



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 10:34 AM UTC

PDB ID : 2WLM / pdb\_00002wlm  
Title : POTASSIUM CHANNEL FROM MAGNETOSPIRILLUM MAGNETO-TACTICUM  
Authors : Clarke, O.B.; Caputo, A.T.; Smith, B.J.; Gulbis, J.M.  
Deposited on : 2009-06-24  
Resolution : 3.61 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                                                             |

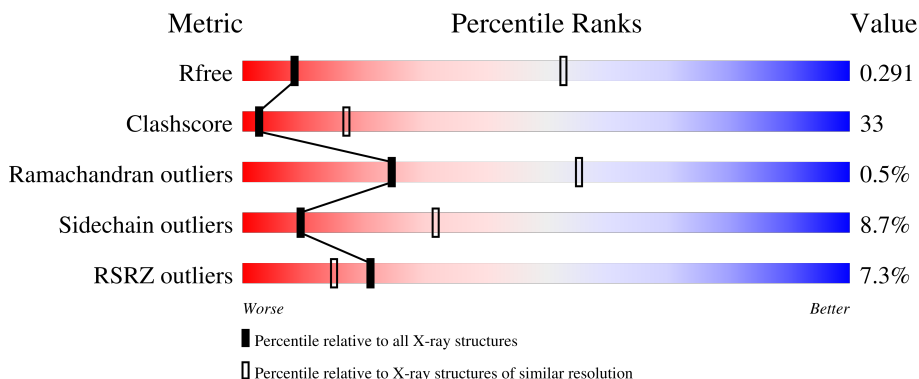
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.61 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                      | 1062 (3.72-3.52)                                      |
| Clashscore            | 190562                      | 1092 (3.72-3.52)                                      |
| Ramachandran outliers | 187476                      | 1057 (3.72-3.52)                                      |
| Sidechain outliers    | 187428                      | 1055 (3.72-3.52)                                      |
| RSRZ outliers         | 180081                      | 1060 (3.72-3.52)                                      |

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     | 301    | <div> <div>5%</div> <div>46% 39% 5% 10%</div> </div> |
| 1   | B     | 301    | <div> <div>9%</div> <div>48% 40% 5% 7%</div> </div>  |
| 1   | C     | 301    | <div> <div>8%</div> <div>47% 41% 5% 7%</div> </div>  |
| 1   | D     | 301    | <div> <div>6%</div> <div>47% 41% 5% 7%</div> </div>  |

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8613 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.

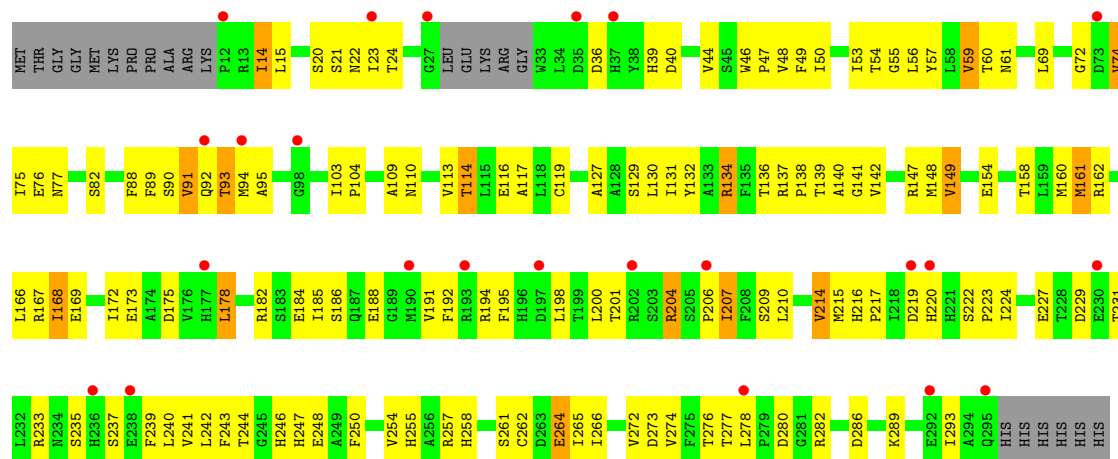
- Molecule 1 is a protein called POTASSIUM CHANNEL.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 271      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2108  | 1361 | 360 | 379 | 8 |         |         |       |
| 1   | B     | 279      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2167  | 1395 | 370 | 394 | 8 |         |         |       |
| 1   | C     | 279      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2167  | 1395 | 370 | 394 | 8 |         |         |       |
| 1   | D     | 279      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2167  | 1393 | 372 | 394 | 8 |         |         |       |

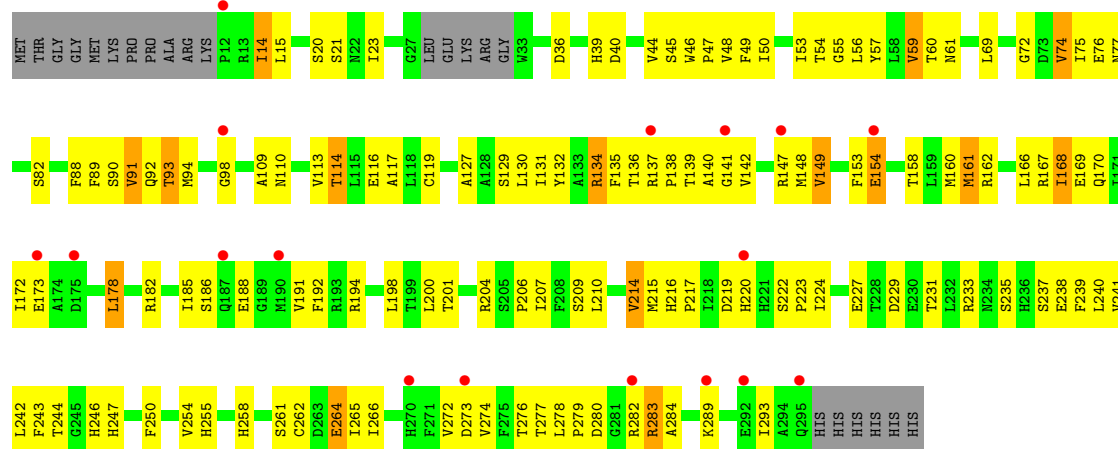
- Molecule 2 is POTASSIUM ION (CCD ID: K) (formula: K).

| Mol | Chain | Residues | Atoms |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 2   | A     | 3        | Total | K | 0       | 0       |
|     |       |          | 3     | 3 |         |         |
| 2   | C     | 1        | Total | K | 0       | 0       |
|     |       |          | 1     | 1 |         |         |





### • Molecule 1: POTASSIUM CHANNEL



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | C 2 2 21                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 99.26Å 151.19Å 294.76Å<br>90.00° 90.00° 90.00°              | Depositor        |
| Resolution (Å)                                                          | 19.97 – 3.61<br>19.97 – 3.61                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 93.7 (19.97-3.61)<br>93.3 (19.97-3.61)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.13                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.22 (at 3.56Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX (PHENIX.REFINE)                                      | Depositor        |
| R, $R_{free}$                                                           | 0.263 , 0.288<br>0.267 , 0.291                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 1239 reflections (5.09%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 81.9                                                        | Xtriage          |
| Anisotropy                                                              | 0.260                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.29 , 118.1                                                | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.87                                                        | EDS              |
| Total number of atoms                                                   | 8613                                                        | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 125.0                                                       | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.44% 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](#)

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

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     | 0.46         | 0/2160      | 0.83        | 1/2940 (0.0%)  |
| 1   | B     | 0.43         | 0/2220      | 0.81        | 2/3021 (0.1%)  |
| 1   | C     | 0.45         | 0/2220      | 0.82        | 2/3021 (0.1%)  |
| 1   | D     | 0.45         | 0/2220      | 0.84        | 0/3022         |
| All | All   | 0.45         | 0/8820      | 0.82        | 5/12004 (0.0%) |

There are no bond length outliers.

All (5) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | B     | 274 | VAL  | CB-CA-C | -5.67 | 104.64      | 111.85   |
| 1   | C     | 207 | ILE  | N-CA-C  | 5.11  | 114.14      | 106.42   |
| 1   | C     | 95  | ALA  | N-CA-C  | -5.05 | 106.90      | 113.16   |
| 1   | A     | 95  | ALA  | N-CA-C  | -5.01 | 107.13      | 113.20   |
| 1   | B     | 207 | ILE  | N-CA-C  | 5.01  | 113.99      | 106.42   |

There are no chirality outliers.

There are no planarity outliers.

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

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 2108  | 0        | 2058     | 152     | 0            |
| 1   | B     | 2167  | 0        | 2118     | 154     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | C     | 2167  | 0        | 2117     | 165     | 0            |
| 1   | D     | 2167  | 0        | 2114     | 169     | 2            |
| 2   | A     | 3     | 0        | 0        | 0       | 0            |
| 2   | C     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 8613  | 0        | 8407     | 568     | 2            |

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 33.

All (568) 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:137:ARG:C    | 1:A:138:PRO:N    | 2.01                     | 1.19              |
| 1:B:137:ARG:C    | 1:B:138:PRO:N    | 2.03                     | 1.16              |
| 1:C:137:ARG:C    | 1:C:138:PRO:N    | 2.07                     | 1.13              |
| 1:D:137:ARG:C    | 1:D:138:PRO:N    | 2.10                     | 1.09              |
| 1:D:168:ILE:H    | 1:D:168:ILE:HD12 | 1.18                     | 1.04              |
| 1:B:168:ILE:HD12 | 1:B:168:ILE:H    | 1.19                     | 1.04              |
| 1:C:168:ILE:HD12 | 1:C:168:ILE:H    | 1.19                     | 1.04              |
| 1:D:274:VAL:HG12 | 1:D:289:LYS:HB2  | 1.38                     | 1.03              |
| 1:A:168:ILE:HD12 | 1:A:168:ILE:H    | 1.18                     | 1.02              |
| 1:B:278:LEU:HD12 | 1:B:282:ARG:HG3  | 1.42                     | 0.99              |
| 1:C:255:HIS:ND1  | 1:D:172:ILE:HD13 | 1.76                     | 0.99              |
| 1:A:278:LEU:HD12 | 1:A:282:ARG:HG3  | 1.45                     | 0.98              |
| 1:A:39:HIS:CD2   | 1:B:249:ALA:HB1  | 1.99                     | 0.97              |
| 1:D:278:LEU:HD12 | 1:D:282:ARG:HG3  | 1.47                     | 0.96              |
| 1:C:242:LEU:HD23 | 1:D:206:PRO:HB3  | 1.48                     | 0.94              |
| 1:C:278:LEU:HD12 | 1:C:282:ARG:HG3  | 1.45                     | 0.94              |
| 1:A:274:VAL:HG12 | 1:A:289:LYS:HB2  | 1.50                     | 0.94              |
| 1:C:274:VAL:HG12 | 1:C:289:LYS:HB2  | 1.50                     | 0.90              |
| 1:C:23:ILE:HD11  | 1:D:283:ARG:HH11 | 1.38                     | 0.88              |
| 1:D:274:VAL:CG1  | 1:D:289:LYS:HB2  | 2.05                     | 0.86              |
| 1:C:23:ILE:CG2   | 1:D:284:ALA:HA   | 2.06                     | 0.85              |
| 1:B:138:PRO:HB3  | 1:B:250:PHE:CD1  | 2.13                     | 0.84              |
| 1:C:22:ASN:O     | 1:C:23:ILE:HD13  | 1.78                     | 0.83              |
| 1:C:23:ILE:CD1   | 1:D:283:ARG:HG2  | 2.08                     | 0.83              |
| 1:C:138:PRO:HB3  | 1:C:250:PHE:CD1  | 2.15                     | 0.82              |
| 1:A:138:PRO:HB3  | 1:A:250:PHE:CD1  | 2.14                     | 0.82              |
| 1:A:36:ASP:OD2   | 1:B:167:ARG:NE   | 2.14                     | 0.81              |
| 1:C:22:ASN:C     | 1:C:23:ILE:HD13  | 2.04                     | 0.81              |
| 1:D:138:PRO:HB3  | 1:D:250:PHE:CD1  | 2.16                     | 0.81              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:242:LEU:CD2  | 1:A:257:ARG:HB3  | 2.10                     | 0.80              |
| 1:A:39:HIS:HD2   | 1:B:249:ALA:HB1  | 1.46                     | 0.80              |
| 1:C:23:ILE:CD1   | 1:D:283:ARG:HH11 | 1.95                     | 0.80              |
| 1:D:283:ARG:HH11 | 1:D:283:ARG:HG2  | 1.47                     | 0.80              |
| 1:A:242:LEU:HD23 | 1:A:257:ARG:HB3  | 1.64                     | 0.80              |
| 1:C:23:ILE:HG23  | 1:D:284:ALA:CA   | 2.11                     | 0.79              |
| 1:B:266:ILE:HD12 | 1:B:293:ILE:HD12 | 1.64                     | 0.79              |
| 1:C:23:ILE:HD12  | 1:D:283:ARG:HG2  | 1.66                     | 0.78              |
| 1:C:23:ILE:HG23  | 1:D:284:ALA:HA   | 1.65                     | 0.78              |
| 1:A:266:ILE:HD12 | 1:A:293:ILE:HD12 | 1.64                     | 0.77              |
| 1:C:266:ILE:HD12 | 1:C:293:ILE:HD12 | 1.66                     | 0.77              |
| 1:B:172:ILE:HG13 | 1:B:246:HIS:HB3  | 1.66                     | 0.77              |
| 1:C:23:ILE:HD11  | 1:D:283:ARG:NH1  | 1.99                     | 0.77              |
| 1:D:172:ILE:HG13 | 1:D:246:HIS:HB3  | 1.66                     | 0.77              |
| 1:A:23:ILE:CG2   | 1:A:24:THR:N     | 2.48                     | 0.76              |
| 1:C:172:ILE:HG13 | 1:C:246:HIS:HB3  | 1.66                     | 0.76              |
| 1:D:266:ILE:HD12 | 1:D:293:ILE:HD12 | 1.66                     | 0.76              |
| 1:A:280:ASP:HB3  | 1:A:282:ARG:HG2  | 1.68                     | 0.76              |
| 1:A:172:ILE:HG13 | 1:A:246:HIS:HB3  | 1.66                     | 0.75              |
| 1:A:56:LEU:O     | 1:A:60:THR:HG23  | 1.87                     | 0.75              |
| 1:C:280:ASP:HB3  | 1:C:282:ARG:HG2  | 1.68                     | 0.75              |
| 1:A:90:SER:O     | 1:A:93:THR:HG22  | 1.87                     | 0.74              |
| 1:C:56:LEU:O     | 1:C:60:THR:HG23  | 1.88                     | 0.74              |
| 1:C:255:HIS:CE1  | 1:D:172:ILE:HD13 | 2.23                     | 0.74              |
| 1:D:90:SER:O     | 1:D:93:THR:HG22  | 1.87                     | 0.74              |
| 1:D:61:ASN:HD21  | 1:D:94:MET:HE1   | 1.53                     | 0.73              |
| 1:D:61:ASN:ND2   | 1:D:94:MET:HE1   | 2.04                     | 0.73              |
| 1:B:56:LEU:O     | 1:B:60:THR:HG23  | 1.88                     | 0.72              |
| 1:D:56:LEU:O     | 1:D:60:THR:HG23  | 1.88                     | 0.72              |
| 1:D:280:ASP:HB3  | 1:D:282:ARG:HG2  | 1.71                     | 0.72              |
| 1:B:90:SER:O     | 1:B:93:THR:HG22  | 1.88                     | 0.72              |
| 1:C:90:SER:O     | 1:C:93:THR:HG22  | 1.89                     | 0.71              |
| 1:B:15:LEU:HD23  | 1:B:21:SER:HA    | 1.72                     | 0.71              |
| 1:A:39:HIS:CD2   | 1:B:249:ALA:CB   | 2.74                     | 0.71              |
| 1:C:23:ILE:CG1   | 1:D:283:ARG:NH1  | 2.53                     | 0.71              |
| 1:C:15:LEU:HD23  | 1:C:21:SER:HA    | 1.71                     | 0.71              |
| 1:C:61:ASN:ND2   | 1:C:94:MET:HE1   | 2.06                     | 0.70              |
| 1:D:15:LEU:HD23  | 1:D:21:SER:HA    | 1.72                     | 0.70              |
| 1:D:201:THR:CG2  | 1:D:217:PRO:HD3  | 2.21                     | 0.70              |
| 1:B:61:ASN:HD21  | 1:B:94:MET:HE1   | 1.56                     | 0.70              |
| 1:C:61:ASN:HD21  | 1:C:94:MET:HE1   | 1.56                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:280:ASP:OD2  | 1:D:282:ARG:HD3  | 1.91                     | 0.70              |
| 1:C:23:ILE:CG2   | 1:D:284:ALA:CA   | 2.68                     | 0.70              |
| 1:C:168:ILE:H    | 1:C:168:ILE:CD1  | 1.94                     | 0.70              |
| 1:C:227:GLU:HG3  | 1:C:231:THR:OG1  | 1.92                     | 0.70              |
| 1:B:158:THR:HG21 | 1:B:215:MET:HB3  | 1.74                     | 0.70              |
| 1:B:280:ASP:OD2  | 1:B:282:ARG:HD3  | 1.91                     | 0.70              |
| 1:C:23:ILE:HG13  | 1:D:283:ARG:NH1  | 2.07                     | 0.69              |
| 1:D:227:GLU:HG3  | 1:D:231:THR:OG1  | 1.92                     | 0.69              |
| 1:B:61:ASN:ND2   | 1:B:94:MET:HE1   | 2.07                     | 0.69              |
| 1:C:280:ASP:OD2  | 1:C:282:ARG:HD3  | 1.92                     | 0.69              |
| 1:A:227:GLU:HG3  | 1:A:231:THR:OG1  | 1.92                     | 0.69              |
| 1:C:158:THR:HG21 | 1:C:215:MET:HB3  | 1.74                     | 0.69              |
| 1:A:44:VAL:CG1   | 1:A:48:VAL:HB    | 2.23                     | 0.69              |
| 1:C:201:THR:CG2  | 1:C:217:PRO:HD3  | 2.23                     | 0.69              |
| 1:A:23:ILE:HG23  | 1:A:24:THR:N     | 2.08                     | 0.68              |
| 1:A:168:ILE:H    | 1:A:168:ILE:CD1  | 1.93                     | 0.68              |
| 1:B:227:GLU:HG3  | 1:B:231:THR:OG1  | 1.94                     | 0.68              |
| 1:D:44:VAL:CG1   | 1:D:48:VAL:HB    | 2.23                     | 0.68              |
| 1:A:280:ASP:OD2  | 1:A:282:ARG:HD3  | 1.92                     | 0.68              |
| 1:A:61:ASN:HD21  | 1:A:94:MET:HE1   | 1.58                     | 0.68              |
| 1:B:280:ASP:HB3  | 1:B:282:ARG:HG2  | 1.75                     | 0.68              |
| 1:D:158:THR:HG21 | 1:D:215:MET:HB3  | 1.73                     | 0.68              |
| 1:B:285:LEU:HD21 | 1:B:287:LEU:HD21 | 1.76                     | 0.68              |
| 1:A:158:THR:HG21 | 1:A:215:MET:HB3  | 1.75                     | 0.68              |
| 1:A:178:LEU:HD13 | 1:A:241:VAL:HG22 | 1.77                     | 0.67              |
| 1:A:61:ASN:ND2   | 1:A:94:MET:HE1   | 2.08                     | 0.67              |
| 1:B:44:VAL:HG13  | 1:B:48:VAL:HB    | 1.77                     | 0.67              |
| 1:C:44:VAL:CG1   | 1:C:48:VAL:HB    | 2.24                     | 0.67              |
| 1:D:61:ASN:HD21  | 1:D:94:MET:CE    | 2.07                     | 0.67              |
| 1:C:20:SER:HA    | 1:D:170:GLN:HE22 | 1.59                     | 0.67              |
| 1:B:229:ASP:OD1  | 1:B:233:ARG:NH1  | 2.28                     | 0.67              |
| 1:D:44:VAL:HG13  | 1:D:48:VAL:HB    | 1.76                     | 0.67              |
| 1:D:178:LEU:HD13 | 1:D:241:VAL:HG22 | 1.77                     | 0.67              |
| 1:B:178:LEU:HD13 | 1:B:241:VAL:HG22 | 1.77                     | 0.67              |
| 1:C:44:VAL:HG13  | 1:C:48:VAL:HB    | 1.77                     | 0.67              |
| 1:A:44:VAL:HG13  | 1:A:48:VAL:HB    | 1.76                     | 0.67              |
| 1:A:201:THR:CG2  | 1:A:217:PRO:HD3  | 2.23                     | 0.67              |
| 1:C:23:ILE:HD12  | 1:D:283:ARG:CG   | 2.25                     | 0.67              |
| 1:B:44:VAL:CG1   | 1:B:48:VAL:HB    | 2.24                     | 0.66              |
| 1:C:272:VAL:CG1  | 1:C:273:ASP:N    | 2.58                     | 0.66              |
| 1:C:23:ILE:HG22  | 1:D:284:ALA:HA   | 1.75                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:168:ILE:H    | 1:B:168:ILE:CD1  | 1.94                     | 0.66              |
| 1:A:39:HIS:HD2   | 1:B:249:ALA:CB   | 2.09                     | 0.66              |
| 1:A:204:ARG:HH11 | 1:A:204:ARG:HG2  | 1.61                     | 0.66              |
| 1:C:178:LEU:HD13 | 1:C:241:VAL:HG22 | 1.78                     | 0.66              |
| 1:D:88:PHE:O     | 1:D:92:GLN:HG3   | 1.96                     | 0.66              |
| 1:C:61:ASN:HD21  | 1:C:94:MET:CE    | 2.09                     | 0.66              |
| 1:A:88:PHE:O     | 1:A:92:GLN:HG3   | 1.97                     | 0.65              |
| 1:C:229:ASP:OD1  | 1:C:233:ARG:NH1  | 2.30                     | 0.65              |
| 1:A:61:ASN:HD21  | 1:A:94:MET:CE    | 2.09                     | 0.65              |
| 1:B:88:PHE:O     | 1:B:92:GLN:HG3   | 1.96                     | 0.65              |
| 1:A:39:HIS:HB2   | 1:B:250:PHE:CZ   | 2.32                     | 0.65              |
| 1:B:200:LEU:HD13 | 1:B:214:VAL:CG1  | 2.26                     | 0.65              |
| 1:B:61:ASN:HD21  | 1:B:94:MET:CE    | 2.09                     | 0.64              |
| 1:B:201:THR:CG2  | 1:B:217:PRO:HD3  | 2.27                     | 0.64              |
| 1:D:229:ASP:OD1  | 1:D:233:ARG:NH1  | 2.30                     | 0.64              |
| 1:C:21:SER:OG    | 1:D:210:LEU:HD11 | 1.97                     | 0.64              |
| 1:A:23:ILE:HG23  | 1:A:24:THR:H     | 1.62                     | 0.64              |
| 1:A:240:LEU:HD21 | 1:B:207:ILE:CD1  | 2.27                     | 0.64              |
| 1:C:88:PHE:O     | 1:C:92:GLN:HG3   | 1.97                     | 0.64              |
| 1:C:23:ILE:CD1   | 1:D:283:ARG:NH1  | 2.57                     | 0.64              |
| 1:A:278:LEU:HD12 | 1:A:282:ARG:CG   | 2.26                     | 0.64              |
| 1:A:200:LEU:HD13 | 1:A:214:VAL:CG1  | 2.29                     | 0.63              |
| 1:B:204:ARG:HG2  | 1:B:204:ARG:HH11 | 1.63                     | 0.63              |
| 1:A:39:HIS:HB2   | 1:B:250:PHE:CE2  | 2.33                     | 0.63              |
| 1:B:278:LEU:HD12 | 1:B:282:ARG:CG   | 2.23                     | 0.63              |
| 1:C:23:ILE:HG23  | 1:D:284:ALA:N    | 2.14                     | 0.63              |
| 1:B:140:ALA:HB1  | 1:B:142:VAL:HG23 | 1.80                     | 0.63              |
| 1:D:127:ALA:O    | 1:D:131:ILE:HG12 | 1.99                     | 0.63              |
| 1:A:229:ASP:OD1  | 1:A:233:ARG:NH1  | 2.32                     | 0.63              |
| 1:B:257:ARG:NH2  | 1:C:248:GLU:OE1  | 2.31                     | 0.63              |
| 1:C:23:ILE:HD12  | 1:D:283:ARG:CB   | 2.29                     | 0.63              |
| 1:D:140:ALA:HB1  | 1:D:142:VAL:HG23 | 1.81                     | 0.63              |
| 1:A:139:THR:O    | 1:A:167:ARG:NH1  | 2.29                     | 0.63              |
| 1:A:240:LEU:HD12 | 1:A:258:HIS:O    | 1.99                     | 0.62              |
| 1:B:139:THR:O    | 1:B:167:ARG:NH1  | 2.27                     | 0.62              |
| 1:D:276:THR:HG22 | 1:D:277:THR:N    | 2.13                     | 0.62              |
| 1:C:204:ARG:HH11 | 1:C:204:ARG:HG2  | 1.63                     | 0.62              |
| 1:C:240:LEU:HD12 | 1:C:258:HIS:O    | 1.99                     | 0.62              |
| 1:A:210:LEU:HD21 | 1:D:21:SER:OG    | 1.99                     | 0.62              |
| 1:B:272:VAL:CG1  | 1:B:273:ASP:N    | 2.60                     | 0.62              |
| 1:D:200:LEU:HD13 | 1:D:214:VAL:CG1  | 2.28                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:127:ALA:O    | 1:A:131:ILE:HG12 | 1.99                     | 0.62              |
| 1:A:140:ALA:HB1  | 1:A:142:VAL:HG23 | 1.79                     | 0.62              |
| 1:C:278:LEU:HD12 | 1:C:282:ARG:CG   | 2.25                     | 0.62              |
| 1:D:272:VAL:CG1  | 1:D:273:ASP:N    | 2.63                     | 0.62              |
| 1:C:200:LEU:HD13 | 1:C:214:VAL:CG1  | 2.29                     | 0.62              |
| 1:B:127:ALA:O    | 1:B:131:ILE:HG12 | 1.99                     | 0.62              |
| 1:D:240:LEU:HD12 | 1:D:258:HIS:O    | 1.98                     | 0.62              |
| 1:B:240:LEU:HD12 | 1:B:258:HIS:O    | 2.00                     | 0.61              |
| 1:D:141:GLY:O    | 1:D:166:LEU:HB2  | 2.00                     | 0.61              |
| 1:A:261:SER:H    | 1:A:264:GLU:HG3  | 1.66                     | 0.61              |
| 1:A:88:PHE:CE2   | 1:D:110:ASN:HB3  | 2.36                     | 0.61              |
| 1:C:127:ALA:O    | 1:C:131:ILE:HG12 | 2.00                     | 0.61              |
| 1:C:141:GLY:O    | 1:C:166:LEU:HB2  | 2.01                     | 0.61              |
| 1:C:140:ALA:HB1  | 1:C:142:VAL:HG23 | 1.81                     | 0.60              |
| 1:B:276:THR:HG22 | 1:B:277:THR:N    | 2.15                     | 0.60              |
| 1:C:261:SER:H    | 1:C:264:GLU:HG3  | 1.66                     | 0.60              |
| 1:D:168:ILE:H    | 1:D:168:ILE:CD1  | 1.93                     | 0.60              |
| 1:D:204:ARG:HG2  | 1:D:204:ARG:HH11 | 1.66                     | 0.60              |
| 1:B:274:VAL:HG12 | 1:B:289:LYS:HB2  | 1.83                     | 0.60              |
| 1:B:278:LEU:CD1  | 1:B:282:ARG:HG3  | 2.27                     | 0.60              |
| 1:B:261:SER:H    | 1:B:264:GLU:HG3  | 1.66                     | 0.60              |
| 1:B:207:ILE:HG22 | 1:B:207:ILE:O    | 2.02                     | 0.60              |
| 1:A:141:GLY:O    | 1:A:166:LEU:HB2  | 2.01                     | 0.60              |
| 1:C:186:SER:OG   | 1:C:188:GLU:OE1  | 2.20                     | 0.60              |
| 1:C:192:PHE:CE1  | 1:C:194:ARG:HB2  | 2.37                     | 0.60              |
| 1:D:283:ARG:HG2  | 1:D:283:ARG:NH1  | 2.15                     | 0.60              |
| 1:D:130:LEU:O    | 1:D:134:ARG:HG2  | 2.02                     | 0.59              |
| 1:A:272:VAL:CG1  | 1:A:273:ASP:N    | 2.64                     | 0.59              |
| 1:C:139:THR:O    | 1:C:167:ARG:NH1  | 2.29                     | 0.59              |
| 1:D:261:SER:H    | 1:D:264:GLU:HG3  | 1.66                     | 0.59              |
| 1:B:75:ILE:HD13  | 1:B:89:PHE:CD2   | 2.38                     | 0.59              |
| 1:B:286:ASP:C    | 1:B:288:GLY:H    | 2.10                     | 0.59              |
| 1:D:132:TYR:C    | 1:D:132:TYR:CD2  | 2.80                     | 0.59              |
| 1:A:93:THR:HG21  | 1:A:116:GLU:OE1  | 2.03                     | 0.59              |
| 1:C:278:LEU:CD1  | 1:C:282:ARG:HG3  | 2.27                     | 0.59              |
| 1:A:114:THR:HG22 | 1:B:91:VAL:HG21  | 1.85                     | 0.59              |
| 1:B:141:GLY:O    | 1:B:166:LEU:HB2  | 2.02                     | 0.59              |
| 1:C:207:ILE:O    | 1:C:207:ILE:HG22 | 2.02                     | 0.59              |
| 1:C:130:LEU:O    | 1:C:134:ARG:HG2  | 2.03                     | 0.59              |
| 1:A:130:LEU:O    | 1:A:134:ARG:HG2  | 2.03                     | 0.58              |
| 1:A:186:SER:OG   | 1:A:188:GLU:OE1  | 2.21                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:173:GLU:HA   | 1:C:206:PRO:HA   | 1.85                     | 0.58              |
| 1:A:74:VAL:HB    | 1:A:109:ALA:HB2  | 1.85                     | 0.58              |
| 1:A:173:GLU:HA   | 1:A:206:PRO:HA   | 1.84                     | 0.58              |
| 1:B:74:VAL:HB    | 1:B:109:ALA:HB2  | 1.85                     | 0.58              |
| 1:B:186:SER:OG   | 1:B:188:GLU:OE1  | 2.21                     | 0.58              |
| 1:D:75:ILE:HD13  | 1:D:89:PHE:CD2   | 2.38                     | 0.58              |
| 1:D:149:VAL:HG12 | 1:D:293:ILE:HD13 | 1.84                     | 0.58              |
| 1:D:186:SER:OG   | 1:D:188:GLU:OE1  | 2.20                     | 0.58              |
| 1:D:139:THR:O    | 1:D:167:ARG:NH1  | 2.27                     | 0.58              |
| 1:C:132:TYR:C    | 1:C:132:TYR:CD2  | 2.82                     | 0.58              |
| 1:B:132:TYR:C    | 1:B:132:TYR:CD2  | 2.82                     | 0.58              |
| 1:C:149:VAL:HG12 | 1:C:293:ILE:HD13 | 1.86                     | 0.58              |
| 1:D:74:VAL:HB    | 1:D:109:ALA:HB2  | 1.86                     | 0.58              |
| 1:D:278:LEU:HD12 | 1:D:282:ARG:CG   | 2.28                     | 0.58              |
| 1:D:93:THR:HG21  | 1:D:116:GLU:OE1  | 2.03                     | 0.57              |
| 1:A:149:VAL:HG12 | 1:A:293:ILE:HD13 | 1.86                     | 0.57              |
| 1:C:21:SER:OG    | 1:D:210:LEU:HD21 | 2.03                     | 0.57              |
| 1:C:75:ILE:HD13  | 1:C:89:PHE:CD2   | 2.38                     | 0.57              |
| 1:A:207:ILE:HD11 | 1:D:242:LEU:HB2  | 1.86                     | 0.57              |
| 1:B:272:VAL:HG12 | 1:B:273:ASP:N    | 2.19                     | 0.57              |
| 1:C:94:MET:HB2   | 1:C:116:GLU:HG2  | 1.86                     | 0.57              |
| 1:A:94:MET:HB2   | 1:A:116:GLU:HG2  | 1.87                     | 0.57              |
| 1:B:149:VAL:HG12 | 1:B:293:ILE:HD13 | 1.87                     | 0.57              |
| 1:C:192:PHE:HE1  | 1:C:194:ARG:HB2  | 1.69                     | 0.57              |
| 1:D:172:ILE:CG1  | 1:D:246:HIS:HB3  | 2.35                     | 0.57              |
| 1:D:207:ILE:HG22 | 1:D:207:ILE:O    | 2.03                     | 0.57              |
| 1:C:74:VAL:HB    | 1:C:109:ALA:HB2  | 1.85                     | 0.57              |
| 1:C:93:THR:HG21  | 1:C:116:GLU:OE1  | 2.04                     | 0.57              |
| 1:C:14:ILE:HD13  | 1:C:14:ILE:N     | 2.20                     | 0.57              |
| 1:C:36:ASP:OD1   | 1:C:39:HIS:HB3   | 2.05                     | 0.57              |
| 1:B:36:ASP:OD1   | 1:B:39:HIS:HB3   | 2.05                     | 0.57              |
| 1:B:185:ILE:CD1  | 1:B:191:VAL:HB   | 2.35                     | 0.57              |
| 1:A:207:ILE:O    | 1:A:207:ILE:HG22 | 2.05                     | 0.57              |
| 1:B:130:LEU:O    | 1:B:134:ARG:HG2  | 2.04                     | 0.57              |
| 1:C:172:ILE:CG1  | 1:C:246:HIS:HB3  | 2.35                     | 0.57              |
| 1:A:46:TRP:O     | 1:A:50:ILE:HG13  | 2.05                     | 0.56              |
| 1:A:75:ILE:HD13  | 1:A:89:PHE:CD2   | 2.40                     | 0.56              |
| 1:B:172:ILE:CG1  | 1:B:246:HIS:HB3  | 2.34                     | 0.56              |
| 1:D:46:TRP:O     | 1:D:50:ILE:HG13  | 2.05                     | 0.56              |
| 1:D:274:VAL:HA   | 1:D:289:LYS:HD2  | 1.86                     | 0.56              |
| 1:A:110:ASN:O    | 1:A:114:THR:HG23 | 2.06                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:132:TYR:C    | 1:A:132:TYR:CD2  | 2.83                     | 0.56              |
| 1:B:75:ILE:CD1   | 1:B:89:PHE:CD2   | 2.89                     | 0.56              |
| 1:C:272:VAL:HG12 | 1:C:273:ASP:N    | 2.19                     | 0.56              |
| 1:D:94:MET:HB2   | 1:D:116:GLU:HG2  | 1.87                     | 0.56              |
| 1:B:46:TRP:O     | 1:B:50:ILE:HG13  | 2.06                     | 0.56              |
| 1:B:93:THR:HG21  | 1:B:116:GLU:OE1  | 2.05                     | 0.56              |
| 1:A:36:ASP:OD1   | 1:A:39:HIS:HB3   | 2.04                     | 0.56              |
| 1:D:75:ILE:CD1   | 1:D:89:PHE:CD2   | 2.89                     | 0.56              |
| 1:C:209:SER:O    | 1:C:210:LEU:HD23 | 2.06                     | 0.55              |
| 1:D:110:ASN:O    | 1:D:114:THR:HG23 | 2.06                     | 0.55              |
| 1:B:94:MET:HB2   | 1:B:116:GLU:HG2  | 1.87                     | 0.55              |
| 1:B:209:SER:O    | 1:B:210:LEU:HD23 | 2.06                     | 0.55              |
| 1:C:185:ILE:CD1  | 1:C:191:VAL:HB   | 2.36                     | 0.55              |
| 1:D:36:ASP:OD1   | 1:D:39:HIS:HB3   | 2.05                     | 0.55              |
| 1:A:209:SER:O    | 1:A:210:LEU:HD23 | 2.07                     | 0.55              |
| 1:D:239:PHE:CE1  | 1:D:265:ILE:HD11 | 2.41                     | 0.55              |
| 1:D:201:THR:HG22 | 1:D:217:PRO:HD3  | 1.87                     | 0.55              |
| 1:A:172:ILE:CG1  | 1:A:246:HIS:HB3  | 2.35                     | 0.55              |
| 1:C:75:ILE:CD1   | 1:C:89:PHE:CD2   | 2.89                     | 0.55              |
| 1:A:172:ILE:HD13 | 1:D:255:HIS:ND1  | 2.22                     | 0.55              |
| 1:A:182:ARG:HA   | 1:A:193:ARG:NH1  | 2.22                     | 0.55              |
| 1:A:161:MET:HE2  | 1:A:162:ARG:N    | 2.21                     | 0.55              |
| 1:D:161:MET:HE2  | 1:D:162:ARG:N    | 2.22                     | 0.55              |
| 1:A:239:PHE:CE1  | 1:A:265:ILE:HD11 | 2.42                     | 0.55              |
| 1:B:161:MET:HE2  | 1:B:162:ARG:N    | 2.22                     | 0.55              |
| 1:C:239:PHE:CE1  | 1:C:265:ILE:HD11 | 2.42                     | 0.55              |
| 1:B:173:GLU:HA   | 1:B:206:PRO:HA   | 1.87                     | 0.55              |
| 1:C:46:TRP:O     | 1:C:50:ILE:HG13  | 2.06                     | 0.55              |
| 1:C:110:ASN:O    | 1:C:114:THR:HG23 | 2.07                     | 0.54              |
| 1:D:209:SER:O    | 1:D:210:LEU:HD23 | 2.07                     | 0.54              |
| 1:B:110:ASN:O    | 1:B:114:THR:HG23 | 2.07                     | 0.54              |
| 1:D:185:ILE:CD1  | 1:D:191:VAL:HB   | 2.36                     | 0.54              |
| 1:D:192:PHE:CE1  | 1:D:194:ARG:HB2  | 2.42                     | 0.54              |
| 1:B:239:PHE:CE1  | 1:B:265:ILE:HD11 | 2.42                     | 0.54              |
| 1:A:75:ILE:CD1   | 1:A:89:PHE:CD2   | 2.91                     | 0.54              |
| 1:A:185:ILE:CD1  | 1:A:191:VAL:HB   | 2.37                     | 0.54              |
| 1:A:138:PRO:HB3  | 1:A:250:PHE:CG   | 2.43                     | 0.54              |
| 1:C:161:MET:HE2  | 1:C:162:ARG:N    | 2.23                     | 0.54              |
| 1:B:14:ILE:N     | 1:B:14:ILE:HD13  | 2.23                     | 0.54              |
| 1:B:138:PRO:HB3  | 1:B:250:PHE:CG   | 2.42                     | 0.54              |
| 1:A:278:LEU:CD1  | 1:A:282:ARG:HG3  | 2.27                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:149:VAL:CG1  | 1:D:293:ILE:HD13 | 2.38                     | 0.53              |
| 1:C:227:GLU:OE2  | 1:C:231:THR:HB   | 2.09                     | 0.53              |
| 1:D:272:VAL:HG12 | 1:D:273:ASP:N    | 2.22                     | 0.53              |
| 1:B:153:PHE:CE2  | 1:B:154:GLU:OE1  | 2.62                     | 0.53              |
| 1:B:21:SER:OG    | 1:C:210:LEU:HD21 | 2.08                     | 0.53              |
| 1:C:257:ARG:CZ   | 1:D:170:GLN:OE1  | 2.57                     | 0.53              |
| 1:C:23:ILE:CG2   | 1:D:284:ALA:C    | 2.82                     | 0.53              |
| 1:C:276:THR:HG22 | 1:C:277:THR:N    | 2.24                     | 0.53              |
| 1:C:21:SER:CB    | 1:D:210:LEU:HD11 | 2.39                     | 0.52              |
| 1:C:138:PRO:HB3  | 1:C:250:PHE:CG   | 2.43                     | 0.52              |
| 1:C:201:THR:HG22 | 1:C:217:PRO:HD3  | 1.92                     | 0.52              |
| 1:D:227:GLU:OE2  | 1:D:231:THR:HB   | 2.10                     | 0.52              |
| 1:A:274:VAL:CG1  | 1:A:289:LYS:HB2  | 2.34                     | 0.52              |
| 1:B:147:ARG:HB2  | 1:B:293:ILE:HD11 | 1.92                     | 0.52              |
| 1:D:278:LEU:HB3  | 1:D:279:PRO:HD2  | 1.91                     | 0.52              |
| 1:D:280:ASP:HB3  | 1:D:282:ARG:CG   | 2.38                     | 0.52              |
| 1:A:39:HIS:HA    | 1:B:250:PHE:CE2  | 2.45                     | 0.52              |
| 1:A:227:GLU:OE2  | 1:A:231:THR:HB   | 2.10                     | 0.52              |
| 1:B:227:GLU:OE2  | 1:B:231:THR:HB   | 2.10                     | 0.52              |
| 1:C:266:ILE:O    | 1:C:266:ILE:HG22 | 2.09                     | 0.51              |
| 1:B:280:ASP:OD1  | 1:B:280:ASP:O    | 2.28                     | 0.51              |
| 1:C:147:ARG:HB2  | 1:C:293:ILE:HD11 | 1.93                     | 0.51              |
| 1:C:280:ASP:HB3  | 1:C:282:ARG:CG   | 2.37                     | 0.51              |
| 1:A:153:PHE:CE2  | 1:A:154:GLU:OE1  | 2.63                     | 0.51              |
| 1:A:272:VAL:HG12 | 1:A:273:ASP:N    | 2.24                     | 0.51              |
| 1:A:39:HIS:HA    | 1:B:250:PHE:HE2  | 1.75                     | 0.51              |
| 1:A:266:ILE:HG22 | 1:A:266:ILE:O    | 2.10                     | 0.51              |
| 1:A:61:ASN:ND2   | 1:A:94:MET:CE    | 2.72                     | 0.51              |
| 1:C:40:ASP:O     | 1:C:44:VAL:HG23  | 2.11                     | 0.51              |
| 1:D:274:VAL:HG12 | 1:D:289:LYS:CB   | 2.27                     | 0.51              |
| 1:D:276:THR:CG2  | 1:D:277:THR:N    | 2.74                     | 0.51              |
| 1:A:147:ARG:HB2  | 1:A:293:ILE:HD11 | 1.92                     | 0.51              |
| 1:A:276:THR:HG22 | 1:A:277:THR:N    | 2.26                     | 0.51              |
| 1:A:280:ASP:HB3  | 1:A:282:ARG:CG   | 2.38                     | 0.51              |
| 1:C:149:VAL:CG1  | 1:C:293:ILE:HD13 | 2.41                     | 0.51              |
| 1:D:138:PRO:HB3  | 1:D:250:PHE:CG   | 2.44                     | 0.51              |
| 1:A:39:HIS:CA    | 1:B:250:PHE:HE2  | 2.24                     | 0.51              |
| 1:D:266:ILE:HG22 | 1:D:266:ILE:O    | 2.11                     | 0.51              |
| 1:B:201:THR:HG22 | 1:B:217:PRO:HD3  | 1.93                     | 0.50              |
| 1:D:137:ARG:CA   | 1:D:138:PRO:N    | 2.73                     | 0.50              |
| 1:B:276:THR:CG2  | 1:B:277:THR:N    | 2.74                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:280:ASP:HB3  | 1:B:282:ARG:CG   | 2.40                     | 0.50              |
| 1:D:153:PHE:CE2  | 1:D:154:GLU:OE1  | 2.64                     | 0.50              |
| 1:D:192:PHE:HE1  | 1:D:194:ARG:HB2  | 1.77                     | 0.50              |
| 1:D:14:ILE:N     | 1:D:14:ILE:HD13  | 2.25                     | 0.50              |
| 1:A:149:VAL:CG1  | 1:A:293:ILE:HD13 | 2.42                     | 0.50              |
| 1:A:110:ASN:O    | 1:A:113:VAL:HB   | 2.11                     | 0.50              |
| 1:B:110:ASN:O    | 1:B:113:VAL:HB   | 2.11                     | 0.50              |
| 1:B:110:ASN:HB3  | 1:C:88:PHE:CD2   | 2.47                     | 0.50              |
| 1:A:93:THR:CG2   | 1:A:94:MET:N     | 2.75                     | 0.49              |
| 1:A:182:ARG:HB3  | 1:A:237:SER:HB3  | 1.94                     | 0.49              |
| 1:C:110:ASN:O    | 1:C:113:VAL:HB   | 2.12                     | 0.49              |
| 1:A:40:ASP:O     | 1:A:44:VAL:HG23  | 2.12                     | 0.49              |
| 1:B:266:ILE:HG22 | 1:B:266:ILE:O    | 2.10                     | 0.49              |
| 1:D:110:ASN:O    | 1:D:113:VAL:HB   | 2.12                     | 0.49              |
| 1:B:149:VAL:CG1  | 1:B:293:ILE:HD13 | 2.43                     | 0.49              |
| 1:D:147:ARG:HB2  | 1:D:293:ILE:HD11 | 1.94                     | 0.49              |
| 1:D:15:LEU:HB2   | 1:D:238:GLU:OE1  | 2.13                     | 0.49              |
| 1:A:284:ALA:HA   | 1:D:23:ILE:HG22  | 1.95                     | 0.48              |
| 1:A:54:THR:O     | 1:A:57:TYR:HB3   | 2.13                     | 0.48              |
| 1:A:207:ILE:CD1  | 1:D:242:LEU:HB2  | 2.42                     | 0.48              |
| 1:B:61:ASN:ND2   | 1:B:94:MET:CE    | 2.72                     | 0.48              |
| 1:D:243:PHE:C    | 1:D:243:PHE:CD2  | 2.91                     | 0.48              |
| 1:C:201:THR:HG23 | 1:C:217:PRO:HD3  | 1.96                     | 0.48              |
| 1:A:181:VAL:HG12 | 1:A:193:ARG:CZ   | 2.43                     | 0.48              |
| 1:A:201:THR:HG22 | 1:A:217:PRO:HD3  | 1.93                     | 0.48              |
| 1:B:54:THR:O     | 1:B:57:TYR:HB3   | 2.14                     | 0.48              |
| 1:D:61:ASN:ND2   | 1:D:94:MET:CE    | 2.71                     | 0.48              |
| 1:D:93:THR:CG2   | 1:D:94:MET:N     | 2.76                     | 0.48              |
| 1:B:40:ASP:O     | 1:B:44:VAL:HG23  | 2.13                     | 0.48              |
| 1:C:24:THR:OG1   | 1:D:278:LEU:HD11 | 2.13                     | 0.48              |
| 1:C:182:ARG:NE   | 1:C:184:GLU:OE2  | 2.38                     | 0.48              |
| 1:D:201:THR:HG23 | 1:D:217:PRO:HD3  | 1.96                     | 0.48              |
| 1:B:286:ASP:C    | 1:B:288:GLY:N    | 2.72                     | 0.48              |
| 1:D:55:GLY:O     | 1:D:59:VAL:HG23  | 2.14                     | 0.48              |
| 1:C:243:PHE:C    | 1:C:243:PHE:CD2  | 2.91                     | 0.48              |
| 1:A:49:PHE:HE2   | 1:A:131:ILE:HD13 | 1.79                     | 0.48              |
| 1:A:243:PHE:CD2  | 1:A:243:PHE:C    | 2.91                     | 0.48              |
| 1:C:257:ARG:HB3  | 1:D:207:ILE:HD11 | 1.95                     | 0.48              |
| 1:D:40:ASP:O     | 1:D:44:VAL:HG23  | 2.13                     | 0.48              |
| 1:B:88:PHE:O     | 1:B:92:GLN:CG    | 2.62                     | 0.47              |
| 1:C:148:MET:HE3  | 1:C:161:MET:HG2  | 1.95                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:182:ARG:HB3  | 1:D:237:SER:HB3  | 1.96                     | 0.47              |
| 1:B:93:THR:CG2   | 1:B:94:MET:N     | 2.76                     | 0.47              |
| 1:B:182:ARG:HB3  | 1:B:237:SER:HB3  | 1.95                     | 0.47              |
| 1:C:173:GLU:O    | 1:C:173:GLU:HG3  | 2.14                     | 0.47              |
| 1:D:54:THR:O     | 1:D:57:TYR:HB3   | 2.14                     | 0.47              |
| 1:B:137:ARG:C    | 1:B:138:PRO:CA   | 2.86                     | 0.47              |
| 1:C:49:PHE:HE2   | 1:C:131:ILE:HD13 | 1.79                     | 0.47              |
| 1:C:130:LEU:HD21 | 1:D:135:PHE:HE2  | 1.80                     | 0.47              |
| 1:A:274:VAL:HA   | 1:A:289:LYS:HD2  | 1.95                     | 0.47              |
| 1:D:49:PHE:HE2   | 1:D:131:ILE:HD13 | 1.79                     | 0.47              |
| 1:D:88:PHE:O     | 1:D:92:GLN:CG    | 2.63                     | 0.47              |
| 1:B:243:PHE:CD2  | 1:B:243:PHE:C    | 2.92                     | 0.47              |
| 1:B:173:GLU:HG3  | 1:B:173:GLU:O    | 2.15                     | 0.47              |
| 1:C:54:THR:O     | 1:C:57:TYR:HB3   | 2.14                     | 0.47              |
| 1:C:175:ASP:OD2  | 1:C:204:ARG:NH1  | 2.47                     | 0.47              |
| 1:C:182:ARG:HB3  | 1:C:237:SER:HB3  | 1.96                     | 0.47              |
| 1:A:23:ILE:HG22  | 1:A:24:THR:N     | 2.26                     | 0.47              |
| 1:A:173:GLU:O    | 1:A:173:GLU:HG3  | 2.15                     | 0.47              |
| 1:A:55:GLY:O     | 1:A:59:VAL:HG23  | 2.15                     | 0.47              |
| 1:A:182:ARG:CB   | 1:A:237:SER:HB3  | 2.45                     | 0.47              |
| 1:A:284:ALA:HA   | 1:D:23:ILE:CG2   | 2.45                     | 0.47              |
| 1:A:148:MET:HE3  | 1:A:161:MET:HG2  | 1.97                     | 0.46              |
| 1:A:170:GLN:HE22 | 1:D:20:SER:HA    | 1.79                     | 0.46              |
| 1:A:244:THR:HG22 | 1:A:255:HIS:HB2  | 1.96                     | 0.46              |
| 1:B:49:PHE:HE2   | 1:B:131:ILE:HD13 | 1.79                     | 0.46              |
| 1:B:110:ASN:HB3  | 1:C:88:PHE:CE2   | 2.50                     | 0.46              |
| 1:D:148:MET:HE3  | 1:D:161:MET:HG2  | 1.96                     | 0.46              |
| 1:A:88:PHE:CD2   | 1:D:110:ASN:HB3  | 2.49                     | 0.46              |
| 1:C:93:THR:CG2   | 1:C:94:MET:N     | 2.77                     | 0.46              |
| 1:D:140:ALA:C    | 1:D:142:VAL:H    | 2.22                     | 0.46              |
| 1:B:148:MET:HE3  | 1:B:161:MET:HG2  | 1.97                     | 0.46              |
| 1:A:204:ARG:HG2  | 1:A:204:ARG:NH1  | 2.30                     | 0.46              |
| 1:B:55:GLY:O     | 1:B:59:VAL:HG23  | 2.15                     | 0.46              |
| 1:D:69:LEU:O     | 1:D:72:GLY:N     | 2.48                     | 0.46              |
| 1:D:182:ARG:CB   | 1:D:237:SER:HB3  | 2.45                     | 0.46              |
| 1:D:222:SER:OG   | 1:D:224:ILE:HG12 | 2.16                     | 0.46              |
| 1:B:140:ALA:C    | 1:B:142:VAL:H    | 2.24                     | 0.46              |
| 1:C:55:GLY:O     | 1:C:59:VAL:HG23  | 2.16                     | 0.46              |
| 1:C:169:GLU:HB2  | 1:C:247:HIS:HE1  | 1.81                     | 0.46              |
| 1:C:182:ARG:CB   | 1:C:237:SER:HB3  | 2.46                     | 0.46              |
| 1:C:69:LEU:O     | 1:C:72:GLY:N     | 2.49                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:116:GLU:O    | 1:C:117:ALA:C    | 2.58                     | 0.46              |
| 1:B:182:ARG:CB   | 1:B:237:SER:HB3  | 2.46                     | 0.46              |
| 1:A:116:GLU:O    | 1:A:117:ALA:C    | 2.59                     | 0.45              |
| 1:C:61:ASN:ND2   | 1:C:94:MET:CE    | 2.72                     | 0.45              |
| 1:D:137:ARG:C    | 1:D:138:PRO:CA   | 2.88                     | 0.45              |
| 1:D:173:GLU:O    | 1:D:173:GLU:HG3  | 2.15                     | 0.45              |
| 1:D:191:VAL:O    | 1:D:191:VAL:HG13 | 2.16                     | 0.45              |
| 1:C:88:PHE:O     | 1:C:92:GLN:CG    | 2.64                     | 0.45              |
| 1:A:49:PHE:CZ    | 1:A:53:ILE:HD11  | 2.52                     | 0.45              |
| 1:A:140:ALA:C    | 1:A:142:VAL:H    | 2.24                     | 0.45              |
| 1:A:201:THR:HG23 | 1:A:217:PRO:HD3  | 1.95                     | 0.45              |
| 1:A:114:THR:CG2  | 1:B:91:VAL:HG21  | 2.47                     | 0.45              |
| 1:B:169:GLU:HB2  | 1:B:247:HIS:HE1  | 1.82                     | 0.45              |
| 1:A:169:GLU:HB2  | 1:A:247:HIS:HE1  | 1.82                     | 0.45              |
| 1:B:69:LEU:O     | 1:B:72:GLY:N     | 2.50                     | 0.45              |
| 1:C:23:ILE:CG1   | 1:D:283:ARG:HG2  | 2.47                     | 0.45              |
| 1:C:140:ALA:C    | 1:C:142:VAL:H    | 2.25                     | 0.45              |
| 1:C:219:ASP:OD1  | 1:C:219:ASP:C    | 2.60                     | 0.45              |
| 1:D:49:PHE:CZ    | 1:D:53:ILE:HD11  | 2.52                     | 0.45              |
| 1:A:69:LEU:O     | 1:A:72:GLY:N     | 2.50                     | 0.45              |
| 1:A:97:ILE:HG22  | 1:D:98:GLY:HA3   | 1.98                     | 0.45              |
| 1:A:110:ASN:HB3  | 1:B:88:PHE:CD2   | 2.52                     | 0.45              |
| 1:A:207:ILE:HG13 | 1:D:242:LEU:HD22 | 1.98                     | 0.45              |
| 1:C:23:ILE:HG23  | 1:D:283:ARG:C    | 2.40                     | 0.45              |
| 1:C:49:PHE:CZ    | 1:C:53:ILE:HD11  | 2.52                     | 0.45              |
| 1:D:169:GLU:HB2  | 1:D:247:HIS:HE1  | 1.82                     | 0.45              |
| 1:A:222:SER:OG   | 1:A:224:ILE:HG12 | 2.17                     | 0.45              |
| 1:B:116:GLU:O    | 1:B:117:ALA:C    | 2.60                     | 0.45              |
| 1:B:191:VAL:HG13 | 1:B:191:VAL:O    | 2.17                     | 0.44              |
| 1:D:116:GLU:O    | 1:D:117:ALA:C    | 2.58                     | 0.44              |
| 1:D:158:THR:HG23 | 1:D:216:HIS:C    | 2.42                     | 0.44              |
| 1:C:255:HIS:ND1  | 1:D:172:ILE:CD1  | 2.65                     | 0.44              |
| 1:C:274:VAL:CG1  | 1:C:289:LYS:HB2  | 2.35                     | 0.44              |
| 1:A:88:PHE:O     | 1:A:92:GLN:CG    | 2.63                     | 0.44              |
| 1:B:158:THR:HG23 | 1:B:216:HIS:C    | 2.43                     | 0.44              |
| 1:C:88:PHE:O     | 1:C:91:VAL:HG22  | 2.16                     | 0.44              |
| 1:C:158:THR:HG23 | 1:C:216:HIS:C    | 2.43                     | 0.44              |
| 1:B:255:HIS:CE1  | 1:C:172:ILE:HD13 | 2.53                     | 0.44              |
| 1:A:158:THR:HG23 | 1:A:216:HIS:C    | 2.43                     | 0.44              |
| 1:A:193:ARG:NH1  | 1:A:236:HIS:O    | 2.50                     | 0.44              |
| 1:A:240:LEU:HD21 | 1:B:207:ILE:HD12 | 1.99                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:138:PRO:HB2  | 1:C:254:VAL:HG12 | 1.99                     | 0.44              |
| 1:C:272:VAL:HG13 | 1:C:273:ASP:H    | 1.83                     | 0.44              |
| 1:D:201:THR:HG22 | 1:D:217:PRO:CD   | 2.48                     | 0.44              |
| 1:A:183:SER:HA   | 1:A:192:PHE:O    | 2.18                     | 0.44              |
| 1:B:88:PHE:O     | 1:B:91:VAL:HG22  | 2.18                     | 0.44              |
| 1:B:219:ASP:OD1  | 1:B:219:ASP:C    | 2.61                     | 0.44              |
| 1:C:93:THR:CG2   | 1:C:116:GLU:OE1  | 2.66                     | 0.44              |
| 1:D:198:LEU:HD22 | 1:D:223:PRO:HD2  | 2.00                     | 0.44              |
| 1:B:49:PHE:CZ    | 1:B:53:ILE:HD11  | 2.52                     | 0.44              |
| 1:B:166:LEU:HD23 | 1:B:166:LEU:HA   | 1.82                     | 0.44              |
| 1:C:222:SER:OG   | 1:C:224:ILE:HG12 | 2.18                     | 0.44              |
| 1:D:93:THR:CG2   | 1:D:116:GLU:OE1  | 2.66                     | 0.44              |
| 1:D:219:ASP:OD1  | 1:D:219:ASP:C    | 2.61                     | 0.44              |
| 1:B:76:GLU:HG3   | 1:B:77:ASN:ND2   | 2.33                     | 0.43              |
| 1:C:244:THR:HG22 | 1:C:255:HIS:CB   | 2.48                     | 0.43              |
| 1:D:138:PRO:HB2  | 1:D:254:VAL:HG12 | 2.00                     | 0.43              |
| 1:A:219:ASP:OD1  | 1:A:219:ASP:C    | 2.61                     | 0.43              |
| 1:C:195:PHE:CD2  | 1:C:195:PHE:N    | 2.86                     | 0.43              |
| 1:A:138:PRO:HB2  | 1:A:254:VAL:HG12 | 2.01                     | 0.43              |
| 1:A:175:ASP:OD1  | 1:A:175:ASP:C    | 2.60                     | 0.43              |
| 1:B:132:TYR:CE1  | 1:B:136:THR:HG21 | 2.54                     | 0.43              |
| 1:B:222:SER:OG   | 1:B:224:ILE:HG12 | 2.17                     | 0.43              |
| 1:C:94:MET:HE2   | 1:C:94:MET:HB3   | 1.85                     | 0.43              |
| 1:A:36:ASP:CG    | 1:A:39:HIS:HB3   | 2.44                     | 0.43              |
| 1:B:242:LEU:HD12 | 1:B:243:PHE:N    | 2.32                     | 0.43              |
| 1:C:76:GLU:HG3   | 1:C:77:ASN:ND2   | 2.33                     | 0.43              |
| 1:C:242:LEU:CD2  | 1:D:206:PRO:HB3  | 2.35                     | 0.43              |
| 1:D:76:GLU:HG3   | 1:D:77:ASN:ND2   | 2.33                     | 0.43              |
| 1:A:88:PHE:O     | 1:A:91:VAL:HG22  | 2.19                     | 0.43              |
| 1:B:175:ASP:C    | 1:B:175:ASP:OD1  | 2.61                     | 0.43              |
| 1:A:76:GLU:HG3   | 1:A:77:ASN:ND2   | 2.33                     | 0.43              |
| 1:A:191:VAL:HG13 | 1:A:191:VAL:O    | 2.18                     | 0.43              |
| 1:B:198:LEU:HB3  | 1:B:216:HIS:ND1  | 2.34                     | 0.43              |
| 1:A:175:ASP:OD2  | 1:A:204:ARG:NH1  | 2.52                     | 0.43              |
| 1:B:138:PRO:HB2  | 1:B:254:VAL:HG12 | 1.99                     | 0.43              |
| 1:B:244:THR:HG22 | 1:B:255:HIS:CB   | 2.49                     | 0.43              |
| 1:A:49:PHE:CE2   | 1:A:131:ILE:HD13 | 2.54                     | 0.43              |
| 1:D:49:PHE:CE2   | 1:D:131:ILE:HD13 | 2.54                     | 0.43              |
| 1:A:93:THR:CG2   | 1:A:116:GLU:OE1  | 2.66                     | 0.43              |
| 1:B:185:ILE:HG22 | 1:B:186:SER:O    | 2.19                     | 0.43              |
| 1:D:88:PHE:O     | 1:D:91:VAL:HG22  | 2.18                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:184:GLU:OE1  | 1:A:194:ARG:HD2  | 2.19                     | 0.42              |
| 1:A:240:LEU:CD2  | 1:B:207:ILE:HD12 | 2.49                     | 0.42              |
| 1:C:184:GLU:O    | 1:C:191:VAL:HA   | 2.19                     | 0.42              |
| 1:A:181:VAL:HG12 | 1:A:193:ARG:NH2  | 2.34                     | 0.42              |
| 1:A:185:ILE:HG22 | 1:A:186:SER:O    | 2.19                     | 0.42              |
| 1:B:257:ARG:HH21 | 1:C:248:GLU:CD   | 2.27                     | 0.42              |
| 1:C:280:ASP:CB   | 1:C:282:ARG:HG2  | 2.45                     | 0.42              |
| 1:D:244:THR:HG22 | 1:D:255:HIS:CB   | 2.49                     | 0.42              |
| 1:A:39:HIS:NE2   | 1:B:169:GLU:CD   | 2.77                     | 0.42              |
| 1:B:161:MET:HE2  | 1:B:161:MET:HB2  | 1.87                     | 0.42              |
| 1:C:204:ARG:HG2  | 1:C:204:ARG:NH1  | 2.32                     | 0.42              |
| 1:A:129:SER:HB3  | 1:B:132:TYR:HD1  | 1.84                     | 0.42              |
| 1:D:109:ALA:O    | 1:D:113:VAL:HG23 | 2.20                     | 0.42              |
| 1:D:242:LEU:HD12 | 1:D:243:PHE:N    | 2.34                     | 0.42              |
| 1:B:49:PHE:CE2   | 1:B:131:ILE:HD13 | 2.54                     | 0.42              |
| 1:B:114:THR:HG22 | 1:C:91:VAL:HG21  | 2.01                     | 0.42              |
| 1:B:181:VAL:HG12 | 1:B:193:ARG:CZ   | 2.50                     | 0.42              |
| 1:C:276:THR:CG2  | 1:C:277:THR:N    | 2.83                     | 0.42              |
| 1:D:278:LEU:CD1  | 1:D:282:ARG:HG3  | 2.33                     | 0.42              |
| 1:B:204:ARG:HG2  | 1:B:204:ARG:NH1  | 2.31                     | 0.42              |
| 1:C:204:ARG:HH11 | 1:C:204:ARG:CG   | 2.32                     | 0.42              |
| 1:C:255:HIS:CE1  | 1:D:172:ILE:CD1  | 2.99                     | 0.42              |
| 1:B:93:THR:CG2   | 1:B:116:GLU:OE1  | 2.68                     | 0.41              |
| 1:B:175:ASP:OD2  | 1:B:204:ARG:NH1  | 2.52                     | 0.41              |
| 1:B:195:PHE:N    | 1:B:195:PHE:CD2  | 2.88                     | 0.41              |
| 1:B:274:VAL:HA   | 1:B:289:LYS:HD2  | 2.03                     | 0.41              |
| 1:C:242:LEU:HD12 | 1:C:243:PHE:N    | 2.34                     | 0.41              |
| 1:D:44:VAL:CG1   | 1:D:45:SER:N     | 2.83                     | 0.41              |
| 1:D:116:GLU:O    | 1:D:119:CYS:HB2  | 2.21                     | 0.41              |
| 1:A:116:GLU:O    | 1:A:119:CYS:HB2  | 2.21                     | 0.41              |
| 1:C:44:VAL:HG11  | 1:C:48:VAL:HG12  | 2.02                     | 0.41              |
| 1:B:201:THR:HG23 | 1:B:217:PRO:HD3  | 2.02                     | 0.41              |
| 1:C:109:ALA:O    | 1:C:113:VAL:HG23 | 2.20                     | 0.41              |
| 1:C:116:GLU:O    | 1:C:119:CYS:HB2  | 2.20                     | 0.41              |
| 1:C:244:THR:HG22 | 1:C:255:HIS:HB3  | 2.02                     | 0.41              |
| 1:C:286:ASP:OD2  | 1:C:289:LYS:HE2  | 2.20                     | 0.41              |
| 1:D:91:VAL:CG2   | 1:D:92:GLN:N     | 2.84                     | 0.41              |
| 1:A:94:MET:HE2   | 1:A:94:MET:HB3   | 1.87                     | 0.41              |
| 1:B:168:ILE:CD1  | 1:B:168:ILE:N    | 2.72                     | 0.41              |
| 1:C:23:ILE:HD12  | 1:D:283:ARG:HB3  | 2.00                     | 0.41              |
| 1:C:185:ILE:HG22 | 1:C:186:SER:O    | 2.20                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:278:LEU:HG   | 1:B:282:ARG:O    | 2.21                     | 0.41              |
| 1:C:166:LEU:HD23 | 1:C:166:LEU:HA   | 1.81                     | 0.41              |
| 1:D:158:THR:CG2  | 1:D:215:MET:HB3  | 2.46                     | 0.41              |
| 1:A:44:VAL:CG1   | 1:A:45:SER:N     | 2.83                     | 0.41              |
| 1:A:129:SER:HB3  | 1:B:132:TYR:CD1  | 2.55                     | 0.41              |
| 1:C:132:TYR:CE1  | 1:C:136:THR:HG21 | 2.56                     | 0.41              |
| 1:B:109:ALA:O    | 1:B:113:VAL:HG23 | 2.21                     | 0.41              |
| 1:B:153:PHE:CE2  | 1:B:154:GLU:HB2  | 2.56                     | 0.41              |
| 1:C:175:ASP:OD1  | 1:C:175:ASP:C    | 2.64                     | 0.41              |
| 1:C:198:LEU:HD22 | 1:C:223:PRO:HD2  | 2.01                     | 0.41              |
| 1:D:185:ILE:HG22 | 1:D:186:SER:O    | 2.21                     | 0.41              |
| 1:A:91:VAL:CG2   | 1:A:92:GLN:N     | 2.84                     | 0.41              |
| 1:A:109:ALA:O    | 1:A:113:VAL:HG23 | 2.21                     | 0.41              |
| 1:B:44:VAL:HG12  | 1:B:45:SER:O     | 2.21                     | 0.41              |
| 1:B:198:LEU:HD22 | 1:B:223:PRO:HD2  | 2.02                     | 0.41              |
| 1:C:49:PHE:CE2   | 1:C:131:ILE:HD13 | 2.55                     | 0.41              |
| 1:C:91:VAL:CG2   | 1:C:92:GLN:N     | 2.83                     | 0.41              |
| 1:C:103:ILE:HG23 | 1:C:104:PRO:HD2  | 2.03                     | 0.41              |
| 1:C:195:PHE:N    | 1:C:195:PHE:HD2  | 2.19                     | 0.41              |
| 1:D:46:TRP:O     | 1:D:47:PRO:C     | 2.64                     | 0.41              |
| 1:D:141:GLY:O    | 1:D:166:LEU:CB   | 2.67                     | 0.41              |
| 1:D:198:LEU:HB3  | 1:D:216:HIS:ND1  | 2.36                     | 0.41              |
| 1:D:204:ARG:HG2  | 1:D:204:ARG:NH1  | 2.32                     | 0.41              |
| 1:A:44:VAL:HG12  | 1:A:45:SER:O     | 2.21                     | 0.41              |
| 1:C:46:TRP:O     | 1:C:47:PRO:C     | 2.64                     | 0.41              |
| 1:D:137:ARG:HA   | 1:D:138:PRO:HD3  | 2.03                     | 0.41              |
| 1:B:46:TRP:O     | 1:B:47:PRO:C     | 2.64                     | 0.40              |
| 1:B:158:THR:CG2  | 1:B:215:MET:HB3  | 2.47                     | 0.40              |
| 1:B:272:VAL:HG13 | 1:B:273:ASP:H    | 1.86                     | 0.40              |
| 1:D:283:ARG:HH11 | 1:D:283:ARG:CG   | 2.18                     | 0.40              |
| 1:B:94:MET:HE2   | 1:B:94:MET:HB3   | 1.85                     | 0.40              |
| 1:B:280:ASP:CB   | 1:B:282:ARG:HG2  | 2.48                     | 0.40              |
| 1:C:242:LEU:HD23 | 1:D:206:PRO:CB   | 2.34                     | 0.40              |
| 1:D:132:TYR:CE1  | 1:D:136:THR:HG21 | 2.56                     | 0.40              |
| 1:A:153:PHE:CE2  | 1:A:154:GLU:HB2  | 2.56                     | 0.40              |
| 1:A:276:THR:CG2  | 1:A:277:THR:N    | 2.84                     | 0.40              |
| 1:B:44:VAL:CG1   | 1:B:45:SER:N     | 2.85                     | 0.40              |
| 1:A:130:LEU:O    | 1:A:131:ILE:C    | 2.64                     | 0.40              |
| 1:A:158:THR:CG2  | 1:A:215:MET:HB3  | 2.47                     | 0.40              |
| 1:A:244:THR:HG22 | 1:A:255:HIS:CB   | 2.51                     | 0.40              |
| 1:B:91:VAL:CG2   | 1:B:92:GLN:N     | 2.84                     | 0.40              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:B:130:LEU:O    | 1:B:131:ILE:C   | 2.65                     | 0.40              |
| 1:D:36:ASP:CG    | 1:D:39:HIS:HB3  | 2.46                     | 0.40              |
| 1:D:244:THR:HG22 | 1:D:255:HIS:HB3 | 2.04                     | 0.40              |
| 1:B:36:ASP:CG    | 1:B:39:HIS:HB3  | 2.47                     | 0.40              |
| 1:B:141:GLY:O    | 1:B:166:LEU:CB  | 2.69                     | 0.40              |
| 1:C:36:ASP:CG    | 1:C:39:HIS:HB3  | 2.47                     | 0.40              |

All (2) 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:D:289:LYS:CE | 1:D:289:LYS:CE[4_555] | 2.01                     | 0.19              |
| 1:D:289:LYS:CE | 1:D:289:LYS:NZ[4_555] | 2.05                     | 0.15              |

## 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     | 265/301 (88%)   | 249 (94%)  | 14 (5%) | 2 (1%)   | 16          | 46 |
| 1   | B     | 273/301 (91%)   | 257 (94%)  | 15 (6%) | 1 (0%)   | 30          | 59 |
| 1   | C     | 273/301 (91%)   | 259 (95%)  | 13 (5%) | 1 (0%)   | 30          | 59 |
| 1   | D     | 273/301 (91%)   | 256 (94%)  | 16 (6%) | 1 (0%)   | 30          | 59 |
| All | All   | 1084/1204 (90%) | 1021 (94%) | 58 (5%) | 5 (0%)   | 24          | 55 |

All (5) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 23  | ILE  |
| 1   | A     | 59  | VAL  |
| 1   | B     | 59  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 59  | VAL  |
| 1   | C     | 59  | 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.

| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 1   | A     | 222/256 (87%)  | 201 (90%) | 21 (10%) | 8           | 30 |
| 1   | B     | 231/256 (90%)  | 212 (92%) | 19 (8%)  | 10          | 34 |
| 1   | C     | 231/256 (90%)  | 211 (91%) | 20 (9%)  | 9           | 32 |
| 1   | D     | 231/256 (90%)  | 211 (91%) | 20 (9%)  | 9           | 32 |
| All | All   | 915/1024 (89%) | 835 (91%) | 80 (9%)  | 9           | 32 |

All (80) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 23  | ILE  |
| 1   | A     | 74  | VAL  |
| 1   | A     | 82  | SER  |
| 1   | A     | 91  | VAL  |
| 1   | A     | 93  | THR  |
| 1   | A     | 114 | THR  |
| 1   | A     | 129 | SER  |
| 1   | A     | 134 | ARG  |
| 1   | A     | 149 | VAL  |
| 1   | A     | 154 | GLU  |
| 1   | A     | 160 | MET  |
| 1   | A     | 161 | MET  |
| 1   | A     | 168 | ILE  |
| 1   | A     | 178 | LEU  |
| 1   | A     | 204 | ARG  |
| 1   | A     | 214 | VAL  |
| 1   | A     | 220 | HIS  |
| 1   | A     | 235 | SER  |
| 1   | A     | 257 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 262 | CYS  |
| 1   | A     | 264 | GLU  |
| 1   | B     | 14  | ILE  |
| 1   | B     | 74  | VAL  |
| 1   | B     | 82  | SER  |
| 1   | B     | 91  | VAL  |
| 1   | B     | 93  | THR  |
| 1   | B     | 114 | THR  |
| 1   | B     | 129 | SER  |
| 1   | B     | 149 | VAL  |
| 1   | B     | 154 | GLU  |
| 1   | B     | 160 | MET  |
| 1   | B     | 161 | MET  |
| 1   | B     | 168 | ILE  |
| 1   | B     | 178 | LEU  |
| 1   | B     | 204 | ARG  |
| 1   | B     | 214 | VAL  |
| 1   | B     | 220 | HIS  |
| 1   | B     | 235 | SER  |
| 1   | B     | 262 | CYS  |
| 1   | B     | 264 | GLU  |
| 1   | C     | 14  | ILE  |
| 1   | C     | 74  | VAL  |
| 1   | C     | 82  | SER  |
| 1   | C     | 91  | VAL  |
| 1   | C     | 93  | THR  |
| 1   | C     | 114 | THR  |
| 1   | C     | 129 | SER  |
| 1   | C     | 134 | ARG  |
| 1   | C     | 149 | VAL  |
| 1   | C     | 154 | GLU  |
| 1   | C     | 160 | MET  |
| 1   | C     | 161 | MET  |
| 1   | C     | 168 | ILE  |
| 1   | C     | 178 | LEU  |
| 1   | C     | 204 | ARG  |
| 1   | C     | 214 | VAL  |
| 1   | C     | 220 | HIS  |
| 1   | C     | 235 | SER  |
| 1   | C     | 262 | CYS  |
| 1   | C     | 264 | GLU  |
| 1   | D     | 14  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 74  | VAL  |
| 1   | D     | 82  | SER  |
| 1   | D     | 91  | VAL  |
| 1   | D     | 93  | THR  |
| 1   | D     | 114 | THR  |
| 1   | D     | 129 | SER  |
| 1   | D     | 134 | ARG  |
| 1   | D     | 149 | VAL  |
| 1   | D     | 154 | GLU  |
| 1   | D     | 160 | MET  |
| 1   | D     | 161 | MET  |
| 1   | D     | 168 | ILE  |
| 1   | D     | 178 | LEU  |
| 1   | D     | 214 | VAL  |
| 1   | D     | 220 | HIS  |
| 1   | D     | 235 | SER  |
| 1   | D     | 262 | CYS  |
| 1   | D     | 264 | GLU  |
| 1   | D     | 283 | ARG  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 61  | ASN  |
| 1   | A     | 77  | ASN  |
| 1   | A     | 170 | GLN  |
| 1   | A     | 258 | HIS  |
| 1   | A     | 270 | HIS  |
| 1   | B     | 61  | ASN  |
| 1   | B     | 77  | ASN  |
| 1   | B     | 196 | HIS  |
| 1   | B     | 258 | HIS  |
| 1   | B     | 270 | HIS  |
| 1   | C     | 61  | ASN  |
| 1   | C     | 77  | ASN  |
| 1   | C     | 258 | HIS  |
| 1   | C     | 270 | HIS  |
| 1   | D     | 61  | ASN  |
| 1   | D     | 77  | ASN  |
| 1   | D     | 258 | HIS  |
| 1   | D     | 270 | HIS  |

### 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](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

There are no such residues in this entry.

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

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 1   | D     | 1                |
| 1   | C     | 1                |
| 1   | B     | 1                |
| 1   | A     | 1                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | D     | 137:ARG   | C      | 138:PRO   | N      | 2.10         |
| 1     | C     | 137:ARG   | C      | 138:PRO   | N      | 2.07         |
| 1     | B     | 137:ARG   | C      | 138:PRO   | N      | 2.03         |
| 1     | A     | 137:ARG   | C      | 138:PRO   | N      | 2.01         |

## 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     | 271/301 (90%)   | 0.53   | 15 (5%) 30 19 | 75, 130, 212, 258     | 0     |
| 1   | B     | 279/301 (92%)   | 0.64   | 26 (9%) 14 12 | 73, 128, 185, 237     | 0     |
| 1   | C     | 279/301 (92%)   | 0.57   | 23 (8%) 17 13 | 53, 106, 205, 302     | 0     |
| 1   | D     | 279/301 (92%)   | 0.56   | 17 (6%) 27 17 | 68, 108, 183, 224     | 0     |
| All | All   | 1108/1204 (92%) | 0.58   | 81 (7%) 21 15 | 53, 121, 199, 302     | 0     |

All (81) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 155 | GLY  | 5.5  |
| 1   | C     | 73  | ASP  | 5.2  |
| 1   | C     | 292 | GLU  | 5.2  |
| 1   | C     | 236 | HIS  | 4.7  |
| 1   | C     | 27  | GLY  | 4.6  |
| 1   | D     | 292 | GLU  | 4.2  |
| 1   | D     | 295 | GLN  | 4.2  |
| 1   | D     | 270 | HIS  | 4.1  |
| 1   | B     | 292 | GLU  | 3.9  |
| 1   | B     | 206 | PRO  | 3.9  |
| 1   | B     | 197 | ASP  | 3.9  |
| 1   | C     | 35  | ASP  | 3.7  |
| 1   | A     | 177 | HIS  | 3.6  |
| 1   | B     | 252 | GLN  | 3.5  |
| 1   | A     | 197 | ASP  | 3.5  |
| 1   | B     | 295 | GLN  | 3.5  |
| 1   | D     | 187 | GLN  | 3.4  |
| 1   | B     | 202 | ARG  | 3.4  |
| 1   | C     | 193 | ARG  | 3.4  |
| 1   | D     | 282 | ARG  | 3.4  |
| 1   | C     | 206 | PRO  | 3.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 255 | HIS  | 3.3  |
| 1   | B     | 73  | ASP  | 3.3  |
| 1   | A     | 252 | GLN  | 3.3  |
| 1   | A     | 220 | HIS  | 3.2  |
| 1   | A     | 175 | ASP  | 3.2  |
| 1   | D     | 98  | GLY  | 3.1  |
| 1   | D     | 289 | LYS  | 3.1  |
| 1   | D     | 154 | GLU  | 3.1  |
| 1   | D     | 141 | GLY  | 3.1  |
| 1   | C     | 12  | PRO  | 3.0  |
| 1   | D     | 137 | ARG  | 3.0  |
| 1   | B     | 173 | GLU  | 3.0  |
| 1   | C     | 202 | ARG  | 3.0  |
| 1   | A     | 22  | ASN  | 3.0  |
| 1   | B     | 155 | GLY  | 3.0  |
| 1   | D     | 12  | PRO  | 2.9  |
| 1   | B     | 284 | ALA  | 2.9  |
| 1   | D     | 147 | ARG  | 2.8  |
| 1   | A     | 292 | GLU  | 2.8  |
| 1   | C     | 177 | HIS  | 2.8  |
| 1   | D     | 190 | MET  | 2.8  |
| 1   | C     | 220 | HIS  | 2.7  |
| 1   | B     | 136 | THR  | 2.7  |
| 1   | A     | 295 | GLN  | 2.7  |
| 1   | B     | 249 | ALA  | 2.7  |
| 1   | C     | 295 | GLN  | 2.7  |
| 1   | B     | 203 | SER  | 2.6  |
| 1   | B     | 220 | HIS  | 2.6  |
| 1   | B     | 99  | TYR  | 2.6  |
| 1   | B     | 154 | GLU  | 2.6  |
| 1   | C     | 23  | ILE  | 2.6  |
| 1   | C     | 92  | GLN  | 2.5  |
| 1   | A     | 283 | ARG  | 2.5  |
| 1   | C     | 197 | ASP  | 2.4  |
| 1   | B     | 281 | GLY  | 2.4  |
| 1   | B     | 250 | PHE  | 2.4  |
| 1   | B     | 247 | HIS  | 2.4  |
| 1   | C     | 278 | LEU  | 2.3  |
| 1   | C     | 190 | MET  | 2.2  |
| 1   | A     | 137 | ARG  | 2.2  |
| 1   | B     | 141 | GLY  | 2.2  |
| 1   | C     | 37  | HIS  | 2.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 169 | GLU  | 2.2  |
| 1   | D     | 273 | ASP  | 2.1  |
| 1   | C     | 94  | MET  | 2.1  |
| 1   | A     | 188 | GLU  | 2.1  |
| 1   | B     | 230 | GLU  | 2.1  |
| 1   | D     | 175 | ASP  | 2.1  |
| 1   | C     | 98  | GLY  | 2.1  |
| 1   | B     | 26  | LEU  | 2.1  |
| 1   | D     | 220 | HIS  | 2.1  |
| 1   | B     | 12  | PRO  | 2.0  |
| 1   | C     | 219 | ASP  | 2.0  |
| 1   | A     | 27  | GLY  | 2.0  |
| 1   | C     | 230 | GLU  | 2.0  |
| 1   | C     | 238 | GLU  | 2.0  |
| 1   | D     | 173 | GLU  | 2.0  |
| 1   | A     | 94  | MET  | 2.0  |
| 1   | B     | 98  | GLY  | 2.0  |
| 1   | B     | 248 | GLU  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 2   | K    | A     | 1298 | 1/1   | 0.78 | 0.08 | 114,114,114,114             | 0     |
| 2   | K    | A     | 1296 | 1/1   | 0.84 | 0.10 | 139,139,139,139             | 0     |
| 2   | K    | A     | 1297 | 1/1   | 0.85 | 0.07 | 120,120,120,120             | 0     |
| 2   | K    | C     | 1299 | 1/1   | 0.92 | 0.13 | 98,98,98,98                 | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.