



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:17 PM GMT

PDB ID : 169L  
Title : PROTEIN FLEXIBILITY AND ADAPTABILITY SEEN IN 25 CRYSTAL FORMS OF T4 LYSOZYME  
Authors : Zhang, X.-J.; Matthews, B.W.  
Deposited on : 1995-03-24  
Resolution : 3.00 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

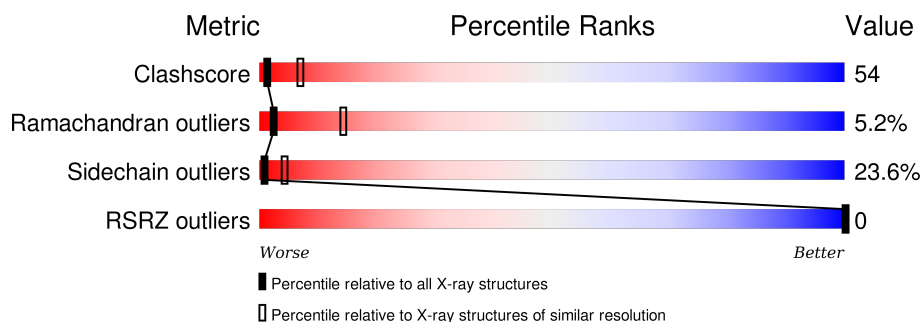
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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)) |
|-----------------------|-----------------------------|---|
| Clashscore            | 102246                      | 1912 (3.00-3.00)                                      |
| Ramachandran outliers | 100387                      | 1853 (3.00-3.00)                                      |
| Sidechain outliers    | 100360                      | 1856 (3.00-3.00)                                      |
| RSRZ outliers         | 91569                       | 1592 (3.00-3.00)                                      |

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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     | 164    |                  |
| 1   | B     | 164    |                  |
| 1   | C     | 164    |                  |
| 1   | D     | 164    |                  |
| 1   | E     | 164    |                  |

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6290 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 T4 LYSOZYME.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | A     | 162      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1258  | 793 | 228 | 230 | 7 |         |         |       |
| 1   | B     | 162      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1258  | 793 | 228 | 230 | 7 |         |         |       |
| 1   | C     | 162      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1258  | 793 | 228 | 230 | 7 |         |         |       |
| 1   | D     | 162      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1258  | 793 | 228 | 230 | 7 |         |         |       |
| 1   | E     | 162      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1258  | 793 | 228 | 230 | 7 |         |         |       |

There are 45 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| A     | 128     | ALA      | GLU    | CONFLICT | UNP P00720 |
| A     | 131     | ALA      | VAL    | CONFLICT | UNP P00720 |
| A     | 132     | ALA      | ASN    | CONFLICT | UNP P00720 |
| A     | 135     | ALA      | LYS    | CONFLICT | UNP P00720 |
| A     | 136     | ALA      | SER    | CONFLICT | UNP P00720 |
| A     | 137     | ALA      | ARG    | CONFLICT | UNP P00720 |
| A     | 139     | ALA      | TYR    | CONFLICT | UNP P00720 |
| A     | 140     | ALA      | ASN    | CONFLICT | UNP P00720 |
| A     | 141     | ALA      | GLN    | CONFLICT | UNP P00720 |
| B     | 128     | ALA      | GLU    | CONFLICT | UNP P00720 |
| B     | 131     | ALA      | VAL    | CONFLICT | UNP P00720 |
| B     | 132     | ALA      | ASN    | CONFLICT | UNP P00720 |
| B     | 135     | ALA      | LYS    | CONFLICT | UNP P00720 |
| B     | 136     | ALA      | SER    | CONFLICT | UNP P00720 |
| B     | 137     | ALA      | ARG    | CONFLICT | UNP P00720 |
| B     | 139     | ALA      | TYR    | CONFLICT | UNP P00720 |
| B     | 140     | ALA      | ASN    | CONFLICT | UNP P00720 |
| B     | 141     | ALA      | GLN    | CONFLICT | UNP P00720 |
| C     | 128     | ALA      | GLU    | CONFLICT | UNP P00720 |

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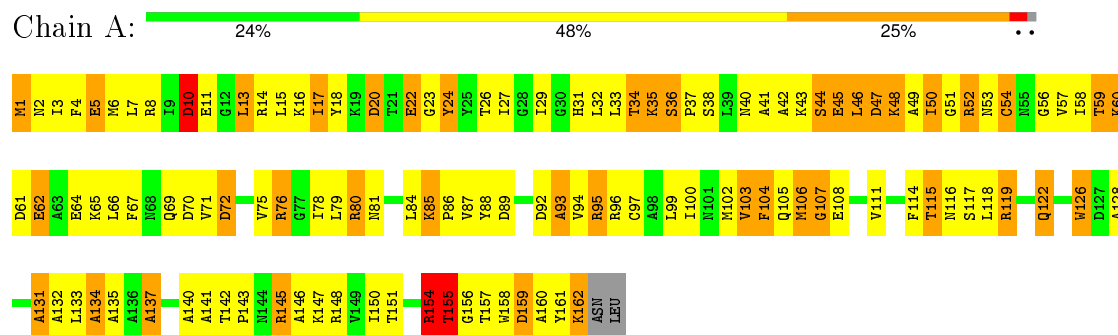
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| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| C     | 131     | ALA      | VAL    | CONFLICT | UNP P00720 |
| C     | 132     | ALA      | ASN    | CONFLICT | UNP P00720 |
| C     | 135     | ALA      | LYS    | CONFLICT | UNP P00720 |
| C     | 136     | ALA      | SER    | CONFLICT | UNP P00720 |
| C     | 137     | ALA      | ARG    | CONFLICT | UNP P00720 |
| C     | 139     | ALA      | TYR    | CONFLICT | UNP P00720 |
| C     | 140     | ALA      | ASN    | CONFLICT | UNP P00720 |
| C     | 141     | ALA      | GLN    | CONFLICT | UNP P00720 |
| D     | 128     | ALA      | GLU    | CONFLICT | UNP P00720 |
| D     | 131     | ALA      | VAL    | CONFLICT | UNP P00720 |
| D     | 132     | ALA      | ASN    | CONFLICT | UNP P00720 |
| D     | 135     | ALA      | LYS    | CONFLICT | UNP P00720 |
| D     | 136     | ALA      | SER    | CONFLICT | UNP P00720 |
| D     | 137     | ALA      | ARG    | CONFLICT | UNP P00720 |
| D     | 139     | ALA      | TYR    | CONFLICT | UNP P00720 |
| D     | 140     | ALA      | ASN    | CONFLICT | UNP P00720 |
| D     | 141     | ALA      | GLN    | CONFLICT | UNP P00720 |
| E     | 128     | ALA      | GLU    | CONFLICT | UNP P00720 |
| E     | 131     | ALA      | VAL    | CONFLICT | UNP P00720 |
| E     | 132     | ALA      | ASN    | CONFLICT | UNP P00720 |
| E     | 135     | ALA      | LYS    | CONFLICT | UNP P00720 |
| E     | 136     | ALA      | SER    | CONFLICT | UNP P00720 |
| E     | 137     | ALA      | ARG    | CONFLICT | UNP P00720 |
| E     | 139     | ALA      | TYR    | CONFLICT | UNP P00720 |
| E     | 140     | ALA      | ASN    | CONFLICT | UNP P00720 |
| E     | 141     | ALA      | GLN    | CONFLICT | UNP P00720 |

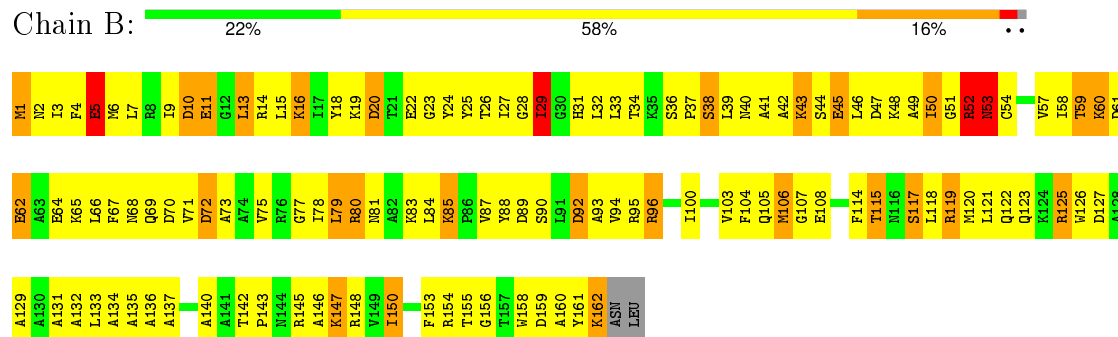
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

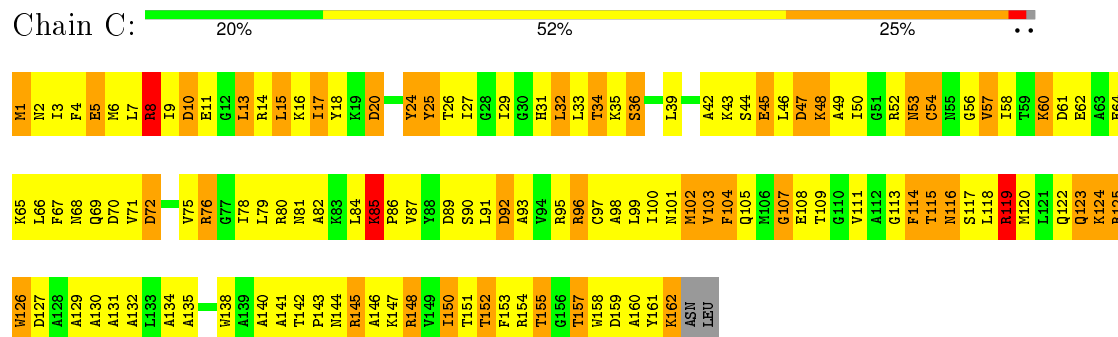
#### • Molecule 1: T4 LYSOZYME



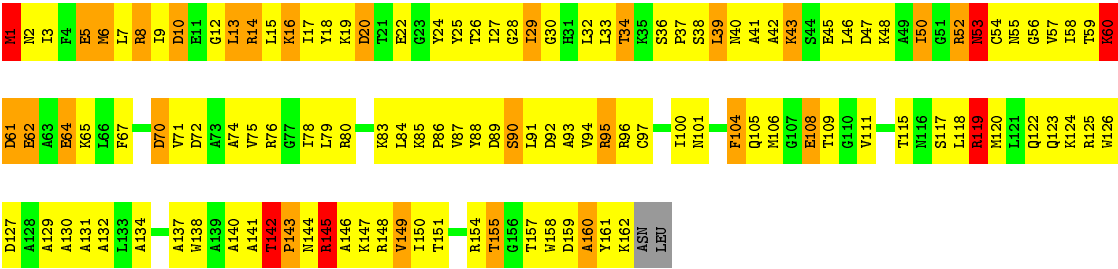
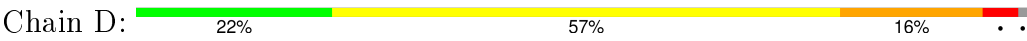
#### • Molecule 1: T4 LYSOZYME



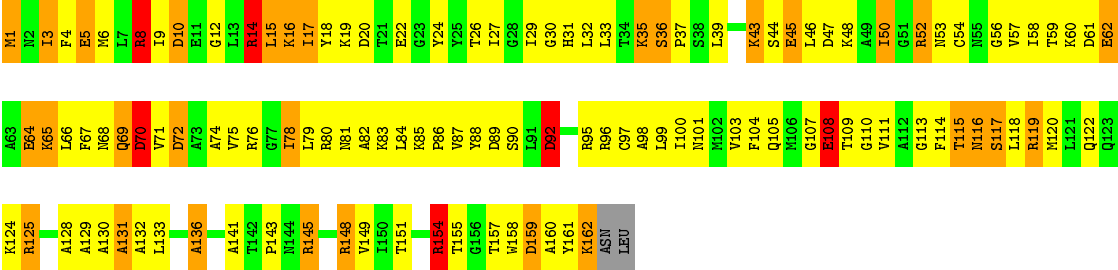
#### • Molecule 1: T4 LYSOZYME



#### • Molecule 1: T4 LYSOZYME



● Molecule 1: T4 LYSOZYME



## 4 Data and refinement statistics

| Property  | Value  | Source           |
|---|--|------------------|
| Space group   | P 1 21 1   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 40.40 Å 112.30 Å 135.20 Å<br>90.00° 91.70° 90.00°            | Depositor        |
| Resolution (Å)  | 6.00 – 3.00<br>51.85 – 2.95                                  | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | (Not available) (6.00-3.00)<br>59.9 (51.85-2.95)             | Depositor<br>EDS |
| $R_{merge}$   | (Not available)  | Depositor        |
| $R_{sym}$   | (Not available)  | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 0.83 (at 2.96 Å)   | Xtriage          |
| Refinement program  | TNT  | Depositor        |
| R, $R_{free}$   | 0.161 , (Not available)<br>(Not available) , (Not available) | Depositor<br>DCC |
| $R_{free}$ test set   | NotAvailable   | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 43.7   | Xtriage          |
| Anisotropy  | 0.260  | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.32 , 115.6   | EDS              |
| Estimated twinning fraction   | 0.125 for h,-k,-l  | Xtriage          |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.24$  | Xtriage          |
| Outliers  | 1 of 15353 reflections (0.007%)                              | Xtriage          |
| $F_o, F_c$ correlation  | 0.89   | EDS              |
| Total number of atoms   | 6290   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 26.0   | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.52% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

| Mol | Chain | Bond lengths |                | Bond angles |                 |
|-----|-------|--------------|----------------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5         |
| 1   | A     | 0.94         | 5/1277 (0.4%)  | 1.50        | 20/1722 (1.2%)  |
| 1   | B     | 0.97         | 7/1277 (0.5%)  | 1.44        | 15/1722 (0.9%)  |
| 1   | C     | 0.92         | 5/1277 (0.4%)  | 1.53        | 23/1722 (1.3%)  |
| 1   | D     | 0.96         | 5/1277 (0.4%)  | 1.55        | 23/1722 (1.3%)  |
| 1   | E     | 0.96         | 6/1277 (0.5%)  | 1.49        | 22/1722 (1.3%)  |
| All | All   | 0.95         | 28/6385 (0.4%) | 1.50        | 103/8610 (1.2%) |

All (28) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1   | B     | 22  | GLU  | CD-OE2 | 7.50 | 1.33        | 1.25     |
| 1   | E     | 5   | GLU  | CD-OE2 | 7.22 | 1.33        | 1.25     |
| 1   | D     | 108 | GLU  | CD-OE2 | 7.21 | 1.33        | 1.25     |
| 1   | D     | 62  | GLU  | CD-OE2 | 7.05 | 1.33        | 1.25     |
| 1   | B     | 62  | GLU  | CD-OE2 | 6.93 | 1.33        | 1.25     |
| 1   | A     | 22  | GLU  | CD-OE2 | 6.86 | 1.33        | 1.25     |
| 1   | E     | 64  | GLU  | CD-OE2 | 6.72 | 1.33        | 1.25     |
| 1   | A     | 45  | GLU  | CD-OE2 | 6.61 | 1.32        | 1.25     |
| 1   | E     | 62  | GLU  | CD-OE2 | 6.60 | 1.32        | 1.25     |
| 1   | A     | 5   | GLU  | CD-OE2 | 6.38 | 1.32        | 1.25     |
| 1   | C     | 45  | GLU  | CD-OE2 | 6.36 | 1.32        | 1.25     |
| 1   | E     | 45  | GLU  | CD-OE2 | 6.26 | 1.32        | 1.25     |
| 1   | A     | 62  | GLU  | CD-OE2 | 6.19 | 1.32        | 1.25     |
| 1   | D     | 64  | GLU  | CD-OE2 | 6.15 | 1.32        | 1.25     |
| 1   | B     | 64  | GLU  | CD-OE2 | 6.10 | 1.32        | 1.25     |
| 1   | E     | 22  | GLU  | CD-OE2 | 6.09 | 1.32        | 1.25     |
| 1   | D     | 5   | GLU  | CD-OE2 | 6.05 | 1.32        | 1.25     |
| 1   | D     | 45  | GLU  | CD-OE2 | 5.92 | 1.32        | 1.25     |
| 1   | B     | 11  | GLU  | CD-OE2 | 5.92 | 1.32        | 1.25     |
| 1   | A     | 108 | GLU  | CD-OE2 | 5.71 | 1.31        | 1.25     |
| 1   | C     | 64  | GLU  | CD-OE2 | 5.59 | 1.31        | 1.25     |
| 1   | B     | 153 | PHE  | CE1-CZ | 5.51 | 1.47        | 1.37     |
| 1   | E     | 108 | GLU  | CD-OE2 | 5.40 | 1.31        | 1.25     |

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| Mol | Chain | Res | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1   | C     | 62  | GLU  | CD-OE2 | 5.34 | 1.31        | 1.25     |
| 1   | B     | 5   | GLU  | CD-OE2 | 5.27 | 1.31        | 1.25     |
| 1   | C     | 5   | GLU  | CD-OE2 | 5.23 | 1.31        | 1.25     |
| 1   | C     | 108 | GLU  | CD-OE2 | 5.21 | 1.31        | 1.25     |
| 1   | B     | 108 | GLU  | CD-OE2 | 5.17 | 1.31        | 1.25     |

All (103) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1   | D     | 142 | THR  | C-N-CD    | -12.14 | 93.88       | 120.60   |
| 1   | C     | 119 | ARG  | NE-CZ-NH1 | 10.16  | 125.38      | 120.30   |
| 1   | D     | 159 | ASP  | CB-CG-OD2 | -10.16 | 109.15      | 118.30   |
| 1   | A     | 92  | ASP  | CB-CG-OD2 | -9.90  | 109.39      | 118.30   |
| 1   | A     | 20  | ASP  | CB-CG-OD2 | -9.13  | 110.09      | 118.30   |
| 1   | E     | 70  | ASP  | CB-CG-OD2 | -9.01  | 110.19      | 118.30   |
| 1   | A     | 61  | ASP  | CB-CG-OD1 | 8.97   | 126.37      | 118.30   |
| 1   | B     | 52  | ARG  | NE-CZ-NH1 | 8.87   | 124.74      | 120.30   |
| 1   | C     | 10  | ASP  | CB-CG-OD1 | 8.69   | 126.12      | 118.30   |
| 1   | D     | 61  | ASP  | CB-CG-OD2 | -7.76  | 111.32      | 118.30   |
| 1   | E     | 148 | ARG  | NE-CZ-NH1 | 7.75   | 124.17      | 120.30   |
| 1   | B     | 52  | ARG  | NE-CZ-NH2 | -7.65  | 116.47      | 120.30   |
| 1   | E     | 70  | ASP  | CB-CG-OD1 | 7.62   | 125.16      | 118.30   |
| 1   | E     | 72  | ASP  | CB-CG-OD2 | -7.58  | 111.48      | 118.30   |
| 1   | C     | 20  | ASP  | CB-CG-OD1 | 7.57   | 125.11      | 118.30   |
| 1   | B     | 10  | ASP  | CB-CG-OD1 | 7.50   | 125.05      | 118.30   |
| 1   | C     | 70  | ASP  | CB-CG-OD2 | -7.49  | 111.56      | 118.30   |
| 1   | A     | 20  | ASP  | CB-CG-OD1 | 7.45   | 125.00      | 118.30   |
| 1   | D     | 10  | ASP  | CB-CG-OD2 | -7.41  | 111.64      | 118.30   |
| 1   | A     | 61  | ASP  | CB-CG-OD2 | -7.35  | 111.69      | 118.30   |
| 1   | C     | 8   | ARG  | NE-CZ-NH2 | -7.32  | 116.64      | 120.30   |
| 1   | B     | 20  | ASP  | CB-CG-OD2 | -7.19  | 111.83      | 118.30   |
| 1   | C     | 154 | ARG  | NE-CZ-NH2 | -7.12  | 116.74      | 120.30   |
| 1   | E     | 10  | ASP  | CB-CG-OD2 | -7.10  | 111.91      | 118.30   |
| 1   | A     | 154 | ARG  | NE-CZ-NH1 | 7.10   | 123.85      | 120.30   |
| 1   | A     | 159 | ASP  | CB-CG-OD2 | -6.89  | 112.10      | 118.30   |
| 1   | D     | 89  | ASP  | CB-CG-OD1 | 6.85   | 124.46      | 118.30   |
| 1   | E     | 92  | ASP  | CB-CG-OD2 | -6.83  | 112.15      | 118.30   |
| 1   | D     | 47  | ASP  | CB-CG-OD2 | -6.82  | 112.16      | 118.30   |
| 1   | E     | 72  | ASP  | CB-CG-OD1 | 6.81   | 124.43      | 118.30   |
| 1   | A     | 10  | ASP  | CB-CG-OD2 | -6.80  | 112.18      | 118.30   |
| 1   | D     | 70  | ASP  | CB-CG-OD1 | 6.79   | 124.41      | 118.30   |
| 1   | C     | 154 | ARG  | NE-CZ-NH1 | 6.76   | 123.68      | 120.30   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | B     | 10  | ASP  | CB-CG-OD2 | -6.71 | 112.26      | 118.30   |
| 1   | E     | 95  | ARG  | NE-CZ-NH2 | -6.65 | 116.98      | 120.30   |
| 1   | D     | 145 | ARG  | NE-CZ-NH1 | 6.62  | 123.61      | 120.30   |
| 1   | B     | 47  | ASP  | CB-CG-OD2 | -6.61 | 112.35      | 118.30   |
| 1   | A     | 8   | ARG  | NE-CZ-NH2 | -6.55 | 117.02      | 120.30   |
| 1   | C     | 47  | ASP  | CB-CG-OD1 | 6.52  | 124.17      | 118.30   |
| 1   | E     | 80  | ARG  | NE-CZ-NH1 | 6.52  | 123.56      | 120.30   |
| 1   | D     | 47  | ASP  | CB-CG-OD1 | 6.44  | 124.10      | 118.30   |
| 1   | B     | 153 | PHE  | CB-CG-CD2 | -6.43 | 116.30      | 120.80   |
| 1   | B     | 95  | ARG  | NE-CZ-NH2 | -6.42 | 117.09      | 120.30   |
| 1   | C     | 10  | ASP  | CB-CG-OD2 | -6.37 | 112.56      | 118.30   |
| 1   | A     | 70  | ASP  | CB-CG-OD2 | -6.37 | 112.57      | 118.30   |
| 1   | E     | 20  | ASP  | CB-CG-OD2 | -6.35 | 112.58      | 118.30   |
| 1   | D     | 95  | ARG  | NE-CZ-NH1 | 6.33  | 123.47      | 120.30   |
| 1   | D     | 119 | ARG  | NE-CZ-NH2 | -6.31 | 117.14      | 120.30   |
| 1   | B     | 80  | ARG  | NE-CZ-NH1 | 6.29  | 123.45      | 120.30   |
| 1   | A     | 76  | ARG  | NE-CZ-NH1 | 6.25  | 123.42      | 120.30   |
| 1   | B     | 153 | PHE  | CB-CG-CD1 | 6.14  | 125.10      | 120.80   |
| 1   | D     | 127 | ASP  | CB-CG-OD2 | -6.10 | 112.81      | 118.30   |
| 1   | C     | 61  | ASP  | CB-CG-OD1 | 6.08  | 123.77      | 118.30   |
| 1   | D     | 125 | ARG  | NE-CZ-NH1 | 6.08  | 123.34      | 120.30   |
| 1   | B     | 61  | ASP  | CB-CG-OD2 | -6.05 | 112.85      | 118.30   |
| 1   | C     | 48  | LYS  | CB-CA-C   | -6.05 | 98.31       | 110.40   |
| 1   | D     | 70  | ASP  | CB-CG-OD2 | -6.04 | 112.86      | 118.30   |
| 1   | A     | 72  | ASP  | CB-CG-OD1 | 5.99  | 123.69      | 118.30   |
| 1   | E     | 95  | ARG  | NE-CZ-NH1 | 5.98  | 123.29      | 120.30   |
| 1   | B     | 20  | ASP  | CB-CG-OD1 | 5.96  | 123.67      | 118.30   |
| 1   | C     | 20  | ASP  | CB-CG-OD2 | -5.91 | 112.98      | 118.30   |
| 1   | D     | 125 | ARG  | NE-CZ-NH2 | -5.82 | 117.39      | 120.30   |
| 1   | C     | 89  | ASP  | CB-CG-OD2 | -5.81 | 113.07      | 118.30   |
| 1   | D     | 1   | MET  | CA-C-N    | -5.81 | 104.42      | 117.20   |
| 1   | A     | 76  | ARG  | NE-CZ-NH2 | -5.79 | 117.41      | 120.30   |
| 1   | E     | 47  | ASP  | CB-CG-OD2 | -5.78 | 113.10      | 118.30   |
| 1   | A     | 159 | ASP  | CB-CG-OD1 | 5.77  | 123.50      | 118.30   |
| 1   | D     | 20  | ASP  | CB-CG-OD1 | 5.75  | 123.48      | 118.30   |
| 1   | A     | 47  | ASP  | CB-CG-OD2 | -5.72 | 113.15      | 118.30   |
| 1   | E     | 125 | ARG  | NE-CZ-NH1 | 5.72  | 123.16      | 120.30   |
| 1   | D     | 20  | ASP  | CB-CG-OD2 | -5.71 | 113.16      | 118.30   |
| 1   | D     | 61  | ASP  | CB-CG-OD1 | 5.64  | 123.38      | 118.30   |
| 1   | C     | 24  | TYR  | CB-CG-CD1 | -5.63 | 117.62      | 121.00   |
| 1   | C     | 72  | ASP  | CB-CG-OD2 | -5.62 | 113.25      | 118.30   |
| 1   | B     | 47  | ASP  | CB-CG-OD1 | 5.59  | 123.33      | 118.30   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | A     | 24  | TYR  | CB-CG-CD1 | -5.54 | 117.67      | 121.00   |
| 1   | C     | 92  | ASP  | CB-CG-OD1 | 5.54  | 123.29      | 118.30   |
| 1   | E     | 61  | ASP  | CB-CG-OD2 | -5.51 | 113.34      | 118.30   |
| 1   | D     | 14  | ARG  | NE-CZ-NH2 | -5.50 | 117.55      | 120.30   |
| 1   | C     | 145 | ARG  | NE-CZ-NH1 | 5.49  | 123.05      | 120.30   |
| 1   | D     | 89  | ASP  | CB-CG-OD2 | -5.47 | 113.37      | 118.30   |
| 1   | E     | 14  | ARG  | NE-CZ-NH1 | 5.41  | 123.00      | 120.30   |
| 1   | B     | 72  | ASP  | CB-CG-OD1 | 5.37  | 123.13      | 118.30   |
| 1   | E     | 8   | ARG  | NE-CZ-NH1 | 5.36  | 122.98      | 120.30   |
| 1   | C     | 4   | PHE  | CB-CG-CD1 | 5.34  | 124.54      | 120.80   |
| 1   | C     | 125 | ARG  | NE-CZ-NH1 | 5.33  | 122.97      | 120.30   |
| 1   | C     | 76  | ARG  | NE-CZ-NH1 | 5.33  | 122.97      | 120.30   |
| 1   | C     | 25  | TYR  | CB-CG-CD1 | -5.29 | 117.83      | 121.00   |
| 1   | A     | 80  | ARG  | NE-CZ-NH1 | 5.27  | 122.94      | 120.30   |
| 1   | A     | 10  | ASP  | CB-CG-OD1 | 5.26  | 123.03      | 118.30   |
| 1   | E     | 159 | ASP  | CB-CG-OD2 | -5.23 | 113.59      | 118.30   |
| 1   | E     | 10  | ASP  | CB-CG-OD1 | 5.20  | 122.98      | 118.30   |
| 1   | A     | 8   | ARG  | NE-CZ-NH1 | 5.18  | 122.89      | 120.30   |
| 1   | E     | 154 | ARG  | NE-CZ-NH2 | -5.17 | 117.71      | 120.30   |
| 1   | C     | 119 | ARG  | NE-CZ-NH2 | -5.17 | 117.72      | 120.30   |
| 1   | D     | 8   | ARG  | CG-CD-NE  | 5.15  | 122.61      | 111.80   |
| 1   | E     | 61  | ASP  | CB-CG-OD1 | 5.14  | 122.93      | 118.30   |
| 1   | C     | 57  | VAL  | CA-CB-CG2 | -5.14 | 103.19      | 110.90   |
| 1   | E     | 59  | THR  | CA-CB-CG2 | -5.14 | 105.20      | 112.40   |
| 1   | E     | 154 | ARG  | NE-CZ-NH1 | 5.08  | 122.84      | 120.30   |
| 1   | A     | 80  | ARG  | NE-CZ-NH2 | -5.06 | 117.77      | 120.30   |
| 1   | D     | 80  | ARG  | NE-CZ-NH1 | 5.03  | 122.82      | 120.30   |
| 1   | B     | 80  | ARG  | NE-CZ-NH2 | -5.01 | 117.80      | 120.30   |

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     | 1258  | 0        | 1287     | 165     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | B     | 1258  | 0        | 1287     | 162     | 0            |
| 1   | C     | 1258  | 0        | 1287     | 145     | 0            |
| 1   | D     | 1258  | 0        | 1287     | 130     | 0            |
| 1   | E     | 1258  | 0        | 1287     | 107     | 0            |
| All | All   | 6290  | 0        | 6435     | 688     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 54.

All (688) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:50:ILE:HD13  | 1:D:62:GLU:HG2   | 1.31                     | 1.11              |
| 1:A:13:LEU:HD21  | 1:A:15:LEU:HD21  | 1.32                     | 1.11              |
| 1:B:50:ILE:HD11  | 1:B:52:ARG:HG2   | 1.17                     | 1.10              |
| 1:A:87:VAL:HG22  | 1:A:122:GLN:HG3  | 1.33                     | 1.10              |
| 1:A:116:ASN:HA   | 1:A:119:ARG:HD3  | 1.38                     | 1.05              |
| 1:D:53:ASN:ND2   | 1:D:53:ASN:H     | 1.52                     | 1.04              |
| 1:D:53:ASN:HD22  | 1:D:53:ASN:N     | 1.55                     | 1.02              |
| 1:C:120:MET:HE1  | 1:C:129:ALA:HA   | 1.41                     | 0.99              |
| 1:B:79:LEU:HA    | 1:B:85:LYS:HG3   | 1.42                     | 0.99              |
| 1:D:120:MET:HE3  | 1:D:129:ALA:HA   | 1.48                     | 0.94              |
| 1:A:81:ASN:ND2   | 1:A:84:LEU:HD12  | 1.83                     | 0.94              |
| 1:A:16:LYS:HB2   | 1:A:57:VAL:HG22  | 1.49                     | 0.93              |
| 1:A:72:ASP:HB3   | 1:A:76:ARG:NH2   | 1.82                     | 0.93              |
| 1:B:120:MET:HE1  | 1:B:129:ALA:HA   | 1.47                     | 0.93              |
| 1:C:53:ASN:H     | 1:C:53:ASN:ND2   | 1.67                     | 0.91              |
| 1:A:1:MET:CE     | 1:A:5:GLU:HB3    | 2.00                     | 0.91              |
| 1:B:120:MET:CE   | 1:B:129:ALA:HA   | 2.01                     | 0.90              |
| 1:C:120:MET:CE   | 1:C:129:ALA:HA   | 2.03                     | 0.89              |
| 1:D:79:LEU:HA    | 1:D:85:LYS:HG3   | 1.54                     | 0.89              |
| 1:B:53:ASN:ND2   | 1:B:53:ASN:H     | 1.70                     | 0.88              |
| 1:C:53:ASN:H     | 1:C:53:ASN:HD22  | 0.88                     | 0.87              |
| 1:E:1:MET:HB3    | 1:E:158:TRP:CD2  | 2.09                     | 0.87              |
| 1:A:52:ARG:NH1   | 1:A:54:CYS:HA    | 1.90                     | 0.87              |
| 1:E:1:MET:HE3    | 1:E:5:GLU:HB3    | 1.56                     | 0.86              |
| 1:D:50:ILE:HD13  | 1:D:62:GLU:CG    | 2.06                     | 0.84              |
| 1:E:116:ASN:HA   | 1:E:119:ARG:HD3  | 1.59                     | 0.84              |
| 1:C:53:ASN:N     | 1:C:53:ASN:HD22  | 1.71                     | 0.84              |
| 1:A:103:VAL:HG23 | 1:A:111:VAL:HG21 | 1.60                     | 0.84              |
| 1:D:14:ARG:HG3   | 1:D:18:TYR:CE2   | 2.12                     | 0.83              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:C:1:MET:HB3   | 1:C:158:TRP:CD2  | 2.14                     | 0.83              |
| 1:D:8:ARG:HH21  | 1:D:9:ILE:HD11   | 1.43                     | 0.83              |
| 1:A:94:VAL:HG22 | 1:A:158:TRP:CZ2  | 2.13                     | 0.83              |
| 1:A:79:LEU:HA   | 1:A:85:LYS:HG3   | 1.61                     | 0.83              |
| 1:A:103:VAL:CG2 | 1:A:111:VAL:HG21 | 2.10                     | 0.82              |
| 1:A:87:VAL:CG2  | 1:A:122:GLN:HG3  | 2.09                     | 0.82              |
| 1:A:116:ASN:HA  | 1:A:119:ARG:CD   | 2.09                     | 0.82              |
| 1:A:145:ARG:HA  | 1:A:148:ARG:NH2  | 1.95                     | 0.81              |
| 1:B:1:MET:HB3   | 1:B:158:TRP:CD2  | 2.15                     | 0.81              |
| 1:B:105:GLN:NE2 | 1:B:145:ARG:HH11 | 1.79                     | 0.81              |
| 1:B:59:THR:HG23 | 1:B:62:GLU:CD    | 2.01                     | 0.81              |
| 1:B:39:LEU:HD11 | 1:B:43:LYS:HD2   | 1.63                     | 0.81              |
| 1:D:1:MET:CE    | 1:D:5:GLU:HB3    | 2.11                     | 0.81              |
| 1:D:119:ARG:O   | 1:D:123:GLN:HG2  | 1.80                     | 0.81              |
| 1:C:72:ASP:HB3  | 1:C:76:ARG:NH2   | 1.95                     | 0.80              |
| 1:E:4:PHE:CE1   | 1:E:29:ILE:HD11  | 2.16                     | 0.80              |
| 1:B:50:ILE:HG13 | 1:B:51:GLY:N     | 1.96                     | 0.80              |
| 1:A:24:TYR:CD1  | 1:A:35:LYS:HB3   | 2.17                     | 0.80              |
| 1:C:148:ARG:HG2 | 1:C:160:ALA:HB1  | 1.64                     | 0.80              |
| 1:C:146:ALA:O   | 1:C:150:ILE:HG13 | 1.82                     | 0.80              |
| 1:D:151:THR:O   | 1:D:155:THR:HG23 | 1.82                     | 0.79              |
| 1:E:155:THR:O   | 1:E:157:THR:HG23 | 1.81                     | 0.79              |
| 1:E:92:ASP:O    | 1:E:96:ARG:HG3   | 1.83                     | 0.79              |
| 1:A:105:GLN:HB2 | 1:A:145:ARG:NH1  | 1.99                     | 0.78              |
| 1:D:14:ARG:O    | 1:D:15:LEU:HD23  | 1.83                     | 0.78              |
| 1:C:20:ASP:OD2  | 1:C:24:TYR:HB2   | 1.83                     | 0.78              |
| 1:A:24:TYR:CE1  | 1:A:35:LYS:HB3   | 2.18                     | 0.78              |
| 1:B:53:ASN:HD22 | 1:B:53:ASN:H     | 1.31                     | 0.78              |
| 1:D:100:ILE:O   | 1:D:104:PHE:HB2  | 1.84                     | 0.78              |
| 1:C:87:VAL:HG22 | 1:C:122:GLN:HG3  | 1.67                     | 0.77              |
| 1:B:1:MET:CE    | 1:B:5:GLU:HB3    | 2.14                     | 0.77              |
| 1:E:120:MET:HE3 | 1:E:129:ALA:HA   | 1.65                     | 0.76              |
| 1:C:1:MET:HE2   | 1:C:5:GLU:HB3    | 1.67                     | 0.76              |
| 1:B:65:LYS:O    | 1:B:69:GLN:HG3   | 1.85                     | 0.76              |
| 1:E:1:MET:CE    | 1:E:5:GLU:HB3    | 2.16                     | 0.76              |
| 1:E:120:MET:HE3 | 1:E:129:ALA:CA   | 2.16                     | 0.76              |
| 1:B:15:LEU:O    | 1:B:27:ILE:HD11  | 1.86                     | 0.75              |
| 1:A:35:LYS:HD3  | 1:E:79:LEU:HD11  | 1.68                     | 0.75              |
| 1:A:1:MET:HE2   | 1:A:5:GLU:HB3    | 1.68                     | 0.75              |
| 1:D:6:MET:HG3   | 1:D:158:TRP:HZ3  | 1.51                     | 0.74              |
| 1:D:1:MET:HE2   | 1:D:5:GLU:HB3    | 1.67                     | 0.74              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:59:THR:HG23  | 1:A:62:GLU:CD    | 2.08                     | 0.74              |
| 1:B:148:ARG:HD2  | 1:B:161:TYR:CE2  | 2.22                     | 0.74              |
| 1:B:50:ILE:CD1   | 1:B:52:ARG:HG2   | 2.10                     | 0.74              |
| 1:A:107:GLY:O    | 1:A:111:VAL:HG23 | 1.86                     | 0.74              |
| 1:B:148:ARG:HB3  | 1:B:161:TYR:CZ   | 2.23                     | 0.74              |
| 1:A:1:MET:HE3    | 1:A:5:GLU:HB3    | 1.69                     | 0.74              |
| 1:E:15:LEU:N     | 1:E:15:LEU:HD23  | 2.03                     | 0.74              |
| 1:B:32:LEU:HD23  | 1:B:33:LEU:N     | 2.03                     | 0.74              |
| 1:D:8:ARG:NH2    | 1:D:9:ILE:HD11   | 2.02                     | 0.74              |
| 1:A:13:LEU:HD21  | 1:A:15:LEU:CD2   | 2.16                     | 0.74              |
| 1:B:120:MET:HE1  | 1:B:132:ALA:HB3  | 1.70                     | 0.74              |
| 1:C:1:MET:CE     | 1:C:5:GLU:HB3    | 2.18                     | 0.74              |
| 1:D:6:MET:HG3    | 1:D:158:TRP:CZ3  | 2.22                     | 0.73              |
| 1:C:1:MET:HB3    | 1:C:158:TRP:CE2  | 2.23                     | 0.73              |
| 1:E:128:ALA:O    | 1:E:131:ALA:HB3  | 1.88                     | 0.73              |
| 1:C:24:TYR:CD1   | 1:C:35:LYS:HB3   | 2.24                     | 0.73              |
| 1:D:130:ALA:CB   | 1:D:154:ARG:HG3  | 2.17                     | 0.73              |
| 1:B:5:GLU:O      | 1:B:9:ILE:HD12   | 1.87                     | 0.73              |
| 1:A:16:LYS:CB    | 1:A:57:VAL:HG22  | 2.17                     | 0.73              |
| 1:E:24:TYR:CE1   | 1:E:35:LYS:HB3   | 2.24                     | 0.73              |
| 1:B:59:THR:HG23  | 1:B:62:GLU:OE1   | 1.88                     | 0.73              |
| 1:C:162:LYS:HB3  | 1:C:162:LYS:NZ   | 2.04                     | 0.72              |
| 1:D:130:ALA:HB2  | 1:D:154:ARG:HG3  | 1.72                     | 0.72              |
| 1:A:81:ASN:O     | 1:A:85:LYS:HB2   | 1.89                     | 0.72              |
| 1:E:87:VAL:HG21  | 1:E:118:LEU:HB3  | 1.70                     | 0.72              |
| 1:B:105:GLN:HE21 | 1:B:145:ARG:HH11 | 1.36                     | 0.72              |
| 1:B:75:VAL:CG2   | 1:B:100:ILE:HD11 | 2.20                     | 0.72              |
| 1:A:60:LYS:HD2   | 1:A:60:LYS:O     | 1.89                     | 0.72              |
| 1:B:146:ALA:O    | 1:B:150:ILE:HG13 | 1.90                     | 0.72              |
| 1:E:39:LEU:O     | 1:E:39:LEU:HD12  | 1.90                     | 0.71              |
| 1:C:100:ILE:O    | 1:C:104:PHE:HB2  | 1.90                     | 0.71              |
| 1:C:3:ILE:HG12   | 1:C:67:PHE:HZ    | 1.55                     | 0.71              |
| 1:C:114:PHE:HB3  | 1:C:117:SER:HB2  | 1.73                     | 0.71              |
| 1:A:105:GLN:HB2  | 1:A:145:ARG:HH12 | 1.55                     | 0.71              |
| 1:C:159:ASP:HA   | 1:C:162:LYS:HE2  | 1.72                     | 0.71              |
| 1:B:120:MET:CB   | 1:B:129:ALA:HB2  | 2.21                     | 0.70              |
| 1:A:88:TYR:O     | 1:A:96:ARG:NE    | 2.25                     | 0.70              |
| 1:B:1:MET:HB3    | 1:B:158:TRP:CG   | 2.26                     | 0.70              |
| 1:B:1:MET:HE3    | 1:B:5:GLU:HG3    | 1.74                     | 0.70              |
| 1:A:87:VAL:HG22  | 1:A:122:GLN:CG   | 2.19                     | 0.70              |
| 1:D:38:SER:HB3   | 1:D:41:ALA:HB2   | 1.74                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:85:LYS:NZ    | 1:A:89:ASP:OD2   | 2.25                     | 0.69              |
| 1:B:105:GLN:HB2  | 1:B:145:ARG:CZ   | 2.22                     | 0.69              |
| 1:B:105:GLN:HB2  | 1:B:145:ARG:NH1  | 2.07                     | 0.69              |
| 1:D:87:VAL:HG11  | 1:D:118:LEU:HD23 | 1.73                     | 0.69              |
| 1:C:76:ARG:O     | 1:C:80:ARG:HD3   | 1.92                     | 0.69              |
| 1:B:38:SER:HG    | 1:B:41:ALA:H     | 1.41                     | 0.69              |
| 1:E:130:ALA:HB2  | 1:E:154:ARG:HG3  | 1.74                     | 0.69              |
| 1:E:100:ILE:O    | 1:E:103:VAL:HG12 | 1.92                     | 0.69              |
| 1:D:1:MET:HB3    | 1:D:158:TRP:CD2  | 2.28                     | 0.68              |
| 1:A:78:ILE:HG23  | 1:A:84:LEU:HB3   | 1.74                     | 0.68              |
| 1:D:61:ASP:O     | 1:D:64:GLU:N     | 2.23                     | 0.68              |
| 1:C:45:GLU:O     | 1:C:48:LYS:HB2   | 1.93                     | 0.68              |
| 1:B:159:ASP:HA   | 1:B:162:LYS:HG2  | 1.74                     | 0.68              |
| 1:C:9:ILE:HG21   | 1:C:161:TYR:HD2  | 1.58                     | 0.68              |
| 1:B:13:LEU:HD12  | 1:B:29:ILE:HG12  | 1.76                     | 0.68              |
| 1:B:120:MET:HB3  | 1:B:129:ALA:HB2  | 1.76                     | 0.68              |
| 1:E:31:HIS:CD2   | 1:E:66:LEU:HD22  | 2.28                     | 0.68              |
| 1:E:8:ARG:NH2    | 1:E:9:ILE:HG13   | 2.09                     | 0.68              |
| 1:C:52:ARG:HG3   | 1:C:53:ASN:N     | 2.09                     | 0.67              |
| 1:E:33:LEU:HD11  | 1:E:46:LEU:HB2   | 1.77                     | 0.67              |
| 1:A:115:THR:HG22 | 1:A:119:ARG:HD2  | 1.75                     | 0.67              |
| 1:B:155:THR:OG1  | 1:B:156:GLY:N    | 2.26                     | 0.67              |
| 1:A:155:THR:OG1  | 1:A:157:THR:N    | 2.27                     | 0.67              |
| 1:E:74:ALA:O     | 1:E:78:ILE:HD12  | 1.94                     | 0.67              |
| 1:C:102:MET:HE3  | 1:C:111:VAL:HG13 | 1.76                     | 0.67              |
| 1:B:50:ILE:HG12  | 1:B:54:CYS:SG    | 2.35                     | 0.66              |
| 1:B:59:THR:N     | 1:B:62:GLU:OE1   | 2.28                     | 0.66              |
| 1:C:151:THR:O    | 1:C:155:THR:HG23 | 1.96                     | 0.66              |
| 1:A:103:VAL:O    | 1:A:107:GLY:N    | 2.28                     | 0.66              |
| 1:B:1:MET:HE2    | 1:B:5:GLU:HB3    | 1.75                     | 0.66              |
| 1:B:38:SER:OG    | 1:B:40:ASN:N     | 2.29                     | 0.66              |
| 1:B:2:ASN:OD1    | 1:B:5:GLU:HB2    | 1.96                     | 0.66              |
| 1:B:120:MET:CE   | 1:B:132:ALA:HB3  | 2.24                     | 0.65              |
| 1:B:105:GLN:NE2  | 1:B:145:ARG:NH1  | 2.43                     | 0.65              |
| 1:E:1:MET:HB3    | 1:E:158:TRP:CG   | 2.31                     | 0.65              |
| 1:B:50:ILE:HD11  | 1:B:52:ARG:CG    | 2.11                     | 0.65              |
| 1:B:125:ARG:O    | 1:B:127:ASP:N    | 2.29                     | 0.65              |
| 1:B:81:ASN:HB3   | 1:B:84:LEU:HB2   | 1.78                     | 0.65              |
| 1:A:33:LEU:HD11  | 1:A:46:LEU:HD13  | 1.77                     | 0.65              |
| 1:A:3:ILE:HD13   | 1:A:71:VAL:HG21  | 1.77                     | 0.65              |
| 1:C:50:ILE:HD11  | 1:C:52:ARG:HG2   | 1.79                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:138:TRP:O    | 1:C:141:ALA:HB3  | 1.96                     | 0.65              |
| 1:B:118:LEU:O    | 1:B:121:LEU:N    | 2.30                     | 0.65              |
| 1:A:115:THR:HG22 | 1:A:116:ASN:N    | 2.11                     | 0.64              |
| 1:E:26:THR:HG22  | 1:E:27:ILE:N     | 2.11                     | 0.64              |
| 1:D:88:TYR:HE2   | 1:D:100:ILE:HD11 | 1.62                     | 0.64              |
| 1:A:20:ASP:OD1   | 1:A:23:GLY:N     | 2.29                     | 0.64              |
| 1:B:39:LEU:O     | 1:B:39:LEU:HD12  | 1.98                     | 0.64              |
| 1:C:13:LEU:HD21  | 1:C:15:LEU:HD21  | 1.80                     | 0.64              |
| 1:D:3:ILE:HG12   | 1:D:67:PHE:HZ    | 1.62                     | 0.64              |
| 1:A:96:ARG:O     | 1:A:100:ILE:HD12 | 1.98                     | 0.63              |
| 1:C:17:ILE:HD12  | 1:C:56:GLY:HA2   | 1.79                     | 0.63              |
| 1:E:81:ASN:OD1   | 1:E:83:LYS:N     | 2.31                     | 0.63              |
| 1:B:75:VAL:HG22  | 1:B:100:ILE:HD11 | 1.79                     | 0.63              |
| 1:A:159:ASP:HA   | 1:A:162:LYS:HE2  | 1.80                     | 0.63              |
| 1:B:79:LEU:CA    | 1:B:85:LYS:HG3   | 2.24                     | 0.63              |
| 1:A:2:ASN:OD1    | 1:A:5:GLU:HB2    | 1.98                     | 0.63              |
| 1:D:60:LYS:O     | 1:D:60:LYS:NZ    | 2.28                     | 0.63              |
| 1:E:4:PHE:HA     | 1:E:67:PHE:CE2   | 2.33                     | 0.63              |
| 1:C:26:THR:HG22  | 1:C:27:ILE:H     | 1.62                     | 0.63              |
| 1:B:44:SER:O     | 1:B:48:LYS:HG3   | 1.98                     | 0.63              |
| 1:D:142:THR:O    | 1:D:144:ASN:N    | 2.31                     | 0.63              |
| 1:A:159:ASP:OD1  | 1:A:162:LYS:HE2  | 1.98                     | 0.62              |
| 1:A:47:ASP:O     | 1:A:51:GLY:N     | 2.30                     | 0.62              |
| 1:E:33:LEU:CD1   | 1:E:46:LEU:HB2   | 2.29                     | 0.62              |
| 1:D:142:THR:N    | 1:D:143:PRO:HD3  | 2.14                     | 0.62              |
| 1:A:94:VAL:HG22  | 1:A:158:TRP:CE2  | 2.34                     | 0.62              |
| 1:B:19:LYS:HA    | 1:B:24:TYR:O     | 1.99                     | 0.62              |
| 1:A:158:TRP:O    | 1:A:162:LYS:HG2  | 1.98                     | 0.62              |
| 1:A:71:VAL:HG12  | 1:A:72:ASP:N     | 2.14                     | 0.62              |
| 1:C:1:MET:HB3    | 1:C:158:TRP:CG   | 2.34                     | 0.62              |
| 1:E:50:ILE:HD13  | 1:E:62:GLU:OE1   | 2.00                     | 0.62              |
| 1:B:79:LEU:HD13  | 1:C:35:LYS:HD2   | 1.79                     | 0.62              |
| 1:A:35:LYS:HD3   | 1:E:79:LEU:CD1   | 2.30                     | 0.62              |
| 1:D:92:ASP:O     | 1:D:96:ARG:HG3   | 2.00                     | 0.62              |
| 1:A:155:THR:OG1  | 1:A:156:GLY:N    | 2.28                     | 0.62              |
| 1:B:158:TRP:O    | 1:B:162:LYS:HG2  | 2.00                     | 0.61              |
| 1:C:26:THR:HG22  | 1:C:27:ILE:N     | 2.15                     | 0.61              |
| 1:B:38:SER:OG    | 1:B:39:LEU:N     | 2.32                     | 0.61              |
| 1:B:93:ALA:HA    | 1:B:96:ARG:HG3   | 1.82                     | 0.61              |
| 1:A:27:ILE:O     | 1:A:31:HIS:HB3   | 2.00                     | 0.61              |
| 1:A:32:LEU:HD23  | 1:A:32:LEU:O     | 2.00                     | 0.61              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:D:10:ASP:HB3  | 1:D:145:ARG:HG3  | 1.81                     | 0.61              |
| 1:C:50:ILE:HG22 | 1:C:66:LEU:HD21  | 1.81                     | 0.61              |
| 1:A:59:THR:HG23 | 1:A:62:GLU:OE1   | 2.01                     | 0.61              |
| 1:B:87:VAL:HG21 | 1:B:118:LEU:HB3  | 1.82                     | 0.61              |
| 1:B:140:ALA:O   | 1:B:143:PRO:HD3  | 2.01                     | 0.61              |
| 1:D:50:ILE:O    | 1:D:50:ILE:HD12  | 2.01                     | 0.61              |
| 1:B:1:MET:HE3   | 1:B:5:GLU:HB3    | 1.83                     | 0.61              |
| 1:A:146:ALA:O   | 1:A:150:ILE:HG13 | 2.01                     | 0.60              |
| 1:C:1:MET:HG3   | 1:C:2:ASN:H      | 1.65                     | 0.60              |
| 1:C:85:LYS:N    | 1:C:86:PRO:HD2   | 2.14                     | 0.60              |
| 1:A:36:SER:O    | 1:A:38:SER:N     | 2.33                     | 0.60              |
| 1:E:116:ASN:O   | 1:E:120:MET:HG3  | 2.02                     | 0.60              |
| 1:C:158:TRP:O   | 1:C:162:LYS:NZ   | 2.33                     | 0.60              |
| 1:C:103:VAL:O   | 1:C:107:GLY:N    | 2.34                     | 0.60              |
| 1:E:71:VAL:O    | 1:E:75:VAL:HG23  | 2.02                     | 0.60              |
| 1:A:52:ARG:HH12 | 1:A:54:CYS:HA    | 1.66                     | 0.60              |
| 1:B:137:ALA:O   | 1:B:140:ALA:N    | 2.35                     | 0.60              |
| 1:C:81:ASN:OD1  | 1:C:82:ALA:N     | 2.34                     | 0.60              |
| 1:D:117:SER:HA  | 1:D:120:MET:HE2  | 1.83                     | 0.60              |
| 1:E:120:MET:CE  | 1:E:129:ALA:HA   | 2.30                     | 0.60              |
| 1:D:8:ARG:CZ    | 1:D:9:ILE:HG13   | 2.31                     | 0.60              |
| 1:C:116:ASN:HA  | 1:C:119:ARG:HD3  | 1.83                     | 0.60              |
| 1:E:44:SER:OG   | 1:E:45:GLU:N     | 2.32                     | 0.60              |
| 1:B:159:ASP:HA  | 1:B:162:LYS:CG   | 2.32                     | 0.59              |
| 1:C:7:LEU:HD22  | 1:C:11:GLU:HG2   | 1.82                     | 0.59              |
| 1:B:123:GLN:HB2 | 1:B:125:ARG:HD3  | 1.83                     | 0.59              |
| 1:A:87:VAL:HA   | 1:A:122:GLN:HG3  | 1.83                     | 0.59              |
| 1:B:94:VAL:HG22 | 1:B:158:TRP:CZ2  | 2.37                     | 0.59              |
| 1:D:46:LEU:O    | 1:D:50:ILE:HG23  | 2.02                     | 0.59              |
| 1:D:124:LYS:HA  | 1:D:126:TRP:CZ3  | 2.37                     | 0.59              |
| 1:B:88:TYR:CE1  | 1:B:96:ARG:HB3   | 2.37                     | 0.59              |
| 1:D:87:VAL:HG22 | 1:D:122:GLN:NE2  | 2.18                     | 0.59              |
| 1:A:88:TYR:CZ   | 1:A:96:ARG:HD2   | 2.37                     | 0.59              |
| 1:A:5:GLU:HA    | 1:A:5:GLU:OE1    | 2.03                     | 0.59              |
| 1:E:98:ALA:HB1  | 1:E:149:VAL:HG13 | 1.84                     | 0.58              |
| 1:D:93:ALA:HB2  | 1:E:19:LYS:NZ    | 2.18                     | 0.58              |
| 1:C:32:LEU:O    | 1:C:32:LEU:HD23  | 2.01                     | 0.58              |
| 1:A:137:ALA:O   | 1:A:140:ALA:HB3  | 2.03                     | 0.58              |
| 1:C:81:ASN:O    | 1:C:85:LYS:HB2   | 2.04                     | 0.58              |
| 1:D:124:LYS:HG2 | 1:D:126:TRP:CH2  | 2.38                     | 0.58              |
| 1:E:32:LEU:C    | 1:E:32:LEU:HD23  | 2.24                     | 0.58              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:B:20:ASP:O    | 1:B:23:GLY:N     | 2.36                     | 0.58              |
| 1:A:45:GLU:HA   | 1:A:45:GLU:OE1   | 2.02                     | 0.58              |
| 1:C:75:VAL:O    | 1:C:78:ILE:N     | 2.37                     | 0.58              |
| 1:C:78:ILE:O    | 1:C:81:ASN:N     | 2.34                     | 0.58              |
| 1:C:71:VAL:HG11 | 1:D:36:SER:HB2   | 1.85                     | 0.58              |
| 1:E:39:LEU:HD11 | 1:E:43:LYS:HD2   | 1.86                     | 0.57              |
| 1:E:50:ILE:HD13 | 1:E:62:GLU:CD    | 2.25                     | 0.57              |
| 1:E:81:ASN:O    | 1:E:85:LYS:HB2   | 2.03                     | 0.57              |
| 1:D:87:VAL:HG22 | 1:D:122:GLN:HE21 | 1.69                     | 0.57              |
| 1:D:13:LEU:HD12 | 1:D:28:GLY:HA2   | 1.85                     | 0.57              |
| 1:B:59:THR:O    | 1:B:62:GLU:HB2   | 2.04                     | 0.57              |
| 1:C:141:ALA:C   | 1:C:143:PRO:HD3  | 2.24                     | 0.57              |
| 1:B:51:GLY:O    | 1:B:52:ARG:HB3   | 2.03                     | 0.57              |
| 1:A:71:VAL:HG11 | 1:B:36:SER:HB2   | 1.85                     | 0.57              |
| 1:B:159:ASP:CA  | 1:B:162:LYS:HG2  | 2.35                     | 0.57              |
| 1:D:141:ALA:C   | 1:D:143:PRO:HD3  | 2.24                     | 0.57              |
| 1:B:120:MET:HB2 | 1:B:129:ALA:HB2  | 1.86                     | 0.57              |
| 1:C:15:LEU:HB3  | 1:C:58:ILE:HG13  | 1.87                     | 0.57              |
| 1:D:58:ILE:HG22 | 1:D:62:GLU:OE1   | 2.04                     | 0.57              |
| 1:D:1:MET:HE3   | 1:D:5:GLU:HB3    | 1.84                     | 0.56              |
| 1:D:16:LYS:HG3  | 1:D:57:VAL:HG22  | 1.87                     | 0.56              |
| 1:B:46:LEU:O    | 1:B:49:ALA:HB3   | 2.05                     | 0.56              |
| 1:B:119:ARG:O   | 1:B:123:GLN:HG2  | 2.05                     | 0.56              |
| 1:C:124:LYS:HA  | 1:C:126:TRP:CZ3  | 2.41                     | 0.56              |
| 1:D:16:LYS:HA   | 1:D:56:GLY:O     | 2.05                     | 0.56              |
| 1:E:120:MET:HE3 | 1:E:129:ALA:N    | 2.19                     | 0.56              |
| 1:B:50:ILE:HG13 | 1:B:51:GLY:H     | 1.68                     | 0.56              |
| 1:B:6:MET:CE    | 1:B:158:TRP:HZ3  | 2.17                     | 0.56              |
| 1:A:65:LYS:NZ   | 1:A:69:GLN:OE1   | 2.29                     | 0.56              |
| 1:A:64:GLU:O    | 1:A:67:PHE:HB3   | 2.05                     | 0.56              |
| 1:C:84:LEU:C    | 1:C:86:PRO:HD2   | 2.26                     | 0.56              |
| 1:B:45:GLU:OE1  | 1:B:45:GLU:HA    | 2.00                     | 0.56              |
| 1:E:159:ASP:OD1 | 1:E:162:LYS:HD2  | 2.04                     | 0.56              |
| 1:B:105:GLN:HB2 | 1:B:145:ARG:NH2  | 2.21                     | 0.56              |
| 1:D:64:GLU:O    | 1:D:67:PHE:HB3   | 2.05                     | 0.56              |
| 1:D:1:MET:HB3   | 1:D:158:TRP:CG   | 2.41                     | 0.56              |
| 1:D:71:VAL:O    | 1:D:75:VAL:HG23  | 2.05                     | 0.56              |
| 1:E:4:PHE:HB2   | 1:E:67:PHE:CD2   | 2.41                     | 0.56              |
| 1:A:95:ARG:HD2  | 1:A:126:TRP:CH2  | 2.40                     | 0.55              |
| 1:C:75:VAL:HG12 | 1:C:79:LEU:HD12  | 1.88                     | 0.55              |
| 1:C:132:ALA:O   | 1:C:135:ALA:HB3  | 2.06                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:84:LEU:HD21  | 1:E:111:VAL:HG12 | 1.87                     | 0.55              |
| 1:D:84:LEU:HD12  | 1:D:108:GLU:HG2  | 1.89                     | 0.55              |
| 1:E:151:THR:HG21 | 1:E:160:ALA:HB2  | 1.87                     | 0.55              |
| 1:C:24:TYR:HB3   | 1:C:32:LEU:HD12  | 1.87                     | 0.55              |
| 1:B:59:THR:H     | 1:B:62:GLU:HB2   | 1.72                     | 0.55              |
| 1:D:67:PHE:O     | 1:D:71:VAL:HG23  | 2.06                     | 0.55              |
| 1:D:85:LYS:N     | 1:D:86:PRO:HD2   | 2.22                     | 0.55              |
| 1:E:158:TRP:O    | 1:E:162:LYS:HG2  | 2.07                     | 0.55              |
| 1:B:75:VAL:HG21  | 1:C:36:SER:HB2   | 1.87                     | 0.55              |
| 1:D:117:SER:HA   | 1:D:120:MET:CE   | 2.37                     | 0.55              |
| 1:D:79:LEU:HD13  | 1:E:35:LYS:HD2   | 1.87                     | 0.55              |
| 1:D:8:ARG:HH21   | 1:D:9:ILE:CD1    | 2.16                     | 0.55              |
| 1:A:95:ARG:NH2   | 1:A:155:THR:O    | 2.39                     | 0.54              |
| 1:A:14:ARG:HG3   | 1:A:18:TYR:CE1   | 2.42                     | 0.54              |
| 1:B:16:LYS:HG3   | 1:B:57:VAL:HG22  | 1.89                     | 0.54              |
| 1:C:50:ILE:C     | 1:C:50:ILE:HD12  | 2.28                     | 0.54              |
| 1:B:59:THR:O     | 1:B:62:GLU:N     | 2.40                     | 0.54              |
| 1:C:148:ARG:CG   | 1:C:160:ALA:HB1  | 2.36                     | 0.54              |
| 1:B:31:HIS:CG    | 1:B:66:LEU:HD22  | 2.43                     | 0.54              |
| 1:C:120:MET:CE   | 1:C:132:ALA:HB3  | 2.37                     | 0.54              |
| 1:E:65:LYS:HG3   | 1:E:66:LEU:N     | 2.17                     | 0.54              |
| 1:C:115:THR:HG22 | 1:C:116:ASN:N    | 2.21                     | 0.54              |
| 1:B:5:GLU:HA     | 1:B:5:GLU:OE1    | 2.06                     | 0.54              |
| 1:C:138:TRP:NE1  | 1:C:146:ALA:HB2  | 2.23                     | 0.54              |
| 1:A:14:ARG:HB2   | 1:A:18:TYR:CE1   | 2.41                     | 0.54              |
| 1:A:100:ILE:O    | 1:A:104:PHE:HB2  | 2.08                     | 0.54              |
| 1:B:32:LEU:C     | 1:B:32:LEU:HD23  | 2.28                     | 0.54              |
| 1:D:17:ILE:HG22  | 1:D:18:TYR:N     | 2.23                     | 0.54              |
| 1:B:53:ASN:N     | 1:B:53:ASN:HD22  | 2.05                     | 0.54              |
| 1:E:65:LYS:O     | 1:E:69:GLN:HG3   | 2.08                     | 0.54              |
| 1:D:140:ALA:O    | 1:D:143:PRO:HG3  | 2.08                     | 0.54              |
| 1:A:119:ARG:NH1  | 1:A:119:ARG:HG2  | 2.23                     | 0.54              |
| 1:E:100:ILE:HA   | 1:E:103:VAL:HG12 | 1.88                     | 0.54              |
| 1:A:27:ILE:HD13  | 1:A:46:LEU:HD11  | 1.89                     | 0.54              |
| 1:E:16:LYS:HG3   | 1:E:57:VAL:HG22  | 1.89                     | 0.54              |
| 1:B:120:MET:SD   | 1:B:129:ALA:HA   | 2.48                     | 0.54              |
| 1:E:14:ARG:C     | 1:E:15:LEU:HD23  | 2.27                     | 0.54              |
| 1:B:43:LYS:O     | 1:B:46:LEU:HB3   | 2.08                     | 0.53              |
| 1:A:46:LEU:O     | 1:A:49:ALA:N     | 2.41                     | 0.53              |
| 1:A:102:MET:O    | 1:A:106:MET:HG3  | 2.09                     | 0.53              |
| 1:C:142:THR:N    | 1:C:143:PRO:HD3  | 2.24                     | 0.53              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:E:26:THR:HG21 | 1:E:30:GLY:HA2  | 1.90                     | 0.53              |
| 1:A:140:ALA:O   | 1:A:143:PRO:HD3 | 2.08                     | 0.53              |
| 1:C:46:LEU:O    | 1:C:49:ALA:HB3  | 2.08                     | 0.53              |
| 1:C:81:ASN:HB3  | 1:C:84:LEU:HB2  | 1.91                     | 0.53              |
| 1:A:79:LEU:CA   | 1:A:85:LYS:HG3  | 2.36                     | 0.53              |
| 1:E:31:HIS:NE2  | 1:E:66:LEU:HD22 | 2.23                     | 0.53              |
| 1:E:72:ASP:O    | 1:E:76:ARG:HG3  | 2.09                     | 0.53              |
| 1:B:148:ARG:HB3 | 1:B:161:TYR:OH  | 2.09                     | 0.53              |
| 1:A:16:LYS:HB2  | 1:A:57:VAL:CG2  | 2.30                     | 0.52              |
| 1:D:148:ARG:HG2 | 1:D:160:ALA:O   | 2.09                     | 0.52              |
| 1:B:68:ASN:O    | 1:B:72:ASP:OD1  | 2.27                     | 0.52              |
| 1:C:69:GLN:O    | 1:C:72:ASP:HB2  | 2.08                     | 0.52              |
| 1:E:26:THR:HG22 | 1:E:27:ILE:H    | 1.75                     | 0.52              |
| 1:A:11:GLU:OE2  | 1:A:145:ARG:NH1 | 2.43                     | 0.52              |
| 1:C:159:ASP:OD1 | 1:C:162:LYS:HE2 | 2.09                     | 0.52              |
| 1:B:52:ARG:NH1  | 1:B:54:CYS:HA   | 2.25                     | 0.52              |
| 1:E:50:ILE:HD11 | 1:E:54:CYS:SG   | 2.49                     | 0.52              |
| 1:A:143:PRO:O   | 1:A:147:LYS:HG3 | 2.10                     | 0.52              |
| 1:C:3:ILE:HG23  | 1:C:67:PHE:HE2  | 1.75                     | 0.52              |
| 1:C:79:LEU:HA   | 1:C:85:LYS:HG3  | 1.91                     | 0.52              |
| 1:A:24:TYR:CE1  | 1:E:96:ARG:NH1  | 2.77                     | 0.52              |
| 1:A:1:MET:CG    | 1:A:2:ASN:H     | 2.23                     | 0.51              |
| 1:C:97:CYS:SG   | 1:D:37:PRO:HG2  | 2.50                     | 0.51              |
| 1:A:145:ARG:CA  | 1:A:148:ARG:NH2 | 2.72                     | 0.51              |
| 1:A:141:ALA:C   | 1:A:143:PRO:HD3 | 2.31                     | 0.51              |
| 1:D:84:LEU:CD1  | 1:D:108:GLU:HG2 | 2.40                     | 0.51              |
| 1:C:162:LYS:HB3 | 1:C:162:LYS:HZ2 | 1.73                     | 0.51              |
| 1:A:95:ARG:CG   | 1:A:95:ARG:HH11 | 2.24                     | 0.51              |
| 1:C:14:ARG:HD2  | 1:C:18:TYR:CD1  | 2.44                     | 0.51              |
| 1:B:114:PHE:HB3 | 1:B:117:SER:HB3 | 1.93                     | 0.51              |
| 1:C:113:GLY:O   | 1:C:115:THR:N   | 2.35                     | 0.51              |
| 1:D:13:LEU:HD11 | 1:D:15:LEU:CD2  | 2.41                     | 0.51              |
| 1:D:33:LEU:C    | 1:D:34:THR:HG22 | 2.31                     | 0.51              |
| 1:E:4:PHE:CD1   | 1:E:29:ILE:HD11 | 2.45                     | 0.51              |
| 1:B:137:ALA:O   | 1:B:140:ALA:HB3 | 2.11                     | 0.51              |
| 1:A:7:LEU:HD12  | 1:A:67:PHE:CE1  | 2.46                     | 0.51              |
| 1:E:148:ARG:HG2 | 1:E:160:ALA:HB1 | 1.93                     | 0.51              |
| 1:C:46:LEU:HG   | 1:C:47:ASP:N    | 2.26                     | 0.51              |
| 1:A:6:MET:O     | 1:A:10:ASP:OD1  | 2.29                     | 0.51              |
| 1:A:87:VAL:HG21 | 1:A:118:LEU:HB3 | 1.93                     | 0.51              |
| 1:A:71:VAL:CG1  | 1:B:36:SER:HB2  | 2.41                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:147:LYS:O    | 1:B:150:ILE:N    | 2.44                     | 0.51              |
| 1:D:87:VAL:HA    | 1:D:90:SER:OG    | 2.11                     | 0.51              |
| 1:A:116:ASN:HD22 | 1:A:119:ARG:CD   | 2.23                     | 0.51              |
| 1:E:85:LYS:HB3   | 1:E:86:PRO:HD3   | 1.92                     | 0.51              |
| 1:C:26:THR:HG23  | 1:C:31:HIS:C     | 2.31                     | 0.51              |
| 1:E:105:GLN:HG2  | 1:E:105:GLN:O    | 2.11                     | 0.51              |
| 1:B:148:ARG:HD2  | 1:B:161:TYR:CZ   | 2.46                     | 0.50              |
| 1:D:38:SER:HB3   | 1:D:41:ALA:CB    | 2.40                     | 0.50              |
| 1:C:162:LYS:HB3  | 1:C:162:LYS:HZ3  | 1.74                     | 0.50              |
| 1:D:8:ARG:NH2    | 1:D:9:ILE:CD1    | 2.71                     | 0.50              |
| 1:C:15:LEU:O     | 1:C:57:VAL:HG13  | 2.12                     | 0.50              |
| 1:B:1:MET:HE3    | 1:B:5:GLU:CG     | 2.39                     | 0.50              |
| 1:C:13:LEU:HD12  | 1:C:29:ILE:HG13  | 1.93                     | 0.50              |
| 1:E:141:ALA:O    | 1:E:143:PRO:HD3  | 2.11                     | 0.50              |
| 1:E:114:PHE:HB3  | 1:E:117:SER:HB2  | 1.92                     | 0.50              |
| 1:C:24:TYR:CE1   | 1:C:35:LYS:HB2   | 2.47                     | 0.50              |
| 1:E:130:ALA:CB   | 1:E:154:ARG:HG3  | 2.42                     | 0.50              |
| 1:C:155:THR:OG1  | 1:C:157:THR:HG23 | 2.11                     | 0.50              |
| 1:C:131:ALA:O    | 1:C:134:ALA:HB3  | 2.12                     | 0.50              |
| 1:C:24:TYR:CE1   | 1:C:35:LYS:CB    | 2.95                     | 0.50              |
| 1:B:10:ASP:OD1   | 1:B:148:ARG:NE   | 2.42                     | 0.50              |
| 1:D:78:ILE:HG23  | 1:D:84:LEU:HB3   | 1.94                     | 0.50              |
| 1:E:64:GLU:O     | 1:E:67:PHE:HB3   | 2.12                     | 0.50              |
| 1:D:20:ASP:OD1   | 1:D:22:GLU:N     | 2.38                     | 0.50              |
| 1:A:40:ASN:OD1   | 1:E:68:ASN:OD1   | 2.29                     | 0.50              |
| 1:B:162:LYS:HB3  | 1:B:162:LYS:NZ   | 2.27                     | 0.50              |
| 1:C:144:ASN:O    | 1:C:147:LYS:HB2  | 2.12                     | 0.50              |
| 1:B:115:THR:HG23 | 1:B:119:ARG:NH1  | 2.27                     | 0.50              |
| 1:B:81:ASN:ND2   | 1:B:84:LEU:HD12  | 2.27                     | 0.50              |
| 1:A:46:LEU:O     | 1:A:49:ALA:HB3   | 2.12                     | 0.50              |
| 1:A:36:SER:C     | 1:A:38:SER:H     | 2.15                     | 0.50              |
| 1:D:17:ILE:CG2   | 1:D:25:TYR:HD1   | 2.25                     | 0.49              |
| 1:D:25:TYR:CE1   | 1:D:39:LEU:HD12  | 2.47                     | 0.49              |
| 1:D:129:ALA:O    | 1:D:132:ALA:HB3  | 2.11                     | 0.49              |
| 1:D:3:ILE:HG12   | 1:D:67:PHE:CZ    | 2.47                     | 0.49              |
| 1:B:18:TYR:HD1   | 1:B:19:LYS:O     | 1.94                     | 0.49              |
| 1:E:133:LEU:O    | 1:E:136:ALA:HB3  | 2.12                     | 0.49              |
| 1:C:1:MET:HE3    | 1:C:5:GLU:HB3    | 1.95                     | 0.49              |
| 1:C:72:ASP:HB3   | 1:C:76:ARG:HH22  | 1.75                     | 0.49              |
| 1:D:17:ILE:O     | 1:D:18:TYR:HB3   | 2.12                     | 0.49              |
| 1:B:7:LEU:HD23   | 1:B:11:GLU:HG2   | 1.95                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:39:LEU:CD1   | 1:B:43:LYS:HD2   | 2.41                     | 0.49              |
| 1:C:32:LEU:HG    | 1:C:33:LEU:N     | 2.24                     | 0.49              |
| 1:C:105:GLN:HB2  | 1:C:145:ARG:CZ   | 2.43                     | 0.49              |
| 1:B:32:LEU:HD23  | 1:B:34:THR:N     | 2.27                     | 0.49              |
| 1:A:38:SER:HB3   | 1:A:41:ALA:HB2   | 1.95                     | 0.49              |
| 1:A:128:ALA:O    | 1:A:131:ALA:HB3  | 2.12                     | 0.49              |
| 1:D:146:ALA:O    | 1:D:150:ILE:HD12 | 2.12                     | 0.49              |
| 1:D:33:LEU:HD13  | 1:D:46:LEU:HB2   | 1.94                     | 0.49              |
| 1:C:5:GLU:O      | 1:C:8:ARG:HB3    | 2.13                     | 0.49              |
| 1:D:67:PHE:O     | 1:D:70:ASP:N     | 2.45                     | 0.49              |
| 1:A:4:PHE:CE1    | 1:A:64:GLU:HA    | 2.48                     | 0.49              |
| 1:E:17:ILE:HD11  | 1:E:56:GLY:HA2   | 1.94                     | 0.49              |
| 1:B:4:PHE:HD1    | 1:B:67:PHE:CD2   | 2.30                     | 0.49              |
| 1:B:115:THR:O    | 1:B:119:ARG:HD2  | 2.12                     | 0.49              |
| 1:A:106:MET:O    | 1:A:107:GLY:O    | 2.31                     | 0.49              |
| 1:C:68:ASN:OD1   | 1:D:40:ASN:OD1   | 2.30                     | 0.49              |
| 1:D:50:ILE:HD13  | 1:D:62:GLU:CD    | 2.33                     | 0.49              |
| 1:B:13:LEU:HG    | 1:B:14:ARG:N     | 2.28                     | 0.49              |
| 1:B:89:ASP:O     | 1:B:96:ARG:NH2   | 2.45                     | 0.48              |
| 1:C:1:MET:HB3    | 1:C:158:TRP:CD1  | 2.48                     | 0.48              |
| 1:A:140:ALA:O    | 1:A:143:PRO:HG3  | 2.14                     | 0.48              |
| 1:C:105:GLN:OE1  | 1:C:145:ARG:HD3  | 2.13                     | 0.48              |
| 1:C:103:VAL:HG23 | 1:C:111:VAL:HG21 | 1.95                     | 0.48              |
| 1:A:20:ASP:OD1   | 1:A:22:GLU:N     | 2.46                     | 0.48              |
| 1:A:103:VAL:HG22 | 1:A:111:VAL:HG21 | 1.95                     | 0.48              |
| 1:A:14:ARG:HG3   | 1:A:18:TYR:CZ    | 2.47                     | 0.48              |
| 1:D:131:ALA:O    | 1:D:134:ALA:HB3  | 2.13                     | 0.48              |
| 1:D:120:MET:CE   | 1:D:129:ALA:HA   | 2.32                     | 0.48              |
| 1:D:28:GLY:O     | 1:D:30:GLY:N     | 2.42                     | 0.48              |
| 1:B:158:TRP:C    | 1:B:162:LYS:HG2  | 2.33                     | 0.48              |
| 1:B:18:TYR:CZ    | 1:B:26:THR:HG22  | 2.49                     | 0.48              |
| 1:C:148:ARG:HB3  | 1:C:161:TYR:CZ   | 2.49                     | 0.48              |
| 1:A:59:THR:HG23  | 1:A:62:GLU:CG    | 2.43                     | 0.48              |
| 1:B:118:LEU:O    | 1:B:121:LEU:HB2  | 2.13                     | 0.48              |
| 1:B:106:MET:HG3  | 1:B:106:MET:O    | 2.13                     | 0.48              |
| 1:D:34:THR:CG2   | 1:D:42:ALA:HA    | 2.42                     | 0.48              |
| 1:C:130:ALA:HB1  | 1:C:150:ILE:CG2  | 2.44                     | 0.48              |
| 1:C:140:ALA:O    | 1:C:143:PRO:HG3  | 2.13                     | 0.48              |
| 1:A:93:ALA:O     | 1:A:96:ARG:HB2   | 2.13                     | 0.48              |
| 1:B:34:THR:HG22  | 1:B:42:ALA:HB2   | 1.96                     | 0.48              |
| 1:C:93:ALA:HA    | 1:C:96:ARG:HG3   | 1.94                     | 0.48              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:E:8:ARG:NH2   | 1:E:9:ILE:CG1    | 2.75                     | 0.48              |
| 1:C:126:TRP:HE3 | 1:C:126:TRP:HA   | 1.78                     | 0.47              |
| 1:D:8:ARG:NH2   | 1:D:9:ILE:CG1    | 2.78                     | 0.47              |
| 1:B:162:LYS:CB  | 1:B:162:LYS:NZ   | 2.77                     | 0.47              |
| 1:E:4:PHE:CA    | 1:E:67:PHE:CE2   | 2.96                     | 0.47              |
| 1:D:15:LEU:HD13 | 1:D:58:ILE:O     | 2.13                     | 0.47              |
| 1:B:105:GLN:CG  | 1:B:145:ARG:NH1  | 2.78                     | 0.47              |
| 1:D:142:THR:N   | 1:D:143:PRO:CD   | 2.78                     | 0.47              |
| 1:A:133:LEU:C   | 1:A:135:ALA:H    | 2.17                     | 0.47              |
| 1:C:39:LEU:HD12 | 1:C:39:LEU:O     | 2.15                     | 0.47              |
| 1:A:3:ILE:HB    | 1:A:97:CYS:SG    | 2.54                     | 0.47              |
| 1:B:129:ALA:O   | 1:B:133:LEU:HD12 | 2.14                     | 0.47              |
| 1:A:51:GLY:O    | 1:A:52:ARG:HB3   | 2.14                     | 0.47              |
| 1:B:131:ALA:O   | 1:B:134:ALA:HB3  | 2.15                     | 0.47              |
| 1:B:60:LYS:HB3  | 1:B:60:LYS:HE3   | 1.47                     | 0.47              |
| 1:D:18:TYR:O    | 1:D:26:THR:N     | 2.41                     | 0.47              |
| 1:D:27:ILE:CD1  | 1:D:58:ILE:HG12  | 2.45                     | 0.47              |
| 1:D:17:ILE:CG2  | 1:D:18:TYR:N     | 2.76                     | 0.47              |
| 1:A:75:VAL:HA   | 1:A:78:ILE:HD12  | 1.96                     | 0.47              |
| 1:B:59:THR:HG23 | 1:B:62:GLU:OE2   | 2.14                     | 0.47              |
| 1:C:114:PHE:HB3 | 1:C:117:SER:CB   | 2.44                     | 0.47              |
| 1:E:8:ARG:HG2   | 1:E:8:ARG:O      | 2.13                     | 0.47              |
| 1:C:7:LEU:HD22  | 1:C:11:GLU:CG    | 2.45                     | 0.47              |
| 1:D:138:TRP:HH2 | 1:D:149:VAL:HG12 | 1.80                     | 0.47              |
| 1:C:87:VAL:HG12 | 1:C:87:VAL:O     | 2.14                     | 0.47              |
| 1:C:87:VAL:O    | 1:C:91:LEU:HG    | 2.15                     | 0.47              |
| 1:C:155:THR:OG1 | 1:C:157:THR:N    | 2.48                     | 0.47              |
| 1:A:33:LEU:C    | 1:A:34:THR:HG22  | 2.35                     | 0.47              |
| 1:D:140:ALA:O   | 1:D:143:PRO:HD3  | 2.14                     | 0.47              |
| 1:A:131:ALA:O   | 1:A:133:LEU:N    | 2.48                     | 0.47              |
| 1:E:120:MET:HE1 | 1:E:132:ALA:HB2  | 1.97                     | 0.47              |
| 1:B:1:MET:HB3   | 1:B:158:TRP:CD1  | 2.50                     | 0.47              |
| 1:D:93:ALA:CB   | 1:E:19:LYS:HZ1   | 2.28                     | 0.47              |
| 1:A:7:LEU:CD1   | 1:A:67:PHE:HE1   | 2.27                     | 0.47              |
| 1:D:8:ARG:O     | 1:D:12:GLY:HA2   | 2.15                     | 0.47              |
| 1:A:148:ARG:HG2 | 1:A:160:ALA:HB1  | 1.97                     | 0.47              |
| 1:A:29:ILE:O    | 1:A:29:ILE:HG22  | 2.14                     | 0.47              |
| 1:E:162:LYS:NZ  | 1:E:162:LYS:CB   | 2.78                     | 0.46              |
| 1:A:45:GLU:OE1  | 1:A:48:LYS:HE2   | 2.14                     | 0.46              |
| 1:B:117:SER:HA  | 1:B:120:MET:HE3  | 1.96                     | 0.46              |
| 1:A:34:THR:HG21 | 1:A:42:ALA:HA    | 1.97                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:105:GLN:CB   | 1:B:145:ARG:NH1  | 2.78                     | 0.46              |
| 1:D:1:MET:HG3    | 1:D:2:ASN:H      | 1.79                     | 0.46              |
| 1:A:34:THR:CG2   | 1:A:42:ALA:HA    | 2.45                     | 0.46              |
| 1:D:93:ALA:HB2   | 1:E:19:LYS:HZ3   | 1.80                     | 0.46              |
| 1:E:4:PHE:HB2    | 1:E:67:PHE:CE2   | 2.51                     | 0.46              |
| 1:A:95:ARG:CD    | 1:A:126:TRP:CH2  | 2.99                     | 0.46              |
| 1:A:26:THR:CG2   | 1:A:27:ILE:N     | 2.79                     | 0.46              |
| 1:A:50:ILE:HG22  | 1:A:66:LEU:HD21  | 1.97                     | 0.46              |
| 1:B:1:MET:HB3    | 1:B:158:TRP:CE2  | 2.48                     | 0.46              |
| 1:D:111:VAL:O    | 1:D:118:LEU:HD11 | 2.16                     | 0.46              |
| 1:E:50:ILE:HD11  | 1:E:52:ARG:HE    | 1.80                     | 0.46              |
| 1:D:124:LYS:HA   | 1:D:126:TRP:CH2  | 2.50                     | 0.46              |
| 1:A:94:VAL:CG2   | 1:A:158:TRP:CE2  | 2.99                     | 0.46              |
| 1:B:105:GLN:NE2  | 1:B:145:ARG:CD   | 2.79                     | 0.46              |
| 1:E:6:MET:HE1    | 1:E:101:ASN:HB3  | 1.98                     | 0.46              |
| 1:B:50:ILE:CG1   | 1:B:51:GLY:N     | 2.74                     | 0.46              |
| 1:B:87:VAL:HG22  | 1:B:122:GLN:HE21 | 1.81                     | 0.46              |
| 1:E:26:THR:CG2   | 1:E:27:ILE:N     | 2.77                     | 0.46              |
| 1:E:58:ILE:HG22  | 1:E:62:GLU:OE1   | 2.16                     | 0.46              |
| 1:B:85:LYS:HE3   | 1:B:89:ASP:OD2   | 2.16                     | 0.46              |
| 1:E:3:ILE:HG23   | 1:E:67:PHE:HE2   | 1.80                     | 0.46              |
| 1:D:9:ILE:HG21   | 1:D:161:TYR:HD2  | 1.81                     | 0.45              |
| 1:A:95:ARG:CG    | 1:A:95:ARG:NH1   | 2.79                     | 0.45              |
| 1:A:133:LEU:O    | 1:A:135:ALA:N    | 2.50                     | 0.45              |
| 1:A:115:THR:HG22 | 1:A:116:ASN:HD22 | 1.81                     | 0.45              |
| 1:D:115:THR:O    | 1:D:119:ARG:HD2  | 2.17                     | 0.45              |
| 1:C:143:PRO:O    | 1:C:147:LYS:HD2  | 2.16                     | 0.45              |
| 1:C:145:ARG:C    | 1:C:147:LYS:H    | 2.18                     | 0.45              |
| 1:C:87:VAL:HG21  | 1:C:118:LEU:HB3  | 1.97                     | 0.45              |
| 1:A:18:TYR:CE1   | 1:A:26:THR:HG22  | 2.52                     | 0.45              |
| 1:A:85:LYS:N     | 1:A:86:PRO:CD    | 2.79                     | 0.45              |
| 1:A:105:GLN:HB2  | 1:A:145:ARG:CZ   | 2.47                     | 0.45              |
| 1:B:105:GLN:HE21 | 1:B:145:ARG:NH1  | 2.09                     | 0.45              |
| 1:C:119:ARG:O    | 1:C:123:GLN:HG2  | 2.17                     | 0.45              |
| 1:A:32:LEU:C     | 1:A:32:LEU:HD23  | 2.36                     | 0.45              |
| 1:A:87:VAL:HA    | 1:A:122:GLN:CG   | 2.47                     | 0.45              |
| 1:A:159:ASP:CA   | 1:A:162:LYS:HE2  | 2.46                     | 0.45              |
| 1:B:18:TYR:CZ    | 1:B:26:THR:CG2   | 3.00                     | 0.45              |
| 1:C:102:MET:CE   | 1:C:111:VAL:HG13 | 2.44                     | 0.45              |
| 1:D:143:PRO:O    | 1:D:147:LYS:HG3  | 2.17                     | 0.45              |
| 1:C:96:ARG:O     | 1:C:100:ILE:HD12 | 2.17                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:120:MET:CE   | 1:E:132:ALA:HB2  | 2.47                     | 0.45              |
| 1:C:3:ILE:HG12   | 1:C:67:PHE:CZ    | 2.43                     | 0.45              |
| 1:B:78:ILE:HG23  | 1:B:84:LEU:HB3   | 1.98                     | 0.45              |
| 1:C:14:ARG:HD2   | 1:C:18:TYR:CG    | 2.51                     | 0.45              |
| 1:A:88:TYR:CE1   | 1:A:96:ARG:HD3   | 2.52                     | 0.45              |
| 1:C:7:LEU:CD2    | 1:C:11:GLU:HG2   | 2.47                     | 0.45              |
| 1:B:70:ASP:O     | 1:B:73:ALA:HB3   | 2.17                     | 0.45              |
| 1:C:72:ASP:O     | 1:C:76:ARG:HB2   | 2.16                     | 0.45              |
| 1:B:1:MET:CB     | 1:B:158:TRP:CG   | 2.97                     | 0.44              |
| 1:B:6:MET:CE     | 1:B:158:TRP:CZ3  | 3.00                     | 0.44              |
| 1:A:117:SER:OG   | 1:A:133:LEU:HD21 | 2.18                     | 0.44              |
| 1:C:120:MET:HE1  | 1:C:132:ALA:HB3  | 1.98                     | 0.44              |
| 1:D:79:LEU:CD1   | 1:E:35:LYS:HD2   | 2.47                     | 0.44              |
| 1:D:94:VAL:O     | 1:D:97:CYS:HB2   | 2.18                     | 0.44              |
| 1:E:33:LEU:HA    | 1:E:33:LEU:HD23  | 1.44                     | 0.44              |
| 1:D:105:GLN:HB2  | 1:D:145:ARG:NH2  | 2.32                     | 0.44              |
| 1:D:20:ASP:OD2   | 1:D:24:TYR:HB2   | 2.16                     | 0.44              |
| 1:C:120:MET:HE2  | 1:C:132:ALA:HB3  | 1.98                     | 0.44              |
| 1:C:24:TYR:CD1   | 1:C:35:LYS:CB    | 2.98                     | 0.44              |
| 1:D:71:VAL:O     | 1:D:74:ALA:HB3   | 2.18                     | 0.44              |
| 1:D:88:TYR:CZ    | 1:D:96:ARG:HD3   | 2.52                     | 0.44              |
| 1:A:79:LEU:HD21  | 1:A:88:TYR:CD2   | 2.52                     | 0.44              |
| 1:E:81:ASN:OD1   | 1:E:82:ALA:N     | 2.50                     | 0.44              |
| 1:A:81:ASN:HD22  | 1:A:84:LEU:HD12  | 1.78                     | 0.44              |
| 1:E:8:ARG:NH2    | 1:E:9:ILE:CD1    | 2.80                     | 0.44              |
| 1:A:95:ARG:CD    | 1:A:126:TRP:CZ3  | 3.01                     | 0.44              |
| 1:A:142:THR:N    | 1:A:143:PRO:HD3  | 2.33                     | 0.44              |
| 1:B:103:VAL:O    | 1:B:107:GLY:N    | 2.51                     | 0.44              |
| 1:A:119:ARG:HH11 | 1:A:119:ARG:CG   | 2.29                     | 0.44              |
| 1:A:103:VAL:HA   | 1:A:111:VAL:HG21 | 1.99                     | 0.44              |
| 1:C:6:MET:SD     | 1:C:158:TRP:HZ3  | 2.41                     | 0.44              |
| 1:A:15:LEU:O     | 1:A:57:VAL:HG13  | 2.17                     | 0.44              |
| 1:C:50:ILE:HD11  | 1:C:54:CYS:SG    | 2.57                     | 0.44              |
| 1:A:2:ASN:OD1    | 1:A:2:ASN:N      | 2.49                     | 0.44              |
| 1:A:47:ASP:HA    | 1:A:54:CYS:SG    | 2.57                     | 0.44              |
| 1:B:1:MET:HE3    | 1:B:5:GLU:CB     | 2.46                     | 0.44              |
| 1:D:13:LEU:HD11  | 1:D:15:LEU:HD21  | 2.00                     | 0.44              |
| 1:A:119:ARG:NH1  | 1:A:119:ARG:CG   | 2.81                     | 0.44              |
| 1:A:114:PHE:HB3  | 1:A:117:SER:HB3  | 1.99                     | 0.44              |
| 1:C:18:TYR:O     | 1:C:25:TYR:HA    | 2.17                     | 0.44              |
| 1:D:143:PRO:O    | 1:D:147:LYS:HD2  | 2.18                     | 0.44              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:A:38:SER:HB3  | 1:A:41:ALA:CB   | 2.48                     | 0.44              |
| 1:C:126:TRP:CE3 | 1:C:126:TRP:HA  | 2.51                     | 0.44              |
| 1:B:3:ILE:HD13  | 1:B:71:VAL:HG11 | 2.00                     | 0.44              |
| 1:D:25:TYR:HE1  | 1:D:39:LEU:HD12 | 1.83                     | 0.43              |
| 1:B:114:PHE:HB3 | 1:B:117:SER:CB  | 2.48                     | 0.43              |
| 1:A:33:LEU:HD23 | 1:A:33:LEU:HA   | 1.76                     | 0.43              |
| 1:D:72:ASP:O    | 1:D:76:ARG:HB2  | 2.19                     | 0.43              |
| 1:C:120:MET:HE2 | 1:C:132:ALA:CB  | 2.48                     | 0.43              |
| 1:B:14:ARG:HB2  | 1:B:18:TYR:CE2  | 2.52                     | 0.43              |
| 1:B:25:TYR:CE2  | 1:B:38:SER:O    | 2.71                     | 0.43              |
| 1:E:1:MET:HE2   | 1:E:5:GLU:C     | 2.38                     | 0.43              |
| 1:E:8:ARG:O     | 1:E:12:GLY:HA2  | 2.17                     | 0.43              |
| 1:C:60:LYS:NZ   | 1:C:60:LYS:O    | 2.40                     | 0.43              |
| 1:B:117:SER:OG  | 1:B:133:LEU:HG  | 2.19                     | 0.43              |
| 1:C:46:LEU:O    | 1:C:49:ALA:N    | 2.51                     | 0.43              |
| 1:D:52:ARG:O    | 1:D:54:CYS:N    | 2.46                     | 0.43              |
| 1:D:39:LEU:HD21 | 1:D:43:LYS:HZ1  | 1.84                     | 0.43              |
| 1:A:115:THR:CG2 | 1:A:119:ARG:HD2 | 2.45                     | 0.43              |
| 1:E:116:ASN:ND2 | 1:E:116:ASN:N   | 2.64                     | 0.43              |
| 1:C:10:ASP:OD1  | 1:C:161:TYR:HE2 | 2.02                     | 0.43              |
| 1:A:155:THR:OG1 | 1:A:157:THR:OG1 | 2.27                     | 0.43              |
| 1:E:67:PHE:O    | 1:E:70:ASP:HB2  | 2.19                     | 0.43              |
| 1:B:46:LEU:HD11 | 1:B:50:ILE:CG2  | 2.49                     | 0.43              |
| 1:B:58:ILE:HB   | 1:B:62:GLU:OE1  | 2.19                     | 0.43              |
| 1:E:14:ARG:HB2  | 1:E:18:TYR:CE1  | 2.54                     | 0.43              |
| 1:C:14:ARG:C    | 1:C:15:LEU:HG   | 2.39                     | 0.43              |
| 1:D:10:ASP:CB   | 1:D:145:ARG:HG3 | 2.49                     | 0.43              |
| 1:A:96:ARG:HB2  | 1:B:37:PRO:HG3  | 2.00                     | 0.43              |
| 1:C:120:MET:HE3 | 1:C:129:ALA:HA  | 1.93                     | 0.42              |
| 1:C:29:ILE:O    | 1:C:29:ILE:HG22 | 2.19                     | 0.42              |
| 1:E:10:ASP:OD1  | 1:E:161:TYR:HE1 | 2.01                     | 0.42              |
| 1:D:29:ILE:O    | 1:D:29:ILE:HG22 | 2.19                     | 0.42              |
| 1:E:8:ARG:NH2   | 1:E:9:ILE:HD11  | 2.34                     | 0.42              |
| 1:E:118:LEU:O   | 1:E:122:GLN:HB2 | 2.19                     | 0.42              |
| 1:E:17:ILE:HG13 | 1:E:56:GLY:CA   | 2.50                     | 0.42              |
| 1:B:4:PHE:HA    | 1:B:67:PHE:CE2  | 2.55                     | 0.42              |
| 1:A:94:VAL:CG2  | 1:A:158:TRP:NE1 | 2.82                     | 0.42              |
| 1:A:71:VAL:CG1  | 1:B:36:SER:CB   | 2.98                     | 0.42              |
| 1:D:148:ARG:HB3 | 1:D:161:TYR:CZ  | 2.54                     | 0.42              |
| 1:A:24:TYR:CE1  | 1:A:35:LYS:CB   | 2.98                     | 0.42              |
| 1:E:36:SER:HA   | 1:E:37:PRO:HD3  | 1.87                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:15:LEU:O     | 1:D:57:VAL:HA    | 2.19                     | 0.42              |
| 1:B:41:ALA:O     | 1:B:45:GLU:N     | 2.42                     | 0.42              |
| 1:E:10:ASP:OD2   | 1:E:101:ASN:ND2  | 2.50                     | 0.42              |
| 1:A:88:TYR:CD1   | 1:A:96:ARG:HD3   | 2.54                     | 0.42              |
| 1:A:65:LYS:HG3   | 1:A:66:LEU:N     | 2.28                     | 0.42              |
| 1:C:34:THR:CG2   | 1:C:42:ALA:HA    | 2.49                     | 0.42              |
| 1:E:145:ARG:HH11 | 1:E:145:ARG:HD2  | 1.71                     | 0.42              |
| 1:C:6:MET:CE     | 1:C:101:ASN:ND2  | 2.83                     | 0.42              |
| 1:E:88:TYR:CZ    | 1:E:96:ARG:HD3   | 2.55                     | 0.42              |
| 1:A:150:ILE:HG22 | 1:A:150:ILE:O    | 2.20                     | 0.42              |
| 1:C:7:LEU:HA     | 1:C:7:LEU:HD23   | 1.89                     | 0.42              |
| 1:A:7:LEU:HD12   | 1:A:67:PHE:CZ    | 2.55                     | 0.42              |
| 1:B:134:ALA:C    | 1:B:136:ALA:H    | 2.23                     | 0.42              |
| 1:B:62:GLU:O     | 1:B:65:LYS:HB3   | 2.19                     | 0.42              |
| 1:D:6:MET:SD     | 1:D:101:ASN:ND2  | 2.87                     | 0.42              |
| 1:B:148:ARG:HD2  | 1:B:161:TYR:CD2  | 2.54                     | 0.42              |
| 1:A:36:SER:HB2   | 1:E:71:VAL:HG12  | 2.02                     | 0.42              |
| 1:B:92:ASP:O     | 1:B:96:ARG:HG2   | 2.20                     | 0.42              |
| 1:D:8:ARG:NE     | 1:D:9:ILE:HG13   | 2.35                     | 0.42              |
| 1:D:91:LEU:HD13  | 1:D:95:ARG:HB3   | 2.02                     | 0.42              |
| 1:C:120:MET:CE   | 1:C:132:ALA:CB   | 2.97                     | 0.42              |
| 1:C:1:MET:HE3    | 1:C:5:GLU:CB     | 2.49                     | 0.42              |
| 1:B:26:THR:CG2   | 1:B:27:ILE:N     | 2.83                     | 0.42              |
| 1:A:131:ALA:O    | 1:A:134:ALA:N    | 2.53                     | 0.42              |
| 1:B:60:LYS:O     | 1:B:60:LYS:NZ    | 2.53                     | 0.41              |
| 1:A:94:VAL:O     | 1:A:97:CYS:HB2   | 2.20                     | 0.41              |
| 1:A:79:LEU:HA    | 1:A:79:LEU:HD23  | 1.72                     | 0.41              |
| 1:D:3:ILE:HG23   | 1:D:67:PHE:HE2   | 1.85                     | 0.41              |
| 1:C:103:VAL:HA   | 1:C:111:VAL:HG21 | 2.02                     | 0.41              |
| 1:D:36:SER:HA    | 1:D:37:PRO:HD3   | 1.90                     | 0.41              |
| 1:C:98:ALA:HB3   | 1:C:153:PHE:CE1  | 2.54                     | 0.41              |
| 1:D:120:MET:HE3  | 1:D:132:ALA:CB   | 2.51                     | 0.41              |
| 1:B:31:HIS:HD2   | 1:B:33:LEU:CD2   | 2.33                     | 0.41              |
| 1:C:71:VAL:CG1   | 1:D:36:SER:HB2   | 2.50                     | 0.41              |
| 1:C:99:LEU:HA    | 1:C:99:LEU:HD12  | 1.75                     | 0.41              |
| 1:E:108:GLU:O    | 1:E:110:GLY:N    | 2.53                     | 0.41              |
| 1:D:32:LEU:HD23  | 1:D:33:LEU:N     | 2.36                     | 0.41              |
| 1:B:58:ILE:HB    | 1:B:59:THR:H     | 1.57                     | 0.41              |
| 1:D:94:VAL:HG22  | 1:D:158:TRP:CE2  | 2.55                     | 0.41              |
| 1:E:79:LEU:O     | 1:E:85:LYS:HB2   | 2.21                     | 0.41              |
| 1:A:44:SER:O     | 1:A:48:LYS:HB2   | 2.21                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:50:ILE:HG12  | 1:C:54:CYS:SG    | 2.60                     | 0.41              |
| 1:E:88:TYR:CE1   | 1:E:96:ARG:HB3   | 2.55                     | 0.41              |
| 1:B:31:HIS:CD2   | 1:B:33:LEU:HD23  | 2.55                     | 0.41              |
| 1:C:111:VAL:C    | 1:C:113:GLY:H    | 2.24                     | 0.41              |
| 1:D:60:LYS:HZ2   | 1:D:60:LYS:C     | 2.18                     | 0.41              |
| 1:E:6:MET:HE1    | 1:E:101:ASN:CB   | 2.51                     | 0.41              |
| 1:C:148:ARG:O    | 1:C:152:THR:OG1  | 2.34                     | 0.41              |
| 1:C:15:LEU:HB3   | 1:C:58:ILE:CG1   | 2.50                     | 0.41              |
| 1:B:77:GLY:O     | 1:B:80:ARG:N     | 2.54                     | 0.41              |
| 1:D:18:TYR:HD1   | 1:D:19:LYS:O     | 2.04                     | 0.41              |
| 1:E:85:LYS:HB3   | 1:E:86:PRO:CD    | 2.51                     | 0.41              |
| 1:C:26:THR:CG2   | 1:C:27:ILE:N     | 2.83                     | 0.41              |
| 1:A:10:ASP:OD1   | 1:A:161:TYR:HE2  | 2.03                     | 0.41              |
| 1:C:92:ASP:OD1   | 1:C:95:ARG:HG3   | 2.20                     | 0.41              |
| 1:A:3:ILE:HD12   | 1:A:100:ILE:HD13 | 2.03                     | 0.41              |
| 1:B:14:ARG:HB2   | 1:B:18:TYR:HE2   | 1.85                     | 0.41              |
| 1:C:3:ILE:HG23   | 1:C:67:PHE:CE2   | 2.54                     | 0.41              |
| 1:B:115:THR:HG23 | 1:B:119:ARG:HH11 | 1.84                     | 0.41              |
| 1:B:52:ARG:O     | 1:B:54:CYS:N     | 2.54                     | 0.41              |
| 1:A:75:VAL:O     | 1:A:78:ILE:N     | 2.54                     | 0.41              |
| 1:E:111:VAL:O    | 1:E:113:GLY:N    | 2.53                     | 0.41              |
| 1:D:14:ARG:HG3   | 1:D:18:TYR:CD2   | 2.53                     | 0.40              |
| 1:A:3:ILE:CD1    | 1:A:71:VAL:CG2   | 2.99                     | 0.40              |
| 1:E:85:LYS:N     | 1:E:86:PRO:HD2   | 2.35                     | 0.40              |
| 1:B:14:ARG:O     | 1:B:28:GLY:HA2   | 2.20                     | 0.40              |
| 1:B:115:THR:O    | 1:B:119:ARG:HG3  | 2.22                     | 0.40              |
| 1:C:75:VAL:HG12  | 1:C:79:LEU:CD1   | 2.51                     | 0.40              |
| 1:D:39:LEU:HD21  | 1:D:43:LYS:NZ    | 2.36                     | 0.40              |
| 1:A:16:LYS:HA    | 1:A:56:GLY:O     | 2.21                     | 0.40              |
| 1:B:46:LEU:HD12  | 1:B:50:ILE:HG23  | 2.02                     | 0.40              |
| 1:A:1:MET:HG3    | 1:A:2:ASN:H      | 1.86                     | 0.40              |
| 1:C:9:ILE:HG22   | 1:C:10:ASP:N     | 2.36                     | 0.40              |
| 1:B:60:LYS:HZ2   | 1:B:60:LYS:C     | 2.24                     | 0.40              |
| 1:A:1:MET:HG3    | 1:A:5:GLU:HB2    | 2.04                     | 0.40              |
| 1:A:88:TYR:CE1   | 1:A:96:ARG:CD    | 3.05                     | 0.40              |
| 1:D:3:ILE:O      | 1:D:6:MET:HB3    | 2.22                     | 0.40              |
| 1:D:155:THR:OG1  | 1:D:157:THR:OG1  | 2.27                     | 0.40              |
| 1:A:114:PHE:O    | 1:A:117:SER:HB3  | 2.21                     | 0.40              |
| 1:E:17:ILE:HG13  | 1:E:56:GLY:HA3   | 2.04                     | 0.40              |
| 1:B:79:LEU:HD22  | 1:C:35:LYS:CD    | 2.52                     | 0.40              |
| 1:B:114:PHE:O    | 1:B:117:SER:N    | 2.55                     | 0.40              |

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| Atom-1         | Atom-2         | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|----------------|--------------------------|-------------------|
| 1:D:1:MET:CB   | 1:D:158:TRP:CG | 3.04                     | 0.40              |
| 1:C:75:VAL:CG1 | 1:C:79:LEU:CD1 | 2.99                     | 0.40              |
| 1:A:7:LEU:CD1  | 1:A:67:PHE:CE1 | 3.05                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed   | Outliers | Percentiles |           |
|-----|-------|---------------|-----------|-----------|----------|-------------|-----------|
| 1   | A     | 160/164 (98%) | 124 (78%) | 22 (14%)  | 14 (9%)  | <b>1</b>    | <b>4</b>  |
| 1   | B     | 160/164 (98%) | 127 (79%) | 26 (16%)  | 7 (4%)   | <b>3</b>    | <b>18</b> |
| 1   | C     | 160/164 (98%) | 128 (80%) | 28 (18%)  | 4 (2%)   | <b>7</b>    | <b>34</b> |
| 1   | D     | 160/164 (98%) | 133 (83%) | 19 (12%)  | 8 (5%)   | <b>3</b>    | <b>15</b> |
| 1   | E     | 160/164 (98%) | 130 (81%) | 21 (13%)  | 9 (6%)   | <b>2</b>    | <b>13</b> |
| All | All   | 800/820 (98%) | 642 (80%) | 116 (14%) | 42 (5%)  | <b>2</b>    | <b>14</b> |

All (42) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 52  | ARG  |
| 1   | A     | 93  | ALA  |
| 1   | A     | 115 | THR  |
| 1   | B     | 52  | ARG  |
| 1   | B     | 126 | TRP  |
| 1   | B     | 160 | ALA  |
| 1   | C     | 114 | PHE  |
| 1   | D     | 29  | ILE  |
| 1   | D     | 143 | PRO  |
| 1   | E     | 3   | ILE  |
| 1   | A     | 107 | GLY  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 126 | TRP  |
| 1   | A     | 132 | ALA  |
| 1   | B     | 115 | THR  |
| 1   | B     | 135 | ALA  |
| 1   | C     | 107 | GLY  |
| 1   | C     | 115 | THR  |
| 1   | E     | 70  | ASP  |
| 1   | E     | 107 | GLY  |
| 1   | E     | 108 | GLU  |
| 1   | E     | 109 | THR  |
| 1   | E     | 115 | THR  |
| 1   | E     | 136 | ALA  |
| 1   | A     | 37  | PRO  |
| 1   | A     | 46  | LEU  |
| 1   | A     | 131 | ALA  |
| 1   | A     | 134 | ALA  |
| 1   | B     | 53  | ASN  |
| 1   | D     | 137 | ALA  |
| 1   | A     | 155 | THR  |
| 1   | D     | 53  | ASN  |
| 1   | D     | 55  | ASN  |
| 1   | D     | 60  | LYS  |
| 1   | D     | 160 | ALA  |
| 1   | E     | 131 | ALA  |
| 1   | A     | 137 | ALA  |
| 1   | A     | 154 | ARG  |
| 1   | D     | 142 | THR  |
| 1   | A     | 17  | ILE  |
| 1   | C     | 85  | LYS  |
| 1   | E     | 17  | ILE  |
| 1   | B     | 29  | ILE  |

### 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.

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| Mol | Chain | Analysed      | Rotameric | Outliers  | Percentiles |   |
|-----|-------|---------------|-----------|-----------|-------------|---|
| 1   | A     | 127/129 (98%) | 97 (76%)  | 30 (24%)  | 1           | 4 |
| 1   | B     | 127/129 (98%) | 99 (78%)  | 28 (22%)  | 1           | 6 |
| 1   | C     | 127/129 (98%) | 92 (72%)  | 35 (28%)  | 0           | 2 |
| 1   | D     | 127/129 (98%) | 101 (80%) | 26 (20%)  | 1           | 7 |
| 1   | E     | 127/129 (98%) | 96 (76%)  | 31 (24%)  | 1           | 4 |
| All | All   | 635/645 (98%) | 485 (76%) | 150 (24%) | 1           | 4 |

All (150) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 1   | MET  |
| 1   | A     | 10  | ASP  |
| 1   | A     | 13  | LEU  |
| 1   | A     | 17  | ILE  |
| 1   | A     | 34  | THR  |
| 1   | A     | 35  | LYS  |
| 1   | A     | 36  | SER  |
| 1   | A     | 43  | LYS  |
| 1   | A     | 44  | SER  |
| 1   | A     | 48  | LYS  |
| 1   | A     | 50  | ILE  |
| 1   | A     | 53  | ASN  |
| 1   | A     | 54  | CYS  |
| 1   | A     | 58  | ILE  |
| 1   | A     | 59  | THR  |
| 1   | A     | 60  | LYS  |
| 1   | A     | 80  | ARG  |
| 1   | A     | 85  | LYS  |
| 1   | A     | 95  | ARG  |
| 1   | A     | 99  | LEU  |
| 1   | A     | 103 | VAL  |
| 1   | A     | 104 | PHE  |
| 1   | A     | 106 | MET  |
| 1   | A     | 119 | ARG  |
| 1   | A     | 122 | GLN  |
| 1   | A     | 145 | ARG  |
| 1   | A     | 151 | THR  |
| 1   | A     | 154 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 155 | THR  |
| 1   | A     | 162 | LYS  |
| 1   | B     | 1   | MET  |
| 1   | B     | 5   | GLU  |
| 1   | B     | 13  | LEU  |
| 1   | B     | 16  | LYS  |
| 1   | B     | 29  | ILE  |
| 1   | B     | 38  | SER  |
| 1   | B     | 43  | LYS  |
| 1   | B     | 45  | GLU  |
| 1   | B     | 50  | ILE  |
| 1   | B     | 53  | ASN  |
| 1   | B     | 59  | THR  |
| 1   | B     | 60  | LYS  |
| 1   | B     | 79  | LEU  |
| 1   | B     | 83  | LYS  |
| 1   | B     | 85  | LYS  |
| 1   | B     | 90  | SER  |
| 1   | B     | 92  | ASP  |
| 1   | B     | 96  | ARG  |
| 1   | B     | 104 | PHE  |
| 1   | B     | 106 | MET  |
| 1   | B     | 117 | SER  |
| 1   | B     | 119 | ARG  |
| 1   | B     | 125 | ARG  |
| 1   | B     | 142 | THR  |
| 1   | B     | 147 | LYS  |
| 1   | B     | 150 | ILE  |
| 1   | B     | 154 | ARG  |
| 1   | B     | 162 | LYS  |
| 1   | C     | 1   | MET  |
| 1   | C     | 8   | ARG  |
| 1   | C     | 13  | LEU  |
| 1   | C     | 15  | LEU  |
| 1   | C     | 16  | LYS  |
| 1   | C     | 17  | ILE  |
| 1   | C     | 32  | LEU  |
| 1   | C     | 34  | THR  |
| 1   | C     | 36  | SER  |
| 1   | C     | 43  | LYS  |
| 1   | C     | 44  | SER  |
| 1   | C     | 53  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 54  | CYS  |
| 1   | C     | 60  | LYS  |
| 1   | C     | 65  | LYS  |
| 1   | C     | 85  | LYS  |
| 1   | C     | 90  | SER  |
| 1   | C     | 96  | ARG  |
| 1   | C     | 102 | MET  |
| 1   | C     | 103 | VAL  |
| 1   | C     | 104 | PHE  |
| 1   | C     | 109 | THR  |
| 1   | C     | 116 | ASN  |
| 1   | C     | 119 | ARG  |
| 1   | C     | 123 | GLN  |
| 1   | C     | 124 | LYS  |
| 1   | C     | 125 | ARG  |
| 1   | C     | 126 | TRP  |
| 1   | C     | 127 | ASP  |
| 1   | C     | 148 | ARG  |
| 1   | C     | 150 | ILE  |
| 1   | C     | 152 | THR  |
| 1   | C     | 155 | THR  |
| 1   | C     | 157 | THR  |
| 1   | C     | 162 | LYS  |
| 1   | D     | 1   | MET  |
| 1   | D     | 6   | MET  |
| 1   | D     | 7   | LEU  |
| 1   | D     | 13  | LEU  |
| 1   | D     | 16  | LYS  |
| 1   | D     | 34  | THR  |
| 1   | D     | 39  | LEU  |
| 1   | D     | 43  | LYS  |
| 1   | D     | 48  | LYS  |
| 1   | D     | 50  | ILE  |
| 1   | D     | 52  | ARG  |
| 1   | D     | 53  | ASN  |
| 1   | D     | 59  | THR  |
| 1   | D     | 60  | LYS  |
| 1   | D     | 65  | LYS  |
| 1   | D     | 83  | LYS  |
| 1   | D     | 90  | SER  |
| 1   | D     | 104 | PHE  |
| 1   | D     | 106 | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 109 | THR  |
| 1   | D     | 119 | ARG  |
| 1   | D     | 142 | THR  |
| 1   | D     | 145 | ARG  |
| 1   | D     | 149 | VAL  |
| 1   | D     | 155 | THR  |
| 1   | D     | 162 | LYS  |
| 1   | E     | 1   | MET  |
| 1   | E     | 8   | ARG  |
| 1   | E     | 14  | ARG  |
| 1   | E     | 15  | LEU  |
| 1   | E     | 16  | LYS  |
| 1   | E     | 35  | LYS  |
| 1   | E     | 36  | SER  |
| 1   | E     | 43  | LYS  |
| 1   | E     | 48  | LYS  |
| 1   | E     | 50  | ILE  |
| 1   | E     | 52  | ARG  |
| 1   | E     | 53  | ASN  |
| 1   | E     | 60  | LYS  |
| 1   | E     | 65  | LYS  |
| 1   | E     | 69  | GLN  |
| 1   | E     | 78  | ILE  |
| 1   | E     | 89  | ASP  |
| 1   | E     | 90  | SER  |
| 1   | E     | 92  | ASP  |
| 1   | E     | 97  | CYS  |
| 1   | E     | 99  | LEU  |
| 1   | E     | 104 | PHE  |
| 1   | E     | 115 | THR  |
| 1   | E     | 116 | ASN  |
| 1   | E     | 117 | SER  |
| 1   | E     | 119 | ARG  |
| 1   | E     | 124 | LYS  |
| 1   | E     | 125 | ARG  |
| 1   | E     | 145 | ARG  |
| 1   | E     | 154 | ARG  |
| 1   | E     | 162 | LYS  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 40  | ASN  |
| 1   | A     | 116 | ASN  |
| 1   | B     | 31  | HIS  |
| 1   | B     | 40  | ASN  |
| 1   | B     | 53  | ASN  |
| 1   | B     | 105 | GLN  |
| 1   | B     | 116 | ASN  |
| 1   | B     | 122 | GLN  |
| 1   | B     | 144 | ASN  |
| 1   | C     | 31  | HIS  |
| 1   | C     | 53  | ASN  |
| 1   | C     | 69  | GLN  |
| 1   | C     | 101 | ASN  |
| 1   | C     | 116 | ASN  |
| 1   | C     | 122 | GLN  |
| 1   | D     | 40  | ASN  |
| 1   | D     | 53  | ASN  |
| 1   | D     | 68  | ASN  |
| 1   | D     | 116 | ASN  |
| 1   | D     | 122 | GLN  |
| 1   | E     | 31  | HIS  |
| 1   | E     | 53  | ASN  |
| 1   | E     | 116 | 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 carbohydrates 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     | 162/164 (98%) | -0.66  | 0 100 100 | 4, 27, 48, 64         | 0     |
| 1   | B     | 162/164 (98%) | -0.52  | 0 100 100 | 5, 29, 49, 64         | 0     |
| 1   | C     | 162/164 (98%) | -0.68  | 0 100 100 | 4, 23, 55, 75         | 0     |
| 1   | D     | 162/164 (98%) | -0.73  | 0 100 100 | 2, 22, 46, 63         | 0     |
| 1   | E     | 162/164 (98%) | -0.72  | 0 100 100 | 5, 21, 45, 60         | 0     |
| All | All   | 810/820 (98%) | -0.66  | 0 100 100 | 2, 24, 49, 75         | 0     |

There are no RSRZ outliers to report.

### 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 carbohydrates 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.