



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:32 PM UTC

PDB ID : 6ERQ / pdb\_00006erq  
Title : Structure of the human mitochondrial transcription initiation complex at the HSP promoter  
Authors : Hillen, H.S.; Morozov, Y.I.; Sarfallah, A.; Temiakov, D.; Cramer, P.  
Deposited on : 2017-10-18  
Resolution : 4.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

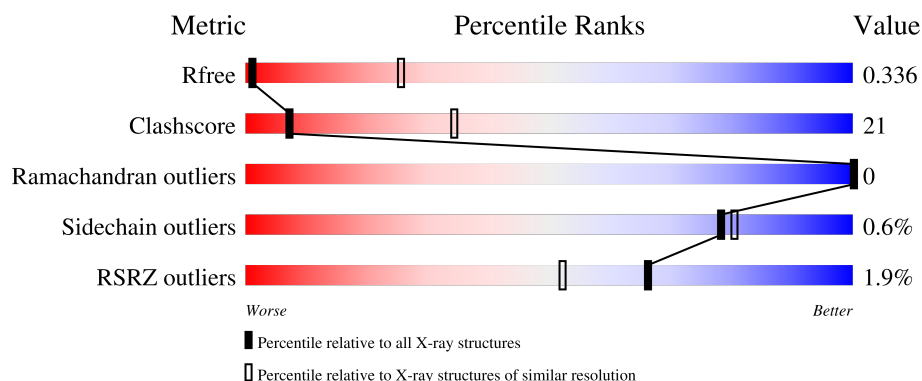
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.50 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                      | 1127 (5.10-3.90)                                      |
| Clashscore            | 190562                      | 1002 (5.06-3.94)                                      |
| Ramachandran outliers | 187476                      | 1060 (5.10-3.90)                                      |
| Sidechain outliers    | 187428                      | 1043 (5.10-3.90)                                      |
| RSRZ outliers         | 180081                      | 1122 (5.10-3.90)                                      |

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

| Mol | Chain | Length | Quality of chain                                                     |
|-----|-------|--------|----------------------------------------------------------------------|
| 1   | C     | 205    | <div> <div></div> <div>67%</div> <div>26%</div> <div>6%</div> </div> |
| 1   | G     | 205    | <div> <div></div> <div>58%</div> <div>36%</div> <div>6%</div> </div> |
| 2   | D     | 50     | <div> <div>16%</div> <div>76%</div> <div>8%</div> </div>             |
| 2   | H     | 50     | <div> <div>30%</div> <div>62%</div> <div>8%</div> </div>             |
| 3   | E     | 50     | <div> <div>18%</div> <div>70%</div> <div>10%</div> </div>            |

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| Mol | Chain | Length | Quality of chain                             |
|-----|-------|--------|----------------------------------------------|
| 3   | I     | 50     | <div><div></div><div>24%64%10%</div></div>   |
| 4   | A     | 1128   | <div><div></div><div>2%58%31%10%</div></div> |
| 4   | B     | 1128   | <div><div></div><div>2%57%32%11%</div></div> |
| 5   | F     | 377    | <div><div></div><div>%51%25%24%</div></div>  |
| 5   | J     | 377    | <div><div></div><div>%48%28%24%</div></div>  |

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 27643 atoms, of which 42 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Transcription factor A, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | C     | 192      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1615  | 1019 | 291 | 300 | 5 |         |         |       |
| 1   | G     | 192      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1615  | 1019 | 291 | 300 | 5 |         |         |       |

There are 6 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| C     | 41      | ASN      | -      | expression tag | UNP Q00059 |
| C     | 42      | ALA      | -      | expression tag | UNP Q00059 |
| C     | 49      | SER      | CYS    | conflict       | UNP Q00059 |
| G     | 41      | ASN      | -      | expression tag | UNP Q00059 |
| G     | 42      | ALA      | -      | expression tag | UNP Q00059 |
| G     | 49      | SER      | CYS    | conflict       | UNP Q00059 |

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

| Mol | Chain | Residues | Atoms |     |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 2   | D     | 46       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 924   | 440 | 175 | 264 | 45 |         |         |       |
| 2   | H     | 46       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 924   | 440 | 175 | 264 | 45 |         |         |       |

- Molecule 3 is a DNA chain called Template DNA.

| Mol | Chain | Residues | Atoms |     |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 3   | E     | 45       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 938   | 444 | 171 | 279 | 44 |         |         |       |
| 3   | I     | 45       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 938   | 444 | 171 | 279 | 44 |         |         |       |

- Molecule 4 is a protein called DNA-directed RNA polymerase, mitochondrial.

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 4   | A     | 1011     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 8028  | 5107 | 1452 | 1418 | 51 |         |         |       |
| 4   | B     | 1002     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 7967  | 5069 | 1443 | 1404 | 51 |         |         |       |

There are 6 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 103     | ASN      | -      | expression tag | UNP O00411 |
| A     | 104     | ALA      | -      | expression tag | UNP O00411 |
| A     | 555     | ALA      | GLU    | conflict       | UNP O00411 |
| B     | 103     | ASN      | -      | expression tag | UNP O00411 |
| B     | 104     | ALA      | -      | expression tag | UNP O00411 |
| B     | 555     | ALA      | GLU    | conflict       | UNP O00411 |

- Molecule 5 is a protein called Dimethyladenosine transferase 2, mitochondrial.

| Mol | Chain | Residues | Atoms |      |    |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|----|-----|-----|---------|---------|-------|
| 5   | F     | 288      | Total | C    | H  | N   | O   | S       | 0       | 0     |
|     |       |          | 2347  | 1506 | 21 | 397 | 408 | 15      |         |       |
| 5   | J     | 288      | Total | C    | H  | N   | O   | S       | 0       | 0     |
|     |       |          | 2347  | 1506 | 21 | 397 | 408 | 15      |         |       |

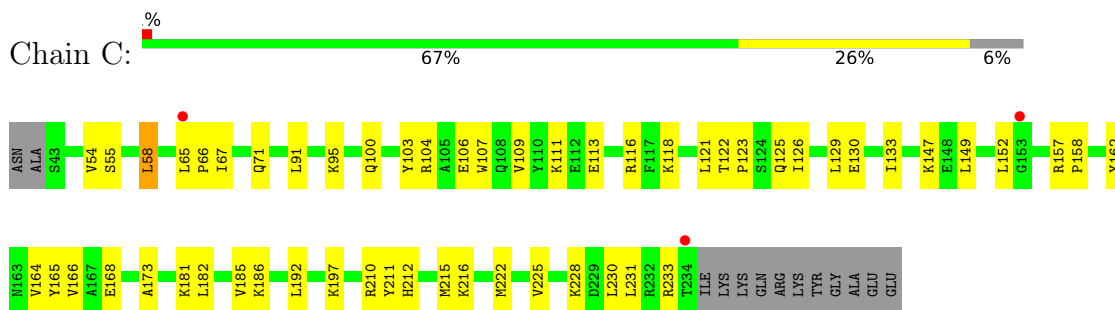
There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| F     | 20      | ASN      | -      | expression tag | UNP Q9H5Q4 |
| F     | 21      | ALA      | -      | expression tag | UNP Q9H5Q4 |
| J     | 20      | ASN      | -      | expression tag | UNP Q9H5Q4 |
| J     | 21      | ALA      | -      | expression tag | UNP Q9H5Q4 |

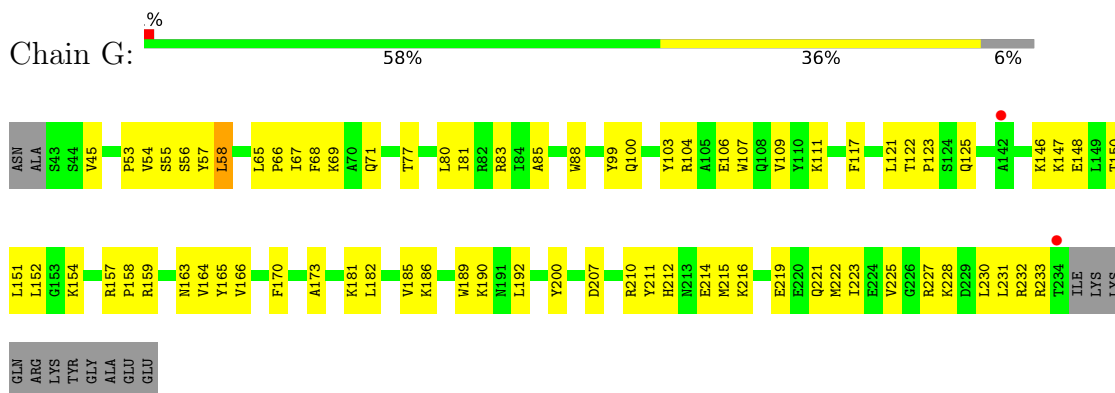
### 3 Residue-property plots

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

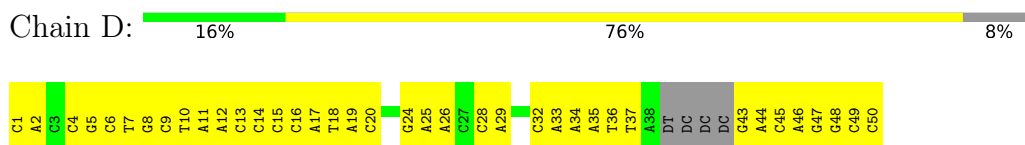
- Molecule 1: Transcription factor A, mitochondrial



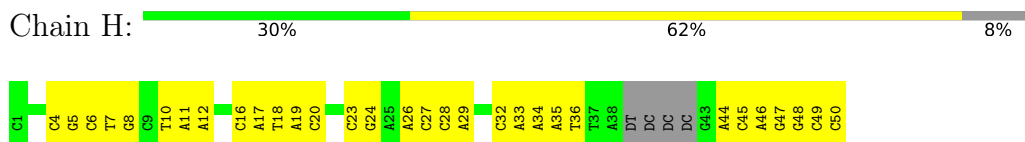
- Molecule 1: Transcription factor A, mitochondrial



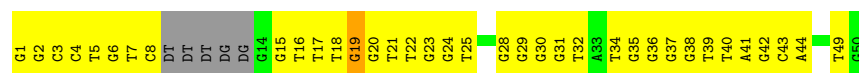
- Molecule 2: Non-Template DNA



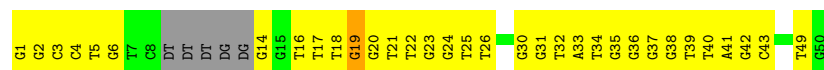
- Molecule 2: Non-Template DNA



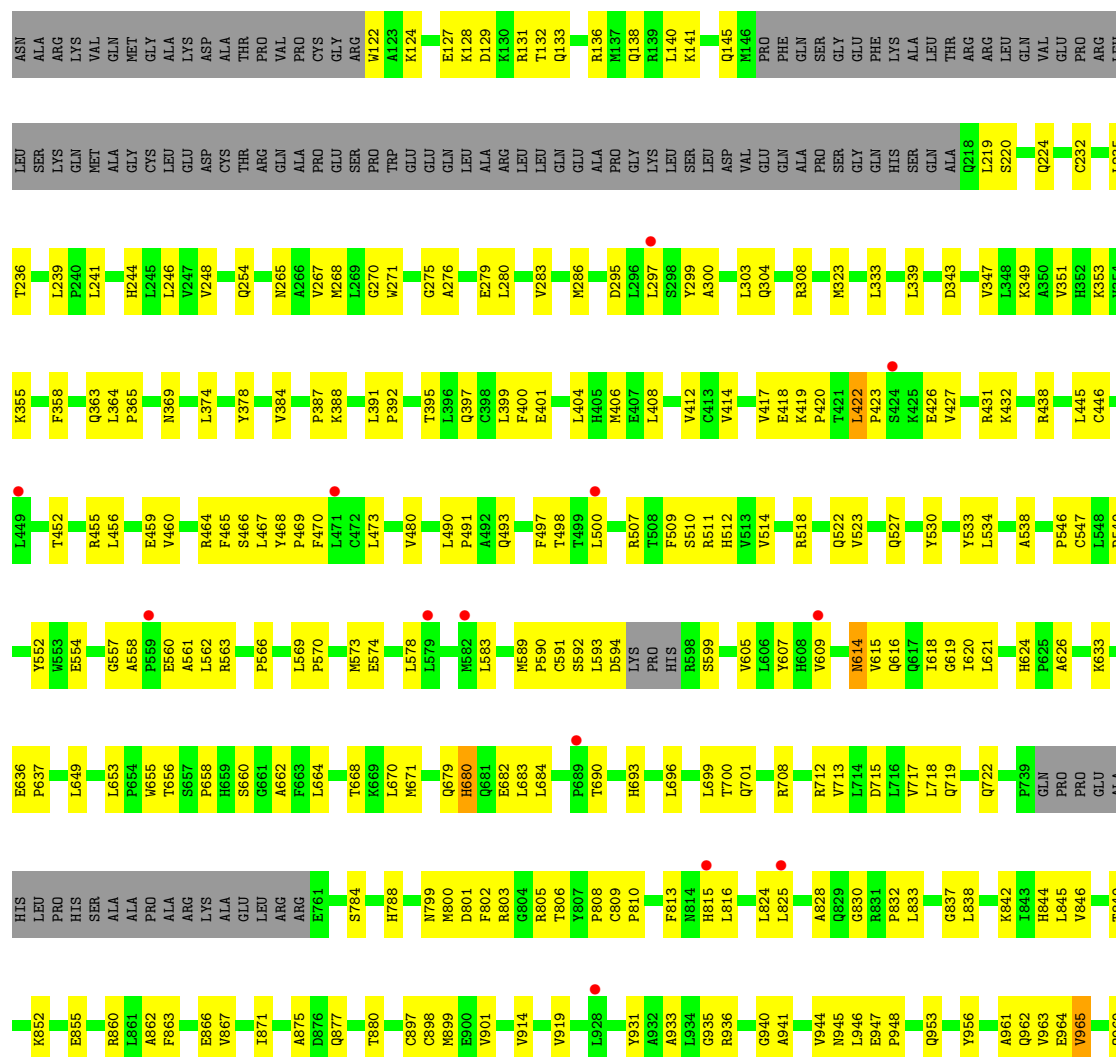
- Molecule 3: Template DNA

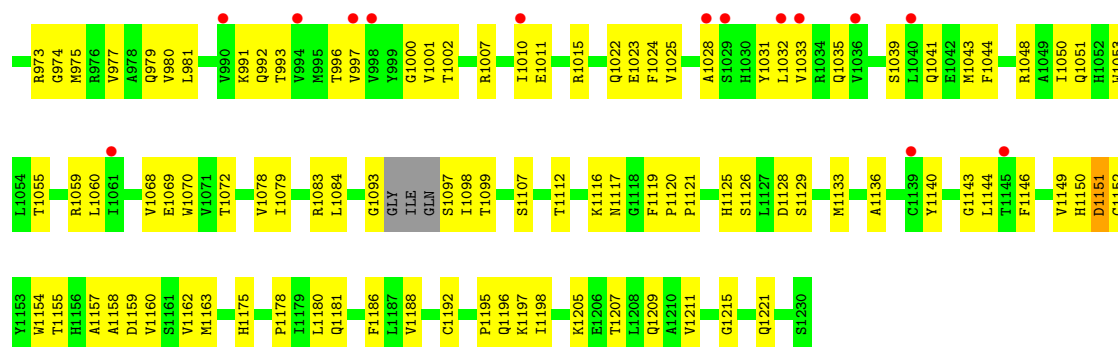


- Molecule 3: Template DNA

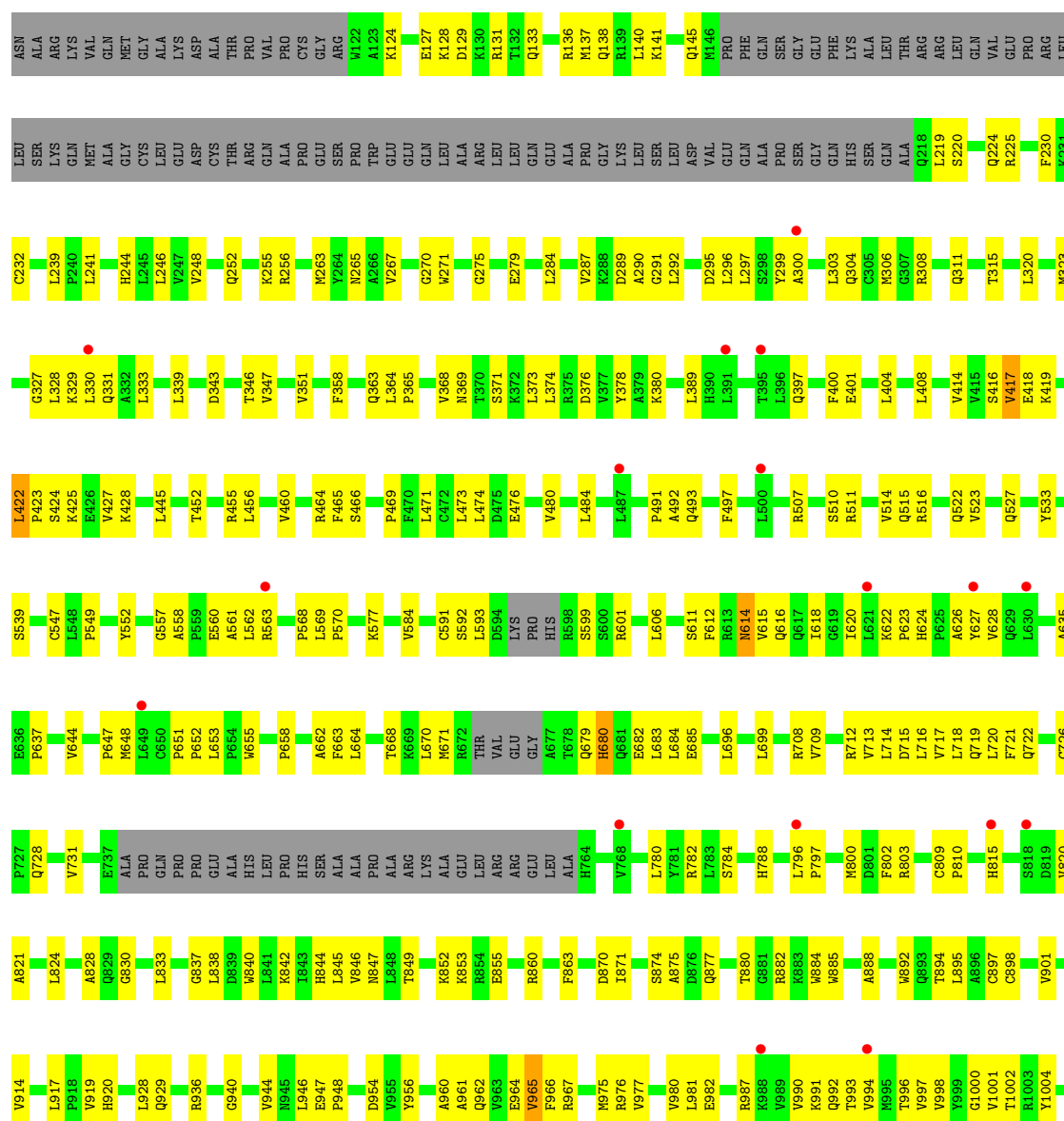


- Molecule 4: DNA-directed RNA polymerase, mitochondrial

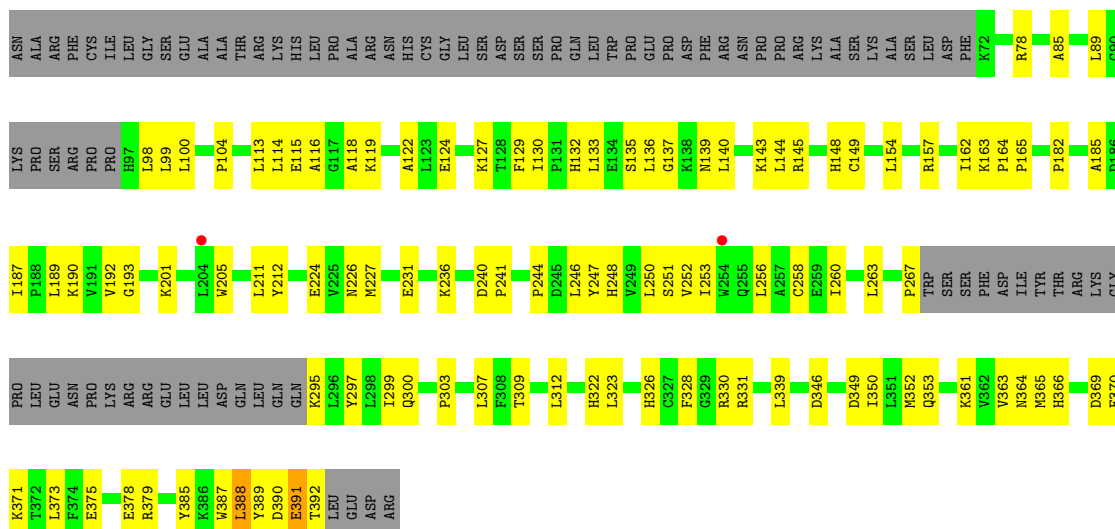




• Molecule 4: DNA-directed RNA polymerase, mitochondrial







## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 1 21 1                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 103.62Å 197.73Å 134.34Å<br>90.00° 99.39° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 49.58 – 4.50<br>49.58 – 4.50                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.1 (49.58-4.50)<br>99.2 (49.58-4.50)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.43 (at 4.45Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX (1.11.1_2575: ???)                                   | Depositor        |
| R, $R_{free}$                                                           | 0.291 , 0.333<br>0.293 , 0.336                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 1573 reflections (5.00%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 248.7                                                       | Xtriage          |
| Anisotropy                                                              | 0.204                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.28 , 278.0                                                | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.90                                                        | EDS              |
| Total number of atoms                                                   | 27643                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 333.0                                                       | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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   | C     | 0.08         | 0/1646  | 0.25        | 0/2202         |
| 1   | G     | 0.08         | 0/1646  | 0.25        | 0/2202         |
| 2   | D     | 0.20         | 0/1035  | 0.37        | 0/1587         |
| 2   | H     | 0.21         | 0/1035  | 0.38        | 0/1587         |
| 3   | E     | 0.21         | 0/1051  | 0.53        | 2/1625 (0.1%)  |
| 3   | I     | 0.23         | 0/1051  | 0.53        | 2/1625 (0.1%)  |
| 4   | A     | 0.09         | 0/8213  | 0.26        | 0/11132        |
| 4   | B     | 0.09         | 0/8150  | 0.26        | 0/11043        |
| 5   | F     | 0.08         | 0/2380  | 0.26        | 0/3213         |
| 5   | J     | 0.08         | 0/2380  | 0.25        | 0/3213         |
| All | All   | 0.11         | 0/28587 | 0.30        | 4/39429 (0.0%) |

There are no bond length outliers.

All (4) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 3   | E     | 19  | DG   | OP2-P-O3' | -9.15 | 80.54       | 108.00   |
| 3   | I     | 19  | DG   | OP2-P-O3' | -9.06 | 80.81       | 108.00   |
| 3   | I     | 19  | DG   | OP1-P-O3' | -7.25 | 86.26       | 108.00   |
| 3   | E     | 19  | DG   | OP1-P-O3' | -7.17 | 86.49       | 108.00   |

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | C     | 1615  | 0        | 1655     | 48      | 0            |
| 1   | G     | 1615  | 0        | 1655     | 84      | 1            |
| 2   | D     | 924   | 0        | 514      | 54      | 1            |
| 2   | H     | 924   | 0        | 514      | 50      | 0            |
| 3   | E     | 938   | 0        | 512      | 66      | 0            |
| 3   | I     | 938   | 0        | 512      | 65      | 1            |
| 4   | A     | 8028  | 0        | 8092     | 322     | 1            |
| 4   | B     | 7967  | 0        | 8032     | 330     | 0            |
| 5   | F     | 2326  | 21       | 2375     | 85      | 0            |
| 5   | J     | 2326  | 21       | 2375     | 95      | 0            |
| All | All   | 27601 | 42       | 26236    | 1113    | 2            |

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 21.

All (1113) 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:363:GLN:HB3  | 4:A:364:LEU:HG   | 1.30                     | 1.13              |
| 4:B:422:LEU:HD12 | 4:B:427:VAL:HG23 | 1.19                     | 1.12              |
| 4:A:422:LEU:HD12 | 4:A:427:VAL:HG23 | 1.29                     | 1.11              |
| 3:E:16:DT:H4'    | 4:A:618:ILE:HG22 | 1.31                     | 1.11              |
| 4:B:363:GLN:HB3  | 4:B:364:LEU:HG   | 1.26                     | 1.09              |
| 4:B:422:LEU:HD22 | 4:B:423:PRO:HD2  | 1.39                     | 1.05              |
| 3:E:15:DG:H2'    | 3:E:16:DT:H72    | 1.38                     | 1.04              |
| 4:A:422:LEU:HD13 | 4:A:423:PRO:HD2  | 1.39                     | 1.03              |
| 5:J:114:LEU:HB3  | 5:J:140:LEU:HD11 | 1.43                     | 1.01              |
| 4:A:944:VAL:HG23 | 4:A:946:LEU:HD13 | 1.42                     | 1.00              |
| 5:F:114:LEU:HB3  | 5:F:140:LEU:HD11 | 1.45                     | 0.96              |
| 3:I:16:DT:H4'    | 4:B:618:ILE:HG22 | 1.46                     | 0.95              |
| 4:A:655:TRP:HB3  | 4:A:696:LEU:HD22 | 1.46                     | 0.95              |
| 4:B:419:LYS:HE2  | 4:B:422:LEU:HD23 | 1.49                     | 0.94              |
| 3:E:39:DT:C2'    | 3:E:40:DT:H72    | 1.97                     | 0.93              |
| 1:G:214:GLU:OE2  | 4:B:133:GLN:NE2  | 2.03                     | 0.92              |
| 4:B:655:TRP:HB3  | 4:B:696:LEU:HD22 | 1.51                     | 0.91              |
| 4:B:299:TYR:HB3  | 4:B:323:MET:HE2  | 1.53                     | 0.90              |
| 4:B:592:SER:HB2  | 4:B:599:SER:HB2  | 1.51                     | 0.90              |
| 5:J:114:LEU:HD11 | 5:J:144:LEU:HD22 | 1.55                     | 0.89              |
| 1:C:121:LEU:HD12 | 1:C:125:GLN:HG2  | 1.54                     | 0.89              |
| 3:E:39:DT:H2''   | 3:E:40:DT:H72    | 1.54                     | 0.88              |
| 3:I:41:DA:H2'    | 3:I:42:DG:C8     | 2.08                     | 0.88              |
| 4:B:592:SER:CB   | 4:B:599:SER:HB2  | 2.04                     | 0.87              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:A:718:LEU:O    | 4:A:722:GLN:HG3   | 1.74                     | 0.87              |
| 4:B:944:VAL:HG23 | 4:B:946:LEU:HD13  | 1.55                     | 0.87              |
| 4:B:256:ARG:HD3  | 4:B:290:ALA:HB2   | 1.57                     | 0.86              |
| 4:B:796:LEU:HD22 | 4:B:810:PRO:HG2   | 1.56                     | 0.86              |
| 1:G:154:LYS:HE3  | 1:G:215:MET:HE1   | 1.57                     | 0.85              |
| 4:B:611:SER:OG   | 5:J:391:GLU:OE1   | 1.95                     | 0.83              |
| 4:B:516:ARG:HH22 | 4:B:562:LEU:HD22  | 1.44                     | 0.83              |
| 1:C:231:LEU:O    | 1:C:233:ARG:NH1   | 2.11                     | 0.82              |
| 5:F:89:LEU:HD11  | 5:F:116:ALA:HB1   | 1.59                     | 0.82              |
| 2:D:43:DG:H4'    | 2:D:44:DA:OP1     | 1.80                     | 0.82              |
| 4:A:246:LEU:HD22 | 4:A:267:VAL:HG21  | 1.62                     | 0.82              |
| 4:A:936:ARG:HB2  | 4:A:1215:GLY:H    | 1.46                     | 0.81              |
| 2:D:34:DA:H2''   | 2:D:35:DA:C8      | 2.15                     | 0.81              |
| 3:I:14:DG:H22    | 4:B:1102:HIS:HA   | 1.45                     | 0.81              |
| 4:A:422:LEU:HD13 | 4:A:423:PRO:CD    | 2.10                     | 0.80              |
| 2:D:35:DA:N1     | 4:A:616:GLN:HG3   | 1.95                     | 0.80              |
| 5:J:100:LEU:HD13 | 5:J:189:LEU:HD11  | 1.62                     | 0.80              |
| 4:A:299:TYR:HB3  | 4:A:323:MET:HE2   | 1.63                     | 0.80              |
| 3:E:41:DA:H2'    | 3:E:42:DG:C8      | 2.15                     | 0.80              |
| 4:B:422:LEU:CD2  | 4:B:423:PRO:HD2   | 2.11                     | 0.80              |
| 1:C:121:LEU:HB2  | 1:C:125:GLN:CG    | 2.12                     | 0.80              |
| 1:C:149:LEU:O    | 1:C:152:LEU:HG    | 1.82                     | 0.79              |
| 3:E:36:DG:H2'    | 3:E:37:DG:C8      | 2.18                     | 0.79              |
| 4:B:996:THR:O    | 4:B:1000:GLY:N    | 2.15                     | 0.79              |
| 4:A:422:LEU:CD1  | 4:A:423:PRO:HD2   | 2.12                     | 0.79              |
| 5:F:244:PRO:HB3  | 5:F:363:VAL:HG21  | 1.65                     | 0.79              |
| 5:F:244:PRO:HB3  | 5:F:363:VAL:CG2   | 2.12                     | 0.79              |
| 4:B:712:ARG:NH2  | 4:B:875:ALA:O     | 2.16                     | 0.78              |
| 4:A:815:HIS:HD2  | 4:A:1149:VAL:HG22 | 1.48                     | 0.78              |
| 3:I:39:DT:C6     | 3:I:40:DT:H72     | 2.18                     | 0.78              |
| 4:B:422:LEU:HD12 | 4:B:427:VAL:CG2   | 2.08                     | 0.78              |
| 4:A:718:LEU:HB3  | 4:A:722:GLN:HE21  | 1.48                     | 0.78              |
| 4:B:363:GLN:HB3  | 4:B:364:LEU:CG    | 2.11                     | 0.78              |
| 5:J:100:LEU:HD22 | 5:J:189:LEU:HD21  | 1.65                     | 0.78              |
| 4:A:852:LYS:HD2  | 4:A:855:GLU:HG3   | 1.65                     | 0.78              |
| 4:B:1069:GLU:HG2 | 4:B:1079:ILE:HG23 | 1.64                     | 0.77              |
| 4:A:936:ARG:HB2  | 4:A:1215:GLY:N    | 2.00                     | 0.77              |
| 3:I:17:DT:OP2    | 4:B:1100:TYR:HA   | 1.83                     | 0.77              |
| 2:H:36:DT:H6     | 5:J:201:LYS:HZ3   | 1.33                     | 0.77              |
| 5:J:349:ASP:OD1  | 5:J:353:GLN:NE2   | 2.17                     | 0.77              |
| 3:I:21:DT:C6     | 3:I:22:DT:H72     | 2.21                     | 0.76              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:B:363:GLN:CB   | 4:B:364:LEU:HG    | 2.12                     | 0.76              |
| 4:A:417:VAL:HG11 | 4:A:718:LEU:HD22  | 1.68                     | 0.76              |
| 2:H:4:DC:H2'     | 2:H:5:DG:C8       | 2.21                     | 0.75              |
| 4:B:422:LEU:HD13 | 4:B:423:PRO:CD    | 2.18                     | 0.74              |
| 5:F:349:ASP:O    | 5:F:353:GLN:HG2   | 1.88                     | 0.74              |
| 4:A:363:GLN:HB3  | 4:A:364:LEU:CG    | 2.14                     | 0.73              |
| 4:B:300:ALA:HB2  | 4:B:333:LEU:HD11  | 1.71                     | 0.73              |
| 3:I:17:DT:C6     | 3:I:18:DT:H72     | 2.22                     | 0.73              |
| 4:A:809:CYS:HB2  | 4:A:810:PRO:HD3   | 1.69                     | 0.73              |
| 5:F:100:LEU:HD13 | 5:F:189:LEU:HD11  | 1.69                     | 0.73              |
| 3:I:20:DG:C8     | 3:I:21:DT:H72     | 2.23                     | 0.73              |
| 2:D:25:DA:H1'    | 2:D:26:DA:H5'     | 1.70                     | 0.72              |
| 4:A:219:LEU:HD23 | 4:A:219:LEU:H     | 1.54                     | 0.72              |
| 3:E:39:DT:H2''   | 3:E:40:DT:C5      | 2.24                     | 0.72              |
| 5:F:114:LEU:HB3  | 5:F:140:LEU:CD1   | 2.20                     | 0.72              |
| 5:J:137:GLY:HA2  | 5:J:144:LEU:HD23  | 1.71                     | 0.72              |
| 1:G:107:TRP:CZ2  | 2:H:24:DG:H5''    | 2.24                     | 0.72              |
| 4:A:940:GLY:O    | 4:A:944:VAL:HG22  | 1.89                     | 0.72              |
| 4:A:1178:PRO:HB2 | 4:A:1181:GLN:HB2  | 1.71                     | 0.72              |
| 1:C:222:MET:HE2  | 1:C:230:LEU:HD12  | 1.71                     | 0.72              |
| 3:E:39:DT:H2''   | 3:E:40:DT:C7      | 2.19                     | 0.72              |
| 2:H:17:DA:H2''   | 2:H:18:DT:H71     | 1.71                     | 0.72              |
| 4:A:363:GLN:CB   | 4:A:364:LEU:HG    | 2.15                     | 0.72              |
| 4:B:306:MET:HG2  | 4:B:311:GLN:HG3   | 1.70                     | 0.72              |
| 4:B:1001:VAL:O   | 4:B:1002:THR:OG1  | 2.04                     | 0.72              |
| 4:A:369:ASN:ND2  | 4:A:690:THR:O     | 2.23                     | 0.71              |
| 4:A:962:GLN:O    | 4:A:965:VAL:HG22  | 1.90                     | 0.71              |
| 5:J:236:LYS:HG2  | 5:J:246:LEU:HD22  | 1.72                     | 0.71              |
| 2:D:18:DT:H2''   | 2:D:19:DA:C8      | 2.25                     | 0.71              |
| 4:A:283:VAL:HA   | 4:A:286:MET:CE    | 2.20                     | 0.71              |
| 4:B:809:CYS:HB2  | 4:B:810:PRO:HD3   | 1.71                     | 0.71              |
| 4:A:718:LEU:C    | 4:A:722:GLN:HG3   | 2.15                     | 0.71              |
| 4:A:815:HIS:CD2  | 4:A:1149:VAL:HG22 | 2.24                     | 0.71              |
| 4:B:658:PRO:HA   | 4:B:670:LEU:HD22  | 1.70                     | 0.71              |
| 3:E:20:DG:C8     | 3:E:21:DT:H72     | 2.25                     | 0.71              |
| 4:A:838:LEU:HG   | 4:A:842:LYS:HE3   | 1.73                     | 0.71              |
| 4:A:992:GLN:HG3  | 4:A:1010:ILE:HG12 | 1.72                     | 0.71              |
| 4:A:422:LEU:CD1  | 4:A:427:VAL:HG23  | 2.14                     | 0.71              |
| 4:A:1001:VAL:O   | 4:A:1002:THR:OG1  | 2.03                     | 0.71              |
| 4:B:962:GLN:O    | 4:B:965:VAL:HG22  | 1.91                     | 0.70              |
| 1:G:58:LEU:HD22  | 3:I:30:DG:N3      | 2.05                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:A:283:VAL:HA   | 4:A:286:MET:HE2  | 1.73                     | 0.70              |
| 4:A:803:ARG:HD3  | 4:A:1125:HIS:ND1 | 2.06                     | 0.70              |
| 1:C:165:TYR:CE1  | 1:C:192:LEU:HD11 | 2.26                     | 0.70              |
| 2:D:36:DT:H2''   | 2:D:37:DT:H5''   | 1.71                     | 0.70              |
| 4:B:219:LEU:HD23 | 4:B:219:LEU:H    | 1.56                     | 0.70              |
| 3:I:36:DG:H2'    | 3:I:37:DG:C8     | 2.26                     | 0.70              |
| 4:B:1004:TYR:HB2 | 4:B:1007:ARG:HB2 | 1.73                     | 0.70              |
| 4:A:239:LEU:HD11 | 4:A:270:GLY:HA3  | 1.73                     | 0.70              |
| 5:J:349:ASP:O    | 5:J:353:GLN:HG2  | 1.92                     | 0.69              |
| 4:A:363:GLN:HA   | 4:A:365:PRO:HD3  | 1.73                     | 0.69              |
| 4:B:424:SER:O    | 4:B:428:LYS:HG3  | 1.92                     | 0.69              |
| 4:B:653:LEU:HG   | 4:B:664:LEU:HD23 | 1.72                     | 0.69              |
| 5:F:114:LEU:HD11 | 5:F:144:LEU:HD22 | 1.75                     | 0.69              |
| 3:E:5:DT:H2''    | 3:E:6:DG:C8      | 2.28                     | 0.69              |
| 1:G:45:VAL:HG21  | 1:G:125:GLN:HB3  | 1.75                     | 0.69              |
| 2:D:37:DT:H72    | 5:F:202:ARG:HH11 | 1.57                     | 0.69              |
| 3:E:18:DT:OP2    | 4:A:1099:THR:N   | 2.26                     | 0.69              |
| 4:B:718:LEU:O    | 4:B:722:GLN:HG3  | 1.93                     | 0.69              |
| 4:B:419:LYS:CE   | 4:B:422:LEU:HD23 | 2.22                     | 0.69              |
| 4:A:232:CYS:SG   | 4:A:473:LEU:HD11 | 2.34                     | 0.68              |
| 4:B:849:THR:HA   | 4:B:888:ALA:HB1  | 1.76                     | 0.68              |
| 4:B:416:SER:HB3  | 4:B:637:PRO:HA   | 1.74                     | 0.68              |
| 4:B:1080:GLN:NE2 | 4:B:1115:GLN:OE1 | 2.27                     | 0.68              |
| 3:E:19:DG:H1'    | 3:E:20:DG:OP1    | 1.93                     | 0.68              |
| 1:G:107:TRP:CH2  | 2:H:24:DG:H5''   | 2.28                     | 0.68              |
| 1:G:165:TYR:CE1  | 1:G:192:LEU:HD11 | 2.29                     | 0.68              |
| 3:I:16:DT:C2     | 4:B:616:GLN:HB3  | 2.28                     | 0.68              |
| 3:I:19:DG:H1'    | 3:I:20:DG:OP1    | 1.93                     | 0.68              |
| 4:B:417:VAL:HG22 | 4:B:784:SER:HA   | 1.75                     | 0.68              |
| 4:A:1011:GLU:O   | 4:A:1015:ARG:HG3 | 1.94                     | 0.68              |
| 4:A:1070:TRP:HA  | 4:A:1186:PHE:CE1 | 2.28                     | 0.68              |
| 3:E:4:DC:C2'     | 3:E:5:DT:H71     | 2.24                     | 0.67              |
| 3:E:35:DG:H2''   | 3:E:36:DG:C8     | 2.28                     | 0.67              |
| 4:B:422:LEU:HD13 | 4:B:423:PRO:HG2  | 1.76                     | 0.67              |
| 1:C:113:GLU:HG2  | 1:C:116:ARG:HH21 | 1.59                     | 0.67              |
| 4:A:1043:MET:HG3 | 4:A:1044:PHE:CD2 | 2.30                     | 0.67              |
| 4:A:467:LEU:HD12 | 4:A:578:LEU:CD1  | 2.23                     | 0.67              |
| 5:F:200:GLU:OE2  | 5:F:230:GLY:N    | 2.23                     | 0.67              |
| 4:A:418:GLU:CD   | 4:A:722:GLN:HG2  | 2.19                     | 0.67              |
| 5:F:100:LEU:HD22 | 5:F:189:LEU:HD21 | 1.75                     | 0.67              |
| 3:I:5:DT:H2''    | 3:I:6:DG:C8      | 2.30                     | 0.67              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:F:240:ASP:HB2  | 5:F:241:PRO:HD2   | 1.76                     | 0.67              |
| 4:A:509:PHE:CE1  | 4:A:566:PRO:HA    | 2.29                     | 0.67              |
| 4:A:300:ALA:HB2  | 4:A:333:LEU:HD11  | 1.77                     | 0.67              |
| 1:G:221:GLN:NE2  | 4:B:140:LEU:HD13  | 2.09                     | 0.67              |
| 4:B:256:ARG:NH2  | 4:B:289:ASP:OD2   | 2.27                     | 0.67              |
| 4:A:1120:PRO:HB2 | 4:A:1121:PRO:HD3  | 1.76                     | 0.67              |
| 2:H:35:DA:N1     | 4:B:616:GLN:HG3   | 2.10                     | 0.66              |
| 4:B:1070:TRP:HA  | 4:B:1186:PHE:CE1  | 2.30                     | 0.66              |
| 4:B:1083:ARG:NH1 | 4:B:1108:ARG:O    | 2.28                     | 0.66              |
| 1:G:146:LYS:HE2  | 3:I:39:DT:OP2     | 1.95                     | 0.66              |
| 4:B:1120:PRO:HB2 | 4:B:1121:PRO:HD3  | 1.77                     | 0.66              |
| 4:A:236:THR:HG23 | 4:A:473:LEU:HD23  | 1.78                     | 0.66              |
| 4:B:592:SER:OG   | 4:B:599:SER:HB2   | 1.95                     | 0.66              |
| 4:B:225:ARG:HD2  | 4:B:465:PHE:CE1   | 2.31                     | 0.66              |
| 4:B:239:LEU:HD11 | 4:B:270:GLY:HA3   | 1.77                     | 0.66              |
| 4:B:993:THR:HA   | 4:B:1010:ILE:CD1  | 2.26                     | 0.66              |
| 4:B:726:CYS:H    | 4:B:731:VAL:HB    | 1.61                     | 0.65              |
| 4:B:940:GLY:O    | 4:B:944:VAL:HG22  | 1.97                     | 0.65              |
| 5:J:114:LEU:HB3  | 5:J:140:LEU:CD1   | 2.21                     | 0.65              |
| 3:E:4:DC:H2"     | 3:E:5:DT:H71      | 1.78                     | 0.65              |
| 4:A:1125:HIS:HA  | 4:A:1128:ASP:OD2  | 1.96                     | 0.65              |
| 4:B:993:THR:HA   | 4:B:1010:ILE:HD11 | 1.79                     | 0.65              |
| 4:B:1015:ARG:CZ  | 4:B:1025:VAL:HG11 | 2.26                     | 0.65              |
| 3:I:21:DT:N1     | 3:I:22:DT:H72     | 2.12                     | 0.65              |
| 4:B:417:VAL:CG2  | 4:B:784:SER:HA    | 2.27                     | 0.65              |
| 5:F:349:ASP:HA   | 5:F:352:MET:CE    | 2.27                     | 0.65              |
| 4:B:940:GLY:HA2  | 4:B:1044:PHE:HE1  | 1.63                     | 0.64              |
| 4:A:138:GLN:HA   | 4:A:141:LYS:HE2   | 1.80                     | 0.64              |
| 5:F:137:GLY:HA2  | 5:F:144:LEU:HD23  | 1.77                     | 0.64              |
| 4:A:418:GLU:CG   | 4:A:722:GLN:HG2   | 2.26                     | 0.64              |
| 4:B:956:TYR:CD1  | 4:B:991:LYS:HA    | 2.32                     | 0.64              |
| 5:J:240:ASP:HB2  | 5:J:241:PRO:HD2   | 1.77                     | 0.64              |
| 4:B:977:VAL:HA   | 4:B:980:VAL:HG22  | 1.79                     | 0.64              |
| 4:B:954:ASP:OD1  | 4:B:987:ARG:NE    | 2.24                     | 0.64              |
| 2:D:35:DA:C2     | 4:A:616:GLN:HG3   | 2.32                     | 0.64              |
| 4:B:699:LEU:HD11 | 4:B:800:MET:HG3   | 1.80                     | 0.64              |
| 4:B:833:LEU:HB3  | 4:B:837:GLY:HA3   | 1.80                     | 0.64              |
| 4:A:1039:SER:O   | 4:A:1043:MET:HG2  | 1.98                     | 0.64              |
| 4:A:832:PRO:O    | 4:A:1158:ALA:HB2  | 1.98                     | 0.63              |
| 4:B:618:ILE:HG13 | 4:B:620:ILE:HD11  | 1.79                     | 0.63              |
| 4:B:129:ASP:O    | 4:B:133:GLN:HG3   | 1.97                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:7:DT:H2'      | 2:D:8:DG:C8       | 2.33                     | 0.63              |
| 4:B:1043:MET:HG3  | 4:B:1044:PHE:CD2  | 2.33                     | 0.63              |
| 5:J:248:HIS:HA    | 5:J:328:PHE:CE1   | 2.33                     | 0.63              |
| 4:B:1147:VAL:CG2  | 4:B:1154:TRP:HB2  | 2.29                     | 0.63              |
| 3:E:18:DT:OP1     | 4:A:1098:ILE:HA   | 1.98                     | 0.63              |
| 4:A:1072:THR:HG22 | 4:A:1126:SER:HB2  | 1.81                     | 0.63              |
| 5:F:137:GLY:CA    | 5:F:144:LEU:HD23  | 2.28                     | 0.63              |
| 5:F:164:PRO:HG2   | 5:F:165:PRO:HD3   | 1.81                     | 0.63              |
| 3:E:16:DT:C2      | 4:A:616:GLN:HB3   | 2.34                     | 0.62              |
| 3:I:31:DG:N7      | 3:I:32:DT:H73     | 2.14                     | 0.62              |
| 4:A:522:GLN:OE1   | 4:A:561:ALA:HB1   | 1.99                     | 0.62              |
| 4:A:1069:GLU:HG2  | 4:A:1079:ILE:HG23 | 1.78                     | 0.62              |
| 5:F:236:LYS:O     | 5:F:251:SER:OG    | 2.17                     | 0.62              |
| 4:A:241:LEU:HD11  | 4:A:460:VAL:HG11  | 1.81                     | 0.62              |
| 4:B:422:LEU:HD13  | 4:B:423:PRO:CG    | 2.29                     | 0.62              |
| 5:J:322:HIS:HB3   | 5:J:389:TYR:CZ    | 2.35                     | 0.62              |
| 1:C:212:HIS:NE2   | 1:C:216:LYS:HE3   | 2.14                     | 0.62              |
| 4:A:607:TYR:CE1   | 5:F:388:LEU:HD13  | 2.34                     | 0.62              |
| 4:A:1083:ARG:HD3  | 4:A:1107:SER:CB   | 2.30                     | 0.62              |
| 1:G:58:LEU:HG     | 3:I:31:DG:N3      | 2.14                     | 0.62              |
| 4:A:414:VAL:HG13  | 4:A:788:HIS:HB2   | 1.81                     | 0.62              |
| 4:B:232:CYS:SG    | 4:B:469:PRO:HB2   | 2.40                     | 0.62              |
| 5:J:137:GLY:CA    | 5:J:144:LEU:HD23  | 2.30                     | 0.62              |
| 2:D:45:DC:H2''    | 2:D:46:DA:C8      | 2.34                     | 0.62              |
| 4:B:680:HIS:NE2   | 4:B:802:PHE:HB2   | 2.15                     | 0.62              |
| 4:B:838:LEU:HG    | 4:B:842:LYS:HE3   | 1.80                     | 0.62              |
| 5:J:164:PRO:HG2   | 5:J:165:PRO:HD3   | 1.82                     | 0.62              |
| 5:F:240:ASP:HB2   | 5:F:241:PRO:CD    | 2.30                     | 0.62              |
| 1:C:233:ARG:HG2   | 3:E:49:DT:P       | 2.40                     | 0.61              |
| 1:G:150:THR:HG21  | 3:I:38:DG:OP2     | 1.99                     | 0.61              |
| 4:A:418:GLU:HG3   | 4:A:722:GLN:HA    | 1.82                     | 0.61              |
| 3:E:34:DT:H2''    | 3:E:35:DG:C8      | 2.35                     | 0.61              |
| 4:A:871:ILE:HG23  | 4:A:898:CYS:SG    | 2.40                     | 0.61              |
| 4:A:713:VAL:HG12  | 4:A:824:LEU:HD23  | 1.82                     | 0.61              |
| 1:G:54:VAL:HG12   | 1:G:58:LEU:HB3    | 1.82                     | 0.61              |
| 3:I:32:DT:H2''    | 3:I:33:DA:C8      | 2.35                     | 0.61              |
| 5:J:240:ASP:HB2   | 5:J:241:PRO:CD    | 2.30                     | 0.61              |
| 1:G:67:ILE:O      | 1:G:71:GLN:HG2    | 1.99                     | 0.61              |
| 4:B:1059:ARG:HG2  | 4:B:1116:LYS:HD3  | 1.83                     | 0.61              |
| 3:I:39:DT:H2'     | 3:I:40:DT:H72     | 1.83                     | 0.61              |
| 2:H:4:DC:H2''     | 2:H:5:DG:O5'      | 2.01                     | 0.61              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:G:159:ARG:HD3  | 2:H:8:DG:H5''     | 1.83                     | 0.61              |
| 5:F:344:PRO:HG3  | 5:F:385:TYR:CD2   | 2.35                     | 0.61              |
| 4:A:124:LYS:O    | 4:A:128:LYS:HG3   | 2.01                     | 0.61              |
| 4:B:683:LEU:CD1  | 4:B:1079:ILE:HG12 | 2.31                     | 0.61              |
| 4:B:124:LYS:O    | 4:B:128:LYS:HG3   | 2.01                     | 0.60              |
| 4:B:1039:SER:O   | 4:B:1043:MET:HG2  | 2.00                     | 0.60              |
| 2:D:36:DT:O4'    | 4:A:615:VAL:HG13  | 2.00                     | 0.60              |
| 4:A:236:THR:CG2  | 4:A:473:LEU:HD23  | 2.31                     | 0.60              |
| 4:A:616:GLN:N    | 4:A:616:GLN:OE1   | 2.34                     | 0.60              |
| 3:E:1:DG:H2''    | 3:E:2:DG:C8       | 2.35                     | 0.60              |
| 4:A:456:LEU:O    | 4:A:460:VAL:HG23  | 2.00                     | 0.60              |
| 4:B:246:LEU:HD22 | 4:B:267:VAL:HG21  | 1.82                     | 0.60              |
| 4:B:1055:THR:O   | 4:B:1059:ARG:HG3  | 2.00                     | 0.60              |
| 2:D:47:DG:H2''   | 2:D:48:DG:C8      | 2.36                     | 0.60              |
| 3:E:38:DG:C2'    | 3:E:39:DT:H71     | 2.32                     | 0.60              |
| 4:B:422:LEU:HD13 | 4:B:423:PRO:HD2   | 1.82                     | 0.60              |
| 3:E:16:DT:C4'    | 4:A:618:ILE:HG22  | 2.20                     | 0.60              |
| 1:G:117:PHE:CZ   | 1:G:121:LEU:HD21  | 2.36                     | 0.60              |
| 2:H:4:DC:H4'     | 2:H:5:DG:OP1      | 2.01                     | 0.60              |
| 4:A:852:LYS:CD   | 4:A:855:GLU:HG3   | 2.31                     | 0.60              |
| 4:B:622:LYS:HD3  | 5:J:388:LEU:CD2   | 2.32                     | 0.60              |
| 2:H:34:DA:H2''   | 2:H:35:DA:C8      | 2.36                     | 0.60              |
| 4:B:622:LYS:HD3  | 5:J:388:LEU:HD22  | 1.84                     | 0.60              |
| 1:G:54:VAL:CG1   | 1:G:58:LEU:HB3    | 2.32                     | 0.60              |
| 4:A:355:LYS:HB3  | 4:A:358:PHE:HB2   | 1.83                     | 0.60              |
| 4:B:1178:PRO:HB2 | 4:B:1181:GLN:HB2  | 1.83                     | 0.60              |
| 3:E:39:DT:H2'    | 3:E:40:DT:H72     | 1.79                     | 0.60              |
| 4:A:941:ALA:HA   | 4:A:946:LEU:HB2   | 1.83                     | 0.60              |
| 2:D:4:DC:H2'     | 2:D:5:DG:C8       | 2.37                     | 0.59              |
| 4:A:846:VAL:HG21 | 4:A:860:ARG:O     | 2.02                     | 0.59              |
| 2:D:4:DC:H2''    | 2:D:5:DG:O5'      | 2.02                     | 0.59              |
| 3:E:7:DT:H2''    | 3:E:8:DC:C5       | 2.37                     | 0.59              |
| 3:E:17:DT:C2'    | 3:E:18:DT:H71     | 2.33                     | 0.59              |
| 4:A:417:VAL:HG11 | 4:A:718:LEU:CD2   | 2.31                     | 0.59              |
| 4:B:474:LEU:HD12 | 4:B:515:GLN:OE1   | 2.03                     | 0.59              |
| 4:B:780:LEU:O    | 4:B:784:SER:OG    | 2.16                     | 0.59              |
| 5:J:236:LYS:HA   | 5:J:246:LEU:HB3   | 1.85                     | 0.59              |
| 4:A:1055:THR:O   | 4:A:1059:ARG:HG3  | 2.03                     | 0.59              |
| 4:A:1150:HIS:NE2 | 4:A:1152:CYS:SG   | 2.73                     | 0.59              |
| 1:C:122:THR:HB   | 1:C:123:PRO:CD    | 2.33                     | 0.59              |
| 4:B:993:THR:CG2  | 4:B:1036:VAL:HG21 | 2.33                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:F:152:PHE:CZ    | 5:F:196:PRO:HD3   | 2.38                     | 0.59              |
| 2:D:37:DT:H72     | 5:F:202:ARG:HD3   | 1.85                     | 0.59              |
| 5:F:349:ASP:HA    | 5:F:352:MET:HE3   | 1.84                     | 0.59              |
| 1:C:121:LEU:CD1   | 1:C:125:GLN:HG2   | 2.30                     | 0.58              |
| 2:D:47:DG:OP1     | 4:A:1112:THR:HG21 | 2.02                     | 0.58              |
| 1:C:168:GLU:OE2   | 4:A:122:TRP:NE1   | 2.37                     | 0.58              |
| 4:B:844:HIS:CG    | 4:B:919:VAL:HG13  | 2.38                     | 0.58              |
| 5:J:322:HIS:HB3   | 5:J:389:TYR:CE2   | 2.37                     | 0.58              |
| 1:C:54:VAL:CG1    | 1:C:58:LEU:HB3    | 2.33                     | 0.58              |
| 1:G:57:TYR:OH     | 2:H:20:DC:H1'     | 2.03                     | 0.58              |
| 4:B:960:ALA:CB    | 4:B:990:VAL:HG21  | 2.33                     | 0.58              |
| 4:A:241:LEU:HD11  | 4:A:460:VAL:CG1   | 2.34                     | 0.58              |
| 4:A:940:GLY:HA2   | 4:A:1044:PHE:CE1  | 2.39                     | 0.58              |
| 4:A:996:THR:O     | 4:A:1000:GLY:N    | 2.33                     | 0.58              |
| 1:G:147:LYS:O     | 1:G:151:LEU:HD13  | 2.04                     | 0.58              |
| 4:B:653:LEU:HG    | 4:B:664:LEU:CD2   | 2.33                     | 0.58              |
| 4:B:992:GLN:HG3   | 4:B:1010:ILE:HG12 | 1.86                     | 0.58              |
| 1:C:121:LEU:HB2   | 1:C:125:GLN:HG2   | 1.85                     | 0.58              |
| 2:D:11:DA:H2''    | 2:D:12:DA:O4'     | 2.03                     | 0.58              |
| 4:A:852:LYS:HB3   | 4:A:855:GLU:HB2   | 1.85                     | 0.58              |
| 4:A:1155:THR:HB   | 4:A:1163:MET:SD   | 2.43                     | 0.58              |
| 4:B:680:HIS:O     | 4:B:684:LEU:HG    | 2.02                     | 0.58              |
| 4:B:936:ARG:HB2   | 4:B:1215:GLY:H    | 1.69                     | 0.58              |
| 5:F:267:PRO:HA    | 5:F:295:LYS:HA    | 1.84                     | 0.58              |
| 4:A:418:GLU:HG3   | 4:A:722:GLN:HG2   | 1.85                     | 0.58              |
| 4:B:796:LEU:CD2   | 4:B:810:PRO:HG2   | 2.31                     | 0.58              |
| 1:G:117:PHE:CE2   | 1:G:121:LEU:HD11  | 2.38                     | 0.58              |
| 4:B:803:ARG:HD3   | 4:B:1125:HIS:ND1  | 2.18                     | 0.58              |
| 4:B:1144:LEU:HD11 | 4:B:1162:VAL:CG1  | 2.34                     | 0.58              |
| 1:C:164:VAL:HG13  | 4:A:122:TRP:CZ2   | 2.39                     | 0.58              |
| 4:A:129:ASP:O     | 4:A:133:GLN:HG3   | 2.04                     | 0.58              |
| 4:B:845:LEU:HD11  | 4:B:898:CYS:SG    | 2.44                     | 0.58              |
| 1:G:65:LEU:HD11   | 1:G:77:THR:HG23   | 1.86                     | 0.57              |
| 4:A:1059:ARG:NE   | 4:A:1116:LYS:HD2  | 2.19                     | 0.57              |
| 2:H:36:DT:H71     | 5:J:201:LYS:NZ    | 2.19                     | 0.57              |
| 4:B:616:GLN:OE1   | 4:B:616:GLN:N     | 2.37                     | 0.57              |
| 2:D:13:DC:H2''    | 2:D:14:DC:C6      | 2.39                     | 0.57              |
| 2:H:36:DT:O4'     | 4:B:615:VAL:HG13  | 2.05                     | 0.57              |
| 4:B:1011:GLU:HG2  | 4:B:1025:VAL:HG22 | 1.85                     | 0.57              |
| 5:J:162:ILE:O     | 5:J:163:LYS:HG3   | 2.04                     | 0.57              |
| 3:I:39:DT:H2''    | 3:I:40:DT:H5'     | 1.85                     | 0.57              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:A:969:GLN:O    | 4:A:973:ARG:HG3   | 2.05                     | 0.57              |
| 4:B:1004:TYR:CB  | 4:B:1007:ARG:HB2  | 2.34                     | 0.57              |
| 1:G:164:VAL:HG12 | 1:G:200:TYR:HD1   | 1.69                     | 0.57              |
| 4:A:1041:GLN:HB3 | 4:A:1048:ARG:HD2  | 1.86                     | 0.57              |
| 4:B:662:ALA:HB3  | 4:B:668:THR:OG1   | 2.04                     | 0.57              |
| 4:B:1004:TYR:HB3 | 4:B:1007:ARG:HD2  | 1.86                     | 0.57              |
| 5:J:263:LEU:HD11 | 5:J:300:GLN:HB2   | 1.85                     | 0.57              |
| 3:I:16:DT:H6     | 3:I:16:DT:OP1     | 1.87                     | 0.57              |
| 4:B:683:LEU:HD12 | 4:B:1079:ILE:HG12 | 1.86                     | 0.57              |
| 2:D:37:DT:C7     | 5:F:202:ARG:HD3   | 2.34                     | 0.57              |
| 3:I:1:DG:H2''    | 3:I:2:DG:C8       | 2.40                     | 0.57              |
| 5:J:89:LEU:HD21  | 5:J:118:ALA:HB2   | 1.85                     | 0.57              |
| 1:G:81:ILE:HG13  | 2:H:19:DA:C2      | 2.40                     | 0.57              |
| 4:A:956:TYR:CD1  | 4:A:991:LYS:HA    | 2.39                     | 0.57              |
| 5:F:212:TYR:CE1  | 5:F:253:ILE:HG23  | 2.40                     | 0.57              |
| 5:J:205:TRP:CE2  | 5:J:250:LEU:HD21  | 2.40                     | 0.57              |
| 4:B:655:TRP:O    | 4:B:696:LEU:HB3   | 2.05                     | 0.57              |
| 4:A:1119:PHE:HB3 | 4:A:1120:PRO:HD3  | 1.87                     | 0.57              |
| 4:B:452:THR:HG23 | 4:B:455:ARG:NH2   | 2.20                     | 0.57              |
| 4:B:533:TYR:OH   | 4:B:549:PRO:HB3   | 2.04                     | 0.57              |
| 4:B:547:CYS:SG   | 4:B:552:TYR:HB2   | 2.45                     | 0.57              |
| 2:D:4:DC:H4'     | 2:D:5:DG:OP1      | 2.05                     | 0.56              |
| 1:G:222:MET:HE2  | 1:G:230:LEU:HD12  | 1.86                     | 0.56              |
| 4:B:1028:ALA:O   | 4:B:1032:LEU:HG   | 2.05                     | 0.56              |
| 4:B:1088:VAL:O   | 4:B:1102:HIS:N    | 2.38                     | 0.56              |
| 4:A:554:GLU:HA   | 4:A:558:ALA:HB2   | 1.87                     | 0.56              |
| 4:A:944:VAL:CG2  | 4:A:946:LEU:HD13  | 2.25                     | 0.56              |
| 4:B:940:GLY:HA2  | 4:B:1044:PHE:CE1  | 2.40                     | 0.56              |
| 1:C:233:ARG:HG2  | 3:E:49:DT:OP1     | 2.04                     | 0.56              |
| 2:H:18:DT:H2''   | 2:H:19:DA:C8      | 2.40                     | 0.56              |
| 4:A:574:GLU:O    | 4:A:578:LEU:HG    | 2.05                     | 0.56              |
| 4:B:287:VAL:HG13 | 4:B:292:LEU:HB2   | 1.87                     | 0.56              |
| 4:B:1041:GLN:HB3 | 4:B:1048:ARG:HD2  | 1.87                     | 0.56              |
| 5:F:194:MET:HG2  | 5:F:228:PHE:CD2   | 2.41                     | 0.56              |
| 1:G:69:LYS:NZ    | 3:I:34:DT:H5'     | 2.20                     | 0.56              |
| 4:A:662:ALA:HB3  | 4:A:668:THR:HG21  | 1.87                     | 0.56              |
| 4:B:327:GLY:O    | 4:B:329:LYS:HE2   | 2.05                     | 0.56              |
| 4:A:653:LEU:HG   | 4:A:664:LEU:HD23  | 1.86                     | 0.56              |
| 1:G:170:PHE:HA   | 1:G:185:VAL:HG21  | 1.86                     | 0.56              |
| 4:A:303:LEU:HD11 | 4:A:323:MET:HE1   | 1.88                     | 0.56              |
| 5:F:375:GLU:O    | 5:F:379:ARG:HG3   | 2.05                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:E:23:DG:H2''    | 3:E:24:DG:H5''    | 1.87                     | 0.56              |
| 3:I:36:DG:H2'     | 3:I:37:DG:H8      | 1.68                     | 0.56              |
| 4:A:452:THR:HG23  | 4:A:455:ARG:NH2   | 2.20                     | 0.56              |
| 4:B:363:GLN:HA    | 4:B:365:PRO:HD3   | 1.86                     | 0.56              |
| 1:G:233:ARG:HG2   | 3:I:49:DT:P       | 2.46                     | 0.56              |
| 4:A:607:TYR:CZ    | 5:F:388:LEU:HD13  | 2.40                     | 0.56              |
| 4:A:690:THR:HA    | 4:A:693:HIS:CE1   | 2.41                     | 0.56              |
| 1:G:159:ARG:HG2   | 2:H:8:DG:H5'      | 1.88                     | 0.56              |
| 2:H:45:DC:H2''    | 2:H:46:DA:C8      | 2.41                     | 0.56              |
| 4:A:708:ARG:HD3   | 4:A:828:ALA:HA    | 1.87                     | 0.56              |
| 4:A:1149:VAL:HG12 | 4:A:1150:HIS:ND1  | 2.21                     | 0.56              |
| 4:B:279:GLU:OE1   | 4:B:279:GLU:N     | 2.39                     | 0.56              |
| 4:B:820:VAL:HG22  | 4:B:892:TRP:CD1   | 2.40                     | 0.56              |
| 2:D:46:DA:H2''    | 2:D:47:DG:C8      | 2.40                     | 0.56              |
| 4:B:138:GLN:HA    | 4:B:141:LYS:HE2   | 1.87                     | 0.56              |
| 4:B:815:HIS:CD2   | 4:B:1149:VAL:HG22 | 2.41                     | 0.56              |
| 4:B:1011:GLU:O    | 4:B:1015:ARG:HG3  | 2.05                     | 0.56              |
| 4:B:1119:PHE:HB3  | 4:B:1120:PRO:HD3  | 1.86                     | 0.56              |
| 1:C:107:TRP:O     | 1:C:111:LYS:HG3   | 2.06                     | 0.55              |
| 2:H:17:DA:H2''    | 2:H:18:DT:C7      | 2.36                     | 0.55              |
| 5:J:78:ARG:NH2    | 5:J:115:GLU:OE1   | 2.39                     | 0.55              |
| 4:A:422:LEU:HD22  | 4:A:423:PRO:HD2   | 1.88                     | 0.55              |
| 4:A:1059:ARG:HE   | 4:A:1116:LYS:HD2  | 1.72                     | 0.55              |
| 4:A:1068:VAL:HG11 | 4:A:1119:PHE:CD1  | 2.42                     | 0.55              |
| 4:B:1125:HIS:HA   | 4:B:1128:ASP:OD2  | 2.06                     | 0.55              |
| 4:B:1205:LYS:HE2  | 4:B:1209:GLN:NE2  | 2.21                     | 0.55              |
| 5:F:239:ALA:O     | 5:F:255:GLN:NE2   | 2.35                     | 0.55              |
| 1:G:186:LYS:HE2   | 3:I:43:DC:H4'     | 1.88                     | 0.55              |
| 1:G:231:LEU:O     | 1:G:233:ARG:NH1   | 2.40                     | 0.55              |
| 5:J:244:PRO:HB3   | 5:J:363:VAL:CG2   | 2.37                     | 0.55              |
| 4:A:467:LEU:HD12  | 4:A:578:LEU:HD11  | 1.89                     | 0.55              |
| 4:A:712:ARG:NH2   | 4:A:875:ALA:O     | 2.38                     | 0.55              |
| 4:B:655:TRP:HB3   | 4:B:696:LEU:CD2   | 2.33                     | 0.55              |
| 4:B:844:HIS:HB2   | 4:B:919:VAL:HG13  | 1.87                     | 0.55              |
| 4:B:852:LYS:HD2   | 4:B:855:GLU:HG3   | 1.89                     | 0.55              |
| 4:B:929:GLN:HA    | 4:B:944:VAL:HG21  | 1.89                     | 0.55              |
| 1:C:55:SER:HA     | 1:C:103:TYR:CD1   | 2.42                     | 0.54              |
| 2:H:47:DG:H2''    | 2:H:48:DG:C8      | 2.42                     | 0.54              |
| 3:I:41:DA:H4'     | 3:I:42:DG:OP1     | 2.07                     | 0.54              |
| 4:A:940:GLY:HA2   | 4:A:1044:PHE:HE1  | 1.72                     | 0.54              |
| 4:B:219:LEU:HD12  | 4:B:224:GLN:NE2   | 2.22                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:28:DC:H2''    | 2:D:29:DA:C8      | 2.43                     | 0.54              |
| 3:E:3:DC:H2''     | 3:E:4:DC:C6       | 2.42                     | 0.54              |
| 4:A:1015:ARG:CZ   | 4:A:1025:VAL:HG11 | 2.38                     | 0.54              |
| 5:F:119:LYS:HE3   | 5:F:143:LYS:HB3   | 1.89                     | 0.54              |
| 4:B:1147:VAL:HG23 | 4:B:1154:TRP:HB2  | 1.89                     | 0.54              |
| 1:C:173:ALA:O     | 1:C:181:LYS:HE3   | 2.08                     | 0.54              |
| 3:E:2:DG:H2''     | 3:E:3:DC:C6       | 2.43                     | 0.54              |
| 3:E:17:DT:H2'     | 3:E:18:DT:H71     | 1.88                     | 0.54              |
| 4:A:591:CYS:O     | 4:A:593:LEU:HD23  | 2.07                     | 0.54              |
| 4:B:815:HIS:HD2   | 4:B:1149:VAL:HG22 | 1.73                     | 0.54              |
| 4:B:830:GLY:HA3   | 4:B:914:VAL:HG12  | 1.90                     | 0.54              |
| 5:F:248:HIS:NE2   | 5:F:250:LEU:HB2   | 2.23                     | 0.54              |
| 4:A:414:VAL:HG22  | 4:A:788:HIS:CG    | 2.43                     | 0.54              |
| 4:B:1084:LEU:HG   | 4:B:1111:ASN:HB2  | 1.90                     | 0.54              |
| 4:B:300:ALA:CB    | 4:B:333:LEU:HD11  | 2.38                     | 0.54              |
| 5:J:236:LYS:O     | 5:J:251:SER:OG    | 2.26                     | 0.54              |
| 1:C:122:THR:HB    | 1:C:123:PRO:HD2   | 1.90                     | 0.53              |
| 3:E:18:DT:P       | 4:A:1098:ILE:HA   | 2.48                     | 0.53              |
| 4:A:808:PRO:CD    | 4:A:816:LEU:HD13  | 2.38                     | 0.53              |
| 4:A:1093:GLY:HA2  | 4:A:1097:SER:CB   | 2.37                     | 0.53              |
| 4:B:936:ARG:HB2   | 4:B:1215:GLY:N    | 2.22                     | 0.53              |
| 2:H:17:DA:C2'     | 2:H:18:DT:H71     | 2.38                     | 0.53              |
| 4:A:589:MET:HB3   | 4:A:605:VAL:HG22  | 1.88                     | 0.53              |
| 4:A:658:PRO:HA    | 4:A:670:LEU:HD22  | 1.90                     | 0.53              |
| 4:A:680:HIS:O     | 4:A:684:LEU:HG    | 2.07                     | 0.53              |
| 4:A:712:ARG:NH2   | 4:A:899:MET:HE2   | 2.23                     | 0.53              |
| 4:A:945:ASN:OD1   | 4:A:953:GLN:N     | 2.32                     | 0.53              |
| 4:B:339:LEU:HB3   | 4:B:343:ASP:HB2   | 1.90                     | 0.53              |
| 4:B:224:GLN:OE1   | 4:B:568:PRO:HB3   | 2.08                     | 0.53              |
| 4:B:1082:TYR:HB2  | 4:B:1115:GLN:HE21 | 1.73                     | 0.53              |
| 1:G:107:TRP:O     | 1:G:111:LYS:HG3   | 2.08                     | 0.53              |
| 4:A:265:ASN:HB3   | 4:A:297:LEU:HD23  | 1.90                     | 0.53              |
| 1:G:152:LEU:HD22  | 1:G:230:LEU:CD1   | 2.38                     | 0.53              |
| 4:A:590:PRO:HB3   | 4:A:599:SER:HB3   | 1.89                     | 0.53              |
| 4:A:1144:LEU:HD22 | 4:A:1159:ASP:CG   | 2.33                     | 0.53              |
| 5:J:256:LEU:O     | 5:J:307:LEU:HD13  | 2.09                     | 0.53              |
| 4:A:815:HIS:HD2   | 4:A:1149:VAL:CG2  | 2.21                     | 0.53              |
| 5:F:144:LEU:HD12  | 5:F:145:ARG:H     | 1.73                     | 0.53              |
| 4:A:956:TYR:CE1   | 4:A:991:LYS:HA    | 2.43                     | 0.53              |
| 4:B:961:ALA:O     | 4:B:964:GLU:HB3   | 2.09                     | 0.53              |
| 3:E:4:DC:H2'      | 3:E:5:DT:H71      | 1.91                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:E:15:DG:H2'    | 3:E:16:DT:C7     | 2.27                     | 0.53              |
| 1:G:222:MET:HB2  | 1:G:231:LEU:HD11 | 1.91                     | 0.53              |
| 4:B:871:ILE:HG23 | 4:B:898:CYS:SG   | 2.49                     | 0.53              |
| 4:B:1015:ARG:HA  | 4:B:1022:GLN:OE1 | 2.09                     | 0.53              |
| 4:A:609:VAL:HG12 | 5:F:341:SER:O    | 2.08                     | 0.53              |
| 4:B:271:TRP:O    | 4:B:275:GLY:N    | 2.42                     | 0.53              |
| 4:A:132:THR:O    | 4:A:136:ARG:HG3  | 2.08                     | 0.52              |
| 4:B:419:LYS:HD3  | 4:B:635:ALA:HB1  | 1.90                     | 0.52              |
| 3:E:4:DC:H2''    | 3:E:5:DT:C6      | 2.44                     | 0.52              |
| 1:G:166:VAL:HA   | 1:G:185:VAL:HG11 | 1.90                     | 0.52              |
| 2:H:7:DT:H2'     | 2:H:8:DG:C8      | 2.44                     | 0.52              |
| 4:A:992:GLN:HG3  | 4:A:1010:ILE:CG1 | 2.37                     | 0.52              |
| 4:A:1188:VAL:O   | 4:A:1192:CYS:HB2 | 2.08                     | 0.52              |
| 1:C:121:LEU:HB2  | 1:C:125:GLN:HG3  | 1.90                     | 0.52              |
| 1:C:158:PRO:HG3  | 1:C:211:TYR:CD2  | 2.44                     | 0.52              |
| 4:A:467:LEU:HD12 | 4:A:578:LEU:HD12 | 1.90                     | 0.52              |
| 5:F:320:PHE:CE2  | 5:F:324:LEU:HD11 | 2.44                     | 0.52              |
| 5:J:144:LEU:HD12 | 5:J:145:ARG:H    | 1.74                     | 0.52              |
| 5:J:263:LEU:CD1  | 5:J:300:GLN:HB2  | 2.39                     | 0.52              |
| 1:G:225:VAL:HG12 | 1:G:225:VAL:O    | 2.10                     | 0.52              |
| 4:B:304:GLN:HG3  | 4:B:346:THR:OG1  | 2.10                     | 0.52              |
| 4:B:981:LEU:HD23 | 4:B:1020:PHE:CE2 | 2.45                     | 0.52              |
| 4:B:562:LEU:HD23 | 4:B:563:ARG:N    | 2.24                     | 0.52              |
| 5:F:260:ILE:HA   | 5:F:300:GLN:O    | 2.09                     | 0.52              |
| 1:G:170:PHE:HE2  | 2:H:10:DT:H4'    | 1.73                     | 0.52              |
| 4:A:279:GLU:N    | 4:A:279:GLU:OE1  | 2.39                     | 0.52              |
| 4:A:662:ALA:HB3  | 4:A:668:THR:OG1  | 2.10                     | 0.52              |
| 1:C:225:VAL:HG12 | 1:C:225:VAL:O    | 2.09                     | 0.52              |
| 5:F:149:CYS:HB2  | 5:F:167:MET:SD   | 2.50                     | 0.52              |
| 1:C:157:ARG:HA   | 1:C:211:TYR:CE1  | 2.45                     | 0.52              |
| 2:D:44:DA:H2''   | 2:D:45:DC:C6     | 2.45                     | 0.52              |
| 1:G:45:VAL:HG21  | 1:G:125:GLN:CB   | 2.40                     | 0.52              |
| 4:A:655:TRP:CE3  | 4:A:670:LEU:HD13 | 2.45                     | 0.52              |
| 4:A:671:MET:SD   | 4:A:684:LEU:HD11 | 2.50                     | 0.52              |
| 4:A:679:GLN:O    | 4:A:682:GLU:HG2  | 2.09                     | 0.52              |
| 4:B:671:MET:SD   | 4:B:680:HIS:ND1  | 2.82                     | 0.52              |
| 3:E:41:DA:H4'    | 3:E:42:DG:OP1    | 2.09                     | 0.52              |
| 1:G:163:ASN:ND2  | 2:H:8:DG:H1'     | 2.24                     | 0.52              |
| 1:G:211:TYR:O    | 1:G:215:MET:HG2  | 2.10                     | 0.52              |
| 4:B:464:ARG:HA   | 4:B:464:ARG:HH11 | 1.75                     | 0.52              |
| 1:G:159:ARG:HD3  | 2:H:8:DG:C5'     | 2.40                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:B:291:GLY:O    | 4:B:292:LEU:HD23 | 2.10                     | 0.52              |
| 1:C:182:LEU:HD21 | 3:E:43:DC:C2     | 2.45                     | 0.51              |
| 4:B:591:CYS:SG   | 4:B:601:ARG:NH2  | 2.73                     | 0.51              |
| 4:B:960:ALA:HB2  | 4:B:990:VAL:HG21 | 1.90                     | 0.51              |
| 3:E:7:DT:H2''    | 3:E:8:DC:C6      | 2.45                     | 0.51              |
| 2:H:46:DA:H2''   | 2:H:47:DG:C8     | 2.45                     | 0.51              |
| 4:A:590:PRO:CB   | 4:A:599:SER:HB3  | 2.40                     | 0.51              |
| 4:A:1150:HIS:HE2 | 4:A:1152:CYS:HG  | 1.53                     | 0.51              |
| 4:B:376:ASP:OD2  | 4:B:1173:ARG:NH1 | 2.40                     | 0.51              |
| 4:B:491:PRO:HB2  | 4:B:493:GLN:CD   | 2.35                     | 0.51              |
| 5:F:137:GLY:O    | 5:F:141:ASP:N    | 2.21                     | 0.51              |
| 4:A:304:GLN:HG2  | 4:A:308:ARG:HH12 | 1.75                     | 0.51              |
| 4:A:547:CYS:SG   | 4:A:552:TYR:HB2  | 2.50                     | 0.51              |
| 4:A:833:LEU:HB3  | 4:A:837:GLY:HA3  | 1.91                     | 0.51              |
| 4:B:844:HIS:CD2  | 4:B:920:HIS:H    | 2.28                     | 0.51              |
| 4:B:846:VAL:HG21 | 4:B:860:ARG:O    | 2.11                     | 0.51              |
| 1:G:100:GLN:O    | 1:G:104:ARG:HG3  | 2.09                     | 0.51              |
| 4:A:400:PHE:CE1  | 4:A:664:LEU:HD13 | 2.45                     | 0.51              |
| 4:A:419:LYS:N    | 4:A:420:PRO:HD3  | 2.25                     | 0.51              |
| 4:B:295:ASP:HA   | 4:B:328:LEU:HD11 | 1.93                     | 0.51              |
| 5:J:375:GLU:O    | 5:J:379:ARG:HG3  | 2.10                     | 0.51              |
| 4:A:351:VAL:HG11 | 4:A:358:PHE:CD2  | 2.44                     | 0.51              |
| 5:J:247:TYR:OH   | 5:J:252:VAL:HG22 | 2.11                     | 0.51              |
| 4:A:355:LYS:CB   | 4:A:358:PHE:HB2  | 2.41                     | 0.51              |
| 2:D:35:DA:H2''   | 2:D:36:DT:H5'    | 1.93                     | 0.51              |
| 5:J:244:PRO:HB3  | 5:J:363:VAL:HG21 | 1.93                     | 0.51              |
| 2:D:25:DA:C1'    | 2:D:26:DA:H5'    | 2.38                     | 0.51              |
| 4:A:562:LEU:HD23 | 4:A:563:ARG:N    | 2.25                     | 0.51              |
| 4:A:931:TYR:CZ   | 4:A:1051:GLN:HG2 | 2.46                     | 0.51              |
| 5:F:348:ARG:O    | 5:F:352:MET:HG3  | 2.11                     | 0.51              |
| 5:J:212:TYR:CE1  | 5:J:253:ILE:HG23 | 2.45                     | 0.51              |
| 5:J:378:GLU:OE2  | 5:J:387:TRP:NE1  | 2.40                     | 0.51              |
| 4:B:612:PHE:HZ   | 5:J:326:HIS:HA   | 1.75                     | 0.51              |
| 2:H:28:DC:H2''   | 2:H:29:DA:C8     | 2.46                     | 0.50              |
| 5:J:98:LEU:O     | 5:J:189:LEU:HD12 | 2.11                     | 0.50              |
| 1:G:221:GLN:HE22 | 4:B:140:LEU:HD13 | 1.74                     | 0.50              |
| 4:B:1139:CYS:HB3 | 4:B:1144:LEU:HB2 | 1.93                     | 0.50              |
| 5:F:149:CYS:SG   | 5:F:154:LEU:HD21 | 2.52                     | 0.50              |
| 3:E:21:DT:C2'    | 3:E:22:DT:H71    | 2.42                     | 0.50              |
| 4:B:929:GLN:HG2  | 4:B:944:VAL:HB   | 1.92                     | 0.50              |
| 1:G:55:SER:HA    | 1:G:103:TYR:CD1  | 2.47                     | 0.50              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:F:182:PRO:HG2  | 5:F:185:ALA:HB2   | 1.94                     | 0.50              |
| 1:G:158:PRO:HG3  | 1:G:211:TYR:CD2   | 2.47                     | 0.50              |
| 4:A:464:ARG:HH11 | 4:A:464:ARG:HA    | 1.76                     | 0.50              |
| 4:A:944:VAL:HG23 | 4:A:946:LEU:CD1   | 2.28                     | 0.50              |
| 4:A:977:VAL:HA   | 4:A:980:VAL:HG22  | 1.94                     | 0.50              |
| 1:C:211:TYR:O    | 1:C:215:MET:HG2   | 2.11                     | 0.50              |
| 3:E:6:DG:H2''    | 3:E:7:DT:H71      | 1.93                     | 0.50              |
| 4:A:397:GLN:O    | 4:A:401:GLU:HG2   | 2.10                     | 0.50              |
| 4:A:569:LEU:N    | 4:A:570:PRO:HD2   | 2.27                     | 0.50              |
| 4:B:133:GLN:O    | 4:B:137:MET:HG2   | 2.11                     | 0.50              |
| 4:A:455:ARG:O    | 4:A:459:GLU:HG3   | 2.12                     | 0.50              |
| 4:A:491:PRO:HB2  | 4:A:493:GLN:CD    | 2.36                     | 0.50              |
| 4:B:343:ASP:O    | 4:B:347:VAL:HG23  | 2.12                     | 0.50              |
| 4:B:870:ASP:HB3  | 4:B:884:TRP:CG    | 2.46                     | 0.50              |
| 4:A:417:VAL:HG22 | 4:A:784:SER:HA    | 1.93                     | 0.50              |
| 4:B:456:LEU:O    | 4:B:460:VAL:HG23  | 2.12                     | 0.50              |
| 5:F:351:LEU:HD23 | 5:F:354:ILE:HD11  | 1.93                     | 0.50              |
| 1:C:54:VAL:HG12  | 1:C:58:LEU:HB3    | 1.92                     | 0.50              |
| 2:H:36:DT:C7     | 5:J:201:LYS:NZ    | 2.75                     | 0.50              |
| 4:B:618:ILE:O    | 4:B:620:ILE:HD12  | 2.12                     | 0.50              |
| 5:F:98:LEU:O     | 5:F:189:LEU:HD12  | 2.11                     | 0.50              |
| 1:G:223:ILE:HD11 | 1:G:231:LEU:HD22  | 1.94                     | 0.49              |
| 3:I:35:DG:H2''   | 3:I:36:DG:C8      | 2.46                     | 0.49              |
| 4:A:802:PHE:O    | 4:A:1078:VAL:HG13 | 2.11                     | 0.49              |
| 4:A:1023:GLU:HG3 | 4:A:1024:PHE:CD2  | 2.47                     | 0.49              |
| 4:A:1053:TRP:CZ2 | 4:A:1211:VAL:HG22 | 2.47                     | 0.49              |
| 4:B:323:MET:SD   | 4:B:330:LEU:HD23  | 2.52                     | 0.49              |
| 1:C:118:LYS:O    | 1:C:125:GLN:HG3   | 2.12                     | 0.49              |
| 4:A:464:ARG:NH1  | 4:A:465:PHE:H     | 2.09                     | 0.49              |
| 4:A:470:PHE:HA   | 4:A:473:LEU:CD1   | 2.42                     | 0.49              |
| 4:A:683:LEU:CD1  | 4:A:1079:ILE:HG12 | 2.42                     | 0.49              |
| 4:A:845:LEU:O    | 4:A:849:THR:HG23  | 2.11                     | 0.49              |
| 4:B:569:LEU:N    | 4:B:570:PRO:HD2   | 2.27                     | 0.49              |
| 4:B:993:THR:O    | 4:B:996:THR:HB    | 2.13                     | 0.49              |
| 5:J:339:LEU:HD21 | 5:J:373:LEU:HD21  | 1.94                     | 0.49              |
| 1:C:106:GLU:HA   | 1:C:109:VAL:HG12  | 1.94                     | 0.49              |
| 3:I:37:DG:H2''   | 3:I:38:DG:C8      | 2.47                     | 0.49              |
| 4:A:469:PRO:O    | 4:A:473:LEU:HG    | 2.12                     | 0.49              |
| 4:A:490:LEU:HD12 | 4:A:491:PRO:HD2   | 1.94                     | 0.49              |
| 4:A:614:ASN:OD1  | 4:A:614:ASN:N     | 2.45                     | 0.49              |
| 4:B:422:LEU:CD1  | 4:B:423:PRO:HD2   | 2.41                     | 0.49              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:D:16:DC:H2''   | 2:D:17:DA:C8      | 2.47                     | 0.49              |
| 1:G:158:PRO:HG3  | 1:G:211:TYR:CG    | 2.47                     | 0.49              |
| 5:F:162:ILE:O    | 5:F:163:LYS:HG3   | 2.13                     | 0.49              |
| 3:I:20:DG:N9     | 3:I:21:DT:H72     | 2.28                     | 0.49              |
| 4:A:363:GLN:HB3  | 4:A:364:LEU:CA    | 2.43                     | 0.49              |
| 4:A:530:TYR:CE1  | 4:A:534:LEU:HD21  | 2.47                     | 0.49              |
| 4:B:418:GLU:HG3  | 4:B:721:PHE:CE2   | 2.48                     | 0.49              |
| 4:B:671:MET:SD   | 4:B:684:LEU:HD11  | 2.52                     | 0.49              |
| 1:G:106:GLU:HA   | 1:G:109:VAL:HG12  | 1.94                     | 0.49              |
| 1:G:152:LEU:HD22 | 1:G:230:LEU:HD13  | 1.95                     | 0.49              |
| 1:G:173:ALA:O    | 1:G:181:LYS:HE3   | 2.12                     | 0.49              |
| 4:A:808:PRO:HD2  | 4:A:816:LEU:HD22  | 1.94                     | 0.49              |
| 4:A:1205:LYS:HE2 | 4:A:1209:GLN:OE1  | 2.12                     | 0.49              |
| 4:B:510:SER:O    | 4:B:514:VAL:HG23  | 2.12                     | 0.49              |
| 3:I:16:DT:OP1    | 3:I:16:DT:H2'     | 2.13                     | 0.49              |
| 4:A:446:CYS:SG   | 4:A:480:VAL:HG21  | 2.53                     | 0.49              |
| 4:A:589:MET:CG   | 4:A:605:VAL:HG22  | 2.42                     | 0.49              |
| 4:A:963:VAL:HG22 | 4:A:1039:SER:OG   | 2.12                     | 0.49              |
| 4:A:1022:GLN:O   | 4:A:1025:VAL:HG12 | 2.11                     | 0.49              |
| 5:J:309:THR:OG1  | 5:J:375:GLU:OE2   | 2.16                     | 0.49              |
| 3:E:40:DT:C2     | 3:E:41:DA:N7      | 2.81                     | 0.49              |
| 4:A:438:ARG:NH1  | 4:A:636:GLU:OE2   | 2.35                     | 0.49              |
| 4:A:662:ALA:CB   | 4:A:668:THR:HG21  | 2.42                     | 0.49              |
| 4:A:713:VAL:O    | 4:A:717:VAL:HG23  | 2.13                     | 0.49              |
| 1:C:100:GLN:O    | 1:C:104:ARG:HG3   | 2.12                     | 0.49              |
| 4:A:1024:PHE:O   | 4:A:1028:ALA:N    | 2.33                     | 0.49              |
| 4:B:464:ARG:NH1  | 4:B:465:PHE:H     | 2.10                     | 0.49              |
| 4:B:874:SER:HB3  | 4:B:885:TRP:HD1   | 1.78                     | 0.49              |
| 5:F:132:HIS:O    | 5:F:135:SER:HB3   | 2.12                     | 0.49              |
| 1:C:129:LEU:HD11 | 1:C:133:ILE:HD11  | 1.95                     | 0.49              |
| 4:A:656:THR:OG1  | 4:A:660:SER:OG    | 2.27                     | 0.49              |
| 4:A:997:VAL:HG22 | 4:A:1033:VAL:HG13 | 1.94                     | 0.49              |
| 5:F:74:TYR:CD1   | 5:F:105:GLY:HA3   | 2.48                     | 0.49              |
| 5:F:248:HIS:CE1  | 5:F:250:LEU:HB2   | 2.48                     | 0.49              |
| 5:J:144:LEU:HD12 | 5:J:145:ARG:N     | 2.28                     | 0.49              |
| 1:C:67:ILE:O     | 1:C:71:GLN:HG2    | 2.13                     | 0.48              |
| 2:D:11:DA:H2'    | 2:D:12:DA:C8      | 2.48                     | 0.48              |
| 1:G:53:PRO:HB3   | 1:G:106:GLU:HB3   | 1.95                     | 0.48              |
| 4:A:830:GLY:HA3  | 4:A:914:VAL:HG12  | 1.96                     | 0.48              |
| 4:A:1120:PRO:CB  | 4:A:1121:PRO:HD3  | 2.42                     | 0.48              |
| 4:B:592:SER:O    | 4:B:593:LEU:HG    | 2.13                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:B:874:SER:HB3  | 4:B:885:TRP:CD1  | 2.48                     | 0.48              |
| 5:F:164:PRO:HG2  | 5:F:165:PRO:CD   | 2.42                     | 0.48              |
| 2:D:15:DC:H2''   | 2:D:16:DC:C5     | 2.47                     | 0.48              |
| 3:E:37:DG:H2'    | 3:E:38:DG:C8     | 2.48                     | 0.48              |
| 5:F:89:LEU:HD11  | 5:F:116:ALA:CB   | 2.39                     | 0.48              |
| 5:J:130:ILE:HD11 | 5:J:148:HIS:HB2  | 1.95                     | 0.48              |
| 4:A:589:MET:HG2  | 4:A:605:VAL:HG22 | 1.94                     | 0.48              |
| 4:A:1136:ALA:HB2 | 4:A:1146:PHE:CE1 | 2.48                     | 0.48              |
| 4:B:232:CYS:SG   | 4:B:473:LEU:HD21 | 2.53                     | 0.48              |
| 4:B:652:PRO:HB3  | 4:B:797:PRO:HB3  | 1.93                     | 0.48              |
| 5:J:182:PRO:HG2  | 5:J:185:ALA:HB2  | 1.93                     | 0.48              |
| 5:J:349:ASP:HA   | 5:J:352:MET:CE   | 2.43                     | 0.48              |
| 1:G:228:LYS:HA   | 1:G:231:LEU:HD13 | 1.96                     | 0.48              |
| 4:A:127:GLU:O    | 4:A:131:ARG:HG3  | 2.14                     | 0.48              |
| 4:B:1120:PRO:CB  | 4:B:1121:PRO:HD3 | 2.43                     | 0.48              |
| 3:E:31:DG:N7     | 3:E:32:DT:H73    | 2.29                     | 0.48              |
| 1:G:65:LEU:HB3   | 1:G:66:PRO:HD3   | 1.94                     | 0.48              |
| 1:G:212:HIS:NE2  | 1:G:216:LYS:HE3  | 2.29                     | 0.48              |
| 4:A:283:VAL:HA   | 4:A:286:MET:HE3  | 1.94                     | 0.48              |
| 4:A:808:PRO:HG3  | 4:A:815:HIS:CE1  | 2.48                     | 0.48              |
| 4:A:838:LEU:CG   | 4:A:842:LYS:HE3  | 2.42                     | 0.48              |
| 4:B:368:VAL:HG11 | 4:B:380:LYS:NZ   | 2.28                     | 0.48              |
| 5:F:144:LEU:HD12 | 5:F:145:ARG:N    | 2.28                     | 0.48              |
| 1:G:80:LEU:CD2   | 1:G:83:ARG:HH21  | 2.27                     | 0.48              |
| 1:G:222:MET:HE3  | 1:G:227:ARG:HB2  | 1.95                     | 0.48              |
| 4:A:422:LEU:HD22 | 4:A:423:PRO:CD   | 2.43                     | 0.48              |
| 3:E:23:DG:H2''   | 3:E:24:DG:C5'    | 2.44                     | 0.48              |
| 4:A:349:LYS:O    | 4:A:353:LYS:HG2  | 2.13                     | 0.48              |
| 4:A:1116:LYS:HG3 | 4:A:1117:ASN:N   | 2.29                     | 0.48              |
| 4:B:241:LEU:HD11 | 4:B:460:VAL:CG1  | 2.44                     | 0.48              |
| 4:B:680:HIS:CD2  | 4:B:802:PHE:HB2  | 2.49                     | 0.48              |
| 5:F:129:PHE:O    | 5:F:133:LEU:HG   | 2.13                     | 0.48              |
| 5:J:350:ILE:HA   | 5:J:353:GLN:HG2  | 1.95                     | 0.48              |
| 4:B:584:VAL:HG22 | 4:B:606:LEU:HD12 | 1.96                     | 0.48              |
| 5:J:260:ILE:HA   | 5:J:300:GLN:O    | 2.14                     | 0.48              |
| 4:A:343:ASP:O    | 4:A:347:VAL:HG23 | 2.14                     | 0.48              |
| 4:B:347:VAL:O    | 4:B:351:VAL:HG23 | 2.13                     | 0.48              |
| 4:B:708:ARG:HD3  | 4:B:828:ALA:HA   | 1.96                     | 0.48              |
| 4:B:992:GLN:HG3  | 4:B:1010:ILE:CG1 | 2.42                     | 0.48              |
| 4:B:1111:ASN:ND2 | 4:B:1114:LYS:HD2 | 2.28                     | 0.48              |
| 4:B:1116:LYS:HG3 | 4:B:1117:ASN:N   | 2.28                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:B:1144:LEU:HD22 | 4:B:1159:ASP:CG   | 2.39                     | 0.48              |
| 5:J:192:VAL:HA    | 5:J:226:ASN:O     | 2.13                     | 0.48              |
| 4:A:961:ALA:O     | 4:A:964:GLU:HB3   | 2.14                     | 0.48              |
| 4:B:820:VAL:O     | 4:B:824:LEU:HG    | 2.14                     | 0.48              |
| 1:G:165:TYR:CD2   | 1:G:189:TRP:HB2   | 2.49                     | 0.47              |
| 1:G:182:LEU:HD23  | 3:I:42:DG:N3      | 2.29                     | 0.47              |
| 3:I:14:DG:N2      | 4:B:1102:HIS:HA   | 2.23                     | 0.47              |
| 4:A:653:LEU:CD1   | 4:A:664:LEU:HA    | 2.44                     | 0.47              |
| 4:A:808:PRO:CG    | 4:A:816:LEU:HD13  | 2.43                     | 0.47              |
| 4:A:947:GLU:OE2   | 4:A:948:PRO:HD2   | 2.14                     | 0.47              |
| 4:B:624:HIS:O     | 4:B:627:TYR:HB3   | 2.14                     | 0.47              |
| 1:G:103:TYR:OH    | 2:H:23:DC:H4'     | 2.13                     | 0.47              |
| 4:A:363:GLN:CB    | 4:A:364:LEU:HA    | 2.43                     | 0.47              |
| 4:A:431:ARG:NH2   | 4:A:637:PRO:HD3   | 2.28                     | 0.47              |
| 4:A:956:TYR:CZ    | 4:A:991:LYS:HG3   | 2.48                     | 0.47              |
| 4:B:464:ARG:HA    | 4:B:464:ARG:NH1   | 2.28                     | 0.47              |
| 4:B:1084:LEU:HD11 | 4:B:1111:ASN:ND2  | 2.30                     | 0.47              |
| 5:F:244:PRO:HB3   | 5:F:363:VAL:HG22  | 1.93                     | 0.47              |
| 5:F:344:PRO:HG3   | 5:F:385:TYR:CE2   | 2.48                     | 0.47              |
| 4:A:1002:THR:H    | 4:A:1007:ARG:NH2  | 2.11                     | 0.47              |
| 3:E:24:DG:H2''    | 3:E:25:DT:C6      | 2.48                     | 0.47              |
| 4:B:658:PRO:CA    | 4:B:670:LEU:HD22  | 2.40                     | 0.47              |
| 3:I:4:DC:H2''     | 3:I:5:DT:C6       | 2.50                     | 0.47              |
| 3:I:37:DG:C2'     | 3:I:38:DG:C8      | 2.97                     | 0.47              |
| 4:A:981:LEU:HD13  | 4:A:1032:LEU:HD21 | 1.97                     | 0.47              |
| 4:B:614:ASN:OD1   | 4:B:614:ASN:N     | 2.47                     | 0.47              |
| 4:B:647:PRO:HG3   | 4:B:796:LEU:HD21  | 1.96                     | 0.47              |
| 5:J:365:MET:HB2   | 5:J:370:PHE:CZ    | 2.49                     | 0.47              |
| 3:I:19:DG:C1'     | 3:I:20:DG:OP1     | 2.63                     | 0.47              |
| 4:A:690:THR:HA    | 4:A:693:HIS:NE2   | 2.29                     | 0.47              |
| 4:A:1041:GLN:CD   | 4:A:1048:ARG:HH11 | 2.22                     | 0.47              |
| 4:B:136:ARG:O     | 4:B:140:LEU:HG    | 2.14                     | 0.47              |
| 4:B:584:VAL:HA    | 4:B:606:LEU:HD12  | 1.95                     | 0.47              |
| 5:F:323:LEU:HG    | 5:F:342:LEU:HD13  | 1.96                     | 0.47              |
| 1:C:107:TRP:CZ2   | 2:D:24:DG:H5''    | 2.50                     | 0.47              |
| 1:C:126:ILE:O     | 1:C:130:GLU:HG3   | 2.15                     | 0.47              |
| 2:H:4:DC:H2''     | 2:H:5:DG:C5'      | 2.45                     | 0.47              |
| 3:I:39:DT:C2'     | 3:I:40:DT:H72     | 2.45                     | 0.47              |
| 4:A:246:LEU:HD22  | 4:A:267:VAL:CG2   | 2.41                     | 0.47              |
| 4:A:268:MET:HG2   | 4:A:280:LEU:HG    | 1.96                     | 0.47              |
| 4:A:518:ARG:HA    | 4:A:523:VAL:HG21  | 1.96                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:A:619:GLY:O     | 4:A:620:ILE:HD13  | 2.15                     | 0.47              |
| 4:A:1059:ARG:HG2  | 4:A:1116:LYS:CB   | 2.44                     | 0.47              |
| 4:A:1144:LEU:HD11 | 4:A:1162:VAL:CG1  | 2.44                     | 0.47              |
| 4:B:626:ALA:HB2   | 5:J:385:TYR:OH    | 2.14                     | 0.47              |
| 4:B:679:GLN:O     | 4:B:682:GLU:HG2   | 2.14                     | 0.47              |
| 4:A:557:GLY:HA3   | 4:A:558:ALA:HA    | 1.47                     | 0.47              |
| 4:B:303:LEU:HD11  | 4:B:323:MET:HE1   | 1.97                     | 0.47              |
| 4:B:422:LEU:CG    | 4:B:423:PRO:HD2   | 2.45                     | 0.47              |
| 4:B:445:LEU:HD12  | 4:B:484:LEU:HD21  | 1.97                     | 0.47              |
| 4:B:1015:ARG:NH2  | 4:B:1025:VAL:HG11 | 2.29                     | 0.47              |
| 1:G:215:MET:HB3   | 1:G:232:ARG:NH2   | 2.30                     | 0.47              |
| 2:H:36:DT:C7      | 5:J:201:LYS:HZ3   | 2.27                     | 0.47              |
| 4:B:507:ARG:HB3   | 4:B:511:ARG:NH1   | 2.30                     | 0.47              |
| 4:B:897:CYS:HA    | 4:B:917:LEU:HD22  | 1.97                     | 0.47              |
| 4:A:683:LEU:HD12  | 4:A:1079:ILE:HG12 | 1.97                     | 0.47              |
| 4:A:877:GLN:HB3   | 4:A:880:THR:OG1   | 2.15                     | 0.47              |
| 4:A:941:ALA:CA    | 4:A:946:LEU:HB2   | 2.45                     | 0.47              |
| 3:I:37:DG:C2'     | 3:I:38:DG:H8      | 2.27                     | 0.46              |
| 4:A:220:SER:O     | 4:A:224:GLN:HG3   | 2.14                     | 0.46              |
| 4:A:363:GLN:HB3   | 4:A:364:LEU:HA    | 1.96                     | 0.46              |
| 5:J:164:PRO:HG2   | 5:J:165:PRO:CD    | 2.44                     | 0.46              |
| 1:C:107:TRP:CH2   | 2:D:24:DG:H4'     | 2.51                     | 0.46              |
| 1:G:163:ASN:CB    | 2:H:8:DG:H1'      | 2.45                     | 0.46              |
| 4:A:1059:ARG:HG2  | 4:A:1116:LYS:CD   | 2.45                     | 0.46              |
| 5:J:132:HIS:O     | 5:J:135:SER:HB3   | 2.15                     | 0.46              |
| 1:C:58:LEU:HD22   | 3:E:30:DG:N3      | 2.30                     | 0.46              |
| 1:C:186:LYS:HG3   | 3:E:44:DA:H5'     | 1.96                     | 0.46              |
| 3:I:4:DC:H2'      | 3:I:5:DT:H72      | 1.98                     | 0.46              |
| 4:A:422:LEU:CD2   | 4:A:423:PRO:HD2   | 2.45                     | 0.46              |
| 4:A:426:GLU:OE2   | 4:A:633:LYS:HG2   | 2.15                     | 0.46              |
| 4:A:507:ARG:HB3   | 4:A:511:ARG:NH1   | 2.30                     | 0.46              |
| 5:J:149:CYS:SG    | 5:J:154:LEU:HD21  | 2.55                     | 0.46              |
| 5:J:346:ASP:HB3   | 5:J:349:ASP:HB3   | 1.96                     | 0.46              |
| 1:G:56:SER:HA     | 1:G:99:TYR:HB3    | 1.96                     | 0.46              |
| 3:I:16:DT:C2'     | 3:I:17:DT:H71     | 2.45                     | 0.46              |
| 4:A:387:PRO:HD3   | 4:A:1143:GLY:HA2  | 1.98                     | 0.46              |
| 4:A:592:SER:O     | 4:A:593:LEU:HG    | 2.15                     | 0.46              |
| 4:B:476:GLU:O     | 4:B:480:VAL:HG23  | 2.15                     | 0.46              |
| 5:J:114:LEU:HD22  | 5:J:140:LEU:HD12  | 1.98                     | 0.46              |
| 2:D:9:DC:H2''     | 2:D:10:DT:H5'     | 1.98                     | 0.46              |
| 2:D:36:DT:OP2     | 5:F:201:LYS:NZ    | 2.43                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:A:400:PHE:HE1   | 4:A:664:LEU:HD13  | 1.80                     | 0.46              |
| 4:A:464:ARG:HA    | 4:A:464:ARG:NH1   | 2.30                     | 0.46              |
| 4:A:562:LEU:HD23  | 4:A:563:ARG:C     | 2.40                     | 0.46              |
| 4:B:853:LYS:HD3   | 4:B:987:ARG:NH1   | 2.30                     | 0.46              |
| 4:B:830:GLY:HA3   | 4:B:914:VAL:CG1   | 2.46                     | 0.46              |
| 3:I:22:DT:H2''    | 3:I:23:DG:C8      | 2.51                     | 0.46              |
| 3:I:23:DG:H2''    | 3:I:24:DG:H5''    | 1.97                     | 0.46              |
| 4:A:830:GLY:HA3   | 4:A:914:VAL:CG1   | 2.46                     | 0.46              |
| 4:A:844:HIS:CG    | 4:A:919:VAL:HG13  | 2.51                     | 0.46              |
| 4:A:1059:ARG:CG   | 4:A:1116:LYS:HB2  | 2.46                     | 0.46              |
| 5:J:119:LYS:HE3   | 5:J:143:LYS:HB3   | 1.96                     | 0.46              |
| 5:J:129:PHE:O     | 5:J:133:LEU:HG    | 2.16                     | 0.46              |
| 5:J:323:LEU:HD23  | 5:J:323:LEU:C     | 2.41                     | 0.46              |
| 1:C:65:LEU:HB3    | 1:C:66:PRO:HD3    | 1.97                     | 0.46              |
| 5:J:85:ALA:HA     | 5:J:113:LEU:CD2   | 2.46                     | 0.46              |
| 3:E:41:DA:H2''    | 3:E:42:DG:O5'     | 2.16                     | 0.46              |
| 5:J:244:PRO:O     | 5:J:331:ARG:NH2   | 2.48                     | 0.46              |
| 2:D:34:DA:H2''    | 2:D:35:DA:H8      | 1.76                     | 0.46              |
| 1:G:122:THR:HB    | 1:G:123:PRO:HD2   | 1.98                     | 0.46              |
| 3:I:3:DC:H2''     | 3:I:4:DC:C6       | 2.51                     | 0.46              |
| 4:A:945:ASN:ND2   | 4:A:953:GLN:O     | 2.49                     | 0.46              |
| 4:B:852:LYS:HE3   | 4:B:863:PHE:CG    | 2.51                     | 0.46              |
| 2:D:4:DC:H2''     | 2:D:5:DG:C5'      | 2.46                     | 0.45              |
| 3:E:19:DG:C1'     | 3:E:20:DG:OP1     | 2.62                     | 0.45              |
| 4:A:523:VAL:O     | 4:A:527:GLN:HG3   | 2.16                     | 0.45              |
| 4:B:300:ALA:HB2   | 4:B:333:LEU:CD1   | 2.43                     | 0.45              |
| 4:B:671:MET:HA    | 4:B:800:MET:O     | 2.16                     | 0.45              |
| 4:B:847:ASN:OD1   | 4:B:860:ARG:NH1   | 2.49                     | 0.45              |
| 4:B:993:THR:HA    | 4:B:1010:ILE:HD13 | 1.95                     | 0.45              |
| 4:B:1144:LEU:HD11 | 4:B:1162:VAL:HG12 | 1.97                     | 0.45              |
| 5:F:346:ASP:HB3   | 5:F:349:ASP:HB3   | 1.97                     | 0.45              |
| 5:F:378:GLU:OE2   | 5:F:387:TRP:NE1   | 2.48                     | 0.45              |
| 4:B:363:GLN:HB3   | 4:B:364:LEU:CA    | 2.45                     | 0.45              |
| 4:B:416:SER:HB3   | 4:B:637:PRO:C     | 2.42                     | 0.45              |
| 5:F:181:VAL:HB    | 5:F:182:PRO:HD2   | 1.99                     | 0.45              |
| 1:G:85:ALA:CB     | 2:H:20:DC:H4'     | 2.46                     | 0.45              |
| 1:G:186:LYS:HD2   | 1:G:190:LYS:HE2   | 1.99                     | 0.45              |
| 4:A:235:LEU:HD13  | 4:A:512:HIS:NE2   | 2.32                     | 0.45              |
| 4:B:557:GLY:HA3   | 4:B:558:ALA:HA    | 1.58                     | 0.45              |
| 2:D:47:DG:H2''    | 2:D:48:DG:H8      | 1.79                     | 0.45              |
| 1:G:58:LEU:HD13   | 3:I:30:DG:N2      | 2.31                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:G:182:LEU:HD22  | 3:I:42:DG:C2      | 2.51                     | 0.45              |
| 1:G:210:ARG:HD2   | 1:G:210:ARG:C     | 2.42                     | 0.45              |
| 4:B:230:PHE:CD2   | 4:B:263:MET:HB3   | 2.51                     | 0.45              |
| 4:B:720:LEU:HD12  | 4:B:892:TRP:HZ2   | 1.80                     | 0.45              |
| 4:B:997:VAL:HG22  | 4:B:1033:VAL:HG13 | 1.99                     | 0.45              |
| 4:B:1204:LEU:O    | 4:B:1208:LEU:HG   | 2.16                     | 0.45              |
| 5:F:247:TYR:OH    | 5:F:252:VAL:HG22  | 2.16                     | 0.45              |
| 3:E:19:DG:C4'     | 3:E:20:DG:OP1     | 2.63                     | 0.45              |
| 1:G:148:GLU:O     | 1:G:152:LEU:HG    | 2.17                     | 0.45              |
| 4:A:456:LEU:HD22  | 4:A:466:SER:HB2   | 1.98                     | 0.45              |
| 4:A:562:LEU:HD23  | 4:A:562:LEU:C     | 2.41                     | 0.45              |
| 4:A:1041:GLN:HG2  | 4:A:1048:ARG:HB2  | 1.97                     | 0.45              |
| 4:B:141:LYS:O     | 4:B:145:GLN:HG3   | 2.16                     | 0.45              |
| 4:B:522:GLN:OE1   | 4:B:561:ALA:HB1   | 2.17                     | 0.45              |
| 4:B:956:TYR:CZ    | 4:B:991:LYS:HG3   | 2.52                     | 0.45              |
| 4:B:1084:LEU:HD11 | 4:B:1111:ASN:CG   | 2.42                     | 0.45              |
| 5:F:127:LYS:HG3   | 5:F:130:ILE:HD12  | 1.98                     | 0.45              |
| 5:F:351:LEU:HA    | 5:F:354:ILE:HG12  | 1.98                     | 0.45              |
| 4:A:470:PHE:HA    | 4:A:473:LEU:HG    | 1.99                     | 0.45              |
| 4:A:594:ASP:OD2   | 4:A:633:LYS:NZ    | 2.28                     | 0.45              |
| 4:A:993:THR:O     | 4:A:996:THR:HB    | 2.17                     | 0.45              |
| 4:B:419:LYS:HD3   | 4:B:635:ALA:CB    | 2.46                     | 0.45              |
| 4:B:644:VAL:HA    | 4:B:663:PHE:CE2   | 2.52                     | 0.45              |
| 1:G:157:ARG:HH12  | 2:H:5:DG:N2       | 2.14                     | 0.45              |
| 3:I:16:DT:H2''    | 3:I:17:DT:H71     | 1.99                     | 0.45              |
| 4:A:347:VAL:O     | 4:A:351:VAL:HG23  | 2.16                     | 0.45              |
| 4:B:425:LYS:HZ2   | 4:B:428:LYS:HD3   | 1.81                     | 0.45              |
| 4:B:497:PHE:CE2   | 4:B:577:LYS:HG2   | 2.52                     | 0.45              |
| 4:B:1023:GLU:HG3  | 4:B:1024:PHE:CD2  | 2.51                     | 0.45              |
| 4:B:1072:THR:HG22 | 4:B:1126:SER:HB2  | 1.99                     | 0.45              |
| 5:F:365:MET:HB2   | 5:F:370:PHE:CZ    | 2.52                     | 0.45              |
| 3:E:3:DC:H2''     | 3:E:4:DC:C5       | 2.52                     | 0.45              |
| 2:H:46:DA:OP1     | 4:B:1059:ARG:NH2  | 2.49                     | 0.45              |
| 4:A:1041:GLN:CD   | 4:A:1048:ARG:HD2  | 2.42                     | 0.45              |
| 4:A:1043:MET:HG3  | 4:A:1044:PHE:CE2  | 2.51                     | 0.45              |
| 4:B:492:ALA:HB1   | 4:B:628:VAL:CG2   | 2.47                     | 0.45              |
| 5:F:89:LEU:CD1    | 5:F:116:ALA:HB1   | 2.39                     | 0.45              |
| 5:F:164:PRO:N     | 5:F:165:PRO:HD2   | 2.32                     | 0.45              |
| 2:D:12:DA:H2''    | 2:D:13:DC:O5'     | 2.17                     | 0.45              |
| 3:E:41:DA:H2'     | 3:E:42:DG:H8      | 1.77                     | 0.45              |
| 4:B:648:MET:SD    | 4:B:797:PRO:HG3   | 2.56                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:B:993:THR:HG21  | 4:B:1036:VAL:HG21 | 1.99                     | 0.45              |
| 4:B:1013:ARG:HH21 | 4:B:1016:GLU:CD   | 2.25                     | 0.45              |
| 5:F:85:ALA:O      | 5:F:89:LEU:HG     | 2.17                     | 0.45              |
| 5:F:189:LEU:HG    | 5:F:190:LYS:N     | 2.32                     | 0.45              |
| 5:F:236:LYS:HG2   | 5:F:246:LEU:HD22  | 1.98                     | 0.45              |
| 5:J:366:HIS:O     | 5:J:369:ASP:HB2   | 2.17                     | 0.45              |
| 1:G:122:THR:HB    | 1:G:123:PRO:CD    | 2.46                     | 0.45              |
| 4:A:1195:PRO:O    | 4:A:1198:ILE:HG13 | 2.17                     | 0.45              |
| 4:B:562:LEU:HD23  | 4:B:562:LEU:C     | 2.42                     | 0.45              |
| 4:B:948:PRO:HD3   | 4:B:1221:GLN:HB3  | 1.98                     | 0.45              |
| 4:B:1188:VAL:O    | 4:B:1192:CYS:HB2  | 2.17                     | 0.45              |
| 5:F:323:LEU:C     | 5:F:323:LEU:HD23  | 2.41                     | 0.45              |
| 5:J:205:TRP:CD2   | 5:J:250:LEU:HD21  | 2.52                     | 0.45              |
| 1:G:58:LEU:HG     | 3:I:31:DG:C4      | 2.52                     | 0.44              |
| 4:A:232:CYS:SG    | 4:A:473:LEU:HD21  | 2.57                     | 0.44              |
| 4:A:1028:ALA:O    | 4:A:1032:LEU:HG   | 2.17                     | 0.44              |
| 4:A:1083:ARG:O    | 4:A:1084:LEU:HD23 | 2.17                     | 0.44              |
| 4:B:244:HIS:O     | 4:B:248:VAL:HG23  | 2.17                     | 0.44              |
| 4:B:612:PHE:CZ    | 5:J:326:HIS:HA    | 2.51                     | 0.44              |
| 1:C:113:GLU:HG2   | 1:C:116:ARG:NH2   | 2.30                     | 0.44              |
| 2:H:36:DT:H71     | 5:J:201:LYS:HZ3   | 1.81                     | 0.44              |
| 4:A:418:GLU:CD    | 4:A:722:GLN:CG    | 2.88                     | 0.44              |
| 4:A:1129:SER:O    | 4:A:1133:MET:HG3  | 2.17                     | 0.44              |
| 4:B:265:ASN:HB3   | 4:B:297:LEU:HD23  | 2.00                     | 0.44              |
| 4:B:1195:PRO:O    | 4:B:1198:ILE:HG13 | 2.17                     | 0.44              |
| 5:J:189:LEU:HG    | 5:J:190:LYS:N     | 2.32                     | 0.44              |
| 4:A:690:THR:HA    | 4:A:693:HIS:CD2   | 2.52                     | 0.44              |
| 4:B:416:SER:HB3   | 4:B:637:PRO:CA    | 2.45                     | 0.44              |
| 5:F:114:LEU:HD22  | 5:F:140:LEU:HD12  | 1.99                     | 0.44              |
| 5:F:126:ASP:HB3   | 5:F:129:PHE:HD2   | 1.82                     | 0.44              |
| 3:E:22:DT:H2''    | 3:E:23:DG:H8      | 1.81                     | 0.44              |
| 2:H:48:DG:H2''    | 2:H:49:DC:C6      | 2.52                     | 0.44              |
| 4:A:497:PHE:CD1   | 4:A:621:LEU:HD11  | 2.52                     | 0.44              |
| 4:A:607:TYR:HE2   | 4:A:624:HIS:HA    | 1.83                     | 0.44              |
| 2:H:49:DC:H2''    | 2:H:50:DC:C6      | 2.52                     | 0.44              |
| 4:A:300:ALA:CB    | 4:A:333:LEU:HD11  | 2.46                     | 0.44              |
| 4:A:549:PRO:HB2   | 4:A:700:THR:HG21  | 2.00                     | 0.44              |
| 4:B:252:GLN:HB2   | 4:B:255:LYS:HB2   | 1.99                     | 0.44              |
| 4:B:782:ARG:HD2   | 4:B:821:ALA:HB2   | 1.99                     | 0.44              |
| 5:F:164:PRO:CD    | 5:F:165:PRO:HD2   | 2.48                     | 0.44              |
| 5:J:127:LYS:HG3   | 5:J:130:ILE:HD12  | 2.00                     | 0.44              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:G:57:TYR:HD1   | 1:G:88:TRP:CG     | 2.35                     | 0.44              |
| 3:I:40:DT:C2     | 3:I:41:DA:N7      | 2.86                     | 0.44              |
| 4:A:801:ASP:OD1  | 4:A:805:ARG:N     | 2.50                     | 0.44              |
| 4:A:1053:TRP:HZ3 | 4:A:1180:LEU:HD22 | 1.83                     | 0.44              |
| 4:B:232:CYS:SG   | 4:B:473:LEU:HD11  | 2.58                     | 0.44              |
| 5:J:389:TYR:HB3  | 5:J:390:ASP:H     | 1.62                     | 0.44              |
| 3:E:21:DT:H2'    | 3:E:22:DT:H71     | 2.00                     | 0.44              |
| 1:G:56:SER:HB2   | 1:G:99:TYR:CB     | 2.48                     | 0.44              |
| 4:A:592:SER:C    | 4:A:593:LEU:HD23  | 2.43                     | 0.44              |
| 4:A:662:ALA:HB3  | 4:A:668:THR:CG2   | 2.48                     | 0.44              |
| 4:A:808:PRO:HD3  | 4:A:816:LEU:HD13  | 1.99                     | 0.44              |
| 4:A:1041:GLN:NE2 | 4:A:1048:ARG:HH11 | 2.16                     | 0.44              |
| 4:B:306:MET:CE   | 4:B:315:THR:HG22  | 2.48                     | 0.44              |
| 4:B:1164:ASN:HB3 | 4:B:1168:ARG:NH1  | 2.32                     | 0.44              |
| 5:F:194:MET:HG2  | 5:F:228:PHE:HD2   | 1.82                     | 0.44              |
| 5:F:380:SER:O    | 5:F:386:LYS:HE2   | 2.18                     | 0.44              |
| 5:J:85:ALA:HA    | 5:J:113:LEU:HD23  | 1.98                     | 0.44              |
| 5:J:391:GLU:HG2  | 5:J:392:THR:O     | 2.18                     | 0.44              |
| 3:E:16:DT:H2''   | 3:E:17:DT:H71     | 2.00                     | 0.44              |
| 3:E:21:DT:C2     | 3:E:22:DT:C5      | 3.06                     | 0.44              |
| 3:E:22:DT:H2''   | 3:E:23:DG:C8      | 2.51                     | 0.44              |
| 1:G:147:LYS:O    | 1:G:151:LEU:HB2   | 2.17                     | 0.44              |
| 4:A:391:LEU:HD22 | 4:A:395:THR:HG21  | 1.99                     | 0.44              |
| 4:B:523:VAL:O    | 4:B:527:GLN:HG3   | 2.17                     | 0.44              |
| 4:B:614:ASN:C    | 4:B:616:GLN:N     | 2.75                     | 0.44              |
| 4:B:994:VAL:HG13 | 4:B:1040:LEU:HD11 | 2.00                     | 0.44              |
| 5:J:164:PRO:N    | 5:J:165:PRO:HD2   | 2.33                     | 0.44              |
| 5:J:227:MET:O    | 5:J:299:ILE:HG12  | 2.18                     | 0.44              |
| 3:E:19:DG:H4'    | 3:E:20:DG:OP2     | 2.18                     | 0.44              |
| 1:G:207:ASP:CG   | 1:G:210:ARG:HH21  | 2.25                     | 0.44              |
| 1:G:219:GLU:O    | 1:G:223:ILE:HG12  | 2.18                     | 0.44              |
| 3:I:4:DC:C2'     | 3:I:5:DT:H72      | 2.47                     | 0.44              |
| 4:B:655:TRP:CE3  | 4:B:670:LEU:HD13  | 2.52                     | 0.44              |
| 4:B:713:VAL:O    | 4:B:717:VAL:HG23  | 2.18                     | 0.44              |
| 4:B:967:ARG:NH2  | 4:B:982:GLU:HG3   | 2.32                     | 0.44              |
| 1:C:210:ARG:C    | 1:C:210:ARG:HD2   | 2.43                     | 0.43              |
| 4:A:1150:HIS:CD2 | 4:A:1151:ASP:H    | 2.36                     | 0.43              |
| 4:B:981:LEU:HD23 | 4:B:1020:PHE:HE2  | 1.83                     | 0.43              |
| 4:B:993:THR:HG22 | 4:B:1036:VAL:HG21 | 1.99                     | 0.43              |
| 3:E:17:DT:H2''   | 3:E:18:DT:C6      | 2.53                     | 0.43              |
| 2:H:16:DC:H2''   | 2:H:17:DA:H8      | 1.83                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:B:241:LEU:HD11  | 4:B:460:VAL:HG11  | 1.99                     | 0.43              |
| 5:F:326:HIS:CG    | 5:F:342:LEU:HD21  | 2.53                     | 0.43              |
| 2:H:32:DC:H2''    | 2:H:33:DA:H8      | 1.82                     | 0.43              |
| 3:I:25:DT:H2''    | 3:I:26:DT:H72     | 2.01                     | 0.43              |
| 4:A:392:PRO:HG2   | 4:A:395:THR:OG1   | 2.18                     | 0.43              |
| 4:A:404:LEU:O     | 4:A:408:LEU:HG    | 2.18                     | 0.43              |
| 4:A:445:LEU:HD21  | 4:A:583:LEU:HD12  | 2.01                     | 0.43              |
| 4:A:701:GLN:CD    | 4:A:1140:TYR:HB2  | 2.43                     | 0.43              |
| 4:A:897:CYS:O     | 4:A:901:VAL:HG23  | 2.19                     | 0.43              |
| 4:A:941:ALA:O     | 4:A:946:LEU:N     | 2.49                     | 0.43              |
| 4:A:1060:LEU:HD11 | 4:A:1207:THR:HG21 | 2.00                     | 0.43              |
| 4:A:1070:TRP:CE2  | 4:A:1078:VAL:HB   | 2.54                     | 0.43              |
| 4:B:584:VAL:HG22  | 4:B:606:LEU:CD1   | 2.48                     | 0.43              |
| 4:B:592:SER:HB2   | 4:B:599:SER:CB    | 2.35                     | 0.43              |
| 4:B:897:CYS:HA    | 4:B:917:LEU:CD2   | 2.48                     | 0.43              |
| 1:C:91:LEU:HG     | 1:C:95:LYS:HB2    | 2.00                     | 0.43              |
| 4:A:271:TRP:O     | 4:A:275:GLY:N     | 2.50                     | 0.43              |
| 4:A:862:ALA:O     | 4:A:866:GLU:HG3   | 2.18                     | 0.43              |
| 4:A:1031:TYR:O    | 4:A:1035:GLN:HG2  | 2.18                     | 0.43              |
| 4:A:1059:ARG:HG2  | 4:A:1116:LYS:HB2  | 2.01                     | 0.43              |
| 4:B:284:LEU:O     | 4:B:287:VAL:HB    | 2.19                     | 0.43              |
| 4:B:422:LEU:HD22  | 4:B:423:PRO:CD    | 2.29                     | 0.43              |
| 2:D:36:DT:C2'     | 2:D:37:DT:H5''    | 2.42                     | 0.43              |
| 3:I:33:DA:H2''    | 3:I:34:DT:C6      | 2.53                     | 0.43              |
| 3:I:42:DG:H2''    | 3:I:43:DC:OP1     | 2.18                     | 0.43              |
| 4:A:219:LEU:HD12  | 4:A:224:GLN:NE2   | 2.33                     | 0.43              |
| 4:B:870:ASP:OD1   | 4:B:882:ARG:NH1   | 2.51                     | 0.43              |
| 1:G:57:TYR:HE2    | 2:H:20:DC:O2      | 2.00                     | 0.43              |
| 2:H:16:DC:H2''    | 2:H:17:DA:C8      | 2.53                     | 0.43              |
| 4:A:996:THR:OG1   | 4:A:1010:ILE:HD11 | 2.18                     | 0.43              |
| 4:B:404:LEU:O     | 4:B:408:LEU:HG    | 2.18                     | 0.43              |
| 4:B:1070:TRP:CZ2  | 4:B:1078:VAL:HG11 | 2.53                     | 0.43              |
| 3:E:16:DT:C6      | 3:E:16:DT:OP1     | 2.72                     | 0.43              |
| 3:I:32:DT:H2''    | 3:I:33:DA:N7      | 2.34                     | 0.43              |
| 4:A:498:THR:HG23  | 4:A:573:MET:HE1   | 2.01                     | 0.43              |
| 4:A:935:GLY:HA3   | 4:A:1050:ILE:HD11 | 2.00                     | 0.43              |
| 4:B:418:GLU:HB2   | 4:B:780:LEU:HD13  | 2.01                     | 0.43              |
| 2:D:32:DC:H2''    | 2:D:33:DA:H8      | 1.83                     | 0.43              |
| 2:D:46:DA:H2''    | 2:D:47:DG:H8      | 1.82                     | 0.43              |
| 4:B:563:ARG:HH12  | 4:B:685:GLU:HG3   | 1.84                     | 0.43              |
| 5:J:346:ASP:HB3   | 5:J:349:ASP:CB    | 2.49                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:I:2:DG:H2''     | 3:I:3:DC:C6       | 2.53                     | 0.43              |
| 4:A:422:LEU:HB3   | 4:A:427:VAL:HG21  | 2.01                     | 0.43              |
| 4:A:961:ALA:O     | 4:A:965:VAL:HG13  | 2.18                     | 0.43              |
| 4:A:975:MET:O     | 4:A:979:GLN:HG3   | 2.18                     | 0.43              |
| 4:A:1157:ALA:HA   | 4:A:1160:VAL:HG23 | 2.00                     | 0.43              |
| 4:B:852:LYS:HE3   | 4:B:863:PHE:CD1   | 2.54                     | 0.43              |
| 2:D:6:DC:C2'      | 2:D:7:DT:H71      | 2.48                     | 0.43              |
| 3:E:1:DG:H2''     | 3:E:2:DG:H8       | 1.78                     | 0.43              |
| 3:E:37:DG:C2'     | 3:E:38:DG:C8      | 3.02                     | 0.43              |
| 2:H:34:DA:H2''    | 2:H:35:DA:H8      | 1.81                     | 0.43              |
| 3:I:18:DT:H2''    | 3:I:19:DG:H8      | 1.84                     | 0.43              |
| 4:A:141:LYS:O     | 4:A:145:GLN:HG3   | 2.19                     | 0.43              |
| 4:A:276:ALA:HB1   | 4:A:279:GLU:OE1   | 2.19                     | 0.43              |
| 4:A:1059:ARG:HG2  | 4:A:1116:LYS:HD3  | 2.01                     | 0.43              |
| 4:B:397:GLN:O     | 4:B:401:GLU:HG2   | 2.19                     | 0.43              |
| 4:B:592:SER:C     | 4:B:593:LEU:HD23  | 2.44                     | 0.43              |
| 4:A:339:LEU:HB3   | 4:A:343:ASP:HB2   | 2.01                     | 0.42              |
| 4:B:651:PRO:HA    | 4:B:652:PRO:HD3   | 1.92                     | 0.42              |
| 4:B:897:CYS:O     | 4:B:901:VAL:HG23  | 2.19                     | 0.42              |
| 2:D:1:DC:H2''     | 2:D:2:DA:H8       | 1.84                     | 0.42              |
| 4:A:374:LEU:HB3   | 4:A:378:TYR:CE2   | 2.54                     | 0.42              |
| 4:A:384:VAL:HG21  | 4:A:546:PRO:HB2   | 2.02                     | 0.42              |
| 4:A:1041:GLN:CG   | 4:A:1048:ARG:HD2  | 2.49                     | 0.42              |
| 4:B:369:ASN:HB3   | 4:B:378:TYR:CD2   | 2.53                     | 0.42              |
| 4:B:373:LEU:HD13  | 4:B:1134:LEU:HD11 | 2.00                     | 0.42              |
| 4:B:456:LEU:HD22  | 4:B:466:SER:HB2   | 2.01                     | 0.42              |
| 4:B:1205:LYS:HE2  | 4:B:1209:GLN:HE22 | 1.83                     | 0.42              |
| 5:F:361:LYS:HB2   | 5:F:364:ASN:ND2   | 2.34                     | 0.42              |
| 2:D:13:DC:H2''    | 2:D:14:DC:C5      | 2.55                     | 0.42              |
| 2:H:6:DC:C2'      | 2:H:7:DT:H71      | 2.48                     | 0.42              |
| 2:H:26:DA:H2''    | 2:H:27:DC:C5      | 2.55                     | 0.42              |
| 4:B:713:VAL:HG12  | 4:B:824:LEU:HD23  | 2.00                     | 0.42              |
| 4:B:1172:VAL:HG21 | 4:B:1223:LYS:HG3  | 2.01                     | 0.42              |
| 5:F:211:LEU:HD23  | 5:F:211:LEU:C     | 2.45                     | 0.42              |
| 5:J:267:PRO:HA    | 5:J:295:LYS:HA    | 2.01                     | 0.42              |
| 3:E:38:DG:H2'     | 3:E:39:DT:H71     | 2.01                     | 0.42              |
| 4:A:933:ALA:HB3   | 4:A:1175:HIS:CE1  | 2.55                     | 0.42              |
| 4:A:1151:ASP:OD1  | 4:A:1151:ASP:N    | 2.53                     | 0.42              |
| 4:B:230:PHE:CE2   | 4:B:263:MET:HB3   | 2.54                     | 0.42              |
| 4:B:320:LEU:HD22  | 4:B:330:LEU:HD21  | 2.02                     | 0.42              |
| 4:B:560:GLU:HA    | 4:B:560:GLU:OE1   | 2.19                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:B:977:VAL:HA    | 4:B:980:VAL:CG2   | 2.48                     | 0.42              |
| 4:B:1084:LEU:HD21 | 4:B:1111:ASN:HD22 | 1.85                     | 0.42              |
| 4:A:497:PHE:HD1   | 4:A:621:LEU:HD11  | 1.84                     | 0.42              |
| 4:A:518:ARG:HA    | 4:A:523:VAL:CG2   | 2.50                     | 0.42              |
| 4:B:331:GLN:HG2   | 4:B:358:PHE:CZ    | 2.55                     | 0.42              |
| 5:J:193:GLY:O     | 5:J:227:MET:HA    | 2.19                     | 0.42              |
| 1:G:68:PHE:HB3    | 1:G:80:LEU:HD22   | 2.00                     | 0.42              |
| 1:G:182:LEU:HB2   | 3:I:42:DG:H21     | 1.83                     | 0.42              |
| 4:A:265:ASN:HD21  | 4:A:295:ASP:CG    | 2.27                     | 0.42              |
| 4:A:418:GLU:OE1   | 4:A:418:GLU:HA    | 2.19                     | 0.42              |
| 4:A:699:LEU:HD11  | 4:A:800:MET:HG3   | 2.02                     | 0.42              |
| 4:A:974:GLY:HA2   | 4:A:979:GLN:NE2   | 2.34                     | 0.42              |
| 4:A:1196:GLN:HA   | 4:A:1197:LYS:HA   | 1.75                     | 0.42              |
| 4:B:425:LYS:O     | 4:B:428:LYS:HB2   | 2.19                     | 0.42              |
| 4:B:562:LEU:HD23  | 4:B:563:ARG:C     | 2.45                     | 0.42              |
| 4:B:849:THR:HG22  | 4:B:894:THR:HG21  | 2.02                     | 0.42              |
| 5:J:231:GLU:OE2   | 5:J:297:TYR:OH    | 2.28                     | 0.42              |
| 2:D:28:DC:H2''    | 2:D:29:DA:H8      | 1.85                     | 0.42              |
| 2:D:48:DG:H2''    | 2:D:49:DC:C6      | 2.53                     | 0.42              |
| 2:H:11:DA:H2'     | 2:H:12:DA:C8      | 2.54                     | 0.42              |
| 2:H:36:DT:H71     | 5:J:201:LYS:HZ2   | 1.84                     | 0.42              |
| 3:I:39:DT:H2'     | 3:I:40:DT:C7      | 2.49                     | 0.42              |
| 4:A:589:MET:CB    | 4:A:605:VAL:HG22  | 2.49                     | 0.42              |
| 2:D:33:DA:H2''    | 2:D:34:DA:H8      | 1.85                     | 0.42              |
| 3:E:25:DT:H5''    | 4:A:254:GLN:HG2   | 2.02                     | 0.42              |
| 1:G:54:VAL:HG22   | 3:I:31:DG:H5'     | 2.01                     | 0.42              |
| 4:B:967:ARG:NH1   | 4:B:982:GLU:HB2   | 2.35                     | 0.42              |
| 2:D:15:DC:H2''    | 2:D:16:DC:H5      | 1.85                     | 0.42              |
| 3:E:23:DG:C2'     | 3:E:24:DG:H5''    | 2.50                     | 0.42              |
| 4:A:510:SER:O     | 4:A:514:VAL:HG23  | 2.18                     | 0.42              |
| 4:A:948:PRO:HD3   | 4:A:1221:GLN:HB3  | 2.02                     | 0.42              |
| 4:B:1070:TRP:CE3  | 4:B:1119:PHE:HE1  | 2.38                     | 0.42              |
| 4:B:1084:LEU:HD21 | 4:B:1111:ASN:ND2  | 2.35                     | 0.42              |
| 4:B:1147:VAL:HG22 | 4:B:1154:TRP:HB2  | 2.01                     | 0.42              |
| 5:J:312:LEU:HD23  | 5:J:371:LYS:HE3   | 2.01                     | 0.42              |
| 3:I:21:DT:C2      | 3:I:22:DT:H72     | 2.54                     | 0.42              |
| 4:A:468:TYR:N     | 4:A:469:PRO:HD2   | 2.35                     | 0.42              |
| 4:A:614:ASN:C     | 4:A:616:GLN:N     | 2.78                     | 0.42              |
| 4:A:813:PHE:CZ    | 4:A:825:LEU:HD21  | 2.54                     | 0.42              |
| 4:B:296:LEU:HG    | 4:B:328:LEU:HD22  | 2.01                     | 0.42              |
| 4:B:414:VAL:HG13  | 4:B:788:HIS:HB2   | 2.02                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:121:LEU:HB2  | 1:C:125:GLN:CB    | 2.50                     | 0.41              |
| 2:H:35:DA:H2''   | 2:H:36:DT:H5'     | 2.02                     | 0.41              |
| 4:A:241:LEU:CD1  | 4:A:460:VAL:HG11  | 2.48                     | 0.41              |
| 4:B:400:PHE:HE1  | 4:B:664:LEU:HD13  | 1.84                     | 0.41              |
| 5:J:349:ASP:HA   | 5:J:352:MET:HE3   | 2.02                     | 0.41              |
| 5:J:361:LYS:HB2  | 5:J:364:ASN:ND2   | 2.35                     | 0.41              |
| 1:C:107:TRP:CE2  | 2:D:24:DG:H5''    | 2.55                     | 0.41              |
| 1:G:170:PHE:CE2  | 2:H:10:DT:H4'     | 2.53                     | 0.41              |
| 4:B:491:PRO:HB2  | 4:B:493:GLN:NE2   | 2.35                     | 0.41              |
| 4:B:845:LEU:HB2  | 4:B:897:CYS:SG    | 2.60                     | 0.41              |
| 4:B:961:ALA:O    | 4:B:965:VAL:HG13  | 2.19                     | 0.41              |
| 4:B:966:PHE:HB3  | 4:B:1035:GLN:HE21 | 1.85                     | 0.41              |
| 4:B:1022:GLN:O   | 4:B:1025:VAL:HG12 | 2.20                     | 0.41              |
| 5:F:164:PRO:CG   | 5:F:165:PRO:CD    | 2.98                     | 0.41              |
| 5:J:136:LEU:O    | 5:J:139:ASN:HB2   | 2.20                     | 0.41              |
| 5:J:258:CYS:SG   | 5:J:303:PRO:HA    | 2.60                     | 0.41              |
| 3:E:28:DG:H2''   | 3:E:29:DG:C8      | 2.54                     | 0.41              |
| 3:I:21:DT:C2     | 3:I:22:DT:C5      | 3.08                     | 0.41              |
| 4:B:371:SER:HB3  | 4:B:374:LEU:HB2   | 2.01                     | 0.41              |
| 4:B:658:PRO:HA   | 4:B:670:LEU:HB2   | 2.01                     | 0.41              |
| 2:D:19:DA:H62    | 2:D:20:DC:N4      | 2.19                     | 0.41              |
| 4:A:388:LYS:HD3  | 4:A:538:ALA:O     | 2.20                     | 0.41              |
| 4:B:389:LEU:O    | 4:B:539:SER:HB3   | 2.21                     | 0.41              |
| 5:F:162:ILE:O    | 5:F:162:ILE:HG22  | 2.20                     | 0.41              |
| 5:F:372:THR:O    | 5:F:376:THR:OG1   | 2.33                     | 0.41              |
| 1:C:147:LYS:NZ   | 2:D:16:DC:H4'     | 2.35                     | 0.41              |
| 4:A:624:HIS:HD2  | 4:A:626:ALA:HB3   | 1.86                     | 0.41              |
| 4:B:300:ALA:CA   | 4:B:333:LEU:HD11  | 2.50                     | 0.41              |
| 4:B:304:GLN:HG2  | 4:B:308:ARG:HH12  | 1.86                     | 0.41              |
| 4:B:400:PHE:CE1  | 4:B:664:LEU:HD13  | 2.56                     | 0.41              |
| 4:B:662:ALA:HB3  | 4:B:668:THR:HG21  | 2.02                     | 0.41              |
| 4:B:683:LEU:HD12 | 4:B:1079:ILE:CD1  | 2.50                     | 0.41              |
| 4:B:844:HIS:CB   | 4:B:919:VAL:HG13  | 2.49                     | 0.41              |
| 4:B:1108:ARG:N   | 4:B:1108:ARG:HD3  | 2.36                     | 0.41              |
| 5:F:83:THR:O     | 5:F:87:ILE:HG13   | 2.21                     | 0.41              |
| 1:C:192:LEU:HB2  | 1:C:197:LYS:HE3   | 2.02                     | 0.41              |
| 4:B:497:PHE:HE2  | 4:B:577:LYS:HG2   | 1.86                     | 0.41              |
| 4:B:728:GLN:CD   | 4:B:728:GLN:H     | 2.28                     | 0.41              |
| 5:J:162:ILE:O    | 5:J:162:ILE:HG22  | 2.20                     | 0.41              |
| 5:J:187:ILE:HD13 | 5:J:224:GLU:HB2   | 2.03                     | 0.41              |
| 1:G:77:THR:HG21  | 3:I:33:DA:N3      | 2.36                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:B:1116:LYS:NZ  | 4:B:1117:ASN:OD1  | 2.49                     | 0.41              |
| 5:J:104:PRO:HG3  | 5:J:122:ALA:HB1   | 2.03                     | 0.41              |
| 5:J:211:LEU:C    | 5:J:211:LEU:HD23  | 2.45                     | 0.41              |
| 4:A:136:ARG:O    | 4:A:140:LEU:HG    | 2.21                     | 0.41              |
| 4:A:701:GLN:NE2  | 4:A:1140:TYR:HB2  | 2.36                     | 0.41              |
| 4:A:799:ASN:O    | 4:A:806:THR:HA    | 2.21                     | 0.41              |
| 4:B:127:GLU:O    | 4:B:131:ARG:HG3   | 2.20                     | 0.41              |
| 4:B:220:SER:O    | 4:B:224:GLN:HG3   | 2.20                     | 0.41              |
| 4:B:716:LEU:CD1  | 4:B:895:LEU:HD21  | 2.51                     | 0.41              |
| 4:B:928:LEU:HG   | 4:B:998:VAL:HG21  | 2.03                     | 0.41              |
| 4:B:975:MET:HE1  | 4:B:1031:TYR:CD1  | 2.56                     | 0.41              |
| 4:B:1196:GLN:HA  | 4:B:1197:LYS:HA   | 1.74                     | 0.41              |
| 5:J:89:LEU:CD1   | 5:J:116:ALA:HB1   | 2.51                     | 0.41              |
| 5:J:104:PRO:HD2  | 5:J:124:GLU:OE1   | 2.20                     | 0.41              |
| 2:D:35:DA:H3'    | 5:F:201:LYS:HZ1   | 1.86                     | 0.41              |
| 2:D:37:DT:C5     | 5:F:202:ARG:HD3   | 2.57                     | 0.41              |
| 1:G:58:LEU:HD13  | 3:I:30:DG:C2      | 2.56                     | 0.41              |
| 1:G:215:MET:HB3  | 1:G:232:ARG:CZ    | 2.51                     | 0.41              |
| 4:A:378:TYR:OH   | 4:A:693:HIS:HB3   | 2.21                     | 0.41              |
| 4:A:1043:MET:HE2 | 4:A:1044:PHE:CZ   | 2.56                     | 0.41              |
| 4:B:363:GLN:CB   | 4:B:364:LEU:HA    | 2.49                     | 0.41              |
| 4:B:369:ASN:HB3  | 4:B:378:TYR:CE2   | 2.56                     | 0.41              |
| 4:B:622:LYS:HG3  | 4:B:623:PRO:HD2   | 2.02                     | 0.41              |
| 2:D:36:DT:C4     | 2:D:37:DT:H73     | 2.55                     | 0.40              |
| 1:G:56:SER:HB2   | 1:G:99:TYR:HB2    | 2.03                     | 0.40              |
| 4:A:399:LEU:HB3  | 4:A:649:LEU:O     | 2.20                     | 0.40              |
| 4:B:363:GLN:HB3  | 4:B:364:LEU:HA    | 2.02                     | 0.40              |
| 4:B:418:GLU:HG3  | 4:B:721:PHE:HE2   | 1.84                     | 0.40              |
| 4:B:840:TRP:CZ3  | 4:B:1160:VAL:HG11 | 2.56                     | 0.40              |
| 5:F:124:GLU:HG3  | 5:F:126:ASP:O     | 2.21                     | 0.40              |
| 5:J:164:PRO:CD   | 5:J:165:PRO:HD2   | 2.51                     | 0.40              |
| 2:D:49:DC:H2''   | 2:D:50:DC:C6      | 2.56                     | 0.40              |
| 3:I:18:DT:H5''   | 5:J:330:ARG:HG2   | 2.03                     | 0.40              |
| 4:A:406:MET:HG3  | 4:A:412:VAL:HG22  | 2.02                     | 0.40              |
| 4:A:500:LEU:HD23 | 4:A:621:LEU:CD1   | 2.51                     | 0.40              |
| 4:A:718:LEU:O    | 4:A:722:GLN:N     | 2.25                     | 0.40              |
| 4:B:709:VAL:HG11 | 4:B:714:LEU:HD22  | 2.03                     | 0.40              |
| 1:C:181:LYS:O    | 1:C:185:VAL:HG23  | 2.22                     | 0.40              |
| 1:C:228:LYS:HA   | 1:C:231:LEU:HD13  | 2.04                     | 0.40              |
| 2:D:32:DC:H2''   | 2:D:33:DA:C8      | 2.55                     | 0.40              |
| 3:E:42:DG:H2''   | 3:E:43:DC:OP1     | 2.21                     | 0.40              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:A:363:GLN:HA   | 4:A:364:LEU:HA    | 1.90                     | 0.40              |
| 4:A:560:GLU:OE1  | 4:A:560:GLU:HA    | 2.20                     | 0.40              |
| 4:A:683:LEU:HD12 | 4:A:1079:ILE:CD1  | 2.51                     | 0.40              |
| 4:A:863:PHE:O    | 4:A:867:VAL:HG22  | 2.21                     | 0.40              |
| 4:A:919:VAL:O    | 4:A:1154:TRP:HA   | 2.21                     | 0.40              |
| 4:B:877:GLN:HB3  | 4:B:880:THR:OG1   | 2.21                     | 0.40              |
| 5:J:99:LEU:HD23  | 5:J:190:LYS:HB3   | 2.03                     | 0.40              |
| 5:J:130:ILE:CD1  | 5:J:148:HIS:HB2   | 2.51                     | 0.40              |
| 2:H:17:DA:H2''   | 2:H:18:DT:C5      | 2.56                     | 0.40              |
| 4:A:533:TYR:OH   | 4:A:549:PRO:HB3   | 2.21                     | 0.40              |
| 4:A:997:VAL:CG2  | 4:A:1033:VAL:HG13 | 2.52                     | 0.40              |
| 4:B:456:LEU:HD12 | 4:B:471:LEU:HD12  | 2.03                     | 0.40              |
| 4:B:715:ASP:O    | 4:B:719:GLN:HG3   | 2.20                     | 0.40              |
| 4:B:947:GLU:OE2  | 4:B:948:PRO:HD2   | 2.22                     | 0.40              |
| 5:F:366:HIS:O    | 5:F:369:ASP:HB2   | 2.22                     | 0.40              |
| 1:C:162:TYR:O    | 1:C:166:VAL:HG23  | 2.21                     | 0.40              |
| 2:H:44:DA:H2''   | 2:H:45:DC:C6      | 2.56                     | 0.40              |
| 3:I:19:DG:C4'    | 3:I:20:DG:OP1     | 2.66                     | 0.40              |
| 4:A:244:HIS:O    | 4:A:248:VAL:HG23  | 2.21                     | 0.40              |
| 4:A:715:ASP:O    | 4:A:719:GLN:HG3   | 2.21                     | 0.40              |
| 4:B:976:ARG:NH2  | 5:J:162:ILE:HG22  | 2.36                     | 0.40              |
| 5:F:349:ASP:HA   | 5:F:352:MET:HE2   | 1.99                     | 0.40              |
| 5:J:244:PRO:HB3  | 5:J:363:VAL:HG22  | 2.04                     | 0.40              |

All (2) 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) |
|---------------|-----------------------|--------------------------|-------------------|
| 2:D:1:DC:O5'  | 1:G:233:ARG:O[2_654]  | 2.02                     | 0.18              |
| 3:I:40:DT:OP1 | 4:A:432:LYS:NZ[2_644] | 2.12                     | 0.08              |

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

The Analysed column shows the number of residues for which the backbone conformation was



analysed, and the total number of residues.

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1   | C     | 190/205 (93%)   | 185 (97%)  | 5 (3%)   | 0        | 100         | 100 |
| 1   | G     | 190/205 (93%)   | 186 (98%)  | 4 (2%)   | 0        | 100         | 100 |
| 4   | A     | 1001/1128 (89%) | 962 (96%)  | 39 (4%)  | 0        | 100         | 100 |
| 4   | B     | 990/1128 (88%)  | 949 (96%)  | 41 (4%)  | 0        | 100         | 100 |
| 5   | F     | 282/377 (75%)   | 272 (96%)  | 10 (4%)  | 0        | 100         | 100 |
| 5   | J     | 282/377 (75%)   | 272 (96%)  | 10 (4%)  | 0        | 100         | 100 |
| All | All   | 2935/3420 (86%) | 2826 (96%) | 109 (4%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1   | C     | 178/188 (95%)   | 177 (99%)  | 1 (1%)   | 78          | 80 |
| 1   | G     | 178/188 (95%)   | 177 (99%)  | 1 (1%)   | 78          | 80 |
| 4   | A     | 865/976 (89%)   | 860 (99%)  | 5 (1%)   | 78          | 80 |
| 4   | B     | 859/976 (88%)   | 854 (99%)  | 5 (1%)   | 78          | 80 |
| 5   | F     | 255/335 (76%)   | 254 (100%) | 1 (0%)   | 84          | 82 |
| 5   | J     | 255/335 (76%)   | 252 (99%)  | 3 (1%)   | 63          | 73 |
| All | All   | 2590/2998 (86%) | 2574 (99%) | 16 (1%)  | 78          | 80 |

All (16) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 58  | LEU  |
| 1   | G     | 58  | LEU  |
| 4   | A     | 422 | LEU  |
| 4   | A     | 614 | ASN  |
| 4   | A     | 680 | HIS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 4   | A     | 965  | VAL  |
| 4   | A     | 1151 | ASP  |
| 4   | B     | 417  | VAL  |
| 4   | B     | 422  | LEU  |
| 4   | B     | 614  | ASN  |
| 4   | B     | 680  | HIS  |
| 4   | B     | 965  | VAL  |
| 5   | F     | 157  | ARG  |
| 5   | J     | 157  | ARG  |
| 5   | J     | 388  | LEU  |
| 5   | J     | 391  | GLU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C     | 108  | GLN  |
| 1   | G     | 221  | GLN  |
| 4   | A     | 249  | HIS  |
| 4   | A     | 252  | GLN  |
| 4   | A     | 629  | GLN  |
| 4   | A     | 722  | GLN  |
| 4   | A     | 773  | HIS  |
| 4   | A     | 812  | HIS  |
| 4   | A     | 815  | HIS  |
| 4   | A     | 1170 | GLN  |
| 4   | B     | 429  | HIS  |
| 4   | B     | 624  | HIS  |
| 4   | B     | 701  | GLN  |
| 4   | B     | 728  | GLN  |
| 4   | B     | 787  | GLN  |
| 4   | B     | 815  | HIS  |
| 4   | B     | 893  | GLN  |
| 4   | B     | 916  | HIS  |
| 4   | B     | 1111 | ASN  |
| 4   | B     | 1156 | HIS  |
| 4   | B     | 1175 | HIS  |
| 4   | B     | 1181 | GLN  |
| 5   | F     | 97   | HIS  |
| 5   | F     | 103  | ASN  |
| 5   | F     | 322  | HIS  |
| 5   | F     | 353  | GLN  |
| 5   | F     | 364  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | J     | 103 | ASN  |
| 5   | J     | 148 | HIS  |
| 5   | J     | 264 | HIS  |
| 5   | J     | 300 | GLN  |
| 5   | J     | 364 | ASN  |
| 5   | J     | 368 | GLN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 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   | C     | 192/205 (93%)   | -0.14  | 3 (1%) 70 55  | 292, 364, 421, 433    | 0     |
| 1   | G     | 192/205 (93%)   | -0.27  | 2 (1%) 79 64  | 335, 409, 458, 512    | 0     |
| 2   | D     | 46/50 (92%)     | 0.06   | 0 100 100     | 344, 408, 562, 599    | 0     |
| 2   | H     | 46/50 (92%)     | 0.19   | 0 100 100     | 342, 419, 482, 500    | 0     |
| 3   | E     | 45/50 (90%)     | -0.04  | 0 100 100     | 329, 373, 481, 547    | 0     |
| 3   | I     | 45/50 (90%)     | 0.14   | 0 100 100     | 336, 408, 504, 549    | 0     |
| 4   | A     | 1011/1128 (89%) | 0.01   | 27 (2%) 56 44 | 225, 300, 360, 402    | 0     |
| 4   | B     | 1002/1128 (88%) | -0.06  | 21 (2%) 63 50 | 245, 308, 366, 420    | 0     |
| 5   | F     | 288/377 (76%)   | -0.20  | 4 (1%) 73 58  | 270, 328, 415, 455    | 0     |
| 5   | J     | 288/377 (76%)   | -0.18  | 2 (0%) 84 71  | 245, 320, 447, 510    | 0     |
| All | All   | 3155/3620 (87%) | -0.07  | 59 (1%) 66 52 | 225, 320, 426, 599    | 0     |

All (59) RSRZ outliers are listed below:

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 5   | F     | 339  | LEU  | 5.4  |
| 4   | A     | 815  | HIS  | 4.3  |
| 4   | B     | 1014 | LEU  | 4.2  |
| 4   | A     | 1032 | LEU  | 4.2  |
| 4   | A     | 1033 | VAL  | 4.1  |
| 4   | B     | 768  | VAL  | 3.8  |
| 5   | F     | 217  | ILE  | 3.7  |
| 1   | C     | 65   | LEU  | 3.5  |
| 4   | B     | 487  | LEU  | 3.4  |
| 4   | B     | 1057 | SER  | 3.3  |
| 4   | A     | 609  | VAL  | 3.3  |
| 4   | A     | 1029 | SER  | 3.3  |
| 4   | B     | 1032 | LEU  | 3.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 4   | B     | 994  | VAL  | 3.2  |
| 4   | A     | 998  | VAL  | 3.1  |
| 5   | F     | 172  | LEU  | 3.0  |
| 4   | A     | 1145 | THR  | 3.0  |
| 4   | A     | 994  | VAL  | 3.0  |
| 4   | A     | 582  | MET  | 3.0  |
| 4   | B     | 649  | LEU  | 3.0  |
| 5   | F     | 173  | PHE  | 2.9  |
| 5   | J     | 254  | TRP  | 2.9  |
| 4   | B     | 815  | HIS  | 2.8  |
| 4   | A     | 297  | LEU  | 2.8  |
| 4   | A     | 1040 | LEU  | 2.8  |
| 4   | B     | 1079 | ILE  | 2.6  |
| 1   | G     | 142  | ALA  | 2.6  |
| 4   | A     | 997  | VAL  | 2.6  |
| 4   | A     | 424  | SER  | 2.6  |
| 4   | B     | 818  | SER  | 2.5  |
| 4   | A     | 579  | LEU  | 2.5  |
| 4   | A     | 825  | LEU  | 2.5  |
| 1   | C     | 234  | THR  | 2.5  |
| 4   | A     | 471  | LEU  | 2.5  |
| 4   | A     | 928  | LEU  | 2.4  |
| 5   | J     | 204  | LEU  | 2.3  |
| 4   | A     | 500  | LEU  | 2.3  |
| 4   | B     | 796  | LEU  | 2.3  |
| 4   | A     | 1061 | ILE  | 2.3  |
| 4   | B     | 300  | ALA  | 2.3  |
| 4   | A     | 1010 | ILE  | 2.3  |
| 4   | B     | 330  | LEU  | 2.3  |
| 4   | B     | 563  | ARG  | 2.3  |
| 4   | A     | 1028 | ALA  | 2.2  |
| 4   | B     | 391  | LEU  | 2.2  |
| 1   | G     | 234  | THR  | 2.2  |
| 4   | A     | 1036 | VAL  | 2.2  |
| 4   | B     | 395  | THR  | 2.2  |
| 4   | B     | 630  | LEU  | 2.2  |
| 4   | A     | 689  | PRO  | 2.1  |
| 4   | B     | 627  | TYR  | 2.1  |
| 4   | A     | 559  | PRO  | 2.1  |
| 4   | B     | 621  | LEU  | 2.1  |
| 4   | A     | 1139 | CYS  | 2.1  |
| 4   | A     | 449  | LEU  | 2.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 4   | B     | 988 | LYS  | 2.1  |
| 1   | C     | 153 | GLY  | 2.0  |
| 4   | A     | 990 | VAL  | 2.0  |
| 4   | B     | 500 | LEU  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.