%</div><div>21%</div><div>18%</div><div>• •</div></div> |

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 10471 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 TBC1 domain family member 7.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | B     | 272      | Total | C    | N   | O   | S  | 0       | 1       | 0     |
|     |       |          | 2200  | 1424 | 368 | 393 | 15 |         |         |       |
| 1   | G     | 272      | Total | C    | N   | O   | S  | 0       | 1       | 0     |
|     |       |          | 2206  | 1427 | 371 | 393 | 15 |         |         |       |
| 1   | E     | 272      | Total | C    | N   | O   | S  | 0       | 1       | 0     |
|     |       |          | 2206  | 1427 | 371 | 393 | 15 |         |         |       |
| 1   | A     | 273      | Total | C    | N   | O   | S  | 0       | 1       | 0     |
|     |       |          | 2212  | 1430 | 372 | 395 | 15 |         |         |       |

- Molecule 2 is a protein called Hamartin.

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 2   | C     | 53       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 402   | 252 | 69 | 81 |         |         |       |
| 2   | H     | 55       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 415   | 259 | 71 | 85 |         |         |       |
| 2   | F     | 54       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 407   | 255 | 70 | 82 |         |         |       |
| 2   | D     | 53       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 402   | 252 | 69 | 81 |         |         |       |

- Molecule 3 is water.

| Mol | Chain | Residues | Atoms |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 3   | B     | 4        | Total | O | 0       | 0       |
|     |       |          | 4     | 4 |         |         |
| 3   | C     | 4        | Total | O | 0       | 0       |
|     |       |          | 4     | 4 |         |         |
| 3   | G     | 6        | Total | O | 0       | 0       |
|     |       |          | 6     | 6 |         |         |
| 3   | H     | 2        | Total | O | 0       | 0       |
|     |       |          | 2     | 2 |         |         |

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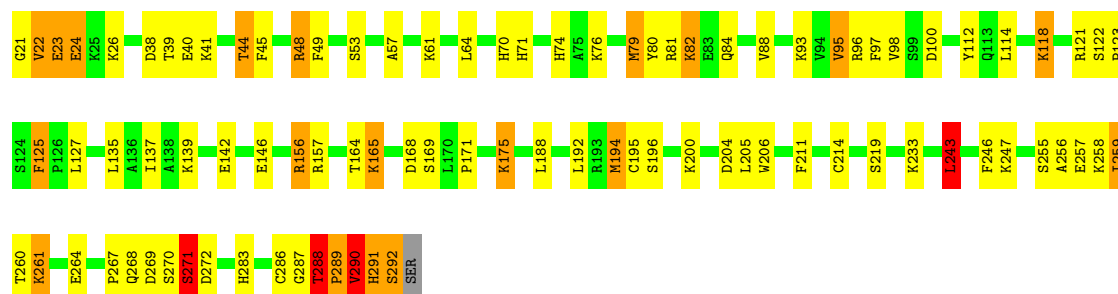
| Mol | Chain | Residues | Atoms      |        | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|---------|---------|
| 3   | E     | 1        | Total<br>1 | O<br>1 | 0       | 0       |
| 3   | F     | 1        | Total<br>1 | O<br>1 | 0       | 0       |
| 3   | A     | 1        | Total<br>1 | O<br>1 | 0       | 0       |
| 3   | D     | 2        | Total<br>2 | O<br>2 | 0       | 0       |

### 3 Residue-property plots [i](#)

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.

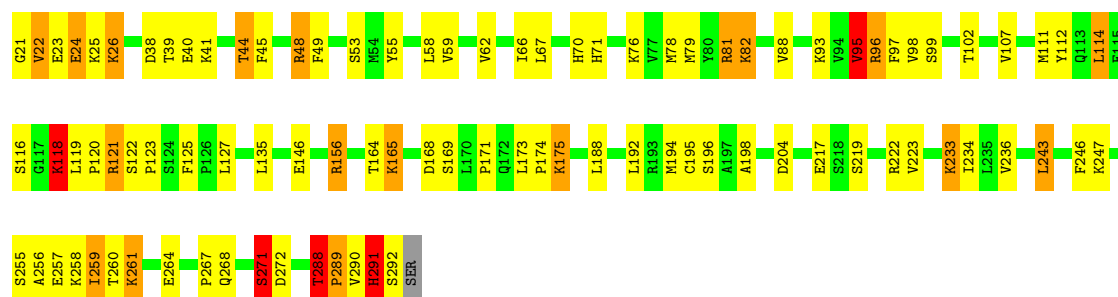
- Molecule 1: TBC1 domain family member 7

Chain B: 



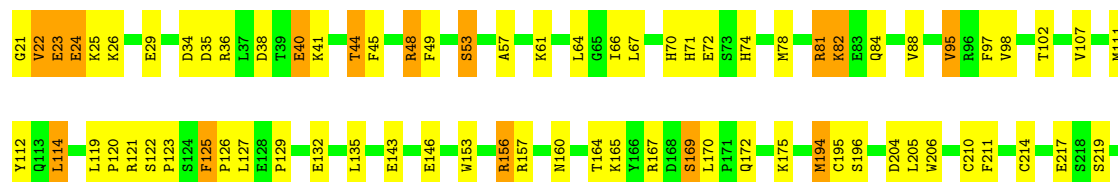
- Molecule 1: TBC1 domain family member 7

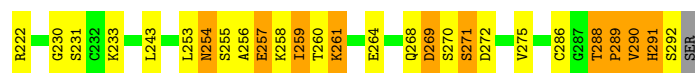
Chain G: 



- Molecule 1: TBC1 domain family member 7

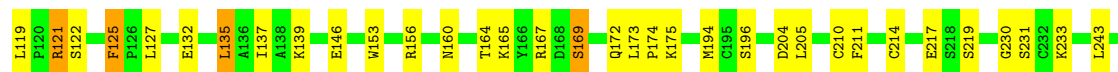
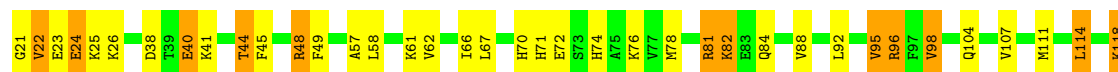
Chain E: 





- Molecule 1: TBC1 domain family member 7

Chain A: 66% 26% 8%



- Molecule 2: Hamartin

Chain C: 45% 54% 36% 5% 5%



- Molecule 2: Hamartin

Chain H: 41% 55% 21% 18% 2%



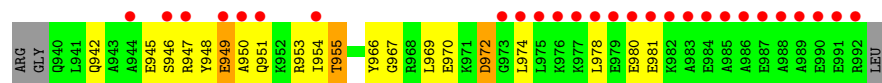
- Molecule 2: Hamartin

Chain F: 43% 61% 29% 7% 1%



- Molecule 2: Hamartin

Chain D: 48% 59% 30% 5% 5%



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 1 21 1                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 56.99Å 145.69Å 114.76Å<br>90.00° 89.65° 90.00°              | Depositor        |
| Resolution (Å)                                                          | 50.00 – 2.81<br>50.00 – 2.81                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 98.0 (50.00-2.81)<br>97.3 (50.00-2.81)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.85 (at 2.81Å)                                             | Xtriage          |
| Refinement program                                                      | REFMAC 5.6.0117                                             | Depositor        |
| R, $R_{free}$                                                           | 0.206 , 0.255<br>0.206 , 0.253                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 2260 reflections (4.97%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 69.9                                                        | Xtriage          |
| Anisotropy                                                              | 0.130                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.30 , 50.9                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$ | Xtriage          |
| Estimated twinning fraction                                             | 0.418 for h,-k,-l                                           | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.93                                                        | EDS              |
| Total number of atoms                                                   | 10471                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 68.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.59% 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     | 1.03         | 1/2269 (0.0%)  | 1.16        | 11/3073 (0.4%)  |
| 1   | B     | 1.02         | 3/2257 (0.1%)  | 1.17        | 9/3058 (0.3%)   |
| 1   | E     | 1.05         | 0/2263         | 1.19        | 15/3065 (0.5%)  |
| 1   | G     | 1.03         | 2/2263 (0.1%)  | 1.19        | 11/3065 (0.4%)  |
| 2   | C     | 0.76         | 0/404          | 1.03        | 0/543           |
| 2   | D     | 0.78         | 0/404          | 1.01        | 0/543           |
| 2   | F     | 0.74         | 0/409          | 1.07        | 0/550           |
| 2   | H     | 0.78         | 0/417          | 1.20        | 3/560 (0.5%)    |
| All | All   | 1.00         | 6/10686 (0.1%) | 1.16        | 49/14457 (0.3%) |

All (6) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 1   | B     | 74  | HIS  | CG-CD2  | 6.00 | 1.42        | 1.35     |
| 1   | B     | 74  | HIS  | ND1-CE1 | 5.66 | 1.38        | 1.32     |
| 1   | A     | 283 | HIS  | CG-CD2  | 5.32 | 1.41        | 1.35     |
| 1   | G     | 289 | PRO  | CA-C    | 5.27 | 1.58        | 1.52     |
| 1   | G     | 288 | THR  | N-CA    | 5.24 | 1.51        | 1.46     |
| 1   | B     | 288 | THR  | N-CA    | 5.13 | 1.51        | 1.46     |

All (49) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | G     | 95  | VAL  | N-CA-C | 13.37 | 123.09      | 110.53   |
| 2   | H     | 941 | LEU  | N-CA-C | -9.11 | 101.23      | 111.71   |
| 2   | H     | 949 | GLU  | N-CA-C | -8.58 | 101.93      | 111.28   |
| 1   | G     | 289 | PRO  | N-CA-C | 8.41  | 123.35      | 111.33   |
| 1   | B     | 289 | PRO  | N-CA-C | 8.39  | 122.96      | 111.22   |
| 1   | G     | 288 | THR  | N-CA-C | 8.28  | 115.67      | 108.22   |
| 1   | E     | 289 | PRO  | N-CA-C | 7.10  | 121.70      | 111.13   |
| 1   | E     | 230 | GLY  | N-CA-C | 6.92  | 125.02      | 115.27   |
| 1   | A     | 288 | THR  | CA-C-N | 6.59  | 127.49      | 120.11   |
| 1   | A     | 288 | THR  | C-N-CA | 6.59  | 127.49      | 120.11   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | E     | 24  | GLU  | N-CA-C   | -6.32 | 104.77      | 113.18   |
| 1   | E     | 170 | LEU  | CA-C-N   | -6.32 | 113.71      | 120.47   |
| 1   | E     | 170 | LEU  | C-N-CA   | -6.32 | 113.71      | 120.47   |
| 1   | A     | 271 | SER  | N-CA-C   | 6.22  | 117.73      | 111.07   |
| 1   | G     | 291 | HIS  | N-CA-C   | 6.10  | 118.84      | 111.40   |
| 1   | E     | 254 | ASN  | N-CA-C   | 6.08  | 118.82      | 111.40   |
| 1   | B     | 24  | GLU  | N-CA-C   | -6.00 | 104.74      | 111.28   |
| 1   | B     | 259 | ILE  | CB-CA-C  | -5.93 | 104.39      | 111.97   |
| 1   | E     | 288 | THR  | CA-C-N   | 5.87  | 126.33      | 120.52   |
| 1   | E     | 288 | THR  | C-N-CA   | 5.87  | 126.33      | 120.52   |
| 1   | A     | 230 | GLY  | N-CA-C   | 5.86  | 122.54      | 114.92   |
| 1   | E     | 259 | ILE  | CB-CA-C  | -5.71 | 104.66      | 111.97   |
| 2   | H     | 939 | GLY  | N-CA-C   | 5.71  | 120.72      | 113.24   |
| 1   | E     | 23  | GLU  | N-CA-C   | -5.66 | 101.98      | 113.29   |
| 1   | G     | 271 | SER  | N-CA-C   | 5.64  | 117.43      | 111.28   |
| 1   | B     | 271 | SER  | N-CA-C   | 5.64  | 117.10      | 111.07   |
| 1   | B     | 290 | VAL  | CB-CA-C  | -5.61 | 103.32      | 111.68   |
| 1   | G     | 259 | ILE  | CB-CA-C  | -5.61 | 104.79      | 111.97   |
| 1   | B     | 288 | THR  | N-CA-C   | 5.58  | 113.24      | 108.22   |
| 1   | A     | 259 | ILE  | CB-CA-C  | -5.51 | 104.91      | 111.97   |
| 1   | B     | 95  | VAL  | CA-C-N   | -5.51 | 113.50      | 122.65   |
| 1   | B     | 95  | VAL  | C-N-CA   | -5.51 | 113.50      | 122.65   |
| 1   | A     | 217 | GLU  | N-CA-C   | 5.43  | 118.71      | 111.75   |
| 1   | A     | 289 | PRO  | N-CA-C   | 5.36  | 118.99      | 111.33   |
| 1   | E     | 49  | PHE  | CA-C-N   | -5.35 | 114.21      | 119.99   |
| 1   | E     | 49  | PHE  | C-N-CA   | -5.35 | 114.21      | 119.99   |
| 1   | A     | 254 | ASN  | N-CA-C   | 5.34  | 117.91      | 111.40   |
| 1   | B     | 243 | LEU  | CA-CB-CG | -5.30 | 97.75       | 116.30   |
| 1   | E     | 53  | SER  | N-CA-C   | 5.28  | 117.72      | 111.33   |
| 1   | G     | 118 | LYS  | N-CA-C   | 5.25  | 117.49      | 109.62   |
| 1   | A     | 71  | HIS  | N-CA-C   | 5.24  | 117.67      | 111.33   |
| 1   | E     | 275 | VAL  | N-CA-C   | 5.20  | 115.92      | 110.62   |
| 1   | A     | 49  | PHE  | CA-C-N   | -5.17 | 114.41      | 119.99   |
| 1   | A     | 49  | PHE  | C-N-CA   | -5.17 | 114.41      | 119.99   |
| 1   | E     | 253 | LEU  | N-CA-C   | 5.16  | 118.02      | 109.46   |
| 1   | G     | 198 | ALA  | CA-C-N   | -5.16 | 114.47      | 120.04   |
| 1   | G     | 198 | ALA  | C-N-CA   | -5.16 | 114.47      | 120.04   |
| 1   | G     | 99  | SER  | N-CA-C   | -5.12 | 101.68      | 108.74   |
| 1   | G     | 223 | VAL  | CB-CA-C  | -5.08 | 105.36      | 112.02   |

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     | 2212  | 0        | 2253     | 103     | 1            |
| 1   | B     | 2200  | 0        | 2237     | 61      | 1            |
| 1   | E     | 2206  | 0        | 2248     | 74      | 2            |
| 1   | G     | 2206  | 0        | 2248     | 102     | 2            |
| 2   | C     | 402   | 0        | 382      | 15      | 0            |
| 2   | D     | 402   | 0        | 383      | 18      | 0            |
| 2   | F     | 407   | 0        | 385      | 20      | 0            |
| 2   | H     | 415   | 0        | 392      | 48      | 0            |
| 3   | A     | 1     | 0        | 0        | 1       | 0            |
| 3   | B     | 4     | 0        | 0        | 0       | 0            |
| 3   | C     | 4     | 0        | 0        | 0       | 0            |
| 3   | D     | 2     | 0        | 0        | 0       | 0            |
| 3   | E     | 1     | 0        | 0        | 0       | 0            |
| 3   | F     | 1     | 0        | 0        | 0       | 0            |
| 3   | G     | 6     | 0        | 0        | 0       | 0            |
| 3   | H     | 2     | 0        | 0        | 0       | 0            |
| All | All   | 10471 | 0        | 10528    | 429     | 3            |

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 (429) 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:121:ARG:HD2 | 1:A:125:PHE:CE2 | 1.20                     | 1.73              |
| 1:A:121:ARG:CD  | 1:A:125:PHE:CE2 | 1.89                     | 1.54              |
| 1:G:22:VAL:C    | 1:G:24:GLU:HB2  | 1.34                     | 1.50              |
| 1:A:21:GLY:C    | 1:A:24:GLU:HG2  | 1.43                     | 1.41              |
| 1:A:121:ARG:HD2 | 1:A:125:PHE:CD2 | 1.57                     | 1.36              |
| 1:A:48:ARG:HD2  | 1:A:289:PRO:O   | 1.25                     | 1.34              |
| 1:A:21:GLY:O    | 1:A:24:GLU:HG3  | 1.16                     | 1.34              |
| 1:A:95:VAL:O    | 1:A:96:ARG:CG   | 1.76                     | 1.32              |
| 1:A:21:GLY:O    | 1:A:24:GLU:CG   | 1.78                     | 1.31              |
| 1:A:21:GLY:C    | 1:A:24:GLU:CG   | 2.04                     | 1.28              |
| 1:G:121:ARG:HG3 | 1:G:125:PHE:CE1 | 1.69                     | 1.27              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:A:95:VAL:O    | 1:A:96:ARG:CD   | 1.86                     | 1.23              |
| 1:A:22:VAL:C    | 1:A:24:GLU:HB3  | 1.65                     | 1.22              |
| 1:A:95:VAL:O    | 1:A:96:ARG:HG3  | 1.24                     | 1.21              |
| 1:A:21:GLY:CA   | 1:A:24:GLU:HG2  | 1.71                     | 1.20              |
| 1:G:23:GLU:N    | 1:G:24:GLU:HB2  | 1.55                     | 1.20              |
| 1:A:48:ARG:CD   | 1:A:289:PRO:O   | 1.89                     | 1.19              |
| 1:A:95:VAL:C    | 1:A:96:ARG:HG3  | 1.48                     | 1.19              |
| 2:D:966:TYR:O   | 2:D:970:GLU:HG2 | 1.43                     | 1.18              |
| 1:A:23:GLU:CB   | 1:A:26:LYS:HB2  | 1.72                     | 1.18              |
| 1:E:48:ARG:HD3  | 1:E:289:PRO:O   | 1.42                     | 1.17              |
| 1:G:45:PHE:HB2  | 1:G:291:HIS:CE1 | 1.80                     | 1.16              |
| 2:F:966:TYR:O   | 2:F:970:GLU:HG2 | 1.46                     | 1.16              |
| 1:A:121:ARG:NE  | 1:A:125:PHE:HE2 | 1.45                     | 1.15              |
| 1:E:48:ARG:CD   | 1:E:289:PRO:O   | 1.96                     | 1.13              |
| 1:A:23:GLU:N    | 1:A:24:GLU:HB3  | 1.61                     | 1.13              |
| 1:A:121:ARG:NE  | 1:A:125:PHE:CE2 | 2.13                     | 1.13              |
| 2:H:942:GLN:O   | 2:H:945:GLU:HG3 | 1.49                     | 1.12              |
| 1:G:45:PHE:CB   | 1:G:291:HIS:HE1 | 1.64                     | 1.10              |
| 2:H:966:TYR:O   | 2:H:970:GLU:HG2 | 1.50                     | 1.10              |
| 2:C:966:TYR:O   | 2:C:970:GLU:HG2 | 1.51                     | 1.09              |
| 2:H:939:GLY:C   | 2:H:942:GLN:HB3 | 1.77                     | 1.09              |
| 2:H:942:GLN:HA  | 2:H:945:GLU:CG  | 1.84                     | 1.07              |
| 1:G:95:VAL:HG11 | 1:G:97:PHE:HD2  | 1.10                     | 1.07              |
| 1:G:22:VAL:C    | 1:G:24:GLU:CB   | 2.28                     | 1.06              |
| 1:E:233:LYS:NZ  | 1:E:286:CYS:SG  | 2.29                     | 1.06              |
| 1:A:233:LYS:NZ  | 1:A:286:CYS:SG  | 2.30                     | 1.05              |
| 2:H:949:GLU:O   | 2:H:952:LYS:HG3 | 1.55                     | 1.04              |
| 1:A:24:GLU:OE2  | 1:A:24:GLU:HA   | 1.55                     | 1.04              |
| 1:G:95:VAL:HG11 | 1:G:97:PHE:CD2  | 1.92                     | 1.04              |
| 1:G:48:ARG:NH2  | 1:G:49:PHE:HE1  | 1.54                     | 1.04              |
| 2:H:945:GLU:O   | 2:H:949:GLU:HG2 | 1.56                     | 1.04              |
| 1:E:21:GLY:O    | 1:E:25:LYS:N    | 1.90                     | 1.04              |
| 1:A:121:ARG:HD2 | 1:A:125:PHE:CZ  | 1.92                     | 1.03              |
| 1:G:45:PHE:CA   | 1:G:291:HIS:HE1 | 1.72                     | 1.02              |
| 1:G:95:VAL:CG1  | 1:G:97:PHE:HD2  | 1.74                     | 1.01              |
| 1:A:121:ARG:CD  | 1:A:125:PHE:CD2 | 2.28                     | 1.00              |
| 1:B:233:LYS:NZ  | 1:B:286:CYS:SG  | 2.34                     | 0.99              |
| 2:H:939:GLY:O   | 2:H:942:GLN:HB3 | 1.63                     | 0.99              |
| 2:H:946:SER:HA  | 2:H:949:GLU:HG3 | 1.45                     | 0.99              |
| 1:A:23:GLU:CB   | 1:A:26:LYS:CB   | 2.41                     | 0.99              |
| 1:G:121:ARG:CG  | 1:G:125:PHE:CE1 | 2.47                     | 0.98              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 2:D:946:SER:O    | 2:D:949:GLU:HG3 | 1.62                     | 0.98              |
| 1:E:21:GLY:O     | 1:E:24:GLU:HB3  | 1.65                     | 0.97              |
| 1:G:257:GLU:O    | 1:G:261:LYS:HG2 | 1.64                     | 0.95              |
| 2:F:946:SER:O    | 2:F:949:GLU:HG3 | 1.64                     | 0.95              |
| 1:A:22:VAL:C     | 1:A:24:GLU:CB   | 2.40                     | 0.95              |
| 2:H:942:GLN:HA   | 2:H:945:GLU:CD  | 1.90                     | 0.94              |
| 1:B:260:THR:O    | 1:B:264:GLU:HG3 | 1.67                     | 0.93              |
| 1:A:121:ARG:HG2  | 1:A:125:PHE:CD2 | 2.03                     | 0.93              |
| 1:G:260:THR:O    | 1:G:264:GLU:HG3 | 1.68                     | 0.92              |
| 2:F:969:LEU:CD2  | 2:F:974:LEU:HB3 | 2.00                     | 0.92              |
| 1:G:45:PHE:HB2   | 1:G:291:HIS:HE1 | 1.18                     | 0.92              |
| 1:A:23:GLU:CB    | 1:A:26:LYS:CG   | 2.48                     | 0.91              |
| 1:B:288:THR:HG22 | 1:B:289:PRO:HD2 | 1.50                     | 0.91              |
| 1:E:121:ARG:HD2  | 1:E:125:PHE:CE1 | 2.05                     | 0.90              |
| 1:A:121:ARG:CG   | 1:A:125:PHE:CD2 | 2.54                     | 0.90              |
| 2:H:942:GLN:HA   | 2:H:945:GLU:HG2 | 1.53                     | 0.90              |
| 1:A:104:GLN:HG2  | 3:A:301:HOH:O   | 1.71                     | 0.89              |
| 1:G:288:THR:HG22 | 1:G:289:PRO:HD2 | 1.53                     | 0.89              |
| 1:G:257:GLU:O    | 1:G:261:LYS:CG  | 2.22                     | 0.87              |
| 1:E:260:THR:O    | 1:E:264:GLU:HG3 | 1.74                     | 0.87              |
| 1:G:24:GLU:HA    | 1:G:24:GLU:OE2  | 1.74                     | 0.87              |
| 1:G:22:VAL:CA    | 1:G:24:GLU:HB2  | 2.04                     | 0.86              |
| 1:G:48:ARG:NE    | 1:G:49:PHE:CZ   | 2.42                     | 0.86              |
| 1:A:23:GLU:CB    | 1:A:26:LYS:CD   | 2.54                     | 0.86              |
| 1:G:291:HIS:N    | 1:G:292:SER:C   | 2.35                     | 0.85              |
| 1:G:291:HIS:H    | 1:G:292:SER:C   | 1.85                     | 0.84              |
| 1:G:45:PHE:CA    | 1:G:291:HIS:CE1 | 2.60                     | 0.84              |
| 1:E:121:ARG:HD2  | 1:E:125:PHE:CZ  | 2.13                     | 0.84              |
| 1:G:23:GLU:N     | 1:G:24:GLU:CB   | 2.39                     | 0.83              |
| 1:G:233:LYS:H    | 1:G:233:LYS:HD2 | 1.41                     | 0.83              |
| 1:E:25:LYS:HE3   | 1:E:29:GLU:OE1  | 1.79                     | 0.82              |
| 1:A:260:THR:O    | 1:A:264:GLU:HG3 | 1.80                     | 0.82              |
| 1:G:45:PHE:CB    | 1:G:291:HIS:CE1 | 2.49                     | 0.82              |
| 1:G:48:ARG:NH2   | 1:G:49:PHE:CE1  | 2.38                     | 0.82              |
| 1:G:291:HIS:CA   | 1:G:292:SER:C   | 2.52                     | 0.82              |
| 1:A:23:GLU:CB    | 1:A:26:LYS:HD2  | 2.11                     | 0.80              |
| 1:G:48:ARG:NE    | 1:G:49:PHE:CE1  | 2.48                     | 0.80              |
| 1:G:21:GLY:O     | 1:G:24:GLU:HB3  | 1.82                     | 0.80              |
| 1:G:291:HIS:HB2  | 1:G:292:SER:C   | 2.06                     | 0.80              |
| 1:G:21:GLY:C     | 1:G:24:GLU:HB3  | 2.06                     | 0.80              |
| 2:H:941:LEU:HD22 | 2:H:941:LEU:O   | 1.82                     | 0.80              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:291:HIS:CB   | 1:G:292:SER:C    | 2.55                     | 0.79              |
| 1:G:24:GLU:OE2   | 1:G:24:GLU:CA    | 2.30                     | 0.79              |
| 1:E:48:ARG:HD2   | 1:E:289:PRO:O    | 1.82                     | 0.79              |
| 2:H:942:GLN:HA   | 2:H:945:GLU:OE1  | 1.84                     | 0.78              |
| 2:H:946:SER:HA   | 2:H:949:GLU:CG   | 2.14                     | 0.78              |
| 1:A:95:VAL:O     | 1:A:96:ARG:HD3   | 1.80                     | 0.78              |
| 1:A:23:GLU:N     | 1:A:24:GLU:CB    | 2.43                     | 0.78              |
| 1:G:95:VAL:CG1   | 1:G:97:PHE:CD2   | 2.60                     | 0.77              |
| 1:A:48:ARG:HD3   | 1:A:289:PRO:O    | 1.82                     | 0.77              |
| 1:B:79:MET:HE1   | 1:B:82:LYS:NZ    | 1.99                     | 0.77              |
| 1:B:288:THR:HG22 | 1:B:289:PRO:CD   | 2.14                     | 0.77              |
| 2:H:940:GLN:N    | 2:H:940:GLN:CD   | 2.43                     | 0.76              |
| 1:A:121:ARG:CZ   | 1:A:125:PHE:CE2  | 2.69                     | 0.76              |
| 2:H:942:GLN:CA   | 2:H:945:GLU:CG   | 2.64                     | 0.76              |
| 1:A:24:GLU:OE2   | 1:A:24:GLU:CA    | 2.34                     | 0.75              |
| 2:H:939:GLY:CA   | 2:H:942:GLN:HB3  | 2.17                     | 0.74              |
| 1:A:290:VAL:HG12 | 1:A:291:HIS:H    | 1.51                     | 0.73              |
| 1:E:21:GLY:O     | 1:E:24:GLU:CB    | 2.36                     | 0.73              |
| 2:C:955:THR:HG22 | 2:F:955:THR:HG22 | 1.71                     | 0.73              |
| 1:A:23:GLU:HA    | 1:A:26:LYS:H     | 1.54                     | 0.72              |
| 1:A:23:GLU:HA    | 1:A:26:LYS:N     | 2.05                     | 0.72              |
| 1:A:121:ARG:HG2  | 1:A:125:PHE:HD2  | 1.49                     | 0.72              |
| 1:E:21:GLY:C     | 1:E:24:GLU:HB3   | 2.15                     | 0.72              |
| 2:H:939:GLY:HA2  | 2:H:942:GLN:NE2  | 2.04                     | 0.71              |
| 2:H:942:GLN:C    | 2:H:945:GLU:HG3  | 2.14                     | 0.71              |
| 2:F:945:GLU:O    | 2:F:949:GLU:HG2  | 1.91                     | 0.71              |
| 1:B:22:VAL:O     | 1:B:23:GLU:CB    | 2.37                     | 0.71              |
| 2:H:939:GLY:O    | 2:H:942:GLN:CB   | 2.39                     | 0.70              |
| 1:E:222:ARG:NH2  | 1:E:272:ASP:OD2  | 2.25                     | 0.70              |
| 1:E:121:ARG:HD2  | 1:E:125:PHE:CD1  | 2.26                     | 0.70              |
| 1:A:22:VAL:CA    | 1:A:24:GLU:HB3   | 2.20                     | 0.70              |
| 2:H:942:GLN:CB   | 2:H:945:GLU:OE1  | 2.40                     | 0.70              |
| 1:A:121:ARG:CZ   | 1:A:125:PHE:HE2  | 2.04                     | 0.70              |
| 2:D:945:GLU:O    | 2:D:949:GLU:HG2  | 1.92                     | 0.70              |
| 2:D:969:LEU:O    | 2:D:972:ASP:O    | 2.10                     | 0.70              |
| 1:E:48:ARG:HD2   | 1:E:288:THR:HG22 | 1.72                     | 0.69              |
| 1:G:45:PHE:HA    | 1:G:291:HIS:CE1  | 2.27                     | 0.69              |
| 2:F:969:LEU:HD22 | 2:F:974:LEU:HB3  | 1.74                     | 0.68              |
| 2:H:951:GLN:O    | 2:H:955:THR:HG23 | 1.93                     | 0.68              |
| 1:G:121:ARG:HG3  | 1:G:125:PHE:CD1  | 2.25                     | 0.68              |
| 1:A:23:GLU:CA    | 1:A:26:LYS:H     | 2.06                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:268:GLN:O    | 1:E:271:SER:OG   | 2.11                     | 0.68              |
| 2:H:946:SER:CA   | 2:H:949:GLU:HG3  | 2.22                     | 0.68              |
| 2:C:972:ASP:OD1  | 2:C:972:ASP:N    | 2.26                     | 0.68              |
| 2:C:949:GLU:HG2  | 2:C:950:ALA:N    | 2.09                     | 0.67              |
| 2:H:940:GLN:CD   | 2:H:940:GLN:H    | 2.00                     | 0.67              |
| 1:E:255:SER:OG   | 1:E:258:LYS:HE2  | 1.95                     | 0.67              |
| 2:H:942:GLN:CA   | 2:H:945:GLU:OE1  | 2.42                     | 0.67              |
| 1:A:95:VAL:O     | 1:A:95:VAL:CG1   | 2.42                     | 0.66              |
| 2:F:969:LEU:O    | 2:F:972:ASP:O    | 2.14                     | 0.66              |
| 1:A:95:VAL:O     | 1:A:96:ARG:HD2   | 1.91                     | 0.66              |
| 1:G:288:THR:HG22 | 1:G:289:PRO:CD   | 2.23                     | 0.66              |
| 2:H:948:TYR:CD1  | 2:H:948:TYR:C    | 2.74                     | 0.66              |
| 1:B:121:ARG:CB   | 1:B:125:PHE:HE2  | 2.09                     | 0.65              |
| 2:H:942:GLN:CA   | 2:H:945:GLU:HG2  | 2.25                     | 0.65              |
| 1:G:121:ARG:CG   | 1:G:125:PHE:HE1  | 2.07                     | 0.65              |
| 2:H:966:TYR:OH   | 1:A:96:ARG:HG2   | 1.97                     | 0.65              |
| 2:H:941:LEU:O    | 2:H:945:GLU:HG2  | 1.97                     | 0.65              |
| 1:B:164:THR:OG1  | 1:B:165:LYS:N    | 2.29                     | 0.65              |
| 2:H:955:THR:HG22 | 2:D:955:THR:HG22 | 1.78                     | 0.65              |
| 1:G:48:ARG:CZ    | 1:G:49:PHE:CE1   | 2.80                     | 0.65              |
| 1:G:233:LYS:H    | 1:G:233:LYS:CD   | 2.10                     | 0.64              |
| 1:B:121:ARG:CB   | 1:B:125:PHE:CE2  | 2.81                     | 0.64              |
| 1:A:121:ARG:NH1  | 1:A:125:PHE:CZ   | 2.65                     | 0.64              |
| 1:G:24:GLU:N     | 1:G:24:GLU:CD    | 2.55                     | 0.64              |
| 1:A:95:VAL:O     | 1:A:95:VAL:HG13  | 1.96                     | 0.64              |
| 1:B:88:VAL:HG13  | 1:B:114:LEU:HD22 | 1.78                     | 0.64              |
| 2:C:969:LEU:O    | 2:C:972:ASP:O    | 2.15                     | 0.64              |
| 1:A:164:THR:OG1  | 1:A:165:LYS:N    | 2.31                     | 0.64              |
| 1:B:257:GLU:O    | 1:B:261:LYS:HG3  | 1.98                     | 0.63              |
| 1:G:48:ARG:HH21  | 1:G:49:PHE:HE1   | 0.75                     | 0.63              |
| 2:F:972:ASP:OD1  | 2:F:972:ASP:N    | 2.32                     | 0.63              |
| 1:G:96:ARG:HD2   | 1:G:96:ARG:N     | 2.14                     | 0.62              |
| 1:G:38:ASP:HB3   | 1:G:41:LYS:HB2   | 1.82                     | 0.62              |
| 2:H:939:GLY:O    | 2:H:942:GLN:CD   | 2.43                     | 0.62              |
| 1:A:292:SER:OG   | 1:A:293:SER:CB   | 2.48                     | 0.61              |
| 1:G:24:GLU:OE2   | 1:G:24:GLU:N     | 2.34                     | 0.61              |
| 1:G:22:VAL:CA    | 1:G:24:GLU:CB    | 2.74                     | 0.61              |
| 1:B:79:MET:HE1   | 1:B:82:LYS:HZ2   | 1.66                     | 0.61              |
| 2:C:988:ALA:HA   | 1:E:126:PRO:HG2  | 1.83                     | 0.61              |
| 1:G:21:GLY:C     | 1:G:24:GLU:CB    | 2.73                     | 0.61              |
| 1:A:21:GLY:HA3   | 1:A:24:GLU:HG2   | 1.75                     | 0.61              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:E:21:GLY:O    | 1:E:24:GLU:CA    | 2.49                     | 0.61              |
| 1:G:121:ARG:HB2 | 1:G:125:PHE:CE1  | 2.37                     | 0.60              |
| 1:E:271:SER:O   | 1:E:272:ASP:C    | 2.43                     | 0.60              |
| 1:E:164:THR:OG1 | 1:E:165:LYS:N    | 2.34                     | 0.60              |
| 1:B:95:VAL:HG12 | 1:B:96:ARG:N     | 2.16                     | 0.60              |
| 1:B:24:GLU:HA   | 1:B:24:GLU:OE2   | 2.01                     | 0.60              |
| 1:B:38:ASP:HB3  | 1:B:41:LYS:HB2   | 1.84                     | 0.60              |
| 1:B:283:HIS:O   | 1:B:287:GLY:N    | 2.32                     | 0.60              |
| 2:H:972:ASP:OD1 | 2:H:972:ASP:N    | 2.34                     | 0.60              |
| 1:G:96:ARG:O    | 1:G:96:ARG:HG2   | 2.01                     | 0.60              |
| 2:F:969:LEU:CD2 | 2:F:974:LEU:CB   | 2.76                     | 0.60              |
| 2:D:972:ASP:OD1 | 2:D:972:ASP:N    | 2.34                     | 0.60              |
| 1:E:22:VAL:C    | 1:E:24:GLU:H     | 2.10                     | 0.59              |
| 1:A:84:GLN:HE21 | 2:D:950:ALA:HB2  | 1.65                     | 0.59              |
| 1:A:21:GLY:C    | 1:A:24:GLU:CB    | 2.75                     | 0.59              |
| 1:A:121:ARG:CD  | 1:A:125:PHE:CZ   | 2.69                     | 0.59              |
| 1:A:255:SER:HB2 | 1:A:258:LYS:H    | 1.68                     | 0.59              |
| 1:G:121:ARG:HB2 | 1:G:125:PHE:HE1  | 1.66                     | 0.58              |
| 1:G:222:ARG:NH2 | 1:G:272:ASP:OD1  | 2.36                     | 0.58              |
| 1:G:255:SER:HB2 | 1:G:258:LYS:HG2  | 1.85                     | 0.58              |
| 1:A:292:SER:OG  | 1:A:293:SER:HB3  | 2.02                     | 0.58              |
| 1:B:257:GLU:O   | 1:B:261:LYS:CG   | 2.50                     | 0.58              |
| 1:E:84:GLN:HE21 | 2:F:950:ALA:HB2  | 1.67                     | 0.58              |
| 1:A:23:GLU:CB   | 1:A:26:LYS:HG3   | 2.30                     | 0.58              |
| 1:B:40:GLU:O    | 1:B:44:THR:HG23  | 2.03                     | 0.58              |
| 1:G:195:CYS:O   | 1:G:256:ALA:HB2  | 2.04                     | 0.58              |
| 2:D:969:LEU:O   | 2:D:969:LEU:HD23 | 2.04                     | 0.58              |
| 2:H:942:GLN:O   | 2:H:945:GLU:CG   | 2.39                     | 0.57              |
| 1:E:95:VAL:O    | 1:E:95:VAL:CG1   | 2.52                     | 0.57              |
| 1:E:88:VAL:HG13 | 1:E:114:LEU:HD22 | 1.86                     | 0.57              |
| 1:B:93:LYS:O    | 1:B:95:VAL:O     | 2.23                     | 0.57              |
| 2:H:942:GLN:CG  | 2:H:945:GLU:OE1  | 2.53                     | 0.57              |
| 2:H:942:GLN:C   | 2:H:945:GLU:CG   | 2.78                     | 0.56              |
| 1:E:121:ARG:HD2 | 1:E:125:PHE:CE2  | 2.39                     | 0.56              |
| 1:E:255:SER:HB2 | 1:E:258:LYS:H    | 1.71                     | 0.56              |
| 1:G:121:ARG:CB  | 1:G:125:PHE:CE1  | 2.88                     | 0.56              |
| 2:H:945:GLU:O   | 2:H:949:GLU:CG   | 2.45                     | 0.56              |
| 2:F:969:LEU:O   | 2:F:969:LEU:HD23 | 2.05                     | 0.56              |
| 1:B:79:MET:HE1  | 1:B:82:LYS:HZ1   | 1.66                     | 0.56              |
| 1:A:57:ALA:O    | 1:A:61:LYS:HG3   | 2.06                     | 0.56              |
| 2:C:949:GLU:O   | 2:C:952:LYS:HG2  | 2.05                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:67:LEU:HD21  | 1:G:78:MET:HG2   | 1.87                     | 0.56              |
| 1:E:21:GLY:O     | 1:E:24:GLU:C     | 2.48                     | 0.56              |
| 2:H:939:GLY:HA2  | 2:H:942:GLN:HB3  | 1.88                     | 0.55              |
| 1:G:121:ARG:CB   | 1:G:125:PHE:HE1  | 2.19                     | 0.55              |
| 1:E:22:VAL:O     | 1:E:23:GLU:CB    | 2.54                     | 0.55              |
| 1:B:255:SER:OG   | 1:B:258:LYS:HE2  | 2.06                     | 0.55              |
| 1:B:268:GLN:O    | 1:B:271:SER:OG   | 2.22                     | 0.55              |
| 1:E:67:LEU:HD21  | 1:E:78:MET:HG2   | 1.89                     | 0.55              |
| 1:E:57:ALA:O     | 1:E:61:LYS:HG3   | 2.07                     | 0.54              |
| 2:F:970:GLU:OE2  | 2:F:974:LEU:HD12 | 2.06                     | 0.54              |
| 1:G:258:LYS:HA   | 1:G:261:LYS:HG3  | 1.87                     | 0.54              |
| 1:G:93:LYS:O     | 1:G:96:ARG:HB3   | 2.07                     | 0.54              |
| 1:E:40:GLU:O     | 1:E:44:THR:HG23  | 2.07                     | 0.54              |
| 1:E:114:LEU:HD12 | 1:E:119:LEU:HD22 | 1.90                     | 0.54              |
| 1:E:95:VAL:HG12  | 1:E:97:PHE:HD2   | 1.72                     | 0.54              |
| 1:B:291:HIS:O    | 1:B:292:SER:C    | 2.50                     | 0.54              |
| 1:A:67:LEU:HD21  | 1:A:78:MET:HG2   | 1.89                     | 0.53              |
| 1:A:268:GLN:O    | 1:A:271:SER:OG   | 2.19                     | 0.53              |
| 1:G:164:THR:OG1  | 1:G:165:LYS:N    | 2.41                     | 0.53              |
| 1:G:291:HIS:HB2  | 1:G:292:SER:O    | 2.07                     | 0.53              |
| 1:A:255:SER:HB3  | 1:A:257:GLU:HB2  | 1.90                     | 0.53              |
| 1:G:95:VAL:HG12  | 1:G:96:ARG:CA    | 2.40                     | 0.52              |
| 1:E:21:GLY:O     | 1:E:24:GLU:N     | 2.41                     | 0.52              |
| 1:E:38:ASP:HB3   | 1:E:41:LYS:HB2   | 1.91                     | 0.52              |
| 2:D:951:GLN:O    | 2:D:955:THR:HG23 | 2.09                     | 0.52              |
| 1:B:195:CYS:O    | 1:B:256:ALA:HB2  | 2.10                     | 0.52              |
| 1:B:255:SER:H    | 1:B:258:LYS:CE   | 2.23                     | 0.52              |
| 1:A:40:GLU:O     | 1:A:44:THR:HG23  | 2.09                     | 0.52              |
| 1:B:112:TYR:CD1  | 1:B:156:ARG:HD3  | 2.44                     | 0.52              |
| 1:A:22:VAL:O     | 1:A:22:VAL:CG2   | 2.57                     | 0.51              |
| 1:B:57:ALA:O     | 1:B:61:LYS:HG3   | 2.10                     | 0.51              |
| 1:E:119:LEU:HD12 | 1:E:120:PRO:HD2  | 1.92                     | 0.51              |
| 1:B:84:GLN:HB2   | 2:C:947:ARG:HG3  | 1.92                     | 0.51              |
| 1:E:66:ILE:O     | 1:E:81:ARG:NH2   | 2.44                     | 0.51              |
| 2:C:951:GLN:O    | 2:C:955:THR:HG23 | 2.10                     | 0.51              |
| 1:E:257:GLU:OE1  | 1:E:261:LYS:NZ   | 2.42                     | 0.50              |
| 2:C:948:TYR:CD1  | 2:C:948:TYR:C    | 2.89                     | 0.50              |
| 1:G:97:PHE:HA    | 1:G:123:PRO:HG3  | 1.93                     | 0.50              |
| 1:G:112:TYR:HD1  | 1:G:156:ARG:HG2  | 1.76                     | 0.50              |
| 2:H:967:GLY:HA2  | 2:H:970:GLU:HG3  | 1.94                     | 0.50              |
| 1:E:210:CYS:O    | 1:E:211:PHE:HB2  | 2.12                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:254:ASN:HB2  | 1:E:258:LYS:NZ   | 2.26                     | 0.50              |
| 1:G:45:PHE:N     | 1:G:291:HIS:CE1  | 2.80                     | 0.50              |
| 1:A:38:ASP:HB3   | 1:A:41:LYS:HB2   | 1.93                     | 0.50              |
| 1:B:97:PHE:HA    | 1:B:123:PRO:HG3  | 1.94                     | 0.50              |
| 2:D:966:TYR:C    | 2:D:970:GLU:HG2  | 2.31                     | 0.50              |
| 1:G:116:SER:O    | 1:G:118:LYS:HG2  | 2.12                     | 0.50              |
| 1:G:22:VAL:N     | 1:G:24:GLU:CB    | 2.75                     | 0.50              |
| 1:A:23:GLU:H     | 1:A:25:LYS:N     | 2.10                     | 0.49              |
| 1:A:107:VAL:O    | 1:A:111:MET:HG3  | 2.12                     | 0.49              |
| 1:G:23:GLU:H     | 1:G:25:LYS:N     | 2.10                     | 0.49              |
| 1:A:88:VAL:HG13  | 1:A:114:LEU:HD22 | 1.93                     | 0.49              |
| 1:A:288:THR:HG22 | 1:A:289:PRO:HD2  | 1.93                     | 0.49              |
| 1:B:24:GLU:OE2   | 1:B:24:GLU:CA    | 2.56                     | 0.49              |
| 1:G:45:PHE:C     | 1:G:45:PHE:CD2   | 2.90                     | 0.49              |
| 1:G:96:ARG:NH1   | 2:D:966:TYR:CE1  | 2.80                     | 0.49              |
| 1:G:233:LYS:O    | 1:G:234:ILE:C    | 2.55                     | 0.49              |
| 1:A:121:ARG:NH1  | 1:A:125:PHE:HZ   | 2.09                     | 0.49              |
| 2:D:946:SER:C    | 2:D:949:GLU:HG3  | 2.36                     | 0.49              |
| 1:B:45:PHE:C     | 1:B:45:PHE:CD2   | 2.91                     | 0.49              |
| 1:E:97:PHE:HA    | 1:E:123:PRO:HG3  | 1.94                     | 0.49              |
| 1:A:23:GLU:CA    | 1:A:24:GLU:C     | 2.86                     | 0.49              |
| 1:A:269:ASP:OD1  | 1:A:269:ASP:N    | 2.39                     | 0.49              |
| 1:E:121:ARG:CD   | 1:E:125:PHE:CZ   | 2.93                     | 0.49              |
| 2:C:969:LEU:O    | 2:C:969:LEU:HD23 | 2.13                     | 0.48              |
| 1:A:23:GLU:N     | 1:A:26:LYS:H     | 2.11                     | 0.48              |
| 1:G:23:GLU:N     | 1:G:24:GLU:CA    | 2.77                     | 0.48              |
| 2:H:940:GLN:N    | 2:H:940:GLN:OE1  | 2.46                     | 0.48              |
| 1:E:48:ARG:HG2   | 1:E:288:THR:CG2  | 2.43                     | 0.48              |
| 2:F:966:TYR:C    | 2:F:970:GLU:HG2  | 2.33                     | 0.48              |
| 1:A:66:ILE:O     | 1:A:81:ARG:NH2   | 2.46                     | 0.48              |
| 1:B:260:THR:O    | 1:B:264:GLU:CG   | 2.53                     | 0.48              |
| 1:G:175:LYS:HA   | 1:G:175:LYS:HD3  | 1.67                     | 0.48              |
| 1:A:23:GLU:HA    | 1:A:24:GLU:C     | 2.38                     | 0.48              |
| 1:A:92:LEU:HB3   | 1:A:98:VAL:HG13  | 1.95                     | 0.48              |
| 1:A:121:ARG:HE   | 1:A:121:ARG:HB3  | 1.50                     | 0.48              |
| 1:G:188:LEU:HD22 | 1:G:247:LYS:HG3  | 1.95                     | 0.48              |
| 1:B:79:MET:O     | 1:B:80:TYR:C     | 2.54                     | 0.47              |
| 1:G:233:LYS:HD2  | 1:G:233:LYS:N    | 2.21                     | 0.47              |
| 1:A:21:GLY:CA    | 1:A:24:GLU:CG    | 2.64                     | 0.47              |
| 1:G:102:THR:HG22 | 1:G:107:VAL:HG23 | 1.96                     | 0.47              |
| 1:G:88:VAL:HG13  | 1:G:114:LEU:HD22 | 1.96                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:107:VAL:O    | 1:G:111:MET:HG3  | 2.15                     | 0.47              |
| 1:A:169:SER:HA   | 1:A:172:GLN:HE21 | 1.79                     | 0.47              |
| 1:G:66:ILE:O     | 1:G:81:ARG:NH2   | 2.47                     | 0.47              |
| 1:G:168:ASP:O    | 1:G:171:PRO:HD2  | 2.15                     | 0.47              |
| 1:A:22:VAL:C     | 1:A:24:GLU:HB2   | 2.36                     | 0.47              |
| 2:F:951:GLN:O    | 2:F:955:THR:HG23 | 2.15                     | 0.47              |
| 2:H:938:ARG:O    | 2:H:942:GLN:HB2  | 2.15                     | 0.46              |
| 2:F:946:SER:C    | 2:F:949:GLU:HG3  | 2.39                     | 0.46              |
| 1:B:194:MET:HE3  | 1:B:194:MET:HA   | 1.98                     | 0.46              |
| 1:G:40:GLU:O     | 1:G:44:THR:HG23  | 2.16                     | 0.46              |
| 1:E:45:PHE:C     | 1:E:45:PHE:CD2   | 2.93                     | 0.46              |
| 1:A:58:LEU:O     | 1:A:62:VAL:HG23  | 2.16                     | 0.46              |
| 2:F:969:LEU:HD21 | 2:F:974:LEU:CB   | 2.44                     | 0.46              |
| 1:E:255:SER:HB3  | 1:E:257:GLU:HB2  | 1.97                     | 0.46              |
| 1:A:121:ARG:CZ   | 1:A:125:PHE:CZ   | 2.99                     | 0.45              |
| 1:A:210:CYS:O    | 1:A:211:PHE:HB2  | 2.16                     | 0.45              |
| 1:B:95:VAL:CG1   | 1:B:96:ARG:N     | 2.79                     | 0.45              |
| 2:H:949:GLU:C    | 2:H:952:LYS:HG3  | 2.37                     | 0.45              |
| 1:B:48:ARG:HG3   | 1:B:289:PRO:O    | 2.16                     | 0.45              |
| 1:A:45:PHE:C     | 1:A:45:PHE:CD2   | 2.95                     | 0.45              |
| 1:G:118:LYS:HE2  | 1:G:118:LYS:HB3  | 1.70                     | 0.45              |
| 1:E:66:ILE:HD13  | 1:E:153:TRP:HB3  | 1.97                     | 0.45              |
| 1:E:269:ASP:OD1  | 1:E:269:ASP:N    | 2.46                     | 0.45              |
| 1:B:21:GLY:CA    | 1:B:24:GLU:HG2   | 2.46                     | 0.45              |
| 1:A:114:LEU:HD12 | 1:A:119:LEU:HD22 | 1.99                     | 0.45              |
| 1:A:292:SER:HA   | 1:A:293:SER:HA   | 1.71                     | 0.45              |
| 1:G:95:VAL:HG12  | 1:G:97:PHE:N     | 2.32                     | 0.45              |
| 1:A:24:GLU:HG3   | 1:A:25:LYS:H     | 1.81                     | 0.45              |
| 1:G:112:TYR:CD1  | 1:G:156:ARG:HD3  | 2.52                     | 0.45              |
| 1:E:95:VAL:O     | 1:E:95:VAL:HG13  | 2.17                     | 0.45              |
| 2:F:947:ARG:HE   | 2:F:947:ARG:HB3  | 1.51                     | 0.45              |
| 1:A:22:VAL:O     | 1:A:22:VAL:HG23  | 2.17                     | 0.45              |
| 1:E:67:LEU:HB3   | 1:E:74:HIS:CD2   | 2.51                     | 0.45              |
| 2:D:953:ARG:O    | 2:D:954:ILE:C    | 2.59                     | 0.45              |
| 1:B:188:LEU:HD22 | 1:B:247:LYS:HG3  | 1.98                     | 0.44              |
| 1:G:23:GLU:CB    | 1:G:26:LYS:HB2   | 2.47                     | 0.44              |
| 1:E:22:VAL:C     | 1:E:24:GLU:N     | 2.71                     | 0.44              |
| 1:G:257:GLU:OE1  | 1:G:261:LYS:HE3  | 2.17                     | 0.44              |
| 1:E:254:ASN:HB2  | 1:E:258:LYS:HZ3  | 1.81                     | 0.44              |
| 1:B:206:TRP:CD1  | 1:B:211:PHE:CE1  | 3.06                     | 0.44              |
| 1:B:255:SER:H    | 1:B:258:LYS:HE2  | 1.82                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:968:ARG:HG2  | 2:F:969:LEU:HD11 | 1.99                     | 0.44              |
| 2:F:948:TYR:CD1  | 2:F:948:TYR:C    | 2.95                     | 0.44              |
| 1:A:281:LEU:HD12 | 1:A:281:LEU:HA   | 1.85                     | 0.44              |
| 1:B:112:TYR:HD1  | 1:B:156:ARG:HG2  | 1.83                     | 0.44              |
| 1:B:246:PHE:CE1  | 1:B:267:PRO:HG2  | 2.52                     | 0.44              |
| 1:B:118:LYS:HB3  | 1:B:118:LYS:HE2  | 1.61                     | 0.44              |
| 1:G:268:GLN:O    | 1:G:271:SER:OG   | 2.26                     | 0.44              |
| 1:A:67:LEU:HB3   | 1:A:74:HIS:CD2   | 2.53                     | 0.44              |
| 1:E:143:GLU:HB2  | 1:E:217:GLU:HG2  | 2.00                     | 0.44              |
| 1:E:107:VAL:O    | 1:E:111:MET:HG3  | 2.18                     | 0.43              |
| 2:F:950:ALA:O    | 2:F:953:ARG:HB2  | 2.18                     | 0.43              |
| 1:B:48:ARG:HD3   | 1:B:49:PHE:CZ    | 2.53                     | 0.43              |
| 1:B:175:LYS:HA   | 1:B:175:LYS:HD3  | 1.77                     | 0.43              |
| 1:E:21:GLY:CA    | 1:E:24:GLU:HB3   | 2.47                     | 0.43              |
| 1:E:205:LEU:HD21 | 1:E:214:CYS:HB2  | 2.00                     | 0.43              |
| 1:B:23:GLU:HA    | 1:B:26:LYS:HB2   | 2.00                     | 0.43              |
| 1:A:82:LYS:HE3   | 1:A:82:LYS:HB2   | 1.77                     | 0.43              |
| 1:B:288:THR:CG2  | 1:B:289:PRO:CD   | 2.93                     | 0.43              |
| 1:G:55:TYR:O     | 1:G:59:VAL:HG23  | 2.18                     | 0.43              |
| 2:H:949:GLU:O    | 2:H:952:LYS:CG   | 2.46                     | 0.43              |
| 1:E:102:THR:HG22 | 1:E:107:VAL:HG23 | 2.01                     | 0.43              |
| 1:B:79:MET:CE    | 1:B:82:LYS:HZ1   | 2.30                     | 0.43              |
| 1:B:168:ASP:O    | 1:B:171:PRO:HD2  | 2.18                     | 0.43              |
| 1:G:217:GLU:CD   | 1:G:217:GLU:H    | 2.26                     | 0.43              |
| 2:H:940:GLN:C    | 2:H:942:GLN:N    | 2.68                     | 0.43              |
| 1:A:21:GLY:HA2   | 1:A:24:GLU:HG2   | 1.83                     | 0.43              |
| 1:B:114:LEU:CD1  | 2:C:957:VAL:HG21 | 2.49                     | 0.43              |
| 1:G:111:MET:HE2  | 1:G:111:MET:HB3  | 1.93                     | 0.43              |
| 1:E:48:ARG:HG2   | 1:E:288:THR:HG21 | 2.00                     | 0.43              |
| 1:E:121:ARG:HD2  | 1:E:125:PHE:CG   | 2.54                     | 0.43              |
| 1:E:290:VAL:HG12 | 1:E:291:HIS:H    | 1.84                     | 0.43              |
| 1:E:22:VAL:HG13  | 1:E:26:LYS:HE2   | 2.00                     | 0.43              |
| 1:E:121:ARG:NH1  | 1:E:125:PHE:CZ   | 2.87                     | 0.43              |
| 1:B:139:LYS:HA   | 1:B:142:GLU:HG3  | 2.00                     | 0.43              |
| 1:G:96:ARG:HD2   | 1:G:96:ARG:H     | 1.84                     | 0.43              |
| 1:E:255:SER:H    | 1:E:258:LYS:CE   | 2.31                     | 0.42              |
| 1:A:24:GLU:CG    | 1:A:25:LYS:H     | 2.32                     | 0.42              |
| 1:A:290:VAL:HG12 | 1:A:291:HIS:N    | 2.26                     | 0.42              |
| 2:D:948:TYR:CD1  | 2:D:948:TYR:C    | 2.95                     | 0.42              |
| 1:G:22:VAL:O     | 1:G:24:GLU:HG2   | 2.19                     | 0.42              |
| 1:B:269:ASP:N    | 1:B:269:ASP:OD1  | 2.52                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:206:TRP:CD1  | 1:E:211:PHE:CE1  | 3.08                     | 0.42              |
| 1:G:173:LEU:N    | 1:G:174:PRO:CD   | 2.83                     | 0.42              |
| 1:G:258:LYS:CA   | 1:G:261:LYS:HG3  | 2.49                     | 0.42              |
| 2:H:939:GLY:HA2  | 2:H:942:GLN:CB   | 2.49                     | 0.42              |
| 1:G:119:LEU:HD12 | 1:G:120:PRO:CD   | 2.50                     | 0.42              |
| 2:H:941:LEU:HD22 | 2:H:941:LEU:C    | 2.45                     | 0.42              |
| 1:E:194:MET:CE   | 1:E:194:MET:HA   | 2.50                     | 0.42              |
| 1:E:195:CYS:O    | 1:E:256:ALA:HB2  | 2.20                     | 0.42              |
| 2:H:946:SER:CA   | 2:H:949:GLU:CG   | 2.90                     | 0.41              |
| 1:A:23:GLU:N     | 1:A:25:LYS:N     | 2.69                     | 0.41              |
| 1:E:21:GLY:HA2   | 1:E:24:GLU:CD    | 2.44                     | 0.41              |
| 2:D:947:ARG:HE   | 2:D:947:ARG:HB3  | 1.62                     | 0.41              |
| 1:G:246:PHE:CE1  | 1:G:267:PRO:HG2  | 2.56                     | 0.41              |
| 1:E:64:LEU:O     | 1:E:157:ARG:NH1  | 2.53                     | 0.41              |
| 1:E:194:MET:HA   | 1:E:194:MET:HE2  | 2.02                     | 0.41              |
| 2:D:967:GLY:HA2  | 2:D:970:GLU:HG3  | 2.01                     | 0.41              |
| 1:B:82:LYS:HB2   | 1:B:82:LYS:HE3   | 1.62                     | 0.41              |
| 1:B:257:GLU:O    | 1:B:261:LYS:HG2  | 2.20                     | 0.41              |
| 1:E:82:LYS:HE3   | 1:E:82:LYS:HB2   | 1.74                     | 0.41              |
| 1:A:66:ILE:HD13  | 1:A:153:TRP:HB3  | 2.01                     | 0.41              |
| 2:D:969:LEU:HD23 | 2:D:969:LEU:C    | 2.45                     | 0.41              |
| 1:B:64:LEU:O     | 1:B:157:ARG:NH1  | 2.53                     | 0.41              |
| 1:B:192:LEU:HD11 | 1:B:243:LEU:HD22 | 2.03                     | 0.41              |
| 1:A:23:GLU:N     | 1:A:24:GLU:CA    | 2.83                     | 0.41              |
| 1:B:205:LEU:HD21 | 1:B:214:CYS:HB2  | 2.03                     | 0.41              |
| 1:B:255:SER:HB2  | 1:B:258:LYS:H    | 1.86                     | 0.41              |
| 1:E:112:TYR:HD1  | 1:E:156:ARG:HG2  | 1.85                     | 0.41              |
| 1:G:58:LEU:O     | 1:G:62:VAL:HG23  | 2.21                     | 0.41              |
| 2:H:939:GLY:CA   | 2:H:942:GLN:NE2  | 2.81                     | 0.41              |
| 1:A:173:LEU:N    | 1:A:174:PRO:CD   | 2.83                     | 0.41              |
| 1:B:84:GLN:HE21  | 2:C:950:ALA:HB2  | 1.86                     | 0.41              |
| 1:B:257:GLU:OE1  | 1:B:257:GLU:HA   | 2.21                     | 0.41              |
| 2:H:948:TYR:CD1  | 2:H:948:TYR:O    | 2.74                     | 0.41              |
| 1:B:114:LEU:HD12 | 2:C:957:VAL:HG21 | 2.03                     | 0.41              |
| 1:G:82:LYS:HE3   | 1:G:82:LYS:HB2   | 1.62                     | 0.41              |
| 1:E:95:VAL:CG1   | 1:E:97:PHE:HD2   | 2.34                     | 0.41              |
| 2:H:954:ILE:HG22 | 2:H:955:THR:N    | 2.35                     | 0.40              |
| 1:A:205:LEU:HD21 | 1:A:214:CYS:HB2  | 2.02                     | 0.40              |
| 1:A:135:LEU:O    | 1:A:139:LYS:HG3  | 2.21                     | 0.40              |
| 1:A:288:THR:HA   | 1:A:289:PRO:HD3  | 1.90                     | 0.40              |
| 1:G:23:GLU:H     | 1:G:26:LYS:H     | 1.69                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:34:ASP:HB3   | 1:E:36:ARG:O     | 2.21                     | 0.40              |
| 1:E:169:SER:HA   | 1:E:172:GLN:HE21 | 1.86                     | 0.40              |
| 1:A:23:GLU:H     | 1:A:26:LYS:H     | 1.69                     | 0.40              |
| 1:A:253:LEU:HD22 | 1:A:258:LYS:HB3  | 2.02                     | 0.40              |
| 1:G:119:LEU:HD12 | 1:G:119:LEU:HA   | 1.86                     | 0.40              |
| 1:G:173:LEU:HD22 | 1:G:236:VAL:CG2  | 2.51                     | 0.40              |
| 1:G:192:LEU:HD11 | 1:G:243:LEU:HD22 | 2.02                     | 0.40              |
| 2:D:950:ALA:O    | 2:D:953:ARG:HB2  | 2.21                     | 0.40              |

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1          | Atom-2                | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------------|--------------------------|-------------------|
| 1:G:24:GLU:OE1  | 1:E:290:VAL:N[1_655]  | 1.80                     | 0.40              |
| 1:G:23:GLU:O    | 1:E:288:THR:O[1_655]  | 1.88                     | 0.32              |
| 1:B:290:VAL:CG2 | 1:A:40:GLU:OE2[1_655] | 2.18                     | 0.02              |

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed       | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|----------|----------|-------------|-----|
| 1   | A     | 272/273 (100%) | 253 (93%) | 18 (7%)  | 1 (0%)   | 30          | 58  |
| 1   | B     | 271/273 (99%)  | 254 (94%) | 16 (6%)  | 1 (0%)   | 30          | 58  |
| 1   | E     | 271/273 (99%)  | 254 (94%) | 17 (6%)  | 0        | 100         | 100 |
| 1   | G     | 271/273 (99%)  | 255 (94%) | 16 (6%)  | 0        | 100         | 100 |
| 2   | C     | 51/56 (91%)    | 43 (84%)  | 6 (12%)  | 2 (4%)   | 2           | 8   |
| 2   | D     | 51/56 (91%)    | 39 (76%)  | 11 (22%) | 1 (2%)   | 6           | 19  |
| 2   | F     | 52/56 (93%)    | 48 (92%)  | 3 (6%)   | 1 (2%)   | 6           | 20  |
| 2   | H     | 53/56 (95%)    | 47 (89%)  | 2 (4%)   | 4 (8%)   | 1           | 1   |

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| Mol | Chain | Analysed        | Favoured   | Allowed | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|---------|----------|-------------|----|
| All | All   | 1292/1316 (98%) | 1193 (92%) | 89 (7%) | 10 (1%)  | 16          | 41 |

All (10) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | H     | 981 | GLU  |
| 2   | H     | 991 | GLU  |
| 2   | F     | 982 | LYS  |
| 2   | D     | 980 | GLU  |
| 1   | B     | 23  | GLU  |
| 2   | C     | 990 | GLU  |
| 2   | H     | 982 | LYS  |
| 2   | H     | 990 | GLU  |
| 1   | A     | 118 | LYS  |
| 2   | C     | 991 | GLU  |

### 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     | 249/249 (100%)  | 207 (83%) | 42 (17%)  | 2           | 7 |
| 1   | B     | 247/249 (99%)   | 207 (84%) | 40 (16%)  | 2           | 8 |
| 1   | E     | 248/249 (100%)  | 207 (84%) | 41 (16%)  | 2           | 7 |
| 1   | G     | 248/249 (100%)  | 208 (84%) | 40 (16%)  | 2           | 8 |
| 2   | C     | 36/45 (80%)     | 26 (72%)  | 10 (28%)  | 0           | 1 |
| 2   | D     | 36/45 (80%)     | 29 (81%)  | 7 (19%)   | 1           | 4 |
| 2   | F     | 36/45 (80%)     | 27 (75%)  | 9 (25%)   | 0           | 2 |
| 2   | H     | 37/45 (82%)     | 23 (62%)  | 14 (38%)  | 0           | 0 |
| All | All   | 1137/1176 (97%) | 934 (82%) | 203 (18%) | 2           | 6 |

All (203) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res   | Type |
|-----|-------|-------|------|
| 1   | B     | 22    | VAL  |
| 1   | B     | 39[A] | THR  |
| 1   | B     | 39[B] | THR  |
| 1   | B     | 44    | THR  |
| 1   | B     | 48    | ARG  |
| 1   | B     | 53    | SER  |
| 1   | B     | 70    | HIS  |
| 1   | B     | 71    | HIS  |
| 1   | B     | 76    | LYS  |
| 1   | B     | 79    | MET  |
| 1   | B     | 81    | ARG  |
| 1   | B     | 82    | LYS  |
| 1   | B     | 98    | VAL  |
| 1   | B     | 100   | ASP  |
| 1   | B     | 118   | LYS  |
| 1   | B     | 122   | SER  |
| 1   | B     | 125   | PHE  |
| 1   | B     | 127   | LEU  |
| 1   | B     | 135   | LEU  |
| 1   | B     | 137   | ILE  |
| 1   | B     | 146   | GLU  |
| 1   | B     | 156   | ARG  |
| 1   | B     | 165   | LYS  |
| 1   | B     | 169   | SER  |
| 1   | B     | 175   | LYS  |
| 1   | B     | 194   | MET  |
| 1   | B     | 196   | SER  |
| 1   | B     | 200   | LYS  |
| 1   | B     | 204   | ASP  |
| 1   | B     | 219   | SER  |
| 1   | B     | 243   | LEU  |
| 1   | B     | 259   | ILE  |
| 1   | B     | 261   | LYS  |
| 1   | B     | 270   | SER  |
| 1   | B     | 271   | SER  |
| 1   | B     | 272   | ASP  |
| 1   | B     | 288   | THR  |
| 1   | B     | 290   | VAL  |
| 1   | B     | 291   | HIS  |
| 1   | B     | 292   | SER  |
| 2   | C     | 941   | LEU  |
| 2   | C     | 942   | GLN  |
| 2   | C     | 949   | GLU  |

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| Mol | Chain | Res   | Type |
|-----|-------|-------|------|
| 2   | C     | 955   | THR  |
| 2   | C     | 972   | ASP  |
| 2   | C     | 974   | LEU  |
| 2   | C     | 975   | LEU  |
| 2   | C     | 976   | LYS  |
| 2   | C     | 980   | GLU  |
| 2   | C     | 981   | GLU  |
| 1   | G     | 22    | VAL  |
| 1   | G     | 24    | GLU  |
| 1   | G     | 26    | LYS  |
| 1   | G     | 39[A] | THR  |
| 1   | G     | 39[B] | THR  |
| 1   | G     | 44    | THR  |
| 1   | G     | 48    | ARG  |
| 1   | G     | 53    | SER  |
| 1   | G     | 70    | HIS  |
| 1   | G     | 71    | HIS  |
| 1   | G     | 76    | LYS  |
| 1   | G     | 79    | MET  |
| 1   | G     | 81    | ARG  |
| 1   | G     | 82    | LYS  |
| 1   | G     | 95    | VAL  |
| 1   | G     | 96    | ARG  |
| 1   | G     | 98    | VAL  |
| 1   | G     | 114   | LEU  |
| 1   | G     | 118   | LYS  |
| 1   | G     | 121   | ARG  |
| 1   | G     | 122   | SER  |
| 1   | G     | 127   | LEU  |
| 1   | G     | 135   | LEU  |
| 1   | G     | 146   | GLU  |
| 1   | G     | 156   | ARG  |
| 1   | G     | 165   | LYS  |
| 1   | G     | 169   | SER  |
| 1   | G     | 175   | LYS  |
| 1   | G     | 194   | MET  |
| 1   | G     | 196   | SER  |
| 1   | G     | 204   | ASP  |
| 1   | G     | 219   | SER  |
| 1   | G     | 233   | LYS  |
| 1   | G     | 243   | LEU  |
| 1   | G     | 259   | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 261 | LYS  |
| 1   | G     | 271 | SER  |
| 1   | G     | 288 | THR  |
| 1   | G     | 290 | VAL  |
| 1   | G     | 291 | HIS  |
| 2   | H     | 940 | GLN  |
| 2   | H     | 941 | LEU  |
| 2   | H     | 942 | GLN  |
| 2   | H     | 945 | GLU  |
| 2   | H     | 946 | SER  |
| 2   | H     | 948 | TYR  |
| 2   | H     | 949 | GLU  |
| 2   | H     | 952 | LYS  |
| 2   | H     | 954 | ILE  |
| 2   | H     | 972 | ASP  |
| 2   | H     | 974 | LEU  |
| 2   | H     | 976 | LYS  |
| 2   | H     | 980 | GLU  |
| 2   | H     | 981 | GLU  |
| 1   | E     | 22  | VAL  |
| 1   | E     | 35  | ASP  |
| 1   | E     | 40  | GLU  |
| 1   | E     | 44  | THR  |
| 1   | E     | 48  | ARG  |
| 1   | E     | 53  | SER  |
| 1   | E     | 70  | HIS  |
| 1   | E     | 71  | HIS  |
| 1   | E     | 72  | GLU  |
| 1   | E     | 81  | ARG  |
| 1   | E     | 82  | LYS  |
| 1   | E     | 95  | VAL  |
| 1   | E     | 98  | VAL  |
| 1   | E     | 114 | LEU  |
| 1   | E     | 122 | SER  |
| 1   | E     | 125 | PHE  |
| 1   | E     | 127 | LEU  |
| 1   | E     | 129 | PRO  |
| 1   | E     | 132 | GLU  |
| 1   | E     | 135 | LEU  |
| 1   | E     | 146 | GLU  |
| 1   | E     | 156 | ARG  |
| 1   | E     | 160 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 167 | ARG  |
| 1   | E     | 169 | SER  |
| 1   | E     | 175 | LYS  |
| 1   | E     | 194 | MET  |
| 1   | E     | 196 | SER  |
| 1   | E     | 204 | ASP  |
| 1   | E     | 219 | SER  |
| 1   | E     | 231 | SER  |
| 1   | E     | 243 | LEU  |
| 1   | E     | 257 | GLU  |
| 1   | E     | 259 | ILE  |
| 1   | E     | 261 | LYS  |
| 1   | E     | 269 | ASP  |
| 1   | E     | 270 | SER  |
| 1   | E     | 271 | SER  |
| 1   | E     | 290 | VAL  |
| 1   | E     | 291 | HIS  |
| 1   | E     | 292 | SER  |
| 2   | F     | 941 | LEU  |
| 2   | F     | 942 | GLN  |
| 2   | F     | 949 | GLU  |
| 2   | F     | 955 | THR  |
| 2   | F     | 972 | ASP  |
| 2   | F     | 974 | LEU  |
| 2   | F     | 975 | LEU  |
| 2   | F     | 978 | LEU  |
| 2   | F     | 981 | GLU  |
| 1   | A     | 22  | VAL  |
| 1   | A     | 24  | GLU  |
| 1   | A     | 40  | GLU  |
| 1   | A     | 44  | THR  |
| 1   | A     | 48  | ARG  |
| 1   | A     | 70  | HIS  |
| 1   | A     | 72  | GLU  |
| 1   | A     | 76  | LYS  |
| 1   | A     | 81  | ARG  |
| 1   | A     | 82  | LYS  |
| 1   | A     | 95  | VAL  |
| 1   | A     | 96  | ARG  |
| 1   | A     | 98  | VAL  |
| 1   | A     | 114 | LEU  |
| 1   | A     | 118 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 121 | ARG  |
| 1   | A     | 122 | SER  |
| 1   | A     | 125 | PHE  |
| 1   | A     | 127 | LEU  |
| 1   | A     | 132 | GLU  |
| 1   | A     | 135 | LEU  |
| 1   | A     | 137 | ILE  |
| 1   | A     | 146 | GLU  |
| 1   | A     | 156 | ARG  |
| 1   | A     | 160 | ASN  |
| 1   | A     | 167 | ARG  |
| 1   | A     | 169 | SER  |
| 1   | A     | 175 | LYS  |
| 1   | A     | 194 | MET  |
| 1   | A     | 196 | SER  |
| 1   | A     | 204 | ASP  |
| 1   | A     | 219 | SER  |
| 1   | A     | 231 | SER  |
| 1   | A     | 243 | LEU  |
| 1   | A     | 259 | ILE  |
| 1   | A     | 269 | ASP  |
| 1   | A     | 270 | SER  |
| 1   | A     | 271 | SER  |
| 1   | A     | 272 | ASP  |
| 1   | A     | 288 | THR  |
| 1   | A     | 291 | HIS  |
| 1   | A     | 293 | SER  |
| 2   | D     | 942 | GLN  |
| 2   | D     | 949 | GLU  |
| 2   | D     | 955 | THR  |
| 2   | D     | 972 | ASP  |
| 2   | D     | 974 | LEU  |
| 2   | D     | 978 | LEU  |
| 2   | D     | 981 | GLU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 172 | GLN  |
| 1   | B     | 283 | HIS  |
| 2   | C     | 940 | GLN  |
| 2   | C     | 942 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 172 | GLN  |
| 1   | G     | 291 | HIS  |
| 2   | H     | 942 | GLN  |
| 1   | E     | 84  | GLN  |
| 1   | E     | 161 | GLN  |
| 1   | E     | 172 | GLN  |
| 2   | F     | 940 | GLN  |
| 2   | F     | 942 | GLN  |
| 1   | A     | 70  | HIS  |
| 1   | A     | 84  | GLN  |
| 1   | A     | 172 | GLN  |
| 2   | D     | 940 | GLN  |
| 2   | D     | 942 | 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 ⓘ

### 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(Å²) | Q<0.9            |          |
|-----|-------|-----------------|--------|----------|-----|----------|------------------|----------|
| 1   | A     | 273/273 (100%)  | -1.15  | 0        | 100 | 100      | 38, 58, 109, 198 | 1 (0%)   |
| 1   | B     | 272/273 (99%)   | -1.20  | 0        | 100 | 100      | 39, 60, 99, 165  | 1 (0%)   |
| 1   | E     | 272/273 (99%)   | -1.12  | 0        | 100 | 100      | 39, 58, 105, 185 | 1 (0%)   |
| 1   | G     | 272/273 (99%)   | -1.14  | 0        | 100 | 100      | 40, 60, 103, 170 | 1 (0%)   |
| 2   | C     | 53/56 (94%)     | 4.71   | 25 (47%) | 0   | 0        | 4, 58, 150, 155  | 21 (39%) |
| 2   | D     | 53/56 (94%)     | 4.18   | 27 (50%) | 0   | 0        | 3, 62, 99, 117   | 25 (47%) |
| 2   | F     | 54/56 (96%)     | 3.51   | 24 (44%) | 0   | 0        | 5, 66, 119, 149  | 21 (38%) |
| 2   | H     | 55/56 (98%)     | 3.93   | 23 (41%) | 0   | 0        | 4, 69, 195, 213  | 22 (40%) |
| All | All   | 1304/1316 (99%) | -0.29  | 99 (7%)  | 20  | 14       | 3, 59, 117, 213  | 93 (7%)  |

All (99) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | C     | 974 | LEU  | 20.0 |
| 2   | C     | 987 | GLU  | 16.6 |
| 2   | D     | 987 | GLU  | 16.4 |
| 2   | D     | 974 | LEU  | 15.1 |
| 2   | F     | 988 | ALA  | 14.4 |
| 2   | C     | 988 | ALA  | 14.2 |
| 2   | F     | 979 | GLU  | 13.9 |
| 2   | C     | 990 | GLU  | 13.7 |
| 2   | H     | 981 | GLU  | 13.3 |
| 2   | H     | 975 | LEU  | 13.3 |
| 2   | H     | 992 | ARG  | 13.2 |
| 2   | C     | 981 | GLU  | 13.1 |
| 2   | C     | 983 | ALA  | 13.1 |
| 2   | C     | 986 | ALA  | 12.9 |
| 2   | F     | 987 | GLU  | 12.9 |
| 2   | H     | 988 | ALA  | 12.9 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | H     | 987 | GLU  | 12.6 |
| 2   | F     | 985 | ALA  | 12.5 |
| 2   | C     | 977 | LYS  | 12.4 |
| 2   | D     | 980 | GLU  | 12.2 |
| 2   | F     | 986 | ALA  | 12.1 |
| 2   | C     | 989 | ALA  | 11.9 |
| 2   | C     | 975 | LEU  | 11.9 |
| 2   | C     | 980 | GLU  | 11.7 |
| 2   | D     | 985 | ALA  | 11.7 |
| 2   | D     | 986 | ALA  | 11.7 |
| 2   | C     | 978 | LEU  | 11.6 |
| 2   | H     | 974 | LEU  | 11.5 |
| 2   | H     | 977 | LYS  | 11.4 |
| 2   | D     | 979 | GLU  | 11.3 |
| 2   | D     | 973 | GLY  | 11.1 |
| 2   | H     | 980 | GLU  | 11.1 |
| 2   | H     | 986 | ALA  | 11.0 |
| 2   | H     | 983 | ALA  | 10.9 |
| 2   | H     | 989 | ALA  | 10.6 |
| 2   | F     | 981 | GLU  | 10.6 |
| 2   | F     | 992 | ARG  | 10.6 |
| 2   | C     | 976 | LYS  | 10.5 |
| 2   | F     | 984 | GLU  | 10.4 |
| 2   | C     | 982 | LYS  | 10.2 |
| 2   | H     | 979 | GLU  | 10.1 |
| 2   | F     | 989 | ALA  | 10.1 |
| 2   | H     | 985 | ALA  | 10.0 |
| 2   | H     | 982 | LYS  | 10.0 |
| 2   | F     | 980 | GLU  | 10.0 |
| 2   | C     | 991 | GLU  | 9.8  |
| 2   | C     | 992 | ARG  | 9.8  |
| 2   | D     | 981 | GLU  | 9.8  |
| 2   | C     | 985 | ALA  | 9.7  |
| 2   | H     | 978 | LEU  | 9.6  |
| 2   | C     | 979 | GLU  | 9.6  |
| 2   | D     | 975 | LEU  | 9.5  |
| 2   | D     | 984 | GLU  | 9.5  |
| 2   | H     | 984 | GLU  | 9.4  |
| 2   | D     | 988 | ALA  | 9.3  |
| 2   | D     | 978 | LEU  | 9.2  |
| 2   | D     | 992 | ARG  | 9.0  |
| 2   | H     | 991 | GLU  | 8.8  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | D     | 983 | ALA  | 8.7  |
| 2   | F     | 993 | LEU  | 8.7  |
| 2   | D     | 991 | GLU  | 8.6  |
| 2   | H     | 990 | GLU  | 8.5  |
| 2   | D     | 990 | GLU  | 8.5  |
| 2   | F     | 983 | ALA  | 8.4  |
| 2   | C     | 984 | GLU  | 8.2  |
| 2   | F     | 991 | GLU  | 7.9  |
| 2   | D     | 976 | LYS  | 7.8  |
| 2   | F     | 982 | LYS  | 7.7  |
| 2   | H     | 976 | LYS  | 7.6  |
| 2   | D     | 989 | ALA  | 7.6  |
| 2   | D     | 977 | LYS  | 6.7  |
| 2   | F     | 990 | GLU  | 6.7  |
| 2   | C     | 973 | GLY  | 6.6  |
| 2   | D     | 982 | LYS  | 6.1  |
| 2   | F     | 975 | LEU  | 5.5  |
| 2   | F     | 978 | LEU  | 5.4  |
| 2   | F     | 944 | ALA  | 4.6  |
| 2   | H     | 946 | SER  | 4.6  |
| 2   | F     | 974 | LEU  | 4.5  |
| 2   | D     | 944 | ALA  | 4.4  |
| 2   | D     | 946 | SER  | 3.8  |
| 2   | F     | 976 | LYS  | 3.7  |
| 2   | C     | 943 | ALA  | 3.7  |
| 2   | H     | 973 | GLY  | 3.6  |
| 2   | F     | 946 | SER  | 3.4  |
| 2   | C     | 946 | SER  | 3.3  |
| 2   | F     | 977 | LYS  | 3.2  |
| 2   | F     | 947 | ARG  | 3.1  |
| 2   | H     | 943 | ALA  | 3.1  |
| 2   | D     | 947 | ARG  | 2.9  |
| 2   | C     | 953 | ARG  | 2.6  |
| 2   | F     | 961 | GLU  | 2.6  |
| 2   | D     | 950 | ALA  | 2.6  |
| 2   | D     | 951 | GLN  | 2.5  |
| 2   | H     | 953 | ARG  | 2.4  |
| 2   | C     | 947 | ARG  | 2.3  |
| 2   | D     | 949 | GLU  | 2.3  |
| 2   | C     | 940 | GLN  | 2.2  |
| 2   | D     | 954 | ILE  | 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.