



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:26 AM UTC

PDB ID : 4A3D / pdb\_00004a3d  
Title : RNA Polymerase II initial transcribing complex with a 6nt DNA-RNA hybrid  
Authors : Cheung, A.C.M.; Sainsbury, S.; Cramer, P.  
Deposited on : 2011-09-30  
Resolution : 3.40 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  
Mogul : 2022.3.0, CSD as543be (2022)  
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

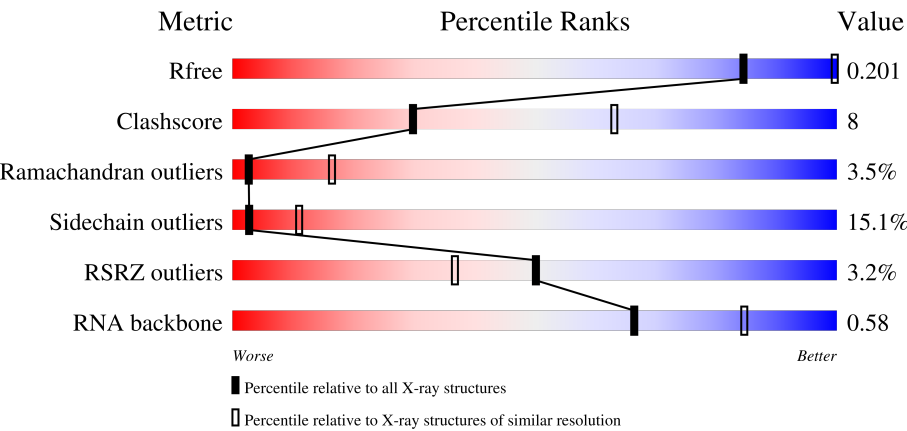
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 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 <sub>free</sub>     | 180053                      | 1001 (3.44-3.36)                                      |
| Clashscore            | 190562                      | 1022 (3.44-3.36)                                      |
| Ramachandran outliers | 187476                      | 1012 (3.44-3.36)                                      |
| Sidechain outliers    | 187428                      | 1012 (3.44-3.36)                                      |
| RSRZ outliers         | 180081                      | 1001 (3.44-3.36)                                      |
| RNA backbone          | 3983                        | 1157 (3.80-3.00)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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     | 1732   | <div><div>2%</div><div><div></div><div>53%</div><div>22%</div><div>5%</div><div>18%</div></div></div> |
| 2   | B     | 1224   | <div><div>4%</div><div><div></div><div>58%</div><div>27%</div><div>5%</div><div>9%</div></div></div>  |
| 3   | C     | 318    | <div><div></div><div><div></div><div>58%</div><div>20%</div><div>5%</div><div>16%</div></div></div>   |
| 4   | D     | 221    | <div><div>5%</div><div><div></div><div>50%</div><div>24%</div><div>5%</div><div>19%</div></div></div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 5   | E     | 215    |                  |
| 6   | F     | 155    |                  |
| 7   | G     | 171    |                  |
| 8   | H     | 146    |                  |
| 9   | I     | 122    |                  |
| 10  | J     | 70     |                  |
| 11  | K     | 120    |                  |
| 12  | L     | 70     |                  |
| 13  | N     | 14     |                  |
| 14  | P     | 6      |                  |
| 15  | T     | 26     |                  |

## 2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 31937 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     | 1422     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 11174 | 7037 | 1954 | 2121 | 62 |         |         |       |

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB2.

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 2   | B     | 1115     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 8859  | 5609 | 1554 | 1641 | 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 SUB-UNIT RPABC 1.

| 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 SUB-UNIT RPABC 2.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6   | F     | 84       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 679   | 434 | 115 | 127 | 3 |         |         |       |

- Molecule 7 is a protein called RPB7, 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 RPABC 3.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8   | H     | 133      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1068  | 673 | 180 | 211 | 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 RPABC 5.

| 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     | 115      | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 920   | 590 | 157 | 171 | 2 |         |         |       |

- Molecule 12 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4.

| 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 DNA chain called NON TEMPLATE DNA 5'-D(\*TP\*AP\*AP\*GP\*TP\*AP\*CP\*TP\*TP \*GP\*AP\*GP\*CP\*TP)-3'.

| Mol | Chain | Residues | Atoms |    |    |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|----|---------|---------|-------|
| 13  | N     | 10       | Total | C  | N  | O  | P  | 0       | 0       | 0     |
|     |       |          | 207   | 99 | 39 | 59 | 10 |         |         |       |

- Molecule 14 is a RNA chain called TRANSCRIPT RNA 5'-R(\*CP\*CP\*AP\*GP\*GP\*AP)-3'.

| Mol | Chain | Residues | Atoms |    |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|---------|-------|
| 14  | P     | 6        | Total | C  | N  | O  | P | 0       | 0       | 0     |
|     |       |          | 130   | 58 | 26 | 40 | 6 |         |         |       |

- Molecule 15 is a DNA chain called TEMPLATE DNA 5'-D(\*AP\*GP\*CP\*TP\*CP\*AP\*AP\*GP\*TP\*AP\*CP \*TP\*TP\*TP\*TP\*TP\*CP\*CP\*TP\*BRUP\*GP\*GP\*TP\*CP\*AP\*TP\*TP)-3'.

| Mol | Chain | Residues | Atoms |    |     |    |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|-----|----|-----|---------|---------|-------|
| 15  | T     | 20       | Total | Br | C   | N  | O   | P       | 0       | 0     |
|     |       |          | 404   | 1  | 194 | 63 | 126 | 20      |         |       |

- Molecule 16 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 16  | A     | 2        | Total | Zn | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 16  | B     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 16  | C     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 16  | I     | 2        | Total | Zn | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 16  | J     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 16  | L     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

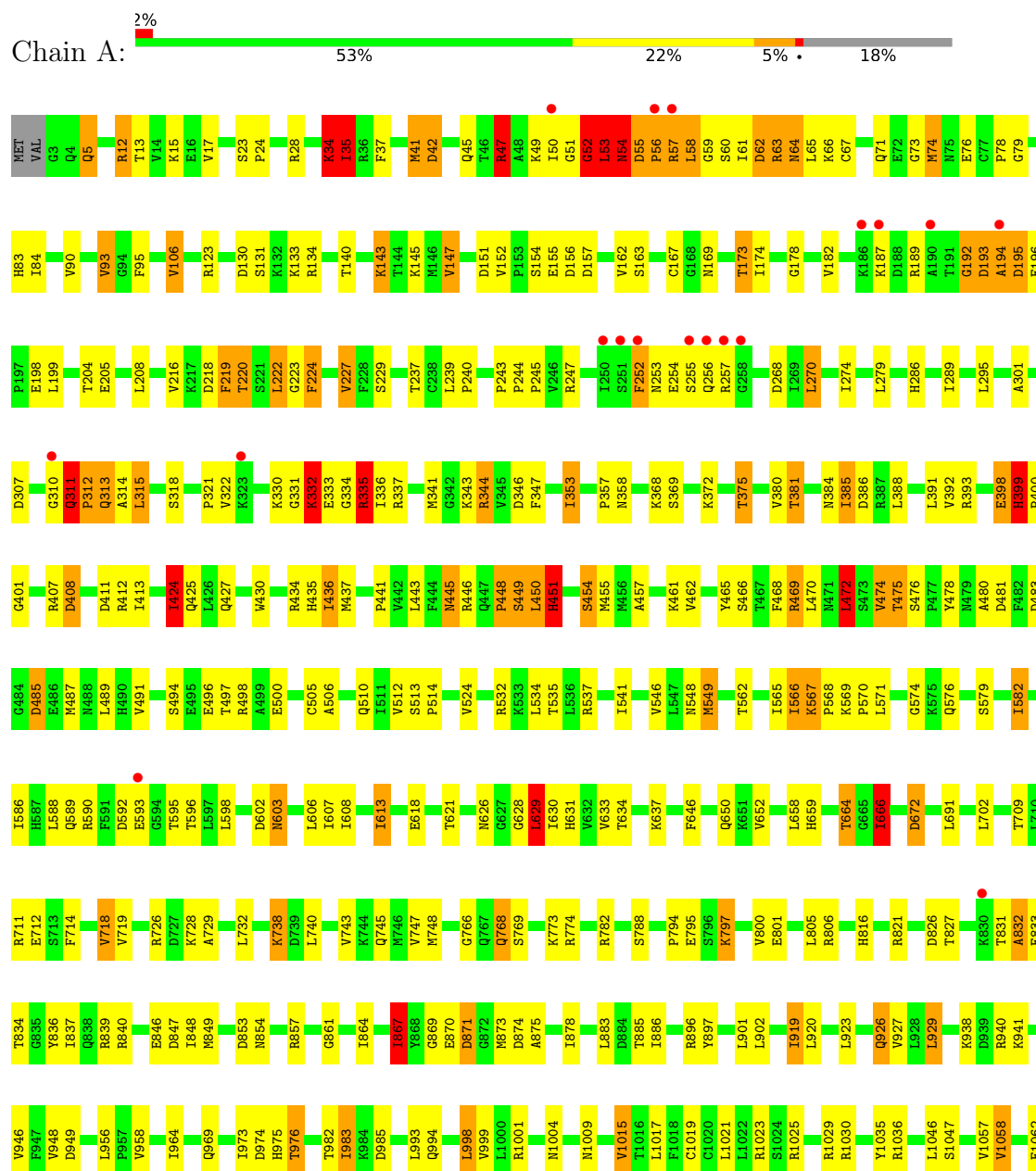
- Molecule 17 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

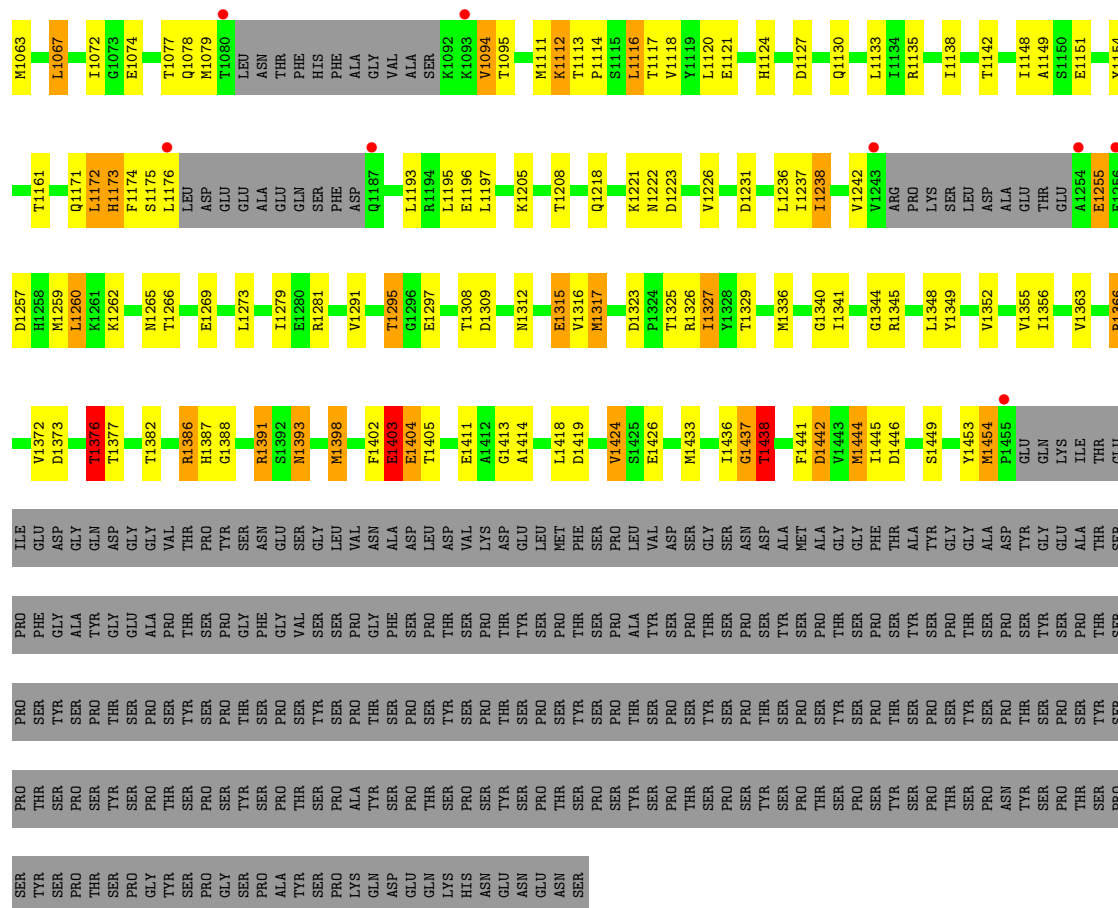
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 17  | A     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

### 3 Residue-property plots

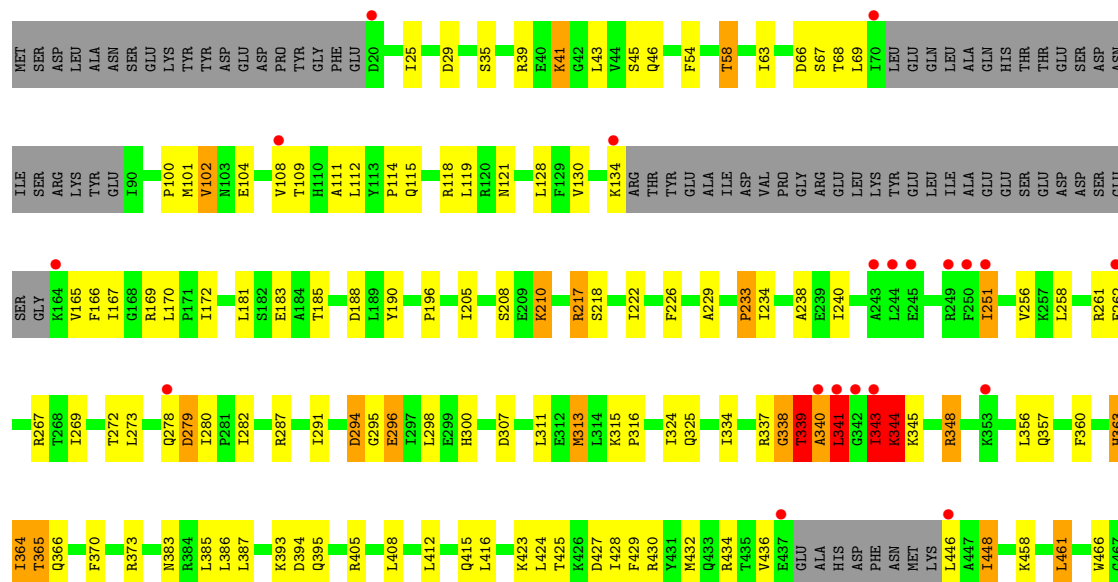
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

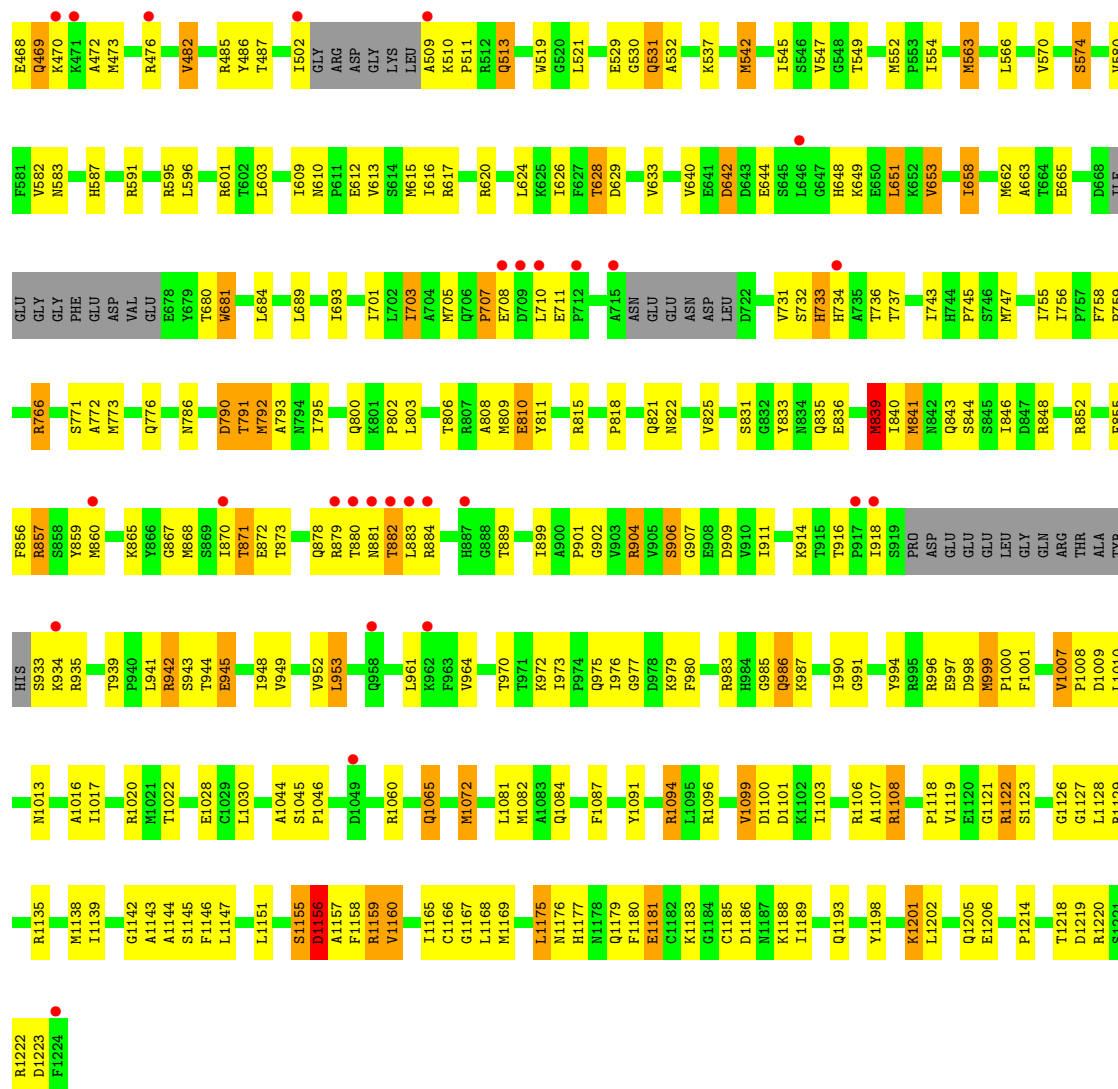




● Molecule 2: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB2

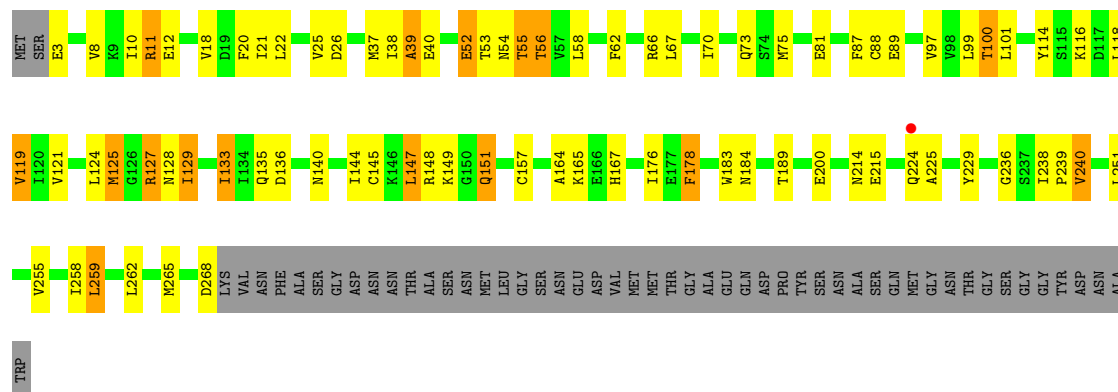




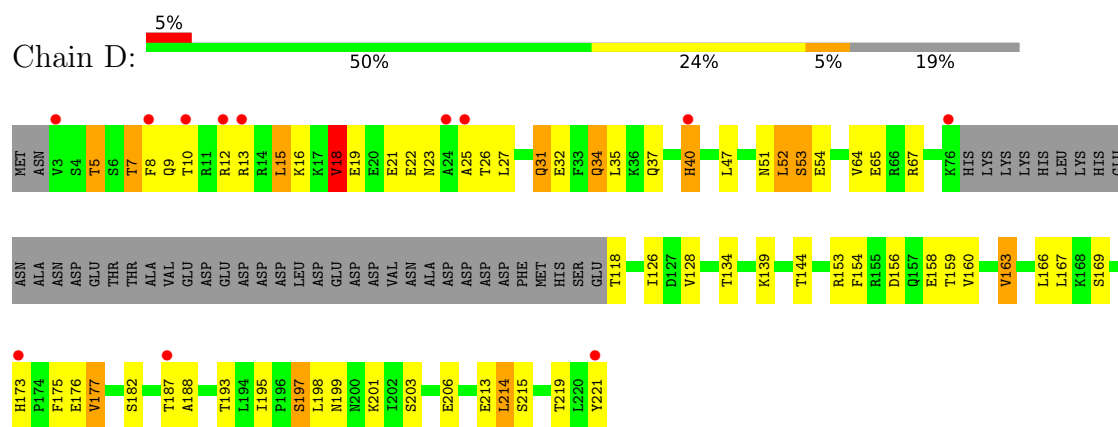


- Molecule 3: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3

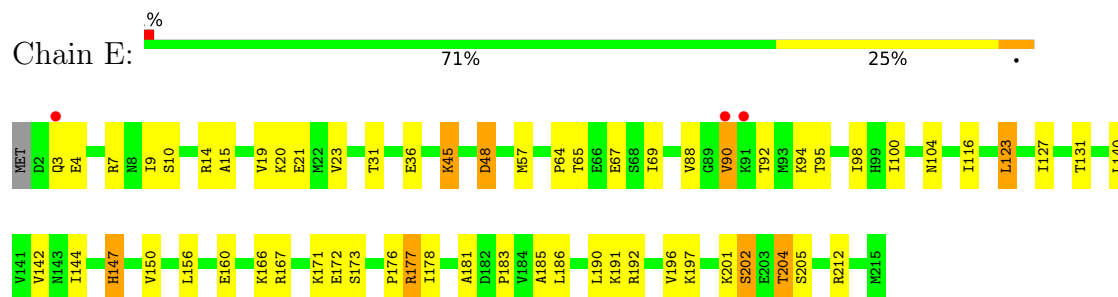
Chain C:



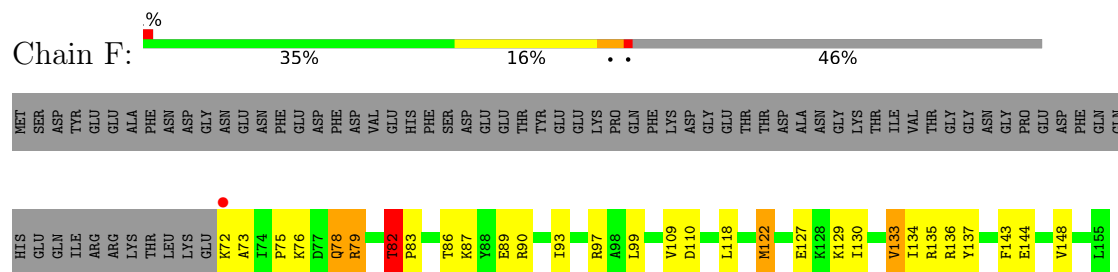
- Molecule 4: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB4



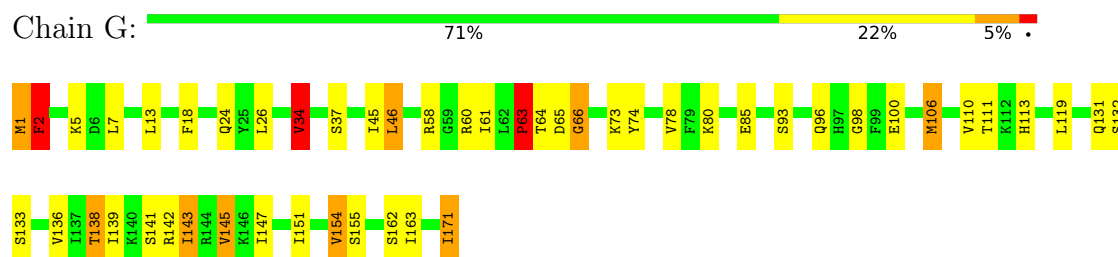
- Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1



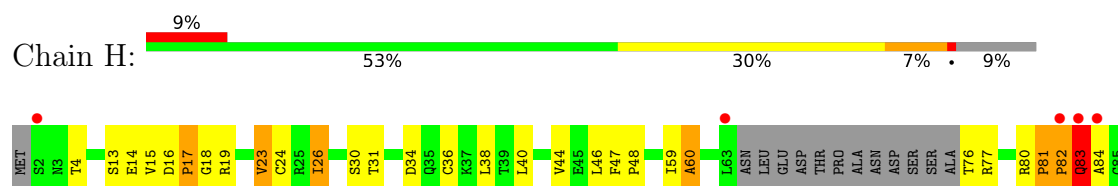
- Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2



- Molecule 7: RPB7, DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7

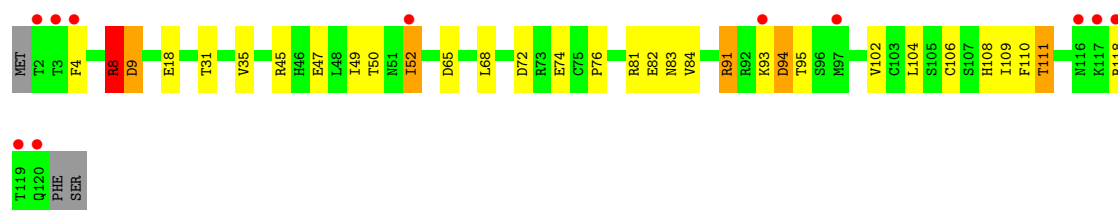


- Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3

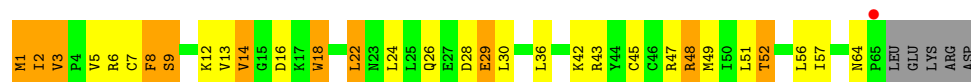




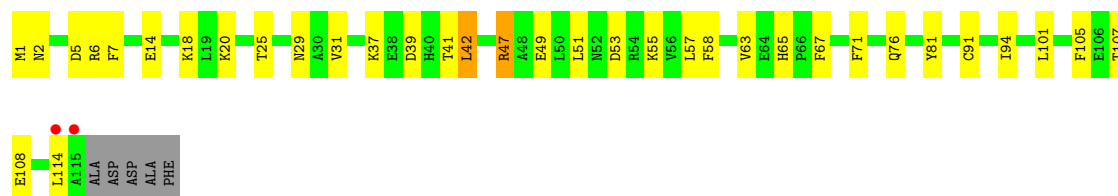
● Molecule 9: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9



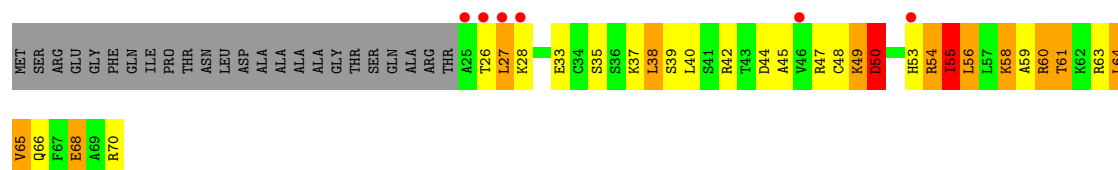
● Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5



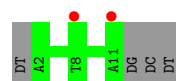
● Molecule 11: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11



● Molecule 12: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4



● Molecule 13: NON TEMPLATE DNA 5'-D(\*TP\*AP\*AP\*GP\*TP\*AP\*CP\*TP\*TP \*GP\*AP\*GP\*CP\*TP)-3'



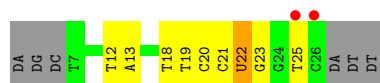
- Molecule 14: TRANSCRIPT RNA 5'-R(\*CP\*CP\*AP\*GP\*GP\*AP)-3'

Chain P:  67% 17% 17%



- Molecule 15: TEMPLATE DNA 5'-D(\*AP\*GP\*CP\*TP\*CP\*AP\*AP\*GP\*TP\*AP\*CP \*TP\*TP\*TP\*TP\*CP\*CP\*TP\*BRUP\*GP\*GP\*TP\*CP\*AP\*TP\*TP)-3'

Chain T:  8% 42% 31% 23%



## 4 Data and refinement statistics

| Property                                                                | Value                                                                         | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------------------------|------------------|
| Space group                                                             | C 2 2 21                                                                      | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 221.91Å 391.36Å 283.92Å<br>90.00° 90.00° 90.00°                               | Depositor        |
| Resolution (Å)                                                          | 49.96 – 3.40<br>49.96 – 3.40                                                  | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 100.0 (49.96-3.40)<br>100.0 (49.96-3.40)                                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.93                                                                          | Depositor        |
| $R_{sym}$                                                               | (Not available)                                                               | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.16 (at 3.40Å)                                                               | Xtriage          |
| Refinement program                                                      | BUSTER 2.11.2                                                                 | Depositor        |
| R, $R_{free}$                                                           | 0.161 , 0.186<br>0.183 , 0.201                                                | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 3331 reflections (1.98%)                                                      | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 95.8                                                                          | Xtriage          |
| Anisotropy                                                              | 0.405                                                                         | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.31 , 103.6                                                                  | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$                   | Xtriage          |
| Estimated twinning fraction                                             | 0.034 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l<br>0.037 for 1/2*h+1/2*k,3/2*h-1/2*k,-l | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.94                                                                          | EDS              |
| Total number of atoms                                                   | 31937                                                                         | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 111.0                                                                         | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.86% 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: BRU, ZN, MG

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     | 0.92         | 13/11374 (0.1%) | 1.56        | 134/15383 (0.9%) |
| 2   | B     | 0.87         | 4/9029 (0.0%)   | 1.45        | 82/12171 (0.7%)  |
| 3   | C     | 0.84         | 0/2133          | 1.42        | 15/2891 (0.5%)   |
| 4   | D     | 0.87         | 2/1444 (0.1%)   | 1.60        | 20/1935 (1.0%)   |
| 5   | E     | 0.83         | 0/1788          | 1.41        | 13/2406 (0.5%)   |
| 6   | F     | 1.00         | 1/691 (0.1%)    | 1.41        | 5/933 (0.5%)     |
| 7   | G     | 0.88         | 1/1368 (0.1%)   | 1.39        | 12/1844 (0.7%)   |
| 8   | H     | 0.86         | 0/1086          | 1.43        | 13/1470 (0.9%)   |
| 9   | I     | 0.82         | 0/989           | 1.37        | 7/1331 (0.5%)    |
| 10  | J     | 0.90         | 0/541           | 1.60        | 8/727 (1.1%)     |
| 11  | K     | 0.77         | 0/938           | 1.34        | 1/1267 (0.1%)    |
| 12  | L     | 0.92         | 0/365           | 1.51        | 5/485 (1.0%)     |
| 13  | N     | 0.47         | 0/232           | 0.67        | 0/356            |
| 14  | P     | 0.82         | 0/145           | 0.71        | 0/224            |
| 15  | T     | 0.55         | 0/426           | 0.65        | 0/652            |
| All | All   | 0.88         | 21/32549 (0.1%) | 1.47        | 315/44075 (0.7%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 2                   |

All (21) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4   | D     | 25  | ALA  | CA-C    | 8.25  | 1.62        | 1.53     |
| 1   | A     | 867 | ILE  | CG1-CD1 | 8.13  | 1.83        | 1.51     |
| 1   | A     | 549 | MET  | SD-CE   | -7.58 | 1.60        | 1.79     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1   | A     | 1454 | MET  | CA-C  | 6.86  | 1.61        | 1.52     |
| 7   | G     | 1    | MET  | C-N   | 6.50  | 1.42        | 1.33     |
| 1   | A     | 54   | ASN  | CA-C  | 6.49  | 1.61        | 1.52     |
| 6   | F     | 122  | MET  | SD-CE | 6.23  | 1.95        | 1.79     |
| 1   | A     | 57   | ARG  | CA-C  | 6.18  | 1.61        | 1.52     |
| 1   | A     | 1398 | MET  | SD-CE | 5.96  | 1.94        | 1.79     |
| 4   | D     | 18   | VAL  | CA-C  | 5.72  | 1.60        | 1.52     |
| 2   | B     | 839  | MET  | SD-CE | -5.70 | 1.65        | 1.79     |
| 1   | A     | 437  | MET  | SD-CE | 5.51  | 1.93        | 1.79     |
| 1   | A     | 52   | GLY  | C-N   | 5.50  | 1.42        | 1.33     |
| 1   | A     | 57   | ARG  | C-N   | 5.39  | 1.41        | 1.33     |
| 2   | B     | 1017 | ILE  | CA-C  | 5.38  | 1.58        | 1.52     |
| 2   | B     | 881  | ASN  | C-N   | 5.37  | 1.40        | 1.33     |
| 1   | A     | 56   | PRO  | C-N   | 5.13  | 1.40        | 1.33     |
| 1   | A     | 332  | LYS  | CA-C  | -5.08 | 1.46        | 1.52     |
| 2   | B     | 1169 | MET  | SD-CE | -5.08 | 1.66        | 1.79     |
| 1   | A     | 1057 | VAL  | C-N   | 5.07  | 1.39        | 1.33     |
| 1   | A     | 53   | LEU  | N-CA  | 5.02  | 1.52        | 1.45     |

All (315) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 4   | D     | 26   | THR  | N-CA-C   | -11.91 | 96.11       | 112.30   |
| 1   | A     | 34   | LYS  | CA-C-N   | 10.02  | 139.73      | 121.70   |
| 1   | A     | 34   | LYS  | C-N-CA   | 10.02  | 139.73      | 121.70   |
| 8   | H     | 92   | ASP  | N-CA-C   | -9.78  | 101.57      | 112.72   |
| 2   | B     | 296  | GLU  | N-CA-C   | -9.70  | 99.76       | 111.69   |
| 3   | C     | 39   | ALA  | N-CA-C   | 9.52   | 125.68      | 112.45   |
| 10  | J     | 5    | VAL  | N-CA-C   | -9.42  | 97.43       | 109.58   |
| 2   | B     | 628  | THR  | CA-C-N   | 9.38   | 135.29      | 121.31   |
| 2   | B     | 628  | THR  | C-N-CA   | 9.38   | 135.29      | 121.31   |
| 4   | D     | 25   | ALA  | CA-C-N   | 8.89   | 136.98      | 122.14   |
| 4   | D     | 25   | ALA  | C-N-CA   | 8.89   | 136.98      | 122.14   |
| 8   | H     | 81   | PRO  | N-CA-C   | 8.75   | 121.37      | 110.70   |
| 1   | A     | 54   | ASN  | CA-CB-CG | 8.51   | 121.11      | 112.60   |
| 2   | B     | 1122 | ARG  | CA-C-N   | 8.40   | 131.88      | 120.54   |
| 2   | B     | 1122 | ARG  | C-N-CA   | 8.40   | 131.88      | 120.54   |
| 4   | D     | 54   | GLU  | N-CA-C   | -8.23  | 102.39      | 111.36   |
| 1   | A     | 42   | ASP  | CA-CB-CG | 8.22   | 120.82      | 112.60   |
| 8   | H     | 129  | TYR  | N-CA-C   | 8.15   | 119.79      | 111.07   |
| 1   | A     | 1403 | GLU  | CA-C-N   | -8.00  | 109.85      | 122.65   |
| 1   | A     | 1403 | GLU  | C-N-CA   | -8.00  | 109.85      | 122.65   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1   | A     | 56   | PRO  | CA-C-N   | 7.96  | 136.73      | 121.54   |
| 1   | A     | 56   | PRO  | C-N-CA   | 7.96  | 136.73      | 121.54   |
| 1   | A     | 194  | ALA  | CA-C-N   | 7.85  | 135.83      | 121.70   |
| 1   | A     | 194  | ALA  | C-N-CA   | 7.85  | 135.83      | 121.70   |
| 4   | D     | 31   | GLN  | N-CA-C   | -7.66 | 103.01      | 111.36   |
| 1   | A     | 143  | LYS  | CA-C-N   | 7.64  | 130.52      | 120.28   |
| 1   | A     | 143  | LYS  | C-N-CA   | 7.64  | 130.52      | 120.28   |
| 1   | A     | 35   | ILE  | N-CA-CB  | 7.64  | 124.49      | 111.50   |
| 1   | A     | 485  | ASP  | CA-CB-CG | 7.56  | 120.16      | 112.60   |
| 2   | B     | 340  | ALA  | CA-C-N   | 7.54  | 135.94      | 121.54   |
| 2   | B     | 340  | ALA  | C-N-CA   | 7.54  | 135.94      | 121.54   |
| 2   | B     | 629  | ASP  | CA-CB-CG | 7.49  | 120.08      | 112.60   |
| 1   | A     | 399  | HIS  | N-CA-CB  | 7.46  | 123.66      | 110.37   |
| 1   | A     | 311  | GLN  | N-CA-C   | 7.33  | 126.01      | 109.81   |
| 2   | B     | 736  | THR  | N-CA-C   | -7.33 | 104.19      | 113.72   |
| 1   | A     | 998  | LEU  | N-CA-C   | 7.32  | 120.60      | 108.96   |
| 1   | A     | 1404 | GLU  | N-CA-C   | 7.29  | 121.89      | 112.92   |
| 2   | B     | 1169 | MET  | CA-C-N   | 7.26  | 130.98      | 120.38   |
| 2   | B     | 1169 | MET  | C-N-CA   | 7.26  | 130.98      | 120.38   |
| 1   | A     | 5    | GLN  | N-CA-C   | 7.19  | 120.03      | 110.53   |
| 6   | F     | 87   | LYS  | CA-C-N   | 7.18  | 129.91      | 120.28   |
| 6   | F     | 87   | LYS  | C-N-CA   | 7.18  | 129.91      | 120.28   |
| 8   | H     | 128  | ASN  | CA-C-N   | 7.15  | 129.73      | 120.44   |
| 8   | H     | 128  | ASN  | C-N-CA   | 7.15  | 129.73      | 120.44   |
| 10  | J     | 9    | SER  | N-CA-C   | 7.15  | 118.72      | 111.07   |
| 3   | C     | 62   | PHE  | CA-C-N   | 7.14  | 129.56      | 120.56   |
| 3   | C     | 62   | PHE  | C-N-CA   | 7.14  | 129.56      | 120.56   |
| 2   | B     | 188  | ASP  | CA-CB-CG | 7.14  | 119.74      | 112.60   |
| 1   | A     | 1419 | ASP  | CA-C-N   | 7.12  | 129.82      | 120.28   |
| 1   | A     | 1419 | ASP  | C-N-CA   | 7.12  | 129.82      | 120.28   |
| 7   | G     | 34   | VAL  | N-CA-C   | 7.05  | 117.66      | 110.82   |
| 3   | C     | 183  | TRP  | N-CA-C   | -7.00 | 97.83       | 109.24   |
| 1   | A     | 53   | LEU  | N-CA-CB  | 6.80  | 120.94      | 110.60   |
| 4   | D     | 51   | ASN  | CA-CB-CG | 6.78  | 119.38      | 112.60   |
| 1   | A     | 64   | ASN  | N-CA-C   | -6.70 | 101.89      | 110.53   |
| 10  | J     | 18   | TRP  | N-CA-C   | 6.66  | 118.42      | 111.03   |
| 2   | B     | 1181 | GLU  | N-CA-C   | 6.63  | 124.92      | 110.80   |
| 7   | G     | 2    | PHE  | CA-CB-CG | 6.62  | 120.42      | 113.80   |
| 1   | A     | 1403 | GLU  | N-CA-C   | 6.58  | 124.81      | 110.80   |
| 3   | C     | 40   | GLU  | N-CA-C   | 6.54  | 121.41      | 113.17   |
| 2   | B     | 294  | ASP  | CA-CB-CG | 6.52  | 119.12      | 112.60   |
| 1   | A     | 219  | PHE  | CA-CB-CG | 6.52  | 120.32      | 113.80   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 2   | B     | 790  | ASP  | CA-CB-CG | 6.52  | 119.12      | 112.60   |
| 2   | B     | 339  | THR  | CA-C-N   | 6.51  | 133.97      | 121.54   |
| 2   | B     | 339  | THR  | C-N-CA   | 6.51  | 133.97      | 121.54   |
| 1   | A     | 897  | TYR  | N-CA-C   | 6.50  | 121.33      | 113.41   |
| 7   | G     | 65   | ASP  | CA-CB-CG | 6.48  | 119.08      | 112.60   |
| 1   | A     | 223  | GLY  | CA-C-N   | 6.47  | 133.91      | 121.54   |
| 1   | A     | 223  | GLY  | C-N-CA   | 6.47  | 133.91      | 121.54   |
| 4   | D     | 163  | VAL  | CA-C-N   | 6.47  | 129.32      | 120.46   |
| 4   | D     | 163  | VAL  | C-N-CA   | 6.47  | 129.32      | 120.46   |
| 1   | A     | 472  | LEU  | N-CA-C   | 6.47  | 119.15      | 111.71   |
| 2   | B     | 102  | VAL  | N-CA-C   | 6.44  | 117.13      | 108.11   |
| 2   | B     | 1156 | ASP  | N-CA-C   | 6.44  | 124.52      | 110.80   |
| 3   | C     | 178  | PHE  | CA-CB-CG | 6.41  | 120.21      | 113.80   |
| 2   | B     | 66   | ASP  | CA-C-N   | 6.39  | 129.67      | 120.79   |
| 2   | B     | 66   | ASP  | C-N-CA   | 6.39  | 129.67      | 120.79   |
| 2   | B     | 1219 | ASP  | CA-CB-CG | 6.38  | 118.98      | 112.60   |
| 4   | D     | 31   | GLN  | CA-C-N   | 6.37  | 128.81      | 120.28   |
| 4   | D     | 31   | GLN  | C-N-CA   | 6.37  | 128.81      | 120.28   |
| 3   | C     | 200  | GLU  | N-CA-C   | 6.36  | 118.30      | 111.36   |
| 2   | B     | 1177 | HIS  | N-CA-C   | -6.36 | 105.56      | 113.38   |
| 3   | C     | 135  | GLN  | CA-C-N   | 6.36  | 131.48      | 121.56   |
| 3   | C     | 135  | GLN  | C-N-CA   | 6.36  | 131.48      | 121.56   |
| 3   | C     | 89   | GLU  | N-CA-C   | -6.34 | 96.73       | 108.02   |
| 2   | B     | 818  | PRO  | N-CA-C   | 6.33  | 120.08      | 111.22   |
| 1   | A     | 341  | MET  | CA-C-N   | 6.28  | 126.44      | 121.61   |
| 1   | A     | 341  | MET  | C-N-CA   | 6.28  | 126.44      | 121.61   |
| 1   | A     | 411  | ASP  | CA-C-N   | 6.22  | 130.39      | 121.50   |
| 1   | A     | 411  | ASP  | C-N-CA   | 6.22  | 130.39      | 121.50   |
| 1   | A     | 408  | ASP  | CA-C-N   | 6.21  | 130.62      | 120.63   |
| 1   | A     | 408  | ASP  | C-N-CA   | 6.21  | 130.62      | 120.63   |
| 1   | A     | 169  | ASN  | N-CA-C   | 6.19  | 119.02      | 110.35   |
| 1   | A     | 334  | GLY  | CA-C-N   | 6.18  | 133.35      | 121.54   |
| 1   | A     | 334  | GLY  | C-N-CA   | 6.18  | 133.35      | 121.54   |
| 2   | B     | 1180 | PHE  | CA-CB-CG | -6.18 | 107.62      | 113.80   |
| 1   | A     | 398  | GLU  | CA-C-O   | -6.17 | 114.84      | 121.56   |
| 1   | A     | 123  | ARG  | CA-C-N   | 6.15  | 128.81      | 120.44   |
| 1   | A     | 123  | ARG  | C-N-CA   | 6.15  | 128.81      | 120.44   |
| 2   | B     | 67   | SER  | N-CA-C   | 6.15  | 118.53      | 111.02   |
| 2   | B     | 363  | HIS  | N-CA-C   | -6.15 | 102.56      | 110.19   |
| 1   | A     | 60   | SER  | N-CA-C   | 6.06  | 118.63      | 109.23   |
| 11  | K     | 53   | ASP  | CA-CB-CG | 6.06  | 118.66      | 112.60   |
| 7   | G     | 106  | MET  | N-CA-C   | 6.06  | 119.53      | 110.14   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 9   | I     | 8    | ARG  | N-CA-C   | -6.06 | 100.13      | 109.76   |
| 4   | D     | 188  | ALA  | N-CA-C   | -6.04 | 105.17      | 112.54   |
| 4   | D     | 18   | VAL  | CA-C-N   | 6.04  | 132.57      | 121.70   |
| 4   | D     | 18   | VAL  | C-N-CA   | 6.04  | 132.57      | 121.70   |
| 2   | B     | 906  | SER  | N-CA-C   | 6.03  | 122.34      | 114.75   |
| 1   | A     | 244  | PRO  | N-CA-C   | 6.02  | 118.05      | 110.70   |
| 1   | A     | 1112 | LYS  | N-CA-C   | 6.02  | 119.10      | 111.69   |
| 8   | H     | 131  | ASN  | N-CA-C   | -6.02 | 104.80      | 111.36   |
| 2   | B     | 338  | GLY  | CA-C-N   | 6.00  | 132.50      | 121.70   |
| 2   | B     | 338  | GLY  | C-N-CA   | 6.00  | 132.50      | 121.70   |
| 1   | A     | 1376 | THR  | CB-CA-C  | 5.98  | 120.90      | 111.39   |
| 2   | B     | 68   | THR  | CB-CA-C  | 5.98  | 117.16      | 109.80   |
| 2   | B     | 642  | ASP  | N-CA-C   | -5.98 | 105.08      | 112.38   |
| 9   | I     | 94   | ASP  | CA-C-N   | 5.96  | 132.93      | 121.54   |
| 9   | I     | 94   | ASP  | C-N-CA   | 5.96  | 132.93      | 121.54   |
| 2   | B     | 707  | PRO  | CA-C-N   | 5.94  | 128.56      | 120.54   |
| 2   | B     | 707  | PRO  | C-N-CA   | 5.94  | 128.56      | 120.54   |
| 1   | A     | 78   | PRO  | N-CA-C   | -5.94 | 101.94      | 111.38   |
| 10  | J     | 14   | VAL  | N-CA-C   | -5.93 | 107.35      | 113.10   |
| 2   | B     | 791  | THR  | N-CA-C   | -5.89 | 100.94      | 109.59   |
| 1   | A     | 794  | PRO  | CA-C-N   | 5.88  | 128.75      | 120.28   |
| 1   | A     | 794  | PRO  | C-N-CA   | 5.88  | 128.75      | 120.28   |
| 1   | A     | 853  | ASP  | CA-CB-CG | 5.88  | 118.48      | 112.60   |
| 5   | E     | 123  | LEU  | CA-C-N   | 5.86  | 125.02      | 120.33   |
| 5   | E     | 123  | LEU  | C-N-CA   | 5.86  | 125.02      | 120.33   |
| 5   | E     | 171  | LYS  | N-CA-C   | -5.85 | 100.75      | 110.17   |
| 1   | A     | 718  | VAL  | CA-C-N   | 5.83  | 128.75      | 120.53   |
| 1   | A     | 718  | VAL  | C-N-CA   | 5.83  | 128.75      | 120.53   |
| 1   | A     | 871  | ASP  | CA-CB-CG | 5.81  | 118.41      | 112.60   |
| 2   | B     | 208  | SER  | N-CA-C   | 5.79  | 119.06      | 110.48   |
| 1   | A     | 424  | ILE  | CA-C-N   | -5.79 | 115.31      | 122.84   |
| 1   | A     | 424  | ILE  | C-N-CA   | -5.79 | 115.31      | 122.84   |
| 1   | A     | 800  | VAL  | CA-C-N   | 5.78  | 128.02      | 120.28   |
| 1   | A     | 800  | VAL  | C-N-CA   | 5.78  | 128.02      | 120.28   |
| 9   | I     | 52   | ILE  | N-CA-CB  | 5.77  | 118.23      | 111.66   |
| 12  | L     | 44   | ASP  | CA-C-N   | 5.76  | 132.54      | 121.54   |
| 12  | L     | 44   | ASP  | C-N-CA   | 5.76  | 132.54      | 121.54   |
| 5   | E     | 95   | THR  | CA-C-N   | 5.76  | 128.00      | 120.28   |
| 5   | E     | 95   | THR  | C-N-CA   | 5.76  | 128.00      | 120.28   |
| 1   | A     | 462  | VAL  | N-CA-CB  | 5.75  | 117.39      | 110.31   |
| 1   | A     | 832  | ALA  | CA-C-N   | 5.75  | 127.92      | 120.44   |
| 1   | A     | 832  | ALA  | C-N-CA   | 5.75  | 127.92      | 120.44   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 2   | B     | 825  | VAL  | N-CA-C   | 5.74  | 116.12      | 107.80   |
| 1   | A     | 728  | LYS  | CA-C-N   | 5.74  | 128.24      | 120.38   |
| 1   | A     | 728  | LYS  | C-N-CA   | 5.74  | 128.24      | 120.38   |
| 1   | A     | 833  | GLU  | CA-C-N   | 5.74  | 127.97      | 120.28   |
| 1   | A     | 833  | GLU  | C-N-CA   | 5.74  | 127.97      | 120.28   |
| 1   | A     | 938  | LYS  | CA-C-N   | 5.74  | 128.28      | 120.54   |
| 1   | A     | 938  | LYS  | C-N-CA   | 5.74  | 128.28      | 120.54   |
| 2   | B     | 703  | ILE  | N-CA-C   | 5.73  | 117.25      | 108.71   |
| 10  | J     | 14   | VAL  | CB-CA-C  | 5.72  | 117.22      | 110.93   |
| 9   | I     | 93   | LYS  | CA-C-N   | 5.71  | 129.39      | 120.82   |
| 9   | I     | 93   | LYS  | C-N-CA   | 5.71  | 129.39      | 120.82   |
| 7   | G     | 141  | SER  | N-CA-C   | 5.71  | 117.66      | 110.24   |
| 4   | D     | 173  | HIS  | CB-CA-C  | 5.67  | 118.33      | 109.42   |
| 4   | D     | 158  | GLU  | CA-C-N   | 5.66  | 127.80      | 120.44   |
| 4   | D     | 158  | GLU  | C-N-CA   | 5.66  | 127.80      | 120.44   |
| 1   | A     | 537  | ARG  | CA-C-N   | 5.66  | 128.64      | 120.38   |
| 1   | A     | 537  | ARG  | C-N-CA   | 5.66  | 128.64      | 120.38   |
| 12  | L     | 49   | LYS  | CA-C-N   | 5.66  | 132.34      | 121.54   |
| 12  | L     | 49   | LYS  | C-N-CA   | 5.66  | 132.34      | 121.54   |
| 1   | A     | 23   | SER  | N-CA-C   | -5.63 | 102.95      | 109.93   |
| 2   | B     | 732  | SER  | N-CA-C   | 5.62  | 116.79      | 108.86   |
| 1   | A     | 34   | LYS  | N-CA-C   | -5.62 | 98.01       | 108.02   |
| 1   | A     | 1138 | ILE  | N-CA-C   | 5.61  | 116.44      | 111.90   |
| 7   | G     | 66   | GLY  | CA-C-N   | 5.61  | 132.26      | 121.54   |
| 7   | G     | 66   | GLY  | C-N-CA   | 5.61  | 132.26      | 121.54   |
| 2   | B     | 343  | ILE  | CA-C-N   | 5.58  | 132.20      | 121.54   |
| 2   | B     | 343  | ILE  | C-N-CA   | 5.58  | 132.20      | 121.54   |
| 1   | A     | 629  | LEU  | N-CA-C   | -5.58 | 105.20      | 111.28   |
| 1   | A     | 602  | ASP  | CA-CB-CG | 5.56  | 118.16      | 112.60   |
| 2   | B     | 1155 | SER  | CA-C-N   | 5.56  | 132.16      | 121.54   |
| 2   | B     | 1155 | SER  | C-N-CA   | 5.56  | 132.16      | 121.54   |
| 2   | B     | 1013 | ASN  | N-CA-C   | 5.56  | 117.67      | 109.50   |
| 1   | A     | 1344 | GLY  | CA-C-N   | 5.54  | 127.65      | 120.44   |
| 1   | A     | 1344 | GLY  | C-N-CA   | 5.54  | 127.65      | 120.44   |
| 1   | A     | 222  | LEU  | N-CA-C   | -5.54 | 103.59      | 110.41   |
| 1   | A     | 496  | GLU  | CA-C-N   | 5.54  | 127.71      | 120.28   |
| 1   | A     | 496  | GLU  | C-N-CA   | 5.54  | 127.71      | 120.28   |
| 1   | A     | 54   | ASN  | CA-C-N   | 5.54  | 135.31      | 121.80   |
| 1   | A     | 54   | ASN  | C-N-CA   | 5.54  | 135.31      | 121.80   |
| 1   | A     | 1072 | ILE  | N-CA-C   | -5.53 | 107.42      | 111.90   |
| 2   | B     | 1017 | ILE  | N-CA-C   | 5.52  | 120.81      | 108.88   |
| 1   | A     | 229  | SER  | N-CA-C   | 5.52  | 117.70      | 107.60   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 2   | B     | 41   | LYS  | N-CA-C   | 5.50  | 117.36      | 111.36   |
| 1   | A     | 218  | ASP  | CA-CB-CG | 5.50  | 118.10      | 112.60   |
| 2   | B     | 755  | ILE  | N-CA-C   | -5.50 | 107.43      | 113.43   |
| 1   | A     | 1269 | GLU  | N-CA-C   | 5.49  | 118.44      | 111.69   |
| 2   | B     | 733  | HIS  | CA-C-N   | 5.48  | 127.89      | 120.38   |
| 2   | B     | 733  | HIS  | C-N-CA   | 5.48  | 127.89      | 120.38   |
| 2   | B     | 1009 | ASP  | N-CA-C   | -5.47 | 105.73      | 112.90   |
| 1   | A     | 57   | ARG  | CA-C-N   | 5.47  | 131.98      | 121.54   |
| 1   | A     | 57   | ARG  | C-N-CA   | 5.47  | 131.98      | 121.54   |
| 1   | A     | 1001 | ARG  | N-CA-C   | 5.46  | 120.60      | 113.88   |
| 1   | A     | 1413 | GLY  | CA-C-N   | 5.46  | 127.87      | 120.38   |
| 1   | A     | 1413 | GLY  | C-N-CA   | 5.46  | 127.87      | 120.38   |
| 1   | A     | 173  | THR  | CB-CA-C  | 5.46  | 120.47      | 111.31   |
| 2   | B     | 945  | GLU  | N-CA-C   | 5.45  | 117.56      | 110.53   |
| 2   | B     | 1185 | CYS  | N-CA-C   | -5.45 | 106.77      | 113.41   |
| 2   | B     | 1180 | PHE  | N-CA-C   | 5.44  | 119.59      | 112.13   |
| 1   | A     | 1231 | ASP  | CA-C-N   | 5.43  | 128.01      | 120.63   |
| 1   | A     | 1231 | ASP  | C-N-CA   | 5.43  | 128.01      | 120.63   |
| 2   | B     | 43   | LEU  | N-CA-C   | 5.43  | 119.90      | 113.28   |
| 2   | B     | 427  | ASP  | N-CA-C   | -5.43 | 106.79      | 113.41   |
| 1   | A     | 399  | HIS  | CA-CB-CG | -5.41 | 108.39      | 113.80   |
| 1   | A     | 874  | ASP  | CA-CB-CG | 5.40  | 118.00      | 112.60   |
| 6   | F     | 82   | THR  | CB-CA-C  | -5.40 | 100.99      | 109.52   |
| 5   | E     | 172  | GLU  | CA-C-N   | 5.40  | 127.83      | 120.54   |
| 5   | E     | 172  | GLU  | C-N-CA   | 5.40  | 127.83      | 120.54   |
| 4   | D     | 214  | LEU  | N-CA-C   | -5.39 | 106.38      | 113.12   |
| 2   | B     | 45   | SER  | CA-C-N   | 5.38  | 127.81      | 120.54   |
| 2   | B     | 45   | SER  | C-N-CA   | 5.38  | 127.81      | 120.54   |
| 1   | A     | 1295 | THR  | CB-CA-C  | 5.37  | 121.12      | 110.17   |
| 1   | A     | 1161 | THR  | N-CA-C   | 5.36  | 118.22      | 109.59   |
| 10  | J     | 16   | ASP  | CA-CB-CG | 5.36  | 117.96      | 112.60   |
| 1   | A     | 224  | PHE  | CA-CB-CG | -5.35 | 108.45      | 113.80   |
| 10  | J     | 8    | PHE  | CA-CB-CG | 5.35  | 119.15      | 113.80   |
| 1   | A     | 510  | GLN  | N-CA-C   | 5.35  | 119.43      | 113.01   |
| 3   | C     | 87   | PHE  | N-CA-C   | 5.34  | 119.78      | 113.16   |
| 8   | H     | 137  | GLN  | CA-C-N   | 5.34  | 127.97      | 120.28   |
| 8   | H     | 137  | GLN  | C-N-CA   | 5.34  | 127.97      | 120.28   |
| 12  | L     | 40   | LEU  | N-CA-C   | 5.34  | 117.58      | 110.53   |
| 2   | B     | 1186 | ASP  | CA-CB-CG | 5.33  | 117.93      | 112.60   |
| 4   | D     | 26   | THR  | CA-C-N   | 5.31  | 130.10      | 122.40   |
| 4   | D     | 26   | THR  | C-N-CA   | 5.31  | 130.10      | 122.40   |
| 2   | B     | 1099 | VAL  | N-CA-CB  | 5.30  | 116.40      | 110.51   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1   | A     | 592  | ASP  | CA-CB-CG | 5.30  | 117.90      | 112.60   |
| 8   | H     | 128  | ASN  | CA-CB-CG | 5.30  | 117.90      | 112.60   |
| 1   | A     | 1205 | LYS  | N-CA-C   | -5.29 | 98.20       | 107.73   |
| 1   | A     | 664  | THR  | CB-CA-C  | 5.28  | 118.82      | 109.89   |
| 1   | A     | 1403 | GLU  | CB-CG-CD | 5.28  | 121.57      | 112.60   |
| 1   | A     | 1117 | THR  | CB-CA-C  | 5.27  | 120.09      | 111.23   |
| 2   | B     | 1065 | GLN  | CB-CA-C  | 5.27  | 118.93      | 110.29   |
| 1   | A     | 310  | GLY  | CA-C-N   | 5.26  | 134.63      | 121.80   |
| 1   | A     | 310  | GLY  | C-N-CA   | 5.26  | 134.63      | 121.80   |
| 2   | B     | 881  | ASN  | CA-C-N   | 5.25  | 127.27      | 120.44   |
| 2   | B     | 881  | ASN  | C-N-CA   | 5.25  | 127.27      | 120.44   |
| 8   | H     | 83   | GLN  | CA-C-N   | 5.25  | 130.76      | 120.99   |
| 8   | H     | 83   | GLN  | C-N-CA   | 5.25  | 130.76      | 120.99   |
| 2   | B     | 628  | THR  | N-CA-C   | -5.25 | 106.88      | 113.28   |
| 5   | E     | 21   | GLU  | CA-C-N   | 5.25  | 127.31      | 120.28   |
| 5   | E     | 21   | GLU  | C-N-CA   | 5.25  | 127.31      | 120.28   |
| 1   | A     | 17   | VAL  | N-CA-CB  | 5.24  | 118.50      | 111.90   |
| 1   | A     | 1266 | THR  | N-CA-C   | -5.24 | 105.47      | 111.07   |
| 1   | A     | 331  | GLY  | CA-C-N   | 5.23  | 131.53      | 121.54   |
| 1   | A     | 331  | GLY  | C-N-CA   | 5.23  | 131.53      | 121.54   |
| 1   | A     | 73   | GLY  | CA-C-N   | 5.23  | 131.52      | 121.54   |
| 1   | A     | 73   | GLY  | C-N-CA   | 5.23  | 131.52      | 121.54   |
| 7   | G     | 63   | PRO  | N-CA-C   | 5.23  | 123.24      | 112.47   |
| 1   | A     | 451  | HIS  | N-CA-CB  | -5.22 | 101.81      | 111.52   |
| 5   | E     | 177  | ARG  | N-CA-C   | 5.21  | 117.46      | 109.07   |
| 1   | A     | 535  | THR  | N-CA-C   | 5.21  | 118.49      | 112.97   |
| 5   | E     | 147  | HIS  | CA-C-N   | 5.21  | 129.47      | 121.19   |
| 5   | E     | 147  | HIS  | C-N-CA   | 5.21  | 129.47      | 121.19   |
| 1   | A     | 666  | ILE  | N-CA-CB  | 5.21  | 119.56      | 110.65   |
| 1   | A     | 47   | ARG  | CA-C-N   | 5.20  | 131.47      | 121.54   |
| 1   | A     | 47   | ARG  | C-N-CA   | 5.20  | 131.47      | 121.54   |
| 2   | B     | 233  | PRO  | CA-C-N   | 5.18  | 128.81      | 121.66   |
| 2   | B     | 233  | PRO  | C-N-CA   | 5.18  | 128.81      | 121.66   |
| 2   | B     | 222  | ILE  | CA-C-N   | 5.18  | 128.94      | 121.18   |
| 2   | B     | 222  | ILE  | C-N-CA   | 5.18  | 128.94      | 121.18   |
| 1   | A     | 969  | GLN  | N-CA-CB  | 5.17  | 117.81      | 110.16   |
| 1   | A     | 24   | PRO  | CA-C-N   | 5.17  | 127.46      | 120.38   |
| 1   | A     | 24   | PRO  | C-N-CA   | 5.17  | 127.46      | 120.38   |
| 3   | C     | 225  | ALA  | N-CA-C   | 5.16  | 116.67      | 108.67   |
| 3   | C     | 262  | LEU  | CA-C-N   | 5.16  | 127.19      | 120.28   |
| 3   | C     | 262  | LEU  | C-N-CA   | 5.16  | 127.19      | 120.28   |
| 9   | I     | 110  | PHE  | CA-CB-CG | 5.15  | 118.95      | 113.80   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 6   | F     | 122  | MET  | CA-C-N   | 5.14  | 127.12      | 120.44   |
| 6   | F     | 122  | MET  | C-N-CA   | 5.14  | 127.12      | 120.44   |
| 2   | B     | 810  | GLU  | CA-C-N   | 5.13  | 129.41      | 120.68   |
| 2   | B     | 810  | GLU  | C-N-CA   | 5.13  | 129.41      | 120.68   |
| 1   | A     | 193  | ASP  | CA-C-N   | 5.12  | 130.91      | 121.70   |
| 1   | A     | 193  | ASP  | C-N-CA   | 5.12  | 130.91      | 121.70   |
| 1   | A     | 1079 | MET  | N-CA-C   | 5.12  | 116.86      | 108.52   |
| 2   | B     | 366  | GLN  | N-CA-C   | -5.12 | 105.93      | 113.61   |
| 1   | A     | 1127 | ASP  | CA-CB-CG | 5.11  | 117.71      | 112.60   |
| 4   | D     | 23   | ASN  | CA-CB-CG | 5.11  | 117.71      | 112.60   |
| 1   | A     | 1315 | GLU  | N-CA-C   | 5.10  | 116.65      | 111.14   |
| 10  | J     | 64   | ASN  | N-CA-C   | 5.10  | 121.08      | 109.81   |
| 1   | A     | 478  | TYR  | CA-C-N   | 5.09  | 129.78      | 122.35   |
| 1   | A     | 478  | TYR  | C-N-CA   | 5.09  | 129.78      | 122.35   |
| 7   | G     | 18   | PHE  | CA-CB-CG | 5.09  | 118.89      | 113.80   |
| 1   | A     | 106  | VAL  | N-CA-CB  | -5.07 | 106.56      | 112.34   |
| 1   | A     | 192  | GLY  | CA-C-N   | 5.07  | 131.22      | 121.54   |
| 1   | A     | 192  | GLY  | C-N-CA   | 5.07  | 131.22      | 121.54   |
| 8   | H     | 145  | ARG  | CA-C-N   | 5.07  | 130.82      | 121.70   |
| 8   | H     | 145  | ARG  | C-N-CA   | 5.07  | 130.82      | 121.70   |
| 2   | B     | 472  | ALA  | CA-C-N   | 5.07  | 131.21      | 121.54   |
| 2   | B     | 472  | ALA  | C-N-CA   | 5.07  | 131.21      | 121.54   |
| 7   | G     | 46   | LEU  | N-CA-C   | 5.07  | 117.77      | 111.24   |
| 2   | B     | 222  | ILE  | N-CA-C   | 5.06  | 115.14      | 107.75   |
| 2   | B     | 681  | TRP  | N-CA-C   | -5.05 | 105.85      | 111.36   |
| 7   | G     | 154  | VAL  | CA-C-N   | 5.05  | 131.04      | 122.65   |
| 7   | G     | 154  | VAL  | C-N-CA   | 5.05  | 131.04      | 122.65   |
| 1   | A     | 268  | ASP  | CA-CB-CG | 5.04  | 117.64      | 112.60   |
| 1   | A     | 408  | ASP  | CA-CB-CG | 5.04  | 117.64      | 112.60   |
| 2   | B     | 210  | LYS  | CA-C-N   | 5.04  | 128.87      | 122.37   |
| 2   | B     | 210  | LYS  | C-N-CA   | 5.04  | 128.87      | 122.37   |
| 1   | A     | 147  | VAL  | N-CA-C   | 5.03  | 115.16      | 108.27   |
| 2   | B     | 663  | ALA  | N-CA-C   | -5.02 | 105.27      | 111.40   |
| 1   | A     | 466  | SER  | N-CA-C   | 5.02  | 120.30      | 113.37   |
| 2   | B     | 296  | GLU  | CA-C-N   | 5.01  | 126.88      | 120.56   |
| 2   | B     | 296  | GLU  | C-N-CA   | 5.01  | 126.88      | 120.56   |
| 5   | E     | 48   | ASP  | CA-CB-CG | 5.01  | 117.61      | 112.60   |
| 1   | A     | 474  | VAL  | CA-C-N   | 5.00  | 127.26      | 120.65   |
| 1   | A     | 474  | VAL  | C-N-CA   | 5.00  | 127.26      | 120.65   |
| 2   | B     | 415  | GLN  | CA-C-N   | 5.00  | 127.40      | 120.29   |
| 2   | B     | 415  | GLN  | C-N-CA   | 5.00  | 127.40      | 120.29   |
| 2   | B     | 998  | ASP  | CA-CB-CG | 5.00  | 117.60      | 112.60   |

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| Mol | Chain | Res | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 3   | C     | 136 | ASP  | CA-CB-CG | 5.00 | 117.60      | 112.60   |

There are no chirality outliers.

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group             |
|-----|-------|-----|------|-------------------|
| 1   | A     | 34  | LYS  | Mainchain,Peptide |

## 5.2 Too-close contacts [i](#)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 11174 | 0        | 11233    | 221     | 0            |
| 2   | B     | 8859  | 0        | 8901     | 172     | 0            |
| 3   | C     | 2095  | 0        | 2051     | 45      | 0            |
| 4   | D     | 1434  | 0        | 1460     | 17      | 0            |
| 5   | E     | 1752  | 0        | 1776     | 27      | 0            |
| 6   | F     | 679   | 0        | 701      | 18      | 0            |
| 7   | G     | 1340  | 0        | 1357     | 27      | 0            |
| 8   | H     | 1068  | 0        | 1040     | 25      | 0            |
| 9   | I     | 971   | 0        | 927      | 15      | 0            |
| 10  | J     | 532   | 0        | 542      | 16      | 0            |
| 11  | K     | 920   | 0        | 929      | 20      | 0            |
| 12  | L     | 363   | 0        | 386      | 16      | 0            |
| 13  | N     | 207   | 0        | 114      | 0       | 0            |
| 14  | P     | 130   | 0        | 66       | 1       | 0            |
| 15  | T     | 404   | 0        | 227      | 9       | 0            |
| 16  | A     | 2     | 0        | 0        | 0       | 0            |
| 16  | B     | 1     | 0        | 0        | 0       | 0            |
| 16  | C     | 1     | 0        | 0        | 0       | 0            |
| 16  | I     | 2     | 0        | 0        | 0       | 0            |
| 16  | J     | 1     | 0        | 0        | 0       | 0            |
| 16  | L     | 1     | 0        | 0        | 0       | 0            |
| 17  | A     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 31937 | 0        | 31710    | 541     | 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 8.

All (541) 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:867:ILE:CG1   | 1:A:867:ILE:CD1   | 1.83                     | 1.53              |
| 1:A:53:LEU:HD23   | 1:A:54:ASN:H      | 1.03                     | 1.13              |
| 7:G:1:MET:HE1     | 7:G:80:LYS:O      | 1.54                     | 1.08              |
| 1:A:1444:MET:HE1  | 6:F:135:ARG:HB2   | 1.45                     | 0.94              |
| 2:B:583:ASN:HD21  | 2:B:628:THR:HG22  | 1.27                     | 0.94              |
| 1:A:1438:THR:HG22 | 2:B:1144:ALA:HB3  | 1.52                     | 0.91              |
| 1:A:53:LEU:HD23   | 1:A:54:ASN:N      | 1.87                     | 0.89              |
| 6:F:76:LYS:HA     | 6:F:79:ARG:HD3    | 1.56                     | 0.86              |
| 1:A:902:LEU:HG    | 1:A:926:GLN:HG3   | 1.59                     | 0.84              |
| 3:C:148:ARG:H     | 3:C:151:GLN:HG3   | 1.43                     | 0.82              |
| 3:C:148:ARG:HD3   | 3:C:149:LYS:HG2   | 1.61                     | 0.81              |
| 1:A:53:LEU:CD2    | 1:A:54:ASN:H      | 1.91                     | 0.80              |
| 2:B:29:ASP:HB3    | 2:B:658:ILE:HG12  | 1.64                     | 0.80              |
| 3:C:147:LEU:HB3   | 3:C:151:GLN:HB2   | 1.66                     | 0.77              |
| 1:A:368:LYS:HE2   | 1:A:399:HIS:HB2   | 1.67                     | 0.77              |
| 2:B:101:MET:HG2   | 2:B:111:ALA:HA    | 1.66                     | 0.76              |
| 6:F:93:ILE:HD11   | 6:F:134:ILE:HD11  | 1.66                     | 0.76              |
| 4:D:40:HIS:HB3    | 7:G:73:LYS:HE3    | 1.68                     | 0.74              |
| 1:A:1116:LEU:HD12 | 1:A:1329:THR:HB   | 1.67                     | 0.74              |
| 8:H:38:LEU:HD11   | 8:H:123:MET:HE2   | 1.70                     | 0.74              |
| 1:A:497:THR:HG22  | 2:B:1146:PHE:HD1  | 1.52                     | 0.74              |
| 4:D:203:SER:HB3   | 4:D:206:GLU:HB2   | 1.70                     | 0.73              |
| 8:H:84:ALA:HA     | 8:H:87:ARG:HB2    | 1.71                     | 0.72              |
| 1:A:726:ARG:HD3   | 1:A:766:GLY:HA3   | 1.72                     | 0.72              |
| 11:K:58:PHE:HB3   | 11:K:76:GLN:HB3   | 1.72                     | 0.72              |
| 6:F:75:PRO:HG2    | 6:F:78:GLN:HB2    | 1.72                     | 0.72              |
| 2:B:1198:TYR:CE2  | 2:B:1201:LYS:HE3  | 2.25                     | 0.70              |
| 3:C:66:ARG:NH2    | 10:J:3:VAL:O      | 2.23                     | 0.70              |
| 3:C:18:VAL:HG23   | 3:C:240:VAL:HB    | 1.74                     | 0.69              |
| 1:A:140:THR:HA    | 1:A:143:LYS:HE2   | 1.75                     | 0.69              |
| 5:E:185:ALA:HA    | 5:E:190:LEU:HD12  | 1.74                     | 0.69              |
| 1:A:1197:LEU:HD11 | 1:A:1238:ILE:HD11 | 1.74                     | 0.69              |
| 3:C:259:LEU:HD22  | 11:K:91:CYS:HB3   | 1.75                     | 0.68              |
| 7:G:138:THR:HG22  | 7:G:139:ILE:H     | 1.59                     | 0.68              |
| 1:A:61:ILE:HG22   | 1:A:62:ASP:H      | 1.58                     | 0.68              |
| 1:A:445:ASN:HB2   | 1:A:455:MET:HG2   | 1.75                     | 0.68              |
| 1:A:870:GLU:HB2   | 5:E:204:THR:HG21  | 1.75                     | 0.68              |
| 1:A:347:PHE:HE1   | 1:A:375:THR:HG22  | 1.60                     | 0.67              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:871:ASP:HB3  | 5:E:204:THR:HG23  | 1.76                     | 0.67              |
| 2:B:114:PRO:HG3  | 2:B:181:LEU:HD11  | 1.76                     | 0.67              |
| 1:A:34:LYS:HB3   | 1:A:83:HIS:CE1    | 2.30                     | 0.66              |
| 5:E:4:GLU:HB3    | 5:E:7:ARG:HE      | 1.59                     | 0.66              |
| 2:B:563:MET:HE1  | 2:B:587:HIS:HB2   | 1.76                     | 0.66              |
| 1:A:1442:ASP:HB2 | 6:F:137:TYR:HE1   | 1.61                     | 0.66              |
| 2:B:428:ILE:HG22 | 2:B:432:MET:HE2   | 1.77                     | 0.66              |
| 2:B:773:MET:HE1  | 2:B:985:GLY:HA2   | 1.79                     | 0.65              |
| 12:L:61:THR:CG2  | 12:L:63:ARG:HG2   | 2.26                     | 0.65              |
| 1:A:388:LEU:O    | 1:A:392:VAL:HG23  | 1.96                     | 0.64              |
| 2:B:296:GLU:O    | 2:B:300:HIS:HD2   | 1.80                     | 0.64              |
| 2:B:996:ARG:HG3  | 2:B:1007:VAL:HG11 | 1.79                     | 0.64              |
| 3:C:56:THR:HG21  | 3:C:145:CYS:SG    | 2.37                     | 0.64              |
| 2:B:806:THR:HG22 | 2:B:808:ALA:H     | 1.63                     | 0.64              |
| 1:A:1433:MET:CE  | 7:G:63:PRO:HB3    | 2.28                     | 0.64              |
| 1:A:1402:PHE:CE1 | 1:A:1403:GLU:HG2  | 2.33                     | 0.64              |
| 1:A:37:PHE:CD2   | 1:A:52:GLY:HA3    | 2.33                     | 0.63              |
| 8:H:82:PRO:C     | 8:H:84:ALA:H      | 2.05                     | 0.63              |
| 12:L:28:LYS:HB2  | 12:L:39:SER:HA    | 1.80                     | 0.63              |
| 3:C:10:ILE:HD12  | 11:K:108:GLU:HB3  | 1.81                     | 0.63              |
| 2:B:999:MET:HG3  | 2:B:1000:PRO:HD2  | 1.80                     | 0.62              |
| 1:A:1193:LEU:HB2 | 1:A:1260:LEU:HD21 | 1.81                     | 0.62              |
| 2:B:269:ILE:HD11 | 2:B:386:LEU:HD21  | 1.82                     | 0.62              |
| 3:C:11:ARG:HH21  | 3:C:229:TYR:HD2   | 1.48                     | 0.62              |
| 4:D:176:GLU:OE2  | 4:D:197:SER:HB2   | 1.99                     | 0.62              |
| 1:A:343:LYS:HD3  | 2:B:1156:ASP:HB2  | 1.82                     | 0.61              |
| 1:A:448:PRO:O    | 1:A:449:SER:HB2   | 2.01                     | 0.61              |
| 1:A:1063:MET:SD  | 1:A:1436:ILE:HG13 | 2.41                     | 0.61              |
| 2:B:843:GLN:HA   | 2:B:846:ILE:HD12  | 1.82                     | 0.61              |
| 11:K:49:GLU:HG3  | 11:K:94:ILE:HG13  | 1.81                     | 0.61              |
| 2:B:841:MET:HB3  | 2:B:846:ILE:HD11  | 1.81                     | 0.61              |
| 2:B:486:TYR:HB3  | 2:B:1096:ARG:CZ   | 2.31                     | 0.61              |
| 1:A:1130:GLN:HA  | 1:A:1133:LEU:HD12 | 1.83                     | 0.61              |
| 1:A:372:LYS:HA   | 1:A:435:HIS:CD2   | 2.36                     | 0.60              |
| 1:A:871:ASP:OD1  | 1:A:1366:ARG:NH2  | 2.34                     | 0.60              |
| 1:A:946:VAL:HG22 | 5:E:201:LYS:HD2   | 1.82                     | 0.60              |
| 1:A:1111:MET:HG3 | 1:A:1114:PRO:HG3  | 1.83                     | 0.60              |
| 3:C:67:LEU:HA    | 3:C:70:ILE:HD12   | 1.82                     | 0.60              |
| 7:G:1:MET:SD     | 7:G:2:PHE:N       | 2.63                     | 0.60              |
| 3:C:184:ASN:HD21 | 3:C:189:THR:H     | 1.50                     | 0.60              |
| 2:B:918:ILE:HD13 | 2:B:935:ARG:HH22  | 1.65                     | 0.60              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:380:VAL:HG13 | 1:A:385:ILE:HG12  | 1.83                     | 0.60              |
| 12:L:61:THR:HG21 | 12:L:63:ARG:HG2   | 1.84                     | 0.60              |
| 1:A:1387:HIS:O   | 1:A:1391:ARG:HG2  | 2.02                     | 0.59              |
| 5:E:4:GLU:HB3    | 5:E:7:ARG:NE      | 2.16                     | 0.59              |
| 1:A:857:ARG:HD3  | 1:A:861:GLY:O     | 2.03                     | 0.59              |
| 1:A:1433:MET:HE3 | 7:G:63:PRO:HB3    | 1.85                     | 0.59              |
| 5:E:202:SER:HB3  | 5:E:205:SER:H     | 1.66                     | 0.59              |
| 2:B:976:ILE:O    | 2:B:990:ILE:HB    | 2.02                     | 0.59              |
| 2:B:839:MET:HE3  | 2:B:1010:LEU:HD21 | 1.83                     | 0.59              |
| 1:A:436:ILE:HD11 | 1:A:491:VAL:HG11  | 1.85                     | 0.59              |
| 1:A:335:ARG:HD2  | 2:B:1206:GLU:OE1  | 2.02                     | 0.58              |
| 1:A:629:LEU:O    | 1:A:633:VAL:HG23  | 2.02                     | 0.58              |
| 1:A:315:LEU:HA   | 1:A:321:PRO:HA    | 1.85                     | 0.58              |
| 1:A:483:ASP:HB2  | 2:B:987:LYS:HE3   | 1.84                     | 0.58              |
| 1:A:588:LEU:HD23 | 1:A:607:ILE:HD12  | 1.86                     | 0.58              |
| 1:A:901:LEU:HD22 | 1:A:919:ILE:HG23  | 1.85                     | 0.58              |
| 2:B:653:VAL:HG22 | 2:B:689:LEU:HB3   | 1.84                     | 0.58              |
| 1:A:566:ILE:HD11 | 8:H:98:TYR:HB2    | 1.85                     | 0.58              |
| 2:B:810:GLU:HA   | 2:B:815:ARG:HH12  | 1.69                     | 0.58              |
| 8:H:47:PHE:HB3   | 8:H:95:TYR:CD2    | 2.38                     | 0.58              |
| 12:L:47:ARG:HH21 | 12:L:54:ARG:HH21  | 1.50                     | 0.58              |
| 5:E:147:HIS:HB3  | 5:E:150:VAL:HG23  | 1.84                     | 0.58              |
| 2:B:792:MET:HA   | 2:B:856:PHE:O     | 2.04                     | 0.58              |
| 4:D:7:THR:HG21   | 7:G:5:LYS:HZ1     | 1.67                     | 0.58              |
| 1:A:590:ARG:NH2  | 1:A:621:THR:OG1   | 2.36                     | 0.57              |
| 1:A:1444:MET:HG2 | 7:G:58:ARG:HB3    | 1.85                     | 0.57              |
| 2:B:363:HIS:O    | 2:B:364:ILE:HB    | 2.02                     | 0.57              |
| 8:H:44:VAL:HG13  | 8:H:48:PRO:HA     | 1.87                     | 0.57              |
| 2:B:519:TRP:HZ2  | 2:B:705:MET:HE1   | 1.70                     | 0.57              |
| 2:B:542:MET:HE1  | 2:B:743:ILE:HD12  | 1.87                     | 0.57              |
| 4:D:40:HIS:HB3   | 7:G:73:LYS:CE     | 2.35                     | 0.57              |
| 1:A:49:LYS:HD2   | 1:A:55:ASP:HB3    | 1.85                     | 0.57              |
| 1:A:5:GLN:O      | 2:B:1159:ARG:NH2  | 2.39                     | 0.56              |
| 2:B:313:MET:HE2  | 2:B:386:LEU:HD22  | 1.87                     | 0.56              |
| 4:D:159:THR:O    | 4:D:163:VAL:HG23  | 2.05                     | 0.56              |
| 7:G:45:ILE:HA    | 7:G:78:VAL:HG12   | 1.88                     | 0.56              |
| 10:J:3:VAL:HG11  | 10:J:18:TRP:HB2   | 1.88                     | 0.56              |
| 6:F:79:ARG:HG2   | 6:F:144:GLU:HB3   | 1.88                     | 0.56              |
| 7:G:34:VAL:O     | 7:G:37:SER:HB3    | 2.06                     | 0.56              |
| 1:A:847:ASP:HB3  | 1:A:1398:MET:HE1  | 1.88                     | 0.56              |
| 11:K:57:LEU:HB2  | 11:K:76:GLN:HG2   | 1.88                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:792:MET:HE2   | 2:B:857:ARG:NH2   | 2.21                     | 0.55              |
| 1:A:388:LEU:HA    | 1:A:391:LEU:HD12  | 1.88                     | 0.55              |
| 3:C:39:ALA:HA     | 3:C:164:ALA:HB3   | 1.87                     | 0.55              |
| 4:D:18:VAL:HG22   | 4:D:19:GLU:HA     | 1.88                     | 0.55              |
| 6:F:118:LEU:O     | 6:F:122:MET:HG3   | 2.06                     | 0.55              |
| 1:A:35:ILE:HA     | 1:A:52:GLY:O      | 2.07                     | 0.55              |
| 1:A:1015:VAL:HG13 | 1:A:1019:CYS:SG   | 2.47                     | 0.55              |
| 2:B:128:LEU:HD21  | 2:B:170:LEU:HB2   | 1.87                     | 0.55              |
| 4:D:167:LEU:HB3   | 4:D:177:VAL:HG22  | 1.87                     | 0.55              |
| 2:B:54:PHE:HA     | 2:B:58:THR:HB     | 1.89                     | 0.55              |
| 10:J:48:ARG:HE    | 10:J:49:MET:CE    | 2.19                     | 0.55              |
| 1:A:344:ARG:HB3   | 2:B:1118:PRO:HB2  | 1.89                     | 0.55              |
| 1:A:608:ILE:HD12  | 1:A:613:ILE:HD13  | 1.89                     | 0.55              |
| 1:A:1376:THR:HG23 | 5:E:212:ARG:HH22  | 1.72                     | 0.55              |
| 8:H:89:LEU:C      | 8:H:91:ASP:H      | 2.14                     | 0.54              |
| 1:A:993:LEU:HD22  | 1:A:1046:LEU:HD22 | 1.88                     | 0.54              |
| 10:J:1:MET:HB2    | 10:J:56:LEU:HB2   | 1.89                     | 0.54              |
| 2:B:280:ILE:HD13  | 2:B:334:ILE:HG12  | 1.89                     | 0.54              |
| 6:F:89:GLU:O      | 6:F:93:ILE:HD12   | 2.06                     | 0.54              |
| 6:F:109:VAL:HG23  | 6:F:127:GLU:OE1   | 2.07                     | 0.54              |
| 1:A:1349:TYR:HA   | 1:A:1372:VAL:HG21 | 1.90                     | 0.54              |
| 2:B:226:PHE:HA    | 2:B:395:GLN:HG3   | 1.87                     | 0.54              |
| 2:B:486:TYR:HB3   | 2:B:1096:ARG:NH2  | 2.22                     | 0.54              |
| 7:G:111:THR:HG22  | 7:G:113:HIS:H     | 1.72                     | 0.54              |
| 1:A:497:THR:HG23  | 2:B:1146:PHE:HA   | 1.89                     | 0.54              |
| 2:B:356:LEU:HA    | 2:B:360:PHE:HB3   | 1.89                     | 0.54              |
| 2:B:1100:ASP:OD2  | 11:K:1:MET:HB3    | 2.08                     | 0.54              |
| 1:A:666:ILE:HD11  | 2:B:1030:LEU:HD13 | 1.90                     | 0.54              |
| 1:A:832:ALA:HB1   | 15:T:18:DT:H2"    | 1.89                     | 0.54              |
| 5:E:94:LYS:HE2    | 5:E:98:ILE:HD11   | 1.90                     | 0.54              |
| 1:A:768:GLN:HG2   | 1:A:816:HIS:HA    | 1.88                     | 0.54              |
| 1:A:1116:LEU:H    | 1:A:1308:THR:HB   | 1.73                     | 0.54              |
| 1:A:1172:LEU:C    | 1:A:1174:PHE:H    | 2.16                     | 0.54              |
| 2:B:343:ILE:O     | 2:B:344:LYS:HB2   | 2.07                     | 0.54              |
| 2:B:338:GLY:CA    | 2:B:339:THR:HB    | 2.38                     | 0.54              |
| 2:B:815:ARG:HG3   | 2:B:815:ARG:HH11  | 1.72                     | 0.54              |
| 1:A:658:LEU:HD23  | 1:A:659:HIS:NE2   | 2.24                     | 0.53              |
| 1:A:982:THR:HB    | 1:A:985:ASP:H     | 1.73                     | 0.53              |
| 1:A:1004:ASN:CG   | 5:E:167:ARG:HD2   | 2.33                     | 0.53              |
| 7:G:131:GLN:HG2   | 7:G:136:VAL:HG22  | 1.90                     | 0.53              |
| 10:J:24:LEU:O     | 10:J:30:LEU:HB2   | 2.08                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:510:LYS:HB2   | 2:B:513:GLN:OE1   | 2.08                     | 0.53              |
| 3:C:52:GLU:HA     | 12:L:64:LEU:HD22  | 1.91                     | 0.53              |
| 6:F:134:ILE:HG22  | 6:F:136:ARG:HG3   | 1.91                     | 0.53              |
| 2:B:408:LEU:HD21  | 2:B:545:ILE:HD13  | 1.91                     | 0.53              |
| 3:C:73:GLN:O      | 3:C:129:ILE:HA    | 2.08                     | 0.53              |
| 2:B:1103:ILE:O    | 2:B:1122:ARG:NH1  | 2.42                     | 0.53              |
| 7:G:119:LEU:HD12  | 7:G:132:SER:HB2   | 1.91                     | 0.53              |
| 10:J:48:ARG:HE    | 10:J:49:MET:HE2   | 1.74                     | 0.52              |
| 1:A:63:ARG:HA     | 1:A:74:MET:HG3    | 1.91                     | 0.52              |
| 1:A:357:PRO:HD2   | 2:B:833:TYR:CZ    | 2.44                     | 0.52              |
| 2:B:291:ILE:HD12  | 2:B:291:ILE:H     | 1.75                     | 0.52              |
| 3:C:164:ALA:HA    | 3:C:167:HIS:O     | 2.09                     | 0.52              |
| 5:E:156:LEU:HD11  | 5:E:197:LYS:HB2   | 1.90                     | 0.52              |
| 1:A:55:ASP:H      | 1:A:56:PRO:HD3    | 1.75                     | 0.52              |
| 1:A:541:ILE:HG22  | 1:A:546:VAL:HG23  | 1.91                     | 0.52              |
| 3:C:37:MET:HE3    | 3:C:176:ILE:HD13  | 1.90                     | 0.52              |
| 2:B:873:THR:O     | 2:B:914:LYS:HA    | 2.09                     | 0.52              |
| 1:A:79:GLY:HA3    | 1:A:243:PRO:HB2   | 1.92                     | 0.52              |
| 5:E:19:VAL:O      | 5:E:23:VAL:HG23   | 2.08                     | 0.52              |
| 2:B:295:GLY:HA2   | 2:B:298:LEU:HB2   | 1.91                     | 0.52              |
| 11:K:5:ASP:HB3    | 11:K:7:PHE:CE2    | 2.45                     | 0.52              |
| 11:K:49:GLU:HG3   | 11:K:94:ILE:CG1   | 2.40                     | 0.52              |
| 1:A:472:LEU:O     | 1:A:475:THR:HB    | 2.10                     | 0.51              |
| 1:A:494:SER:HB3   | 1:A:497:THR:OG1   | 2.10                     | 0.51              |
| 1:A:646:PHE:O     | 1:A:650:GLN:HG2   | 2.10                     | 0.51              |
| 2:B:101:MET:HB3   | 2:B:109:THR:HG22  | 1.90                     | 0.51              |
| 2:B:166:PHE:HZ    | 2:B:169:ARG:HG2   | 1.74                     | 0.51              |
| 1:A:446:ARG:HD2   | 1:A:480:ALA:HB2   | 1.92                     | 0.51              |
| 1:A:1095:THR:HG23 | 1:A:1113:THR:HG23 | 1.92                     | 0.51              |
| 2:B:530:GLY:O     | 2:B:532:ALA:N     | 2.44                     | 0.51              |
| 5:E:64:PRO:HB2    | 5:E:69:ILE:HD11   | 1.93                     | 0.51              |
| 11:K:55:LYS:HB3   | 11:K:81:TYR:CD2   | 2.45                     | 0.51              |
| 1:A:1149:ALA:HB2  | 9:I:47:GLU:HA     | 1.92                     | 0.51              |
| 2:B:238:ALA:HB3   | 2:B:256:VAL:HB    | 1.93                     | 0.51              |
| 2:B:373:ARG:HG2   | 2:B:566:LEU:HD23  | 1.92                     | 0.51              |
| 2:B:882:THR:C     | 2:B:884:ARG:H     | 2.19                     | 0.51              |
| 1:A:870:GLU:HB2   | 5:E:204:THR:CG2   | 2.40                     | 0.51              |
| 1:A:95:PHE:CE1    | 1:A:1414:ALA:HB2  | 2.45                     | 0.51              |
| 1:A:254:GLU:HB3   | 2:B:935:ARG:HH21  | 1.76                     | 0.51              |
| 1:A:51:GLY:HA2    | 1:A:56:PRO:HA     | 1.93                     | 0.51              |
| 2:B:684:LEU:HA    | 2:B:689:LEU:HD12  | 1.93                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:F:73:ALA:HB2    | 6:F:143:PHE:CZ    | 2.46                     | 0.51              |
| 1:A:52:GLY:N      | 1:A:56:PRO:HB3    | 2.26                     | 0.51              |
| 2:B:773:MET:CE    | 2:B:985:GLY:HA2   | 2.40                     | 0.51              |
| 2:B:852:ARG:HH22  | 12:L:70:ARG:C     | 2.19                     | 0.51              |
| 5:E:15:ALA:O      | 5:E:19:VAL:HG23   | 2.11                     | 0.51              |
| 9:I:65:ASP:HB3    | 9:I:68:LEU:HD12   | 1.94                     | 0.51              |
| 2:B:904:ARG:HG3   | 2:B:948:ILE:HG13  | 1.93                     | 0.50              |
| 1:A:497:THR:CG2   | 2:B:1146:PHE:HD1  | 2.23                     | 0.50              |
| 1:A:1095:THR:HG21 | 1:A:1112:LYS:HB2  | 1.93                     | 0.50              |
| 3:C:99:LEU:HB2    | 3:C:157:CYS:HB2   | 1.94                     | 0.50              |
| 1:A:714:PHE:O     | 1:A:718:VAL:HG23  | 2.12                     | 0.50              |
| 1:A:64:ASN:O      | 1:A:65:LEU:HB3    | 2.12                     | 0.50              |
| 2:B:701:ILE:HD11  | 2:B:703:ILE:HD11  | 1.94                     | 0.50              |
| 8:H:17:PRO:HB3    | 8:H:24:CYS:SG     | 2.52                     | 0.50              |
| 1:A:940:ARG:HB3   | 1:A:941:LYS:HE2   | 1.92                     | 0.50              |
| 2:B:710:LEU:HA    | 2:B:733:HIS:HB3   | 1.93                     | 0.50              |
| 2:B:902:GLY:O     | 12:L:65:VAL:HG11  | 2.11                     | 0.50              |
| 1:A:1402:PHE:CD1  | 1:A:1403:GLU:HG2  | 2.47                     | 0.50              |
| 1:A:1444:MET:HB2  | 6:F:133:VAL:HG12  | 1.92                     | 0.50              |
| 2:B:1122:ARG:HB3  | 15:T:23:DG:OP1    | 2.12                     | 0.50              |
| 2:B:35:SER:HA     | 2:B:811:TYR:HE1   | 1.77                     | 0.50              |
| 2:B:1201:LYS:HD3  | 2:B:1205:GLN:OE1  | 2.11                     | 0.50              |
| 3:C:116:LYS:HD3   | 3:C:140:ASN:HA    | 1.93                     | 0.50              |
| 1:A:315:LEU:H     | 1:A:315:LEU:HD12  | 1.76                     | 0.49              |
| 1:A:1348:LEU:O    | 1:A:1352:VAL:HG23 | 2.11                     | 0.49              |
| 2:B:1008:PRO:HB3  | 2:B:1087:PHE:HE1  | 1.77                     | 0.49              |
| 2:B:1072:MET:HB3  | 2:B:1081:LEU:HD12 | 1.94                     | 0.49              |
| 2:B:430:ARG:HB3   | 2:B:434:ARG:HH21  | 1.77                     | 0.49              |
| 2:B:338:GLY:HA2   | 2:B:339:THR:HB    | 1.94                     | 0.49              |
| 7:G:1:MET:CG      | 7:G:2:PHE:N       | 2.76                     | 0.49              |
| 1:A:252:PHE:HD1   | 1:A:256:GLN:HB3   | 1.78                     | 0.49              |
| 2:B:705:MET:HE2   | 2:B:745:PRO:HB3   | 1.94                     | 0.49              |
| 1:A:37:PHE:HD2    | 1:A:52:GLY:HA3    | 1.77                     | 0.49              |
| 1:A:1193:LEU:HB2  | 1:A:1260:LEU:CD2  | 2.42                     | 0.49              |
| 1:A:1433:MET:HE1  | 7:G:63:PRO:HB3    | 1.94                     | 0.49              |
| 2:B:1135:ARG:HG2  | 2:B:1139:ILE:HD11 | 1.94                     | 0.49              |
| 3:C:75:MET:HB3    | 3:C:128:ASN:HB3   | 1.95                     | 0.49              |
| 7:G:142:ARG:HB3   | 7:G:171:ILE:HD12  | 1.95                     | 0.49              |
| 2:B:574:SER:HB3   | 2:B:591:ARG:HE    | 1.77                     | 0.49              |
| 2:B:806:THR:HB    | 2:B:809:MET:HG3   | 1.94                     | 0.49              |
| 1:A:1116:LEU:HG   | 1:A:1327:ILE:HD11 | 1.95                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:114:TYR:HB2   | 3:C:116:LYS:HG2   | 1.93                     | 0.49              |
| 1:A:1312:ASN:O    | 1:A:1316:VAL:HG23 | 2.12                     | 0.49              |
| 2:B:640:VAL:HG22  | 2:B:651:LEU:HG    | 1.95                     | 0.49              |
| 1:A:227:VAL:HG12  | 4:D:15:LEU:HD23   | 1.95                     | 0.48              |
| 2:B:217:ARG:HH21  | 2:B:405:ARG:HG3   | 1.78                     | 0.48              |
| 2:B:933:SER:O     | 2:B:935:ARG:N     | 2.45                     | 0.48              |
| 1:A:568:PRO:HG2   | 8:H:46:LEU:HD12   | 1.95                     | 0.48              |
| 8:H:23:VAL:HG11   | 8:H:121:LEU:HD22  | 1.95                     | 0.48              |
| 1:A:875:ALA:HB2   | 1:A:1366:ARG:HD2  | 1.95                     | 0.48              |
| 1:A:919:ILE:HG12  | 1:A:983:ILE:HD13  | 1.94                     | 0.48              |
| 2:B:693:ILE:HG21  | 2:B:701:ILE:HD13  | 1.95                     | 0.48              |
| 2:B:916:THR:O     | 2:B:935:ARG:HG2   | 2.12                     | 0.48              |
| 3:C:38:ILE:HG13   | 3:C:176:ILE:HD12  | 1.96                     | 0.48              |
| 4:D:195:ILE:HG22  | 4:D:198:LEU:HG    | 1.94                     | 0.48              |
| 8:H:40:LEU:HD13   | 8:H:123:MET:HG3   | 1.95                     | 0.48              |
| 2:B:840:ILE:HG21  | 2:B:994:TYR:HD2   | 1.79                     | 0.48              |
| 8:H:80:ARG:HG2    | 11:K:57:LEU:HD22  | 1.95                     | 0.48              |
| 1:A:216:VAL:O     | 1:A:220:THR:HB    | 2.12                     | 0.48              |
| 1:A:929:LEU:HD21  | 1:A:983:ILE:HG21  | 1.96                     | 0.48              |
| 1:A:66:LYS:HB3    | 1:A:71:GLN:O      | 2.13                     | 0.48              |
| 2:B:258:LEU:HB2   | 2:B:385:LEU:HD21  | 1.96                     | 0.48              |
| 1:A:738:LYS:HA    | 8:H:19:ARG:HH12   | 1.79                     | 0.48              |
| 2:B:977:GLY:HA3   | 2:B:1099:VAL:HB   | 1.95                     | 0.48              |
| 1:A:55:ASP:N      | 1:A:56:PRO:HD3    | 2.28                     | 0.48              |
| 1:A:55:ASP:HA     | 1:A:58:LEU:HB2    | 1.96                     | 0.48              |
| 11:K:63:VAL:HG12  | 11:K:71:PHE:HB3   | 1.96                     | 0.48              |
| 7:G:85:GLU:HB3    | 7:G:147:ILE:HD12  | 1.96                     | 0.47              |
| 10:J:9:SER:HB2    | 10:J:45:CYS:HB2   | 1.95                     | 0.47              |
| 1:A:154:SER:HB3   | 1:A:162:VAL:HG23  | 1.95                     | 0.47              |
| 1:A:1436:ILE:O    | 1:A:1437:GLY:C    | 2.56                     | 0.47              |
| 1:A:12:ARG:HB3    | 2:B:1218:THR:HB   | 1.96                     | 0.47              |
| 1:A:579:SER:HA    | 1:A:582:ILE:HG13  | 1.97                     | 0.47              |
| 2:B:800:GLN:HB2   | 2:B:821:GLN:HA    | 1.96                     | 0.47              |
| 1:A:1279:ILE:HG23 | 1:A:1308:THR:HG23 | 1.96                     | 0.47              |
| 2:B:486:TYR:HB3   | 2:B:1096:ARG:NE   | 2.28                     | 0.47              |
| 2:B:542:MET:HG3   | 2:B:747:MET:HB3   | 1.95                     | 0.47              |
| 12:L:27:LEU:HD13  | 12:L:37:LYS:HG2   | 1.95                     | 0.47              |
| 12:L:68:GLU:HB2   | 12:L:70:ARG:HD2   | 1.96                     | 0.47              |
| 1:A:836:TYR:CE2   | 1:A:840:ARG:HD2   | 2.50                     | 0.47              |
| 1:A:1345:ARG:HG3  | 1:A:1376:THR:HG21 | 1.96                     | 0.47              |
| 7:G:1:MET:CE      | 7:G:80:LYS:O      | 2.45                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:54:ASN:HB3   | 1:A:247:ARG:HH12 | 1.80                     | 0.47              |
| 1:A:475:THR:HG21 | 2:B:836:GLU:OE2  | 2.14                     | 0.47              |
| 1:A:497:THR:HG22 | 2:B:1146:PHE:CD1 | 2.42                     | 0.47              |
| 2:B:345:LYS:HA   | 2:B:348:ARG:HD2  | 1.96                     | 0.47              |
| 5:E:176:PRO:O    | 5:E:212:ARG:HA   | 2.14                     | 0.47              |
| 9:I:106:CYS:SG   | 9:I:108:HIS:HB3  | 2.55                     | 0.47              |
| 1:A:709:THR:HG22 | 1:A:711:ARG:H    | 1.80                     | 0.47              |
| 4:D:8:PHE:HZ     | 4:D:37:GLN:NE2   | 2.13                     | 0.47              |
| 4:D:144:THR:HG21 | 7:G:46:LEU:HD13  | 1.97                     | 0.47              |
| 2:B:705:MET:H    | 2:B:710:LEU:HD12 | 1.79                     | 0.47              |
| 1:A:253:ASN:HB3  | 2:B:935:ARG:NE   | 2.29                     | 0.47              |
| 8:H:115:TYR:CE1  | 8:H:124:ARG:HG3  | 2.49                     | 0.47              |
| 1:A:448:PRO:HG3  | 15:T:19:DT:O2    | 2.13                     | 0.46              |
| 3:C:8:VAL:HG11   | 11:K:105:PHE:HD1 | 1.80                     | 0.46              |
| 9:I:102:VAL:HG22 | 9:I:109:ILE:HG12 | 1.97                     | 0.46              |
| 1:A:353:ILE:HG21 | 1:A:487:MET:HE3  | 1.96                     | 0.46              |
| 1:A:956:LEU:HD21 | 1:A:1017:LEU:HG  | 1.96                     | 0.46              |
| 1:A:745:GLN:HA   | 1:A:748:MET:HE3  | 1.98                     | 0.46              |
| 3:C:18:VAL:HG12  | 3:C:20:PHE:HD1   | 1.81                     | 0.46              |
| 3:C:58:LEU:HD21  | 10:J:57:ILE:HD12 | 1.97                     | 0.46              |
| 4:D:5:THR:HG21   | 7:G:74:TYR:OH    | 2.15                     | 0.46              |
| 9:I:83:ASN:HA    | 9:I:104:LEU:HG   | 1.98                     | 0.46              |
| 1:A:1074:GLU:O   | 1:A:1077:THR:HB  | 2.16                     | 0.46              |
| 2:B:210:LYS:HD3  | 2:B:482:VAL:HG13 | 1.97                     | 0.46              |
| 3:C:100:THR:HG22 | 3:C:119:VAL:HG22 | 1.97                     | 0.46              |
| 1:A:923:LEU:O    | 1:A:927:VAL:HG23 | 2.16                     | 0.46              |
| 1:A:1386:ARG:HB3 | 1:A:1403:GLU:HG3 | 1.97                     | 0.46              |
| 2:B:882:THR:HG21 | 2:B:935:ARG:HA   | 1.98                     | 0.46              |
| 5:E:65:THR:O     | 5:E:69:ILE:HD12  | 2.16                     | 0.46              |
| 1:A:567:LYS:HA   | 1:A:568:PRO:C    | 2.41                     | 0.46              |
| 1:A:1446:ASP:HB3 | 1:A:1449:SER:OG  | 2.15                     | 0.46              |
| 2:B:662:MET:HA   | 2:B:665:GLU:HB2  | 1.97                     | 0.46              |
| 2:B:756:ILE:O    | 2:B:759:PRO:HD3  | 2.15                     | 0.46              |
| 1:A:565:ILE:O    | 1:A:570:PRO:HA   | 2.16                     | 0.46              |
| 1:A:1345:ARG:HG2 | 1:A:1372:VAL:CG1 | 2.45                     | 0.46              |
| 3:C:165:LYS:O    | 11:K:6:ARG:NH1   | 2.46                     | 0.46              |
| 2:B:582:VAL:HG22 | 2:B:626:ILE:HB   | 1.97                     | 0.46              |
| 2:B:803:LEU:HG   | 10:J:52:THR:HG21 | 1.98                     | 0.46              |
| 9:I:72:ASP:O     | 9:I:81:ARG:HG2   | 2.16                     | 0.46              |
| 1:A:311:GLN:O    | 1:A:312:PRO:C    | 2.59                     | 0.45              |
| 1:A:353:ILE:HG22 | 1:A:468:PHE:HB2  | 1.98                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:291:ILE:HD12 | 2:B:291:ILE:N    | 2.30                     | 0.45              |
| 1:A:399:HIS:O    | 1:A:401:GLY:N    | 2.48                     | 0.45              |
| 1:A:457:ALA:HB3  | 1:A:506:ALA:HA   | 1.97                     | 0.45              |
| 2:B:1001:PHE:HE2 | 3:C:178:PHE:HB3  | 1.81                     | 0.45              |
| 8:H:93:TYR:HA    | 8:H:145:ARG:HB3  | 1.99                     | 0.45              |
| 1:A:448:PRO:O    | 1:A:449:SER:CB   | 2.63                     | 0.45              |
| 1:A:875:ALA:HA   | 1:A:878:ILE:HD12 | 1.99                     | 0.45              |
| 2:B:793:ALA:HB3  | 2:B:856:PHE:HB2  | 1.98                     | 0.45              |
| 2:B:901:PRO:O    | 12:L:60:ARG:HA   | 2.17                     | 0.45              |
| 2:B:394:ASP:OD2  | 9:I:91:ARG:HD2   | 2.17                     | 0.45              |
| 1:A:883:LEU:HD23 | 1:A:1021:LEU:HB2 | 1.97                     | 0.45              |
| 1:A:1151:GLU:HG2 | 9:I:45:ARG:HG3   | 1.99                     | 0.45              |
| 2:B:233:PRO:HG2  | 2:B:234:ILE:HD12 | 1.99                     | 0.45              |
| 2:B:468:GLU:HG2  | 2:B:469:GLN:HB2  | 1.99                     | 0.45              |
| 6:F:89:GLU:C     | 6:F:93:ILE:HD12  | 2.42                     | 0.45              |
| 7:G:98:GLY:HA3   | 7:G:110:VAL:O    | 2.17                     | 0.45              |
| 1:A:187:LYS:HE3  | 1:A:198:GLU:HB2  | 1.99                     | 0.45              |
| 1:A:446:ARG:HB2  | 1:A:487:MET:SD   | 2.57                     | 0.45              |
| 4:D:31:GLN:O     | 4:D:34:GLN:HB2   | 2.17                     | 0.45              |
| 1:A:254:GLU:H    | 2:B:935:ARG:HH21 | 1.65                     | 0.45              |
| 1:A:53:LEU:O     | 1:A:54:ASN:C     | 2.60                     | 0.45              |
| 5:E:88:VAL:HB    | 5:E:116:ILE:HG12 | 1.97                     | 0.45              |
| 8:H:30:SER:HB3   | 8:H:36:CYS:HB3   | 1.98                     | 0.45              |
| 1:A:35:ILE:HG13  | 1:A:56:PRO:HG2   | 1.99                     | 0.45              |
| 1:A:743:VAL:O    | 1:A:747:VAL:HG23 | 2.16                     | 0.45              |
| 2:B:563:MET:HE3  | 2:B:580:VAL:HB   | 1.99                     | 0.45              |
| 9:I:50:THR:HG22  | 9:I:52:ILE:H     | 1.81                     | 0.45              |
| 3:C:70:ILE:HD11  | 3:C:144:ILE:HG12 | 1.98                     | 0.44              |
| 3:C:148:ARG:N    | 3:C:151:GLN:HG3  | 2.22                     | 0.44              |
| 10:J:28:ASP:C    | 10:J:30:LEU:H    | 2.24                     | 0.44              |
| 1:A:1154:TYR:CE1 | 9:I:18:GLU:HG3   | 2.53                     | 0.44              |
| 3:C:11:ARG:HE    | 3:C:21:ILE:HD11  | 1.83                     | 0.44              |
| 1:A:347:PHE:H    | 2:B:1107:ALA:HA  | 1.82                     | 0.44              |
| 1:A:869:GLY:O    | 5:E:204:THR:HG21 | 2.18                     | 0.44              |
| 1:A:1393:ASN:ND2 | 1:A:1393:ASN:H   | 2.15                     | 0.44              |
| 3:C:97:VAL:HG21  | 3:C:129:ILE:HG23 | 1.99                     | 0.44              |
| 5:E:90:VAL:HG23  | 5:E:123:LEU:HD11 | 1.98                     | 0.44              |
| 1:A:534:LEU:O    | 1:A:574:GLY:HA3  | 2.17                     | 0.44              |
| 1:A:994:GLN:HE22 | 1:A:1023:ARG:HE  | 1.66                     | 0.44              |
| 6:F:130:ILE:HB   | 6:F:148:VAL:HG21 | 1.99                     | 0.44              |
| 2:B:365:THR:HG21 | 2:B:370:PHE:CG   | 2.51                     | 0.44              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B:617:ARG:HG3  | 2:B:624:LEU:HD12  | 2.00                     | 0.44              |
| 2:B:1166:CYS:O   | 2:B:1168:LEU:N    | 2.42                     | 0.44              |
| 8:H:105:GLU:HB3  | 8:H:113:ALA:HB3   | 2.00                     | 0.44              |
| 1:A:548:ASN:HD21 | 11:K:47:ARG:HH21  | 1.65                     | 0.44              |
| 1:A:589:GLN:HG2  | 1:A:606:LEU:HD13  | 1.99                     | 0.44              |
| 1:A:974:ASP:C    | 1:A:976:THR:H     | 2.25                     | 0.44              |
| 1:A:1148:ILE:HA  | 9:I:49:ILE:HD12   | 2.00                     | 0.44              |
| 3:C:55:THR:HB    | 3:C:151:GLN:HA    | 1.99                     | 0.44              |
| 15:T:12:DT:H2'   | 15:T:13:DA:C8     | 2.52                     | 0.44              |
| 1:A:270:LEU:HD12 | 1:A:274:ILE:HD11  | 1.98                     | 0.44              |
| 4:D:7:THR:HG23   | 7:G:7:LEU:HD23    | 1.99                     | 0.44              |
| 10:J:36:LEU:HD11 | 10:J:51:LEU:HB2   | 2.00                     | 0.44              |
| 14:P:8:G:H2'     | 14:P:9:G:H8       | 1.81                     | 0.44              |
| 1:A:1441:PHE:CZ  | 6:F:89:GLU:HA     | 2.53                     | 0.44              |
| 2:B:1158:PHE:HE2 | 2:B:1160:VAL:HG13 | 1.83                     | 0.44              |
| 3:C:133:ILE:HG21 | 3:C:236:GLY:HA3   | 2.00                     | 0.44              |
| 7:G:143:ILE:HG22 | 7:G:145:VAL:HG22  | 1.99                     | 0.44              |
| 1:A:514:PRO:HG2  | 1:A:1067:LEU:HD11 | 1.98                     | 0.44              |
| 2:B:509:ALA:C    | 2:B:511:PRO:HD3   | 2.43                     | 0.44              |
| 2:B:865:LYS:HB2  | 2:B:961:LEU:HD21  | 2.00                     | 0.44              |
| 1:A:62:ASP:HB2   | 1:A:65:LEU:HD22   | 1.99                     | 0.43              |
| 1:A:449:SER:HA   | 1:A:454:SER:HB3   | 1.98                     | 0.43              |
| 1:A:1345:ARG:HD2 | 1:A:1373:ASP:OD1  | 2.18                     | 0.43              |
| 2:B:190:TYR:CZ   | 2:B:196:PRO:HG3   | 2.53                     | 0.43              |
| 15:T:21:DC:H2'   | 15:T:22:BRU:H6    | 2.00                     | 0.43              |
| 1:A:332:LYS:HZ2  | 15:T:19:DT:P      | 2.41                     | 0.43              |
| 1:A:344:ARG:HG2  | 2:B:1127:GLY:O    | 2.18                     | 0.43              |
| 1:A:451:HIS:CD2  | 1:A:1074:GLU:HG3  | 2.52                     | 0.43              |
| 1:A:449:SER:HA   | 1:A:454:SER:CB    | 2.49                     | 0.43              |
| 1:A:875:ALA:HB2  | 1:A:1366:ARG:CD   | 2.48                     | 0.43              |
| 1:A:41:MET:HB3   | 1:A:49:LYS:HA     | 2.00                     | 0.43              |
| 1:A:151:ASP:HA   | 1:A:163:SER:HA    | 1.99                     | 0.43              |
| 1:A:407:ARG:HG2  | 1:A:430:TRP:CZ2   | 2.53                     | 0.43              |
| 1:A:1323:ASP:CG  | 1:A:1326:ARG:HG3  | 2.44                     | 0.43              |
| 1:A:1345:ARG:HG2 | 1:A:1372:VAL:HG12 | 2.01                     | 0.43              |
| 2:B:167:ILE:HG22 | 2:B:167:ILE:O     | 2.18                     | 0.43              |
| 7:G:93:SER:OG    | 7:G:100:GLU:HB2   | 2.19                     | 0.43              |
| 15:T:19:DT:H2'   | 15:T:20:DC:C6     | 2.54                     | 0.43              |
| 1:A:239:LEU:HD12 | 1:A:240:PRO:HD2   | 2.01                     | 0.43              |
| 1:A:1025:ARG:O   | 1:A:1035:TYR:HE2  | 2.02                     | 0.43              |
| 2:B:980:PHE:CD1  | 2:B:1094:ARG:HA   | 2.54                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:K:65:HIS:HE1   | 11:K:67:PHE:CG    | 2.35                     | 0.43              |
| 1:A:130:ASP:HB3   | 1:A:133:LYS:HB2   | 2.00                     | 0.43              |
| 8:H:16:ASP:HA     | 8:H:17:PRO:HD3    | 1.92                     | 0.43              |
| 1:A:450:LEU:H     | 1:A:450:LEU:HG    | 1.71                     | 0.43              |
| 1:A:774:ARG:HH21  | 1:A:797:LYS:HB2   | 1.83                     | 0.43              |
| 1:A:1438:THR:HB   | 2:B:1142:GLY:O    | 2.19                     | 0.43              |
| 2:B:983:ARG:HD2   | 2:B:1091:TYR:HD2  | 1.84                     | 0.43              |
| 8:H:4:THR:HA      | 8:H:60:ALA:HB2    | 2.00                     | 0.43              |
| 1:A:729:ALA:HA    | 1:A:732:LEU:HD12  | 2.01                     | 0.43              |
| 1:A:1348:LEU:HG   | 1:A:1372:VAL:HG22 | 2.00                     | 0.43              |
| 2:B:802:PRO:HA    | 2:B:822:ASN:HD21  | 1.84                     | 0.43              |
| 2:B:899:ILE:CG2   | 2:B:949:VAL:HG21  | 2.49                     | 0.43              |
| 3:C:251:LEU:O     | 3:C:255:VAL:HG23  | 2.19                     | 0.43              |
| 6:F:82:THR:HG22   | 6:F:83:PRO:HD2    | 2.01                     | 0.43              |
| 2:B:859:TYR:OH    | 2:B:941:LEU:HD12  | 2.19                     | 0.43              |
| 2:B:952:VAL:HB    | 12:L:58:LYS:HB2   | 2.01                     | 0.43              |
| 12:L:49:LYS:O     | 12:L:50:ASP:HB2   | 2.19                     | 0.43              |
| 1:A:873:MET:C     | 1:A:1058:VAL:HG22 | 2.44                     | 0.43              |
| 2:B:115:GLN:O     | 2:B:119:LEU:HD12  | 2.19                     | 0.43              |
| 8:H:15:VAL:HG22   | 8:H:26:ILE:HG13   | 2.00                     | 0.43              |
| 2:B:424:LEU:HD11  | 2:B:448:ILE:HG22  | 2.01                     | 0.42              |
| 2:B:521:LEU:HD22  | 2:B:633:VAL:HG12  | 2.01                     | 0.42              |
| 2:B:1143:ALA:HB1  | 2:B:1146:PHE:HB3  | 2.01                     | 0.42              |
| 5:E:181:ALA:HA    | 5:E:186:LEU:HD21  | 2.01                     | 0.42              |
| 1:A:413:ILE:HD13  | 1:A:424:ILE:HD11  | 2.01                     | 0.42              |
| 1:A:481:ASP:OD1   | 1:A:485:ASP:OD1   | 2.37                     | 0.42              |
| 1:A:871:ASP:CG    | 1:A:1366:ARG:HH22 | 2.28                     | 0.42              |
| 1:A:358:ASN:HB2   | 11:K:65:HIS:HD2   | 1.84                     | 0.42              |
| 1:A:709:THR:HB    | 1:A:712:GLU:H     | 1.83                     | 0.42              |
| 1:A:873:MET:HB3   | 1:A:878:ILE:HD11  | 2.01                     | 0.42              |
| 1:A:1259:MET:HA   | 1:A:1262:LYS:HD2  | 1.99                     | 0.42              |
| 1:A:1356:ILE:HG21 | 1:A:1363:VAL:HG23 | 1.99                     | 0.42              |
| 2:B:226:PHE:HA    | 2:B:395:GLN:CG    | 2.49                     | 0.42              |
| 2:B:766:ARG:NH2   | 2:B:1020:ARG:HD3  | 2.33                     | 0.42              |
| 1:A:598:LEU:HD23  | 1:A:598:LEU:HA    | 1.83                     | 0.42              |
| 3:C:184:ASN:ND2   | 3:C:189:THR:O     | 2.52                     | 0.42              |
| 1:A:541:ILE:HG21  | 1:A:549:MET:CE    | 2.49                     | 0.42              |
| 1:A:1340:GLY:HA2  | 5:E:183:PRO:HD2   | 2.01                     | 0.42              |
| 1:A:1444:MET:HB2  | 1:A:1444:MET:HE2  | 1.62                     | 0.42              |
| 3:C:148:ARG:HG3   | 3:C:151:GLN:HG3   | 2.01                     | 0.42              |
| 2:B:102:VAL:HG13  | 2:B:112:LEU:HD22  | 2.02                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:J:48:ARG:HH21  | 10:J:49:MET:HE1   | 1.85                     | 0.42              |
| 1:A:562:THR:O     | 1:A:576:GLN:NE2   | 2.53                     | 0.42              |
| 2:B:165:VAL:O     | 2:B:167:ILE:HD12  | 2.20                     | 0.42              |
| 2:B:986:GLN:OE1   | 2:B:1016:ALA:HB1  | 2.20                     | 0.42              |
| 1:A:469:ARG:NH2   | 2:B:991:GLY:O     | 2.52                     | 0.42              |
| 2:B:642:ASP:HA    | 2:B:649:LYS:HA    | 2.02                     | 0.42              |
| 1:A:194:ALA:HA    | 1:A:195:ASP:C     | 2.45                     | 0.42              |
| 1:A:1221:LYS:HB3  | 1:A:1222:ASN:H    | 1.72                     | 0.42              |
| 2:B:383:ASN:O     | 2:B:387:LEU:HB2   | 2.19                     | 0.42              |
| 2:B:792:MET:HG2   | 2:B:855:PHE:CZ    | 2.55                     | 0.42              |
| 2:B:857:ARG:NH1   | 2:B:945:GLU:OE2   | 2.52                     | 0.42              |
| 3:C:125:MET:HE3   | 3:C:125:MET:HA    | 2.02                     | 0.42              |
| 1:A:58:LEU:HB3    | 1:A:59:GLY:H      | 1.45                     | 0.42              |
| 2:B:583:ASN:ND2   | 2:B:628:THR:HG22  | 2.12                     | 0.42              |
| 6:F:99:LEU:HD23   | 7:G:66:GLY:HA2    | 2.01                     | 0.42              |
| 8:H:38:LEU:HD13   | 8:H:125:LEU:HD13  | 2.02                     | 0.42              |
| 12:L:38:LEU:HD21  | 12:L:48:CYS:HA    | 2.02                     | 0.42              |
| 2:B:69:LEU:HD11   | 2:B:425:THR:HG23  | 2.01                     | 0.41              |
| 3:C:99:LEU:HB3    | 3:C:118:LEU:HD22  | 2.01                     | 0.41              |
| 1:A:381:THR:HG22  | 1:A:384:ASN:CG    | 2.46                     | 0.41              |
| 2:B:311:LEU:HB3   | 9:I:4:PHE:HE2     | 1.85                     | 0.41              |
| 3:C:99:LEU:HD12   | 3:C:118:LEU:HB3   | 2.02                     | 0.41              |
| 15:T:25:DT:H6     | 15:T:25:DT:H2'    | 1.64                     | 0.41              |
| 1:A:313:GLN:O     | 1:A:314:ALA:C     | 2.63                     | 0.41              |
| 1:A:595:THR:OG1   | 1:A:603:ASN:HB3   | 2.20                     | 0.41              |
| 1:A:867:ILE:CD1   | 1:A:867:ILE:CB    | 2.87                     | 0.41              |
| 2:B:205:ILE:HD13  | 2:B:461:LEU:HB3   | 2.02                     | 0.41              |
| 2:B:279:ASP:OD1   | 2:B:279:ASP:N     | 2.53                     | 0.41              |
| 2:B:425:THR:HA    | 2:B:428:ILE:HD12  | 2.01                     | 0.41              |
| 5:E:156:LEU:HD23  | 5:E:160:GLU:HB3   | 2.03                     | 0.41              |
| 9:I:76:PRO:HD2    | 9:I:108:HIS:HD2   | 1.84                     | 0.41              |
| 11:K:39:ASP:OD1   | 11:K:41:THR:HB    | 2.20                     | 0.41              |
| 5:E:10:SER:O      | 5:E:14:ARG:HG3    | 2.19                     | 0.41              |
| 5:E:167:ARG:HA    | 5:E:167:ARG:HD3   | 1.78                     | 0.41              |
| 8:H:82:PRO:HB2    | 8:H:83:GLN:H      | 1.65                     | 0.41              |
| 1:A:37:PHE:O      | 1:A:53:LEU:HB2    | 2.21                     | 0.41              |
| 1:A:133:LYS:HE3   | 1:A:1391:ARG:HH12 | 1.85                     | 0.41              |
| 1:A:399:HIS:HB3   | 1:A:400:PRO:HD3   | 2.02                     | 0.41              |
| 1:A:1196:GLU:HA   | 1:A:1236:LEU:O    | 2.21                     | 0.41              |
| 1:A:1094:VAL:HG22 | 1:A:1113:THR:HB   | 2.02                     | 0.41              |
| 2:B:39:ARG:HE     | 2:B:665:GLU:HG2   | 1.86                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:273:LEU:HD12  | 2:B:280:ILE:HD12  | 2.01                     | 0.41              |
| 2:B:563:MET:CE    | 2:B:580:VAL:HB    | 2.51                     | 0.41              |
| 3:C:149:LYS:C     | 3:C:151:GLN:H     | 2.28                     | 0.41              |
| 4:D:175:PHE:HZ    | 7:G:85:GLU:HG3    | 1.86                     | 0.41              |
| 9:I:111:THR:HG21  | 9:I:118:ARG:HD2   | 2.03                     | 0.41              |
| 1:A:626:ASN:O     | 1:A:631:HIS:ND1   | 2.53                     | 0.41              |
| 1:A:1036:ARG:HH11 | 1:A:1036:ARG:HG2  | 1.85                     | 0.41              |
| 1:A:1418:LEU:HD23 | 2:B:1222:ARG:HD3  | 2.03                     | 0.41              |
| 2:B:758:PHE:CE1   | 2:B:1044:ALA:HA   | 2.56                     | 0.41              |
| 2:B:841:MET:HG2   | 2:B:1010:LEU:HD12 | 2.01                     | 0.41              |
| 12:L:27:LEU:HD22  | 12:L:37:LYS:HE3   | 2.02                     | 0.41              |
| 1:A:497:THR:CG2   | 2:B:1146:PHE:CD1  | 3.02                     | 0.41              |
| 1:A:1317:MET:HE2  | 5:E:142:VAL:HG11  | 2.02                     | 0.41              |
| 2:B:509:ALA:O     | 2:B:511:PRO:HD3   | 2.20                     | 0.41              |
| 2:B:681:TRP:HA    | 2:B:684:LEU:HD12  | 2.03                     | 0.41              |
| 2:B:848:ARG:HD2   | 10:J:8:PHE:O      | 2.20                     | 0.41              |
| 2:B:899:ILE:HG21  | 2:B:949:VAL:HG21  | 2.03                     | 0.41              |
| 2:B:953:LEU:HD11  | 12:L:55:ILE:HG22  | 2.03                     | 0.41              |
| 3:C:75:MET:HE1    | 3:C:239:PRO:HG3   | 2.03                     | 0.41              |
| 1:A:1424:VAL:HG22 | 1:A:1436:ILE:HD11 | 2.03                     | 0.41              |
| 2:B:100:PRO:HG3   | 2:B:172:ILE:HG13  | 2.03                     | 0.41              |
| 2:B:341:LEU:HD11  | 2:B:343:ILE:HB    | 2.02                     | 0.41              |
| 2:B:871:THR:HG22  | 2:B:872:GLU:H     | 1.86                     | 0.41              |
| 2:B:1082:MET:HA   | 3:C:189:THR:HA    | 2.03                     | 0.41              |
| 8:H:125:LEU:HG    | 8:H:130:ARG:HH22  | 1.85                     | 0.41              |
| 10:J:22:LEU:O     | 10:J:26:GLN:HG2   | 2.20                     | 0.41              |
| 1:A:93:VAL:HG13   | 1:A:301:ALA:HB1   | 2.03                     | 0.41              |
| 1:A:369:SER:HB3   | 11:K:2:ASN:OD1    | 2.21                     | 0.41              |
| 1:A:441:PRO:HD2   | 1:A:498:ARG:CZ    | 2.51                     | 0.41              |
| 2:B:315:LYS:N     | 2:B:316:PRO:HD2   | 2.36                     | 0.41              |
| 2:B:1119:VAL:HG23 | 2:B:1126:GLY:HA2  | 2.03                     | 0.41              |
| 3:C:125:MET:HB2   | 3:C:127:ARG:NE    | 2.36                     | 0.41              |
| 10:J:1:MET:HE3    | 10:J:1:MET:HB3    | 1.87                     | 0.41              |
| 10:J:43:ARG:O     | 10:J:47:ARG:HG3   | 2.21                     | 0.41              |
| 1:A:93:VAL:HG22   | 1:A:301:ALA:HA    | 2.04                     | 0.40              |
| 1:A:346:ASP:HB3   | 2:B:1108:ARG:H    | 1.86                     | 0.40              |
| 1:A:243:PRO:HB2   | 1:A:245:PRO:HD2   | 2.02                     | 0.40              |
| 1:A:586:ILE:HD11  | 1:A:637:LYS:HG2   | 2.03                     | 0.40              |
| 2:B:986:GLN:NE2   | 2:B:1022:THR:HG21 | 2.36                     | 0.40              |
| 3:C:255:VAL:HG21  | 11:K:94:ILE:HG21  | 2.03                     | 0.40              |
| 4:D:154:PHE:HB2   | 4:D:160:VAL:HG22  | 2.04                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 8:H:104:PHE:CE1  | 8:H:136:LYS:HG3  | 2.57                     | 0.40              |
| 9:I:8:ARG:O      | 9:I:9:ASP:CB     | 2.69                     | 0.40              |
| 2:B:904:ARG:NH1  | 12:L:66:GLN:O    | 2.55                     | 0.40              |
| 3:C:258:ILE:HG13 | 11:K:42:LEU:HD21 | 2.03                     | 0.40              |
| 6:F:97:ARG:HD2   | 6:F:97:ARG:HA    | 1.82                     | 0.40              |
| 1:A:982:THR:H    | 1:A:985:ASP:HB2  | 1.86                     | 0.40              |
| 1:A:1402:PHE:CE1 | 1:A:1403:GLU:CG  | 3.04                     | 0.40              |
| 2:B:121:ASN:ND2  | 2:B:860:MET:HE2  | 2.36                     | 0.40              |
| 2:B:610:ASN:HB3  | 2:B:613:VAL:HG23 | 2.03                     | 0.40              |
| 2:B:1129:ARG:HB3 | 15:T:21:DC:OP1   | 2.22                     | 0.40              |
| 8:H:38:LEU:CD1   | 8:H:123:MET:HE2  | 2.46                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1   | A     | 1414/1732 (82%) | 1236 (87%) | 126 (9%) | 52 (4%)  | 2           | 16  |
| 2   | B     | 1095/1224 (90%) | 968 (88%)  | 85 (8%)  | 42 (4%)  | 2           | 15  |
| 3   | C     | 264/318 (83%)   | 242 (92%)  | 20 (8%)  | 2 (1%)   | 16          | 44  |
| 4   | D     | 174/221 (79%)   | 148 (85%)  | 17 (10%) | 9 (5%)   | 1           | 10  |
| 5   | E     | 212/215 (99%)   | 195 (92%)  | 13 (6%)  | 4 (2%)   | 6           | 26  |
| 6   | F     | 82/155 (53%)    | 75 (92%)   | 7 (8%)   | 0        | 100         | 100 |
| 7   | G     | 169/171 (99%)   | 158 (94%)  | 8 (5%)   | 3 (2%)   | 6           | 26  |
| 8   | H     | 129/146 (88%)   | 106 (82%)  | 14 (11%) | 9 (7%)   | 1           | 6   |
| 9   | I     | 117/122 (96%)   | 98 (84%)   | 16 (14%) | 3 (3%)   | 4           | 21  |
| 10  | J     | 63/70 (90%)     | 51 (81%)   | 9 (14%)  | 3 (5%)   | 2           | 11  |
| 11  | K     | 113/120 (94%)   | 109 (96%)  | 4 (4%)   | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|----------|-------------|----|
| 12  | L     | 44/70 (63%)     | 27 (61%)   | 9 (20%)  | 8 (18%)  | 0           | 0  |
| All | All   | 3876/4564 (85%) | 3413 (88%) | 328 (8%) | 135 (4%) | 3           | 16 |

All (135) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 57   | ARG  |
| 1   | A     | 58   | LEU  |
| 1   | A     | 76   | GLU  |
| 1   | A     | 189  | ARG  |
| 1   | A     | 195  | ASP  |
| 1   | A     | 257  | ARG  |
| 1   | A     | 318  | SER  |
| 1   | A     | 399  | HIS  |
| 1   | A     | 449  | SER  |
| 1   | A     | 628  | GLY  |
| 1   | A     | 1377 | THR  |
| 1   | A     | 1403 | GLU  |
| 1   | A     | 1405 | THR  |
| 2   | B     | 108  | VAL  |
| 2   | B     | 229  | ALA  |
| 2   | B     | 307  | ASP  |
| 2   | B     | 344  | LYS  |
| 2   | B     | 473  | MET  |
| 2   | B     | 531  | GLN  |
| 2   | B     | 772  | ALA  |
| 2   | B     | 867  | GLY  |
| 2   | B     | 943  | SER  |
| 2   | B     | 1046 | PRO  |
| 2   | B     | 1181 | GLU  |
| 4   | D     | 18   | VAL  |
| 4   | D     | 53   | SER  |
| 4   | D     | 199  | ASN  |
| 9   | I     | 9    | ASP  |
| 9   | I     | 95   | THR  |
| 12  | L     | 50   | ASP  |
| 12  | L     | 53   | HIS  |
| 1   | A     | 47   | ARG  |
| 1   | A     | 54   | ASN  |
| 1   | A     | 167  | CYS  |
| 1   | A     | 178  | GLY  |
| 1   | A     | 193  | ASP  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 224  | PHE  |
| 1   | A     | 286  | HIS  |
| 1   | A     | 332  | LYS  |
| 1   | A     | 672  | ASP  |
| 1   | A     | 1175 | SER  |
| 1   | A     | 1281 | ARG  |
| 2   | B     | 262  | GLU  |
| 2   | B     | 282  | ILE  |
| 2   | B     | 339  | THR  |
| 2   | B     | 341  | LEU  |
| 2   | B     | 466  | TRP  |
| 2   | B     | 707  | PRO  |
| 2   | B     | 731  | VAL  |
| 2   | B     | 792  | MET  |
| 2   | B     | 879  | ARG  |
| 2   | B     | 1175 | LEU  |
| 2   | B     | 1176 | ASN  |
| 4   | D     | 16   | LYS  |
| 4   | D     | 52   | LEU  |
| 4   | D     | 169  | SER  |
| 5   | E     | 36   | GLU  |
| 7   | G     | 2    | PHE  |
| 8   | H     | 17   | PRO  |
| 8   | H     | 81   | PRO  |
| 8   | H     | 82   | PRO  |
| 8   | H     | 83   | GLN  |
| 8   | H     | 90   | ALA  |
| 10  | J     | 6    | ARG  |
| 12  | L     | 45   | ALA  |
| 12  | L     | 56   | LEU  |
| 1   | A     | 335  | ARG  |
| 1   | A     | 975  | HIS  |
| 1   | A     | 1173 | HIS  |
| 2   | B     | 58   | THR  |
| 2   | B     | 340  | ALA  |
| 2   | B     | 343  | ILE  |
| 2   | B     | 711  | GLU  |
| 2   | B     | 1156 | ASP  |
| 2   | B     | 1157 | ALA  |
| 2   | B     | 1167 | GLY  |
| 4   | D     | 22   | GLU  |
| 5   | E     | 45   | LYS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 5   | E     | 48   | ASP  |
| 7   | G     | 154  | VAL  |
| 8   | H     | 18   | GLY  |
| 12  | L     | 59   | ALA  |
| 1   | A     | 42   | ASP  |
| 1   | A     | 52   | GLY  |
| 1   | A     | 74   | MET  |
| 1   | A     | 465  | TYR  |
| 1   | A     | 569  | LYS  |
| 1   | A     | 846  | GLU  |
| 1   | A     | 958  | VAL  |
| 1   | A     | 1255 | GLU  |
| 1   | A     | 1437 | GLY  |
| 1   | A     | 1438 | THR  |
| 2   | B     | 648  | HIS  |
| 2   | B     | 883  | LEU  |
| 2   | B     | 942  | ARG  |
| 2   | B     | 1108 | ARG  |
| 2   | B     | 1155 | SER  |
| 3   | C     | 88   | CYS  |
| 9   | I     | 91   | ARG  |
| 10  | J     | 29   | GLU  |
| 12  | L     | 26   | THR  |
| 12  | L     | 55   | ILE  |
| 12  | L     | 64   | LEU  |
| 1   | A     | 156  | ASP  |
| 1   | A     | 311  | GLN  |
| 1   | A     | 336  | ILE  |
| 1   | A     | 567  | LYS  |
| 1   | A     | 1171 | GLN  |
| 1   | A     | 1366 | ARG  |
| 2   | B     | 251  | ILE  |
| 2   | B     | 469  | GLN  |
| 2   | B     | 880  | THR  |
| 2   | B     | 907  | GLY  |
| 2   | B     | 1223 | ASP  |
| 4   | D     | 21   | GLU  |
| 8   | H     | 60   | ALA  |
| 8   | H     | 128  | ASN  |
| 10  | J     | 2    | ILE  |
| 1   | A     | 35   | ILE  |
| 1   | A     | 55   | ASP  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 155  | GLU  |
| 1   | A     | 885  | THR  |
| 3   | C     | 214  | ASN  |
| 4   | D     | 15   | LEU  |
| 1   | A     | 196  | GLU  |
| 1   | A     | 1388 | GLY  |
| 5   | E     | 90   | VAL  |
| 7   | G     | 63   | PRO  |
| 2   | B     | 364  | ILE  |
| 1   | A     | 192  | GLY  |
| 1   | A     | 312  | PRO  |
| 2   | B     | 1121 | GLY  |
| 1   | A     | 448  | PRO  |
| 2   | B     | 1214 | PRO  |
| 8   | H     | 59   | ILE  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed        | Rotameric  | Outliers  | Percentiles |    |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 1   | A     | 1240/1519 (82%) | 1040 (84%) | 200 (16%) | 2           | 10 |
| 2   | B     | 966/1061 (91%)  | 824 (85%)  | 142 (15%) | 3           | 12 |
| 3   | C     | 234/274 (85%)   | 204 (87%)  | 30 (13%)  | 4           | 17 |
| 4   | D     | 160/200 (80%)   | 123 (77%)  | 37 (23%)  | 1           | 2  |
| 5   | E     | 196/197 (100%)  | 173 (88%)  | 23 (12%)  | 5           | 20 |
| 6   | F     | 74/137 (54%)    | 65 (88%)   | 9 (12%)   | 5           | 19 |
| 7   | G     | 152/152 (100%)  | 134 (88%)  | 18 (12%)  | 5           | 20 |
| 8   | H     | 117/128 (91%)   | 101 (86%)  | 16 (14%)  | 3           | 14 |
| 9   | I     | 113/116 (97%)   | 105 (93%)  | 8 (7%)    | 13          | 39 |
| 10  | J     | 60/65 (92%)     | 48 (80%)   | 12 (20%)  | 1           | 4  |
| 11  | K     | 99/102 (97%)    | 86 (87%)   | 13 (13%)  | 4           | 16 |
| 12  | L     | 40/57 (70%)     | 26 (65%)   | 14 (35%)  | 0           | 0  |

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| Mol | Chain | Analysed        | Rotameric  | Outliers  | Percentiles        |
|-----|-------|-----------------|------------|-----------|--------------------|
| All | All   | 3451/4008 (86%) | 2929 (85%) | 522 (15%) | <b>3</b> <b>11</b> |

All (522) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 12  | ARG  |
| 1   | A     | 13  | THR  |
| 1   | A     | 15  | LYS  |
| 1   | A     | 28  | ARG  |
| 1   | A     | 34  | LYS  |
| 1   | A     | 41  | MET  |
| 1   | A     | 45  | GLN  |
| 1   | A     | 47  | ARG  |
| 1   | A     | 50  | ILE  |
| 1   | A     | 53  | LEU  |
| 1   | A     | 54  | ASN  |
| 1   | A     | 62  | ASP  |
| 1   | A     | 63  | ARG  |
| 1   | A     | 67  | CYS  |
| 1   | A     | 84  | ILE  |
| 1   | A     | 90  | VAL  |
| 1   | A     | 93  | VAL  |
| 1   | A     | 106 | VAL  |
| 1   | A     | 131 | SER  |
| 1   | A     | 134 | ARG  |
| 1   | A     | 145 | LYS  |
| 1   | A     | 147 | VAL  |
| 1   | A     | 152 | VAL  |
| 1   | A     | 157 | ASP  |
| 1   | A     | 173 | THR  |
| 1   | A     | 174 | ILE  |
| 1   | A     | 182 | VAL  |
| 1   | A     | 199 | LEU  |
| 1   | A     | 204 | THR  |
| 1   | A     | 205 | GLU  |
| 1   | A     | 208 | LEU  |
| 1   | A     | 219 | PHE  |
| 1   | A     | 220 | THR  |
| 1   | A     | 222 | LEU  |
| 1   | A     | 227 | VAL  |
| 1   | A     | 237 | THR  |
| 1   | A     | 252 | PHE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 255 | SER  |
| 1   | A     | 270 | LEU  |
| 1   | A     | 279 | LEU  |
| 1   | A     | 289 | ILE  |
| 1   | A     | 295 | LEU  |
| 1   | A     | 307 | ASP  |
| 1   | A     | 313 | GLN  |
| 1   | A     | 315 | LEU  |
| 1   | A     | 322 | VAL  |
| 1   | A     | 330 | LYS  |
| 1   | A     | 333 | GLU  |
| 1   | A     | 335 | ARG  |
| 1   | A     | 337 | ARG  |
| 1   | A     | 344 | ARG  |
| 1   | A     | 353 | ILE  |
| 1   | A     | 375 | THR  |
| 1   | A     | 381 | THR  |
| 1   | A     | 385 | ILE  |
| 1   | A     | 386 | ASP  |
| 1   | A     | 393 | ARG  |
| 1   | A     | 398 | GLU  |
| 1   | A     | 408 | ASP  |
| 1   | A     | 412 | ARG  |
| 1   | A     | 424 | ILE  |
| 1   | A     | 425 | GLN  |
| 1   | A     | 427 | GLN  |
| 1   | A     | 434 | ARG  |
| 1   | A     | 436 | ILE  |
| 1   | A     | 443 | LEU  |
| 1   | A     | 445 | ASN  |
| 1   | A     | 450 | LEU  |
| 1   | A     | 451 | HIS  |
| 1   | A     | 454 | SER  |
| 1   | A     | 461 | LYS  |
| 1   | A     | 469 | ARG  |
| 1   | A     | 470 | LEU  |
| 1   | A     | 472 | LEU  |
| 1   | A     | 474 | VAL  |
| 1   | A     | 475 | THR  |
| 1   | A     | 476 | SER  |
| 1   | A     | 489 | LEU  |
| 1   | A     | 500 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 505 | CYS  |
| 1   | A     | 512 | VAL  |
| 1   | A     | 513 | SER  |
| 1   | A     | 524 | VAL  |
| 1   | A     | 532 | ARG  |
| 1   | A     | 566 | ILE  |
| 1   | A     | 571 | LEU  |
| 1   | A     | 582 | ILE  |
| 1   | A     | 593 | GLU  |
| 1   | A     | 596 | THR  |
| 1   | A     | 603 | ASN  |
| 1   | A     | 613 | ILE  |
| 1   | A     | 618 | GLU  |
| 1   | A     | 629 | LEU  |
| 1   | A     | 630 | ILE  |
| 1   | A     | 634 | THR  |
| 1   | A     | 652 | VAL  |
| 1   | A     | 664 | THR  |
| 1   | A     | 666 | ILE  |
| 1   | A     | 672 | ASP  |
| 1   | A     | 691 | LEU  |
| 1   | A     | 702 | LEU  |
| 1   | A     | 719 | VAL  |
| 1   | A     | 738 | LYS  |
| 1   | A     | 740 | LEU  |
| 1   | A     | 768 | GLN  |
| 1   | A     | 769 | SER  |
| 1   | A     | 773 | LYS  |
| 1   | A     | 782 | ARG  |
| 1   | A     | 788 | SER  |
| 1   | A     | 795 | GLU  |
| 1   | A     | 797 | LYS  |
| 1   | A     | 801 | GLU  |
| 1   | A     | 805 | LEU  |
| 1   | A     | 806 | ARG  |
| 1   | A     | 821 | ARG  |
| 1   | A     | 826 | ASP  |
| 1   | A     | 827 | THR  |
| 1   | A     | 831 | THR  |
| 1   | A     | 834 | THR  |
| 1   | A     | 837 | ILE  |
| 1   | A     | 839 | ARG  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 848  | ILE  |
| 1   | A     | 849  | MET  |
| 1   | A     | 854  | ASN  |
| 1   | A     | 864  | ILE  |
| 1   | A     | 867  | ILE  |
| 1   | A     | 886  | ILE  |
| 1   | A     | 896  | ARG  |
| 1   | A     | 919  | ILE  |
| 1   | A     | 920  | LEU  |
| 1   | A     | 926  | GLN  |
| 1   | A     | 929  | LEU  |
| 1   | A     | 948  | VAL  |
| 1   | A     | 949  | ASP  |
| 1   | A     | 964  | ILE  |
| 1   | A     | 973  | ILE  |
| 1   | A     | 976  | THR  |
| 1   | A     | 983  | ILE  |
| 1   | A     | 998  | LEU  |
| 1   | A     | 999  | VAL  |
| 1   | A     | 1009 | ASN  |
| 1   | A     | 1015 | VAL  |
| 1   | A     | 1029 | ARG  |
| 1   | A     | 1030 | ARG  |
| 1   | A     | 1047 | SER  |
| 1   | A     | 1058 | VAL  |
| 1   | A     | 1062 | GLU  |
| 1   | A     | 1067 | LEU  |
| 1   | A     | 1078 | GLN  |
| 1   | A     | 1094 | VAL  |
| 1   | A     | 1116 | LEU  |
| 1   | A     | 1118 | VAL  |
| 1   | A     | 1120 | LEU  |
| 1   | A     | 1121 | GLU  |
| 1   | A     | 1124 | HIS  |
| 1   | A     | 1135 | ARG  |
| 1   | A     | 1142 | THR  |
| 1   | A     | 1172 | LEU  |
| 1   | A     | 1173 | HIS  |
| 1   | A     | 1176 | LEU  |
| 1   | A     | 1195 | LEU  |
| 1   | A     | 1208 | THR  |
| 1   | A     | 1218 | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1223 | ASP  |
| 1   | A     | 1226 | VAL  |
| 1   | A     | 1237 | ILE  |
| 1   | A     | 1238 | ILE  |
| 1   | A     | 1242 | VAL  |
| 1   | A     | 1255 | GLU  |
| 1   | A     | 1257 | ASP  |
| 1   | A     | 1260 | LEU  |
| 1   | A     | 1265 | ASN  |
| 1   | A     | 1273 | LEU  |
| 1   | A     | 1291 | VAL  |
| 1   | A     | 1295 | THR  |
| 1   | A     | 1297 | GLU  |
| 1   | A     | 1309 | ASP  |
| 1   | A     | 1315 | GLU  |
| 1   | A     | 1317 | MET  |
| 1   | A     | 1325 | THR  |
| 1   | A     | 1327 | ILE  |
| 1   | A     | 1336 | MET  |
| 1   | A     | 1341 | ILE  |
| 1   | A     | 1355 | VAL  |
| 1   | A     | 1376 | THR  |
| 1   | A     | 1382 | THR  |
| 1   | A     | 1386 | ARG  |
| 1   | A     | 1391 | ARG  |
| 1   | A     | 1393 | ASN  |
| 1   | A     | 1403 | GLU  |
| 1   | A     | 1404 | GLU  |
| 1   | A     | 1411 | GLU  |
| 1   | A     | 1424 | VAL  |
| 1   | A     | 1426 | GLU  |
| 1   | A     | 1438 | THR  |
| 1   | A     | 1442 | ASP  |
| 1   | A     | 1444 | MET  |
| 1   | A     | 1445 | ILE  |
| 1   | A     | 1453 | TYR  |
| 1   | A     | 1454 | MET  |
| 2   | B     | 25   | ILE  |
| 2   | B     | 41   | LYS  |
| 2   | B     | 46   | GLN  |
| 2   | B     | 63   | ILE  |
| 2   | B     | 104  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 118 | ARG  |
| 2   | B     | 130 | VAL  |
| 2   | B     | 134 | LYS  |
| 2   | B     | 183 | GLU  |
| 2   | B     | 185 | THR  |
| 2   | B     | 217 | ARG  |
| 2   | B     | 218 | SER  |
| 2   | B     | 240 | ILE  |
| 2   | B     | 251 | ILE  |
| 2   | B     | 261 | ARG  |
| 2   | B     | 267 | ARG  |
| 2   | B     | 272 | THR  |
| 2   | B     | 278 | GLN  |
| 2   | B     | 279 | ASP  |
| 2   | B     | 287 | ARG  |
| 2   | B     | 294 | ASP  |
| 2   | B     | 313 | MET  |
| 2   | B     | 324 | ILE  |
| 2   | B     | 325 | GLN  |
| 2   | B     | 337 | ARG  |
| 2   | B     | 341 | LEU  |
| 2   | B     | 343 | ILE  |
| 2   | B     | 344 | LYS  |
| 2   | B     | 348 | ARG  |
| 2   | B     | 357 | GLN  |
| 2   | B     | 365 | THR  |
| 2   | B     | 393 | LYS  |
| 2   | B     | 412 | LEU  |
| 2   | B     | 416 | LEU  |
| 2   | B     | 423 | LYS  |
| 2   | B     | 429 | PHE  |
| 2   | B     | 436 | VAL  |
| 2   | B     | 446 | LEU  |
| 2   | B     | 448 | ILE  |
| 2   | B     | 458 | LYS  |
| 2   | B     | 461 | LEU  |
| 2   | B     | 470 | LYS  |
| 2   | B     | 476 | ARG  |
| 2   | B     | 482 | VAL  |
| 2   | B     | 485 | ARG  |
| 2   | B     | 487 | THR  |
| 2   | B     | 502 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 513 | GLN  |
| 2   | B     | 529 | GLU  |
| 2   | B     | 531 | GLN  |
| 2   | B     | 537 | LYS  |
| 2   | B     | 542 | MET  |
| 2   | B     | 547 | VAL  |
| 2   | B     | 549 | THR  |
| 2   | B     | 552 | MET  |
| 2   | B     | 554 | ILE  |
| 2   | B     | 563 | MET  |
| 2   | B     | 570 | VAL  |
| 2   | B     | 574 | SER  |
| 2   | B     | 595 | ARG  |
| 2   | B     | 596 | LEU  |
| 2   | B     | 601 | ARG  |
| 2   | B     | 603 | LEU  |
| 2   | B     | 609 | ILE  |
| 2   | B     | 612 | GLU  |
| 2   | B     | 615 | MET  |
| 2   | B     | 616 | ILE  |
| 2   | B     | 620 | ARG  |
| 2   | B     | 644 | GLU  |
| 2   | B     | 651 | LEU  |
| 2   | B     | 653 | VAL  |
| 2   | B     | 658 | ILE  |
| 2   | B     | 680 | THR  |
| 2   | B     | 708 | GLU  |
| 2   | B     | 734 | HIS  |
| 2   | B     | 737 | THR  |
| 2   | B     | 766 | ARG  |
| 2   | B     | 771 | SER  |
| 2   | B     | 776 | GLN  |
| 2   | B     | 786 | ASN  |
| 2   | B     | 790 | ASP  |
| 2   | B     | 791 | THR  |
| 2   | B     | 795 | ILE  |
| 2   | B     | 831 | SER  |
| 2   | B     | 835 | GLN  |
| 2   | B     | 839 | MET  |
| 2   | B     | 841 | MET  |
| 2   | B     | 844 | SER  |
| 2   | B     | 857 | ARG  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 868  | MET  |
| 2   | B     | 870  | ILE  |
| 2   | B     | 871  | THR  |
| 2   | B     | 878  | GLN  |
| 2   | B     | 882  | THR  |
| 2   | B     | 889  | THR  |
| 2   | B     | 904  | ARG  |
| 2   | B     | 906  | SER  |
| 2   | B     | 909  | ASP  |
| 2   | B     | 911  | ILE  |
| 2   | B     | 934  | LYS  |
| 2   | B     | 939  | THR  |
| 2   | B     | 942  | ARG  |
| 2   | B     | 944  | THR  |
| 2   | B     | 953  | LEU  |
| 2   | B     | 964  | VAL  |
| 2   | B     | 970  | THR  |
| 2   | B     | 972  | LYS  |
| 2   | B     | 973  | ILE  |
| 2   | B     | 975  | GLN  |
| 2   | B     | 979  | LYS  |
| 2   | B     | 986  | GLN  |
| 2   | B     | 997  | GLU  |
| 2   | B     | 999  | MET  |
| 2   | B     | 1007 | VAL  |
| 2   | B     | 1028 | GLU  |
| 2   | B     | 1045 | SER  |
| 2   | B     | 1060 | ARG  |
| 2   | B     | 1065 | GLN  |
| 2   | B     | 1072 | MET  |
| 2   | B     | 1084 | GLN  |
| 2   | B     | 1094 | ARG  |
| 2   | B     | 1101 | ASP  |
| 2   | B     | 1106 | ARG  |
| 2   | B     | 1123 | SER  |
| 2   | B     | 1128 | LEU  |
| 2   | B     | 1138 | MET  |
| 2   | B     | 1145 | SER  |
| 2   | B     | 1147 | LEU  |
| 2   | B     | 1151 | LEU  |
| 2   | B     | 1156 | ASP  |
| 2   | B     | 1159 | ARG  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 1160 | VAL  |
| 2   | B     | 1165 | ILE  |
| 2   | B     | 1175 | LEU  |
| 2   | B     | 1179 | GLN  |
| 2   | B     | 1183 | LYS  |
| 2   | B     | 1188 | LYS  |
| 2   | B     | 1189 | ILE  |
| 2   | B     | 1193 | GLN  |
| 2   | B     | 1201 | LYS  |
| 2   | B     | 1202 | LEU  |
| 2   | B     | 1220 | ARG  |
| 3   | C     | 3    | GLU  |
| 3   | C     | 11   | ARG  |
| 3   | C     | 12   | GLU  |
| 3   | C     | 22   | LEU  |
| 3   | C     | 25   | VAL  |
| 3   | C     | 26   | ASP  |
| 3   | C     | 52   | GLU  |
| 3   | C     | 53   | THR  |
| 3   | C     | 54   | ASN  |
| 3   | C     | 55   | THR  |
| 3   | C     | 56   | THR  |
| 3   | C     | 81   | GLU  |
| 3   | C     | 100  | THR  |
| 3   | C     | 101  | LEU  |
| 3   | C     | 119  | VAL  |
| 3   | C     | 121  | VAL  |
| 3   | C     | 124  | LEU  |
| 3   | C     | 125  | MET  |
| 3   | C     | 127  | ARG  |
| 3   | C     | 129  | ILE  |
| 3   | C     | 133  | ILE  |
| 3   | C     | 147  | LEU  |
| 3   | C     | 151  | GLN  |
| 3   | C     | 215  | GLU  |
| 3   | C     | 224  | GLN  |
| 3   | C     | 238  | ILE  |
| 3   | C     | 240  | VAL  |
| 3   | C     | 259  | LEU  |
| 3   | C     | 265  | MET  |
| 3   | C     | 268  | ASP  |
| 4   | D     | 5    | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | D     | 7   | THR  |
| 4   | D     | 9   | GLN  |
| 4   | D     | 10  | THR  |
| 4   | D     | 12  | ARG  |
| 4   | D     | 13  | ARG  |
| 4   | D     | 18  | VAL  |
| 4   | D     | 27  | LEU  |
| 4   | D     | 32  | GLU  |
| 4   | D     | 34  | GLN  |
| 4   | D     | 35  | LEU  |
| 4   | D     | 40  | HIS  |
| 4   | D     | 47  | LEU  |
| 4   | D     | 52  | LEU  |
| 4   | D     | 53  | SER  |
| 4   | D     | 64  | VAL  |
| 4   | D     | 65  | GLU  |
| 4   | D     | 67  | ARG  |
| 4   | D     | 118 | THR  |
| 4   | D     | 126 | ILE  |
| 4   | D     | 128 | VAL  |
| 4   | D     | 134 | THR  |
| 4   | D     | 139 | LYS  |
| 4   | D     | 153 | ARG  |
| 4   | D     | 156 | ASP  |
| 4   | D     | 166 | LEU  |
| 4   | D     | 177 | VAL  |
| 4   | D     | 182 | SER  |
| 4   | D     | 187 | THR  |
| 4   | D     | 193 | THR  |
| 4   | D     | 197 | SER  |
| 4   | D     | 201 | LYS  |
| 4   | D     | 213 | GLU  |
| 4   | D     | 214 | LEU  |
| 4   | D     | 215 | SER  |
| 4   | D     | 219 | THR  |
| 4   | D     | 221 | TYR  |
| 5   | E     | 3   | GLN  |
| 5   | E     | 9   | ILE  |
| 5   | E     | 20  | LYS  |
| 5   | E     | 31  | THR  |
| 5   | E     | 45  | LYS  |
| 5   | E     | 57  | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | E     | 67  | GLU  |
| 5   | E     | 92  | THR  |
| 5   | E     | 100 | ILE  |
| 5   | E     | 104 | ASN  |
| 5   | E     | 127 | ILE  |
| 5   | E     | 131 | THR  |
| 5   | E     | 140 | LEU  |
| 5   | E     | 144 | ILE  |
| 5   | E     | 166 | LYS  |
| 5   | E     | 173 | SER  |
| 5   | E     | 177 | ARG  |
| 5   | E     | 178 | ILE  |
| 5   | E     | 191 | LYS  |
| 5   | E     | 192 | ARG  |
| 5   | E     | 196 | VAL  |
| 5   | E     | 202 | SER  |
| 5   | E     | 204 | THR  |
| 6   | F     | 72  | LYS  |
| 6   | F     | 78  | GLN  |
| 6   | F     | 79  | ARG  |
| 6   | F     | 82  | THR  |
| 6   | F     | 86  | THR  |
| 6   | F     | 90  | ARG  |
| 6   | F     | 110 | ASP  |
| 6   | F     | 129 | LYS  |
| 6   | F     | 133 | VAL  |
| 7   | G     | 13  | LEU  |
| 7   | G     | 24  | GLN  |
| 7   | G     | 26  | LEU  |
| 7   | G     | 34  | VAL  |
| 7   | G     | 60  | ARG  |
| 7   | G     | 61  | ILE  |
| 7   | G     | 64  | THR  |
| 7   | G     | 96  | GLN  |
| 7   | G     | 106 | MET  |
| 7   | G     | 133 | SER  |
| 7   | G     | 138 | THR  |
| 7   | G     | 143 | ILE  |
| 7   | G     | 145 | VAL  |
| 7   | G     | 151 | ILE  |
| 7   | G     | 155 | SER  |
| 7   | G     | 162 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | G     | 163 | ILE  |
| 7   | G     | 171 | ILE  |
| 8   | H     | 13  | SER  |
| 8   | H     | 14  | GLU  |
| 8   | H     | 23  | VAL  |
| 8   | H     | 26  | ILE  |
| 8   | H     | 31  | THR  |
| 8   | H     | 34  | ASP  |
| 8   | H     | 76  | THR  |
| 8   | H     | 77  | ARG  |
| 8   | H     | 83  | GLN  |
| 8   | H     | 89  | LEU  |
| 8   | H     | 92  | ASP  |
| 8   | H     | 103 | LYS  |
| 8   | H     | 128 | ASN  |
| 8   | H     | 130 | ARG  |
| 8   | H     | 135 | LEU  |
| 8   | H     | 138 | GLU  |
| 9   | I     | 8   | ARG  |
| 9   | I     | 31  | THR  |
| 9   | I     | 35  | VAL  |
| 9   | I     | 74  | GLU  |
| 9   | I     | 82  | GLU  |
| 9   | I     | 84  | VAL  |
| 9   | I     | 94  | ASP  |
| 9   | I     | 111 | THR  |
| 10  | J     | 1   | MET  |
| 10  | J     | 2   | ILE  |
| 10  | J     | 3   | VAL  |
| 10  | J     | 7   | CYS  |
| 10  | J     | 12  | LYS  |
| 10  | J     | 13  | VAL  |
| 10  | J     | 14  | VAL  |
| 10  | J     | 22  | LEU  |
| 10  | J     | 29  | GLU  |
| 10  | J     | 42  | LYS  |
| 10  | J     | 48  | ARG  |
| 10  | J     | 52  | THR  |
| 11  | K     | 14  | GLU  |
| 11  | K     | 18  | LYS  |
| 11  | K     | 20  | LYS  |
| 11  | K     | 25  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11  | K     | 29  | ASN  |
| 11  | K     | 31  | VAL  |
| 11  | K     | 37  | LYS  |
| 11  | K     | 42  | LEU  |
| 11  | K     | 47  | ARG  |
| 11  | K     | 51  | LEU  |
| 11  | K     | 101 | LEU  |
| 11  | K     | 107 | THR  |
| 11  | K     | 114 | LEU  |
| 12  | L     | 27  | LEU  |
| 12  | L     | 33  | GLU  |
| 12  | L     | 35  | SER  |
| 12  | L     | 38  | LEU  |
| 12  | L     | 42  | ARG  |
| 12  | L     | 50  | ASP  |
| 12  | L     | 54  | ARG  |
| 12  | L     | 55  | ILE  |
| 12  | L     | 56  | LEU  |
| 12  | L     | 58  | LYS  |
| 12  | L     | 60  | ARG  |
| 12  | L     | 61  | THR  |
| 12  | L     | 65  | VAL  |
| 12  | L     | 68  | GLU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 18  | GLN  |
| 1   | A     | 54  | ASN  |
| 1   | A     | 282 | ASN  |
| 1   | A     | 390 | GLN  |
| 1   | A     | 394 | ASN  |
| 1   | A     | 399 | HIS  |
| 1   | A     | 425 | GLN  |
| 1   | A     | 451 | HIS  |
| 1   | A     | 479 | ASN  |
| 1   | A     | 517 | ASN  |
| 1   | A     | 545 | GLN  |
| 1   | A     | 548 | ASN  |
| 1   | A     | 603 | ASN  |
| 1   | A     | 760 | GLN  |
| 1   | A     | 811 | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 838  | GLN  |
| 1   | A     | 965  | GLN  |
| 1   | A     | 966  | ASN  |
| 1   | A     | 969  | GLN  |
| 1   | A     | 994  | GLN  |
| 1   | A     | 1106 | ASN  |
| 1   | A     | 1128 | GLN  |
| 1   | A     | 1140 | HIS  |
| 1   | A     | 1173 | HIS  |
| 1   | A     | 1232 | ASN  |
| 1   | A     | 1270 | ASN  |
| 1   | A     | 1393 | ASN  |
| 1   | A     | 1427 | ASN  |
| 2   | B     | 46   | GLN  |
| 2   | B     | 278  | GLN  |
| 2   | B     | 300  | HIS  |
| 2   | B     | 357  | GLN  |
| 2   | B     | 433  | GLN  |
| 2   | B     | 538  | ASN  |
| 2   | B     | 686  | ASN  |
| 2   | B     | 786  | ASN  |
| 2   | B     | 842  | ASN  |
| 2   | B     | 1025 | HIS  |
| 2   | B     | 1117 | GLN  |
| 2   | B     | 1176 | ASN  |
| 2   | B     | 1177 | HIS  |
| 3   | C     | 112  | ASN  |
| 3   | C     | 131  | HIS  |
| 3   | C     | 135  | GLN  |
| 3   | C     | 184  | ASN  |
| 3   | C     | 203  | GLN  |
| 3   | C     | 214  | ASN  |
| 3   | C     | 231  | ASN  |
| 4   | D     | 37   | GLN  |
| 4   | D     | 132  | GLN  |
| 4   | D     | 143  | ASN  |
| 5   | E     | 3    | GLN  |
| 5   | E     | 32   | GLN  |
| 5   | E     | 54   | GLN  |
| 5   | E     | 115  | ASN  |
| 5   | E     | 146  | HIS  |
| 5   | E     | 179  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | G     | 53  | ASN  |
| 7   | G     | 71  | ASN  |
| 8   | H     | 35  | GLN  |
| 8   | H     | 52  | GLN  |
| 8   | H     | 83  | GLN  |
| 8   | H     | 131 | ASN  |
| 9   | I     | 83  | ASN  |
| 9   | I     | 89  | GLN  |
| 9   | I     | 108 | HIS  |
| 10  | J     | 26  | GLN  |
| 10  | J     | 64  | ASN  |
| 11  | K     | 44  | ASN  |
| 11  | K     | 76  | GLN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed  | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------|-------------------|-----------------|
| 14  | P     | 5/6 (83%) | 1 (20%)           | 0               |

All (1) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 14  | P     | 8   | G    |

There are no RNA pucker outliers to report.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link  | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|-------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |       | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 15  | BRU  | T     | 22  | 15,14 | 18,21,22     | 1.00 | 1 (5%)      | 25,30,33    | 1.66 | 6 (24%)     |



In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link  | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|-------|---------|-----------|---------|
| 15  | BRU  | T     | 22  | 15,14 | -       | 0/7/21/22 | 0/2/2/2 |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 15  | T     | 22  | BRU  | C4-N3 | -2.26 | 1.34        | 1.38     |

All (6) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 15  | T     | 22  | BRU  | O4'-C1'-N1 | 4.22  | 115.35      | 107.86   |
| 15  | T     | 22  | BRU  | BR-C5-C4   | 2.83  | 121.28      | 118.02   |
| 15  | T     | 22  | BRU  | N3-C2-N1   | 2.75  | 118.48      | 114.89   |
| 15  | T     | 22  | BRU  | BR-C5-C6   | -2.63 | 116.96      | 120.64   |
| 15  | T     | 22  | BRU  | C2'-C1'-N1 | -2.23 | 108.25      | 113.81   |
| 15  | T     | 22  | BRU  | O2-C2-N3   | -2.12 | 117.57      | 121.49   |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 15  | T     | 22  | BRU  | 1       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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 [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 2   | B     | 2                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | B     | 934:LYS   | C      | 935:ARG   | N      | 5.39         |
| 1     | B     | 351:TYR   | C      | 352:ALA   | N      | 3.28         |

## 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     | 1422/1732 (82%) | -0.20  | 26 (1%) 67 53  | 52, 96, 155, 215      | 0     |
| 2   | B     | 1115/1224 (91%) | 0.09   | 48 (4%) 40 29  | 56, 111, 174, 201     | 0     |
| 3   | C     | 266/318 (83%)   | -0.40  | 1 (0%) 88 81   | 68, 97, 135, 165      | 0     |
| 4   | D     | 178/221 (80%)   | 0.01   | 12 (6%) 24 19  | 77, 110, 162, 182     | 0     |
| 5   | E     | 214/215 (99%)   | 0.03   | 3 (1%) 73 59   | 72, 128, 170, 191     | 0     |
| 6   | F     | 84/155 (54%)    | -0.59  | 1 (1%) 76 63   | 55, 76, 106, 122      | 0     |
| 7   | G     | 171/171 (100%)  | -0.16  | 0 100 100      | 65, 96, 134, 153      | 0     |
| 8   | H     | 133/146 (91%)   | 0.55   | 13 (9%) 13 13  | 110, 136, 175, 195    | 0     |
| 9   | I     | 119/122 (97%)   | 0.26   | 11 (9%) 14 14  | 107, 137, 173, 189    | 0     |
| 10  | J     | 65/70 (92%)     | -0.28  | 1 (1%) 72 57   | 73, 94, 129, 142      | 0     |
| 11  | K     | 115/120 (95%)   | -0.42  | 2 (1%) 69 54   | 63, 95, 135, 151      | 0     |
| 12  | L     | 46/70 (65%)     | 1.12   | 6 (13%) 7 8    | 92, 161, 182, 184     | 0     |
| 13  | N     | 10/14 (71%)     | 0.91   | 2 (20%) 3 4    | 158, 184, 239, 246    | 0     |
| 14  | P     | 6/6 (100%)      | -0.76  | 0 100 100      | 75, 90, 111, 138      | 0     |
| 15  | T     | 19/26 (73%)     | 0.75   | 2 (10%) 11 12  | 105, 152, 246, 248    | 0     |
| All | All   | 3963/4610 (85%) | -0.06  | 128 (3%) 50 37 | 52, 105, 168, 248     | 0     |

All (128) RSRZ outliers are listed below:

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | A     | 251  | SER  | 8.3  |
| 12  | L     | 27   | LEU  | 7.6  |
| 8   | H     | 63   | LEU  | 6.5  |
| 2   | B     | 446  | LEU  | 6.4  |
| 2   | B     | 1224 | PHE  | 6.0  |
| 2   | B     | 509  | ALA  | 5.7  |
| 12  | L     | 26   | THR  | 5.6  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | A     | 1243 | VAL  | 5.5  |
| 2   | B     | 502  | ILE  | 5.5  |
| 2   | B     | 882  | THR  | 5.1  |
| 12  | L     | 25   | ALA  | 5.1  |
| 2   | B     | 251  | ILE  | 5.0  |
| 2   | B     | 709  | ASP  | 4.9  |
| 1   | A     | 1080 | THR  | 4.8  |
| 11  | K     | 114  | LEU  | 4.6  |
| 9   | I     | 120  | GLN  | 4.4  |
| 8   | H     | 132  | LEU  | 4.3  |
| 2   | B     | 883  | LEU  | 4.3  |
| 1   | A     | 1176 | LEU  | 4.3  |
| 1   | A     | 194  | ALA  | 4.3  |
| 2   | B     | 70   | ILE  | 4.3  |
| 2   | B     | 243  | ALA  | 4.1  |
| 4   | D     | 25   | ALA  | 4.0  |
| 2   | B     | 708  | GLU  | 4.0  |
| 1   | A     | 56   | PRO  | 4.0  |
| 2   | B     | 134  | LYS  | 3.9  |
| 4   | D     | 3    | VAL  | 3.9  |
| 15  | T     | 26   | DC   | 3.9  |
| 4   | D     | 76   | LYS  | 3.7  |
| 10  | J     | 65   | PRO  | 3.6  |
| 1   | A     | 190  | ALA  | 3.5  |
| 2   | B     | 870  | ILE  | 3.5  |
| 12  | L     | 28   | LYS  | 3.4  |
| 2   | B     | 342  | GLY  | 3.4  |
| 2   | B     | 341  | LEU  | 3.4  |
| 8   | H     | 2    | SER  | 3.4  |
| 2   | B     | 343  | ILE  | 3.4  |
| 2   | B     | 715  | ALA  | 3.3  |
| 2   | B     | 710  | LEU  | 3.3  |
| 4   | D     | 24   | ALA  | 3.3  |
| 2   | B     | 958  | GLN  | 3.3  |
| 1   | A     | 252  | PHE  | 3.3  |
| 2   | B     | 262  | GLU  | 3.3  |
| 1   | A     | 250  | ILE  | 3.2  |
| 9   | I     | 52   | ILE  | 3.2  |
| 4   | D     | 221  | TYR  | 3.2  |
| 8   | H     | 139  | ASN  | 3.1  |
| 1   | A     | 1187 | GLN  | 3.1  |
| 2   | B     | 470  | LYS  | 3.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 2   | B     | 879  | ARG  | 3.0  |
| 1   | A     | 1455 | PRO  | 3.0  |
| 2   | B     | 881  | ASN  | 3.0  |
| 2   | B     | 340  | ALA  | 2.9  |
| 8   | H     | 82   | PRO  | 2.9  |
| 4   | D     | 187  | THR  | 2.9  |
| 1   | A     | 830  | LYS  | 2.9  |
| 6   | F     | 72   | LYS  | 2.8  |
| 2   | B     | 108  | VAL  | 2.7  |
| 4   | D     | 173  | HIS  | 2.7  |
| 8   | H     | 90   | ALA  | 2.7  |
| 2   | B     | 712  | PRO  | 2.7  |
| 8   | H     | 135  | LEU  | 2.7  |
| 2   | B     | 918  | ILE  | 2.7  |
| 11  | K     | 115  | ALA  | 2.7  |
| 2   | B     | 250  | PHE  | 2.6  |
| 2   | B     | 476  | ARG  | 2.6  |
| 2   | B     | 1049 | ASP  | 2.6  |
| 4   | D     | 10   | THR  | 2.6  |
| 1   | A     | 310  | GLY  | 2.6  |
| 2   | B     | 249  | ARG  | 2.6  |
| 12  | L     | 46   | VAL  | 2.6  |
| 9   | I     | 119  | THR  | 2.6  |
| 2   | B     | 646  | LEU  | 2.5  |
| 5   | E     | 3    | GLN  | 2.5  |
| 1   | A     | 255  | SER  | 2.5  |
| 13  | N     | 11   | DA   | 2.5  |
| 4   | D     | 8    | PHE  | 2.5  |
| 1   | A     | 1093 | LYS  | 2.5  |
| 1   | A     | 1254 | ALA  | 2.5  |
| 2   | B     | 164  | LYS  | 2.5  |
| 2   | B     | 437  | GLU  | 2.4  |
| 1   | A     | 57   | ARG  | 2.4  |
| 2   | B     | 244  | LEU  | 2.4  |
| 2   | B     | 917  | PRO  | 2.4  |
| 9   | I     | 118  | ARG  | 2.4  |
| 5   | E     | 90   | VAL  | 2.4  |
| 9   | I     | 3    | THR  | 2.4  |
| 8   | H     | 84   | ALA  | 2.4  |
| 8   | H     | 136  | LYS  | 2.4  |
| 9   | I     | 117  | LYS  | 2.3  |
| 5   | E     | 91   | LYS  | 2.3  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | A     | 258  | GLY  | 2.3  |
| 1   | A     | 50   | ILE  | 2.3  |
| 2   | B     | 880  | THR  | 2.3  |
| 8   | H     | 89   | LEU  | 2.3  |
| 9   | I     | 116  | ASN  | 2.3  |
| 8   | H     | 86   | ASP  | 2.3  |
| 2   | B     | 734  | HIS  | 2.2  |
| 4   | D     | 40   | HIS  | 2.2  |
| 2   | B     | 962  | LYS  | 2.2  |
| 1   | A     | 323  | LYS  | 2.2  |
| 4   | D     | 13   | ARG  | 2.2  |
| 13  | N     | 8    | DT   | 2.2  |
| 1   | A     | 256  | GLN  | 2.2  |
| 8   | H     | 83   | GLN  | 2.2  |
| 2   | B     | 245  | GLU  | 2.2  |
| 1   | A     | 186  | LYS  | 2.2  |
| 12  | L     | 53   | HIS  | 2.2  |
| 9   | I     | 2    | THR  | 2.1  |
| 8   | H     | 129  | TYR  | 2.1  |
| 2   | B     | 934  | LYS  | 2.1  |
| 2   | B     | 20   | ASP  | 2.1  |
| 1   | A     | 187  | LYS  | 2.1  |
| 2   | B     | 278  | GLN  | 2.1  |
| 3   | C     | 224  | GLN  | 2.1  |
| 2   | B     | 887  | HIS  | 2.1  |
| 2   | B     | 860  | MET  | 2.1  |
| 1   | A     | 593  | GLU  | 2.1  |
| 2   | B     | 353  | LYS  | 2.0  |
| 2   | B     | 471  | LYS  | 2.0  |
| 4   | D     | 12   | ARG  | 2.0  |
| 9   | I     | 4    | PHE  | 2.0  |
| 9   | I     | 93   | LYS  | 2.0  |
| 1   | A     | 257  | ARG  | 2.0  |
| 2   | B     | 884  | ARG  | 2.0  |
| 9   | I     | 97   | MET  | 2.0  |
| 15  | T     | 25   | DT   | 2.0  |
| 1   | A     | 1256 | GLU  | 2.0  |

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

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(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 15  | BRU  | T     | 22  | 20/21 | 0.96 | 0.08 | 107,109,114,121            | 0     |

### 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(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 16  | ZN   | I     | 1122 | 1/1   | 0.99 | 0.03 | 182,182,182,182            | 0     |
| 16  | ZN   | L     | 1071 | 1/1   | 0.99 | 0.04 | 163,163,163,163            | 0     |
| 16  | ZN   | B     | 2225 | 1/1   | 1.00 | 0.04 | 77,77,77,77                | 0     |
| 16  | ZN   | C     | 1269 | 1/1   | 1.00 | 0.02 | 88,88,88,88                | 0     |
| 16  | ZN   | I     | 1121 | 1/1   | 1.00 | 0.04 | 121,121,121,121            | 0     |
| 16  | ZN   | A     | 2456 | 1/1   | 1.00 | 0.02 | 133,133,133,133            | 0     |
| 16  | ZN   | J     | 1066 | 1/1   | 1.00 | 0.03 | 91,91,91,91                | 0     |
| 16  | ZN   | A     | 2457 | 1/1   | 1.00 | 0.03 | 67,67,67,67                | 0     |
| 17  | MG   | A     | 2458 | 1/1   | 1.00 | 0.02 | 64,64,64,64                | 0     |

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

There are no such residues in this entry.