



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:55 AM UTC

PDB ID : 1KB5 / pdb\_00001kb5  
Title : MURINE T-CELL RECEPTOR VARIABLE DOMAIN/FAB COMPLEX  
Authors : Housset, D.; Mazza, G.; Gregoire, C.; Piras, C.; Malissen, B.; Fontecilla-Camps, J.C.  
Deposited on : 1997-04-06  
Resolution : 2.50 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

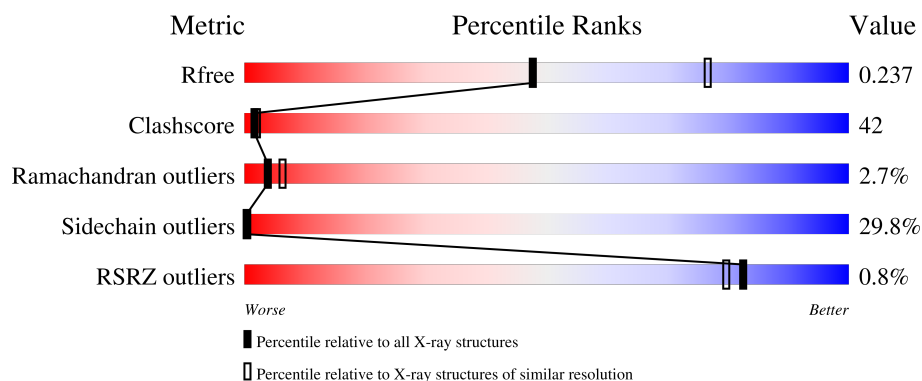
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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                      | 5829 (2.50-2.50)                                      |
| Clashscore            | 190562                      | 6492 (2.50-2.50)                                      |
| Ramachandran outliers | 187476                      | 6378 (2.50-2.50)                                      |
| Sidechain outliers    | 187428                      | 6380 (2.50-2.50)                                      |
| RSRZ outliers         | 180081                      | 5833 (2.50-2.50)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain                                                        |
|-----|-------|--------|-------------------------------------------------------------------------|
| 1   | A     | 115    | <div> <div>19%</div> <div>48%</div> <div>29%</div> <div>.</div> </div>  |
| 2   | B     | 117    | <div> <div>19%</div> <div>47%</div> <div>28%</div> <div>6%</div> </div> |
| 3   | L     | 214    | <div> <div>26%</div> <div>46%</div> <div>27%</div> <div>.</div> </div>  |
| 4   | H     | 219    | <div> <div>31%</div> <div>46%</div> <div>21%</div> <div>.</div> </div>  |

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5438 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 KB5-C20 T-CELL ANTIGEN RECEPTOR.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | A     | 115      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 904   | 572 | 153 | 177 | 2 |         |         |       |

- Molecule 2 is a protein called KB5-C20 T-CELL ANTIGEN RECEPTOR.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2   | B     | 117      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 941   | 596 | 167 | 173 | 5 |         |         |       |

There are 8 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment   | Reference  |
|-------|---------|----------|--------|-----------|------------|
| B     | 100     | TRP      | -      | insertion | UNP P04214 |
| B     | 101     | GLY      | TYR    | conflict  | UNP P04214 |
| B     | 102     | ALA      | ASN    | conflict  | UNP P04214 |
| B     | 104     | ALA      | -      | insertion | UNP P04214 |
| B     | 105     | GLU      | -      | insertion | UNP P04214 |
| B     | 105A    | THR      | PRO    | conflict  | UNP P04214 |
| B     | 109     | GLY      | ALA    | conflict  | UNP P04214 |
| B     | 110     | SER      | ALA    | conflict  | UNP P04214 |

- Molecule 3 is a protein called ANTIBODY DESIRE-1.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3   | L     | 214      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1661  | 1036 | 280 | 338 | 7 |         |         |       |

There are 5 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| L     | 27      | LYS      | GLU    | conflict | UNP P01837 |
| L     | 55      | GLY      | ALA    | conflict | UNP P01837 |

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| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| L     | 96      | TYR      | LEU    | conflict | UNP P01837 |
| L     | 100     | GLY      | ALA    | conflict | UNP P01837 |
| L     | 106     | ILE      | LEU    | conflict | UNP P01837 |

- Molecule 4 is a protein called ANTIBODY DESIRE-1.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 4   | H     | 219      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1666  | 1052 | 270 | 337 | 7 |         |         |       |

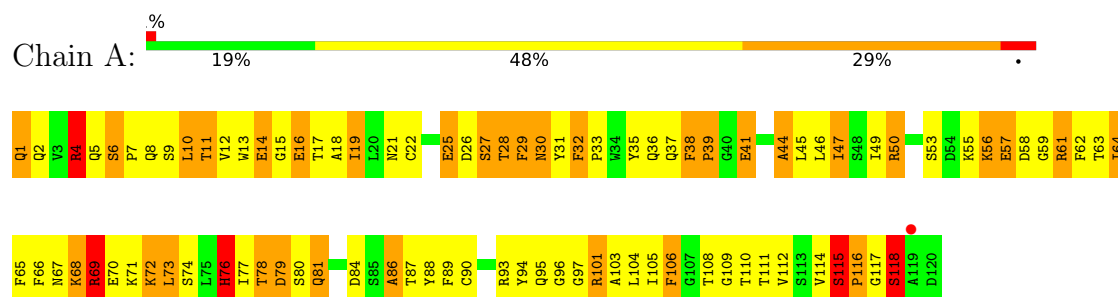
- Molecule 5 is water.

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 5   | A     | 53       | Total | O  | 0       | 0       |
|     |       |          | 53    | 53 |         |         |
| 5   | B     | 54       | Total | O  | 0       | 0       |
|     |       |          | 54    | 54 |         |         |
| 5   | L     | 74       | Total | O  | 0       | 0       |
|     |       |          | 74    | 74 |         |         |
| 5   | H     | 85       | Total | O  | 0       | 0       |
|     |       |          | 85    | 85 |         |         |

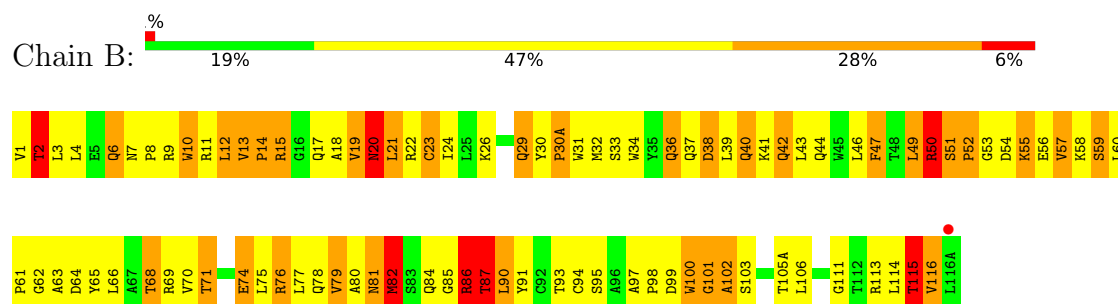
### 3 Residue-property plots

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.

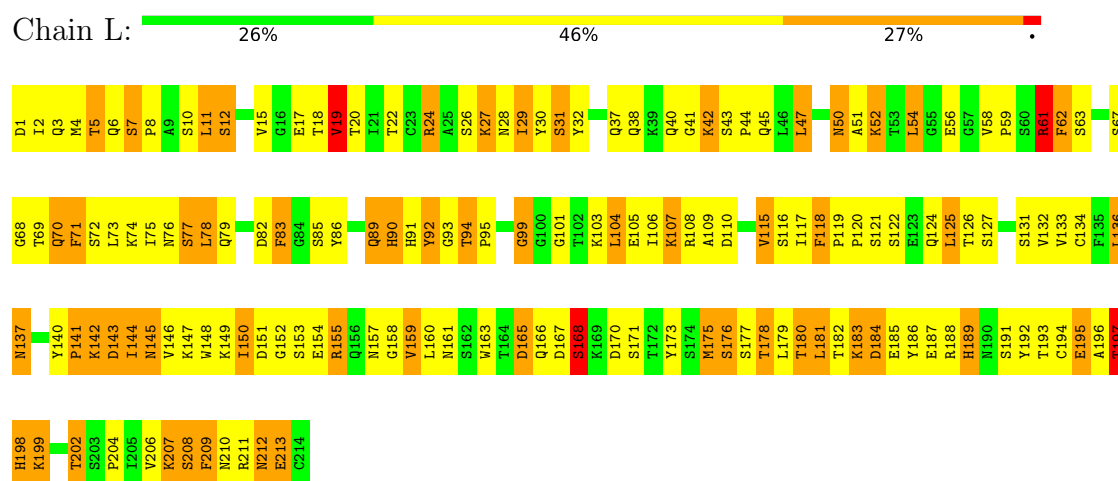
#### • Molecule 1: KB5-C20 T-CELL ANTIGEN RECEPTOR



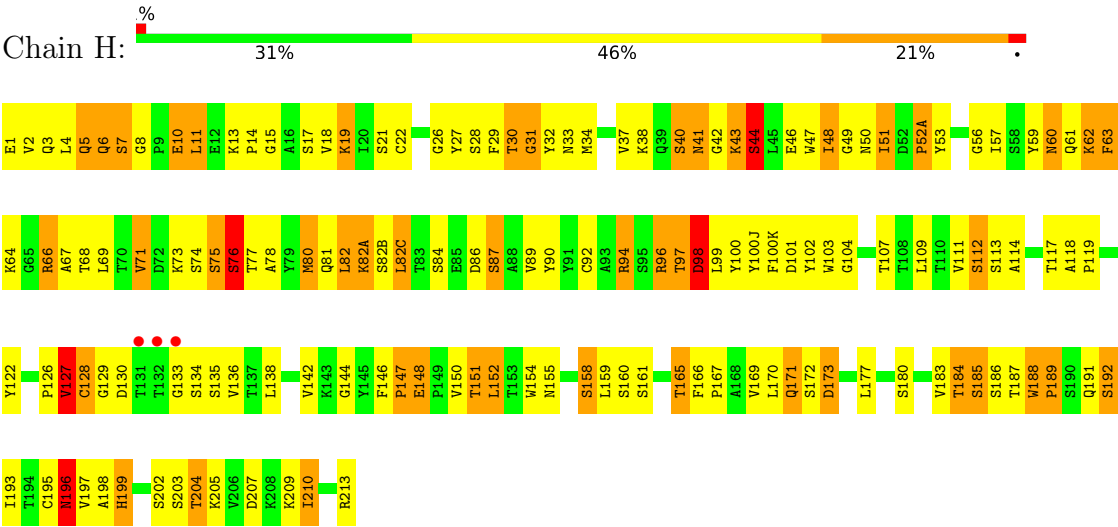
#### • Molecule 2: KB5-C20 T-CELL ANTIGEN RECEPTOR



#### • Molecule 3: ANTIBODY DESIRE-1



#### • Molecule 4: ANTIBODY DESIRE-1



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 21 2                                                   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 187.31 Å 80.95 Å 52.08 Å<br>90.00° 90.00° 90.00°            | Depositor        |
| Resolution (Å)                                                          | 10.00 – 2.50<br>10.00 – 2.50                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | (Not available) (10.00-2.50)<br>71.5 (10.00-2.50)           | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | 0.09                                                        | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.12 (at 2.50 Å)                                            | Xtriage          |
| Refinement program                                                      | REFMAC                                                      | Depositor        |
| R, $R_{free}$                                                           | 0.219 , (Not available)<br>0.222 , 0.237                    | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 1056 reflections (5.12%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 49.2                                                        | Xtriage          |
| Anisotropy                                                              | 0.238                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.41 , 162.6                                                | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.93                                                        | EDS              |
| Total number of atoms                                                   | 5438                                                        | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 48.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.59% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

| Mol | Chain | Bond lengths |               | Bond angles |                 |
|-----|-------|--------------|---------------|-------------|-----------------|
|     |       | RMSZ         | # $ Z  > 5$   | RMSZ        | # $ Z  > 5$     |
| 1   | A     | 0.99         | 1/927 (0.1%)  | 2.50        | 54/1256 (4.3%)  |
| 2   | B     | 0.95         | 1/963 (0.1%)  | 2.33        | 42/1310 (3.2%)  |
| 3   | L     | 0.90         | 1/1700 (0.1%) | 2.03        | 58/2304 (2.5%)  |
| 4   | H     | 0.86         | 1/1708 (0.1%) | 1.97        | 60/2328 (2.6%)  |
| All | All   | 0.91         | 4/5298 (0.1%) | 2.16        | 214/7198 (3.0%) |

All (4) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 2   | B     | 116 | VAL  | N-CA  | -7.63 | 1.36        | 1.46     |
| 3   | L     | 29  | ILE  | C-O   | 5.97  | 1.29        | 1.23     |
| 4   | H     | 98  | ASP  | N-CA  | 5.46  | 1.53        | 1.45     |
| 1   | A     | 118 | SER  | N-CA  | -5.22 | 1.39        | 1.46     |

All (214) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|--------|-------------|----------|
| 2   | B     | 115 | THR  | CA-C-N   | 26.36  | 169.42      | 121.97   |
| 2   | B     | 115 | THR  | C-N-CA   | 26.36  | 169.42      | 121.97   |
| 1   | A     | 116 | PRO  | CA-C-N   | 20.14  | 160.88      | 121.41   |
| 1   | A     | 116 | PRO  | C-N-CA   | 20.14  | 160.88      | 121.41   |
| 1   | A     | 93  | ARG  | CD-NE-CZ | 19.41  | 151.57      | 124.40   |
| 1   | A     | 76  | HIS  | CA-CB-CG | 15.88  | 129.69      | 113.80   |
| 1   | A     | 29  | PHE  | CA-CB-CG | 14.42  | 128.22      | 113.80   |
| 3   | L     | 140 | TYR  | CA-C-O   | -13.80 | 107.16      | 119.72   |
| 3   | L     | 29  | ILE  | CA-C-O   | -12.68 | 111.67      | 121.68   |
| 3   | L     | 91  | HIS  | CA-CB-CG | 11.90  | 125.70      | 113.80   |
| 1   | A     | 6   | SER  | O-C-N    | 11.69  | 130.18      | 121.88   |
| 2   | B     | 86  | ARG  | CD-NE-CZ | 11.14  | 140.00      | 124.40   |
| 1   | A     | 6   | SER  | CA-C-O   | -11.13 | 108.81      | 120.28   |
| 4   | H     | 53  | TYR  | N-CA-C   | 10.62  | 122.54      | 110.97   |
| 2   | B     | 20  | ASN  | CA-CB-CG | 10.37  | 122.97      | 112.60   |
| 4   | H     | 188 | TRP  | CA-C-O   | -10.09 | 109.06      | 120.46   |

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| Mol | Chain | Res    | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 2   | B     | 91     | TYR  | N-CA-C    | 10.07 | 125.65      | 109.24   |
| 4   | H     | 98     | ASP  | CA-CB-CG  | 10.01 | 122.61      | 112.60   |
| 1   | A     | 4      | ARG  | CD-NE-CZ  | 9.84  | 138.17      | 124.40   |
| 4   | H     | 97     | THR  | CA-C-N    | -9.77 | 107.06      | 122.29   |
| 4   | H     | 97     | THR  | C-N-CA    | -9.77 | 107.06      | 122.29   |
| 1   | A     | 29     | PHE  | N-CA-C    | -9.74 | 94.81       | 110.20   |
| 3   | L     | 94     | THR  | CA-C-O    | -9.72 | 109.99      | 120.88   |
| 1   | A     | 116    | PRO  | N-CA-C    | 9.70  | 126.80      | 111.38   |
| 1   | A     | 97     | GLY  | N-CA-C    | 9.40  | 122.74      | 111.93   |
| 2   | B     | 100    | TRP  | CA-C-N    | 9.26  | 132.88      | 122.42   |
| 2   | B     | 100    | TRP  | C-N-CA    | 9.26  | 132.88      | 122.42   |
| 1   | A     | 117    | GLY  | CA-C-N    | 9.14  | 138.99      | 121.54   |
| 1   | A     | 117    | GLY  | C-N-CA    | 9.14  | 138.99      | 121.54   |
| 4   | H     | 66     | ARG  | CD-NE-CZ  | 9.08  | 137.12      | 124.40   |
| 2   | B     | 74     | GLU  | CB-CG-CD  | 8.98  | 127.87      | 112.60   |
| 3   | L     | 208    | SER  | N-CA-C    | 8.98  | 120.11      | 108.34   |
| 4   | H     | 196    | ASN  | CA-CB-CG  | 8.87  | 121.47      | 112.60   |
| 1   | A     | 116    | PRO  | CA-C-O    | 8.87  | 132.49      | 121.67   |
| 4   | H     | 189    | PRO  | N-CA-CB   | 8.84  | 112.32      | 102.60   |
| 3   | L     | 19     | VAL  | N-CA-CB   | 8.60  | 127.95      | 111.62   |
| 1   | A     | 69     | ARG  | CD-NE-CZ  | 8.46  | 136.24      | 124.40   |
| 1   | A     | 96     | GLY  | CA-C-N    | 8.27  | 127.96      | 120.10   |
| 1   | A     | 96     | GLY  | C-N-CA    | 8.27  | 127.96      | 120.10   |
| 2   | B     | 2      | THR  | N-CA-CB   | 8.26  | 124.45      | 110.49   |
| 4   | H     | 97     | THR  | CA-C-O    | -8.16 | 111.78      | 120.42   |
| 4   | H     | 100(K) | PHE  | CA-C-N    | 8.08  | 136.97      | 121.54   |
| 4   | H     | 100(K) | PHE  | C-N-CA    | 8.08  | 136.97      | 121.54   |
| 3   | L     | 141    | PRO  | N-CA-CB   | 8.02  | 111.42      | 102.60   |
| 2   | B     | 7      | ASN  | CA-C-O    | -7.96 | 110.49      | 120.04   |
| 3   | L     | 195    | GLU  | N-CA-C    | 7.87  | 121.79      | 108.02   |
| 2   | B     | 102    | ALA  | CA-C-N    | 7.84  | 134.70      | 122.78   |
| 2   | B     | 102    | ALA  | C-N-CA    | 7.84  | 134.70      | 122.78   |
| 1   | A     | 7      | PRO  | N-CA-CB   | 7.80  | 111.18      | 102.60   |
| 2   | B     | 87     | THR  | CB-CA-C   | 7.77  | 122.56      | 109.75   |
| 3   | L     | 202    | THR  | N-CA-C    | -7.75 | 103.97      | 113.50   |
| 4   | H     | 94     | ARG  | NE-CZ-NH2 | 7.73  | 126.16      | 119.20   |
| 3   | L     | 95     | PRO  | N-CA-CB   | 7.73  | 111.11      | 102.60   |
| 4   | H     | 43     | LYS  | CA-C-N    | 7.71  | 132.07      | 121.05   |
| 4   | H     | 43     | LYS  | C-N-CA    | 7.71  | 132.07      | 121.05   |
| 1   | A     | 19     | ILE  | N-CA-CB   | 7.69  | 121.64      | 111.64   |
| 4   | H     | 98     | ASP  | CB-CA-C   | 7.56  | 123.14      | 109.99   |
| 3   | L     | 61     | ARG  | CD-NE-CZ  | 7.55  | 134.97      | 124.40   |

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| Mol | Chain | Res    | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 4   | H     | 146    | PHE  | CA-C-O    | -7.54 | 109.83      | 120.16   |
| 1   | A     | 61     | ARG  | CD-NE-CZ  | 7.45  | 134.82      | 124.40   |
| 4   | H     | 188    | TRP  | O-C-N     | 7.38  | 128.14      | 121.80   |
| 1   | A     | 64     | ILE  | CB-CA-C   | -7.35 | 100.61      | 110.98   |
| 2   | B     | 115    | THR  | N-CA-CB   | 7.30  | 121.66      | 110.49   |
| 4   | H     | 52(A)  | PRO  | CA-C-N    | 7.27  | 130.25      | 120.65   |
| 4   | H     | 52(A)  | PRO  | C-N-CA    | 7.27  | 130.25      | 120.65   |
| 3   | L     | 213    | GLU  | N-CA-C    | 7.26  | 119.80      | 110.65   |
| 1   | A     | 106    | PHE  | N-CA-C    | 7.26  | 121.66      | 109.76   |
| 3   | L     | 61     | ARG  | N-CA-C    | -7.18 | 103.18      | 112.23   |
| 3   | L     | 29     | ILE  | CA-C-N    | -7.18 | 107.83      | 121.54   |
| 3   | L     | 29     | ILE  | C-N-CA    | -7.18 | 107.83      | 121.54   |
| 4   | H     | 146    | PHE  | O-C-N     | 7.17  | 129.56      | 121.32   |
| 2   | B     | 40     | GLN  | CA-C-O    | 7.15  | 129.20      | 120.55   |
| 2   | B     | 8      | PRO  | N-CA-CB   | 7.12  | 110.43      | 102.60   |
| 4   | H     | 100(K) | PHE  | CA-C-O    | 7.11  | 128.19      | 120.58   |
| 2   | B     | 42     | GLN  | CB-CA-C   | 7.05  | 121.71      | 109.65   |
| 4   | H     | 112    | SER  | N-CA-C    | 7.05  | 119.65      | 109.14   |
| 3   | L     | 99     | GLY  | N-CA-C    | -7.05 | 101.50      | 112.85   |
| 3   | L     | 110    | ASP  | CA-CB-CG  | 6.96  | 119.56      | 112.60   |
| 2   | B     | 40     | GLN  | CA-C-N    | 6.84  | 134.60      | 121.54   |
| 2   | B     | 40     | GLN  | C-N-CA    | 6.84  | 134.60      | 121.54   |
| 3   | L     | 50     | ASN  | CA-CB-CG  | 6.80  | 119.40      | 112.60   |
| 3   | L     | 62     | PHE  | CA-CB-CG  | -6.79 | 107.00      | 113.80   |
| 3   | L     | 125    | LEU  | N-CA-C    | -6.78 | 103.58      | 110.97   |
| 4   | H     | 112    | SER  | CA-C-O    | 6.78  | 129.10      | 121.51   |
| 3   | L     | 212    | ASN  | CA-CB-CG  | 6.77  | 119.37      | 112.60   |
| 1   | A     | 15     | GLY  | CA-C-O    | 6.72  | 125.55      | 119.83   |
| 2   | B     | 101    | GLY  | CA-C-O    | -6.72 | 112.19      | 120.92   |
| 3   | L     | 94     | THR  | O-C-N     | 6.71  | 129.04      | 121.53   |
| 4   | H     | 94     | ARG  | NE-CZ-NH1 | -6.69 | 114.81      | 121.50   |
| 1   | A     | 116    | PRO  | O-C-N     | -6.66 | 114.87      | 123.06   |
| 4   | H     | 165    | THR  | CB-CA-C   | 6.62  | 120.83      | 109.51   |
| 1   | A     | 16     | GLU  | N-CA-C    | 6.58  | 119.21      | 110.53   |
| 3   | L     | 107    | LYS  | CA-CB-CG  | 6.56  | 127.22      | 114.10   |
| 1   | A     | 66     | PHE  | N-CA-C    | 6.54  | 120.06      | 109.40   |
| 3   | L     | 137    | ASN  | CA-CB-CG  | 6.52  | 119.12      | 112.60   |
| 3   | L     | 150    | ILE  | CB-CA-C   | 6.52  | 118.71      | 111.80   |
| 4   | H     | 60     | ASN  | N-CA-C    | -6.43 | 100.91      | 110.23   |
| 3   | L     | 8      | PRO  | N-CA-CB   | 6.40  | 109.64      | 102.60   |
| 1   | A     | 9      | SER  | CB-CA-C   | -6.39 | 102.76      | 110.94   |
| 2   | B     | 98     | PRO  | N-CA-CB   | 6.34  | 108.90      | 103.19   |

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| Mol | Chain | Res    | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|----------|-------|-------------|----------|
| 1   | A     | 65     | PHE  | CA-CB-CG | 6.30  | 120.10      | 113.80   |
| 4   | H     | 147    | PRO  | N-CA-CB  | 6.27  | 109.49      | 102.60   |
| 2   | B     | 29     | GLN  | CA-C-N   | 6.25  | 129.73      | 122.85   |
| 2   | B     | 29     | GLN  | C-N-CA   | 6.25  | 129.73      | 122.85   |
| 3   | L     | 197    | THR  | N-CA-CB  | 6.20  | 120.29      | 110.55   |
| 4   | H     | 96     | ARG  | CA-CB-CG | 6.18  | 126.47      | 114.10   |
| 4   | H     | 96     | ARG  | N-CA-CB  | 6.18  | 118.65      | 110.25   |
| 1   | A     | 28     | THR  | CA-C-O   | 6.14  | 129.29      | 120.51   |
| 4   | H     | 148    | GLU  | N-CA-C   | 6.12  | 123.33      | 109.81   |
| 2   | B     | 20     | ASN  | CB-CA-C  | 6.07  | 121.70      | 109.38   |
| 3   | L     | 159    | VAL  | N-CA-C   | 6.05  | 116.58      | 107.80   |
| 4   | H     | 76     | SER  | N-CA-C   | -6.03 | 102.94      | 111.56   |
| 1   | A     | 57     | GLU  | N-CA-C   | 6.02  | 119.01      | 109.50   |
| 4   | H     | 15     | GLY  | N-CA-C   | -6.02 | 106.78      | 114.37   |
| 4   | H     | 67     | ALA  | CA-C-O   | -6.00 | 114.64      | 121.72   |
| 3   | L     | 185    | GLU  | N-CA-C   | -5.99 | 104.83      | 111.36   |
| 2   | B     | 10     | TRP  | CA-CB-CG | 5.98  | 124.96      | 113.60   |
| 2   | B     | 19     | VAL  | CB-CA-C  | -5.97 | 104.76      | 111.45   |
| 2   | B     | 97     | ALA  | CA-C-N   | 5.97  | 126.32      | 119.93   |
| 2   | B     | 97     | ALA  | C-N-CA   | 5.97  | 126.32      | 119.93   |
| 3   | L     | 29     | ILE  | N-CA-C   | -5.95 | 101.24      | 109.46   |
| 3   | L     | 41     | GLY  | N-CA-C   | -5.95 | 107.18      | 114.92   |
| 4   | H     | 100(K) | PHE  | N-CA-C   | 5.91  | 117.93      | 108.41   |
| 3   | L     | 29     | ILE  | O-C-N    | -5.90 | 116.63      | 122.12   |
| 2   | B     | 52     | PRO  | N-CA-CB  | 5.88  | 108.53      | 103.36   |
| 4   | H     | 8      | GLY  | CA-C-N   | 5.84  | 125.75      | 119.85   |
| 4   | H     | 8      | GLY  | C-N-CA   | 5.84  | 125.75      | 119.85   |
| 4   | H     | 89     | VAL  | CA-C-N   | -5.81 | 114.98      | 123.00   |
| 4   | H     | 89     | VAL  | C-N-CA   | -5.81 | 114.98      | 123.00   |
| 3   | L     | 59     | PRO  | N-CA-CB  | 5.80  | 108.84      | 103.39   |
| 3   | L     | 76     | ASN  | CA-C-O   | -5.80 | 115.11      | 121.89   |
| 3   | L     | 92     | TYR  | CA-C-O   | -5.75 | 114.14      | 120.70   |
| 4   | H     | 173    | ASP  | N-CA-C   | 5.75  | 119.59      | 112.47   |
| 2   | B     | 50     | ARG  | N-CA-C   | 5.72  | 118.38      | 111.40   |
| 1   | A     | 41     | GLU  | CB-CG-CD | 5.71  | 122.31      | 112.60   |
| 1   | A     | 32     | PHE  | CA-C-N   | 5.71  | 126.15      | 119.99   |
| 1   | A     | 32     | PHE  | C-N-CA   | 5.71  | 126.15      | 119.99   |
| 3   | L     | 7      | SER  | CA-C-O   | -5.67 | 113.49      | 119.50   |
| 4   | H     | 41     | ASN  | N-CA-CB  | -5.67 | 103.51      | 112.63   |
| 1   | A     | 81     | GLN  | O-C-N    | 5.65  | 125.96      | 121.55   |
| 3   | L     | 198    | HIS  | CA-C-N   | 5.65  | 128.62      | 120.38   |
| 3   | L     | 198    | HIS  | C-N-CA   | 5.65  | 128.62      | 120.38   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2   | B     | 115 | THR  | CA-C-O   | 5.64  | 128.64      | 121.82   |
| 4   | H     | 92  | CYS  | N-CA-C   | -5.64 | 101.35      | 110.32   |
| 3   | L     | 79  | GLN  | CA-C-N   | 5.63  | 125.48      | 119.28   |
| 3   | L     | 79  | GLN  | C-N-CA   | 5.63  | 125.48      | 119.28   |
| 1   | A     | 32  | PHE  | CA-CB-CG | -5.63 | 108.17      | 113.80   |
| 4   | H     | 104 | GLY  | N-CA-C   | -5.59 | 103.96      | 112.51   |
| 4   | H     | 147 | PRO  | CA-N-CD  | -5.58 | 103.68      | 111.50   |
| 3   | L     | 107 | LYS  | CA-C-N   | 5.57  | 130.96      | 122.11   |
| 3   | L     | 107 | LYS  | C-N-CA   | 5.57  | 130.96      | 122.11   |
| 3   | L     | 167 | ASP  | CA-CB-CG | 5.55  | 118.15      | 112.60   |
| 3   | L     | 30  | TYR  | CB-CA-C  | 5.51  | 121.40      | 110.42   |
| 2   | B     | 82  | MET  | N-CA-C   | 5.49  | 117.18      | 108.67   |
| 3   | L     | 31  | SER  | N-CA-C   | -5.48 | 105.29      | 112.41   |
| 4   | H     | 210 | ILE  | N-CA-CB  | 5.47  | 117.08      | 110.95   |
| 2   | B     | 18  | ALA  | N-CA-C   | 5.47  | 118.19      | 107.57   |
| 3   | L     | 184 | ASP  | N-CA-C   | -5.42 | 105.28      | 111.14   |
| 3   | L     | 83  | PHE  | N-CA-C   | -5.42 | 103.34      | 110.33   |
| 3   | L     | 24  | ARG  | CD-NE-CZ | 5.41  | 131.97      | 124.40   |
| 1   | A     | 103 | ALA  | N-CA-C   | 5.41  | 117.19      | 109.14   |
| 2   | B     | 47  | PHE  | CA-CB-CG | 5.40  | 119.20      | 113.80   |
| 1   | A     | 115 | SER  | CA-C-N   | 5.37  | 125.28      | 119.85   |
| 1   | A     | 115 | SER  | C-N-CA   | 5.37  | 125.28      | 119.85   |
| 2   | B     | 7   | ASN  | O-C-N    | 5.37  | 126.71      | 121.66   |
| 3   | L     | 180 | THR  | CA-C-O   | 5.36  | 126.03      | 120.30   |
| 1   | A     | 44  | ALA  | N-CA-C   | 5.36  | 117.14      | 108.41   |
| 1   | A     | 30  | ASN  | CA-CB-CG | 5.32  | 117.92      | 112.60   |
| 1   | A     | 12  | VAL  | N-CA-CB  | -5.31 | 102.74      | 111.45   |
| 3   | L     | 50  | ASN  | N-CA-C   | -5.30 | 104.12      | 111.28   |
| 4   | H     | 42  | GLY  | CA-C-N   | 5.30  | 131.66      | 121.54   |
| 4   | H     | 42  | GLY  | C-N-CA   | 5.30  | 131.66      | 121.54   |
| 2   | B     | 91  | TYR  | CB-CA-C  | -5.29 | 101.02      | 109.75   |
| 1   | A     | 87  | THR  | CA-C-O   | 5.29  | 126.14      | 120.38   |
| 2   | B     | 98  | PRO  | CA-C-N   | 5.26  | 127.33      | 120.28   |
| 2   | B     | 98  | PRO  | C-N-CA   | 5.26  | 127.33      | 120.28   |
| 4   | H     | 44  | SER  | N-CA-C   | 5.25  | 117.96      | 110.24   |
| 1   | A     | 116 | PRO  | N-CA-CB  | 5.24  | 108.21      | 103.33   |
| 2   | B     | 53  | GLY  | N-CA-C   | -5.23 | 107.58      | 115.32   |
| 3   | L     | 209 | PHE  | CA-CB-CG | 5.21  | 119.00      | 113.80   |
| 4   | H     | 199 | HIS  | CA-C-N   | 5.20  | 126.34      | 119.84   |
| 4   | H     | 199 | HIS  | C-N-CA   | 5.20  | 126.34      | 119.84   |
| 2   | B     | 6   | GLN  | N-CA-C   | 5.19  | 117.08      | 108.20   |
| 3   | L     | 168 | SER  | CA-C-O   | 5.19  | 126.06      | 119.78   |

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| Mol | Chain | Res   | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-------|------|-----------|-------|-------------|----------|
| 3   | L     | 95    | PRO  | CA-N-CD   | -5.19 | 104.24      | 111.50   |
| 3   | L     | 204   | PRO  | N-CA-CB   | 5.18  | 108.26      | 103.39   |
| 4   | H     | 34    | MET  | N-CA-CB   | 5.18  | 118.84      | 110.65   |
| 4   | H     | 130   | ASP  | N-CA-CB   | 5.18  | 119.24      | 110.49   |
| 4   | H     | 100   | TYR  | C-N-CA    | 5.17  | 134.62      | 121.70   |
| 3   | L     | 202   | THR  | CA-C-O    | 5.16  | 124.82      | 119.14   |
| 4   | H     | 31    | GLY  | O-C-N     | -5.16 | 115.99      | 122.70   |
| 1   | A     | 95    | GLN  | CA-C-N    | 5.15  | 130.60      | 122.51   |
| 1   | A     | 95    | GLN  | C-N-CA    | 5.15  | 130.60      | 122.51   |
| 1   | A     | 79    | ASP  | CA-C-O    | -5.14 | 114.61      | 120.32   |
| 1   | A     | 110   | THR  | CA-C-O    | -5.13 | 115.27      | 120.71   |
| 1   | A     | 38    | PHE  | CA-CB-CG  | -5.11 | 108.69      | 113.80   |
| 4   | H     | 33    | ASN  | CA-CB-CG  | 5.11  | 117.71      | 112.60   |
| 3   | L     | 118   | PHE  | CA-C-N    | 5.09  | 125.62      | 120.38   |
| 3   | L     | 118   | PHE  | C-N-CA    | 5.09  | 125.62      | 120.38   |
| 2   | B     | 30(A) | PRO  | N-CA-CB   | 5.08  | 108.03      | 103.20   |
| 3   | L     | 19    | VAL  | CA-CB-CG2 | 5.07  | 119.01      | 110.40   |
| 4   | H     | 63    | PHE  | CA-CB-CG  | -5.06 | 108.74      | 113.80   |
| 4   | H     | 133   | GLY  | N-CA-C    | -5.05 | 107.56      | 114.64   |
| 4   | H     | 185   | SER  | CA-C-N    | 5.05  | 130.30      | 122.26   |
| 4   | H     | 185   | SER  | C-N-CA    | 5.05  | 130.30      | 122.26   |
| 1   | A     | 11    | THR  | CA-C-N    | -5.05 | 115.44      | 122.71   |
| 1   | A     | 11    | THR  | C-N-CA    | -5.05 | 115.44      | 122.71   |
| 4   | H     | 189   | PRO  | CA-N-CD   | -5.05 | 104.43      | 111.50   |
| 1   | A     | 118   | SER  | N-CA-C    | 5.05  | 121.55      | 110.80   |
| 2   | B     | 71    | THR  | CB-CA-C   | -5.03 | 101.84      | 114.11   |
| 1   | A     | 29    | PHE  | CA-C-O    | -5.02 | 115.33      | 121.05   |
| 4   | H     | 134   | SER  | N-CA-C    | 5.02  | 119.25      | 113.38   |
| 1   | A     | 29    | PHE  | CA-C-N    | -5.01 | 114.38      | 122.24   |
| 1   | A     | 29    | PHE  | C-N-CA    | -5.01 | 114.38      | 122.24   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 904   | 0        | 861      | 83      | 0            |
| 2   | B     | 941   | 0        | 936      | 103     | 0            |
| 3   | L     | 1661  | 0        | 1586     | 151     | 2            |
| 4   | H     | 1666  | 0        | 1618     | 110     | 0            |
| 5   | A     | 53    | 0        | 0        | 6       | 0            |
| 5   | B     | 54    | 0        | 0        | 8       | 0            |
| 5   | H     | 85    | 0        | 0        | 8       | 0            |
| 5   | L     | 74    | 0        | 0        | 15      | 0            |
| All | All   | 5438  | 0        | 5001     | 423     | 2            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 42.

All (423) 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:B:113:ARG:HH21 | 2:B:115:THR:HG21 | 1.25                     | 1.00              |
| 3:L:119:PRO:HG2  | 4:H:213:ARG:HH12 | 1.29                     | 0.95              |
| 3:L:42:LYS:HZ2   | 3:L:43:SER:H     | 1.07                     | 0.93              |
| 4:H:199:HIS:HB3  | 4:H:204:THR:HB   | 1.51                     | 0.93              |
| 2:B:22:ARG:HH21  | 2:B:74:GLU:HG3   | 1.34                     | 0.92              |
| 1:A:11:THR:HG23  | 1:A:116:PRO:HG2  | 1.52                     | 0.92              |
| 3:L:119:PRO:HD2  | 4:H:213:ARG:HH22 | 1.36                     | 0.91              |
| 3:L:145:ASN:HB3  | 3:L:197:THR:HG22 | 1.51                     | 0.91              |
| 1:A:4:ARG:HH22   | 1:A:25:GLU:HB2   | 1.35                     | 0.91              |
| 3:L:187:GLU:HA   | 3:L:211:ARG:HD3  | 1.53                     | 0.90              |
| 4:H:51:ILE:HG12  | 4:H:57:ILE:HG12  | 1.54                     | 0.88              |
| 3:L:42:LYS:HZ2   | 3:L:43:SER:N     | 1.72                     | 0.88              |
| 3:L:155:ARG:HD3  | 3:L:179:LEU:HD11 | 1.56                     | 0.88              |
| 1:A:115:SER:N    | 1:A:116:PRO:HD3  | 1.90                     | 0.87              |
| 2:B:21:LEU:HD23  | 2:B:77:LEU:HD23  | 1.59                     | 0.84              |
| 2:B:80:ALA:O     | 2:B:81:ASN:HB2   | 1.76                     | 0.83              |
| 1:A:61:ARG:HD2   | 1:A:79:ASP:HB3   | 1.60                     | 0.81              |
| 2:B:13:VAL:HB    | 2:B:19:VAL:CG2   | 2.09                     | 0.81              |
| 1:A:29:PHE:HE1   | 1:A:105:ILE:HD13 | 1.47                     | 0.80              |
| 2:B:99:ASP:O     | 2:B:100:TRP:HB2  | 1.81                     | 0.80              |
| 2:B:22:ARG:HH21  | 2:B:74:GLU:CG    | 1.94                     | 0.79              |
| 2:B:22:ARG:NH2   | 2:B:74:GLU:HG3   | 1.97                     | 0.78              |
| 3:L:28:ASN:ND2   | 3:L:68:GLY:HA2   | 2.00                     | 0.76              |
| 3:L:122:SER:HA   | 3:L:125:LEU:HD12 | 1.66                     | 0.76              |
| 3:L:141:PRO:HG2  | 3:L:199:LYS:HE2  | 1.66                     | 0.76              |
| 3:L:183:LYS:HD3  | 3:L:187:GLU:HG3  | 1.66                     | 0.75              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:L:22:THR:HG22  | 3:L:72:SER:OG     | 1.86                     | 0.75              |
| 1:A:61:ARG:NH1   | 1:A:79:ASP:O      | 2.18                     | 0.75              |
| 3:L:147:LYS:HG2  | 3:L:154:GLU:HG3   | 1.69                     | 0.74              |
| 4:H:87:SER:HA    | 4:H:109:LEU:O     | 1.87                     | 0.74              |
| 2:B:36:GLN:HG2   | 2:B:46:LEU:HD21   | 1.69                     | 0.73              |
| 3:L:28:ASN:HD22  | 3:L:68:GLY:HA2    | 1.50                     | 0.73              |
| 3:L:187:GLU:HA   | 3:L:211:ARG:CD    | 2.18                     | 0.73              |
| 1:A:104:LEU:HD12 | 2:B:106:LEU:HD23  | 1.69                     | 0.73              |
| 3:L:42:LYS:NZ    | 3:L:43:SER:H      | 1.84                     | 0.72              |
| 2:B:66:LEU:HD23  | 2:B:78:GLN:HE21   | 1.53                     | 0.72              |
| 3:L:150:ILE:HG13 | 3:L:192:TYR:CE1   | 2.25                     | 0.72              |
| 3:L:155:ARG:HB2  | 3:L:155:ARG:HH11  | 1.54                     | 0.72              |
| 3:L:83:PHE:HB3   | 3:L:106:ILE:CD1   | 2.20                     | 0.72              |
| 1:A:1:GLN:HB3    | 1:A:4:ARG:HD3     | 1.70                     | 0.72              |
| 3:L:183:LYS:HA   | 3:L:186:TYR:HB3   | 1.71                     | 0.71              |
| 3:L:61:ARG:HG2   | 3:L:61:ARG:HH11   | 1.55                     | 0.71              |
| 4:H:138:LEU:HD23 | 4:H:210:ILE:HG21  | 1.70                     | 0.71              |
| 2:B:13:VAL:HB    | 2:B:19:VAL:HG23   | 1.72                     | 0.71              |
| 3:L:11:LEU:HD13  | 3:L:104:LEU:HD23  | 1.72                     | 0.70              |
| 1:A:4:ARG:NH2    | 1:A:25:GLU:HB2    | 2.06                     | 0.70              |
| 3:L:119:PRO:HG2  | 4:H:213:ARG:NH1   | 2.05                     | 0.70              |
| 1:A:5:GLN:HE22   | 1:A:90:CYS:H      | 1.39                     | 0.69              |
| 3:L:27:LYS:HD3   | 5:L:229:HOH:O     | 1.91                     | 0.69              |
| 3:L:12:SER:HA    | 3:L:105:GLU:O     | 1.93                     | 0.69              |
| 4:H:30:THR:HA    | 4:H:52(A):PRO:HB2 | 1.75                     | 0.68              |
| 1:A:5:GLN:NE2    | 1:A:90:CYS:H      | 1.92                     | 0.68              |
| 3:L:193:THR:HG23 | 3:L:206:VAL:HG23  | 1.76                     | 0.68              |
| 1:A:47:ILE:HG23  | 1:A:64:ILE:HD11   | 1.76                     | 0.67              |
| 3:L:175:MET:HG2  | 3:L:176:SER:N     | 2.07                     | 0.67              |
| 2:B:31:TRP:CZ3   | 2:B:50:ARG:HD2    | 2.29                     | 0.67              |
| 1:A:116:PRO:HB3  | 1:A:118:SER:HA    | 1.77                     | 0.66              |
| 3:L:47:LEU:HA    | 3:L:58:VAL:HG21   | 1.76                     | 0.66              |
| 3:L:83:PHE:HE1   | 3:L:168:SER:HG    | 1.44                     | 0.66              |
| 3:L:144:ILE:HD12 | 3:L:198:HIS:HB2   | 1.78                     | 0.66              |
| 4:H:94:ARG:NH1   | 4:H:102:TYR:HD2   | 1.94                     | 0.66              |
| 3:L:86:TYR:O     | 3:L:101:GLY:HA2   | 1.96                     | 0.66              |
| 4:H:187:THR:O    | 4:H:191:GLN:HB2   | 1.96                     | 0.66              |
| 1:A:10:LEU:CD1   | 1:A:112:VAL:HG13  | 2.26                     | 0.65              |
| 1:A:49:ILE:HG21  | 1:A:64:ILE:HG21   | 1.78                     | 0.65              |
| 2:B:49:LEU:H     | 2:B:49:LEU:HD12   | 1.62                     | 0.65              |
| 1:A:11:THR:HG23  | 1:A:116:PRO:CG    | 2.26                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:L:12:SER:HB2   | 3:L:105:GLU:HB3  | 1.79                     | 0.65              |
| 3:L:136:LEU:HD23 | 3:L:196:ALA:HB2  | 1.78                     | 0.65              |
| 1:A:49:ILE:HD12  | 1:A:56:LYS:HB2   | 1.80                     | 0.64              |
| 4:H:51:ILE:HG21  | 4:H:71:VAL:HG23  | 1.80                     | 0.64              |
| 4:H:155:ASN:HB2  | 4:H:159:LEU:HB2  | 1.78                     | 0.64              |
| 3:L:83:PHE:HB3   | 3:L:106:ILE:HD11 | 1.76                     | 0.64              |
| 2:B:79:VAL:HG21  | 2:B:82:MET:HE3   | 1.79                     | 0.64              |
| 2:B:113:ARG:NH2  | 2:B:115:THR:HG21 | 2.07                     | 0.64              |
| 2:B:4:LEU:HD22   | 2:B:23:CYS:SG    | 2.39                     | 0.63              |
| 2:B:57:VAL:HG12  | 2:B:66:LEU:HA    | 1.79                     | 0.63              |
| 3:L:3:GLN:HB3    | 3:L:26:SER:HB3   | 1.79                     | 0.63              |
| 3:L:170:ASP:O    | 3:L:171:SER:HB2  | 1.97                     | 0.63              |
| 4:H:40:SER:O     | 4:H:43:LYS:HB2   | 1.99                     | 0.63              |
| 2:B:66:LEU:HD23  | 2:B:78:GLN:NE2   | 2.13                     | 0.63              |
| 1:A:116:PRO:HB3  | 1:A:118:SER:CA   | 2.29                     | 0.62              |
| 2:B:113:ARG:HH21 | 2:B:115:THR:CG2  | 2.07                     | 0.62              |
| 1:A:69:ARG:HG2   | 1:A:69:ARG:HH11  | 1.62                     | 0.62              |
| 2:B:49:LEU:HD13  | 2:B:75:LEU:HD11  | 1.81                     | 0.62              |
| 2:B:80:ALA:O     | 2:B:81:ASN:CB    | 2.46                     | 0.62              |
| 2:B:101:GLY:O    | 2:B:103:SER:N    | 2.33                     | 0.62              |
| 3:L:119:PRO:HD2  | 4:H:213:ARG:NH2  | 2.11                     | 0.62              |
| 1:A:1:GLN:NE2    | 1:A:4:ARG:HB3    | 2.14                     | 0.62              |
| 1:A:5:GLN:NE2    | 1:A:109:GLY:H    | 1.97                     | 0.62              |
| 3:L:90:HIS:HD2   | 3:L:92:TYR:H     | 1.48                     | 0.62              |
| 4:H:188:TRP:CG   | 4:H:189:PRO:HA   | 2.35                     | 0.61              |
| 3:L:50:ASN:O     | 3:L:52:LYS:N     | 2.32                     | 0.61              |
| 4:H:138:LEU:HB3  | 4:H:210:ILE:HD13 | 1.81                     | 0.61              |
| 4:H:152:LEU:HB2  | 4:H:197:VAL:HG22 | 1.82                     | 0.61              |
| 4:H:38:LYS:HB2   | 4:H:90:TYR:CE1   | 2.36                     | 0.60              |
| 4:H:94:ARG:HH12  | 4:H:102:TYR:HD2  | 1.49                     | 0.60              |
| 1:A:2:GLN:OE1    | 1:A:26:ASP:HB2   | 2.00                     | 0.60              |
| 4:H:138:LEU:HD21 | 4:H:188:TRP:CD2  | 2.36                     | 0.60              |
| 3:L:141:PRO:HG2  | 3:L:199:LYS:CE   | 2.31                     | 0.60              |
| 2:B:22:ARG:HA    | 2:B:76:ARG:HA    | 1.84                     | 0.60              |
| 4:H:10:GLU:HG3   | 4:H:18:VAL:HG21  | 1.84                     | 0.60              |
| 1:A:45:LEU:HD12  | 1:A:46:LEU:N     | 2.16                     | 0.60              |
| 1:A:101:ARG:NE   | 4:H:98:ASP:OD1   | 2.31                     | 0.60              |
| 1:A:80:SER:HB3   | 1:A:114:VAL:CG1  | 2.32                     | 0.59              |
| 1:A:13:TRP:O     | 1:A:16:GLU:HB2   | 2.02                     | 0.59              |
| 3:L:125:LEU:O    | 3:L:126:THR:C    | 2.46                     | 0.59              |
| 4:H:50:ASN:O     | 4:H:57:ILE:HG23  | 2.03                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:18:ALA:O     | 1:A:76:HIS:HA    | 2.02                     | 0.59              |
| 3:L:159:VAL:HA   | 3:L:178:THR:O    | 2.02                     | 0.59              |
| 3:L:108:ARG:HG2  | 3:L:109:ALA:N    | 2.18                     | 0.59              |
| 2:B:36:GLN:NE2   | 2:B:65:TYR:OH    | 2.35                     | 0.59              |
| 1:A:101:ARG:HB2  | 4:H:98:ASP:OD1   | 2.03                     | 0.59              |
| 4:H:1:GLU:O      | 4:H:26:GLY:HA3   | 2.03                     | 0.59              |
| 3:L:115:VAL:CG1  | 3:L:207:LYS:HB2  | 2.33                     | 0.58              |
| 1:A:80:SER:HB3   | 1:A:114:VAL:HG11 | 1.84                     | 0.58              |
| 3:L:90:HIS:HE1   | 5:L:230:HOH:O    | 1.87                     | 0.58              |
| 4:H:150:VAL:HG23 | 4:H:198:ALA:O    | 2.03                     | 0.58              |
| 1:A:61:ARG:CD    | 1:A:79:ASP:HB3   | 2.31                     | 0.58              |
| 4:H:41:ASN:HB3   | 4:H:43:LYS:HG3   | 1.85                     | 0.57              |
| 1:A:50:ARG:HB3   | 5:B:137:HOH:O    | 2.04                     | 0.57              |
| 3:L:108:ARG:HG2  | 3:L:109:ALA:H    | 1.69                     | 0.57              |
| 1:A:116:PRO:HB3  | 1:A:118:SER:H    | 1.70                     | 0.57              |
| 4:H:38:LYS:CB    | 4:H:48:ILE:HD11  | 2.34                     | 0.57              |
| 3:L:117:ILE:HD11 | 3:L:132:VAL:HG11 | 1.87                     | 0.56              |
| 2:B:32:MET:SD    | 5:B:134:HOH:O    | 2.57                     | 0.56              |
| 3:L:70:GLN:HE21  | 3:L:71:PHE:N     | 2.03                     | 0.56              |
| 3:L:2:ILE:HD13   | 3:L:29:ILE:CG2   | 2.35                     | 0.56              |
| 4:H:7:SER:HB3    | 4:H:21:SER:H     | 1.70                     | 0.56              |
| 4:H:154:TRP:O    | 4:H:155:ASN:HB2  | 2.04                     | 0.56              |
| 4:H:86:ASP:HB2   | 4:H:111:VAL:HG21 | 1.88                     | 0.56              |
| 1:A:67:ASN:HB3   | 1:A:72:LYS:HB3   | 1.86                     | 0.56              |
| 2:B:31:TRP:HZ3   | 5:B:117:HOH:O    | 1.89                     | 0.56              |
| 2:B:51:SER:O     | 2:B:54:ASP:HB2   | 2.05                     | 0.56              |
| 3:L:3:GLN:HB2    | 5:L:237:HOH:O    | 2.06                     | 0.56              |
| 1:A:115:SER:N    | 1:A:116:PRO:CD   | 2.67                     | 0.56              |
| 3:L:144:ILE:HD11 | 3:L:196:ALA:HB1  | 1.89                     | 0.55              |
| 1:A:10:LEU:HD11  | 1:A:112:VAL:HG13 | 1.87                     | 0.55              |
| 2:B:42:GLN:HB3   | 5:H:217:HOH:O    | 2.06                     | 0.55              |
| 3:L:193:THR:HG23 | 3:L:206:VAL:CG2  | 2.36                     | 0.55              |
| 3:L:124:GLN:HG3  | 4:H:122:TYR:CZ   | 2.41                     | 0.55              |
| 3:L:83:PHE:HB3   | 3:L:106:ILE:HD12 | 1.87                     | 0.55              |
| 3:L:115:VAL:HG12 | 3:L:207:LYS:HB2  | 1.88                     | 0.55              |
| 4:H:155:ASN:O    | 4:H:158:SER:HB3  | 2.07                     | 0.55              |
| 2:B:55:LYS:HA    | 2:B:68:THR:HA    | 1.89                     | 0.55              |
| 2:B:59:SER:O     | 4:H:56:GLY:HA2   | 2.06                     | 0.55              |
| 3:L:27:LYS:HE3   | 5:L:276:HOH:O    | 2.07                     | 0.55              |
| 4:H:18:VAL:HG11  | 4:H:109:LEU:CD1  | 2.37                     | 0.55              |
| 3:L:86:TYR:HE2   | 3:L:104:LEU:HD12 | 1.72                     | 0.55              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:A:1:GLN:HA     | 5:A:153:HOH:O      | 2.07                     | 0.54              |
| 1:A:29:PHE:CE1   | 1:A:105:ILE:HD13   | 2.37                     | 0.54              |
| 4:H:18:VAL:HG11  | 4:H:109:LEU:HD13   | 1.88                     | 0.54              |
| 4:H:43:LYS:HD2   | 5:H:247:HOH:O      | 2.06                     | 0.54              |
| 2:B:49:LEU:HD12  | 2:B:49:LEU:N       | 2.22                     | 0.54              |
| 3:L:181:LEU:HD23 | 5:L:231:HOH:O      | 2.07                     | 0.54              |
| 4:H:38:LYS:HB2   | 4:H:48:ILE:HD11    | 1.89                     | 0.54              |
| 3:L:148:TRP:O    | 3:L:154:GLU:HA     | 2.07                     | 0.54              |
| 1:A:10:LEU:HD12  | 1:A:10:LEU:O       | 2.06                     | 0.54              |
| 4:H:18:VAL:O     | 4:H:81:GLN:HG3     | 2.08                     | 0.54              |
| 1:A:4:ARG:NH1    | 5:A:136:HOH:O      | 2.39                     | 0.54              |
| 1:A:32:PHE:HB3   | 1:A:73:LEU:HD21    | 1.90                     | 0.54              |
| 3:L:19:VAL:HG23  | 3:L:78:LEU:HD21    | 1.89                     | 0.54              |
| 3:L:183:LYS:CD   | 3:L:187:GLU:HG3    | 2.37                     | 0.54              |
| 2:B:62:GLY:HA2   | 2:B:84:GLN:OE1     | 2.08                     | 0.53              |
| 2:B:79:VAL:HG21  | 2:B:82:MET:CE      | 2.38                     | 0.53              |
| 3:L:195:GLU:HG2  | 3:L:206:VAL:HB     | 1.91                     | 0.53              |
| 4:H:84:SER:HB2   | 5:H:231:HOH:O      | 2.07                     | 0.53              |
| 4:H:68:THR:OG1   | 4:H:82(A):LYS:HE2  | 2.08                     | 0.53              |
| 3:L:134:CYS:HB2  | 3:L:148:TRP:CH2    | 2.43                     | 0.53              |
| 4:H:99:LEU:HB3   | 4:H:100(J):TYR:CD2 | 2.44                     | 0.53              |
| 2:B:17:GLN:NE2   | 5:B:129:HOH:O      | 2.41                     | 0.53              |
| 2:B:85:GLY:H     | 2:B:116:VAL:HG21   | 1.73                     | 0.53              |
| 3:L:119:PRO:CG   | 4:H:213:ARG:HH12   | 2.11                     | 0.53              |
| 4:H:154:TRP:CZ3  | 4:H:210:ILE:HD11   | 2.44                     | 0.53              |
| 4:H:1:GLU:HG2    | 4:H:2:VAL:H        | 1.74                     | 0.53              |
| 1:A:62:PHE:CE1   | 1:A:77:ILE:HG23    | 2.43                     | 0.53              |
| 4:H:196:ASN:HB3  | 4:H:207:ASP:OD1    | 2.09                     | 0.53              |
| 3:L:207:LYS:HE2  | 5:L:245:HOH:O      | 2.09                     | 0.52              |
| 4:H:11:LEU:HG    | 4:H:147:PRO:HG3    | 1.92                     | 0.52              |
| 3:L:136:LEU:CD2  | 3:L:196:ALA:HB2    | 2.40                     | 0.52              |
| 4:H:171:GLN:O    | 4:H:172:SER:C      | 2.52                     | 0.52              |
| 1:A:36:GLN:HG3   | 1:A:88:TYR:CE2     | 2.44                     | 0.52              |
| 1:A:45:LEU:HD12  | 1:A:46:LEU:H       | 1.74                     | 0.52              |
| 3:L:105:GLU:HG2  | 3:L:106:ILE:N      | 2.24                     | 0.52              |
| 3:L:31:SER:O     | 3:L:50:ASN:HA      | 2.10                     | 0.52              |
| 3:L:119:PRO:CD   | 4:H:213:ARG:HH22   | 2.15                     | 0.52              |
| 2:B:11:ARG:HG3   | 5:B:165:HOH:O      | 2.09                     | 0.52              |
| 4:H:138:LEU:HD21 | 4:H:188:TRP:CE2    | 2.45                     | 0.52              |
| 3:L:210:ASN:HB2  | 3:L:213:GLU:HB2    | 1.91                     | 0.52              |
| 4:H:59:TYR:HB2   | 4:H:64:LYS:HD2     | 1.93                     | 0.51              |

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| Atom-1           | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|---------------------|--------------------------|-------------------|
| 3:L:150:ILE:HG23 | 5:L:255:HOH:O       | 2.10                     | 0.51              |
| 3:L:184:ASP:O    | 3:L:188:ARG:HB2     | 2.10                     | 0.51              |
| 3:L:28:ASN:HD22  | 3:L:68:GLY:CA       | 2.20                     | 0.51              |
| 2:B:37:GLN:OE1   | 2:B:43:LEU:HD13     | 2.10                     | 0.51              |
| 3:L:158:GLY:O    | 3:L:179:LEU:HA      | 2.11                     | 0.51              |
| 3:L:186:TYR:CE2  | 3:L:211:ARG:HG3     | 2.46                     | 0.51              |
| 3:L:186:TYR:HH   | 3:L:209:PHE:HE1     | 1.58                     | 0.51              |
| 1:A:114:VAL:O    | 1:A:115:SER:HB3     | 2.10                     | 0.51              |
| 2:B:70:VAL:HG12  | 2:B:71:THR:HG23     | 1.93                     | 0.51              |
| 2:B:84:GLN:O     | 2:B:86:ARG:NH1      | 2.44                     | 0.51              |
| 3:L:2:ILE:HB     | 3:L:90:HIS:CE1      | 2.46                     | 0.51              |
| 5:L:268:HOH:O    | 4:H:61:GLN:HB2      | 2.10                     | 0.51              |
| 1:A:76:HIS:HB3   | 5:A:124:HOH:O       | 2.10                     | 0.50              |
| 2:B:93:THR:CB    | 2:B:106:LEU:HD11    | 2.41                     | 0.50              |
| 3:L:136:LEU:HD21 | 3:L:146:VAL:HG22    | 1.94                     | 0.50              |
| 1:A:114:VAL:C    | 1:A:116:PRO:HD3     | 2.37                     | 0.50              |
| 4:H:142:VAL:CG2  | 4:H:197:VAL:HG21    | 2.42                     | 0.50              |
| 2:B:85:GLY:H     | 2:B:116:VAL:CG2     | 2.25                     | 0.50              |
| 3:L:125:LEU:CD2  | 3:L:183:LYS:HG3     | 2.42                     | 0.50              |
| 3:L:19:VAL:HG12  | 3:L:20:THR:H        | 1.76                     | 0.50              |
| 2:B:70:VAL:HB    | 2:B:74:GLU:HB3      | 1.94                     | 0.49              |
| 2:B:22:ARG:NH2   | 2:B:74:GLU:CG       | 2.66                     | 0.49              |
| 2:B:10:TRP:O     | 2:B:10:TRP:CD1      | 2.65                     | 0.49              |
| 2:B:34:TRP:HE1   | 2:B:75:LEU:HG       | 1.77                     | 0.49              |
| 3:L:108:ARG:NH2  | 5:L:236:HOH:O       | 2.45                     | 0.49              |
| 3:L:143:ASP:O    | 3:L:198:HIS:HD2     | 1.95                     | 0.49              |
| 3:L:18:THR:HG22  | 5:L:278:HOH:O       | 2.13                     | 0.49              |
| 1:A:21:ASN:ND2   | 5:A:159:HOH:O       | 2.45                     | 0.49              |
| 4:H:27:TYR:CZ    | 4:H:94:ARG:HD2      | 2.47                     | 0.49              |
| 3:L:125:LEU:HD23 | 3:L:183:LYS:HG3     | 1.95                     | 0.49              |
| 3:L:86:TYR:CE2   | 3:L:104:LEU:HD12    | 2.47                     | 0.49              |
| 4:H:75:SER:O     | 4:H:76:SER:HB2      | 2.12                     | 0.49              |
| 1:A:8:GLN:NE2    | 1:A:108:THR:OG1     | 2.45                     | 0.48              |
| 1:A:45:LEU:HD23  | 2:B:105(A):THR:HG23 | 1.94                     | 0.48              |
| 2:B:55:LYS:HB3   | 2:B:68:THR:HG23     | 1.95                     | 0.48              |
| 3:L:11:LEU:O     | 3:L:104:LEU:HA      | 2.12                     | 0.48              |
| 2:B:6:GLN:HE22   | 2:B:111:GLY:HA2     | 1.77                     | 0.48              |
| 4:H:188:TRP:CD2  | 4:H:189:PRO:HA      | 2.48                     | 0.48              |
| 2:B:37:GLN:HB2   | 2:B:43:LEU:CD1      | 2.43                     | 0.48              |
| 3:L:37:GLN:HE22  | 3:L:82:ASP:HA       | 1.79                     | 0.48              |
| 3:L:210:ASN:HD22 | 3:L:213:GLU:HB2     | 1.78                     | 0.48              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 2:B:21:LEU:HD21  | 2:B:79:VAL:CG1     | 2.44                     | 0.48              |
| 1:A:10:LEU:HD12  | 1:A:10:LEU:C       | 2.39                     | 0.48              |
| 1:A:57:GLU:HG3   | 1:A:58:ASP:N       | 2.28                     | 0.48              |
| 2:B:19:VAL:HG11  | 2:B:114:LEU:HD21   | 1.96                     | 0.48              |
| 2:B:64:ASP:HB2   | 2:B:80:ALA:O       | 2.14                     | 0.48              |
| 2:B:22:ARG:HG3   | 2:B:76:ARG:HD3     | 1.96                     | 0.48              |
| 4:H:94:ARG:NH1   | 4:H:101:ASP:OD2    | 2.47                     | 0.48              |
| 1:A:31:TYR:CE2   | 1:A:33:PRO:HG3     | 2.49                     | 0.48              |
| 3:L:145:ASN:CB   | 3:L:197:THR:HG22   | 2.34                     | 0.48              |
| 2:B:100:TRP:CE2  | 3:L:31:SER:HB2     | 2.48                     | 0.47              |
| 3:L:50:ASN:ND2   | 5:L:216:HOH:O      | 2.41                     | 0.47              |
| 1:A:78:THR:HB    | 5:A:171:HOH:O      | 2.14                     | 0.47              |
| 3:L:119:PRO:CB   | 3:L:120:PRO:CD     | 2.92                     | 0.47              |
| 3:L:210:ASN:ND2  | 3:L:213:GLU:OE1    | 2.47                     | 0.47              |
| 1:A:58:ASP:O     | 1:A:59:GLY:C       | 2.56                     | 0.47              |
| 2:B:93:THR:OG1   | 2:B:106:LEU:HD11   | 2.14                     | 0.47              |
| 2:B:116:VAL:HA   | 5:B:132:HOH:O      | 2.12                     | 0.47              |
| 3:L:131:SER:HA   | 3:L:179:LEU:O      | 2.14                     | 0.47              |
| 3:L:195:GLU:HG3  | 3:L:206:VAL:HG23   | 1.97                     | 0.47              |
| 4:H:18:VAL:HG22  | 4:H:19:LYS:N       | 2.28                     | 0.47              |
| 4:H:135:SER:HA   | 4:H:184:THR:HA     | 1.96                     | 0.47              |
| 3:L:3:GLN:HB3    | 3:L:26:SER:CB      | 2.45                     | 0.47              |
| 4:H:29:PHE:HZ    | 4:H:71:VAL:HG22    | 1.79                     | 0.47              |
| 3:L:5:THR:HG22   | 3:L:24:ARG:HD3     | 1.96                     | 0.47              |
| 3:L:206:VAL:O    | 3:L:207:LYS:HD3    | 2.13                     | 0.47              |
| 2:B:10:TRP:O     | 2:B:10:TRP:HD1     | 1.98                     | 0.47              |
| 2:B:99:ASP:O     | 2:B:100:TRP:CB     | 2.55                     | 0.47              |
| 3:L:136:LEU:N    | 3:L:136:LEU:HD12   | 2.30                     | 0.47              |
| 4:H:46:GLU:OE2   | 4:H:62:LYS:HE2     | 2.14                     | 0.47              |
| 3:L:10:SER:O     | 3:L:11:LEU:HB3     | 2.15                     | 0.47              |
| 3:L:106:ILE:H    | 3:L:166:GLN:HE22   | 1.63                     | 0.47              |
| 1:A:62:PHE:CE1   | 1:A:77:ILE:HG12    | 2.50                     | 0.47              |
| 1:A:104:LEU:HD12 | 2:B:106:LEU:CD2    | 2.42                     | 0.47              |
| 1:A:116:PRO:CB   | 1:A:118:SER:H      | 2.27                     | 0.47              |
| 3:L:44:PRO:HG2   | 4:H:103:TRP:CZ3    | 2.50                     | 0.47              |
| 4:H:30:THR:O     | 4:H:32:TYR:N       | 2.48                     | 0.47              |
| 4:H:18:VAL:HG12  | 4:H:82(C):LEU:HD11 | 1.97                     | 0.47              |
| 1:A:84:ASP:HB2   | 1:A:114:VAL:HG21   | 1.95                     | 0.46              |
| 2:B:19:VAL:HG12  | 2:B:20:ASN:N       | 2.30                     | 0.46              |
| 3:L:42:LYS:NZ    | 3:L:42:LYS:HA      | 2.30                     | 0.46              |
| 4:H:166:PHE:O    | 4:H:167:PRO:C      | 2.57                     | 0.46              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:A:101:ARG:HD3  | 3:L:32:TYR:CZ      | 2.50                     | 0.46              |
| 3:L:83:PHE:HE1   | 3:L:168:SER:OG     | 1.97                     | 0.46              |
| 3:L:90:HIS:C     | 3:L:90:HIS:CD2     | 2.93                     | 0.46              |
| 3:L:121:SER:OG   | 4:H:122:TYR:HB3    | 2.15                     | 0.46              |
| 1:A:67:ASN:O     | 1:A:68:LYS:C       | 2.58                     | 0.46              |
| 2:B:21:LEU:N     | 2:B:21:LEU:HD22    | 2.31                     | 0.46              |
| 2:B:30:TYR:N     | 2:B:30(A):PRO:HD3  | 2.31                     | 0.46              |
| 4:H:51:ILE:CG1   | 4:H:57:ILE:HG12    | 2.38                     | 0.46              |
| 1:A:116:PRO:HB3  | 1:A:118:SER:OG     | 2.16                     | 0.46              |
| 2:B:13:VAL:HA    | 2:B:14:PRO:HD3     | 1.77                     | 0.46              |
| 4:H:60:ASN:HB3   | 4:H:63:PHE:HD2     | 1.81                     | 0.46              |
| 1:A:35:TYR:O     | 1:A:88:TYR:HA      | 2.16                     | 0.46              |
| 1:A:116:PRO:HB3  | 1:A:118:SER:N      | 2.31                     | 0.46              |
| 3:L:165:ASP:O    | 3:L:166:GLN:C      | 2.60                     | 0.46              |
| 2:B:14:PRO:HG2   | 2:B:17:GLN:HB2     | 1.98                     | 0.45              |
| 2:B:13:VAL:HG11  | 2:B:82:MET:HG2     | 1.98                     | 0.45              |
| 4:H:17:SER:O     | 4:H:81:GLN:NE2     | 2.49                     | 0.45              |
| 2:B:87:THR:HB    | 2:B:113:ARG:HA     | 1.97                     | 0.45              |
| 3:L:54:LEU:HD21  | 3:L:62:PHE:O       | 2.17                     | 0.45              |
| 4:H:18:VAL:H     | 4:H:82(C):LEU:HD11 | 1.81                     | 0.45              |
| 1:A:10:LEU:HD12  | 1:A:112:VAL:HG13   | 1.96                     | 0.45              |
| 4:H:38:LYS:HB3   | 4:H:48:ILE:HD11    | 1.97                     | 0.45              |
| 3:L:210:ASN:HB3  | 3:L:213:GLU:H      | 1.82                     | 0.45              |
| 4:H:6:GLN:HB3    | 4:H:21:SER:O       | 2.16                     | 0.45              |
| 4:H:184:THR:O    | 4:H:186:SER:N      | 2.50                     | 0.45              |
| 1:A:14:GLU:HG3   | 1:A:81:GLN:HA      | 1.99                     | 0.45              |
| 1:A:29:PHE:HA    | 1:A:94:TYR:HA      | 1.98                     | 0.45              |
| 3:L:210:ASN:O    | 3:L:211:ARG:C      | 2.60                     | 0.45              |
| 2:B:60:LEU:HB3   | 2:B:61:PRO:HD2     | 1.99                     | 0.45              |
| 4:H:14:PRO:HA    | 4:H:82(C):LEU:O    | 2.17                     | 0.44              |
| 4:H:22:CYS:HB3   | 4:H:78:ALA:HB3     | 1.99                     | 0.44              |
| 3:L:89:GLN:HG2   | 3:L:90:HIS:O       | 2.18                     | 0.44              |
| 4:H:2:VAL:HG13   | 4:H:27:TYR:CD2     | 2.52                     | 0.44              |
| 2:B:21:LEU:CD2   | 2:B:77:LEU:HD23    | 2.38                     | 0.44              |
| 2:B:85:GLY:HA3   | 2:B:116:VAL:HG23   | 1.98                     | 0.44              |
| 4:H:43:LYS:HB3   | 4:H:44:SER:H       | 1.50                     | 0.44              |
| 2:B:100:TRP:HH2  | 3:L:32:TYR:CD1     | 2.35                     | 0.44              |
| 3:L:117:ILE:HG22 | 3:L:207:LYS:HB3    | 1.99                     | 0.44              |
| 2:B:21:LEU:O     | 2:B:76:ARG:HB3     | 2.17                     | 0.44              |
| 2:B:40:GLN:HE21  | 2:B:42:GLN:CD      | 2.26                     | 0.44              |
| 3:L:61:ARG:HH11  | 3:L:61:ARG:CG      | 2.27                     | 0.44              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:L:145:ASN:O    | 3:L:196:ALA:HA    | 2.17                     | 0.44              |
| 4:H:154:TRP:HZ3  | 4:H:210:ILE:HD11  | 1.80                     | 0.44              |
| 3:L:77:SER:O     | 3:L:78:LEU:C      | 2.61                     | 0.44              |
| 4:H:142:VAL:HG22 | 4:H:197:VAL:HG21  | 2.00                     | 0.44              |
| 4:H:32:TYR:O     | 4:H:52(A):PRO:HD2 | 2.18                     | 0.44              |
| 1:A:27:SER:HA    | 1:A:71:LYS:HD3    | 1.99                     | 0.44              |
| 2:B:13:VAL:HG23  | 2:B:14:PRO:HD2    | 1.99                     | 0.44              |
| 2:B:62:GLY:O     | 2:B:63:ALA:HB2    | 2.18                     | 0.44              |
| 4:H:138:LEU:HD23 | 4:H:210:ILE:CG2   | 2.44                     | 0.44              |
| 3:L:142:LYS:HB2  | 3:L:173:TYR:CE2   | 2.53                     | 0.43              |
| 4:H:136:VAL:HG13 | 4:H:138:LEU:CD1   | 2.48                     | 0.43              |
| 2:B:6:GLN:NE2    | 2:B:111:GLY:HA2   | 2.33                     | 0.43              |
| 2:B:37:GLN:HB2   | 2:B:43:LEU:HD12   | 2.00                     | 0.43              |
| 2:B:87:THR:HG22  | 5:B:157:HOH:O     | 2.16                     | 0.43              |
| 3:L:155:ARG:HH11 | 3:L:155:ARG:CB    | 2.28                     | 0.43              |
| 1:A:49:ILE:HG22  | 1:A:64:ILE:HD13   | 1.99                     | 0.43              |
| 2:B:56:GLU:OE2   | 3:L:94:THR:N      | 2.40                     | 0.43              |
| 3:L:42:LYS:HZ2   | 3:L:42:LYS:CA     | 2.31                     | 0.43              |
| 3:L:131:SER:OG   | 3:L:180:THR:HG23  | 2.18                     | 0.43              |
| 4:H:61:GLN:HB3   | 5:H:221:HOH:O     | 2.18                     | 0.43              |
| 1:A:44:ALA:O     | 1:A:45:LEU:C      | 2.59                     | 0.43              |
| 1:A:106:PHE:HB3  | 5:A:126:HOH:O     | 2.18                     | 0.43              |
| 3:L:5:THR:HB     | 5:L:217:HOH:O     | 2.19                     | 0.43              |
| 3:L:143:ASP:O    | 3:L:198:HIS:CD2   | 2.72                     | 0.43              |
| 3:L:210:ASN:CB   | 3:L:213:GLU:HB2   | 2.48                     | 0.43              |
| 4:H:202:SER:O    | 4:H:203:SER:C     | 2.60                     | 0.43              |
| 1:A:61:ARG:HA    | 1:A:78:THR:HG22   | 1.99                     | 0.43              |
| 3:L:44:PRO:HG2   | 4:H:103:TRP:CH2   | 2.54                     | 0.43              |
| 4:H:126:PRO:O    | 4:H:127:VAL:C     | 2.62                     | 0.43              |
| 2:B:31:TRP:CE2   | 2:B:50:ARG:HG3    | 2.54                     | 0.43              |
| 3:L:210:ASN:HB2  | 5:L:244:HOH:O     | 2.18                     | 0.43              |
| 4:H:40:SER:O     | 4:H:41:ASN:HB3    | 2.19                     | 0.43              |
| 1:A:37:GLN:HE22  | 2:B:37:GLN:HE22   | 1.67                     | 0.42              |
| 1:A:106:PHE:CE2  | 2:B:43:LEU:HD23   | 2.53                     | 0.42              |
| 2:B:11:ARG:HB3   | 2:B:114:LEU:CD2   | 2.49                     | 0.42              |
| 3:L:118:PHE:HA   | 3:L:119:PRO:HD3   | 1.76                     | 0.42              |
| 3:L:38:GLN:NE2   | 3:L:42:LYS:O      | 2.43                     | 0.42              |
| 3:L:71:PHE:N     | 3:L:71:PHE:CD1    | 2.87                     | 0.42              |
| 3:L:117:ILE:HD12 | 3:L:148:TRP:HZ3   | 1.83                     | 0.42              |
| 3:L:142:LYS:HB2  | 3:L:173:TYR:CD2   | 2.54                     | 0.42              |
| 4:H:184:THR:C    | 4:H:186:SER:H     | 2.27                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:14:PRO:O     | 2:B:15:ARG:HB2   | 2.19                     | 0.42              |
| 2:B:60:LEU:HD13  | 2:B:65:TYR:HE2   | 1.84                     | 0.42              |
| 2:B:22:ARG:HG3   | 2:B:76:ARG:CG    | 2.50                     | 0.42              |
| 3:L:148:TRP:NE1  | 3:L:177:SER:OG   | 2.43                     | 0.42              |
| 2:B:38:ASP:OD1   | 2:B:40:GLN:OE1   | 2.37                     | 0.42              |
| 4:H:28:SER:O     | 4:H:29:PHE:C     | 2.63                     | 0.42              |
| 2:B:52:PRO:HB3   | 2:B:71:THR:HA    | 2.01                     | 0.42              |
| 4:H:112:SER:OG   | 4:H:113:SER:N    | 2.52                     | 0.42              |
| 3:L:178:THR:HG22 | 5:L:225:HOH:O    | 2.19                     | 0.42              |
| 4:H:13:LYS:O     | 4:H:14:PRO:C     | 2.63                     | 0.42              |
| 2:B:69:ARG:HD2   | 2:B:74:GLU:O     | 2.20                     | 0.42              |
| 3:L:161:ASN:OD1  | 3:L:177:SER:HA   | 2.20                     | 0.42              |
| 4:H:192:SER:O    | 4:H:193:ILE:HD13 | 2.20                     | 0.42              |
| 1:A:35:TYR:OH    | 2:B:106:LEU:HB3  | 2.20                     | 0.41              |
| 4:H:148:GLU:HB2  | 5:H:218:HOH:O    | 2.20                     | 0.41              |
| 3:L:20:THR:HA    | 3:L:73:LEU:O     | 2.20                     | 0.41              |
| 4:H:75:SER:HB2   | 4:H:77:THR:OG1   | 2.19                     | 0.41              |
| 4:H:94:ARG:NH1   | 4:H:101:ASP:HB3  | 2.35                     | 0.41              |
| 2:B:114:LEU:HD23 | 2:B:114:LEU:HA   | 1.94                     | 0.41              |
| 4:H:29:PHE:CZ    | 4:H:71:VAL:HG22  | 2.55                     | 0.41              |
| 4:H:118:ALA:HB1  | 4:H:119:PRO:HD2  | 2.02                     | 0.41              |
| 4:H:147:PRO:HB2  | 5:H:218:HOH:O    | 2.19                     | 0.41              |
| 4:H:154:TRP:HZ3  | 4:H:210:ILE:CD1  | 2.32                     | 0.41              |
| 1:A:21:ASN:O     | 1:A:22:CYS:HB2   | 2.20                     | 0.41              |
| 1:A:106:PHE:CZ   | 2:B:43:LEU:HD23  | 2.56                     | 0.41              |
| 2:B:38:ASP:O     | 2:B:41:LYS:HA    | 2.20                     | 0.41              |
| 2:B:77:LEU:CD2   | 2:B:90:LEU:HD22  | 2.51                     | 0.41              |
| 2:B:93:THR:HB    | 2:B:106:LEU:HD11 | 2.03                     | 0.41              |
| 3:L:82:ASP:HA    | 5:L:288:HOH:O    | 2.19                     | 0.41              |
| 3:L:149:LYS:HA   | 3:L:153:SER:O    | 2.21                     | 0.41              |
| 3:L:163:TRP:CZ2  | 3:L:175:MET:HE3  | 2.55                     | 0.41              |
| 1:A:38:PHE:O     | 1:A:39:PRO:C     | 2.62                     | 0.41              |
| 3:L:151:ASP:OD2  | 3:L:189:HIS:HD2  | 2.04                     | 0.41              |
| 3:L:155:ARG:HE   | 3:L:181:LEU:HD23 | 1.85                     | 0.41              |
| 4:H:188:TRP:CD1  | 4:H:189:PRO:HA   | 2.55                     | 0.41              |
| 2:B:90:LEU:CD1   | 2:B:114:LEU:HD12 | 2.51                     | 0.41              |
| 4:H:47:TRP:O     | 4:H:60:ASN:HB2   | 2.20                     | 0.41              |
| 3:L:42:LYS:HZ2   | 3:L:42:LYS:HA    | 1.84                     | 0.41              |
| 3:L:148:TRP:CZ3  | 3:L:194:CYS:HB2  | 2.56                     | 0.41              |
| 4:H:47:TRP:CZ2   | 4:H:49:GLY:HA2   | 2.56                     | 0.41              |
| 2:B:12:LEU:C     | 2:B:12:LEU:HD12  | 2.46                     | 0.41              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 2:B:22:ARG:HG3   | 2:B:76:ARG:CD      | 2.51                     | 0.41              |
| 2:B:51:SER:HA    | 2:B:52:PRO:HD3     | 1.88                     | 0.41              |
| 3:L:28:ASN:ND2   | 3:L:29:ILE:O       | 2.54                     | 0.41              |
| 3:L:56:GLU:H     | 3:L:56:GLU:CD      | 2.28                     | 0.41              |
| 3:L:160:LEU:HD11 | 5:H:277:HOH:O      | 2.21                     | 0.41              |
| 4:H:18:VAL:O     | 4:H:81:GLN:HA      | 2.20                     | 0.41              |
| 4:H:37:VAL:HA    | 4:H:46:GLU:O       | 2.21                     | 0.41              |
| 4:H:69:LEU:HD13  | 4:H:80:MET:HG3     | 2.02                     | 0.41              |
| 4:H:151:THR:O    | 4:H:151:THR:HG22   | 2.20                     | 0.41              |
| 1:A:2:GLN:HG3    | 1:A:29:PHE:CZ      | 2.56                     | 0.41              |
| 1:A:38:PHE:CE1   | 1:A:86:ALA:HB2     | 2.57                     | 0.41              |
| 2:B:10:TRP:CD2   | 2:B:113:ARG:HD3    | 2.56                     | 0.41              |
| 3:L:144:ILE:HG13 | 3:L:145:ASN:N      | 2.34                     | 0.41              |
| 2:B:85:GLY:CA    | 2:B:116:VAL:HG23   | 2.52                     | 0.40              |
| 3:L:186:TYR:OH   | 3:L:209:PHE:HE1    | 2.04                     | 0.40              |
| 4:H:5:GLN:HG3    | 5:H:237:HOH:O      | 2.21                     | 0.40              |
| 1:A:4:ARG:HH22   | 1:A:25:GLU:CB      | 2.19                     | 0.40              |
| 3:L:4:MET:HB2    | 3:L:99:GLY:HA2     | 2.04                     | 0.40              |
| 3:L:146:VAL:HA   | 3:L:195:GLU:O      | 2.21                     | 0.40              |
| 1:A:1:GLN:O      | 1:A:4:ARG:NE       | 2.54                     | 0.40              |
| 1:A:5:GLN:HE22   | 1:A:89:PHE:HA      | 1.87                     | 0.40              |
| 1:A:17:THR:HG23  | 1:A:78:THR:HA      | 2.04                     | 0.40              |
| 2:B:41:LYS:NZ    | 5:B:135:HOH:O      | 2.54                     | 0.40              |
| 2:B:60:LEU:HB3   | 2:B:61:PRO:CD      | 2.51                     | 0.40              |
| 3:L:108:ARG:HD3  | 3:L:109:ALA:O      | 2.22                     | 0.40              |
| 4:H:82:LEU:HB3   | 4:H:82(C):LEU:HD21 | 2.04                     | 0.40              |
| 4:H:152:LEU:C    | 4:H:152:LEU:HD12   | 2.47                     | 0.40              |
| 4:H:188:TRP:CD1  | 4:H:191:GLN:O      | 2.75                     | 0.40              |

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

| Atom-1         | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|------------------------|--------------------------|-------------------|
| 3:L:1:ASP:CB   | 3:L:157:ASN:ND2[3_558] | 1.76                     | 0.44              |
| 3:L:17:GLU:OE2 | 3:L:152:GLY:O[3_557]   | 2.06                     | 0.14              |



## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 1   | A     | 113/115 (98%) | 93 (82%)  | 15 (13%) | 5 (4%)   | 2           | 2  |
| 2   | B     | 115/117 (98%) | 99 (86%)  | 12 (10%) | 4 (4%)   | 3           | 4  |
| 3   | L     | 212/214 (99%) | 191 (90%) | 19 (9%)  | 2 (1%)   | 14          | 27 |
| 4   | H     | 217/219 (99%) | 177 (82%) | 33 (15%) | 7 (3%)   | 3           | 4  |
| All | All   | 657/665 (99%) | 560 (85%) | 79 (12%) | 18 (3%)  | 4           | 6  |

All (18) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 115 | SER  |
| 2   | B     | 2   | THR  |
| 2   | B     | 102 | ALA  |
| 3   | L     | 51  | ALA  |
| 4   | H     | 127 | VAL  |
| 1   | A     | 118 | SER  |
| 2   | B     | 15  | ARG  |
| 4   | H     | 31  | GLY  |
| 4   | H     | 114 | ALA  |
| 1   | A     | 86  | ALA  |
| 1   | A     | 68  | LYS  |
| 4   | H     | 128 | CYS  |
| 4   | H     | 144 | GLY  |
| 1   | A     | 39  | PRO  |
| 4   | H     | 185 | SER  |
| 2   | B     | 14  | PRO  |
| 4   | H     | 129 | GLY  |
| 3   | L     | 93  | GLY  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed       | Rotameric | Outliers  | Percentiles |   |
|-----|-------|----------------|-----------|-----------|-------------|---|
| 1   | A     | 98/98 (100%)   | 72 (74%)  | 26 (26%)  | 0           | 1 |
| 2   | B     | 102/102 (100%) | 66 (65%)  | 36 (35%)  | 0           | 0 |
| 3   | L     | 188/188 (100%) | 131 (70%) | 57 (30%)  | 0           | 0 |
| 4   | H     | 190/190 (100%) | 137 (72%) | 53 (28%)  | 0           | 1 |
| All | All   | 578/578 (100%) | 406 (70%) | 172 (30%) | 0           | 0 |

All (172) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 1   | GLN  |
| 1   | A     | 4   | ARG  |
| 1   | A     | 6   | SER  |
| 1   | A     | 10  | LEU  |
| 1   | A     | 14  | GLU  |
| 1   | A     | 19  | ILE  |
| 1   | A     | 25  | GLU  |
| 1   | A     | 27  | SER  |
| 1   | A     | 28  | THR  |
| 1   | A     | 30  | ASN  |
| 1   | A     | 41  | GLU  |
| 1   | A     | 47  | ILE  |
| 1   | A     | 50  | ARG  |
| 1   | A     | 53  | SER  |
| 1   | A     | 55  | LYS  |
| 1   | A     | 56  | LYS  |
| 1   | A     | 63  | THR  |
| 1   | A     | 69  | ARG  |
| 1   | A     | 70  | GLU  |
| 1   | A     | 72  | LYS  |
| 1   | A     | 73  | LEU  |
| 1   | A     | 74  | SER  |
| 1   | A     | 76  | HIS  |
| 1   | A     | 78  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 101 | ARG  |
| 1   | A     | 111 | THR  |
| 2   | B     | 1   | VAL  |
| 2   | B     | 2   | THR  |
| 2   | B     | 3   | LEU  |
| 2   | B     | 9   | ARG  |
| 2   | B     | 12  | LEU  |
| 2   | B     | 13  | VAL  |
| 2   | B     | 20  | ASN  |
| 2   | B     | 21  | LEU  |
| 2   | B     | 23  | CYS  |
| 2   | B     | 24  | ILE  |
| 2   | B     | 26  | LYS  |
| 2   | B     | 29  | GLN  |
| 2   | B     | 33  | SER  |
| 2   | B     | 36  | GLN  |
| 2   | B     | 38  | ASP  |
| 2   | B     | 39  | LEU  |
| 2   | B     | 44  | GLN  |
| 2   | B     | 47  | PHE  |
| 2   | B     | 49  | LEU  |
| 2   | B     | 50  | ARG  |
| 2   | B     | 51  | SER  |
| 2   | B     | 55  | LYS  |
| 2   | B     | 57  | VAL  |
| 2   | B     | 58  | LYS  |
| 2   | B     | 59  | SER  |
| 2   | B     | 68  | THR  |
| 2   | B     | 76  | ARG  |
| 2   | B     | 79  | VAL  |
| 2   | B     | 81  | ASN  |
| 2   | B     | 82  | MET  |
| 2   | B     | 86  | ARG  |
| 2   | B     | 87  | THR  |
| 2   | B     | 90  | LEU  |
| 2   | B     | 94  | CYS  |
| 2   | B     | 95  | SER  |
| 2   | B     | 115 | THR  |
| 3   | L     | 5   | THR  |
| 3   | L     | 6   | GLN  |
| 3   | L     | 7   | SER  |
| 3   | L     | 11  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | L     | 12  | SER  |
| 3   | L     | 15  | VAL  |
| 3   | L     | 19  | VAL  |
| 3   | L     | 27  | LYS  |
| 3   | L     | 40  | GLN  |
| 3   | L     | 42  | LYS  |
| 3   | L     | 45  | GLN  |
| 3   | L     | 47  | LEU  |
| 3   | L     | 52  | LYS  |
| 3   | L     | 54  | LEU  |
| 3   | L     | 61  | ARG  |
| 3   | L     | 63  | SER  |
| 3   | L     | 67  | SER  |
| 3   | L     | 69  | THR  |
| 3   | L     | 70  | GLN  |
| 3   | L     | 71  | PHE  |
| 3   | L     | 74  | LYS  |
| 3   | L     | 75  | ILE  |
| 3   | L     | 77  | SER  |
| 3   | L     | 78  | LEU  |
| 3   | L     | 85  | SER  |
| 3   | L     | 89  | GLN  |
| 3   | L     | 90  | HIS  |
| 3   | L     | 103 | LYS  |
| 3   | L     | 104 | LEU  |
| 3   | L     | 107 | LYS  |
| 3   | L     | 115 | VAL  |
| 3   | L     | 116 | SER  |
| 3   | L     | 127 | SER  |
| 3   | L     | 133 | VAL  |
| 3   | L     | 136 | LEU  |
| 3   | L     | 137 | ASN  |
| 3   | L     | 142 | LYS  |
| 3   | L     | 143 | ASP  |
| 3   | L     | 144 | ILE  |
| 3   | L     | 145 | ASN  |
| 3   | L     | 155 | ARG  |
| 3   | L     | 165 | ASP  |
| 3   | L     | 168 | SER  |
| 3   | L     | 175 | MET  |
| 3   | L     | 176 | SER  |
| 3   | L     | 178 | THR  |

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| Mol | Chain | Res   | Type |
|-----|-------|-------|------|
| 3   | L     | 181   | LEU  |
| 3   | L     | 182   | THR  |
| 3   | L     | 183   | LYS  |
| 3   | L     | 189   | HIS  |
| 3   | L     | 191   | SER  |
| 3   | L     | 197   | THR  |
| 3   | L     | 199   | LYS  |
| 3   | L     | 202   | THR  |
| 3   | L     | 207   | LYS  |
| 3   | L     | 208   | SER  |
| 3   | L     | 212   | ASN  |
| 4   | H     | 3     | GLN  |
| 4   | H     | 4     | LEU  |
| 4   | H     | 5     | GLN  |
| 4   | H     | 6     | GLN  |
| 4   | H     | 7     | SER  |
| 4   | H     | 10    | GLU  |
| 4   | H     | 11    | LEU  |
| 4   | H     | 19    | LYS  |
| 4   | H     | 30    | THR  |
| 4   | H     | 40    | SER  |
| 4   | H     | 44    | SER  |
| 4   | H     | 48    | ILE  |
| 4   | H     | 51    | ILE  |
| 4   | H     | 62    | LYS  |
| 4   | H     | 66    | ARG  |
| 4   | H     | 71    | VAL  |
| 4   | H     | 73    | LYS  |
| 4   | H     | 74    | SER  |
| 4   | H     | 75    | SER  |
| 4   | H     | 76    | SER  |
| 4   | H     | 80    | MET  |
| 4   | H     | 82    | LEU  |
| 4   | H     | 82(A) | LYS  |
| 4   | H     | 82(B) | SER  |
| 4   | H     | 82(C) | LEU  |
| 4   | H     | 87    | SER  |
| 4   | H     | 96    | ARG  |
| 4   | H     | 97    | THR  |
| 4   | H     | 98    | ASP  |
| 4   | H     | 107   | THR  |
| 4   | H     | 117   | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | H     | 127 | VAL  |
| 4   | H     | 128 | CYS  |
| 4   | H     | 151 | THR  |
| 4   | H     | 152 | LEU  |
| 4   | H     | 158 | SER  |
| 4   | H     | 160 | SER  |
| 4   | H     | 161 | SER  |
| 4   | H     | 165 | THR  |
| 4   | H     | 169 | VAL  |
| 4   | H     | 170 | LEU  |
| 4   | H     | 171 | GLN  |
| 4   | H     | 173 | ASP  |
| 4   | H     | 177 | LEU  |
| 4   | H     | 180 | SER  |
| 4   | H     | 183 | VAL  |
| 4   | H     | 184 | THR  |
| 4   | H     | 192 | SER  |
| 4   | H     | 195 | CYS  |
| 4   | H     | 196 | ASN  |
| 4   | H     | 204 | THR  |
| 4   | H     | 205 | LYS  |
| 4   | H     | 209 | LYS  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 5   | GLN  |
| 1   | A     | 8   | GLN  |
| 1   | A     | 37  | GLN  |
| 2   | B     | 36  | GLN  |
| 2   | B     | 37  | GLN  |
| 2   | B     | 40  | GLN  |
| 2   | B     | 44  | GLN  |
| 2   | B     | 78  | GLN  |
| 3   | L     | 28  | ASN  |
| 3   | L     | 45  | GLN  |
| 3   | L     | 70  | GLN  |
| 3   | L     | 90  | HIS  |
| 3   | L     | 145 | ASN  |
| 3   | L     | 189 | HIS  |
| 3   | L     | 210 | ASN  |
| 4   | H     | 3   | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | H     | 5   | GLN  |
| 4   | H     | 61  | GLN  |
| 4   | H     | 81  | GLN  |
| 4   | H     | 164 | HIS  |
| 4   | H     | 171 | GLN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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

There are no ligands in this entry.

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

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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

| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2      | OWAB(Å <sup>2</sup> ) | Q<0.9  |
|-----|-------|----------------|--------|--------------|-----------------------|--------|
| 1   | A     | 115/115 (100%) | -0.20  | 1 (0%) 81 78 | 30, 48, 65, 88        | 3 (2%) |
| 2   | B     | 117/117 (100%) | -0.21  | 1 (0%) 81 78 | 35, 49, 72, 75        | 0      |
| 3   | L     | 214/214 (100%) | -0.31  | 0 100 100    | 28, 44, 60, 75        | 2 (0%) |
| 4   | H     | 219/219 (100%) | -0.19  | 3 (1%) 73 70 | 33, 50, 64, 84        | 0      |
| All | All   | 665/665 (100%) | -0.24  | 5 (0%) 82 80 | 28, 48, 66, 88        | 5 (0%) |

All (5) RSRZ outliers are listed below:

| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 4   | H     | 131    | THR  | 3.3  |
| 4   | H     | 132    | THR  | 3.0  |
| 2   | B     | 116(A) | LEU  | 2.1  |
| 1   | A     | 119    | ALA  | 2.0  |
| 4   | H     | 133    | GLY  | 2.0  |

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

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

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.