



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:47 PM UTC

PDB ID : 3WWK / pdb\_00003wwk  
Title : Crystal structure of CLEC-2 in complex with rhodocytin  
Authors : Nagae, M.; Morita-Matsumoto, K.; Kato, M.; Kato-Kaneko, M.; Kato, Y.; Yamaguchi, Y.  
Deposited on : 2014-06-20  
Resolution : 2.98 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Xtriage (Phenix)               | : | 2.0                                                              |
| EDS                            | : | 3.0                                                              |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4                           | : | 9.0.010 (Gargrove)                                               |
| Density-Fitness                | : | 1.0.12                                                           |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

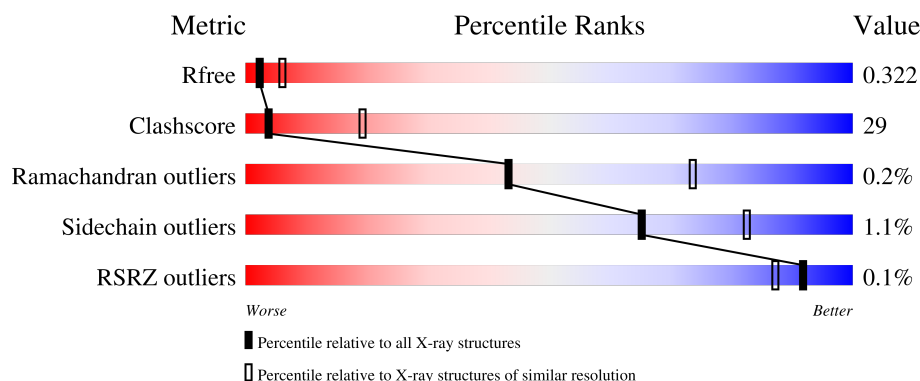
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.98 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                      | 3580 (3.00-2.96)                                      |
| Clashscore            | 190562                      | 3904 (3.00-2.96)                                      |
| Ramachandran outliers | 187476                      | 3761 (3.00-2.96)                                      |
| Sidechain outliers    | 187428                      | 3764 (3.00-2.96)                                      |
| RSRZ outliers         | 180081                      | 3579 (3.00-2.96)                                      |

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   | C     | 128    | <div> <div>73%</div> <div>22%</div> <div>5%</div> </div>              |
| 1   | F     | 128    | <div> <div>%</div> <div>68%</div> <div>27%</div> <div>5%</div> </div> |
| 1   | I     | 128    | <div> <div>73%</div> <div>23%</div> <div>5%</div> </div>              |
| 1   | L     | 128    | <div> <div>45%</div> <div>49%</div> <div>• 5%</div> </div>            |
| 2   | A     | 136    | <div> <div>66%</div> <div>26%</div> <div>• • •</div> </div>           |

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| Mol | Chain | Length | Quality of chain                                                                                    |
|-----|-------|--------|-----------------------------------------------------------------------------------------------------|
| 2   | D     | 136    |  62% 28% 6% . .   |
| 2   | G     | 136    |  66% 27% . . .    |
| 2   | J     | 136    |  31% 52% 10% . 7% |
| 3   | B     | 146    |  57% 23% . . 16%  |
| 3   | E     | 146    |  66% 17% . 16%    |
| 3   | H     | 146    |  60% 22% . . 16%  |
| 3   | K     | 146    |  62% 20% . . 16%  |

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12453 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 C-type lectin domain family 1 member B.

| Mol | Chain | Residues | Atoms |     |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 1   | C     | 122      | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1023  | 644 | 180 | 188 | 11 |         |         |       |
| 1   | I     | 122      | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1023  | 644 | 180 | 188 | 11 |         |         |       |
| 1   | L     | 122      | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1023  | 644 | 180 | 188 | 11 |         |         |       |
| 1   | F     | 122      | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1023  | 644 | 180 | 188 | 11 |         |         |       |

There are 12 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| C     | 94      | GLY      | -      | expression tag      | UNP Q9P126 |
| C     | 95      | SER      | -      | expression tag      | UNP Q9P126 |
| C     | 99      | SER      | CYS    | engineered mutation | UNP Q9P126 |
| I     | 94      | GLY      | -      | expression tag      | UNP Q9P126 |
| I     | 95      | SER      | -      | expression tag      | UNP Q9P126 |
| I     | 99      | SER      | CYS    | engineered mutation | UNP Q9P126 |
| L     | 94      | GLY      | -      | expression tag      | UNP Q9P126 |
| L     | 95      | SER      | -      | expression tag      | UNP Q9P126 |
| L     | 99      | SER      | CYS    | engineered mutation | UNP Q9P126 |
| F     | 94      | GLY      | -      | expression tag      | UNP Q9P126 |
| F     | 95      | SER      | -      | expression tag      | UNP Q9P126 |
| F     | 99      | SER      | CYS    | engineered mutation | UNP Q9P126 |

- Molecule 2 is a protein called Snaclec rhodocytin subunit alpha.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2   | A     | 133      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1092  | 688 | 180 | 216 | 8 |         |         |       |
| 2   | D     | 133      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1092  | 688 | 180 | 216 | 8 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2   | G     | 133      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1092  | 688 | 180 | 216 | 8 |         |         |       |
| 2   | J     | 127      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1045  | 661 | 174 | 202 | 8 |         |         |       |

- Molecule 3 is a protein called Snaclec rhodocytin subunit beta.

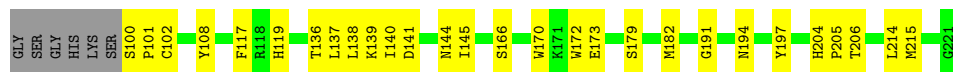
| Mol | Chain | Residues | Atoms |     |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 3   | B     | 123      | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1010  | 642 | 177 | 181 | 10 |         |         |       |
| 3   | E     | 123      | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1010  | 642 | 177 | 181 | 10 |         |         |       |
| 3   | H     | 123      | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1010  | 642 | 177 | 181 | 10 |         |         |       |
| 3   | K     | 123      | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1010  | 642 | 177 | 181 | 10 |         |         |       |

### 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: C-type lectin domain family 1 member B

Chain C: 

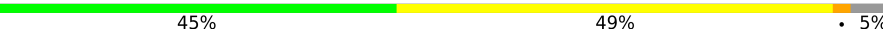


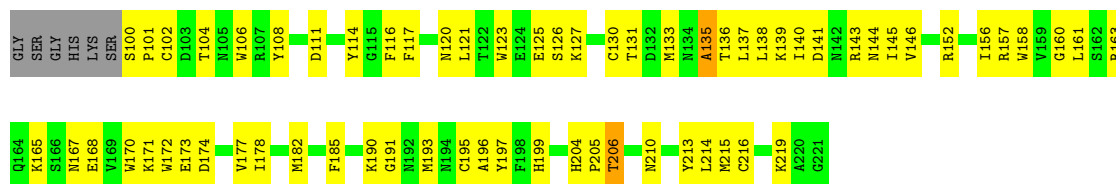
- Molecule 1: C-type lectin domain family 1 member B

Chain I: 



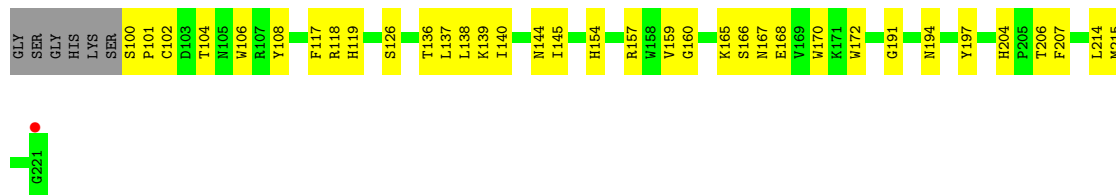
- Molecule 1: C-type lectin domain family 1 member B

Chain L: 



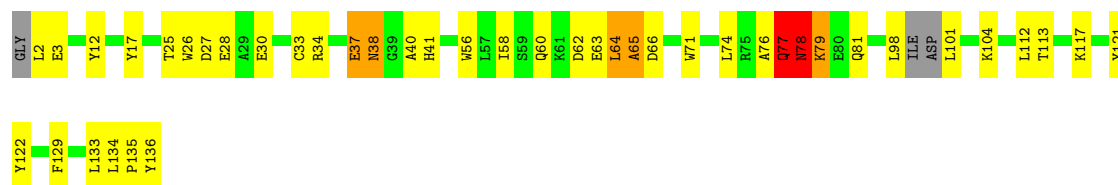
- Molecule 1: C-type lectin domain family 1 member B

Chain F: 

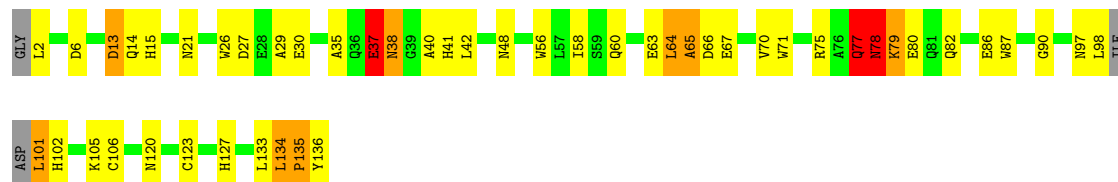


- Molecule 2: Snaclec rhodocytin subunit alpha

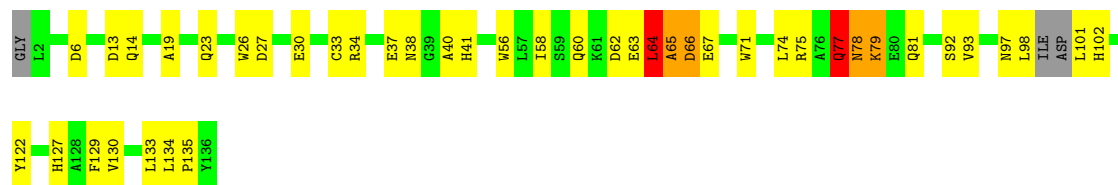
Chain A: 



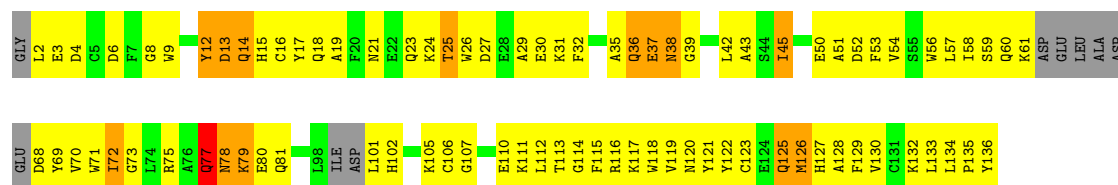
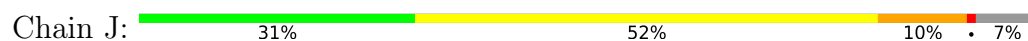
• Molecule 2: Snaclec rhodocytin subunit alpha



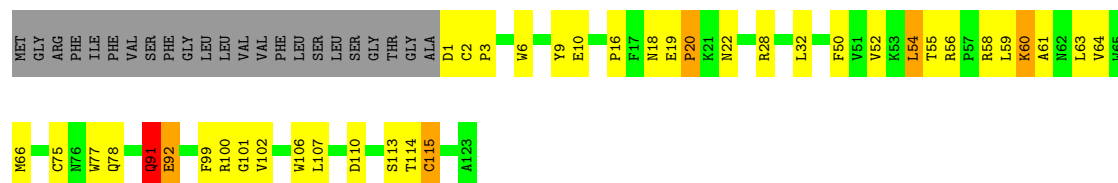
• Molecule 2: Snaclec rhodocytin subunit alpha



• Molecule 2: Snaclec rhodocytin subunit alpha

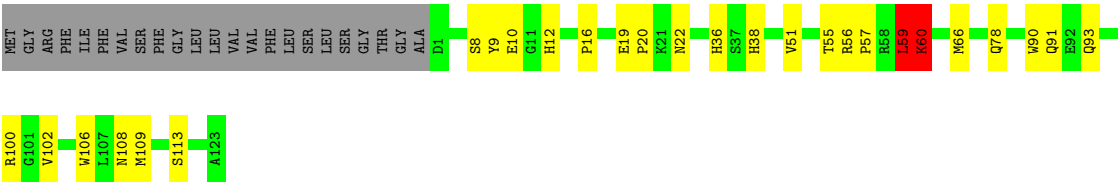


• Molecule 3: Snaclec rhodocytin subunit beta

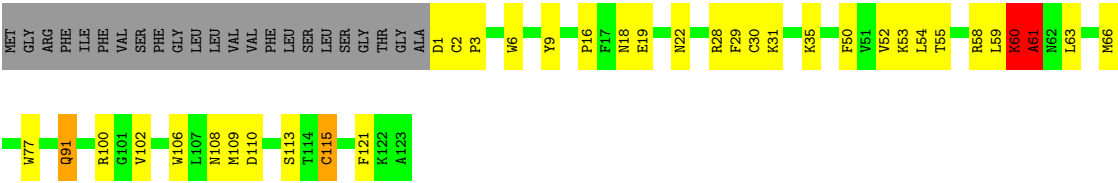


• Molecule 3: Snaclec rhodocytin subunit beta

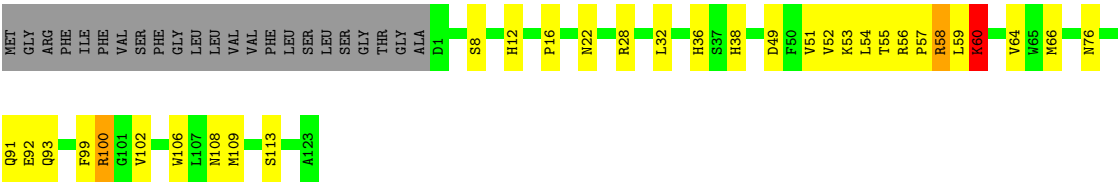




• Molecule 3: Snaclec rhodocytin subunit beta



• Molecule 3: Snaclec rhodocytin subunit beta





## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | C 1 2 1                                                     | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 130.85Å 117.07Å 152.24Å<br>90.00° 115.78° 90.00°            | Depositor        |
| Resolution (Å)                                                          | 37.56 – 2.98<br>37.56 – 2.98                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 98.0 (37.56-2.98)<br>98.3 (37.56-2.98)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | 0.10                                                        | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 3.97 (at 3.01Å)                                             | Xtriage          |
| Refinement program                                                      | REFMAC 5.8.0049                                             | Depositor        |
| R, $R_{free}$                                                           | 0.282 , 0.325<br>0.282 , 0.322                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 2117 reflections (3.55%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 50.4                                                        | Xtriage          |
| Anisotropy                                                              | 0.587                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.25 , 18.3                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$ | Xtriage          |
| Estimated twinning fraction                                             | 0.347 for h,-k,-h-l                                         | Xtriage          |
| Reported twinning fraction                                              | 0.649 for H, K, L<br>0.351 for -H, -K, H+L                  | Depositor        |
| Outliers                                                                | 2 of 41626 reflections (0.005%)                             | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.94                                                        | EDS              |
| Total number of atoms                                                   | 12453                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 60.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% 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   | C     | 0.59         | 0/1052         | 0.82        | 0/1415          |
| 1   | F     | 0.58         | 0/1052         | 0.81        | 0/1415          |
| 1   | I     | 0.61         | 0/1052         | 0.80        | 0/1415          |
| 1   | L     | 0.71         | 0/1052         | 0.94        | 1/1415 (0.1%)   |
| 2   | A     | 0.71         | 1/1121 (0.1%)  | 1.17        | 5/1513 (0.3%)   |
| 2   | D     | 0.70         | 0/1121         | 1.34        | 15/1513 (1.0%)  |
| 2   | G     | 0.67         | 1/1121 (0.1%)  | 1.16        | 11/1513 (0.7%)  |
| 2   | J     | 0.69         | 0/1073         | 1.25        | 8/1446 (0.6%)   |
| 3   | B     | 0.83         | 3/1045 (0.3%)  | 1.11        | 8/1416 (0.6%)   |
| 3   | E     | 0.71         | 0/1045         | 1.08        | 4/1416 (0.3%)   |
| 3   | H     | 0.79         | 1/1045 (0.1%)  | 1.18        | 12/1416 (0.8%)  |
| 3   | K     | 0.75         | 2/1045 (0.2%)  | 1.10        | 5/1416 (0.4%)   |
| All | All   | 0.70         | 8/12824 (0.1%) | 1.08        | 69/17309 (0.4%) |

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 |
|-----|-------|---------------------|---------------------|
| 2   | A     | 0                   | 6                   |
| 2   | D     | 0                   | 6                   |
| 2   | G     | 0                   | 5                   |
| 2   | J     | 0                   | 4                   |
| 3   | B     | 0                   | 2                   |
| 3   | E     | 0                   | 2                   |
| 3   | H     | 0                   | 3                   |
| 3   | K     | 0                   | 2                   |
| All | All   | 0                   | 30                  |

All (8) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 3   | B     | 91  | GLN  | CA-C  | -9.13 | 1.41        | 1.52     |
| 3   | K     | 58  | ARG  | CA-C  | -7.07 | 1.43        | 1.52     |
| 3   | H     | 91  | GLN  | CA-C  | -7.06 | 1.43        | 1.52     |
| 3   | B     | 60  | LYS  | CA-C  | -6.04 | 1.45        | 1.53     |
| 3   | K     | 60  | LYS  | CA-C  | 5.49  | 1.59        | 1.53     |
| 2   | G     | 66  | ASP  | CA-C  | 5.43  | 1.60        | 1.52     |
| 3   | B     | 115 | CYS  | CA-C  | -5.26 | 1.45        | 1.52     |
| 2   | A     | 78  | ASN  | N-CA  | -5.19 | 1.39        | 1.46     |

All (69) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 2   | A     | 79  | LYS  | N-CA-C  | 16.75  | 132.82      | 112.38   |
| 3   | E     | 60  | LYS  | N-CA-C  | 16.00  | 136.46      | 111.81   |
| 3   | K     | 60  | LYS  | N-CA-C  | 14.66  | 134.08      | 108.56   |
| 2   | D     | 79  | LYS  | N-CA-C  | 14.37  | 130.70      | 112.89   |
| 2   | A     | 78  | ASN  | N-CA-CB | -13.34 | 89.60       | 110.28   |
| 2   | D     | 77  | GLN  | N-CA-C  | 12.33  | 129.05      | 112.90   |
| 3   | H     | 60  | LYS  | N-CA-C  | 12.15  | 126.03      | 110.24   |
| 2   | D     | 78  | ASN  | N-CA-C  | -10.83 | 87.72       | 110.80   |
| 2   | A     | 38  | ASN  | N-CA-C  | -10.76 | 90.72       | 108.48   |
| 3   | K     | 58  | ARG  | N-CA-C  | 10.51  | 133.19      | 110.80   |
| 3   | H     | 61  | ALA  | N-CA-C  | 9.94   | 131.97      | 110.80   |
| 2   | G     | 38  | ASN  | N-CA-C  | -9.72  | 92.44       | 108.48   |
| 3   | H     | 18  | ASN  | N-CA-C  | 9.50   | 125.49      | 111.81   |
| 2   | J     | 79  | LYS  | N-CA-C  | 9.34   | 122.65      | 111.82   |
| 2   | G     | 64  | LEU  | CA-C-N  | -9.03  | 107.72      | 122.08   |
| 2   | G     | 64  | LEU  | C-N-CA  | -9.03  | 107.72      | 122.08   |
| 2   | D     | 37  | GLU  | N-CA-C  | 8.70   | 123.51      | 110.64   |
| 2   | J     | 38  | ASN  | N-CA-C  | -8.70  | 92.28       | 110.80   |
| 2   | J     | 12  | TYR  | CB-CA-C | -8.48  | 100.92      | 111.43   |
| 2   | D     | 13  | ASP  | N-CA-C  | 8.39   | 120.73      | 110.91   |
| 3   | E     | 60  | LYS  | CB-CA-C | -8.35  | 97.03       | 111.23   |
| 2   | D     | 134 | LEU  | CA-C-N  | 8.26   | 128.19      | 119.85   |
| 2   | D     | 134 | LEU  | C-N-CA  | 8.26   | 128.19      | 119.85   |
| 2   | G     | 135 | PRO  | CA-C-N  | 7.90   | 135.92      | 121.70   |
| 2   | G     | 135 | PRO  | C-N-CA  | 7.90   | 135.92      | 121.70   |
| 2   | J     | 25  | THR  | CB-CA-C | -7.69  | 96.51       | 109.65   |
| 2   | G     | 64  | LEU  | N-CA-C  | -7.46  | 96.25       | 108.41   |
| 2   | A     | 78  | ASN  | N-CA-C  | 7.24   | 120.21      | 111.82   |
| 3   | K     | 58  | ARG  | CB-CA-C | -7.11  | 96.26       | 110.42   |
| 2   | D     | 38  | ASN  | N-CA-C  | -7.09  | 95.70       | 110.80   |
| 2   | J     | 39  | GLY  | N-CA-C  | -6.93  | 96.76       | 113.18   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | H     | 60  | LYS  | CA-C-N  | 6.77  | 134.47      | 121.54   |
| 3   | H     | 60  | LYS  | C-N-CA  | 6.77  | 134.47      | 121.54   |
| 3   | B     | 92  | GLU  | N-CA-C  | 6.75  | 125.17      | 110.80   |
| 2   | G     | 135 | PRO  | N-CA-C  | 6.74  | 121.54      | 110.55   |
| 2   | G     | 97  | ASN  | N-CA-C  | 6.68  | 120.66      | 111.71   |
| 2   | D     | 102 | HIS  | N-CA-C  | 6.61  | 120.41      | 107.98   |
| 3   | H     | 60  | LYS  | CA-C-O  | 6.47  | 128.43      | 121.44   |
| 2   | D     | 38  | ASN  | CA-C-N  | -6.32 | 109.02      | 121.41   |
| 2   | D     | 38  | ASN  | C-N-CA  | -6.32 | 109.02      | 121.41   |
| 2   | G     | 77  | GLN  | CA-C-N  | -6.22 | 112.59      | 122.29   |
| 2   | G     | 77  | GLN  | C-N-CA  | -6.22 | 112.59      | 122.29   |
| 3   | H     | 18  | ASN  | CB-CA-C | -6.20 | 103.50      | 111.50   |
| 2   | J     | 12  | TYR  | N-CA-C  | 6.16  | 117.67      | 107.20   |
| 3   | H     | 60  | LYS  | CB-CA-C | -6.03 | 98.97       | 109.64   |
| 2   | D     | 78  | ASN  | CB-CA-C | 6.01  | 122.37      | 110.42   |
| 2   | D     | 101 | LEU  | CA-C-N  | -5.83 | 113.01      | 122.34   |
| 2   | D     | 101 | LEU  | C-N-CA  | -5.83 | 113.01      | 122.34   |
| 3   | K     | 60  | LYS  | CB-CA-C | -5.80 | 102.97      | 112.03   |
| 3   | E     | 60  | LYS  | N-CA-CB | -5.76 | 102.84      | 111.25   |
| 3   | B     | 19  | GLU  | CA-C-N  | 5.74  | 127.28      | 120.23   |
| 3   | B     | 19  | GLU  | C-N-CA  | 5.74  | 127.28      | 120.23   |
| 3   | H     | 19  | GLU  | CA-C-N  | 5.65  | 126.53      | 119.98   |
| 3   | H     | 19  | GLU  | C-N-CA  | 5.65  | 126.53      | 119.98   |
| 2   | J     | 113 | THR  | CB-CA-C | 5.59  | 119.43      | 110.09   |
| 2   | A     | 77  | GLN  | N-CA-C  | 5.55  | 122.62      | 110.80   |
| 2   | G     | 79  | LYS  | N-CA-C  | 5.47  | 119.57      | 113.01   |
| 3   | B     | 20  | PRO  | CA-C-N  | 5.32  | 130.92      | 122.62   |
| 3   | B     | 20  | PRO  | C-N-CA  | 5.32  | 130.92      | 122.62   |
| 2   | J     | 45  | ILE  | CB-CA-C | -5.28 | 102.63      | 111.29   |
| 3   | B     | 61  | ALA  | N-CA-C  | 5.21  | 121.90      | 110.80   |
| 3   | B     | 54  | LEU  | CA-C-N  | 5.20  | 127.68      | 120.29   |
| 3   | B     | 54  | LEU  | C-N-CA  | 5.20  | 127.68      | 120.29   |
| 3   | E     | 59  | LEU  | N-CA-C  | 5.16  | 119.15      | 113.21   |
| 2   | D     | 135 | PRO  | N-CA-C  | 5.15  | 119.57      | 111.38   |
| 3   | H     | 115 | CYS  | N-CA-CB | -5.13 | 103.60      | 111.56   |
| 3   | K     | 100 | ARG  | CA-C-O  | -5.13 | 116.11      | 121.55   |
| 3   | H     | 19  | GLU  | CB-CA-C | -5.07 | 100.19      | 110.17   |
| 1   | L     | 135 | ALA  | N-CA-C  | 5.01  | 117.74      | 109.72   |

There are no chirality outliers.

All (30) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group             |
|-----|-------|-----|------|-------------------|
| 2   | A     | 37  | GLU  | Peptide           |
| 2   | A     | 64  | LEU  | Peptide           |
| 2   | A     | 65  | ALA  | Peptide           |
| 2   | A     | 77  | GLN  | Mainchain,Peptide |
| 2   | A     | 78  | ASN  | Peptide           |
| 3   | B     | 60  | LYS  | Peptide           |
| 3   | B     | 91  | GLN  | Peptide           |
| 2   | D     | 37  | GLU  | Peptide           |
| 2   | D     | 64  | LEU  | Peptide           |
| 2   | D     | 65  | ALA  | Peptide           |
| 2   | D     | 77  | GLN  | Peptide           |
| 2   | D     | 78  | ASN  | Mainchain,Peptide |
| 3   | E     | 59  | LEU  | Peptide           |
| 3   | E     | 60  | LYS  | Peptide           |
| 2   | G     | 37  | GLU  | Peptide           |
| 2   | G     | 64  | LEU  | Peptide           |
| 2   | G     | 65  | ALA  | Peptide           |
| 2   | G     | 77  | GLN  | Peptide           |
| 2   | G     | 78  | ASN  | Peptide           |
| 3   | H     | 60  | LYS  | Mainchain,Peptide |
| 3   | H     | 91  | GLN  | Peptide           |
| 2   | J     | 36  | GLN  | Peptide           |
| 2   | J     | 37  | GLU  | Peptide           |
| 2   | J     | 77  | GLN  | Peptide           |
| 2   | J     | 78  | ASN  | Peptide           |
| 3   | K     | 58  | ARG  | Mainchain         |
| 3   | K     | 60  | LYS  | Peptide           |

## 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   | C     | 1023  | 0        | 947      | 25      | 0            |
| 1   | F     | 1023  | 0        | 947      | 38      | 0            |
| 1   | I     | 1023  | 0        | 947      | 19      | 0            |
| 1   | L     | 1023  | 0        | 947      | 131     | 0            |
| 2   | A     | 1092  | 0        | 984      | 67      | 0            |
| 2   | D     | 1092  | 0        | 984      | 67      | 1            |
| 2   | G     | 1092  | 0        | 984      | 43      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | J     | 1045  | 0        | 947      | 186     | 1            |
| 3   | B     | 1010  | 0        | 932      | 41      | 0            |
| 3   | E     | 1010  | 0        | 930      | 31      | 0            |
| 3   | H     | 1010  | 0        | 932      | 32      | 0            |
| 3   | K     | 1010  | 0        | 932      | 35      | 0            |
| All | All   | 12453 | 0        | 11413    | 686     | 1            |

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 29.

All (686) 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) |
|-----------------|------------------|--------------------------|-------------------|
| 2:J:45:ILE:HD11 | 2:J:51:ALA:CB    | 1.57                     | 1.34              |
| 2:G:78:ASN:OD1  | 2:G:79:LYS:HA    | 1.30                     | 1.28              |
| 1:L:196:ALA:HA  | 1:L:204:HIS:O    | 1.08                     | 1.25              |
| 1:L:130:CYS:HB3 | 1:L:136:THR:N    | 1.49                     | 1.25              |
| 2:J:45:ILE:CD1  | 2:J:51:ALA:HB2   | 1.70                     | 1.22              |
| 1:L:130:CYS:HB3 | 1:L:135:ALA:C    | 1.62                     | 1.22              |
| 2:J:17:TYR:CE1  | 2:J:132:LYS:HD2  | 1.75                     | 1.20              |
| 3:K:16:PRO:HB2  | 3:K:59:LEU:CD1   | 1.70                     | 1.20              |
| 2:J:18:GLN:O    | 2:J:130:VAL:HG13 | 1.40                     | 1.20              |
| 2:J:78:ASN:OD1  | 2:J:79:LYS:HA    | 1.42                     | 1.20              |
| 1:L:196:ALA:CA  | 1:L:204:HIS:O    | 1.90                     | 1.19              |
| 2:G:78:ASN:OD1  | 2:G:79:LYS:CA    | 1.91                     | 1.18              |
| 1:L:130:CYS:C   | 1:L:135:ALA:HB3  | 1.69                     | 1.17              |
| 1:L:130:CYS:O   | 1:L:135:ALA:HB3  | 1.43                     | 1.17              |
| 2:J:26:TRP:CD1  | 2:J:71:TRP:CE3   | 2.33                     | 1.16              |
| 2:J:110:GLU:HG3 | 2:J:119:VAL:HG21 | 1.20                     | 1.13              |
| 1:L:195:CYS:O   | 1:L:206:THR:N    | 1.80                     | 1.13              |
| 2:G:78:ASN:OD1  | 2:G:79:LYS:C     | 1.91                     | 1.13              |
| 1:L:130:CYS:CA  | 1:L:135:ALA:HB3  | 1.79                     | 1.13              |
| 2:J:112:LEU:O   | 2:J:112:LEU:HG   | 1.48                     | 1.13              |
| 3:B:20:PRO:HB2  | 3:B:114:THR:HG22 | 1.26                     | 1.12              |
| 2:J:45:ILE:HG21 | 2:J:118:TRP:CZ2  | 1.83                     | 1.12              |
| 2:A:38:ASN:ND2  | 2:A:136:TYR:HB3  | 1.64                     | 1.12              |
| 2:D:78:ASN:HD22 | 2:D:79:LYS:HA    | 1.12                     | 1.12              |
| 2:J:15:HIS:CD2  | 2:J:134:LEU:HD12 | 1.86                     | 1.11              |
| 2:J:68:ASP:O    | 2:J:111:LYS:HB2  | 1.51                     | 1.11              |
| 1:C:139:LYS:HE3 | 1:C:141:ASP:OD2  | 1.50                     | 1.10              |
| 1:L:130:CYS:O   | 1:L:135:ALA:CB   | 1.98                     | 1.10              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:J:26:TRP:HD1   | 2:J:71:TRP:CE3   | 1.69                     | 1.08              |
| 1:L:130:CYS:O    | 1:L:135:ALA:N    | 1.86                     | 1.08              |
| 2:J:6:ASP:O      | 2:J:9:TRP:O      | 1.73                     | 1.06              |
| 2:J:45:ILE:CG2   | 2:J:118:TRP:HZ2  | 1.68                     | 1.06              |
| 2:D:78:ASN:ND2   | 2:D:79:LYS:HA    | 1.68                     | 1.06              |
| 2:J:45:ILE:CG2   | 2:J:45:ILE:O     | 1.95                     | 1.05              |
| 1:F:137:LEU:CD2  | 1:F:214:LEU:HD11 | 1.86                     | 1.05              |
| 2:J:45:ILE:HG21  | 2:J:118:TRP:HZ2  | 0.93                     | 1.04              |
| 1:L:170:TRP:CH2  | 1:L:205:PRO:HB3  | 1.90                     | 1.04              |
| 2:J:126:MET:O    | 2:J:127:HIS:CD2  | 2.11                     | 1.04              |
| 2:J:110:GLU:CG   | 2:J:119:VAL:HG21 | 1.87                     | 1.03              |
| 2:J:78:ASN:OD1   | 2:J:79:LYS:CA    | 2.07                     | 1.03              |
| 2:A:81:GLN:HG3   | 2:A:98:LEU:HD12  | 1.03                     | 1.02              |
| 2:D:56:TRP:O     | 2:D:60:GLN:HG2   | 1.60                     | 1.02              |
| 1:F:138:LEU:HD13 | 1:F:215:MET:HG3  | 1.37                     | 1.02              |
| 2:A:38:ASN:HD22  | 2:A:136:TYR:HB3  | 1.20                     | 1.01              |
| 3:K:16:PRO:HB2   | 3:K:59:LEU:HD13  | 1.39                     | 1.01              |
| 1:L:130:CYS:O    | 1:L:135:ALA:CA   | 2.07                     | 1.01              |
| 3:K:60:LYS:O     | 3:K:60:LYS:HG2   | 1.58                     | 1.01              |
| 1:L:130:CYS:HA   | 1:L:135:ALA:HB3  | 1.37                     | 1.00              |
| 2:J:68:ASP:HA    | 2:J:111:LYS:CG   | 1.92                     | 1.00              |
| 1:L:130:CYS:CA   | 1:L:135:ALA:CB   | 2.40                     | 1.00              |
| 3:E:91:GLN:HG3   | 3:E:93:GLN:NE2   | 1.77                     | 0.99              |
| 2:J:17:TYR:HE1   | 2:J:132:LYS:HD2  | 0.86                     | 0.99              |
| 1:L:126:SER:HB3  | 1:L:137:LEU:HD21 | 1.41                     | 0.99              |
| 2:J:17:TYR:HE1   | 2:J:132:LYS:CD   | 1.76                     | 0.99              |
| 1:L:130:CYS:CB   | 1:L:135:ALA:C    | 2.36                     | 0.98              |
| 1:L:130:CYS:C    | 1:L:135:ALA:CB   | 2.35                     | 0.98              |
| 1:L:156:ILE:O    | 1:L:157:ARG:HG2  | 1.63                     | 0.98              |
| 2:J:45:ILE:O     | 2:J:45:ILE:HG23  | 1.18                     | 0.98              |
| 3:K:16:PRO:HB2   | 3:K:59:LEU:HD11  | 1.43                     | 0.98              |
| 1:L:126:SER:HB3  | 1:L:214:LEU:CD1  | 1.95                     | 0.97              |
| 1:F:137:LEU:HD23 | 1:F:214:LEU:HD11 | 1.46                     | 0.97              |
| 1:L:126:SER:CB   | 1:L:214:LEU:HD12 | 1.94                     | 0.97              |
| 2:D:78:ASN:HD22  | 2:D:79:LYS:CA    | 1.77                     | 0.97              |
| 3:H:60:LYS:HG3   | 3:H:60:LYS:O     | 1.64                     | 0.97              |
| 2:A:81:GLN:HG3   | 2:A:98:LEU:CD1   | 1.96                     | 0.96              |
| 2:J:12:TYR:O     | 2:J:12:TYR:CD2   | 2.18                     | 0.96              |
| 2:A:81:GLN:CG    | 2:A:98:LEU:HD12  | 1.95                     | 0.96              |
| 2:J:126:MET:O    | 2:J:127:HIS:HD2  | 1.45                     | 0.95              |
| 1:L:167:ASN:ND2  | 1:L:191:GLY:O    | 1.99                     | 0.95              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:78:ASN:ND2   | 2:D:79:LYS:CA    | 2.28                     | 0.95              |
| 1:L:130:CYS:HA   | 1:L:135:ALA:CB   | 1.96                     | 0.95              |
| 2:A:58:ILE:HG23  | 2:A:64:LEU:HD22  | 1.49                     | 0.94              |
| 1:L:131:THR:N    | 1:L:135:ALA:O    | 2.01                     | 0.93              |
| 2:J:23:GLN:HA    | 2:J:127:HIS:O    | 1.67                     | 0.93              |
| 2:J:15:HIS:HB2   | 2:J:17:TYR:CZ    | 2.03                     | 0.93              |
| 3:B:20:PRO:HB2   | 3:B:114:THR:CG2  | 1.97                     | 0.93              |
| 2:J:53:PHE:O     | 2:J:53:PHE:CD2   | 2.21                     | 0.93              |
| 2:J:78:ASN:OD1   | 2:J:79:LYS:C     | 2.11                     | 0.93              |
| 3:E:16:PRO:HB2   | 3:E:59:LEU:HD13  | 1.49                     | 0.92              |
| 1:L:130:CYS:C    | 1:L:135:ALA:CA   | 2.43                     | 0.90              |
| 1:L:126:SER:CB   | 1:L:214:LEU:CD1  | 2.48                     | 0.90              |
| 2:A:78:ASN:ND2   | 2:A:79:LYS:HA    | 1.86                     | 0.90              |
| 2:D:26:TRP:CE3   | 2:D:27:ASP:OD1   | 2.23                     | 0.90              |
| 2:G:78:ASN:CG    | 2:G:79:LYS:HA    | 1.96                     | 0.90              |
| 2:D:15:HIS:CD2   | 2:D:134:LEU:HB3  | 2.07                     | 0.90              |
| 2:J:15:HIS:CD2   | 2:J:134:LEU:CD1  | 2.54                     | 0.90              |
| 1:C:136:THR:HG23 | 1:C:173:GLU:HG2  | 1.52                     | 0.90              |
| 2:J:71:TRP:CZ3   | 2:J:106:CYS:HB2  | 2.08                     | 0.89              |
| 1:L:126:SER:CB   | 1:L:137:LEU:HD21 | 2.01                     | 0.89              |
| 1:L:126:SER:OG   | 1:L:214:LEU:HD12 | 1.73                     | 0.88              |
| 3:E:56:ARG:O     | 3:E:60:LYS:HB3   | 1.73                     | 0.88              |
| 2:J:26:TRP:HD1   | 2:J:71:TRP:CD2   | 1.91                     | 0.88              |
| 2:J:58:ILE:HD13  | 2:J:70:VAL:HG21  | 1.56                     | 0.88              |
| 2:J:68:ASP:HA    | 2:J:111:LYS:HG3  | 1.55                     | 0.88              |
| 2:J:56:TRP:O     | 2:J:57:LEU:HD12  | 1.74                     | 0.88              |
| 3:H:28:ARG:O     | 3:H:31:LYS:N     | 2.07                     | 0.87              |
| 3:B:55:THR:HG21  | 3:B:101:GLY:HA2  | 1.56                     | 0.87              |
| 3:B:52:VAL:O     | 3:B:56:ARG:HG3   | 1.75                     | 0.86              |
| 3:K:52:VAL:O     | 3:K:56:ARG:HG3   | 1.73                     | 0.86              |
| 3:B:20:PRO:HA    | 3:B:115:CYS:O    | 1.75                     | 0.85              |
| 2:J:45:ILE:HD11  | 2:J:51:ALA:HB2   | 0.86                     | 0.85              |
| 3:H:28:ARG:O     | 3:H:29:PHE:C     | 2.20                     | 0.84              |
| 1:F:100:SER:HB2  | 1:F:101:PRO:HD3  | 1.59                     | 0.84              |
| 2:J:14:GLN:O     | 2:J:135:PRO:HD2  | 1.76                     | 0.84              |
| 2:A:81:GLN:HG2   | 2:A:98:LEU:HB2   | 1.60                     | 0.83              |
| 2:D:40:ALA:HB2   | 2:D:133:LEU:HB2  | 1.60                     | 0.83              |
| 2:J:26:TRP:NE1   | 2:J:72:ILE:O     | 2.10                     | 0.83              |
| 1:L:130:CYS:CB   | 1:L:136:THR:N    | 2.37                     | 0.83              |
| 1:L:130:CYS:C    | 1:L:135:ALA:C    | 2.46                     | 0.83              |
| 1:L:170:TRP:HH2  | 1:L:205:PRO:HB3  | 1.39                     | 0.83              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:126:SER:HB3  | 1:F:214:LEU:HD13 | 1.60                     | 0.83              |
| 2:J:12:TYR:O     | 2:J:17:TYR:HE2   | 1.61                     | 0.83              |
| 3:K:16:PRO:HD3   | 3:K:54:LEU:HD21  | 1.61                     | 0.83              |
| 2:J:15:HIS:NE2   | 2:J:134:LEU:CD1  | 2.42                     | 0.82              |
| 2:J:56:TRP:O     | 2:J:56:TRP:CD2   | 2.32                     | 0.82              |
| 2:A:78:ASN:HD22  | 2:A:79:LYS:HA    | 1.43                     | 0.82              |
| 3:K:16:PRO:CB    | 3:K:59:LEU:HD13  | 2.08                     | 0.82              |
| 2:J:15:HIS:NE2   | 2:J:134:LEU:HD13 | 1.94                     | 0.82              |
| 1:L:100:SER:HB2  | 1:L:101:PRO:HD3  | 1.61                     | 0.82              |
| 1:L:170:TRP:CZ2  | 1:L:205:PRO:HB3  | 2.13                     | 0.82              |
| 2:J:2:LEU:HD23   | 2:J:4:ASP:H      | 1.45                     | 0.82              |
| 1:F:100:SER:HB2  | 1:F:101:PRO:CD   | 2.10                     | 0.81              |
| 2:J:110:GLU:HG3  | 2:J:119:VAL:CG2  | 2.08                     | 0.81              |
| 1:L:100:SER:HB2  | 1:L:101:PRO:CD   | 2.10                     | 0.81              |
| 1:L:170:TRP:CH2  | 1:L:205:PRO:CB   | 2.64                     | 0.81              |
| 1:L:195:CYS:O    | 1:L:205:PRO:HA   | 1.80                     | 0.81              |
| 3:B:20:PRO:CB    | 3:B:114:THR:HG22 | 2.09                     | 0.80              |
| 1:C:100:SER:OG   | 1:C:101:PRO:CD   | 2.30                     | 0.80              |
| 1:C:197:TYR:CE2  | 1:C:206:THR:HG21 | 2.17                     | 0.80              |
| 1:L:156:ILE:CG2  | 1:L:157:ARG:N    | 2.44                     | 0.80              |
| 1:L:156:ILE:HG22 | 1:L:157:ARG:N    | 1.97                     | 0.80              |
| 2:G:98:LEU:O     | 2:G:101:LEU:HD12 | 1.82                     | 0.79              |
| 2:A:38:ASN:HD21  | 2:A:136:TYR:C    | 1.91                     | 0.79              |
| 2:J:53:PHE:O     | 2:J:53:PHE:CG    | 2.35                     | 0.79              |
| 2:D:21:ASN:ND2   | 2:D:63:GLU:HG2   | 1.97                     | 0.79              |
| 1:L:138:LEU:HD13 | 1:L:215:MET:HG3  | 1.65                     | 0.79              |
| 3:E:16:PRO:HB2   | 3:E:59:LEU:CD1   | 2.12                     | 0.79              |
| 2:D:71:TRP:CD1   | 2:D:127:HIS:HB2  | 2.17                     | 0.78              |
| 2:G:58:ILE:HG23  | 2:G:64:LEU:HD22  | 1.64                     | 0.78              |
| 3:E:56:ARG:HB3   | 3:E:57:PRO:HD3   | 1.66                     | 0.78              |
| 1:L:158:TRP:HZ3  | 1:L:195:CYS:HB3  | 1.46                     | 0.78              |
| 2:D:71:TRP:HZ3   | 2:D:106:CYS:CB   | 1.97                     | 0.78              |
| 2:J:19:ALA:HB1   | 2:J:58:ILE:HG12  | 1.64                     | 0.78              |
| 2:J:110:GLU:CD   | 2:J:119:VAL:HG21 | 2.08                     | 0.78              |
| 1:F:137:LEU:CD2  | 1:F:214:LEU:CD1  | 2.61                     | 0.77              |
| 2:D:26:TRP:CZ3   | 2:D:27:ASP:OD1   | 2.37                     | 0.77              |
| 2:J:116:ARG:NH1  | 2:J:116:ARG:HB3  | 2.00                     | 0.77              |
| 2:J:68:ASP:C     | 2:J:111:LYS:HB2  | 2.10                     | 0.77              |
| 2:J:68:ASP:O     | 2:J:111:LYS:CB   | 2.33                     | 0.76              |
| 1:I:100:SER:OG   | 1:I:101:PRO:CD   | 2.34                     | 0.76              |
| 1:L:190:LYS:HG2  | 1:L:193:MET:HE2  | 1.66                     | 0.76              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:126:SER:HB3  | 1:L:214:LEU:HD11 | 1.65                     | 0.76              |
| 1:L:196:ALA:CB   | 1:L:204:HIS:O    | 2.33                     | 0.75              |
| 2:J:18:GLN:O     | 2:J:130:VAL:CG1  | 2.29                     | 0.75              |
| 2:J:112:LEU:O    | 2:J:112:LEU:CG   | 2.31                     | 0.75              |
| 2:G:133:LEU:HG   | 2:G:134:LEU:O    | 1.86                     | 0.75              |
| 2:J:56:TRP:O     | 2:J:56:TRP:CE3   | 2.40                     | 0.75              |
| 1:I:166:SER:HB3  | 1:I:191:GLY:O    | 1.86                     | 0.75              |
| 2:J:23:GLN:HG2   | 2:J:127:HIS:HA   | 1.69                     | 0.75              |
| 2:J:12:TYR:HB3   | 2:J:17:TYR:CD2   | 2.22                     | 0.74              |
| 1:L:141:ASP:HA   | 1:L:182:MET:HG3  | 1.67                     | 0.74              |
| 2:D:38:ASN:ND2   | 2:D:136:TYR:O    | 2.19                     | 0.74              |
| 1:C:100:SER:OG   | 1:C:101:PRO:HD3  | 1.86                     | 0.73              |
| 2:J:52:ASP:OD1   | 2:J:116:ARG:NH2  | 2.21                     | 0.73              |
| 2:A:117:LYS:HD3  | 3:B:91:GLN:NE2   | 2.03                     | 0.73              |
| 2:J:45:ILE:CG2   | 2:J:118:TRP:CZ2  | 2.54                     | 0.73              |
| 1:F:157:ARG:HD2  | 1:F:215:MET:HE2  | 1.69                     | 0.73              |
| 2:J:2:LEU:CD2    | 2:J:4:ASP:H      | 2.01                     | 0.73              |
| 1:F:159:VAL:HG22 | 1:F:160:GLY:H    | 1.52                     | 0.73              |
| 2:A:58:ILE:HG23  | 2:A:64:LEU:CD2   | 2.19                     | 0.73              |
| 2:D:26:TRP:HE3   | 2:D:27:ASP:OD1   | 1.68                     | 0.72              |
| 2:A:79:LYS:HD2   | 2:A:79:LYS:O     | 1.88                     | 0.72              |
| 1:L:156:ILE:C    | 1:L:157:ARG:CG   | 2.62                     | 0.72              |
| 2:A:66:ASP:OD1   | 2:A:66:ASP:O     | 2.08                     | 0.72              |
| 1:L:130:CYS:C    | 1:L:135:ALA:O    | 2.33                     | 0.72              |
| 1:F:166:SER:HB3  | 1:F:191:GLY:O    | 1.89                     | 0.72              |
| 3:H:63:LEU:C     | 3:H:115:CYS:SG   | 2.73                     | 0.72              |
| 2:J:68:ASP:HA    | 2:J:111:LYS:CB   | 2.18                     | 0.72              |
| 1:L:156:ILE:O    | 1:L:157:ARG:CG   | 2.37                     | 0.71              |
| 2:A:113:THR:CG2  | 2:A:117:LYS:HB2  | 2.19                     | 0.71              |
| 2:A:38:ASN:ND2   | 2:A:136:TYR:OXT  | 2.23                     | 0.71              |
| 2:D:58:ILE:HG23  | 2:D:64:LEU:HD22  | 1.72                     | 0.71              |
| 1:L:126:SER:HB3  | 1:L:214:LEU:HD12 | 1.60                     | 0.71              |
| 2:J:35:ALA:O     | 2:J:37:GLU:OE1   | 2.09                     | 0.71              |
| 3:B:55:THR:CG2   | 3:B:101:GLY:HA2  | 2.21                     | 0.71              |
| 2:G:75:ARG:HD3   | 2:G:77:GLN:HE22  | 1.54                     | 0.71              |
| 2:G:98:LEU:O     | 2:G:101:LEU:CD1  | 2.38                     | 0.70              |
| 3:H:63:LEU:C     | 3:H:115:CYS:HG   | 1.99                     | 0.70              |
| 2:J:125:GLN:HA   | 2:J:125:GLN:HE21 | 1.57                     | 0.70              |
| 1:I:100:SER:OG   | 1:I:101:PRO:HD3  | 1.92                     | 0.69              |
| 2:J:68:ASP:HA    | 2:J:111:LYS:HB2  | 1.74                     | 0.69              |
| 3:H:52:VAL:HA    | 3:H:55:THR:OG1   | 1.92                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:J:106:CYS:N    | 2:J:123:CYS:SG   | 2.65                     | 0.69              |
| 2:J:26:TRP:CD1   | 2:J:71:TRP:HE3   | 2.09                     | 0.69              |
| 1:L:139:LYS:NZ   | 1:L:174:ASP:OD2  | 2.25                     | 0.69              |
| 2:A:81:GLN:CG    | 2:A:98:LEU:HB2   | 2.23                     | 0.68              |
| 1:L:127:LYS:HZ1  | 1:L:173:GLU:CD   | 2.01                     | 0.68              |
| 2:A:2:LEU:O      | 2:A:3:GLU:HG2    | 1.92                     | 0.68              |
| 1:C:139:LYS:CE   | 1:C:141:ASP:OD2  | 2.38                     | 0.68              |
| 1:L:138:LEU:CD1  | 1:L:215:MET:HG3  | 2.22                     | 0.68              |
| 2:A:78:ASN:ND2   | 2:A:79:LYS:HD2   | 2.09                     | 0.68              |
| 1:L:158:TRP:CZ3  | 1:L:195:CYS:HB3  | 2.29                     | 0.67              |
| 2:A:113:THR:HG21 | 2:A:117:LYS:HB2  | 1.75                     | 0.67              |
| 2:J:116:ARG:HB3  | 2:J:116:ARG:HH11 | 1.57                     | 0.67              |
| 1:L:193:MET:HB3  | 1:L:206:THR:HA   | 1.76                     | 0.67              |
| 2:D:71:TRP:CH2   | 2:D:123:CYS:HA   | 2.28                     | 0.67              |
| 2:J:30:GLU:OE1   | 2:J:42:LEU:HD12  | 1.95                     | 0.67              |
| 1:L:195:CYS:HB2  | 1:L:206:THR:O    | 1.94                     | 0.67              |
| 2:A:56:TRP:O     | 2:A:60:GLN:HG2   | 1.94                     | 0.67              |
| 2:J:45:ILE:CD1   | 2:J:51:ALA:CB    | 2.47                     | 0.67              |
| 1:I:118:ARG:NH2  | 2:G:6:ASP:OD1    | 2.26                     | 0.67              |
| 2:A:30:GLU:OE1   | 2:A:41:HIS:HD2   | 1.78                     | 0.66              |
| 2:J:17:TYR:CE1   | 2:J:132:LYS:CD   | 2.63                     | 0.66              |
| 1:L:163:ARG:HD2  | 1:L:168:GLU:O    | 1.94                     | 0.66              |
| 1:L:190:LYS:H    | 1:L:193:MET:HE3  | 1.60                     | 0.66              |
| 2:G:30:GLU:OE1   | 2:G:41:HIS:HD2   | 1.79                     | 0.66              |
| 2:A:25:THR:HG23  | 2:A:28:GLU:H     | 1.61                     | 0.66              |
| 2:D:71:TRP:HZ3   | 2:D:106:CYS:HB3  | 1.59                     | 0.66              |
| 2:J:53:PHE:CD2   | 2:J:53:PHE:C     | 2.74                     | 0.66              |
| 2:A:135:PRO:O    | 2:A:136:TYR:HB2  | 1.95                     | 0.66              |
| 3:K:16:PRO:CB    | 3:K:59:LEU:CD1   | 2.59                     | 0.65              |
| 1:L:140:ILE:O    | 1:L:172:TRP:CZ2  | 2.49                     | 0.65              |
| 2:A:78:ASN:CB    | 2:A:79:LYS:HA    | 2.26                     | 0.65              |
| 1:L:163:ARG:CD   | 1:L:168:GLU:O    | 2.45                     | 0.65              |
| 2:D:71:TRP:HZ3   | 2:D:106:CYS:HB2  | 1.60                     | 0.65              |
| 2:J:12:TYR:O     | 2:J:17:TYR:CE2   | 2.47                     | 0.65              |
| 2:J:2:LEU:HD23   | 2:J:3:GLU:N      | 2.11                     | 0.65              |
| 1:L:195:CYS:N    | 1:L:206:THR:O    | 2.27                     | 0.65              |
| 1:L:143:ARG:HG2  | 1:L:185:PHE:CE2  | 2.31                     | 0.65              |
| 2:J:71:TRP:HZ3   | 2:J:106:CYS:HB2  | 1.62                     | 0.64              |
| 2:J:68:ASP:CA    | 2:J:111:LYS:HB2  | 2.28                     | 0.64              |
| 1:C:197:TYR:HE2  | 1:C:206:THR:HG21 | 1.60                     | 0.64              |
| 2:J:12:TYR:HB3   | 2:J:17:TYR:HD2   | 1.63                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:J:16:CYS:N     | 2:J:133:LEU:O    | 2.31                     | 0.64              |
| 1:C:166:SER:HB3  | 1:C:191:GLY:O    | 1.98                     | 0.64              |
| 2:J:45:ILE:CG1   | 2:J:51:ALA:HB2   | 2.27                     | 0.64              |
| 2:J:80:GLU:O     | 2:J:105:LYS:NZ   | 2.18                     | 0.64              |
| 2:J:12:TYR:O     | 2:J:12:TYR:HD2   | 1.77                     | 0.63              |
| 2:J:45:ILE:HD11  | 2:J:51:ALA:HB1   | 1.72                     | 0.63              |
| 1:L:138:LEU:HD13 | 1:L:215:MET:CG   | 2.27                     | 0.63              |
| 1:L:126:SER:CB   | 1:L:214:LEU:HD11 | 2.23                     | 0.63              |
| 2:G:30:GLU:O     | 2:G:34:ARG:HG2   | 1.98                     | 0.63              |
| 2:J:56:TRP:O     | 2:J:56:TRP:CG    | 2.49                     | 0.63              |
| 1:L:143:ARG:HG2  | 1:L:185:PHE:CZ   | 2.34                     | 0.63              |
| 1:F:159:VAL:HG22 | 1:F:160:GLY:N    | 2.13                     | 0.63              |
| 2:A:25:THR:HG22  | 2:A:28:GLU:CD    | 2.23                     | 0.62              |
| 1:C:141:ASP:OD1  | 1:C:172:TRP:NE1  | 2.32                     | 0.62              |
| 2:D:78:ASN:HD22  | 2:D:79:LYS:C     | 2.07                     | 0.62              |
| 3:H:16:PRO:HG2   | 3:H:58:ARG:HD3   | 1.82                     | 0.62              |
| 2:J:32:PHE:CE1   | 2:J:36:GLN:HG3   | 2.33                     | 0.62              |
| 1:L:195:CYS:O    | 1:L:205:PRO:CA   | 2.47                     | 0.62              |
| 2:D:21:ASN:HD22  | 2:D:63:GLU:HG2   | 1.63                     | 0.62              |
| 2:J:12:TYR:CD2   | 2:J:12:TYR:C     | 2.75                     | 0.62              |
| 2:A:33:CYS:O     | 2:A:40:ALA:HB3   | 2.00                     | 0.61              |
| 2:G:75:ARG:HD3   | 2:G:77:GLN:NE2   | 2.13                     | 0.61              |
| 2:J:125:GLN:HE21 | 2:J:125:GLN:CA   | 2.13                     | 0.61              |
| 1:L:140:ILE:HG23 | 1:L:145:ILE:HG23 | 1.83                     | 0.61              |
| 2:A:38:ASN:ND2   | 2:A:136:TYR:CB   | 2.53                     | 0.61              |
| 2:D:97:ASN:C     | 2:D:98:LEU:HD12  | 2.25                     | 0.61              |
| 2:J:23:GLN:HA    | 2:J:127:HIS:C    | 2.25                     | 0.61              |
| 2:J:68:ASP:CA    | 2:J:111:LYS:HG3  | 2.27                     | 0.61              |
| 2:A:63:GLU:O     | 2:A:65:ALA:HB2   | 2.01                     | 0.61              |
| 3:H:63:LEU:O     | 3:H:115:CYS:SG   | 2.53                     | 0.61              |
| 2:J:68:ASP:HA    | 2:J:111:LYS:CD   | 2.30                     | 0.61              |
| 2:D:71:TRP:CZ3   | 2:D:106:CYS:CB   | 2.84                     | 0.61              |
| 2:D:78:ASN:ND2   | 2:D:79:LYS:CB    | 2.63                     | 0.61              |
| 1:C:140:ILE:HG23 | 1:C:145:ILE:HG23 | 1.82                     | 0.60              |
| 3:B:16:PRO:HG2   | 3:B:58:ARG:HD3   | 1.82                     | 0.60              |
| 2:G:67:GLU:OE2   | 2:G:127:HIS:HD2  | 1.84                     | 0.60              |
| 2:J:26:TRP:CD1   | 2:J:71:TRP:CD2   | 2.78                     | 0.60              |
| 1:C:100:SER:OG   | 1:C:101:PRO:HD2  | 2.02                     | 0.60              |
| 2:A:117:LYS:HD3  | 3:B:91:GLN:HE21  | 1.64                     | 0.60              |
| 2:J:58:ILE:HD11  | 2:J:70:VAL:HG11  | 1.84                     | 0.60              |
| 2:A:77:GLN:HG3   | 3:B:78:GLN:HE21  | 1.66                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:78:ASN:HD22  | 2:A:79:LYS:CA    | 2.15                     | 0.60              |
| 1:L:190:LYS:H    | 1:L:193:MET:CE   | 2.14                     | 0.60              |
| 3:H:16:PRO:HB2   | 3:H:59:LEU:HD13  | 1.83                     | 0.60              |
| 2:D:65:ALA:H     | 2:D:67:GLU:N     | 2.00                     | 0.60              |
| 3:B:9:TYR:CZ     | 3:B:10:GLU:HG2   | 2.37                     | 0.60              |
| 3:E:91:GLN:CG    | 3:E:93:GLN:NE2   | 2.61                     | 0.60              |
| 2:A:78:ASN:ND2   | 2:A:79:LYS:CD    | 2.65                     | 0.59              |
| 2:A:78:ASN:CG    | 2:A:79:LYS:HA    | 2.26                     | 0.59              |
| 2:D:134:LEU:HD12 | 2:D:134:LEU:O    | 2.03                     | 0.59              |
| 2:D:26:TRP:HD1   | 2:D:71:TRP:CE3   | 2.21                     | 0.59              |
| 2:J:69:TYR:CE2   | 2:J:121:TYR:CZ   | 2.91                     | 0.59              |
| 3:K:56:ARG:HB2   | 3:K:57:PRO:HD3   | 1.84                     | 0.59              |
| 2:D:13:ASP:OD1   | 2:D:13:ASP:O     | 2.19                     | 0.59              |
| 2:D:71:TRP:CZ3   | 2:D:106:CYS:HB3  | 2.38                     | 0.59              |
| 1:F:206:THR:HG22 | 1:F:207:PHE:N    | 2.17                     | 0.59              |
| 3:H:16:PRO:HD3   | 3:H:54:LEU:HD21  | 1.83                     | 0.59              |
| 2:J:15:HIS:HB2   | 2:J:17:TYR:OH    | 2.00                     | 0.59              |
| 2:D:58:ILE:CG2   | 2:D:64:LEU:HD22  | 2.32                     | 0.59              |
| 1:I:100:SER:OG   | 1:I:101:PRO:HD2  | 2.03                     | 0.59              |
| 2:G:56:TRP:O     | 2:G:60:GLN:HG2   | 2.03                     | 0.59              |
| 3:B:16:PRO:HB2   | 3:B:59:LEU:HD13  | 1.84                     | 0.59              |
| 2:J:125:GLN:HA   | 2:J:125:GLN:NE2  | 2.18                     | 0.58              |
| 2:A:25:THR:HG22  | 2:A:28:GLU:CG    | 2.33                     | 0.58              |
| 2:A:78:ASN:ND2   | 2:A:79:LYS:CA    | 2.64                     | 0.58              |
| 1:F:138:LEU:HD22 | 1:F:215:MET:SD   | 2.43                     | 0.58              |
| 3:B:16:PRO:HB2   | 3:B:59:LEU:CD1   | 2.33                     | 0.58              |
| 1:I:140:ILE:HG23 | 1:I:145:ILE:HG23 | 1.84                     | 0.58              |
| 2:D:78:ASN:CG    | 2:D:79:LYS:HA    | 2.26                     | 0.58              |
| 2:J:12:TYR:HB3   | 2:J:17:TYR:CE2   | 2.39                     | 0.58              |
| 3:B:63:LEU:O     | 3:B:115:CYS:HB2  | 2.04                     | 0.57              |
| 2:J:26:TRP:HE3   | 2:J:27:ASP:OD1   | 1.87                     | 0.57              |
| 2:J:78:ASN:CG    | 2:J:79:LYS:HA    | 2.25                     | 0.57              |
| 1:F:138:LEU:O    | 1:F:159:VAL:HG22 | 2.04                     | 0.57              |
| 1:F:140:ILE:HG23 | 1:F:145:ILE:HG23 | 1.85                     | 0.57              |
| 1:L:195:CYS:O    | 1:L:205:PRO:C    | 2.46                     | 0.57              |
| 1:C:136:THR:HG22 | 1:C:137:LEU:O    | 2.04                     | 0.57              |
| 1:I:138:LEU:HD13 | 1:I:215:MET:HG3  | 1.85                     | 0.57              |
| 2:D:78:ASN:CB    | 2:D:79:LYS:HA    | 2.34                     | 0.57              |
| 1:F:166:SER:HA   | 1:F:194:ASN:OD1  | 2.05                     | 0.57              |
| 2:D:64:LEU:HD21  | 2:D:70:VAL:HG21  | 1.85                     | 0.57              |
| 2:J:58:ILE:CD1   | 2:J:70:VAL:HG11  | 2.35                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:J:12:TYR:HD2   | 2:J:17:TYR:HE2   | 1.52                     | 0.56              |
| 1:C:138:LEU:HD13 | 1:C:215:MET:HG3  | 1.86                     | 0.56              |
| 2:D:6:ASP:OD1    | 1:F:118:ARG:NH2  | 2.38                     | 0.56              |
| 3:B:63:LEU:HD11  | 3:B:107:LEU:HD12 | 1.86                     | 0.56              |
| 2:J:19:ALA:CB    | 2:J:58:ILE:HG12  | 2.34                     | 0.56              |
| 2:J:68:ASP:O     | 2:J:111:LYS:N    | 2.38                     | 0.56              |
| 1:L:123:TRP:HZ2  | 1:L:160:GLY:O    | 1.88                     | 0.56              |
| 1:L:130:CYS:HA   | 1:L:135:ALA:HB1  | 1.86                     | 0.56              |
| 1:L:165:LYS:HB2  | 1:L:168:GLU:HG3  | 1.87                     | 0.56              |
| 1:F:136:THR:HG22 | 1:F:137:LEU:O    | 2.05                     | 0.56              |
| 2:J:54:VAL:HG12  | 2:J:54:VAL:O     | 2.03                     | 0.56              |
| 2:D:40:ALA:HB2   | 2:D:133:LEU:HD13 | 1.86                     | 0.56              |
| 2:J:75:ARG:HG3   | 2:J:106:CYS:SG   | 2.45                     | 0.56              |
| 3:K:28:ARG:HG2   | 3:K:32:LEU:HD13  | 1.86                     | 0.56              |
| 1:L:156:ILE:CG2  | 1:L:157:ARG:H    | 2.19                     | 0.56              |
| 2:D:120:ASN:H    | 3:E:90:TRP:HZ3   | 1.54                     | 0.56              |
| 2:A:78:ASN:HD21  | 2:A:79:LYS:CD    | 2.19                     | 0.56              |
| 3:K:60:LYS:O     | 3:K:60:LYS:CG    | 2.39                     | 0.56              |
| 2:D:71:TRP:CZ3   | 2:D:106:CYS:HB2  | 2.41                     | 0.55              |
| 2:J:25:THR:HG22  | 2:J:27:ASP:H     | 1.72                     | 0.55              |
| 2:A:98:LEU:HD22  | 2:A:101:LEU:HD22 | 1.89                     | 0.55              |
| 2:G:79:LYS:O     | 2:G:79:LYS:HG3   | 2.06                     | 0.55              |
| 2:D:86:GLU:OE2   | 2:D:90:GLY:HA2   | 2.06                     | 0.55              |
| 2:J:71:TRP:CE3   | 2:J:107:GLY:O    | 2.59                     | 0.55              |
| 2:J:81:GLN:HA    | 2:J:105:LYS:NZ   | 2.22                     | 0.55              |
| 1:L:170:TRP:HH2  | 1:L:205:PRO:CB   | 2.10                     | 0.55              |
| 2:A:25:THR:HG22  | 2:A:28:GLU:OE1   | 2.07                     | 0.55              |
| 2:D:77:GLN:CG    | 3:E:78:GLN:HG3   | 2.37                     | 0.55              |
| 2:J:21:ASN:HB3   | 2:J:61:LYS:HD2   | 1.89                     | 0.55              |
| 2:G:122:TYR:HE2  | 3:K:102:VAL:HG21 | 1.70                     | 0.55              |
| 1:L:126:SER:HB2  | 1:L:137:LEU:HD21 | 1.87                     | 0.55              |
| 1:L:126:SER:CA   | 1:L:214:LEU:HD11 | 2.37                     | 0.55              |
| 1:L:120:ASN:O    | 1:L:121:LEU:HD23 | 2.06                     | 0.55              |
| 2:G:63:GLU:O     | 2:G:65:ALA:HB2   | 2.06                     | 0.54              |
| 3:B:100:ARG:NH2  | 3:E:108:ASN:OD1  | 2.40                     | 0.54              |
| 3:H:35:LYS:HG2   | 3:H:121:PHE:CE1  | 2.41                     | 0.54              |
| 2:J:4:ASP:OD1    | 1:L:157:ARG:NH2  | 2.38                     | 0.54              |
| 1:F:100:SER:CB   | 1:F:101:PRO:CD   | 2.83                     | 0.54              |
| 1:I:102:CYS:SG   | 1:I:108:TYR:HB2  | 2.48                     | 0.54              |
| 2:G:122:TYR:CE2  | 3:K:102:VAL:HG21 | 2.43                     | 0.54              |
| 2:J:19:ALA:HA    | 2:J:130:VAL:HG22 | 1.88                     | 0.54              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 2:J:2:LEU:HD21   | 2:J:4:ASP:HB2   | 1.89                     | 0.54              |
| 2:J:27:ASP:O     | 2:J:31:LYS:HG3  | 2.08                     | 0.54              |
| 2:J:119:VAL:HG12 | 2:J:120:ASN:O   | 2.08                     | 0.54              |
| 3:E:91:GLN:HG3   | 3:E:93:GLN:HE22 | 1.71                     | 0.54              |
| 2:J:8:GLY:O      | 2:J:18:GLN:CD   | 2.51                     | 0.54              |
| 2:J:30:GLU:HB2   | 2:J:42:LEU:HD12 | 1.90                     | 0.54              |
| 2:J:58:ILE:HG22  | 2:J:58:ILE:O    | 2.08                     | 0.53              |
| 2:D:66:ASP:OD1   | 2:D:66:ASP:O    | 2.26                     | 0.53              |
| 3:H:60:LYS:O     | 3:H:60:LYS:CG   | 2.46                     | 0.53              |
| 3:H:110:ASP:OD1  | 3:H:110:ASP:C   | 2.51                     | 0.53              |
| 2:J:30:GLU:HA    | 2:J:42:LEU:HG   | 1.90                     | 0.53              |
| 1:L:121:LEU:O    | 1:L:158:TRP:NE1 | 2.41                     | 0.53              |
| 2:D:80:GLU:HG2   | 2:D:82:GLN:O    | 2.09                     | 0.53              |
| 1:L:158:TRP:HZ2  | 1:L:210:ASN:O   | 1.91                     | 0.53              |
| 1:L:170:TRP:CZ2  | 1:L:205:PRO:CB  | 2.90                     | 0.53              |
| 2:G:26:TRP:HE3   | 2:G:27:ASP:OD1  | 1.91                     | 0.53              |
| 2:J:2:LEU:HD23   | 2:J:4:ASP:N     | 2.19                     | 0.53              |
| 2:A:113:THR:HG22 | 2:A:113:THR:O   | 2.09                     | 0.53              |
| 3:B:91:GLN:OE1   | 3:B:92:GLU:HB2  | 2.08                     | 0.53              |
| 3:E:56:ARG:O     | 3:E:60:LYS:CB   | 2.52                     | 0.53              |
| 2:J:78:ASN:OD1   | 2:J:79:LYS:O    | 2.26                     | 0.53              |
| 1:F:102:CYS:SG   | 1:F:108:TYR:HB2 | 2.49                     | 0.53              |
| 2:D:78:ASN:CB    | 2:D:105:LYS:HE3 | 2.38                     | 0.53              |
| 3:H:28:ARG:O     | 3:H:30:CYS:N    | 2.41                     | 0.53              |
| 1:L:127:LYS:NZ   | 1:L:173:GLU:OE2 | 2.40                     | 0.53              |
| 3:B:64:VAL:HG11  | 3:B:99:PHE:CZ   | 2.43                     | 0.53              |
| 1:F:157:ARG:CD   | 1:F:215:MET:HE2 | 2.37                     | 0.53              |
| 2:J:68:ASP:HA    | 2:J:111:LYS:HD2 | 1.90                     | 0.53              |
| 2:A:78:ASN:HD22  | 2:A:79:LYS:C    | 2.16                     | 0.52              |
| 2:A:2:LEU:O      | 2:A:3:GLU:CG    | 2.56                     | 0.52              |
| 2:J:71:TRP:HE3   | 2:J:107:GLY:O   | 1.91                     | 0.52              |
| 1:L:100:SER:CB   | 1:L:101:PRO:CD  | 2.83                     | 0.52              |
| 1:L:156:ILE:HG23 | 1:L:197:TYR:HB2 | 1.91                     | 0.52              |
| 2:A:37:GLU:HB2   | 2:A:38:ASN:O    | 2.10                     | 0.52              |
| 3:E:60:LYS:O     | 3:E:60:LYS:HG3  | 2.08                     | 0.52              |
| 2:G:23:GLN:HG2   | 2:G:127:HIS:HA  | 1.91                     | 0.52              |
| 3:E:60:LYS:O     | 3:E:60:LYS:CG   | 2.54                     | 0.52              |
| 2:J:16:CYS:HB2   | 2:J:133:LEU:HB3 | 1.90                     | 0.52              |
| 1:L:102:CYS:SG   | 1:L:108:TYR:HB2 | 2.50                     | 0.52              |
| 3:B:110:ASP:C    | 3:B:110:ASP:OD1 | 2.52                     | 0.52              |
| 3:E:9:TYR:CZ     | 3:E:10:GLU:HG2  | 2.44                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:E:22:ASN:HA    | 3:E:113:SER:O    | 2.10                     | 0.52              |
| 3:K:16:PRO:CB    | 3:K:59:LEU:HD11  | 2.30                     | 0.52              |
| 1:L:139:LYS:HA   | 1:L:172:TRP:CE3  | 2.45                     | 0.52              |
| 1:L:126:SER:HB3  | 1:L:137:LEU:CD2  | 2.29                     | 0.52              |
| 1:L:130:CYS:CB   | 1:L:135:ALA:CB   | 2.87                     | 0.52              |
| 2:G:26:TRP:CE3   | 2:G:27:ASP:OD1   | 2.63                     | 0.52              |
| 3:H:22:ASN:HA    | 3:H:113:SER:O    | 2.10                     | 0.51              |
| 1:L:123:TRP:CZ2  | 1:L:160:GLY:O    | 2.64                     | 0.51              |
| 3:B:20:PRO:C     | 3:B:114:THR:HG23 | 2.34                     | 0.51              |
| 3:E:19:GLU:CD    | 3:E:20:PRO:HD2   | 2.35                     | 0.51              |
| 2:G:14:GLN:O     | 2:G:134:LEU:CD2  | 2.59                     | 0.51              |
| 2:J:119:VAL:HG13 | 3:K:93:GLN:HE22  | 1.75                     | 0.51              |
| 2:A:79:LYS:O     | 2:A:79:LYS:CD    | 2.58                     | 0.51              |
| 1:C:102:CYS:SG   | 1:C:108:TYR:HB2  | 2.50                     | 0.51              |
| 3:E:66:MET:HE1   | 3:E:106:TRP:CD1  | 2.44                     | 0.51              |
| 3:H:61:ALA:HB2   | 3:H:102:VAL:HG13 | 1.91                     | 0.51              |
| 3:K:51:VAL:O     | 3:K:55:THR:HG23  | 2.10                     | 0.51              |
| 2:D:29:ALA:HB1   | 2:D:42:LEU:HD21  | 1.91                     | 0.51              |
| 2:J:26:TRP:CE3   | 2:J:27:ASP:OD1   | 2.63                     | 0.51              |
| 1:L:138:LEU:HD22 | 1:L:215:MET:HE3  | 1.91                     | 0.51              |
| 3:K:66:MET:HE1   | 3:K:106:TRP:CD1  | 2.46                     | 0.51              |
| 1:L:136:THR:HG22 | 1:L:137:LEU:O    | 2.11                     | 0.51              |
| 2:A:30:GLU:OE1   | 2:A:41:HIS:CD2   | 2.63                     | 0.51              |
| 3:B:22:ASN:HA    | 3:B:113:SER:O    | 2.11                     | 0.51              |
| 2:D:78:ASN:HB2   | 2:D:105:LYS:HE3  | 1.91                     | 0.51              |
| 1:L:127:LYS:NZ   | 1:L:173:GLU:OE1  | 2.43                     | 0.51              |
| 3:B:28:ARG:HE    | 3:B:32:LEU:HD11  | 1.75                     | 0.51              |
| 3:K:22:ASN:HA    | 3:K:113:SER:O    | 2.11                     | 0.51              |
| 2:J:3:GLU:HG3    | 1:L:116:PHE:CD2  | 2.46                     | 0.51              |
| 1:L:111:ASP:OD2  | 1:L:219:LYS:HE3  | 2.11                     | 0.51              |
| 1:F:214:LEU:HG   | 1:F:215:MET:N    | 2.25                     | 0.51              |
| 3:K:93:GLN:HG3   | 3:K:93:GLN:O     | 2.09                     | 0.50              |
| 1:L:177:VAL:HG12 | 1:L:178:ILE:O    | 2.11                     | 0.50              |
| 2:J:24:LYS:HD3   | 2:J:29:ALA:HA    | 1.93                     | 0.50              |
| 2:J:77:GLN:O     | 3:K:76:ASN:HB2   | 2.12                     | 0.50              |
| 1:L:130:CYS:CA   | 1:L:135:ALA:HB1  | 2.36                     | 0.50              |
| 3:H:35:LYS:HG2   | 3:H:121:PHE:CZ   | 2.46                     | 0.50              |
| 2:A:98:LEU:HA    | 2:A:101:LEU:HD13 | 1.93                     | 0.50              |
| 1:C:197:TYR:CE1  | 1:C:204:HIS:HB2  | 2.46                     | 0.50              |
| 2:A:66:ASP:O     | 2:A:66:ASP:CG    | 2.54                     | 0.50              |
| 2:D:64:LEU:N     | 2:D:65:ALA:HA    | 2.26                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:78:ASN:HD21  | 2:A:79:LYS:HD2   | 1.77                     | 0.50              |
| 2:J:12:TYR:HD2   | 2:J:17:TYR:CE2   | 2.30                     | 0.50              |
| 1:F:138:LEU:O    | 1:F:159:VAL:CG2  | 2.59                     | 0.50              |
| 3:B:66:MET:HE1   | 3:B:106:TRP:CD1  | 2.47                     | 0.50              |
| 2:G:81:GLN:CD    | 2:G:101:LEU:HD11 | 2.37                     | 0.50              |
| 2:J:126:MET:C    | 2:J:127:HIS:CD2  | 2.89                     | 0.50              |
| 2:J:114:GLY:O    | 2:J:115:PHE:HB2  | 2.12                     | 0.50              |
| 2:J:54:VAL:O     | 2:J:54:VAL:CG1   | 2.60                     | 0.49              |
| 3:H:61:ALA:HB2   | 3:H:102:VAL:CG1  | 2.42                     | 0.49              |
| 2:J:15:HIS:NE2   | 2:J:134:LEU:HD12 | 2.12                     | 0.49              |
| 1:L:156:ILE:C    | 1:L:157:ARG:HG3  | 2.36                     | 0.49              |
| 1:F:197:TYR:CE1  | 1:F:204:HIS:HB2  | 2.47                     | 0.49              |
| 2:A:66:ASP:OD1   | 2:A:66:ASP:C     | 2.56                     | 0.49              |
| 1:C:214:LEU:C    | 1:C:214:LEU:HD12 | 2.38                     | 0.49              |
| 2:J:81:GLN:HA    | 2:J:105:LYS:HZ2  | 1.77                     | 0.49              |
| 1:L:135:ALA:HB1  | 1:L:216:CYS:HB3  | 1.94                     | 0.49              |
| 2:D:135:PRO:O    | 2:D:136:TYR:HB3  | 2.13                     | 0.49              |
| 2:J:117:LYS:HD2  | 3:K:91:GLN:HE21  | 1.78                     | 0.49              |
| 2:J:126:MET:HE3  | 2:J:126:MET:HB3  | 1.70                     | 0.49              |
| 2:A:40:ALA:HB2   | 2:A:133:LEU:HD13 | 1.94                     | 0.49              |
| 3:H:61:ALA:O     | 3:K:109:MET:HE2  | 2.13                     | 0.49              |
| 2:J:37:GLU:OE1   | 2:J:37:GLU:N     | 2.46                     | 0.49              |
| 1:F:159:VAL:CG2  | 1:F:160:GLY:H    | 2.24                     | 0.49              |
| 1:I:179:SER:OG   | 1:I:182:MET:HG2  | 2.13                     | 0.48              |
| 2:J:81:GLN:OE1   | 2:J:101:LEU:HD22 | 2.13                     | 0.48              |
| 1:I:197:TYR:CE1  | 1:I:204:HIS:HB2  | 2.48                     | 0.48              |
| 2:J:71:TRP:CZ2   | 2:J:122:TYR:O    | 2.66                     | 0.48              |
| 1:L:156:ILE:HG23 | 1:L:157:ARG:H    | 1.78                     | 0.48              |
| 1:I:165:LYS:HB2  | 1:I:168:GLU:HG3  | 1.95                     | 0.48              |
| 2:J:129:PHE:CD1  | 2:J:129:PHE:N    | 2.81                     | 0.48              |
| 2:D:38:ASN:HD21  | 2:D:136:TYR:C    | 2.16                     | 0.48              |
| 2:J:18:GLN:C     | 2:J:130:VAL:HG13 | 2.28                     | 0.48              |
| 2:J:32:PHE:O     | 2:J:36:GLN:HG2   | 2.13                     | 0.48              |
| 2:G:30:GLU:OE1   | 2:G:41:HIS:CD2   | 2.63                     | 0.48              |
| 2:J:25:THR:HG22  | 2:J:26:TRP:N     | 2.28                     | 0.48              |
| 1:L:123:TRP:CD1  | 1:L:137:LEU:HD13 | 2.48                     | 0.48              |
| 2:A:74:LEU:HD11  | 3:B:77:TRP:HB3   | 1.96                     | 0.48              |
| 3:E:56:ARG:NH1   | 3:E:102:VAL:O    | 2.47                     | 0.48              |
| 1:L:130:CYS:CA   | 1:L:135:ALA:C    | 2.85                     | 0.48              |
| 1:C:179:SER:OG   | 1:C:182:MET:HG2  | 2.14                     | 0.48              |
| 2:A:26:TRP:HE3   | 2:A:27:ASP:OD1   | 1.97                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:71:TRP:NE1   | 2:D:127:HIS:HB2  | 2.27                     | 0.48              |
| 3:H:66:MET:HE1   | 3:H:106:TRP:CD1  | 2.49                     | 0.48              |
| 2:J:30:GLU:HB2   | 2:J:42:LEU:CD1   | 2.44                     | 0.48              |
| 1:L:117:PHE:CZ   | 1:L:133:MET:HE1  | 2.48                     | 0.48              |
| 2:J:2:LEU:HD21   | 2:J:4:ASP:CG     | 2.39                     | 0.48              |
| 2:J:57:LEU:C     | 2:J:59:SER:H     | 2.22                     | 0.48              |
| 2:A:79:LYS:O     | 2:A:79:LYS:CG    | 2.62                     | 0.48              |
| 3:B:9:TYR:HB2    | 3:B:50:PHE:CZ    | 2.49                     | 0.48              |
| 3:B:55:THR:CG2   | 3:B:101:GLY:CA   | 2.90                     | 0.48              |
| 2:A:62:ASP:C     | 2:A:64:LEU:H     | 2.22                     | 0.47              |
| 2:J:32:PHE:CD1   | 2:J:32:PHE:C     | 2.91                     | 0.47              |
| 1:L:130:CYS:HB3  | 1:L:135:ALA:CB   | 2.44                     | 0.47              |
| 2:G:33:CYS:O     | 2:G:40:ALA:HB3   | 2.14                     | 0.47              |
| 1:L:130:CYS:CB   | 1:L:135:ALA:HB1  | 2.43                     | 0.47              |
| 3:H:9:TYR:HB2    | 3:H:50:PHE:CZ    | 2.48                     | 0.47              |
| 2:J:71:TRP:HZ3   | 2:J:106:CYS:C    | 2.22                     | 0.47              |
| 2:D:38:ASN:HB2   | 2:D:133:LEU:HD11 | 1.96                     | 0.47              |
| 2:J:58:ILE:C     | 2:J:60:GLN:H     | 2.22                     | 0.47              |
| 3:H:100:ARG:C    | 3:H:102:VAL:H    | 2.22                     | 0.47              |
| 1:C:166:SER:HA   | 1:C:194:ASN:OD1  | 2.15                     | 0.47              |
| 3:H:50:PHE:O     | 3:H:53:LYS:HB3   | 2.14                     | 0.47              |
| 2:A:30:GLU:O     | 2:A:34:ARG:HG2   | 2.15                     | 0.47              |
| 2:J:38:ASN:HB2   | 2:J:133:LEU:HD11 | 1.97                     | 0.47              |
| 3:E:109:MET:HE2  | 3:E:109:MET:HA   | 1.97                     | 0.47              |
| 2:A:78:ASN:OD1   | 2:A:78:ASN:N     | 2.30                     | 0.46              |
| 2:J:30:GLU:OE1   | 2:J:42:LEU:HB2   | 2.15                     | 0.46              |
| 3:B:54:LEU:HD12  | 3:B:58:ARG:NH1   | 2.30                     | 0.46              |
| 2:J:45:ILE:HG22  | 2:J:118:TRP:CZ2  | 2.48                     | 0.46              |
| 3:K:56:ARG:O     | 3:K:57:PRO:C     | 2.58                     | 0.46              |
| 3:B:100:ARG:C    | 3:B:102:VAL:H    | 2.23                     | 0.46              |
| 2:A:65:ALA:O     | 2:A:66:ASP:HB3   | 2.15                     | 0.46              |
| 2:D:26:TRP:HZ3   | 2:D:27:ASP:OD1   | 1.95                     | 0.46              |
| 1:F:170:TRP:CZ3  | 1:F:194:ASN:O    | 2.68                     | 0.46              |
| 3:B:9:TYR:CE2    | 3:B:10:GLU:HG2   | 2.50                     | 0.46              |
| 2:D:63:GLU:HG3   | 2:D:63:GLU:O     | 2.14                     | 0.46              |
| 2:J:2:LEU:HD21   | 2:J:4:ASP:CB     | 2.46                     | 0.46              |
| 2:J:15:HIS:CB    | 2:J:17:TYR:CZ    | 2.89                     | 0.46              |
| 3:K:49:ASP:O     | 3:K:53:LYS:HG3   | 2.16                     | 0.46              |
| 1:C:100:SER:CB   | 1:C:101:PRO:CD   | 2.94                     | 0.46              |
| 2:D:78:ASN:ND2   | 2:D:79:LYS:HB2   | 2.31                     | 0.46              |
| 1:F:206:THR:HG22 | 1:F:207:PHE:H    | 1.78                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:B:9:TYR:CE1    | 3:B:10:GLU:HG2   | 2.50                     | 0.45              |
| 2:D:35:ALA:C     | 2:D:37:GLU:H     | 2.23                     | 0.45              |
| 1:I:170:TRP:CZ3  | 1:I:194:ASN:O    | 2.69                     | 0.45              |
| 2:G:65:ALA:O     | 2:G:66:ASP:HB2   | 2.16                     | 0.45              |
| 2:J:2:LEU:HA     | 1:L:152:ARG:O    | 2.16                     | 0.45              |
| 2:J:12:TYR:CD2   | 2:J:17:TYR:HE2   | 2.32                     | 0.45              |
| 2:J:50:GLU:OE1   | 2:J:132:LYS:NZ   | 2.44                     | 0.45              |
| 1:L:193:MET:HB3  | 1:L:206:THR:CA   | 2.46                     | 0.45              |
| 1:C:170:TRP:CZ3  | 1:C:194:ASN:O    | 2.69                     | 0.45              |
| 2:G:14:GLN:O     | 2:G:134:LEU:HD23 | 2.16                     | 0.45              |
| 2:J:8:GLY:O      | 2:J:18:GLN:NE2   | 2.49                     | 0.45              |
| 2:J:56:TRP:C     | 2:J:57:LEU:HD12  | 2.41                     | 0.45              |
| 1:L:127:LYS:NZ   | 1:L:173:GLU:CD   | 2.71                     | 0.45              |
| 1:I:100:SER:CB   | 1:I:101:PRO:CD   | 2.95                     | 0.45              |
| 2:D:77:GLN:HG3   | 3:E:78:GLN:HG3   | 1.99                     | 0.45              |
| 2:J:102:HIS:O    | 2:J:102:HIS:ND1  | 2.50                     | 0.45              |
| 1:L:161:LEU:HD12 | 1:L:171:LYS:C    | 2.41                     | 0.45              |
| 3:B:20:PRO:C     | 3:B:114:THR:CG2  | 2.89                     | 0.45              |
| 2:G:79:LYS:O     | 2:G:79:LYS:CG    | 2.64                     | 0.45              |
| 3:K:36:HIS:NE2   | 3:K:38:HIS:NE2   | 2.62                     | 0.45              |
| 2:D:77:GLN:HG2   | 3:E:78:GLN:HG3   | 1.99                     | 0.45              |
| 1:L:139:LYS:HE3  | 1:L:172:TRP:CD1  | 2.51                     | 0.45              |
| 2:D:2:LEU:HD21   | 1:F:154:HIS:CE1  | 2.52                     | 0.45              |
| 3:E:9:TYR:CE2    | 3:E:10:GLU:HG2   | 2.52                     | 0.45              |
| 2:J:26:TRP:HZ2   | 2:J:73:GLY:C     | 2.25                     | 0.45              |
| 2:J:12:TYR:CE2   | 2:J:13:ASP:HB3   | 2.52                     | 0.45              |
| 1:L:190:LYS:CG   | 1:L:193:MET:HE2  | 2.43                     | 0.45              |
| 2:A:71:TRP:HB2   | 2:A:129:PHE:HB3  | 1.99                     | 0.44              |
| 2:D:13:ASP:O     | 2:D:14:GLN:HB2   | 2.18                     | 0.44              |
| 1:L:214:LEU:HD23 | 1:L:215:MET:N    | 2.32                     | 0.44              |
| 1:C:179:SER:HG   | 1:C:182:MET:HG2  | 1.82                     | 0.44              |
| 2:G:19:ALA:HB2   | 2:G:130:VAL:HG22 | 1.99                     | 0.44              |
| 2:A:12:TYR:HB3   | 2:A:17:TYR:CE2   | 2.53                     | 0.44              |
| 2:A:78:ASN:HD21  | 2:A:79:LYS:HD3   | 1.82                     | 0.44              |
| 3:E:36:HIS:NE2   | 3:E:38:HIS:CE1   | 2.85                     | 0.44              |
| 2:J:21:ASN:HB3   | 2:J:61:LYS:HB2   | 1.99                     | 0.44              |
| 3:K:92:GLU:O     | 3:K:92:GLU:HG3   | 2.18                     | 0.44              |
| 1:L:126:SER:CA   | 1:L:214:LEU:CD1  | 2.93                     | 0.44              |
| 2:J:135:PRO:O    | 2:J:136:TYR:HB2  | 2.16                     | 0.44              |
| 1:L:123:TRP:O    | 1:L:137:LEU:HD11 | 2.17                     | 0.44              |
| 1:L:204:HIS:HA   | 1:L:205:PRO:HD3  | 1.67                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:J:71:TRP:HZ3   | 2:J:106:CYS:CB   | 2.28                     | 0.44              |
| 3:K:59:LEU:HD23  | 3:K:64:VAL:HG22  | 1.99                     | 0.44              |
| 1:L:157:ARG:HA   | 1:L:213:TYR:O    | 2.17                     | 0.44              |
| 1:F:139:LYS:HA   | 1:F:172:TRP:CE3  | 2.53                     | 0.44              |
| 1:F:206:THR:CG2  | 1:F:207:PHE:N    | 2.80                     | 0.44              |
| 1:I:214:LEU:C    | 1:I:214:LEU:HD12 | 2.42                     | 0.44              |
| 3:H:61:ALA:O     | 3:K:109:MET:CE   | 2.66                     | 0.44              |
| 2:J:71:TRP:CH2   | 2:J:123:CYS:HA   | 2.53                     | 0.44              |
| 1:F:166:SER:O    | 1:F:167:ASN:OD1  | 2.35                     | 0.44              |
| 3:H:1:ASP:CG     | 3:H:2:CYS:N      | 2.75                     | 0.44              |
| 3:K:100:ARG:C    | 3:K:102:VAL:H    | 2.25                     | 0.44              |
| 2:G:93:VAL:HG13  | 2:G:93:VAL:O     | 2.17                     | 0.44              |
| 2:G:134:LEU:HD23 | 2:G:134:LEU:HA   | 1.68                     | 0.44              |
| 2:J:23:GLN:HB3   | 2:J:126:MET:C    | 2.42                     | 0.44              |
| 1:L:121:LEU:HB3  | 1:L:125:GLU:CB   | 2.48                     | 0.44              |
| 1:F:137:LEU:HD21 | 1:F:214:LEU:HD11 | 1.89                     | 0.44              |
| 1:F:165:LYS:HB2  | 1:F:168:GLU:HG3  | 1.99                     | 0.44              |
| 3:B:18:ASN:OD1   | 3:B:18:ASN:O     | 2.35                     | 0.44              |
| 2:D:71:TRP:HH2   | 2:D:123:CYS:HA   | 1.79                     | 0.44              |
| 2:G:102:HIS:CG   | 2:G:102:HIS:O    | 2.69                     | 0.44              |
| 2:A:58:ILE:CG2   | 2:A:64:LEU:HD22  | 2.33                     | 0.43              |
| 1:L:121:LEU:HB2  | 1:L:126:SER:OG   | 2.18                     | 0.43              |
| 1:L:141:ASP:CA   | 1:L:182:MET:HG3  | 2.45                     | 0.43              |
| 2:A:121:TYR:CE1  | 3:E:56:ARG:HD3   | 2.53                     | 0.43              |
| 3:H:60:LYS:HA    | 3:H:61:ALA:HA    | 1.70                     | 0.43              |
| 2:J:15:HIS:HA    | 2:J:135:PRO:CD   | 2.48                     | 0.43              |
| 2:J:30:GLU:OE1   | 2:J:42:LEU:CD1   | 2.65                     | 0.43              |
| 2:J:37:GLU:O     | 2:J:37:GLU:HG2   | 2.18                     | 0.43              |
| 2:D:86:GLU:HG2   | 2:D:87:TRP:O     | 2.19                     | 0.43              |
| 1:I:117:PHE:HB3  | 1:I:119:HIS:HD2  | 1.83                     | 0.43              |
| 2:D:40:ALA:CB    | 2:D:133:LEU:HB2  | 2.38                     | 0.43              |
| 1:I:166:SER:HA   | 1:I:194:ASN:OD1  | 2.18                     | 0.43              |
| 2:G:102:HIS:O    | 2:G:102:HIS:CD2  | 2.71                     | 0.43              |
| 2:J:15:HIS:HB2   | 2:J:17:TYR:CE1   | 2.50                     | 0.43              |
| 2:A:104:LYS:HG3  | 2:A:122:TYR:CE1  | 2.53                     | 0.43              |
| 3:B:28:ARG:HH22  | 2:G:92:SER:HB3   | 1.84                     | 0.43              |
| 3:E:8:SER:HA     | 3:E:12:HIS:O     | 2.19                     | 0.43              |
| 3:E:51:VAL:O     | 3:E:55:THR:HG23  | 2.19                     | 0.43              |
| 3:E:100:ARG:C    | 3:E:102:VAL:H    | 2.26                     | 0.43              |
| 2:D:75:ARG:HG3   | 2:D:105:LYS:O    | 2.19                     | 0.43              |
| 2:J:70:VAL:CG1   | 2:J:130:VAL:HG23 | 2.49                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:J:15:HIS:CB    | 2:J:17:TYR:CE1   | 3.02                     | 0.43              |
| 3:K:8:SER:HA     | 3:K:12:HIS:O     | 2.18                     | 0.43              |
| 2:A:76:ALA:HB1   | 3:B:75:CYS:HB3   | 2.01                     | 0.42              |
| 1:I:139:LYS:HA   | 1:I:172:TRP:CE3  | 2.53                     | 0.42              |
| 2:G:78:ASN:H     | 2:G:79:LYS:HA    | 1.83                     | 0.42              |
| 2:G:81:GLN:OE1   | 2:G:101:LEU:HD11 | 2.19                     | 0.42              |
| 1:L:130:CYS:HB3  | 1:L:135:ALA:CA   | 2.44                     | 0.42              |
| 2:A:26:TRP:CE3   | 2:A:27:ASP:OD1   | 2.71                     | 0.42              |
| 2:D:30:GLU:OE2   | 2:D:41:HIS:CD2   | 2.71                     | 0.42              |
| 2:J:26:TRP:HD1   | 2:J:71:TRP:CG    | 2.36                     | 0.42              |
| 2:A:112:LEU:HD22 | 3:E:57:PRO:HB2   | 2.01                     | 0.42              |
| 1:I:136:THR:HG22 | 1:I:137:LEU:O    | 2.19                     | 0.42              |
| 2:J:30:GLU:OE1   | 2:J:42:LEU:CG    | 2.67                     | 0.42              |
| 2:J:71:TRP:CH2   | 2:J:122:TYR:O    | 2.72                     | 0.42              |
| 1:F:137:LEU:HD21 | 1:F:214:LEU:CD1  | 2.47                     | 0.42              |
| 1:C:117:PHE:HB3  | 1:C:119:HIS:HD2  | 1.83                     | 0.42              |
| 1:L:121:LEU:HB3  | 1:L:125:GLU:HB3  | 2.01                     | 0.42              |
| 1:L:143:ARG:O    | 1:L:146:VAL:HB   | 2.20                     | 0.42              |
| 1:F:104:THR:O    | 1:F:106:TRP:HD1  | 2.02                     | 0.42              |
| 2:D:64:LEU:O     | 2:D:64:LEU:HD23  | 2.20                     | 0.42              |
| 2:D:120:ASN:N    | 3:E:90:TRP:HZ3   | 2.17                     | 0.42              |
| 1:L:130:CYS:CB   | 1:L:136:THR:CA   | 2.98                     | 0.42              |
| 3:B:16:PRO:HG2   | 3:B:58:ARG:CD    | 2.49                     | 0.42              |
| 2:G:71:TRP:HB2   | 2:G:129:PHE:HB3  | 2.00                     | 0.42              |
| 3:H:108:ASN:O    | 3:H:109:MET:HE2  | 2.19                     | 0.42              |
| 3:K:108:ASN:H    | 3:K:108:ASN:ND2  | 2.18                     | 0.42              |
| 3:B:9:TYR:CZ     | 3:B:10:GLU:CG    | 3.03                     | 0.42              |
| 3:B:16:PRO:HG3   | 3:B:58:ARG:HD2   | 2.01                     | 0.42              |
| 2:J:17:TYR:O     | 2:J:18:GLN:HB2   | 2.19                     | 0.42              |
| 2:G:67:GLU:OE2   | 2:G:127:HIS:CD2  | 2.68                     | 0.42              |
| 1:L:130:CYS:HB3  | 1:L:135:ALA:HB1  | 2.00                     | 0.42              |
| 1:C:205:PRO:O    | 1:C:206:THR:HG23 | 2.19                     | 0.42              |
| 3:E:91:GLN:CG    | 3:E:93:GLN:HE22  | 2.29                     | 0.42              |
| 1:I:104:THR:O    | 1:I:106:TRP:HD1  | 2.03                     | 0.42              |
| 2:G:13:ASP:O     | 2:G:14:GLN:HB2   | 2.18                     | 0.42              |
| 2:J:19:ALA:CB    | 2:J:130:VAL:HG22 | 2.50                     | 0.42              |
| 2:J:68:ASP:O     | 2:J:111:LYS:CA   | 2.67                     | 0.42              |
| 3:K:64:VAL:HG11  | 3:K:99:PHE:CZ    | 2.55                     | 0.42              |
| 1:L:116:PHE:HD1  | 1:L:215:MET:HB3  | 1.85                     | 0.42              |
| 1:L:195:CYS:C    | 1:L:206:THR:H    | 2.09                     | 0.42              |
| 1:F:159:VAL:CG2  | 1:F:160:GLY:N    | 2.82                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:139:LYS:HA   | 1:C:172:TRP:CE3  | 2.55                     | 0.41              |
| 1:C:141:ASP:OD1  | 1:C:172:TRP:CE2  | 2.73                     | 0.41              |
| 1:L:116:PHE:CD1  | 1:L:215:MET:HB3  | 2.55                     | 0.41              |
| 1:L:156:ILE:HG12 | 1:L:199:HIS:HB2  | 2.02                     | 0.41              |
| 3:K:109:MET:HE2  | 3:K:109:MET:HA   | 2.01                     | 0.41              |
| 1:F:117:PHE:HB3  | 1:F:119:HIS:HD2  | 1.85                     | 0.41              |
| 2:J:78:ASN:H     | 2:J:79:LYS:HA    | 1.84                     | 0.41              |
| 3:K:108:ASN:H    | 3:K:108:ASN:HD22 | 1.68                     | 0.41              |
| 1:L:133:MET:HE3  | 1:L:133:MET:HB2  | 1.92                     | 0.41              |
| 1:L:170:TRP:CZ2  | 1:L:205:PRO:CG   | 3.04                     | 0.41              |
| 2:D:26:TRP:CD1   | 2:D:71:TRP:CE3   | 3.05                     | 0.41              |
| 2:G:74:LEU:HD11  | 3:H:77:TRP:HB3   | 2.02                     | 0.41              |
| 2:J:71:TRP:CZ3   | 2:J:106:CYS:CB   | 2.91                     | 0.41              |
| 2:D:30:GLU:OE2   | 2:D:41:HIS:HD2   | 2.03                     | 0.41              |
| 2:J:70:VAL:HA    | 2:J:128:ALA:O    | 2.20                     | 0.41              |
| 2:A:25:THR:CG2   | 2:A:28:GLU:HG3   | 2.51                     | 0.41              |
| 2:J:15:HIS:HA    | 2:J:135:PRO:HD2  | 2.03                     | 0.41              |
| 2:G:62:ASP:C     | 2:G:64:LEU:H     | 2.28                     | 0.41              |
| 3:H:3:PRO:HG2    | 3:H:6:TRP:CD1    | 2.55                     | 0.41              |
| 2:J:53:PHE:HE2   | 2:J:57:LEU:HD21  | 1.86                     | 0.41              |
| 3:B:3:PRO:HG2    | 3:B:6:TRP:CD1    | 2.56                     | 0.41              |
| 3:E:9:TYR:CE2    | 3:E:10:GLU:CG    | 3.03                     | 0.41              |
| 3:H:100:ARG:NH2  | 3:H:102:VAL:HG21 | 2.36                     | 0.41              |
| 2:J:24:LYS:N     | 2:J:127:HIS:O    | 2.53                     | 0.41              |
| 2:J:117:LYS:HD3  | 3:K:91:GLN:HA    | 2.02                     | 0.41              |
| 1:L:156:ILE:CG2  | 1:L:197:TYR:HB2  | 2.51                     | 0.41              |
| 2:G:58:ILE:CG2   | 2:G:64:LEU:HD22  | 2.45                     | 0.41              |
| 3:H:28:ARG:C     | 3:H:30:CYS:N     | 2.75                     | 0.41              |
| 1:L:114:TYR:OH   | 1:L:145:ILE:HD13 | 2.20                     | 0.41              |
| 2:J:14:GLN:O     | 2:J:135:PRO:CD   | 2.59                     | 0.40              |
| 1:L:126:SER:HA   | 1:L:214:LEU:CD1  | 2.51                     | 0.40              |
| 1:F:206:THR:CG2  | 1:F:207:PHE:H    | 2.34                     | 0.40              |
| 2:D:26:TRP:HD1   | 2:D:71:TRP:HE3   | 1.67                     | 0.40              |
| 2:J:9:TRP:CZ3    | 2:J:133:LEU:N    | 2.89                     | 0.40              |
| 2:J:78:ASN:OD1   | 2:J:78:ASN:C     | 2.63                     | 0.40              |
| 1:L:104:THR:O    | 1:L:106:TRP:HD1  | 2.04                     | 0.40              |
| 3:B:1:ASP:CG     | 3:B:2:CYS:N      | 2.75                     | 0.40              |
| 1:L:126:SER:HA   | 1:L:214:LEU:HD11 | 2.03                     | 0.40              |
| 2:D:78:ASN:HB3   | 2:D:105:LYS:HE3  | 2.02                     | 0.40              |
| 3:H:28:ARG:HA    | 3:H:31:LYS:HB2   | 2.04                     | 0.40              |
| 2:J:43:ALA:HB3   | 2:J:72:ILE:HG22  | 2.04                     | 0.40              |

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| Atom-1        | Atom-2         | Interatomic distance (Å) | Clash overlap (Å) |
|---------------|----------------|--------------------------|-------------------|
| 3:B:9:TYR:CE2 | 3:B:10:GLU:CG  | 3.05                     | 0.40              |
| 2:J:105:LYS:C | 2:J:123:CYS:SG | 3.04                     | 0.40              |

All (1) 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) |
|----------------|-----------------------|--------------------------|-------------------|
| 2:D:48:ASN:ND2 | 2:J:52:ASP:OD2[3_545] | 2.16                     | 0.04              |

## 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   | C     | 120/128 (94%)   | 117 (98%)  | 3 (2%)   | 0        | 100         | 100 |
| 1   | F     | 120/128 (94%)   | 117 (98%)  | 3 (2%)   | 0        | 100         | 100 |
| 1   | I     | 120/128 (94%)   | 118 (98%)  | 2 (2%)   | 0        | 100         | 100 |
| 1   | L     | 120/128 (94%)   | 115 (96%)  | 5 (4%)   | 0        | 100         | 100 |
| 2   | A     | 129/136 (95%)   | 114 (88%)  | 15 (12%) | 0        | 100         | 100 |
| 2   | D     | 129/136 (95%)   | 113 (88%)  | 15 (12%) | 1 (1%)   | 16          | 47  |
| 2   | G     | 129/136 (95%)   | 117 (91%)  | 12 (9%)  | 0        | 100         | 100 |
| 2   | J     | 121/136 (89%)   | 103 (85%)  | 17 (14%) | 1 (1%)   | 16          | 47  |
| 3   | B     | 121/146 (83%)   | 113 (93%)  | 8 (7%)   | 0        | 100         | 100 |
| 3   | E     | 121/146 (83%)   | 112 (93%)  | 9 (7%)   | 0        | 100         | 100 |
| 3   | H     | 121/146 (83%)   | 113 (93%)  | 7 (6%)   | 1 (1%)   | 16          | 47  |
| 3   | K     | 121/146 (83%)   | 112 (93%)  | 9 (7%)   | 0        | 100         | 100 |
| All | All   | 1472/1640 (90%) | 1364 (93%) | 105 (7%) | 3 (0%)   | 43          | 73  |

All (3) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | H     | 61  | ALA  |
| 2   | D     | 78  | ASN  |
| 2   | J     | 13  | ASP  |

### 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   | C     | 110/114 (96%)   | 109 (99%)  | 1 (1%)   | 70          | 85  |
| 1   | F     | 110/114 (96%)   | 109 (99%)  | 1 (1%)   | 70          | 85  |
| 1   | I     | 110/114 (96%)   | 109 (99%)  | 1 (1%)   | 70          | 85  |
| 1   | L     | 110/114 (96%)   | 108 (98%)  | 2 (2%)   | 51          | 76  |
| 2   | A     | 116/118 (98%)   | 114 (98%)  | 2 (2%)   | 53          | 77  |
| 2   | D     | 116/118 (98%)   | 114 (98%)  | 2 (2%)   | 53          | 77  |
| 2   | G     | 116/118 (98%)   | 115 (99%)  | 1 (1%)   | 70          | 85  |
| 2   | J     | 111/118 (94%)   | 106 (96%)  | 5 (4%)   | 24          | 57  |
| 3   | B     | 109/127 (86%)   | 109 (100%) | 0        | 100         | 100 |
| 3   | E     | 109/127 (86%)   | 109 (100%) | 0        | 100         | 100 |
| 3   | H     | 109/127 (86%)   | 109 (100%) | 0        | 100         | 100 |
| 3   | K     | 109/127 (86%)   | 109 (100%) | 0        | 100         | 100 |
| All | All   | 1335/1436 (93%) | 1320 (99%) | 15 (1%)  | 65          | 82  |

All (15) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 144 | ASN  |
| 2   | A     | 78  | ASN  |
| 2   | A     | 134 | LEU  |
| 2   | D     | 78  | ASN  |
| 2   | D     | 101 | LEU  |
| 1   | I     | 144 | ASN  |
| 2   | G     | 64  | LEU  |
| 2   | J     | 14  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | J     | 72  | ILE  |
| 2   | J     | 77  | GLN  |
| 2   | J     | 125 | GLN  |
| 2   | J     | 126 | MET  |
| 1   | L     | 144 | ASN  |
| 1   | L     | 206 | THR  |
| 1   | F     | 144 | ASN  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 105 | ASN  |
| 1   | C     | 119 | HIS  |
| 1   | C     | 144 | ASN  |
| 1   | C     | 200 | ASN  |
| 2   | A     | 36  | GLN  |
| 2   | A     | 38  | ASN  |
| 2   | A     | 41  | HIS  |
| 2   | A     | 78  | ASN  |
| 2   | A     | 81  | GLN  |
| 3   | B     | 76  | ASN  |
| 3   | B     | 78  | GLN  |
| 3   | B     | 103 | HIS  |
| 2   | D     | 23  | GLN  |
| 2   | D     | 36  | GLN  |
| 2   | D     | 41  | HIS  |
| 2   | D     | 48  | ASN  |
| 2   | D     | 77  | GLN  |
| 2   | D     | 78  | ASN  |
| 3   | E     | 38  | HIS  |
| 3   | E     | 76  | ASN  |
| 3   | E     | 78  | GLN  |
| 3   | E     | 93  | GLN  |
| 1   | I     | 105 | ASN  |
| 1   | I     | 119 | HIS  |
| 1   | I     | 144 | ASN  |
| 1   | I     | 200 | ASN  |
| 2   | G     | 23  | GLN  |
| 2   | G     | 36  | GLN  |
| 2   | G     | 41  | HIS  |
| 2   | G     | 77  | GLN  |
| 2   | G     | 127 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | H     | 70  | ASN  |
| 3   | H     | 76  | ASN  |
| 3   | H     | 103 | HIS  |
| 2   | J     | 14  | GLN  |
| 2   | J     | 36  | GLN  |
| 2   | J     | 41  | HIS  |
| 2   | J     | 48  | ASN  |
| 2   | J     | 60  | GLN  |
| 2   | J     | 125 | GLN  |
| 2   | J     | 127 | HIS  |
| 3   | K     | 33  | GLN  |
| 3   | K     | 70  | ASN  |
| 3   | K     | 76  | ASN  |
| 3   | K     | 91  | GLN  |
| 3   | K     | 93  | GLN  |
| 3   | K     | 108 | ASN  |
| 1   | L     | 105 | ASN  |
| 1   | L     | 200 | ASN  |
| 1   | L     | 204 | HIS  |
| 1   | F     | 119 | HIS  |
| 1   | F     | 144 | ASN  |
| 1   | F     | 200 | 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   | C     | 122/128 (95%)   | -1.10  | 0 100 100    | 38, 76, 92, 96        | 8 (6%)  |
| 1   | F     | 122/128 (95%)   | -0.85  | 1 (0%) 82 67 | 47, 87, 103, 108      | 8 (6%)  |
| 1   | I     | 122/128 (95%)   | -1.28  | 0 100 100    | 31, 62, 80, 87        | 8 (6%)  |
| 1   | L     | 122/128 (95%)   | -1.15  | 0 100 100    | 38, 71, 84, 93        | 8 (6%)  |
| 2   | A     | 133/136 (97%)   | -1.33  | 0 100 100    | 41, 53, 63, 69        | 0       |
| 2   | D     | 133/136 (97%)   | -1.17  | 0 100 100    | 46, 70, 80, 86        | 0       |
| 2   | G     | 133/136 (97%)   | -1.37  | 0 100 100    | 39, 50, 59, 63        | 0       |
| 2   | J     | 127/136 (93%)   | -1.07  | 0 100 100    | 44, 72, 82, 102       | 0       |
| 3   | B     | 123/146 (84%)   | -1.44  | 0 100 100    | 36, 44, 57, 61        | 0       |
| 3   | E     | 123/146 (84%)   | -1.40  | 0 100 100    | 37, 47, 67, 72        | 0       |
| 3   | H     | 123/146 (84%)   | -1.42  | 0 100 100    | 35, 42, 56, 61        | 0       |
| 3   | K     | 123/146 (84%)   | -1.43  | 0 100 100    | 37, 45, 64, 67        | 0       |
| All | All   | 1506/1640 (91%) | -1.25  | 1 (0%) 92 87 | 31, 58, 89, 108       | 32 (2%) |

All (1) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | F     | 221 | GLY  | 2.4  |

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 6.3 Carbohydrates ⓘ

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.