



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 07:42 PM UTC

PDB ID : 9N5B / pdb\_00009n5b  
Title : RNA polymerase II elongation complex containing 8-oxoG at +1 site, apo form  
Authors : Oh, J.; Wang, D.  
Deposited on : 2025-02-04  
Resolution : 3.10 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>.

---

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

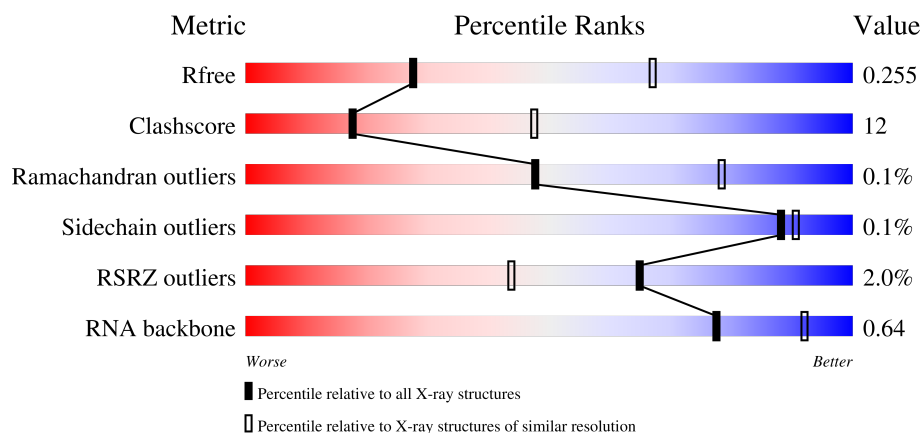
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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                      | 1456 (3.10-3.10)                                      |
| Clashscore            | 190562                      | 1539 (3.10-3.10)                                      |
| Ramachandran outliers | 187476                      | 1467 (3.10-3.10)                                      |
| Sidechain outliers    | 187428                      | 1467 (3.10-3.10)                                      |
| RSRZ outliers         | 180081                      | 1456 (3.10-3.10)                                      |
| RNA backbone          | 3983                        | 1022 (3.32-2.88)                                      |

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   | R     | 9      | <div> <div>6%</div> <div>56%</div> <div>33%</div> <div>11%</div> </div> |
| 2   | T     | 29     | <div> <div>24%</div> <div>66%</div> <div>10%</div> </div>               |
| 3   | N     | 18     | <div> <div>6%</div> <div>33%</div> <div>50%</div> <div>17%</div> </div> |
| 4   | A     | 1733   | <div> <div>2%</div> <div>55%</div> <div>25%</div> <div>20%</div> </div> |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain    |
|-----|-------|--------|---------------------|
| 5   | B     | 1224   | <br>% 68% 24% 8%    |
| 6   | C     | 318    | <br>64% 20% 16%     |
| 7   | E     | 215    | <br>2% 68% 31% .    |
| 8   | F     | 155    | <br>% 39% 16% 45%   |
| 9   | H     | 146    | <br>3% 60% 32% 9%   |
| 10  | I     | 122    | <br>2% 68% 29% .    |
| 11  | J     | 70     | <br>60% 33% 7%      |
| 12  | K     | 120    | <br>72% 22% 5%      |
| 13  | L     | 70     | <br>10% 43% 19% 39% |

## 2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 29047 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 RNA chain called RNA.

| Mol | Chain | Residues | Atoms |    |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|---------|-------|
| 1   | R     | 9        | Total | C  | N  | O  | P | 0       | 0       | 0     |
|     |       |          | 195   | 88 | 40 | 59 | 8 |         |         |       |

- Molecule 2 is a DNA chain called Template strand DNA.

| Mol | Chain | Residues | Atoms |     |    |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|---------|-------|
| 2   | T     | 26       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 521   | 250 | 80 | 165 | 26 |         |         |       |

- Molecule 3 is a DNA chain called Non-template strand DNA.

| Mol | Chain | Residues | Atoms |     |    |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|----|---------|---------|-------|
| 3   | N     | 15       | Total | C   | N  | O  | P  | 0       | 0       | 0     |
|     |       |          | 317   | 148 | 71 | 83 | 15 |         |         |       |

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB1.

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 4   | A     | 1385     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 10827 | 6830 | 1894 | 2043 | 60 |         |         |       |

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit RPB2.

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 5   | B     | 1121     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 8849  | 5601 | 1550 | 1645 | 53 |         |         |       |

- Molecule 6 is a protein called DNA-directed RNA polymerase II subunit RPB3.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 6   | C     | 267      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2101  | 1320 | 349 | 419 | 13 |         |         |       |

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 7   | E     | 213      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1740  | 1105 | 307 | 317 | 11 |         |         |       |

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8   | F     | 86       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 684   | 437 | 115 | 129 | 3 |         |         |       |

- Molecule 9 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 9   | H     | 133      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1064  | 670 | 179 | 211 | 4 |         |         |       |

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit RPB9.

| Mol | Chain | Residues | Atoms |     |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 10  | I     | 118      | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 952   | 585 | 173 | 184 | 10 |         |         |       |

- Molecule 11 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 11  | J     | 65       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 532   | 339 | 93 | 94 | 6 |         |         |       |

- Molecule 12 is a protein called DNA-directed RNA polymerase II subunit RPB11.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12  | K     | 114      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 919   | 590 | 156 | 171 | 2 |         |         |       |

- Molecule 13 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 13  | L     | 43       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 337   | 208 | 66 | 59 | 4 |         |         |       |

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

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

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

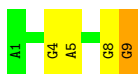
| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 15  | A     | 1        | Total<br>1 | Mg<br>1 | 0       | 0       |

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

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

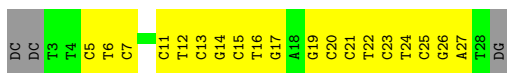
- Molecule 1: RNA

Chain R:



- Molecule 2: Template strand DNA

Chain T:



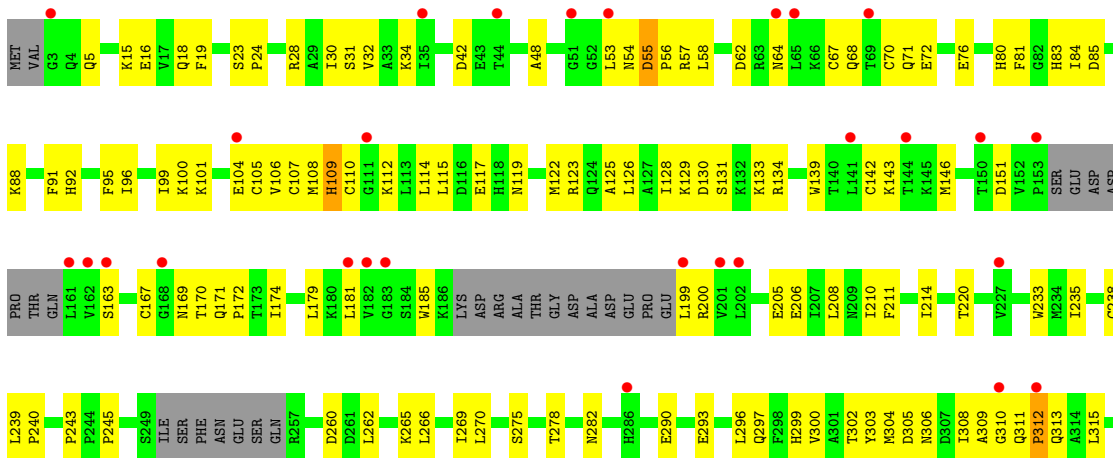
- Molecule 3: Non-template strand DNA

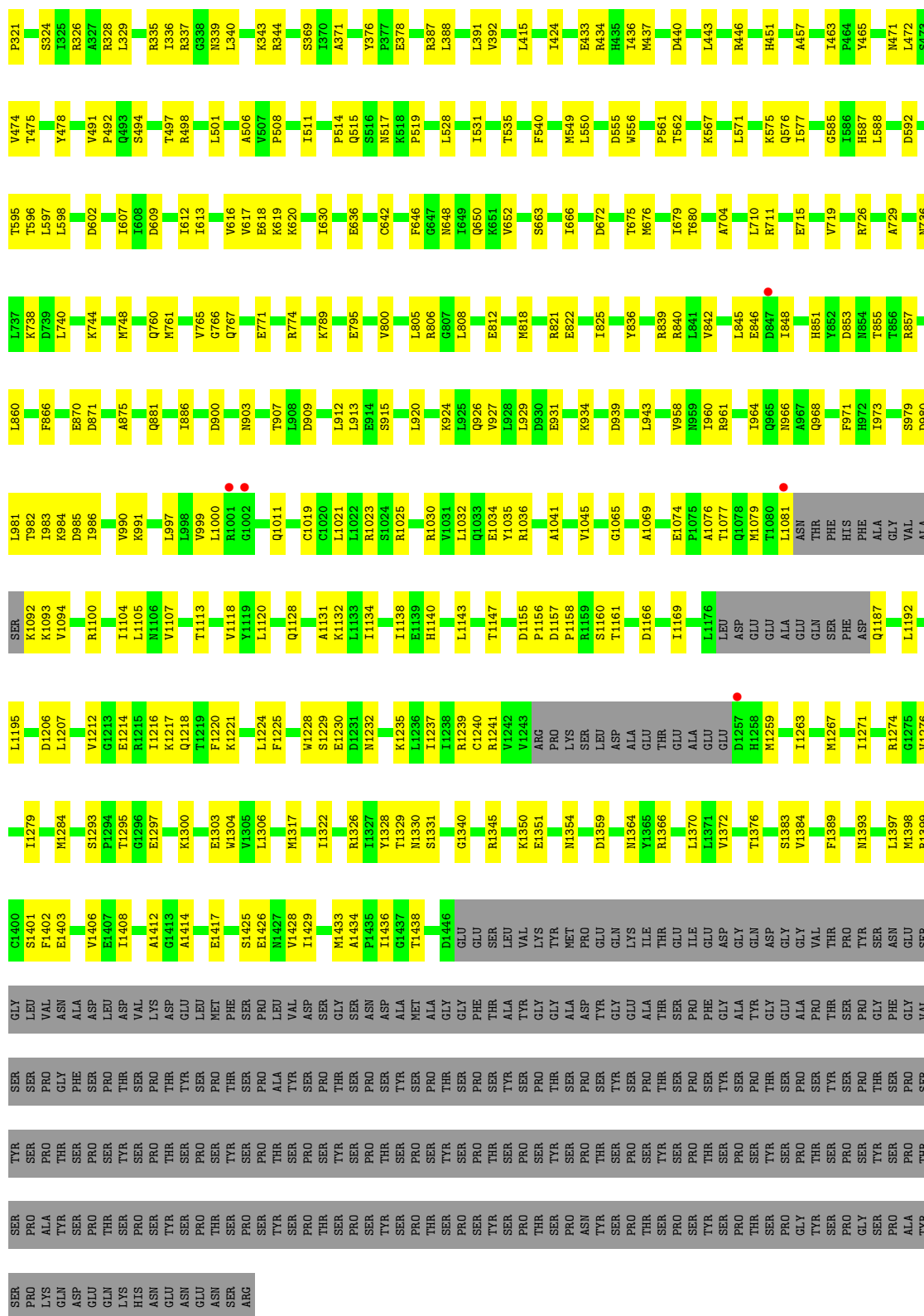
Chain N:



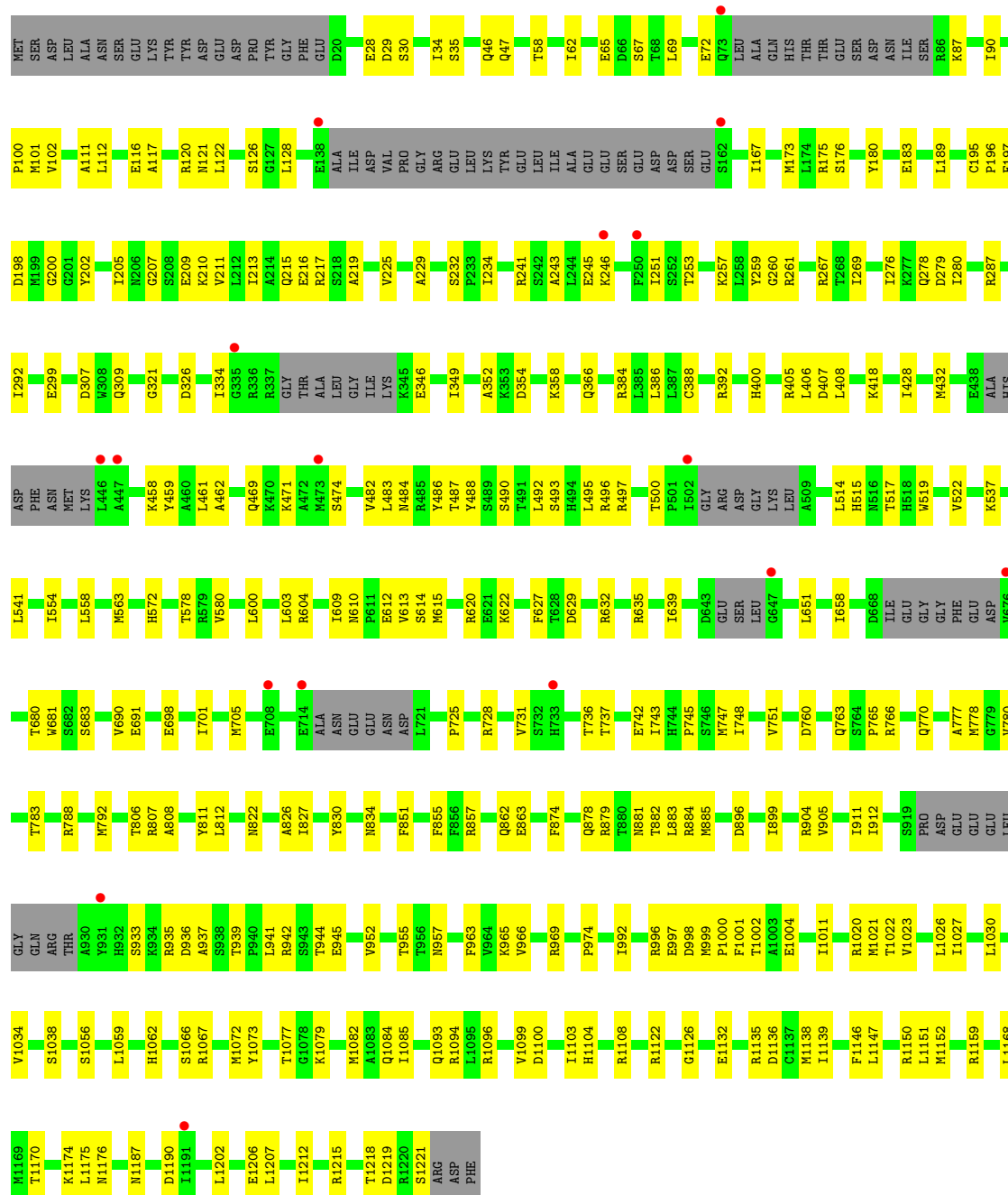
- Molecule 4: DNA-directed RNA polymerase II subunit RPB1

Chain A:



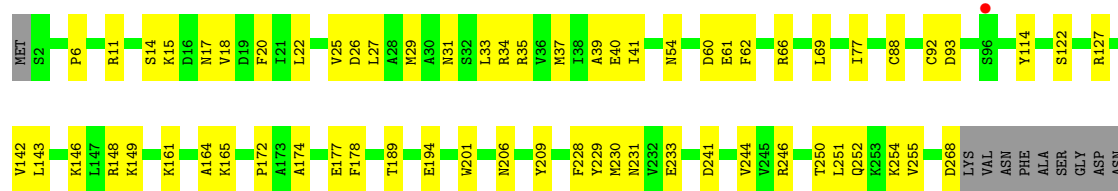






• Molecule 6: DNA-directed RNA polymerase II subunit RPB3

Chain C: 64% 20% 16%



ASN THR ASP ALA SER ASN MET LEU GLY SER ASN GLU ASP VAL MET MET THR MET GLY ALA GLU GLN ASP PRO TYR SER ASN ASN ALA SER GLN MET MET GLY ASN THR THR GLY SER GLY TYR ASP ASP ASN ALA TRP

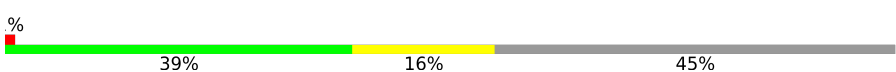
- Molecule 7: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E: 

MET ASP Q3 V19 V23 K24 Y28 E34 L37 P38 L39 K43 Y46 C47 D48 R52 P53 Q54 R55 K56 M57 M58 S59 P64 M75 G76 S77 L78 W79 V80 E81 F82 C83 D84 E85 P86 S87 V88 G89 V90 K91 T92 M93 F96 V97 I100 Q101

F105 Q106 T107 G108 I109 Q113 N114 T117 P118 M121 K122 L123 V124 T125 S126 I127 P128 P129 T134 F135 L140 P151 R152 H153 S157 E160 K166 R167 R177 P183 V184 A185 L190 Y208 R212 W215

- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F: 

MET SER THR TRR GLU ALA PHE ASN ASP GLY ASN GLU ASN PHE GLU PHE T81 T82 P83 Y84 M85 T86 E89 R92 R97 A98 L99 S102 L111 E114 K128 R135 R136 P139 D140 G141 E144 D145 W146 E149 E150 L151 D154 LEU

HIS GLU GLN ILE ARG LYS THR L69 K76 D77 Q78 R79 A80 T81 T82 P83 Y84 M85 T86 E89 R92 R97 A98 L99 S102 L111 E114 K128 R135 R136 P139 D140 G141 E144 D145 W146 E149 E150 L151 D154 LEU

- Molecule 9: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H: 

MET S2 L5 D8 I9 F10 V15 C24 E27 A28 A29 S30 Q33 C36 K37 L38 T39 L40 V44 P48 T56 S61 S62 L63 ASN LEU GLU ASP THR PRO ALA ASN ASP SER SER ALA T76 P81 P82 L89 A90 D91 D92 Y93 D94 Y95

V96 A101 Y102 F104 A113 V114 Y115 S117 M123 R124 L125 E126 Y129 R130 N131 N133 K136 Q137 E138 N139 R145 R146

- Molecule 10: DNA-directed RNA polymerase II subunit RPB9

Chain I: 

MET T2 T3 F4 R5 G10 N11 M12 M13 Y15 D19 R24 E36 E47 L48 T49 T50 N51 I52 E53 E54 Q60 D61 E62 G63 S64 T67 R70 S71 D72 R73 C78 H79 S80 N83 Q87 S88 Q89 Q90 S96 M97 V98 S107 T111 S112

D113 T119 G119 PHE SER

- Molecule 11: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J: 



- Molecule 12: DNA-directed RNA polymerase II subunit RPB11



- Molecule 13: DNA-directed RNA polymerases I, II, and III subunit RPABC4



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | C 1 2 1                                                     | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 157.84Å 221.72Å 190.84Å<br>90.00° 97.41° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 46.28 – 3.10<br>46.28 – 3.10                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.9 (46.28-3.10)<br>99.8 (46.28-3.10)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.41                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.37 (at 3.12Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX (1.19.2_4158: ???)                                   | Depositor        |
| R, $R_{free}$                                                           | 0.213 , 0.256<br>0.214 , 0.255                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 2000 reflections (1.54%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 67.3                                                        | Xtriage          |
| Anisotropy                                                              | 0.595                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.31 , 65.9                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.92                                                        | EDS              |
| Total number of atoms                                                   | 29047                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 86.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% 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 [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: MG, SOG, 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   | R     | 0.18         | 0/219       | 0.35        | 0/341       |
| 2   | T     | 0.26         | 0/551       | 0.51        | 0/843       |
| 3   | N     | 0.25         | 0/359       | 0.48        | 0/553       |
| 4   | A     | 0.18         | 0/11017     | 0.40        | 0/14903     |
| 5   | B     | 0.18         | 0/9020      | 0.39        | 0/12172     |
| 6   | C     | 0.18         | 0/2139      | 0.37        | 0/2899      |
| 7   | E     | 0.16         | 0/1776      | 0.37        | 0/2390      |
| 8   | F     | 0.16         | 0/696       | 0.35        | 0/943       |
| 9   | H     | 0.19         | 0/1082      | 0.46        | 0/1466      |
| 10  | I     | 0.17         | 0/970       | 0.36        | 0/1308      |
| 11  | J     | 0.17         | 0/541       | 0.39        | 0/727       |
| 12  | K     | 0.17         | 0/937       | 0.34        | 0/1265      |
| 13  | L     | 0.23         | 0/339       | 0.51        | 0/450       |
| All | All   | 0.18         | 0/29646     | 0.40        | 0/40260     |

There are no bond length outliers.

There are no bond angle outliers.

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   | R     | 195   | 0        | 99       | 3       | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | T     | 521   | 0        | 297      | 13      | 0            |
| 3   | N     | 317   | 0        | 166      | 11      | 0            |
| 4   | A     | 10827 | 0        | 10873    | 319     | 1            |
| 5   | B     | 8849  | 0        | 8810     | 216     | 0            |
| 6   | C     | 2101  | 0        | 2056     | 50      | 0            |
| 7   | E     | 1740  | 0        | 1766     | 48      | 0            |
| 8   | F     | 684   | 0        | 692      | 17      | 0            |
| 9   | H     | 1064  | 0        | 1029     | 33      | 0            |
| 10  | I     | 952   | 0        | 897      | 25      | 1            |
| 11  | J     | 532   | 0        | 542      | 21      | 0            |
| 12  | K     | 919   | 0        | 929      | 20      | 0            |
| 13  | L     | 337   | 0        | 352      | 10      | 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            |
| All | All   | 29047 | 0        | 28508    | 711     | 1            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (711) 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:1224:LEU:HD21 | 4:A:1240:CYS:HB3  | 1.57                     | 0.87              |
| 4:A:1329:THR:HG22 | 4:A:1331:SER:H    | 1.40                     | 0.86              |
| 12:K:24:ASP:OD2   | 12:K:74:ARG:NH1   | 2.09                     | 0.85              |
| 4:A:106:VAL:O     | 4:A:171:GLN:NE2   | 2.10                     | 0.85              |
| 5:B:1099:VAL:HG12 | 5:B:1103:ILE:HD11 | 1.62                     | 0.81              |
| 4:A:666:ILE:HG23  | 5:B:1026:LEU:HB2  | 1.60                     | 0.81              |
| 10:I:50:THR:HG22  | 10:I:52:ILE:H     | 1.46                     | 0.81              |
| 11:J:8:PHE:H      | 11:J:49:MET:HE3   | 1.44                     | 0.81              |
| 6:C:66:ARG:NH2    | 11:J:3:VAL:O      | 2.14                     | 0.80              |
| 4:A:607:ILE:HG12  | 4:A:612:ILE:HG22  | 1.63                     | 0.79              |
| 7:E:59:SER:HB3    | 7:E:81:GLU:HA     | 1.64                     | 0.79              |
| 4:A:108:MET:SD    | 4:A:171:GLN:NE2   | 2.55                     | 0.78              |
| 6:C:35:ARG:NH1    | 12:K:41:THR:OG1   | 2.17                     | 0.77              |
| 4:A:91:PHE:H      | 4:A:297:GLN:HE22  | 1.31                     | 0.76              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:B:46:GLN:OE1    | 5:B:408:LEU:HD21  | 1.86                     | 0.74              |
| 4:A:575:LYS:HB3   | 4:A:612:ILE:HD11  | 1.69                     | 0.74              |
| 12:K:100:ALA:O    | 12:K:104:ASN:ND2  | 2.19                     | 0.74              |
| 5:B:705:MET:HE2   | 5:B:745:PRO:HB3   | 1.70                     | 0.73              |
| 12:K:32:VAL:HG22  | 12:K:74:ARG:HG3   | 1.71                     | 0.73              |
| 4:A:636:GLU:OE2   | 4:A:966:ASN:ND2   | 2.22                     | 0.72              |
| 9:H:36:CYS:HA     | 9:H:126:GLU:O     | 1.89                     | 0.72              |
| 4:A:806:ARG:NH2   | 5:B:725:PRO:O     | 2.22                     | 0.72              |
| 4:A:30:ILE:HD12   | 5:B:1170:THR:HG21 | 1.71                     | 0.72              |
| 5:B:34:ILE:HD13   | 5:B:747:MET:HE3   | 1.71                     | 0.72              |
| 5:B:822:ASN:O     | 11:J:48:ARG:NH1   | 2.23                     | 0.72              |
| 6:C:31:ASN:OD1    | 6:C:34:ARG:NH1    | 2.22                     | 0.71              |
| 7:E:185:ALA:HA    | 7:E:190:LEU:HD23  | 1.73                     | 0.70              |
| 3:N:11:DA:H2'     | 3:N:12:DG:C8      | 2.26                     | 0.70              |
| 4:A:491:VAL:O     | 5:B:1150:ARG:NH2  | 2.25                     | 0.70              |
| 4:A:243:PRO:HB2   | 4:A:245:PRO:HD2   | 1.72                     | 0.70              |
| 5:B:519:TRP:CZ2   | 5:B:705:MET:HE1   | 2.27                     | 0.70              |
| 5:B:969:ARG:NH1   | 6:C:61:GLU:OE1    | 2.24                     | 0.70              |
| 6:C:11:ARG:HH21   | 6:C:229:TYR:HD2   | 1.40                     | 0.70              |
| 4:A:535:THR:HG21  | 4:A:617:VAL:HG23  | 1.74                     | 0.70              |
| 4:A:108:MET:HE3   | 4:A:210:ILE:HD13  | 1.73                     | 0.70              |
| 4:A:1192:LEU:HD11 | 4:A:1239:ARG:HB3  | 1.74                     | 0.69              |
| 4:A:875:ALA:HB2   | 4:A:1366:ARG:HD2  | 1.74                     | 0.69              |
| 4:A:1134:ILE:O    | 4:A:1138:ILE:HG22 | 1.92                     | 0.69              |
| 5:B:1002:THR:HG23 | 5:B:1004:GLU:H    | 1.57                     | 0.69              |
| 9:H:40:LEU:HD13   | 9:H:123:MET:HE3   | 1.73                     | 0.69              |
| 6:C:22:LEU:HG     | 6:C:25:VAL:HG21   | 1.75                     | 0.68              |
| 4:A:1214:GLU:O    | 4:A:1218:GLN:NE2  | 2.27                     | 0.68              |
| 4:A:596:THR:HG22  | 4:A:597:LEU:H     | 1.57                     | 0.68              |
| 5:B:213:ILE:O     | 5:B:215:GLN:NE2   | 2.25                     | 0.68              |
| 9:H:38:LEU:HD11   | 9:H:123:MET:HE2   | 1.76                     | 0.67              |
| 6:C:11:ARG:NH2    | 6:C:206:ASN:OD1   | 2.27                     | 0.67              |
| 7:E:56:LYS:HD3    | 7:E:84:ASP:HB2    | 1.75                     | 0.67              |
| 4:A:337:ARG:NH2   | 5:B:1132:GLU:OE1  | 2.27                     | 0.67              |
| 11:J:37:SER:OG    | 11:J:47:ARG:NH2   | 2.28                     | 0.67              |
| 5:B:101:MET:HG2   | 5:B:111:ALA:HA    | 1.75                     | 0.67              |
| 5:B:205:ILE:HG13  | 5:B:461:LEU:HB3   | 1.75                     | 0.67              |
| 8:F:82:THR:O      | 8:F:136:ARG:NH1   | 2.21                     | 0.67              |
| 4:A:433:GLU:OE1   | 5:B:1108:ARG:NH1  | 2.28                     | 0.66              |
| 4:A:550:LEU:HD21  | 4:A:561:PRO:HD2   | 1.76                     | 0.66              |
| 11:J:9:SER:OG     | 11:J:48:ARG:NH2   | 2.28                     | 0.66              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:J:13:VAL:O     | 11:J:17:LYS:NZ    | 2.28                     | 0.66              |
| 4:A:1206:ASP:O    | 4:A:1274:ARG:NH1  | 2.28                     | 0.66              |
| 5:B:770:GLN:HE22  | 5:B:1093:GLN:HE22 | 1.44                     | 0.66              |
| 5:B:792:MET:HG3   | 5:B:855:PHE:HE1   | 1.61                     | 0.66              |
| 4:A:115:LEU:HD23  | 4:A:142:CYS:HB3   | 1.77                     | 0.66              |
| 4:A:871:ASP:OD1   | 4:A:1366:ARG:NH2  | 2.28                     | 0.66              |
| 4:A:711:ARG:NH2   | 10:I:87:GLN:OE1   | 2.28                     | 0.66              |
| 5:B:862:GLN:HG2   | 5:B:963:PHE:HD1   | 1.60                     | 0.66              |
| 8:F:128:LYS:NZ    | 8:F:151:LEU:O     | 2.26                     | 0.66              |
| 4:A:853:ASP:OD1   | 4:A:855:THR:OG1   | 2.10                     | 0.65              |
| 5:B:276:ILE:HG21  | 5:B:280:ILE:HD11  | 1.78                     | 0.65              |
| 4:A:821:ARG:O     | 4:A:825:ILE:HG12  | 1.95                     | 0.65              |
| 5:B:612:GLU:O     | 5:B:632:ARG:NH2   | 2.26                     | 0.65              |
| 4:A:71:GLN:OE1    | 5:B:1176:ASN:ND2  | 2.29                     | 0.65              |
| 4:A:886:ILE:HD11  | 4:A:943:LEU:HB3   | 1.77                     | 0.65              |
| 4:A:5:GLN:O       | 5:B:1159:ARG:NH2  | 2.30                     | 0.65              |
| 5:B:639:ILE:HD11  | 5:B:691:GLU:HB2   | 1.77                     | 0.65              |
| 4:A:1345:ARG:HG2  | 4:A:1372:VAL:HG12 | 1.79                     | 0.64              |
| 10:I:10:CYS:O     | 10:I:12:ASN:N     | 2.31                     | 0.64              |
| 4:A:555:ASP:OD1   | 4:A:648:ASN:ND2   | 2.30                     | 0.64              |
| 4:A:1267:MET:HA   | 4:A:1271:ILE:HD12 | 1.79                     | 0.64              |
| 4:A:326:ARG:HG3   | 4:A:1406:VAL:HG11 | 1.78                     | 0.64              |
| 5:B:198:ASP:OD2   | 5:B:202:TYR:OH    | 2.15                     | 0.64              |
| 9:H:103:LYS:HB3   | 9:H:115:TYR:HD1   | 1.64                     | 0.63              |
| 5:B:229:ALA:O     | 5:B:261:ARG:NH2   | 2.30                     | 0.63              |
| 5:B:998:ASP:OD1   | 6:C:35:ARG:NH2    | 2.31                     | 0.63              |
| 10:I:111:THR:HG22 | 10:I:113:ASP:H    | 1.62                     | 0.63              |
| 4:A:107:CYS:HA    | 4:A:171:GLN:HE21  | 1.64                     | 0.63              |
| 4:A:1113:THR:O    | 4:A:1330:ASN:ND2  | 2.31                     | 0.63              |
| 5:B:299:GLU:OE2   | 5:B:572:HIS:ND1   | 2.21                     | 0.63              |
| 4:A:715:GLU:OE2   | 4:A:774:ARG:NH1   | 2.31                     | 0.63              |
| 5:B:857:ARG:NH1   | 5:B:945:GLU:OE2   | 2.31                     | 0.63              |
| 5:B:806:THR:HG22  | 5:B:808:ALA:H     | 1.64                     | 0.63              |
| 5:B:904:ARG:NH1   | 13:L:66:GLN:O     | 2.31                     | 0.62              |
| 5:B:1187:ASN:ND2  | 5:B:1190:ASP:O    | 2.29                     | 0.62              |
| 4:A:67:CYS:O      | 4:A:70:CYS:N      | 2.30                     | 0.62              |
| 4:A:167:CYS:SG    | 4:A:169:ASN:ND2   | 2.68                     | 0.62              |
| 10:I:63:GLY:O     | 10:I:70:ARG:NH2   | 2.33                     | 0.62              |
| 4:A:1107:VAL:HG22 | 4:A:1383:SER:HB3  | 1.81                     | 0.62              |
| 5:B:260:GLY:O     | 5:B:267:ARG:NH1   | 2.29                     | 0.62              |
| 5:B:610:ASN:HB3   | 5:B:613:VAL:HG23  | 1.80                     | 0.62              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:A:18:GLN:NE2    | 4:A:19:PHE:O      | 2.28                     | 0.62              |
| 7:E:77:SER:HB2    | 7:E:105:PHE:HD2   | 1.65                     | 0.62              |
| 4:A:378:GLU:OE1   | 4:A:434:ARG:NH1   | 2.32                     | 0.62              |
| 5:B:29:ASP:HB3    | 5:B:658:ILE:HG12  | 1.82                     | 0.61              |
| 5:B:558:LEU:HB3   | 5:B:563:MET:HG3   | 1.82                     | 0.61              |
| 2:T:6:DT:H2"      | 2:T:7:DC:C5       | 2.35                     | 0.61              |
| 2:T:22:DT:OP1     | 4:A:344:ARG:NH1   | 2.34                     | 0.61              |
| 6:C:143:LEU:HD21  | 6:C:146:LYS:HE3   | 1.83                     | 0.61              |
| 5:B:522:VAL:HG21  | 5:B:537:LYS:HB3   | 1.82                     | 0.61              |
| 4:A:72:GLU:HB3    | 4:A:76:GLU:HB3    | 1.82                     | 0.61              |
| 5:B:766:ARG:HG3   | 5:B:1022:THR:HG22 | 1.83                     | 0.61              |
| 4:A:100:LYS:O     | 4:A:104:GLU:N     | 2.33                     | 0.60              |
| 5:B:46:GLN:NE2    | 5:B:47:GLN:HG2    | 2.16                     | 0.60              |
| 4:A:315:LEU:HA    | 4:A:321:PRO:HA    | 1.84                     | 0.60              |
| 4:A:562:THR:O     | 4:A:576:GLN:NE2   | 2.34                     | 0.60              |
| 5:B:69:LEU:HB3    | 5:B:432:MET:HE1   | 1.83                     | 0.60              |
| 4:A:54:ASN:C      | 4:A:56:PRO:HD3    | 2.26                     | 0.60              |
| 4:A:269:ILE:HD13  | 4:A:299:HIS:HB3   | 1.83                     | 0.60              |
| 5:B:629:ASP:HB2   | 5:B:632:ARG:HD3   | 1.83                     | 0.60              |
| 4:A:1350:LYS:O    | 4:A:1354:ASN:ND2  | 2.26                     | 0.60              |
| 4:A:134:ARG:NH2   | 4:A:220:THR:O     | 2.34                     | 0.60              |
| 4:A:596:THR:HG22  | 4:A:597:LEU:N     | 2.16                     | 0.60              |
| 4:A:1118:VAL:HB   | 4:A:1306:LEU:HB2  | 1.84                     | 0.60              |
| 5:B:896:ASP:OD2   | 13:L:58:LYS:NZ    | 2.34                     | 0.60              |
| 6:C:40:GLU:OE2    | 6:C:254:LYS:NZ    | 2.34                     | 0.59              |
| 4:A:302:THR:OG1   | 4:A:306:ASN:OD1   | 2.19                     | 0.59              |
| 4:A:531:ILE:O     | 4:A:535:THR:OG1   | 2.19                     | 0.59              |
| 4:A:146:MET:SD    | 4:A:146:MET:N     | 2.75                     | 0.59              |
| 2:T:25:DC:OP1     | 5:B:857:ARG:NH2   | 2.35                     | 0.59              |
| 5:B:1077:THR:HG22 | 5:B:1079:LYS:H    | 1.67                     | 0.59              |
| 6:C:93:ASP:O      | 6:C:127:ARG:NH2   | 2.35                     | 0.59              |
| 4:A:129:LYS:HA    | 4:A:134:ARG:HH11  | 1.67                     | 0.59              |
| 4:A:1293:SER:OG   | 4:A:1297:GLU:OE1  | 2.20                     | 0.59              |
| 6:C:54:ASN:ND2    | 6:C:60:ASP:OD1    | 2.35                     | 0.58              |
| 11:J:8:PHE:CD1    | 11:J:49:MET:HE1   | 2.38                     | 0.58              |
| 4:A:42:ASP:OD1    | 4:A:42:ASP:N      | 2.35                     | 0.58              |
| 4:A:903:ASN:O     | 4:A:907:THR:OG1   | 2.14                     | 0.58              |
| 4:A:1161:THR:HG21 | 4:A:1166:ASP:HB2  | 1.85                     | 0.58              |
| 7:E:101:GLN:O     | 7:E:101:GLN:NE2   | 2.37                     | 0.58              |
| 4:A:771:GLU:N     | 4:A:822:GLU:OE1   | 2.30                     | 0.58              |
| 4:A:704:ALA:HB2   | 4:A:710:LEU:HD13  | 1.85                     | 0.58              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:A:262:LEU:O    | 4:A:266:LEU:HG    | 2.04                     | 0.58              |
| 4:A:337:ARG:HH21 | 4:A:337:ARG:HG2   | 1.69                     | 0.58              |
| 10:I:60:GLN:NE2  | 10:I:107:SER:OG   | 2.30                     | 0.58              |
| 4:A:174:ILE:HD11 | 4:A:181:LEU:HB3   | 1.87                     | 0.57              |
| 4:A:848:ILE:HG21 | 4:A:1370:LEU:HD11 | 1.86                     | 0.57              |
| 5:B:519:TRP:HZ2  | 5:B:705:MET:HE1   | 1.66                     | 0.57              |
| 5:B:1072:MET:HG3 | 5:B:1085:ILE:HB   | 1.86                     | 0.57              |
| 3:N:12:DG:H1'    | 3:N:13:DA:N7      | 2.18                     | 0.57              |
| 5:B:175:ARG:HG3  | 5:B:200:GLY:HA3   | 1.86                     | 0.57              |
| 9:H:5:LEU:HB3    | 9:H:133:ASN:HB2   | 1.86                     | 0.57              |
| 4:A:329:LEU:HA   | 4:A:335:ARG:H     | 1.68                     | 0.57              |
| 4:A:392:VAL:HG12 | 4:A:424:ILE:HD13  | 1.86                     | 0.57              |
| 4:A:170:THR:OG1  | 4:A:185:TRP:NE1   | 2.38                     | 0.57              |
| 4:A:1235:LYS:HB3 | 4:A:1237:ILE:HD11 | 1.86                     | 0.57              |
| 5:B:173:MET:O    | 5:B:176:SER:OG    | 2.14                     | 0.57              |
| 5:B:334:ILE:HG21 | 5:B:352:ALA:HB2   | 1.86                     | 0.57              |
| 7:E:78:LEU:HD23  | 7:E:107:THR:HB    | 1.86                     | 0.57              |
| 5:B:905:VAL:HG23 | 5:B:941:LEU:HD11  | 1.85                     | 0.57              |
| 6:C:142:VAL:HG13 | 11:J:15:GLY:HA3   | 1.85                     | 0.57              |
| 4:A:744:LYS:HG2  | 4:A:748:MET:HE2   | 1.87                     | 0.57              |
| 5:B:232:SER:O    | 5:B:261:ARG:NH2   | 2.37                     | 0.57              |
| 6:C:27:LEU:HD12  | 6:C:228:PHE:HE2   | 1.70                     | 0.57              |
| 4:A:42:ASP:OD1   | 4:A:48:ALA:N      | 2.38                     | 0.56              |
| 4:A:587:HIS:HA   | 4:A:607:ILE:O     | 2.04                     | 0.56              |
| 6:C:88:CYS:HB3   | 6:C:92:CYS:HB3    | 1.87                     | 0.56              |
| 12:K:8:GLU:O     | 12:K:37:LYS:HE3   | 2.05                     | 0.56              |
| 4:A:913:LEU:HD22 | 4:A:915:SER:H     | 1.69                     | 0.56              |
| 4:A:997:LEU:O    | 4:A:1011:GLN:NE2  | 2.38                     | 0.56              |
| 4:A:1155:ASP:O   | 4:A:1241:ARG:NH2  | 2.30                     | 0.56              |
| 5:B:629:ASP:O    | 5:B:632:ARG:NH1   | 2.38                     | 0.56              |
| 5:B:834:ASN:HD22 | 5:B:1011:ILE:HG22 | 1.71                     | 0.56              |
| 10:I:60:GLN:HE22 | 10:I:107:SER:HG   | 1.49                     | 0.56              |
| 4:A:68:GLN:NE2   | 4:A:70:CYS:HB2    | 2.20                     | 0.56              |
| 4:A:105:CYS:SG   | 4:A:114:LEU:HB2   | 2.44                     | 0.56              |
| 4:A:146:MET:O    | 4:A:171:GLN:N     | 2.23                     | 0.56              |
| 7:E:93:MET:O     | 7:E:97:VAL:HG23   | 2.06                     | 0.56              |
| 7:E:101:GLN:HB2  | 7:E:127:ILE:HG21  | 1.88                     | 0.56              |
| 7:E:157:SER:HB3  | 7:E:160:GLU:HG3   | 1.88                     | 0.56              |
| 2:T:20:DC:H2'    | 2:T:21:DC:C6      | 2.41                     | 0.56              |
| 5:B:515:HIS:ND1  | 5:B:517:THR:OG1   | 2.34                     | 0.56              |
| 5:B:487:THR:OG1  | 5:B:777:ALA:O     | 2.24                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:A:117:GLU:HG2  | 4:A:123:ARG:HG3   | 1.87                     | 0.56              |
| 4:A:999:VAL:HG12 | 4:A:1000:LEU:HD12 | 1.87                     | 0.56              |
| 5:B:603:LEU:HB3  | 5:B:609:ILE:HG13  | 1.88                     | 0.56              |
| 5:B:259:TYR:OH   | 5:B:279:ASP:OD2   | 2.19                     | 0.55              |
| 5:B:102:VAL:HG13 | 5:B:112:LEU:HD22  | 1.88                     | 0.55              |
| 7:E:151:PRO:HD2  | 7:E:153:HIS:HE1   | 1.69                     | 0.55              |
| 4:A:72:GLU:HG3   | 4:A:76:GLU:HG2    | 1.86                     | 0.55              |
| 4:A:1212:VAL:O   | 4:A:1216:ILE:HG13 | 2.07                     | 0.55              |
| 4:A:392:VAL:HG13 | 4:A:415:LEU:CD1   | 2.37                     | 0.55              |
| 4:A:391:LEU:HD11 | 4:A:437:MET:HE1   | 1.88                     | 0.55              |
| 4:A:666:ILE:HD11 | 5:B:1030:LEU:HD22 | 1.88                     | 0.55              |
| 5:B:217:ARG:NH1  | 5:B:407:ASP:OD1   | 2.39                     | 0.55              |
| 9:H:5:LEU:O      | 9:H:133:ASN:ND2   | 2.38                     | 0.55              |
| 4:A:1131:ALA:HB3 | 4:A:1284:MET:HE3  | 1.87                     | 0.55              |
| 5:B:912:ILE:HB   | 5:B:939:THR:HB    | 1.89                     | 0.55              |
| 5:B:1104:HIS:NE2 | 5:B:1126:GLY:O    | 2.36                     | 0.55              |
| 4:A:105:CYS:O    | 4:A:106:VAL:HG23  | 2.06                     | 0.55              |
| 5:B:728:ARG:NH2  | 5:B:760:ASP:OD2   | 2.28                     | 0.55              |
| 6:C:6:PRO:HB3    | 6:C:25:VAL:HG22   | 1.89                     | 0.54              |
| 5:B:751:VAL:HG23 | 5:B:812:LEU:HD22  | 1.90                     | 0.54              |
| 6:C:60:ASP:OD2   | 13:L:60:ARG:NH1   | 2.40                     | 0.54              |
| 5:B:28:GLU:OE1   | 5:B:807:ARG:NH1   | 2.39                     | 0.54              |
| 5:B:72:GLU:HA    | 5:B:87:LYS:HA     | 1.88                     | 0.54              |
| 5:B:996:ARG:NH2  | 6:C:174:ALA:O     | 2.40                     | 0.54              |
| 6:C:177:GLU:HB2  | 6:C:231:ASN:HB3   | 1.89                     | 0.54              |
| 7:E:88:VAL:HG23  | 7:E:92:THR:HB     | 1.90                     | 0.54              |
| 9:H:44:VAL:HG13  | 9:H:48:PRO:HA     | 1.90                     | 0.54              |
| 4:A:471:ASN:O    | 4:A:474:VAL:HG12  | 2.07                     | 0.54              |
| 5:B:881:ASN:HD21 | 5:B:933:SER:HG    | 1.55                     | 0.54              |
| 4:A:311:GLN:N    | 4:A:312:PRO:HD3   | 2.22                     | 0.54              |
| 6:C:62:PHE:O     | 6:C:66:ARG:HG3    | 2.08                     | 0.54              |
| 8:F:128:LYS:HD2  | 8:F:149:GLU:HA    | 1.90                     | 0.54              |
| 4:A:24:PRO:HB3   | 4:A:238:CYS:HB3   | 1.88                     | 0.54              |
| 4:A:592:ASP:O    | 4:A:595:THR:OG1   | 2.26                     | 0.54              |
| 4:A:392:VAL:HG13 | 4:A:415:LEU:HD11  | 1.88                     | 0.54              |
| 4:A:618:GLU:OE2  | 4:A:620:LYS:HB2   | 2.07                     | 0.54              |
| 4:A:32:VAL:HG12  | 4:A:32:VAL:O      | 2.07                     | 0.54              |
| 4:A:335:ARG:HD2  | 5:B:1202:LEU:HD12 | 1.89                     | 0.53              |
| 6:C:165:LYS:O    | 12:K:6:ARG:NH1    | 2.41                     | 0.53              |
| 5:B:604:ARG:NH1  | 5:B:691:GLU:OE2   | 2.37                     | 0.53              |
| 5:B:997:GLU:HG2  | 6:C:39:ALA:HB2    | 1.91                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:B:1103:ILE:O   | 5:B:1122:ARG:NH1 | 2.38                     | 0.53              |
| 4:A:613:ILE:HG23 | 9:H:117:SER:HB2  | 1.90                     | 0.53              |
| 4:A:1187:GLN:N   | 4:A:1187:GLN:OE1 | 2.41                     | 0.53              |
| 5:B:955:THR:OG1  | 13:L:54:ARG:O    | 2.25                     | 0.53              |
| 7:E:124:VAL:HG23 | 7:E:125:PRO:HD3  | 1.90                     | 0.53              |
| 4:A:851:HIS:CD2  | 8:F:139:PRO:HG3  | 2.43                     | 0.53              |
| 5:B:620:ARG:NH2  | 10:I:89:GLN:OE1  | 2.42                     | 0.53              |
| 5:B:1138:MET:HE2 | 5:B:1146:PHE:CD2 | 2.43                     | 0.53              |
| 5:B:234:ILE:HD12 | 5:B:257:LYS:HB3  | 1.90                     | 0.53              |
| 4:A:378:GLU:OE2  | 4:A:387:ARG:NH2  | 2.38                     | 0.53              |
| 4:A:1340:GLY:HA2 | 7:E:183:PRO:HD2  | 1.90                     | 0.53              |
| 6:C:252:GLN:OE1  | 12:K:102:LYS:NZ  | 2.34                     | 0.53              |
| 11:J:23:ASN:O    | 11:J:27:GLU:HB3  | 2.09                     | 0.53              |
| 4:A:575:LYS:NZ   | 4:A:602:ASP:OD2  | 2.40                     | 0.53              |
| 5:B:35:SER:HG    | 5:B:811:TYR:HH   | 1.54                     | 0.53              |
| 4:A:736:ASN:O    | 4:A:736:ASN:ND2  | 2.42                     | 0.53              |
| 5:B:287:ARG:NH1  | 5:B:321:GLY:O    | 2.41                     | 0.53              |
| 4:A:130:ASP:HB3  | 4:A:133:LYS:HB2  | 1.90                     | 0.52              |
| 7:E:121:MET:O    | 7:E:124:VAL:HG22 | 2.10                     | 0.52              |
| 4:A:16:GLU:OE2   | 5:B:1221:SER:N   | 2.39                     | 0.52              |
| 4:A:789:LYS:HG3  | 10:I:67:THR:HB   | 1.91                     | 0.52              |
| 5:B:680:THR:O    | 5:B:683:SER:OG   | 2.25                     | 0.52              |
| 4:A:1143:LEU:O   | 4:A:1147:THR:OG1 | 2.23                     | 0.52              |
| 4:A:1232:ASN:O   | 4:A:1232:ASN:ND2 | 2.41                     | 0.52              |
| 5:B:1082:MET:HA  | 6:C:189:THR:HA   | 1.91                     | 0.52              |
| 9:H:89:LEU:HD13  | 9:H:91:ASP:H     | 1.74                     | 0.52              |
| 4:A:675:THR:OG1  | 4:A:736:ASN:OD1  | 2.27                     | 0.52              |
| 4:A:34:LYS:HG2   | 4:A:83:HIS:CE1   | 2.44                     | 0.52              |
| 4:A:517:ASN:OD1  | 4:A:1364:ASN:ND2 | 2.41                     | 0.52              |
| 5:B:243:ALA:HA   | 5:B:251:ILE:HG13 | 1.90                     | 0.52              |
| 6:C:250:THR:O    | 6:C:254:LYS:HG3  | 2.08                     | 0.52              |
| 6:C:14:SER:OG    | 6:C:15:LYS:N     | 2.42                     | 0.52              |
| 4:A:122:MET:O    | 4:A:126:LEU:HG   | 2.08                     | 0.52              |
| 4:A:1398:MET:O   | 4:A:1401:SER:OG  | 2.28                     | 0.52              |
| 5:B:999:MET:HG3  | 5:B:1000:PRO:HD2 | 1.92                     | 0.52              |
| 7:E:135:PHE:HD2  | 7:E:140:LEU:HD21 | 1.74                     | 0.52              |
| 3:N:6:DG:H2"     | 3:N:7:DA:C8      | 2.45                     | 0.52              |
| 4:A:821:ARG:HH21 | 5:B:514:LEU:HD13 | 1.75                     | 0.52              |
| 9:H:137:GLN:OE1  | 9:H:139:ASN:ND2  | 2.43                     | 0.52              |
| 4:A:457:ALA:HB3  | 4:A:506:ALA:HA   | 1.92                     | 0.52              |
| 5:B:936:ASP:OD1  | 5:B:937:ALA:N    | 2.42                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:A:900:ASP:HA   | 4:A:926:GLN:HE22  | 1.76                     | 0.51              |
| 4:A:1166:ASP:HA  | 4:A:1169:ILE:HD13 | 1.92                     | 0.51              |
| 5:B:780:VAL:HG11 | 11:J:56:LEU:HD13  | 1.93                     | 0.51              |
| 4:A:982:THR:HG22 | 4:A:984:LYS:H     | 1.75                     | 0.51              |
| 8:F:82:THR:HG22  | 8:F:84:TYR:H      | 1.75                     | 0.51              |
| 4:A:1328:TYR:OH  | 4:A:1351:GLU:OE1  | 2.27                     | 0.51              |
| 12:K:21:ILE:HG12 | 12:K:33:ILE:HG12  | 1.92                     | 0.51              |
| 3:N:5:DC:N4      | 3:N:6:DG:O6       | 2.44                     | 0.51              |
| 4:A:76:GLU:OE2   | 5:B:1159:ARG:NH1  | 2.43                     | 0.51              |
| 4:A:1220:PHE:HE1 | 4:A:1224:LEU:HD22 | 1.75                     | 0.51              |
| 4:A:1398:MET:N   | 4:A:1426:GLU:OE2  | 2.43                     | 0.51              |
| 5:B:760:ASP:OD1  | 5:B:760:ASP:N     | 2.34                     | 0.51              |
| 4:A:55:ASP:N     | 4:A:56:PRO:HD3    | 2.26                     | 0.51              |
| 5:B:1023:VAL:O   | 5:B:1027:ILE:HG13 | 2.10                     | 0.51              |
| 7:E:46:TYR:CE1   | 7:E:58:MET:HG2    | 2.46                     | 0.51              |
| 10:I:50:THR:O    | 10:I:90:GLN:NE2   | 2.42                     | 0.51              |
| 4:A:278:THR:O    | 4:A:282:ASN:HB2   | 2.11                     | 0.51              |
| 4:A:585:GLY:N    | 4:A:609:ASP:OD1   | 2.40                     | 0.51              |
| 7:E:39:LEU:O     | 7:E:43:LYS:HG3    | 2.10                     | 0.51              |
| 8:F:81:THR:OG1   | 8:F:144:GLU:OE1   | 2.25                     | 0.51              |
| 4:A:1259:MET:HG2 | 4:A:1263:ILE:HD13 | 1.93                     | 0.51              |
| 5:B:216:GLU:OE1  | 5:B:500:THR:OG1   | 2.25                     | 0.51              |
| 5:B:635:ARG:NH1  | 5:B:742:GLU:OE2   | 2.43                     | 0.51              |
| 7:E:96:PHE:O     | 7:E:100:ILE:HG12  | 2.11                     | 0.51              |
| 4:A:1021:LEU:O   | 4:A:1025:ARG:HG3  | 2.11                     | 0.51              |
| 4:A:1076:ALA:HA  | 4:A:1079:MET:HG3  | 1.93                     | 0.51              |
| 5:B:189:LEU:HD13 | 5:B:196:PRO:HA    | 1.93                     | 0.51              |
| 5:B:1056:SER:HB3 | 5:B:1066:SER:HB2  | 1.93                     | 0.51              |
| 4:A:308:ILE:HG22 | 4:A:309:ALA:H     | 1.76                     | 0.50              |
| 4:A:376:TYR:CZ   | 4:A:498:ARG:HD2   | 2.45                     | 0.50              |
| 4:A:443:LEU:HD12 | 4:A:501:LEU:HD11  | 1.93                     | 0.50              |
| 5:B:1207:LEU:HB3 | 5:B:1212:ILE:HB   | 1.93                     | 0.50              |
| 4:A:371:ALA:HA   | 4:A:436:ILE:HG22  | 1.93                     | 0.50              |
| 4:A:514:PRO:HB3  | 4:A:875:ALA:HB3   | 1.93                     | 0.50              |
| 5:B:736:THR:HG23 | 5:B:737:THR:HG23  | 1.93                     | 0.50              |
| 5:B:778:MET:HE1  | 5:B:1094:ARG:HD3  | 1.91                     | 0.50              |
| 4:A:602:ASP:HB3  | 4:A:616:VAL:HG23  | 1.92                     | 0.50              |
| 5:B:69:LEU:HB2   | 5:B:90:ILE:HB     | 1.94                     | 0.50              |
| 6:C:31:ASN:O     | 6:C:35:ARG:HG3    | 2.12                     | 0.50              |
| 10:I:5:ARG:NH2   | 10:I:36:GLU:OE2   | 2.44                     | 0.50              |
| 11:J:14:VAL:HB   | 11:J:50:ILE:HD11  | 1.93                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 12:K:49:GLU:HG3  | 12:K:94:ILE:CG1  | 2.40                     | 0.50              |
| 4:A:108:MET:O    | 4:A:110:CYS:N    | 2.45                     | 0.50              |
| 4:A:646:PHE:O    | 4:A:650:GLN:HG3  | 2.10                     | 0.50              |
| 9:H:93:TYR:CD2   | 9:H:145:ARG:HB2  | 2.46                     | 0.50              |
| 4:A:265:LYS:O    | 4:A:269:ILE:HG12 | 2.12                     | 0.50              |
| 4:A:960:ILE:HG22 | 4:A:964:ILE:HD13 | 1.93                     | 0.50              |
| 9:H:133:ASN:OD1  | 9:H:133:ASN:N    | 2.45                     | 0.50              |
| 4:A:99:ILE:HD12  | 4:A:211:PHE:HE2  | 1.77                     | 0.50              |
| 4:A:881:GLN:NE2  | 4:A:958:VAL:O    | 2.42                     | 0.50              |
| 1:R:4:G:H2'      | 1:R:5:A:C8       | 2.46                     | 0.50              |
| 4:A:1229:SER:OG  | 4:A:1230:GLU:N   | 2.45                     | 0.50              |
| 5:B:307:ASP:OD2  | 5:B:392:ARG:NH1  | 2.44                     | 0.50              |
| 5:B:346:GLU:HA   | 5:B:349:ILE:HD13 | 1.92                     | 0.50              |
| 6:C:244:VAL:HG11 | 12:K:105:PHE:CZ  | 2.47                     | 0.50              |
| 7:E:100:ILE:HG23 | 7:E:105:PHE:HB2  | 1.94                     | 0.50              |
| 5:B:830:TYR:CZ   | 5:B:1000:PRO:HD3 | 2.47                     | 0.49              |
| 6:C:241:ASP:N    | 6:C:241:ASP:OD1  | 2.43                     | 0.49              |
| 4:A:434:ARG:HE   | 4:A:437:MET:HE3  | 1.77                     | 0.49              |
| 5:B:46:GLN:CD    | 5:B:47:GLN:HG2   | 2.37                     | 0.49              |
| 7:E:48:ASP:OD2   | 7:E:52:ARG:N     | 2.38                     | 0.49              |
| 10:I:98:VAL:HG11 | 10:I:113:ASP:HB2 | 1.95                     | 0.49              |
| 4:A:1074:GLU:O   | 4:A:1077:THR:OG1 | 2.28                     | 0.49              |
| 6:C:178:PHE:CE1  | 6:C:230:MET:HE2  | 2.47                     | 0.49              |
| 4:A:57:ARG:HA    | 4:A:68:GLN:HB3   | 1.94                     | 0.49              |
| 4:A:451:HIS:NE2  | 4:A:515:GLN:OE1  | 2.45                     | 0.49              |
| 4:A:517:ASN:O    | 4:A:517:ASN:ND2  | 2.45                     | 0.49              |
| 5:B:635:ARG:HH12 | 5:B:742:GLU:CD   | 2.21                     | 0.49              |
| 6:C:77:ILE:HG13  | 6:C:161:LYS:HE3  | 1.94                     | 0.49              |
| 10:I:13:MET:HE2  | 10:I:15:TYR:CE2  | 2.47                     | 0.49              |
| 2:T:25:DC:P      | 5:B:942:ARG:HH22 | 2.36                     | 0.49              |
| 6:C:148:ARG:NH1  | 11:J:64:ASN:O    | 2.45                     | 0.49              |
| 9:H:56:THR:HB    | 9:H:145:ARG:HB3  | 1.94                     | 0.49              |
| 4:A:853:ASP:OD2  | 4:A:857:ARG:NH2  | 2.45                     | 0.49              |
| 5:B:578:THR:HG23 | 5:B:622:LYS:C    | 2.38                     | 0.49              |
| 6:C:246:ARG:O    | 6:C:250:THR:OG1  | 2.29                     | 0.49              |
| 9:H:8:ASP:OD2    | 9:H:9:ILE:N      | 2.42                     | 0.49              |
| 4:A:101:LYS:HG3  | 4:A:139:TRP:CD1  | 2.48                     | 0.49              |
| 4:A:549:MET:HG2  | 4:A:652:VAL:HG13 | 1.95                     | 0.49              |
| 4:A:1019:CYS:O   | 4:A:1023:ARG:HG3 | 2.13                     | 0.49              |
| 5:B:997:GLU:CD   | 5:B:997:GLU:H    | 2.20                     | 0.49              |
| 7:E:128:PRO:N    | 7:E:129:PRO:HD2  | 2.28                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:A:808:LEU:O     | 5:B:728:ARG:NH1   | 2.46                     | 0.48              |
| 4:A:979:SER:OG    | 4:A:980:ASP:N     | 2.46                     | 0.48              |
| 8:F:86:THR:OG1    | 8:F:89:GLU:HG2    | 2.13                     | 0.48              |
| 9:H:94:ASP:N      | 9:H:94:ASP:OD1    | 2.46                     | 0.48              |
| 4:A:675:THR:O     | 4:A:679:ILE:HG13  | 2.13                     | 0.48              |
| 4:A:860:LEU:HD11  | 4:A:1393:ASN:HB2  | 1.95                     | 0.48              |
| 9:H:5:LEU:HD21    | 9:H:61:SER:HB2    | 1.94                     | 0.48              |
| 5:B:957:ASN:OD1   | 5:B:957:ASN:N     | 2.46                     | 0.48              |
| 7:E:121:MET:HE1   | 7:E:134:THR:HG21  | 1.95                     | 0.48              |
| 10:I:4:PHE:HE1    | 10:I:13:MET:HG3   | 1.79                     | 0.48              |
| 2:T:11:DC:H2''    | 2:T:12:DT:C6      | 2.48                     | 0.48              |
| 5:B:100:PRO:HA    | 5:B:126:SER:HB3   | 1.95                     | 0.48              |
| 5:B:121:ASN:HA    | 5:B:207:GLY:HA3   | 1.96                     | 0.48              |
| 8:F:140:ASP:OD1   | 8:F:141:GLY:N     | 2.47                     | 0.48              |
| 4:A:260:ASP:OD2   | 4:A:328:ARG:NH2   | 2.46                     | 0.48              |
| 5:B:459:TYR:CE2   | 5:B:469:GLN:HA    | 2.48                     | 0.48              |
| 5:B:944:THR:OG1   | 5:B:1122:ARG:NH2  | 2.46                     | 0.48              |
| 4:A:939:ASP:OD1   | 4:A:1023:ARG:NH1  | 2.47                     | 0.48              |
| 5:B:471:LYS:O     | 5:B:474:SER:N     | 2.41                     | 0.48              |
| 9:H:136:LYS:H     | 9:H:136:LYS:HD2   | 1.77                     | 0.48              |
| 10:I:61:ASP:O     | 10:I:64:SER:OG    | 2.32                     | 0.48              |
| 11:J:6:ARG:HD3    | 11:J:11:GLY:O     | 2.14                     | 0.48              |
| 4:A:340:LEU:HD13  | 4:A:1429:ILE:HG23 | 1.95                     | 0.48              |
| 5:B:269:ILE:HD11  | 5:B:386:LEU:HD21  | 1.96                     | 0.48              |
| 4:A:760:GLN:HG2   | 4:A:765:VAL:HA    | 1.96                     | 0.48              |
| 13:L:47:ARG:NH1   | 13:L:54:ARG:HE    | 2.12                     | 0.48              |
| 2:T:16:DT:H2'     | 2:T:17:DG:C8      | 2.48                     | 0.47              |
| 4:A:23:SER:HB3    | 4:A:233:TRP:CZ2   | 2.49                     | 0.47              |
| 4:A:28:ARG:NH2    | 4:A:85:ASP:OD1    | 2.45                     | 0.47              |
| 4:A:846:GLU:OE2   | 4:A:1425:SER:OG   | 2.31                     | 0.47              |
| 12:K:24:ASP:OD1   | 12:K:25:THR:N     | 2.46                     | 0.47              |
| 3:N:12:DG:H1'     | 3:N:13:DA:C5      | 2.49                     | 0.47              |
| 4:A:208:LEU:HD23  | 4:A:235:ILE:HD11  | 1.96                     | 0.47              |
| 4:A:540:PHE:HB3   | 4:A:571:LEU:HG    | 1.97                     | 0.47              |
| 4:A:961:ARG:NH1   | 4:A:1025:ARG:HH12 | 2.12                     | 0.47              |
| 5:B:519:TRP:CH2   | 5:B:705:MET:HE1   | 2.49                     | 0.47              |
| 6:C:114:TYR:OH    | 11:J:19:GLU:OE2   | 2.22                     | 0.47              |
| 11:J:48:ARG:NE    | 11:J:49:MET:HE2   | 2.29                     | 0.47              |
| 4:A:472:LEU:O     | 4:A:475:THR:OG1   | 2.30                     | 0.47              |
| 5:B:1002:THR:HG23 | 5:B:1004:GLU:N    | 2.27                     | 0.47              |
| 4:A:306:ASN:ND2   | 4:A:313:GLN:O     | 2.47                     | 0.47              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:A:870:GLU:HG2   | 7:E:208:TYR:CG    | 2.49                     | 0.47              |
| 4:A:929:LEU:HD21  | 4:A:983:ILE:HD13  | 1.96                     | 0.47              |
| 5:B:276:ILE:HG22  | 5:B:278:GLN:H     | 1.80                     | 0.47              |
| 1:R:8:G:H2'       | 1:R:9:G:C8        | 2.50                     | 0.47              |
| 4:A:5:GLN:HB2     | 5:B:1175:LEU:HD13 | 1.96                     | 0.47              |
| 4:A:1438:THR:CG2  | 8:F:92:ARG:HB2    | 2.45                     | 0.47              |
| 5:B:354:ASP:O     | 5:B:358:LYS:HB2   | 2.15                     | 0.47              |
| 5:B:1135:ARG:O    | 5:B:1139:ILE:HG13 | 2.15                     | 0.47              |
| 7:E:55:ARG:NH2    | 7:E:113:GLN:OE1   | 2.48                     | 0.47              |
| 7:E:85:GLU:N      | 7:E:85:GLU:OE1    | 2.48                     | 0.47              |
| 10:I:97:MET:HE2   | 10:I:97:MET:HB3   | 1.87                     | 0.47              |
| 11:J:7:CYS:HA     | 11:J:49:MET:HG3   | 1.96                     | 0.47              |
| 3:N:5:DC:H2'      | 3:N:6:DG:C8       | 2.50                     | 0.47              |
| 3:N:8:DG:OP2      | 4:A:143:LYS:NZ    | 2.37                     | 0.47              |
| 5:B:736:THR:OG1   | 5:B:737:THR:N     | 2.46                     | 0.47              |
| 6:C:251:LEU:O     | 6:C:255:VAL:HG23  | 2.14                     | 0.47              |
| 9:H:146:ARG:HD2   | 9:H:146:ARG:H     | 1.79                     | 0.47              |
| 10:I:71:SER:OG    | 10:I:83:ASN:OD1   | 2.27                     | 0.47              |
| 5:B:225:VAL:HG11  | 5:B:388:CYS:HB3   | 1.96                     | 0.47              |
| 6:C:18:VAL:HG12   | 6:C:20:PHE:HD2    | 1.80                     | 0.47              |
| 4:A:672:ASP:OD1   | 4:A:736:ASN:ND2   | 2.34                     | 0.47              |
| 5:B:100:PRO:O     | 5:B:180:TYR:OH    | 2.22                     | 0.47              |
| 5:B:681:TRP:CH2   | 5:B:690:VAL:HG11  | 2.50                     | 0.47              |
| 5:B:1219:ASP:OD1  | 5:B:1219:ASP:N    | 2.47                     | 0.47              |
| 7:E:77:SER:OG     | 7:E:106:GLN:N     | 2.48                     | 0.47              |
| 10:I:19:ASP:HB3   | 10:I:24:ARG:HB2   | 1.97                     | 0.47              |
| 11:J:3:VAL:HG11   | 11:J:18:TRP:HB2   | 1.97                     | 0.47              |
| 4:A:125:ALA:O     | 4:A:128:ILE:HG22  | 2.14                     | 0.46              |
| 5:B:211:VAL:HG13  | 5:B:495:LEU:HD23  | 1.96                     | 0.46              |
| 4:A:58:LEU:HA     | 4:A:58:LEU:HD23   | 1.56                     | 0.46              |
| 4:A:88:LYS:NZ     | 4:A:205:GLU:HB2   | 2.30                     | 0.46              |
| 4:A:1138:ILE:HG12 | 4:A:1279:ILE:HG21 | 1.96                     | 0.46              |
| 12:K:49:GLU:HG3   | 12:K:94:ILE:HG13  | 1.96                     | 0.46              |
| 4:A:679:ILE:HG23  | 4:A:729:ALA:HB1   | 1.96                     | 0.46              |
| 5:B:458:LYS:O     | 5:B:462:ALA:N     | 2.40                     | 0.46              |
| 5:B:745:PRO:O     | 5:B:748:ILE:HG12  | 2.15                     | 0.46              |
| 5:B:486:TYR:OH    | 5:B:1096:ARG:HB3  | 2.16                     | 0.46              |
| 5:B:884:ARG:HH11  | 5:B:935:ARG:HD3   | 1.80                     | 0.46              |
| 4:A:501:LEU:HD21  | 5:B:1146:PHE:CD1  | 2.50                     | 0.46              |
| 4:A:866:PHE:H     | 7:E:208:TYR:HH    | 1.63                     | 0.46              |
| 6:C:33:LEU:HG     | 6:C:37:MET:HE2    | 1.96                     | 0.46              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:A:434:ARG:NH2   | 4:A:440:ASP:OD2   | 2.49                     | 0.46              |
| 4:A:630:ILE:HG23  | 4:A:642:CYS:SG    | 2.56                     | 0.46              |
| 4:A:1094:VAL:HA   | 4:A:1113:THR:HG21 | 1.98                     | 0.46              |
| 5:B:69:LEU:HD12   | 5:B:432:MET:HE2   | 1.96                     | 0.46              |
| 6:C:33:LEU:O      | 6:C:37:MET:HG3    | 2.16                     | 0.46              |
| 2:T:14:DG:H2''    | 2:T:15:DC:C5      | 2.51                     | 0.46              |
| 4:A:1376:THR:HG22 | 7:E:212:ARG:HH12  | 1.80                     | 0.46              |
| 13:L:31:CYS:SG    | 13:L:32:ALA:N     | 2.89                     | 0.46              |
| 4:A:290:GLU:HA    | 4:A:293:GLU:CD    | 2.41                     | 0.46              |
| 4:A:663:SER:OG    | 5:B:827:ILE:O     | 2.31                     | 0.46              |
| 10:I:78:CYS:SG    | 10:I:80:SER:OG    | 2.69                     | 0.46              |
| 4:A:446:ARG:HD3   | 4:A:478:TYR:O     | 2.16                     | 0.45              |
| 4:A:836:TYR:O     | 4:A:840:ARG:HG3   | 2.16                     | 0.45              |
| 5:B:202:TYR:CD2   | 5:B:483:LEU:HD11  | 2.50                     | 0.45              |
| 5:B:999:MET:HE2   | 5:B:1011:ILE:HD12 | 1.98                     | 0.45              |
| 10:I:51:ASN:O     | 10:I:54:GLU:HG2   | 2.16                     | 0.45              |
| 4:A:15:LYS:HD3    | 5:B:1218:THR:O    | 2.16                     | 0.45              |
| 4:A:511:ILE:O     | 4:A:519:PRO:HA    | 2.15                     | 0.45              |
| 4:A:1412:ALA:HA   | 4:A:1417:GLU:HG3  | 1.97                     | 0.45              |
| 8:F:99:LEU:O      | 8:F:102:SER:OG    | 2.31                     | 0.45              |
| 5:B:486:TYR:CZ    | 5:B:1096:ARG:HB3  | 2.51                     | 0.45              |
| 5:B:558:LEU:HD13  | 5:B:580:VAL:HG11  | 1.99                     | 0.45              |
| 4:A:508:PRO:O     | 4:A:511:ILE:HG13  | 2.16                     | 0.45              |
| 4:A:1438:THR:HG23 | 8:F:92:ARG:HB2    | 1.98                     | 0.45              |
| 4:A:199:LEU:HB3   | 4:A:200:ARG:H     | 1.58                     | 0.45              |
| 4:A:715:GLU:O     | 4:A:719:VAL:HG23  | 2.16                     | 0.45              |
| 5:B:1000:PRO:HB2  | 5:B:1072:MET:HE3  | 1.97                     | 0.45              |
| 13:L:29:TYR:HE2   | 13:L:58:LYS:HG3   | 1.82                     | 0.45              |
| 4:A:110:CYS:SG    | 4:A:112:LYS:HD2   | 2.57                     | 0.45              |
| 4:A:1397:LEU:HB2  | 4:A:1426:GLU:HG3  | 1.98                     | 0.45              |
| 4:A:1402:PHE:O    | 4:A:1403:GLU:HG3  | 2.15                     | 0.45              |
| 4:A:842:VAL:HG11  | 5:B:1136:ASP:CG   | 2.42                     | 0.45              |
| 4:A:1120:LEU:HD21 | 4:A:1131:ALA:HB2  | 1.99                     | 0.45              |
| 4:A:1428:VAL:HG13 | 5:B:1151:LEU:CD2  | 2.46                     | 0.45              |
| 5:B:878:GLN:O     | 5:B:882:THR:N     | 2.42                     | 0.45              |
| 5:B:879:ARG:HB2   | 5:B:885:MET:HE2   | 1.98                     | 0.45              |
| 9:H:102:TYR:CZ    | 9:H:115:TYR:HB3   | 2.51                     | 0.45              |
| 10:I:96:SER:HB2   | 10:I:98:VAL:HG23  | 1.99                     | 0.45              |
| 3:N:11:DA:H3'     | 3:N:12:DG:H2'     | 1.99                     | 0.45              |
| 1:R:4:G:H2'       | 1:R:5:A:H8        | 1.82                     | 0.45              |
| 4:A:339:ASN:O     | 4:A:343:LYS:HE2   | 2.16                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:B:698:GLU:HA   | 5:B:701:ILE:HG12  | 1.99                     | 0.45              |
| 5:B:1084:GLN:HG2 | 6:C:201:TRP:CH2   | 2.52                     | 0.45              |
| 4:A:100:LYS:HE2  | 4:A:100:LYS:HB3   | 1.70                     | 0.45              |
| 4:A:598:LEU:HD11 | 9:H:124:ARG:HB3   | 1.99                     | 0.45              |
| 4:A:1218:GLN:HA  | 4:A:1221:LYS:HG3  | 1.99                     | 0.45              |
| 2:T:23:DC:H2''   | 2:T:24:DT:H5'     | 1.98                     | 0.44              |
| 4:A:62:ASP:HB3   | 4:A:64:ASN:OD1    | 2.17                     | 0.44              |
| 4:A:265:LYS:HG3  | 4:A:303:TYR:HB2   | 1.99                     | 0.44              |
| 5:B:116:GLU:OE2  | 5:B:120:ARG:NH1   | 2.50                     | 0.44              |
| 5:B:770:GLN:NE2  | 5:B:1093:GLN:HE22 | 2.11                     | 0.44              |
| 5:B:904:ARG:NH2  | 13:L:68:GLU:OE2   | 2.51                     | 0.44              |
| 4:A:666:ILE:HG23 | 5:B:1026:LEU:CB   | 2.41                     | 0.44              |
| 4:A:1036:ARG:NH1 | 4:A:1036:ARG:HB2  | 2.32                     | 0.44              |
| 9:H:129:TYR:O    | 9:H:131:ASN:ND2   | 2.50                     | 0.44              |
| 5:B:863:GLU:OE2  | 5:B:874:PHE:N     | 2.47                     | 0.44              |
| 9:H:24:CYS:SG    | 9:H:44:VAL:HG21   | 2.57                     | 0.44              |
| 4:A:549:MET:SD   | 4:A:577:ILE:HG21  | 2.57                     | 0.44              |
| 4:A:550:LEU:HD23 | 4:A:556:TRP:CZ2   | 2.53                     | 0.44              |
| 4:A:588:LEU:HB3  | 4:A:607:ILE:HD12  | 2.00                     | 0.44              |
| 4:A:1157:ASP:HB3 | 4:A:1160:SER:O    | 2.16                     | 0.44              |
| 8:F:146:TRP:HB3  | 8:F:151:LEU:HD21  | 1.98                     | 0.44              |
| 11:J:8:PHE:N     | 11:J:49:MET:HE3   | 2.22                     | 0.44              |
| 4:A:860:LEU:CD1  | 4:A:1393:ASN:HB2  | 2.47                     | 0.44              |
| 4:A:1030:ARG:HG2 | 4:A:1034:GLU:OE2  | 2.18                     | 0.44              |
| 4:A:1303:GLU:CD  | 4:A:1326:ARG:HH12 | 2.24                     | 0.44              |
| 5:B:287:ARG:HG2  | 5:B:292:ILE:HA    | 2.00                     | 0.44              |
| 6:C:69:LEU:HD12  | 11:J:6:ARG:HG3    | 2.00                     | 0.44              |
| 12:K:61:TYR:HA   | 12:K:72:LYS:O     | 2.18                     | 0.44              |
| 4:A:53:LEU:HA    | 4:A:53:LEU:HD12   | 1.75                     | 0.44              |
| 4:A:68:GLN:HE21  | 4:A:80:HIS:CD2    | 2.36                     | 0.44              |
| 4:A:239:LEU:HD12 | 4:A:240:PRO:HD2   | 2.00                     | 0.44              |
| 4:A:1093:LYS:N   | 4:A:1093:LYS:HD2  | 2.33                     | 0.44              |
| 4:A:296:LEU:O    | 4:A:300:VAL:HG23  | 2.18                     | 0.44              |
| 4:A:982:THR:HG22 | 4:A:984:LYS:N     | 2.33                     | 0.44              |
| 5:B:46:GLN:HE22  | 5:B:47:GLN:HG2    | 1.83                     | 0.44              |
| 5:B:899:ILE:O    | 5:B:952:VAL:HG21  | 2.17                     | 0.44              |
| 4:A:618:GLU:OE1  | 4:A:619:LYS:N     | 2.51                     | 0.44              |
| 4:A:648:ASN:O    | 4:A:652:VAL:HG23  | 2.17                     | 0.44              |
| 4:A:913:LEU:HD21 | 4:A:981:LEU:O     | 2.18                     | 0.44              |
| 4:A:1317:MET:HA  | 4:A:1322:ILE:HD11 | 1.99                     | 0.44              |
| 10:I:73:ARG:O    | 10:I:83:ASN:ND2   | 2.51                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:A:1434:ALA:HB3 | 4:A:1436:ILE:HD12 | 2.00                     | 0.44              |
| 5:B:128:LEU:HB3  | 5:B:167:ILE:HG22  | 1.99                     | 0.44              |
| 9:H:81:PRO:HA    | 9:H:82:PRO:HD3    | 1.83                     | 0.44              |
| 4:A:845:LEU:HD12 | 4:A:1069:ALA:HB2  | 1.99                     | 0.43              |
| 5:B:197:PHE:O    | 5:B:488:TYR:OH    | 2.27                     | 0.43              |
| 6:C:41:ILE:HD11  | 6:C:172:PRO:HG2   | 2.00                     | 0.43              |
| 7:E:23:VAL:HG12  | 7:E:28:TYR:HB2    | 2.00                     | 0.43              |
| 4:A:80:HIS:O     | 4:A:243:PRO:HB3   | 2.18                     | 0.43              |
| 4:A:443:LEU:HB2  | 4:A:501:LEU:HD11  | 2.00                     | 0.43              |
| 4:A:839:ARG:NH2  | 4:A:1402:PHE:HA   | 2.34                     | 0.43              |
| 5:B:484:ASN:OD1  | 5:B:490:SER:OG    | 2.35                     | 0.43              |
| 5:B:1020:ARG:H   | 5:B:1020:ARG:HG2  | 1.71                     | 0.43              |
| 6:C:17:ASN:OD1   | 6:C:233:GLU:HG3   | 2.18                     | 0.43              |
| 9:H:30:SER:HB2   | 9:H:33:GLN:HB3    | 1.99                     | 0.43              |
| 4:A:443:LEU:HD13 | 5:B:1146:PHE:CZ   | 2.54                     | 0.43              |
| 4:A:765:VAL:CG2  | 4:A:800:VAL:HB    | 2.49                     | 0.43              |
| 4:A:934:LYS:HE3  | 4:A:934:LYS:HB2   | 1.61                     | 0.43              |
| 4:A:328:ARG:HD3  | 5:B:1206:GLU:OE1  | 2.17                     | 0.43              |
| 4:A:767:GLN:NE2  | 4:A:774:ARG:HG2   | 2.34                     | 0.43              |
| 4:A:1433:MET:HE2 | 4:A:1433:MET:HB3  | 1.88                     | 0.43              |
| 5:B:1100:ASP:HA  | 5:B:1103:ILE:HG12 | 2.00                     | 0.43              |
| 9:H:103:LYS:HD3  | 9:H:104:PHE:N     | 2.33                     | 0.43              |
| 4:A:71:GLN:HE21  | 5:B:1174:LYS:HB3  | 1.83                     | 0.43              |
| 4:A:275:SER:O    | 4:A:278:THR:HB    | 2.18                     | 0.43              |
| 4:A:305:ASP:OD1  | 4:A:306:ASN:N     | 2.51                     | 0.43              |
| 4:A:1128:GLN:HB3 | 4:A:1304:TRP:CE2  | 2.53                     | 0.43              |
| 5:B:183:GLU:OE1  | 5:B:183:GLU:N     | 2.49                     | 0.43              |
| 5:B:245:GLU:HG3  | 5:B:246:LYS:HE2   | 2.00                     | 0.43              |
| 4:A:304:MET:O    | 4:A:324:SER:HB2   | 2.18                     | 0.43              |
| 4:A:567:LYS:HB2  | 9:H:96:VAL:HB     | 2.01                     | 0.43              |
| 4:A:800:VAL:HG13 | 4:A:812:GLU:CD    | 2.43                     | 0.43              |
| 4:A:1041:ALA:O   | 4:A:1045:VAL:HG23 | 2.18                     | 0.43              |
| 5:B:309:GLN:OE1  | 5:B:392:ARG:NH2   | 2.51                     | 0.43              |
| 12:K:91:CYS:O    | 12:K:95:ILE:HG13  | 2.18                     | 0.43              |
| 4:A:34:LYS:HE2   | 4:A:83:HIS:CE1    | 2.54                     | 0.43              |
| 4:A:528:LEU:O    | 4:A:531:ILE:HG22  | 2.19                     | 0.43              |
| 4:A:939:ASP:OD2  | 4:A:1023:ARG:HD2  | 2.19                     | 0.43              |
| 5:B:952:VAL:HG22 | 5:B:966:VAL:HG13  | 2.01                     | 0.43              |
| 11:J:44:TYR:O    | 11:J:48:ARG:HG3   | 2.19                     | 0.43              |
| 4:A:57:ARG:CA    | 4:A:68:GLN:HB3    | 2.49                     | 0.43              |
| 4:A:676:MET:O    | 4:A:680:THR:HG22  | 2.19                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:A:1399:ARG:HB3  | 4:A:1408:ILE:HD13 | 2.01                     | 0.43              |
| 5:B:117:ALA:HA    | 5:B:122:LEU:HB2   | 2.00                     | 0.43              |
| 5:B:600:LEU:HB3   | 5:B:615:MET:SD    | 2.59                     | 0.43              |
| 9:H:113:ALA:HA    | 9:H:125:LEU:O     | 2.18                     | 0.43              |
| 4:A:1081:LEU:HD23 | 4:A:1081:LEU:HA   | 1.87                     | 0.43              |
| 5:B:30:SER:HB3    | 5:B:743:ILE:O     | 2.19                     | 0.43              |
| 13:L:40:LEU:HD23  | 13:L:44:ASP:HB3   | 1.99                     | 0.43              |
| 4:A:1092:LYS:C    | 4:A:1093:LYS:HD2  | 2.44                     | 0.43              |
| 5:B:210:LYS:NZ    | 5:B:482:VAL:HG22  | 2.34                     | 0.43              |
| 7:E:19:VAL:O      | 7:E:23:VAL:HG23   | 2.19                     | 0.43              |
| 9:H:27:GLU:OE1    | 9:H:39:THR:HG23   | 2.19                     | 0.43              |
| 4:A:96:ILE:O      | 4:A:99:ILE:HB     | 2.18                     | 0.42              |
| 4:A:1300:LYS:HB2  | 4:A:1300:LYS:HE2  | 1.57                     | 0.42              |
| 5:B:326:ASP:OD1   | 5:B:326:ASP:N     | 2.52                     | 0.42              |
| 5:B:492:LEU:O     | 5:B:496:ARG:HG3   | 2.19                     | 0.42              |
| 6:C:26:ASP:OD1    | 6:C:26:ASP:N      | 2.50                     | 0.42              |
| 4:A:269:ILE:HD12  | 4:A:300:VAL:HG22  | 2.00                     | 0.42              |
| 4:A:1134:ILE:HB   | 4:A:1306:LEU:HD11 | 2.01                     | 0.42              |
| 6:C:39:ALA:HA     | 6:C:164:ALA:HB3   | 2.01                     | 0.42              |
| 10:I:5:ARG:HD3    | 10:I:36:GLU:OE2   | 2.18                     | 0.42              |
| 4:A:23:SER:HB3    | 4:A:233:TRP:CE2   | 2.53                     | 0.42              |
| 4:A:210:ILE:O     | 4:A:214:ILE:HG12  | 2.19                     | 0.42              |
| 4:A:575:LYS:HB3   | 4:A:612:ILE:CD1   | 2.46                     | 0.42              |
| 4:A:726:ARG:HD3   | 4:A:766:GLY:HA3   | 2.00                     | 0.42              |
| 5:B:778:MET:CE    | 5:B:1094:ARG:HD3  | 2.49                     | 0.42              |
| 5:B:1067:ARG:NE   | 6:C:194:GLU:OE1   | 2.47                     | 0.42              |
| 4:A:115:LEU:HD12  | 4:A:119:ASN:HB2   | 2.01                     | 0.42              |
| 4:A:607:ILE:HA    | 4:A:612:ILE:HA    | 2.01                     | 0.42              |
| 4:A:986:ILE:O     | 4:A:990:VAL:HG23  | 2.20                     | 0.42              |
| 4:A:1295:THR:HB   | 4:A:1297:GLU:OE1  | 2.19                     | 0.42              |
| 5:B:522:VAL:CG2   | 5:B:537:LYS:HB3   | 2.49                     | 0.42              |
| 5:B:851:PHE:O     | 5:B:974:PRO:HD3   | 2.20                     | 0.42              |
| 4:A:738:LYS:HB2   | 4:A:740:LEU:HG    | 2.01                     | 0.42              |
| 4:A:1157:ASP:OD2  | 4:A:1160:SER:HB3  | 2.19                     | 0.42              |
| 5:B:493:SER:OG    | 5:B:497:ARG:NH2   | 2.53                     | 0.42              |
| 5:B:519:TRP:NE1   | 5:B:742:GLU:OE1   | 2.47                     | 0.42              |
| 5:B:763:GLN:HG3   | 5:B:765:PRO:HD2   | 2.00                     | 0.42              |
| 5:B:911:ILE:HD13  | 5:B:941:LEU:HD23  | 2.00                     | 0.42              |
| 7:E:46:TYR:CD1    | 7:E:58:MET:HE2    | 2.55                     | 0.42              |
| 4:A:58:LEU:HD21   | 4:A:80:HIS:O      | 2.20                     | 0.42              |
| 4:A:795:GLU:HG2   | 5:B:731:VAL:HG11  | 2.02                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:A:1239:ARG:HH12 | 4:A:1241:ARG:HH12 | 1.67                     | 0.42              |
| 5:B:58:THR:O      | 5:B:62:ILE:HG13   | 2.19                     | 0.42              |
| 5:B:651:LEU:H     | 5:B:651:LEU:HD12  | 1.84                     | 0.42              |
| 7:E:79:TRP:HD1    | 7:E:100:ILE:HD11  | 1.83                     | 0.42              |
| 12:K:65:HIS:ND1   | 12:K:66:PRO:HD2   | 2.34                     | 0.42              |
| 3:N:10:DG:H2''    | 3:N:11:DA:H8      | 1.85                     | 0.42              |
| 13:L:41:SER:N     | 13:L:44:ASP:OD2   | 2.52                     | 0.42              |
| 2:T:12:DT:H2''    | 2:T:13:DC:H5'     | 2.02                     | 0.42              |
| 2:T:25:DC:OP2     | 5:B:942:ARG:NH2   | 2.41                     | 0.42              |
| 4:A:84:ILE:HG23   | 4:A:239:LEU:HB3   | 2.01                     | 0.42              |
| 4:A:1025:ARG:O    | 4:A:1035:TYR:OH   | 2.37                     | 0.42              |
| 5:B:1152:MET:HE3  | 5:B:1152:MET:HB3  | 1.98                     | 0.42              |
| 7:E:177:ARG:HD3   | 7:E:215:MET:SD    | 2.60                     | 0.42              |
| 8:F:97:ARG:HD2    | 8:F:97:ARG:HA     | 1.68                     | 0.42              |
| 8:F:135:ARG:NH2   | 8:F:145:ASP:OD2   | 2.35                     | 0.42              |
| 4:A:388:LEU:HD23  | 4:A:388:LEU:HA    | 1.87                     | 0.42              |
| 7:E:46:TYR:HD1    | 7:E:58:MET:HE2    | 1.83                     | 0.42              |
| 4:A:95:PHE:CE2    | 4:A:1414:ALA:HB2  | 2.55                     | 0.42              |
| 4:A:931:GLU:OE2   | 4:A:991:LYS:NZ    | 2.38                     | 0.42              |
| 4:A:1217:LYS:HE3  | 4:A:1228:TRP:CZ3  | 2.55                     | 0.42              |
| 5:B:209:GLU:HB2   | 5:B:483:LEU:HB2   | 2.02                     | 0.42              |
| 5:B:428:ILE:O     | 5:B:432:MET:HG2   | 2.20                     | 0.42              |
| 5:B:541:LEU:HD23  | 5:B:541:LEU:HA    | 1.92                     | 0.42              |
| 5:B:614:SER:OG    | 5:B:627:PHE:HB2   | 2.20                     | 0.42              |
| 10:I:47:GLU:OE1   | 10:I:50:THR:HG23  | 2.20                     | 0.42              |
| 12:K:20:LYS:O     | 12:K:33:ILE:HA    | 2.20                     | 0.42              |
| 4:A:336:ILE:HG21  | 4:A:1401:SER:HA   | 2.02                     | 0.41              |
| 4:A:463:ILE:HD12  | 4:A:465:TYR:H     | 1.85                     | 0.41              |
| 4:A:494:SER:O     | 4:A:498:ARG:HG3   | 2.19                     | 0.41              |
| 5:B:554:ILE:O     | 5:B:558:LEU:HG    | 2.20                     | 0.41              |
| 5:B:992:ILE:HD11  | 12:K:66:PRO:HB2   | 2.02                     | 0.41              |
| 5:B:1023:VAL:HG12 | 5:B:1027:ILE:HD11 | 2.02                     | 0.41              |
| 3:N:15:DA:P       | 7:E:117:THR:HG21  | 2.59                     | 0.41              |
| 4:A:53:LEU:HB3    | 4:A:54:ASN:H      | 1.61                     | 0.41              |
| 4:A:310:GLY:C     | 4:A:312:PRO:HD3   | 2.45                     | 0.41              |
| 5:B:963:PHE:CE2   | 5:B:965:LYS:HE3   | 2.55                     | 0.41              |
| 5:B:1135:ARG:NH2  | 5:B:1136:ASP:OD1  | 2.53                     | 0.41              |
| 5:B:1168:LEU:HD21 | 5:B:1215:ARG:HG2  | 2.01                     | 0.41              |
| 7:E:118:PRO:O     | 7:E:122:LYS:HG2   | 2.20                     | 0.41              |
| 10:I:60:GLN:NE2   | 10:I:107:SER:HG   | 2.11                     | 0.41              |
| 5:B:400:HIS:NE2   | 5:B:517:THR:HG21  | 2.36                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 5:B:883:LEU:HD12  | 5:B:884:ARG:H    | 1.85                     | 0.41              |
| 7:E:46:TYR:CD1    | 7:E:58:MET:HG2   | 2.56                     | 0.41              |
| 7:E:78:LEU:HD21   | 7:E:109:ILE:HD12 | 2.02                     | 0.41              |
| 7:E:90:VAL:HG13   | 7:E:123:LEU:HD21 | 2.02                     | 0.41              |
| 11:J:16:ASP:OD1   | 11:J:16:ASP:N    | 2.37                     | 0.41              |
| 12:K:54:ARG:HE    | 12:K:54:ARG:HB2  | 1.59                     | 0.41              |
| 2:T:26:DG:H1'     | 2:T:27:DA:H5'    | 2.01                     | 0.41              |
| 4:A:1128:GLN:O    | 4:A:1132:LYS:HG3 | 2.21                     | 0.41              |
| 5:B:219:ALA:HB2   | 5:B:405:ARG:HG2  | 2.01                     | 0.41              |
| 5:B:408:LEU:HD12  | 5:B:408:LEU:HA   | 1.80                     | 0.41              |
| 5:B:1034:VAL:HG22 | 5:B:1059:LEU:HB2 | 2.03                     | 0.41              |
| 7:E:64:PRO:HB3    | 7:E:75:MET:HG2   | 2.01                     | 0.41              |
| 12:K:58:PHE:HB3   | 12:K:76:GLN:HB3  | 2.01                     | 0.41              |
| 4:A:172:PRO:HB3   | 4:A:185:TRP:CG   | 2.56                     | 0.41              |
| 4:A:845:LEU:O     | 4:A:1065:GLY:HA3 | 2.19                     | 0.41              |
| 9:H:76:THR:OG1    | 9:H:77:ARG:N     | 2.53                     | 0.41              |
| 4:A:597:LEU:HD13  | 9:H:103:LYS:HG3  | 2.01                     | 0.41              |
| 4:A:1195:LEU:HD11 | 4:A:1267:MET:HE1 | 2.02                     | 0.41              |
| 4:A:1225:PHE:O    | 4:A:1240:CYS:HA  | 2.20                     | 0.41              |
| 5:B:358:LYS:HA    | 5:B:366:GLN:HG2  | 2.01                     | 0.41              |
| 5:B:384:ARG:HA    | 5:B:384:ARG:HD3  | 1.84                     | 0.41              |
| 6:C:268:ASP:OD1   | 6:C:268:ASP:N    | 2.54                     | 0.41              |
| 9:H:101:ALA:HB2   | 9:H:116:TYR:CE2  | 2.55                     | 0.41              |
| 4:A:206:GLU:HG3   | 4:A:210:ILE:HD11 | 2.03                     | 0.41              |
| 5:B:209:GLU:OE2   | 5:B:788:ARG:NH2  | 2.46                     | 0.41              |
| 5:B:241:ARG:HG2   | 5:B:253:THR:HG22 | 2.02                     | 0.41              |
| 7:E:166:LYS:HG2   | 7:E:167:ARG:HD2  | 2.03                     | 0.41              |
| 4:A:1384:VAL:HA   | 4:A:1389:PHE:HD2 | 1.85                     | 0.41              |
| 5:B:195:CYS:SG    | 5:B:783:THR:OG1  | 2.65                     | 0.41              |
| 7:E:24:LYS:HE3    | 7:E:24:LYS:HB2   | 1.87                     | 0.41              |
| 8:F:77:ASP:OD1    | 8:F:77:ASP:N     | 2.40                     | 0.41              |
| 4:A:151:ASP:CG    | 4:A:163:SER:H    | 2.28                     | 0.41              |
| 4:A:179:LEU:HD23  | 4:A:297:GLN:HG3  | 2.03                     | 0.41              |
| 4:A:369:SER:OG    | 12:K:2:ASN:ND2   | 2.40                     | 0.41              |
| 4:A:1032:LEU:HD23 | 4:A:1032:LEU:HA  | 1.84                     | 0.41              |
| 4:A:1079:MET:HG2  | 4:A:1359:ASP:OD2 | 2.21                     | 0.41              |
| 5:B:406:LEU:HD23  | 5:B:406:LEU:HA   | 1.87                     | 0.41              |
| 6:C:93:ASP:OD1    | 6:C:122:SER:HB2  | 2.21                     | 0.41              |
| 7:E:46:TYR:OH     | 7:E:57:MET:HB3   | 2.21                     | 0.41              |
| 7:E:64:PRO:HD3    | 7:E:76:GLY:HA2   | 2.03                     | 0.41              |
| 8:F:76:LYS:HA     | 8:F:79:ARG:HE    | 1.86                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:A:982:THR:O     | 4:A:985:ASP:HB2   | 2.21                     | 0.41              |
| 4:A:1100:ARG:O    | 4:A:1104:ILE:HG13 | 2.21                     | 0.41              |
| 4:A:1140:HIS:HB2  | 4:A:1276:VAL:O    | 2.20                     | 0.41              |
| 4:A:1295:THR:HB   | 4:A:1297:GLU:CD   | 2.46                     | 0.41              |
| 5:B:65:GLU:O      | 5:B:67:SER:N      | 2.54                     | 0.41              |
| 5:B:418:LYS:HE3   | 5:B:418:LYS:HB3   | 1.86                     | 0.41              |
| 5:B:1001:PHE:CZ   | 5:B:1073:TYR:HB2  | 2.56                     | 0.41              |
| 6:C:11:ARG:HD3    | 6:C:209:TYR:CE1   | 2.57                     | 0.41              |
| 4:A:31:SER:HA     | 4:A:81:PHE:O      | 2.21                     | 0.40              |
| 4:A:92:HIS:CE1    | 4:A:304:MET:HE3   | 2.56                     | 0.40              |
| 4:A:108:MET:HB2   | 4:A:109:HIS:ND1   | 2.36                     | 0.40              |
| 4:A:666:ILE:CD1   | 5:B:1030:LEU:HD22 | 2.51                     | 0.40              |
| 4:A:924:LYS:O     | 4:A:927:VAL:HG22  | 2.20                     | 0.40              |
| 4:A:1105:LEU:HD22 | 4:A:1384:VAL:HG21 | 2.02                     | 0.40              |
| 5:B:102:VAL:CG1   | 5:B:112:LEU:HD22  | 2.51                     | 0.40              |
| 5:B:515:HIS:CE1   | 5:B:517:THR:HG1   | 2.34                     | 0.40              |
| 5:B:826:ALA:HB3   | 5:B:1011:ILE:HG12 | 2.01                     | 0.40              |
| 2:T:5:DC:H2''     | 2:T:6:DT:H5'      | 2.03                     | 0.40              |
| 4:A:492:PRO:HB3   | 4:A:497:THR:HG22  | 2.03                     | 0.40              |
| 4:A:761:MET:HG3   | 5:B:1021:MET:HG2  | 2.03                     | 0.40              |
| 4:A:926:GLN:O     | 4:A:926:GLN:HG3   | 2.21                     | 0.40              |
| 5:B:1038:SER:HB3  | 5:B:1062:HIS:NE2  | 2.37                     | 0.40              |
| 9:H:10:PHE:HB3    | 9:H:28:ALA:HB1    | 2.03                     | 0.40              |
| 9:H:103:LYS:HB3   | 9:H:115:TYR:CD1   | 2.49                     | 0.40              |
| 4:A:270:LEU:HD23  | 4:A:270:LEU:HA    | 1.92                     | 0.40              |
| 4:A:302:THR:HA    | 4:A:305:ASP:O     | 2.21                     | 0.40              |
| 4:A:818:MET:HG3   | 5:B:514:LEU:O     | 2.21                     | 0.40              |
| 4:A:1156:PRO:O    | 4:A:1158:PRO:HD3  | 2.22                     | 0.40              |
| 4:A:1428:VAL:HG22 | 5:B:1147:LEU:HD11 | 2.03                     | 0.40              |
| 6:C:149:LYS:HE3   | 6:C:149:LYS:HB3   | 1.89                     | 0.40              |
| 8:F:111:LEU:HD12  | 8:F:114:GLU:O     | 2.21                     | 0.40              |
| 3:N:15:DA:OP2     | 7:E:117:THR:HG21  | 2.21                     | 0.40              |
| 4:A:964:ILE:O     | 4:A:968:GLN:HG3   | 2.21                     | 0.40              |
| 4:A:1207:LEU:HD23 | 4:A:1207:LEU:HA   | 1.92                     | 0.40              |
| 7:E:34:GLU:O      | 7:E:37:LEU:HD23   | 2.22                     | 0.40              |
| 7:E:46:TYR:HD2    | 7:E:53:PRO:CB     | 2.34                     | 0.40              |
| 4:A:909:ASP:HB3   | 4:A:912:LEU:HG    | 2.03                     | 0.40              |
| 4:A:971:PHE:O     | 4:A:973:ILE:N     | 2.54                     | 0.40              |
| 4:A:1345:ARG:HG2  | 4:A:1372:VAL:CG1  | 2.50                     | 0.40              |
| 6:C:29:MET:HE3    | 6:C:29:MET:HB2    | 1.92                     | 0.40              |
| 7:E:86:PRO:O      | 7:E:114:ASN:HB2   | 2.21                     | 0.40              |



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

| Atom-1        | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------|------------------------|--------------------------|-------------------|
| 4:A:920:LEU:O | 10:I:24:ARG:NH2[4_546] | 2.16                     | 0.04              |

## 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 |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 4   | A     | 1371/1733 (79%) | 1292 (94%) | 76 (6%)  | 3 (0%)   | 43          | 73  |
| 5   | B     | 1101/1224 (90%) | 1027 (93%) | 74 (7%)  | 0        | 100         | 100 |
| 6   | C     | 265/318 (83%)   | 256 (97%)  | 9 (3%)   | 0        | 100         | 100 |
| 7   | E     | 211/215 (98%)   | 196 (93%)  | 15 (7%)  | 0        | 100         | 100 |
| 8   | F     | 84/155 (54%)    | 81 (96%)   | 3 (4%)   | 0        | 100         | 100 |
| 9   | H     | 129/146 (88%)   | 115 (89%)  | 14 (11%) | 0        | 100         | 100 |
| 10  | I     | 116/122 (95%)   | 105 (90%)  | 10 (9%)  | 1 (1%)   | 14          | 44  |
| 11  | J     | 63/70 (90%)     | 60 (95%)   | 3 (5%)   | 0        | 100         | 100 |
| 12  | K     | 112/120 (93%)   | 109 (97%)  | 3 (3%)   | 0        | 100         | 100 |
| 13  | L     | 41/70 (59%)     | 39 (95%)   | 2 (5%)   | 0        | 100         | 100 |
| All | All   | 3493/4173 (84%) | 3280 (94%) | 209 (6%) | 4 (0%)   | 48          | 78  |

All (4) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | A     | 55  | ASP  |
| 4   | A     | 109 | HIS  |
| 10  | I     | 11  | ASN  |
| 4   | A     | 312 | 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 |     |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 4   | A     | 1193/1520 (78%) | 1191 (100%) | 2 (0%)   | 87          | 89  |
| 5   | B     | 955/1061 (90%)  | 955 (100%)  | 0        | 100         | 100 |
| 6   | C     | 235/274 (86%)   | 235 (100%)  | 0        | 100         | 100 |
| 7   | E     | 194/197 (98%)   | 194 (100%)  | 0        | 100         | 100 |
| 8   | F     | 73/137 (53%)    | 73 (100%)   | 0        | 100         | 100 |
| 9   | H     | 116/128 (91%)   | 116 (100%)  | 0        | 100         | 100 |
| 10  | I     | 110/116 (95%)   | 110 (100%)  | 0        | 100         | 100 |
| 11  | J     | 60/65 (92%)     | 60 (100%)   | 0        | 100         | 100 |
| 12  | K     | 99/102 (97%)    | 99 (100%)   | 0        | 100         | 100 |
| 13  | L     | 37/57 (65%)     | 36 (97%)    | 1 (3%)   | 39          | 67  |
| All | All   | 3072/3657 (84%) | 3069 (100%) | 3 (0%)   | 88          | 90  |

All (3) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | A     | 131 | SER  |
| 4   | A     | 805 | LEU  |
| 13  | L     | 43  | THR  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | A     | 118 | HIS  |
| 4   | A     | 171 | GLN  |
| 4   | A     | 209 | ASN  |
| 4   | A     | 282 | ASN  |
| 4   | A     | 297 | GLN  |
| 4   | A     | 390 | GLN  |
| 4   | A     | 394 | ASN  |
| 4   | A     | 435 | HIS  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 4   | A     | 510  | GLN  |
| 4   | A     | 603  | ASN  |
| 4   | A     | 698  | GLN  |
| 4   | A     | 741  | ASN  |
| 4   | A     | 968  | GLN  |
| 4   | A     | 1106 | ASN  |
| 4   | A     | 1124 | HIS  |
| 4   | A     | 1187 | GLN  |
| 4   | A     | 1387 | HIS  |
| 4   | A     | 1427 | ASN  |
| 5   | B     | 667  | GLN  |
| 5   | B     | 842  | ASN  |
| 5   | B     | 881  | ASN  |
| 5   | B     | 1093 | GLN  |
| 7   | E     | 63   | ASN  |
| 9   | H     | 33   | GLN  |
| 9   | H     | 139  | ASN  |
| 12  | K     | 92   | ASN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed  | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------|-------------------|-----------------|
| 1   | R     | 8/9 (88%) | 1 (12%)           | 0               |

All (1) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | R     | 9   | G    |

There are no RNA pucker outliers to report.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 2   | 8OG  | T     | 19  | 2    | 22,25,26     | 4.25 | 17 (77%)    | 26,37,40    | 2.43 | 9 (34%)     |

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   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 2   | 8OG  | T     | 19  | 2    | -       | 6/7/21/22 | 0/3/3/3 |

All (17) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | T     | 19  | 8OG  | C8-N7   | 7.31  | 1.51        | 1.38     |
| 2   | T     | 19  | 8OG  | C8-N9   | 6.57  | 1.52        | 1.40     |
| 2   | T     | 19  | 8OG  | C4-N3   | 6.43  | 1.49        | 1.34     |
| 2   | T     | 19  | 8OG  | C2-N3   | 6.28  | 1.48        | 1.33     |
| 2   | T     | 19  | 8OG  | C2-N2   | 5.83  | 1.47        | 1.34     |
| 2   | T     | 19  | 8OG  | C5-N7   | 4.61  | 1.45        | 1.37     |
| 2   | T     | 19  | 8OG  | C2-N1   | 4.55  | 1.48        | 1.37     |
| 2   | T     | 19  | 8OG  | O4'-C1' | -4.51 | 1.32        | 1.42     |
| 2   | T     | 19  | 8OG  | C6-N1   | 4.47  | 1.47        | 1.38     |
| 2   | T     | 19  | 8OG  | O3'-C3' | 3.98  | 1.51        | 1.43     |
| 2   | T     | 19  | 8OG  | C4-N9   | 3.96  | 1.46        | 1.39     |
| 2   | T     | 19  | 8OG  | C2'-C1' | 3.69  | 1.62        | 1.52     |
| 2   | T     | 19  | 8OG  | C5-C4   | 3.66  | 1.42        | 1.37     |
| 2   | T     | 19  | 8OG  | C5-C6   | 3.54  | 1.52        | 1.41     |
| 2   | T     | 19  | 8OG  | C5'-C4' | -3.23 | 1.41        | 1.51     |
| 2   | T     | 19  | 8OG  | O6-C6   | -2.38 | 1.19        | 1.23     |
| 2   | T     | 19  | 8OG  | C3'-C4' | 2.16  | 1.58        | 1.53     |

All (9) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2   | T     | 19  | 8OG  | C2-N3-C4 | 7.14  | 124.60      | 112.30   |
| 2   | T     | 19  | 8OG  | N1-C2-N3 | -4.28 | 115.50      | 123.32   |
| 2   | T     | 19  | 8OG  | N9-C4-N3 | 4.17  | 131.34      | 126.13   |
| 2   | T     | 19  | 8OG  | O6-C6-C5 | -3.88 | 117.89      | 127.26   |
| 2   | T     | 19  | 8OG  | N2-C2-N1 | 3.46  | 124.06      | 116.76   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2   | T     | 19  | 8OG  | C5-C6-N1 | 3.25  | 121.05      | 112.13   |
| 2   | T     | 19  | 8OG  | O8-C8-N9 | 2.38  | 129.24      | 126.00   |
| 2   | T     | 19  | 8OG  | N7-C8-N9 | -2.33 | 104.02      | 106.61   |
| 2   | T     | 19  | 8OG  | C2-N1-C6 | -2.32 | 120.91      | 125.11   |

There are no chirality outliers.

All (6) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | T     | 19  | 8OG  | O4'-C1'-N9-C8   |
| 2   | T     | 19  | 8OG  | C2'-C1'-N9-C8   |
| 2   | T     | 19  | 8OG  | O4'-C4'-C5'-O5' |
| 2   | T     | 19  | 8OG  | C3'-C4'-C5'-O5' |
| 2   | T     | 19  | 8OG  | C2'-C1'-N9-C4   |
| 2   | T     | 19  | 8OG  | O4'-C1'-N9-C4   |

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1   | R     | 9/9 (100%)      | -0.09  | 0 100 100     | 70, 82, 137, 137      | 0     |
| 2   | T     | 25/29 (86%)     | 0.89   | 0 100 100     | 71, 185, 229, 244     | 0     |
| 3   | N     | 15/18 (83%)     | 1.08   | 1 (6%) 24 13  | 169, 211, 234, 237    | 0     |
| 4   | A     | 1385/1733 (79%) | 0.16   | 33 (2%) 59 38 | 39, 77, 154, 266      | 0     |
| 5   | B     | 1121/1224 (91%) | 0.05   | 17 (1%) 72 52 | 37, 69, 128, 195      | 0     |
| 6   | C     | 267/318 (83%)   | -0.12  | 1 (0%) 88 76  | 41, 66, 98, 133       | 0     |
| 7   | E     | 213/215 (99%)   | 0.28   | 4 (1%) 66 45  | 58, 104, 168, 202     | 0     |
| 8   | F     | 86/155 (55%)    | -0.04  | 1 (1%) 76 58  | 60, 84, 118, 174      | 0     |
| 9   | H     | 133/146 (91%)   | 0.44   | 4 (3%) 52 31  | 71, 103, 145, 175     | 0     |
| 10  | I     | 118/122 (96%)   | 0.17   | 3 (2%) 58 37  | 50, 84, 119, 137      | 0     |
| 11  | J     | 65/70 (92%)     | -0.20  | 0 100 100     | 50, 61, 95, 123       | 0     |
| 12  | K     | 114/120 (95%)   | -0.22  | 0 100 100     | 44, 72, 101, 138      | 0     |
| 13  | L     | 43/70 (61%)     | 1.09   | 7 (16%) 4 2   | 63, 128, 178, 218     | 0     |
| All | All   | 3594/4229 (84%) | 0.12   | 71 (1%) 65 44 | 37, 76, 149, 266      | 0     |

All (71) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 9   | H     | 139 | ASN  | 5.1  |
| 5   | B     | 714 | GLU  | 4.3  |
| 5   | B     | 335 | GLY  | 4.0  |
| 13  | L     | 45  | ALA  | 4.0  |
| 4   | A     | 69  | THR  | 3.8  |
| 7   | E     | 93  | MET  | 3.6  |
| 13  | L     | 46  | VAL  | 3.6  |
| 4   | A     | 182 | VAL  | 3.5  |
| 4   | A     | 141 | LEU  | 3.2  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 4   | A     | 1257 | ASP  | 3.1  |
| 5   | B     | 733  | HIS  | 3.0  |
| 4   | A     | 161  | LEU  | 3.0  |
| 4   | A     | 144  | THR  | 3.0  |
| 4   | A     | 1081 | LEU  | 3.0  |
| 13  | L     | 32   | ALA  | 2.9  |
| 4   | A     | 104  | GLU  | 2.9  |
| 9   | H     | 63   | LEU  | 2.8  |
| 5   | B     | 473  | MET  | 2.7  |
| 4   | A     | 111  | GLY  | 2.7  |
| 5   | B     | 73   | GLN  | 2.7  |
| 4   | A     | 65   | LEU  | 2.7  |
| 13  | L     | 40   | LEU  | 2.7  |
| 4   | A     | 1002 | GLY  | 2.7  |
| 10  | I     | 119  | THR  | 2.7  |
| 4   | A     | 202  | LEU  | 2.6  |
| 4   | A     | 53   | LEU  | 2.6  |
| 9   | H     | 15   | VAL  | 2.6  |
| 5   | B     | 250  | PHE  | 2.5  |
| 4   | A     | 162  | VAL  | 2.5  |
| 4   | A     | 163  | SER  | 2.5  |
| 7   | E     | 83   | CYS  | 2.5  |
| 4   | A     | 310  | GLY  | 2.4  |
| 10  | I     | 49   | ILE  | 2.4  |
| 4   | A     | 312  | PRO  | 2.4  |
| 13  | L     | 39   | SER  | 2.4  |
| 5   | B     | 246  | LYS  | 2.4  |
| 4   | A     | 153  | PRO  | 2.4  |
| 10  | I     | 4    | PHE  | 2.4  |
| 9   | H     | 104  | PHE  | 2.3  |
| 4   | A     | 286  | HIS  | 2.3  |
| 4   | A     | 199  | LEU  | 2.3  |
| 7   | E     | 88   | VAL  | 2.3  |
| 4   | A     | 227  | VAL  | 2.3  |
| 4   | A     | 847  | ASP  | 2.3  |
| 4   | A     | 3    | GLY  | 2.2  |
| 4   | A     | 150  | THR  | 2.2  |
| 6   | C     | 96   | SER  | 2.2  |
| 4   | A     | 51   | GLY  | 2.2  |
| 4   | A     | 183  | GLY  | 2.2  |
| 13  | L     | 28   | LYS  | 2.2  |
| 5   | B     | 162  | SER  | 2.2  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 5   | B     | 138  | GLU  | 2.2  |
| 5   | B     | 676  | VAL  | 2.2  |
| 5   | B     | 502  | ILE  | 2.2  |
| 5   | B     | 1191 | ILE  | 2.2  |
| 5   | B     | 446  | LEU  | 2.2  |
| 4   | A     | 44   | THR  | 2.1  |
| 4   | A     | 201  | VAL  | 2.1  |
| 4   | A     | 181  | LEU  | 2.1  |
| 4   | A     | 35   | ILE  | 2.1  |
| 8   | F     | 69   | LEU  | 2.1  |
| 4   | A     | 1001 | ARG  | 2.1  |
| 5   | B     | 647  | GLY  | 2.1  |
| 4   | A     | 64   | ASN  | 2.1  |
| 7   | E     | 92   | THR  | 2.1  |
| 5   | B     | 708  | GLU  | 2.1  |
| 3   | N     | 16   | DA   | 2.1  |
| 5   | B     | 447  | ALA  | 2.1  |
| 5   | B     | 931  | TYR  | 2.0  |
| 4   | A     | 168  | GLY  | 2.0  |
| 13  | L     | 66   | GLN  | 2.0  |

## 6.2 Non-standard residues in protein, DNA, RNA chains [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 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 2   | 8OG  | T     | 19  | 23/24 | 0.89 | 0.12 | 75,94,132,135              | 0     |

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

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



| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 14  | ZN   | L     | 101  | 1/1   | 0.93 | 0.11 | 200,200,200,200             | 0     |
| 14  | ZN   | A     | 1801 | 1/1   | 0.94 | 0.09 | 217,217,217,217             | 0     |
| 15  | MG   | A     | 1803 | 1/1   | 0.96 | 0.06 | 76,76,76,76                 | 0     |
| 14  | ZN   | B     | 1301 | 1/1   | 0.98 | 0.04 | 121,121,121,121             | 0     |
| 14  | ZN   | I     | 202  | 1/1   | 0.99 | 0.06 | 139,139,139,139             | 0     |
| 14  | ZN   | A     | 1802 | 1/1   | 0.99 | 0.02 | 108,108,108,108             | 0     |
| 14  | ZN   | I     | 201  | 1/1   | 0.99 | 0.03 | 93,93,93,93                 | 0     |
| 14  | ZN   | C     | 401  | 1/1   | 1.00 | 0.03 | 82,82,82,82                 | 0     |
| 14  | ZN   | J     | 101  | 1/1   | 1.00 | 0.05 | 69,69,69,69                 | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.