



## Full wwPDB EM Validation Report ⓘ

May 10, 2026 – 12:28 AM JST

PDB ID : 9K13 / pdb\_00009k13  
EMDB ID : EMD-61963  
Title : A cryo-EM structure of *B. oleracea* RNA polymerase V in complex with 2U scaffold at 3.04 Angstrom  
Authors : Xie, G.; Du, X.; Du, J.  
Deposited on : 2024-10-16  
Resolution : 3.04 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>  
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:

EMDB validation analysis : **FAILED**  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : **NOT EXECUTED**  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

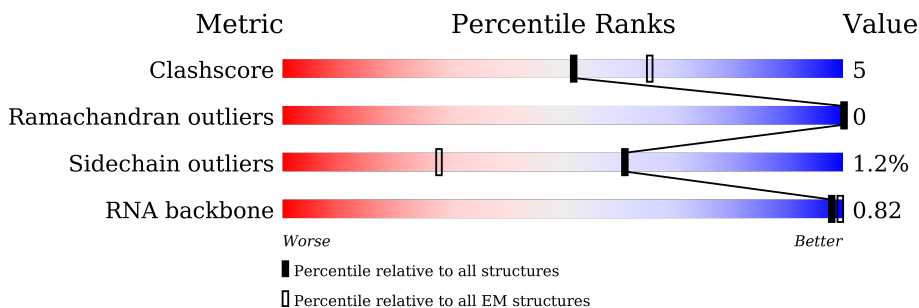
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.04 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) | EM structures<br>(#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore            | 229148                      | 23984                       |
| Ramachandran outliers | 224038                      | 23583                       |
| Sidechain outliers    | 223484                      | 23102                       |
| RNA backbone          | 8273                        | 3508                        |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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  $\leq 5\%$ .

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | T     | 34     | 26% 24% 50%      |
| 2   | N     | 34     | 41% 15% 44%      |
| 3   | P     | 20     | 10% 30% 60%      |
| 4   | A     | 2032   | 36% 5% 58%       |
| 5   | C     | 319    | 83% 7% 10%       |
| 6   | F     | 144    | 48% 8% 44%       |
| 7   | J     | 71     | 82% 7% 11%       |
| 8   | K     | 116    | 84% 9% 7%        |

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| Mol | Chain | Length | Quality of chain                                                                                    |
|-----|-------|--------|-----------------------------------------------------------------------------------------------------|
| 9   | L     | 51     | <br>76% 12% 12%   |
| 10  | H     | 146    | <br>72% 24% • •   |
| 11  | I     | 114    | <br>62% 21% • 15% |
| 12  | E     | 230    | <br>61% 29% • 9%  |
| 13  | B     | 1169   | <br>76% 7% 17%    |

## 2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 23483 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 DNA chain called DNA (34-MER).

| Mol | Chain | Residues | Atoms |     |    |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|-------|
| 1   | T     | 17       | Total | C   | N  | O   | P  | 0       | 0     |
|     |       |          | 345   | 164 | 64 | 100 | 17 |         |       |

- Molecule 2 is a DNA chain called DNA (34-MER).

| Mol | Chain | Residues | Atoms |     |    |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|-------|
| 2   | N     | 19       | Total | C   | N  | O   | P  | 0       | 0     |
|     |       |          | 392   | 186 | 72 | 115 | 19 |         |       |

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

| Mol | Chain | Residues | Atoms |    |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|-------|
| 3   | P     | 8        | Total | C  | N  | O  | P | 0       | 0     |
|     |       |          | 171   | 76 | 30 | 57 | 8 |         |       |

- Molecule 4 is a protein called DNA-directed RNA polymerase V largest subunit.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 4   | A     | 844      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6608  | 4175 | 1136 | 1253 | 44 |         |       |

- Molecule 5 is a protein called DNA-directed RNA polymerase RpoA/D/Rpb3-type domain-containing protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 5   | C     | 287      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2256  | 1418 | 380 | 445 | 13 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference      |
|-------|---------|----------|--------|----------|----------------|
| C     | 2       | THR      | SER    | conflict | UNP A0A0D3D418 |

- Molecule 6 is a protein called DNA-directed RNA polymerase RpoA/D/Rpb3-type domain-containing protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6   | F     | 80       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 660   | 420 | 114 | 122 | 4 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference      |
|-------|---------|----------|--------|----------|----------------|
| F     | 51      | GLU      | ASP    | conflict | UNP A0A0D3BZZ8 |

- Molecule 7 is a protein called DNA-directed RNA polymerase II, IV and V subunit 10.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 7   | J     | 63       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 507   | 324 | 85 | 91 | 7 |         |       |

- Molecule 8 is a protein called DNA-directed RNA polymerase RBP11-like dimerisation domain-containing protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8   | K     | 108      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 890   | 565 | 156 | 167 | 2 |         |       |

- Molecule 9 is a protein called DNA-directed RNA polymerase II, IV and V subunit 12.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 9   | L     | 45       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 365   | 224 | 70 | 67 | 4 |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference      |
|-------|---------|----------|--------|----------|----------------|
| L     | 18      | GLU      | LYS    | conflict | UNP A0A0D2ZPP3 |
| L     | 32      | CYS      | ARG    | conflict | UNP A0A0D2ZPP3 |

- Molecule 10 is a protein called DNA-directed RNA polymerase II, IV and V subunit 8.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10  | H     | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1129  | 729 | 183 | 208 | 9 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 11  | I     | 97       | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 787   | 482 | 150 | 143 | 12 |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference      |
|-------|---------|----------|--------|----------|----------------|
| I     | 20      | ARG      | LYS    | conflict | UNP A0A0D3A7P5 |
| I     | 40      | ASP      | ASN    | conflict | UNP A0A0D3A7P5 |

- Molecule 12 is a protein called RNA polymerase subunit H/Rpb5 C-terminal domain-containing protein.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 12  | E     | 209      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1706  | 1085 | 303 | 316 | 2 |         |       |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference      |
|-------|---------|----------|--------|----------|----------------|
| E     | 101     | GLY      | SER    | conflict | UNP A0A0D3DTU3 |
| E     | 182     | GLN      | HIS    | conflict | UNP A0A0D3DTU3 |
| E     | 210     | ILE      | VAL    | conflict | UNP A0A0D3DTU3 |

- Molecule 13 is a protein called DNA-directed RNA polymerase IV and V subunit 2.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 13  | B     | 967      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 7660  | 4827 | 1357 | 1432 | 44 |         |       |

- Molecule 14 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 14  | A     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 15 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms      |         | AltConf |
|-----|-------|----------|------------|---------|---------|
| 15  | A     | 1        | Total<br>1 | Zn<br>1 | 0       |
| 15  | C     | 1        | Total<br>1 | Zn<br>1 | 0       |
| 15  | J     | 1        | Total<br>1 | Zn<br>1 | 0       |
| 15  | L     | 1        | Total<br>1 | Zn<br>1 | 0       |
| 15  | I     | 2        | Total<br>2 | Zn<br>2 | 0       |



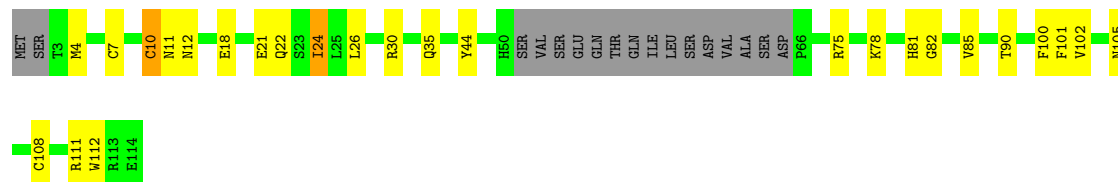




Chain H:  72% 24% 4%



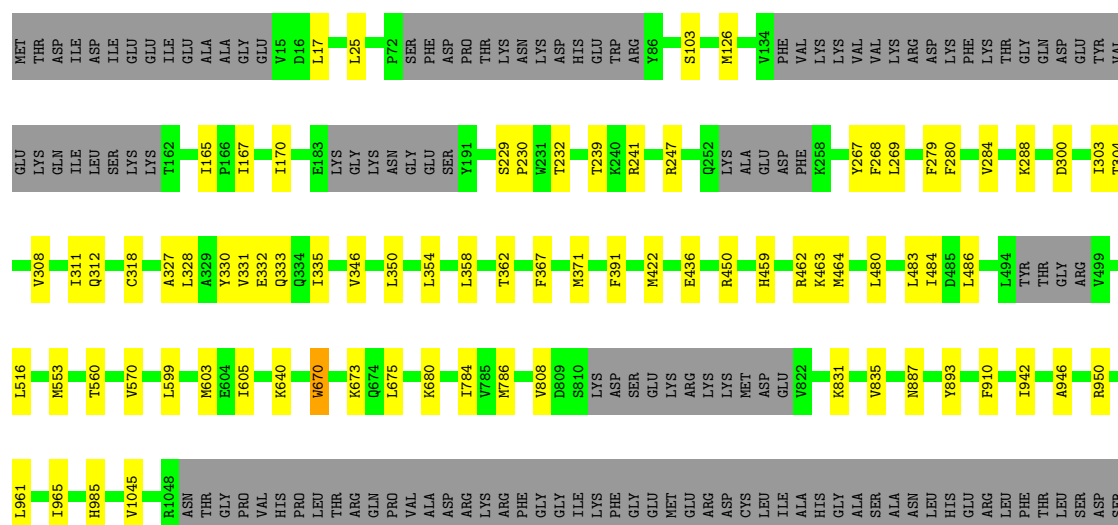
• Molecule 11: DNA-directed RNA polymerase subunit



• Molecule 12: RNA polymerase subunit H/Rpb5 C-terminal domain-containing protein



• Molecule 13: DNA-directed RNA polymerase IV and V subunit 2



SER  
GLN  
MET  
HIS  
ILE  
CYS  
ARG  
ASN  
CYS  
LYS  
SER  
ALA  
ALA  
ASN  
VAL  
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GLU  
ARG  
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ALA  
SER  
SER  
GLY  
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TYR  
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ASN  
LEU  
CYS

## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 46670                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TALOS ARCTICA                       | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 1.5625                                  | Depositor |
| Minimum defocus (nm)                 | 1000                                    | Depositor |
| Maximum defocus (nm)                 | 2500                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K3 (6k x 4k)                      | Depositor |

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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   | T     | 0.19         | 0/385       | 0.36        | 0/588          |
| 2   | N     | 0.20         | 0/438       | 0.37        | 0/672          |
| 3   | P     | 0.07         | 0/190       | 0.17        | 0/294          |
| 4   | A     | 0.16         | 0/6720      | 0.42        | 0/9070         |
| 5   | C     | 0.13         | 0/2286      | 0.37        | 0/3087         |
| 6   | F     | 0.15         | 0/673       | 0.40        | 0/905          |
| 7   | J     | 0.14         | 0/515       | 0.36        | 0/696          |
| 8   | K     | 0.15         | 0/908       | 0.31        | 0/1224         |
| 9   | L     | 0.15         | 0/369       | 0.37        | 0/493          |
| 10  | H     | 0.15         | 0/1155      | 0.46        | 0/1557         |
| 11  | I     | 0.14         | 0/804       | 0.42        | 1/1081 (0.1%)  |
| 12  | E     | 0.14         | 0/1732      | 0.43        | 0/2332         |
| 13  | B     | 0.14         | 0/7809      | 0.35        | 0/10524        |
| All | All   | 0.15         | 0/23984     | 0.39        | 1/32523 (0.0%) |

There are no bond length outliers.

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|-----|------|--------|-------|------------------------|---------------------|
| 11  | I     | 24  | ILE  | N-CA-C | -5.43 | 108.56                 | 113.71              |

There are no chirality outliers.

There are no planarity outliers.

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

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | T     | 345   | 0        | 192      | 8       | 0            |
| 2   | N     | 392   | 0        | 216      | 3       | 0            |
| 3   | P     | 171   | 0        | 87       | 5       | 0            |
| 4   | A     | 6608  | 0        | 6661     | 85      | 0            |
| 5   | C     | 2256  | 0        | 2269     | 18      | 0            |
| 6   | F     | 660   | 0        | 669      | 9       | 0            |
| 7   | J     | 507   | 0        | 512      | 4       | 0            |
| 8   | K     | 890   | 0        | 883      | 9       | 0            |
| 9   | L     | 365   | 0        | 364      | 4       | 0            |
| 10  | H     | 1129  | 0        | 1128     | 23      | 0            |
| 11  | I     | 787   | 0        | 736      | 20      | 0            |
| 12  | E     | 1706  | 0        | 1759     | 48      | 0            |
| 13  | B     | 7660  | 0        | 7600     | 47      | 0            |
| 14  | A     | 1     | 0        | 0        | 0       | 0            |
| 15  | A     | 1     | 0        | 0        | 0       | 0            |
| 15  | C     | 1     | 0        | 0        | 0       | 0            |
| 15  | I     | 2     | 0        | 0        | 0       | 0            |
| 15  | J     | 1     | 0        | 0        | 0       | 0            |
| 15  | L     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 23483 | 0        | 23076    | 252     | 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 5.

All (252) 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) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:A:940:HIS:CE1   | 4:A:989:CYS:SG    | 2.63                     | 0.92              |
| 4:A:885:ARG:HE    | 12:E:22:LEU:HB2   | 1.40                     | 0.86              |
| 4:A:804:SER:HA    | 12:E:189:GLN:HB3  | 1.62                     | 0.82              |
| 12:E:135:LYS:HA   | 12:E:138:LYS:HE3  | 1.71                     | 0.73              |
| 1:T:17:DA:H61     | 3:P:20:U:H3       | 1.37                     | 0.72              |
| 13:B:247:ARG:HH12 | 13:B:267:TYR:HB2  | 1.53                     | 0.71              |
| 11:I:100:PHE:HE1  | 11:I:111:ARG:HB3  | 1.57                     | 0.69              |
| 13:B:670:TRP:H    | 13:B:675:LEU:HD23 | 1.57                     | 0.69              |
| 5:C:114:THR:HG22  | 5:C:116:GLN:H     | 1.58                     | 0.68              |
| 8:K:78:THR:HG23   | 8:K:80:GLN:H      | 1.57                     | 0.68              |
| 13:B:350:LEU:HD22 | 13:B:354:LEU:HD22 | 1.76                     | 0.67              |
| 12:E:166:LEU:HD21 | 12:E:215:TYR:HA   | 1.77                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:E:121:ILE:HG13 | 12:E:123:GLY:H    | 1.61                     | 0.66              |
| 4:A:335:ASN:HB2   | 4:A:338:GLU:HG3   | 1.78                     | 0.66              |
| 4:A:953:MET:HE3   | 4:A:953:MET:H     | 1.61                     | 0.65              |
| 12:E:63:LEU:HD21  | 12:E:67:ARG:HH21  | 1.62                     | 0.65              |
| 11:I:21:GLU:HG2   | 11:I:22:GLN:HG2   | 1.77                     | 0.65              |
| 4:A:534:LYS:HB3   | 10:H:49:VAL:HG23  | 1.79                     | 0.64              |
| 4:A:1096:LEU:HD11 | 12:E:35:ARG:HB2   | 1.80                     | 0.63              |
| 13:B:247:ARG:NH1  | 13:B:267:TYR:HB2  | 2.14                     | 0.63              |
| 11:I:78:LYS:HZ1   | 11:I:108:CYS:HA   | 1.64                     | 0.62              |
| 12:E:85:HIS:CE1   | 12:E:88:ASP:H     | 2.17                     | 0.62              |
| 4:A:1017:LEU:HD11 | 11:I:18:GLU:HB3   | 1.80                     | 0.62              |
| 12:E:36:TYR:HB3   | 12:E:40:ARG:HH21  | 1.65                     | 0.61              |
| 4:A:686:ILE:HD12  | 4:A:686:ILE:H     | 1.65                     | 0.61              |
| 4:A:896:ALA:HB1   | 4:A:1048:ILE:HD13 | 1.81                     | 0.60              |
| 6:F:61:THR:HB     | 6:F:116:ARG:HH11  | 1.66                     | 0.60              |
| 4:A:904:LYS:HE2   | 4:A:1046:ALA:H    | 1.68                     | 0.58              |
| 6:F:126:TRP:HE1   | 6:F:130:GLU:HB3   | 1.67                     | 0.58              |
| 12:E:85:HIS:CE1   | 12:E:87:SER:H     | 2.22                     | 0.58              |
| 4:A:363:LEU:HD23  | 4:A:366:LEU:HD12  | 1.86                     | 0.57              |
| 4:A:951:ILE:HD11  | 4:A:1038:LYS:HD3  | 1.86                     | 0.57              |
| 12:E:171:LEU:HD12 | 12:E:175:GLU:HB3  | 1.85                     | 0.57              |
| 4:A:592:LYS:HB3   | 4:A:596:GLU:HG3   | 1.87                     | 0.57              |
| 4:A:1133:SER:O    | 4:A:1137:ARG:HG2  | 2.04                     | 0.57              |
| 12:E:121:ILE:HG13 | 12:E:122:THR:N    | 2.20                     | 0.57              |
| 13:B:599:LEU:HD13 | 13:B:603:MET:HE1  | 1.87                     | 0.56              |
| 4:A:1111:SER:HB3  | 4:A:1114:GLN:HG2  | 1.87                     | 0.56              |
| 4:A:594:PRO:O     | 4:A:595:LYS:HD3   | 2.05                     | 0.56              |
| 8:K:58:PHE:HB3    | 8:K:76:HIS:HB2    | 1.86                     | 0.56              |
| 10:H:8:PHE:HB3    | 10:H:62:MET:HB2   | 1.87                     | 0.56              |
| 12:E:107:THR:O    | 12:E:111:VAL:HG22 | 2.04                     | 0.56              |
| 10:H:41:MET:HE2   | 10:H:43:LEU:HD22  | 1.87                     | 0.56              |
| 4:A:502:MET:HE2   | 4:A:541:PHE:HB2   | 1.86                     | 0.56              |
| 4:A:950:ASN:O     | 4:A:950:ASN:ND2   | 2.26                     | 0.56              |
| 5:C:288:LEU:HD22  | 8:K:98:LEU:HD11   | 1.88                     | 0.56              |
| 1:T:19:DC:H2'     | 1:T:20:DG:H8      | 1.70                     | 0.56              |
| 11:I:85:VAL:HG13  | 11:I:102:VAL:HG13 | 1.87                     | 0.55              |
| 5:C:33:MET:HE2    | 8:K:45:ILE:HD11   | 1.88                     | 0.55              |
| 4:A:950:ASN:HD22  | 4:A:950:ASN:C     | 2.12                     | 0.55              |
| 12:E:66:PHE:HA    | 12:E:69:VAL:HG12  | 1.87                     | 0.55              |
| 12:E:94:LYS:HG2   | 12:E:121:ILE:HD13 | 1.89                     | 0.55              |
| 12:E:187:GLU:HA   | 12:E:190:LEU:HD12 | 1.89                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:A:1088:TRP:O    | 4:A:1092:ILE:HG22 | 2.06                     | 0.55              |
| 13:B:335:ILE:HD12 | 13:B:346:VAL:HG12 | 1.89                     | 0.55              |
| 4:A:895:SER:O     | 4:A:899:VAL:HG23  | 2.07                     | 0.54              |
| 11:I:102:VAL:HB   | 11:I:111:ARG:HG2  | 1.88                     | 0.54              |
| 13:B:961:LEU:O    | 13:B:965:ILE:HG23 | 2.06                     | 0.54              |
| 4:A:918:GLU:HG3   | 4:A:991:PHE:CE2   | 2.42                     | 0.54              |
| 4:A:412:ILE:HG21  | 4:A:446:LEU:HD21  | 1.88                     | 0.54              |
| 4:A:964:ILE:HD12  | 4:A:1032:LEU:HD21 | 1.89                     | 0.54              |
| 12:E:133:THR:HG22 | 12:E:135:LYS:H    | 1.72                     | 0.54              |
| 10:H:61:ALA:HB3   | 10:H:142:LEU:HB2  | 1.90                     | 0.54              |
| 11:I:75:ARG:HA    | 11:I:82:GLY:HA2   | 1.90                     | 0.54              |
| 13:B:165:ILE:HD12 | 13:B:436:GLU:HG3  | 1.89                     | 0.54              |
| 13:B:239:THR:HG22 | 13:B:241:ARG:H    | 1.72                     | 0.53              |
| 4:A:542:PHE:HE1   | 4:A:570:PHE:HB3   | 1.74                     | 0.53              |
| 1:T:8:DA:H2''     | 1:T:9:DG:C8       | 2.43                     | 0.53              |
| 9:L:32:CYS:HB3    | 9:L:34:TYR:HD1    | 1.73                     | 0.53              |
| 4:A:950:ASN:O     | 4:A:951:ILE:HD13  | 2.08                     | 0.53              |
| 1:T:8:DA:H2''     | 1:T:9:DG:N7       | 2.24                     | 0.53              |
| 5:C:33:MET:CE     | 8:K:45:ILE:HD11   | 2.39                     | 0.52              |
| 4:A:1002:MET:HE3  | 4:A:1002:MET:H    | 1.73                     | 0.52              |
| 4:A:950:ASN:HB2   | 11:I:90:THR:HG21  | 1.91                     | 0.52              |
| 12:E:200:VAL:HG23 | 12:E:205:LEU:HB2  | 1.91                     | 0.52              |
| 4:A:953:MET:H     | 4:A:953:MET:CE    | 2.21                     | 0.52              |
| 4:A:553:LEU:HD22  | 4:A:588:ILE:HD11  | 1.92                     | 0.52              |
| 4:A:1066:ARG:HG3  | 4:A:1067:ARG:N    | 2.25                     | 0.52              |
| 4:A:362:TYR:HD1   | 6:F:95:THR:HG21   | 1.74                     | 0.51              |
| 4:A:1123:CYS:O    | 4:A:1127:GLN:HG2  | 2.10                     | 0.51              |
| 12:E:37:TYR:O     | 12:E:40:ARG:HG2   | 2.11                     | 0.51              |
| 1:T:7:DA:C8       | 1:T:7:DA:H5'      | 2.46                     | 0.51              |
| 13:B:126:MET:HG3  | 13:B:167:ILE:HG22 | 1.93                     | 0.51              |
| 13:B:784:ILE:HG22 | 13:B:942:ILE:HG22 | 1.93                     | 0.51              |
| 10:H:100:ILE:HG12 | 10:H:100:ILE:O    | 2.11                     | 0.50              |
| 5:C:115:ASP:HB3   | 5:C:158:ARG:HH21  | 1.76                     | 0.50              |
| 5:C:62:LEU:HD11   | 7:J:2:ILE:HD11    | 1.92                     | 0.50              |
| 2:N:11:DT:H1'     | 2:N:12:DG:N7      | 2.26                     | 0.50              |
| 13:B:229:SER:HB3  | 13:B:230:PRO:HD3  | 1.92                     | 0.50              |
| 10:H:130:ILE:HG23 | 10:H:133:PHE:HD2  | 1.76                     | 0.50              |
| 13:B:268:PHE:CE2  | 13:B:269:LEU:HD12 | 2.47                     | 0.50              |
| 4:A:1089:ARG:HD3  | 12:E:153:THR:HG23 | 1.93                     | 0.50              |
| 12:E:105:VAL:O    | 12:E:109:ARG:HG3  | 2.12                     | 0.49              |
| 4:A:645:MET:HE2   | 4:A:649:LEU:HG    | 1.94                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:A:885:ARG:NH1   | 4:A:886:CYS:HB2   | 2.28                     | 0.49              |
| 13:B:280:PHE:HA   | 13:B:284:VAL:HG12 | 1.95                     | 0.49              |
| 4:A:885:ARG:NE    | 12:E:22:LEU:HB2   | 2.18                     | 0.49              |
| 13:B:300:ASP:HB3  | 13:B:303:ILE:HG12 | 1.94                     | 0.49              |
| 13:B:553:MET:HE2  | 13:B:570:VAL:HG21 | 1.95                     | 0.49              |
| 11:I:24:ILE:HB    | 11:I:26:LEU:HG    | 1.95                     | 0.48              |
| 12:E:63:LEU:HD21  | 12:E:67:ARG:NH2   | 2.28                     | 0.48              |
| 13:B:946:ALA:O    | 13:B:950:ARG:HG2  | 2.13                     | 0.48              |
| 4:A:878:ILE:HD11  | 4:A:1110:TYR:HD1  | 1.78                     | 0.48              |
| 10:H:142:LEU:HD12 | 10:H:142:LEU:H    | 1.77                     | 0.48              |
| 12:E:36:TYR:HB3   | 12:E:40:ARG:NH2   | 2.28                     | 0.48              |
| 13:B:450:ARG:HH11 | 13:B:450:ARG:HG2  | 1.78                     | 0.48              |
| 4:A:792:THR:HG23  | 4:A:794:ASP:H     | 1.78                     | 0.48              |
| 4:A:362:TYR:O     | 4:A:366:LEU:HG    | 2.13                     | 0.48              |
| 10:H:98:TYR:CZ    | 10:H:113:TYR:HB3  | 2.49                     | 0.48              |
| 12:E:39:ALA:HA    | 12:E:155:LEU:O    | 2.13                     | 0.48              |
| 4:A:531:LYS:HD3   | 10:H:77:PHE:HE2   | 1.79                     | 0.48              |
| 11:I:4:MET:HE2    | 13:B:304:THR:HG23 | 1.96                     | 0.48              |
| 13:B:165:ILE:HG23 | 13:B:436:GLU:HG2  | 1.96                     | 0.48              |
| 3:P:15:G:H2'      | 3:P:16:A:C8       | 2.49                     | 0.47              |
| 4:A:868:PHE:CE2   | 4:A:870:ASN:HB3   | 2.49                     | 0.47              |
| 4:A:879:LEU:HD13  | 4:A:1102:ILE:HD12 | 1.96                     | 0.47              |
| 4:A:964:ILE:O     | 4:A:968:VAL:HG12  | 2.14                     | 0.47              |
| 6:F:98:LEU:O      | 6:F:102:MET:HE3   | 2.15                     | 0.47              |
| 10:H:97:LEU:HD21  | 10:H:100:ILE:HB   | 1.94                     | 0.47              |
| 5:C:80:ARG:O      | 5:C:84:MET:HG3    | 2.14                     | 0.47              |
| 5:C:176:HIS:CD2   | 9:L:51:ARG:HG3    | 2.49                     | 0.47              |
| 13:B:367:PHE:O    | 13:B:371:MET:HG3  | 2.14                     | 0.47              |
| 4:A:1162:LEU:HD12 | 4:A:1172:LEU:HB2  | 1.97                     | 0.47              |
| 13:B:480:LEU:O    | 13:B:484:ILE:HG23 | 2.14                     | 0.47              |
| 13:B:887:ASN:HB2  | 13:B:893:TYR:HE2  | 1.78                     | 0.47              |
| 4:A:1029:TYR:CE2  | 4:A:1033:LEU:HD11 | 2.49                     | 0.47              |
| 5:C:237:TYR:CZ    | 5:C:258:ILE:HD13  | 2.50                     | 0.47              |
| 6:F:61:THR:HB     | 6:F:116:ARG:NH1   | 2.30                     | 0.47              |
| 3:P:15:G:H2'      | 3:P:16:A:H8       | 1.80                     | 0.47              |
| 4:A:879:LEU:HD22  | 4:A:1102:ILE:HD11 | 1.97                     | 0.47              |
| 4:A:642:ILE:O     | 4:A:646:VAL:HG23  | 2.15                     | 0.46              |
| 1:T:6:DC:H2''     | 1:T:7:DA:C8       | 2.50                     | 0.46              |
| 12:E:135:LYS:HD2  | 12:E:138:LYS:NZ   | 2.30                     | 0.46              |
| 4:A:1096:LEU:HD21 | 12:E:34:HIS:HB3   | 1.96                     | 0.46              |
| 11:I:81:HIS:HD2   | 11:I:105:ASN:HB2  | 1.80                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:I:105:ASN:HB3  | 11:I:108:CYS:HB2  | 1.97                     | 0.46              |
| 4:A:465:ALA:O     | 4:A:469:VAL:HG23  | 2.15                     | 0.46              |
| 12:E:61:LEU:HD11  | 12:E:66:PHE:HD1   | 1.80                     | 0.46              |
| 13:B:463:LYS:HD2  | 13:B:463:LYS:HA   | 1.70                     | 0.46              |
| 7:J:3:ILE:HD12    | 7:J:4:PRO:HD2     | 1.98                     | 0.46              |
| 13:B:459:HIS:HB3  | 13:B:462:ARG:O    | 2.15                     | 0.46              |
| 12:E:169:ARG:HB2  | 12:E:212:LYS:HE3  | 1.97                     | 0.46              |
| 13:B:831:LYS:HG3  | 13:B:835:VAL:H    | 1.79                     | 0.46              |
| 12:E:150:PHE:HE1  | 12:E:201:ARG:HD3  | 1.81                     | 0.46              |
| 13:B:327:ALA:O    | 13:B:331:VAL:HG23 | 2.15                     | 0.46              |
| 4:A:885:ARG:HH11  | 4:A:886:CYS:HB2   | 1.80                     | 0.46              |
| 4:A:1155:MET:HE3  | 4:A:1155:MET:HB2  | 1.80                     | 0.46              |
| 4:A:950:ASN:ND2   | 4:A:950:ASN:C     | 2.72                     | 0.45              |
| 4:A:1127:GLN:O    | 4:A:1131:ARG:HG3  | 2.15                     | 0.45              |
| 10:H:66:LEU:HD12  | 10:H:85:LEU:HD13  | 1.97                     | 0.45              |
| 4:A:643:SER:OG    | 4:A:644:PRO:HD3   | 2.15                     | 0.45              |
| 4:A:686:ILE:HD12  | 4:A:686:ILE:N     | 2.29                     | 0.45              |
| 12:E:46:MET:HA    | 12:E:202:TYR:CZ   | 2.51                     | 0.45              |
| 13:B:232:THR:HG23 | 13:B:247:ARG:HB3  | 1.97                     | 0.45              |
| 13:B:358:LEU:HD12 | 13:B:358:LEU:HA   | 1.86                     | 0.45              |
| 5:C:261:LYS:HE3   | 5:C:261:LYS:HB2   | 1.77                     | 0.45              |
| 4:A:323:SER:HA    | 4:A:457:LEU:O     | 2.17                     | 0.45              |
| 11:I:11:ASN:HB3   | 13:B:288:LYS:HG2  | 1.98                     | 0.45              |
| 3:P:16:A:H2'      | 3:P:17:C:C6       | 2.53                     | 0.44              |
| 4:A:961:GLU:O     | 4:A:964:ILE:HG22  | 2.17                     | 0.44              |
| 10:H:31:GLU:OE1   | 10:H:42:HIS:HB3   | 2.16                     | 0.44              |
| 10:H:112:MET:HE2  | 10:H:123:LEU:HD23 | 2.00                     | 0.44              |
| 4:A:1133:SER:HB2  | 12:E:219:LEU:HD22 | 1.99                     | 0.44              |
| 12:E:197:ASP:HB3  | 12:E:200:VAL:HG12 | 1.98                     | 0.44              |
| 4:A:510:LYS:O     | 4:A:514:GLN:HG3   | 2.18                     | 0.44              |
| 11:I:26:LEU:HD22  | 11:I:35:GLN:HB2   | 2.00                     | 0.44              |
| 5:C:297:LEU:HD23  | 8:K:84:MET:SD     | 2.57                     | 0.44              |
| 4:A:675:LEU:HD21  | 4:A:684:ILE:HD11  | 1.99                     | 0.44              |
| 4:A:900:ARG:HD2   | 4:A:900:ARG:O     | 2.18                     | 0.44              |
| 12:E:56:LEU:HG    | 12:E:57:GLU:CD    | 2.43                     | 0.44              |
| 12:E:135:LYS:HE2  | 12:E:135:LYS:HB3  | 1.91                     | 0.44              |
| 4:A:890:TYR:HA    | 4:A:893:GLU:OE2   | 2.17                     | 0.44              |
| 13:B:229:SER:CB   | 13:B:230:PRO:HD3  | 2.48                     | 0.44              |
| 5:C:200:MET:HE2   | 5:C:255:LEU:HD11  | 2.00                     | 0.43              |
| 10:H:85:LEU:HD12  | 10:H:86:ALA:N     | 2.33                     | 0.43              |
| 11:I:75:ARG:HD2   | 11:I:75:ARG:C     | 2.43                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:I:10:CYS:HB3   | 11:I:12:ASN:OD1   | 2.18                     | 0.43              |
| 10:H:26:LYS:HB3   | 10:H:48:GLU:OE2   | 2.19                     | 0.43              |
| 10:H:56:ASP:HB3   | 10:H:145:LYS:HE2  | 2.01                     | 0.43              |
| 12:E:66:PHE:HE2   | 12:E:70:TYR:HD2   | 1.66                     | 0.43              |
| 4:A:591:GLU:HA    | 6:F:137:TRP:O     | 2.19                     | 0.43              |
| 10:H:145:LYS:HA   | 10:H:145:LYS:HD3  | 1.84                     | 0.43              |
| 11:I:30:ARG:NH2   | 13:B:312:GLN:HA   | 2.33                     | 0.43              |
| 4:A:1037:ILE:HD13 | 4:A:1037:ILE:HA   | 1.89                     | 0.43              |
| 4:A:916:LEU:HA    | 11:I:44:TYR:O     | 2.19                     | 0.43              |
| 4:A:542:PHE:CE1   | 4:A:570:PHE:HB3   | 2.52                     | 0.43              |
| 7:J:48:MET:HE3    | 7:J:48:MET:HB3    | 1.90                     | 0.43              |
| 10:H:89:TYR:HB3   | 10:H:143:MET:O    | 2.19                     | 0.43              |
| 13:B:328:LEU:HD12 | 13:B:328:LEU:H    | 1.84                     | 0.43              |
| 5:C:285:ILE:HG21  | 8:K:102:LYS:HB2   | 2.01                     | 0.43              |
| 10:H:97:LEU:HA    | 10:H:114:VAL:HG12 | 2.00                     | 0.43              |
| 1:T:6:DC:C4       | 1:T:7:DA:N6       | 2.87                     | 0.43              |
| 12:E:61:LEU:HD12  | 12:E:62:SER:O     | 2.18                     | 0.43              |
| 4:A:395:LYS:HG2   | 4:A:398:GLN:HE22  | 1.84                     | 0.42              |
| 11:I:101:PHE:HB2  | 11:I:112:TRP:CZ3  | 2.54                     | 0.42              |
| 13:B:330:TYR:HA   | 13:B:333:GLN:HG2  | 2.01                     | 0.42              |
| 10:H:14:VAL:HG22  | 10:H:55:GLY:H     | 1.82                     | 0.42              |
| 2:N:19:DA:H5'     | 2:N:19:DA:H8      | 1.84                     | 0.42              |
| 4:A:605:GLN:HB3   | 4:A:606:PRO:HD3   | 2.01                     | 0.42              |
| 5:C:40:VAL:HG13   | 5:C:44:GLU:HB2    | 2.01                     | 0.42              |
| 13:B:318:CYS:HB2  | 13:B:330:TYR:CD1  | 2.55                     | 0.42              |
| 12:E:64:GLN:O     | 12:E:68:THR:HG23  | 2.19                     | 0.42              |
| 4:A:726:LYS:NZ    | 4:A:726:LYS:HB2   | 2.35                     | 0.42              |
| 4:A:1141:LYS:HB3  | 4:A:1141:LYS:HE2  | 1.82                     | 0.42              |
| 2:N:30:DA:H2''    | 2:N:31:DG:C8      | 2.54                     | 0.42              |
| 4:A:646:VAL:HG13  | 4:A:659:LEU:HD11  | 2.02                     | 0.42              |
| 9:L:27:ILE:HG23   | 9:L:37:LEU:HD12   | 2.02                     | 0.42              |
| 4:A:1161:MET:C    | 4:A:1162:LEU:HD23 | 2.45                     | 0.41              |
| 4:A:362:TYR:CD1   | 6:F:95:THR:HG21   | 2.54                     | 0.41              |
| 4:A:1066:ARG:HG3  | 4:A:1068:GLY:H    | 1.83                     | 0.41              |
| 5:C:59:SER:O      | 5:C:160:GLN:HG2   | 2.20                     | 0.41              |
| 10:H:94:HIS:HE1   | 10:H:138:ARG:HB3  | 1.84                     | 0.41              |
| 13:B:483:LEU:HD12 | 13:B:483:LEU:HA   | 1.87                     | 0.41              |
| 13:B:786:MET:HE1  | 13:B:910:PHE:CZ   | 2.55                     | 0.41              |
| 1:T:20:DG:H2'     | 1:T:21:DT:C6      | 2.56                     | 0.41              |
| 13:B:362:THR:HG23 | 13:B:560:THR:HB   | 2.03                     | 0.41              |
| 4:A:792:THR:OG1   | 6:F:119:PRO:HG3   | 2.21                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:E:46:MET:HA    | 12:E:202:TYR:OH   | 2.21                     | 0.41              |
| 12:E:129:GLN:HE22 | 12:E:152:ILE:HD13 | 1.86                     | 0.41              |
| 4:A:674:MET:HE2   | 4:A:695:LEU:HG    | 2.03                     | 0.41              |
| 4:A:973:LYS:HA    | 4:A:973:LYS:HD2   | 1.92                     | 0.41              |
| 4:A:1026:ASN:OD1  | 4:A:1027:THR:HG23 | 2.21                     | 0.41              |
| 5:C:14:ILE:HG13   | 8:K:108:GLU:HB3   | 2.02                     | 0.41              |
| 10:H:11:ILE:HG22  | 10:H:59:THR:HB    | 2.01                     | 0.41              |
| 12:E:217:GLY:O    | 12:E:221:GLU:HG3  | 2.20                     | 0.41              |
| 13:B:603:MET:HE3  | 13:B:605:ILE:HD11 | 2.03                     | 0.41              |
| 12:E:66:PHE:CE2   | 12:E:70:TYR:HD2   | 2.39                     | 0.41              |
| 12:E:144:THR:HG23 | 12:E:145:PHE:CD2  | 2.56                     | 0.41              |
| 13:B:463:LYS:HG3  | 13:B:464:MET:SD   | 2.60                     | 0.41              |
| 3:P:18:G:H2'      | 3:P:19:U:C6       | 2.56                     | 0.41              |
| 4:A:532:SER:HA    | 10:H:90:GLU:O     | 2.21                     | 0.41              |
| 6:F:65:MET:HG3    | 6:F:131:LEU:HB2   | 2.02                     | 0.41              |
| 9:L:35:ARG:HE     | 13:B:103:SER:HB2  | 1.85                     | 0.41              |
| 12:E:102:LYS:HA   | 12:E:130:ASN:HD21 | 1.86                     | 0.41              |
| 13:B:25:LEU:HD13  | 13:B:673:LYS:NZ   | 2.36                     | 0.41              |
| 4:A:953:MET:HE3   | 4:A:953:MET:N     | 2.34                     | 0.41              |
| 12:E:93:VAL:O     | 12:E:94:LYS:HD3   | 2.21                     | 0.41              |
| 4:A:457:LEU:HD23  | 4:A:457:LEU:HA    | 1.87                     | 0.40              |
| 12:E:34:HIS:HB2   | 12:E:67:ARG:HH22  | 1.86                     | 0.40              |
| 4:A:499:LEU:HB3   | 4:A:577:LEU:HD21  | 2.04                     | 0.40              |
| 12:E:53:GLU:HG2   | 12:E:86:ARG:HA    | 2.03                     | 0.40              |
| 13:B:17:LEU:H     | 13:B:680:LYS:HE2  | 1.86                     | 0.40              |
| 13:B:308:VAL:HA   | 13:B:311:ILE:HG22 | 2.02                     | 0.40              |
| 13:B:516:LEU:HD23 | 13:B:516:LEU:HA   | 1.96                     | 0.40              |
| 13:B:640:LYS:HD3  | 13:B:640:LYS:HA   | 1.75                     | 0.40              |
| 12:E:92:LYS:HG3   | 12:E:121:ILE:HA   | 2.03                     | 0.40              |
| 4:A:594:PRO:C     | 4:A:595:LYS:HD3   | 2.47                     | 0.40              |
| 13:B:332:GLU:OE2  | 13:B:346:VAL:HG13 | 2.21                     | 0.40              |
| 5:C:175:ASP:HA    | 8:K:10:PHE:CZ     | 2.57                     | 0.40              |
| 5:C:297:LEU:HD12  | 5:C:297:LEU:HA    | 1.92                     | 0.40              |
| 7:J:24:LEU:HD23   | 7:J:24:LEU:HA     | 1.91                     | 0.40              |
| 11:I:7:CYS:HB3    | 11:I:12:ASN:H     | 1.86                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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 |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 4   | A     | 834/2032 (41%)  | 796 (95%)  | 38 (5%)  | 0        | 100         | 100 |
| 5   | C     | 283/319 (89%)   | 277 (98%)  | 6 (2%)   | 0        | 100         | 100 |
| 6   | F     | 78/144 (54%)    | 71 (91%)   | 7 (9%)   | 0        | 100         | 100 |
| 7   | J     | 61/71 (86%)     | 58 (95%)   | 3 (5%)   | 0        | 100         | 100 |
| 8   | K     | 106/116 (91%)   | 105 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 9   | L     | 43/51 (84%)     | 40 (93%)   | 3 (7%)   | 0        | 100         | 100 |
| 10  | H     | 139/146 (95%)   | 124 (89%)  | 15 (11%) | 0        | 100         | 100 |
| 11  | I     | 93/114 (82%)    | 87 (94%)   | 6 (6%)   | 0        | 100         | 100 |
| 12  | E     | 207/230 (90%)   | 197 (95%)  | 10 (5%)  | 0        | 100         | 100 |
| 13  | B     | 953/1169 (82%)  | 918 (96%)  | 35 (4%)  | 0        | 100         | 100 |
| All | All   | 2797/4392 (64%) | 2673 (96%) | 124 (4%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 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 PDB entries followed by that with respect to all EM entries.

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 |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 4   | A     | 749/1709 (44%) | 738 (98%)  | 11 (2%)  | 57          | 77  |
| 5   | C     | 253/276 (92%)  | 252 (100%) | 1 (0%)   | 84          | 87  |
| 6   | F     | 72/128 (56%)   | 72 (100%)  | 0        | 100         | 100 |
| 7   | J     | 56/63 (89%)    | 56 (100%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 8   | K     | 98/105 (93%)    | 98 (100%)  | 0        | 100         | 100 |
| 9   | L     | 40/46 (87%)     | 40 (100%)  | 0        | 100         | 100 |
| 10  | H     | 123/127 (97%)   | 121 (98%)  | 2 (2%)   | 55          | 76  |
| 11  | I     | 85/101 (84%)    | 84 (99%)   | 1 (1%)   | 63          | 79  |
| 12  | E     | 190/209 (91%)   | 183 (96%)  | 7 (4%)   | 30          | 61  |
| 13  | B     | 846/1026 (82%)  | 837 (99%)  | 9 (1%)   | 65          | 80  |
| All | All   | 2512/3790 (66%) | 2481 (99%) | 31 (1%)  | 61          | 79  |

All (31) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 4   | A     | 324  | SER  |
| 4   | A     | 343  | MET  |
| 4   | A     | 430  | VAL  |
| 4   | A     | 535  | SER  |
| 4   | A     | 541  | PHE  |
| 4   | A     | 649  | LEU  |
| 4   | A     | 864  | CYS  |
| 4   | A     | 950  | ASN  |
| 4   | A     | 981  | MET  |
| 4   | A     | 1049 | ILE  |
| 4   | A     | 1139 | VAL  |
| 5   | C     | 288  | LEU  |
| 10  | H     | 14   | VAL  |
| 10  | H     | 132  | HIS  |
| 11  | I     | 10   | CYS  |
| 12  | E     | 36   | TYR  |
| 12  | E     | 103  | VAL  |
| 12  | E     | 115  | ILE  |
| 12  | E     | 162  | HIS  |
| 12  | E     | 181  | LYS  |
| 12  | E     | 190  | LEU  |
| 12  | E     | 193  | ILE  |
| 13  | B     | 170  | ILE  |
| 13  | B     | 279  | PHE  |
| 13  | B     | 391  | PHE  |
| 13  | B     | 422  | MET  |
| 13  | B     | 486  | LEU  |
| 13  | B     | 670  | TRP  |
| 13  | B     | 808  | VAL  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 13  | B     | 985  | HIS  |
| 13  | B     | 1045 | VAL  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 4   | A     | 1011 | ASN  |
| 5   | C     | 69   | HIS  |
| 8   | K     | 44   | ASN  |
| 8   | K     | 51   | HIS  |
| 11  | I     | 31   | ASN  |
| 12  | E     | 85   | HIS  |
| 12  | E     | 129  | GLN  |
| 13  | B     | 251  | ASN  |
| 13  | B     | 333  | GLN  |
| 13  | B     | 529  | ASN  |
| 13  | B     | 714  | GLN  |
| 13  | B     | 951  | GLN  |
| 13  | B     | 1039 | HIS  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed   | Backbone Outliers | Pucker Outliers |
|-----|-------|------------|-------------------|-----------------|
| 3   | P     | 7/20 (35%) | 0                 | 0               |

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.



## 5.6 Ligand geometry

Of 7 ligands modelled in this entry, 7 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.