



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:22 AM UTC

PDB ID : 3K1F / pdb\_00003k1f  
Title : Crystal structure of RNA Polymerase II in complex with TFIIB  
Authors : Kostrewa, D.; Zeller, M.E.; Armache, K.-J.; Seizl, M.; Leike, K.; Thomm, M.; Cramer, P.  
Deposited on : 2009-09-27  
Resolution : 4.30 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

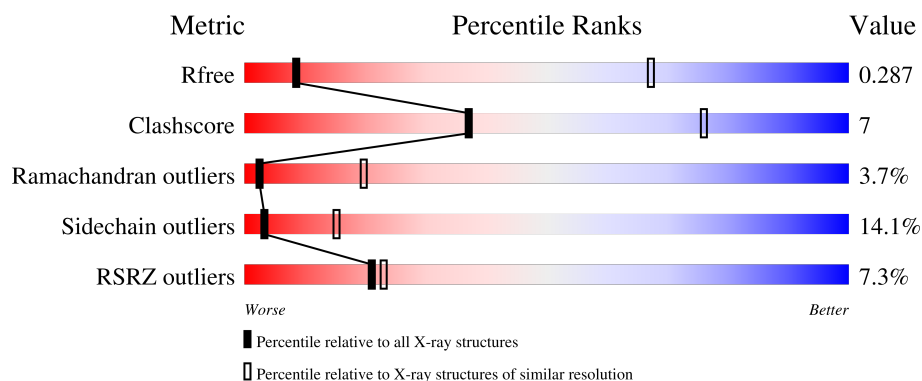
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.30 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                      | 1052 (4.70-3.90)                                      |
| Clashscore            | 190562                      | 1097 (4.70-3.90)                                      |
| Ramachandran outliers | 187476                      | 1001 (4.70-3.90)                                      |
| Sidechain outliers    | 187428                      | 1007 (4.72-3.88)                                      |
| RSRZ outliers         | 180081                      | 1049 (4.70-3.90)                                      |

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     | 1733   | <div> <div>4%</div> <div>56% 21% 5% 18%</div> </div> |
| 2   | B     | 1224   | <div> <div>9%</div> <div>61% 25% 5% 8%</div> </div>  |
| 3   | C     | 318    | <div> <div>3%</div> <div>60% 21% .. 16%</div> </div> |
| 4   | D     | 221    | <div> <div>8%</div> <div>56% 22% . 19%</div> </div>  |
| 5   | E     | 215    | <div> <div>8%</div> <div>72% 23% .</div> </div>      |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 6   | F     | 155    |                  |
| 7   | G     | 171    |                  |
| 8   | H     | 146    |                  |
| 9   | I     | 122    |                  |
| 10  | J     | 70     |                  |
| 11  | K     | 120    |                  |
| 12  | L     | 70     |                  |
| 13  | M     | 197    |                  |

## 2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 32332 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 DNA-directed RNA polymerase II subunit RPB1.

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 1   | A     | 1416     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 11143 | 7021 | 1949 | 2111 | 62 |         |         |       |

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 2   | B     | 1120     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 8910  | 5639 | 1560 | 1656 | 55 |         |         |       |

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 3   | C     | 266      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2095  | 1317 | 348 | 417 | 13 |         |         |       |

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 4   | D     | 178      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1434  | 887 | 257 | 288 | 2 |         |         |       |

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 5   | E     | 214      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1752  | 1111 | 309 | 321 | 11 |         |         |       |

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6   | F     | 87       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 705   | 451 | 119 | 132 | 3 |         |         |       |

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7   | G     | 171      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1340  | 861 | 222 | 249 | 8 |         |         |       |

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8   | H     | 134      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1076  | 677 | 182 | 213 | 4 |         |         |       |

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

| Mol | Chain | Residues | Atoms |     |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 9   | I     | 119      | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 971   | 596 | 179 | 186 | 10 |         |         |       |

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 10  | J     | 65       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 532   | 339 | 93 | 94 | 6 |         |         |       |

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 11  | K     | 114      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 919   | 590 | 156 | 171 | 2 |         |         |       |

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 12  | L     | 46       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 363   | 224 | 72 | 63 | 4 |         |         |       |

- Molecule 13 is a protein called Transcription initiation factor IIB.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13  | M     | 185      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1083  | 662 | 207 | 210 | 4 |         |         |       |

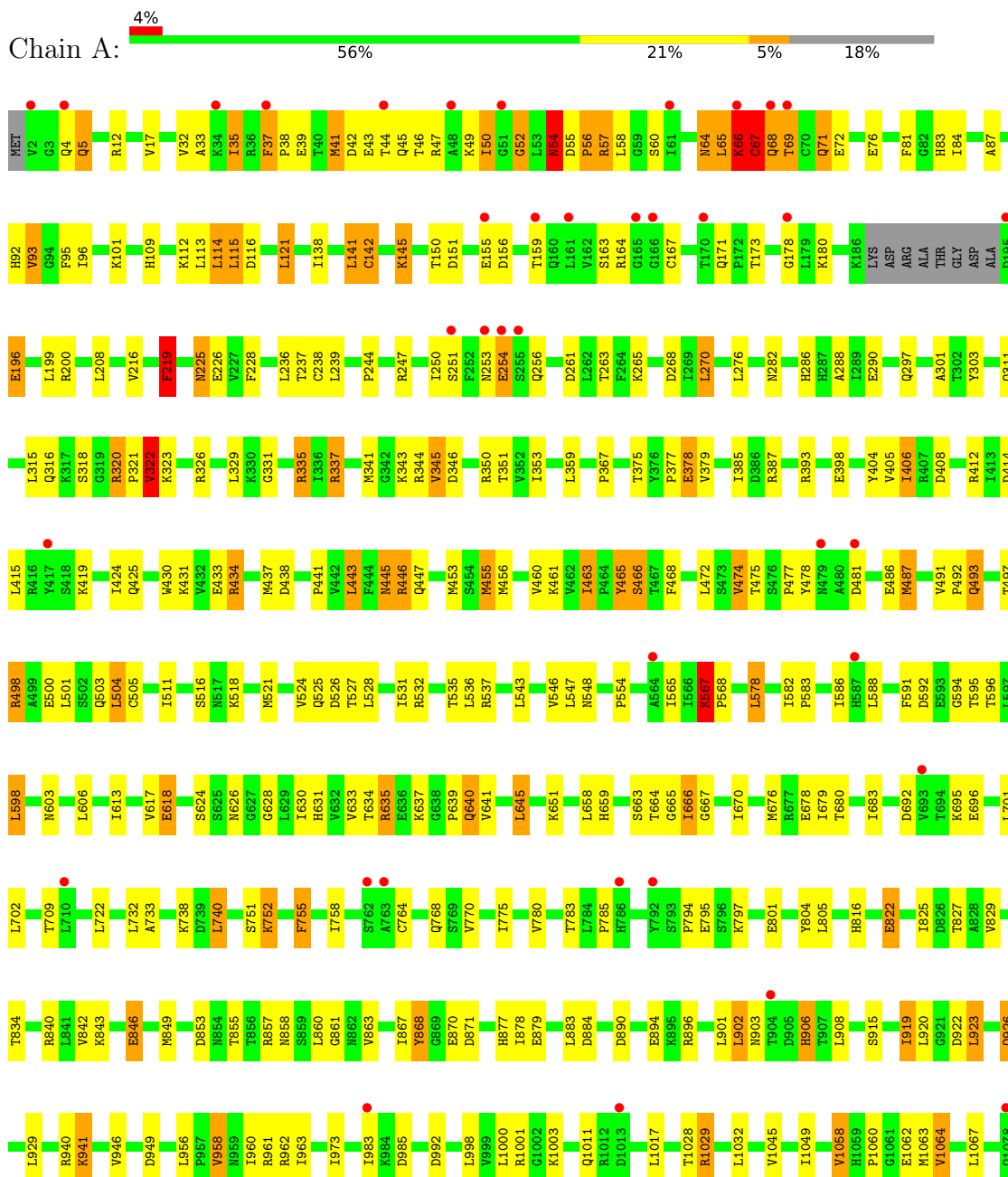
- Molecule 14 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 14  | A     | 2        | Total<br>2 | Zn<br>2 | 0       | 0       |
| 14  | B     | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 14  | C     | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 14  | I     | 2        | Total<br>2 | Zn<br>2 | 0       | 0       |
| 14  | J     | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 14  | L     | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 14  | M     | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |

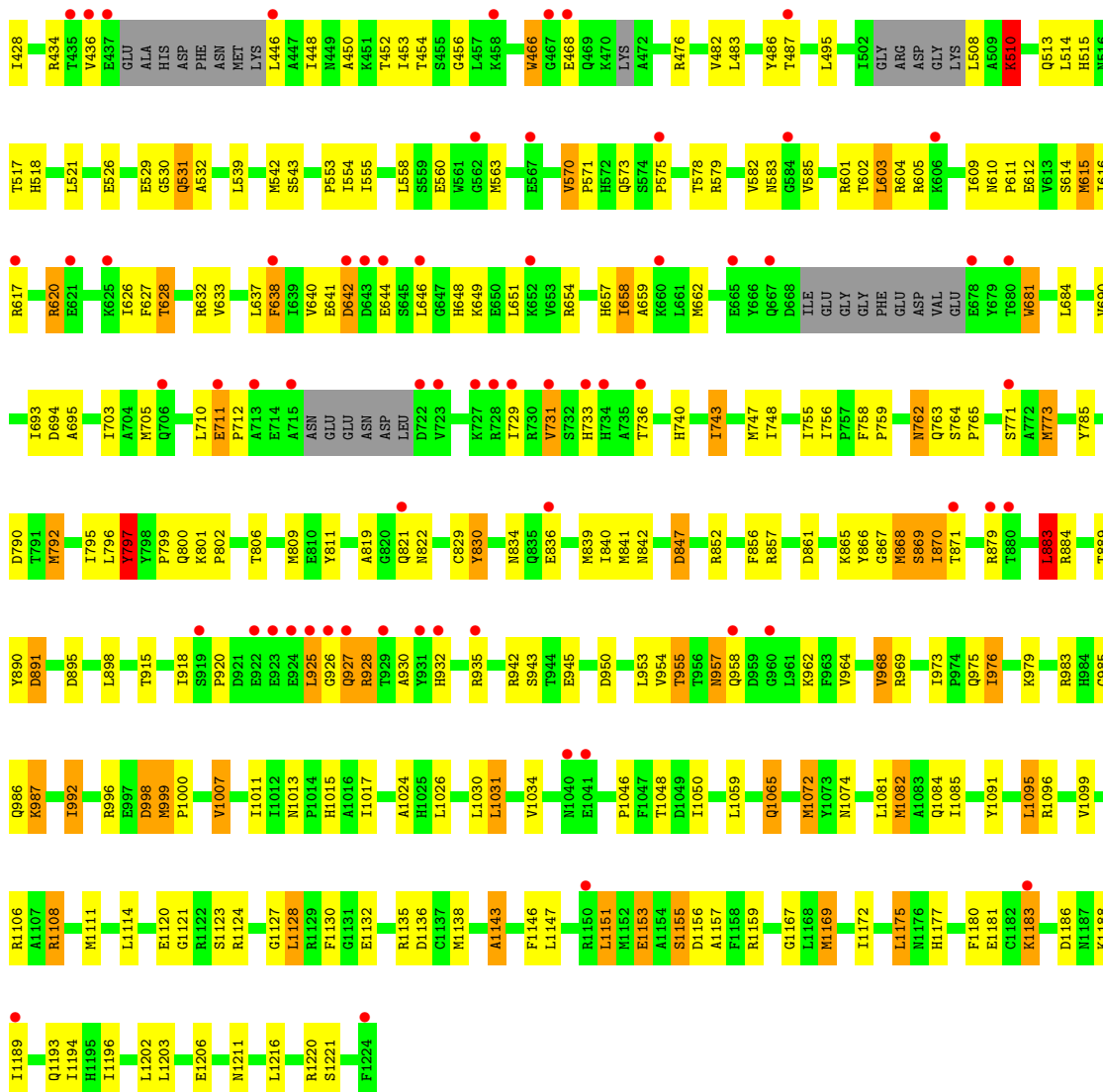
### 3 Residue-property plots

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

- Molecule 1: DNA-directed RNA polymerase II subunit RPB1



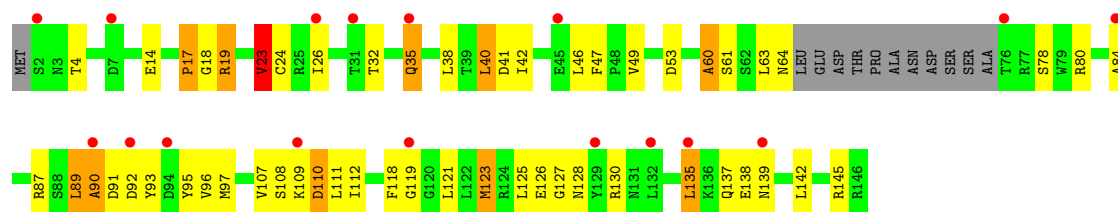




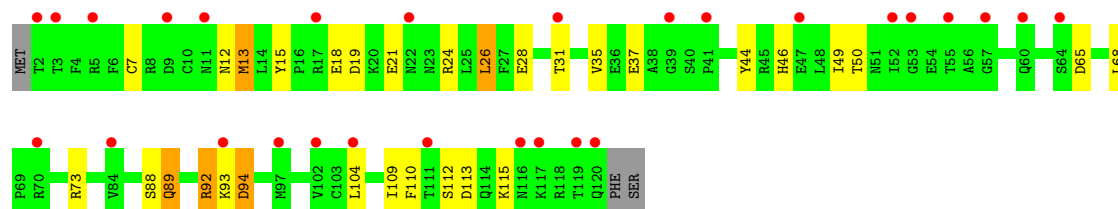




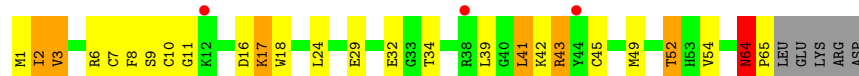
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



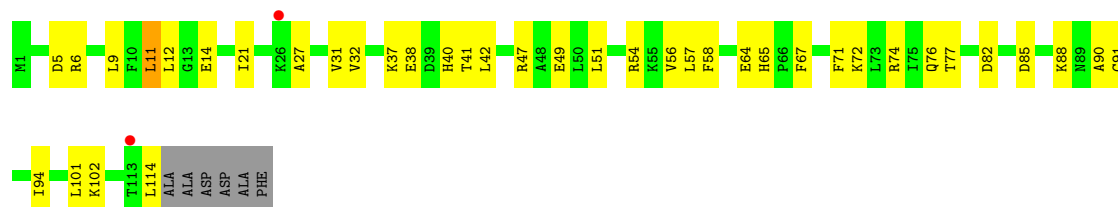
- Molecule 9: DNA-directed RNA polymerase II subunit RPB9



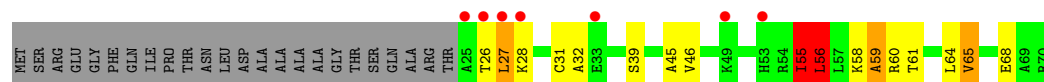
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



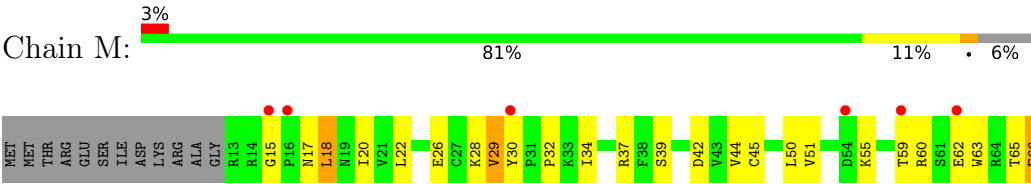
- Molecule 11: DNA-directed RNA polymerase II subunit RPB11



- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4



● Molecule 13: Transcription initiation factor IIB



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | C 2 2 21                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 220.97Å 408.27Å 275.24Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 39.69 – 4.30<br>39.69 – 4.30                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.4 (39.69-4.30)<br>96.7 (39.69-4.30)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | 0.13                                                        | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.41 (at 4.28Å)                                             | Xtriage          |
| Refinement program                                                      | BUSTER 2.7.0                                                | Depositor        |
| R, $R_{free}$                                                           | 0.220 , 0.255<br>0.250 , 0.287                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 2058 reflections (2.45%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 81.9                                                        | Xtriage          |
| Anisotropy                                                              | 0.780                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.29 , 153.6                                                | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.83                                                        | EDS              |
| Total number of atoms                                                   | 32332                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 124.0                                                       | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.92% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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     | 0.79         | 0/11342 | 1.44        | 67/15337 (0.4%)  |
| 2   | B     | 0.80         | 0/9084  | 1.38        | 57/12251 (0.5%)  |
| 3   | C     | 0.78         | 0/2133  | 1.38        | 16/2891 (0.6%)   |
| 4   | D     | 0.75         | 0/1444  | 1.45        | 10/1935 (0.5%)   |
| 5   | E     | 0.76         | 0/1788  | 1.35        | 8/2406 (0.3%)    |
| 6   | F     | 0.77         | 0/717   | 1.43        | 11/967 (1.1%)    |
| 7   | G     | 0.73         | 0/1368  | 1.37        | 8/1844 (0.4%)    |
| 8   | H     | 0.82         | 0/1094  | 1.32        | 9/1481 (0.6%)    |
| 9   | I     | 0.77         | 0/989   | 1.40        | 5/1331 (0.4%)    |
| 10  | J     | 0.78         | 0/541   | 1.49        | 4/727 (0.6%)     |
| 11  | K     | 0.77         | 0/937   | 1.36        | 4/1265 (0.3%)    |
| 12  | L     | 0.89         | 0/365   | 1.39        | 3/485 (0.6%)     |
| 13  | M     | 0.76         | 0/449   | 1.26        | 2/609 (0.3%)     |
| All | All   | 0.79         | 0/32251 | 1.40        | 204/43529 (0.5%) |

There are no bond length outliers.

All (204) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1   | A     | 244  | PRO  | N-CA-C   | 8.61  | 121.21      | 110.70   |
| 2   | B     | 1136 | ASP  | CA-CB-CG | 7.15  | 119.75      | 112.60   |
| 1   | A     | 56   | PRO  | N-CA-C   | -7.08 | 105.50      | 114.35   |
| 1   | A     | 219  | PHE  | CA-CB-CG | 7.00  | 120.80      | 113.80   |
| 1   | A     | 288  | ALA  | N-CA-C   | -6.78 | 106.20      | 114.75   |
| 2   | B     | 998  | ASP  | CA-CB-CG | 6.71  | 119.31      | 112.60   |
| 3   | C     | 121  | VAL  | N-CA-C   | 6.69  | 116.84      | 110.42   |
| 2   | B     | 628  | THR  | CA-C-N   | 6.63  | 130.56      | 120.82   |
| 2   | B     | 628  | THR  | C-N-CA   | 6.63  | 130.56      | 120.82   |
| 2   | B     | 1186 | ASP  | CA-CB-CG | 6.62  | 119.22      | 112.60   |
| 3   | C     | 191  | TYR  | N-CA-C   | 6.58  | 119.26      | 109.59   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1   | A     | 56   | PRO  | CA-C-N   | 6.54  | 134.02      | 121.54   |
| 1   | A     | 56   | PRO  | C-N-CA   | 6.54  | 134.02      | 121.54   |
| 1   | A     | 524  | VAL  | N-CA-C   | 6.51  | 118.20      | 108.96   |
| 1   | A     | 54   | ASN  | CA-CB-CG | 6.48  | 119.08      | 112.60   |
| 13  | M     | 42   | ASP  | CA-CB-CG | 6.45  | 119.05      | 112.60   |
| 9   | I     | 110  | PHE  | CA-CB-CG | 6.38  | 120.18      | 113.80   |
| 5   | E     | 5    | ASN  | CA-C-N   | 6.36  | 128.71      | 120.44   |
| 5   | E     | 5    | ASN  | C-N-CA   | 6.36  | 128.71      | 120.44   |
| 1   | A     | 1406 | VAL  | CA-C-N   | 6.36  | 129.05      | 120.65   |
| 1   | A     | 1406 | VAL  | C-N-CA   | 6.36  | 129.05      | 120.65   |
| 6   | F     | 154  | ASP  | CA-CB-CG | 6.36  | 118.96      | 112.60   |
| 1   | A     | 1331 | SER  | CA-C-N   | 6.33  | 129.05      | 120.38   |
| 1   | A     | 1331 | SER  | C-N-CA   | 6.33  | 129.05      | 120.38   |
| 2   | B     | 879  | ARG  | CA-C-N   | 6.23  | 128.63      | 120.28   |
| 2   | B     | 879  | ARG  | C-N-CA   | 6.23  | 128.63      | 120.28   |
| 1   | A     | 466  | SER  | N-CA-C   | 6.20  | 124.01      | 110.80   |
| 8   | H     | 110  | ASP  | CA-C-N   | 6.17  | 129.60      | 120.90   |
| 8   | H     | 110  | ASP  | C-N-CA   | 6.17  | 129.60      | 120.90   |
| 1   | A     | 846  | GLU  | CA-C-N   | 6.11  | 130.47      | 120.63   |
| 1   | A     | 846  | GLU  | C-N-CA   | 6.11  | 130.47      | 120.63   |
| 1   | A     | 1419 | ASP  | CA-C-N   | 6.10  | 129.06      | 120.28   |
| 1   | A     | 1419 | ASP  | C-N-CA   | 6.10  | 129.06      | 120.28   |
| 2   | B     | 869  | SER  | N-CA-C   | 6.09  | 119.76      | 111.17   |
| 4   | D     | 35   | LEU  | N-CA-C   | 6.07  | 118.39      | 111.11   |
| 7   | G     | 22   | MET  | N-CA-C   | -6.05 | 104.63      | 112.68   |
| 11  | K     | 40   | HIS  | CA-C-N   | 6.05  | 128.70      | 120.54   |
| 11  | K     | 40   | HIS  | C-N-CA   | 6.05  | 128.70      | 120.54   |
| 1   | A     | 804  | TYR  | CA-C-N   | 6.03  | 128.28      | 120.44   |
| 1   | A     | 804  | TYR  | C-N-CA   | 6.03  | 128.28      | 120.44   |
| 6   | F     | 71   | GLU  | N-CA-C   | -6.02 | 104.64      | 112.23   |
| 1   | A     | 491  | VAL  | N-CA-C   | 6.01  | 113.03      | 107.56   |
| 1   | A     | 537  | ARG  | N-CA-C   | -5.98 | 105.81      | 113.23   |
| 1   | A     | 37   | PHE  | CA-CB-CG | 5.97  | 119.77      | 113.80   |
| 2   | B     | 1095 | LEU  | CA-C-N   | 5.96  | 128.26      | 120.28   |
| 2   | B     | 1095 | LEU  | C-N-CA   | 5.96  | 128.26      | 120.28   |
| 3   | C     | 40   | GLU  | N-CA-C   | 5.95  | 121.58      | 113.37   |
| 5   | E     | 163  | GLU  | CB-CG-CD | 5.91  | 122.65      | 112.60   |
| 1   | A     | 915  | SER  | CA-C-N   | 5.89  | 126.52      | 119.98   |
| 1   | A     | 915  | SER  | C-N-CA   | 5.89  | 126.52      | 119.98   |
| 6   | F     | 154  | ASP  | CA-C-N   | 5.89  | 132.30      | 121.70   |
| 6   | F     | 154  | ASP  | C-N-CA   | 5.89  | 132.30      | 121.70   |
| 2   | B     | 839  | MET  | N-CA-C   | 5.87  | 118.06      | 108.55   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 3   | C     | 60   | ASP  | CA-CB-CG | 5.86  | 118.46      | 112.60   |
| 1   | A     | 1121 | GLU  | N-CA-C   | -5.85 | 102.68      | 109.93   |
| 2   | B     | 890  | TYR  | CA-C-N   | 5.84  | 132.70      | 121.54   |
| 2   | B     | 890  | TYR  | C-N-CA   | 5.84  | 132.70      | 121.54   |
| 2   | B     | 830  | TYR  | N-CA-C   | 5.83  | 114.35      | 108.75   |
| 9   | I     | 31   | THR  | N-CA-C   | -5.83 | 106.00      | 113.23   |
| 3   | C     | 136  | ASP  | CA-C-N   | 5.80  | 127.97      | 120.44   |
| 3   | C     | 136  | ASP  | C-N-CA   | 5.80  | 127.97      | 120.44   |
| 7   | G     | 17   | PHE  | CA-CB-CG | 5.80  | 119.60      | 113.80   |
| 3   | C     | 96   | SER  | N-CA-C   | 5.78  | 118.89      | 109.24   |
| 9   | I     | 94   | ASP  | N-CA-C   | 5.74  | 118.40      | 111.40   |
| 1   | A     | 1003 | LYS  | N-CA-C   | 5.74  | 117.61      | 111.36   |
| 8   | H     | 23   | VAL  | N-CA-C   | 5.71  | 116.35      | 108.12   |
| 1   | A     | 1109 | LYS  | N-CA-C   | -5.71 | 105.81      | 112.89   |
| 7   | G     | 155  | SER  | N-CA-C   | -5.71 | 103.68      | 111.56   |
| 7   | G     | 32   | GLU  | CA-C-N   | 5.64  | 128.40      | 120.28   |
| 7   | G     | 32   | GLU  | C-N-CA   | 5.64  | 128.40      | 120.28   |
| 12  | L     | 65   | VAL  | N-CA-C   | 5.63  | 116.33      | 108.89   |
| 2   | B     | 927  | GLN  | CA-C-N   | 5.63  | 128.14      | 120.54   |
| 2   | B     | 927  | GLN  | C-N-CA   | 5.63  | 128.14      | 120.54   |
| 2   | B     | 1074 | ASN  | CA-CB-CG | 5.61  | 118.21      | 112.60   |
| 2   | B     | 681  | TRP  | N-CA-C   | -5.60 | 104.80      | 111.69   |
| 7   | G     | 34   | VAL  | N-CA-C   | 5.60  | 116.38      | 111.56   |
| 4   | D     | 157  | GLN  | CA-C-N   | 5.55  | 128.17      | 120.63   |
| 4   | D     | 157  | GLN  | C-N-CA   | 5.55  | 128.17      | 120.63   |
| 1   | A     | 375  | THR  | N-CA-C   | 5.54  | 118.12      | 108.76   |
| 2   | B     | 25   | ILE  | N-CA-C   | 5.53  | 116.55      | 108.58   |
| 2   | B     | 66   | ASP  | CA-C-N   | 5.53  | 129.11      | 120.82   |
| 2   | B     | 66   | ASP  | C-N-CA   | 5.53  | 129.11      | 120.82   |
| 2   | B     | 870  | ILE  | CA-C-N   | 5.52  | 128.61      | 120.82   |
| 2   | B     | 870  | ILE  | C-N-CA   | 5.52  | 128.61      | 120.82   |
| 6   | F     | 103  | MET  | N-CA-C   | -5.52 | 106.58      | 113.15   |
| 3   | C     | 136  | ASP  | N-CA-C   | 5.50  | 118.05      | 110.35   |
| 2   | B     | 304  | ASP  | CA-CB-CG | 5.49  | 118.09      | 112.60   |
| 8   | H     | 90   | ALA  | N-CA-C   | -5.49 | 107.16      | 112.97   |
| 4   | D     | 172  | LEU  | CA-C-N   | 5.48  | 128.46      | 120.51   |
| 4   | D     | 172  | LEU  | C-N-CA   | 5.48  | 128.46      | 120.51   |
| 2   | B     | 1121 | GLY  | CA-C-N   | 5.47  | 127.61      | 120.28   |
| 2   | B     | 1121 | GLY  | C-N-CA   | 5.47  | 127.61      | 120.28   |
| 2   | B     | 1221 | SER  | CA-C-N   | 5.46  | 127.92      | 120.54   |
| 2   | B     | 1221 | SER  | C-N-CA   | 5.46  | 127.92      | 120.54   |
| 1   | A     | 81   | PHE  | N-CA-C   | 5.46  | 117.74      | 110.53   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 11  | K     | 71   | PHE  | CA-CB-CG | 5.44  | 119.24      | 113.80   |
| 1   | A     | 829  | VAL  | CA-C-N   | 5.43  | 127.87      | 120.54   |
| 1   | A     | 829  | VAL  | C-N-CA   | 5.43  | 127.87      | 120.54   |
| 12  | L     | 65   | VAL  | N-CA-CB  | 5.43  | 116.45      | 110.53   |
| 1   | A     | 345  | VAL  | N-CA-C   | 5.42  | 117.45      | 108.99   |
| 6   | F     | 114  | GLU  | N-CA-C   | 5.41  | 117.55      | 108.73   |
| 9   | I     | 92   | ARG  | CA-C-N   | 5.41  | 127.47      | 120.44   |
| 9   | I     | 92   | ARG  | C-N-CA   | 5.41  | 127.47      | 120.44   |
| 1   | A     | 871  | ASP  | CA-CB-CG | 5.38  | 117.98      | 112.60   |
| 10  | J     | 41   | LEU  | CA-C-N   | 5.37  | 131.80      | 121.54   |
| 10  | J     | 41   | LEU  | C-N-CA   | 5.37  | 131.80      | 121.54   |
| 1   | A     | 985  | ASP  | CA-CB-CG | 5.36  | 117.96      | 112.60   |
| 6   | F     | 81   | THR  | CA-C-N   | 5.36  | 128.28      | 120.51   |
| 6   | F     | 81   | THR  | C-N-CA   | 5.36  | 128.28      | 120.51   |
| 2   | B     | 638  | PHE  | CA-CB-CG | 5.35  | 119.15      | 113.80   |
| 3   | C     | 133  | ILE  | CB-CA-C  | 5.33  | 117.16      | 111.35   |
| 7   | G     | 18   | PHE  | CA-CB-CG | 5.31  | 119.11      | 113.80   |
| 2   | B     | 762  | ASN  | N-CA-C   | 5.31  | 118.39      | 109.95   |
| 2   | B     | 1120 | GLU  | CB-CG-CD | 5.31  | 121.62      | 112.60   |
| 1   | A     | 1233 | ASP  | N-CA-C   | 5.31  | 117.14      | 110.24   |
| 8   | H     | 40   | LEU  | N-CA-C   | 5.30  | 117.72      | 108.76   |
| 2   | B     | 282  | ILE  | CA-C-N   | 5.29  | 127.23      | 120.56   |
| 2   | B     | 282  | ILE  | C-N-CA   | 5.29  | 127.23      | 120.56   |
| 1   | A     | 640  | GLN  | CA-C-N   | 5.29  | 127.22      | 120.56   |
| 1   | A     | 640  | GLN  | C-N-CA   | 5.29  | 127.22      | 120.56   |
| 2   | B     | 968  | VAL  | CA-C-N   | 5.28  | 130.51      | 122.65   |
| 2   | B     | 968  | VAL  | C-N-CA   | 5.28  | 130.51      | 122.65   |
| 2   | B     | 1065 | GLN  | CA-C-N   | 5.28  | 127.66      | 120.54   |
| 2   | B     | 1065 | GLN  | C-N-CA   | 5.28  | 127.66      | 120.54   |
| 12  | L     | 56   | LEU  | N-CA-C   | 5.27  | 122.03      | 110.80   |
| 1   | A     | 67   | CYS  | N-CA-C   | -5.27 | 99.57       | 110.80   |
| 1   | A     | 1365 | TYR  | CA-C-N   | 5.27  | 127.66      | 120.54   |
| 1   | A     | 1365 | TYR  | C-N-CA   | 5.27  | 127.66      | 120.54   |
| 3   | C     | 225  | ALA  | CA-C-N   | 5.27  | 131.26      | 121.62   |
| 3   | C     | 225  | ALA  | C-N-CA   | 5.27  | 131.26      | 121.62   |
| 1   | A     | 65   | LEU  | CA-C-N   | 5.27  | 131.60      | 121.54   |
| 1   | A     | 65   | LEU  | C-N-CA   | 5.27  | 131.60      | 121.54   |
| 2   | B     | 276  | ILE  | CA-C-N   | 5.27  | 127.29      | 120.44   |
| 2   | B     | 276  | ILE  | C-N-CA   | 5.27  | 127.29      | 120.44   |
| 6   | F     | 132  | LEU  | CA-C-N   | 5.26  | 130.09      | 123.10   |
| 6   | F     | 132  | LEU  | C-N-CA   | 5.26  | 130.09      | 123.10   |
| 1   | A     | 225  | ASN  | CA-C-N   | 5.25  | 128.05      | 120.38   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1   | A     | 225  | ASN  | C-N-CA   | 5.25  | 128.05      | 120.38   |
| 1   | A     | 1393 | ASN  | CA-CB-CG | 5.25  | 117.85      | 112.60   |
| 3   | C     | 52   | GLU  | N-CA-C   | -5.24 | 105.71      | 112.68   |
| 7   | G     | 166  | ASP  | N-CA-C   | 5.24  | 117.05      | 110.24   |
| 1   | A     | 961  | ARG  | CA-C-N   | 5.23  | 127.24      | 120.44   |
| 1   | A     | 961  | ARG  | C-N-CA   | 5.23  | 127.24      | 120.44   |
| 2   | B     | 370  | PHE  | CA-CB-CG | 5.23  | 119.03      | 113.80   |
| 2   | B     | 1220 | ARG  | N-CA-C   | 5.23  | 117.28      | 110.53   |
| 3   | C     | 202  | PRO  | N-CA-C   | 5.22  | 119.28      | 111.14   |
| 1   | A     | 755  | PHE  | CA-C-N   | 5.21  | 127.13      | 120.56   |
| 1   | A     | 755  | PHE  | C-N-CA   | 5.21  | 127.13      | 120.56   |
| 1   | A     | 870  | GLU  | CB-CG-CD | 5.20  | 121.43      | 112.60   |
| 3   | C     | 20   | PHE  | N-CA-C   | 5.18  | 116.95      | 109.07   |
| 1   | A     | 142  | CYS  | N-CA-C   | 5.18  | 118.42      | 112.57   |
| 1   | A     | 1312 | ASN  | CA-C-N   | 5.18  | 128.59      | 120.82   |
| 1   | A     | 1312 | ASN  | C-N-CA   | 5.18  | 128.59      | 120.82   |
| 2   | B     | 1099 | VAL  | CA-C-N   | 5.17  | 127.72      | 120.28   |
| 2   | B     | 1099 | VAL  | C-N-CA   | 5.17  | 127.72      | 120.28   |
| 4   | D     | 127  | ASP  | CA-C-N   | 5.16  | 127.15      | 120.70   |
| 4   | D     | 127  | ASP  | C-N-CA   | 5.16  | 127.15      | 120.70   |
| 2   | B     | 1130 | PHE  | N-CA-C   | -5.16 | 97.56       | 107.57   |
| 4   | D     | 26   | THR  | CA-C-N   | 5.15  | 131.38      | 121.54   |
| 4   | D     | 26   | THR  | C-N-CA   | 5.15  | 131.38      | 121.54   |
| 1   | A     | 678  | GLU  | CA-C-N   | 5.14  | 127.04      | 120.56   |
| 1   | A     | 678  | GLU  | C-N-CA   | 5.14  | 127.04      | 120.56   |
| 2   | B     | 932  | HIS  | N-CA-C   | 5.14  | 118.33      | 111.24   |
| 2   | B     | 889  | THR  | N-CA-C   | 5.12  | 117.99      | 110.30   |
| 3   | C     | 40   | GLU  | CA-C-N   | -5.12 | 118.90      | 122.59   |
| 3   | C     | 40   | GLU  | C-N-CA   | -5.12 | 118.90      | 122.59   |
| 1   | A     | 1427 | ASN  | CA-C-N   | 5.11  | 127.00      | 120.56   |
| 1   | A     | 1427 | ASN  | C-N-CA   | 5.11  | 127.00      | 120.56   |
| 8   | H     | 90   | ALA  | CA-C-N   | 5.11  | 130.50      | 120.99   |
| 8   | H     | 90   | ALA  | C-N-CA   | 5.11  | 130.50      | 120.99   |
| 10  | J     | 17   | LYS  | N-CA-C   | 5.10  | 117.58      | 111.71   |
| 2   | B     | 1143 | ALA  | CA-C-N   | 5.09  | 127.36      | 120.38   |
| 2   | B     | 1143 | ALA  | C-N-CA   | 5.09  | 127.36      | 120.38   |
| 1   | A     | 639  | PRO  | CA-C-N   | 5.09  | 127.10      | 120.28   |
| 1   | A     | 639  | PRO  | C-N-CA   | 5.09  | 127.10      | 120.28   |
| 1   | A     | 64   | ASN  | CA-C-N   | 5.08  | 131.25      | 121.54   |
| 1   | A     | 64   | ASN  | C-N-CA   | 5.08  | 131.25      | 121.54   |
| 2   | B     | 694  | ASP  | CA-CB-CG | 5.08  | 117.68      | 112.60   |
| 2   | B     | 847  | ASP  | CA-CB-CG | 5.08  | 117.68      | 112.60   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 5   | E     | 53   | PRO  | N-CA-C   | 5.07  | 119.17      | 110.95   |
| 2   | B     | 868  | MET  | CA-C-N   | 5.07  | 130.02      | 122.82   |
| 2   | B     | 868  | MET  | C-N-CA   | 5.07  | 130.02      | 122.82   |
| 1   | A     | 1029 | ARG  | CA-C-N   | 5.07  | 127.38      | 120.54   |
| 1   | A     | 1029 | ARG  | C-N-CA   | 5.07  | 127.38      | 120.54   |
| 1   | A     | 1308 | THR  | N-CA-C   | 5.07  | 117.50      | 109.50   |
| 2   | B     | 510  | LYS  | N-CA-C   | 5.07  | 121.00      | 109.81   |
| 2   | B     | 1153 | GLU  | CB-CG-CD | 5.07  | 121.21      | 112.60   |
| 5   | E     | 152  | LYS  | CA-C-N   | 5.06  | 129.13      | 122.30   |
| 5   | E     | 152  | LYS  | C-N-CA   | 5.06  | 129.13      | 122.30   |
| 10  | J     | 64   | ASN  | N-CA-C   | 5.06  | 121.00      | 109.81   |
| 13  | M     | 51   | VAL  | N-CA-CB  | 5.06  | 117.19      | 110.26   |
| 5   | E     | 165  | LEU  | CA-C-N   | 5.06  | 127.47      | 120.29   |
| 5   | E     | 165  | LEU  | C-N-CA   | 5.06  | 127.47      | 120.29   |
| 2   | B     | 1206 | GLU  | CB-CG-CD | 5.05  | 121.18      | 112.60   |
| 6   | F     | 145  | ASP  | CA-CB-CG | 5.05  | 117.65      | 112.60   |
| 4   | D     | 171  | GLY  | N-CA-C   | -5.04 | 108.32      | 115.43   |
| 2   | B     | 957  | ASN  | N-CA-C   | 5.03  | 114.93      | 108.34   |
| 2   | B     | 320  | ASP  | CA-CB-CG | 5.03  | 117.63      | 112.60   |
| 11  | K     | 82   | ASP  | CA-CB-CG | 5.02  | 117.62      | 112.60   |
| 1   | A     | 1102 | LYS  | CA-C-N   | 5.02  | 126.97      | 120.44   |
| 1   | A     | 1102 | LYS  | C-N-CA   | 5.02  | 126.97      | 120.44   |
| 8   | H     | 127  | GLY  | CA-C-N   | 5.01  | 131.11      | 121.54   |
| 8   | H     | 127  | GLY  | C-N-CA   | 5.01  | 131.11      | 121.54   |
| 1   | A     | 173  | THR  | CB-CA-C  | 5.01  | 119.68      | 111.41   |

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     | 11143 | 0        | 11217    | 174     | 0            |
| 2   | B     | 8910  | 0        | 8926     | 141     | 0            |
| 3   | C     | 2095  | 0        | 2051     | 31      | 0            |
| 4   | D     | 1434  | 0        | 1460     | 17      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 5   | E     | 1752  | 0        | 1776     | 27      | 0            |
| 6   | F     | 705   | 0        | 731      | 16      | 0            |
| 7   | G     | 1340  | 0        | 1357     | 29      | 0            |
| 8   | H     | 1076  | 0        | 1046     | 24      | 0            |
| 9   | I     | 971   | 0        | 927      | 13      | 0            |
| 10  | J     | 532   | 0        | 542      | 14      | 0            |
| 11  | K     | 919   | 0        | 929      | 15      | 0            |
| 12  | L     | 363   | 0        | 386      | 5       | 0            |
| 13  | M     | 1083  | 0        | 578      | 12      | 0            |
| 14  | A     | 2     | 0        | 0        | 0       | 0            |
| 14  | B     | 1     | 0        | 0        | 0       | 0            |
| 14  | C     | 1     | 0        | 0        | 0       | 0            |
| 14  | I     | 2     | 0        | 0        | 0       | 0            |
| 14  | J     | 1     | 0        | 0        | 0       | 0            |
| 14  | L     | 1     | 0        | 0        | 0       | 0            |
| 14  | M     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 32332 | 0        | 31926    | 454     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (454) 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:567:LYS:HB2  | 1:A:568:PRO:HD3   | 1.48                     | 0.94              |
| 1:A:465:TYR:HB3  | 2:B:976:ILE:HG21  | 1.60                     | 0.83              |
| 1:A:768:GLN:HG2  | 1:A:816:HIS:HA    | 1.62                     | 0.82              |
| 1:A:225:ASN:HD22 | 1:A:228:PHE:H     | 1.28                     | 0.81              |
| 3:C:142:VAL:H    | 10:J:16:ASP:HB3   | 1.46                     | 0.79              |
| 2:B:866:TYR:HB2  | 2:B:870:ILE:HB    | 1.67                     | 0.75              |
| 11:K:38:GLU:HG3  | 11:K:42:LEU:HD22  | 1.69                     | 0.75              |
| 1:A:250:ILE:HD13 | 13:M:62:GLU:HG2   | 1.68                     | 0.74              |
| 2:B:983:ARG:HD2  | 2:B:1091:TYR:HB3  | 1.70                     | 0.72              |
| 1:A:853:ASP:OD1  | 1:A:855:THR:HG22  | 1.90                     | 0.72              |
| 6:F:99:LEU:O     | 6:F:103:MET:HG2   | 1.88                     | 0.72              |
| 1:A:343:LYS:HE3  | 2:B:1151:LEU:HD23 | 1.72                     | 0.71              |
| 12:L:27:LEU:HD12 | 12:L:59:ALA:HB1   | 1.73                     | 0.70              |
| 2:B:583:ASN:HD21 | 2:B:628:THR:HG22  | 1.57                     | 0.70              |
| 2:B:1138:MET:HE3 | 2:B:1143:ALA:HB3  | 1.75                     | 0.69              |
| 11:K:49:GLU:HG3  | 11:K:94:ILE:HG12  | 1.73                     | 0.69              |
| 3:C:39:ALA:HA    | 3:C:164:ALA:HB3   | 1.75                     | 0.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:666:ILE:HD11  | 2:B:1030:LEU:HD13 | 1.76                     | 0.68              |
| 2:B:999:MET:HG3   | 2:B:1000:PRO:HD2  | 1.76                     | 0.67              |
| 2:B:865:LYS:HE2   | 2:B:869:SER:H     | 1.58                     | 0.67              |
| 1:A:958:VAL:HG11  | 1:A:1049:ILE:HG23 | 1.77                     | 0.67              |
| 2:B:710:LEU:HA    | 2:B:733:HIS:HB3   | 1.78                     | 0.66              |
| 1:A:567:LYS:HB3   | 8:H:96:VAL:H      | 1.61                     | 0.65              |
| 1:A:855:THR:CG2   | 1:A:857:ARG:HE    | 2.09                     | 0.65              |
| 1:A:640:GLN:HE21  | 1:A:641:VAL:HG23  | 1.61                     | 0.65              |
| 5:E:185:ALA:HA    | 5:E:190:LEU:HD12  | 1.78                     | 0.65              |
| 3:C:66:ARG:NH2    | 10:J:3:VAL:O      | 2.30                     | 0.65              |
| 3:C:99:LEU:HD12   | 3:C:118:LEU:HB3   | 1.77                     | 0.65              |
| 3:C:254:LYS:HB3   | 11:K:42:LEU:HD11  | 1.78                     | 0.65              |
| 8:H:95:TYR:HE2    | 8:H:97:MET:HG3    | 1.62                     | 0.64              |
| 2:B:25:ILE:HG21   | 2:B:658:ILE:HD13  | 1.77                     | 0.64              |
| 1:A:93:VAL:HG13   | 1:A:301:ALA:HB1   | 1.79                     | 0.64              |
| 6:F:124:GLU:HB3   | 6:F:130:ILE:HG13  | 1.79                     | 0.64              |
| 2:B:1111:MET:HG3  | 13:M:55:LYS:HG2   | 1.78                     | 0.64              |
| 1:A:121:LEU:HB3   | 1:A:141:LEU:HD21  | 1.80                     | 0.64              |
| 1:A:740:LEU:HD23  | 8:H:19:ARG:HH12   | 1.63                     | 0.63              |
| 1:A:946:VAL:HG22  | 5:E:201:LYS:HD2   | 1.81                     | 0.63              |
| 3:C:136:ASP:HB2   | 3:C:141:GLY:H     | 1.64                     | 0.63              |
| 3:C:259:LEU:HD21  | 11:K:91:CYS:HB3   | 1.79                     | 0.63              |
| 10:J:64:ASN:HB3   | 10:J:65:PRO:HD3   | 1.81                     | 0.62              |
| 1:A:225:ASN:ND2   | 1:A:228:PHE:H     | 1.98                     | 0.62              |
| 8:H:38:LEU:HD11   | 8:H:123:MET:HE2   | 1.82                     | 0.62              |
| 1:A:1124:HIS:HB3  | 1:A:1130:GLN:HG2  | 1.82                     | 0.62              |
| 7:G:85:GLU:HB3    | 7:G:147:ILE:HD12  | 1.82                     | 0.61              |
| 1:A:567:LYS:HB2   | 1:A:568:PRO:CD    | 2.27                     | 0.61              |
| 1:A:37:PHE:HB2    | 1:A:52:GLY:HA3    | 1.83                     | 0.61              |
| 1:A:855:THR:HG21  | 1:A:857:ARG:HE    | 1.65                     | 0.61              |
| 1:A:41:MET:HA     | 1:A:49:LYS:HA     | 1.82                     | 0.60              |
| 9:I:7:CYS:HB3     | 9:I:12:ASN:H      | 1.65                     | 0.60              |
| 1:A:445:ASN:HB2   | 1:A:455:MET:HG2   | 1.82                     | 0.60              |
| 1:A:1120:LEU:HD13 | 1:A:1125:ALA:HA   | 1.84                     | 0.60              |
| 1:A:350:ARG:HE    | 1:A:486:GLU:HB3   | 1.67                     | 0.59              |
| 3:C:70:ILE:HG12   | 3:C:142:VAL:HG11  | 1.83                     | 0.59              |
| 5:E:156:LEU:HD12  | 5:E:195:VAL:HB    | 1.84                     | 0.59              |
| 10:J:32:GLU:CD    | 10:J:32:GLU:H     | 2.10                     | 0.59              |
| 1:A:1224:LEU:HD11 | 1:A:1240:CYS:HB3  | 1.82                     | 0.59              |
| 1:A:1336:MET:HE2  | 1:A:1381:LEU:HB2  | 1.83                     | 0.59              |
| 6:F:109:VAL:HG21  | 6:F:124:GLU:HA    | 1.84                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:101:MET:HG2   | 2:B:111:ALA:HA    | 1.84                     | 0.59              |
| 2:B:925:LEU:HG    | 13:M:22:LEU:HD12  | 1.85                     | 0.59              |
| 1:A:345:VAL:HG12  | 2:B:1155:SER:HB2  | 1.85                     | 0.59              |
| 1:A:868:TYR:HD2   | 1:A:1058:VAL:HG21 | 1.67                     | 0.59              |
| 7:G:9:LEU:HD23    | 7:G:30:LEU:HD12   | 1.85                     | 0.58              |
| 1:A:755:PHE:HA    | 1:A:758:ILE:HD12  | 1.85                     | 0.58              |
| 1:A:1127:ASP:HB3  | 1:A:1130:GLN:HB3  | 1.84                     | 0.58              |
| 10:J:8:PHE:H      | 10:J:49:MET:HE3   | 1.67                     | 0.58              |
| 2:B:319:GLU:HG2   | 9:I:15:TYR:HE2    | 1.69                     | 0.58              |
| 2:B:925:LEU:HB3   | 2:B:928:ARG:HB3   | 1.85                     | 0.58              |
| 4:D:37:GLN:HE21   | 4:D:47:LEU:HD22   | 1.68                     | 0.58              |
| 1:A:785:PRO:HB2   | 2:B:703:ILE:HD12  | 1.86                     | 0.58              |
| 10:J:3:VAL:HG11   | 10:J:18:TRP:HB2   | 1.84                     | 0.58              |
| 1:A:692:ASP:HA    | 1:A:695:LYS:HD2   | 1.86                     | 0.57              |
| 8:H:95:TYR:CE2    | 8:H:97:MET:HG3    | 2.39                     | 0.57              |
| 2:B:238:ALA:HB3   | 2:B:256:VAL:HB    | 1.86                     | 0.57              |
| 1:A:150:THR:O     | 1:A:163:SER:HA    | 2.05                     | 0.57              |
| 1:A:902:LEU:HG    | 1:A:926:GLN:HG3   | 1.86                     | 0.56              |
| 2:B:226:PHE:HA    | 2:B:395:GLN:HG3   | 1.86                     | 0.56              |
| 1:A:49:LYS:HD2    | 1:A:55:ASP:HB3    | 1.85                     | 0.56              |
| 1:A:1441:PHE:CZ   | 6:F:89:GLU:HA     | 2.40                     | 0.56              |
| 2:B:705:MET:H     | 2:B:710:LEU:HD12  | 1.71                     | 0.56              |
| 1:A:567:LYS:CB    | 1:A:568:PRO:HD3   | 2.30                     | 0.56              |
| 2:B:999:MET:HG2   | 2:B:1007:VAL:HG13 | 1.87                     | 0.56              |
| 6:F:94:LEU:HD13   | 6:F:122:MET:HE2   | 1.87                     | 0.56              |
| 2:B:1124:ARG:HH12 | 13:M:60:ARG:HB2   | 1.71                     | 0.56              |
| 1:A:446:ARG:HG3   | 1:A:487:MET:HG2   | 1.87                     | 0.56              |
| 1:A:1407:GLU:CD   | 1:A:1407:GLU:H    | 2.13                     | 0.56              |
| 1:A:535:THR:HG21  | 1:A:617:VAL:HG23  | 1.88                     | 0.55              |
| 2:B:526:GLU:HG3   | 2:B:771:SER:HB3   | 1.89                     | 0.55              |
| 2:B:365:THR:HG21  | 2:B:370:PHE:HB2   | 1.89                     | 0.55              |
| 2:B:570:VAL:HB    | 2:B:573:GLN:HB3   | 1.89                     | 0.55              |
| 11:K:12:LEU:HA    | 11:K:37:LYS:HG3   | 1.88                     | 0.55              |
| 1:A:1342:GLU:HG3  | 5:E:198:ILE:HG21  | 1.88                     | 0.55              |
| 5:E:100:ILE:HG23  | 5:E:105:PHE:HB2   | 1.88                     | 0.55              |
| 2:B:530:GLY:O     | 2:B:532:ALA:N     | 2.40                     | 0.55              |
| 1:A:567:LYS:H     | 8:H:96:VAL:HB     | 1.72                     | 0.55              |
| 2:B:428:ILE:HG12  | 2:B:448:ILE:HG23  | 1.88                     | 0.55              |
| 3:C:177:GLU:HB2   | 3:C:231:ASN:HB3   | 1.89                     | 0.55              |
| 2:B:227:LYS:HE2   | 2:B:395:GLN:H     | 1.73                     | 0.54              |
| 2:B:1072:MET:HB3  | 2:B:1081:LEU:HD12 | 1.89                     | 0.54              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 8:H:40:LEU:HD13   | 8:H:123:MET:HG3  | 1.89                     | 0.54              |
| 5:E:88:VAL:HG11   | 5:E:110:PHE:HZ   | 1.73                     | 0.54              |
| 7:G:1:MET:HE1     | 7:G:79:PHE:HA    | 1.89                     | 0.54              |
| 12:L:55:ILE:HG12  | 12:L:56:LEU:H    | 1.72                     | 0.54              |
| 2:B:1167:GLY:HA3  | 2:B:1216:LEU:H   | 1.72                     | 0.54              |
| 2:B:114:PRO:HG3   | 2:B:181:LEU:HD11 | 1.89                     | 0.54              |
| 2:B:763:GLN:HG2   | 2:B:765:PRO:HD2  | 1.91                     | 0.54              |
| 1:A:532:ARG:HG3   | 1:A:618:GLU:HB3  | 1.90                     | 0.53              |
| 1:A:492:PRO:HG3   | 1:A:501:LEU:HD12 | 1.90                     | 0.53              |
| 2:B:364:ILE:HG12  | 2:B:585:VAL:HG13 | 1.90                     | 0.53              |
| 5:E:24:LYS:HD2    | 5:E:30:ILE:HG22  | 1.91                     | 0.53              |
| 2:B:521:LEU:HA    | 2:B:543:SER:HB3  | 1.89                     | 0.53              |
| 1:A:49:LYS:HZ2    | 1:A:60:SER:HA    | 1.72                     | 0.53              |
| 1:A:387:ARG:HH12  | 1:A:434:ARG:HH11 | 1.57                     | 0.53              |
| 1:A:405:VAL:HG23  | 1:A:415:LEU:HD11 | 1.91                     | 0.53              |
| 6:F:138:LEU:HD23  | 6:F:139:PRO:HD2  | 1.90                     | 0.53              |
| 7:G:45:ILE:HA     | 7:G:78:VAL:HG12  | 1.91                     | 0.53              |
| 1:A:596:THR:C     | 1:A:598:LEU:H    | 2.17                     | 0.52              |
| 6:F:74:ILE:HD11   | 6:F:142:SER:HB3  | 1.90                     | 0.52              |
| 1:A:320:ARG:HE    | 1:A:323:LYS:HE3  | 1.74                     | 0.52              |
| 1:A:1433:MET:HG3  | 7:G:63:PRO:HB2   | 1.92                     | 0.52              |
| 1:A:87:ALA:HB3    | 1:A:276:LEU:HD23 | 1.92                     | 0.52              |
| 1:A:583:PRO:O     | 1:A:586:ILE:HG12 | 2.10                     | 0.52              |
| 7:G:111:THR:HG22  | 7:G:114:LEU:HD22 | 1.91                     | 0.52              |
| 8:H:91:ASP:C      | 8:H:93:TYR:H     | 2.17                     | 0.52              |
| 1:A:1211:GLN:HE22 | 1:A:1274:ARG:HD2 | 1.74                     | 0.52              |
| 2:B:241:ARG:HA    | 2:B:253:THR:HG22 | 1.92                     | 0.52              |
| 1:A:949:ASP:HB2   | 1:A:1290:LYS:HD3 | 1.91                     | 0.52              |
| 1:A:1187:GLN:HA   | 1:A:1244:ARG:HE  | 1.73                     | 0.52              |
| 10:J:7:CYS:HA     | 10:J:49:MET:HG2  | 1.92                     | 0.52              |
| 1:A:42:ASP:HA     | 1:A:46:THR:O     | 2.09                     | 0.52              |
| 7:G:114:LEU:HG    | 7:G:162:SER:HB3  | 1.92                     | 0.52              |
| 1:A:337:ARG:HA    | 1:A:341:MET:HB2  | 1.93                     | 0.52              |
| 2:B:121:ASN:HD22  | 2:B:207:GLY:HA3  | 1.75                     | 0.52              |
| 1:A:680:THR:HA    | 1:A:683:ILE:HD12 | 1.92                     | 0.51              |
| 1:A:315:LEU:HA    | 1:A:321:PRO:HA   | 1.92                     | 0.51              |
| 2:B:637:LEU:HB2   | 2:B:693:ILE:HD13 | 1.92                     | 0.51              |
| 4:D:202:ILE:HG21  | 4:D:207:LEU:HD13 | 1.92                     | 0.51              |
| 3:C:51:VAL:HA     | 3:C:155:LEU:HD23 | 1.92                     | 0.51              |
| 11:K:27:ALA:HB3   | 11:K:74:ARG:HH12 | 1.74                     | 0.51              |
| 1:A:115:LEU:HD12  | 1:A:142:CYS:HB3  | 1.91                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:378:GLU:O     | 1:A:431:LYS:HA    | 2.11                     | 0.51              |
| 2:B:521:LEU:HD22  | 2:B:633:VAL:HG12  | 1.92                     | 0.51              |
| 1:A:531:ILE:HD11  | 1:A:578:LEU:HD21  | 1.93                     | 0.51              |
| 1:A:667:GLY:HA2   | 1:A:670:ILE:HD12  | 1.92                     | 0.51              |
| 2:B:35:SER:HA     | 2:B:811:TYR:HE2   | 1.75                     | 0.50              |
| 1:A:1161:THR:HG23 | 1:A:1239:ARG:HH21 | 1.76                     | 0.50              |
| 2:B:412:LEU:HB3   | 2:B:466:TRP:HZ2   | 1.77                     | 0.50              |
| 1:A:56:PRO:HD2    | 1:A:58:LEU:HG     | 1.92                     | 0.50              |
| 2:B:1106:ARG:HG2  | 2:B:1127:GLY:HA2  | 1.94                     | 0.50              |
| 13:M:63:TRP:HA    | 13:M:66:PHE:HD2   | 1.76                     | 0.50              |
| 1:A:351:THR:HG22  | 1:A:468:PHE:CD1   | 2.45                     | 0.50              |
| 1:A:696:GLU:HB3   | 1:A:702:LEU:HB2   | 1.94                     | 0.50              |
| 2:B:514:LEU:HD12  | 2:B:518:HIS:HD2   | 1.75                     | 0.50              |
| 1:A:216:VAL:HA    | 1:A:219:PHE:HB2   | 1.92                     | 0.50              |
| 1:A:770:VAL:HG13  | 1:A:822:GLU:HG3   | 1.93                     | 0.50              |
| 4:D:180:LEU:HD11  | 4:D:198:LEU:HD21  | 1.94                     | 0.50              |
| 6:F:103:MET:HG3   | 7:G:15:PRO:HG2    | 1.94                     | 0.50              |
| 4:D:207:LEU:HA    | 4:D:210:ILE:HD12  | 1.93                     | 0.50              |
| 1:A:528:LEU:HD23  | 1:A:751:SER:HA    | 1.94                     | 0.49              |
| 2:B:420:LEU:HD21  | 2:B:456:GLY:HA3   | 1.93                     | 0.49              |
| 3:C:97:VAL:HG11   | 3:C:130:GLY:HA3   | 1.94                     | 0.49              |
| 8:H:40:LEU:HD11   | 8:H:97:MET:HE1    | 1.94                     | 0.49              |
| 11:K:58:PHE:HB3   | 11:K:76:GLN:HB3   | 1.94                     | 0.49              |
| 2:B:800:GLN:HB2   | 2:B:821:GLN:HA    | 1.93                     | 0.49              |
| 2:B:979:LYS:HB3   | 2:B:1095:LEU:HB2  | 1.92                     | 0.49              |
| 2:B:405:ARG:CZ    | 2:B:632:ARG:HG2   | 2.43                     | 0.49              |
| 6:F:128:LYS:HD2   | 6:F:149:GLU:HA    | 1.95                     | 0.49              |
| 1:A:472:LEU:O     | 1:A:475:THR:HG22  | 2.12                     | 0.49              |
| 2:B:840:ILE:HG12  | 2:B:992:ILE:HG22  | 1.94                     | 0.49              |
| 3:C:142:VAL:N     | 10:J:16:ASP:HB3   | 2.23                     | 0.49              |
| 1:A:752:LYS:HG3   | 2:B:1015:HIS:HB3  | 1.94                     | 0.49              |
| 3:C:196:ASP:O     | 3:C:200:GLU:HB2   | 2.12                     | 0.49              |
| 2:B:64:CYS:HA     | 2:B:67:SER:HB3    | 1.95                     | 0.49              |
| 2:B:644:GLU:HB3   | 2:B:648:HIS:O     | 2.12                     | 0.49              |
| 9:I:19:ASP:HB3    | 9:I:24:ARG:HG3    | 1.95                     | 0.49              |
| 2:B:703:ILE:HA    | 2:B:740:HIS:O     | 2.13                     | 0.48              |
| 1:A:406:ILE:HG13  | 1:A:412:ARG:HG3   | 1.95                     | 0.48              |
| 4:D:32:GLU:HB3    | 7:G:5:LYS:HE2     | 1.96                     | 0.48              |
| 7:G:21:ARG:HD2    | 7:G:24:GLN:HB2    | 1.94                     | 0.48              |
| 12:L:28:LYS:HB3   | 12:L:39:SER:HA    | 1.95                     | 0.48              |
| 9:I:73:ARG:HH12   | 9:I:112:SER:HA    | 1.79                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:E:101:GLN:HG3   | 5:E:127:ILE:HD13  | 1.95                     | 0.48              |
| 1:A:1121:GLU:HB3  | 1:A:1124:HIS:HD2  | 1.78                     | 0.48              |
| 2:B:487:THR:HG21  | 2:B:819:ALA:HB2   | 1.94                     | 0.48              |
| 2:B:601:ARG:HG3   | 2:B:615:MET:HE1   | 1.94                     | 0.48              |
| 2:B:602:THR:HA    | 2:B:605:ARG:HB2   | 1.96                     | 0.48              |
| 4:D:25:ALA:HB2    | 7:G:84:GLY:HA3    | 1.96                     | 0.48              |
| 4:D:139:LYS:HA    | 4:D:142:LYS:HD2   | 1.95                     | 0.48              |
| 5:E:78:LEU:HD12   | 5:E:107:THR:HB    | 1.94                     | 0.48              |
| 5:E:77:SER:HB2    | 5:E:105:PHE:HA    | 1.96                     | 0.48              |
| 4:D:48:ILE:HG21   | 7:G:4:ILE:HB      | 1.96                     | 0.48              |
| 1:A:637:LYS:HB3   | 1:A:641:VAL:HG11  | 1.96                     | 0.47              |
| 1:A:923:LEU:HA    | 1:A:926:GLN:HB2   | 1.96                     | 0.47              |
| 2:B:842:ASN:HD21  | 2:B:996:ARG:HG3   | 1.78                     | 0.47              |
| 5:E:193:GLY:H     | 5:E:214:CYS:HB3   | 1.79                     | 0.47              |
| 1:A:1377:THR:HG22 | 5:E:176:PRO:HB3   | 1.97                     | 0.47              |
| 1:A:346:ASP:CG    | 2:B:1108:ARG:HA   | 2.39                     | 0.47              |
| 2:B:603:LEU:HD12  | 2:B:609:ILE:HG12  | 1.95                     | 0.47              |
| 1:A:71:GLN:HE21   | 13:M:18:LEU:HD23  | 1.80                     | 0.47              |
| 1:A:594:GLY:H     | 1:A:603:ASN:HD22  | 1.62                     | 0.47              |
| 6:F:72:LYS:HB2    | 6:F:142:SER:HA    | 1.96                     | 0.47              |
| 2:B:762:ASN:HD22  | 2:B:1024:ALA:HB3  | 1.79                     | 0.47              |
| 7:G:96:GLN:H      | 7:G:96:GLN:HE21   | 1.63                     | 0.47              |
| 10:J:43:ARG:HG3   | 10:J:45:CYS:SG    | 2.54                     | 0.47              |
| 2:B:1082:MET:HA   | 3:C:189:THR:HA    | 1.97                     | 0.47              |
| 5:E:56:LYS:HE2    | 5:E:84:ASP:H      | 1.79                     | 0.47              |
| 3:C:174:ALA:HB1   | 10:J:11:GLY:HA3   | 1.96                     | 0.47              |
| 4:D:138:ASN:HB3   | 4:D:141:LEU:HB3   | 1.96                     | 0.47              |
| 2:B:883:LEU:HD23  | 2:B:884:ARG:H     | 1.79                     | 0.47              |
| 8:H:47:PHE:CD2    | 8:H:95:TYR:HD1    | 2.33                     | 0.47              |
| 10:J:17:LYS:HG2   | 10:J:41:LEU:HD21  | 1.97                     | 0.47              |
| 1:A:1219:THR:HG21 | 1:A:1271:ILE:HG12 | 1.97                     | 0.46              |
| 1:A:441:PRO:HG2   | 1:A:498:ARG:HB2   | 1.97                     | 0.46              |
| 1:A:443:LEU:HD22  | 1:A:455:MET:HE2   | 1.98                     | 0.46              |
| 1:A:775:ILE:O     | 1:A:797:LYS:HD2   | 2.15                     | 0.46              |
| 2:B:555:ILE:HA    | 2:B:558:LEU:HD12  | 1.96                     | 0.46              |
| 2:B:802:PRO:HA    | 2:B:822:ASN:HD21  | 1.79                     | 0.46              |
| 2:B:211:VAL:HG21  | 2:B:483:LEU:HD13  | 1.98                     | 0.46              |
| 8:H:4:THR:HA      | 8:H:60:ALA:HB2    | 1.97                     | 0.46              |
| 1:A:32:VAL:O      | 1:A:57:ARG:HD2    | 2.15                     | 0.46              |
| 2:B:1159:ARG:HD3  | 2:B:1193:GLN:HB2  | 1.98                     | 0.46              |
| 4:D:52:LEU:H      | 4:D:182:SER:HB3   | 1.80                     | 0.46              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:D:206:GLU:HA   | 4:D:209:ARG:HD2   | 1.98                     | 0.46              |
| 1:A:963:ILE:HG22 | 1:A:1045:VAL:HG22 | 1.98                     | 0.46              |
| 1:A:1060:PRO:HD2 | 6:F:86:THR:HG21   | 1.96                     | 0.46              |
| 2:B:640:VAL:HA   | 2:B:651:LEU:HA    | 1.96                     | 0.46              |
| 3:C:148:ARG:HB3  | 3:C:151:GLN:NE2   | 2.31                     | 0.46              |
| 3:C:175:ALA:HB2  | 10:J:10:CYS:HB2   | 1.97                     | 0.46              |
| 7:G:143:ILE:HG22 | 7:G:145:VAL:HG22  | 1.97                     | 0.46              |
| 1:A:83:HIS:HB2   | 1:A:238:CYS:SG    | 2.55                     | 0.46              |
| 1:A:453:MET:HB3  | 1:A:477:PRO:HB3   | 1.97                     | 0.46              |
| 1:A:857:ARG:HD3  | 1:A:861:GLY:O     | 2.16                     | 0.46              |
| 2:B:515:HIS:HD2  | 2:B:517:THR:OG1   | 1.99                     | 0.46              |
| 2:B:553:PRO:HG2  | 2:B:554:ILE:HD12  | 1.96                     | 0.46              |
| 2:B:582:VAL:HG22 | 2:B:626:ILE:HB    | 1.97                     | 0.46              |
| 2:B:979:LYS:HE2  | 2:B:987:LYS:HB2   | 1.96                     | 0.46              |
| 2:B:234:ILE:HG23 | 2:B:258:LEU:H     | 1.81                     | 0.46              |
| 11:K:90:ALA:O    | 11:K:94:ILE:HG13  | 2.16                     | 0.46              |
| 1:A:17:VAL:HB    | 1:A:1419:ASP:HB3  | 1.96                     | 0.46              |
| 1:A:1152:ILE:HB  | 9:I:44:TYR:HB3    | 1.97                     | 0.46              |
| 2:B:122:LEU:HD22 | 2:B:958:GLN:HG3   | 1.98                     | 0.46              |
| 2:B:796:LEU:HD23 | 2:B:799:PRO:HA    | 1.97                     | 0.46              |
| 2:B:927:GLN:HA   | 2:B:930:ALA:HB3   | 1.98                     | 0.46              |
| 2:B:1180:PHE:H   | 2:B:1188:LYS:HE3  | 1.81                     | 0.46              |
| 5:E:90:VAL:HA    | 5:E:120:ALA:HB2   | 1.96                     | 0.46              |
| 1:A:54:ASN:HB3   | 1:A:247:ARG:HH12  | 1.80                     | 0.46              |
| 1:A:445:ASN:HB2  | 1:A:455:MET:HA    | 1.98                     | 0.46              |
| 2:B:614:SER:HB3  | 2:B:627:PHE:HB2   | 1.97                     | 0.46              |
| 5:E:168:TYR:HB3  | 5:E:170:LEU:HD21  | 1.98                     | 0.46              |
| 1:A:1317:MET:HG3 | 1:A:1327:ILE:HG21 | 1.97                     | 0.46              |
| 2:B:620:ARG:HH21 | 9:I:89:GLN:HG2    | 1.81                     | 0.46              |
| 2:B:942:ARG:HB2  | 2:B:945:GLU:HB2   | 1.98                     | 0.46              |
| 4:D:203:SER:HB3  | 4:D:206:GLU:HB2   | 1.97                     | 0.46              |
| 5:E:100:ILE:HA   | 5:E:105:PHE:HD1   | 1.80                     | 0.46              |
| 11:K:65:HIS:HD2  | 11:K:67:PHE:HB2   | 1.80                     | 0.46              |
| 1:A:377:PRO:HD3  | 1:A:493:GLN:OE1   | 2.16                     | 0.45              |
| 2:B:123:THR:HG23 | 2:B:205:ILE:HA    | 1.98                     | 0.45              |
| 2:B:276:ILE:HG23 | 2:B:336:ARG:HB2   | 1.98                     | 0.45              |
| 4:D:40:HIS:ND1   | 7:G:6:ASP:HB3     | 2.30                     | 0.45              |
| 2:B:834:ASN:O    | 2:B:1013:ASN:HB2  | 2.16                     | 0.45              |
| 8:H:125:LEU:HG   | 8:H:126:GLU:H     | 1.80                     | 0.45              |
| 1:A:55:ASP:C     | 1:A:57:ARG:H      | 2.25                     | 0.45              |
| 1:A:456:MET:HB2  | 1:A:478:TYR:OH    | 2.16                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:633:VAL:HG11  | 1:A:645:LEU:HD22  | 1.97                     | 0.45              |
| 1:A:722:LEU:HD21  | 1:A:794:PRO:HB3   | 1.97                     | 0.45              |
| 8:H:41:ASP:HB3    | 8:H:121:LEU:HD22  | 1.98                     | 0.45              |
| 1:A:55:ASP:N      | 1:A:56:PRO:HD3    | 2.31                     | 0.45              |
| 1:A:683:ILE:HG21  | 1:A:801:GLU:HB2   | 1.98                     | 0.45              |
| 2:B:170:LEU:HG    | 2:B:171:PRO:HD2   | 1.98                     | 0.45              |
| 2:B:282:ILE:HA    | 2:B:285:ILE:HD12  | 1.99                     | 0.45              |
| 7:G:112:LYS:HA    | 7:G:115:MET:HE3   | 1.99                     | 0.45              |
| 8:H:42:ILE:HD13   | 8:H:49:VAL:HG21   | 1.99                     | 0.45              |
| 1:A:329:LEU:HA    | 1:A:335:ARG:HB3   | 1.97                     | 0.45              |
| 1:A:446:ARG:HB3   | 1:A:446:ARG:HH11  | 1.82                     | 0.45              |
| 1:A:511:ILE:HA    | 1:A:521:MET:HE3   | 1.99                     | 0.45              |
| 7:G:130:TYR:O     | 7:G:136:VAL:HA    | 2.17                     | 0.45              |
| 1:A:353:ILE:HG21  | 1:A:487:MET:HG3   | 1.98                     | 0.45              |
| 2:B:801:LYS:O     | 10:J:52:THR:HG23  | 2.17                     | 0.45              |
| 2:B:1034:VAL:HG22 | 2:B:1059:LEU:HB2  | 1.99                     | 0.45              |
| 3:C:252:GLN:HE22  | 11:K:102:LYS:HE3  | 1.82                     | 0.45              |
| 4:D:167:LEU:HD21  | 4:D:214:LEU:HD21  | 1.99                     | 0.45              |
| 1:A:1260:LEU:HA   | 1:A:1263:ILE:HD12 | 1.98                     | 0.45              |
| 2:B:806:THR:H     | 2:B:809:MET:HE3   | 1.82                     | 0.45              |
| 2:B:999:MET:HE2   | 2:B:1011:ILE:HD12 | 1.99                     | 0.45              |
| 1:A:855:THR:HG23  | 1:A:857:ARG:HE    | 1.82                     | 0.44              |
| 1:A:857:ARG:HG2   | 1:A:863:VAL:HA    | 1.99                     | 0.44              |
| 1:A:858:ASN:HD21  | 1:A:860:LEU:HD12  | 1.82                     | 0.44              |
| 1:A:1148:ILE:HG23 | 9:I:49:ILE:HB     | 1.99                     | 0.44              |
| 2:B:950:ASP:HB2   | 2:B:969:ARG:HG3   | 1.98                     | 0.44              |
| 13:M:37:ARG:HD3   | 13:M:37:ARG:HA    | 1.89                     | 0.44              |
| 1:A:261:ASP:HB3   | 1:A:322:VAL:HG22  | 1.99                     | 0.44              |
| 5:E:62:ALA:HB3    | 5:E:78:LEU:HD23   | 1.98                     | 0.44              |
| 5:E:97:VAL:HG21   | 5:E:123:LEU:HB3   | 1.98                     | 0.44              |
| 5:E:198:ILE:HD11  | 5:E:212:ARG:HB2   | 1.99                     | 0.44              |
| 13:M:62:GLU:HA    | 13:M:65:THR:HG22  | 1.98                     | 0.44              |
| 7:G:96:GLN:H      | 7:G:96:GLN:NE2    | 2.15                     | 0.44              |
| 1:A:1444:MET:HG3  | 7:G:60:ARG:HA     | 2.00                     | 0.44              |
| 2:B:1084:GLN:HG2  | 3:C:201:TRP:CZ2   | 2.52                     | 0.44              |
| 7:G:46:LEU:HD11   | 7:G:79:PHE:HB2    | 2.00                     | 0.44              |
| 1:A:1210:GLY:O    | 1:A:1214:GLU:HG2  | 2.18                     | 0.44              |
| 2:B:124:TYR:HB2   | 2:B:204:ILE:HB    | 2.00                     | 0.44              |
| 2:B:168:GLY:H     | 2:B:450:ALA:HB1   | 1.83                     | 0.44              |
| 2:B:792:MET:HE2   | 2:B:857:ARG:HH21  | 1.80                     | 0.44              |
| 2:B:797:TYR:HB2   | 2:B:852:ARG:O     | 2.17                     | 0.44              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:E:154:ILE:O    | 5:E:196:VAL:HA    | 2.18                     | 0.44              |
| 11:K:85:ASP:HA   | 11:K:88:LYS:HD2   | 1.99                     | 0.44              |
| 1:A:38:PRO:HB3   | 1:A:270:LEU:HB3   | 1.99                     | 0.44              |
| 10:J:1:MET:N     | 10:J:54:VAL:O     | 2.51                     | 0.44              |
| 1:A:658:LEU:HD23 | 1:A:659:HIS:CD2   | 2.52                     | 0.44              |
| 2:B:898:LEU:HD21 | 2:B:964:VAL:HG21  | 1.98                     | 0.44              |
| 1:A:849:MET:HB3  | 1:A:1063:MET:SD   | 2.57                     | 0.43              |
| 2:B:711:GLU:H    | 2:B:712:PRO:HD2   | 1.83                     | 0.43              |
| 2:B:918:ILE:HB   | 2:B:935:ARG:HG2   | 1.99                     | 0.43              |
| 2:B:1169:MET:HE3 | 2:B:1169:MET:H    | 1.83                     | 0.43              |
| 1:A:180:LYS:HE2  | 1:A:297:GLN:HG2   | 1.99                     | 0.43              |
| 2:B:773:MET:HE2  | 2:B:985:GLY:HA2   | 1.99                     | 0.43              |
| 13:M:29:VAL:HG23 | 13:M:32:PRO:HB3   | 2.00                     | 0.43              |
| 1:A:84:ILE:HB    | 1:A:239:LEU:HB3   | 1.99                     | 0.43              |
| 1:A:940:ARG:HG2  | 1:A:941:LYS:HE3   | 2.00                     | 0.43              |
| 1:A:1340:GLY:HA2 | 5:E:183:PRO:HD2   | 1.99                     | 0.43              |
| 8:H:135:LEU:HD22 | 8:H:137:GLN:HE21  | 1.83                     | 0.43              |
| 13:M:30:TYR:O    | 13:M:32:PRO:HD3   | 2.18                     | 0.43              |
| 1:A:631:HIS:HE1  | 1:A:879:GLU:HG2   | 1.83                     | 0.43              |
| 1:A:1447:GLU:HG3 | 7:G:56:ILE:HG12   | 2.01                     | 0.43              |
| 2:B:642:ASP:HA   | 2:B:649:LYS:HA    | 2.00                     | 0.43              |
| 3:C:51:VAL:HG21  | 3:C:60:ASP:HB3    | 2.00                     | 0.43              |
| 3:C:238:ILE:HG13 | 3:C:239:PRO:HD2   | 2.00                     | 0.43              |
| 7:G:1:MET:HE2    | 7:G:2:PHE:HA      | 2.00                     | 0.43              |
| 1:A:254:GLU:HB2  | 2:B:918:ILE:HG21  | 2.01                     | 0.43              |
| 1:A:554:PRO:HG3  | 1:A:651:LYS:HE3   | 2.00                     | 0.43              |
| 1:A:592:ASP:H    | 1:A:595:THR:HG21  | 1.83                     | 0.43              |
| 1:A:640:GLN:CD   | 1:A:640:GLN:H     | 2.26                     | 0.43              |
| 2:B:315:LYS:HE3  | 9:I:13:MET:HE1    | 1.99                     | 0.43              |
| 8:H:87:ARG:HB2   | 8:H:89:LEU:HD11   | 2.00                     | 0.43              |
| 1:A:114:LEU:HD11 | 1:A:171:GLN:HG3   | 2.01                     | 0.43              |
| 1:A:453:MET:HB3  | 1:A:477:PRO:CB    | 2.49                     | 0.43              |
| 3:C:194:GLU:HB3  | 3:C:195:GLN:HE21  | 1.84                     | 0.43              |
| 1:A:497:THR:HG23 | 2:B:1146:PHE:HA   | 2.00                     | 0.43              |
| 1:A:500:GLU:O    | 1:A:504:LEU:HB2   | 2.19                     | 0.43              |
| 2:B:1138:MET:HB2 | 2:B:1147:LEU:HD13 | 2.00                     | 0.43              |
| 2:B:365:THR:HG22 | 2:B:374:LYS:HE3   | 2.00                     | 0.43              |
| 2:B:756:ILE:O    | 2:B:759:PRO:HD3   | 2.19                     | 0.43              |
| 2:B:925:LEU:HB3  | 2:B:928:ARG:CB    | 2.48                     | 0.43              |
| 8:H:97:MET:HE3   | 8:H:142:LEU:HD23  | 2.01                     | 0.43              |
| 8:H:118:PHE:HE1  | 8:H:123:MET:HB2   | 1.84                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:I:26:LEU:HG     | 9:I:37:GLU:HA     | 2.00                     | 0.43              |
| 12:L:32:ALA:HB3   | 12:L:55:ILE:HG13  | 1.99                     | 0.43              |
| 1:A:709:THR:HG23  | 9:I:94:ASP:HA     | 2.01                     | 0.43              |
| 2:B:659:ALA:HA    | 2:B:662:MET:HE2   | 2.01                     | 0.43              |
| 1:A:408:ASP:H     | 1:A:430:TRP:CD1   | 2.37                     | 0.43              |
| 7:G:129:SER:HB3   | 7:G:138:THR:HG23  | 2.01                     | 0.43              |
| 1:A:998:LEU:HA    | 1:A:1011:GLN:HE22 | 1.84                     | 0.42              |
| 4:D:37:GLN:NE2    | 4:D:48:ILE:HG12   | 2.34                     | 0.42              |
| 12:L:31:CYS:SG    | 12:L:55:ILE:HD11  | 2.58                     | 0.42              |
| 1:A:12:ARG:O      | 2:B:1194:ILE:HG22 | 2.20                     | 0.42              |
| 2:B:120:ARG:HG2   | 2:B:955:THR:HG21  | 2.01                     | 0.42              |
| 2:B:331:LEU:HA    | 2:B:334:ILE:HD12  | 2.00                     | 0.42              |
| 2:B:420:LEU:HD22  | 2:B:453:ILE:HA    | 2.01                     | 0.42              |
| 5:E:180:ARG:HH21  | 5:E:192:ARG:HH11  | 1.66                     | 0.42              |
| 6:F:102:SER:C     | 6:F:104:ASN:H     | 2.26                     | 0.42              |
| 1:A:867:ILE:HG12  | 1:A:1000:LEU:HD11 | 2.00                     | 0.42              |
| 3:C:84:ARG:HD2    | 11:K:11:LEU:HD11  | 2.01                     | 0.42              |
| 1:A:326:ARG:HG3   | 1:A:1406:VAL:HG11 | 2.02                     | 0.42              |
| 2:B:308:TRP:HA    | 2:B:311:LEU:HB2   | 2.01                     | 0.42              |
| 7:G:143:ILE:HG13  | 7:G:170:ALA:HA    | 2.01                     | 0.42              |
| 1:A:50:ILE:H      | 1:A:50:ILE:HG13   | 1.74                     | 0.42              |
| 1:A:663:SER:CB    | 2:B:1085:ILE:HA   | 2.50                     | 0.42              |
| 1:A:679:ILE:HD11  | 1:A:733:ALA:HB2   | 2.01                     | 0.42              |
| 2:B:515:HIS:CD2   | 2:B:517:THR:H     | 2.37                     | 0.42              |
| 8:H:23:VAL:HG21   | 8:H:121:LEU:HD21  | 2.02                     | 0.42              |
| 1:A:92:HIS:CG     | 1:A:95:PHE:HD1    | 2.38                     | 0.42              |
| 1:A:635:ARG:NH2   | 1:A:877:HIS:HA    | 2.34                     | 0.42              |
| 1:A:853:ASP:CG    | 1:A:855:THR:HG22  | 2.44                     | 0.42              |
| 2:B:22:SER:HB3    | 2:B:654:ARG:HH11  | 1.85                     | 0.42              |
| 1:A:1428:VAL:HG11 | 2:B:1135:ARG:HD2  | 2.02                     | 0.42              |
| 2:B:1167:GLY:HA3  | 2:B:1216:LEU:N    | 2.35                     | 0.42              |
| 3:C:164:ALA:HA    | 3:C:167:HIS:O     | 2.20                     | 0.42              |
| 6:F:103:MET:HB2   | 7:G:15:PRO:HB2    | 2.01                     | 0.42              |
| 1:A:567:LYS:CB    | 1:A:568:PRO:CD    | 2.95                     | 0.42              |
| 1:A:1438:THR:HG23 | 6:F:92:ARG:HB2    | 2.02                     | 0.42              |
| 2:B:169:ARG:HB2   | 2:B:454:THR:HG23  | 2.01                     | 0.42              |
| 2:B:758:PHE:HZ    | 2:B:1031:LEU:HD13 | 1.83                     | 0.42              |
| 4:D:29:LEU:HB3    | 4:D:33:PHE:HB2    | 2.01                     | 0.42              |
| 7:G:13:LEU:HD22   | 7:G:17:PHE:HB2    | 2.02                     | 0.42              |
| 1:A:114:LEU:HD22  | 1:A:145:LYS:HB3   | 2.01                     | 0.42              |
| 1:A:606:LEU:HG    | 1:A:613:ILE:HD13  | 2.02                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:956:LEU:HD11  | 1:A:1017:LEU:HG   | 2.02                     | 0.42              |
| 3:C:87:PHE:CD1    | 3:C:87:PHE:N      | 2.88                     | 0.42              |
| 7:G:30:LEU:HD11   | 7:G:74:TYR:CD2    | 2.53                     | 0.42              |
| 11:K:56:VAL:HG22  | 11:K:77:THR:HG22  | 2.01                     | 0.42              |
| 13:M:63:TRP:HA    | 13:M:66:PHE:CD2   | 2.55                     | 0.42              |
| 1:A:42:ASP:HB3    | 1:A:45:GLN:HA     | 2.02                     | 0.41              |
| 1:A:543:LEU:O     | 1:A:547:LEU:HG    | 2.20                     | 0.41              |
| 1:A:1256:GLU:HA   | 1:A:1259:MET:HB3  | 2.02                     | 0.41              |
| 2:B:324:ILE:HD13  | 2:B:330:ALA:HA    | 2.02                     | 0.41              |
| 8:H:80:ARG:HG2    | 11:K:57:LEU:HD22  | 2.02                     | 0.41              |
| 8:H:93:TYR:HA     | 8:H:145:ARG:HB3   | 2.02                     | 0.41              |
| 2:B:610:ASN:HA    | 2:B:611:PRO:HD3   | 1.92                     | 0.41              |
| 2:B:856:PHE:HA    | 2:B:968:VAL:O     | 2.20                     | 0.41              |
| 2:B:1172:ILE:HG12 | 2:B:1183:LYS:HE2  | 2.02                     | 0.41              |
| 3:C:70:ILE:HG23   | 3:C:142:VAL:HG21  | 2.01                     | 0.41              |
| 8:H:63:LEU:HB3    | 8:H:90:ALA:H      | 1.85                     | 0.41              |
| 1:A:35:ILE:HA     | 1:A:52:GLY:O      | 2.20                     | 0.41              |
| 2:B:542:MET:HE2   | 2:B:747:MET:HE2   | 2.02                     | 0.41              |
| 2:B:847:ASP:OD2   | 11:K:6:ARG:NH2    | 2.53                     | 0.41              |
| 1:A:701:LEU:HA    | 9:I:115:LYS:HE3   | 2.02                     | 0.41              |
| 2:B:259:TYR:HB2   | 2:B:268:THR:HG23  | 2.02                     | 0.41              |
| 2:B:401:PHE:HB3   | 2:B:695:ALA:HB1   | 2.02                     | 0.41              |
| 2:B:681:TRP:HA    | 2:B:684:LEU:HD12  | 2.02                     | 0.41              |
| 5:E:165:LEU:HD23  | 5:E:170:LEU:HD12  | 2.02                     | 0.41              |
| 1:A:825:ILE:HD13  | 2:B:513:GLN:HE21  | 1.85                     | 0.41              |
| 1:A:1193:LEU:HB2  | 1:A:1260:LEU:HD23 | 2.02                     | 0.41              |
| 2:B:275:TYR:HD2   | 2:B:355:ILE:HD11  | 1.84                     | 0.41              |
| 2:B:638:PHE:HA    | 2:B:690:VAL:HG12  | 2.02                     | 0.41              |
| 3:C:201:TRP:HA    | 3:C:202:PRO:HD3   | 1.92                     | 0.41              |
| 5:E:97:VAL:HG13   | 5:E:127:ILE:HG12  | 2.02                     | 0.41              |
| 1:A:254:GLU:HG2   | 2:B:920:PRO:HG2   | 2.03                     | 0.41              |
| 1:A:518:LYS:HB3   | 1:A:626:ASN:HD22  | 1.84                     | 0.41              |
| 2:B:211:VAL:HG11  | 2:B:495:LEU:HA    | 2.01                     | 0.41              |
| 2:B:637:LEU:HA    | 2:B:743:ILE:HD11  | 2.02                     | 0.41              |
| 5:E:66:GLU:HA     | 5:E:69:ILE:HD12   | 2.01                     | 0.41              |
| 5:E:77:SER:HB3    | 5:E:105:PHE:HD2   | 1.85                     | 0.41              |
| 1:A:350:ARG:HB2   | 2:B:1128:LEU:HD11 | 2.02                     | 0.41              |
| 1:A:503:GLN:NE2   | 6:F:90:ARG:HH21   | 2.19                     | 0.41              |
| 2:B:425:THR:HA    | 2:B:428:ILE:HD12  | 2.02                     | 0.41              |
| 8:H:17:PRO:HB3    | 8:H:24:CYS:SG     | 2.60                     | 0.41              |
| 1:A:66:LYS:HG2    | 13:M:18:LEU:HD22  | 2.03                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:474:VAL:HG23  | 1:A:521:MET:SD    | 2.61                     | 0.41              |
| 1:A:1389:PHE:C    | 1:A:1391:ARG:H    | 2.29                     | 0.41              |
| 2:B:172:ILE:HG12  | 2:B:178:ASN:HD22  | 1.86                     | 0.41              |
| 3:C:41:ILE:HB     | 3:C:172:PRO:HG2   | 2.02                     | 0.41              |
| 3:C:73:GLN:HB2    | 3:C:131:HIS:HB2   | 2.03                     | 0.41              |
| 9:I:92:ARG:HG2    | 9:I:93:LYS:HD3    | 2.03                     | 0.41              |
| 1:A:665:GLY:HA2   | 2:B:1026:LEU:HD22 | 2.03                     | 0.41              |
| 2:B:654:ARG:H     | 2:B:657:HIS:HD2   | 1.68                     | 0.41              |
| 3:C:46:ILE:HA     | 3:C:159:ALA:HA    | 2.03                     | 0.41              |
| 5:E:18:THR:HG23   | 5:E:143:ASN:HD22  | 1.86                     | 0.41              |
| 1:A:43:GLU:HB3    | 1:A:50:ILE:HG23   | 2.02                     | 0.40              |
| 7:G:49:LEU:HD21   | 7:G:77:VAL:HG23   | 2.02                     | 0.40              |
| 1:A:1398:MET:HE3  | 1:A:1425:SER:H    | 1.86                     | 0.40              |
| 7:G:3:PHE:HB2     | 7:G:78:VAL:HG23   | 2.03                     | 0.40              |
| 1:A:367:PRO:HA    | 1:A:463:ILE:O     | 2.21                     | 0.40              |
| 1:A:567:LYS:HB3   | 8:H:96:VAL:N      | 2.33                     | 0.40              |
| 1:A:1224:LEU:HD12 | 1:A:1242:VAL:H    | 1.86                     | 0.40              |
| 2:B:830:TYR:CZ    | 2:B:1000:PRO:HD3  | 2.56                     | 0.40              |
| 3:C:73:GLN:HB3    | 3:C:131:HIS:H     | 1.87                     | 0.40              |
| 4:D:37:GLN:HE21   | 4:D:47:LEU:HA     | 1.86                     | 0.40              |
| 6:F:82:THR:HG22   | 6:F:84:TYR:H      | 1.87                     | 0.40              |
| 9:I:65:ASP:HB3    | 9:I:68:LEU:HD12   | 2.02                     | 0.40              |
| 1:A:901:LEU:HD22  | 1:A:919:ILE:HG12  | 2.03                     | 0.40              |
| 2:B:486:TYR:HB3   | 2:B:1096:ARG:NH2  | 2.36                     | 0.40              |
| 1:A:33:ALA:HA     | 1:A:57:ARG:NH1    | 2.36                     | 0.40              |
| 1:A:49:LYS:HB3    | 1:A:54:ASN:O      | 2.21                     | 0.40              |
| 1:A:404:TYR:HD2   | 1:A:414:ASP:HA    | 1.87                     | 0.40              |

There are no symmetry-related clashes.

## 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     | 1406/1733 (81%) | 1215 (86%) | 137 (10%) | 54 (4%)  | 2           | 19  |
| 2   | B     | 1102/1224 (90%) | 938 (85%)  | 126 (11%) | 38 (3%)  | 3           | 21  |
| 3   | C     | 264/318 (83%)   | 219 (83%)  | 37 (14%)  | 8 (3%)   | 3           | 22  |
| 4   | D     | 174/221 (79%)   | 147 (84%)  | 20 (12%)  | 7 (4%)   | 2           | 18  |
| 5   | E     | 212/215 (99%)   | 192 (91%)  | 16 (8%)   | 4 (2%)   | 6           | 32  |
| 6   | F     | 85/155 (55%)    | 74 (87%)   | 11 (13%)  | 0        | 100         | 100 |
| 7   | G     | 169/171 (99%)   | 145 (86%)  | 21 (12%)  | 3 (2%)   | 6           | 33  |
| 8   | H     | 130/146 (89%)   | 97 (75%)   | 18 (14%)  | 15 (12%) | 0           | 5   |
| 9   | I     | 117/122 (96%)   | 96 (82%)   | 19 (16%)  | 2 (2%)   | 7           | 35  |
| 10  | J     | 63/70 (90%)     | 51 (81%)   | 7 (11%)   | 5 (8%)   | 1           | 9   |
| 11  | K     | 112/120 (93%)   | 101 (90%)  | 10 (9%)   | 1 (1%)   | 14          | 49  |
| 12  | L     | 44/70 (63%)     | 34 (77%)   | 5 (11%)   | 5 (11%)  | 0           | 5   |
| 13  | M     | 54/197 (27%)    | 43 (80%)   | 8 (15%)   | 3 (6%)   | 1           | 15  |
| All | All   | 3932/4762 (83%) | 3352 (85%) | 435 (11%) | 145 (4%) | 2           | 20  |

All (145) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 57   | ARG  |
| 1   | A     | 65   | LEU  |
| 1   | A     | 66   | LYS  |
| 1   | A     | 167  | CYS  |
| 1   | A     | 311  | GLN  |
| 1   | A     | 567  | LYS  |
| 1   | A     | 780  | VAL  |
| 1   | A     | 846  | GLU  |
| 1   | A     | 1206 | ASP  |
| 1   | A     | 1405 | THR  |
| 2   | B     | 282  | ILE  |
| 2   | B     | 531  | GLN  |
| 2   | B     | 731  | VAL  |
| 2   | B     | 785  | TYR  |
| 2   | B     | 891  | ASP  |
| 2   | B     | 895  | ASP  |
| 3   | C     | 149  | LYS  |
| 4   | D     | 18   | VAL  |
| 4   | D     | 27   | LEU  |
| 7   | G     | 20   | PRO  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 7   | G     | 139  | ILE  |
| 7   | G     | 154  | VAL  |
| 8   | H     | 128  | ASN  |
| 10  | J     | 64   | ASN  |
| 12  | L     | 55   | ILE  |
| 1   | A     | 5    | GLN  |
| 1   | A     | 52   | GLY  |
| 1   | A     | 54   | ASN  |
| 1   | A     | 68   | GLN  |
| 1   | A     | 72   | GLU  |
| 1   | A     | 178  | GLY  |
| 1   | A     | 282  | ASN  |
| 1   | A     | 322  | VAL  |
| 1   | A     | 331  | GLY  |
| 1   | A     | 624  | SER  |
| 1   | A     | 903  | ASN  |
| 1   | A     | 1242 | VAL  |
| 1   | A     | 1280 | GLU  |
| 1   | A     | 1365 | TYR  |
| 1   | A     | 1403 | GLU  |
| 2   | B     | 45   | SER  |
| 2   | B     | 245  | GLU  |
| 2   | B     | 367  | LEU  |
| 2   | B     | 468  | GLU  |
| 2   | B     | 476  | ARG  |
| 2   | B     | 575  | PRO  |
| 2   | B     | 797  | TYR  |
| 2   | B     | 926  | GLY  |
| 2   | B     | 1046 | PRO  |
| 2   | B     | 1153 | GLU  |
| 2   | B     | 1155 | SER  |
| 2   | B     | 1157 | ALA  |
| 2   | B     | 1175 | LEU  |
| 3   | C     | 142  | VAL  |
| 3   | C     | 175  | ALA  |
| 3   | C     | 184  | ASN  |
| 4   | D     | 20   | GLU  |
| 4   | D     | 53   | SER  |
| 4   | D     | 199  | ASN  |
| 5   | E     | 3    | GLN  |
| 5   | E     | 141  | VAL  |
| 8   | H     | 92   | ASP  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 10  | J     | 2    | ILE  |
| 12  | L     | 46   | VAL  |
| 12  | L     | 56   | LEU  |
| 13  | M     | 17   | ASN  |
| 1   | A     | 4    | GLN  |
| 1   | A     | 67   | CYS  |
| 1   | A     | 71   | GLN  |
| 1   | A     | 286  | HIS  |
| 1   | A     | 318  | SER  |
| 1   | A     | 466  | SER  |
| 1   | A     | 525  | GLN  |
| 1   | A     | 591  | PHE  |
| 1   | A     | 628  | GLY  |
| 1   | A     | 868  | TYR  |
| 1   | A     | 906  | HIS  |
| 1   | A     | 920  | LEU  |
| 2   | B     | 248  | SER  |
| 2   | B     | 335  | GLY  |
| 2   | B     | 641  | GLU  |
| 2   | B     | 711  | GLU  |
| 2   | B     | 883  | LEU  |
| 8   | H     | 18   | GLY  |
| 8   | H     | 78   | SER  |
| 8   | H     | 108  | SER  |
| 8   | H     | 109  | LYS  |
| 8   | H     | 110  | ASP  |
| 9   | I     | 21   | GLU  |
| 9   | I     | 88   | SER  |
| 10  | J     | 42   | LYS  |
| 12  | L     | 45   | ALA  |
| 13  | M     | 28   | LYS  |
| 1   | A     | 47   | ARG  |
| 1   | A     | 69   | THR  |
| 1   | A     | 156  | ASP  |
| 1   | A     | 196  | GLU  |
| 1   | A     | 253  | ASN  |
| 1   | A     | 290  | GLU  |
| 1   | A     | 465  | TYR  |
| 1   | A     | 922  | ASP  |
| 1   | A     | 1255 | GLU  |
| 2   | B     | 58   | THR  |
| 2   | B     | 962  | LYS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 1017 | ILE  |
| 2   | B     | 1082 | MET  |
| 2   | B     | 1108 | ARG  |
| 3   | C     | 110  | THR  |
| 3   | C     | 141  | GLY  |
| 5   | E     | 104  | ASN  |
| 8   | H     | 35   | GLN  |
| 8   | H     | 84   | ALA  |
| 8   | H     | 139  | ASN  |
| 10  | J     | 6    | ARG  |
| 10  | J     | 9    | SER  |
| 11  | K     | 64   | GLU  |
| 12  | L     | 59   | ALA  |
| 13  | M     | 15   | GLY  |
| 1   | A     | 35   | ILE  |
| 1   | A     | 958  | VAL  |
| 1   | A     | 1377 | THR  |
| 2   | B     | 642  | ASP  |
| 2   | B     | 792  | MET  |
| 2   | B     | 1156 | ASP  |
| 2   | B     | 1181 | GLU  |
| 3   | C     | 167  | HIS  |
| 3   | C     | 174  | ALA  |
| 4   | D     | 5    | THR  |
| 4   | D     | 119  | ARG  |
| 5   | E     | 148  | GLU  |
| 8   | H     | 60   | ALA  |
| 8   | H     | 61   | SER  |
| 2   | B     | 100  | PRO  |
| 1   | A     | 1327 | ILE  |
| 2   | B     | 510  | LYS  |
| 2   | B     | 867  | GLY  |
| 8   | H     | 107  | VAL  |
| 1   | A     | 1437 | GLY  |
| 8   | H     | 17   | PRO  |
| 1   | A     | 424  | ILE  |
| 8   | H     | 119  | GLY  |
| 1   | A     | 1454 | MET  |
| 1   | A     | 1064 | VAL  |
| 2   | B     | 571  | PRO  |
| 2   | B     | 764  | SER  |

### 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     | 1239/1520 (82%) | 1048 (85%) | 191 (15%) | 2           | 13 |
| 2   | B     | 972/1061 (92%)  | 842 (87%)  | 130 (13%) | 4           | 16 |
| 3   | C     | 234/274 (85%)   | 206 (88%)  | 28 (12%)  | 5           | 19 |
| 4   | D     | 160/200 (80%)   | 137 (86%)  | 23 (14%)  | 3           | 15 |
| 5   | E     | 196/197 (100%)  | 177 (90%)  | 19 (10%)  | 8           | 25 |
| 6   | F     | 77/137 (56%)    | 66 (86%)   | 11 (14%)  | 3           | 15 |
| 7   | G     | 152/152 (100%)  | 128 (84%)  | 24 (16%)  | 2           | 13 |
| 8   | H     | 118/128 (92%)   | 102 (86%)  | 16 (14%)  | 3           | 16 |
| 9   | I     | 113/116 (97%)   | 102 (90%)  | 11 (10%)  | 8           | 25 |
| 10  | J     | 60/65 (92%)     | 52 (87%)   | 8 (13%)   | 4           | 16 |
| 11  | K     | 99/102 (97%)    | 85 (86%)   | 14 (14%)  | 3           | 15 |
| 12  | L     | 40/57 (70%)     | 31 (78%)   | 9 (22%)   | 1           | 6  |
| 13  | M     | 52/62 (84%)     | 41 (79%)   | 11 (21%)  | 1           | 6  |
| All | All   | 3512/4071 (86%) | 3017 (86%) | 495 (14%) | 3           | 15 |

All (495) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 5   | GLN  |
| 1   | A     | 39  | GLU  |
| 1   | A     | 41  | MET  |
| 1   | A     | 44  | THR  |
| 1   | A     | 50  | ILE  |
| 1   | A     | 64  | ASN  |
| 1   | A     | 66  | LYS  |
| 1   | A     | 67  | CYS  |
| 1   | A     | 68  | GLN  |
| 1   | A     | 69  | THR  |
| 1   | A     | 76  | GLU  |
| 1   | A     | 93  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 96  | ILE  |
| 1   | A     | 101 | LYS  |
| 1   | A     | 109 | HIS  |
| 1   | A     | 112 | LYS  |
| 1   | A     | 113 | LEU  |
| 1   | A     | 114 | LEU  |
| 1   | A     | 115 | LEU  |
| 1   | A     | 116 | ASP  |
| 1   | A     | 121 | LEU  |
| 1   | A     | 138 | ILE  |
| 1   | A     | 141 | LEU  |
| 1   | A     | 145 | LYS  |
| 1   | A     | 151 | ASP  |
| 1   | A     | 155 | GLU  |
| 1   | A     | 159 | THR  |
| 1   | A     | 164 | ARG  |
| 1   | A     | 196 | GLU  |
| 1   | A     | 199 | LEU  |
| 1   | A     | 200 | ARG  |
| 1   | A     | 208 | LEU  |
| 1   | A     | 219 | PHE  |
| 1   | A     | 226 | GLU  |
| 1   | A     | 236 | LEU  |
| 1   | A     | 237 | THR  |
| 1   | A     | 251 | SER  |
| 1   | A     | 254 | GLU  |
| 1   | A     | 256 | GLN  |
| 1   | A     | 263 | THR  |
| 1   | A     | 265 | LYS  |
| 1   | A     | 268 | ASP  |
| 1   | A     | 270 | LEU  |
| 1   | A     | 303 | TYR  |
| 1   | A     | 316 | GLN  |
| 1   | A     | 320 | ARG  |
| 1   | A     | 322 | VAL  |
| 1   | A     | 335 | ARG  |
| 1   | A     | 337 | ARG  |
| 1   | A     | 344 | ARG  |
| 1   | A     | 359 | LEU  |
| 1   | A     | 378 | GLU  |
| 1   | A     | 379 | VAL  |
| 1   | A     | 385 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 393 | ARG  |
| 1   | A     | 398 | GLU  |
| 1   | A     | 406 | ILE  |
| 1   | A     | 419 | LYS  |
| 1   | A     | 425 | GLN  |
| 1   | A     | 433 | GLU  |
| 1   | A     | 434 | ARG  |
| 1   | A     | 437 | MET  |
| 1   | A     | 438 | ASP  |
| 1   | A     | 443 | LEU  |
| 1   | A     | 445 | ASN  |
| 1   | A     | 446 | ARG  |
| 1   | A     | 447 | GLN  |
| 1   | A     | 455 | MET  |
| 1   | A     | 460 | VAL  |
| 1   | A     | 461 | LYS  |
| 1   | A     | 463 | ILE  |
| 1   | A     | 474 | VAL  |
| 1   | A     | 481 | ASP  |
| 1   | A     | 487 | MET  |
| 1   | A     | 493 | GLN  |
| 1   | A     | 498 | ARG  |
| 1   | A     | 504 | LEU  |
| 1   | A     | 505 | CYS  |
| 1   | A     | 516 | SER  |
| 1   | A     | 526 | ASP  |
| 1   | A     | 527 | THR  |
| 1   | A     | 536 | LEU  |
| 1   | A     | 546 | VAL  |
| 1   | A     | 548 | ASN  |
| 1   | A     | 565 | ILE  |
| 1   | A     | 567 | LYS  |
| 1   | A     | 578 | LEU  |
| 1   | A     | 582 | ILE  |
| 1   | A     | 588 | LEU  |
| 1   | A     | 598 | LEU  |
| 1   | A     | 618 | GLU  |
| 1   | A     | 630 | ILE  |
| 1   | A     | 634 | THR  |
| 1   | A     | 635 | ARG  |
| 1   | A     | 645 | LEU  |
| 1   | A     | 664 | THR  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 666  | ILE  |
| 1   | A     | 676  | MET  |
| 1   | A     | 732  | LEU  |
| 1   | A     | 738  | LYS  |
| 1   | A     | 740  | LEU  |
| 1   | A     | 752  | LYS  |
| 1   | A     | 764  | CYS  |
| 1   | A     | 783  | THR  |
| 1   | A     | 795  | GLU  |
| 1   | A     | 805  | LEU  |
| 1   | A     | 822  | GLU  |
| 1   | A     | 827  | THR  |
| 1   | A     | 834  | THR  |
| 1   | A     | 840  | ARG  |
| 1   | A     | 842  | VAL  |
| 1   | A     | 843  | LYS  |
| 1   | A     | 878  | ILE  |
| 1   | A     | 883  | LEU  |
| 1   | A     | 884  | ASP  |
| 1   | A     | 890  | ASP  |
| 1   | A     | 894  | GLU  |
| 1   | A     | 896  | ARG  |
| 1   | A     | 902  | LEU  |
| 1   | A     | 906  | HIS  |
| 1   | A     | 908  | LEU  |
| 1   | A     | 919  | ILE  |
| 1   | A     | 923  | LEU  |
| 1   | A     | 926  | GLN  |
| 1   | A     | 929  | LEU  |
| 1   | A     | 941  | LYS  |
| 1   | A     | 960  | ILE  |
| 1   | A     | 962  | ARG  |
| 1   | A     | 973  | ILE  |
| 1   | A     | 983  | ILE  |
| 1   | A     | 992  | ASP  |
| 1   | A     | 1001 | ARG  |
| 1   | A     | 1028 | THR  |
| 1   | A     | 1029 | ARG  |
| 1   | A     | 1032 | LEU  |
| 1   | A     | 1058 | VAL  |
| 1   | A     | 1062 | GLU  |
| 1   | A     | 1064 | VAL  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1067 | LEU  |
| 1   | A     | 1079 | MET  |
| 1   | A     | 1094 | VAL  |
| 1   | A     | 1116 | LEU  |
| 1   | A     | 1120 | LEU  |
| 1   | A     | 1136 | SER  |
| 1   | A     | 1143 | LEU  |
| 1   | A     | 1148 | ILE  |
| 1   | A     | 1150 | SER  |
| 1   | A     | 1155 | ASP  |
| 1   | A     | 1159 | ARG  |
| 1   | A     | 1161 | THR  |
| 1   | A     | 1167 | GLU  |
| 1   | A     | 1187 | GLN  |
| 1   | A     | 1195 | LEU  |
| 1   | A     | 1196 | GLU  |
| 1   | A     | 1205 | LYS  |
| 1   | A     | 1207 | LEU  |
| 1   | A     | 1218 | GLN  |
| 1   | A     | 1223 | ASP  |
| 1   | A     | 1226 | VAL  |
| 1   | A     | 1237 | ILE  |
| 1   | A     | 1255 | GLU  |
| 1   | A     | 1266 | THR  |
| 1   | A     | 1274 | ARG  |
| 1   | A     | 1291 | VAL  |
| 1   | A     | 1295 | THR  |
| 1   | A     | 1297 | GLU  |
| 1   | A     | 1316 | VAL  |
| 1   | A     | 1322 | ILE  |
| 1   | A     | 1323 | ASP  |
| 1   | A     | 1333 | ILE  |
| 1   | A     | 1334 | ASP  |
| 1   | A     | 1341 | ILE  |
| 1   | A     | 1351 | GLU  |
| 1   | A     | 1356 | ILE  |
| 1   | A     | 1370 | LEU  |
| 1   | A     | 1371 | LEU  |
| 1   | A     | 1381 | LEU  |
| 1   | A     | 1382 | THR  |
| 1   | A     | 1385 | THR  |
| 1   | A     | 1393 | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1397 | LEU  |
| 1   | A     | 1405 | THR  |
| 1   | A     | 1406 | VAL  |
| 1   | A     | 1420 | ASP  |
| 1   | A     | 1424 | VAL  |
| 1   | A     | 1433 | MET  |
| 1   | A     | 1442 | ASP  |
| 1   | A     | 1443 | VAL  |
| 1   | A     | 1444 | MET  |
| 1   | A     | 1445 | ILE  |
| 1   | A     | 1453 | TYR  |
| 2   | B     | 21   | GLU  |
| 2   | B     | 40   | GLU  |
| 2   | B     | 44   | VAL  |
| 2   | B     | 46   | GLN  |
| 2   | B     | 47   | GLN  |
| 2   | B     | 58   | THR  |
| 2   | B     | 63   | ILE  |
| 2   | B     | 102  | VAL  |
| 2   | B     | 104  | GLU  |
| 2   | B     | 123  | THR  |
| 2   | B     | 128  | LEU  |
| 2   | B     | 134  | LYS  |
| 2   | B     | 167  | ILE  |
| 2   | B     | 170  | LEU  |
| 2   | B     | 183  | GLU  |
| 2   | B     | 191  | LYS  |
| 2   | B     | 192  | LEU  |
| 2   | B     | 222  | ILE  |
| 2   | B     | 223  | VAL  |
| 2   | B     | 228  | LYS  |
| 2   | B     | 240  | ILE  |
| 2   | B     | 251  | ILE  |
| 2   | B     | 261  | ARG  |
| 2   | B     | 272  | THR  |
| 2   | B     | 273  | LEU  |
| 2   | B     | 277  | LYS  |
| 2   | B     | 280  | ILE  |
| 2   | B     | 289  | LEU  |
| 2   | B     | 291  | ILE  |
| 2   | B     | 305  | VAL  |
| 2   | B     | 312  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 323 | VAL  |
| 2   | B     | 331 | LEU  |
| 2   | B     | 346 | GLU  |
| 2   | B     | 347 | LYS  |
| 2   | B     | 355 | ILE  |
| 2   | B     | 357 | GLN  |
| 2   | B     | 365 | THR  |
| 2   | B     | 371 | GLU  |
| 2   | B     | 373 | ARG  |
| 2   | B     | 387 | LEU  |
| 2   | B     | 390 | LEU  |
| 2   | B     | 391 | ASP  |
| 2   | B     | 393 | LYS  |
| 2   | B     | 398 | ARG  |
| 2   | B     | 401 | PHE  |
| 2   | B     | 416 | LEU  |
| 2   | B     | 420 | LEU  |
| 2   | B     | 423 | LYS  |
| 2   | B     | 424 | LEU  |
| 2   | B     | 427 | ASP  |
| 2   | B     | 434 | ARG  |
| 2   | B     | 436 | VAL  |
| 2   | B     | 446 | LEU  |
| 2   | B     | 452 | THR  |
| 2   | B     | 466 | TRP  |
| 2   | B     | 482 | VAL  |
| 2   | B     | 508 | LEU  |
| 2   | B     | 510 | LYS  |
| 2   | B     | 529 | GLU  |
| 2   | B     | 531 | GLN  |
| 2   | B     | 539 | LEU  |
| 2   | B     | 560 | GLU  |
| 2   | B     | 563 | MET  |
| 2   | B     | 570 | VAL  |
| 2   | B     | 578 | THR  |
| 2   | B     | 579 | ARG  |
| 2   | B     | 603 | LEU  |
| 2   | B     | 604 | ARG  |
| 2   | B     | 612 | GLU  |
| 2   | B     | 615 | MET  |
| 2   | B     | 616 | ILE  |
| 2   | B     | 617 | ARG  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 620  | ARG  |
| 2   | B     | 646  | LEU  |
| 2   | B     | 658  | ILE  |
| 2   | B     | 729  | ILE  |
| 2   | B     | 731  | VAL  |
| 2   | B     | 736  | THR  |
| 2   | B     | 743  | ILE  |
| 2   | B     | 748  | ILE  |
| 2   | B     | 755  | ILE  |
| 2   | B     | 773  | MET  |
| 2   | B     | 790  | ASP  |
| 2   | B     | 795  | ILE  |
| 2   | B     | 797  | TYR  |
| 2   | B     | 829  | CYS  |
| 2   | B     | 836  | GLU  |
| 2   | B     | 841  | MET  |
| 2   | B     | 861  | ASP  |
| 2   | B     | 868  | MET  |
| 2   | B     | 871  | THR  |
| 2   | B     | 883  | LEU  |
| 2   | B     | 891  | ASP  |
| 2   | B     | 915  | THR  |
| 2   | B     | 925  | LEU  |
| 2   | B     | 928  | ARG  |
| 2   | B     | 943  | SER  |
| 2   | B     | 953  | LEU  |
| 2   | B     | 954  | VAL  |
| 2   | B     | 955  | THR  |
| 2   | B     | 957  | ASN  |
| 2   | B     | 973  | ILE  |
| 2   | B     | 975  | GLN  |
| 2   | B     | 976  | ILE  |
| 2   | B     | 986  | GLN  |
| 2   | B     | 987  | LYS  |
| 2   | B     | 992  | ILE  |
| 2   | B     | 998  | ASP  |
| 2   | B     | 999  | MET  |
| 2   | B     | 1007 | VAL  |
| 2   | B     | 1031 | LEU  |
| 2   | B     | 1048 | THR  |
| 2   | B     | 1050 | ILE  |
| 2   | B     | 1065 | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 1072 | MET  |
| 2   | B     | 1114 | LEU  |
| 2   | B     | 1123 | SER  |
| 2   | B     | 1128 | LEU  |
| 2   | B     | 1132 | GLU  |
| 2   | B     | 1151 | LEU  |
| 2   | B     | 1169 | MET  |
| 2   | B     | 1175 | LEU  |
| 2   | B     | 1177 | HIS  |
| 2   | B     | 1183 | LYS  |
| 2   | B     | 1189 | ILE  |
| 2   | B     | 1196 | ILE  |
| 2   | B     | 1202 | LEU  |
| 2   | B     | 1203 | LEU  |
| 2   | B     | 1211 | ASN  |
| 3   | C     | 11   | ARG  |
| 3   | C     | 14   | SER  |
| 3   | C     | 22   | LEU  |
| 3   | C     | 25   | VAL  |
| 3   | C     | 29   | MET  |
| 3   | C     | 43   | THR  |
| 3   | C     | 44   | LEU  |
| 3   | C     | 56   | THR  |
| 3   | C     | 60   | ASP  |
| 3   | C     | 76   | ASP  |
| 3   | C     | 77   | ILE  |
| 3   | C     | 78   | GLU  |
| 3   | C     | 111  | THR  |
| 3   | C     | 120  | ILE  |
| 3   | C     | 127  | ARG  |
| 3   | C     | 129  | ILE  |
| 3   | C     | 133  | ILE  |
| 3   | C     | 136  | ASP  |
| 3   | C     | 146  | LYS  |
| 3   | C     | 186  | LEU  |
| 3   | C     | 195  | GLN  |
| 3   | C     | 197  | SER  |
| 3   | C     | 203  | GLN  |
| 3   | C     | 214  | ASN  |
| 3   | C     | 215  | GLU  |
| 3   | C     | 224  | GLN  |
| 3   | C     | 262  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 265 | MET  |
| 4   | D     | 11  | ARG  |
| 4   | D     | 17  | LYS  |
| 4   | D     | 28  | GLN  |
| 4   | D     | 34  | GLN  |
| 4   | D     | 40  | HIS  |
| 4   | D     | 43  | GLU  |
| 4   | D     | 47  | LEU  |
| 4   | D     | 50  | LEU  |
| 4   | D     | 57  | LEU  |
| 4   | D     | 65  | GLU  |
| 4   | D     | 120 | GLU  |
| 4   | D     | 139 | LYS  |
| 4   | D     | 148 | LEU  |
| 4   | D     | 152 | SER  |
| 4   | D     | 156 | ASP  |
| 4   | D     | 165 | GLN  |
| 4   | D     | 187 | THR  |
| 4   | D     | 200 | ASN  |
| 4   | D     | 202 | ILE  |
| 4   | D     | 206 | GLU  |
| 4   | D     | 213 | GLU  |
| 4   | D     | 214 | LEU  |
| 4   | D     | 220 | LEU  |
| 5   | E     | 14  | ARG  |
| 5   | E     | 30  | ILE  |
| 5   | E     | 33  | GLU  |
| 5   | E     | 81  | GLU  |
| 5   | E     | 92  | THR  |
| 5   | E     | 98  | ILE  |
| 5   | E     | 104 | ASN  |
| 5   | E     | 107 | THR  |
| 5   | E     | 116 | ILE  |
| 5   | E     | 123 | LEU  |
| 5   | E     | 148 | GLU  |
| 5   | E     | 149 | LEU  |
| 5   | E     | 170 | LEU  |
| 5   | E     | 179 | GLN  |
| 5   | E     | 184 | VAL  |
| 5   | E     | 188 | LEU  |
| 5   | E     | 195 | VAL  |
| 5   | E     | 198 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | E     | 205 | SER  |
| 6   | F     | 70  | LYS  |
| 6   | F     | 78  | GLN  |
| 6   | F     | 79  | ARG  |
| 6   | F     | 96  | THR  |
| 6   | F     | 109 | VAL  |
| 6   | F     | 112 | GLU  |
| 6   | F     | 118 | LEU  |
| 6   | F     | 119 | ARG  |
| 6   | F     | 122 | MET  |
| 6   | F     | 138 | LEU  |
| 6   | F     | 155 | LEU  |
| 7   | G     | 1   | MET  |
| 7   | G     | 12  | THR  |
| 7   | G     | 21  | ARG  |
| 7   | G     | 26  | LEU  |
| 7   | G     | 46  | LEU  |
| 7   | G     | 52  | ASP  |
| 7   | G     | 54  | ILE  |
| 7   | G     | 60  | ARG  |
| 7   | G     | 87  | VAL  |
| 7   | G     | 90  | THR  |
| 7   | G     | 91  | VAL  |
| 7   | G     | 96  | GLN  |
| 7   | G     | 101 | VAL  |
| 7   | G     | 106 | MET  |
| 7   | G     | 113 | HIS  |
| 7   | G     | 114 | LEU  |
| 7   | G     | 119 | LEU  |
| 7   | G     | 138 | THR  |
| 7   | G     | 141 | SER  |
| 7   | G     | 145 | VAL  |
| 7   | G     | 154 | VAL  |
| 7   | G     | 157 | ILE  |
| 7   | G     | 160 | ILE  |
| 7   | G     | 165 | GLU  |
| 8   | H     | 14  | GLU  |
| 8   | H     | 19  | ARG  |
| 8   | H     | 23  | VAL  |
| 8   | H     | 26  | ILE  |
| 8   | H     | 32  | THR  |
| 8   | H     | 35  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | H     | 46  | LEU  |
| 8   | H     | 53  | ASP  |
| 8   | H     | 64  | ASN  |
| 8   | H     | 89  | LEU  |
| 8   | H     | 111 | LEU  |
| 8   | H     | 112 | ILE  |
| 8   | H     | 123 | MET  |
| 8   | H     | 130 | ARG  |
| 8   | H     | 135 | LEU  |
| 8   | H     | 138 | GLU  |
| 9   | I     | 13  | MET  |
| 9   | I     | 18  | GLU  |
| 9   | I     | 26  | LEU  |
| 9   | I     | 28  | GLU  |
| 9   | I     | 35  | VAL  |
| 9   | I     | 46  | HIS  |
| 9   | I     | 50  | THR  |
| 9   | I     | 89  | GLN  |
| 9   | I     | 104 | LEU  |
| 9   | I     | 109 | ILE  |
| 9   | I     | 113 | ASP  |
| 10  | J     | 2   | ILE  |
| 10  | J     | 3   | VAL  |
| 10  | J     | 24  | LEU  |
| 10  | J     | 29  | GLU  |
| 10  | J     | 34  | THR  |
| 10  | J     | 39  | LEU  |
| 10  | J     | 43  | ARG  |
| 10  | J     | 52  | THR  |
| 11  | K     | 5   | ASP  |
| 11  | K     | 9   | LEU  |
| 11  | K     | 11  | LEU  |
| 11  | K     | 14  | GLU  |
| 11  | K     | 21  | ILE  |
| 11  | K     | 31  | VAL  |
| 11  | K     | 32  | VAL  |
| 11  | K     | 41  | THR  |
| 11  | K     | 47  | ARG  |
| 11  | K     | 51  | LEU  |
| 11  | K     | 54  | ARG  |
| 11  | K     | 72  | LYS  |
| 11  | K     | 101 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11  | K     | 114 | LEU  |
| 12  | L     | 26  | THR  |
| 12  | L     | 27  | LEU  |
| 12  | L     | 55  | ILE  |
| 12  | L     | 58  | LYS  |
| 12  | L     | 60  | ARG  |
| 12  | L     | 61  | THR  |
| 12  | L     | 64  | LEU  |
| 12  | L     | 65  | VAL  |
| 12  | L     | 68  | GLU  |
| 13  | M     | 18  | LEU  |
| 13  | M     | 20  | ILE  |
| 13  | M     | 26  | GLU  |
| 13  | M     | 29  | VAL  |
| 13  | M     | 34  | ILE  |
| 13  | M     | 39  | SER  |
| 13  | M     | 44  | VAL  |
| 13  | M     | 45  | CYS  |
| 13  | M     | 50  | LEU  |
| 13  | M     | 59  | THR  |
| 13  | M     | 66  | PHE  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (112) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 54  | ASN  |
| 1   | A     | 64  | ASN  |
| 1   | A     | 71  | GLN  |
| 1   | A     | 118 | HIS  |
| 1   | A     | 225 | ASN  |
| 1   | A     | 253 | ASN  |
| 1   | A     | 256 | GLN  |
| 1   | A     | 316 | GLN  |
| 1   | A     | 339 | ASN  |
| 1   | A     | 358 | ASN  |
| 1   | A     | 425 | GLN  |
| 1   | A     | 471 | ASN  |
| 1   | A     | 503 | GLN  |
| 1   | A     | 517 | ASN  |
| 1   | A     | 587 | HIS  |
| 1   | A     | 603 | ASN  |
| 1   | A     | 626 | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 631  | HIS  |
| 1   | A     | 640  | GLN  |
| 1   | A     | 650  | GLN  |
| 1   | A     | 659  | HIS  |
| 1   | A     | 736  | ASN  |
| 1   | A     | 741  | ASN  |
| 1   | A     | 742  | ASN  |
| 1   | A     | 745  | GLN  |
| 1   | A     | 768  | GLN  |
| 1   | A     | 926  | GLN  |
| 1   | A     | 965  | GLN  |
| 1   | A     | 968  | GLN  |
| 1   | A     | 969  | GLN  |
| 1   | A     | 1052 | GLN  |
| 1   | A     | 1070 | GLN  |
| 1   | A     | 1124 | HIS  |
| 1   | A     | 1171 | GLN  |
| 1   | A     | 1188 | GLN  |
| 1   | A     | 1211 | GLN  |
| 1   | A     | 1218 | GLN  |
| 1   | A     | 1270 | ASN  |
| 1   | A     | 1312 | ASN  |
| 1   | A     | 1354 | ASN  |
| 2   | B     | 121  | ASN  |
| 2   | B     | 178  | ASN  |
| 2   | B     | 206  | ASN  |
| 2   | B     | 255  | GLN  |
| 2   | B     | 306  | ASN  |
| 2   | B     | 513  | GLN  |
| 2   | B     | 515  | HIS  |
| 2   | B     | 516  | ASN  |
| 2   | B     | 518  | HIS  |
| 2   | B     | 531  | GLN  |
| 2   | B     | 657  | HIS  |
| 2   | B     | 822  | ASN  |
| 2   | B     | 842  | ASN  |
| 2   | B     | 843  | GLN  |
| 2   | B     | 862  | GLN  |
| 2   | B     | 878  | GLN  |
| 2   | B     | 951  | GLN  |
| 2   | B     | 957  | ASN  |
| 2   | B     | 986  | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 1015 | HIS  |
| 2   | B     | 1025 | HIS  |
| 2   | B     | 1040 | ASN  |
| 2   | B     | 1074 | ASN  |
| 2   | B     | 1076 | HIS  |
| 2   | B     | 1097 | HIS  |
| 2   | B     | 1161 | HIS  |
| 2   | B     | 1193 | GLN  |
| 2   | B     | 1195 | HIS  |
| 2   | B     | 1205 | GLN  |
| 2   | B     | 1211 | ASN  |
| 3   | C     | 17   | ASN  |
| 3   | C     | 54   | ASN  |
| 3   | C     | 79   | GLN  |
| 3   | C     | 102  | GLN  |
| 3   | C     | 131  | HIS  |
| 3   | C     | 184  | ASN  |
| 3   | C     | 195  | GLN  |
| 3   | C     | 224  | GLN  |
| 3   | C     | 231  | ASN  |
| 4   | D     | 34   | GLN  |
| 4   | D     | 37   | GLN  |
| 4   | D     | 41   | GLN  |
| 4   | D     | 132  | GLN  |
| 4   | D     | 143  | ASN  |
| 4   | D     | 179  | GLN  |
| 5   | E     | 5    | ASN  |
| 5   | E     | 8    | ASN  |
| 5   | E     | 54   | GLN  |
| 5   | E     | 99   | HIS  |
| 5   | E     | 106  | GLN  |
| 5   | E     | 113  | GLN  |
| 5   | E     | 115  | ASN  |
| 5   | E     | 143  | ASN  |
| 6   | F     | 78   | GLN  |
| 7   | G     | 14   | HIS  |
| 7   | G     | 24   | GLN  |
| 7   | G     | 71   | ASN  |
| 7   | G     | 96   | GLN  |
| 7   | G     | 102  | GLN  |
| 7   | G     | 126  | ASN  |
| 7   | G     | 131  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | H     | 33  | GLN  |
| 8   | H     | 83  | GLN  |
| 8   | H     | 128 | ASN  |
| 8   | H     | 137 | GLN  |
| 9   | I     | 12  | ASN  |
| 10  | J     | 53  | HIS  |
| 11  | K     | 2   | ASN  |
| 11  | K     | 65  | HIS  |
| 11  | K     | 96  | ASN  |
| 13  | M     | 17  | ASN  |
| 13  | M     | 19  | 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 ⓘ

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 13  | M     | 2                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | M     | 68:ASN    | C      | 84:UNK    | N      | 13.19        |
| 1     | M     | 99:UNK    | C      | 102:UNK   | N      | 11.41        |

## 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     | 1416/1733 (81%) | 0.64   | 67 (4%) 36 32  | 53, 106, 168, 238     | 0     |
| 2   | B     | 1120/1224 (91%) | 0.84   | 111 (9%) 13 16 | 53, 122, 192, 238     | 0     |
| 3   | C     | 266/318 (83%)   | 0.60   | 8 (3%) 52 40   | 63, 117, 167, 202     | 0     |
| 4   | D     | 178/221 (80%)   | 1.01   | 18 (10%) 12 16 | 65, 132, 190, 228     | 0     |
| 5   | E     | 214/215 (99%)   | 0.88   | 18 (8%) 17 20  | 74, 138, 210, 245     | 0     |
| 6   | F     | 87/155 (56%)    | 0.48   | 2 (2%) 61 48   | 56, 88, 114, 128      | 0     |
| 7   | G     | 171/171 (100%)  | 0.62   | 5 (2%) 53 41   | 64, 108, 146, 188     | 0     |
| 8   | H     | 134/146 (91%)   | 1.12   | 17 (12%) 8 12  | 101, 144, 209, 224    | 0     |
| 9   | I     | 119/122 (97%)   | 1.40   | 28 (23%) 2 5   | 103, 170, 220, 232    | 0     |
| 10  | J     | 65/70 (92%)     | 0.66   | 3 (4%) 37 33   | 78, 114, 152, 177     | 0     |
| 11  | K     | 114/120 (95%)   | 0.56   | 2 (1%) 67 53   | 74, 120, 143, 198     | 0     |
| 12  | L     | 46/70 (65%)     | 1.29   | 7 (15%) 5 10   | 81, 152, 165, 202     | 0     |
| 13  | M     | 56/197 (28%)    | 0.97   | 6 (10%) 11 15  | 89, 117, 157, 174     | 0     |
| All | All   | 3986/4762 (83%) | 0.77   | 292 (7%) 21 23 | 53, 118, 192, 245     | 0     |

All (292) RSRZ outliers are listed below:

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 4   | D     | 4    | SER  | 7.9  |
| 1   | A     | 1254 | ALA  | 7.4  |
| 1   | A     | 69   | THR  | 7.0  |
| 12  | L     | 27   | LEU  | 6.8  |
| 2   | B     | 266  | ALA  | 5.2  |
| 2   | B     | 250  | PHE  | 5.0  |
| 12  | L     | 26   | THR  | 4.8  |
| 9   | I     | 119  | THR  | 4.5  |
| 2   | B     | 731  | VAL  | 4.4  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 2   | B     | 715  | ALA  | 4.4  |
| 2   | B     | 723  | VAL  | 4.3  |
| 2   | B     | 446  | LEU  | 4.3  |
| 1   | A     | 1455 | PRO  | 4.3  |
| 1   | A     | 2    | VAL  | 4.2  |
| 1   | A     | 1204 | ASP  | 4.2  |
| 2   | B     | 108  | VAL  | 4.2  |
| 12  | L     | 25   | ALA  | 4.2  |
| 2   | B     | 468  | GLU  | 4.1  |
| 13  | M     | 30   | TYR  | 4.1  |
| 9   | I     | 52   | ILE  | 4.0  |
| 8   | H     | 31   | THR  | 4.0  |
| 8   | H     | 135  | LEU  | 3.9  |
| 5   | E     | 49   | SER  | 3.8  |
| 1   | A     | 155  | GLU  | 3.8  |
| 1   | A     | 587  | HIS  | 3.8  |
| 2   | B     | 265  | SER  | 3.8  |
| 8   | H     | 7    | ASP  | 3.7  |
| 2   | B     | 169  | ARG  | 3.7  |
| 11  | K     | 113  | THR  | 3.7  |
| 2   | B     | 646  | LEU  | 3.7  |
| 1   | A     | 1244 | ARG  | 3.7  |
| 2   | B     | 351  | TYR  | 3.7  |
| 8   | H     | 2    | SER  | 3.7  |
| 8   | H     | 92   | ASP  | 3.7  |
| 8   | H     | 94   | ASP  | 3.7  |
| 2   | B     | 164  | LYS  | 3.6  |
| 2   | B     | 652  | LYS  | 3.6  |
| 1   | A     | 1187 | GLN  | 3.6  |
| 1   | A     | 254  | GLU  | 3.6  |
| 2   | B     | 879  | ARG  | 3.6  |
| 2   | B     | 575  | PRO  | 3.5  |
| 4   | D     | 3    | VAL  | 3.5  |
| 1   | A     | 159  | THR  | 3.5  |
| 1   | A     | 1222 | ASN  | 3.5  |
| 1   | A     | 1173 | HIS  | 3.4  |
| 2   | B     | 926  | GLY  | 3.4  |
| 8   | H     | 132  | LEU  | 3.4  |
| 1   | A     | 1284 | MET  | 3.4  |
| 2   | B     | 132  | VAL  | 3.4  |
| 5   | E     | 11   | ARG  | 3.4  |
| 5   | E     | 95   | THR  | 3.4  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 8   | H     | 139  | ASN  | 3.4  |
| 2   | B     | 924  | GLU  | 3.3  |
| 2   | B     | 369  | GLY  | 3.3  |
| 2   | B     | 727  | LYS  | 3.3  |
| 4   | D     | 76   | LYS  | 3.3  |
| 4   | D     | 220  | LEU  | 3.3  |
| 2   | B     | 734  | HIS  | 3.3  |
| 2   | B     | 1183 | LYS  | 3.3  |
| 2   | B     | 927  | GLN  | 3.3  |
| 9   | I     | 53   | GLY  | 3.2  |
| 2   | B     | 70   | ILE  | 3.2  |
| 1   | A     | 1172 | LEU  | 3.2  |
| 1   | A     | 44   | THR  | 3.2  |
| 9   | I     | 60   | GLN  | 3.2  |
| 2   | B     | 305  | VAL  | 3.2  |
| 2   | B     | 319  | GLU  | 3.1  |
| 8   | H     | 119  | GLY  | 3.1  |
| 2   | B     | 263  | GLY  | 3.1  |
| 1   | A     | 763  | ALA  | 3.1  |
| 1   | A     | 710  | LEU  | 3.1  |
| 4   | D     | 212  | LYS  | 3.1  |
| 1   | A     | 1164 | PRO  | 3.1  |
| 5   | E     | 44   | ALA  | 3.1  |
| 1   | A     | 1165 | GLU  | 3.1  |
| 4   | D     | 118  | THR  | 3.1  |
| 2   | B     | 643  | ASP  | 3.0  |
| 2   | B     | 935  | ARG  | 3.0  |
| 4   | D     | 7    | THR  | 2.9  |
| 5   | E     | 152  | LYS  | 2.9  |
| 2   | B     | 24   | PRO  | 2.9  |
| 2   | B     | 251  | ILE  | 2.9  |
| 5   | E     | 91   | LYS  | 2.9  |
| 1   | A     | 51   | GLY  | 2.9  |
| 9   | I     | 9    | ASP  | 2.9  |
| 8   | H     | 109  | LYS  | 2.9  |
| 2   | B     | 736  | THR  | 2.9  |
| 9   | I     | 55   | THR  | 2.9  |
| 2   | B     | 925  | LEU  | 2.9  |
| 9   | I     | 41   | PRO  | 2.8  |
| 2   | B     | 133  | LYS  | 2.8  |
| 2   | B     | 584  | GLY  | 2.8  |
| 13  | M     | 15   | GLY  | 2.8  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 2   | B     | 722  | ASP  | 2.8  |
| 4   | D     | 9    | GLN  | 2.8  |
| 12  | L     | 53   | HIS  | 2.8  |
| 4   | D     | 5    | THR  | 2.8  |
| 2   | B     | 313  | MET  | 2.8  |
| 2   | B     | 359  | GLU  | 2.8  |
| 2   | B     | 606  | LYS  | 2.7  |
| 1   | A     | 564  | ALA  | 2.7  |
| 2   | B     | 922  | GLU  | 2.7  |
| 2   | B     | 958  | GLN  | 2.7  |
| 5   | E     | 86   | PRO  | 2.7  |
| 1   | A     | 1162 | VAL  | 2.7  |
| 2   | B     | 403  | LYS  | 2.7  |
| 2   | B     | 1041 | GLU  | 2.7  |
| 2   | B     | 358  | LYS  | 2.7  |
| 2   | B     | 621  | GLU  | 2.7  |
| 1   | A     | 251  | SER  | 2.7  |
| 2   | B     | 327  | ARG  | 2.7  |
| 12  | L     | 28   | LYS  | 2.7  |
| 1   | A     | 4    | GLN  | 2.7  |
| 2   | B     | 665  | GLU  | 2.7  |
| 2   | B     | 871  | THR  | 2.7  |
| 9   | I     | 3    | THR  | 2.7  |
| 8   | H     | 84   | ALA  | 2.6  |
| 1   | A     | 983  | ILE  | 2.6  |
| 2   | B     | 733  | HIS  | 2.6  |
| 5   | E     | 123  | LEU  | 2.6  |
| 5   | E     | 3    | GLN  | 2.6  |
| 2   | B     | 303  | TYR  | 2.6  |
| 5   | E     | 211  | TYR  | 2.6  |
| 8   | H     | 129  | TYR  | 2.6  |
| 2   | B     | 166  | PHE  | 2.6  |
| 5   | E     | 103  | LYS  | 2.6  |
| 1   | A     | 1243 | VAL  | 2.6  |
| 4   | D     | 18   | VAL  | 2.6  |
| 2   | B     | 458  | LYS  | 2.6  |
| 1   | A     | 417  | TYR  | 2.6  |
| 6   | F     | 69   | LEU  | 2.6  |
| 9   | I     | 17   | ARG  | 2.6  |
| 9   | I     | 11   | ASN  | 2.6  |
| 9   | I     | 39   | GLY  | 2.6  |
| 3   | C     | 148  | ARG  | 2.6  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 5   | E     | 7    | ARG  | 2.6  |
| 2   | B     | 711  | GLU  | 2.6  |
| 9   | I     | 117  | LYS  | 2.5  |
| 7   | G     | 33   | GLU  | 2.5  |
| 9   | I     | 5    | ARG  | 2.5  |
| 2   | B     | 644  | GLU  | 2.5  |
| 2   | B     | 660  | LYS  | 2.5  |
| 9   | I     | 84   | VAL  | 2.5  |
| 2   | B     | 66   | ASP  | 2.5  |
| 4   | D     | 46   | GLU  | 2.5  |
| 2   | B     | 362  | PRO  | 2.5  |
| 2   | B     | 436  | VAL  | 2.5  |
| 2   | B     | 27   | ALA  | 2.5  |
| 9   | I     | 120  | GLN  | 2.5  |
| 5   | E     | 43   | LYS  | 2.5  |
| 7   | G     | 126  | ASN  | 2.5  |
| 3   | C     | 10   | ILE  | 2.5  |
| 9   | I     | 70   | ARG  | 2.5  |
| 1   | A     | 37   | PHE  | 2.5  |
| 3   | C     | 13   | ALA  | 2.5  |
| 2   | B     | 836  | GLU  | 2.4  |
| 2   | B     | 960  | GLY  | 2.4  |
| 2   | B     | 929  | THR  | 2.4  |
| 1   | A     | 253  | ASN  | 2.4  |
| 2   | B     | 90   | ILE  | 2.4  |
| 10  | J     | 44   | TYR  | 2.4  |
| 9   | I     | 111  | THR  | 2.4  |
| 9   | I     | 93   | LYS  | 2.4  |
| 3   | C     | 266  | ASP  | 2.4  |
| 2   | B     | 249  | ARG  | 2.4  |
| 7   | G     | 162  | SER  | 2.4  |
| 1   | A     | 1257 | ASP  | 2.4  |
| 1   | A     | 792  | TYR  | 2.4  |
| 1   | A     | 904  | THR  | 2.4  |
| 2   | B     | 21   | GLU  | 2.4  |
| 3   | C     | 149  | LYS  | 2.4  |
| 13  | M     | 16   | PRO  | 2.4  |
| 1   | A     | 178  | GLY  | 2.4  |
| 4   | D     | 26   | THR  | 2.4  |
| 8   | H     | 90   | ALA  | 2.4  |
| 1   | A     | 1013 | ASP  | 2.4  |
| 2   | B     | 642  | ASP  | 2.4  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 3   | C     | 15   | LYS  | 2.4  |
| 11  | K     | 26   | LYS  | 2.4  |
| 2   | B     | 678  | GLU  | 2.3  |
| 2   | B     | 638  | PHE  | 2.3  |
| 2   | B     | 880  | THR  | 2.3  |
| 2   | B     | 931  | TYR  | 2.3  |
| 1   | A     | 165  | GLY  | 2.3  |
| 2   | B     | 437  | GLU  | 2.3  |
| 8   | H     | 45   | GLU  | 2.3  |
| 1   | A     | 1080 | THR  | 2.3  |
| 8   | H     | 76   | THR  | 2.3  |
| 1   | A     | 34   | LYS  | 2.3  |
| 5   | E     | 56   | LYS  | 2.3  |
| 2   | B     | 328  | GLU  | 2.3  |
| 2   | B     | 625  | LYS  | 2.3  |
| 9   | I     | 2    | THR  | 2.3  |
| 1   | A     | 1256 | GLU  | 2.3  |
| 2   | B     | 567  | GLU  | 2.3  |
| 1   | A     | 66   | LYS  | 2.3  |
| 1   | A     | 1205 | LYS  | 2.3  |
| 9   | I     | 64   | SER  | 2.3  |
| 1   | A     | 61   | ILE  | 2.3  |
| 1   | A     | 1275 | GLY  | 2.3  |
| 2   | B     | 326  | ASP  | 2.3  |
| 1   | A     | 1078 | GLN  | 2.3  |
| 4   | D     | 121  | LYS  | 2.3  |
| 4   | D     | 137  | ASN  | 2.3  |
| 1   | A     | 1092 | LYS  | 2.3  |
| 1   | A     | 693  | VAL  | 2.3  |
| 13  | M     | 62   | GLU  | 2.3  |
| 2   | B     | 248  | SER  | 2.3  |
| 9   | I     | 102  | VAL  | 2.3  |
| 2   | B     | 729  | ILE  | 2.2  |
| 2   | B     | 315  | LYS  | 2.2  |
| 2   | B     | 229  | ALA  | 2.2  |
| 1   | A     | 68   | GLN  | 2.2  |
| 1   | A     | 481  | ASP  | 2.2  |
| 3   | C     | 208  | GLU  | 2.2  |
| 8   | H     | 26   | ILE  | 2.2  |
| 1   | A     | 1109 | LYS  | 2.2  |
| 2   | B     | 562  | GLY  | 2.2  |
| 1   | A     | 1234 | GLU  | 2.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 2   | B     | 109  | THR  | 2.2  |
| 2   | B     | 243  | ALA  | 2.2  |
| 2   | B     | 667  | GLN  | 2.2  |
| 4   | D     | 122  | GLU  | 2.2  |
| 7   | G     | 167  | TYR  | 2.2  |
| 2   | B     | 713  | ALA  | 2.2  |
| 13  | M     | 54   | ASP  | 2.2  |
| 1   | A     | 166  | GLY  | 2.2  |
| 2   | B     | 728  | ARG  | 2.2  |
| 5   | E     | 114  | ASN  | 2.2  |
| 2   | B     | 487  | THR  | 2.2  |
| 1   | A     | 1163 | ILE  | 2.2  |
| 12  | L     | 33   | GLU  | 2.2  |
| 9   | I     | 97   | MET  | 2.2  |
| 10  | J     | 38   | ARG  | 2.2  |
| 2   | B     | 1189 | ILE  | 2.2  |
| 4   | D     | 10   | THR  | 2.2  |
| 1   | A     | 1175 | SER  | 2.2  |
| 2   | B     | 325  | GLN  | 2.2  |
| 2   | B     | 923  | GLU  | 2.2  |
| 2   | B     | 467  | GLY  | 2.1  |
| 2   | B     | 1040 | ASN  | 2.1  |
| 9   | I     | 116  | ASN  | 2.1  |
| 10  | J     | 12   | LYS  | 2.1  |
| 1   | A     | 1377 | THR  | 2.1  |
| 2   | B     | 435  | THR  | 2.1  |
| 1   | A     | 255  | SER  | 2.1  |
| 2   | B     | 919  | SER  | 2.1  |
| 1   | A     | 1230 | GLU  | 2.1  |
| 3   | C     | 37   | MET  | 2.1  |
| 4   | D     | 176  | GLU  | 2.1  |
| 9   | I     | 47   | GLU  | 2.1  |
| 2   | B     | 268  | THR  | 2.1  |
| 9   | I     | 31   | THR  | 2.1  |
| 8   | H     | 35   | GLN  | 2.1  |
| 2   | B     | 1224 | PHE  | 2.1  |
| 9   | I     | 104  | LEU  | 2.1  |
| 2   | B     | 306  | ASN  | 2.1  |
| 1   | A     | 1454 | MET  | 2.1  |
| 2   | B     | 680  | THR  | 2.1  |
| 13  | M     | 59   | THR  | 2.1  |
| 1   | A     | 1214 | GLU  | 2.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 4   | D     | 22   | GLU  | 2.1  |
| 5   | E     | 215  | MET  | 2.1  |
| 1   | A     | 1272 | THR  | 2.1  |
| 5   | E     | 102  | GLU  | 2.1  |
| 2   | B     | 771  | SER  | 2.1  |
| 1   | A     | 1217 | LYS  | 2.1  |
| 1   | A     | 170  | THR  | 2.1  |
| 5   | E     | 67   | GLU  | 2.1  |
| 1   | A     | 161  | LEU  | 2.0  |
| 1   | A     | 195  | ASP  | 2.0  |
| 9   | I     | 57   | GLY  | 2.0  |
| 2   | B     | 215  | GLN  | 2.0  |
| 7   | G     | 128  | PRO  | 2.0  |
| 1   | A     | 762  | SER  | 2.0  |
| 2   | B     | 617  | ARG  | 2.0  |
| 2   | B     | 1150 | ARG  | 2.0  |
| 2   | B     | 244  | LEU  | 2.0  |
| 1   | A     | 48   | ALA  | 2.0  |
| 2   | B     | 111  | ALA  | 2.0  |
| 2   | B     | 932  | HIS  | 2.0  |
| 1   | A     | 479  | ASN  | 2.0  |
| 2   | B     | 706  | GLN  | 2.0  |
| 9   | I     | 22   | ASN  | 2.0  |
| 2   | B     | 191  | LYS  | 2.0  |
| 2   | B     | 264  | SER  | 2.0  |
| 2   | B     | 270  | LYS  | 2.0  |
| 1   | A     | 786  | HIS  | 2.0  |
| 2   | B     | 407  | ASP  | 2.0  |
| 6   | F     | 154  | ASP  | 2.0  |
| 2   | B     | 821  | GLN  | 2.0  |
| 12  | L     | 49   | LYS  | 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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 14  | ZN   | L     | 3005 | 1/1   | 0.98 | 0.08 | 190,190,190,190             | 0     |
| 14  | ZN   | A     | 3008 | 1/1   | 0.99 | 0.06 | 65,65,65,65                 | 0     |
| 14  | ZN   | B     | 3007 | 1/1   | 0.99 | 0.06 | 78,78,78,78                 | 0     |
| 14  | ZN   | I     | 3004 | 1/1   | 0.99 | 0.04 | 196,196,196,196             | 0     |
| 14  | ZN   | J     | 3001 | 1/1   | 0.99 | 0.09 | 124,124,124,124             | 0     |
| 14  | ZN   | A     | 3006 | 1/1   | 0.99 | 0.07 | 130,130,130,130             | 0     |
| 14  | ZN   | I     | 3003 | 1/1   | 1.00 | 0.09 | 151,151,151,151             | 0     |
| 14  | ZN   | C     | 3002 | 1/1   | 1.00 | 0.05 | 62,62,62,62                 | 0     |
| 14  | ZN   | M     | 3009 | 1/1   | 1.00 | 0.06 | 71,71,71,71                 | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.