



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 27, 2026 – 08:45 PM UTC

PDB ID : 9S9G / pdb\_00009s9g  
Title : S. islandicus CdvA filament (X-ray)  
Authors : Salzer, R.; Lowe, J.; Bellini, D.  
Deposited on : 2025-08-06  
Resolution : 2.85 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

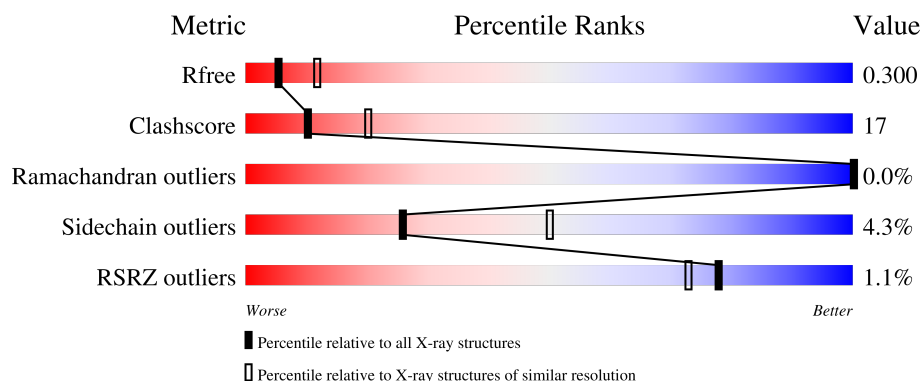
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.85 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 1407 (2.88-2.84)                                      |
| Clashscore            | 190562                      | 1446 (2.88-2.84)                                      |
| Ramachandran outliers | 187476                      | 1406 (2.88-2.84)                                      |
| Sidechain outliers    | 187428                      | 1407 (2.88-2.84)                                      |
| RSRZ outliers         | 180081                      | 1408 (2.88-2.84)                                      |

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

| Mol | Chain | Length | Quality of chain                                                                                  |
|-----|-------|--------|---------------------------------------------------------------------------------------------------|
| 1   | A     | 238    | <div> <div>0%</div> <div> <div>59%</div> <div>21%</div> <div>•</div> <div>18%</div> </div> </div> |
| 1   | B     | 238    | <div> <div>51%</div> <div>28%</div> <div>•</div> <div>18%</div> </div>                            |
| 1   | C     | 238    | <div> <div>51%</div> <div>28%</div> <div>•</div> <div>18%</div> </div>                            |
| 1   | D     | 238    | <div> <div>2%</div> <div>55%</div> <div>26%</div> <div>•</div> <div>18%</div> </div>              |
| 1   | E     | 238    | <div> <div>0%</div> <div>52%</div> <div>29%</div> <div>•</div> <div>18%</div> </div>              |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 1   | F     | 238    | <div> <div>2%</div> <div>51%</div> <div>29%</div> <div>•</div> <div>18%</div> </div> |
| 1   | G     | 238    | <div> <div>%</div> <div>50%</div> <div>30%</div> <div>•</div> <div>18%</div> </div>  |
| 1   | H     | 238    | <div> <div>%</div> <div>53%</div> <div>27%</div> <div>•</div> <div>18%</div> </div>  |
| 1   | I     | 238    | <div> <div>50%</div> <div>29%</div> <div>•</div> <div>19%</div> </div>               |
| 1   | J     | 238    | <div> <div>%</div> <div>52%</div> <div>26%</div> <div>•</div> <div>19%</div> </div>  |
| 1   | K     | 238    | <div> <div>%</div> <div>51%</div> <div>28%</div> <div>•</div> <div>19%</div> </div>  |
| 1   | L     | 238    | <div> <div>48%</div> <div>31%</div> <div>•</div> <div>19%</div> </div>               |
| 1   | M     | 238    | <div> <div>%</div> <div>47%</div> <div>30%</div> <div>•</div> <div>20%</div> </div>  |
| 1   | N     | 238    | <div> <div>%</div> <div>54%</div> <div>27%</div> <div>•</div> <div>19%</div> </div>  |

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 21978 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.

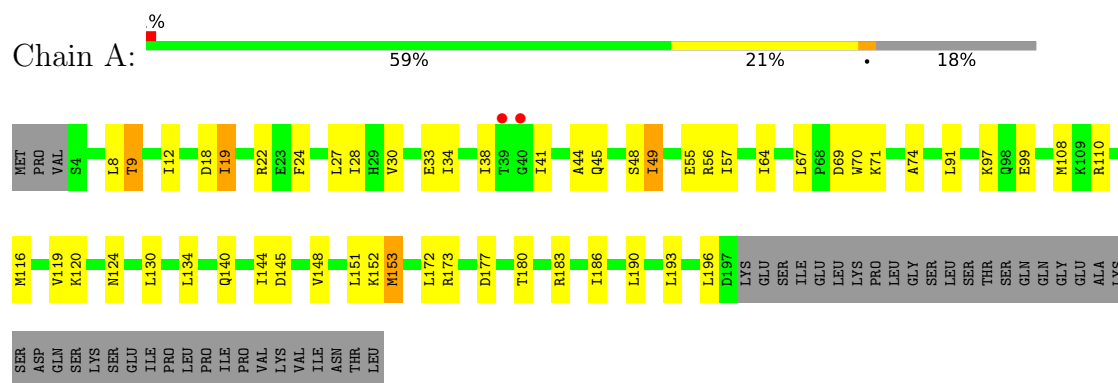
- Molecule 1 is a protein called Cell division protein CdvA.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 194      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1573  | 990  | 268 | 309 | 6 |         |         |       |
| 1   | B     | 194      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1572  | 991  | 268 | 307 | 6 |         |         |       |
| 1   | C     | 195      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1580  | 995  | 269 | 310 | 6 |         |         |       |
| 1   | D     | 195      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1580  | 995  | 269 | 310 | 6 |         |         |       |
| 1   | E     | 194      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1573  | 990  | 268 | 309 | 6 |         |         |       |
| 1   | F     | 196      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1587  | 1000 | 270 | 311 | 6 |         |         |       |
| 1   | G     | 195      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1580  | 995  | 269 | 310 | 6 |         |         |       |
| 1   | H     | 194      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1572  | 991  | 268 | 307 | 6 |         |         |       |
| 1   | I     | 193      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1565  | 986  | 267 | 306 | 6 |         |         |       |
| 1   | J     | 193      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1565  | 986  | 267 | 306 | 6 |         |         |       |
| 1   | K     | 193      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1565  | 986  | 267 | 306 | 6 |         |         |       |
| 1   | L     | 192      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1558  | 982  | 266 | 304 | 6 |         |         |       |
| 1   | M     | 190      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1543  | 973  | 264 | 300 | 6 |         |         |       |
| 1   | N     | 193      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1565  | 986  | 267 | 306 | 6 |         |         |       |

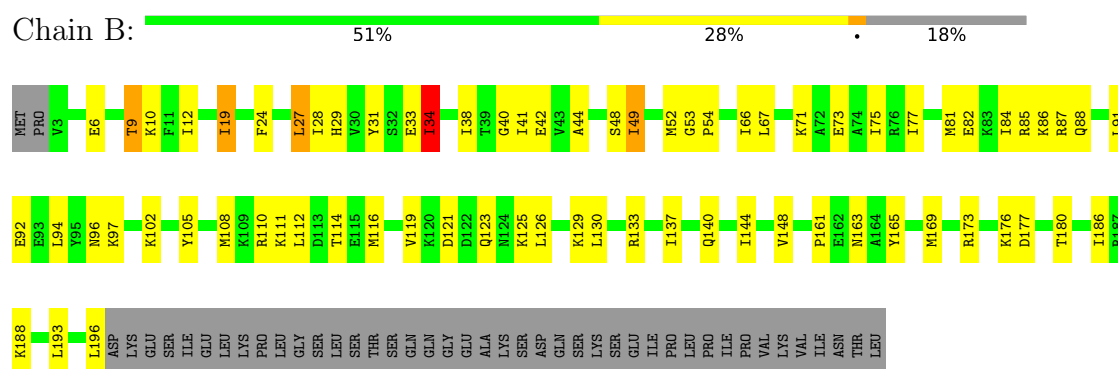
### 3 Residue-property plots [i](#)

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

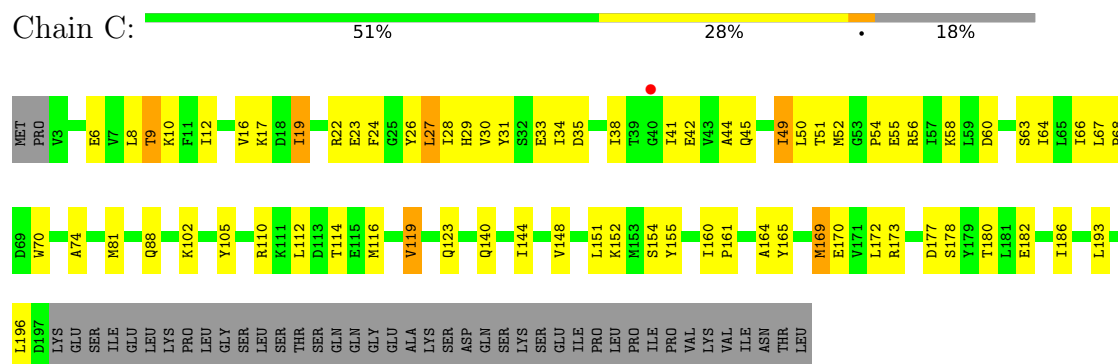
#### • Molecule 1: Cell division protein CdvA



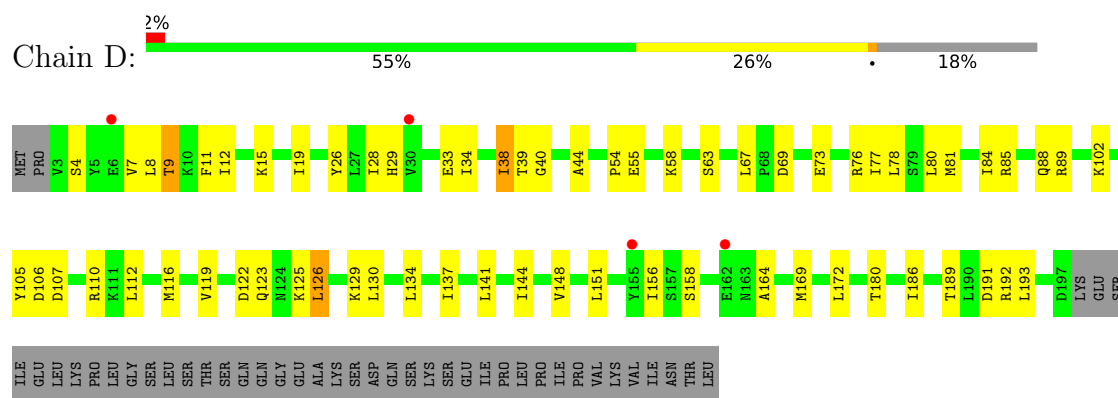
#### • Molecule 1: Cell division protein CdvA



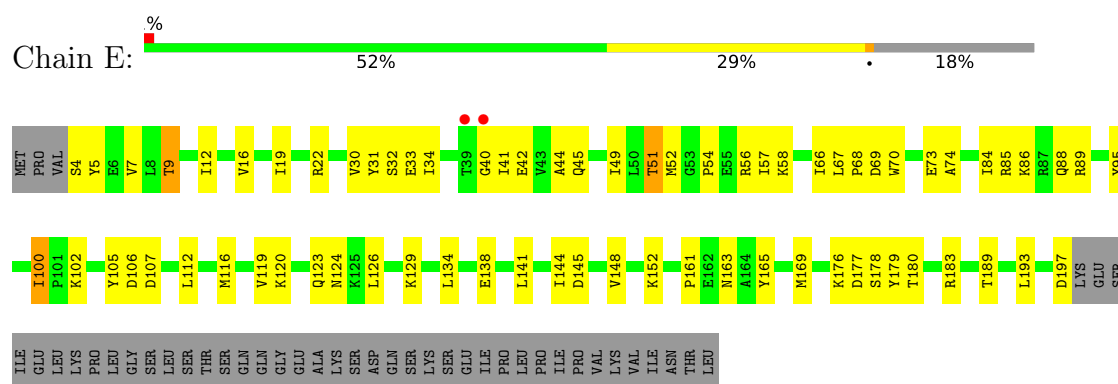
#### • Molecule 1: Cell division protein CdvA



- Molecule 1: Cell division protein CdvA



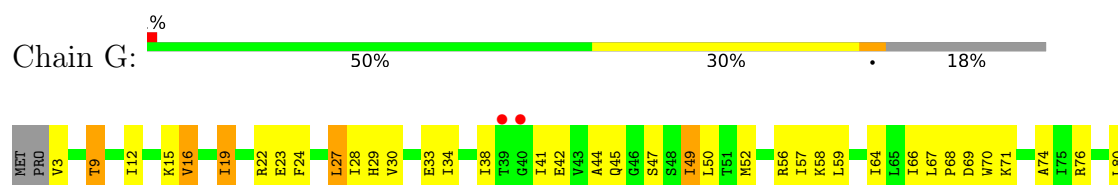
- Molecule 1: Cell division protein CdvA

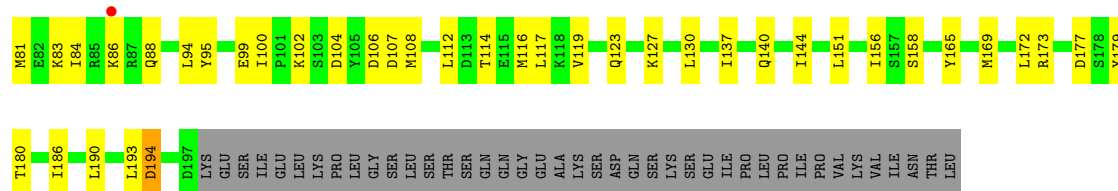


- Molecule 1: Cell division protein CdvA

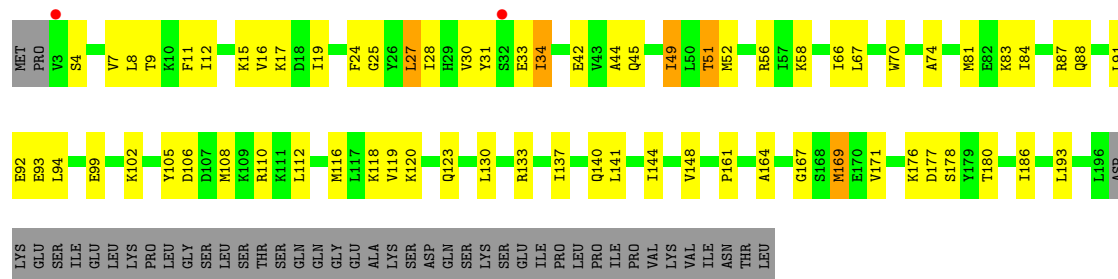


- Molecule 1: Cell division protein CdvA

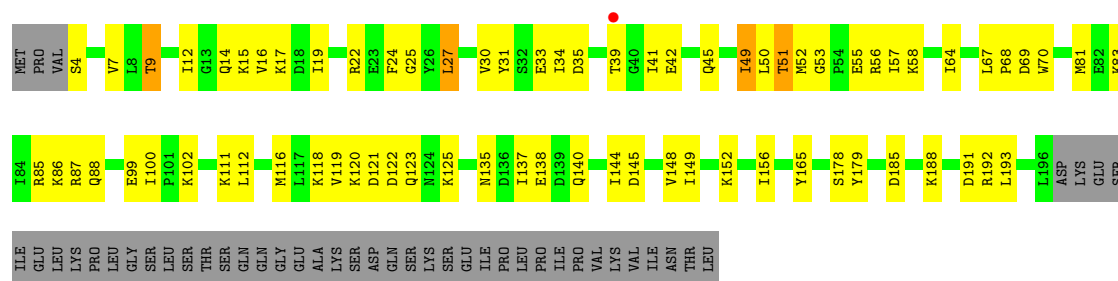




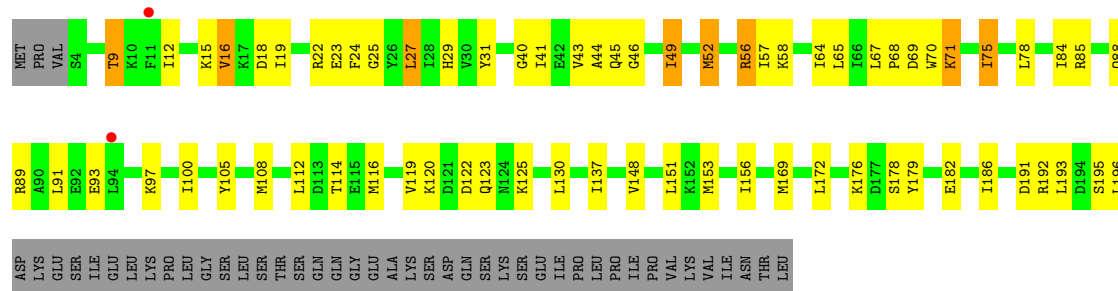
• Molecule 1: Cell division protein CdvA



• Molecule 1: Cell division protein CdvA

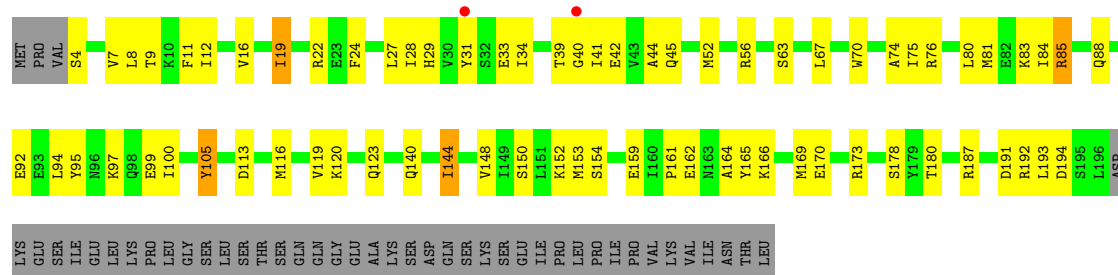


• Molecule 1: Cell division protein CdvA

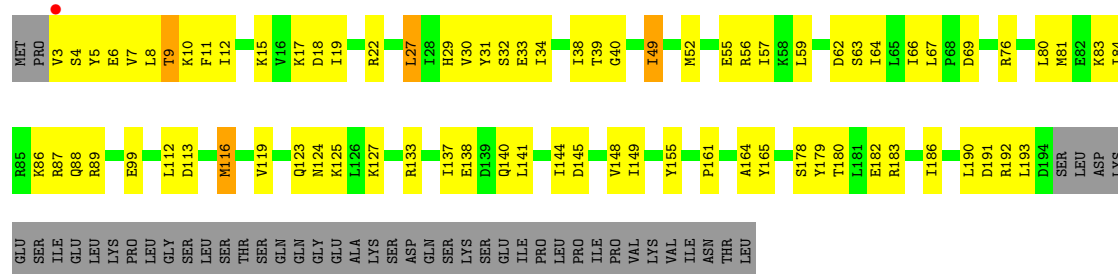


• Molecule 1: Cell division protein CdvA





• Molecule 1: Cell division protein CdvA





## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 1 21 1                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 71.03Å 102.72Å 328.55Å<br>90.00° 92.35° 90.00°              | Depositor        |
| Resolution (Å)                                                          | 52.62 – 2.85<br>52.62 – 2.85                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 33.2 (52.62-2.85)<br>33.2 (52.62-2.85)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 1.67                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.49 (at 2.86Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX (1.17.1_3660)                                        | Depositor        |
| R, $R_{free}$                                                           | 0.226 , 0.298<br>0.228 , 0.300                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 1872 reflections (1.69%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 83.4                                                        | Xtriage          |
| Anisotropy                                                              | 0.061                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.29 , 47.3                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$ | Xtriage          |
| Estimated twinning fraction                                             | 0.000 for h,-k,-l                                           | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.95                                                        | EDS              |
| Total number of atoms                                                   | 21978                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 68.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.56 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.7337e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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

| Mol | Chain | Bond lengths |                | Bond angles |                |
|-----|-------|--------------|----------------|-------------|----------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5        |
| 1   | A     | 0.51         | 0/1591         | 0.78        | 0/2129         |
| 1   | B     | 0.46         | 0/1590         | 0.76        | 1/2128 (0.0%)  |
| 1   | C     | 0.50         | 0/1598         | 0.76        | 0/2139         |
| 1   | D     | 0.48         | 0/1598         | 0.75        | 1/2139 (0.0%)  |
| 1   | E     | 0.51         | 0/1591         | 0.79        | 0/2129         |
| 1   | F     | 0.49         | 0/1606         | 0.79        | 0/2150         |
| 1   | G     | 0.53         | 0/1598         | 0.82        | 0/2139         |
| 1   | H     | 0.45         | 0/1590         | 0.74        | 0/2128         |
| 1   | I     | 0.46         | 0/1583         | 0.77        | 0/2118         |
| 1   | J     | 0.53         | 1/1583 (0.1%)  | 0.81        | 3/2118 (0.1%)  |
| 1   | K     | 0.53         | 0/1583         | 0.80        | 0/2118         |
| 1   | L     | 0.47         | 0/1576         | 0.74        | 0/2109         |
| 1   | M     | 0.49         | 0/1561         | 0.80        | 0/2088         |
| 1   | N     | 0.52         | 0/1583         | 0.75        | 0/2118         |
| All | All   | 0.50         | 1/22231 (0.0%) | 0.78        | 5/29750 (0.0%) |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | J     | 46  | GLY  | C-O   | -5.84 | 1.21        | 1.24     |

All (5) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | J     | 52  | MET  | CB-CG-SD  | -8.04 | 88.59       | 112.70   |
| 1   | J     | 56  | ARG  | NE-CZ-NH1 | -6.05 | 115.45      | 121.50   |
| 1   | B     | 34  | ILE  | N-CA-C    | 5.39  | 116.16      | 110.72   |
| 1   | J     | 52  | MET  | CG-SD-CE  | -5.07 | 89.74       | 100.90   |
| 1   | D     | 126 | LEU  | CB-CG-CD1 | -5.03 | 95.61       | 110.70   |

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     | 1573  | 0        | 1619     | 44      | 1            |
| 1   | B     | 1572  | 0        | 1624     | 65      | 0            |
| 1   | C     | 1580  | 0        | 1628     | 56      | 0            |
| 1   | D     | 1580  | 0        | 1628     | 53      | 0            |
| 1   | E     | 1573  | 0        | 1619     | 57      | 0            |
| 1   | F     | 1587  | 0        | 1636     | 70      | 0            |
| 1   | G     | 1580  | 0        | 1628     | 63      | 0            |
| 1   | H     | 1572  | 0        | 1624     | 51      | 0            |
| 1   | I     | 1565  | 0        | 1615     | 58      | 0            |
| 1   | J     | 1565  | 0        | 1615     | 56      | 0            |
| 1   | K     | 1565  | 0        | 1615     | 54      | 0            |
| 1   | L     | 1558  | 0        | 1608     | 58      | 1            |
| 1   | M     | 1543  | 0        | 1595     | 63      | 0            |
| 1   | N     | 1565  | 0        | 1615     | 48      | 0            |
| All | All   | 21978 | 0        | 22669    | 765     | 1            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

All (765) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:19:ILE:HD11 | 1:A:67:LEU:HA    | 1.49                     | 0.94              |
| 1:H:19:ILE:HD11 | 1:H:67:LEU:HA    | 1.50                     | 0.94              |
| 1:G:57:ILE:HD12 | 1:G:64:ILE:HD11  | 1.50                     | 0.93              |
| 1:I:19:ILE:HD11 | 1:I:67:LEU:HA    | 1.51                     | 0.92              |
| 1:K:28:ILE:HD11 | 1:K:44:ALA:HB2   | 1.52                     | 0.91              |
| 1:D:88:GLN:HG3  | 1:D:112:LEU:HD13 | 1.51                     | 0.90              |
| 1:M:84:ILE:HG21 | 1:M:116:MET:HB2  | 1.55                     | 0.89              |
| 1:K:19:ILE:HD11 | 1:K:67:LEU:HA    | 1.53                     | 0.89              |
| 1:C:34:ILE:HA   | 1:K:83:LYS:HE2   | 1.53                     | 0.88              |
| 1:J:19:ILE:HD11 | 1:J:67:LEU:HA    | 1.53                     | 0.88              |
| 1:D:107:ASP:OD1 | 1:D:110:ARG:NH1  | 2.06                     | 0.87              |
| 1:A:56:ARG:HH12 | 1:A:69:ASP:HB3   | 1.38                     | 0.86              |
| 1:C:60:ASP:HB3  | 1:C:63:SER:HB3   | 1.57                     | 0.84              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:19:ILE:HD11  | 1:E:67:LEU:HA    | 1.60                     | 0.84              |
| 1:G:28:ILE:HD11  | 1:G:44:ALA:HB2   | 1.60                     | 0.83              |
| 1:C:49:ILE:HD11  | 1:G:144:ILE:HG12 | 1.59                     | 0.83              |
| 1:D:9:THR:HA     | 1:D:12:ILE:HG13  | 1.61                     | 0.83              |
| 1:D:28:ILE:HD11  | 1:D:44:ALA:HB2   | 1.59                     | 0.83              |
| 1:K:88:GLN:NE2   | 1:K:113:ASP:OD1  | 2.13                     | 0.82              |
| 1:H:12:ILE:HG22  | 1:H:27:LEU:HD11  | 1.61                     | 0.82              |
| 1:J:85:ARG:HD3   | 1:J:89:ARG:HH11  | 1.45                     | 0.81              |
| 1:F:12:ILE:HD11  | 1:F:29:HIS:HA    | 1.63                     | 0.81              |
| 1:I:88:GLN:HG3   | 1:I:112:LEU:HD23 | 1.63                     | 0.81              |
| 1:I:33:GLU:HG2   | 1:I:34:ILE:H     | 1.45                     | 0.81              |
| 1:A:33:GLU:HG2   | 1:A:34:ILE:H     | 1.44                     | 0.80              |
| 1:H:33:GLU:HG3   | 1:H:34:ILE:H     | 1.46                     | 0.80              |
| 1:A:172:LEU:HD21 | 1:B:28:ILE:HD13  | 1.62                     | 0.80              |
| 1:F:183:ARG:HG2  | 1:F:187:ARG:HE   | 1.46                     | 0.79              |
| 1:N:19:ILE:HD11  | 1:N:67:LEU:HA    | 1.63                     | 0.79              |
| 1:M:134:LEU:HD13 | 1:M:186:ILE:HG21 | 1.63                     | 0.79              |
| 1:I:15:LYS:HB3   | 1:I:17:LYS:HZ3   | 1.48                     | 0.79              |
| 1:F:52:MET:HE3   | 1:F:56:ARG:HB2   | 1.63                     | 0.78              |
| 1:G:58:LYS:HB2   | 1:G:67:LEU:HD11  | 1.65                     | 0.78              |
| 1:H:91:LEU:HD11  | 1:H:108:MET:HE3  | 1.63                     | 0.78              |
| 1:F:107:ASP:OD1  | 1:F:110:ARG:NH2  | 2.17                     | 0.78              |
| 1:B:28:ILE:HD11  | 1:B:44:ALA:HB2   | 1.66                     | 0.77              |
| 1:E:85:ARG:HE    | 1:E:116:MET:HE1  | 1.49                     | 0.77              |
| 1:H:123:GLN:HG3  | 1:H:193:LEU:HD21 | 1.66                     | 0.77              |
| 1:E:88:GLN:HG3   | 1:E:112:LEU:HD13 | 1.67                     | 0.77              |
| 1:E:58:LYS:HB2   | 1:E:67:LEU:HD11  | 1.67                     | 0.76              |
| 1:I:12:ILE:HG22  | 1:I:27:LEU:HD11  | 1.64                     | 0.76              |
| 1:C:19:ILE:HD11  | 1:C:67:LEU:HA    | 1.67                     | 0.76              |
| 1:N:116:MET:HA   | 1:N:119:VAL:HG12 | 1.67                     | 0.76              |
| 1:F:58:LYS:HB2   | 1:F:67:LEU:HD11  | 1.66                     | 0.76              |
| 1:J:58:LYS:HB2   | 1:J:67:LEU:HD11  | 1.67                     | 0.76              |
| 1:H:81:MET:HE2   | 1:H:119:VAL:HG23 | 1.68                     | 0.76              |
| 1:M:140:GLN:O    | 1:M:144:ILE:HG13 | 1.87                     | 0.75              |
| 1:E:126:LEU:HD23 | 1:E:129:LYS:HD3  | 1.67                     | 0.75              |
| 1:B:19:ILE:HD11  | 1:B:67:LEU:HA    | 1.69                     | 0.75              |
| 1:C:33:GLU:HG3   | 1:C:34:ILE:H     | 1.52                     | 0.74              |
| 1:B:33:GLU:HG3   | 1:B:34:ILE:H     | 1.52                     | 0.73              |
| 1:C:24:PHE:CE2   | 1:C:66:ILE:HG21  | 2.23                     | 0.73              |
| 1:K:12:ILE:HD11  | 1:K:29:HIS:HA    | 1.70                     | 0.73              |
| 1:A:48:SER:HA    | 1:B:140:GLN:HE22 | 1.54                     | 0.72              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:140:GLN:O    | 1:N:144:ILE:HG13 | 1.88                     | 0.72              |
| 1:H:31:TYR:HE1   | 1:H:42:GLU:HB2   | 1.53                     | 0.72              |
| 1:N:52:MET:HE3   | 1:N:56:ARG:HB2   | 1.70                     | 0.72              |
| 1:K:148:VAL:HG12 | 1:K:152:LYS:HE3  | 1.72                     | 0.72              |
| 1:M:19:ILE:HD11  | 1:M:67:LEU:HA    | 1.70                     | 0.72              |
| 1:G:33:GLU:HG2   | 1:G:34:ILE:H     | 1.55                     | 0.72              |
| 1:H:84:ILE:HG21  | 1:H:116:MET:HB2  | 1.71                     | 0.71              |
| 1:D:19:ILE:HD11  | 1:D:67:LEU:HA    | 1.72                     | 0.71              |
| 1:B:19:ILE:HD11  | 1:B:67:LEU:HD23  | 1.72                     | 0.71              |
| 1:E:9:THR:HA     | 1:E:12:ILE:HG13  | 1.73                     | 0.71              |
| 1:A:130:LEU:HD11 | 1:A:186:ILE:HG23 | 1.73                     | 0.70              |
| 1:B:123:GLN:HE22 | 1:B:196:LEU:HD21 | 1.56                     | 0.70              |
| 1:B:102:LYS:HA   | 1:B:105:TYR:HB3  | 1.73                     | 0.70              |
| 1:H:140:GLN:O    | 1:H:144:ILE:HG13 | 1.91                     | 0.70              |
| 1:F:83:LYS:HG3   | 1:F:87:ARG:HH12  | 1.56                     | 0.70              |
| 1:H:28:ILE:HD11  | 1:H:44:ALA:HB2   | 1.72                     | 0.70              |
| 1:M:130:LEU:HD23 | 1:M:190:LEU:HD13 | 1.71                     | 0.70              |
| 1:I:50:LEU:HD11  | 1:I:52:MET:HE3   | 1.74                     | 0.70              |
| 1:H:58:LYS:HB2   | 1:H:67:LEU:HD11  | 1.72                     | 0.70              |
| 1:F:102:LYS:HE2  | 1:F:106:ASP:OD2  | 1.92                     | 0.69              |
| 1:E:84:ILE:HG21  | 1:E:116:MET:HB2  | 1.74                     | 0.69              |
| 1:F:28:ILE:HD11  | 1:F:44:ALA:HB2   | 1.74                     | 0.69              |
| 1:M:12:ILE:HD11  | 1:M:30:VAL:HG12  | 1.75                     | 0.69              |
| 1:F:152:LYS:NZ   | 1:I:99:GLU:OE1   | 2.22                     | 0.69              |
| 1:I:83:LYS:HG2   | 1:I:86:LYS:HE2   | 1.72                     | 0.69              |
| 1:B:24:PHE:CE2   | 1:B:66:ILE:HG21  | 2.27                     | 0.69              |
| 1:A:140:GLN:O    | 1:A:144:ILE:HG13 | 1.92                     | 0.68              |
| 1:E:100:ILE:HD12 | 1:E:105:TYR:HB2  | 1.75                     | 0.68              |
| 1:L:33:GLU:HG2   | 1:L:34:ILE:H     | 1.56                     | 0.68              |
| 1:B:12:ILE:HG12  | 1:B:27:LEU:HD11  | 1.75                     | 0.68              |
| 1:K:81:MET:HE1   | 1:K:120:LYS:HE2  | 1.74                     | 0.68              |
| 1:G:84:ILE:HG21  | 1:G:116:MET:HB2  | 1.75                     | 0.68              |
| 1:F:88:GLN:HG3   | 1:F:112:LEU:HD23 | 1.74                     | 0.68              |
| 1:D:191:ASP:OD1  | 1:D:192:ARG:N    | 2.26                     | 0.68              |
| 1:L:119:VAL:O    | 1:L:123:GLN:N    | 2.23                     | 0.68              |
| 1:F:83:LYS:HA    | 1:F:86:LYS:HZ2   | 1.59                     | 0.67              |
| 1:D:81:MET:HE2   | 1:D:119:VAL:HG23 | 1.74                     | 0.67              |
| 1:B:116:MET:HA   | 1:B:119:VAL:HG12 | 1.76                     | 0.67              |
| 1:J:91:LEU:HD11  | 1:J:108:MET:HE3  | 1.75                     | 0.67              |
| 1:J:88:GLN:HG3   | 1:J:112:LEU:HD13 | 1.77                     | 0.67              |
| 1:G:9:THR:HA     | 1:G:12:ILE:HG13  | 1.77                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:123:GLN:HG3  | 1:C:193:LEU:HD11 | 1.77                     | 0.67              |
| 1:A:56:ARG:HG2   | 1:A:56:ARG:O     | 1.94                     | 0.66              |
| 1:F:94:LEU:HA    | 1:F:97:LYS:HD3   | 1.75                     | 0.66              |
| 1:E:56:ARG:HH12  | 1:E:69:ASP:HB3   | 1.61                     | 0.66              |
| 1:G:127:LYS:HE3  | 1:G:190:LEU:HD11 | 1.78                     | 0.66              |
| 1:M:41:ILE:HG23  | 1:M:52:MET:HG3   | 1.79                     | 0.65              |
| 1:H:88:GLN:HG3   | 1:H:112:LEU:HD13 | 1.77                     | 0.65              |
| 1:L:12:ILE:HD11  | 1:L:29:HIS:HA    | 1.78                     | 0.65              |
| 1:D:126:LEU:HA   | 1:D:129:LYS:HE3  | 1.79                     | 0.65              |
| 1:F:124:ASN:HA   | 1:F:127:LYS:HD3  | 1.78                     | 0.65              |
| 1:A:24:PHE:CE1   | 1:A:45:GLN:HG2   | 2.32                     | 0.65              |
| 1:C:28:ILE:HD11  | 1:C:44:ALA:HB2   | 1.79                     | 0.65              |
| 1:I:191:ASP:OD1  | 1:I:192:ARG:N    | 2.30                     | 0.65              |
| 1:N:170:GLU:OE2  | 1:N:173:ARG:NH2  | 2.30                     | 0.65              |
| 1:A:19:ILE:HD12  | 1:A:19:ILE:H     | 1.62                     | 0.64              |
| 1:L:56:ARG:HH12  | 1:L:69:ASP:HB3   | 1.63                     | 0.64              |
| 1:C:165:TYR:CE1  | 1:C:169:MET:HE2  | 2.32                     | 0.64              |
| 1:F:19:ILE:HD11  | 1:F:67:LEU:HA    | 1.79                     | 0.64              |
| 1:J:84:ILE:HG21  | 1:J:116:MET:HB2  | 1.79                     | 0.64              |
| 1:D:40:GLY:HA2   | 1:D:54:PRO:HD3   | 1.80                     | 0.63              |
| 1:H:56:ARG:NE    | 1:H:67:LEU:O     | 2.23                     | 0.63              |
| 1:J:93:GLU:HG2   | 1:J:97:LYS:HE2   | 1.79                     | 0.63              |
| 1:C:12:ILE:HA    | 1:C:27:LEU:HG    | 1.81                     | 0.63              |
| 1:D:8:LEU:O      | 1:D:11:PHE:N     | 2.26                     | 0.63              |
| 1:H:24:PHE:CE1   | 1:H:45:GLN:HG2   | 2.33                     | 0.63              |
| 1:J:137:ILE:HG23 | 1:J:179:TYR:CD1  | 2.34                     | 0.63              |
| 1:K:123:GLN:HG3  | 1:K:193:LEU:HD11 | 1.79                     | 0.63              |
| 1:M:183:ARG:HH21 | 1:M:187:ARG:HH12 | 1.45                     | 0.63              |
| 1:C:28:ILE:HD13  | 1:G:172:LEU:HD21 | 1.81                     | 0.62              |
| 1:E:106:ASP:OD1  | 1:E:107:ASP:N    | 2.32                     | 0.62              |
| 1:L:56:ARG:HG2   | 1:L:66:ILE:HG23  | 1.81                     | 0.62              |
| 1:M:40:GLY:HA2   | 1:M:54:PRO:HD3   | 1.80                     | 0.62              |
| 1:K:33:GLU:HG3   | 1:K:34:ILE:H     | 1.63                     | 0.62              |
| 1:N:8:LEU:HB3    | 1:N:30:VAL:HG21  | 1.81                     | 0.62              |
| 1:J:12:ILE:HG12  | 1:J:27:LEU:HD11  | 1.81                     | 0.62              |
| 1:I:81:MET:HE2   | 1:I:119:VAL:HG23 | 1.81                     | 0.61              |
| 1:M:100:ILE:HD12 | 1:M:105:TYR:HB2  | 1.80                     | 0.61              |
| 1:N:56:ARG:HH11  | 1:N:68:PRO:HA    | 1.64                     | 0.61              |
| 1:A:97:LYS:HG3   | 1:A:99:GLU:HG3   | 1.83                     | 0.61              |
| 1:G:24:PHE:CE2   | 1:G:45:GLN:HG2   | 2.34                     | 0.61              |
| 1:I:15:LYS:HB3   | 1:I:17:LYS:NZ    | 2.16                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:130:LEU:HD23 | 1:A:190:LEU:HD13 | 1.82                     | 0.61              |
| 1:B:91:LEU:HD11  | 1:B:108:MET:HE3  | 1.82                     | 0.61              |
| 1:K:119:VAL:O    | 1:K:123:GLN:N    | 2.29                     | 0.61              |
| 1:C:16:VAL:HG12  | 1:C:64:ILE:HG23  | 1.82                     | 0.61              |
| 1:D:33:GLU:HG3   | 1:D:34:ILE:H     | 1.66                     | 0.61              |
| 1:F:83:LYS:HE3   | 1:F:87:ARG:NH1   | 2.16                     | 0.61              |
| 1:I:81:MET:O     | 1:I:85:ARG:HG2   | 2.00                     | 0.61              |
| 1:C:140:GLN:O    | 1:C:144:ILE:HG13 | 2.01                     | 0.60              |
| 1:G:3:VAL:HG13   | 1:G:59:LEU:HD11  | 1.81                     | 0.60              |
| 1:M:88:GLN:NE2   | 1:M:113:ASP:OD1  | 2.34                     | 0.60              |
| 1:H:144:ILE:O    | 1:H:148:VAL:HG13 | 2.02                     | 0.60              |
| 1:N:84:ILE:HG21  | 1:N:116:MET:HB2  | 1.83                     | 0.60              |
| 1:I:16:VAL:HG22  | 1:I:25:GLY:O     | 2.01                     | 0.60              |
| 1:M:83:LYS:HG2   | 1:M:86:LYS:HE2   | 1.84                     | 0.60              |
| 1:A:91:LEU:HD11  | 1:A:108:MET:HE3  | 1.84                     | 0.60              |
| 1:I:119:VAL:O    | 1:I:123:GLN:N    | 2.30                     | 0.60              |
| 1:E:138:GLU:OE2  | 1:E:183:ARG:HD2  | 2.02                     | 0.60              |
| 1:J:44:ALA:HA    | 1:J:49:ILE:HG22  | 1.84                     | 0.60              |
| 1:J:122:ASP:HA   | 1:J:125:LYS:HD2  | 1.83                     | 0.60              |
| 1:M:106:ASP:OD1  | 1:M:107:ASP:N    | 2.34                     | 0.60              |
| 1:I:144:ILE:O    | 1:I:148:VAL:HG13 | 2.02                     | 0.60              |
| 1:F:93:GLU:O     | 1:F:97:LYS:HG3   | 2.01                     | 0.59              |
| 1:I:121:ASP:O    | 1:I:125:LYS:HG2  | 2.02                     | 0.59              |
| 1:J:52:MET:CG    | 1:J:56:ARG:HD3   | 2.32                     | 0.59              |
| 1:J:43:VAL:HG11  | 1:J:52:MET:SD    | 2.42                     | 0.59              |
| 1:J:191:ASP:OD1  | 1:J:192:ARG:N    | 2.35                     | 0.59              |
| 1:B:33:GLU:CG    | 1:B:34:ILE:H     | 2.14                     | 0.59              |
| 1:D:148:VAL:HG12 | 1:D:172:LEU:HD13 | 1.85                     | 0.59              |
| 1:H:133:ARG:O    | 1:H:137:ILE:HG13 | 2.02                     | 0.59              |
| 1:C:19:ILE:HD11  | 1:C:67:LEU:HD23  | 1.84                     | 0.59              |
| 1:F:33:GLU:HG2   | 1:F:34:ILE:H     | 1.68                     | 0.59              |
| 1:B:87:ARG:HG2   | 1:B:112:LEU:HD21 | 1.84                     | 0.59              |
| 1:F:97:LYS:HE2   | 1:F:99:GLU:OE2   | 2.03                     | 0.59              |
| 1:I:12:ILE:HA    | 1:I:27:LEU:HG    | 1.83                     | 0.59              |
| 1:L:87:ARG:HG2   | 1:L:112:LEU:HD11 | 1.84                     | 0.59              |
| 1:J:44:ALA:CB    | 1:J:49:ILE:HG22  | 2.32                     | 0.59              |
| 1:H:33:GLU:CG    | 1:H:34:ILE:H     | 2.14                     | 0.58              |
| 1:M:49:ILE:HG13  | 1:M:49:ILE:O     | 2.01                     | 0.58              |
| 1:G:94:LEU:HG    | 1:G:100:ILE:HB   | 1.84                     | 0.58              |
| 1:G:119:VAL:O    | 1:G:123:GLN:N    | 2.23                     | 0.58              |
| 1:H:102:LYS:HE2  | 1:H:106:ASP:OD2  | 2.03                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:33:GLU:OE2   | 1:I:111:LYS:NZ   | 2.36                     | 0.58              |
| 1:E:70:TRP:O     | 1:E:74:ALA:N     | 2.33                     | 0.58              |
| 1:F:106:ASP:O    | 1:F:110:ARG:HG3  | 2.03                     | 0.58              |
| 1:K:116:MET:HA   | 1:K:119:VAL:HG22 | 1.84                     | 0.58              |
| 1:K:191:ASP:OD1  | 1:K:192:ARG:N    | 2.36                     | 0.58              |
| 1:M:152:LYS:O    | 1:M:156:ILE:N    | 2.30                     | 0.58              |
| 1:B:81:MET:HE2   | 1:B:119:VAL:HG13 | 1.86                     | 0.58              |
| 1:C:172:LEU:HD21 | 1:G:28:ILE:HD13  | 1.85                     | 0.58              |
| 1:G:83:LYS:HA    | 1:G:86:LYS:HE2   | 1.86                     | 0.58              |
| 1:F:153:MET:HE1  | 1:I:87:ARG:HE    | 1.68                     | 0.58              |
| 1:A:8:LEU:HB3    | 1:A:30:VAL:HG21  | 1.86                     | 0.58              |
| 1:E:141:LEU:HD23 | 1:E:144:ILE:HD11 | 1.86                     | 0.58              |
| 1:E:120:LYS:HE2  | 1:E:124:ASN:ND2  | 2.19                     | 0.57              |
| 1:A:116:MET:HA   | 1:A:119:VAL:HG12 | 1.85                     | 0.57              |
| 1:E:12:ILE:HD11  | 1:E:30:VAL:HG23  | 1.86                     | 0.57              |
| 1:J:89:ARG:NH1   | 1:K:194:ASP:HB3  | 2.19                     | 0.57              |
| 1:N:9:THR:HA     | 1:N:12:ILE:HG13  | 1.85                     | 0.57              |
| 1:A:56:ARG:HH22  | 1:A:69:ASP:N     | 2.02                     | 0.57              |
| 1:J:148:VAL:HG12 | 1:J:172:LEU:HD13 | 1.85                     | 0.57              |
| 1:L:141:LEU:HD23 | 1:L:144:ILE:HD11 | 1.85                     | 0.57              |
| 1:K:140:GLN:O    | 1:K:144:ILE:HG13 | 2.04                     | 0.57              |
| 1:K:162:GLU:OE1  | 1:K:166:LYS:NZ   | 2.24                     | 0.57              |
| 1:L:12:ILE:HA    | 1:L:27:LEU:HD11  | 1.87                     | 0.57              |
| 1:H:141:LEU:HD11 | 1:H:176:LYS:HG3  | 1.87                     | 0.57              |
| 1:C:9:THR:HA     | 1:C:12:ILE:HG23  | 1.86                     | 0.57              |
| 1:G:19:ILE:HD11  | 1:G:67:LEU:HA    | 1.87                     | 0.57              |
| 1:L:137:ILE:O    | 1:L:141:LEU:N    | 2.33                     | 0.57              |
| 1:N:153:MET:HA   | 1:N:156:ILE:HD12 | 1.86                     | 0.57              |
| 1:C:110:ARG:O    | 1:C:114:THR:OG1  | 2.19                     | 0.56              |
| 1:E:73:GLU:HB3   | 1:E:126:LEU:HD13 | 1.87                     | 0.56              |
| 1:F:116:MET:HA   | 1:F:119:VAL:HG12 | 1.87                     | 0.56              |
| 1:L:56:ARG:NH1   | 1:L:69:ASP:HB3   | 2.20                     | 0.56              |
| 1:G:70:TRP:CE2   | 1:G:186:ILE:HD11 | 2.40                     | 0.56              |
| 1:C:56:ARG:HH21  | 1:C:68:PRO:HA    | 1.69                     | 0.56              |
| 1:F:82:GLU:OE2   | 1:F:192:ARG:NH1  | 2.39                     | 0.56              |
| 1:M:41:ILE:HG23  | 1:M:52:MET:CG    | 2.35                     | 0.56              |
| 1:M:152:LYS:C    | 1:M:156:ILE:HG12 | 2.31                     | 0.56              |
| 1:A:56:ARG:HH12  | 1:A:69:ASP:CB    | 2.15                     | 0.56              |
| 1:M:24:PHE:HE1   | 1:M:43:VAL:HG11  | 1.70                     | 0.56              |
| 1:F:124:ASN:HD22 | 1:F:127:LYS:HD3  | 1.70                     | 0.56              |
| 1:F:144:ILE:O    | 1:F:148:VAL:HG13 | 2.06                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:131:LYS:HG2  | 1:F:134:LEU:HD23 | 1.88                     | 0.56              |
| 1:I:140:GLN:O    | 1:I:144:ILE:HG13 | 2.05                     | 0.56              |
| 1:J:123:GLN:HG3  | 1:J:193:LEU:HD11 | 1.87                     | 0.56              |
| 1:L:127:LYS:HG3  | 1:L:190:LEU:HD21 | 1.87                     | 0.56              |
| 1:M:18:ASP:HB2   | 1:M:22:ARG:O     | 2.06                     | 0.56              |
| 1:C:31:TYR:HE1   | 1:C:42:GLU:HB2   | 1.70                     | 0.56              |
| 1:B:49:ILE:HG13  | 1:B:49:ILE:O     | 2.05                     | 0.55              |
| 1:E:40:GLY:HA2   | 1:E:54:PRO:HD3   | 1.87                     | 0.55              |
| 1:F:183:ARG:HG2  | 1:F:187:ARG:NE   | 2.18                     | 0.55              |
| 1:F:191:ASP:OD1  | 1:F:192:ARG:N    | 2.40                     | 0.55              |
| 1:A:70:TRP:O     | 1:A:74:ALA:N     | 2.31                     | 0.55              |
| 1:H:15:LYS:NZ    | 1:H:17:LYS:HE3   | 2.21                     | 0.55              |
| 1:I:49:ILE:O     | 1:I:49:ILE:HG13  | 2.04                     | 0.55              |
| 1:F:83:LYS:HE3   | 1:F:87:ARG:HH12  | 1.71                     | 0.55              |
| 1:N:83:LYS:HA    | 1:N:86:LYS:HG2   | 1.87                     | 0.55              |
| 1:E:116:MET:HA   | 1:E:119:VAL:HG12 | 1.89                     | 0.55              |
| 1:N:27:LEU:HD13  | 1:N:41:ILE:HD11  | 1.88                     | 0.55              |
| 1:G:12:ILE:HD11  | 1:G:30:VAL:HG23  | 1.89                     | 0.55              |
| 1:H:19:ILE:CD1   | 1:H:67:LEU:HA    | 2.32                     | 0.55              |
| 1:I:42:GLU:OE1   | 1:I:51:THR:HG22  | 2.07                     | 0.55              |
| 1:L:137:ILE:HG23 | 1:L:179:TYR:CD1  | 2.42                     | 0.55              |
| 1:M:22:ARG:NH2   | 1:M:182:GLU:OE1  | 2.30                     | 0.55              |
| 1:H:116:MET:HA   | 1:H:119:VAL:HG22 | 1.89                     | 0.54              |
| 1:B:165:TYR:CZ   | 1:B:169:MET:HG3  | 2.43                     | 0.54              |
| 1:L:52:MET:SD    | 1:L:56:ARG:HD2   | 2.47                     | 0.54              |
| 1:G:106:ASP:OD1  | 1:G:107:ASP:N    | 2.39                     | 0.54              |
| 1:B:12:ILE:HD13  | 1:B:29:HIS:HA    | 1.89                     | 0.54              |
| 1:B:40:GLY:HA2   | 1:B:54:PRO:HD3   | 1.89                     | 0.54              |
| 1:C:22:ARG:HD2   | 1:G:47:SER:OG    | 2.07                     | 0.54              |
| 1:E:22:ARG:HH22  | 1:E:179:TYR:HA   | 1.73                     | 0.54              |
| 1:H:119:VAL:O    | 1:H:123:GLN:N    | 2.35                     | 0.54              |
| 1:M:151:LEU:HD23 | 1:M:169:MET:SD   | 2.47                     | 0.54              |
| 1:B:88:GLN:HG3   | 1:B:112:LEU:HD23 | 1.90                     | 0.54              |
| 1:H:83:LYS:HE3   | 1:H:87:ARG:NH1   | 2.23                     | 0.54              |
| 1:M:22:ARG:HD2   | 1:N:47:SER:OG    | 2.06                     | 0.54              |
| 1:H:4:SER:HB2    | 1:H:7:VAL:HG22   | 1.90                     | 0.54              |
| 1:I:152:LYS:O    | 1:I:156:ILE:HG12 | 2.07                     | 0.54              |
| 1:J:44:ALA:HB2   | 1:J:49:ILE:HG22  | 1.89                     | 0.54              |
| 1:M:19:ILE:HD12  | 1:M:19:ILE:H     | 1.73                     | 0.54              |
| 1:H:49:ILE:O     | 1:H:49:ILE:HG13  | 2.07                     | 0.54              |
| 1:K:116:MET:HG3  | 1:K:116:MET:O    | 2.08                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:81:MET:HG2   | 1:C:119:VAL:HG21 | 1.89                     | 0.53              |
| 1:L:19:ILE:HG12  | 1:L:66:ILE:O     | 2.08                     | 0.53              |
| 1:B:41:ILE:HD11  | 1:B:54:PRO:HA    | 1.90                     | 0.53              |
| 1:D:164:ALA:HB1  | 1:F:12:ILE:CG2   | 2.39                     | 0.53              |
| 1:E:116:MET:O    | 1:E:116:MET:HG2  | 2.08                     | 0.53              |
| 1:J:137:ILE:HG23 | 1:J:179:TYR:HD1  | 1.74                     | 0.53              |
| 1:N:34:ILE:H     | 1:N:34:ILE:HD12  | 1.74                     | 0.53              |
| 1:F:81:MET:HE3   | 1:F:116:MET:HE3  | 1.90                     | 0.53              |
| 1:H:161:PRO:HG2  | 1:H:164:ALA:HB3  | 1.90                     | 0.53              |
| 1:J:195:SER:HB3  | 1:K:85:ARG:NH2   | 2.24                     | 0.53              |
| 1:D:106:ASP:O    | 1:D:110:ARG:HG3  | 2.07                     | 0.53              |
| 1:J:70:TRP:CZ3   | 1:J:71:LYS:HG2   | 2.44                     | 0.53              |
| 1:K:27:LEU:HD12  | 1:K:42:GLU:O     | 2.08                     | 0.53              |
| 1:L:140:GLN:O    | 1:L:144:ILE:HG12 | 2.09                     | 0.53              |
| 1:D:85:ARG:HH11  | 1:D:89:ARG:HH22  | 1.56                     | 0.53              |
| 1:H:70:TRP:O     | 1:H:74:ALA:N     | 2.38                     | 0.53              |
| 1:I:123:GLN:HG3  | 1:I:193:LEU:HD21 | 1.91                     | 0.53              |
| 1:E:56:ARG:O     | 1:E:56:ARG:HG2   | 2.09                     | 0.53              |
| 1:E:123:GLN:HG3  | 1:E:193:LEU:HD21 | 1.91                     | 0.53              |
| 1:K:170:GLU:HG3  | 1:K:173:ARG:HH21 | 1.74                     | 0.53              |
| 1:M:177:ASP:HA   | 1:M:180:THR:HB   | 1.91                     | 0.53              |
| 1:D:85:ARG:HH11  | 1:D:89:ARG:NH2   | 2.07                     | 0.53              |
| 1:F:183:ARG:O    | 1:F:187:ARG:HG3  | 2.09                     | 0.53              |
| 1:I:9:THR:HA     | 1:I:12:ILE:HG23  | 1.91                     | 0.53              |
| 1:A:130:LEU:CD1  | 1:A:186:ILE:HG23 | 2.39                     | 0.52              |
| 1:G:130:LEU:HD23 | 1:G:190:LEU:HD13 | 1.91                     | 0.52              |
| 1:L:11:PHE:O     | 1:L:27:LEU:HD21  | 2.09                     | 0.52              |
| 1:M:134:LEU:HD13 | 1:M:186:ILE:CG2  | 2.38                     | 0.52              |
| 1:D:122:ASP:HA   | 1:D:125:LYS:HE3  | 1.90                     | 0.52              |
| 1:A:9:THR:HA     | 1:A:12:ILE:HG13  | 1.92                     | 0.52              |
| 1:B:123:GLN:CD   | 1:B:193:LEU:HD11 | 2.35                     | 0.52              |
| 1:C:144:ILE:HG12 | 1:G:49:ILE:HD11  | 1.91                     | 0.52              |
| 1:D:80:LEU:HD22  | 1:I:34:ILE:HG22  | 1.91                     | 0.52              |
| 1:E:102:LYS:HA   | 1:E:105:TYR:HB3  | 1.91                     | 0.52              |
| 1:C:81:MET:HE3   | 1:C:196:LEU:HD13 | 1.90                     | 0.52              |
| 1:D:151:LEU:HD23 | 1:D:169:MET:SD   | 2.50                     | 0.52              |
| 1:H:31:TYR:CE1   | 1:H:42:GLU:HB2   | 2.39                     | 0.52              |
| 1:H:123:GLN:CG   | 1:H:193:LEU:HD21 | 2.37                     | 0.52              |
| 1:J:44:ALA:CA    | 1:J:49:ILE:HG22  | 2.39                     | 0.52              |
| 1:M:97:LYS:HB3   | 1:M:99:GLU:HG3   | 1.90                     | 0.52              |
| 1:D:88:GLN:CG    | 1:D:112:LEU:HD13 | 2.34                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:11:PHE:CE1   | 1:K:63:SER:HA    | 2.44                     | 0.52              |
| 1:J:19:ILE:HD12  | 1:J:19:ILE:H     | 1.75                     | 0.52              |
| 1:A:12:ILE:HD11  | 1:A:30:VAL:HG23  | 1.92                     | 0.52              |
| 1:A:145:ASP:HA   | 1:A:148:VAL:HG22 | 1.92                     | 0.52              |
| 1:D:123:GLN:HG3  | 1:D:193:LEU:HD21 | 1.92                     | 0.52              |
| 1:M:116:MET:O    | 1:M:119:VAL:HG12 | 2.09                     | 0.52              |
| 1:F:176:LYS:HE2  | 1:F:180:THR:HG21 | 1.92                     | 0.51              |
| 1:G:94:LEU:HD12  | 1:G:99:GLU:HB2   | 1.91                     | 0.51              |
| 1:L:49:ILE:HG13  | 1:L:49:ILE:O     | 2.08                     | 0.51              |
| 1:B:6:GLU:O      | 1:B:10:LYS:HG3   | 2.10                     | 0.51              |
| 1:B:33:GLU:OE2   | 1:B:34:ILE:HG13  | 2.10                     | 0.51              |
| 1:H:92:GLU:OE2   | 1:H:105:TYR:OH   | 2.28                     | 0.51              |
| 1:I:145:ASP:O    | 1:I:148:VAL:HG22 | 2.10                     | 0.51              |
| 1:J:22:ARG:HG3   | 1:J:178:SER:OG   | 2.10                     | 0.51              |
| 1:L:191:ASP:OD1  | 1:L:192:ARG:N    | 2.44                     | 0.51              |
| 1:N:19:ILE:HD11  | 1:N:67:LEU:HD23  | 1.92                     | 0.51              |
| 1:B:81:MET:O     | 1:B:85:ARG:HG2   | 2.10                     | 0.51              |
| 1:B:82:GLU:HG3   | 1:B:86:LYS:NZ    | 2.25                     | 0.51              |
| 1:J:52:MET:HG3   | 1:J:56:ARG:HH21  | 1.75                     | 0.51              |
| 1:J:151:LEU:HD23 | 1:J:169:MET:HG2  | 1.91                     | 0.51              |
| 1:C:29:HIS:HB3   | 1:C:42:GLU:HB3   | 1.92                     | 0.51              |
| 1:M:71:LYS:O     | 1:M:75:ILE:HG23  | 2.09                     | 0.51              |
| 1:F:83:LYS:HA    | 1:F:86:LYS:HG2   | 1.93                     | 0.51              |
| 1:N:74:ALA:O     | 1:N:78:LEU:HD13  | 2.11                     | 0.51              |
| 1:C:34:ILE:CA    | 1:K:83:LYS:HE2   | 2.32                     | 0.51              |
| 1:B:71:LYS:O     | 1:B:75:ILE:HG22  | 2.11                     | 0.51              |
| 1:H:148:VAL:HB   | 1:H:169:MET:HE1  | 1.91                     | 0.51              |
| 1:B:9:THR:HA     | 1:B:12:ILE:HG13  | 1.92                     | 0.51              |
| 1:B:173:ARG:HH11 | 1:B:176:LYS:HD3  | 1.76                     | 0.51              |
| 1:G:27:LEU:HD13  | 1:G:41:ILE:HD11  | 1.92                     | 0.51              |
| 1:E:45:GLN:O     | 1:E:45:GLN:HG2   | 2.11                     | 0.51              |
| 1:H:33:GLU:OE2   | 1:H:34:ILE:HG13  | 2.11                     | 0.51              |
| 1:J:120:LYS:NZ   | 1:J:196:LEU:HA   | 2.26                     | 0.51              |
| 1:C:170:GLU:OE2  | 1:C:173:ARG:NH2  | 2.43                     | 0.51              |
| 1:I:33:GLU:HG2   | 1:I:34:ILE:HD12  | 1.93                     | 0.51              |
| 1:F:83:LYS:CA    | 1:F:86:LYS:HZ2   | 2.23                     | 0.50              |
| 1:I:24:PHE:CE1   | 1:I:45:GLN:HG2   | 2.45                     | 0.50              |
| 1:K:70:TRP:O     | 1:K:74:ALA:N     | 2.37                     | 0.50              |
| 1:B:84:ILE:HG21  | 1:B:116:MET:HB2  | 1.93                     | 0.50              |
| 1:F:85:ARG:NH2   | 1:F:197:ASP:O    | 2.44                     | 0.50              |
| 1:G:104:ASP:HB3  | 1:G:108:MET:HE2  | 1.94                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:24:PHE:CE1   | 1:J:45:GLN:HB3   | 2.45                     | 0.50              |
| 1:A:151:LEU:HD13 | 1:B:29:HIS:HB2   | 1.94                     | 0.50              |
| 1:H:177:ASP:OD1  | 1:H:178:SER:N    | 2.45                     | 0.50              |
| 1:D:73:GLU:OE2   | 1:D:76:ARG:NH2   | 2.39                     | 0.50              |
| 1:G:16:VAL:HG12  | 1:G:64:ILE:HG23  | 1.94                     | 0.50              |
| 1:K:28:ILE:CD1   | 1:K:44:ALA:HB2   | 2.35                     | 0.50              |
| 1:L:5:TYR:CE1    | 1:L:32:SER:HB3   | 2.47                     | 0.50              |
| 1:I:19:ILE:HD12  | 1:I:19:ILE:H     | 1.76                     | 0.50              |
| 1:B:29:HIS:HB3   | 1:B:42:GLU:HB3   | 1.94                     | 0.50              |
| 1:E:56:ARG:HH22  | 1:E:69:ASP:N     | 2.10                     | 0.50              |
| 1:D:172:LEU:HD21 | 1:F:28:ILE:HD13  | 1.93                     | 0.49              |
| 1:E:86:LYS:O     | 1:E:89:ARG:HB3   | 2.11                     | 0.49              |
| 1:M:106:ASP:HB2  | 1:M:110:ARG:NH2  | 2.27                     | 0.49              |
| 1:B:133:ARG:O    | 1:B:137:ILE:HG13 | 2.12                     | 0.49              |
| 1:B:144:ILE:O    | 1:B:148:VAL:HG23 | 2.12                     | 0.49              |
| 1:D:164:ALA:HB1  | 1:F:12:ILE:HG22  | 1.95                     | 0.49              |
| 1:K:150:SER:HA   | 1:K:153:MET:HE3  | 1.94                     | 0.49              |
| 1:E:95:TYR:HB2   | 1:E:100:ILE:HD11 | 1.93                     | 0.49              |
| 1:F:27:LEU:HD13  | 1:F:41:ILE:HD11  | 1.93                     | 0.49              |
| 1:F:93:GLU:OE1   | 1:F:97:LYS:HD2   | 2.13                     | 0.49              |
| 1:G:33:GLU:HG2   | 1:G:34:ILE:N     | 2.22                     | 0.49              |
| 1:M:144:ILE:O    | 1:M:148:VAL:HG23 | 2.12                     | 0.49              |
| 1:C:6:GLU:O      | 1:C:10:LYS:HG3   | 2.12                     | 0.49              |
| 1:D:73:GLU:HG3   | 1:D:126:LEU:HD11 | 1.94                     | 0.49              |
| 1:E:42:GLU:OE1   | 1:E:51:THR:HG23  | 2.12                     | 0.49              |
| 1:G:12:ILE:HA    | 1:G:27:LEU:HG    | 1.94                     | 0.49              |
| 1:G:88:GLN:HG3   | 1:G:112:LEU:HD13 | 1.94                     | 0.49              |
| 1:K:152:LYS:HA   | 1:K:165:TYR:HE2  | 1.77                     | 0.49              |
| 1:M:106:ASP:O    | 1:M:110:ARG:HG3  | 2.12                     | 0.49              |
| 1:B:87:ARG:HH22  | 1:B:111:LYS:NZ   | 2.10                     | 0.49              |
| 1:G:95:TYR:HA    | 1:G:100:ILE:HG22 | 1.94                     | 0.49              |
| 1:G:140:GLN:O    | 1:G:144:ILE:HG13 | 2.12                     | 0.49              |
| 1:K:148:VAL:CG1  | 1:K:152:LYS:HE3  | 2.42                     | 0.49              |
| 1:D:11:PHE:CE1   | 1:D:63:SER:HA    | 2.48                     | 0.49              |
| 1:D:130:LEU:HD11 | 1:D:186:ILE:HG23 | 1.95                     | 0.49              |
| 1:B:94:LEU:HD23  | 1:B:97:LYS:HD3   | 1.95                     | 0.49              |
| 1:B:110:ARG:O    | 1:B:114:THR:OG1  | 2.23                     | 0.49              |
| 1:B:140:GLN:O    | 1:B:144:ILE:HG13 | 2.12                     | 0.49              |
| 1:N:130:LEU:HD22 | 1:N:186:ILE:HG23 | 1.95                     | 0.49              |
| 1:F:12:ILE:HG13  | 1:F:27:LEU:CD1   | 2.42                     | 0.49              |
| 1:L:124:ASN:OD1  | 1:L:125:LYS:N    | 2.46                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:130:LEU:HD11 | 1:M:186:ILE:HG23 | 1.94                     | 0.49              |
| 1:B:161:PRO:HB2  | 1:B:163:ASN:OD1  | 2.12                     | 0.49              |
| 1:D:29:HIS:HD2   | 1:F:160:ILE:HD11 | 1.77                     | 0.49              |
| 1:H:8:LEU:O      | 1:H:11:PHE:N     | 2.32                     | 0.49              |
| 1:J:64:ILE:O     | 1:J:65:LEU:HD23  | 2.11                     | 0.49              |
| 1:E:52:MET:HE3   | 1:E:56:ARG:HD2   | 1.95                     | 0.48              |
| 1:N:40:GLY:HA2   | 1:N:54:PRO:HD3   | 1.94                     | 0.48              |
| 1:A:144:ILE:O    | 1:A:148:VAL:HG13 | 2.13                     | 0.48              |
| 1:C:144:ILE:O    | 1:C:148:VAL:HG23 | 2.12                     | 0.48              |
| 1:E:145:ASP:HA   | 1:E:148:VAL:HG22 | 1.95                     | 0.48              |
| 1:J:119:VAL:O    | 1:J:123:GLN:N    | 2.45                     | 0.48              |
| 1:L:155:TYR:HB2  | 1:L:165:TYR:CD2  | 2.48                     | 0.48              |
| 1:A:55:GLU:H     | 1:A:55:GLU:CD    | 2.20                     | 0.48              |
| 1:C:70:TRP:O     | 1:C:74:ALA:N     | 2.36                     | 0.48              |
| 1:L:123:GLN:HG3  | 1:L:193:LEU:HD11 | 1.96                     | 0.48              |
| 1:B:116:MET:HE3  | 1:B:116:MET:HB3  | 1.83                     | 0.48              |
| 1:D:15:LYS:HE3   | 1:D:26:TYR:OH    | 2.13                     | 0.48              |
| 1:G:70:TRP:CH2   | 1:G:71:LYS:HD3   | 2.48                     | 0.48              |
| 1:A:134:LEU:HD11 | 1:A:183:ARG:HG3  | 1.95                     | 0.48              |
| 1:H:52:MET:HE3   | 1:H:56:ARG:HB2   | 1.95                     | 0.48              |
| 1:K:84:ILE:HG22  | 1:K:116:MET:HE2  | 1.96                     | 0.48              |
| 1:D:58:LYS:HB2   | 1:D:67:LEU:HD11  | 1.96                     | 0.48              |
| 1:F:83:LYS:HA    | 1:F:86:LYS:NZ    | 2.29                     | 0.48              |
| 1:G:116:MET:HG2  | 1:G:116:MET:O    | 2.13                     | 0.48              |
| 1:L:12:ILE:CD1   | 1:L:29:HIS:HA    | 2.44                     | 0.48              |
| 1:L:22:ARG:NH2   | 1:L:182:GLU:OE1  | 2.35                     | 0.48              |
| 1:L:83:LYS:HA    | 1:L:86:LYS:HE2   | 1.96                     | 0.48              |
| 1:C:161:PRO:HG2  | 1:C:164:ALA:HB3  | 1.96                     | 0.48              |
| 1:I:118:LYS:NZ   | 1:I:122:ASP:OD2  | 2.47                     | 0.48              |
| 1:M:127:LYS:HZ2  | 1:M:193:LEU:HD23 | 1.78                     | 0.48              |
| 1:N:49:ILE:O     | 1:N:49:ILE:HG13  | 2.13                     | 0.48              |
| 1:H:102:LYS:HA   | 1:H:105:TYR:HB3  | 1.96                     | 0.48              |
| 1:E:56:ARG:HH12  | 1:E:69:ASP:CB    | 2.27                     | 0.48              |
| 1:J:12:ILE:HD13  | 1:J:29:HIS:HA    | 1.95                     | 0.48              |
| 1:N:163:ASN:OD1  | 1:N:164:ALA:N    | 2.46                     | 0.48              |
| 1:A:41:ILE:HD13  | 1:A:57:ILE:HD11  | 1.94                     | 0.47              |
| 1:C:24:PHE:CE1   | 1:C:45:GLN:HB3   | 2.49                     | 0.47              |
| 1:C:41:ILE:CD1   | 1:C:54:PRO:HA    | 2.44                     | 0.47              |
| 1:F:130:LEU:CD1  | 1:F:186:ILE:HD12 | 2.44                     | 0.47              |
| 1:K:24:PHE:O     | 1:K:45:GLN:HA    | 2.14                     | 0.47              |
| 1:L:182:GLU:O    | 1:L:186:ILE:HG13 | 2.14                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:100:ILE:HD11 | 1:N:108:MET:CE   | 2.44                     | 0.47              |
| 1:F:94:LEU:HA    | 1:F:97:LYS:CD    | 2.41                     | 0.47              |
| 1:B:96:ASN:OD1   | 1:B:97:LYS:N     | 2.47                     | 0.47              |
| 1:B:121:ASP:OD1  | 1:B:125:LYS:HE3  | 2.14                     | 0.47              |
| 1:J:130:LEU:HD11 | 1:J:186:ILE:HG23 | 1.96                     | 0.47              |
| 1:J:70:TRP:CH2   | 1:J:71:LYS:HG2   | 2.49                     | 0.47              |
| 1:M:19:ILE:CD1   | 1:M:68:PRO:HD3   | 2.45                     | 0.47              |
| 1:N:77:ILE:HG22  | 1:N:81:MET:HE2   | 1.96                     | 0.47              |
| 1:K:41:ILE:HG22  | 1:K:52:MET:O     | 2.14                     | 0.47              |
| 1:F:83:LYS:CG    | 1:F:87:ARG:HH12  | 2.27                     | 0.47              |
| 1:G:144:ILE:HG23 | 1:G:172:LEU:HD22 | 1.96                     | 0.47              |
| 1:L:8:LEU:HB3    | 1:L:30:VAL:HG21  | 1.97                     | 0.47              |
| 1:M:22:ARG:HG3   | 1:M:178:SER:OG   | 2.15                     | 0.47              |
| 1:A:110:ARG:HD3  | 1:A:110:ARG:C    | 2.40                     | 0.47              |
| 1:C:102:LYS:HA   | 1:C:105:TYR:HB3  | 1.97                     | 0.47              |
| 1:E:5:TYR:CE1    | 1:E:32:SER:HB3   | 2.50                     | 0.47              |
| 1:H:4:SER:O      | 1:H:7:VAL:HG22   | 2.15                     | 0.47              |
| 1:N:22:ARG:HG3   | 1:N:178:SER:OG   | 2.14                     | 0.47              |
| 1:N:41:ILE:CD1   | 1:N:57:ILE:HD11  | 2.45                     | 0.47              |
| 1:I:41:ILE:HD12  | 1:I:57:ILE:HD13  | 1.96                     | 0.47              |
| 1:L:27:LEU:O     | 1:L:27:LEU:HG    | 2.14                     | 0.47              |
| 1:M:95:TYR:HB2   | 1:M:100:ILE:HD11 | 1.96                     | 0.47              |
| 1:B:33:GLU:HG3   | 1:B:34:ILE:N     | 2.25                     | 0.47              |
| 1:B:92:GLU:OE2   | 1:B:105:TYR:OH   | 2.27                     | 0.47              |
| 1:C:33:GLU:HG3   | 1:C:34:ILE:N     | 2.27                     | 0.47              |
| 1:E:57:ILE:HD13  | 1:E:66:ILE:HG13  | 1.97                     | 0.47              |
| 1:L:69:ASP:OD1   | 1:L:69:ASP:N     | 2.48                     | 0.47              |
| 1:M:130:LEU:HD21 | 1:M:190:LEU:HB2  | 1.97                     | 0.47              |
| 1:B:81:MET:CE    | 1:B:119:VAL:HG13 | 2.45                     | 0.47              |
| 1:D:141:LEU:HD23 | 1:D:144:ILE:HD11 | 1.97                     | 0.47              |
| 1:K:12:ILE:CD1   | 1:K:29:HIS:HA    | 2.41                     | 0.47              |
| 1:M:44:ALA:HA    | 1:M:49:ILE:HA    | 1.97                     | 0.47              |
| 1:C:8:LEU:HB3    | 1:C:30:VAL:HG21  | 1.96                     | 0.46              |
| 1:E:56:ARG:HG2   | 1:E:66:ILE:HG23  | 1.97                     | 0.46              |
| 1:H:33:GLU:HG3   | 1:H:34:ILE:N     | 2.25                     | 0.46              |
| 1:J:68:PRO:HB2   | 1:J:70:TRP:CD1   | 2.50                     | 0.46              |
| 1:K:31:TYR:HB2   | 1:K:40:GLY:O     | 2.14                     | 0.46              |
| 1:M:69:ASP:N     | 1:M:69:ASP:OD1   | 2.46                     | 0.46              |
| 1:C:26:TYR:N     | 1:C:26:TYR:CD1   | 2.83                     | 0.46              |
| 1:F:12:ILE:HG13  | 1:F:27:LEU:HD11  | 1.97                     | 0.46              |
| 1:L:15:LYS:NZ    | 1:L:17:LYS:HE3   | 2.30                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:76:ARG:O     | 1:L:80:LEU:HD13  | 2.16                     | 0.46              |
| 1:C:177:ASP:OD1  | 1:C:178:SER:N    | 2.48                     | 0.46              |
| 1:L:127:LYS:HE3  | 1:L:193:LEU:HD23 | 1.98                     | 0.46              |
| 1:I:33:GLU:HG2   | 1:I:34:ILE:N     | 2.22                     | 0.46              |
| 1:N:152:LYS:HG2  | 1:N:165:TYR:OH   | 2.16                     | 0.46              |
| 1:B:82:GLU:HG3   | 1:B:86:LYS:HZ2   | 1.80                     | 0.46              |
| 1:C:24:PHE:CD2   | 1:C:66:ILE:HG21  | 2.50                     | 0.46              |
| 1:G:12:ILE:HD13  | 1:G:29:HIS:HA    | 1.97                     | 0.46              |
| 1:J:9:THR:HA     | 1:J:12:ILE:HG13  | 1.97                     | 0.46              |
| 1:N:107:ASP:HA   | 1:N:110:ARG:NH1  | 2.30                     | 0.46              |
| 1:G:66:ILE:HA    | 1:G:66:ILE:HD13  | 1.69                     | 0.46              |
| 1:I:53:GLY:HA3   | 1:I:55:GLU:OE1   | 2.16                     | 0.46              |
| 1:I:57:ILE:CG2   | 1:I:64:ILE:HD11  | 2.45                     | 0.46              |
| 1:J:78:LEU:HD23  | 1:J:78:LEU:HA    | 1.79                     | 0.46              |
| 1:K:81:MET:HE2   | 1:K:81:MET:HB3   | 1.59                     | 0.46              |
| 1:L:161:PRO:HG2  | 1:L:164:ALA:HB3  | 1.98                     | 0.46              |
| 1:B:126:LEU:HD23 | 1:B:129:LYS:HD3  | 1.98                     | 0.46              |
| 1:D:4:SER:HB2    | 1:D:7:VAL:HG12   | 1.96                     | 0.46              |
| 1:I:31:TYR:CE2   | 1:I:42:GLU:HB2   | 2.50                     | 0.46              |
| 1:N:151:LEU:HD23 | 1:N:169:MET:SD   | 2.55                     | 0.46              |
| 1:F:29:HIS:HB3   | 1:F:42:GLU:HB3   | 1.98                     | 0.46              |
| 1:I:50:LEU:HD11  | 1:I:52:MET:CE    | 2.44                     | 0.46              |
| 1:J:18:ASP:HB2   | 1:J:22:ARG:O     | 2.16                     | 0.46              |
| 1:E:73:GLU:HB3   | 1:E:126:LEU:CD1  | 2.45                     | 0.46              |
| 1:G:70:TRP:CZ3   | 1:G:71:LYS:HD3   | 2.51                     | 0.46              |
| 1:K:92:GLU:OE2   | 1:K:105:TYR:OH   | 2.28                     | 0.46              |
| 1:M:41:ILE:HD13  | 1:M:57:ILE:HD11  | 1.97                     | 0.46              |
| 1:E:141:LEU:O    | 1:E:144:ILE:HG12 | 2.14                     | 0.46              |
| 1:G:29:HIS:HB3   | 1:G:42:GLU:HB3   | 1.98                     | 0.46              |
| 1:D:85:ARG:HD2   | 1:D:88:GLN:NE2   | 2.31                     | 0.45              |
| 1:D:144:ILE:O    | 1:D:148:VAL:HG13 | 2.15                     | 0.45              |
| 1:E:41:ILE:HG22  | 1:E:52:MET:O     | 2.16                     | 0.45              |
| 1:G:193:LEU:HD23 | 1:G:193:LEU:HA   | 1.70                     | 0.45              |
| 1:J:31:TYR:HB2   | 1:J:40:GLY:O     | 2.15                     | 0.45              |
| 1:K:9:THR:O      | 1:K:12:ILE:HG22  | 2.16                     | 0.45              |
| 1:N:116:MET:O    | 1:N:116:MET:HG2  | 2.15                     | 0.45              |
| 1:A:33:GLU:HG2   | 1:A:34:ILE:N     | 2.24                     | 0.45              |
| 1:G:49:ILE:O     | 1:G:49:ILE:HG13  | 2.17                     | 0.45              |
| 1:G:173:ARG:CZ   | 1:G:177:ASP:HB3  | 2.46                     | 0.45              |
| 1:H:167:GLY:O    | 1:H:171:VAL:HG23 | 2.16                     | 0.45              |
| 1:N:44:ALA:CB    | 1:N:49:ILE:HG22  | 2.46                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:152:LYS:HA   | 1:N:165:TYR:HE2  | 1.81                     | 0.45              |
| 1:J:29:HIS:HD2   | 1:J:31:TYR:CD1   | 2.34                     | 0.45              |
| 1:K:144:ILE:O    | 1:K:148:VAL:HG23 | 2.16                     | 0.45              |
| 1:M:15:LYS:HG2   | 1:M:23:GLU:OE2   | 2.16                     | 0.45              |
| 1:G:165:TYR:CZ   | 1:G:169:MET:HE2  | 2.52                     | 0.45              |
| 1:L:133:ARG:O    | 1:L:137:ILE:HG13 | 2.17                     | 0.45              |
| 1:L:145:ASP:O    | 1:L:149:ILE:HG13 | 2.16                     | 0.45              |
| 1:C:24:PHE:O     | 1:C:45:GLN:HA    | 2.16                     | 0.45              |
| 1:D:141:LEU:O    | 1:D:144:ILE:HG12 | 2.17                     | 0.45              |
| 1:E:69:ASP:N     | 1:E:69:ASP:OD1   | 2.50                     | 0.45              |
| 1:N:6:GLU:O      | 1:N:10:LYS:HG2   | 2.16                     | 0.45              |
| 1:J:116:MET:O    | 1:J:119:VAL:HG12 | 2.17                     | 0.45              |
| 1:L:56:ARG:HG2   | 1:L:56:ARG:O     | 2.16                     | 0.45              |
| 1:M:127:LYS:NZ   | 1:M:193:LEU:HD23 | 2.32                     | 0.45              |
| 1:M:163:ASN:OD1  | 1:M:164:ALA:N    | 2.49                     | 0.45              |
| 1:I:120:LYS:HA   | 1:I:123:GLN:HB3  | 1.99                     | 0.45              |
| 1:L:3:VAL:HG11   | 1:L:59:LEU:CD1   | 2.47                     | 0.45              |
| 1:N:116:MET:HE2  | 1:N:116:MET:HB3  | 1.75                     | 0.45              |
| 1:F:81:MET:HB3   | 1:F:81:MET:HE2   | 1.72                     | 0.45              |
| 1:L:137:ILE:HG23 | 1:L:179:TYR:HD1  | 1.82                     | 0.45              |
| 1:B:52:MET:HG2   | 1:B:53:GLY:N     | 2.32                     | 0.45              |
| 1:G:76:ARG:CD    | 1:G:80:LEU:HD22  | 2.47                     | 0.45              |
| 1:G:116:MET:HE2  | 1:G:116:MET:HB3  | 1.80                     | 0.45              |
| 1:G:137:ILE:HG23 | 1:G:179:TYR:CD1  | 2.51                     | 0.45              |
| 1:I:12:ILE:HA    | 1:I:27:LEU:CG    | 2.47                     | 0.45              |
| 1:I:22:ARG:HG3   | 1:I:178:SER:OG   | 2.15                     | 0.45              |
| 1:F:83:LYS:O     | 1:F:86:LYS:HG2   | 2.17                     | 0.45              |
| 1:L:3:VAL:HG11   | 1:L:59:LEU:HD11  | 1.98                     | 0.45              |
| 1:G:19:ILE:HD12  | 1:G:19:ILE:H     | 1.82                     | 0.44              |
| 1:H:94:LEU:HD22  | 1:H:99:GLU:HB2   | 1.99                     | 0.44              |
| 1:I:56:ARG:C     | 1:I:57:ILE:HD12  | 2.42                     | 0.44              |
| 1:M:24:PHE:CE1   | 1:M:45:GLN:HG2   | 2.52                     | 0.44              |
| 1:M:180:THR:O    | 1:M:183:ARG:HB3  | 2.18                     | 0.44              |
| 1:D:126:LEU:O    | 1:D:130:LEU:N    | 2.43                     | 0.44              |
| 1:E:66:ILE:N     | 1:E:66:ILE:HD12  | 2.31                     | 0.44              |
| 1:F:19:ILE:CD1   | 1:F:67:LEU:HA    | 2.47                     | 0.44              |
| 1:F:40:GLY:HA2   | 1:F:54:PRO:HD3   | 1.99                     | 0.44              |
| 1:H:27:LEU:HG    | 1:H:27:LEU:O     | 2.17                     | 0.44              |
| 1:L:57:ILE:HG21  | 1:L:64:ILE:HD11  | 1.99                     | 0.44              |
| 1:D:11:PHE:CZ    | 1:D:63:SER:HA    | 2.52                     | 0.44              |
| 1:F:123:GLN:HG3  | 1:F:193:LEU:HD13 | 1.98                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:83:LYS:HB3   | 1:L:83:LYS:HE3   | 1.59                     | 0.44              |
| 1:N:66:ILE:HD13  | 1:N:66:ILE:HA    | 1.73                     | 0.44              |
| 1:I:58:LYS:HB2   | 1:I:67:LEU:HD11  | 2.00                     | 0.44              |
| 1:B:73:GLU:O     | 1:B:77:ILE:HG12  | 2.17                     | 0.44              |
| 1:D:116:MET:O    | 1:D:116:MET:HG2  | 2.16                     | 0.44              |
| 1:K:170:GLU:CG   | 1:K:173:ARG:HH21 | 2.30                     | 0.44              |
| 1:A:18:ASP:OD2   | 1:A:22:ARG:NH1   | 2.51                     | 0.44              |
| 1:F:55:GLU:H     | 1:F:55:GLU:CD    | 2.25                     | 0.44              |
| 1:G:165:TYR:CD1  | 1:G:165:TYR:C    | 2.96                     | 0.44              |
| 1:N:56:ARG:NH1   | 1:N:68:PRO:HA    | 2.31                     | 0.44              |
| 1:A:193:LEU:O    | 1:A:196:LEU:N    | 2.47                     | 0.44              |
| 1:E:85:ARG:HH22  | 1:E:197:ASP:C    | 2.25                     | 0.44              |
| 1:C:154:SER:HB3  | 1:C:160:ILE:HG13 | 2.00                     | 0.44              |
| 1:K:161:PRO:HG2  | 1:K:164:ALA:HB3  | 1.98                     | 0.44              |
| 1:L:138:GLU:OE2  | 1:L:183:ARG:NE   | 2.44                     | 0.44              |
| 1:C:182:GLU:O    | 1:C:186:ILE:HG13 | 2.18                     | 0.44              |
| 1:D:73:GLU:CG    | 1:D:126:LEU:HD11 | 2.47                     | 0.44              |
| 1:I:4:SER:OG     | 1:I:7:VAL:HG12   | 2.18                     | 0.44              |
| 1:L:81:MET:HG2   | 1:L:119:VAL:HG21 | 2.00                     | 0.44              |
| 1:A:193:LEU:O    | 1:A:196:LEU:HB2  | 2.18                     | 0.43              |
| 1:D:38:ILE:HD13  | 1:D:38:ILE:HG21  | 1.83                     | 0.43              |
| 1:E:152:LYS:HE2  | 1:E:152:LYS:HB3  | 1.85                     | 0.43              |
| 1:F:130:LEU:HD12 | 1:F:186:ILE:HD12 | 1.99                     | 0.43              |
| 1:G:19:ILE:HD11  | 1:G:68:PRO:HD3   | 1.99                     | 0.43              |
| 1:I:57:ILE:HG21  | 1:I:64:ILE:HD11  | 2.00                     | 0.43              |
| 1:K:56:ARG:NE    | 1:K:67:LEU:O     | 2.31                     | 0.43              |
| 1:K:94:LEU:HB2   | 1:K:100:ILE:HD11 | 1.98                     | 0.43              |
| 1:N:24:PHE:O     | 1:N:45:GLN:HA    | 2.18                     | 0.43              |
| 1:E:31:TYR:HE1   | 1:E:42:GLU:HB2   | 1.83                     | 0.43              |
| 1:E:144:ILE:HD12 | 1:E:176:LYS:HB2  | 1.98                     | 0.43              |
| 1:F:130:LEU:HD11 | 1:F:186:ILE:HG23 | 2.00                     | 0.43              |
| 1:I:14:GLN:O     | 1:I:16:VAL:HG13  | 2.18                     | 0.43              |
| 1:L:9:THR:O      | 1:L:12:ILE:HG22  | 2.18                     | 0.43              |
| 1:L:31:TYR:HB2   | 1:L:40:GLY:O     | 2.19                     | 0.43              |
| 1:E:52:MET:SD    | 1:E:56:ARG:HD2   | 2.58                     | 0.43              |
| 1:F:84:ILE:HG21  | 1:F:116:MET:HB2  | 1.99                     | 0.43              |
| 1:I:33:GLU:CG    | 1:I:34:ILE:HD12  | 2.48                     | 0.43              |
| 1:I:135:ASN:HA   | 1:I:138:GLU:HG2  | 2.00                     | 0.43              |
| 1:K:80:LEU:HD23  | 1:K:80:LEU:HA    | 1.74                     | 0.43              |
| 1:K:97:LYS:HE2   | 1:K:99:GLU:OE2   | 2.18                     | 0.43              |
| 1:N:83:LYS:O     | 1:N:86:LYS:HG2   | 2.18                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:153:MET:HE2  | 1:A:153:MET:HB3  | 1.65                     | 0.43              |
| 1:C:22:ARG:HG3   | 1:C:178:SER:OG   | 2.18                     | 0.43              |
| 1:D:102:LYS:HA   | 1:D:105:TYR:HB3  | 2.00                     | 0.43              |
| 1:D:137:ILE:HG22 | 1:D:141:LEU:HD12 | 2.00                     | 0.43              |
| 1:G:24:PHE:CE1   | 1:G:66:ILE:HG21  | 2.53                     | 0.43              |
| 1:G:194:ASP:OD1  | 1:G:194:ASP:N    | 2.48                     | 0.43              |
| 1:I:55:GLU:CD    | 1:I:55:GLU:H     | 2.26                     | 0.43              |
| 1:E:33:GLU:HG3   | 1:E:34:ILE:H     | 1.84                     | 0.43              |
| 1:A:120:LYS:NZ   | 1:A:124:ASN:HD21 | 2.16                     | 0.43              |
| 1:B:130:LEU:HD11 | 1:B:186:ILE:HG12 | 2.01                     | 0.43              |
| 1:B:188:LYS:HA   | 1:B:188:LYS:HD2  | 1.68                     | 0.43              |
| 1:C:88:GLN:HG3   | 1:C:112:LEU:HD23 | 2.01                     | 0.43              |
| 1:D:85:ARG:HH21  | 1:D:88:GLN:HE22  | 1.66                     | 0.43              |
| 1:F:131:LYS:O    | 1:F:134:LEU:N    | 2.52                     | 0.43              |
| 1:M:130:LEU:HD12 | 1:M:130:LEU:HA   | 1.74                     | 0.43              |
| 1:C:116:MET:O    | 1:C:116:MET:HG2  | 2.18                     | 0.43              |
| 1:G:15:LYS:HG2   | 1:G:23:GLU:OE2   | 2.18                     | 0.43              |
| 1:I:185:ASP:OD1  | 1:I:188:LYS:HE2  | 2.19                     | 0.43              |
| 1:L:6:GLU:O      | 1:L:10:LYS:HG3   | 2.19                     | 0.43              |
| 1:L:56:ARG:HG3   | 1:L:67:LEU:O     | 2.17                     | 0.43              |
| 1:C:29:HIS:HB2   | 1:G:151:LEU:HD13 | 2.00                     | 0.43              |
| 1:D:69:ASP:N     | 1:D:69:ASP:OD1   | 2.51                     | 0.43              |
| 1:E:4:SER:HB2    | 1:E:7:VAL:HG23   | 2.01                     | 0.43              |
| 1:J:100:ILE:HD13 | 1:J:105:TYR:HB2  | 2.00                     | 0.43              |
| 1:N:83:LYS:HB3   | 1:N:83:LYS:HE3   | 1.62                     | 0.43              |
| 1:F:94:LEU:HD23  | 1:F:97:LYS:HD3   | 2.00                     | 0.43              |
| 1:F:156:ILE:C    | 1:F:158:SER:H    | 2.25                     | 0.43              |
| 1:G:22:ARG:NH2   | 1:G:179:TYR:HA   | 2.34                     | 0.43              |
| 1:M:113:ASP:O    | 1:M:117:LEU:N    | 2.48                     | 0.43              |
| 1:M:148:VAL:HG13 | 1:M:169:MET:SD   | 2.59                     | 0.43              |
| 1:B:193:LEU:O    | 1:B:196:LEU:HG   | 2.19                     | 0.43              |
| 1:F:52:MET:CG    | 1:F:56:ARG:HD3   | 2.49                     | 0.43              |
| 1:F:70:TRP:CE2   | 1:F:186:ILE:HD11 | 2.54                     | 0.43              |
| 1:G:186:ILE:HD12 | 1:G:186:ILE:HG23 | 1.74                     | 0.43              |
| 1:L:4:SER:O      | 1:L:7:VAL:HG22   | 2.19                     | 0.43              |
| 1:L:22:ARG:HG3   | 1:L:178:SER:OG   | 2.19                     | 0.43              |
| 1:L:88:GLN:NE2   | 1:L:113:ASP:OD1  | 2.51                     | 0.43              |
| 1:B:73:GLU:HB3   | 1:B:126:LEU:CD1  | 2.48                     | 0.42              |
| 1:B:130:LEU:HD11 | 1:B:186:ILE:HG23 | 2.01                     | 0.42              |
| 1:I:83:LYS:HA    | 1:I:86:LYS:HG2   | 2.01                     | 0.42              |
| 1:M:9:THR:HA     | 1:M:12:ILE:HG13  | 2.00                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:28:ILE:HG23  | 1:N:172:LEU:HD11 | 2.01                     | 0.42              |
| 1:N:24:PHE:CD2   | 1:N:66:ILE:HG21  | 2.54                     | 0.42              |
| 1:B:24:PHE:CZ    | 1:B:66:ILE:HG21  | 2.53                     | 0.42              |
| 1:C:31:TYR:CE1   | 1:C:42:GLU:HB2   | 2.51                     | 0.42              |
| 1:K:154:SER:O    | 1:K:159:GLU:HG2  | 2.18                     | 0.42              |
| 1:M:79:SER:HA    | 1:M:82:GLU:OE1   | 2.19                     | 0.42              |
| 1:N:31:TYR:CE2   | 1:N:42:GLU:HB2   | 2.54                     | 0.42              |
| 1:E:177:ASP:OD1  | 1:E:178:SER:N    | 2.52                     | 0.42              |
| 1:H:42:GLU:OE1   | 1:H:51:THR:HG23  | 2.18                     | 0.42              |
| 1:M:22:ARG:HH12  | 1:M:179:TYR:HA   | 1.83                     | 0.42              |
| 1:D:55:GLU:H     | 1:D:55:GLU:CD    | 2.26                     | 0.42              |
| 1:A:71:LYS:HD2   | 1:A:71:LYS:HA    | 1.88                     | 0.42              |
| 1:E:120:LYS:HD3  | 1:E:120:LYS:C    | 2.44                     | 0.42              |
| 1:I:68:PRO:HB2   | 1:I:70:TRP:CD1   | 2.54                     | 0.42              |
| 1:I:69:ASP:OD1   | 1:I:69:ASP:N     | 2.52                     | 0.42              |
| 1:M:66:ILE:N     | 1:M:66:ILE:HD12  | 2.35                     | 0.42              |
| 1:M:106:ASP:HB2  | 1:M:110:ARG:CZ   | 2.49                     | 0.42              |
| 1:E:134:LEU:HD12 | 1:E:134:LEU:HA   | 1.74                     | 0.42              |
| 1:F:140:GLN:HG2  | 1:F:179:TYR:CZ   | 2.55                     | 0.42              |
| 1:G:50:LEU:HD11  | 1:G:52:MET:HE3   | 2.00                     | 0.42              |
| 1:I:165:TYR:CD1  | 1:I:165:TYR:C    | 2.98                     | 0.42              |
| 1:K:24:PHE:CE2   | 1:K:45:GLN:HG2   | 2.55                     | 0.42              |
| 1:C:152:LYS:O    | 1:C:155:TYR:N    | 2.53                     | 0.42              |
| 1:F:153:MET:HE2  | 1:F:153:MET:HB3  | 1.78                     | 0.42              |
| 1:L:84:ILE:HG21  | 1:L:116:MET:HB2  | 2.02                     | 0.42              |
| 1:A:27:LEU:HD13  | 1:A:41:ILE:HD11  | 2.01                     | 0.42              |
| 1:E:68:PRO:HB2   | 1:E:70:TRP:CD1   | 2.55                     | 0.42              |
| 1:I:31:TYR:HE2   | 1:I:42:GLU:HB2   | 1.84                     | 0.42              |
| 1:J:91:LEU:HG    | 1:J:105:TYR:CD1  | 2.55                     | 0.42              |
| 1:L:55:GLU:H     | 1:L:55:GLU:CD    | 2.27                     | 0.42              |
| 1:N:100:ILE:HD11 | 1:N:108:MET:HE1  | 2.02                     | 0.42              |
| 1:D:134:LEU:HA   | 1:D:134:LEU:HD12 | 1.69                     | 0.42              |
| 1:F:167:GLY:O    | 1:F:171:VAL:HG23 | 2.19                     | 0.42              |
| 1:F:168:SER:O    | 1:F:171:VAL:HB   | 2.20                     | 0.42              |
| 1:I:145:ASP:O    | 1:I:149:ILE:HG13 | 2.20                     | 0.42              |
| 1:J:15:LYS:HD2   | 1:J:23:GLU:CD    | 2.45                     | 0.42              |
| 1:M:102:LYS:HA   | 1:M:105:TYR:HB3  | 2.02                     | 0.42              |
| 1:C:17:LYS:HE2   | 1:C:23:GLU:OE1   | 2.20                     | 0.42              |
| 1:F:131:LYS:O    | 1:F:135:ASN:N    | 2.44                     | 0.42              |
| 1:H:118:LYS:HA   | 1:H:118:LYS:HD2  | 1.89                     | 0.42              |
| 1:N:6:GLU:HG2    | 1:N:10:LYS:HE2   | 2.02                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:77:ILE:HG23  | 1:D:81:MET:HE3   | 2.02                     | 0.41              |
| 1:D:80:LEU:HD21  | 1:I:35:ASP:HA    | 2.02                     | 0.41              |
| 1:D:84:ILE:HG23  | 1:D:112:LEU:HD22 | 2.02                     | 0.41              |
| 1:E:95:TYR:OH    | 1:E:102:LYS:HD3  | 2.20                     | 0.41              |
| 1:H:66:ILE:N     | 1:H:66:ILE:HD12  | 2.34                     | 0.41              |
| 1:L:62:ASP:OD1   | 1:L:63:SER:N     | 2.52                     | 0.41              |
| 1:A:116:MET:O    | 1:A:116:MET:HG2  | 2.20                     | 0.41              |
| 1:B:27:LEU:O     | 1:B:27:LEU:HG    | 2.20                     | 0.41              |
| 1:C:55:GLU:H     | 1:C:55:GLU:CD    | 2.28                     | 0.41              |
| 1:D:78:LEU:C     | 1:D:78:LEU:HD23  | 2.45                     | 0.41              |
| 1:G:81:MET:HG2   | 1:G:119:VAL:HG21 | 2.02                     | 0.41              |
| 1:K:8:LEU:HD23   | 1:K:8:LEU:HA     | 1.86                     | 0.41              |
| 1:N:88:GLN:NE2   | 1:N:113:ASP:OD1  | 2.52                     | 0.41              |
| 1:D:116:MET:HA   | 1:D:119:VAL:HG22 | 2.01                     | 0.41              |
| 1:J:69:ASP:OD1   | 1:J:69:ASP:N     | 2.54                     | 0.41              |
| 1:K:22:ARG:HG3   | 1:K:178:SER:OG   | 2.20                     | 0.41              |
| 1:K:95:TYR:HB2   | 1:K:105:TYR:CD1  | 2.56                     | 0.41              |
| 1:L:140:GLN:HG2  | 1:L:179:TYR:OH   | 2.21                     | 0.41              |
| 1:M:27:LEU:HA    | 1:M:43:VAL:HG23  | 2.01                     | 0.41              |
| 1:B:44:ALA:HB2   | 1:B:49:ILE:HG22  | 2.02                     | 0.41              |
| 1:B:177:ASP:HA   | 1:B:180:THR:OG1  | 2.19                     | 0.41              |
| 1:E:52:MET:HE2   | 1:E:52:MET:HB3   | 1.73                     | 0.41              |
| 1:H:130:LEU:HD11 | 1:H:186:ILE:HG23 | 2.03                     | 0.41              |
| 1:C:34:ILE:HG12  | 1:K:83:LYS:NZ    | 2.35                     | 0.41              |
| 1:D:156:ILE:C    | 1:D:158:SER:H    | 2.28                     | 0.41              |
| 1:I:137:ILE:HG23 | 1:I:179:TYR:CD1  | 2.56                     | 0.41              |
| 1:L:127:LYS:CE   | 1:L:193:LEU:HD23 | 2.51                     | 0.41              |
| 1:E:165:TYR:CZ   | 1:E:169:MET:HG3  | 2.56                     | 0.41              |
| 1:F:8:LEU:HD23   | 1:F:8:LEU:HA     | 1.92                     | 0.41              |
| 1:G:19:ILE:CD1   | 1:G:68:PRO:HD3   | 2.50                     | 0.41              |
| 1:J:153:MET:HE3  | 1:J:153:MET:HB3  | 1.92                     | 0.41              |
| 1:M:55:GLU:H     | 1:M:55:GLU:CD    | 2.28                     | 0.41              |
| 1:N:41:ILE:HG21  | 1:N:41:ILE:HD13  | 1.88                     | 0.41              |
| 1:C:35:ASP:HA    | 1:K:80:LEU:HD21  | 2.03                     | 0.41              |
| 1:E:52:MET:CE    | 1:E:56:ARG:HD2   | 2.51                     | 0.41              |
| 1:N:18:ASP:HB2   | 1:N:22:ARG:O     | 2.21                     | 0.41              |
| 1:A:144:ILE:HG12 | 1:B:49:ILE:HD11  | 2.02                     | 0.41              |
| 1:B:31:TYR:HE2   | 1:B:42:GLU:OE1   | 2.03                     | 0.41              |
| 1:B:82:GLU:C     | 1:B:86:LYS:HZ2   | 2.29                     | 0.41              |
| 1:E:161:PRO:HB2  | 1:E:163:ASN:OD1  | 2.21                     | 0.41              |
| 1:F:177:ASP:OD1  | 1:F:178:SER:N    | 2.54                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:70:TRP:O     | 1:G:74:ALA:N     | 2.46                     | 0.41              |
| 1:H:12:ILE:HA    | 1:H:27:LEU:HG    | 2.02                     | 0.41              |
| 1:J:22:ARG:NH2   | 1:J:182:GLU:OE1  | 2.50                     | 0.41              |
| 1:J:75:ILE:HD12  | 1:J:75:ILE:HA    | 1.81                     | 0.41              |
| 1:M:43:VAL:CG1   | 1:M:52:MET:HE1   | 2.51                     | 0.41              |
| 1:A:49:ILE:HG12  | 1:B:144:ILE:HG12 | 2.01                     | 0.41              |
| 1:A:116:MET:HE2  | 1:A:116:MET:HB3  | 1.70                     | 0.41              |
| 1:A:140:GLN:NE2  | 1:B:49:ILE:O     | 2.53                     | 0.41              |
| 1:B:116:MET:HA   | 1:B:119:VAL:CG1  | 2.48                     | 0.41              |
| 1:B:119:VAL:O    | 1:B:123:GLN:N    | 2.44                     | 0.41              |
| 1:C:151:LEU:HD23 | 1:C:169:MET:SD   | 2.60                     | 0.41              |
| 1:E:44:ALA:HA    | 1:E:49:ILE:HA    | 2.02                     | 0.41              |
| 1:G:95:TYR:HD1   | 1:G:100:ILE:HG23 | 1.86                     | 0.41              |
| 1:G:156:ILE:C    | 1:G:158:SER:H    | 2.28                     | 0.41              |
| 1:J:41:ILE:HD12  | 1:J:57:ILE:HD13  | 2.03                     | 0.41              |
| 1:J:88:GLN:HG3   | 1:J:112:LEU:CD1  | 2.49                     | 0.41              |
| 1:J:176:LYS:HB3  | 1:J:176:LYS:HE2  | 1.76                     | 0.41              |
| 1:J:195:SER:HB3  | 1:K:85:ARG:HH21  | 1.85                     | 0.41              |
| 1:L:18:ASP:HB2   | 1:L:22:ARG:O     | 2.21                     | 0.41              |
| 1:M:31:TYR:HE2   | 1:M:42:GLU:OE1   | 2.03                     | 0.41              |
| 1:M:133:ARG:O    | 1:M:137:ILE:HG13 | 2.20                     | 0.41              |
| 1:N:15:LYS:HG3   | 1:N:23:GLU:OE2   | 2.21                     | 0.41              |
| 1:A:57:ILE:HG23  | 1:A:64:ILE:HG13  | 2.03                     | 0.41              |
| 1:C:50:LEU:HD11  | 1:C:52:MET:HE3   | 2.02                     | 0.41              |
| 1:F:131:LYS:HA   | 1:F:134:LEU:CB   | 2.51                     | 0.41              |
| 1:K:75:ILE:HD12  | 1:K:76:ARG:N     | 2.36                     | 0.41              |
| 1:M:138:GLU:HA   | 1:M:141:LEU:HB2  | 2.02                     | 0.41              |
| 1:N:71:LYS:HA    | 1:N:74:ALA:HB3   | 2.02                     | 0.41              |
| 1:C:177:ASP:HA   | 1:C:180:THR:OG1  | 2.20                     | 0.40              |
| 1:G:56:ARG:NH2   | 1:G:69:ASP:HB3   | 2.36                     | 0.40              |
| 1:G:76:ARG:HD2   | 1:G:80:LEU:HD22  | 2.03                     | 0.40              |
| 1:H:120:LYS:HA   | 1:H:123:GLN:HB3  | 2.03                     | 0.40              |
| 1:J:16:VAL:HG23  | 1:J:25:GLY:O     | 2.22                     | 0.40              |
| 1:K:148:VAL:CG1  | 1:K:169:MET:HE1  | 2.51                     | 0.40              |
| 1:M:116:MET:HA   | 1:M:119:VAL:HG12 | 2.03                     | 0.40              |
| 1:C:34:ILE:HG12  | 1:K:83:LYS:HZ3   | 1.86                     | 0.40              |
| 1:E:126:LEU:HD23 | 1:E:126:LEU:HA   | 1.93                     | 0.40              |
| 1:I:116:MET:HA   | 1:I:119:VAL:HG22 | 2.02                     | 0.40              |
| 1:J:116:MET:HE3  | 1:J:116:MET:HB3  | 1.77                     | 0.40              |
| 1:A:28:ILE:HD11  | 1:A:44:ALA:HB2   | 2.04                     | 0.40              |
| 1:A:173:ARG:CZ   | 1:A:177:ASP:OD1  | 2.69                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:16:VAL:HG22  | 1:H:25:GLY:O     | 2.21                     | 0.40              |
| 1:H:106:ASP:O    | 1:H:110:ARG:N    | 2.35                     | 0.40              |
| 1:K:4:SER:O      | 1:K:7:VAL:HG22   | 2.21                     | 0.40              |
| 1:C:8:LEU:HA     | 1:C:8:LEU:HD23   | 1.87                     | 0.40              |
| 1:F:193:LEU:HD23 | 1:F:193:LEU:HA   | 1.88                     | 0.40              |
| 1:H:141:LEU:CD1  | 1:H:176:LYS:HG3  | 2.51                     | 0.40              |
| 1:K:33:GLU:CG    | 1:K:34:ILE:H     | 2.33                     | 0.40              |
| 1:M:29:HIS:HB3   | 1:M:42:GLU:HB3   | 2.03                     | 0.40              |
| 1:G:114:THR:O    | 1:G:117:LEU:HB3  | 2.22                     | 0.40              |
| 1:J:52:MET:HG3   | 1:J:56:ARG:HD3   | 2.02                     | 0.40              |
| 1:J:156:ILE:HD13 | 1:J:156:ILE:HA   | 1.96                     | 0.40              |
| 1:L:89:ARG:HD3   | 1:L:89:ARG:HA    | 1.86                     | 0.40              |
| 1:L:145:ASP:HA   | 1:L:148:VAL:HG22 | 2.04                     | 0.40              |
| 1:N:44:ALA:HB2   | 1:N:49:ILE:HG22  | 2.04                     | 0.40              |

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1         | Atom-2                | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------------|--------------------------|-------------------|
| 1:A:152:LYS:NZ | 1:L:99:GLU:OE1[2_556] | 2.17                     | 0.03              |

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | A     | 192/238 (81%) | 188 (98%) | 4 (2%)  | 0        | 100         | 100 |
| 1   | B     | 192/238 (81%) | 189 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 1   | C     | 193/238 (81%) | 189 (98%) | 4 (2%)  | 0        | 100         | 100 |
| 1   | D     | 193/238 (81%) | 191 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 1   | E     | 192/238 (81%) | 190 (99%) | 2 (1%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|---------|----------|-------------|-----|
| 1   | F     | 194/238 (82%)   | 190 (98%)  | 3 (2%)  | 1 (0%)   | 24          | 42  |
| 1   | G     | 193/238 (81%)   | 190 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 1   | H     | 192/238 (81%)   | 190 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 1   | I     | 191/238 (80%)   | 188 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 1   | J     | 191/238 (80%)   | 187 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 1   | K     | 191/238 (80%)   | 187 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 1   | L     | 190/238 (80%)   | 186 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 1   | M     | 188/238 (79%)   | 187 (100%) | 1 (0%)  | 0        | 100         | 100 |
| 1   | N     | 191/238 (80%)   | 188 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| All | All   | 2683/3332 (80%) | 2640 (98%) | 42 (2%) | 1 (0%)   | 100         | 100 |

All (1) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 46  | GLY  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 1   | A     | 177/218 (81%) | 171 (97%) | 6 (3%)   | 32          | 58 |
| 1   | B     | 177/218 (81%) | 170 (96%) | 7 (4%)   | 28          | 53 |
| 1   | C     | 178/218 (82%) | 169 (95%) | 9 (5%)   | 21          | 43 |
| 1   | D     | 178/218 (82%) | 173 (97%) | 5 (3%)   | 38          | 62 |
| 1   | E     | 177/218 (81%) | 171 (97%) | 6 (3%)   | 32          | 58 |
| 1   | F     | 179/218 (82%) | 167 (93%) | 12 (7%)  | 15          | 31 |
| 1   | G     | 178/218 (82%) | 169 (95%) | 9 (5%)   | 21          | 43 |
| 1   | H     | 177/218 (81%) | 168 (95%) | 9 (5%)   | 21          | 43 |
| 1   | I     | 176/218 (81%) | 168 (96%) | 8 (4%)   | 24          | 48 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1   | J     | 176/218 (81%)   | 169 (96%)  | 7 (4%)   | 28          | 53 |
| 1   | K     | 176/218 (81%)   | 168 (96%)  | 8 (4%)   | 24          | 48 |
| 1   | L     | 175/218 (80%)   | 168 (96%)  | 7 (4%)   | 28          | 53 |
| 1   | M     | 173/218 (79%)   | 164 (95%)  | 9 (5%)   | 21          | 43 |
| 1   | N     | 176/218 (81%)   | 171 (97%)  | 5 (3%)   | 38          | 62 |
| All | All   | 2473/3052 (81%) | 2366 (96%) | 107 (4%) | 26          | 50 |

All (107) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 9   | THR  |
| 1   | A     | 19  | ILE  |
| 1   | A     | 38  | ILE  |
| 1   | A     | 49  | ILE  |
| 1   | A     | 153 | MET  |
| 1   | A     | 180 | THR  |
| 1   | B     | 9   | THR  |
| 1   | B     | 19  | ILE  |
| 1   | B     | 27  | LEU  |
| 1   | B     | 34  | ILE  |
| 1   | B     | 38  | ILE  |
| 1   | B     | 48  | SER  |
| 1   | B     | 49  | ILE  |
| 1   | C     | 9   | THR  |
| 1   | C     | 19  | ILE  |
| 1   | C     | 27  | LEU  |
| 1   | C     | 38  | ILE  |
| 1   | C     | 49  | ILE  |
| 1   | C     | 51  | THR  |
| 1   | C     | 58  | LYS  |
| 1   | C     | 119 | VAL  |
| 1   | C     | 169 | MET  |
| 1   | D     | 9   | THR  |
| 1   | D     | 38  | ILE  |
| 1   | D     | 39  | THR  |
| 1   | D     | 180 | THR  |
| 1   | D     | 189 | THR  |
| 1   | E     | 9   | THR  |
| 1   | E     | 16  | VAL  |
| 1   | E     | 51  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 100 | ILE  |
| 1   | E     | 180 | THR  |
| 1   | E     | 189 | THR  |
| 1   | F     | 9   | THR  |
| 1   | F     | 23  | GLU  |
| 1   | F     | 27  | LEU  |
| 1   | F     | 34  | ILE  |
| 1   | F     | 38  | ILE  |
| 1   | F     | 39  | THR  |
| 1   | F     | 94  | LEU  |
| 1   | F     | 138 | GLU  |
| 1   | F     | 148 | VAL  |
| 1   | F     | 156 | ILE  |
| 1   | F     | 169 | MET  |
| 1   | F     | 180 | THR  |
| 1   | G     | 9   | THR  |
| 1   | G     | 16  | VAL  |
| 1   | G     | 19  | ILE  |
| 1   | G     | 27  | LEU  |
| 1   | G     | 38  | ILE  |
| 1   | G     | 49  | ILE  |
| 1   | G     | 102 | LYS  |
| 1   | G     | 180 | THR  |
| 1   | G     | 194 | ASP  |
| 1   | H     | 9   | THR  |
| 1   | H     | 27  | LEU  |
| 1   | H     | 30  | VAL  |
| 1   | H     | 34  | ILE  |
| 1   | H     | 49  | ILE  |
| 1   | H     | 51  | THR  |
| 1   | H     | 93  | GLU  |
| 1   | H     | 169 | MET  |
| 1   | H     | 180 | THR  |
| 1   | I     | 9   | THR  |
| 1   | I     | 27  | LEU  |
| 1   | I     | 30  | VAL  |
| 1   | I     | 39  | THR  |
| 1   | I     | 49  | ILE  |
| 1   | I     | 51  | THR  |
| 1   | I     | 100 | ILE  |
| 1   | I     | 102 | LYS  |
| 1   | J     | 9   | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | J     | 16  | VAL  |
| 1   | J     | 27  | LEU  |
| 1   | J     | 49  | ILE  |
| 1   | J     | 71  | LYS  |
| 1   | J     | 75  | ILE  |
| 1   | J     | 114 | THR  |
| 1   | K     | 16  | VAL  |
| 1   | K     | 19  | ILE  |
| 1   | K     | 39  | THR  |
| 1   | K     | 85  | ARG  |
| 1   | K     | 105 | TYR  |
| 1   | K     | 144 | ILE  |
| 1   | K     | 180 | THR  |
| 1   | K     | 187 | ARG  |
| 1   | L     | 9   | THR  |
| 1   | L     | 27  | LEU  |
| 1   | L     | 38  | ILE  |
| 1   | L     | 39  | THR  |
| 1   | L     | 49  | ILE  |
| 1   | L     | 116 | MET  |
| 1   | L     | 180 | THR  |
| 1   | M     | 19  | ILE  |
| 1   | M     | 38  | ILE  |
| 1   | M     | 39  | THR  |
| 1   | M     | 43  | VAL  |
| 1   | M     | 49  | ILE  |
| 1   | M     | 102 | LYS  |
| 1   | M     | 119 | VAL  |
| 1   | M     | 180 | THR  |
| 1   | M     | 189 | THR  |
| 1   | N     | 9   | THR  |
| 1   | N     | 38  | ILE  |
| 1   | N     | 39  | THR  |
| 1   | N     | 51  | THR  |
| 1   | N     | 180 | THR  |

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

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 29  | HIS  |
| 1   | A     | 124 | ASN  |
| 1   | B     | 123 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 140 | GLN  |
| 1   | D     | 88  | GLN  |
| 1   | D     | 135 | ASN  |
| 1   | F     | 124 | ASN  |
| 1   | F     | 140 | GLN  |
| 1   | G     | 88  | GLN  |
| 1   | G     | 140 | GLN  |
| 1   | H     | 45  | GLN  |
| 1   | I     | 135 | ASN  |
| 1   | J     | 29  | HIS  |
| 1   | L     | 98  | GLN  |
| 1   | L     | 143 | HIS  |
| 1   | M     | 143 | HIS  |
| 1   | N     | 88  | GLN  |
| 1   | N     | 124 | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

### 5.7 Other polymers ⓘ

There are no such residues in this entry.

### 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1   | A     | 194/238 (81%)   | -0.22  | 2 (1%) 79 74  | 31, 52, 98, 146       | 0     |
| 1   | B     | 194/238 (81%)   | -0.22  | 0 100 100     | 41, 72, 126, 218      | 0     |
| 1   | C     | 195/238 (81%)   | -0.39  | 1 (0%) 87 85  | 23, 48, 104, 129      | 0     |
| 1   | D     | 195/238 (81%)   | -0.18  | 4 (2%) 63 55  | 34, 72, 122, 147      | 0     |
| 1   | E     | 194/238 (81%)   | -0.36  | 2 (1%) 79 74  | 25, 53, 111, 148      | 0     |
| 1   | F     | 196/238 (82%)   | -0.08  | 4 (2%) 65 57  | 36, 82, 125, 147      | 0     |
| 1   | G     | 195/238 (81%)   | -0.25  | 3 (1%) 72 65  | 24, 47, 94, 145       | 0     |
| 1   | H     | 194/238 (81%)   | -0.37  | 2 (1%) 79 74  | 30, 62, 114, 144      | 0     |
| 1   | I     | 193/238 (81%)   | -0.33  | 1 (0%) 87 85  | 26, 65, 111, 170      | 0     |
| 1   | J     | 193/238 (81%)   | -0.29  | 2 (1%) 79 74  | 35, 69, 114, 139      | 0     |
| 1   | K     | 193/238 (81%)   | -0.22  | 2 (1%) 79 74  | 29, 58, 103, 156      | 0     |
| 1   | L     | 192/238 (80%)   | -0.28  | 1 (0%) 87 85  | 33, 66, 115, 182      | 0     |
| 1   | M     | 190/238 (79%)   | -0.19  | 2 (1%) 78 73  | 44, 77, 121, 151      | 0     |
| 1   | N     | 193/238 (81%)   | -0.27  | 3 (1%) 70 64  | 37, 70, 118, 166      | 0     |
| All | All   | 2711/3332 (81%) | -0.26  | 29 (1%) 78 73 | 23, 64, 117, 218      | 0     |

All (29) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | G     | 40  | GLY  | 4.3  |
| 1   | A     | 40  | GLY  | 4.1  |
| 1   | E     | 39  | THR  | 3.6  |
| 1   | A     | 39  | THR  | 3.1  |
| 1   | G     | 39  | THR  | 2.8  |
| 1   | D     | 162 | GLU  | 2.6  |
| 1   | E     | 40  | GLY  | 2.6  |
| 1   | J     | 94  | LEU  | 2.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | F     | 77  | ILE  | 2.4  |
| 1   | F     | 31  | TYR  | 2.4  |
| 1   | I     | 39  | THR  | 2.4  |
| 1   | K     | 31  | TYR  | 2.4  |
| 1   | G     | 86  | LYS  | 2.3  |
| 1   | N     | 40  | GLY  | 2.3  |
| 1   | D     | 155 | TYR  | 2.3  |
| 1   | J     | 11  | PHE  | 2.2  |
| 1   | F     | 40  | GLY  | 2.2  |
| 1   | H     | 32  | SER  | 2.2  |
| 1   | N     | 151 | LEU  | 2.2  |
| 1   | C     | 40  | GLY  | 2.1  |
| 1   | F     | 189 | THR  | 2.1  |
| 1   | M     | 193 | LEU  | 2.1  |
| 1   | N     | 196 | LEU  | 2.1  |
| 1   | D     | 6   | GLU  | 2.1  |
| 1   | D     | 30  | VAL  | 2.1  |
| 1   | L     | 3   | VAL  | 2.1  |
| 1   | M     | 191 | ASP  | 2.1  |
| 1   | H     | 3   | VAL  | 2.0  |
| 1   | K     | 40  | GLY  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.