



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:33 AM UTC

PDB ID : 1P1Z / pdb\_00001p1z  
Title : X-RAY CRYSTAL STRUCTURE OF THE LECTIN-LIKE NATURAL KILLER CELL RECEPTOR LY-49C BOUND TO ITS MHC CLASS I LIG- AND H-2Kb  
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Deposited on : 2003-04-14  
Resolution : 3.26 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

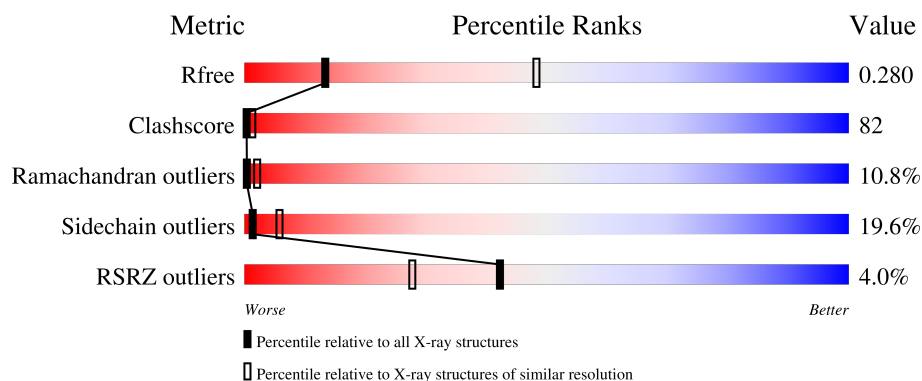
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.26 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                      | 1605 (3.30-3.22)                                      |
| Clashscore            | 190562                      | 1660 (3.30-3.22)                                      |
| Ramachandran outliers | 187476                      | 1630 (3.30-3.22)                                      |
| Sidechain outliers    | 187428                      | 1629 (3.30-3.22)                                      |
| RSRZ outliers         | 180081                      | 1605 (3.30-3.22)                                      |

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     | 274    |                  |
| 2   | B     | 99     |                  |
| 3   | P     | 8      |                  |
| 4   | D     | 120    |                  |

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3926 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 H-2 class I histocompatibility antigen, K-B alpha chain.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 255      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2072  | 1312 | 361 | 390 | 9 |         |         |       |

- Molecule 2 is a protein called Beta-2-microglobulin.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2   | B     | 97       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 803   | 515 | 136 | 146 | 6 |         |         |       |

- Molecule 3 is a protein called Ovalbumin peptide.

| Mol | Chain | Residues | Atoms |    |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|---------|-------|
| 3   | P     | 8        | Total | C  | N  | O  | 0       | 0       | 0     |
|     |       |          | 68    | 45 | 10 | 13 |         |         |       |

- Molecule 4 is a protein called LY49-C antigen.

| Mol | Chain | Residues | Atoms |     |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 4   | D     | 118      | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 983   | 637 | 161 | 174 | 11 |         |         |       |

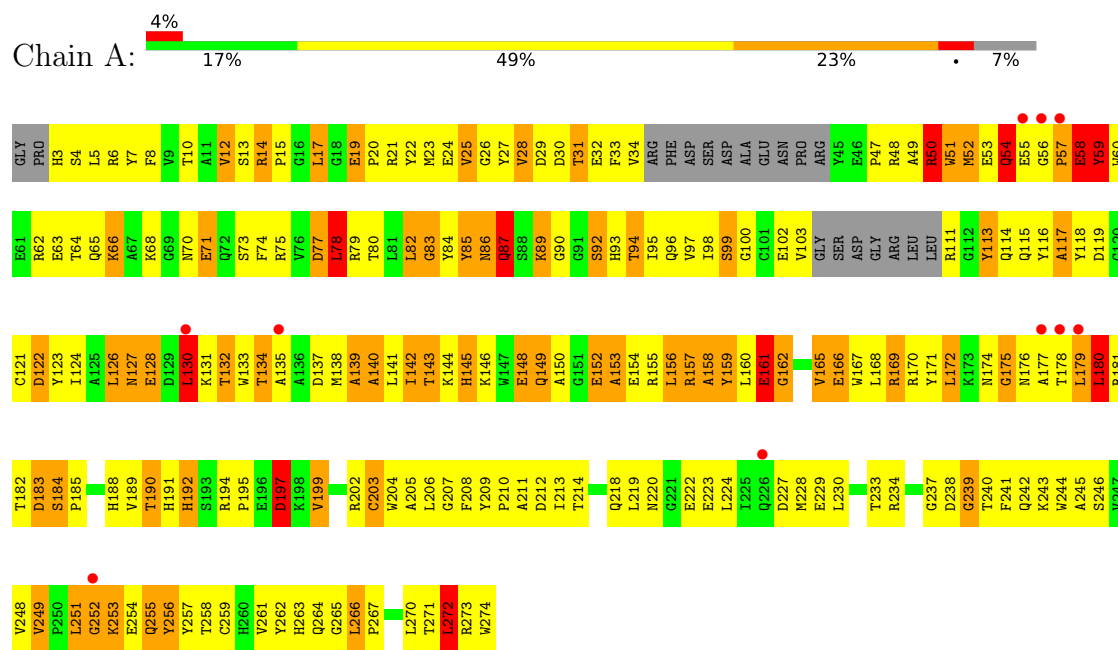
There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| D     | 144     | VAL      | LYS    | conflict | UNP Q64329 |

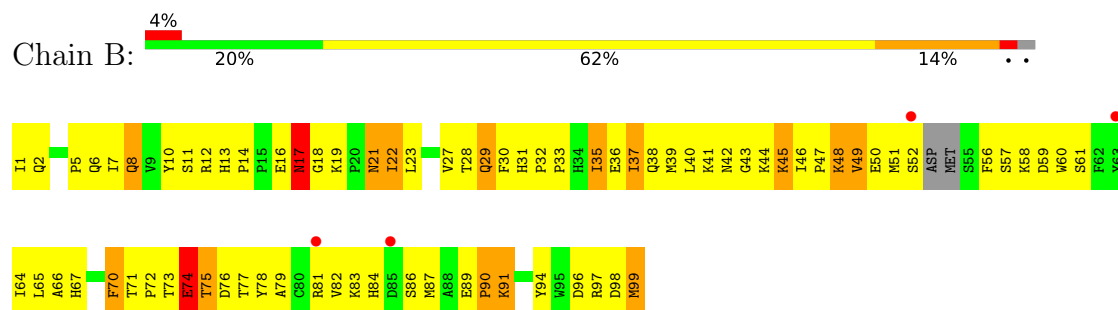
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: H-2 class I histocompatibility antigen, K-B alpha chain



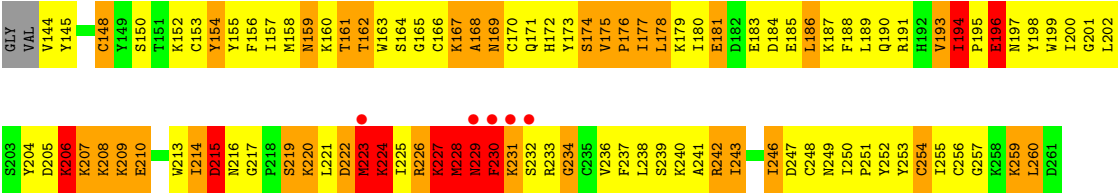
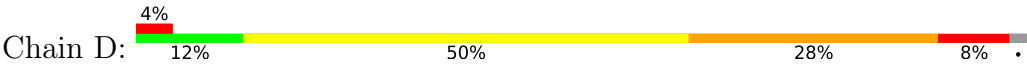
- Molecule 2: Beta-2-microglobulin



- Molecule 3: Ovalbumin peptide



- Molecule 4: LY49-C antigen



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 43 21 2                                                   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 149.05Å 149.05Å 64.38Å<br>90.00° 90.00° 90.00°              | Depositor        |
| Resolution (Å)                                                          | 50.00 – 3.26<br>50.00 – 3.26                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | (Not available) (50.00-3.26)<br>99.4 (50.00-3.26)           | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.10                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.90 (at 3.25Å)                                             | Xtriage          |
| Refinement program                                                      | CNS 1.0                                                     | Depositor        |
| R, $R_{free}$                                                           | 0.263 , 0.316<br>0.260 , 0.280                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 558 reflections (4.75%)                                     | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 79.2                                                        | Xtriage          |
| Anisotropy                                                              | 0.053                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.31 , 86.5                                                 | 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                                                   | 3926                                                        | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 52.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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

| Mol | Chain | Bond lengths |               | Bond angles |                |
|-----|-------|--------------|---------------|-------------|----------------|
|     |       | RMSZ         | $\# Z  > 5$   | RMSZ        | $\# Z  > 5$    |
| 1   | A     | 0.63         | 0/2126        | 1.32        | 31/2885 (1.1%) |
| 2   | B     | 0.68         | 0/828         | 1.35        | 10/1122 (0.9%) |
| 3   | P     | 0.70         | 0/68          | 1.00        | 0/88           |
| 4   | D     | 0.80         | 1/1011 (0.1%) | 1.55        | 26/1362 (1.9%) |
| All | All   | 0.69         | 1/4033 (0.0%) | 1.38        | 67/5457 (1.2%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 2                   |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 4   | D     | 223 | MET  | SD-CE | 5.07 | 1.92        | 1.79     |

All (67) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 4   | D     | 224 | LYS  | N-CA-C | -15.14 | 94.88       | 113.20   |
| 1   | A     | 82  | LEU  | N-CA-C | -11.97 | 98.31       | 111.36   |
| 2   | B     | 89  | GLU  | CA-C-N | 11.63  | 131.76      | 119.78   |
| 2   | B     | 89  | GLU  | C-N-CA | 11.63  | 131.76      | 119.78   |
| 1   | A     | 59  | TYR  | N-CA-C | -10.82 | 87.75       | 110.80   |
| 1   | A     | 28  | VAL  | N-CA-C | -10.04 | 92.07       | 107.73   |
| 4   | D     | 230 | PHE  | N-CA-C | -9.59  | 94.35       | 107.88   |
| 1   | A     | 62  | ARG  | N-CA-C | -9.19  | 101.27      | 111.28   |
| 1   | A     | 197 | ASP  | N-CA-C | 8.61   | 123.27      | 111.39   |
| 4   | D     | 220 | LYS  | N-CA-C | -8.10  | 103.54      | 113.50   |
| 1   | A     | 89  | LYS  | N-CA-C | -7.80  | 103.75      | 112.57   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | B     | 74  | GLU  | N-CA-C  | -7.74 | 101.78      | 112.30   |
| 1   | A     | 149 | GLN  | N-CA-C  | -7.59 | 104.12      | 113.15   |
| 1   | A     | 57  | PRO  | N-CA-C  | -7.42 | 97.19       | 112.47   |
| 4   | D     | 178 | LEU  | N-CA-C  | 7.34  | 120.05      | 110.43   |
| 4   | D     | 222 | ASP  | N-CA-C  | -7.34 | 98.69       | 109.11   |
| 2   | B     | 71  | THR  | CA-C-N  | 7.25  | 127.01      | 119.76   |
| 2   | B     | 71  | THR  | C-N-CA  | 7.25  | 127.01      | 119.76   |
| 1   | A     | 31  | THR  | N-CA-C  | 7.14  | 121.32      | 109.46   |
| 4   | D     | 234 | GLY  | N-CA-C  | 7.13  | 130.08      | 113.18   |
| 4   | D     | 164 | SER  | N-CA-C  | -6.73 | 103.59      | 112.34   |
| 1   | A     | 58  | GLU  | N-CA-C  | -6.71 | 96.51       | 110.80   |
| 1   | A     | 203 | CYS  | N-CA-C  | -6.68 | 100.60      | 110.48   |
| 4   | D     | 254 | CYS  | N-CA-C  | 6.68  | 120.40      | 109.72   |
| 1   | A     | 153 | ALA  | N-CA-C  | -6.65 | 103.96      | 111.07   |
| 4   | D     | 173 | TYR  | N-CA-C  | -6.64 | 103.50      | 112.26   |
| 4   | D     | 226 | ARG  | N-CA-C  | -6.47 | 97.01       | 110.80   |
| 1   | A     | 19  | GLU  | CA-C-N  | 6.40  | 126.74      | 119.83   |
| 1   | A     | 19  | GLU  | C-N-CA  | 6.40  | 126.74      | 119.83   |
| 4   | D     | 227 | LYS  | N-CA-C  | 6.39  | 124.42      | 110.80   |
| 1   | A     | 148 | GLU  | N-CA-C  | -6.37 | 105.63      | 113.41   |
| 1   | A     | 113 | TYR  | N-CA-C  | 6.37  | 120.66      | 109.96   |
| 1   | A     | 184 | SER  | CA-C-N  | 6.11  | 126.02      | 119.85   |
| 1   | A     | 184 | SER  | C-N-CA  | 6.11  | 126.02      | 119.85   |
| 4   | D     | 223 | MET  | N-CA-C  | -6.05 | 97.90       | 110.80   |
| 4   | D     | 219 | SER  | N-CA-C  | -6.04 | 100.42      | 109.96   |
| 1   | A     | 12  | VAL  | N-CA-C  | 5.99  | 121.80      | 109.34   |
| 4   | D     | 215 | ASP  | N-CA-C  | -5.85 | 105.91      | 113.16   |
| 2   | B     | 28  | THR  | N-CA-C  | 5.74  | 117.70      | 109.14   |
| 2   | B     | 37  | ILE  | CB-CA-C | -5.71 | 103.25      | 111.19   |
| 4   | D     | 206 | LYS  | CA-C-N  | -5.68 | 112.22      | 120.29   |
| 4   | D     | 206 | LYS  | C-N-CA  | -5.68 | 112.22      | 120.29   |
| 4   | D     | 162 | THR  | N-CA-C  | -5.62 | 103.50      | 110.41   |
| 2   | B     | 90  | PRO  | N-CA-C  | 5.62  | 120.14      | 111.21   |
| 4   | D     | 181 | GLU  | N-CA-C  | 5.57  | 117.43      | 111.36   |
| 1   | A     | 85  | TYR  | N-CA-C  | 5.46  | 119.63      | 112.92   |
| 4   | D     | 154 | TYR  | N-CA-C  | 5.45  | 118.59      | 110.14   |
| 1   | A     | 71  | GLU  | N-CA-C  | -5.45 | 102.38      | 111.37   |
| 1   | A     | 92  | SER  | N-CA-C  | -5.45 | 102.69      | 110.59   |
| 1   | A     | 143 | THR  | N-CA-C  | -5.40 | 99.29       | 110.80   |
| 1   | A     | 256 | TYR  | N-CA-C  | -5.39 | 99.33       | 110.80   |
| 1   | A     | 166 | GLU  | N-CA-C  | -5.37 | 105.12      | 110.97   |
| 4   | D     | 194 | ILE  | CA-C-N  | 5.36  | 126.54      | 119.84   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 4   | D     | 194 | ILE  | C-N-CA | 5.36  | 126.54      | 119.84   |
| 1   | A     | 25  | VAL  | CA-C-N | -5.34 | 118.02      | 121.65   |
| 1   | A     | 25  | VAL  | C-N-CA | -5.34 | 118.02      | 121.65   |
| 2   | B     | 45  | LYS  | CA-C-N | -5.27 | 118.19      | 123.04   |
| 2   | B     | 45  | LYS  | C-N-CA | -5.27 | 118.19      | 123.04   |
| 4   | D     | 229 | ASN  | N-CA-C | -5.27 | 99.58       | 110.80   |
| 4   | D     | 148 | CYS  | N-CA-C | 5.27  | 117.08      | 109.07   |
| 4   | D     | 175 | VAL  | CA-C-N | 5.27  | 126.42      | 119.84   |
| 4   | D     | 175 | VAL  | C-N-CA | 5.27  | 126.42      | 119.84   |
| 1   | A     | 117 | ALA  | N-CA-C | -5.22 | 101.36      | 109.24   |
| 4   | D     | 242 | ARG  | N-CA-C | 5.20  | 117.10      | 109.24   |
| 1   | A     | 127 | ASN  | N-CA-C | 5.14  | 117.16      | 110.53   |
| 1   | A     | 272 | LEU  | N-CA-C | 5.14  | 117.00      | 109.24   |
| 1   | A     | 161 | GLU  | N-CA-C | -5.02 | 105.72      | 111.14   |

There are no chirality outliers.

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | A     | 262 | TYR  | Sidechain |
| 1   | A     | 59  | TYR  | Sidechain |

## 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     | 2072  | 0        | 1968     | 346     | 0            |
| 2   | B     | 803   | 0        | 776      | 119     | 0            |
| 3   | P     | 68    | 0        | 74       | 27      | 0            |
| 4   | D     | 983   | 0        | 949      | 186     | 0            |
| All | All   | 3926  | 0        | 3767     | 632     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 82.

All (632) 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) |
|------------------|------------------|--------------------------|-------------------|
| 3:P:7:LYS:H      | 3:P:7:LYS:HD2    | 1.03                     | 1.16              |
| 1:A:29:ASP:HA    | 4:D:230:PHE:CZ   | 1.81                     | 1.13              |
| 4:D:157:ILE:HB   | 4:D:254:CYS:HB2  | 1.24                     | 1.12              |
| 2:B:38:GLN:HB2   | 2:B:81:ARG:HB3   | 1.29                     | 1.12              |
| 2:B:2:GLN:NE2    | 2:B:86:SER:HA    | 1.65                     | 1.10              |
| 2:B:29:GLN:HA    | 2:B:61:SER:HB2   | 1.33                     | 1.09              |
| 3:P:7:LYS:H      | 3:P:7:LYS:CD     | 1.63                     | 1.08              |
| 2:B:83:LYS:HG3   | 2:B:90:PRO:HG3   | 1.27                     | 1.08              |
| 4:D:224:LYS:O    | 4:D:227:LYS:HE3  | 1.53                     | 1.07              |
| 2:B:38:GLN:HE22  | 2:B:45:LYS:HG3   | 1.20                     | 1.06              |
| 4:D:227:LYS:HE2  | 4:D:227:LYS:HA   | 1.04                     | 1.04              |
| 4:D:177:ILE:HD11 | 4:D:214:ILE:HG13 | 1.39                     | 1.03              |
| 4:D:227:LYS:HA   | 4:D:227:LYS:CE   | 1.89                     | 1.01              |
| 1:A:128:GLU:HG3  | 4:D:223:MET:HE3  | 1.40                     | 1.01              |
| 4:D:169:ASN:HD22 | 4:D:169:ASN:N    | 1.54                     | 0.99              |
| 4:D:177:ILE:HD13 | 4:D:177:ILE:H    | 1.26                     | 0.98              |
| 2:B:73:THR:HG22  | 2:B:74:GLU:H     | 1.26                     | 0.97              |
| 1:A:172:LEU:H    | 1:A:172:LEU:HD22 | 1.30                     | 0.97              |
| 4:D:148:CYS:CB   | 4:D:153:CYS:HA   | 1.95                     | 0.97              |
| 4:D:227:LYS:HE2  | 4:D:227:LYS:CA   | 1.94                     | 0.97              |
| 2:B:2:GLN:HE21   | 2:B:86:SER:HA    | 1.14                     | 0.97              |
| 4:D:239:SER:HB2  | 4:D:242:ARG:HB2  | 1.46                     | 0.96              |
| 4:D:169:ASN:H    | 4:D:169:ASN:ND2  | 1.55                     | 0.95              |
| 4:D:148:CYS:HB3  | 4:D:153:CYS:HA   | 1.48                     | 0.95              |
| 4:D:223:MET:HA   | 4:D:225:ILE:HG22 | 1.45                     | 0.93              |
| 1:A:29:ASP:HA    | 4:D:230:PHE:HZ   | 1.23                     | 0.93              |
| 4:D:226:ARG:O    | 4:D:228:MET:N    | 2.01                     | 0.92              |
| 1:A:99:SER:OG    | 1:A:114:GLN:NE2  | 2.02                     | 0.92              |
| 1:A:27:TYR:HA    | 1:A:31:THR:O     | 1.68                     | 0.92              |
| 1:A:28:VAL:HG11  | 1:A:179:LEU:HD22 | 1.51                     | 0.91              |
| 3:P:7:LYS:HD2    | 3:P:7:LYS:N      | 1.84                     | 0.91              |
| 2:B:97:ARG:HG3   | 2:B:98:ASP:N     | 1.86                     | 0.89              |
| 4:D:246:ILE:HG12 | 4:D:247:ASP:H    | 1.39                     | 0.88              |
| 4:D:259:LYS:H    | 4:D:259:LYS:HD2  | 1.36                     | 0.88              |
| 1:A:179:LEU:O    | 1:A:180:LEU:HD12 | 1.77                     | 0.84              |
| 4:D:224:LYS:O    | 4:D:227:LYS:CE   | 2.24                     | 0.84              |
| 1:A:93:HIS:HD2   | 1:A:118:TYR:OH   | 1.59                     | 0.84              |
| 2:B:31:HIS:ND1   | 2:B:32:PRO:HA    | 1.93                     | 0.83              |
| 2:B:50:GLU:HB2   | 2:B:67:HIS:CD2   | 2.14                     | 0.83              |
| 1:A:229:GLU:HB3  | 1:A:246:SER:OG   | 1.78                     | 0.83              |
| 1:A:4:SER:OG     | 4:D:230:PHE:HE1  | 1.60                     | 0.83              |
| 1:A:116:TYR:HB2  | 1:A:124:ILE:HG22 | 1.59                     | 0.82              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:273:ARG:O    | 1:A:274:TRP:HB3  | 1.79                     | 0.82              |
| 1:A:87:GLN:HG2   | 1:A:93:HIS:NE2   | 1.95                     | 0.82              |
| 1:A:33:PHE:CD1   | 1:A:34:VAL:HG13  | 2.15                     | 0.82              |
| 2:B:11:SER:HB2   | 2:B:21:ASN:HD22  | 1.45                     | 0.82              |
| 2:B:83:LYS:CG    | 2:B:90:PRO:HG3   | 2.09                     | 0.82              |
| 1:A:28:VAL:CG1   | 1:A:179:LEU:HD22 | 2.10                     | 0.81              |
| 4:D:228:MET:O    | 4:D:229:ASN:HB2  | 1.77                     | 0.81              |
| 2:B:73:THR:HG22  | 2:B:74:GLU:N     | 1.92                     | 0.81              |
| 1:A:15:PRO:C     | 1:A:17:LEU:H     | 1.88                     | 0.81              |
| 1:A:128:GLU:HG3  | 4:D:223:MET:CE   | 2.11                     | 0.81              |
| 1:A:4:SER:OG     | 4:D:230:PHE:CE1  | 2.34                     | 0.81              |
| 1:A:5:LEU:HB2    | 1:A:168:LEU:HD13 | 1.63                     | 0.80              |
| 2:B:32:PRO:HB2   | 2:B:33:PRO:HD2   | 1.63                     | 0.80              |
| 2:B:73:THR:HG21  | 2:B:75:THR:HG23  | 1.62                     | 0.80              |
| 4:D:224:LYS:O    | 4:D:224:LYS:HG2  | 1.78                     | 0.80              |
| 4:D:223:MET:SD   | 4:D:225:ILE:HG21 | 2.22                     | 0.80              |
| 2:B:73:THR:O     | 2:B:97:ARG:NH2   | 2.14                     | 0.79              |
| 4:D:204:TYR:CD2  | 4:D:233:ARG:HD2  | 2.18                     | 0.79              |
| 1:A:30:ASP:OD1   | 4:D:231:LYS:HE2  | 1.80                     | 0.79              |
| 1:A:117:ALA:HB2  | 2:B:60:TRP:CE2   | 2.18                     | 0.79              |
| 1:A:4:SER:HG     | 4:D:230:PHE:HE1  | 0.79                     | 0.79              |
| 2:B:38:GLN:CB    | 2:B:81:ARG:HB3   | 2.10                     | 0.78              |
| 2:B:21:ASN:N     | 2:B:70:PHE:O     | 2.16                     | 0.78              |
| 4:D:223:MET:C    | 4:D:225:ILE:H    | 1.91                     | 0.78              |
| 1:A:58:GLU:CD    | 1:A:58:GLU:O     | 2.27                     | 0.78              |
| 1:A:80:THR:HG1   | 1:A:84:TYR:HE2   | 1.33                     | 0.77              |
| 4:D:178:LEU:HB2  | 4:D:255:ILE:HG22 | 1.65                     | 0.77              |
| 4:D:259:LYS:HD2  | 4:D:259:LYS:N    | 1.99                     | 0.77              |
| 1:A:51:TRP:HB2   | 1:A:174:ASN:O    | 1.85                     | 0.77              |
| 1:A:24:GLU:CD    | 3:P:2:ILE:HD13   | 2.10                     | 0.76              |
| 1:A:47:PRO:HG3   | 1:A:60:TRP:HZ2   | 1.49                     | 0.76              |
| 4:D:223:MET:SD   | 4:D:225:ILE:CG2  | 2.74                     | 0.76              |
| 1:A:185:PRO:HB3  | 1:A:208:PHE:HB3  | 1.68                     | 0.75              |
| 4:D:194:ILE:HG23 | 4:D:198:TYR:OH   | 1.85                     | 0.75              |
| 3:P:7:LYS:CD     | 3:P:7:LYS:N      | 2.40                     | 0.75              |
| 4:D:177:ILE:H    | 4:D:177:ILE:CD1  | 1.98                     | 0.75              |
| 1:A:237:GLY:HA3  | 2:B:12:ARG:CZ    | 2.17                     | 0.75              |
| 4:D:197:ASN:ND2  | 4:D:237:PHE:CE2  | 2.55                     | 0.75              |
| 4:D:214:ILE:HD13 | 4:D:214:ILE:O    | 1.86                     | 0.75              |
| 2:B:41:LYS:HG3   | 2:B:78:TYR:CE2   | 2.22                     | 0.74              |
| 1:A:229:GLU:HB3  | 1:A:246:SER:HG   | 1.49                     | 0.74              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:P:3:ILE:HD13   | 3:P:4:ASN:N      | 2.02                     | 0.74              |
| 4:D:202:LEU:O    | 4:D:236:VAL:HG23 | 1.88                     | 0.74              |
| 1:A:7:TYR:OH     | 3:P:1:SER:HB3    | 1.87                     | 0.74              |
| 4:D:169:ASN:HD22 | 4:D:169:ASN:H    | 0.81                     | 0.74              |
| 4:D:230:PHE:O    | 4:D:232:SER:N    | 2.19                     | 0.74              |
| 4:D:193:VAL:HG13 | 4:D:198:TYR:CE2  | 2.23                     | 0.74              |
| 1:A:79:ARG:HA    | 1:A:82:LEU:HD23  | 1.69                     | 0.74              |
| 4:D:177:ILE:HD13 | 4:D:177:ILE:N    | 2.00                     | 0.74              |
| 2:B:11:SER:HB2   | 2:B:21:ASN:ND2   | 2.03                     | 0.73              |
| 2:B:12:ARG:HD2   | 2:B:22:ILE:HD12  | 1.69                     | 0.73              |
| 4:D:229:ASN:HD21 | 4:D:233:ARG:NE   | 1.87                     | 0.72              |
| 1:A:21:ARG:NH2   | 1:A:23:MET:HE3   | 2.03                     | 0.72              |
| 2:B:12:ARG:HD2   | 2:B:22:ILE:CD1   | 2.19                     | 0.72              |
| 2:B:73:THR:HG22  | 2:B:75:THR:H     | 1.55                     | 0.72              |
| 2:B:83:LYS:HE3   | 2:B:90:PRO:CG    | 2.20                     | 0.72              |
| 1:A:272:LEU:HD12 | 1:A:272:LEU:N    | 2.04                     | 0.72              |
| 1:A:47:PRO:HG3   | 1:A:60:TRP:CZ2   | 2.24                     | 0.72              |
| 1:A:52:MET:HA    | 1:A:52:MET:CE    | 2.19                     | 0.72              |
| 1:A:66:LYS:HB2   | 1:A:66:LYS:NZ    | 2.05                     | 0.71              |
| 4:D:148:CYS:HB2  | 4:D:152:LYS:O    | 1.90                     | 0.71              |
| 1:A:122:ASP:OD2  | 4:D:242:ARG:HD2  | 1.88                     | 0.71              |
| 2:B:48:LYS:NZ    | 2:B:48:LYS:HA    | 2.03                     | 0.71              |
| 1:A:233:THR:HB   | 1:A:243:LYS:HZ3  | 1.55                     | 0.71              |
| 1:A:137:ASP:OD2  | 1:A:139:ALA:HB3  | 1.91                     | 0.71              |
| 1:A:175:GLY:C    | 1:A:177:ALA:H    | 1.98                     | 0.71              |
| 1:A:188:HIS:CD2  | 1:A:204:TRP:HB2  | 2.26                     | 0.71              |
| 2:B:5:PRO:HA     | 2:B:30:PHE:HB3   | 1.72                     | 0.71              |
| 2:B:48:LYS:HA    | 2:B:48:LYS:HZ3   | 1.54                     | 0.71              |
| 1:A:73:SER:OG    | 3:P:7:LYS:HE3    | 1.90                     | 0.71              |
| 2:B:38:GLN:NE2   | 2:B:45:LYS:HG3   | 2.01                     | 0.71              |
| 1:A:66:LYS:HB2   | 1:A:66:LYS:HZ2   | 1.56                     | 0.70              |
| 1:A:29:ASP:CA    | 4:D:230:PHE:HZ   | 2.01                     | 0.70              |
| 1:A:126:LEU:HD13 | 1:A:130:LEU:HB3  | 1.73                     | 0.70              |
| 1:A:159:TYR:CZ   | 3:P:3:ILE:HB     | 2.26                     | 0.70              |
| 1:A:33:PHE:HA    | 1:A:49:ALA:HB2   | 1.74                     | 0.70              |
| 1:A:168:LEU:O    | 1:A:172:LEU:HD22 | 1.92                     | 0.70              |
| 1:A:169:ARG:HA   | 1:A:172:LEU:HD23 | 1.73                     | 0.70              |
| 2:B:17:ASN:HA    | 2:B:72:PRO:HG2   | 1.72                     | 0.70              |
| 1:A:3:HIS:O      | 1:A:103:VAL:HG22 | 1.91                     | 0.70              |
| 1:A:82:LEU:HD12  | 1:A:87:GLN:HB3   | 1.73                     | 0.70              |
| 4:D:194:ILE:HD12 | 4:D:195:PRO:HD2  | 1.74                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:7:TYR:CE2    | 3:P:2:ILE:HA     | 2.27                     | 0.70              |
| 1:A:172:LEU:HD22 | 1:A:172:LEU:N    | 2.05                     | 0.69              |
| 1:A:162:GLY:O    | 1:A:165:VAL:HG23 | 1.92                     | 0.69              |
| 1:A:230:LEU:HD23 | 1:A:245:ALA:HB2  | 1.74                     | 0.69              |
| 4:D:239:SER:CB   | 4:D:242:ARG:HB2  | 2.19                     | 0.69              |
| 2:B:73:THR:CG2   | 2:B:75:THR:HG23  | 2.21                     | 0.69              |
| 4:D:177:ILE:CD1  | 4:D:214:ILE:HG13 | 2.21                     | 0.69              |
| 4:D:178:LEU:HG   | 4:D:179:LYS:N    | 2.05                     | 0.69              |
| 1:A:169:ARG:C    | 1:A:171:TYR:H    | 2.00                     | 0.69              |
| 4:D:144:VAL:HG22 | 4:D:158:MET:HG3  | 1.73                     | 0.69              |
| 4:D:208:LYS:HD3  | 4:D:210:GLU:CD   | 2.18                     | 0.69              |
| 1:A:29:ASP:HA    | 4:D:230:PHE:CE1  | 2.27                     | 0.69              |
| 1:A:21:ARG:HH21  | 1:A:23:MET:HE3   | 1.57                     | 0.69              |
| 2:B:39:MET:HG3   | 2:B:49:VAL:CG2   | 2.22                     | 0.69              |
| 4:D:166:CYS:HB3  | 4:D:177:ILE:HG22 | 1.75                     | 0.69              |
| 1:A:77:ASP:HA    | 1:A:80:THR:HG22  | 1.75                     | 0.69              |
| 4:D:178:LEU:CD1  | 4:D:257:GLY:HA3  | 2.23                     | 0.68              |
| 1:A:92:SER:O     | 1:A:93:HIS:ND1   | 2.26                     | 0.68              |
| 4:D:170:CYS:SG   | 4:D:177:ILE:HA   | 2.32                     | 0.68              |
| 1:A:128:GLU:CG   | 4:D:223:MET:HE3  | 2.21                     | 0.68              |
| 1:A:29:ASP:HB3   | 4:D:231:LYS:CD   | 2.24                     | 0.68              |
| 2:B:42:ASN:O     | 2:B:44:LYS:N     | 2.23                     | 0.68              |
| 4:D:225:ILE:C    | 4:D:227:LYS:N    | 2.50                     | 0.68              |
| 1:A:59:TYR:CE1   | 1:A:63:GLU:OE1   | 2.47                     | 0.68              |
| 2:B:96:ASP:O     | 2:B:99:MET:N     | 2.27                     | 0.68              |
| 1:A:29:ASP:HB3   | 4:D:231:LYS:HD3  | 1.77                     | 0.67              |
| 1:A:266:LEU:HD21 | 1:A:270:LEU:CD1  | 2.25                     | 0.67              |
| 1:A:29:ASP:HB3   | 4:D:231:LYS:CG   | 2.24                     | 0.67              |
| 1:A:167:TRP:O    | 1:A:171:TYR:HD2  | 1.78                     | 0.67              |
| 2:B:73:THR:CG2   | 2:B:74:GLU:H     | 2.05                     | 0.67              |
| 1:A:237:GLY:HA3  | 2:B:12:ARG:NH2   | 2.08                     | 0.67              |
| 2:B:19:LYS:O     | 2:B:72:PRO:HD2   | 1.94                     | 0.67              |
| 1:A:77:ASP:HA    | 1:A:80:THR:CG2   | 2.25                     | 0.66              |
| 1:A:111:ARG:NH1  | 1:A:111:ARG:HB2  | 2.11                     | 0.66              |
| 4:D:223:MET:CA   | 4:D:225:ILE:HG22 | 2.22                     | 0.66              |
| 2:B:97:ARG:HG3   | 2:B:98:ASP:H     | 1.58                     | 0.66              |
| 1:A:152:GLU:HG2  | 1:A:155:ARG:HD2  | 1.77                     | 0.66              |
| 4:D:204:TYR:OH   | 4:D:209:LYS:HG3  | 1.94                     | 0.66              |
| 1:A:12:VAL:HG12  | 1:A:12:VAL:O     | 1.96                     | 0.66              |
| 1:A:27:TYR:CA    | 1:A:31:THR:O     | 2.44                     | 0.66              |
| 4:D:207:LYS:C    | 4:D:209:LYS:H    | 2.03                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:12:VAL:HG22  | 1:A:94:THR:HB    | 1.78                     | 0.66              |
| 3:P:5:PHE:CD1    | 3:P:5:PHE:N      | 2.63                     | 0.66              |
| 1:A:204:TRP:HZ2  | 2:B:99:MET:O     | 1.79                     | 0.66              |
| 4:D:198:TYR:O    | 4:D:237:PHE:HB2  | 1.96                     | 0.65              |
| 2:B:39:MET:HG3   | 2:B:49:VAL:HG23  | 1.79                     | 0.65              |
| 4:D:178:LEU:HD13 | 4:D:257:GLY:HA3  | 1.78                     | 0.65              |
| 1:A:158:ALA:O    | 1:A:160:LEU:N    | 2.28                     | 0.65              |
| 1:A:168:LEU:O    | 1:A:172:LEU:CD2  | 2.44                     | 0.65              |
| 1:A:233:THR:HB   | 1:A:243:LYS:NZ   | 2.11                     | 0.65              |
| 4:D:204:TYR:CE2  | 4:D:233:ARG:HD2  | 2.32                     | 0.65              |
| 1:A:63:GLU:O     | 1:A:66:LYS:HB2   | 1.97                     | 0.64              |
| 4:D:157:ILE:CB   | 4:D:254:CYS:HB2  | 2.15                     | 0.64              |
| 1:A:154:GLU:C    | 1:A:156:LEU:N    | 2.51                     | 0.64              |
| 1:A:52:MET:HA    | 1:A:52:MET:HE2   | 1.78                     | 0.64              |
| 2:B:42:ASN:C     | 2:B:44:LYS:H     | 2.05                     | 0.64              |
| 4:D:166:CYS:CB   | 4:D:177:ILE:HG22 | 2.27                     | 0.64              |
| 4:D:187:LYS:O    | 4:D:191:ARG:HG3  | 1.98                     | 0.64              |
| 2:B:7:ILE:CG1    | 2:B:82:VAL:HG21  | 2.28                     | 0.64              |
| 4:D:144:VAL:HG22 | 4:D:158:MET:CG   | 2.27                     | 0.64              |
| 4:D:161:THR:O    | 4:D:251:PRO:HA   | 1.98                     | 0.64              |
| 1:A:185:PRO:CB   | 1:A:208:PHE:HB3  | 2.28                     | 0.64              |
| 2:B:38:GLN:HB2   | 2:B:81:ARG:CB    | 2.19                     | 0.64              |
| 1:A:85:TYR:C     | 1:A:87:GLN:H     | 2.05                     | 0.64              |
| 1:A:159:TYR:CE2  | 3:P:3:ILE:HB     | 2.33                     | 0.64              |
| 1:A:99:SER:HA    | 1:A:113:TYR:O    | 1.97                     | 0.63              |
| 1:A:213:ILE:HG12 | 1:A:214:THR:N    | 2.11                     | 0.63              |
| 1:A:178:THR:O    | 1:A:181:ARG:HG2  | 1.99                     | 0.63              |
| 1:A:19:GLU:HB3   | 1:A:20:PRO:CD    | 2.29                     | 0.63              |
| 1:A:111:ARG:CB   | 1:A:111:ARG:HH11 | 2.12                     | 0.63              |
| 1:A:29:ASP:HB3   | 4:D:231:LYS:HG2  | 1.81                     | 0.63              |
| 4:D:223:MET:C    | 4:D:225:ILE:N    | 2.50                     | 0.63              |
| 1:A:15:PRO:HG3   | 1:A:90:GLY:O     | 1.99                     | 0.63              |
| 2:B:39:MET:CG    | 2:B:49:VAL:HG21  | 2.29                     | 0.63              |
| 2:B:73:THR:HG22  | 2:B:75:THR:N     | 2.14                     | 0.63              |
| 1:A:237:GLY:HA3  | 2:B:12:ARG:NE    | 2.14                     | 0.62              |
| 2:B:60:TRP:NE1   | 4:D:242:ARG:NH1  | 2.48                     | 0.62              |
| 1:A:142:ILE:HG23 | 1:A:142:ILE:O    | 1.98                     | 0.62              |
| 1:A:153:ALA:HB3  | 1:A:154:GLU:OE1  | 1.99                     | 0.62              |
| 1:A:87:GLN:NE2   | 1:A:118:TYR:OH   | 2.32                     | 0.62              |
| 1:A:99:SER:HG    | 1:A:114:GLN:HE22 | 1.43                     | 0.62              |
| 1:A:117:ALA:HB2  | 2:B:60:TRP:CZ2   | 2.35                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:167:TRP:CG   | 3:P:1:SER:HG     | 2.18                     | 0.62              |
| 1:A:185:PRO:CA   | 1:A:208:PHE:HB3  | 2.30                     | 0.62              |
| 1:A:224:LEU:O    | 1:A:228:MET:HG3  | 2.00                     | 0.62              |
| 1:A:169:ARG:HA   | 1:A:172:LEU:CD2  | 2.29                     | 0.61              |
| 2:B:13:HIS:HB3   | 2:B:14:PRO:HD2   | 1.82                     | 0.61              |
| 4:D:152:LYS:HE2  | 4:D:185:GLU:OE2  | 2.01                     | 0.61              |
| 1:A:238:ASP:O    | 1:A:240:THR:N    | 2.31                     | 0.61              |
| 1:A:7:TYR:CD2    | 3:P:2:ILE:HG13   | 2.36                     | 0.61              |
| 1:A:172:LEU:O    | 1:A:175:GLY:N    | 2.34                     | 0.61              |
| 4:D:180:ILE:O    | 4:D:219:SER:OG   | 2.14                     | 0.61              |
| 1:A:169:ARG:O    | 1:A:171:TYR:N    | 2.34                     | 0.61              |
| 1:A:175:GLY:C    | 1:A:177:ALA:N    | 2.52                     | 0.61              |
| 2:B:96:ASP:O     | 2:B:97:ARG:C     | 2.43                     | 0.61              |
| 4:D:224:LYS:HG2  | 4:D:227:LYS:HE3  | 1.83                     | 0.60              |
| 1:A:197:ASP:OD2  | 1:A:197:ASP:N    | 2.30                     | 0.60              |
| 2:B:16:GLU:O     | 2:B:17:ASN:O     | 2.19                     | 0.60              |
| 4:D:157:ILE:HG22 | 4:D:159:ASN:H    | 1.66                     | 0.60              |
| 2:B:98:ASP:O     | 2:B:99:MET:C     | 2.44                     | 0.60              |
| 3:P:3:ILE:HD13   | 3:P:4:ASN:H      | 1.66                     | 0.60              |
| 1:A:10:THR:O     | 1:A:22:TYR:HA    | 2.02                     | 0.60              |
| 1:A:77:ASP:O     | 1:A:78:LEU:C     | 2.44                     | 0.60              |
| 1:A:158:ALA:O    | 1:A:159:TYR:C    | 2.45                     | 0.60              |
| 1:A:190:THR:HB   | 1:A:192:HIS:NE2  | 2.16                     | 0.60              |
| 4:D:190:GLN:O    | 4:D:240:LYS:HE3  | 2.02                     | 0.59              |
| 2:B:17:ASN:CA    | 2:B:72:PRO:HG2   | 2.32                     | 0.59              |
| 4:D:202:LEU:HD23 | 4:D:236:VAL:HG21 | 1.83                     | 0.59              |
| 2:B:7:ILE:C      | 2:B:8:GLN:HG2    | 2.26                     | 0.59              |
| 4:D:166:CYS:O    | 4:D:167:LYS:C    | 2.45                     | 0.59              |
| 1:A:80:THR:OG1   | 1:A:84:TYR:CE2   | 2.55                     | 0.59              |
| 1:A:219:LEU:O    | 1:A:220:ASN:HB2  | 2.02                     | 0.59              |
| 2:B:41:LYS:HE2   | 2:B:78:TYR:OH    | 2.03                     | 0.59              |
| 1:A:234:ARG:HD2  | 2:B:10:TYR:CD2   | 2.37                     | 0.59              |
| 4:D:224:LYS:O    | 4:D:224:LYS:CG   | 2.49                     | 0.59              |
| 1:A:78:LEU:HA    | 1:A:95:ILE:HD11  | 1.84                     | 0.59              |
| 2:B:27:VAL:HG21  | 2:B:37:ILE:HD12  | 1.84                     | 0.59              |
| 1:A:64:THR:O     | 1:A:65:GLN:C     | 2.44                     | 0.59              |
| 1:A:127:ASN:HD21 | 1:A:133:TRP:C    | 2.11                     | 0.59              |
| 1:A:5:LEU:CB     | 1:A:168:LEU:HD13 | 2.31                     | 0.59              |
| 1:A:207:GLY:HA2  | 1:A:240:THR:HB   | 1.84                     | 0.58              |
| 1:A:251:LEU:HD23 | 1:A:252:GLY:H    | 1.68                     | 0.58              |
| 4:D:144:VAL:N    | 4:D:156:PHE:O    | 2.35                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:244:TRP:CZ3  | 1:A:246:SER:HB3  | 2.38                     | 0.58              |
| 3:P:5:PHE:H      | 3:P:5:PHE:HD1    | 1.50                     | 0.58              |
| 2:B:7:ILE:HD12   | 2:B:7:ILE:H      | 1.68                     | 0.58              |
| 4:D:259:LYS:O    | 4:D:260:LEU:HD22 | 2.03                     | 0.58              |
| 1:A:29:ASP:CA    | 4:D:230:PHE:CZ   | 2.71                     | 0.58              |
| 2:B:11:SER:CB    | 2:B:21:ASN:HD22  | 2.16                     | 0.58              |
| 4:D:233:ARG:HG3  | 4:D:234:GLY:H    | 1.68                     | 0.58              |
| 2:B:2:GLN:HE21   | 2:B:86:SER:CA    | 2.03                     | 0.58              |
| 4:D:148:CYS:HB2  | 4:D:153:CYS:HA   | 1.82                     | 0.58              |
| 4:D:178:LEU:CG   | 4:D:179:LYS:N    | 2.66                     | 0.58              |
| 1:A:211:ALA:HB2  | 1:A:241:PHE:CE1  | 2.39                     | 0.58              |
| 1:A:33:PHE:HA    | 1:A:49:ALA:CB    | 2.34                     | 0.58              |
| 1:A:116:TYR:CB   | 1:A:124:ILE:HG22 | 2.30                     | 0.58              |
| 4:D:175:VAL:O    | 4:D:256:CYS:HB3  | 2.03                     | 0.58              |
| 4:D:205:ASP:O    | 4:D:206:LYS:C    | 2.46                     | 0.58              |
| 2:B:29:GLN:HA    | 2:B:61:SER:CB    | 2.22                     | 0.58              |
| 1:A:66:LYS:NZ    | 1:A:66:LYS:CB    | 2.66                     | 0.57              |
| 2:B:32:PRO:HD2   | 2:B:84:HIS:NE2   | 2.19                     | 0.57              |
| 2:B:57:SER:OG    | 2:B:59:ASP:OD2   | 2.21                     | 0.57              |
| 4:D:229:ASN:ND2  | 4:D:233:ARG:NE   | 2.53                     | 0.57              |
| 1:A:139:ALA:C    | 1:A:141:LEU:N    | 2.61                     | 0.57              |
| 1:A:189:VAL:HG22 | 1:A:203:CYS:HA   | 1.86                     | 0.57              |
| 2:B:73:THR:HG21  | 2:B:76:ASP:H     | 1.69                     | 0.57              |
| 4:D:204:TYR:CD2  | 4:D:233:ARG:CD   | 2.87                     | 0.57              |
| 1:A:139:ALA:O    | 1:A:141:LEU:N    | 2.38                     | 0.57              |
| 3:P:2:ILE:HG23   | 3:P:3:ILE:O      | 2.05                     | 0.57              |
| 1:A:128:GLU:CD   | 1:A:128:GLU:H    | 2.12                     | 0.57              |
| 4:D:227:LYS:O    | 4:D:227:LYS:HD3  | 2.05                     | 0.57              |
| 1:A:192:HIS:CD2  | 1:A:192:HIS:N    | 2.73                     | 0.57              |
| 4:D:194:ILE:CD1  | 4:D:195:PRO:HD2  | 2.35                     | 0.57              |
| 1:A:78:LEU:HD22  | 1:A:95:ILE:CD1   | 2.35                     | 0.57              |
| 1:A:171:TYR:O    | 1:A:172:LEU:C    | 2.48                     | 0.57              |
| 1:A:111:ARG:NH1  | 1:A:111:ARG:CB   | 2.68                     | 0.56              |
| 1:A:152:GLU:HA   | 1:A:155:ARG:HB2  | 1.86                     | 0.56              |
| 2:B:17:ASN:ND2   | 2:B:97:ARG:HH12  | 2.03                     | 0.56              |
| 1:A:77:ASP:CA    | 1:A:80:THR:HG22  | 2.35                     | 0.56              |
| 1:A:138:MET:O    | 1:A:141:LEU:HB3  | 2.05                     | 0.56              |
| 1:A:70:ASN:O     | 1:A:71:GLU:C     | 2.46                     | 0.56              |
| 1:A:168:LEU:O    | 1:A:171:TYR:HB2  | 2.05                     | 0.56              |
| 1:A:243:LYS:HG2  | 1:A:244:TRP:N    | 2.19                     | 0.56              |
| 1:A:258:THR:HG22 | 1:A:273:ARG:HG2  | 1.86                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:30:ASP:CG    | 4:D:231:LYS:HE2  | 2.31                     | 0.56              |
| 1:A:135:ALA:HB1  | 1:A:140:ALA:HB3  | 1.88                     | 0.56              |
| 1:A:178:THR:C    | 1:A:180:LEU:H    | 2.14                     | 0.56              |
| 2:B:46:ILE:HG22  | 2:B:48:LYS:O     | 2.06                     | 0.56              |
| 1:A:118:TYR:O    | 1:A:119:ASP:HB2  | 2.06                     | 0.56              |
| 1:A:273:ARG:O    | 1:A:274:TRP:CB   | 2.50                     | 0.56              |
| 1:A:28:VAL:CG1   | 1:A:28:VAL:O     | 2.53                     | 0.56              |
| 1:A:100:GLY:O    | 1:A:113:TYR:N    | 2.25                     | 0.56              |
| 1:A:185:PRO:HB3  | 1:A:208:PHE:CB   | 2.34                     | 0.55              |
| 1:A:97:VAL:HA    | 1:A:115:GLN:O    | 2.07                     | 0.55              |
| 4:D:225:ILE:O    | 4:D:227:LYS:N    | 2.34                     | 0.55              |
| 4:D:227:LYS:HE2  | 4:D:227:LYS:C    | 2.31                     | 0.55              |
| 4:D:178:LEU:HD12 | 4:D:179:LYS:H    | 1.72                     | 0.55              |
| 1:A:111:ARG:HH11 | 1:A:111:ARG:HB3  | 1.72                     | 0.55              |
| 4:D:227:LYS:CE   | 4:D:227:LYS:O    | 2.54                     | 0.55              |
| 1:A:167:TRP:HB3  | 1:A:171:TYR:CE2  | 2.42                     | 0.55              |
| 1:A:191:HIS:C    | 1:A:192:HIS:HD2  | 2.15                     | 0.55              |
| 1:A:156:LEU:O    | 1:A:157:ARG:C    | 2.50                     | 0.55              |
| 1:A:199:VAL:HG22 | 1:A:249:VAL:HG22 | 1.89                     | 0.55              |
| 2:B:96:ASP:O     | 2:B:99:MET:HB2   | 2.06                     | 0.55              |
| 1:A:211:ALA:HB2  | 1:A:241:PHE:CD1  | 2.42                     | 0.55              |
| 4:D:196:GLU:HG3  | 4:D:253:TYR:CE2  | 2.41                     | 0.55              |
| 1:A:123:TYR:HD2  | 1:A:124:ILE:HB   | 1.71                     | 0.55              |
| 1:A:167:TRP:HB3  | 1:A:171:TYR:HE2  | 1.72                     | 0.55              |
| 1:A:206:LEU:HD23 | 1:A:242:GLN:HB2  | 1.88                     | 0.55              |
| 1:A:254:GLU:O    | 1:A:256:TYR:N    | 2.39                     | 0.55              |
| 4:D:250:ILE:HG21 | 4:D:252:TYR:CZ   | 2.42                     | 0.55              |
| 4:D:163:TRP:C    | 4:D:165:GLY:N    | 2.62                     | 0.54              |
| 4:D:193:VAL:CG1  | 4:D:198:TYR:CE2  | 2.90                     | 0.54              |
| 4:D:177:ILE:HD11 | 4:D:214:ILE:CG1  | 2.26                     | 0.54              |
| 1:A:34:VAL:HA    | 1:A:47:PRO:HA    | 1.88                     | 0.54              |
| 1:A:158:ALA:O    | 1:A:161:GLU:N    | 2.40                     | 0.54              |
| 1:A:213:ILE:CG1  | 1:A:214:THR:N    | 2.71                     | 0.54              |
| 4:D:223:MET:SD   | 4:D:225:ILE:HG22 | 2.48                     | 0.54              |
| 1:A:14:ARG:NE    | 1:A:19:GLU:O     | 2.39                     | 0.54              |
| 1:A:15:PRO:C     | 1:A:17:LEU:N     | 2.58                     | 0.54              |
| 1:A:31:THR:HG22  | 1:A:32:GLU:O     | 2.07                     | 0.54              |
| 1:A:251:LEU:O    | 1:A:252:GLY:C    | 2.50                     | 0.54              |
| 2:B:41:LYS:HE2   | 2:B:78:TYR:CE2   | 2.43                     | 0.54              |
| 2:B:35:ILE:CD1   | 2:B:84:HIS:HB2   | 2.38                     | 0.54              |
| 3:P:2:ILE:HG23   | 3:P:3:ILE:N      | 2.22                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:127:ASN:ND2  | 1:A:132:THR:O    | 2.40                     | 0.54              |
| 4:D:178:LEU:CD1  | 4:D:179:LYS:H    | 2.21                     | 0.54              |
| 1:A:167:TRP:C    | 1:A:171:TYR:HD2  | 2.16                     | 0.53              |
| 1:A:145:HIS:HA   | 1:A:148:GLU:OE2  | 2.08                     | 0.53              |
| 3:P:6:GLU:O      | 3:P:7:LYS:C      | 2.52                     | 0.53              |
| 1:A:14:ARG:H     | 1:A:14:ARG:HD3   | 1.73                     | 0.53              |
| 1:A:28:VAL:O     | 1:A:29:ASP:HB2   | 2.09                     | 0.53              |
| 4:D:197:ASN:O    | 4:D:252:TYR:HB3  | 2.08                     | 0.53              |
| 1:A:56:GLY:O     | 1:A:59:TYR:HB3   | 2.08                     | 0.53              |
| 4:D:229:ASN:HD21 | 4:D:233:ARG:CZ   | 2.21                     | 0.53              |
| 1:A:51:TRP:CZ2   | 1:A:179:LEU:HD21 | 2.44                     | 0.53              |
| 1:A:153:ALA:CB   | 1:A:154:GLU:OE1  | 2.57                     | 0.53              |
| 1:A:211:ALA:HB2  | 1:A:241:PHE:CZ   | 2.44                     | 0.53              |
| 1:A:63:GLU:OE2   | 1:A:66:LYS:HE3   | 2.09                     | 0.53              |
| 2:B:31:HIS:ND1   | 2:B:32:PRO:CA    | 2.70                     | 0.53              |
| 4:D:225:ILE:C    | 4:D:227:LYS:H    | 2.09                     | 0.53              |
| 2:B:7:ILE:HD12   | 2:B:7:ILE:N      | 2.23                     | 0.53              |
| 2:B:18:GLY:N     | 2:B:72:PRO:O     | 2.30                     | 0.52              |
| 2:B:38:GLN:HB3   | 2:B:40:LEU:HD21  | 1.91                     | 0.52              |
| 1:A:50:ARG:O     | 1:A:52:MET:N     | 2.42                     | 0.52              |
| 1:A:169:ARG:C    | 1:A:171:TYR:N    | 2.64                     | 0.52              |
| 2:B:5:PRO:CA     | 2:B:30:PHE:HB3   | 2.40                     | 0.52              |
| 4:D:145:TYR:CD1  | 4:D:145:TYR:C    | 2.87                     | 0.52              |
| 1:A:52:MET:HA    | 1:A:52:MET:HE3   | 1.92                     | 0.52              |
| 1:A:14:ARG:HG2   | 1:A:14:ARG:O     | 2.10                     | 0.52              |
| 4:D:167:LYS:HA   | 4:D:177:ILE:HG23 | 1.92                     | 0.52              |
| 1:A:154:GLU:O    | 1:A:156:LEU:N    | 2.43                     | 0.52              |
| 2:B:73:THR:CG2   | 2:B:75:THR:CG2   | 2.88                     | 0.52              |
| 1:A:92:SER:C     | 1:A:93:HIS:HD1   | 2.17                     | 0.52              |
| 4:D:168:ALA:O    | 4:D:169:ASN:C    | 2.51                     | 0.52              |
| 4:D:178:LEU:CG   | 4:D:179:LYS:H    | 2.23                     | 0.52              |
| 1:A:30:ASP:OD2   | 4:D:230:PHE:HE2  | 1.92                     | 0.52              |
| 2:B:83:LYS:HE3   | 2:B:90:PRO:HG3   | 1.91                     | 0.52              |
| 4:D:246:ILE:HG12 | 4:D:247:ASP:N    | 2.18                     | 0.52              |
| 4:D:227:LYS:O    | 4:D:227:LYS:CD   | 2.58                     | 0.52              |
| 1:A:58:GLU:CD    | 1:A:58:GLU:C     | 2.78                     | 0.52              |
| 1:A:77:ASP:OD1   | 3:P:7:LYS:HA     | 2.10                     | 0.51              |
| 4:D:190:GLN:HG2  | 4:D:239:SER:O    | 2.10                     | 0.51              |
| 1:A:154:GLU:O    | 1:A:155:ARG:C    | 2.52                     | 0.51              |
| 4:D:190:GLN:O    | 4:D:240:LYS:CE   | 2.58                     | 0.51              |
| 1:A:212:ASP:OD2  | 4:D:232:SER:HA   | 2.10                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:65:LEU:HD12  | 2:B:66:ALA:N     | 2.26                     | 0.51              |
| 2:B:79:ALA:CB    | 2:B:94:TYR:HA    | 2.40                     | 0.51              |
| 4:D:148:CYS:HB3  | 4:D:154:TYR:H    | 1.75                     | 0.51              |
| 1:A:7:TYR:HD1    | 1:A:25:VAL:O     | 1.93                     | 0.51              |
| 1:A:258:THR:HG22 | 1:A:273:ARG:CG   | 2.41                     | 0.51              |
| 2:B:79:ALA:HB2   | 2:B:94:TYR:HA    | 1.92                     | 0.51              |
| 1:A:139:ALA:C    | 1:A:141:LEU:H    | 2.19                     | 0.51              |
| 1:A:144:LYS:O    | 1:A:146:LYS:N    | 2.43                     | 0.51              |
| 1:A:126:LEU:HD22 | 1:A:130:LEU:HA   | 1.93                     | 0.51              |
| 1:A:121:CYS:SG   | 2:B:1:ILE:HG12   | 2.51                     | 0.51              |
| 1:A:271:THR:O    | 1:A:271:THR:CG2  | 2.59                     | 0.51              |
| 2:B:40:LEU:HA    | 2:B:44:LYS:O     | 2.10                     | 0.51              |
| 1:A:202:ARG:HD2  | 1:A:204:TRP:CE2  | 2.45                     | 0.51              |
| 1:A:53:GLU:C     | 1:A:55:GLU:H     | 2.19                     | 0.51              |
| 1:A:86:ASN:O     | 1:A:87:GLN:O     | 2.29                     | 0.51              |
| 1:A:4:SER:HB2    | 1:A:102:GLU:HA   | 1.92                     | 0.50              |
| 1:A:202:ARG:HD2  | 1:A:204:TRP:CZ2  | 2.46                     | 0.50              |
| 4:D:148:CYS:HB3  | 4:D:153:CYS:CA   | 2.32                     | 0.50              |
| 1:A:244:TRP:HZ3  | 1:A:246:SER:HB3  | 1.76                     | 0.50              |
| 1:A:123:TYR:CD2  | 1:A:124:ILE:HB   | 2.47                     | 0.50              |
| 1:A:63:GLU:O     | 1:A:66:LYS:N     | 2.45                     | 0.50              |
| 1:A:266:LEU:HD21 | 1:A:270:LEU:HD13 | 1.93                     | 0.50              |
| 1:A:148:GLU:C    | 1:A:150:ALA:H    | 2.19                     | 0.50              |
| 1:A:205:ALA:O    | 1:A:242:GLN:HA   | 2.11                     | 0.50              |
| 1:A:77:ASP:O     | 1:A:79:ARG:N     | 2.44                     | 0.49              |
| 1:A:154:GLU:C    | 1:A:156:LEU:H    | 2.18                     | 0.49              |
| 4:D:181:GLU:HA   | 4:D:219:SER:OG   | 2.12                     | 0.49              |
| 1:A:230:LEU:CD2  | 1:A:245:ALA:HB2  | 2.42                     | 0.49              |
| 4:D:160:LYS:HA   | 4:D:252:TYR:O    | 2.12                     | 0.49              |
| 1:A:22:TYR:OH    | 1:A:24:GLU:HG3   | 2.11                     | 0.49              |
| 1:A:127:ASN:OD1  | 1:A:134:THR:CG2  | 2.60                     | 0.49              |
| 1:A:271:THR:O    | 1:A:271:THR:HG23 | 2.11                     | 0.49              |
| 4:D:190:GLN:HB3  | 4:D:240:LYS:O    | 2.13                     | 0.49              |
| 1:A:28:VAL:HG11  | 1:A:179:LEU:CD2  | 2.34                     | 0.49              |
| 1:A:93:HIS:CD2   | 1:A:118:TYR:OH   | 2.51                     | 0.49              |
| 4:D:144:VAL:HG13 | 4:D:158:MET:HB2  | 1.93                     | 0.49              |
| 1:A:63:GLU:O     | 1:A:64:THR:C     | 2.54                     | 0.49              |
| 2:B:76:ASP:C     | 2:B:77:THR:CG2   | 2.86                     | 0.49              |
| 4:D:234:GLY:C    | 4:D:248:CYS:SG   | 2.96                     | 0.49              |
| 1:A:29:ASP:OD1   | 4:D:230:PHE:CE1  | 2.65                     | 0.49              |
| 1:A:33:PHE:HD1   | 1:A:34:VAL:HG13  | 1.73                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:213:ILE:HG12 | 1:A:214:THR:H    | 1.78                     | 0.49              |
| 1:A:63:GLU:OE2   | 1:A:66:LYS:CE    | 2.61                     | 0.48              |
| 2:B:49:VAL:HG13  | 2:B:49:VAL:O     | 2.13                     | 0.48              |
| 4:D:144:VAL:CG2  | 4:D:158:MET:HG3  | 2.42                     | 0.48              |
| 1:A:191:HIS:HB2  | 1:A:274:TRP:CE2  | 2.48                     | 0.48              |
| 2:B:76:ASP:C     | 2:B:77:THR:HG23  | 2.38                     | 0.48              |
| 4:D:246:ILE:CG1  | 4:D:247:ASP:H    | 2.18                     | 0.48              |
| 1:A:185:PRO:HD2  | 1:A:266:LEU:HD13 | 1.95                     | 0.48              |
| 1:A:208:PHE:HB2  | 1:A:263:HIS:CD2  | 2.48                     | 0.48              |
| 4:D:226:ARG:HB2  | 4:D:228:MET:CE   | 2.43                     | 0.48              |
| 1:A:103:VAL:HG13 | 1:A:168:LEU:HD23 | 1.95                     | 0.48              |
| 2:B:17:ASN:O     | 2:B:18:GLY:C     | 2.57                     | 0.48              |
| 4:D:178:LEU:HD12 | 4:D:257:GLY:HA3  | 1.94                     | 0.48              |
| 1:A:202:ARG:HD2  | 1:A:204:TRP:NE1  | 2.28                     | 0.48              |
| 3:P:3:ILE:CD1    | 3:P:4:ASN:H      | 2.26                     | 0.48              |
| 1:A:8:PHE:CE2    | 1:A:98:ILE:HG23  | 2.48                     | 0.48              |
| 1:A:19:GLU:HB3   | 1:A:20:PRO:HD2   | 1.94                     | 0.48              |
| 1:A:57:PRO:O     | 1:A:58:GLU:CB    | 2.62                     | 0.48              |
| 2:B:42:ASN:C     | 2:B:44:LYS:N     | 2.67                     | 0.48              |
| 4:D:169:ASN:N    | 4:D:169:ASN:ND2  | 2.28                     | 0.48              |
| 1:A:77:ASP:O     | 1:A:80:THR:HG22  | 2.14                     | 0.48              |
| 3:P:7:LYS:H      | 3:P:7:LYS:HD3    | 1.66                     | 0.48              |
| 1:A:130:LEU:H    | 1:A:130:LEU:HG   | 1.32                     | 0.48              |
| 1:A:171:TYR:O    | 1:A:174:ASN:N    | 2.35                     | 0.48              |
| 4:D:161:THR:C    | 4:D:251:PRO:HA   | 2.39                     | 0.48              |
| 1:A:222:GLU:C    | 1:A:223:GLU:O    | 2.55                     | 0.47              |
| 2:B:97:ARG:CG    | 2:B:98:ASP:N     | 2.66                     | 0.47              |
| 4:D:180:ILE:HB   | 4:D:221:LEU:HD22 | 1.95                     | 0.47              |
| 4:D:207:LYS:C    | 4:D:209:LYS:N    | 2.71                     | 0.47              |
| 1:A:139:ALA:O    | 1:A:142:ILE:N    | 2.38                     | 0.47              |
| 1:A:211:ALA:HB2  | 1:A:241:PHE:CG   | 2.49                     | 0.47              |
| 2:B:73:THR:CG2   | 2:B:76:ASP:H     | 2.27                     | 0.47              |
| 1:A:157:ARG:O    | 1:A:158:ALA:O    | 2.32                     | 0.47              |
| 4:D:204:TYR:CD1  | 4:D:204:TYR:C    | 2.93                     | 0.47              |
| 4:D:238:LEU:HD23 | 4:D:239:SER:N    | 2.30                     | 0.47              |
| 4:D:222:ASP:OD1  | 4:D:222:ASP:O    | 2.32                     | 0.47              |
| 1:A:30:ASP:H     | 4:D:231:LYS:HD3  | 1.79                     | 0.47              |
| 4:D:169:ASN:HA   | 4:D:172:HIS:HB3  | 1.96                     | 0.47              |
| 1:A:15:PRO:O     | 1:A:17:LEU:N     | 2.47                     | 0.47              |
| 3:P:3:ILE:HD13   | 3:P:4:ASN:C      | 2.38                     | 0.47              |
| 2:B:35:ILE:HD12  | 2:B:83:LYS:O     | 2.15                     | 0.47              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:A:52:MET:CE    | 1:A:52:MET:CA   | 2.92                     | 0.47              |
| 4:D:208:LYS:O    | 4:D:209:LYS:C   | 2.58                     | 0.47              |
| 1:A:50:ARG:HD3   | 1:A:50:ARG:HA   | 1.42                     | 0.46              |
| 1:A:73:SER:OG    | 3:P:7:LYS:CE    | 2.63                     | 0.46              |
| 1:A:156:LEU:O    | 1:A:158:ALA:N   | 2.48                     | 0.46              |
| 1:A:259:CYS:O    | 1:A:271:THR:HA  | 2.14                     | 0.46              |
| 4:D:227:LYS:O    | 4:D:228:MET:C   | 2.57                     | 0.46              |
| 1:A:22:TYR:OH    | 1:A:24:GLU:CG   | 2.63                     | 0.46              |
| 1:A:213:ILE:CG1  | 1:A:214:THR:H   | 2.28                     | 0.46              |
| 2:B:21:ASN:O     | 2:B:70:PHE:N    | 2.37                     | 0.46              |
| 4:D:178:LEU:HG   | 4:D:179:LYS:H   | 1.77                     | 0.46              |
| 4:D:194:ILE:CG1  | 4:D:195:PRO:HD2 | 2.45                     | 0.46              |
| 1:A:4:SER:O      | 1:A:29:ASP:N    | 2.48                     | 0.46              |
| 1:A:74:PHE:HA    | 1:A:77:ASP:HB2  | 1.96                     | 0.46              |
| 1:A:85:TYR:C     | 1:A:87:GLN:N    | 2.71                     | 0.46              |
| 2:B:41:LYS:O     | 2:B:44:LYS:HB2  | 2.15                     | 0.46              |
| 2:B:73:THR:CG2   | 2:B:75:THR:H    | 2.26                     | 0.46              |
| 1:A:74:PHE:O     | 1:A:77:ASP:HB2  | 2.15                     | 0.46              |
| 1:A:266:LEU:O    | 1:A:267:PRO:C   | 2.59                     | 0.46              |
| 2:B:41:LYS:O     | 2:B:42:ASN:HB2  | 2.16                     | 0.46              |
| 2:B:70:PHE:CD2   | 2:B:78:TYR:CE1  | 3.04                     | 0.46              |
| 1:A:85:TYR:O     | 1:A:87:GLN:N    | 2.49                     | 0.46              |
| 1:A:130:LEU:HD12 | 1:A:157:ARG:HD3 | 1.98                     | 0.46              |
| 2:B:16:GLU:HB2   | 2:B:19:LYS:HG2  | 1.97                     | 0.46              |
| 4:D:179:LYS:HE2  | 4:D:217:GLY:O   | 2.16                     | 0.46              |
| 4:D:198:TYR:O    | 4:D:237:PHE:CB  | 2.64                     | 0.46              |
| 1:A:21:ARG:NH2   | 1:A:23:MET:CE   | 2.77                     | 0.46              |
| 1:A:27:TYR:HB3   | 1:A:29:ASP:O    | 2.16                     | 0.46              |
| 1:A:59:TYR:CD2   | 1:A:60:TRP:N    | 2.84                     | 0.46              |
| 1:A:77:ASP:OD1   | 3:P:8:LEU:N     | 2.39                     | 0.46              |
| 1:A:181:ARG:HH22 | 1:A:239:GLY:HA3 | 1.80                     | 0.46              |
| 1:A:206:LEU:CD2  | 1:A:242:GLN:HB2 | 2.46                     | 0.46              |
| 2:B:7:ILE:CG2    | 2:B:8:GLN:N     | 2.79                     | 0.46              |
| 1:A:59:TYR:CD2   | 1:A:60:TRP:CD1  | 3.04                     | 0.46              |
| 1:A:126:LEU:HD23 | 1:A:126:LEU:HA  | 1.64                     | 0.46              |
| 1:A:243:LYS:HG2  | 1:A:244:TRP:H   | 1.80                     | 0.46              |
| 4:D:230:PHE:CD2  | 4:D:231:LYS:N   | 2.84                     | 0.46              |
| 1:A:57:PRO:O     | 1:A:58:GLU:HB3  | 2.15                     | 0.46              |
| 1:A:211:ALA:HB2  | 1:A:241:PHE:CE2 | 2.50                     | 0.46              |
| 2:B:51:MET:O     | 2:B:52:SER:O    | 2.34                     | 0.46              |
| 3:P:2:ILE:HG12   | 3:P:3:ILE:H     | 1.81                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:227:LYS:O    | 4:D:228:MET:O    | 2.33                     | 0.46              |
| 1:A:96:GLN:O     | 1:A:97:VAL:HG23  | 2.15                     | 0.45              |
| 1:A:137:ASP:O    | 1:A:138:MET:C    | 2.59                     | 0.45              |
| 1:A:209:TYR:CD2  | 1:A:209:TYR:C    | 2.94                     | 0.45              |
| 2:B:35:ILE:HG23  | 2:B:35:ILE:O     | 2.15                     | 0.45              |
| 4:D:228:MET:O    | 4:D:229:ASN:CB   | 2.55                     | 0.45              |
| 1:A:219:LEU:HD22 | 1:A:257:TYR:CE2  | 2.51                     | 0.45              |
| 4:D:154:TYR:OH   | 4:D:185:GLU:OE2  | 2.32                     | 0.45              |
| 4:D:226:ARG:O    | 4:D:227:LYS:C    | 2.50                     | 0.45              |
| 1:A:70:ASN:O     | 1:A:73:SER:N     | 2.49                     | 0.45              |
| 2:B:7:ILE:HG12   | 2:B:82:VAL:HG21  | 1.99                     | 0.45              |
| 4:D:169:ASN:O    | 4:D:170:CYS:C    | 2.57                     | 0.45              |
| 1:A:50:ARG:C     | 1:A:52:MET:N     | 2.75                     | 0.45              |
| 1:A:161:GLU:O    | 1:A:165:VAL:HG21 | 2.16                     | 0.45              |
| 1:A:167:TRP:O    | 1:A:168:LEU:C    | 2.59                     | 0.45              |
| 1:A:52:MET:SD    | 1:A:55:GLU:HG3   | 2.56                     | 0.45              |
| 1:A:97:VAL:HG22  | 1:A:116:TYR:CG   | 2.52                     | 0.45              |
| 2:B:97:ARG:CG    | 2:B:98:ASP:H     | 2.28                     | 0.45              |
| 4:D:185:GLU:O    | 4:D:186:LEU:C    | 2.60                     | 0.45              |
| 4:D:207:LYS:O    | 4:D:209:LYS:N    | 2.48                     | 0.44              |
| 1:A:194:ARG:HG3  | 1:A:195:PRO:HD2  | 1.99                     | 0.44              |
| 1:A:211:ALA:HB2  | 1:A:241:PHE:CD2  | 2.52                     | 0.44              |
| 2:B:32:PRO:HB2   | 2:B:33:PRO:CD    | 2.40                     | 0.44              |
| 2:B:87:MET:SD    | 2:B:91:LYS:HE3   | 2.57                     | 0.44              |
| 4:D:175:VAL:HG12 | 4:D:256:CYS:HB3  | 1.98                     | 0.44              |
| 1:A:28:VAL:O     | 1:A:28:VAL:HG13  | 2.18                     | 0.44              |
| 1:A:122:ASP:CG   | 4:D:242:ARG:HD2  | 2.43                     | 0.44              |
| 2:B:59:ASP:O     | 2:B:60:TRP:HB2   | 2.17                     | 0.44              |
| 3:P:3:ILE:CD1    | 3:P:4:ASN:N      | 2.79                     | 0.44              |
| 2:B:17:ASN:C     | 2:B:19:LYS:N     | 2.74                     | 0.44              |
| 1:A:13:SER:HB3   | 1:A:78:LEU:HG    | 1.99                     | 0.44              |
| 1:A:51:TRP:HZ2   | 1:A:179:LEU:HD21 | 1.83                     | 0.44              |
| 4:D:199:TRP:HE3  | 4:D:236:VAL:O    | 2.00                     | 0.44              |
| 4:D:202:LEU:HD13 | 4:D:213:TRP:CD2  | 2.53                     | 0.44              |
| 1:A:7:TYR:HA     | 1:A:25:VAL:O     | 2.17                     | 0.44              |
| 1:A:202:ARG:NH1  | 1:A:244:TRP:CZ3  | 2.86                     | 0.44              |
| 2:B:27:VAL:HG12  | 2:B:30:PHE:CD2   | 2.53                     | 0.44              |
| 2:B:83:LYS:HE3   | 2:B:90:PRO:HG2   | 1.98                     | 0.44              |
| 2:B:96:ASP:OD2   | 2:B:98:ASP:HB2   | 2.18                     | 0.44              |
| 4:D:243:ILE:HD13 | 4:D:243:ILE:HA   | 1.68                     | 0.44              |
| 1:A:59:TYR:CE2   | 1:A:60:TRP:CD1   | 3.05                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:116:TYR:CG   | 1:A:124:ILE:HG22 | 2.52                     | 0.43              |
| 2:B:7:ILE:C      | 2:B:8:GLN:CG     | 2.91                     | 0.43              |
| 4:D:215:ASP:OD1  | 4:D:217:GLY:N    | 2.47                     | 0.43              |
| 1:A:14:ARG:HG3   | 1:A:14:ARG:HH11  | 1.83                     | 0.43              |
| 1:A:77:ASP:C     | 1:A:79:ARG:N     | 2.77                     | 0.43              |
| 1:A:161:GLU:O    | 1:A:165:VAL:CG2  | 2.66                     | 0.43              |
| 2:B:50:GLU:HB2   | 2:B:67:HIS:NE2   | 2.33                     | 0.43              |
| 4:D:162:THR:O    | 4:D:165:GLY:HA3  | 2.18                     | 0.43              |
| 4:D:179:LYS:HG3  | 4:D:181:GLU:HG2  | 2.00                     | 0.43              |
| 1:A:263:HIS:ND1  | 1:A:264:GLN:N    | 2.66                     | 0.43              |
| 4:D:229:ASN:ND2  | 4:D:233:ARG:HE   | 2.15                     | 0.43              |
| 1:A:12:VAL:HG22  | 1:A:94:THR:CB    | 2.46                     | 0.43              |
| 1:A:22:TYR:CD2   | 1:A:22:TYR:C     | 2.96                     | 0.43              |
| 1:A:130:LEU:HD12 | 1:A:157:ARG:CD   | 2.49                     | 0.43              |
| 1:A:137:ASP:C    | 1:A:139:ALA:N    | 2.77                     | 0.43              |
| 1:A:6:ARG:HA     | 1:A:100:GLY:HA3  | 1.99                     | 0.43              |
| 2:B:23:LEU:HD13  | 2:B:70:PHE:CE1   | 2.54                     | 0.43              |
| 4:D:200:ILE:O    | 4:D:200:ILE:HG13 | 2.17                     | 0.43              |
| 4:D:154:TYR:C    | 4:D:155:TYR:CD2  | 2.97                     | 0.43              |
| 1:A:266:LEU:HD21 | 1:A:270:LEU:HD12 | 1.97                     | 0.43              |
| 4:D:166:CYS:HB2  | 4:D:177:ILE:HG22 | 1.99                     | 0.43              |
| 1:A:65:GLN:OE1   | 1:A:65:GLN:HA    | 2.18                     | 0.43              |
| 1:A:263:HIS:O    | 1:A:266:LEU:HB2  | 2.19                     | 0.43              |
| 2:B:60:TRP:HE1   | 4:D:242:ARG:NH1  | 2.17                     | 0.43              |
| 1:A:74:PHE:O     | 1:A:78:LEU:N     | 2.47                     | 0.42              |
| 1:A:142:ILE:O    | 1:A:142:ILE:CG2  | 2.66                     | 0.42              |
| 1:A:202:ARG:HG3  | 1:A:202:ARG:HH11 | 1.84                     | 0.42              |
| 1:A:209:TYR:HA   | 1:A:210:PRO:C    | 2.44                     | 0.42              |
| 1:A:78:LEU:HD22  | 1:A:95:ILE:HD12  | 2.01                     | 0.42              |
| 1:A:213:ILE:HD11 | 1:A:261:VAL:HG13 | 2.01                     | 0.42              |
| 1:A:183:ASP:O    | 1:A:208:PHE:HA   | 2.20                     | 0.42              |
| 1:A:194:ARG:HD2  | 1:A:248:VAL:HG13 | 2.02                     | 0.42              |
| 1:A:230:LEU:HD12 | 4:D:249:ASN:OD1  | 2.19                     | 0.42              |
| 1:A:237:GLY:CA   | 2:B:12:ARG:NH2   | 2.79                     | 0.42              |
| 1:A:123:TYR:CE2  | 1:A:140:ALA:HA   | 2.55                     | 0.42              |
| 1:A:166:GLU:O    | 1:A:167:TRP:C    | 2.63                     | 0.42              |
| 1:A:127:ASN:OD1  | 1:A:134:THR:HG22 | 2.18                     | 0.42              |
| 1:A:152:GLU:O    | 1:A:156:LEU:HB2  | 2.20                     | 0.42              |
| 4:D:167:LYS:N    | 4:D:177:ILE:CG2  | 2.83                     | 0.42              |
| 4:D:222:ASP:C    | 4:D:224:LYS:H    | 2.28                     | 0.42              |
| 1:A:184:SER:HB3  | 1:A:266:LEU:CD1  | 2.50                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:65:GLN:O     | 1:A:68:LYS:HB2   | 2.20                     | 0.42              |
| 1:A:146:LYS:O    | 1:A:149:GLN:N    | 2.53                     | 0.42              |
| 1:A:255:GLN:O    | 1:A:256:TYR:HD1  | 2.01                     | 0.42              |
| 4:D:152:LYS:HD3  | 4:D:154:TYR:OH   | 2.20                     | 0.42              |
| 4:D:238:LEU:HD23 | 4:D:238:LEU:C    | 2.45                     | 0.42              |
| 1:A:185:PRO:HB3  | 1:A:208:PHE:CG   | 2.55                     | 0.42              |
| 1:A:52:MET:CE    | 1:A:55:GLU:HG3   | 2.49                     | 0.42              |
| 1:A:238:ASP:O    | 1:A:240:THR:HG23 | 2.19                     | 0.42              |
| 4:D:206:LYS:NZ   | 4:D:206:LYS:CB   | 2.83                     | 0.42              |
| 1:A:208:PHE:CD2  | 1:A:263:HIS:CD2  | 3.08                     | 0.41              |
| 4:D:163:TRP:C    | 4:D:165:GLY:H    | 2.27                     | 0.41              |
| 4:D:180:ILE:CG2  | 4:D:221:LEU:HD22 | 2.50                     | 0.41              |
| 1:A:26:GLY:C     | 1:A:33:PHE:CD2   | 2.98                     | 0.41              |
| 1:A:178:THR:C    | 1:A:180:LEU:N    | 2.78                     | 0.41              |
| 1:A:208:PHE:CD2  | 1:A:263:HIS:HD2  | 2.38                     | 0.41              |
| 2:B:41:LYS:HE2   | 2:B:78:TYR:CZ    | 2.54                     | 0.41              |
| 2:B:79:ALA:HB2   | 2:B:94:TYR:CD1   | 2.55                     | 0.41              |
| 4:D:198:TYR:HB3  | 4:D:255:ILE:HG13 | 2.01                     | 0.41              |
| 1:A:54:GLN:HB3   | 1:A:174:ASN:HD22 | 1.86                     | 0.41              |
| 1:A:181:ARG:NH1  | 1:A:183:ASP:OD2  | 2.53                     | 0.41              |
| 4:D:178:LEU:CB   | 4:D:255:ILE:HG22 | 2.43                     | 0.41              |
| 1:A:4:SER:HA     | 1:A:168:LEU:HD21 | 2.02                     | 0.41              |
| 2:B:41:LYS:CG    | 2:B:78:TYR:CE2   | 2.99                     | 0.41              |
| 1:A:19:GLU:HG3   | 1:A:75:ARG:NH1   | 2.34                     | 0.41              |
| 1:A:74:PHE:HA    | 1:A:77:ASP:OD2   | 2.20                     | 0.41              |
| 1:A:74:PHE:O     | 1:A:75:ARG:C     | 2.64                     | 0.41              |
| 1:A:82:LEU:O     | 1:A:83:GLY:O     | 2.38                     | 0.41              |
| 1:A:191:HIS:C    | 1:A:192:HIS:CD2  | 2.96                     | 0.41              |
| 1:A:203:CYS:O    | 1:A:244:TRP:HB2  | 2.21                     | 0.41              |
| 1:A:127:ASN:ND2  | 1:A:133:TRP:O    | 2.46                     | 0.41              |
| 4:D:175:VAL:HA   | 4:D:176:PRO:HD2  | 1.76                     | 0.41              |
| 1:A:205:ALA:O    | 1:A:208:PHE:HE1  | 2.04                     | 0.41              |
| 2:B:12:ARG:HB3   | 2:B:22:ILE:HD12  | 2.02                     | 0.41              |
| 1:A:7:TYR:C      | 1:A:8:PHE:HD2    | 2.29                     | 0.41              |
| 1:A:22:TYR:CZ    | 1:A:24:GLU:HG3   | 2.55                     | 0.41              |
| 1:A:82:LEU:O     | 1:A:83:GLY:C     | 2.62                     | 0.41              |
| 1:A:97:VAL:HG21  | 1:A:116:TYR:CE2  | 2.56                     | 0.41              |
| 1:A:123:TYR:CZ   | 1:A:140:ALA:HA   | 2.56                     | 0.41              |
| 1:A:167:TRP:O    | 1:A:171:TYR:CD2  | 2.66                     | 0.41              |
| 4:D:171:GLN:O    | 4:D:174:SER:N    | 2.50                     | 0.41              |
| 4:D:227:LYS:CE   | 4:D:227:LYS:C    | 2.92                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:50:ARG:C     | 1:A:52:MET:H     | 2.28                     | 0.41              |
| 1:A:172:LEU:O    | 1:A:176:ASN:N    | 2.54                     | 0.41              |
| 1:A:218:GLN:HG2  | 1:A:222:GLU:O    | 2.20                     | 0.41              |
| 1:A:238:ASP:C    | 1:A:240:THR:N    | 2.79                     | 0.41              |
| 4:D:239:SER:C    | 4:D:241:ALA:N    | 2.76                     | 0.41              |
| 2:B:56:PHE:HA    | 2:B:61:SER:O     | 2.22                     | 0.40              |
| 4:D:144:VAL:CG1  | 4:D:158:MET:HB2  | 2.50                     | 0.40              |
| 4:D:179:LYS:HA   | 4:D:213:TRP:CZ3  | 2.56                     | 0.40              |
| 2:B:83:LYS:HG3   | 2:B:90:PRO:CG    | 2.20                     | 0.40              |
| 1:A:66:LYS:CB    | 1:A:66:LYS:HZ3   | 2.35                     | 0.40              |
| 1:A:114:GLN:NE2  | 1:A:114:GLN:HA   | 2.37                     | 0.40              |
| 1:A:144:LYS:C    | 1:A:146:LYS:H    | 2.30                     | 0.40              |
| 1:A:152:GLU:HG2  | 1:A:155:ARG:HB2  | 2.02                     | 0.40              |
| 1:A:265:GLY:O    | 1:A:266:LEU:HD12 | 2.21                     | 0.40              |
| 4:D:193:VAL:HG12 | 4:D:194:ILE:O    | 2.21                     | 0.40              |
| 4:D:260:LEU:HD22 | 4:D:260:LEU:HA   | 1.86                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |   |
|-----|-------|---------------|-----------|----------|----------|-------------|---|
| 1   | A     | 249/274 (91%) | 167 (67%) | 56 (22%) | 26 (10%) | 0           | 2 |
| 2   | B     | 93/99 (94%)   | 77 (83%)  | 11 (12%) | 5 (5%)   | 1           | 9 |
| 3   | P     | 6/8 (75%)     | 3 (50%)   | 2 (33%)  | 1 (17%)  | 0           | 1 |
| 4   | D     | 116/120 (97%) | 75 (65%)  | 23 (20%) | 18 (16%) | 0           | 1 |
| All | All   | 464/501 (93%) | 322 (69%) | 92 (20%) | 50 (11%) | 0           | 2 |

All (50) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 58  | GLU  |
| 1   | A     | 87  | GLN  |
| 1   | A     | 130 | LEU  |
| 1   | A     | 139 | ALA  |
| 1   | A     | 145 | HIS  |
| 1   | A     | 158 | ALA  |
| 1   | A     | 159 | TYR  |
| 1   | A     | 170 | ARG  |
| 1   | A     | 253 | LYS  |
| 1   | A     | 255 | GLN  |
| 2   | B     | 17  | ASN  |
| 4   | D     | 150 | SER  |
| 4   | D     | 168 | ALA  |
| 4   | D     | 174 | SER  |
| 4   | D     | 183 | GLU  |
| 4   | D     | 206 | LYS  |
| 4   | D     | 209 | LYS  |
| 4   | D     | 227 | LYS  |
| 4   | D     | 229 | ASN  |
| 4   | D     | 231 | LYS  |
| 4   | D     | 246 | ILE  |
| 1   | A     | 131 | LYS  |
| 1   | A     | 140 | ALA  |
| 1   | A     | 157 | ARG  |
| 1   | A     | 180 | LEU  |
| 1   | A     | 252 | GLY  |
| 2   | B     | 35  | ILE  |
| 2   | B     | 47  | PRO  |
| 4   | D     | 201 | GLY  |
| 4   | D     | 228 | MET  |
| 1   | A     | 50  | ARG  |
| 1   | A     | 51  | TRP  |
| 1   | A     | 54  | GLN  |
| 1   | A     | 83  | GLY  |
| 1   | A     | 175 | GLY  |
| 1   | A     | 182 | THR  |
| 2   | B     | 43  | GLY  |
| 2   | B     | 49  | VAL  |
| 3   | P     | 7   | LYS  |
| 1   | A     | 78  | LEU  |
| 1   | A     | 162 | GLY  |
| 4   | D     | 189 | LEU  |
| 4   | D     | 196 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | D     | 208 | LYS  |
| 1   | A     | 77  | ASP  |
| 1   | A     | 179 | LEU  |
| 4   | D     | 167 | LYS  |
| 1   | A     | 239 | GLY  |
| 4   | D     | 193 | VAL  |
| 4   | D     | 176 | PRO  |

### 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     | 214/232 (92%) | 174 (81%) | 40 (19%) | 1           | 7  |
| 2   | B     | 90/94 (96%)   | 75 (83%)  | 15 (17%) | 2           | 10 |
| 3   | P     | 8/8 (100%)    | 6 (75%)   | 2 (25%)  | 0           | 2  |
| 4   | D     | 107/111 (96%) | 82 (77%)  | 25 (23%) | 1           | 3  |
| All | All   | 419/445 (94%) | 337 (80%) | 82 (20%) | 1           | 6  |

All (82) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 14  | ARG  |
| 1   | A     | 17  | LEU  |
| 1   | A     | 48  | ARG  |
| 1   | A     | 50  | ARG  |
| 1   | A     | 52  | MET  |
| 1   | A     | 54  | GLN  |
| 1   | A     | 58  | GLU  |
| 1   | A     | 66  | LYS  |
| 1   | A     | 78  | LEU  |
| 1   | A     | 86  | ASN  |
| 1   | A     | 87  | GLN  |
| 1   | A     | 89  | LYS  |
| 1   | A     | 94  | THR  |
| 1   | A     | 99  | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 122 | ASP  |
| 1   | A     | 126 | LEU  |
| 1   | A     | 128 | GLU  |
| 1   | A     | 130 | LEU  |
| 1   | A     | 132 | THR  |
| 1   | A     | 134 | THR  |
| 1   | A     | 142 | ILE  |
| 1   | A     | 143 | THR  |
| 1   | A     | 152 | GLU  |
| 1   | A     | 156 | LEU  |
| 1   | A     | 161 | GLU  |
| 1   | A     | 165 | VAL  |
| 1   | A     | 169 | ARG  |
| 1   | A     | 172 | LEU  |
| 1   | A     | 180 | LEU  |
| 1   | A     | 183 | ASP  |
| 1   | A     | 190 | THR  |
| 1   | A     | 192 | HIS  |
| 1   | A     | 197 | ASP  |
| 1   | A     | 199 | VAL  |
| 1   | A     | 227 | ASP  |
| 1   | A     | 249 | VAL  |
| 1   | A     | 251 | LEU  |
| 1   | A     | 253 | LYS  |
| 1   | A     | 266 | LEU  |
| 1   | A     | 272 | LEU  |
| 2   | B     | 6   | GLN  |
| 2   | B     | 8   | GLN  |
| 2   | B     | 17  | ASN  |
| 2   | B     | 21  | ASN  |
| 2   | B     | 22  | ILE  |
| 2   | B     | 29  | GLN  |
| 2   | B     | 36  | GLU  |
| 2   | B     | 48  | LYS  |
| 2   | B     | 58  | LYS  |
| 2   | B     | 64  | ILE  |
| 2   | B     | 70  | PHE  |
| 2   | B     | 74  | GLU  |
| 2   | B     | 75  | THR  |
| 2   | B     | 91  | LYS  |
| 2   | B     | 99  | MET  |
| 3   | P     | 3   | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | P     | 5   | PHE  |
| 4   | D     | 159 | ASN  |
| 4   | D     | 161 | THR  |
| 4   | D     | 169 | ASN  |
| 4   | D     | 177 | ILE  |
| 4   | D     | 184 | ASP  |
| 4   | D     | 186 | LEU  |
| 4   | D     | 188 | PHE  |
| 4   | D     | 194 | ILE  |
| 4   | D     | 196 | GLU  |
| 4   | D     | 206 | LYS  |
| 4   | D     | 207 | LYS  |
| 4   | D     | 210 | GLU  |
| 4   | D     | 214 | ILE  |
| 4   | D     | 215 | ASP  |
| 4   | D     | 216 | ASN  |
| 4   | D     | 220 | LYS  |
| 4   | D     | 223 | MET  |
| 4   | D     | 224 | LYS  |
| 4   | D     | 227 | LYS  |
| 4   | D     | 228 | MET  |
| 4   | D     | 229 | ASN  |
| 4   | D     | 230 | PHE  |
| 4   | D     | 243 | ILE  |
| 4   | D     | 259 | LYS  |
| 4   | D     | 260 | LEU  |

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     | 70  | ASN  |
| 1   | A     | 86  | ASN  |
| 1   | A     | 87  | GLN  |
| 1   | A     | 93  | HIS  |
| 1   | A     | 114 | GLN  |
| 1   | A     | 174 | ASN  |
| 1   | A     | 260 | HIS  |
| 2   | B     | 2   | GLN  |
| 2   | B     | 6   | GLN  |
| 2   | B     | 13  | HIS  |
| 2   | B     | 17  | ASN  |
| 2   | B     | 21  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 29  | GLN  |
| 2   | B     | 67  | HIS  |
| 3   | P     | 4   | ASN  |
| 4   | D     | 169 | ASN  |
| 4   | D     | 190 | GLN  |
| 4   | D     | 229 | ASN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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

There are no ligands in this entry.

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

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

| Mol | Chain | Analysed      | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|---------------|--------|---------------|-----------------------|-------|
| 1   | A     | 255/274 (93%) | 0.20   | 10 (3%) 43 29 | 18, 50, 84, 128       | 0     |
| 2   | B     | 97/99 (97%)   | 0.17   | 4 (4%) 41 27  | 16, 46, 81, 110       | 0     |
| 3   | P     | 8/8 (100%)    | 0.25   | 0 100 100     | 52, 54, 66, 74        | 0     |
| 4   | D     | 118/120 (98%) | 0.27   | 5 (4%) 40 26  | 22, 48, 94, 142       | 0     |
| All | All   | 478/501 (95%) | 0.21   | 19 (3%) 42 28 | 16, 49, 86, 142       | 0     |

All (19) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 4   | D     | 230 | PHE  | 6.1  |
| 2   | B     | 52  | SER  | 4.3  |
| 1   | A     | 179 | LEU  | 3.5  |
| 4   | D     | 232 | SER  | 3.4  |
| 1   | A     | 56  | GLY  | 3.0  |
| 2   | B     | 85  | ASP  | 2.9  |
| 1   | A     | 178 | THR  | 2.9  |
| 1   | A     | 57  | PRO  | 2.4  |
| 2   | B     | 63  | TYR  | 2.4  |
| 1   | A     | 55  | GLU  | 2.4  |
| 4   | D     | 223 | MET  | 2.4  |
| 2   | B     | 81  | ARG  | 2.4  |
| 1   | A     | 252 | GLY  | 2.3  |
| 4   | D     | 229 | ASN  | 2.3  |
| 1   | A     | 130 | LEU  | 2.2  |
| 4   | D     | 231 | LYS  | 2.2  |
| 1   | A     | 226 | GLN  | 2.1  |
| 1   | A     | 135 | ALA  | 2.1  |
| 1   | A     | 177 | ALA  | 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.