



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 01:02 PM EDT

PDB ID : 3M3Y / pdb\_00003m3y  
Title : RNA polymerase II elongation complex C  
Authors : Wang, D.; Zhu, G.; Huang, X.; Lippard, S.J.  
Deposited on : 2010-03-10  
Resolution : 3.18 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                           | : | 9.0.015 (Gargrove)                                               |
| Density-Fitness                | : | 1.0.12                                                           |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.50                                                             |

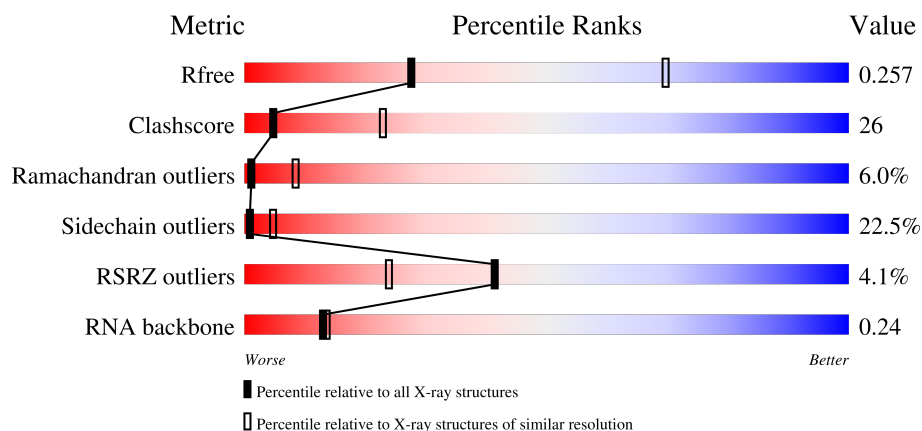
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.18 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 2001 (3.20-3.16)                                      |
| Clashscore            | 190562                      | 2119 (3.20-3.16)                                      |
| Ramachandran outliers | 187476                      | 2070 (3.20-3.16)                                      |
| Sidechain outliers    | 187428                      | 2069 (3.20-3.16)                                      |
| RSRZ outliers         | 180081                      | 2001 (3.20-3.16)                                      |
| RNA backbone          | 3983                        | 1138 (3.46-2.90)                                      |

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

| Mol | Chain | Length | Quality of chain                                                                                                             |
|-----|-------|--------|------------------------------------------------------------------------------------------------------------------------------|
| 1   | A     | 1733   | <div> <div>3%</div> <div> <div></div> <div>38%</div> <div>30%</div> <div>11%</div> <div>•</div> <div>20%</div> </div> </div> |
| 2   | B     | 1224   | <div> <div>3%</div> <div> <div></div> <div>43%</div> <div>33%</div> <div>11%</div> <div>•</div> <div>10%</div> </div> </div> |
| 3   | C     | 318    | <div> <div></div> <div> <div></div> <div>38%</div> <div>32%</div> <div>12%</div> <div>•</div> <div>16%</div> </div> </div>   |
| 4   | E     | 215    | <div> <div>2%</div> <div> <div></div> <div>52%</div> <div>38%</div> <div>9%</div> <div>•</div> </div> </div>                 |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 5   | F     | 155    |                  |
| 6   | H     | 146    |                  |
| 7   | I     | 122    |                  |
| 8   | J     | 70     |                  |
| 9   | K     | 120    |                  |
| 10  | L     | 70     |                  |
| 11  | R     | 11     |                  |
| 12  | T     | 28     |                  |
| 13  | N     | 14     |                  |

## 2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 29241 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     | 1395     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 10969 | 6917 | 1923 | 2068 | 61 |         |         |       |

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

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 2   | B     | 1106     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 8792  | 5568 | 1538 | 1631 | 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 polymerases I, II, and III subunit RPABC1.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 4   | E     | 214      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1752  | 1111 | 309 | 321 | 11 |         |         |       |

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 5   | F     | 84       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 679   | 434 | 115 | 127 | 3 |         |         |       |

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6   | H     | 133      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1068  | 673 | 180 | 211 | 4 |         |         |       |

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB9.

| Mol | Chain | Residues | Atoms |     |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 7   | I     | 119      | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 971   | 596 | 179 | 186 | 10 |         |         |       |

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 8   | J     | 65       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 532   | 339 | 93 | 94 | 6 |         |         |       |

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB11.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 9   | K     | 114      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 919   | 590 | 156 | 171 | 2 |         |         |       |

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 10  | L     | 46       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 363   | 224 | 72 | 63 | 4 |         |         |       |

- Molecule 11 is a RNA chain called RNA (5'-R(\*AP\*UP\*GP\*GP\*AP\*GP\*AP\*GP\*GP\*AP\*C)-3').

| Mol | Chain | Residues | Atoms |     |    |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|----|---------|---------|-------|
| 11  | R     | 11       | Total | C   | N  | O  | P  | 0       | 0       | 0     |
|     |       |          | 240   | 108 | 50 | 72 | 10 |         |         |       |

- Molecule 12 is a DNA chain called DNA (28-MER).

| Mol | Chain | Residues | Atoms |     |    |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|---------|-------|
| 12  | T     | 28       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 550   | 265 | 92 | 166 | 27 |         |         |       |

- Molecule 13 is a DNA chain called DNA (5'-D(\*GP\*TP\*GP\*GP\*TP\*TP\*AP\*TP\*GP\*GP\*GP\*TP\*AP\*G)-3').

| Mol | Chain | Residues | Atoms |     |    |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|----|---------|---------|-------|
| 13  | N     | 14       | Total | C   | N  | O  | P  | 0       | 0       | 0     |
|     |       |          | 293   | 140 | 55 | 85 | 13 |         |         |       |

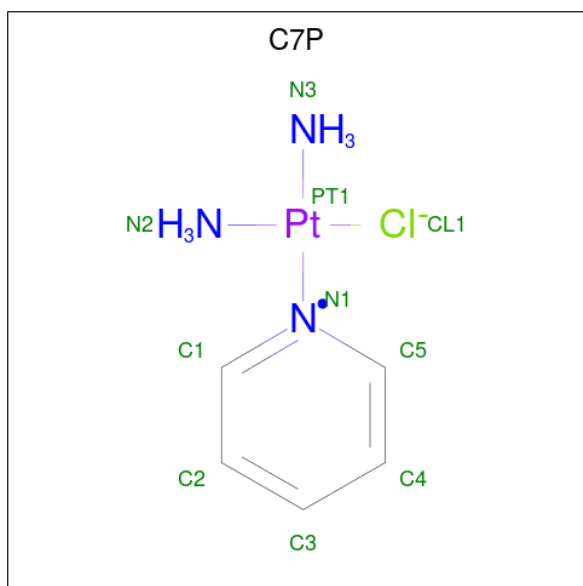
- Molecule 14 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 15  | A     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 16 is cis-diammine(pyridine)chloroplatinum(II) (CCD ID: C7P) (formula: C<sub>5</sub>H<sub>11</sub>ClN<sub>3</sub>Pt).

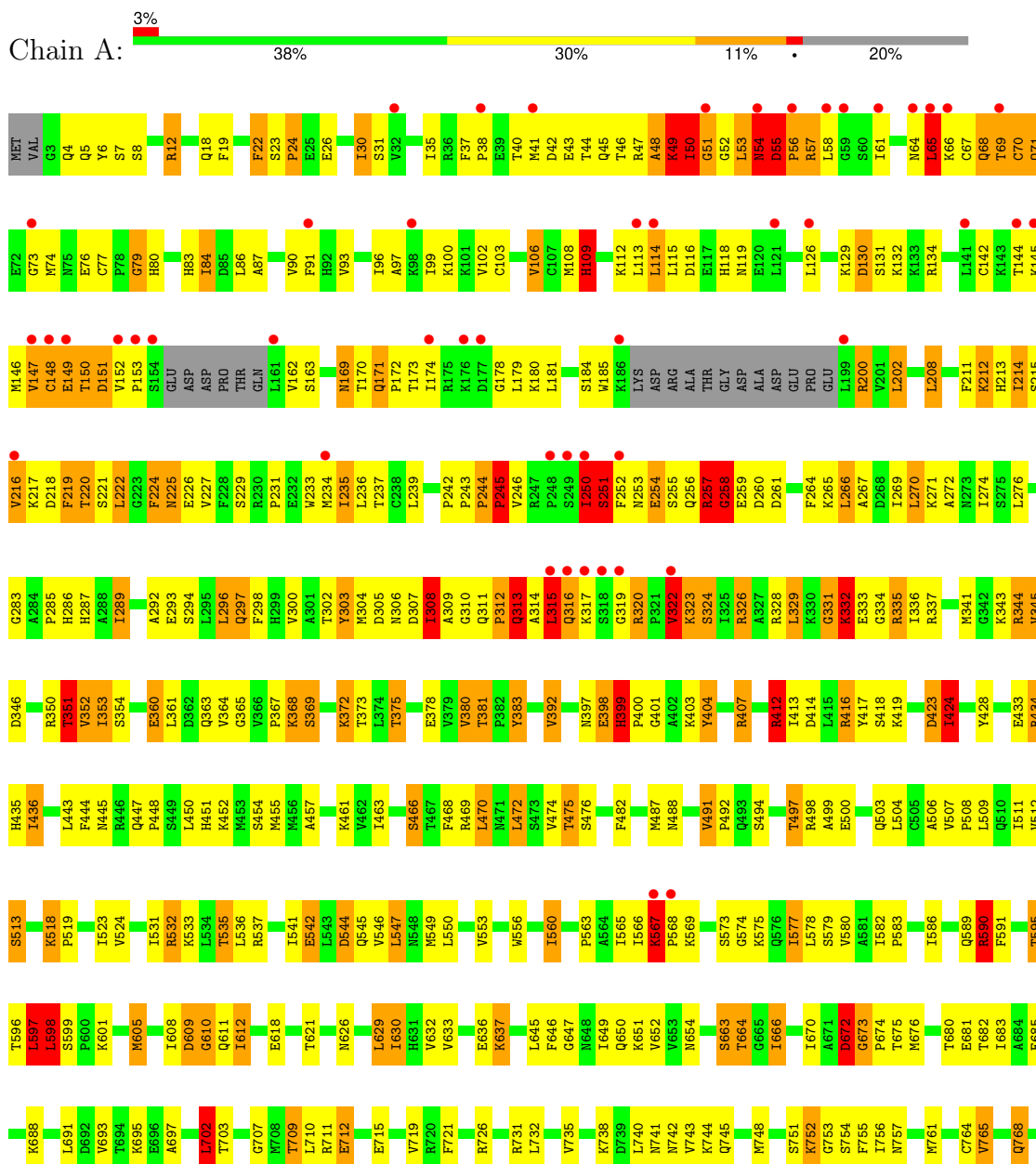


| Mol | Chain | Residues | Atoms |   |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|----|---------|---------|
| 16  | T     | 1        | Total | C | N | Pt | 0       | 0       |
|     |       |          | 9     | 5 | 3 | 1  |         |         |

### 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.

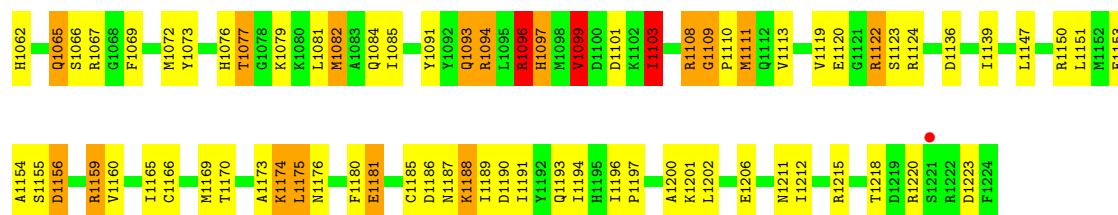
- Molecule 1: DNA-directed RNA polymerase II subunit RPB1





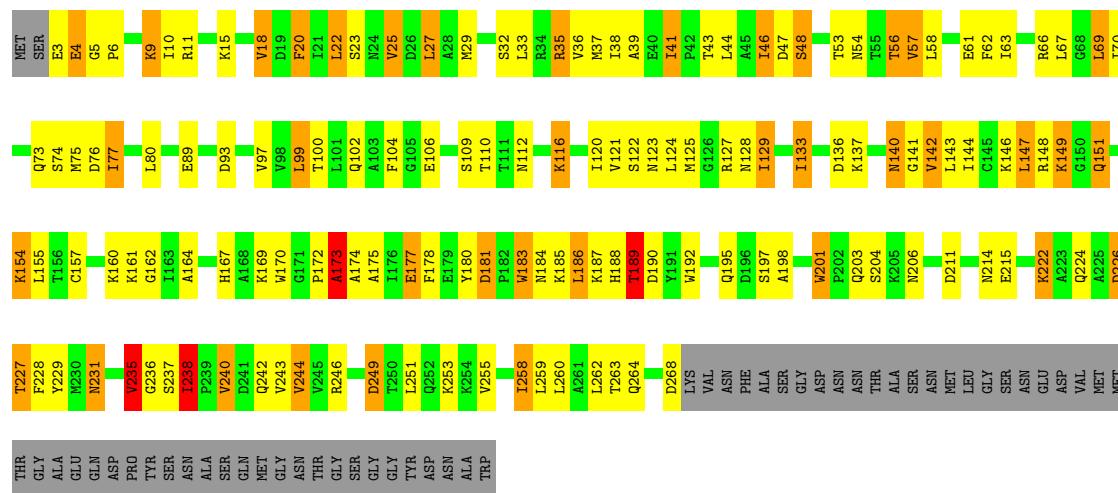






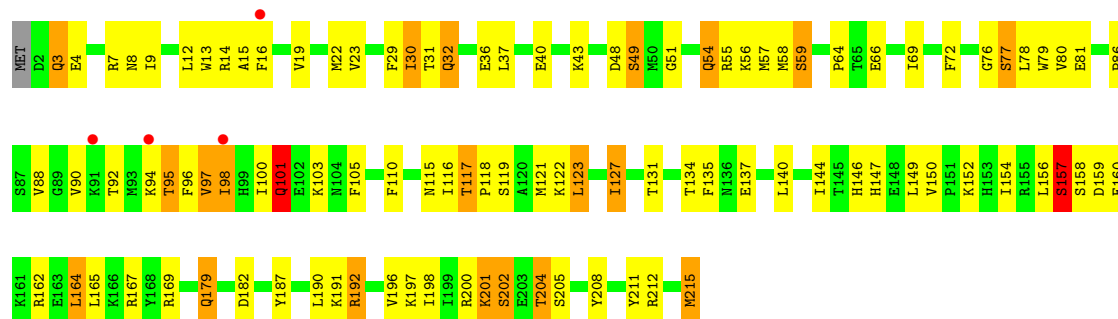
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C: 38% 32% 12% 16%



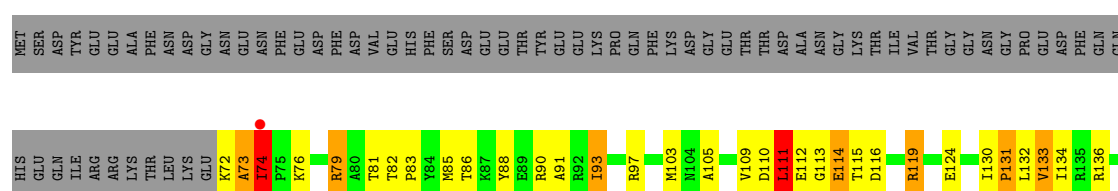
• Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E: 2% 52% 38% 9%



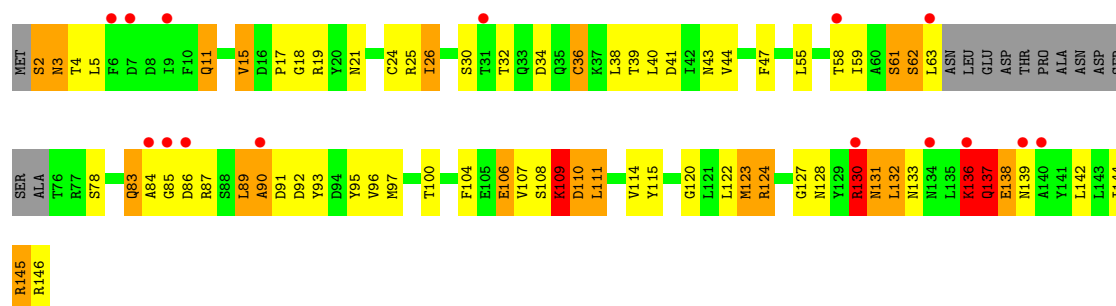
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F: 27% 21% 5% 46%

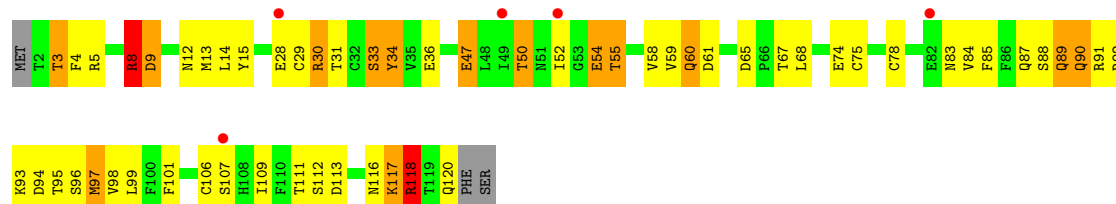




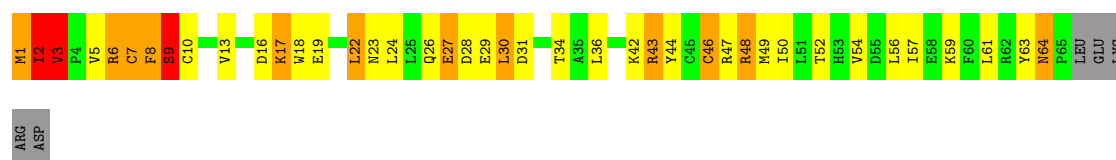
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3



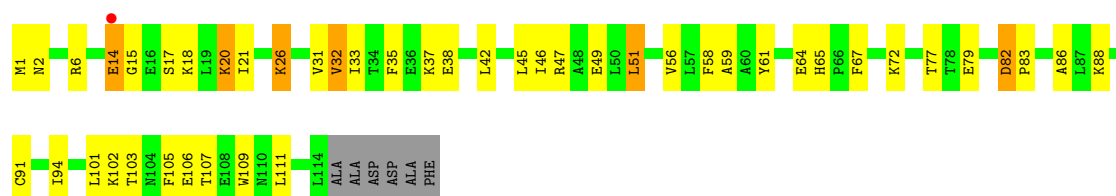
- Molecule 7: DNA-directed RNA polymerase II subunit RPB9



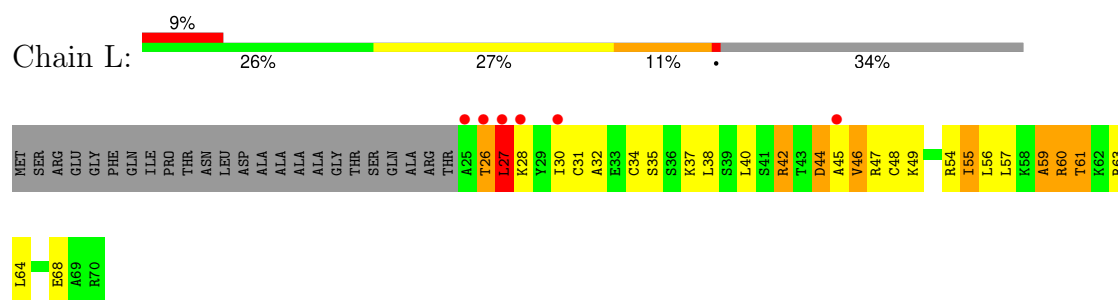
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5



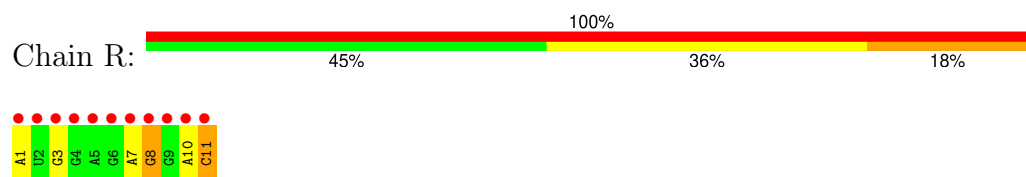
- Molecule 9: DNA-directed RNA polymerase II subunit RPB11



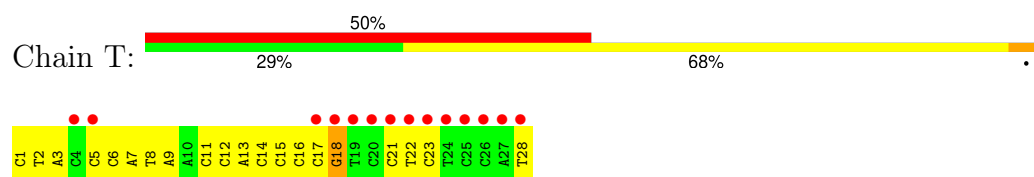
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC4



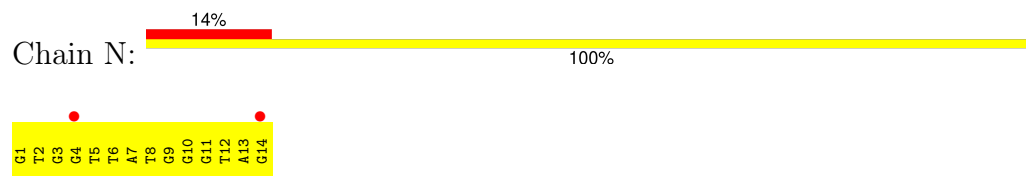
- Molecule 11: RNA (5'-R(\*AP\*UP\*GP\*GP\*AP\*GP\*AP\*GP\*GP\*AP\*C)-3')



- Molecule 12: DNA (28-MER)



- Molecule 13: DNA (5'-D(\*GP\*TP\*GP\*GP\*TP\*TP\*AP\*TP\*GP\*GP\*GP\*TP\*AP\*G)-3')



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | C 1 2 1                                                     | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 169.48Å 223.12Å 193.81Å<br>90.00° 101.47° 90.00°            | Depositor        |
| Resolution (Å)                                                          | 40.00 – 3.18<br>40.00 – 3.18                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 98.6 (40.00-3.18)<br>98.5 (40.00-3.18)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | 0.12                                                        | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.51 (at 3.18Å)                                             | Xtriage          |
| Refinement program                                                      | REFMAC 5.5.0102                                             | Depositor        |
| R, $R_{free}$                                                           | 0.207 , 0.255<br>0.222 , 0.257                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 5827 reflections (4.95%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 77.3                                                        | Xtriage          |
| Anisotropy                                                              | 0.083                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.28 , 68.6                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.92                                                        | EDS              |
| Total number of atoms                                                   | 29241                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 116.0                                                       | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% 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: C7P, MG, ZN

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

| Mol | Chain | Bond lengths |                 | Bond angles |                  |
|-----|-------|--------------|-----------------|-------------|------------------|
|     |       | RMSZ         | $\# Z  > 5$     | RMSZ        | $\# Z  > 5$      |
| 1   | A     | 0.94         | 4/11163 (0.0%)  | 1.21        | 66/15091 (0.4%)  |
| 2   | B     | 1.07         | 9/8963 (0.1%)   | 1.30        | 66/12086 (0.5%)  |
| 3   | C     | 1.03         | 2/2133 (0.1%)   | 1.26        | 11/2891 (0.4%)   |
| 4   | E     | 0.76         | 0/1788          | 1.09        | 4/2406 (0.2%)    |
| 5   | F     | 0.88         | 0/691           | 1.13        | 3/933 (0.3%)     |
| 6   | H     | 0.86         | 0/1086          | 1.15        | 7/1470 (0.5%)    |
| 7   | I     | 1.05         | 0/989           | 1.20        | 6/1331 (0.5%)    |
| 8   | J     | 1.04         | 0/541           | 1.36        | 4/727 (0.6%)     |
| 9   | K     | 0.96         | 1/937 (0.1%)    | 1.10        | 3/1265 (0.2%)    |
| 10  | L     | 1.24         | 1/365 (0.3%)    | 1.52        | 8/485 (1.6%)     |
| 11  | R     | 0.94         | 0/270           | 1.48        | 4/421 (1.0%)     |
| 12  | T     | 0.65         | 0/612           | 1.13        | 2/937 (0.2%)     |
| 13  | N     | 0.15         | 0/329           | 0.34        | 0/509            |
| All | All   | 0.97         | 17/29867 (0.1%) | 1.23        | 184/40552 (0.5%) |

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                   | 3                   |
| 2   | B     | 0                   | 5                   |
| 4   | E     | 0                   | 1                   |
| 6   | H     | 0                   | 3                   |
| 8   | J     | 0                   | 1                   |
| 10  | L     | 0                   | 1                   |
| All | All   | 0                   | 14                  |

All (17) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 2   | B     | 436  | VAL  | CA-CB | 6.80  | 1.63        | 1.54     |
| 1   | A     | 352  | VAL  | CA-CB | -6.41 | 1.47        | 1.54     |
| 2   | B     | 477  | ALA  | CA-CB | 5.99  | 1.63        | 1.53     |
| 9   | K     | 32   | VAL  | CA-CB | 5.95  | 1.60        | 1.53     |
| 2   | B     | 1165 | ILE  | CA-CB | 5.71  | 1.62        | 1.54     |
| 2   | B     | 65   | GLU  | N-CA  | 5.58  | 1.53        | 1.46     |
| 1   | A     | 315  | LEU  | CA-C  | 5.40  | 1.60        | 1.52     |
| 2   | B     | 1099 | VAL  | CA-CB | -5.29 | 1.47        | 1.54     |
| 3   | C     | 181  | ASP  | C-O   | -5.22 | 1.21        | 1.23     |
| 10  | L     | 26   | THR  | CA-CB | 5.18  | 1.62        | 1.53     |
| 2   | B     | 1007 | VAL  | C-O   | -5.15 | 1.20        | 1.24     |
| 1   | A     | 150  | THR  | CA-C  | 5.13  | 1.55        | 1.52     |
| 2   | B     | 487  | THR  | CA-C  | -5.10 | 1.46        | 1.52     |
| 1   | A     | 250  | ILE  | N-CA  | 5.10  | 1.52        | 1.46     |
| 2   | B     | 976  | ILE  | CA-C  | -5.06 | 1.46        | 1.53     |
| 2   | B     | 460  | ALA  | CA-CB | -5.05 | 1.45        | 1.53     |
| 3   | C     | 235  | VAL  | CA-CB | -5.04 | 1.48        | 1.54     |

All (184) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 2   | B     | 1109 | GLY  | CA-C-N      | 10.99  | 131.08      | 119.76   |
| 2   | B     | 1109 | GLY  | C-N-CA      | 10.99  | 131.08      | 119.76   |
| 2   | B     | 37   | PHE  | N-CA-C      | -10.77 | 96.44       | 110.33   |
| 2   | B     | 1007 | VAL  | N-CA-C      | -10.63 | 100.47      | 109.19   |
| 2   | B     | 167  | ILE  | CB-CA-C     | -10.62 | 96.51       | 111.38   |
| 2   | B     | 211  | VAL  | CB-CA-C     | -10.20 | 96.07       | 110.96   |
| 1   | A     | 598  | LEU  | N-CA-C      | -9.53  | 100.15      | 114.64   |
| 1   | A     | 513  | SER  | CA-C-N      | 9.52   | 129.27      | 119.56   |
| 1   | A     | 513  | SER  | C-N-CA      | 9.52   | 129.27      | 119.56   |
| 2   | B     | 711  | GLU  | CA-C-N      | -9.42  | 110.68      | 120.85   |
| 2   | B     | 711  | GLU  | C-N-CA      | -9.42  | 110.68      | 120.85   |
| 5   | F     | 74   | ILE  | CA-C-N      | 9.39   | 131.57      | 119.84   |
| 5   | F     | 74   | ILE  | C-N-CA      | 9.39   | 131.57      | 119.84   |
| 1   | A     | 399  | HIS  | CA-C-N      | -8.99  | 108.60      | 119.84   |
| 1   | A     | 399  | HIS  | C-N-CA      | -8.99  | 108.60      | 119.84   |
| 11  | R     | 8    | G    | C4'-C3'-C2' | -8.88  | 93.72       | 102.60   |
| 2   | B     | 363  | HIS  | N-CA-C      | -8.62  | 99.80       | 110.41   |
| 1   | A     | 331  | GLY  | N-CA-C      | 8.56   | 123.50      | 112.54   |
| 2   | B     | 361  | LEU  | CA-C-N      | 8.45   | 128.14      | 119.19   |
| 2   | B     | 361  | LEU  | C-N-CA      | 8.45   | 128.14      | 119.19   |
| 2   | B     | 780  | VAL  | CB-CA-C     | -8.16  | 102.46      | 111.35   |
| 2   | B     | 1099 | VAL  | CB-CA-C     | -7.96  | 101.39      | 112.14   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 2   | B     | 714  | GLU  | N-CA-C     | 7.89  | 122.07      | 108.02   |
| 2   | B     | 1156 | ASP  | N-CA-C     | 7.71  | 122.44      | 112.26   |
| 1   | A     | 149  | GLU  | N-CA-C     | 7.60  | 119.25      | 108.00   |
| 9   | K     | 64   | GLU  | N-CA-C     | 7.42  | 119.37      | 111.28   |
| 4   | E     | 117  | THR  | CA-C-N     | 7.36  | 129.04      | 119.84   |
| 4   | E     | 117  | THR  | C-N-CA     | 7.36  | 129.04      | 119.84   |
| 2   | B     | 739  | THR  | N-CA-C     | -7.34 | 105.50      | 114.75   |
| 6   | H     | 36   | CYS  | N-CA-C     | 7.33  | 120.36      | 107.61   |
| 12  | T     | 18   | DG   | N9-C1'-C2' | -7.30 | 102.54      | 113.50   |
| 8   | J     | 3    | VAL  | CA-C-N     | 7.28  | 127.71      | 119.93   |
| 8   | J     | 3    | VAL  | C-N-CA     | 7.28  | 127.71      | 119.93   |
| 1   | A     | 973  | ILE  | N-CA-C     | 7.26  | 118.28      | 108.11   |
| 7   | I     | 84   | VAL  | N-CA-C     | -7.25 | 98.05       | 108.42   |
| 1   | A     | 1444 | MET  | N-CA-C     | 7.25  | 117.59      | 108.45   |
| 6   | H     | 84   | ALA  | N-CA-C     | 7.25  | 120.61      | 111.69   |
| 1   | A     | 566  | ILE  | CB-CA-C    | -7.20 | 105.59      | 111.71   |
| 2   | B     | 780  | VAL  | N-CA-C     | 7.19  | 117.75      | 108.12   |
| 10  | L     | 64   | LEU  | N-CA-C     | 7.17  | 122.00      | 109.96   |
| 1   | A     | 1392 | SER  | N-CA-C     | 7.09  | 119.58      | 110.65   |
| 8   | J     | 3    | VAL  | CB-CA-C    | -7.07 | 98.50       | 111.36   |
| 1   | A     | 626  | ASN  | N-CA-C     | 7.04  | 118.85      | 111.03   |
| 2   | B     | 866  | TYR  | N-CA-C     | 6.89  | 125.47      | 110.80   |
| 4   | E     | 115  | ASN  | N-CA-C     | 6.89  | 118.66      | 108.60   |
| 1   | A     | 1207 | LEU  | N-CA-C     | 6.86  | 119.69      | 108.52   |
| 10  | L     | 63   | ARG  | CA-C-N     | -6.84 | 111.96      | 122.09   |
| 10  | L     | 63   | ARG  | C-N-CA     | -6.84 | 111.96      | 122.09   |
| 2   | B     | 478  | GLY  | N-CA-C     | -6.83 | 96.98       | 113.18   |
| 2   | B     | 636  | PRO  | CA-C-N     | 6.83  | 134.00      | 121.70   |
| 2   | B     | 636  | PRO  | C-N-CA     | 6.83  | 134.00      | 121.70   |
| 1   | A     | 229  | SER  | N-CA-C     | 6.71  | 118.44      | 107.23   |
| 1   | A     | 582  | ILE  | CA-C-N     | 6.70  | 128.21      | 119.84   |
| 1   | A     | 582  | ILE  | C-N-CA     | 6.70  | 128.21      | 119.84   |
| 2   | B     | 1096 | ARG  | N-CA-C     | -6.65 | 101.72      | 110.43   |
| 1   | A     | 921  | GLY  | N-CA-C     | -6.64 | 105.56      | 111.67   |
| 1   | A     | 595  | THR  | N-CA-C     | 6.60  | 120.06      | 110.42   |
| 2   | B     | 382  | ILE  | CB-CA-C    | -6.59 | 103.40      | 112.04   |
| 1   | A     | 450  | LEU  | N-CA-C     | 6.52  | 120.44      | 112.23   |
| 1   | A     | 999  | VAL  | N-CA-C     | -6.51 | 106.47      | 111.62   |
| 2   | B     | 610  | ASN  | CA-C-N     | 6.50  | 127.96      | 119.84   |
| 2   | B     | 610  | ASN  | C-N-CA     | 6.50  | 127.96      | 119.84   |
| 2   | B     | 798  | TYR  | CA-C-N     | 6.46  | 127.92      | 119.84   |
| 2   | B     | 798  | TYR  | C-N-CA     | 6.46  | 127.92      | 119.84   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | A     | 412  | ARG  | N-CA-C      | 6.45  | 117.64      | 108.54   |
| 2   | B     | 711  | GLU  | N-CA-C      | 6.44  | 124.05      | 109.81   |
| 10  | L     | 27   | LEU  | N-CA-C      | 6.43  | 120.13      | 109.46   |
| 1   | A     | 200  | ARG  | N-CA-C      | 6.42  | 118.94      | 109.69   |
| 1   | A     | 597  | LEU  | CB-CA-C     | -6.42 | 97.65       | 110.42   |
| 2   | B     | 1007 | VAL  | CB-CA-C     | 6.38  | 115.58      | 109.33   |
| 2   | B     | 698  | GLU  | N-CA-C      | -6.37 | 104.39      | 111.71   |
| 7   | I     | 8    | ARG  | N-CA-C      | -6.35 | 101.08      | 110.48   |
| 1   | A     | 345  | VAL  | N-CA-C      | 6.34  | 119.41      | 108.95   |
| 1   | A     | 360  | GLU  | N-CA-C      | -6.34 | 102.61      | 110.41   |
| 2   | B     | 982  | SER  | N-CA-C      | -6.31 | 99.94       | 109.79   |
| 1   | A     | 491  | VAL  | CA-C-N      | 6.30  | 126.06      | 119.76   |
| 1   | A     | 491  | VAL  | C-N-CA      | 6.30  | 126.06      | 119.76   |
| 1   | A     | 673  | GLY  | CA-C-N      | 6.29  | 127.71      | 119.84   |
| 1   | A     | 673  | GLY  | C-N-CA      | 6.29  | 127.71      | 119.84   |
| 2   | B     | 195  | CYS  | CA-C-N      | -6.26 | 114.44      | 120.83   |
| 2   | B     | 195  | CYS  | C-N-CA      | -6.26 | 114.44      | 120.83   |
| 1   | A     | 1332 | PHE  | N-CA-C      | -6.25 | 105.69      | 113.38   |
| 1   | A     | 1319 | VAL  | CA-C-N      | 6.21  | 126.18      | 120.03   |
| 1   | A     | 1319 | VAL  | C-N-CA      | 6.21  | 126.18      | 120.03   |
| 1   | A     | 524  | VAL  | N-CA-C      | 6.19  | 118.84      | 108.81   |
| 10  | L     | 63   | ARG  | N-CA-C      | -6.17 | 101.05      | 110.30   |
| 1   | A     | 821  | ARG  | N-CA-C      | -6.13 | 104.71      | 111.82   |
| 6   | H     | 145  | ARG  | N-CA-C      | 6.12  | 118.65      | 108.13   |
| 1   | A     | 313  | GLN  | N-CA-C      | 6.06  | 123.70      | 110.80   |
| 2   | B     | 751  | VAL  | N-CA-C      | 6.06  | 121.94      | 109.34   |
| 7   | I     | 31   | THR  | N-CA-C      | -6.04 | 105.93      | 113.55   |
| 1   | A     | 598  | LEU  | N-CA-CB     | 6.03  | 120.65      | 111.06   |
| 1   | A     | 993  | LEU  | N-CA-C      | -5.97 | 103.54      | 111.24   |
| 3   | C     | 238  | ILE  | CA-C-N      | -5.96 | 113.82      | 120.14   |
| 3   | C     | 238  | ILE  | C-N-CA      | -5.96 | 113.82      | 120.14   |
| 1   | A     | 351  | THR  | CB-CA-C     | -5.92 | 99.71       | 111.91   |
| 10  | L     | 68   | GLU  | N-CA-C      | -5.92 | 101.52      | 110.28   |
| 1   | A     | 151  | ASP  | N-CA-C      | 5.91  | 116.04      | 108.24   |
| 3   | C     | 198  | ALA  | N-CA-C      | 5.91  | 117.72      | 111.28   |
| 1   | A     | 886  | ILE  | N-CA-C      | 5.88  | 119.31      | 111.44   |
| 1   | A     | 672  | ASP  | N-CA-C      | 5.87  | 117.90      | 110.33   |
| 2   | B     | 184  | ALA  | N-CA-C      | 5.86  | 119.45      | 110.20   |
| 6   | H     | 137  | GLN  | N-CA-C      | 5.85  | 119.21      | 110.14   |
| 11  | R     | 10   | A    | O4'-C1'-C2' | -5.82 | 101.78      | 107.60   |
| 2   | B     | 616  | ILE  | CB-CA-C     | -5.75 | 104.71      | 111.09   |
| 2   | B     | 165  | VAL  | N-CA-C      | 5.73  | 115.91      | 108.35   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | B     | 883  | LEU  | CA-CB-CG    | 5.70  | 136.23      | 116.30   |
| 2   | B     | 1056 | SER  | N-CA-C      | 5.67  | 118.20      | 111.33   |
| 11  | R     | 10   | A    | C4'-C3'-C2' | -5.67 | 96.93       | 102.60   |
| 1   | A     | 885  | THR  | N-CA-C      | -5.65 | 105.88      | 112.89   |
| 2   | B     | 911  | ILE  | CB-CA-C     | -5.64 | 104.68      | 112.24   |
| 9   | K     | 82   | ASP  | CA-C-N      | 5.63  | 126.88      | 119.84   |
| 9   | K     | 82   | ASP  | C-N-CA      | 5.63  | 126.88      | 119.84   |
| 2   | B     | 99   | LYS  | N-CA-C      | -5.59 | 102.00      | 110.39   |
| 1   | A     | 74   | MET  | N-CA-C      | -5.56 | 105.11      | 113.89   |
| 1   | A     | 1237 | ILE  | N-CA-C      | 5.55  | 116.12      | 108.12   |
| 1   | A     | 590  | ARG  | N-CA-C      | 5.53  | 122.57      | 110.80   |
| 2   | B     | 66   | ASP  | N-CA-C      | -5.53 | 105.26      | 111.28   |
| 2   | B     | 606  | LYS  | N-CA-C      | -5.49 | 106.30      | 114.64   |
| 1   | A     | 250  | ILE  | N-CA-C      | 5.48  | 120.74      | 109.34   |
| 1   | A     | 827  | THR  | N-CA-C      | -5.47 | 106.28      | 113.12   |
| 2   | B     | 871  | THR  | CB-CA-C     | -5.46 | 104.66      | 111.43   |
| 1   | A     | 239  | LEU  | CA-C-N      | 5.45  | 125.37      | 119.76   |
| 1   | A     | 239  | LEU  | C-N-CA      | 5.45  | 125.37      | 119.76   |
| 3   | C     | 104  | PHE  | N-CA-C      | -5.45 | 100.14      | 109.24   |
| 1   | A     | 916  | GLY  | N-CA-C      | 5.44  | 119.26      | 112.73   |
| 10  | L     | 32   | ALA  | N-CA-C      | 5.42  | 117.00      | 111.14   |
| 3   | C     | 173  | ALA  | N-CA-C      | 5.42  | 122.33      | 110.80   |
| 3   | C     | 20   | PHE  | N-CA-C      | 5.42  | 118.09      | 109.81   |
| 11  | R     | 11   | C    | C4'-C3'-C2' | -5.39 | 97.21       | 102.60   |
| 6   | H     | 109  | LYS  | CA-C-N      | 5.39  | 131.40      | 121.70   |
| 6   | H     | 109  | LYS  | C-N-CA      | 5.39  | 131.40      | 121.70   |
| 7   | I     | 78   | CYS  | CB-CA-C     | -5.39 | 100.84      | 110.70   |
| 3   | C     | 201  | TRP  | CA-C-N      | -5.36 | 113.14      | 119.84   |
| 3   | C     | 201  | TRP  | C-N-CA      | -5.36 | 113.14      | 119.84   |
| 2   | B     | 1055 | ILE  | N-CA-C      | -5.36 | 105.39      | 110.42   |
| 12  | T     | 18   | DG   | N3-C4-C5    | -5.36 | 120.37      | 128.40   |
| 1   | A     | 332  | LYS  | N-CA-C      | -5.33 | 99.45       | 110.80   |
| 3   | C     | 155  | LEU  | N-CA-C      | 5.32  | 115.30      | 108.34   |
| 8   | J     | 50   | ILE  | CB-CA-C     | -5.32 | 105.44      | 111.55   |
| 2   | B     | 779  | GLY  | N-CA-C      | -5.31 | 103.63      | 110.69   |
| 1   | A     | 407  | ARG  | N-CA-C      | 5.30  | 118.58      | 110.36   |
| 1   | A     | 919  | ILE  | CB-CA-C     | 5.29  | 116.38      | 111.30   |
| 2   | B     | 593  | PRO  | N-CA-C      | -5.28 | 106.84      | 114.18   |
| 1   | A     | 56   | PRO  | N-CA-C      | -5.26 | 101.62      | 112.47   |
| 1   | A     | 251  | SER  | N-CA-C      | 5.25  | 121.98      | 110.80   |
| 2   | B     | 276  | ILE  | N-CA-C      | 5.23  | 115.38      | 107.80   |
| 2   | B     | 767  | ASN  | N-CA-C      | -5.23 | 105.58      | 111.28   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1   | A     | 1412 | ALA  | N-CA-C   | -5.22 | 106.41      | 112.89   |
| 2   | B     | 422  | LYS  | N-CA-C   | -5.22 | 105.27      | 111.69   |
| 1   | A     | 1406 | VAL  | N-CA-C   | 5.21  | 116.68      | 111.00   |
| 1   | A     | 1403 | GLU  | N-CA-C   | 5.20  | 121.88      | 110.80   |
| 2   | B     | 1009 | ASP  | N-CA-C   | -5.20 | 106.44      | 112.89   |
| 7   | I     | 85   | PHE  | N-CA-C   | 5.19  | 116.69      | 108.96   |
| 7   | I     | 118  | ARG  | N-CA-C   | 5.18  | 116.67      | 108.96   |
| 1   | A     | 171  | GLN  | CA-C-N   | 5.14  | 125.12      | 120.03   |
| 1   | A     | 171  | GLN  | C-N-CA   | 5.14  | 125.12      | 120.03   |
| 2   | B     | 609  | ILE  | N-CA-C   | -5.14 | 101.08      | 108.48   |
| 3   | C     | 189  | THR  | CB-CA-C  | -5.13 | 101.23      | 110.36   |
| 3   | C     | 243  | VAL  | N-CA-CB  | 5.11  | 115.98      | 110.62   |
| 2   | B     | 168  | GLY  | N-CA-C   | 5.09  | 125.25      | 113.18   |
| 10  | L     | 40   | LEU  | N-CA-C   | 5.09  | 117.72      | 110.24   |
| 2   | B     | 1096 | ARG  | CA-C-O   | -5.09 | 116.27      | 121.87   |
| 6   | H     | 85   | GLY  | N-CA-C   | -5.08 | 107.65      | 115.73   |
| 2   | B     | 472  | ALA  | N-CA-C   | -5.08 | 105.02      | 111.11   |
| 1   | A     | 315  | LEU  | CA-C-N   | 5.08  | 130.84      | 121.70   |
| 1   | A     | 315  | LEU  | C-N-CA   | 5.08  | 130.84      | 121.70   |
| 2   | B     | 640  | VAL  | CB-CA-C  | -5.07 | 106.11      | 111.23   |
| 5   | F     | 105  | ALA  | N-CA-C   | -5.07 | 102.89      | 110.20   |
| 2   | B     | 902  | GLY  | N-CA-C   | 5.07  | 118.81      | 112.73   |
| 1   | A     | 702  | LEU  | CA-CB-CG | 5.06  | 134.02      | 116.30   |
| 4   | E     | 157  | SER  | N-CA-C   | 5.06  | 117.59      | 108.48   |
| 1   | A     | 399  | HIS  | N-CA-CB  | 5.06  | 119.37      | 110.37   |
| 2   | B     | 574  | SER  | CA-C-N   | 5.06  | 125.13      | 119.87   |
| 2   | B     | 574  | SER  | C-N-CA   | 5.06  | 125.13      | 119.87   |
| 2   | B     | 900  | ALA  | CA-C-N   | 5.05  | 126.15      | 119.84   |
| 2   | B     | 900  | ALA  | C-N-CA   | 5.05  | 126.15      | 119.84   |
| 2   | B     | 918  | ILE  | N-CA-C   | 5.04  | 115.11      | 107.75   |
| 1   | A     | 743  | VAL  | N-CA-C   | -5.04 | 105.48      | 110.62   |
| 2   | B     | 791  | THR  | N-CA-C   | -5.03 | 102.61      | 110.10   |
| 2   | B     | 971  | THR  | N-CA-C   | -5.03 | 101.52      | 109.76   |
| 2   | B     | 1001 | PHE  | N-CA-C   | 5.02  | 117.63      | 109.24   |
| 1   | A     | 258  | GLY  | N-CA-C   | 5.02  | 125.07      | 113.18   |
| 2   | B     | 1022 | THR  | CB-CA-C  | 5.02  | 119.12      | 111.70   |

There are no chirality outliers.

All (14) planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group   |
|-----|-------|------|------|---------|
| 1   | A     | 1391 | ARG  | Peptide |

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| Mol | Chain | Res  | Type | Group   |
|-----|-------|------|------|---------|
| 1   | A     | 252  | PHE  | Peptide |
| 1   | A     | 71   | GLN  | Peptide |
| 2   | B     | 1076 | HIS  | Peptide |
| 2   | B     | 245  | GLU  | Peptide |
| 2   | B     | 265  | SER  | Peptide |
| 2   | B     | 644  | GLU  | Peptide |
| 2   | B     | 882  | THR  | Peptide |
| 4   | E     | 157  | SER  | Peptide |
| 6   | H     | 136  | LYS  | Peptide |
| 6   | H     | 138  | GLU  | Peptide |
| 6   | H     | 61   | SER  | Peptide |
| 8   | J     | 64   | ASN  | Peptide |
| 10  | L     | 42   | ARG  | Peptide |

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 10969 | 0        | 11071    | 613     | 0            |
| 2   | B     | 8792  | 0        | 8824     | 479     | 0            |
| 3   | C     | 2095  | 0        | 2051     | 119     | 0            |
| 4   | E     | 1752  | 0        | 1776     | 67      | 0            |
| 5   | F     | 679   | 0        | 701      | 27      | 0            |
| 6   | H     | 1068  | 0        | 1040     | 74      | 0            |
| 7   | I     | 971   | 0        | 927      | 42      | 0            |
| 8   | J     | 532   | 0        | 543      | 43      | 0            |
| 9   | K     | 919   | 0        | 929      | 25      | 0            |
| 10  | L     | 363   | 0        | 387      | 13      | 0            |
| 11  | R     | 240   | 0        | 122      | 2       | 0            |
| 12  | T     | 550   | 0        | 316      | 66      | 0            |
| 13  | N     | 293   | 0        | 161      | 75      | 0            |
| 14  | A     | 2     | 0        | 0        | 0       | 0            |
| 14  | B     | 1     | 0        | 0        | 0       | 0            |
| 14  | C     | 1     | 0        | 0        | 0       | 0            |
| 14  | I     | 2     | 0        | 0        | 0       | 0            |
| 14  | J     | 1     | 0        | 0        | 0       | 0            |
| 14  | L     | 1     | 0        | 0        | 0       | 0            |
| 15  | A     | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 16  | T     | 9     | 0        | 5        | 0       | 0            |
| All | All   | 29241 | 0        | 28853    | 1478    | 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 26.

All (1478) 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) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:T:2:DT:H2''    | 12:T:3:DA:C5'     | 1.47                     | 1.44              |
| 12:T:2:DT:C2'     | 12:T:3:DA:H5'     | 1.42                     | 1.43              |
| 1:A:567:LYS:CG    | 1:A:568:PRO:HD2   | 1.60                     | 1.30              |
| 13:N:1:DG:H2''    | 13:N:2:DT:C7      | 1.71                     | 1.19              |
| 12:T:8:DT:H2''    | 12:T:9:DA:C8      | 1.79                     | 1.18              |
| 2:B:747:MET:HE3   | 2:B:747:MET:HA    | 1.23                     | 1.18              |
| 1:A:567:LYS:HB3   | 6:H:96:VAL:H      | 1.03                     | 1.17              |
| 1:A:567:LYS:HG3   | 1:A:568:PRO:CD    | 1.78                     | 1.13              |
| 13:N:1:DG:H2''    | 13:N:2:DT:C5      | 1.84                     | 1.12              |
| 1:A:320:ARG:HG3   | 1:A:320:ARG:HH11  | 1.12                     | 1.11              |
| 5:F:93:ILE:HD11   | 5:F:134:ILE:HD11  | 1.28                     | 1.10              |
| 1:A:423:ASP:O     | 1:A:424:ILE:HB    | 1.50                     | 1.09              |
| 12:T:1:DC:H2''    | 12:T:2:DT:OP2     | 1.45                     | 1.08              |
| 12:T:7:DA:C2      | 12:T:8:DT:C4      | 2.41                     | 1.07              |
| 1:A:1116:LEU:HD13 | 1:A:1329:THR:HG23 | 1.29                     | 1.06              |
| 1:A:630:ILE:HD12  | 1:A:630:ILE:H     | 1.21                     | 1.06              |
| 1:A:567:LYS:HB3   | 6:H:96:VAL:N      | 1.72                     | 1.05              |
| 1:A:315:LEU:HB3   | 1:A:316:GLN:HA    | 1.39                     | 1.04              |
| 2:B:254:LEU:HD23  | 2:B:381:MET:HE1   | 1.33                     | 1.04              |
| 1:A:214:ILE:HG22  | 1:A:215:SER:H     | 1.21                     | 1.04              |
| 1:A:53:LEU:HD23   | 1:A:54:ASN:H      | 1.19                     | 1.02              |
| 2:B:541:LEU:HD12  | 2:B:747:MET:HE1   | 1.38                     | 1.01              |
| 1:A:412:ARG:HG3   | 1:A:412:ARG:HH11  | 1.22                     | 1.01              |
| 13:N:4:DG:H1'     | 13:N:5:DT:H5''    | 1.44                     | 1.00              |
| 2:B:25:ILE:HG23   | 2:B:29:ASP:HB2    | 1.43                     | 0.99              |
| 1:A:344:ARG:HG3   | 1:A:344:ARG:HH11  | 1.23                     | 0.99              |
| 2:B:485:ARG:HG2   | 2:B:485:ARG:HH11  | 1.27                     | 0.99              |
| 1:A:503:GLN:NE2   | 5:F:90:ARG:HH21   | 1.58                     | 0.99              |
| 1:A:853:ASP:OD1   | 1:A:855:THR:HB    | 1.63                     | 0.98              |
| 1:A:855:THR:HG21  | 1:A:857:ARG:HE    | 1.27                     | 0.98              |
| 13:N:4:DG:C2      | 13:N:5:DT:C2      | 2.51                     | 0.98              |
| 4:E:90:VAL:HG23   | 4:E:123:LEU:HD21  | 1.47                     | 0.96              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:T:2:DT:H2'     | 12:T:3:DA:C8      | 2.00                     | 0.96              |
| 3:C:73:GLN:HE21   | 3:C:75:MET:H      | 0.99                     | 0.95              |
| 13:N:4:DG:N2      | 13:N:5:DT:C2      | 2.33                     | 0.95              |
| 2:B:744:HIS:CD2   | 2:B:746:SER:H     | 1.85                     | 0.95              |
| 2:B:744:HIS:HD2   | 2:B:746:SER:H     | 1.02                     | 0.95              |
| 4:E:15:ALA:O      | 4:E:19:VAL:HG23   | 1.67                     | 0.94              |
| 7:I:111:THR:HG22  | 7:I:113:ASP:H     | 1.32                     | 0.94              |
| 1:A:961:ARG:HH11  | 1:A:961:ARG:HB3   | 1.30                     | 0.94              |
| 1:A:1364:ASN:ND2  | 1:A:1366:ARG:HG2  | 1.82                     | 0.94              |
| 13:N:3:DG:H2''    | 13:N:4:DG:OP2     | 1.67                     | 0.94              |
| 13:N:1:DG:C2'     | 13:N:2:DT:C7      | 2.46                     | 0.93              |
| 3:C:222:LYS:HA    | 3:C:222:LYS:HE3   | 1.47                     | 0.93              |
| 1:A:1116:LEU:HD13 | 1:A:1329:THR:CG2  | 1.98                     | 0.93              |
| 1:A:780:VAL:HG22  | 2:B:699:GLU:OE2   | 1.70                     | 0.92              |
| 2:B:423:LYS:O     | 2:B:427:ASP:HB2   | 1.70                     | 0.91              |
| 2:B:175:ARG:HH11  | 2:B:175:ARG:HG3   | 1.35                     | 0.91              |
| 2:B:801:LYS:O     | 8:J:52:THR:HG23   | 1.69                     | 0.91              |
| 2:B:363:HIS:O     | 2:B:364:ILE:HB    | 1.69                     | 0.91              |
| 1:A:1029:ARG:HH11 | 1:A:1029:ARG:CG   | 1.83                     | 0.90              |
| 13:N:4:DG:C6      | 13:N:5:DT:C4      | 2.59                     | 0.90              |
| 13:N:13:DA:H8     | 13:N:13:DA:OP2    | 1.54                     | 0.90              |
| 1:A:503:GLN:HE21  | 5:F:90:ARG:HH21   | 1.18                     | 0.90              |
| 12:T:8:DT:C2'     | 12:T:9:DA:C8      | 2.54                     | 0.90              |
| 12:T:6:DC:C2      | 12:T:7:DA:N7      | 2.40                     | 0.89              |
| 1:A:351:THR:HG23  | 2:B:1103:ILE:HG12 | 1.54                     | 0.89              |
| 1:A:380:VAL:HG12  | 1:A:428:TYR:HA    | 1.54                     | 0.89              |
| 2:B:175:ARG:HH11  | 2:B:175:ARG:CG    | 1.86                     | 0.88              |
| 1:A:313:GLN:HB2   | 1:A:322:VAL:HG22  | 1.54                     | 0.88              |
| 1:A:436:ILE:HD11  | 1:A:491:VAL:HG11  | 1.53                     | 0.88              |
| 2:B:260:GLY:O     | 2:B:267:ARG:HD3   | 1.72                     | 0.88              |
| 12:T:7:DA:C2      | 12:T:8:DT:N3      | 2.42                     | 0.88              |
| 6:H:40:LEU:HD13   | 6:H:123:MET:HB2   | 1.55                     | 0.88              |
| 10:L:47:ARG:NH1   | 10:L:54:ARG:HE    | 1.70                     | 0.87              |
| 1:A:783:THR:HG21  | 1:A:796:SER:O     | 1.75                     | 0.87              |
| 8:J:44:TYR:HA     | 8:J:47:ARG:HB3    | 1.55                     | 0.87              |
| 1:A:567:LYS:HG3   | 1:A:568:PRO:HD2   | 0.89                     | 0.87              |
| 1:A:412:ARG:HH11  | 1:A:412:ARG:CG    | 1.87                     | 0.87              |
| 2:B:986:GLN:NE2   | 2:B:1022:THR:HG21 | 1.90                     | 0.87              |
| 12:T:8:DT:H2''    | 12:T:9:DA:H8      | 1.39                     | 0.87              |
| 1:A:532:ARG:HH11  | 1:A:532:ARG:CG    | 1.88                     | 0.86              |
| 1:A:171:GLN:HG2   | 1:A:172:PRO:HD2   | 1.56                     | 0.86              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:N:6:DT:C2      | 13:N:7:DA:C5      | 2.63                     | 0.86              |
| 2:B:175:ARG:HG3   | 2:B:175:ARG:NH1   | 1.90                     | 0.86              |
| 1:A:1161:THR:HG22 | 1:A:1163:ILE:H    | 1.38                     | 0.86              |
| 13:N:5:DT:H2''    | 13:N:6:DT:C6      | 2.11                     | 0.86              |
| 6:H:89:LEU:HD23   | 6:H:92:ASP:H      | 1.40                     | 0.85              |
| 2:B:635:ARG:HG2   | 2:B:635:ARG:O     | 1.76                     | 0.85              |
| 2:B:63:ILE:O      | 2:B:67:SER:HB2    | 1.77                     | 0.85              |
| 1:A:901:LEU:H     | 1:A:926:GLN:HE21  | 1.20                     | 0.85              |
| 13:N:5:DT:H2'     | 13:N:6:DT:H71     | 1.57                     | 0.85              |
| 1:A:630:ILE:HD12  | 1:A:630:ILE:N     | 1.92                     | 0.85              |
| 1:A:567:LYS:CB    | 1:A:568:PRO:CD    | 2.55                     | 0.84              |
| 12:T:6:DC:C2      | 12:T:7:DA:C8      | 2.66                     | 0.84              |
| 13:N:13:DA:OP2    | 13:N:13:DA:C8     | 2.30                     | 0.84              |
| 2:B:120:ARG:HD2   | 2:B:955:THR:HG21  | 1.57                     | 0.84              |
| 2:B:254:LEU:CD2   | 2:B:381:MET:HE1   | 2.06                     | 0.84              |
| 1:A:412:ARG:HG3   | 1:A:412:ARG:NH1   | 1.88                     | 0.84              |
| 2:B:1051:THR:HG22 | 2:B:1054:GLY:H    | 1.42                     | 0.84              |
| 13:N:12:DT:H2''   | 13:N:13:DA:OP2    | 1.75                     | 0.84              |
| 1:A:567:LYS:CG    | 1:A:568:PRO:CD    | 2.47                     | 0.83              |
| 12:T:6:DC:H2''    | 12:T:7:DA:OP2     | 1.77                     | 0.83              |
| 3:C:54:ASN:OD1    | 3:C:56:THR:HB     | 1.79                     | 0.83              |
| 2:B:822:ASN:HD22  | 8:J:52:THR:HG21   | 1.43                     | 0.83              |
| 1:A:567:LYS:HB2   | 1:A:568:PRO:CD    | 2.09                     | 0.82              |
| 1:A:821:ARG:O     | 1:A:825:ILE:HG12  | 1.79                     | 0.82              |
| 1:A:902:LEU:HD11  | 1:A:926:GLN:HG3   | 1.60                     | 0.82              |
| 2:B:1002:THR:HG23 | 2:B:1004:GLU:H    | 1.44                     | 0.82              |
| 8:J:10:CYS:SG     | 8:J:46:CYS:SG     | 2.77                     | 0.82              |
| 1:A:244:PRO:HB2   | 1:A:245:PRO:HD3   | 1.62                     | 0.82              |
| 1:A:50:ILE:HG22   | 1:A:52:GLY:H      | 1.44                     | 0.82              |
| 1:A:1116:LEU:CD1  | 1:A:1329:THR:HG23 | 2.08                     | 0.82              |
| 2:B:732:SER:HB2   | 2:B:734:HIS:NE2   | 1.94                     | 0.82              |
| 1:A:472:LEU:O     | 1:A:475:THR:HB    | 1.79                     | 0.81              |
| 1:A:344:ARG:HG3   | 1:A:344:ARG:NH1   | 1.91                     | 0.81              |
| 8:J:23:ASN:HB3    | 8:J:27:GLU:OE2    | 1.80                     | 0.81              |
| 1:A:503:GLN:NE2   | 5:F:90:ARG:NH2    | 2.28                     | 0.81              |
| 3:C:73:GLN:NE2    | 3:C:75:MET:H      | 1.76                     | 0.81              |
| 3:C:37:MET:HA     | 3:C:41:ILE:HD11   | 1.61                     | 0.81              |
| 3:C:73:GLN:HE21   | 3:C:75:MET:N      | 1.76                     | 0.81              |
| 13:N:1:DG:H2''    | 13:N:2:DT:H71     | 1.58                     | 0.81              |
| 1:A:265:LYS:C     | 1:A:267:ALA:H     | 1.86                     | 0.80              |
| 1:A:55:ASP:O      | 1:A:56:PRO:C      | 2.22                     | 0.80              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:565:ILE:HG23  | 1:A:567:LYS:HE3   | 1.62                     | 0.80              |
| 2:B:230:ALA:H     | 2:B:231:PRO:CD    | 1.95                     | 0.80              |
| 2:B:747:MET:HA    | 2:B:747:MET:CE    | 2.08                     | 0.80              |
| 1:A:261:ASP:OD2   | 1:A:323:LYS:HD2   | 1.82                     | 0.80              |
| 12:T:6:DC:H1'     | 12:T:7:DA:C8      | 2.18                     | 0.79              |
| 1:A:902:LEU:CD1   | 1:A:926:GLN:HG3   | 2.12                     | 0.79              |
| 2:B:378:LEU:O     | 2:B:382:ILE:HG12  | 1.82                     | 0.79              |
| 1:A:57:ARG:HA     | 1:A:68:GLN:HB3    | 1.65                     | 0.79              |
| 1:A:315:LEU:CB    | 1:A:316:GLN:HA    | 2.11                     | 0.79              |
| 2:B:778:MET:HE1   | 2:B:853:SER:HB3   | 1.62                     | 0.79              |
| 1:A:351:THR:CG2   | 2:B:1103:ILE:HG12 | 2.12                     | 0.79              |
| 1:A:320:ARG:HG3   | 1:A:320:ARG:NH1   | 1.91                     | 0.79              |
| 1:A:567:LYS:CB    | 1:A:568:PRO:HD2   | 2.12                     | 0.79              |
| 13:N:5:DT:C2'     | 13:N:6:DT:H71     | 2.12                     | 0.79              |
| 1:A:115:LEU:HD22  | 1:A:119:ASN:HB2   | 1.65                     | 0.79              |
| 2:B:519:TRP:CZ2   | 2:B:705:MET:HE1   | 2.17                     | 0.79              |
| 13:N:6:DT:O2      | 13:N:7:DA:C5      | 2.36                     | 0.79              |
| 2:B:732:SER:HB2   | 2:B:734:HIS:CD2   | 2.19                     | 0.78              |
| 6:H:89:LEU:CD2    | 6:H:92:ASP:H      | 1.96                     | 0.78              |
| 7:I:92:ARG:HG2    | 7:I:93:LYS:H      | 1.47                     | 0.78              |
| 2:B:29:ASP:HB3    | 2:B:658:ILE:HG12  | 1.63                     | 0.78              |
| 1:A:744:LYS:HE2   | 1:A:748:MET:HE3   | 1.63                     | 0.78              |
| 1:A:53:LEU:HD23   | 1:A:54:ASN:N      | 1.98                     | 0.78              |
| 1:A:567:LYS:CB    | 6:H:96:VAL:H      | 1.92                     | 0.78              |
| 1:A:630:ILE:H     | 1:A:630:ILE:CD1   | 1.97                     | 0.78              |
| 13:N:5:DT:H2'     | 13:N:6:DT:C7      | 2.14                     | 0.78              |
| 13:N:6:DT:C2      | 13:N:7:DA:C6      | 2.71                     | 0.78              |
| 4:E:116:ILE:CG2   | 4:E:121:MET:HG3   | 2.15                     | 0.77              |
| 1:A:1364:ASN:HD22 | 1:A:1366:ARG:HG2  | 1.46                     | 0.77              |
| 1:A:470:LEU:HD21  | 1:A:487:MET:HE3   | 1.67                     | 0.77              |
| 1:A:1364:ASN:HD21 | 1:A:1366:ARG:HH11 | 1.30                     | 0.77              |
| 1:A:215:SER:C     | 1:A:217:LYS:H     | 1.92                     | 0.77              |
| 1:A:37:PHE:HB2    | 1:A:52:GLY:HA3    | 1.67                     | 0.76              |
| 1:A:296:LEU:HG    | 1:A:296:LEU:O     | 1.83                     | 0.76              |
| 1:A:901:LEU:HB2   | 1:A:926:GLN:HG2   | 1.67                     | 0.76              |
| 1:A:855:THR:CG2   | 1:A:857:ARG:HE    | 1.97                     | 0.76              |
| 1:A:1322:ILE:HG12 | 1:A:1323:ASP:N    | 2.00                     | 0.76              |
| 2:B:644:GLU:HA    | 2:B:644:GLU:OE1   | 1.84                     | 0.76              |
| 2:B:778:MET:CE    | 2:B:853:SER:HB3   | 2.14                     | 0.76              |
| 1:A:1029:ARG:HH11 | 1:A:1029:ARG:HG3  | 1.50                     | 0.76              |
| 1:A:315:LEU:HB3   | 1:A:316:GLN:CA    | 2.14                     | 0.76              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 8:J:7:CYS:HA     | 8:J:49:MET:HG2    | 1.66                     | 0.76              |
| 13:N:4:DG:C2     | 13:N:5:DT:N1      | 2.54                     | 0.76              |
| 1:A:741:ASN:HD22 | 1:A:744:LYS:H     | 1.31                     | 0.76              |
| 4:E:19:VAL:O     | 4:E:23:VAL:HG23   | 1.86                     | 0.76              |
| 1:A:114:LEU:O    | 1:A:115:LEU:HG    | 1.86                     | 0.76              |
| 2:B:590:HIS:HD2  | 2:B:596:LEU:HD22  | 1.50                     | 0.75              |
| 7:I:8:ARG:O      | 7:I:9:ASP:HB2     | 1.85                     | 0.75              |
| 13:N:13:DA:H2''  | 13:N:14:DG:C8     | 2.20                     | 0.75              |
| 2:B:515:HIS:HD2  | 2:B:517:THR:H     | 1.34                     | 0.75              |
| 1:A:67:CYS:O     | 1:A:68:GLN:HG3    | 1.87                     | 0.75              |
| 1:A:1063:MET:SD  | 1:A:1436:ILE:HG13 | 2.26                     | 0.75              |
| 2:B:416:LEU:HD11 | 2:B:460:ALA:CB    | 2.17                     | 0.75              |
| 9:K:65:HIS:HD2   | 9:K:67:PHE:H      | 1.30                     | 0.75              |
| 5:F:85:MET:HE1   | 5:F:148:VAL:HG13  | 1.69                     | 0.75              |
| 1:A:1383:SER:O   | 1:A:1388:GLY:HA3  | 1.86                     | 0.75              |
| 2:B:100:PRO:O    | 2:B:101:MET:HG3   | 1.86                     | 0.74              |
| 2:B:641:GLU:HB3  | 2:B:643:ASP:OD1   | 1.87                     | 0.74              |
| 3:C:123:ASN:HD21 | 3:C:125:MET:HB3   | 1.52                     | 0.74              |
| 7:I:92:ARG:HG2   | 7:I:93:LYS:N      | 2.00                     | 0.74              |
| 1:A:882:SER:HB3  | 1:A:953:ASN:OD1   | 1.88                     | 0.74              |
| 1:A:565:ILE:HG23 | 1:A:567:LYS:HG2   | 1.70                     | 0.74              |
| 2:B:241:ARG:HA   | 2:B:253:THR:HG22  | 1.69                     | 0.74              |
| 12:T:6:DC:N1     | 12:T:7:DA:N7      | 2.35                     | 0.74              |
| 1:A:265:LYS:HZ1  | 1:A:302:THR:HG23  | 1.52                     | 0.74              |
| 2:B:313:MET:HE2  | 2:B:390:LEU:HG    | 1.69                     | 0.74              |
| 1:A:244:PRO:HB2  | 1:A:245:PRO:CD    | 2.17                     | 0.74              |
| 6:H:63:LEU:C     | 6:H:90:ALA:HB3    | 2.12                     | 0.74              |
| 1:A:961:ARG:HB3  | 1:A:961:ARG:NH1   | 2.01                     | 0.74              |
| 2:B:969:ARG:NH1  | 3:C:61:GLU:OE1    | 2.21                     | 0.74              |
| 1:A:108:MET:O    | 1:A:109:HIS:HB2   | 1.87                     | 0.74              |
| 1:A:1206:ASP:H   | 1:A:1274:ARG:HH12 | 1.34                     | 0.74              |
| 4:E:147:HIS:HD2  | 4:E:149:LEU:H     | 1.35                     | 0.73              |
| 1:A:961:ARG:HH11 | 1:A:961:ARG:CB    | 1.99                     | 0.73              |
| 2:B:129:PHE:CE2  | 2:B:166:PHE:HB2   | 2.23                     | 0.73              |
| 2:B:1103:ILE:O   | 2:B:1103:ILE:HG22 | 1.86                     | 0.73              |
| 3:C:148:ARG:HG2  | 3:C:149:LYS:N     | 2.02                     | 0.73              |
| 1:A:392:VAL:HG11 | 1:A:424:ILE:HG21  | 1.70                     | 0.73              |
| 3:C:116:LYS:HD3  | 3:C:140:ASN:HB3   | 1.68                     | 0.73              |
| 1:A:596:THR:O    | 1:A:598:LEU:N     | 2.22                     | 0.73              |
| 6:H:47:PHE:HB3   | 6:H:95:TYR:CD1    | 2.23                     | 0.73              |
| 1:A:1435:PRO:O   | 1:A:1436:ILE:HD12 | 1.89                     | 0.73              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B:642:ASP:HB3  | 2:B:649:LYS:HG3   | 1.70                     | 0.73              |
| 2:B:900:ALA:HB3  | 10:L:61:THR:HG23  | 1.69                     | 0.73              |
| 8:J:8:PHE:H      | 8:J:49:MET:HE3    | 1.53                     | 0.73              |
| 1:A:1129:GLU:HA  | 1:A:1132:LYS:HE2  | 1.71                     | 0.73              |
| 4:E:198:ILE:CD1  | 4:E:212:ARG:HG3   | 2.17                     | 0.73              |
| 2:B:705:MET:HE3  | 2:B:742:GLU:HG2   | 1.71                     | 0.73              |
| 2:B:29:ASP:OD2   | 2:B:655:LYS:HE2   | 1.89                     | 0.73              |
| 6:H:2:SER:O      | 6:H:3:ASN:HB2     | 1.88                     | 0.73              |
| 1:A:68:GLN:HE21  | 1:A:70:CYS:HB3    | 1.54                     | 0.72              |
| 1:A:317:LYS:O    | 12:T:28:DT:H4'    | 1.89                     | 0.72              |
| 1:A:1430:LEU:O   | 2:B:1196:ILE:HG22 | 1.88                     | 0.72              |
| 2:B:287:ARG:NH2  | 2:B:294:ASP:OD2   | 2.23                     | 0.72              |
| 1:A:869:GLY:O    | 4:E:204:THR:HG21  | 1.90                     | 0.72              |
| 1:A:709:THR:HB   | 1:A:712:GLU:H     | 1.54                     | 0.72              |
| 2:B:516:ASN:H    | 2:B:516:ASN:HD22  | 1.36                     | 0.72              |
| 6:H:63:LEU:C     | 6:H:90:ALA:CB     | 2.62                     | 0.72              |
| 12:T:6:DC:C1'    | 12:T:7:DA:C8      | 2.72                     | 0.72              |
| 1:A:553:VAL:HG23 | 1:A:652:VAL:CG2   | 2.20                     | 0.72              |
| 2:B:485:ARG:HH11 | 2:B:485:ARG:CG    | 2.02                     | 0.72              |
| 1:A:946:VAL:HG22 | 4:E:201:LYS:HD3   | 1.71                     | 0.72              |
| 2:B:229:ALA:HB1  | 2:B:231:PRO:HD2   | 1.70                     | 0.72              |
| 2:B:519:TRP:HZ2  | 2:B:705:MET:HE1   | 1.52                     | 0.72              |
| 2:B:881:ASN:HA   | 2:B:883:LEU:HD23  | 1.72                     | 0.72              |
| 1:A:858:ASN:C    | 1:A:858:ASN:HD22  | 1.98                     | 0.72              |
| 2:B:345:LYS:O    | 2:B:348:ARG:HG2   | 1.89                     | 0.72              |
| 2:B:428:ILE:HG13 | 2:B:448:ILE:HD13  | 1.71                     | 0.72              |
| 2:B:636:PRO:HB3  | 2:B:743:ILE:HG13  | 1.71                     | 0.71              |
| 12:T:8:DT:O4     | 13:N:7:DA:N1      | 2.23                     | 0.71              |
| 1:A:423:ASP:O    | 1:A:424:ILE:CB    | 2.32                     | 0.71              |
| 2:B:705:MET:HE2  | 2:B:745:PRO:HB3   | 1.69                     | 0.71              |
| 13:N:1:DG:C2'    | 13:N:2:DT:H73     | 2.19                     | 0.71              |
| 13:N:4:DG:C1'    | 13:N:5:DT:H5''    | 2.20                     | 0.71              |
| 3:C:39:ALA:HA    | 3:C:164:ALA:HB3   | 1.73                     | 0.71              |
| 7:I:5:ARG:HD3    | 7:I:36:GLU:OE2    | 1.90                     | 0.71              |
| 12:T:9:DA:C2     | 13:N:7:DA:C2      | 2.78                     | 0.71              |
| 1:A:871:ASP:OD1  | 1:A:1366:ARG:NH2  | 2.23                     | 0.71              |
| 3:C:148:ARG:HG2  | 3:C:149:LYS:H     | 1.55                     | 0.71              |
| 12:T:7:DA:N1     | 12:T:8:DT:C4      | 2.59                     | 0.71              |
| 1:A:214:ILE:HG22 | 1:A:215:SER:N     | 1.99                     | 0.71              |
| 1:A:256:GLN:HA   | 1:A:257:ARG:HB3   | 1.72                     | 0.71              |
| 1:A:567:LYS:HE2  | 6:H:97:MET:HG2    | 1.72                     | 0.71              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:1187:ASN:HD21 | 2:B:1190:ASP:H    | 1.38                     | 0.71              |
| 13:N:6:DT:N3      | 13:N:7:DA:N6      | 2.38                     | 0.71              |
| 1:A:1029:ARG:HH11 | 1:A:1029:ARG:HG2  | 1.55                     | 0.70              |
| 2:B:25:ILE:CG2    | 2:B:29:ASP:HB2    | 2.20                     | 0.70              |
| 13:N:4:DG:N1      | 13:N:5:DT:C4      | 2.60                     | 0.70              |
| 1:A:922:ASP:O     | 1:A:923:LEU:HG    | 1.92                     | 0.70              |
| 1:A:353:ILE:HD13  | 1:A:487:MET:HE2   | 1.72                     | 0.70              |
| 1:A:532:ARG:HH11  | 1:A:532:ARG:HG2   | 1.56                     | 0.70              |
| 2:B:408:LEU:HD21  | 2:B:545:ILE:HD13  | 1.73                     | 0.70              |
| 12:T:1:DC:C2'     | 12:T:2:DT:OP2     | 2.30                     | 0.70              |
| 2:B:789:MET:HE2   | 2:B:965:LYS:HB2   | 1.73                     | 0.70              |
| 2:B:986:GLN:HE21  | 2:B:1022:THR:HG21 | 1.55                     | 0.70              |
| 1:A:726:ARG:HG2   | 1:A:726:ARG:O     | 1.90                     | 0.70              |
| 3:C:162:GLY:HA3   | 3:C:170:TRP:CE2   | 2.25                     | 0.70              |
| 3:C:69:LEU:HB2    | 8:J:5:VAL:CG1     | 2.21                     | 0.70              |
| 3:C:32:SER:O      | 3:C:36:VAL:HG23   | 1.91                     | 0.69              |
| 3:C:56:THR:CG2    | 3:C:58:LEU:H      | 2.05                     | 0.69              |
| 1:A:86:LEU:HD12   | 1:A:236:LEU:O     | 1.91                     | 0.69              |
| 2:B:744:HIS:HD2   | 2:B:746:SER:N     | 1.84                     | 0.69              |
| 1:A:650:GLN:O     | 1:A:654:ASN:HB2   | 1.92                     | 0.69              |
| 1:A:1029:ARG:HG2  | 1:A:1029:ARG:NH1  | 2.06                     | 0.69              |
| 1:A:42:ASP:HB3    | 1:A:45:GLN:HA     | 1.74                     | 0.69              |
| 4:E:116:ILE:HG21  | 4:E:121:MET:HG3   | 1.75                     | 0.69              |
| 2:B:167:ILE:HD13  | 2:B:167:ILE:N     | 2.07                     | 0.69              |
| 12:T:6:DC:N1      | 12:T:7:DA:C8      | 2.60                     | 0.69              |
| 1:A:134:ARG:HD3   | 1:A:221:SER:O     | 1.92                     | 0.69              |
| 3:C:70:ILE:HD11   | 3:C:144:ILE:HD11  | 1.73                     | 0.69              |
| 3:C:27:LEU:HD12   | 3:C:228:PHE:HE2   | 1.56                     | 0.69              |
| 1:A:341:MET:HE2   | 1:A:843:LYS:HZ1   | 1.56                     | 0.68              |
| 3:C:142:VAL:H     | 8:J:16:ASP:HB3    | 1.58                     | 0.68              |
| 3:C:66:ARG:NH2    | 8:J:3:VAL:O       | 2.26                     | 0.68              |
| 4:E:72:PHE:CE2    | 4:E:157:SER:HB3   | 2.28                     | 0.68              |
| 1:A:64:ASN:O      | 1:A:66:LYS:N      | 2.27                     | 0.68              |
| 1:A:711:ARG:HG2   | 7:I:97:MET:HE3    | 1.74                     | 0.68              |
| 1:A:1206:ASP:H    | 1:A:1274:ARG:NH1  | 1.90                     | 0.68              |
| 1:A:55:ASP:O      | 1:A:57:ARG:N      | 2.25                     | 0.68              |
| 2:B:121:ASN:HD22  | 2:B:207:GLY:HA3   | 1.59                     | 0.68              |
| 4:E:55:ARG:C      | 4:E:57:MET:H      | 2.00                     | 0.68              |
| 6:H:131:ASN:C     | 6:H:133:ASN:H     | 2.02                     | 0.68              |
| 1:A:91:PHE:HB2    | 1:A:297:GLN:OE1   | 1.94                     | 0.68              |
| 1:A:260:ASP:OD1   | 1:A:261:ASP:N     | 2.25                     | 0.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:875:ALA:HB2   | 1:A:1366:ARG:HD2  | 1.74                     | 0.68              |
| 1:A:901:LEU:H     | 1:A:926:GLN:NE2   | 1.92                     | 0.68              |
| 1:A:1134:ILE:O    | 1:A:1138:ILE:HG12 | 1.94                     | 0.68              |
| 6:H:89:LEU:C      | 6:H:91:ASP:H      | 2.02                     | 0.68              |
| 13:N:9:DG:H2''    | 13:N:10:DG:C8     | 2.29                     | 0.68              |
| 1:A:399:HIS:O     | 1:A:401:GLY:N     | 2.27                     | 0.68              |
| 1:A:1325:THR:HG22 | 1:A:1326:ARG:HG3  | 1.76                     | 0.68              |
| 1:A:1437:GLY:O    | 1:A:1439:GLY:N    | 2.27                     | 0.68              |
| 13:N:2:DT:H2''    | 13:N:3:DG:C8      | 2.28                     | 0.68              |
| 1:A:1336:MET:HE2  | 1:A:1380:GLY:HA2  | 1.76                     | 0.68              |
| 2:B:476:ARG:O     | 2:B:478:GLY:N     | 2.26                     | 0.68              |
| 1:A:50:ILE:HG22   | 1:A:52:GLY:N      | 2.09                     | 0.67              |
| 13:N:4:DG:N1      | 13:N:5:DT:N3      | 2.41                     | 0.67              |
| 1:A:90:VAL:HB     | 1:A:297:GLN:NE2   | 2.09                     | 0.67              |
| 3:C:99:LEU:HD23   | 3:C:99:LEU:N      | 2.08                     | 0.67              |
| 1:A:51:GLY:HA2    | 1:A:56:PRO:HG3    | 1.74                     | 0.67              |
| 1:A:1189:SER:OG   | 1:A:1190:PRO:HD2  | 1.94                     | 0.67              |
| 2:B:1077:THR:HG23 | 2:B:1079:LYS:H    | 1.59                     | 0.67              |
| 1:A:343:LYS:NZ    | 2:B:1156:ASP:OD2  | 2.28                     | 0.67              |
| 1:A:532:ARG:HH11  | 1:A:532:ARG:HG3   | 1.58                     | 0.67              |
| 1:A:1336:MET:CE   | 1:A:1380:GLY:HA2  | 2.24                     | 0.67              |
| 3:C:22:LEU:HD22   | 3:C:25:VAL:HG21   | 1.77                     | 0.67              |
| 1:A:70:CYS:HA     | 2:B:1174:LYS:HD3  | 1.77                     | 0.67              |
| 1:A:256:GLN:HB3   | 1:A:257:ARG:HD2   | 1.77                     | 0.67              |
| 2:B:640:VAL:HG12  | 2:B:640:VAL:O     | 1.93                     | 0.67              |
| 1:A:500:GLU:OE2   | 1:A:1438:THR:HG21 | 1.95                     | 0.67              |
| 2:B:211:VAL:O     | 2:B:480:SER:HA    | 1.93                     | 0.67              |
| 13:N:4:DG:C5      | 13:N:5:DT:C5      | 2.83                     | 0.67              |
| 13:N:9:DG:H2''    | 13:N:10:DG:N7     | 2.09                     | 0.67              |
| 1:A:53:LEU:CD2    | 1:A:54:ASN:H      | 2.03                     | 0.67              |
| 1:A:1397:LEU:HB2  | 1:A:1426:GLU:OE2  | 1.94                     | 0.67              |
| 2:B:473:MET:C     | 2:B:475:SER:H     | 2.02                     | 0.67              |
| 4:E:147:HIS:CD2   | 4:E:149:LEU:H     | 2.12                     | 0.67              |
| 2:B:843:GLN:HB2   | 2:B:993:THR:HB    | 1.77                     | 0.66              |
| 2:B:880:THR:CG2   | 2:B:880:THR:O     | 2.43                     | 0.66              |
| 1:A:542:GLU:OE1   | 1:A:569:LYS:NZ    | 2.28                     | 0.66              |
| 1:A:609:ASP:O     | 1:A:611:GLN:N     | 2.28                     | 0.66              |
| 2:B:788:ARG:NH1   | 2:B:790:ASP:OD1   | 2.28                     | 0.66              |
| 7:I:111:THR:CG2   | 7:I:113:ASP:HB3   | 2.25                     | 0.66              |
| 9:K:49:GLU:HG3    | 9:K:94:ILE:CG1    | 2.25                     | 0.66              |
| 1:A:875:ALA:HA    | 1:A:878:ILE:HD12  | 1.77                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1206:ASP:N    | 1:A:1274:ARG:HH12 | 1.92                     | 0.66              |
| 1:A:1435:PRO:C    | 1:A:1436:ILE:HD12 | 2.21                     | 0.66              |
| 13:N:6:DT:N3      | 13:N:7:DA:C6      | 2.64                     | 0.66              |
| 1:A:1029:ARG:O    | 1:A:1033:GLN:HB2  | 1.96                     | 0.66              |
| 2:B:470:LYS:O     | 2:B:471:LYS:HG3   | 1.96                     | 0.66              |
| 2:B:1084:GLN:NE2  | 3:C:192:TRP:H     | 1.94                     | 0.66              |
| 12:T:6:DC:H1'     | 12:T:7:DA:H8      | 1.59                     | 0.66              |
| 1:A:378:GLU:OE1   | 1:A:434:ARG:NH1   | 2.27                     | 0.65              |
| 2:B:1028:GLU:O    | 2:B:1032:SER:HB2  | 1.95                     | 0.65              |
| 3:C:56:THR:HG22   | 3:C:58:LEU:H      | 1.59                     | 0.65              |
| 1:A:761:MET:HG3   | 2:B:1021:MET:HG2  | 1.77                     | 0.65              |
| 1:A:871:ASP:HB3   | 4:E:204:THR:HG23  | 1.78                     | 0.65              |
| 2:B:230:ALA:H     | 2:B:231:PRO:HD3   | 1.60                     | 0.65              |
| 1:A:1116:LEU:H    | 1:A:1308:THR:HB   | 1.61                     | 0.65              |
| 2:B:365:THR:HG23  | 2:B:367:LEU:H     | 1.61                     | 0.65              |
| 5:F:93:ILE:HD11   | 5:F:134:ILE:CD1   | 2.16                     | 0.65              |
| 1:A:6:TYR:HD2     | 1:A:7:SER:N       | 1.94                     | 0.65              |
| 3:C:69:LEU:HB2    | 8:J:5:VAL:HG11    | 1.77                     | 0.65              |
| 1:A:470:LEU:HD21  | 1:A:487:MET:CE    | 2.25                     | 0.65              |
| 1:A:1438:THR:H    | 5:F:88:TYR:HB3    | 1.60                     | 0.65              |
| 2:B:482:VAL:C     | 2:B:483:LEU:O     | 2.36                     | 0.65              |
| 1:A:269:ILE:HD11  | 1:A:300:VAL:HA    | 1.78                     | 0.65              |
| 2:B:1023:VAL:O    | 2:B:1027:ILE:HG13 | 1.97                     | 0.65              |
| 1:A:12:ARG:HB3    | 2:B:1218:THR:HB   | 1.79                     | 0.65              |
| 1:A:545:GLN:HG2   | 1:A:549:MET:HE3   | 1.79                     | 0.65              |
| 1:A:1341:ILE:HG22 | 4:E:182:ASP:OD2   | 1.95                     | 0.65              |
| 2:B:299:GLU:OE2   | 2:B:571:PRO:HD2   | 1.97                     | 0.65              |
| 1:A:541:ILE:HG22  | 1:A:546:VAL:HG23  | 1.79                     | 0.65              |
| 1:A:1036:ARG:HG3  | 1:A:1036:ARG:HH11 | 1.62                     | 0.65              |
| 1:A:567:LYS:HD3   | 6:H:95:TYR:CG     | 2.31                     | 0.64              |
| 2:B:282:ILE:HD12  | 2:B:382:ILE:HD12  | 1.79                     | 0.64              |
| 4:E:12:LEU:HD11   | 4:E:58:MET:HE1    | 1.79                     | 0.64              |
| 4:E:64:PRO:CG     | 4:E:76:GLY:HA2    | 2.26                     | 0.64              |
| 6:H:89:LEU:O      | 6:H:91:ASP:N      | 2.30                     | 0.64              |
| 3:C:222:LYS:HA    | 3:C:222:LYS:CE    | 2.21                     | 0.64              |
| 1:A:537:ARG:HD3   | 6:H:120:GLY:O     | 1.96                     | 0.64              |
| 1:A:809:THR:HB    | 1:A:810:PRO:HD2   | 1.78                     | 0.64              |
| 2:B:770:GLN:CG    | 2:B:770:GLN:O     | 2.45                     | 0.64              |
| 2:B:955:THR:HG23  | 10:L:54:ARG:O     | 1.96                     | 0.64              |
| 1:A:185:TRP:HZ3   | 1:A:200:ARG:HG2   | 1.62                     | 0.64              |
| 2:B:25:ILE:HG22   | 2:B:26:THR:N      | 2.12                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:102:VAL:HG11  | 2:B:122:LEU:HD13  | 1.78                     | 0.64              |
| 4:E:135:PHE:HD2   | 4:E:140:LEU:HD21  | 1.61                     | 0.64              |
| 7:I:8:ARG:O       | 7:I:9:ASP:CB      | 2.45                     | 0.64              |
| 13:N:4:DG:C4      | 13:N:5:DT:C6      | 2.85                     | 0.64              |
| 1:A:451:HIS:CD2   | 1:A:1074:GLU:HG3  | 2.33                     | 0.64              |
| 1:A:567:LYS:NZ    | 6:H:95:TYR:CZ     | 2.59                     | 0.64              |
| 1:A:1156:PRO:O    | 1:A:1158:PRO:HD3  | 1.98                     | 0.64              |
| 1:A:351:THR:HG22  | 1:A:352:VAL:H     | 1.63                     | 0.64              |
| 1:A:928:LEU:O     | 1:A:931:GLU:HB3   | 1.98                     | 0.64              |
| 1:A:1291:VAL:HG22 | 1:A:1292:PRO:HD2  | 1.80                     | 0.64              |
| 1:A:1111:MET:HE1  | 1:A:1330:ASN:OD1  | 1.98                     | 0.64              |
| 2:B:167:ILE:O     | 2:B:168:GLY:O     | 2.15                     | 0.64              |
| 12:T:6:DC:C2      | 12:T:7:DA:C5      | 2.86                     | 0.64              |
| 1:A:353:ILE:HD13  | 1:A:487:MET:CE    | 2.28                     | 0.63              |
| 3:C:123:ASN:ND2   | 3:C:125:MET:HB3   | 2.13                     | 0.63              |
| 2:B:647:GLY:C     | 2:B:648:HIS:ND1   | 2.57                     | 0.63              |
| 2:B:822:ASN:O     | 8:J:48:ARG:NH1    | 2.31                     | 0.63              |
| 4:E:96:PHE:C      | 4:E:98:ILE:H      | 2.07                     | 0.63              |
| 1:A:265:LYS:C     | 1:A:267:ALA:N     | 2.55                     | 0.63              |
| 2:B:864:LYS:HD2   | 2:B:865:LYS:N     | 2.13                     | 0.63              |
| 1:A:870:GLU:OE1   | 4:E:202:SER:HB2   | 1.98                     | 0.63              |
| 2:B:482:VAL:O     | 2:B:483:LEU:O     | 2.16                     | 0.63              |
| 4:E:198:ILE:HD11  | 4:E:212:ARG:HG3   | 1.80                     | 0.63              |
| 1:A:353:ILE:HG22  | 1:A:468:PHE:HB2   | 1.80                     | 0.63              |
| 1:A:532:ARG:CG    | 1:A:532:ARG:NH1   | 2.55                     | 0.63              |
| 1:A:567:LYS:HB2   | 1:A:568:PRO:HD3   | 1.79                     | 0.63              |
| 1:A:828:ALA:HB1   | 2:B:530:GLY:HA2   | 1.80                     | 0.63              |
| 2:B:770:GLN:O     | 2:B:770:GLN:HG3   | 1.98                     | 0.63              |
| 1:A:114:LEU:HD12  | 1:A:145:LYS:HB3   | 1.80                     | 0.63              |
| 1:A:874:ASP:HB2   | 1:A:1058:VAL:HG23 | 1.81                     | 0.63              |
| 1:A:1173:HIS:O    | 1:A:1174:PHE:HB3  | 1.99                     | 0.63              |
| 3:C:177:GLU:HG3   | 3:C:231:ASN:HB3   | 1.80                     | 0.63              |
| 1:A:1140:HIS:HB2  | 1:A:1276:VAL:O    | 1.99                     | 0.63              |
| 1:A:215:SER:C     | 1:A:217:LYS:N     | 2.57                     | 0.62              |
| 2:B:732:SER:CB    | 2:B:734:HIS:CD2   | 2.82                     | 0.62              |
| 2:B:899:ILE:HG21  | 2:B:949:VAL:HG21  | 1.80                     | 0.62              |
| 2:B:25:ILE:HD11   | 2:B:653:VAL:HB    | 1.81                     | 0.62              |
| 2:B:363:HIS:O     | 2:B:364:ILE:CB    | 2.45                     | 0.62              |
| 1:A:1155:ASP:OD2  | 1:A:1161:THR:HG23 | 1.98                     | 0.62              |
| 1:A:261:ASP:HB3   | 1:A:323:LYS:HG3   | 1.82                     | 0.62              |
| 1:A:567:LYS:HB2   | 6:H:95:TYR:HA     | 1.80                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:516:ASN:H     | 2:B:516:ASN:ND2   | 1.97                     | 0.62              |
| 1:A:567:LYS:CE    | 6:H:97:MET:HG2    | 2.29                     | 0.62              |
| 1:A:768:GLN:CG    | 1:A:816:HIS:HA    | 2.29                     | 0.62              |
| 2:B:203:PHE:HE1   | 2:B:212:LEU:HD12  | 1.64                     | 0.62              |
| 6:H:89:LEU:CD2    | 6:H:92:ASP:N      | 2.62                     | 0.62              |
| 13:N:4:DG:N3      | 13:N:5:DT:C6      | 2.67                     | 0.62              |
| 1:A:565:ILE:HG23  | 1:A:567:LYS:CE    | 2.30                     | 0.62              |
| 2:B:25:ILE:HG23   | 2:B:29:ASP:CB     | 2.25                     | 0.62              |
| 1:A:1410:PHE:HD2  | 2:B:1212:ILE:HD11 | 1.64                     | 0.62              |
| 6:H:83:GLN:HB3    | 6:H:86:ASP:OD1    | 2.00                     | 0.62              |
| 12:T:6:DC:C2'     | 12:T:7:DA:OP2     | 2.48                     | 0.62              |
| 1:A:265:LYS:NZ    | 1:A:302:THR:HG23  | 2.15                     | 0.61              |
| 1:A:795:GLU:HG3   | 2:B:731:VAL:HG11  | 1.82                     | 0.61              |
| 13:N:4:DG:N2      | 13:N:5:DT:O2      | 2.33                     | 0.61              |
| 1:A:22:PHE:HB2    | 2:B:1211:ASN:OD1  | 2.00                     | 0.61              |
| 1:A:320:ARG:HH11  | 1:A:320:ARG:CG    | 2.02                     | 0.61              |
| 1:A:369:SER:HB3   | 9:K:2:ASN:OD1     | 1.99                     | 0.61              |
| 2:B:361:LEU:HD21  | 2:B:377:PHE:CD2   | 2.36                     | 0.61              |
| 2:B:708:GLU:O     | 2:B:710:LEU:N     | 2.33                     | 0.61              |
| 2:B:880:THR:O     | 2:B:880:THR:HG23  | 1.99                     | 0.61              |
| 2:B:1159:ARG:HG3  | 2:B:1193:GLN:HE21 | 1.66                     | 0.61              |
| 1:A:57:ARG:CA     | 1:A:68:GLN:HB3    | 2.30                     | 0.61              |
| 1:A:1308:THR:CG2  | 1:A:1310:GLY:O    | 2.49                     | 0.61              |
| 2:B:638:PHE:CD2   | 2:B:653:VAL:HG21  | 2.35                     | 0.61              |
| 2:B:879:ARG:HG2   | 2:B:880:THR:N     | 2.15                     | 0.61              |
| 4:E:77:SER:HB2    | 4:E:105:PHE:HD2   | 1.65                     | 0.61              |
| 12:T:2:DT:OP2     | 12:T:2:DT:H71     | 2.00                     | 0.61              |
| 6:H:26:ILE:O      | 6:H:39:THR:HA     | 2.00                     | 0.61              |
| 1:A:508:PRO:O     | 1:A:511:ILE:HG13  | 2.00                     | 0.61              |
| 2:B:766:ARG:NH2   | 2:B:1020:ARG:HG2  | 2.16                     | 0.61              |
| 2:B:708:GLU:O     | 2:B:709:ASP:C     | 2.44                     | 0.61              |
| 2:B:751:VAL:CG1   | 2:B:752:ALA:N     | 2.63                     | 0.61              |
| 2:B:789:MET:HE2   | 2:B:965:LYS:CB    | 2.30                     | 0.61              |
| 3:C:74:SER:O      | 3:C:77:ILE:HB     | 2.01                     | 0.61              |
| 1:A:1424:VAL:HG11 | 2:B:1139:ILE:HD13 | 1.82                     | 0.61              |
| 2:B:422:LYS:O     | 2:B:425:THR:HG22  | 2.01                     | 0.61              |
| 12:T:7:DA:H2''    | 12:T:8:DT:H5''    | 1.82                     | 0.61              |
| 1:A:106:VAL:HG21  | 1:A:214:ILE:HD12  | 1.81                     | 0.60              |
| 1:A:331:GLY:O     | 1:A:332:LYS:HB3   | 1.99                     | 0.60              |
| 1:A:1436:ILE:O    | 1:A:1437:GLY:C    | 2.43                     | 0.60              |
| 2:B:570:VAL:HB    | 2:B:573:GLN:HG2   | 1.84                     | 0.60              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 6:H:145:ARG:HD2  | 6:H:146:ARG:HD2   | 1.83                     | 0.60              |
| 1:A:901:LEU:N    | 1:A:926:GLN:HE21  | 1.95                     | 0.60              |
| 1:A:929:LEU:HD21 | 1:A:983:ILE:HG23  | 1.83                     | 0.60              |
| 1:A:4:GLN:HE22   | 2:B:1159:ARG:H    | 1.50                     | 0.60              |
| 1:A:283:GLY:O    | 1:A:285:PRO:HD3   | 2.02                     | 0.60              |
| 1:A:399:HIS:O    | 1:A:400:PRO:C     | 2.41                     | 0.60              |
| 2:B:95:ILE:HD12  | 2:B:130:VAL:HG22  | 1.83                     | 0.60              |
| 7:I:111:THR:CG2  | 7:I:113:ASP:H     | 2.12                     | 0.60              |
| 13:N:1:DG:H2'    | 13:N:2:DT:H73     | 1.82                     | 0.60              |
| 2:B:864:LYS:HD3  | 2:B:870:ILE:O     | 2.02                     | 0.60              |
| 1:A:53:LEU:HD11  | 1:A:266:LEU:O     | 2.01                     | 0.60              |
| 2:B:173:MET:O    | 2:B:176:SER:HB3   | 2.02                     | 0.60              |
| 2:B:797:TYR:O    | 8:J:1:MET:HG3     | 2.01                     | 0.60              |
| 2:B:570:VAL:HG21 | 2:B:573:GLN:HE21  | 1.67                     | 0.60              |
| 2:B:1001:PHE:HE1 | 3:C:178:PHE:HB3   | 1.66                     | 0.60              |
| 4:E:179:GLN:O    | 4:E:182:ASP:HB2   | 2.01                     | 0.60              |
| 1:A:666:ILE:HD11 | 2:B:1030:LEU:HD13 | 1.83                     | 0.59              |
| 1:A:715:GLU:O    | 1:A:719:VAL:HG23  | 2.02                     | 0.59              |
| 2:B:234:ILE:HG21 | 2:B:257:LYS:HD3   | 1.85                     | 0.59              |
| 1:A:848:ILE:HG21 | 1:A:1370:LEU:HD11 | 1.83                     | 0.59              |
| 1:A:963:ILE:HD13 | 1:A:1048:ASN:HB3  | 1.83                     | 0.59              |
| 1:A:1256:GLU:HA  | 1:A:1259:MET:HB2  | 1.85                     | 0.59              |
| 1:A:809:THR:HB   | 1:A:810:PRO:CD    | 2.32                     | 0.59              |
| 1:A:858:ASN:HD22 | 1:A:860:LEU:H     | 1.50                     | 0.59              |
| 2:B:185:THR:O    | 2:B:188:ASP:HB2   | 2.01                     | 0.59              |
| 2:B:293:PRO:HG2  | 2:B:296:GLU:HB3   | 1.84                     | 0.59              |
| 3:C:3:GLU:HG3    | 3:C:4:GLU:N       | 2.17                     | 0.59              |
| 3:C:20:PHE:HE1   | 3:C:22:LEU:HD12   | 1.67                     | 0.59              |
| 12:T:8:DT:H3     | 13:N:7:DA:H2      | 1.46                     | 0.59              |
| 13:N:4:DG:C2     | 13:N:5:DT:C6      | 2.91                     | 0.59              |
| 2:B:313:MET:CE   | 2:B:390:LEU:HG    | 2.33                     | 0.59              |
| 4:E:100:ILE:O    | 4:E:101:GLN:C     | 2.45                     | 0.59              |
| 5:F:110:ASP:O    | 5:F:111:LEU:C     | 2.46                     | 0.59              |
| 2:B:373:ARG:HD2  | 2:B:566:LEU:HD23  | 1.85                     | 0.59              |
| 2:B:1153:GLU:N   | 2:B:1153:GLU:OE2  | 2.36                     | 0.59              |
| 8:J:57:ILE:O     | 8:J:61:LEU:HG     | 2.01                     | 0.59              |
| 1:A:503:GLN:HE22 | 5:F:90:ARG:NH2    | 1.99                     | 0.59              |
| 2:B:953:LEU:HD11 | 10:L:55:ILE:HG22  | 1.85                     | 0.59              |
| 3:C:260:LEU:HG   | 3:C:264:GLN:HE21  | 1.67                     | 0.59              |
| 5:F:93:ILE:CD1   | 5:F:134:ILE:HD11  | 2.17                     | 0.59              |
| 13:N:1:DG:C2'    | 13:N:2:DT:H71     | 2.25                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:173:THR:HB    | 1:A:184:SER:HB3   | 1.84                     | 0.58              |
| 1:A:765:VAL:HG22  | 1:A:800:VAL:HB    | 1.84                     | 0.58              |
| 1:A:995:GLU:OE2   | 1:A:995:GLU:HA    | 2.01                     | 0.58              |
| 2:B:322:PHE:CZ    | 7:I:30:ARG:HG2    | 2.37                     | 0.58              |
| 2:B:1081:LEU:O    | 3:C:189:THR:HG23  | 2.03                     | 0.58              |
| 4:E:13:TRP:O      | 4:E:16:PHE:HB3    | 2.03                     | 0.58              |
| 4:E:135:PHE:CD2   | 4:E:140:LEU:HD21  | 2.38                     | 0.58              |
| 5:F:109:VAL:HG22  | 5:F:124:GLU:HG3   | 1.85                     | 0.58              |
| 12:T:12:DC:H2''   | 12:T:13:DA:C8     | 2.37                     | 0.58              |
| 2:B:747:MET:HE3   | 2:B:747:MET:CA    | 2.14                     | 0.58              |
| 1:A:929:LEU:HD21  | 1:A:983:ILE:CG2   | 2.34                     | 0.58              |
| 2:B:998:ASP:OD1   | 3:C:35:ARG:NH2    | 2.29                     | 0.58              |
| 8:J:16:ASP:OD1    | 8:J:17:LYS:HG2    | 2.04                     | 0.58              |
| 3:C:102:GLN:HG2   | 3:C:154:LYS:HD3   | 1.86                     | 0.58              |
| 6:H:83:GLN:O      | 6:H:87:ARG:HG3    | 2.03                     | 0.58              |
| 7:I:47:GLU:OE1    | 7:I:50:THR:HG22   | 2.02                     | 0.58              |
| 13:N:1:DG:C2'     | 13:N:2:DT:C5      | 2.76                     | 0.58              |
| 1:A:261:ASP:HB3   | 1:A:323:LYS:CG    | 2.33                     | 0.58              |
| 1:A:341:MET:HE2   | 1:A:843:LYS:NZ    | 2.19                     | 0.58              |
| 1:A:215:SER:O     | 1:A:217:LYS:N     | 2.37                     | 0.58              |
| 2:B:882:THR:H     | 2:B:883:LEU:HB3   | 1.67                     | 0.58              |
| 2:B:1166:CYS:O    | 2:B:1215:ARG:HD3  | 2.04                     | 0.58              |
| 12:T:8:DT:C4      | 13:N:7:DA:N1      | 2.72                     | 0.58              |
| 13:N:6:DT:H1'     | 13:N:7:DA:C8      | 2.38                     | 0.58              |
| 1:A:317:LYS:HB3   | 12:T:28:DT:O3'    | 2.04                     | 0.58              |
| 1:A:532:ARG:HG3   | 1:A:532:ARG:NH1   | 2.14                     | 0.58              |
| 1:A:1312:ASN:O    | 1:A:1316:VAL:HG23 | 2.04                     | 0.58              |
| 4:E:127:ILE:O     | 4:E:127:ILE:HG12  | 2.04                     | 0.58              |
| 1:A:563:PRO:HB2   | 1:A:565:ILE:O     | 2.04                     | 0.57              |
| 1:A:1342:GLU:OE2  | 4:E:212:ARG:NH1   | 2.37                     | 0.57              |
| 1:A:567:LYS:CD    | 6:H:95:TYR:CD1    | 2.87                     | 0.57              |
| 2:B:555:ILE:HD12  | 2:B:587:HIS:CE1   | 2.39                     | 0.57              |
| 7:I:111:THR:HG21  | 7:I:113:ASP:HB3   | 1.86                     | 0.57              |
| 12:T:3:DA:H8      | 12:T:3:DA:OP2     | 1.87                     | 0.57              |
| 1:A:492:PRO:HB2   | 1:A:497:THR:CG2   | 2.33                     | 0.57              |
| 2:B:778:MET:CE    | 2:B:853:SER:CB    | 2.83                     | 0.57              |
| 3:C:184:ASN:OD1   | 3:C:187:LYS:HA    | 2.04                     | 0.57              |
| 1:A:37:PHE:HB2    | 1:A:52:GLY:CA     | 2.33                     | 0.57              |
| 1:A:567:LYS:HD3   | 6:H:95:TYR:CD1    | 2.39                     | 0.57              |
| 1:A:1308:THR:HG21 | 1:A:1310:GLY:O    | 2.04                     | 0.57              |
| 2:B:249:ARG:HG3   | 2:B:251:ILE:HG12  | 1.85                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:590:HIS:CD2   | 2:B:596:LEU:HD22  | 2.37                     | 0.57              |
| 2:B:1077:THR:CG2  | 2:B:1079:LYS:H    | 2.18                     | 0.57              |
| 2:B:899:ILE:HG22  | 2:B:900:ALA:N     | 2.20                     | 0.57              |
| 6:H:115:TYR:CE2   | 6:H:124:ARG:HG3   | 2.40                     | 0.57              |
| 1:A:868:TYR:CE1   | 1:A:1064:VAL:HG21 | 2.39                     | 0.57              |
| 1:A:1293:SER:HB2  | 1:A:1299:VAL:HG23 | 1.87                     | 0.57              |
| 2:B:269:ILE:HD11  | 2:B:386:LEU:HD21  | 1.87                     | 0.57              |
| 6:H:131:ASN:O     | 6:H:133:ASN:N     | 2.36                     | 0.57              |
| 1:A:307:ASP:O     | 1:A:308:ILE:C     | 2.48                     | 0.57              |
| 1:A:332:LYS:H     | 1:A:337:ARG:HB2   | 1.69                     | 0.57              |
| 1:A:302:THR:HA    | 1:A:305:ASP:O     | 2.05                     | 0.57              |
| 1:A:304:MET:O     | 1:A:324:SER:HB2   | 2.05                     | 0.57              |
| 1:A:365:GLY:O     | 1:A:468:PHE:HA    | 2.05                     | 0.57              |
| 2:B:122:LEU:CD2   | 2:B:958:GLN:HB2   | 2.35                     | 0.57              |
| 2:B:332:ASP:C     | 2:B:334:ILE:H     | 2.12                     | 0.57              |
| 2:B:1082:MET:O    | 3:C:189:THR:HG22  | 2.05                     | 0.57              |
| 1:A:211:PHE:O     | 1:A:214:ILE:HG12  | 2.05                     | 0.56              |
| 2:B:195:CYS:HB3   | 2:B:782:LEU:HD22  | 1.87                     | 0.56              |
| 1:A:457:ALA:HB3   | 1:A:506:ALA:HA    | 1.87                     | 0.56              |
| 2:B:996:ARG:HH22  | 3:C:173:ALA:HB1   | 1.71                     | 0.56              |
| 8:J:24:LEU:HB3    | 8:J:30:LEU:HD12   | 1.86                     | 0.56              |
| 1:A:780:VAL:CG2   | 2:B:699:GLU:OE2   | 2.48                     | 0.56              |
| 1:A:1319:VAL:HG12 | 1:A:1320:PRO:O    | 2.05                     | 0.56              |
| 1:A:1342:GLU:HG2  | 4:E:212:ARG:HH11  | 1.69                     | 0.56              |
| 3:C:185:LYS:NZ    | 3:C:211:ASP:O     | 2.31                     | 0.56              |
| 6:H:47:PHE:CB     | 6:H:95:TYR:CD1    | 2.87                     | 0.56              |
| 7:I:120:GLN:OE1   | 7:I:120:GLN:HA    | 2.05                     | 0.56              |
| 12:T:7:DA:OP2     | 12:T:7:DA:H8      | 1.89                     | 0.56              |
| 1:A:1338:VAL:HG12 | 1:A:1339:LEU:HD23 | 1.88                     | 0.56              |
| 1:A:40:THR:HG21   | 1:A:259:GLU:CD    | 2.31                     | 0.56              |
| 2:B:31:TRP:HA     | 2:B:34:ILE:HD12   | 1.88                     | 0.56              |
| 2:B:37:PHE:O      | 2:B:38:PHE:HB2    | 2.06                     | 0.56              |
| 2:B:1096:ARG:O    | 2:B:1097:HIS:CD2  | 2.59                     | 0.56              |
| 1:A:768:GLN:HG3   | 1:A:816:HIS:HA    | 1.88                     | 0.56              |
| 2:B:65:GLU:N      | 2:B:67:SER:HB3    | 2.21                     | 0.56              |
| 2:B:515:HIS:H     | 2:B:518:HIS:CD2   | 2.24                     | 0.56              |
| 2:B:1065:GLN:NE2  | 2:B:1069:PHE:HD1  | 2.03                     | 0.56              |
| 1:A:541:ILE:N     | 1:A:541:ILE:HD12  | 2.20                     | 0.56              |
| 6:H:44:VAL:O      | 6:H:44:VAL:CG1    | 2.53                     | 0.56              |
| 7:I:111:THR:HG22  | 7:I:113:ASP:N     | 2.11                     | 0.56              |
| 12:T:11:DC:C5     | 12:T:12:DC:N4     | 2.74                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:636:PRO:O     | 2:B:691:GLU:O     | 2.24                     | 0.56              |
| 4:E:117:THR:O     | 4:E:119:SER:N     | 2.39                     | 0.56              |
| 6:H:17:PRO:O      | 6:H:19:ARG:N      | 2.38                     | 0.56              |
| 1:A:424:ILE:HG22  | 1:A:424:ILE:O     | 2.05                     | 0.56              |
| 1:A:1332:PHE:CE1  | 1:A:1348:LEU:HD13 | 2.40                     | 0.56              |
| 2:B:58:THR:O      | 2:B:62:ILE:HG12   | 2.04                     | 0.56              |
| 2:B:278:GLN:HG2   | 2:B:279:ASP:H     | 1.70                     | 0.56              |
| 2:B:911:ILE:HG22  | 2:B:912:ILE:HG13  | 1.87                     | 0.56              |
| 2:B:1084:GLN:HE22 | 3:C:192:TRP:N     | 2.04                     | 0.56              |
| 6:H:89:LEU:C      | 6:H:91:ASP:N      | 2.63                     | 0.56              |
| 1:A:224:PHE:CE2   | 1:A:231:PRO:HG3   | 2.41                     | 0.56              |
| 1:A:401:GLY:C     | 1:A:435:HIS:CD2   | 2.84                     | 0.56              |
| 1:A:596:THR:C     | 1:A:598:LEU:H     | 2.14                     | 0.56              |
| 1:A:777:PHE:CD1   | 1:A:781:ASP:HA    | 2.40                     | 0.56              |
| 4:E:64:PRO:CD     | 4:E:76:GLY:HA2    | 2.36                     | 0.55              |
| 12:T:6:DC:C6      | 12:T:7:DA:N7      | 2.74                     | 0.55              |
| 1:A:541:ILE:HG22  | 1:A:546:VAL:CG2   | 2.36                     | 0.55              |
| 13:N:4:DG:C4      | 13:N:5:DT:C5      | 2.94                     | 0.55              |
| 1:A:345:VAL:HB    | 2:B:1154:ALA:HB1  | 1.87                     | 0.55              |
| 1:A:414:ASP:OD1   | 1:A:416:ARG:HG2   | 2.06                     | 0.55              |
| 1:A:565:ILE:HG12  | 1:A:567:LYS:HZ1   | 1.71                     | 0.55              |
| 1:A:709:THR:HG23  | 7:I:94:ASP:HA     | 1.88                     | 0.55              |
| 1:A:907:THR:HG22  | 1:A:908:LEU:N     | 2.21                     | 0.55              |
| 5:F:132:LEU:O     | 5:F:148:VAL:HG23  | 2.07                     | 0.55              |
| 1:A:76:GLU:OE2    | 2:B:1159:ARG:NH1  | 2.40                     | 0.55              |
| 1:A:381:THR:HG23  | 1:A:383:TYR:H     | 1.72                     | 0.55              |
| 2:B:492:LEU:HB3   | 2:B:751:VAL:HG21  | 1.88                     | 0.55              |
| 2:B:642:ASP:HA    | 2:B:649:LYS:HA    | 1.89                     | 0.55              |
| 6:H:104:PHE:CZ    | 6:H:136:LYS:HA    | 2.42                     | 0.55              |
| 2:B:1065:GLN:HE22 | 2:B:1067:ARG:HB2  | 1.70                     | 0.55              |
| 1:A:754:SER:N     | 1:A:757:ASN:HD22  | 2.04                     | 0.55              |
| 2:B:526:GLU:HG3   | 2:B:771:SER:HB3   | 1.89                     | 0.55              |
| 5:F:73:ALA:O      | 5:F:74:ILE:HG12   | 2.06                     | 0.55              |
| 6:H:109:LYS:NZ    | 6:H:111:LEU:HD12  | 2.20                     | 0.55              |
| 2:B:203:PHE:CE1   | 2:B:212:LEU:HD12  | 2.41                     | 0.55              |
| 2:B:999:MET:HG3   | 2:B:1000:PRO:HD2  | 1.88                     | 0.55              |
| 4:E:116:ILE:HG22  | 4:E:121:MET:HG3   | 1.85                     | 0.55              |
| 7:I:15:TYR:CE1    | 7:I:30:ARG:HD3    | 2.41                     | 0.55              |
| 7:I:47:GLU:OE1    | 7:I:50:THR:CG2    | 2.54                     | 0.55              |
| 1:A:482:PHE:HB2   | 2:B:838:SER:HB3   | 1.87                     | 0.55              |
| 1:A:401:GLY:CA    | 1:A:435:HIS:HD2   | 2.20                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:28:GLU:C      | 2:B:30:SER:H      | 2.14                     | 0.55              |
| 3:C:251:LEU:O     | 3:C:255:VAL:HG23  | 2.07                     | 0.55              |
| 13:N:4:DG:C6      | 13:N:5:DT:C5      | 2.95                     | 0.55              |
| 2:B:541:LEU:HD12  | 2:B:747:MET:CE    | 2.26                     | 0.55              |
| 3:C:162:GLY:HA3   | 3:C:170:TRP:CD2   | 2.41                     | 0.55              |
| 4:E:54:GLN:HA     | 4:E:54:GLN:OE1    | 2.05                     | 0.55              |
| 1:A:244:PRO:O     | 1:A:246:VAL:N     | 2.39                     | 0.54              |
| 6:H:106:GLU:C     | 6:H:108:SER:H     | 2.14                     | 0.54              |
| 1:A:50:ILE:C      | 1:A:52:GLY:H      | 2.15                     | 0.54              |
| 1:A:261:ASP:HB3   | 1:A:323:LYS:CD    | 2.37                     | 0.54              |
| 12:T:6:DC:C4      | 12:T:7:DA:N6      | 2.75                     | 0.54              |
| 1:A:645:LEU:HD11  | 1:A:649:ILE:HD11  | 1.89                     | 0.54              |
| 2:B:315:LYS:CG    | 7:I:13:MET:HE1    | 2.38                     | 0.54              |
| 1:A:265:LYS:O     | 1:A:267:ALA:N     | 2.40                     | 0.54              |
| 1:A:574:GLY:O     | 1:A:577:ILE:HD12  | 2.06                     | 0.54              |
| 1:A:786:HIS:HE1   | 2:B:742:GLU:OE1   | 1.91                     | 0.54              |
| 1:A:1431:GLY:HA3  | 2:B:1197:PRO:HD3  | 1.88                     | 0.54              |
| 6:H:108:SER:O     | 6:H:109:LYS:HB2   | 2.07                     | 0.54              |
| 13:N:6:DT:O2      | 13:N:7:DA:C4      | 2.60                     | 0.54              |
| 1:A:86:LEU:HD13   | 1:A:90:VAL:HG22   | 1.89                     | 0.54              |
| 1:A:361:LEU:HD22  | 1:A:646:PHE:CD1   | 2.43                     | 0.54              |
| 1:A:586:ILE:HD11  | 1:A:637:LYS:HG3   | 1.90                     | 0.54              |
| 1:A:1155:ASP:OD1  | 1:A:1162:VAL:HG23 | 2.07                     | 0.54              |
| 12:T:2:DT:O2      | 13:N:13:DA:N1     | 2.40                     | 0.54              |
| 1:A:424:ILE:O     | 1:A:424:ILE:CG2   | 2.54                     | 0.54              |
| 9:K:47:ARG:HH11   | 9:K:47:ARG:HB3    | 1.72                     | 0.54              |
| 1:A:56:PRO:O      | 1:A:58:LEU:N      | 2.41                     | 0.54              |
| 1:A:84:ILE:HD11   | 1:A:270:LEU:HG    | 1.90                     | 0.54              |
| 1:A:372:LYS:HA    | 1:A:435:HIS:ND1   | 2.23                     | 0.54              |
| 2:B:1002:THR:HG23 | 2:B:1004:GLU:N    | 2.20                     | 0.54              |
| 7:I:92:ARG:CG     | 7:I:93:LYS:H      | 2.20                     | 0.54              |
| 12:T:7:DA:N1      | 12:T:8:DT:O4      | 2.40                     | 0.54              |
| 2:B:322:PHE:HZ    | 7:I:30:ARG:HG2    | 1.72                     | 0.54              |
| 3:C:22:LEU:CD2    | 3:C:25:VAL:HG21   | 2.37                     | 0.54              |
| 1:A:364:VAL:O     | 1:A:364:VAL:HG13  | 2.06                     | 0.54              |
| 1:A:984:LYS:O     | 1:A:988:LEU:HB3   | 2.08                     | 0.54              |
| 2:B:473:MET:O     | 2:B:475:SER:N     | 2.41                     | 0.54              |
| 12:T:6:DC:C1'     | 12:T:7:DA:H8      | 2.17                     | 0.54              |
| 1:A:67:CYS:C      | 1:A:68:GLN:HG3    | 2.33                     | 0.53              |
| 1:A:565:ILE:HG12  | 1:A:567:LYS:NZ    | 2.23                     | 0.53              |
| 1:A:1400:CYS:O    | 1:A:1405:THR:HG23 | 2.07                     | 0.53              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:C:141:GLY:O    | 3:C:142:VAL:HB    | 2.07                     | 0.53              |
| 1:A:315:LEU:HD12 | 1:A:319:GLY:O     | 2.07                     | 0.53              |
| 1:A:565:ILE:CG2  | 1:A:567:LYS:HG2   | 2.38                     | 0.53              |
| 1:A:751:SER:OG   | 2:B:1015:HIS:HE1  | 1.92                     | 0.53              |
| 1:A:608:ILE:O    | 1:A:609:ASP:O     | 2.26                     | 0.53              |
| 1:A:1230:GLU:O   | 1:A:1233:ASP:HB2  | 2.08                     | 0.53              |
| 2:B:1084:GLN:HG2 | 3:C:201:TRP:CH2   | 2.43                     | 0.53              |
| 3:C:56:THR:HG22  | 3:C:58:LEU:N      | 2.22                     | 0.53              |
| 9:K:61:TYR:HA    | 9:K:72:LYS:O      | 2.08                     | 0.53              |
| 1:A:151:ASP:CG   | 1:A:163:SER:HA    | 2.34                     | 0.53              |
| 1:A:305:ASP:HA   | 1:A:326:ARG:HB2   | 1.90                     | 0.53              |
| 1:A:44:THR:HG22  | 1:A:44:THR:O      | 2.08                     | 0.53              |
| 1:A:335:ARG:O    | 1:A:335:ARG:HG3   | 2.09                     | 0.53              |
| 2:B:1065:GLN:NE2 | 2:B:1067:ARG:HB2  | 2.23                     | 0.53              |
| 2:B:1096:ARG:O   | 2:B:1097:HIS:CG   | 2.61                     | 0.53              |
| 3:C:175:ALA:HB3  | 8:J:43:ARG:CZ     | 2.39                     | 0.53              |
| 13:N:6:DT:H2''   | 13:N:7:DA:OP2     | 2.09                     | 0.53              |
| 1:A:218:ASP:O    | 1:A:222:LEU:HG    | 2.09                     | 0.53              |
| 1:A:848:ILE:HD11 | 1:A:1374:VAL:HG21 | 1.90                     | 0.53              |
| 2:B:36:ALA:C     | 2:B:37:PHE:O      | 2.42                     | 0.53              |
| 9:K:21:ILE:HG12  | 9:K:33:ILE:HG12   | 1.91                     | 0.53              |
| 13:N:6:DT:C4     | 13:N:7:DA:N6      | 2.77                     | 0.53              |
| 2:B:65:GLU:H     | 2:B:67:SER:HB3    | 1.73                     | 0.53              |
| 2:B:1109:GLY:O   | 2:B:1111:MET:HE2  | 2.09                     | 0.53              |
| 13:N:5:DT:C2'    | 13:N:6:DT:C7      | 2.81                     | 0.53              |
| 1:A:215:SER:HB3  | 1:A:218:ASP:HB2   | 1.90                     | 0.53              |
| 4:E:55:ARG:O     | 4:E:57:MET:N      | 2.42                     | 0.53              |
| 12:T:3:DA:N1     | 13:N:12:DT:C4     | 2.77                     | 0.53              |
| 1:A:828:ALA:CB   | 2:B:530:GLY:HA2   | 2.38                     | 0.52              |
| 2:B:637:LEU:HD13 | 2:B:740:HIS:HB3   | 1.91                     | 0.52              |
| 2:B:751:VAL:HG13 | 2:B:752:ALA:N     | 2.23                     | 0.52              |
| 4:E:32:GLN:HE21  | 4:E:32:GLN:HA     | 1.74                     | 0.52              |
| 12:T:2:DT:H2'    | 12:T:3:DA:H8      | 1.65                     | 0.52              |
| 1:A:550:LEU:HD11 | 1:A:580:VAL:HG21  | 1.90                     | 0.52              |
| 6:H:83:GLN:O     | 6:H:86:ASP:HB3    | 2.10                     | 0.52              |
| 12:T:21:DC:H2''  | 12:T:22:DT:H5'    | 1.90                     | 0.52              |
| 1:A:577:ILE:HD12 | 1:A:578:LEU:H     | 1.73                     | 0.52              |
| 2:B:256:VAL:HG11 | 2:B:382:ILE:HD13  | 1.92                     | 0.52              |
| 1:A:870:GLU:HB2  | 4:E:204:THR:HG21  | 1.91                     | 0.52              |
| 8:J:1:MET:N      | 8:J:57:ILE:H      | 2.07                     | 0.52              |
| 1:A:77:CYS:C     | 1:A:79:GLY:H      | 2.17                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:R:7:A:H2'      | 11:R:8:G:O4'      | 2.10                     | 0.52              |
| 1:A:91:PHE:HA     | 1:A:235:ILE:HG22  | 1.92                     | 0.52              |
| 2:B:114:PRO:HG2   | 2:B:181:LEU:HD11  | 1.91                     | 0.52              |
| 2:B:487:THR:HG23  | 2:B:488:TYR:N     | 2.25                     | 0.52              |
| 2:B:635:ARG:O     | 2:B:636:PRO:O     | 2.26                     | 0.52              |
| 2:B:778:MET:HE1   | 2:B:853:SER:CB    | 2.35                     | 0.52              |
| 4:E:156:LEU:HD23  | 4:E:197:LYS:HB2   | 1.92                     | 0.52              |
| 1:A:1194:ARG:NH2  | 1:A:1237:ILE:HD13 | 2.24                     | 0.52              |
| 2:B:325:GLN:NE2   | 7:I:12:ASN:OD1    | 2.43                     | 0.52              |
| 6:H:40:LEU:CD1    | 6:H:123:MET:HB2   | 2.32                     | 0.52              |
| 12:T:7:DA:OP2     | 12:T:7:DA:H2'     | 2.10                     | 0.52              |
| 13:N:3:DG:C2'     | 13:N:4:DG:OP2     | 2.50                     | 0.52              |
| 1:A:225:ASN:C     | 1:A:225:ASN:HD22  | 2.18                     | 0.52              |
| 1:A:1032:LEU:O    | 1:A:1036:ARG:HG2  | 2.10                     | 0.52              |
| 6:H:104:PHE:CD2   | 6:H:114:VAL:HG12  | 2.44                     | 0.52              |
| 12:T:8:DT:N3      | 13:N:7:DA:C2      | 2.74                     | 0.52              |
| 1:A:65:LEU:C      | 1:A:66:LYS:HG3    | 2.34                     | 0.52              |
| 1:A:511:ILE:O     | 1:A:519:PRO:HA    | 2.10                     | 0.52              |
| 1:A:855:THR:HG21  | 1:A:857:ARG:NE    | 2.11                     | 0.52              |
| 2:B:25:ILE:HG22   | 2:B:26:THR:O      | 2.10                     | 0.52              |
| 2:B:986:GLN:HE21  | 2:B:1022:THR:CG2  | 2.23                     | 0.52              |
| 2:B:1103:ILE:O    | 2:B:1122:ARG:NH1  | 2.42                     | 0.52              |
| 3:C:69:LEU:CB     | 8:J:5:VAL:CG1     | 2.88                     | 0.52              |
| 1:A:276:LEU:HD11  | 1:A:293:GLU:HG2   | 1.92                     | 0.51              |
| 1:A:1193:LEU:HD12 | 1:A:1194:ARG:N    | 2.25                     | 0.51              |
| 2:B:64:CYS:O      | 2:B:65:GLU:CD     | 2.53                     | 0.51              |
| 3:C:147:LEU:HB3   | 3:C:151:GLN:HB2   | 1.92                     | 0.51              |
| 1:A:289:ILE:O     | 1:A:293:GLU:HG3   | 2.10                     | 0.51              |
| 1:A:404:TYR:HA    | 1:A:413:ILE:O     | 2.11                     | 0.51              |
| 1:A:969:GLN:C     | 1:A:971:PHE:H     | 2.18                     | 0.51              |
| 2:B:62:ILE:HG23   | 2:B:418:LYS:HG3   | 1.91                     | 0.51              |
| 2:B:169:ARG:HG3   | 2:B:454:THR:HG23  | 1.91                     | 0.51              |
| 2:B:475:SER:O     | 2:B:476:ARG:C     | 2.52                     | 0.51              |
| 3:C:242:GLN:HE21  | 3:C:246:ARG:HE    | 1.57                     | 0.51              |
| 2:B:487:THR:CG2   | 2:B:488:TYR:N     | 2.73                     | 0.51              |
| 2:B:605:ARG:HH21  | 2:B:639:ILE:HG12  | 1.76                     | 0.51              |
| 2:B:681:TRP:O     | 2:B:684:LEU:HB2   | 2.10                     | 0.51              |
| 9:K:83:PRO:O      | 9:K:86:ALA:HB3    | 2.10                     | 0.51              |
| 1:A:23:SER:O      | 1:A:26:GLU:N      | 2.43                     | 0.51              |
| 1:A:1067:LEU:HD12 | 1:A:1067:LEU:O    | 2.10                     | 0.51              |
| 1:A:1355:VAL:HG12 | 1:A:1356:ILE:HD13 | 1.92                     | 0.51              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B:254:LEU:HD23 | 2:B:381:MET:CE    | 2.23                     | 0.51              |
| 2:B:911:ILE:HG23 | 2:B:966:VAL:HG11  | 1.92                     | 0.51              |
| 4:E:164:LEU:HD13 | 4:E:211:TYR:CE2   | 2.46                     | 0.51              |
| 9:K:37:LYS:O     | 9:K:38:GLU:HG2    | 2.11                     | 0.51              |
| 10:L:44:ASP:O    | 10:L:46:VAL:N     | 2.43                     | 0.51              |
| 2:B:489:SER:HA   | 2:B:492:LEU:HB2   | 1.93                     | 0.51              |
| 1:A:24:PRO:HB3   | 1:A:237:THR:HB    | 1.92                     | 0.51              |
| 1:A:30:ILE:HG12  | 2:B:1170:THR:HG21 | 1.92                     | 0.51              |
| 1:A:596:THR:O    | 1:A:597:LEU:C     | 2.52                     | 0.51              |
| 1:A:856:THR:HB   | 1:A:865:GLN:HB2   | 1.93                     | 0.51              |
| 1:A:1423:GLY:O   | 1:A:1424:VAL:C    | 2.53                     | 0.51              |
| 6:H:5:LEU:HD11   | 6:H:61:SER:HB3    | 1.93                     | 0.51              |
| 7:I:60:GLN:HE21  | 7:I:60:GLN:HA     | 1.75                     | 0.51              |
| 12:T:7:DA:C2     | 12:T:8:DT:C5      | 2.97                     | 0.51              |
| 1:A:244:PRO:C    | 1:A:246:VAL:H     | 2.19                     | 0.51              |
| 2:B:952:VAL:HG13 | 2:B:966:VAL:HG22  | 1.93                     | 0.51              |
| 2:B:1072:MET:HE2 | 2:B:1085:ILE:CB   | 2.41                     | 0.51              |
| 9:K:49:GLU:HG3   | 9:K:94:ILE:HG13   | 1.93                     | 0.51              |
| 12:T:3:DA:C2     | 13:N:12:DT:N3     | 2.73                     | 0.51              |
| 1:A:68:GLN:C     | 1:A:70:CYS:H      | 2.19                     | 0.51              |
| 1:A:225:ASN:C    | 1:A:225:ASN:ND2   | 2.69                     | 0.51              |
| 1:A:858:ASN:ND2  | 1:A:860:LEU:H     | 2.08                     | 0.51              |
| 1:A:870:GLU:HG2  | 4:E:208:TYR:CG    | 2.46                     | 0.51              |
| 2:B:487:THR:H    | 2:B:490:SER:HB3   | 1.76                     | 0.51              |
| 2:B:639:ILE:HD11 | 2:B:691:GLU:HB2   | 1.91                     | 0.51              |
| 3:C:133:ILE:CD1  | 3:C:237:SER:HA    | 2.41                     | 0.51              |
| 6:H:131:ASN:C    | 6:H:133:ASN:N     | 2.69                     | 0.51              |
| 2:B:485:ARG:HG2  | 2:B:485:ARG:NH1   | 2.08                     | 0.51              |
| 6:H:137:GLN:C    | 6:H:139:ASN:H     | 2.18                     | 0.51              |
| 12:T:7:DA:N3     | 12:T:8:DT:C5      | 2.78                     | 0.51              |
| 1:A:507:VAL:N    | 1:A:508:PRO:CD    | 2.73                     | 0.51              |
| 1:A:1121:GLU:O   | 1:A:1124:HIS:O    | 2.29                     | 0.51              |
| 6:H:2:SER:HA     | 6:H:62:SER:HB3    | 1.93                     | 0.51              |
| 6:H:109:LYS:HB2  | 6:H:110:ASP:O     | 2.11                     | 0.51              |
| 2:B:778:MET:HE1  | 2:B:1094:ARG:HD3  | 1.93                     | 0.50              |
| 6:H:41:ASP:OD2   | 6:H:122:LEU:N     | 2.39                     | 0.50              |
| 7:I:111:THR:HG22 | 7:I:113:ASP:HB3   | 1.93                     | 0.50              |
| 13:N:12:DT:H1'   | 13:N:13:DA:C8     | 2.46                     | 0.50              |
| 13:N:13:DA:H8    | 13:N:13:DA:P      | 2.35                     | 0.50              |
| 1:A:276:LEU:HD13 | 1:A:292:ALA:O     | 2.11                     | 0.50              |
| 2:B:120:ARG:CD   | 2:B:955:THR:HG21  | 2.35                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:E:97:VAL:HG12   | 4:E:97:VAL:O      | 2.11                     | 0.50              |
| 1:A:596:THR:C     | 1:A:598:LEU:N     | 2.67                     | 0.50              |
| 1:A:693:VAL:HG21  | 1:A:721:PHE:HE1   | 1.75                     | 0.50              |
| 2:B:398:ARG:HB3   | 2:B:398:ARG:NH1   | 2.27                     | 0.50              |
| 6:H:131:ASN:OD1   | 6:H:132:LEU:N     | 2.42                     | 0.50              |
| 9:K:49:GLU:HG3    | 9:K:94:ILE:HG12   | 1.92                     | 0.50              |
| 1:A:920:LEU:HD23  | 1:A:921:GLY:N     | 2.27                     | 0.50              |
| 2:B:839:MET:CE    | 2:B:1010:LEU:HD21 | 2.41                     | 0.50              |
| 1:A:256:GLN:CA    | 1:A:257:ARG:HB3   | 2.41                     | 0.50              |
| 1:A:472:LEU:HD11  | 2:B:835:GLN:NE2   | 2.27                     | 0.50              |
| 1:A:553:VAL:CG2   | 1:A:652:VAL:CG2   | 2.88                     | 0.50              |
| 1:A:647:GLY:O     | 1:A:651:LYS:HG3   | 2.11                     | 0.50              |
| 1:A:868:TYR:CZ    | 1:A:1064:VAL:HG21 | 2.46                     | 0.50              |
| 1:A:1101:LEU:HD13 | 1:A:1355:VAL:HG11 | 1.94                     | 0.50              |
| 2:B:911:ILE:HD11  | 2:B:941:LEU:HD23  | 1.92                     | 0.50              |
| 12:T:7:DA:C2      | 12:T:8:DT:C2      | 3.00                     | 0.50              |
| 1:A:87:ALA:HB3    | 1:A:276:LEU:HD23  | 1.94                     | 0.50              |
| 1:A:731:ARG:HG3   | 1:A:755:PHE:CZ    | 2.46                     | 0.50              |
| 2:B:176:SER:O     | 2:B:182:SER:HB3   | 2.12                     | 0.50              |
| 2:B:878:GLN:O     | 2:B:879:ARG:C     | 2.55                     | 0.50              |
| 13:N:5:DT:H2"     | 13:N:6:DT:C5      | 2.46                     | 0.50              |
| 1:A:114:LEU:HD11  | 1:A:171:GLN:HE21  | 1.77                     | 0.50              |
| 1:A:219:PHE:O     | 1:A:222:LEU:N     | 2.43                     | 0.50              |
| 1:A:482:PHE:CD1   | 2:B:836:GLU:HB2   | 2.46                     | 0.50              |
| 2:B:981:ALA:O     | 2:B:1093:GLN:HG2  | 2.11                     | 0.50              |
| 5:F:79:ARG:HG2    | 5:F:144:GLU:HB3   | 1.93                     | 0.50              |
| 12:T:14:DC:H2"    | 12:T:15:DC:OP2    | 2.12                     | 0.50              |
| 3:C:124:LEU:HD22  | 3:C:129:ILE:HG22  | 1.93                     | 0.50              |
| 4:E:179:GLN:HA    | 4:E:179:GLN:NE2   | 2.27                     | 0.50              |
| 4:E:179:GLN:HE22  | 4:E:215:MET:HE2   | 1.76                     | 0.50              |
| 1:A:65:LEU:O      | 1:A:66:LYS:HG3    | 2.11                     | 0.50              |
| 2:B:63:ILE:O      | 2:B:67:SER:CB     | 2.55                     | 0.50              |
| 2:B:680:THR:O     | 2:B:681:TRP:C     | 2.53                     | 0.50              |
| 2:B:797:TYR:CE2   | 3:C:62:PHE:CD2    | 3.00                     | 0.50              |
| 4:E:72:PHE:HE2    | 4:E:157:SER:HB3   | 1.77                     | 0.50              |
| 8:J:48:ARG:HE     | 8:J:49:MET:HE2    | 1.77                     | 0.50              |
| 12:T:5:DC:C4      | 12:T:6:DC:C4      | 2.99                     | 0.50              |
| 1:A:1053:PHE:O    | 1:A:1056:SER:N    | 2.36                     | 0.49              |
| 2:B:118:ARG:HH22  | 2:B:194:GLU:CD    | 2.20                     | 0.49              |
| 7:I:59:VAL:HG12   | 7:I:61:ASP:H      | 1.76                     | 0.49              |
| 1:A:852:TYR:CE2   | 1:A:1060:PRO:HB2  | 2.46                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1193:LEU:HD12 | 1:A:1193:LEU:C    | 2.36                     | 0.49              |
| 2:B:636:PRO:HB3   | 2:B:637:LEU:HA    | 1.93                     | 0.49              |
| 1:A:560:ILE:N     | 6:H:78:SER:HB2    | 2.28                     | 0.49              |
| 1:A:1198:ASP:O    | 1:A:1202:MET:HG2  | 2.12                     | 0.49              |
| 2:B:471:LYS:HD2   | 2:B:471:LYS:O     | 2.11                     | 0.49              |
| 2:B:563:MET:HG3   | 2:B:563:MET:O     | 2.13                     | 0.49              |
| 2:B:574:SER:HB3   | 2:B:591:ARG:HH22  | 1.78                     | 0.49              |
| 2:B:863:GLU:OE1   | 2:B:962:LYS:HB3   | 2.12                     | 0.49              |
| 12:T:6:DC:N3      | 12:T:7:DA:C5      | 2.79                     | 0.49              |
| 1:A:567:LYS:HD2   | 6:H:95:TYR:CD1    | 2.48                     | 0.49              |
| 1:A:907:THR:HG22  | 1:A:908:LEU:H     | 1.78                     | 0.49              |
| 1:A:1410:PHE:CD2  | 2:B:1212:ILE:HD11 | 2.45                     | 0.49              |
| 2:B:1096:ARG:O    | 2:B:1097:HIS:CB   | 2.59                     | 0.49              |
| 3:C:76:ASP:OD2    | 3:C:128:ASN:HB3   | 2.12                     | 0.49              |
| 7:I:99:LEU:HB2    | 7:I:112:SER:HB3   | 1.93                     | 0.49              |
| 1:A:303:TYR:O     | 1:A:303:TYR:CG    | 2.66                     | 0.49              |
| 1:A:518:LYS:HB2   | 1:A:519:PRO:HD2   | 1.93                     | 0.49              |
| 1:A:697:ALA:HB2   | 1:A:702:LEU:HD23  | 1.93                     | 0.49              |
| 1:A:1194:ARG:HH21 | 1:A:1237:ILE:HD13 | 1.76                     | 0.49              |
| 2:B:361:LEU:N     | 2:B:362:PRO:HD3   | 2.27                     | 0.49              |
| 7:I:47:GLU:HG2    | 7:I:50:THR:HG23   | 1.94                     | 0.49              |
| 13:N:4:DG:C2'     | 13:N:5:DT:H5''    | 2.42                     | 0.49              |
| 1:A:322:VAL:C     | 1:A:323:LYS:HD3   | 2.37                     | 0.49              |
| 1:A:350:ARG:HG3   | 1:A:488:ASN:OD1   | 2.13                     | 0.49              |
| 2:B:356:LEU:HA    | 2:B:360:PHE:HB3   | 1.95                     | 0.49              |
| 2:B:487:THR:HG22  | 2:B:489:SER:N     | 2.28                     | 0.49              |
| 7:I:33:SER:O      | 7:I:34:TYR:O      | 2.30                     | 0.49              |
| 2:B:764:SER:O     | 2:B:765:PRO:C     | 2.55                     | 0.49              |
| 3:C:18:VAL:HG22   | 3:C:240:VAL:HB    | 1.95                     | 0.49              |
| 4:E:59:SER:HB3    | 4:E:81:GLU:HA     | 1.95                     | 0.49              |
| 1:A:103:CYS:O     | 1:A:174:ILE:HD12  | 2.13                     | 0.49              |
| 1:A:550:LEU:HG    | 1:A:556:TRP:CE2   | 2.47                     | 0.49              |
| 1:A:560:ILE:H     | 6:H:78:SER:HB2    | 1.78                     | 0.49              |
| 1:A:784:LEU:HB3   | 1:A:786:HIS:HD2   | 1.76                     | 0.49              |
| 2:B:211:VAL:HG13  | 2:B:495:LEU:HD23  | 1.94                     | 0.49              |
| 2:B:906:SER:HA    | 2:B:946:ASN:HB2   | 1.93                     | 0.49              |
| 1:A:565:ILE:HG23  | 1:A:567:LYS:CG    | 2.40                     | 0.49              |
| 2:B:487:THR:O     | 2:B:490:SER:HB3   | 2.12                     | 0.49              |
| 6:H:109:LYS:HB3   | 6:H:110:ASP:CB    | 2.43                     | 0.49              |
| 12:T:2:DT:C3'     | 12:T:3:DA:H5'     | 2.32                     | 0.49              |
| 1:A:401:GLY:N     | 1:A:435:HIS:HD2   | 2.10                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:493:SER:OG    | 2:B:775:LYS:HE2   | 2.13                     | 0.49              |
| 8:J:1:MET:HB2     | 8:J:56:LEU:HD12   | 1.94                     | 0.49              |
| 1:A:494:SER:O     | 1:A:498:ARG:HG2   | 2.12                     | 0.48              |
| 1:A:605:MET:HA    | 1:A:605:MET:CE    | 2.43                     | 0.48              |
| 1:A:977:LYS:HE3   | 1:A:977:LYS:HA    | 1.94                     | 0.48              |
| 1:A:1342:GLU:HG2  | 4:E:212:ARG:NH1   | 2.28                     | 0.48              |
| 1:A:1386:ARG:HE   | 1:A:1403:GLU:HG2  | 1.78                     | 0.48              |
| 2:B:197:PHE:CE1   | 2:B:817:LEU:HD11  | 2.48                     | 0.48              |
| 2:B:254:LEU:CD2   | 2:B:381:MET:CE    | 2.87                     | 0.48              |
| 1:A:590:ARG:O     | 1:A:591:PHE:HB2   | 2.12                     | 0.48              |
| 1:A:1392:SER:O    | 1:A:1394:THR:N    | 2.46                     | 0.48              |
| 2:B:25:ILE:CG2    | 2:B:26:THR:N      | 2.76                     | 0.48              |
| 2:B:100:PRO:HD2   | 2:B:180:TYR:CE1   | 2.48                     | 0.48              |
| 2:B:724:ASP:HB3   | 2:B:727:LYS:HG3   | 1.95                     | 0.48              |
| 1:A:55:ASP:N      | 1:A:56:PRO:HD2    | 2.28                     | 0.48              |
| 1:A:218:ASP:O     | 1:A:222:LEU:CD1   | 2.61                     | 0.48              |
| 1:A:574:GLY:HA2   | 1:A:577:ILE:HD11  | 1.95                     | 0.48              |
| 1:A:663:SER:HB2   | 2:B:827:ILE:O     | 2.13                     | 0.48              |
| 1:A:836:TYR:O     | 1:A:837:ILE:C     | 2.56                     | 0.48              |
| 1:A:869:GLY:O     | 1:A:870:GLU:HB2   | 2.12                     | 0.48              |
| 2:B:519:TRP:CH2   | 2:B:705:MET:HE1   | 2.48                     | 0.48              |
| 2:B:562:GLY:HA3   | 2:B:590:HIS:CE1   | 2.49                     | 0.48              |
| 2:B:635:ARG:C     | 2:B:636:PRO:O     | 2.56                     | 0.48              |
| 2:B:760:ASP:OD1   | 2:B:760:ASP:N     | 2.36                     | 0.48              |
| 2:B:879:ARG:O     | 2:B:880:THR:C     | 2.56                     | 0.48              |
| 6:H:91:ASP:O      | 6:H:92:ASP:OD2    | 2.31                     | 0.48              |
| 12:T:7:DA:C4      | 12:T:8:DT:C5      | 3.01                     | 0.48              |
| 13:N:2:DT:H2''    | 13:N:3:DG:O5'     | 2.13                     | 0.48              |
| 1:A:260:ASP:CG    | 1:A:261:ASP:H     | 2.21                     | 0.48              |
| 1:A:800:VAL:HA    | 1:A:812:GLU:HG2   | 1.96                     | 0.48              |
| 1:A:1293:SER:HB2  | 1:A:1299:VAL:CG2  | 2.43                     | 0.48              |
| 1:A:1438:THR:N    | 5:F:88:TYR:HB3    | 2.27                     | 0.48              |
| 2:B:65:GLU:CG     | 2:B:66:ASP:H      | 2.26                     | 0.48              |
| 2:B:834:ASN:ND2   | 2:B:1011:ILE:HG22 | 2.29                     | 0.48              |
| 2:B:973:ILE:HG23  | 2:B:974:PRO:HD2   | 1.94                     | 0.48              |
| 2:B:1010:LEU:HD12 | 2:B:1010:LEU:HA   | 1.51                     | 0.48              |
| 2:B:1072:MET:HE2  | 2:B:1085:ILE:HB   | 1.94                     | 0.48              |
| 3:C:206:ASN:ND2   | 3:C:229:TYR:CB    | 2.76                     | 0.48              |
| 1:A:546:VAL:O     | 1:A:550:LEU:HB2   | 2.12                     | 0.48              |
| 1:A:1356:ILE:HD13 | 1:A:1356:ILE:N    | 2.28                     | 0.48              |
| 2:B:840:ILE:HG12  | 2:B:992:ILE:HG22  | 1.95                     | 0.48              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:868:TYR:CZ    | 1:A:1064:VAL:CG2 | 2.97                     | 0.48              |
| 2:B:100:PRO:C     | 2:B:101:MET:HG3  | 2.38                     | 0.48              |
| 2:B:532:ALA:HB1   | 2:B:536:VAL:HG23 | 1.95                     | 0.48              |
| 1:A:346:ASP:OD1   | 2:B:1108:ARG:HA  | 2.13                     | 0.48              |
| 1:A:1110:ASN:ND2  | 1:A:1110:ASN:H   | 2.11                     | 0.48              |
| 2:B:287:ARG:NH1   | 2:B:324:ILE:O    | 2.44                     | 0.48              |
| 2:B:470:LYS:C     | 2:B:472:ALA:H    | 2.22                     | 0.48              |
| 2:B:591:ARG:O     | 2:B:592:ASN:CB   | 2.61                     | 0.48              |
| 2:B:806:THR:HG22  | 2:B:808:ALA:H    | 1.78                     | 0.48              |
| 3:C:231:ASN:C     | 3:C:231:ASN:ND2  | 2.71                     | 0.48              |
| 1:A:224:PHE:CZ    | 1:A:231:PRO:HG3  | 2.49                     | 0.48              |
| 1:A:407:ARG:HD2   | 1:A:413:ILE:HD11 | 1.95                     | 0.48              |
| 1:A:752:LYS:HD3   | 2:B:1019:SER:HB3 | 1.95                     | 0.48              |
| 1:A:1364:ASN:HD22 | 1:A:1366:ARG:CG  | 2.22                     | 0.48              |
| 1:A:1386:ARG:NE   | 1:A:1403:GLU:HG2 | 2.28                     | 0.48              |
| 2:B:211:VAL:CG2   | 2:B:483:LEU:HD23 | 2.43                     | 0.48              |
| 2:B:315:LYS:HG2   | 7:I:13:MET:HE1   | 1.94                     | 0.48              |
| 2:B:734:HIS:O     | 2:B:735:ALA:HB3  | 2.12                     | 0.48              |
| 1:A:1159:ARG:NH1  | 1:A:1159:ARG:HB3 | 2.28                     | 0.48              |
| 2:B:706:GLN:O     | 2:B:710:LEU:HB2  | 2.14                     | 0.48              |
| 2:B:783:THR:HG22  | 8:J:63:TYR:HE1   | 1.79                     | 0.48              |
| 3:C:99:LEU:HD23   | 3:C:99:LEU:H     | 1.77                     | 0.48              |
| 5:F:116:ASP:HB3   | 5:F:119:ARG:HB2  | 1.95                     | 0.48              |
| 6:H:15:VAL:HA     | 6:H:26:ILE:HD12  | 1.95                     | 0.48              |
| 1:A:1098:VAL:N    | 1:A:1099:PRO:HD2 | 2.29                     | 0.48              |
| 2:B:778:MET:HE3   | 2:B:853:SER:HB3  | 1.92                     | 0.48              |
| 3:C:73:GLN:NE2    | 3:C:75:MET:N     | 2.49                     | 0.48              |
| 3:C:262:LEU:CD1   | 9:K:88:LYS:HG2   | 2.44                     | 0.48              |
| 1:A:567:LYS:HD2   | 6:H:95:TYR:CE1   | 2.49                     | 0.47              |
| 1:A:629:LEU:HD22  | 1:A:633:VAL:HG23 | 1.94                     | 0.47              |
| 1:A:871:ASP:HB3   | 4:E:205:SER:HB3  | 1.95                     | 0.47              |
| 2:B:770:GLN:O     | 2:B:770:GLN:CD   | 2.57                     | 0.47              |
| 2:B:1037:LEU:HD13 | 2:B:1062:HIS:HB3 | 1.95                     | 0.47              |
| 13:N:2:DT:C2'     | 13:N:3:DG:C8     | 2.95                     | 0.47              |
| 1:A:8:SER:HB3     | 2:B:1180:PHE:HE1 | 1.79                     | 0.47              |
| 1:A:664:THR:HG23  | 1:A:742:ASN:HB2  | 1.95                     | 0.47              |
| 2:B:121:ASN:ND2   | 2:B:207:GLY:HA3  | 2.28                     | 0.47              |
| 2:B:778:MET:HG2   | 2:B:794:ASN:HB3  | 1.96                     | 0.47              |
| 2:B:957:ASN:CG    | 2:B:958:GLN:N    | 2.73                     | 0.47              |
| 12:T:5:DC:C5      | 12:T:6:DC:C4     | 3.03                     | 0.47              |
| 1:A:852:TYR:CD2   | 1:A:1060:PRO:HB2 | 2.50                     | 0.47              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:982:THR:O    | 1:A:983:ILE:C     | 2.57                     | 0.47              |
| 1:A:1312:ASN:ND2 | 1:A:1314:SER:OG   | 2.47                     | 0.47              |
| 2:B:227:LYS:H    | 2:B:395:GLN:HG3   | 1.79                     | 0.47              |
| 2:B:334:ILE:HG22 | 2:B:334:ILE:O     | 2.14                     | 0.47              |
| 2:B:365:THR:HG23 | 2:B:367:LEU:N     | 2.28                     | 0.47              |
| 1:A:96:ILE:O     | 1:A:97:ALA:C      | 2.58                     | 0.47              |
| 1:A:108:MET:HE2  | 1:A:202:LEU:HD21  | 1.96                     | 0.47              |
| 1:A:974:ASP:OD1  | 1:A:977:LYS:HB2   | 2.14                     | 0.47              |
| 1:A:1277:GLU:O   | 1:A:1278:ASN:HB2  | 2.13                     | 0.47              |
| 2:B:515:HIS:CD2  | 2:B:517:THR:H     | 2.22                     | 0.47              |
| 2:B:826:ALA:O    | 2:B:1011:ILE:HA   | 2.14                     | 0.47              |
| 2:B:951:GLN:HG2  | 10:L:57:LEU:HD22  | 1.95                     | 0.47              |
| 2:B:1110:PRO:O   | 2:B:1119:VAL:HG13 | 2.14                     | 0.47              |
| 3:C:9:LYS:HB2    | 3:C:9:LYS:HE2     | 1.62                     | 0.47              |
| 3:C:167:HIS:HD2  | 3:C:169:LYS:H     | 1.62                     | 0.47              |
| 4:E:192:ARG:O    | 4:E:192:ARG:HG3   | 2.14                     | 0.47              |
| 13:N:3:DG:OP2    | 13:N:3:DG:H2'     | 2.14                     | 0.47              |
| 13:N:10:DG:H2''  | 13:N:11:DG:OP2    | 2.14                     | 0.47              |
| 1:A:43:GLU:O     | 1:A:43:GLU:HG2    | 2.14                     | 0.47              |
| 1:A:553:VAL:HG23 | 1:A:652:VAL:HG23  | 1.96                     | 0.47              |
| 1:A:672:ASP:HB3  | 1:A:675:THR:H     | 1.79                     | 0.47              |
| 3:C:172:PRO:O    | 3:C:235:VAL:HG23  | 2.14                     | 0.47              |
| 1:A:100:LYS:HG3  | 1:A:181:LEU:HD22  | 1.95                     | 0.47              |
| 1:A:261:ASP:HB3  | 1:A:323:LYS:HD2   | 1.96                     | 0.47              |
| 1:A:550:LEU:HD12 | 1:A:550:LEU:HA    | 1.58                     | 0.47              |
| 2:B:862:GLN:HE21 | 2:B:961:LEU:CD1   | 2.28                     | 0.47              |
| 3:C:244:VAL:HG21 | 9:K:105:PHE:CZ    | 2.50                     | 0.47              |
| 1:A:328:ARG:HD3  | 2:B:1206:GLU:OE1  | 2.14                     | 0.47              |
| 1:A:445:ASN:CG   | 1:A:455:MET:HE3   | 2.40                     | 0.47              |
| 1:A:492:PRO:CB   | 1:A:497:THR:HG23  | 2.44                     | 0.47              |
| 1:A:535:THR:O    | 1:A:536:LEU:C     | 2.58                     | 0.47              |
| 1:A:754:SER:H    | 1:A:757:ASN:HD22  | 1.61                     | 0.47              |
| 1:A:1293:SER:HB3 | 1:A:1297:GLU:O    | 2.15                     | 0.47              |
| 2:B:412:LEU:O    | 2:B:413:LEU:C     | 2.57                     | 0.47              |
| 3:C:29:MET:HA    | 9:K:45:LEU:CD1    | 2.45                     | 0.47              |
| 4:E:167:ARG:HD3  | 4:E:167:ARG:HA    | 1.59                     | 0.47              |
| 8:J:36:LEU:HD13  | 8:J:47:ARG:HG3    | 1.96                     | 0.47              |
| 12:T:6:DC:N4     | 12:T:7:DA:N6      | 2.62                     | 0.47              |
| 1:A:378:GLU:OE1  | 1:A:434:ARG:HD3   | 2.14                     | 0.47              |
| 1:A:567:LYS:CB   | 6:H:95:TYR:HA     | 2.45                     | 0.47              |
| 1:A:636:GLU:OE2  | 1:A:962:ARG:HD2   | 2.15                     | 0.47              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B:620:ARG:CZ   | 7:I:68:LEU:HD21   | 2.44                     | 0.47              |
| 1:A:208:LEU:HD21 | 1:A:212:LYS:NZ    | 2.30                     | 0.47              |
| 1:A:243:PRO:O    | 1:A:244:PRO:C     | 2.57                     | 0.47              |
| 1:A:499:ALA:O    | 1:A:503:GLN:HG2   | 2.14                     | 0.47              |
| 1:A:896:ARG:HD2  | 1:A:897:TYR:CE1   | 2.50                     | 0.47              |
| 2:B:473:MET:C    | 2:B:475:SER:N     | 2.72                     | 0.47              |
| 2:B:512:ARG:HB3  | 2:B:533:CYS:O     | 2.15                     | 0.47              |
| 2:B:552:MET:N    | 2:B:553:PRO:HD2   | 2.30                     | 0.47              |
| 2:B:797:TYR:CE2  | 3:C:62:PHE:HD2    | 2.32                     | 0.47              |
| 2:B:807:ARG:HG2  | 2:B:1045:SER:OG   | 2.14                     | 0.47              |
| 3:C:76:ASP:OD2   | 3:C:128:ASN:N     | 2.46                     | 0.47              |
| 13:N:4:DG:N1     | 13:N:5:DT:C2      | 2.81                     | 0.47              |
| 1:A:1128:GLN:HB2 | 1:A:1304:TRP:NE1  | 2.30                     | 0.47              |
| 2:B:102:VAL:HG22 | 2:B:112:LEU:HB2   | 1.97                     | 0.47              |
| 2:B:115:GLN:HE21 | 2:B:119:LEU:HD11  | 1.81                     | 0.47              |
| 3:C:47:ASP:O     | 3:C:48:SER:HB2    | 2.15                     | 0.47              |
| 4:E:76:GLY:O     | 4:E:77:SER:C      | 2.58                     | 0.47              |
| 10:L:47:ARG:NH1  | 10:L:54:ARG:NE    | 2.52                     | 0.47              |
| 2:B:784:ASN:OD1  | 2:B:788:ARG:HD2   | 2.13                     | 0.46              |
| 2:B:957:ASN:ND2  | 2:B:959:ASP:HB2   | 2.30                     | 0.46              |
| 3:C:190:ASP:C    | 3:C:190:ASP:OD1   | 2.58                     | 0.46              |
| 2:B:860:MET:HG2  | 2:B:861:ASP:H     | 1.80                     | 0.46              |
| 4:E:64:PRO:HD3   | 4:E:76:GLY:HA2    | 1.97                     | 0.46              |
| 9:K:51:LEU:CD1   | 9:K:59:ALA:HB3    | 2.45                     | 0.46              |
| 1:A:312:PRO:C    | 1:A:313:GLN:HE21  | 2.23                     | 0.46              |
| 1:A:741:ASN:ND2  | 1:A:744:LYS:H     | 2.07                     | 0.46              |
| 1:A:855:THR:HG22 | 1:A:857:ARG:HG3   | 1.96                     | 0.46              |
| 1:A:899:VAL:HB   | 1:A:929:LEU:HD13  | 1.98                     | 0.46              |
| 1:A:1353:TYR:HD1 | 1:A:1368:MET:HE1  | 1.79                     | 0.46              |
| 2:B:258:LEU:HD12 | 2:B:269:ILE:HG12  | 1.98                     | 0.46              |
| 2:B:331:LEU:O    | 2:B:334:ILE:HB    | 2.15                     | 0.46              |
| 2:B:744:HIS:O    | 2:B:747:MET:HB2   | 2.15                     | 0.46              |
| 2:B:778:MET:O    | 2:B:819:ALA:HB1   | 2.16                     | 0.46              |
| 5:F:113:GLY:O    | 5:F:115:THR:HG23  | 2.15                     | 0.46              |
| 1:A:68:GLN:NE2   | 1:A:70:CYS:HB3    | 2.27                     | 0.46              |
| 1:A:253:ASN:O    | 1:A:254:GLU:HB2   | 2.15                     | 0.46              |
| 1:A:472:LEU:HD21 | 2:B:835:GLN:HB2   | 1.97                     | 0.46              |
| 1:A:1166:ASP:HA  | 1:A:1169:ILE:HD13 | 1.98                     | 0.46              |
| 6:H:93:TYR:HB3   | 6:H:144:ILE:O     | 2.16                     | 0.46              |
| 6:H:109:LYS:HB3  | 6:H:110:ASP:CG    | 2.40                     | 0.46              |
| 1:A:372:LYS:HD3  | 1:A:397:ASN:HA    | 1.97                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:545:ILE:HG13  | 2:B:633:VAL:HG13  | 1.96                     | 0.46              |
| 2:B:780:VAL:HG21  | 8:J:56:LEU:HD13   | 1.97                     | 0.46              |
| 2:B:1079:LYS:HE2  | 3:C:188:HIS:CE1   | 2.51                     | 0.46              |
| 3:C:236:GLY:C     | 3:C:238:ILE:H     | 2.23                     | 0.46              |
| 1:A:573:SER:O     | 1:A:574:GLY:C     | 2.59                     | 0.46              |
| 1:A:1209:MET:SD   | 1:A:1236:LEU:HB3  | 2.55                     | 0.46              |
| 1:A:1420:ASP:HB3  | 1:A:1422:ARG:HG2  | 1.97                     | 0.46              |
| 2:B:217:ARG:NH1   | 2:B:407:ASP:OD1   | 2.48                     | 0.46              |
| 2:B:485:ARG:CG    | 2:B:485:ARG:NH1   | 2.68                     | 0.46              |
| 2:B:592:ASN:H     | 2:B:593:PRO:HD3   | 1.80                     | 0.46              |
| 6:H:47:PHE:CB     | 6:H:95:TYR:HD1    | 2.27                     | 0.46              |
| 9:K:20:LYS:O      | 9:K:33:ILE:HA     | 2.15                     | 0.46              |
| 1:A:134:ARG:CD    | 1:A:221:SER:O     | 2.63                     | 0.46              |
| 1:A:351:THR:HG21  | 1:A:466:SER:O     | 2.16                     | 0.46              |
| 1:A:738:LYS:HB3   | 6:H:19:ARG:HH22   | 1.81                     | 0.46              |
| 1:A:1308:THR:HG22 | 1:A:1310:GLY:O    | 2.14                     | 0.46              |
| 1:A:1424:VAL:HG11 | 2:B:1139:ILE:CD1  | 2.46                     | 0.46              |
| 2:B:1077:THR:HG23 | 2:B:1079:LYS:HB2  | 1.98                     | 0.46              |
| 1:A:965:GLN:HA    | 1:A:968:GLN:HG2   | 1.98                     | 0.46              |
| 1:A:1392:SER:C    | 1:A:1394:THR:H    | 2.24                     | 0.46              |
| 2:B:198:ASP:OD1   | 2:B:485:ARG:NH2   | 2.46                     | 0.46              |
| 2:B:1001:PHE:CE2  | 2:B:1073:TYR:HB2  | 2.50                     | 0.46              |
| 13:N:4:DG:C5      | 13:N:5:DT:C7      | 2.98                     | 0.46              |
| 1:A:351:THR:HG22  | 1:A:352:VAL:N     | 2.29                     | 0.46              |
| 1:A:500:GLU:O     | 1:A:504:LEU:HB2   | 2.15                     | 0.46              |
| 1:A:1412:ALA:HA   | 1:A:1417:GLU:HG3  | 1.97                     | 0.46              |
| 1:A:1443:VAL:O    | 1:A:1444:MET:HG3  | 2.16                     | 0.46              |
| 2:B:176:SER:OG    | 2:B:177:LYS:N     | 2.48                     | 0.46              |
| 2:B:1065:GLN:HE21 | 2:B:1069:PHE:HD1  | 1.63                     | 0.46              |
| 2:B:1072:MET:HE2  | 2:B:1085:ILE:HG21 | 1.98                     | 0.46              |
| 1:A:579:SER:HB3   | 1:A:611:GLN:HA    | 1.97                     | 0.46              |
| 1:A:856:THR:O     | 1:A:856:THR:HG22  | 2.15                     | 0.46              |
| 1:A:856:THR:HG22  | 1:A:864:ILE:HB    | 1.97                     | 0.46              |
| 1:A:910:PRO:HA    | 1:A:916:GLY:HA3   | 1.97                     | 0.46              |
| 1:A:1035:TYR:O    | 1:A:1037:LEU:N    | 2.49                     | 0.46              |
| 2:B:28:GLU:C      | 2:B:30:SER:N      | 2.74                     | 0.46              |
| 2:B:416:LEU:HD11  | 2:B:460:ALA:HB3   | 1.94                     | 0.46              |
| 2:B:635:ARG:O     | 2:B:636:PRO:C     | 2.59                     | 0.46              |
| 2:B:642:ASP:CB    | 2:B:649:LYS:HG3   | 2.42                     | 0.46              |
| 2:B:766:ARG:HA    | 2:B:766:ARG:HD3   | 1.74                     | 0.46              |
| 2:B:864:LYS:HD2   | 2:B:865:LYS:H     | 1.81                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:996:ARG:HG3   | 2:B:1007:VAL:HG11 | 1.98                     | 0.46              |
| 2:B:1187:ASN:HD22 | 2:B:1188:LYS:N    | 2.14                     | 0.46              |
| 3:C:69:LEU:O      | 8:J:6:ARG:NH1     | 2.49                     | 0.46              |
| 4:E:119:SER:HB2   | 13:N:12:DT:H5''   | 1.98                     | 0.46              |
| 12:T:1:DC:N4      | 13:N:13:DA:N6     | 2.63                     | 0.46              |
| 1:A:31:SER:CB     | 1:A:83:HIS:HD2    | 2.28                     | 0.45              |
| 1:A:180:LYS:HE3   | 1:A:294:SER:HB3   | 1.97                     | 0.45              |
| 1:A:1073:GLY:O    | 1:A:1076:ALA:HB3  | 2.16                     | 0.45              |
| 2:B:830:TYR:CZ    | 2:B:1000:PRO:HD3  | 2.51                     | 0.45              |
| 2:B:1159:ARG:HE   | 2:B:1193:GLN:NE2  | 2.15                     | 0.45              |
| 5:F:130:ILE:HA    | 5:F:131:PRO:HD3   | 1.87                     | 0.45              |
| 9:K:51:LEU:HD13   | 9:K:59:ALA:HB3    | 1.98                     | 0.45              |
| 1:A:23:SER:O      | 1:A:24:PRO:C      | 2.59                     | 0.45              |
| 1:A:214:ILE:CG2   | 1:A:215:SER:N     | 2.70                     | 0.45              |
| 1:A:360:GLU:HB2   | 1:A:363:GLN:HG3   | 1.98                     | 0.45              |
| 1:A:492:PRO:HB2   | 1:A:497:THR:HG23  | 1.98                     | 0.45              |
| 1:A:1107:VAL:HG23 | 1:A:1383:SER:HB3  | 1.97                     | 0.45              |
| 2:B:230:ALA:N     | 2:B:231:PRO:CD    | 2.73                     | 0.45              |
| 1:A:53:LEU:CD1    | 1:A:266:LEU:O     | 2.65                     | 0.45              |
| 1:A:868:TYR:CE1   | 1:A:1064:VAL:CG2  | 2.98                     | 0.45              |
| 2:B:486:TYR:CE2   | 2:B:1096:ARG:HG2  | 2.52                     | 0.45              |
| 3:C:180:TYR:O     | 3:C:181:ASP:C     | 2.59                     | 0.45              |
| 12:T:7:DA:C2'     | 12:T:8:DT:H5''    | 2.45                     | 0.45              |
| 13:N:4:DG:H2''    | 13:N:5:DT:C5'     | 2.46                     | 0.45              |
| 1:A:709:THR:CG2   | 7:I:94:ASP:HA     | 2.46                     | 0.45              |
| 1:A:753:GLY:HA2   | 1:A:757:ASN:ND2   | 2.31                     | 0.45              |
| 1:A:1297:GLU:CD   | 1:A:1297:GLU:H    | 2.24                     | 0.45              |
| 2:B:551:PRO:C     | 2:B:553:PRO:HD2   | 2.41                     | 0.45              |
| 3:C:33:LEU:HG     | 3:C:37:MET:HE2    | 1.98                     | 0.45              |
| 3:C:186:LEU:HB3   | 3:C:188:HIS:CD2   | 2.50                     | 0.45              |
| 3:C:186:LEU:CB    | 3:C:188:HIS:HD2   | 2.29                     | 0.45              |
| 1:A:351:THR:HG21  | 2:B:1103:ILE:HG12 | 1.96                     | 0.45              |
| 1:A:852:TYR:O     | 5:F:81:THR:HG22   | 2.17                     | 0.45              |
| 1:A:1372:VAL:O    | 1:A:1376:THR:HB   | 2.16                     | 0.45              |
| 1:A:1444:MET:HB2  | 5:F:133:VAL:HG12  | 1.97                     | 0.45              |
| 2:B:957:ASN:HD21  | 2:B:959:ASP:HB2   | 1.80                     | 0.45              |
| 3:C:67:LEU:HD23   | 3:C:144:ILE:HD11  | 1.98                     | 0.45              |
| 1:A:43:GLU:OE1    | 1:A:43:GLU:N      | 2.48                     | 0.45              |
| 1:A:265:LYS:HZ1   | 1:A:303:TYR:N     | 2.14                     | 0.45              |
| 1:A:962:ARG:O     | 1:A:966:ASN:HB2   | 2.16                     | 0.45              |
| 2:B:65:GLU:HG2    | 2:B:66:ASP:H      | 1.80                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B:175:ARG:HH11 | 2:B:175:ARG:HG2   | 1.78                     | 0.45              |
| 2:B:845:SER:HB2  | 8:J:8:PHE:HB3     | 1.98                     | 0.45              |
| 2:B:872:GLU:HG2  | 2:B:916:THR:HB    | 1.99                     | 0.45              |
| 2:B:999:MET:HE3  | 2:B:1011:ILE:CD1  | 2.46                     | 0.45              |
| 3:C:238:ILE:HG23 | 3:C:242:GLN:HB2   | 1.99                     | 0.45              |
| 4:E:29:PHE:C     | 4:E:30:ILE:HD12   | 2.42                     | 0.45              |
| 12:T:2:DT:H3'    | 12:T:2:DT:H6      | 1.82                     | 0.45              |
| 1:A:272:ALA:O    | 1:A:296:LEU:HB2   | 2.17                     | 0.45              |
| 1:A:375:THR:HG21 | 1:A:433:GLU:OE1   | 2.16                     | 0.45              |
| 1:A:472:LEU:HD11 | 2:B:835:GLN:HE22  | 1.80                     | 0.45              |
| 2:B:706:GLN:O    | 2:B:707:PRO:C     | 2.58                     | 0.45              |
| 3:C:97:VAL:HG21  | 3:C:129:ILE:HG23  | 1.97                     | 0.45              |
| 3:C:238:ILE:HD11 | 3:C:246:ARG:NH1   | 2.32                     | 0.45              |
| 4:E:79:TRP:HB2   | 4:E:105:PHE:CD1   | 2.51                     | 0.45              |
| 1:A:151:ASP:OD2  | 1:A:163:SER:HA    | 2.17                     | 0.45              |
| 1:A:504:LEU:CD1  | 5:F:91:ALA:HB2    | 2.47                     | 0.45              |
| 1:A:1365:TYR:CD2 | 1:A:1365:TYR:C    | 2.94                     | 0.45              |
| 3:C:142:VAL:HG13 | 8:J:5:VAL:HG23    | 1.98                     | 0.45              |
| 5:F:114:GLU:OE1  | 5:F:119:ARG:HG3   | 2.17                     | 0.45              |
| 6:H:11:GLN:HE21  | 6:H:11:GLN:HB2    | 1.60                     | 0.45              |
| 12:T:2:DT:O2     | 13:N:13:DA:C2     | 2.69                     | 0.45              |
| 13:N:14:DG:OP2   | 13:N:14:DG:H2'    | 2.17                     | 0.45              |
| 2:B:370:PHE:HD2  | 2:B:373:ARG:HG3   | 1.81                     | 0.45              |
| 2:B:647:GLY:O    | 2:B:648:HIS:ND1   | 2.50                     | 0.45              |
| 2:B:708:GLU:O    | 2:B:712:PRO:HD3   | 2.16                     | 0.45              |
| 12:T:16:DC:H2''  | 12:T:17:DC:C5     | 2.52                     | 0.45              |
| 1:A:313:GLN:HB3  | 1:A:314:ALA:H     | 1.42                     | 0.45              |
| 1:A:1258:HIS:O   | 1:A:1262:LYS:NZ   | 2.47                     | 0.45              |
| 2:B:167:ILE:HG21 | 2:B:453:ILE:HD12  | 1.99                     | 0.45              |
| 6:H:110:ASP:O    | 6:H:111:LEU:HG    | 2.16                     | 0.45              |
| 6:H:127:GLY:HA3  | 6:H:130:ARG:CZ    | 2.47                     | 0.45              |
| 13:N:5:DT:C2'    | 13:N:6:DT:C5      | 2.99                     | 0.45              |
| 1:A:219:PHE:HB3  | 1:A:224:PHE:HB2   | 1.99                     | 0.44              |
| 1:A:1349:TYR:O   | 1:A:1350:LYS:C    | 2.58                     | 0.44              |
| 2:B:1093:GLN:HG2 | 2:B:1093:GLN:H    | 1.70                     | 0.44              |
| 3:C:99:LEU:N     | 3:C:99:LEU:CD2    | 2.76                     | 0.44              |
| 5:F:136:ARG:O    | 5:F:143:PHE:HA    | 2.17                     | 0.44              |
| 6:H:109:LYS:HZ3  | 6:H:111:LEU:HD12  | 1.81                     | 0.44              |
| 8:J:8:PHE:H      | 8:J:49:MET:CE     | 2.26                     | 0.44              |
| 1:A:242:PRO:HA   | 1:A:243:PRO:HD3   | 1.81                     | 0.44              |
| 1:A:1130:GLN:O   | 1:A:1134:ILE:HD12 | 2.17                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1323:ASP:C   | 1:A:1325:THR:H   | 2.24                     | 0.44              |
| 2:B:228:LYS:HB3  | 2:B:228:LYS:HE2  | 1.73                     | 0.44              |
| 2:B:793:ALA:HB3  | 2:B:856:PHE:HB2  | 1.98                     | 0.44              |
| 1:A:783:THR:CG2  | 1:A:784:LEU:N    | 2.80                     | 0.44              |
| 1:A:1194:ARG:NH2 | 1:A:1237:ILE:CD1 | 2.80                     | 0.44              |
| 1:A:1206:ASP:N   | 1:A:1206:ASP:OD2 | 2.51                     | 0.44              |
| 1:A:251:SER:HB2  | 11:R:1:A:N3      | 2.32                     | 0.44              |
| 1:A:960:ILE:O    | 1:A:961:ARG:C    | 2.61                     | 0.44              |
| 2:B:764:SER:O    | 2:B:766:ARG:N    | 2.51                     | 0.44              |
| 2:B:382:ILE:HG12 | 2:B:382:ILE:H    | 1.65                     | 0.44              |
| 2:B:420:LEU:HD23 | 2:B:420:LEU:HA   | 1.83                     | 0.44              |
| 3:C:127:ARG:HE   | 3:C:127:ARG:HB2  | 1.54                     | 0.44              |
| 8:J:22:LEU:HA    | 8:J:22:LEU:HD12  | 1.59                     | 0.44              |
| 1:A:5:GLN:O      | 2:B:1159:ARG:NH2 | 2.50                     | 0.44              |
| 1:A:417:TYR:O    | 1:A:418:SER:HB3  | 2.18                     | 0.44              |
| 1:A:547:LEU:HB3  | 9:K:58:PHE:CE1   | 2.52                     | 0.44              |
| 1:A:858:ASN:C    | 1:A:858:ASN:ND2  | 2.70                     | 0.44              |
| 2:B:797:TYR:HB3  | 2:B:798:TYR:CD1  | 2.53                     | 0.44              |
| 2:B:1181:GLU:H   | 2:B:1181:GLU:HG2 | 1.55                     | 0.44              |
| 12:T:5:DC:C4     | 12:T:6:DC:N3     | 2.85                     | 0.44              |
| 13:N:1:DG:H2''   | 13:N:2:DT:C6     | 2.46                     | 0.44              |
| 2:B:475:SER:C    | 2:B:477:ALA:N    | 2.75                     | 0.44              |
| 2:B:857:ARG:O    | 2:B:967:ARG:HA   | 2.18                     | 0.44              |
| 8:J:52:THR:HG22  | 8:J:52:THR:O     | 2.17                     | 0.44              |
| 12:T:22:DT:C2'   | 12:T:23:DC:O5'   | 2.65                     | 0.44              |
| 2:B:43:LEU:HD23  | 2:B:43:LEU:HA    | 1.76                     | 0.44              |
| 2:B:217:ARG:NH2  | 2:B:405:ARG:HG3  | 2.33                     | 0.44              |
| 2:B:792:MET:HE3  | 2:B:792:MET:HB2  | 1.91                     | 0.44              |
| 2:B:1169:MET:HE3 | 2:B:1169:MET:HB2 | 1.79                     | 0.44              |
| 4:E:190:LEU:HD11 | 4:E:196:VAL:HG13 | 2.00                     | 0.44              |
| 4:E:197:LYS:HG3  | 4:E:211:TYR:CE2  | 2.53                     | 0.44              |
| 9:K:109:TRP:C    | 9:K:111:LEU:H    | 2.25                     | 0.44              |
| 1:A:472:LEU:HD21 | 2:B:835:GLN:CB   | 2.48                     | 0.44              |
| 2:B:1109:GLY:HA3 | 2:B:1110:PRO:HD2 | 1.67                     | 0.44              |
| 1:A:114:LEU:HD11 | 1:A:171:GLN:NE2  | 2.33                     | 0.43              |
| 1:A:302:THR:HG21 | 1:A:313:GLN:OE1  | 2.18                     | 0.43              |
| 1:A:328:ARG:C    | 1:A:329:LEU:HD23 | 2.42                     | 0.43              |
| 1:A:835:GLY:HA3  | 12:T:18:DG:H1'   | 1.98                     | 0.43              |
| 1:A:1312:ASN:OD1 | 1:A:1315:GLU:HG3 | 2.18                     | 0.43              |
| 2:B:493:SER:HA   | 2:B:751:VAL:HG11 | 1.99                     | 0.43              |
| 2:B:547:VAL:N    | 2:B:612:GLU:OE2  | 2.39                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:636:PRO:CB    | 2:B:637:LEU:HA    | 2.48                     | 0.43              |
| 3:C:69:LEU:HB3    | 8:J:6:ARG:HD3     | 2.00                     | 0.43              |
| 1:A:22:PHE:CB     | 2:B:1211:ASN:OD1  | 2.65                     | 0.43              |
| 1:A:91:PHE:N      | 1:A:297:GLN:HE22  | 2.15                     | 0.43              |
| 1:A:577:ILE:H     | 1:A:577:ILE:HG13  | 1.57                     | 0.43              |
| 2:B:242:SER:HB2   | 2:B:252:SER:O     | 2.17                     | 0.43              |
| 2:B:778:MET:CE    | 2:B:1094:ARG:HD3  | 2.48                     | 0.43              |
| 2:B:913:GLY:HA2   | 2:B:938:SER:OG    | 2.18                     | 0.43              |
| 3:C:44:LEU:HD12   | 3:C:160:LYS:C     | 2.43                     | 0.43              |
| 3:C:112:ASN:HD21  | 3:C:146:LYS:HD3   | 1.83                     | 0.43              |
| 3:C:129:ILE:HA    | 3:C:129:ILE:HD12  | 1.74                     | 0.43              |
| 1:A:610:GLY:O     | 1:A:611:GLN:NE2   | 2.51                     | 0.43              |
| 1:A:973:ILE:HD12  | 1:A:974:ASP:H     | 1.83                     | 0.43              |
| 1:A:1155:ASP:HA   | 1:A:1156:PRO:HD3  | 1.75                     | 0.43              |
| 2:B:96:TYR:HB2    | 2:B:129:PHE:HB2   | 2.01                     | 0.43              |
| 2:B:453:ILE:O     | 2:B:454:THR:C     | 2.61                     | 0.43              |
| 2:B:518:HIS:O     | 2:B:519:TRP:C     | 2.60                     | 0.43              |
| 2:B:724:ASP:HA    | 2:B:725:PRO:HD3   | 1.90                     | 0.43              |
| 2:B:1084:GLN:NE2  | 3:C:192:TRP:N     | 2.60                     | 0.43              |
| 1:A:269:ILE:HD13  | 1:A:300:VAL:HG22  | 2.00                     | 0.43              |
| 1:A:533:LYS:HD3   | 1:A:745:GLN:NE2   | 2.33                     | 0.43              |
| 1:A:598:LEU:HD23  | 1:A:598:LEU:HA    | 1.74                     | 0.43              |
| 1:A:825:ILE:HD12  | 2:B:512:ARG:HB2   | 2.00                     | 0.43              |
| 1:A:913:LEU:HD11  | 1:A:981:LEU:O     | 2.18                     | 0.43              |
| 2:B:597:MET:HE1   | 2:B:615:MET:HB2   | 2.00                     | 0.43              |
| 4:E:88:VAL:HG11   | 4:E:110:PHE:CE2   | 2.53                     | 0.43              |
| 13:N:7:DA:H2"     | 13:N:8:DT:C6      | 2.54                     | 0.43              |
| 1:A:112:LYS:HG2   | 1:A:113:LEU:N     | 2.34                     | 0.43              |
| 1:A:352:VAL:CG2   | 2:B:1099:VAL:HG13 | 2.48                     | 0.43              |
| 1:A:1156:PRO:HD2  | 1:A:1157:ASP:H    | 1.83                     | 0.43              |
| 2:B:549:THR:O     | 2:B:628:THR:CG2   | 2.67                     | 0.43              |
| 2:B:983:ARG:NH1   | 2:B:1091:TYR:HB3  | 2.32                     | 0.43              |
| 2:B:1058:LEU:HD23 | 2:B:1058:LEU:HA   | 1.87                     | 0.43              |
| 3:C:56:THR:HG23   | 3:C:58:LEU:H      | 1.83                     | 0.43              |
| 3:C:142:VAL:N     | 8:J:16:ASP:HB3    | 2.31                     | 0.43              |
| 7:I:111:THR:CG2   | 7:I:113:ASP:CB    | 2.93                     | 0.43              |
| 1:A:99:ILE:HD13   | 1:A:235:ILE:HG23  | 1.99                     | 0.43              |
| 1:A:354:SER:HA    | 1:A:482:PHE:CD2   | 2.53                     | 0.43              |
| 2:B:121:ASN:HD22  | 2:B:121:ASN:HA    | 1.61                     | 0.43              |
| 5:F:83:PRO:HA     | 5:F:146:TRP:CZ3   | 2.53                     | 0.43              |
| 1:A:754:SER:O     | 1:A:755:PHE:C     | 2.60                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:842:VAL:HG11  | 2:B:1136:ASP:CG   | 2.44                     | 0.43              |
| 2:B:476:ARG:C     | 2:B:478:GLY:H     | 2.27                     | 0.43              |
| 3:C:133:ILE:HD13  | 3:C:236:GLY:C     | 2.43                     | 0.43              |
| 4:E:88:VAL:HG11   | 4:E:110:PHE:HE2   | 1.84                     | 0.43              |
| 5:F:76:LYS:O      | 5:F:79:ARG:HD3    | 2.18                     | 0.43              |
| 1:A:629:LEU:HD13  | 1:A:645:LEU:HD21  | 1.99                     | 0.43              |
| 1:A:1143:LEU:HD23 | 1:A:1267:MET:O    | 2.19                     | 0.43              |
| 2:B:483:LEU:HD23  | 2:B:483:LEU:HA    | 1.93                     | 0.43              |
| 6:H:83:GLN:C      | 6:H:87:ARG:HG3    | 2.43                     | 0.43              |
| 8:J:3:VAL:HG11    | 8:J:18:TRP:HB2    | 2.01                     | 0.43              |
| 1:A:211:PHE:O     | 1:A:213:HIS:N     | 2.52                     | 0.43              |
| 1:A:873:MET:HE1   | 1:A:1057:VAL:HG22 | 2.01                     | 0.43              |
| 1:A:979:SER:OG    | 1:A:981:LEU:HD12  | 2.19                     | 0.43              |
| 1:A:1017:LEU:HB2  | 4:E:205:SER:C     | 2.43                     | 0.43              |
| 2:B:293:PRO:HG2   | 2:B:296:GLU:CB    | 2.48                     | 0.43              |
| 2:B:1021:MET:HB2  | 2:B:1021:MET:HE3  | 1.50                     | 0.43              |
| 2:B:1060:ARG:HD2  | 2:B:1060:ARG:HA   | 1.69                     | 0.43              |
| 3:C:5:GLY:HA3     | 3:C:6:PRO:HD2     | 1.87                     | 0.43              |
| 3:C:77:ILE:HD12   | 3:C:161:LYS:HG3   | 2.01                     | 0.43              |
| 6:H:106:GLU:C     | 6:H:108:SER:N     | 2.77                     | 0.43              |
| 1:A:31:SER:OG     | 1:A:83:HIS:HD2    | 2.02                     | 0.43              |
| 1:A:129:LYS:O     | 1:A:130:ASP:HB3   | 2.19                     | 0.43              |
| 1:A:368:LYS:HB2   | 1:A:368:LYS:HE2   | 1.75                     | 0.43              |
| 2:B:64:CYS:O      | 2:B:65:GLU:HB3    | 2.18                     | 0.43              |
| 2:B:229:ALA:HB1   | 2:B:231:PRO:CD    | 2.44                     | 0.43              |
| 2:B:274:PRO:HB2   | 2:B:359:GLU:HB3   | 2.01                     | 0.43              |
| 2:B:801:LYS:O     | 8:J:52:THR:CG2    | 2.54                     | 0.43              |
| 2:B:911:ILE:HD13  | 2:B:911:ILE:HG21  | 1.60                     | 0.43              |
| 2:B:1200:ALA:O    | 2:B:1201:LYS:C    | 2.59                     | 0.43              |
| 8:J:8:PHE:N       | 8:J:49:MET:HE3    | 2.26                     | 0.43              |
| 1:A:19:PHE:HE1    | 1:A:1396:ALA:HB3  | 1.84                     | 0.42              |
| 1:A:261:ASP:CG    | 1:A:323:LYS:HD2   | 2.41                     | 0.42              |
| 2:B:168:GLY:HA2   | 2:B:454:THR:OG1   | 2.19                     | 0.42              |
| 2:B:293:PRO:C     | 2:B:294:ASP:O     | 2.59                     | 0.42              |
| 2:B:541:LEU:HB2   | 2:B:747:MET:HE2   | 1.99                     | 0.42              |
| 2:B:634:TYR:CD1   | 2:B:692:TYR:HB3   | 2.54                     | 0.42              |
| 3:C:183:TRP:O     | 3:C:184:ASN:C     | 2.61                     | 0.42              |
| 13:N:6:DT:C2      | 13:N:7:DA:N7      | 2.87                     | 0.42              |
| 1:A:398:GLU:O     | 1:A:399:HIS:C     | 2.61                     | 0.42              |
| 1:A:981:LEU:HD21  | 1:A:1039:LYS:HA   | 2.02                     | 0.42              |
| 1:A:1019:CYS:O    | 1:A:1020:CYS:C    | 2.60                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1437:GLY:O    | 1:A:1440:ALA:N    | 2.43                     | 0.42              |
| 4:E:22:MET:HB2    | 4:E:187:TYR:CE1   | 2.54                     | 0.42              |
| 4:E:157:SER:O     | 4:E:159:ASP:N     | 2.52                     | 0.42              |
| 1:A:313:GLN:HB2   | 1:A:322:VAL:CG2   | 2.37                     | 0.42              |
| 1:A:598:LEU:O     | 1:A:599:SER:C     | 2.62                     | 0.42              |
| 1:A:836:TYR:CZ    | 1:A:840:ARG:HD2   | 2.53                     | 0.42              |
| 1:A:992:ASP:O     | 1:A:995:GLU:HB2   | 2.19                     | 0.42              |
| 1:A:1159:ARG:HB3  | 1:A:1159:ARG:HH11 | 1.84                     | 0.42              |
| 2:B:642:ASP:O     | 2:B:644:GLU:N     | 2.52                     | 0.42              |
| 3:C:226:ASP:O     | 3:C:227:THR:O     | 2.37                     | 0.42              |
| 4:E:122:LYS:HB3   | 4:E:123:LEU:HD23  | 2.02                     | 0.42              |
| 4:E:157:SER:N     | 4:E:160:GLU:OE1   | 2.52                     | 0.42              |
| 6:H:43:ASN:OD1    | 6:H:43:ASN:C      | 2.62                     | 0.42              |
| 7:I:101:PHE:O     | 7:I:109:ILE:HA    | 2.20                     | 0.42              |
| 1:A:116:ASP:C     | 1:A:118:HIS:N     | 2.76                     | 0.42              |
| 1:A:269:ILE:CD1   | 1:A:300:VAL:HG22  | 2.49                     | 0.42              |
| 1:A:323:LYS:O     | 1:A:324:SER:CB    | 2.66                     | 0.42              |
| 3:C:246:ARG:HA    | 3:C:249:ASP:HB2   | 2.02                     | 0.42              |
| 4:E:48:ASP:O      | 4:E:49:SER:C      | 2.61                     | 0.42              |
| 7:I:96:SER:C      | 7:I:98:VAL:H      | 2.28                     | 0.42              |
| 1:A:783:THR:HG23  | 1:A:815:PHE:HZ    | 1.84                     | 0.42              |
| 1:A:969:GLN:O     | 1:A:971:PHE:N     | 2.52                     | 0.42              |
| 2:B:212:LEU:HD23  | 2:B:480:SER:HB3   | 2.02                     | 0.42              |
| 2:B:542:MET:SD    | 2:B:747:MET:HG3   | 2.59                     | 0.42              |
| 2:B:1034:VAL:O    | 2:B:1035:ALA:C    | 2.62                     | 0.42              |
| 3:C:63:ILE:HA     | 3:C:66:ARG:HG3    | 2.00                     | 0.42              |
| 6:H:25:ARG:NH2    | 6:H:41:ASP:OD2    | 2.52                     | 0.42              |
| 6:H:38:LEU:HG     | 6:H:39:THR:N      | 2.34                     | 0.42              |
| 7:I:117:LYS:C     | 7:I:118:ARG:HG2   | 2.45                     | 0.42              |
| 1:A:902:LEU:H     | 1:A:902:LEU:HG    | 1.37                     | 0.42              |
| 1:A:1157:ASP:O    | 1:A:1158:PRO:C    | 2.62                     | 0.42              |
| 1:A:1433:MET:HE3  | 1:A:1439:GLY:HA2  | 2.01                     | 0.42              |
| 2:B:382:ILE:O     | 2:B:383:ASN:C     | 2.62                     | 0.42              |
| 2:B:1002:THR:HG22 | 2:B:1006:ILE:H    | 1.85                     | 0.42              |
| 2:B:1124:ARG:HE   | 2:B:1124:ARG:HB2  | 1.66                     | 0.42              |
| 3:C:69:LEU:CB     | 8:J:5:VAL:HG13    | 2.50                     | 0.42              |
| 3:C:142:VAL:H     | 8:J:16:ASP:CB     | 2.28                     | 0.42              |
| 4:E:96:PHE:C      | 4:E:98:ILE:N      | 2.70                     | 0.42              |
| 7:I:58:VAL:HG11   | 7:I:109:ILE:HD11  | 2.02                     | 0.42              |
| 1:A:380:VAL:CG1   | 1:A:428:TYR:HA    | 2.37                     | 0.42              |
| 2:B:515:HIS:HD2   | 2:B:517:THR:N     | 2.11                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:880:THR:O     | 2:B:881:ASN:C     | 2.62                     | 0.42              |
| 3:C:143:LEU:HG    | 8:J:2:ILE:HD11    | 2.00                     | 0.42              |
| 8:J:48:ARG:NH2    | 8:J:49:MET:HE1    | 2.34                     | 0.42              |
| 1:A:1060:PRO:HD2  | 5:F:86:THR:HG21   | 2.02                     | 0.42              |
| 1:A:1115:SER:HB3  | 1:A:1330:ASN:ND2  | 2.35                     | 0.42              |
| 2:B:400:HIS:CE1   | 2:B:517:THR:HG21  | 2.55                     | 0.42              |
| 2:B:413:LEU:HD23  | 2:B:413:LEU:HA    | 1.81                     | 0.42              |
| 2:B:638:PHE:CE2   | 2:B:653:VAL:HG21  | 2.54                     | 0.42              |
| 2:B:1027:ILE:HG23 | 2:B:1052:VAL:HG22 | 2.02                     | 0.42              |
| 3:C:43:THR:HG22   | 3:C:44:LEU:N      | 2.35                     | 0.42              |
| 6:H:91:ASP:O      | 6:H:92:ASP:CG     | 2.63                     | 0.42              |
| 8:J:8:PHE:O       | 8:J:9:SER:C       | 2.63                     | 0.42              |
| 1:A:257:ARG:HG2   | 1:A:258:GLY:N     | 2.34                     | 0.42              |
| 1:A:1349:TYR:CD2  | 1:A:1349:TYR:C    | 2.97                     | 0.42              |
| 2:B:35:SER:O      | 2:B:37:PHE:O      | 2.38                     | 0.42              |
| 2:B:756:ILE:HG12  | 2:B:770:GLN:HG2   | 2.01                     | 0.42              |
| 2:B:1187:ASN:HD21 | 2:B:1190:ASP:N    | 2.12                     | 0.42              |
| 4:E:3:GLN:HB2     | 4:E:4:GLU:H       | 1.63                     | 0.42              |
| 6:H:107:VAL:HG12  | 6:H:107:VAL:O     | 2.20                     | 0.42              |
| 10:L:27:LEU:HD22  | 10:L:37:LYS:NZ    | 2.35                     | 0.42              |
| 1:A:401:GLY:C     | 1:A:435:HIS:HD2   | 2.25                     | 0.42              |
| 1:A:1110:ASN:C    | 1:A:1110:ASN:HD22 | 2.28                     | 0.42              |
| 2:B:120:ARG:HD2   | 2:B:955:THR:CG2   | 2.39                     | 0.42              |
| 2:B:314:LEU:O     | 2:B:317:CYS:HB2   | 2.19                     | 0.42              |
| 2:B:685:LEU:HD21  | 2:B:692:TYR:CE1   | 2.54                     | 0.42              |
| 2:B:804:GLY:HA2   | 2:B:1042:GLY:O    | 2.20                     | 0.42              |
| 2:B:839:MET:HE1   | 2:B:1010:LEU:HD21 | 2.02                     | 0.42              |
| 2:B:862:GLN:HE21  | 2:B:961:LEU:HD13  | 1.85                     | 0.42              |
| 13:N:4:DG:C2      | 13:N:5:DT:N3      | 2.80                     | 0.42              |
| 1:A:99:ILE:CD1    | 1:A:235:ILE:HG23  | 2.50                     | 0.41              |
| 1:A:775:ILE:H     | 1:A:775:ILE:HG12  | 1.69                     | 0.41              |
| 1:A:808:LEU:O     | 2:B:728:ARG:NH1   | 2.53                     | 0.41              |
| 1:A:821:ARG:HH11  | 1:A:821:ARG:HD3   | 1.69                     | 0.41              |
| 1:A:943:LEU:O     | 1:A:946:VAL:N     | 2.51                     | 0.41              |
| 2:B:310:MET:O     | 2:B:313:MET:HB2   | 2.21                     | 0.41              |
| 10:L:59:ALA:O     | 10:L:60:ARG:HB3   | 2.19                     | 0.41              |
| 1:A:77:CYS:C      | 1:A:79:GLY:N      | 2.78                     | 0.41              |
| 1:A:804:TYR:O     | 2:B:761:HIS:ND1   | 2.48                     | 0.41              |
| 2:B:288:ALA:HB1   | 2:B:331:LEU:HD13  | 2.02                     | 0.41              |
| 2:B:301:ILE:HG21  | 2:B:314:LEU:HD11  | 2.02                     | 0.41              |
| 2:B:332:ASP:C     | 2:B:334:ILE:N     | 2.75                     | 0.41              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:B:429:PHE:HA    | 2:B:432:MET:HE2  | 2.02                     | 0.41              |
| 2:B:1002:THR:HG21 | 2:B:1006:ILE:CG1 | 2.50                     | 0.41              |
| 2:B:1056:SER:O    | 2:B:1066:SER:HB2 | 2.20                     | 0.41              |
| 6:H:40:LEU:HD12   | 6:H:41:ASP:H     | 1.84                     | 0.41              |
| 1:A:322:VAL:HB    | 1:A:323:LYS:H    | 1.29                     | 0.41              |
| 2:B:35:SER:O      | 2:B:39:ARG:HB2   | 2.20                     | 0.41              |
| 2:B:185:THR:HG23  | 2:B:188:ASP:OD2  | 2.21                     | 0.41              |
| 12:T:7:DA:H2      | 12:T:8:DT:N3     | 2.07                     | 0.41              |
| 1:A:785:PRO:HD2   | 1:A:786:HIS:CD2  | 2.55                     | 0.41              |
| 2:B:122:LEU:HD21  | 2:B:958:GLN:HB2  | 2.02                     | 0.41              |
| 2:B:195:CYS:SG    | 2:B:783:THR:HB   | 2.60                     | 0.41              |
| 2:B:311:LEU:HB3   | 7:I:4:PHE:HZ     | 1.85                     | 0.41              |
| 4:E:7:ARG:O       | 4:E:8:ASN:C      | 2.63                     | 0.41              |
| 10:L:59:ALA:O     | 10:L:60:ARG:CB   | 2.68                     | 0.41              |
| 1:A:53:LEU:HD23   | 1:A:54:ASN:HB3   | 2.01                     | 0.41              |
| 1:A:1060:PRO:HD2  | 5:F:86:THR:CG2   | 2.49                     | 0.41              |
| 2:B:402:GLY:HA2   | 2:B:695:ALA:HB3  | 2.01                     | 0.41              |
| 2:B:542:MET:SD    | 2:B:636:PRO:HG3  | 2.61                     | 0.41              |
| 2:B:778:MET:HE3   | 2:B:853:SER:CB   | 2.50                     | 0.41              |
| 6:H:62:SER:HB2    | 6:H:63:LEU:H     | 1.41                     | 0.41              |
| 13:N:12:DT:H2"    | 13:N:13:DA:C8    | 2.55                     | 0.41              |
| 1:A:848:ILE:HD11  | 1:A:1374:VAL:CG2 | 2.49                     | 0.41              |
| 2:B:258:LEU:HB2   | 2:B:385:LEU:HD21 | 2.01                     | 0.41              |
| 2:B:500:THR:HA    | 2:B:501:PRO:HD3  | 1.94                     | 0.41              |
| 2:B:522:VAL:HG12  | 2:B:523:CYS:N    | 2.35                     | 0.41              |
| 2:B:798:TYR:CZ    | 3:C:62:PHE:HE2   | 2.38                     | 0.41              |
| 7:I:87:GLN:O      | 7:I:88:SER:C     | 2.63                     | 0.41              |
| 1:A:255:SER:O     | 1:A:256:GLN:HB2  | 2.21                     | 0.41              |
| 1:A:335:ARG:NH1   | 2:B:1206:GLU:OE1 | 2.54                     | 0.41              |
| 1:A:444:PHE:O     | 1:A:455:MET:HA   | 2.21                     | 0.41              |
| 1:A:683:ILE:HD13  | 1:A:683:ILE:HA   | 1.72                     | 0.41              |
| 1:A:1130:GLN:HE21 | 1:A:1130:GLN:HB3 | 1.71                     | 0.41              |
| 1:A:1284:MET:HE3  | 1:A:1284:MET:HB2 | 1.72                     | 0.41              |
| 1:A:1376:THR:HG23 | 4:E:212:ARG:HH22 | 1.85                     | 0.41              |
| 2:B:898:LEU:HD23  | 2:B:898:LEU:HA   | 1.82                     | 0.41              |
| 3:C:102:GLN:CG    | 3:C:154:LYS:HD3  | 2.48                     | 0.41              |
| 1:A:7:SER:HB3     | 2:B:1193:GLN:OE1 | 2.19                     | 0.41              |
| 1:A:149:GLU:HB3   | 1:A:150:THR:H    | 1.63                     | 0.41              |
| 1:A:233:TRP:C     | 1:A:235:ILE:H    | 2.28                     | 0.41              |
| 1:A:553:VAL:CG2   | 1:A:652:VAL:HG23 | 2.51                     | 0.41              |
| 1:A:575:LYS:HD3   | 1:A:612:ILE:HD11 | 2.02                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:709:THR:HG21 | 7:I:93:LYS:O     | 2.20                     | 0.41              |
| 2:B:398:ARG:HB3  | 2:B:398:ARG:CZ   | 2.50                     | 0.41              |
| 2:B:402:GLY:CA   | 2:B:695:ALA:HB3  | 2.51                     | 0.41              |
| 2:B:956:THR:HB   | 10:L:46:VAL:HG21 | 2.03                     | 0.41              |
| 6:H:44:VAL:O     | 6:H:44:VAL:HG12  | 2.19                     | 0.41              |
| 7:I:54:GLU:O     | 7:I:89:GLN:HB2   | 2.20                     | 0.41              |
| 8:J:1:MET:H2     | 8:J:57:ILE:H     | 1.66                     | 0.41              |
| 1:A:322:VAL:HG12 | 1:A:323:LYS:HE2  | 2.03                     | 0.41              |
| 1:A:544:ASP:HB2  | 9:K:47:ARG:HH21  | 1.86                     | 0.41              |
| 1:A:666:ILE:H    | 1:A:666:ILE:HG13 | 1.70                     | 0.41              |
| 1:A:782:ARG:NH2  | 7:I:67:THR:CG2   | 2.84                     | 0.41              |
| 1:A:834:THR:HG21 | 1:A:1077:THR:HA  | 2.03                     | 0.41              |
| 1:A:1015:VAL:O   | 1:A:1015:VAL:CG1 | 2.66                     | 0.41              |
| 1:A:1036:ARG:HG3 | 1:A:1036:ARG:NH1 | 2.31                     | 0.41              |
| 1:A:1118:VAL:HB  | 1:A:1306:LEU:HB2 | 2.01                     | 0.41              |
| 2:B:173:MET:HE2  | 2:B:201:GLY:O    | 2.21                     | 0.41              |
| 2:B:203:PHE:HE1  | 2:B:212:LEU:CD1  | 2.33                     | 0.41              |
| 2:B:212:LEU:HD21 | 2:B:466:TRP:CH2  | 2.55                     | 0.41              |
| 2:B:367:LEU:HB3  | 2:B:368:GLU:H    | 1.58                     | 0.41              |
| 2:B:373:ARG:HE   | 2:B:567:GLU:CD   | 2.27                     | 0.41              |
| 2:B:619:ILE:H    | 2:B:619:ILE:HG12 | 1.73                     | 0.41              |
| 2:B:744:HIS:HA   | 2:B:745:PRO:HD2  | 1.96                     | 0.41              |
| 2:B:834:ASN:O    | 2:B:1013:ASN:HB2 | 2.21                     | 0.41              |
| 2:B:864:LYS:HG2  | 2:B:871:THR:HG23 | 2.03                     | 0.41              |
| 2:B:893:LEU:HD21 | 2:B:910:VAL:HG12 | 2.03                     | 0.41              |
| 3:C:73:GLN:NE2   | 3:C:75:MET:HB2   | 2.36                     | 0.41              |
| 3:C:93:ASP:OD1   | 3:C:122:SER:HB2  | 2.21                     | 0.41              |
| 3:C:133:ILE:HD13 | 3:C:237:SER:HA   | 2.03                     | 0.41              |
| 3:C:259:LEU:HD12 | 3:C:259:LEU:HA   | 1.80                     | 0.41              |
| 3:C:259:LEU:HD13 | 9:K:91:CYS:HB2   | 2.02                     | 0.41              |
| 7:I:55:THR:O     | 7:I:55:THR:CG2   | 2.68                     | 0.41              |
| 12:T:7:DA:C6     | 12:T:8:DT:O4     | 2.74                     | 0.41              |
| 12:T:17:DC:H2'   | 12:T:17:DC:O2    | 2.21                     | 0.41              |
| 1:A:40:THR:HG22  | 1:A:41:MET:HG3   | 2.02                     | 0.41              |
| 1:A:260:ASP:CG   | 1:A:261:ASP:N    | 2.79                     | 0.41              |
| 1:A:851:HIS:CD2  | 1:A:857:ARG:HB2  | 2.55                     | 0.41              |
| 1:A:1280:GLU:O   | 1:A:1281:ARG:C   | 2.64                     | 0.41              |
| 2:B:619:ILE:HG13 | 7:I:65:ASP:HB2   | 2.03                     | 0.41              |
| 2:B:817:LEU:N    | 2:B:818:PRO:CD   | 2.84                     | 0.41              |
| 2:B:1173:ALA:C   | 2:B:1175:LEU:H   | 2.28                     | 0.41              |
| 3:C:181:ASP:CG   | 3:C:186:LEU:HD13 | 2.46                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:556:TRP:O     | 9:K:26:LYS:HD3    | 2.21                     | 0.40              |
| 1:A:707:GLY:O     | 1:A:1281:ARG:HD2  | 2.22                     | 0.40              |
| 1:A:1062:GLU:O    | 1:A:1064:VAL:N    | 2.53                     | 0.40              |
| 1:A:1279:ILE:HD13 | 1:A:1279:ILE:N    | 2.36                     | 0.40              |
| 1:A:1436:ILE:C    | 1:A:1437:GLY:O    | 2.64                     | 0.40              |
| 2:B:412:LEU:HA    | 2:B:412:LEU:HD23  | 1.83                     | 0.40              |
| 2:B:610:ASN:HA    | 2:B:611:PRO:HD3   | 1.95                     | 0.40              |
| 2:B:762:ASN:HD22  | 2:B:762:ASN:HA    | 1.66                     | 0.40              |
| 3:C:46:ILE:HG23   | 3:C:157:CYS:HB3   | 2.03                     | 0.40              |
| 3:C:57:VAL:HG11   | 8:J:57:ILE:HG13   | 2.02                     | 0.40              |
| 6:H:30:SER:HB2    | 6:H:36:CYS:SG     | 2.61                     | 0.40              |
| 10:L:48:CYS:O     | 10:L:49:LYS:HG2   | 2.21                     | 0.40              |
| 12:T:7:DA:N3      | 12:T:8:DT:C6      | 2.89                     | 0.40              |
| 1:A:86:LEU:CD1    | 1:A:236:LEU:O     | 2.67                     | 0.40              |
| 1:A:332:LYS:C     | 1:A:334:GLY:H     | 2.29                     | 0.40              |
| 1:A:541:ILE:HG23  | 1:A:545:GLN:NE2   | 2.37                     | 0.40              |
| 1:A:1279:ILE:N    | 1:A:1279:ILE:CD1  | 2.84                     | 0.40              |
| 2:B:605:ARG:NE    | 2:B:691:GLU:OE2   | 2.54                     | 0.40              |
| 3:C:244:VAL:HG21  | 9:K:105:PHE:CE1   | 2.56                     | 0.40              |
| 1:A:152:VAL:HA    | 1:A:153:PRO:HD3   | 1.92                     | 0.40              |
| 1:A:632:VAL:HG13  | 1:A:962:ARG:HD3   | 2.02                     | 0.40              |
| 2:B:1072:MET:HE2  | 2:B:1085:ILE:CG2  | 2.51                     | 0.40              |
| 3:C:80:LEU:O      | 3:C:161:LYS:HE2   | 2.21                     | 0.40              |
| 3:C:262:LEU:HD13  | 9:K:88:LYS:HG2    | 2.02                     | 0.40              |
| 9:K:14:GLU:O      | 9:K:15:GLY:C      | 2.65                     | 0.40              |
| 10:L:55:ILE:O     | 10:L:56:LEU:HB2   | 2.20                     | 0.40              |
| 1:A:43:GLU:OE1    | 1:A:46:THR:HB     | 2.22                     | 0.40              |
| 1:A:50:ILE:C      | 1:A:52:GLY:N      | 2.80                     | 0.40              |
| 1:A:1129:GLU:HA   | 1:A:1132:LYS:CE   | 2.46                     | 0.40              |
| 1:A:1169:ILE:H    | 1:A:1169:ILE:HD12 | 1.86                     | 0.40              |
| 2:B:199:MET:SD    | 2:B:199:MET:N     | 2.95                     | 0.40              |
| 2:B:214:ALA:HB2   | 2:B:408:LEU:HD13  | 2.03                     | 0.40              |
| 2:B:563:MET:HE1   | 2:B:588:GLY:CA    | 2.51                     | 0.40              |
| 2:B:578:THR:HB    | 2:B:593:PRO:HG3   | 2.04                     | 0.40              |
| 2:B:624:LEU:HD12  | 2:B:624:LEU:C     | 2.47                     | 0.40              |
| 2:B:744:HIS:CD2   | 2:B:744:HIS:C     | 3.00                     | 0.40              |
| 2:B:801:LYS:O     | 2:B:801:LYS:HG2   | 2.21                     | 0.40              |
| 3:C:44:LEU:HD12   | 3:C:160:LYS:O     | 2.20                     | 0.40              |
| 3:C:76:ASP:HB2    | 3:C:129:ILE:HD13  | 2.04                     | 0.40              |
| 3:C:258:ILE:HG12  | 9:K:35:PHE:HE2    | 1.87                     | 0.40              |
| 6:H:106:GLU:OE1   | 6:H:108:SER:HA    | 2.21                     | 0.40              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 8:J:30:LEU:HD22  | 8:J:34:THR:HG21   | 2.04                     | 0.40              |
| 1:A:23:SER:HA    | 1:A:24:PRO:HD2    | 1.91                     | 0.40              |
| 1:A:48:ALA:C     | 1:A:49:LYS:HE2    | 2.47                     | 0.40              |
| 1:A:102:VAL:HG12 | 1:A:102:VAL:O     | 2.21                     | 0.40              |
| 1:A:447:GLN:HB3  | 1:A:448:PRO:HA    | 2.03                     | 0.40              |
| 1:A:664:THR:HA   | 1:A:742:ASN:HD22  | 1.86                     | 0.40              |
| 1:A:1143:LEU:O   | 1:A:1146:VAL:HG23 | 2.22                     | 0.40              |
| 2:B:492:LEU:HD23 | 2:B:492:LEU:HA    | 1.61                     | 0.40              |
| 2:B:879:ARG:CG   | 2:B:880:THR:N     | 2.84                     | 0.40              |
| 3:C:186:LEU:HB2  | 3:C:188:HIS:HD2   | 1.85                     | 0.40              |
| 4:E:95:THR:O     | 4:E:98:ILE:HG22   | 2.21                     | 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     | 1383/1733 (80%) | 1094 (79%) | 201 (14%) | 88 (6%)  | 1           | 7   |
| 2   | B     | 1088/1224 (89%) | 900 (83%)  | 126 (12%) | 62 (6%)  | 1           | 9   |
| 3   | C     | 264/318 (83%)   | 226 (86%)  | 30 (11%)  | 8 (3%)   | 3           | 20  |
| 4   | E     | 212/215 (99%)   | 173 (82%)  | 28 (13%)  | 11 (5%)  | 1           | 11  |
| 5   | F     | 82/155 (53%)    | 63 (77%)   | 13 (16%)  | 6 (7%)   | 1           | 5   |
| 6   | H     | 129/146 (88%)   | 94 (73%)   | 23 (18%)  | 12 (9%)  | 0           | 2   |
| 7   | I     | 117/122 (96%)   | 97 (83%)   | 13 (11%)  | 7 (6%)   | 1           | 8   |
| 8   | J     | 63/70 (90%)     | 52 (82%)   | 6 (10%)   | 5 (8%)   | 1           | 4   |
| 9   | K     | 112/120 (93%)   | 105 (94%)  | 7 (6%)    | 0        | 100         | 100 |
| 10  | L     | 44/70 (63%)     | 25 (57%)   | 10 (23%)  | 9 (20%)  | 0           | 0   |
| All | All   | 3494/4173 (84%) | 2829 (81%) | 457 (13%) | 208 (6%) | 1           | 8   |

All (208) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 50   | ILE  |
| 1   | A     | 55   | ASP  |
| 1   | A     | 57   | ARG  |
| 1   | A     | 65   | LEU  |
| 1   | A     | 73   | GLY  |
| 1   | A     | 109  | HIS  |
| 1   | A     | 148  | CYS  |
| 1   | A     | 169  | ASN  |
| 1   | A     | 216  | VAL  |
| 1   | A     | 226  | GLU  |
| 1   | A     | 245  | PRO  |
| 1   | A     | 250  | ILE  |
| 1   | A     | 258  | GLY  |
| 1   | A     | 286  | HIS  |
| 1   | A     | 308  | ILE  |
| 1   | A     | 315  | LEU  |
| 1   | A     | 399  | HIS  |
| 1   | A     | 424  | ILE  |
| 1   | A     | 567  | LYS  |
| 1   | A     | 597  | LEU  |
| 1   | A     | 609  | ASP  |
| 1   | A     | 610  | GLY  |
| 1   | A     | 846  | GLU  |
| 1   | A     | 923  | LEU  |
| 1   | A     | 972  | HIS  |
| 1   | A     | 994  | GLN  |
| 1   | A     | 1014 | ALA  |
| 1   | A     | 1036 | ARG  |
| 1   | A     | 1393 | ASN  |
| 1   | A     | 1403 | GLU  |
| 1   | A     | 1438 | THR  |
| 2   | B     | 65   | GLU  |
| 2   | B     | 168  | GLY  |
| 2   | B     | 229  | ALA  |
| 2   | B     | 230  | ALA  |
| 2   | B     | 245  | GLU  |
| 2   | B     | 266  | ALA  |
| 2   | B     | 395  | GLN  |
| 2   | B     | 436  | VAL  |
| 2   | B     | 469  | GLN  |
| 2   | B     | 473  | MET  |
| 2   | B     | 474  | SER  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 477  | ALA  |
| 2   | B     | 483  | LEU  |
| 2   | B     | 531  | GLN  |
| 2   | B     | 592  | ASN  |
| 2   | B     | 629  | ASP  |
| 2   | B     | 636  | PRO  |
| 2   | B     | 645  | SER  |
| 2   | B     | 708  | GLU  |
| 2   | B     | 709  | ASP  |
| 2   | B     | 713  | ALA  |
| 2   | B     | 733  | HIS  |
| 2   | B     | 734  | HIS  |
| 2   | B     | 751  | VAL  |
| 2   | B     | 866  | TYR  |
| 2   | B     | 879  | ARG  |
| 2   | B     | 881  | ASN  |
| 2   | B     | 1046 | PRO  |
| 2   | B     | 1097 | HIS  |
| 2   | B     | 1223 | ASP  |
| 3   | C     | 173  | ALA  |
| 4   | E     | 49   | SER  |
| 4   | E     | 59   | SER  |
| 4   | E     | 118  | PRO  |
| 5   | F     | 73   | ALA  |
| 6   | H     | 90   | ALA  |
| 6   | H     | 109  | LYS  |
| 6   | H     | 111  | LEU  |
| 6   | H     | 131  | ASN  |
| 6   | H     | 132  | LEU  |
| 6   | H     | 138  | GLU  |
| 7   | I     | 34   | TYR  |
| 8   | J     | 2    | ILE  |
| 10  | L     | 34   | CYS  |
| 10  | L     | 35   | SER  |
| 10  | L     | 45   | ALA  |
| 10  | L     | 59   | ALA  |
| 10  | L     | 60   | ARG  |
| 1   | A     | 130  | ASP  |
| 1   | A     | 224  | PHE  |
| 1   | A     | 257  | ARG  |
| 1   | A     | 266  | LEU  |
| 1   | A     | 298  | PHE  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 309  | ALA  |
| 1   | A     | 322  | VAL  |
| 1   | A     | 324  | SER  |
| 1   | A     | 837  | ILE  |
| 1   | A     | 1123 | GLY  |
| 1   | A     | 1174 | PHE  |
| 1   | A     | 1234 | GLU  |
| 1   | A     | 1257 | ASP  |
| 1   | A     | 1388 | GLY  |
| 1   | A     | 1420 | ASP  |
| 2   | B     | 67   | SER  |
| 2   | B     | 249  | ARG  |
| 2   | B     | 288  | ALA  |
| 2   | B     | 466  | TRP  |
| 2   | B     | 643  | ASP  |
| 2   | B     | 737  | THR  |
| 2   | B     | 880  | THR  |
| 2   | B     | 1021 | MET  |
| 2   | B     | 1103 | ILE  |
| 2   | B     | 1185 | CYS  |
| 3   | C     | 48   | SER  |
| 3   | C     | 142  | VAL  |
| 3   | C     | 174  | ALA  |
| 3   | C     | 227  | THR  |
| 4   | E     | 56   | LYS  |
| 4   | E     | 77   | SER  |
| 5   | F     | 111  | LEU  |
| 6   | H     | 3    | ASN  |
| 6   | H     | 62   | SER  |
| 6   | H     | 136  | LYS  |
| 7   | I     | 3    | THR  |
| 7   | I     | 9    | ASP  |
| 7   | I     | 54   | GLU  |
| 7   | I     | 97   | MET  |
| 8   | J     | 8    | PHE  |
| 8   | J     | 30   | LEU  |
| 10  | L     | 46   | VAL  |
| 1   | A     | 35   | ILE  |
| 1   | A     | 54   | ASN  |
| 1   | A     | 131  | SER  |
| 1   | A     | 142  | CYS  |
| 1   | A     | 214  | ILE  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 251  | SER  |
| 1   | A     | 673  | GLY  |
| 1   | A     | 674  | PRO  |
| 1   | A     | 852  | TYR  |
| 1   | A     | 1127 | ASP  |
| 1   | A     | 1278 | ASN  |
| 2   | B     | 364  | ILE  |
| 2   | B     | 468  | GLU  |
| 2   | B     | 471  | LYS  |
| 2   | B     | 480  | SER  |
| 2   | B     | 555  | ILE  |
| 2   | B     | 732  | SER  |
| 2   | B     | 735  | ALA  |
| 2   | B     | 792  | MET  |
| 2   | B     | 864  | LYS  |
| 4   | E     | 101  | GLN  |
| 4   | E     | 158  | SER  |
| 5   | F     | 114  | GLU  |
| 6   | H     | 128  | ASN  |
| 7   | I     | 90   | GLN  |
| 8   | J     | 9    | SER  |
| 8   | J     | 19   | GLU  |
| 10  | L     | 44   | ASP  |
| 1   | A     | 48   | ALA  |
| 1   | A     | 49   | LYS  |
| 1   | A     | 69   | THR  |
| 1   | A     | 147  | VAL  |
| 1   | A     | 178  | GLY  |
| 1   | A     | 219  | PHE  |
| 1   | A     | 220  | THR  |
| 1   | A     | 404  | TYR  |
| 1   | A     | 423  | ASP  |
| 1   | A     | 583  | PRO  |
| 1   | A     | 958  | VAL  |
| 1   | A     | 1093 | LYS  |
| 2   | B     | 367  | LEU  |
| 2   | B     | 479  | VAL  |
| 2   | B     | 561  | TRP  |
| 2   | B     | 644  | GLU  |
| 2   | B     | 711  | GLU  |
| 2   | B     | 1108 | ARG  |
| 4   | E     | 97   | VAL  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 6   | H     | 130  | ARG  |
| 7   | I     | 47   | GLU  |
| 1   | A     | 24   | PRO  |
| 1   | A     | 51   | GLY  |
| 1   | A     | 234  | MET  |
| 1   | A     | 254  | GLU  |
| 1   | A     | 903  | ASN  |
| 1   | A     | 970  | THR  |
| 1   | A     | 1151 | GLU  |
| 2   | B     | 333  | PHE  |
| 2   | B     | 413  | LEU  |
| 2   | B     | 476  | ARG  |
| 2   | B     | 707  | PRO  |
| 3   | C     | 214  | ASN  |
| 3   | C     | 215  | GLU  |
| 4   | E     | 36   | GLU  |
| 6   | H     | 18   | GLY  |
| 10  | L     | 26   | THR  |
| 1   | A     | 38   | PRO  |
| 1   | A     | 1062 | GLU  |
| 2   | B     | 233  | PRO  |
| 2   | B     | 1175 | LEU  |
| 3   | C     | 136  | ASP  |
| 4   | E     | 51   | GLY  |
| 5   | F     | 74   | ILE  |
| 5   | F     | 154  | ASP  |
| 1   | A     | 79   | GLY  |
| 1   | A     | 244  | PRO  |
| 1   | A     | 1156 | PRO  |
| 1   | A     | 1424 | VAL  |
| 1   | A     | 1437 | GLY  |
| 2   | B     | 467  | GLY  |
| 1   | A     | 794  | PRO  |
| 5   | F     | 131  | PRO  |
| 1   | A     | 312  | PRO  |
| 1   | A     | 990  | VAL  |
| 10  | L     | 30   | ILE  |
| 1   | A     | 310  | GLY  |
| 1   | A     | 772  | GLY  |
| 4   | E     | 86   | PRO  |

### 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     | 1218/1520 (80%) | 937 (77%)  | 281 (23%) | 1           | 4 |
| 2   | B     | 960/1061 (90%)  | 749 (78%)  | 211 (22%) | 1           | 5 |
| 3   | C     | 234/274 (85%)   | 177 (76%)  | 57 (24%)  | 1           | 3 |
| 4   | E     | 196/197 (100%)  | 154 (79%)  | 42 (21%)  | 1           | 6 |
| 5   | F     | 74/137 (54%)    | 59 (80%)   | 15 (20%)  | 1           | 6 |
| 6   | H     | 117/128 (91%)   | 94 (80%)   | 23 (20%)  | 1           | 7 |
| 7   | I     | 113/116 (97%)   | 90 (80%)   | 23 (20%)  | 1           | 6 |
| 8   | J     | 60/65 (92%)     | 39 (65%)   | 21 (35%)  | 0           | 0 |
| 9   | K     | 99/102 (97%)    | 78 (79%)   | 21 (21%)  | 1           | 6 |
| 10  | L     | 40/57 (70%)     | 33 (82%)   | 7 (18%)   | 2           | 9 |
| All | All   | 3111/3657 (85%) | 2410 (78%) | 701 (22%) | 1           | 5 |

All (701) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 12  | ARG  |
| 1   | A     | 18  | GLN  |
| 1   | A     | 22  | PHE  |
| 1   | A     | 30  | ILE  |
| 1   | A     | 47  | ARG  |
| 1   | A     | 49  | LYS  |
| 1   | A     | 50  | ILE  |
| 1   | A     | 53  | LEU  |
| 1   | A     | 54  | ASN  |
| 1   | A     | 55  | ASP  |
| 1   | A     | 61  | ILE  |
| 1   | A     | 65  | LEU  |
| 1   | A     | 68  | GLN  |
| 1   | A     | 69  | THR  |
| 1   | A     | 70  | CYS  |
| 1   | A     | 71  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 80  | HIS  |
| 1   | A     | 84  | ILE  |
| 1   | A     | 93  | VAL  |
| 1   | A     | 106 | VAL  |
| 1   | A     | 109 | HIS  |
| 1   | A     | 114 | LEU  |
| 1   | A     | 126 | LEU  |
| 1   | A     | 132 | LYS  |
| 1   | A     | 144 | THR  |
| 1   | A     | 146 | MET  |
| 1   | A     | 147 | VAL  |
| 1   | A     | 148 | CYS  |
| 1   | A     | 162 | VAL  |
| 1   | A     | 169 | ASN  |
| 1   | A     | 170 | THR  |
| 1   | A     | 179 | LEU  |
| 1   | A     | 202 | LEU  |
| 1   | A     | 208 | LEU  |
| 1   | A     | 212 | LYS  |
| 1   | A     | 216 | VAL  |
| 1   | A     | 220 | THR  |
| 1   | A     | 222 | LEU  |
| 1   | A     | 225 | ASN  |
| 1   | A     | 227 | VAL  |
| 1   | A     | 235 | ILE  |
| 1   | A     | 245 | PRO  |
| 1   | A     | 250 | ILE  |
| 1   | A     | 257 | ARG  |
| 1   | A     | 264 | PHE  |
| 1   | A     | 270 | LEU  |
| 1   | A     | 271 | LYS  |
| 1   | A     | 274 | ILE  |
| 1   | A     | 287 | HIS  |
| 1   | A     | 289 | ILE  |
| 1   | A     | 296 | LEU  |
| 1   | A     | 297 | GLN  |
| 1   | A     | 303 | TYR  |
| 1   | A     | 306 | ASN  |
| 1   | A     | 308 | ILE  |
| 1   | A     | 311 | GLN  |
| 1   | A     | 313 | GLN  |
| 1   | A     | 315 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 316 | GLN  |
| 1   | A     | 320 | ARG  |
| 1   | A     | 322 | VAL  |
| 1   | A     | 323 | LYS  |
| 1   | A     | 326 | ARG  |
| 1   | A     | 329 | LEU  |
| 1   | A     | 332 | LYS  |
| 1   | A     | 333 | GLU  |
| 1   | A     | 335 | ARG  |
| 1   | A     | 336 | ILE  |
| 1   | A     | 344 | ARG  |
| 1   | A     | 351 | THR  |
| 1   | A     | 353 | ILE  |
| 1   | A     | 367 | PRO  |
| 1   | A     | 368 | LYS  |
| 1   | A     | 369 | SER  |
| 1   | A     | 372 | LYS  |
| 1   | A     | 373 | THR  |
| 1   | A     | 375 | THR  |
| 1   | A     | 380 | VAL  |
| 1   | A     | 381 | THR  |
| 1   | A     | 383 | TYR  |
| 1   | A     | 392 | VAL  |
| 1   | A     | 398 | GLU  |
| 1   | A     | 403 | LYS  |
| 1   | A     | 412 | ARG  |
| 1   | A     | 416 | ARG  |
| 1   | A     | 419 | LYS  |
| 1   | A     | 424 | ILE  |
| 1   | A     | 434 | ARG  |
| 1   | A     | 436 | ILE  |
| 1   | A     | 443 | LEU  |
| 1   | A     | 452 | LYS  |
| 1   | A     | 454 | SER  |
| 1   | A     | 461 | LYS  |
| 1   | A     | 463 | ILE  |
| 1   | A     | 466 | SER  |
| 1   | A     | 469 | ARG  |
| 1   | A     | 470 | LEU  |
| 1   | A     | 472 | LEU  |
| 1   | A     | 474 | VAL  |
| 1   | A     | 475 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 476 | SER  |
| 1   | A     | 497 | THR  |
| 1   | A     | 509 | LEU  |
| 1   | A     | 512 | VAL  |
| 1   | A     | 513 | SER  |
| 1   | A     | 518 | LYS  |
| 1   | A     | 523 | ILE  |
| 1   | A     | 531 | ILE  |
| 1   | A     | 532 | ARG  |
| 1   | A     | 535 | THR  |
| 1   | A     | 542 | GLU  |
| 1   | A     | 544 | ASP  |
| 1   | A     | 547 | LEU  |
| 1   | A     | 560 | ILE  |
| 1   | A     | 567 | LYS  |
| 1   | A     | 577 | ILE  |
| 1   | A     | 589 | GLN  |
| 1   | A     | 590 | ARG  |
| 1   | A     | 595 | THR  |
| 1   | A     | 598 | LEU  |
| 1   | A     | 601 | LYS  |
| 1   | A     | 605 | MET  |
| 1   | A     | 612 | ILE  |
| 1   | A     | 618 | GLU  |
| 1   | A     | 621 | THR  |
| 1   | A     | 629 | LEU  |
| 1   | A     | 630 | ILE  |
| 1   | A     | 637 | LYS  |
| 1   | A     | 663 | SER  |
| 1   | A     | 664 | THR  |
| 1   | A     | 666 | ILE  |
| 1   | A     | 670 | ILE  |
| 1   | A     | 672 | ASP  |
| 1   | A     | 676 | MET  |
| 1   | A     | 680 | THR  |
| 1   | A     | 681 | GLU  |
| 1   | A     | 682 | THR  |
| 1   | A     | 685 | GLU  |
| 1   | A     | 688 | LYS  |
| 1   | A     | 691 | LEU  |
| 1   | A     | 695 | LYS  |
| 1   | A     | 702 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 703 | THR  |
| 1   | A     | 709 | THR  |
| 1   | A     | 710 | LEU  |
| 1   | A     | 712 | GLU  |
| 1   | A     | 732 | LEU  |
| 1   | A     | 735 | VAL  |
| 1   | A     | 740 | LEU  |
| 1   | A     | 752 | LYS  |
| 1   | A     | 756 | ILE  |
| 1   | A     | 764 | CYS  |
| 1   | A     | 765 | VAL  |
| 1   | A     | 768 | GLN  |
| 1   | A     | 780 | VAL  |
| 1   | A     | 783 | THR  |
| 1   | A     | 801 | GLU  |
| 1   | A     | 803 | SER  |
| 1   | A     | 805 | LEU  |
| 1   | A     | 821 | ARG  |
| 1   | A     | 829 | VAL  |
| 1   | A     | 830 | LYS  |
| 1   | A     | 834 | THR  |
| 1   | A     | 838 | GLN  |
| 1   | A     | 855 | THR  |
| 1   | A     | 856 | THR  |
| 1   | A     | 858 | ASN  |
| 1   | A     | 867 | ILE  |
| 1   | A     | 879 | GLU  |
| 1   | A     | 884 | ASP  |
| 1   | A     | 885 | THR  |
| 1   | A     | 886 | ILE  |
| 1   | A     | 895 | LYS  |
| 1   | A     | 896 | ARG  |
| 1   | A     | 902 | LEU  |
| 1   | A     | 904 | THR  |
| 1   | A     | 911 | SER  |
| 1   | A     | 914 | GLU  |
| 1   | A     | 919 | ILE  |
| 1   | A     | 922 | ASP  |
| 1   | A     | 926 | GLN  |
| 1   | A     | 932 | GLU  |
| 1   | A     | 936 | LEU  |
| 1   | A     | 940 | ARG  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 941  | LYS  |
| 1   | A     | 949  | ASP  |
| 1   | A     | 960  | ILE  |
| 1   | A     | 961  | ARG  |
| 1   | A     | 965  | GLN  |
| 1   | A     | 976  | THR  |
| 1   | A     | 977  | LYS  |
| 1   | A     | 982  | THR  |
| 1   | A     | 994  | GLN  |
| 1   | A     | 995  | GLU  |
| 1   | A     | 996  | ASN  |
| 1   | A     | 999  | VAL  |
| 1   | A     | 1000 | LEU  |
| 1   | A     | 1001 | ARG  |
| 1   | A     | 1015 | VAL  |
| 1   | A     | 1017 | LEU  |
| 1   | A     | 1029 | ARG  |
| 1   | A     | 1033 | GLN  |
| 1   | A     | 1034 | GLU  |
| 1   | A     | 1047 | SER  |
| 1   | A     | 1048 | ASN  |
| 1   | A     | 1050 | GLU  |
| 1   | A     | 1058 | VAL  |
| 1   | A     | 1064 | VAL  |
| 1   | A     | 1081 | LEU  |
| 1   | A     | 1092 | LYS  |
| 1   | A     | 1093 | LYS  |
| 1   | A     | 1095 | THR  |
| 1   | A     | 1101 | LEU  |
| 1   | A     | 1110 | ASN  |
| 1   | A     | 1111 | MET  |
| 1   | A     | 1116 | LEU  |
| 1   | A     | 1128 | GLN  |
| 1   | A     | 1130 | GLN  |
| 1   | A     | 1146 | VAL  |
| 1   | A     | 1159 | ARG  |
| 1   | A     | 1165 | GLU  |
| 1   | A     | 1167 | GLU  |
| 1   | A     | 1171 | GLN  |
| 1   | A     | 1172 | LEU  |
| 1   | A     | 1187 | GLN  |
| 1   | A     | 1192 | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1193 | LEU  |
| 1   | A     | 1205 | LYS  |
| 1   | A     | 1206 | ASP  |
| 1   | A     | 1208 | THR  |
| 1   | A     | 1219 | THR  |
| 1   | A     | 1227 | ILE  |
| 1   | A     | 1237 | ILE  |
| 1   | A     | 1238 | ILE  |
| 1   | A     | 1243 | VAL  |
| 1   | A     | 1257 | ASP  |
| 1   | A     | 1259 | MET  |
| 1   | A     | 1261 | LYS  |
| 1   | A     | 1262 | LYS  |
| 1   | A     | 1264 | GLU  |
| 1   | A     | 1267 | MET  |
| 1   | A     | 1269 | GLU  |
| 1   | A     | 1273 | LEU  |
| 1   | A     | 1274 | ARG  |
| 1   | A     | 1277 | GLU  |
| 1   | A     | 1279 | ILE  |
| 1   | A     | 1280 | GLU  |
| 1   | A     | 1285 | MET  |
| 1   | A     | 1288 | ASP  |
| 1   | A     | 1291 | VAL  |
| 1   | A     | 1295 | THR  |
| 1   | A     | 1297 | GLU  |
| 1   | A     | 1299 | VAL  |
| 1   | A     | 1300 | LYS  |
| 1   | A     | 1322 | ILE  |
| 1   | A     | 1325 | THR  |
| 1   | A     | 1329 | THR  |
| 1   | A     | 1333 | ILE  |
| 1   | A     | 1335 | ILE  |
| 1   | A     | 1336 | MET  |
| 1   | A     | 1345 | ARG  |
| 1   | A     | 1350 | LYS  |
| 1   | A     | 1354 | ASN  |
| 1   | A     | 1355 | VAL  |
| 1   | A     | 1356 | ILE  |
| 1   | A     | 1359 | ASP  |
| 1   | A     | 1374 | VAL  |
| 1   | A     | 1376 | THR  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1384 | VAL  |
| 1   | A     | 1385 | THR  |
| 1   | A     | 1386 | ARG  |
| 1   | A     | 1391 | ARG  |
| 1   | A     | 1393 | ASN  |
| 1   | A     | 1400 | CYS  |
| 1   | A     | 1403 | GLU  |
| 1   | A     | 1406 | VAL  |
| 1   | A     | 1407 | GLU  |
| 1   | A     | 1411 | GLU  |
| 1   | A     | 1422 | ARG  |
| 1   | A     | 1426 | GLU  |
| 1   | A     | 1445 | ILE  |
| 2   | B     | 20   | ASP  |
| 2   | B     | 28   | GLU  |
| 2   | B     | 46   | GLN  |
| 2   | B     | 58   | THR  |
| 2   | B     | 61   | ASP  |
| 2   | B     | 63   | ILE  |
| 2   | B     | 65   | GLU  |
| 2   | B     | 66   | ASP  |
| 2   | B     | 67   | SER  |
| 2   | B     | 70   | ILE  |
| 2   | B     | 94   | LYS  |
| 2   | B     | 97   | VAL  |
| 2   | B     | 98   | THR  |
| 2   | B     | 102  | VAL  |
| 2   | B     | 108  | VAL  |
| 2   | B     | 120  | ARG  |
| 2   | B     | 133  | LYS  |
| 2   | B     | 134  | LYS  |
| 2   | B     | 167  | ILE  |
| 2   | B     | 169  | ARG  |
| 2   | B     | 175  | ARG  |
| 2   | B     | 179  | CYS  |
| 2   | B     | 181  | LEU  |
| 2   | B     | 183  | GLU  |
| 2   | B     | 194  | GLU  |
| 2   | B     | 217  | ARG  |
| 2   | B     | 222  | ILE  |
| 2   | B     | 225  | VAL  |
| 2   | B     | 234  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 239 | GLU  |
| 2   | B     | 242 | SER  |
| 2   | B     | 245 | GLU  |
| 2   | B     | 246 | LYS  |
| 2   | B     | 249 | ARG  |
| 2   | B     | 252 | SER  |
| 2   | B     | 258 | LEU  |
| 2   | B     | 268 | THR  |
| 2   | B     | 272 | THR  |
| 2   | B     | 275 | TYR  |
| 2   | B     | 276 | ILE  |
| 2   | B     | 284 | ILE  |
| 2   | B     | 292 | ILE  |
| 2   | B     | 294 | ASP  |
| 2   | B     | 305 | VAL  |
| 2   | B     | 310 | MET  |
| 2   | B     | 313 | MET  |
| 2   | B     | 315 | LYS  |
| 2   | B     | 319 | GLU  |
| 2   | B     | 323 | VAL  |
| 2   | B     | 324 | ILE  |
| 2   | B     | 328 | GLU  |
| 2   | B     | 331 | LEU  |
| 2   | B     | 334 | ILE  |
| 2   | B     | 345 | LYS  |
| 2   | B     | 346 | GLU  |
| 2   | B     | 350 | GLN  |
| 2   | B     | 354 | ASP  |
| 2   | B     | 361 | LEU  |
| 2   | B     | 365 | THR  |
| 2   | B     | 366 | GLN  |
| 2   | B     | 367 | LEU  |
| 2   | B     | 368 | GLU  |
| 2   | B     | 382 | ILE  |
| 2   | B     | 384 | ARG  |
| 2   | B     | 387 | LEU  |
| 2   | B     | 393 | LYS  |
| 2   | B     | 394 | ASP  |
| 2   | B     | 395 | GLN  |
| 2   | B     | 398 | ARG  |
| 2   | B     | 415 | GLN  |
| 2   | B     | 425 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 426 | LYS  |
| 2   | B     | 428 | ILE  |
| 2   | B     | 436 | VAL  |
| 2   | B     | 437 | GLU  |
| 2   | B     | 448 | ILE  |
| 2   | B     | 454 | THR  |
| 2   | B     | 455 | SER  |
| 2   | B     | 461 | LEU  |
| 2   | B     | 468 | GLU  |
| 2   | B     | 471 | LYS  |
| 2   | B     | 474 | SER  |
| 2   | B     | 479 | VAL  |
| 2   | B     | 482 | VAL  |
| 2   | B     | 483 | LEU  |
| 2   | B     | 485 | ARG  |
| 2   | B     | 487 | THR  |
| 2   | B     | 498 | THR  |
| 2   | B     | 502 | ILE  |
| 2   | B     | 512 | ARG  |
| 2   | B     | 513 | GLN  |
| 2   | B     | 516 | ASN  |
| 2   | B     | 527 | THR  |
| 2   | B     | 531 | GLN  |
| 2   | B     | 544 | CYS  |
| 2   | B     | 549 | THR  |
| 2   | B     | 552 | MET  |
| 2   | B     | 554 | ILE  |
| 2   | B     | 563 | MET  |
| 2   | B     | 567 | GLU  |
| 2   | B     | 570 | VAL  |
| 2   | B     | 574 | SER  |
| 2   | B     | 578 | THR  |
| 2   | B     | 598 | GLU  |
| 2   | B     | 604 | ARG  |
| 2   | B     | 606 | LYS  |
| 2   | B     | 609 | ILE  |
| 2   | B     | 617 | ARG  |
| 2   | B     | 619 | ILE  |
| 2   | B     | 624 | LEU  |
| 2   | B     | 633 | VAL  |
| 2   | B     | 635 | ARG  |
| 2   | B     | 637 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 639 | ILE  |
| 2   | B     | 644 | GLU  |
| 2   | B     | 651 | LEU  |
| 2   | B     | 653 | VAL  |
| 2   | B     | 655 | LYS  |
| 2   | B     | 666 | TYR  |
| 2   | B     | 690 | VAL  |
| 2   | B     | 706 | GLN  |
| 2   | B     | 708 | GLU  |
| 2   | B     | 710 | LEU  |
| 2   | B     | 731 | VAL  |
| 2   | B     | 732 | SER  |
| 2   | B     | 739 | THR  |
| 2   | B     | 742 | GLU  |
| 2   | B     | 743 | ILE  |
| 2   | B     | 747 | MET  |
| 2   | B     | 751 | VAL  |
| 2   | B     | 764 | SER  |
| 2   | B     | 780 | VAL  |
| 2   | B     | 786 | ASN  |
| 2   | B     | 787 | VAL  |
| 2   | B     | 789 | MET  |
| 2   | B     | 790 | ASP  |
| 2   | B     | 791 | THR  |
| 2   | B     | 792 | MET  |
| 2   | B     | 795 | ILE  |
| 2   | B     | 815 | ARG  |
| 2   | B     | 825 | VAL  |
| 2   | B     | 827 | ILE  |
| 2   | B     | 844 | SER  |
| 2   | B     | 864 | LYS  |
| 2   | B     | 865 | LYS  |
| 2   | B     | 868 | MET  |
| 2   | B     | 871 | THR  |
| 2   | B     | 879 | ARG  |
| 2   | B     | 880 | THR  |
| 2   | B     | 881 | ASN  |
| 2   | B     | 882 | THR  |
| 2   | B     | 893 | LEU  |
| 2   | B     | 894 | ASP  |
| 2   | B     | 899 | ILE  |
| 2   | B     | 901 | PRO  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 904  | ARG  |
| 2   | B     | 939  | THR  |
| 2   | B     | 943  | SER  |
| 2   | B     | 944  | THR  |
| 2   | B     | 955  | THR  |
| 2   | B     | 957  | ASN  |
| 2   | B     | 963  | PHE  |
| 2   | B     | 969  | ARG  |
| 2   | B     | 970  | THR  |
| 2   | B     | 976  | ILE  |
| 2   | B     | 983  | ARG  |
| 2   | B     | 987  | LYS  |
| 2   | B     | 992  | ILE  |
| 2   | B     | 996  | ARG  |
| 2   | B     | 997  | GLU  |
| 2   | B     | 1002 | THR  |
| 2   | B     | 1004 | GLU  |
| 2   | B     | 1006 | ILE  |
| 2   | B     | 1007 | VAL  |
| 2   | B     | 1021 | MET  |
| 2   | B     | 1028 | GLU  |
| 2   | B     | 1032 | SER  |
| 2   | B     | 1046 | PRO  |
| 2   | B     | 1051 | THR  |
| 2   | B     | 1055 | ILE  |
| 2   | B     | 1057 | LYS  |
| 2   | B     | 1065 | GLN  |
| 2   | B     | 1077 | THR  |
| 2   | B     | 1082 | MET  |
| 2   | B     | 1093 | GLN  |
| 2   | B     | 1094 | ARG  |
| 2   | B     | 1096 | ARG  |
| 2   | B     | 1099 | VAL  |
| 2   | B     | 1101 | ASP  |
| 2   | B     | 1103 | ILE  |
| 2   | B     | 1111 | MET  |
| 2   | B     | 1113 | VAL  |
| 2   | B     | 1120 | GLU  |
| 2   | B     | 1122 | ARG  |
| 2   | B     | 1123 | SER  |
| 2   | B     | 1147 | LEU  |
| 2   | B     | 1150 | ARG  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 1151 | LEU  |
| 2   | B     | 1155 | SER  |
| 2   | B     | 1159 | ARG  |
| 2   | B     | 1160 | VAL  |
| 2   | B     | 1174 | LYS  |
| 2   | B     | 1176 | ASN  |
| 2   | B     | 1181 | GLU  |
| 2   | B     | 1186 | ASP  |
| 2   | B     | 1188 | LYS  |
| 2   | B     | 1189 | ILE  |
| 2   | B     | 1191 | ILE  |
| 2   | B     | 1194 | ILE  |
| 2   | B     | 1202 | LEU  |
| 2   | B     | 1220 | ARG  |
| 3   | C     | 4    | GLU  |
| 3   | C     | 9    | LYS  |
| 3   | C     | 10   | ILE  |
| 3   | C     | 11   | ARG  |
| 3   | C     | 15   | LYS  |
| 3   | C     | 18   | VAL  |
| 3   | C     | 22   | LEU  |
| 3   | C     | 23   | SER  |
| 3   | C     | 25   | VAL  |
| 3   | C     | 27   | LEU  |
| 3   | C     | 35   | ARG  |
| 3   | C     | 38   | ILE  |
| 3   | C     | 41   | ILE  |
| 3   | C     | 46   | ILE  |
| 3   | C     | 53   | THR  |
| 3   | C     | 56   | THR  |
| 3   | C     | 57   | VAL  |
| 3   | C     | 69   | LEU  |
| 3   | C     | 77   | ILE  |
| 3   | C     | 89   | GLU  |
| 3   | C     | 99   | LEU  |
| 3   | C     | 100  | THR  |
| 3   | C     | 106  | GLU  |
| 3   | C     | 109  | SER  |
| 3   | C     | 110  | THR  |
| 3   | C     | 116  | LYS  |
| 3   | C     | 120  | ILE  |
| 3   | C     | 121  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 129 | ILE  |
| 3   | C     | 133 | ILE  |
| 3   | C     | 137 | LYS  |
| 3   | C     | 140 | ASN  |
| 3   | C     | 147 | LEU  |
| 3   | C     | 149 | LYS  |
| 3   | C     | 151 | GLN  |
| 3   | C     | 154 | LYS  |
| 3   | C     | 177 | GLU  |
| 3   | C     | 183 | TRP  |
| 3   | C     | 186 | LEU  |
| 3   | C     | 189 | THR  |
| 3   | C     | 195 | GLN  |
| 3   | C     | 197 | SER  |
| 3   | C     | 203 | GLN  |
| 3   | C     | 204 | SER  |
| 3   | C     | 222 | LYS  |
| 3   | C     | 224 | GLN  |
| 3   | C     | 226 | ASP  |
| 3   | C     | 231 | ASN  |
| 3   | C     | 235 | VAL  |
| 3   | C     | 238 | ILE  |
| 3   | C     | 240 | VAL  |
| 3   | C     | 244 | VAL  |
| 3   | C     | 249 | ASP  |
| 3   | C     | 253 | LYS  |
| 3   | C     | 258 | ILE  |
| 3   | C     | 263 | THR  |
| 3   | C     | 268 | ASP  |
| 4   | E     | 3   | GLN  |
| 4   | E     | 9   | ILE  |
| 4   | E     | 14  | ARG  |
| 4   | E     | 30  | ILE  |
| 4   | E     | 31  | THR  |
| 4   | E     | 32  | GLN  |
| 4   | E     | 37  | LEU  |
| 4   | E     | 40  | GLU  |
| 4   | E     | 43  | LYS  |
| 4   | E     | 54  | GLN  |
| 4   | E     | 66  | GLU  |
| 4   | E     | 69  | ILE  |
| 4   | E     | 78  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | E     | 80  | VAL  |
| 4   | E     | 92  | THR  |
| 4   | E     | 94  | LYS  |
| 4   | E     | 95  | THR  |
| 4   | E     | 98  | ILE  |
| 4   | E     | 101 | GLN  |
| 4   | E     | 103 | LYS  |
| 4   | E     | 123 | LEU  |
| 4   | E     | 127 | ILE  |
| 4   | E     | 131 | THR  |
| 4   | E     | 134 | THR  |
| 4   | E     | 137 | GLU  |
| 4   | E     | 144 | ILE  |
| 4   | E     | 146 | HIS  |
| 4   | E     | 150 | VAL  |
| 4   | E     | 152 | LYS  |
| 4   | E     | 154 | ILE  |
| 4   | E     | 162 | ARG  |
| 4   | E     | 164 | LEU  |
| 4   | E     | 165 | LEU  |
| 4   | E     | 169 | ARG  |
| 4   | E     | 179 | GLN  |
| 4   | E     | 191 | LYS  |
| 4   | E     | 192 | ARG  |
| 4   | E     | 200 | ARG  |
| 4   | E     | 201 | LYS  |
| 4   | E     | 202 | SER  |
| 4   | E     | 204 | THR  |
| 4   | E     | 215 | MET  |
| 5   | F     | 72  | LYS  |
| 5   | F     | 74  | ILE  |
| 5   | F     | 79  | ARG  |
| 5   | F     | 82  | THR  |
| 5   | F     | 93  | ILE  |
| 5   | F     | 97  | ARG  |
| 5   | F     | 103 | MET  |
| 5   | F     | 111 | LEU  |
| 5   | F     | 112 | GLU  |
| 5   | F     | 119 | ARG  |
| 5   | F     | 133 | VAL  |
| 5   | F     | 140 | ASP  |
| 5   | F     | 149 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | F     | 150 | GLU  |
| 5   | F     | 155 | LEU  |
| 6   | H     | 2   | SER  |
| 6   | H     | 4   | THR  |
| 6   | H     | 11  | GLN  |
| 6   | H     | 15  | VAL  |
| 6   | H     | 21  | ASN  |
| 6   | H     | 24  | CYS  |
| 6   | H     | 26  | ILE  |
| 6   | H     | 32  | THR  |
| 6   | H     | 34  | ASP  |
| 6   | H     | 55  | LEU  |
| 6   | H     | 58  | THR  |
| 6   | H     | 59  | ILE  |
| 6   | H     | 83  | GLN  |
| 6   | H     | 89  | LEU  |
| 6   | H     | 100 | THR  |
| 6   | H     | 106 | GLU  |
| 6   | H     | 110 | ASP  |
| 6   | H     | 123 | MET  |
| 6   | H     | 124 | ARG  |
| 6   | H     | 130 | ARG  |
| 6   | H     | 136 | LYS  |
| 6   | H     | 137 | GLN  |
| 6   | H     | 142 | LEU  |
| 7   | I     | 3   | THR  |
| 7   | I     | 8   | ARG  |
| 7   | I     | 14  | LEU  |
| 7   | I     | 28  | GLU  |
| 7   | I     | 29  | CYS  |
| 7   | I     | 30  | ARG  |
| 7   | I     | 33  | SER  |
| 7   | I     | 50  | THR  |
| 7   | I     | 52  | ILE  |
| 7   | I     | 55  | THR  |
| 7   | I     | 60  | GLN  |
| 7   | I     | 74  | GLU  |
| 7   | I     | 75  | CYS  |
| 7   | I     | 83  | ASN  |
| 7   | I     | 89  | GLN  |
| 7   | I     | 90  | GLN  |
| 7   | I     | 91  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | I     | 95  | THR  |
| 7   | I     | 106 | CYS  |
| 7   | I     | 107 | SER  |
| 7   | I     | 116 | ASN  |
| 7   | I     | 117 | LYS  |
| 7   | I     | 118 | ARG  |
| 8   | J     | 1   | MET  |
| 8   | J     | 2   | ILE  |
| 8   | J     | 3   | VAL  |
| 8   | J     | 6   | ARG  |
| 8   | J     | 7   | CYS  |
| 8   | J     | 9   | SER  |
| 8   | J     | 13  | VAL  |
| 8   | J     | 17  | LYS  |
| 8   | J     | 22  | LEU  |
| 8   | J     | 26  | GLN  |
| 8   | J     | 27  | GLU  |
| 8   | J     | 28  | ASP  |
| 8   | J     | 29  | GLU  |
| 8   | J     | 31  | ASP  |
| 8   | J     | 42  | LYS  |
| 8   | J     | 43  | ARG  |
| 8   | J     | 46  | CYS  |
| 8   | J     | 48  | ARG  |
| 8   | J     | 54  | VAL  |
| 8   | J     | 59  | LYS  |
| 8   | J     | 64  | ASN  |
| 9   | K     | 1   | MET  |
| 9   | K     | 6   | ARG  |
| 9   | K     | 14  | GLU  |
| 9   | K     | 17  | SER  |
| 9   | K     | 18  | LYS  |
| 9   | K     | 20  | LYS  |
| 9   | K     | 26  | LYS  |
| 9   | K     | 31  | VAL  |
| 9   | K     | 32  | VAL  |
| 9   | K     | 42  | LEU  |
| 9   | K     | 46  | ILE  |
| 9   | K     | 51  | LEU  |
| 9   | K     | 56  | VAL  |
| 9   | K     | 77  | THR  |
| 9   | K     | 79  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | K     | 82  | ASP  |
| 9   | K     | 101 | LEU  |
| 9   | K     | 102 | LYS  |
| 9   | K     | 103 | THR  |
| 9   | K     | 106 | GLU  |
| 9   | K     | 107 | THR  |
| 10  | L     | 27  | LEU  |
| 10  | L     | 28  | LYS  |
| 10  | L     | 31  | CYS  |
| 10  | L     | 38  | LEU  |
| 10  | L     | 42  | ARG  |
| 10  | L     | 55  | ILE  |
| 10  | L     | 61  | THR  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (110) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 4   | GLN  |
| 1   | A     | 68  | GLN  |
| 1   | A     | 75  | ASN  |
| 1   | A     | 83  | HIS  |
| 1   | A     | 169 | ASN  |
| 1   | A     | 171 | GLN  |
| 1   | A     | 225 | ASN  |
| 1   | A     | 273 | ASN  |
| 1   | A     | 297 | GLN  |
| 1   | A     | 311 | GLN  |
| 1   | A     | 316 | GLN  |
| 1   | A     | 339 | ASN  |
| 1   | A     | 390 | GLN  |
| 1   | A     | 394 | ASN  |
| 1   | A     | 425 | GLN  |
| 1   | A     | 435 | HIS  |
| 1   | A     | 451 | HIS  |
| 1   | A     | 503 | GLN  |
| 1   | A     | 517 | ASN  |
| 1   | A     | 545 | GLN  |
| 1   | A     | 589 | GLN  |
| 1   | A     | 611 | GLN  |
| 1   | A     | 698 | GLN  |
| 1   | A     | 736 | ASN  |
| 1   | A     | 741 | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 742  | ASN  |
| 1   | A     | 745  | GLN  |
| 1   | A     | 757  | ASN  |
| 1   | A     | 768  | GLN  |
| 1   | A     | 786  | HIS  |
| 1   | A     | 858  | ASN  |
| 1   | A     | 906  | HIS  |
| 1   | A     | 926  | GLN  |
| 1   | A     | 968  | GLN  |
| 1   | A     | 1033 | GLN  |
| 1   | A     | 1110 | ASN  |
| 1   | A     | 1130 | GLN  |
| 1   | A     | 1171 | GLN  |
| 1   | A     | 1203 | ASN  |
| 1   | A     | 1270 | ASN  |
| 1   | A     | 1312 | ASN  |
| 1   | A     | 1364 | ASN  |
| 1   | A     | 1378 | GLN  |
| 1   | A     | 1393 | ASN  |
| 1   | A     | 1432 | GLN  |
| 2   | B     | 103  | ASN  |
| 2   | B     | 115  | GLN  |
| 2   | B     | 121  | ASN  |
| 2   | B     | 178  | ASN  |
| 2   | B     | 215  | GLN  |
| 2   | B     | 255  | GLN  |
| 2   | B     | 325  | GLN  |
| 2   | B     | 350  | GLN  |
| 2   | B     | 366  | GLN  |
| 2   | B     | 383  | ASN  |
| 2   | B     | 395  | GLN  |
| 2   | B     | 433  | GLN  |
| 2   | B     | 515  | HIS  |
| 2   | B     | 516  | ASN  |
| 2   | B     | 518  | HIS  |
| 2   | B     | 531  | GLN  |
| 2   | B     | 573  | GLN  |
| 2   | B     | 587  | HIS  |
| 2   | B     | 590  | HIS  |
| 2   | B     | 657  | HIS  |
| 2   | B     | 686  | ASN  |
| 2   | B     | 744  | HIS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 762  | ASN  |
| 2   | B     | 794  | ASN  |
| 2   | B     | 822  | ASN  |
| 2   | B     | 835  | GLN  |
| 2   | B     | 843  | GLN  |
| 2   | B     | 862  | GLN  |
| 2   | B     | 957  | ASN  |
| 2   | B     | 975  | GLN  |
| 2   | B     | 984  | HIS  |
| 2   | B     | 1015 | HIS  |
| 2   | B     | 1065 | GLN  |
| 2   | B     | 1084 | GLN  |
| 2   | B     | 1093 | GLN  |
| 2   | B     | 1117 | GLN  |
| 2   | B     | 1179 | GLN  |
| 2   | B     | 1187 | ASN  |
| 2   | B     | 1193 | GLN  |
| 3   | C     | 73   | GLN  |
| 3   | C     | 79   | GLN  |
| 3   | C     | 112  | ASN  |
| 3   | C     | 123  | ASN  |
| 3   | C     | 128  | ASN  |
| 3   | C     | 167  | HIS  |
| 3   | C     | 188  | HIS  |
| 3   | C     | 206  | ASN  |
| 3   | C     | 224  | GLN  |
| 3   | C     | 242  | GLN  |
| 3   | C     | 264  | GLN  |
| 3   | C     | 267  | GLN  |
| 4   | E     | 32   | GLN  |
| 4   | E     | 63   | ASN  |
| 4   | E     | 147  | HIS  |
| 4   | E     | 179  | GLN  |
| 6   | H     | 11   | GLN  |
| 6   | H     | 133  | ASN  |
| 6   | H     | 137  | GLN  |
| 7   | I     | 12   | ASN  |
| 7   | I     | 60   | GLN  |
| 7   | I     | 83   | ASN  |
| 7   | I     | 114  | GLN  |
| 9   | K     | 65   | HIS  |
| 9   | K     | 76   | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | K     | 89  | ASN  |

### 5.3.3 RNA [i](#)

| Mol | Chain | Analysed    | Backbone Outliers | Pucker Outliers |
|-----|-------|-------------|-------------------|-----------------|
| 11  | R     | 10/11 (90%) | 2 (20%)           | 0               |

All (2) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11  | R     | 3   | G    |
| 11  | R     | 11  | C    |

There are no RNA pucker outliers to report.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 9 are monoatomic - leaving 1 for Mogul analysis.

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 | $\# Z  > 2$ |
| 16  | C7P  | T     | 29  | 12   | 5,9,10       | 1.10 | 0           | 2,11,14     | 0.58 | 0           |

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   |
|-----|------|-------|-----|------|---------|----------|---------|
| 16  | C7P  | T     | 29  | 12   | -       | -        | 0/1/1/1 |

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](#)

There are no chain breaks in this entry.

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

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

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ > 2 |     |     | OWAB(Å <sup>2</sup> ) | Q < 0.9 |
|-----|-------|-----------------|--------|-----------|-----|-----|-----------------------|---------|
| 1   | A     | 1395/1733 (80%) | 0.27   | 55 (3%)   | 43  | 25  | 47, 104, 216, 308     | 0       |
| 2   | B     | 1106/1224 (90%) | 0.03   | 32 (2%)   | 53  | 34  | 43, 86, 154, 209      | 0       |
| 3   | C     | 266/318 (83%)   | -0.15  | 0         | 100 | 100 | 62, 91, 135, 158      | 0       |
| 4   | E     | 214/215 (99%)   | 0.52   | 4 (1%)    | 66  | 45  | 81, 159, 224, 242     | 0       |
| 5   | F     | 84/155 (54%)    | -0.00  | 2 (2%)    | 59  | 39  | 77, 110, 142, 150     | 0       |
| 6   | H     | 133/146 (91%)   | 0.94   | 15 (11%)  | 10  | 6   | 101, 153, 199, 211    | 0       |
| 7   | I     | 119/122 (97%)   | 0.61   | 5 (4%)    | 40  | 23  | 74, 118, 158, 172     | 0       |
| 8   | J     | 65/70 (92%)     | -0.41  | 0         | 100 | 100 | 56, 73, 100, 116      | 0       |
| 9   | K     | 114/120 (95%)   | -0.07  | 1 (0%)    | 81  | 64  | 59, 103, 131, 141     | 0       |
| 10  | L     | 46/70 (65%)     | 1.08   | 6 (13%)   | 7   | 5   | 72, 143, 173, 182     | 0       |
| 11  | R     | 11/11 (100%)    | 3.64   | 11 (100%) | 0   | 0   | 140, 156, 209, 217    | 0       |
| 12  | T     | 28/28 (100%)    | 2.51   | 14 (50%)  | 0   | 1   | 146, 280, 387, 396    | 0       |
| 13  | N     | 14/14 (100%)    | 1.69   | 2 (14%)   | 6   | 4   | 308, 349, 380, 385    | 0       |
| All | All   | 3595/4226 (85%) | 0.23   | 147 (4%)  | 41  | 24  | 43, 103, 202, 396     | 0       |

All (147) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | B     | 477 | ALA  | 7.5  |
| 10  | L     | 27  | LEU  | 5.6  |
| 2   | B     | 335 | GLY  | 5.2  |
| 1   | A     | 141 | LEU  | 5.1  |
| 10  | L     | 28  | LYS  | 4.8  |
| 1   | A     | 318 | SER  | 4.8  |
| 6   | H     | 63  | LEU  | 4.7  |
| 6   | H     | 84  | ALA  | 4.7  |
| 12  | T     | 26  | DC   | 4.5  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 12  | T     | 20  | DC   | 4.5  |
| 11  | R     | 8   | G    | 4.4  |
| 12  | T     | 21  | DC   | 4.4  |
| 11  | R     | 7   | A    | 4.4  |
| 11  | R     | 10  | A    | 4.3  |
| 1   | A     | 69  | THR  | 4.3  |
| 11  | R     | 11  | C    | 4.3  |
| 2   | B     | 70  | ILE  | 4.1  |
| 6   | H     | 140 | ALA  | 4.0  |
| 2   | B     | 643 | ASP  | 4.0  |
| 12  | T     | 25  | DC   | 3.9  |
| 2   | B     | 509 | ALA  | 3.9  |
| 12  | T     | 22  | DT   | 3.9  |
| 11  | R     | 6   | G    | 3.9  |
| 11  | R     | 9   | G    | 3.8  |
| 12  | T     | 24  | DT   | 3.8  |
| 10  | L     | 25  | ALA  | 3.7  |
| 2   | B     | 709 | ASP  | 3.7  |
| 1   | A     | 65  | LEU  | 3.7  |
| 12  | T     | 19  | DT   | 3.7  |
| 6   | H     | 139 | ASN  | 3.6  |
| 12  | T     | 18  | DG   | 3.6  |
| 2   | B     | 446 | LEU  | 3.5  |
| 1   | A     | 51  | GLY  | 3.5  |
| 2   | B     | 646 | LEU  | 3.5  |
| 12  | T     | 23  | DC   | 3.4  |
| 11  | R     | 2   | U    | 3.4  |
| 11  | R     | 5   | A    | 3.4  |
| 12  | T     | 27  | DA   | 3.4  |
| 6   | H     | 85  | GLY  | 3.3  |
| 1   | A     | 250 | ILE  | 3.2  |
| 1   | A     | 59  | GLY  | 3.2  |
| 10  | L     | 26  | THR  | 3.1  |
| 12  | T     | 28  | DT   | 3.1  |
| 6   | H     | 31  | THR  | 3.0  |
| 1   | A     | 154 | SER  | 3.0  |
| 7   | I     | 49  | ILE  | 3.0  |
| 6   | H     | 6   | PHE  | 3.0  |
| 10  | L     | 45  | ALA  | 3.0  |
| 11  | R     | 3   | G    | 3.0  |
| 2   | B     | 715 | ALA  | 2.9  |
| 2   | B     | 866 | TYR  | 2.9  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 6   | H     | 134  | ASN  | 2.9  |
| 1   | A     | 315  | LEU  | 2.9  |
| 2   | B     | 250  | PHE  | 2.9  |
| 7   | I     | 82   | GLU  | 2.8  |
| 1   | A     | 216  | VAL  | 2.8  |
| 6   | H     | 90   | ALA  | 2.8  |
| 1   | A     | 144  | THR  | 2.8  |
| 6   | H     | 130  | ARG  | 2.8  |
| 1   | A     | 317  | LYS  | 2.8  |
| 1   | A     | 322  | VAL  | 2.7  |
| 2   | B     | 473  | MET  | 2.7  |
| 1   | A     | 1081 | LEU  | 2.7  |
| 11  | R     | 1    | A    | 2.7  |
| 2   | B     | 474  | SER  | 2.7  |
| 1   | A     | 174  | ILE  | 2.6  |
| 1   | A     | 252  | PHE  | 2.6  |
| 12  | T     | 4    | DC   | 2.6  |
| 2   | B     | 710  | LEU  | 2.6  |
| 5   | F     | 155  | LEU  | 2.6  |
| 2   | B     | 816  | GLU  | 2.6  |
| 2   | B     | 733  | HIS  | 2.6  |
| 11  | R     | 4    | G    | 2.6  |
| 6   | H     | 136  | LYS  | 2.5  |
| 1   | A     | 1445 | ILE  | 2.5  |
| 4   | E     | 98   | ILE  | 2.5  |
| 1   | A     | 98   | LYS  | 2.5  |
| 1   | A     | 186  | LYS  | 2.5  |
| 1   | A     | 58   | LEU  | 2.5  |
| 13  | N     | 4    | DG   | 2.4  |
| 1   | A     | 121  | LEU  | 2.4  |
| 1   | A     | 73   | GLY  | 2.4  |
| 2   | B     | 731  | VAL  | 2.4  |
| 1   | A     | 126  | LEU  | 2.4  |
| 1   | A     | 54   | ASN  | 2.4  |
| 2   | B     | 334  | ILE  | 2.4  |
| 1   | A     | 64   | ASN  | 2.4  |
| 1   | A     | 114  | LEU  | 2.4  |
| 1   | A     | 153  | PRO  | 2.4  |
| 2   | B     | 865  | LYS  | 2.4  |
| 1   | A     | 41   | MET  | 2.4  |
| 1   | A     | 249  | SER  | 2.4  |
| 2   | B     | 1221 | SER  | 2.4  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | A     | 145  | LYS  | 2.3  |
| 4   | E     | 91   | LYS  | 2.3  |
| 1   | A     | 149  | GLU  | 2.3  |
| 9   | K     | 14   | GLU  | 2.3  |
| 5   | F     | 74   | ILE  | 2.3  |
| 2   | B     | 881  | ASN  | 2.3  |
| 1   | A     | 161  | LEU  | 2.3  |
| 2   | B     | 879  | ARG  | 2.3  |
| 2   | B     | 167  | ILE  | 2.3  |
| 10  | L     | 30   | ILE  | 2.3  |
| 12  | T     | 5    | DC   | 2.3  |
| 1   | A     | 234  | MET  | 2.3  |
| 1   | A     | 199  | LEU  | 2.3  |
| 6   | H     | 7    | ASP  | 2.3  |
| 1   | A     | 567  | LYS  | 2.3  |
| 1   | A     | 32   | VAL  | 2.3  |
| 1   | A     | 1403 | GLU  | 2.3  |
| 1   | A     | 148  | CYS  | 2.3  |
| 1   | A     | 61   | ILE  | 2.2  |
| 2   | B     | 90   | ILE  | 2.2  |
| 1   | A     | 568  | PRO  | 2.2  |
| 1   | A     | 152  | VAL  | 2.2  |
| 7   | I     | 52   | ILE  | 2.2  |
| 1   | A     | 1176 | LEU  | 2.2  |
| 2   | B     | 447  | ALA  | 2.2  |
| 1   | A     | 176  | LYS  | 2.2  |
| 4   | E     | 94   | LYS  | 2.2  |
| 4   | E     | 16   | PHE  | 2.2  |
| 13  | N     | 14   | DG   | 2.2  |
| 2   | B     | 870  | ILE  | 2.2  |
| 1   | A     | 1330 | ASN  | 2.2  |
| 2   | B     | 708  | GLU  | 2.2  |
| 7   | I     | 28   | GLU  | 2.2  |
| 1   | A     | 177  | ASP  | 2.2  |
| 1   | A     | 319  | GLY  | 2.2  |
| 12  | T     | 17   | DC   | 2.1  |
| 1   | A     | 66   | LYS  | 2.1  |
| 1   | A     | 1273 | LEU  | 2.1  |
| 6   | H     | 9    | ILE  | 2.1  |
| 2   | B     | 472  | ALA  | 2.1  |
| 2   | B     | 248  | SER  | 2.1  |
| 6   | H     | 86   | ASP  | 2.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | B     | 277 | LYS  | 2.1  |
| 6   | H     | 58  | THR  | 2.1  |
| 1   | A     | 91  | PHE  | 2.1  |
| 1   | A     | 38  | PRO  | 2.0  |
| 1   | A     | 56  | PRO  | 2.0  |
| 1   | A     | 113 | LEU  | 2.0  |
| 7   | I     | 107 | SER  | 2.0  |
| 1   | A     | 248 | PRO  | 2.0  |
| 1   | A     | 316 | GLN  | 2.0  |
| 1   | A     | 147 | VAL  | 2.0  |
| 2   | B     | 132 | VAL  | 2.0  |
| 2   | B     | 883 | LEU  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 16  | C7P  | T     | 29   | 9/10  | 0.88 | 0.29 | 205,229,260,269            | 1     |
| 15  | MG   | A     | 2001 | 1/1   | 0.93 | 0.09 | 67,67,67,67                | 0     |
| 14  | ZN   | A     | 1734 | 1/1   | 0.96 | 0.09 | 113,113,113,113            | 0     |
| 14  | ZN   | L     | 105  | 1/1   | 0.98 | 0.05 | 101,101,101,101            | 1     |
| 14  | ZN   | A     | 1735 | 1/1   | 0.98 | 0.07 | 83,83,83,83                | 0     |
| 14  | ZN   | B     | 1307 | 1/1   | 0.98 | 0.06 | 92,92,92,92                | 0     |
| 14  | ZN   | J     | 101  | 1/1   | 0.99 | 0.07 | 61,61,61,61                | 0     |
| 14  | ZN   | I     | 204  | 1/1   | 0.99 | 0.11 | 59,59,59,59                | 0     |
| 14  | ZN   | I     | 203  | 1/1   | 1.00 | 0.05 | 74,74,74,74                | 0     |
| 14  | ZN   | C     | 319  | 1/1   | 1.00 | 0.09 | 63,63,63,63                | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.