



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:30 AM UTC

PDB ID : 2FO1 / pdb\_00002fo1  
Title : Crystal Structure of the CSL-Notch-Mastermind ternary complex bound to DNA  
Authors : Wilson, J.J.; Kovall, R.A.  
Deposited on : 2006-01-12  
Resolution : 3.12 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

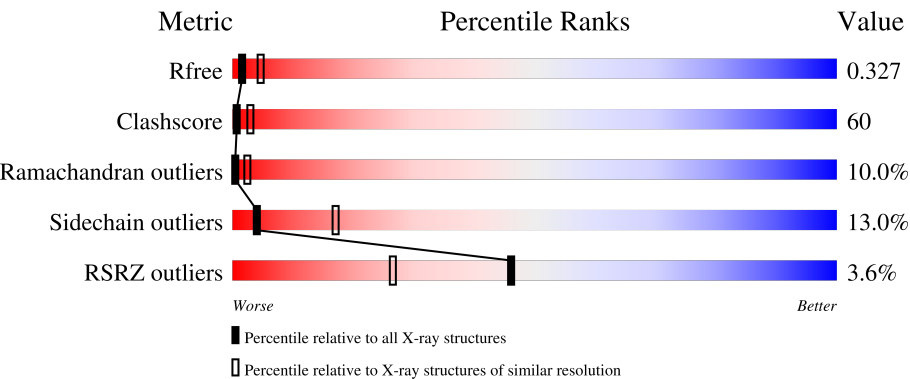
|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                             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

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.12 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                      | 1816 (3.14-3.10)                                      |
| Clashscore            | 190562                      | 1906 (3.14-3.10)                                      |
| Ramachandran outliers | 187476                      | 1802 (3.14-3.10)                                      |
| Sidechain outliers    | 187428                      | 1802 (3.14-3.10)                                      |
| RSRZ outliers         | 180081                      | 1816 (3.14-3.10)                                      |

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   | B     | 15     | <div><div></div><div></div><div></div><div></div><div></div></div> <div>33%60%7%</div>                   |
| 2   | C     | 15     | <div><div></div><div></div><div></div><div></div><div></div></div> <div>33%60%7%</div>                   |
| 3   | A     | 477    | <div><div></div><div></div><div></div><div></div><div></div><div></div></div> <div>3%32%45%13%•8%</div>  |
| 4   | D     | 85     | <div><div></div><div></div><div></div><div></div><div></div><div></div></div> <div>6%16%47%9%•26%</div>  |
| 5   | E     | 373    | <div><div></div><div></div><div></div><div></div><div></div><div></div></div> <div>2%15%43%19%•20%</div> |

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6939 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a DNA chain called 5'-D(\*TP\*TP\*AP\*CP\*TP\*GP\*TP\*GP\*GP\*GP\*AP\*AP\*AP\*GP\*A)-3'.

| Mol | Chain | Residues | Atoms |     |    |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|----|---------|---------|-------|
| 1   | B     | 15       | Total | C   | N  | O  | P  | 0       | 0       | 0     |
|     |       |          | 311   | 149 | 61 | 87 | 14 |         |         |       |

- Molecule 2 is a DNA chain called 5'-D(\*AP\*AP\*TP\*CP\*TP\*TP\*TP\*CP\*CP\*CP\*AP\*CP\*AP\*GP\*T)-3'.

| Mol | Chain | Residues | Atoms |     |    |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|----|---------|---------|-------|
| 2   | C     | 15       | Total | C   | N  | O  | P  | 0       | 0       | 0     |
|     |       |          | 298   | 145 | 50 | 89 | 14 |         |         |       |

- Molecule 3 is a protein called Lin-12 and glp-1 phenotype protein 1, isoform b.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 3   | A     | 439      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3497  | 2218 | 608 | 654 | 17 |         |         |       |

There are 5 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment          | Reference   |
|-------|---------|----------|--------|------------------|-------------|
| A     | 187     | GLY      | -      | cloning artifact | GB 22532887 |
| A     | 188     | PRO      | -      | cloning artifact | GB 22532887 |
| A     | 189     | LEU      | -      | cloning artifact | GB 22532887 |
| A     | 190     | GLY      | -      | cloning artifact | GB 22532887 |
| A     | 191     | SER      | -      | cloning artifact | GB 22532887 |

- Molecule 4 is a protein called Protein lag-3.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 4   | D     | 63       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 524   | 316 | 102 | 105 | 1 |         |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment          | Reference  |
|-------|---------|----------|--------|------------------|------------|
| D     | 48      | SER      | -      | cloning artifact | UNP Q09260 |

- Molecule 5 is a protein called Lin-12 protein.

| Mol | Chain | Residues | Atoms |      |     |     |   |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|----|---------|---------|-------|
| 5   | E     | 297      | Total | C    | N   | O   | S | Se | 0       | 0       | 0     |
|     |       |          | 2309  | 1420 | 427 | 445 | 3 | 14 |         |         |       |

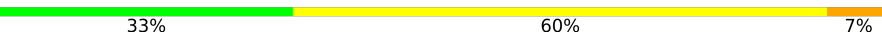
There are 16 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment          | Reference  |
|-------|---------|----------|--------|------------------|------------|
| E     | 929     | GLY      | -      | cloning artifact | UNP P14585 |
| E     | 930     | SER      | -      | cloning artifact | UNP P14585 |
| E     | 939     | MSE      | MET    | modified residue | UNP P14585 |
| E     | 946     | MSE      | MET    | modified residue | UNP P14585 |
| E     | 949     | MSE      | MET    | modified residue | UNP P14585 |
| E     | 1090    | MSE      | MET    | modified residue | UNP P14585 |
| E     | 1099    | MSE      | MET    | modified residue | UNP P14585 |
| E     | 1114    | MSE      | MET    | modified residue | UNP P14585 |
| E     | 1142    | MSE      | MET    | modified residue | UNP P14585 |
| E     | 1143    | MSE      | MET    | modified residue | UNP P14585 |
| E     | 1146    | MSE      | MET    | modified residue | UNP P14585 |
| E     | 1164    | MSE      | MET    | modified residue | UNP P14585 |
| E     | 1168    | MSE      | MET    | modified residue | UNP P14585 |
| E     | 1220    | MSE      | MET    | modified residue | UNP P14585 |
| E     | 1246    | MSE      | MET    | modified residue | UNP P14585 |
| E     | 1258    | MSE      | MET    | modified residue | UNP P14585 |

### 3 Residue-property plots

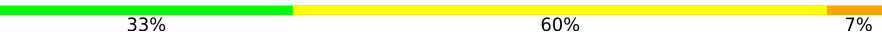
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

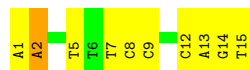
- Molecule 1: 5'-D(\*TP\*TP\*AP\*CP\*TP\*GP\*TP\*GP\*GP\*GP\*AP\*AP\*AP\*GP\*A)-3'

Chain B: 



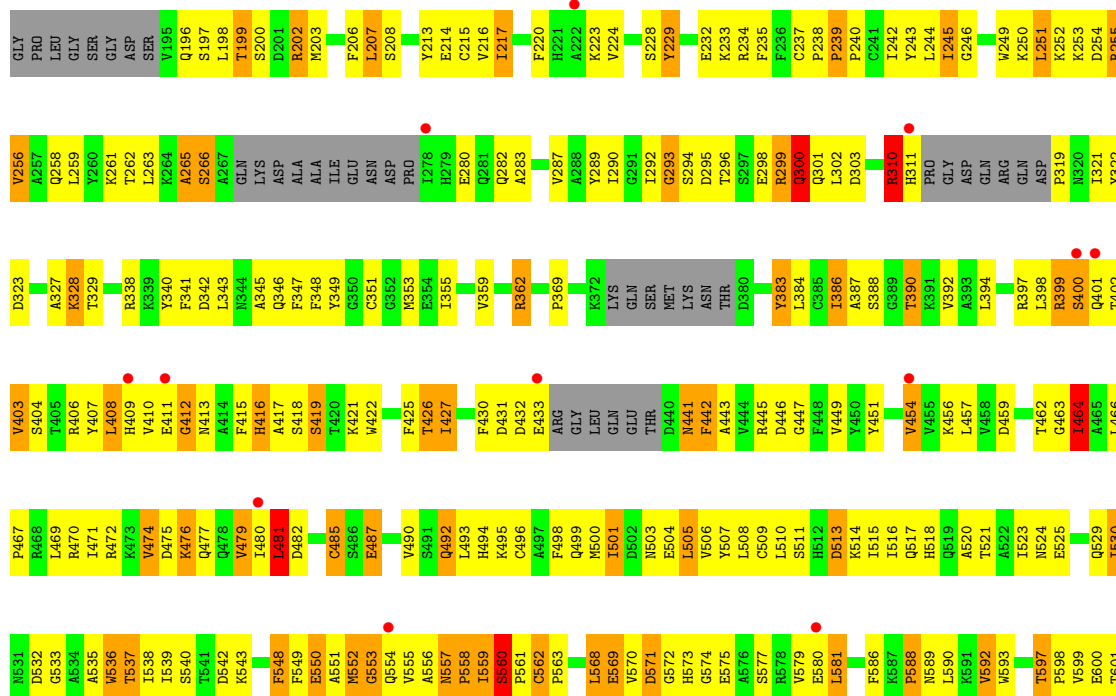
- Molecule 2: 5'-D(\*AP\*AP\*TP\*CP\*TP\*TP\*TP\*CP\*CP\*CP\*AP\*CP\*AP\*GP\*T)-3'

Chain C: 



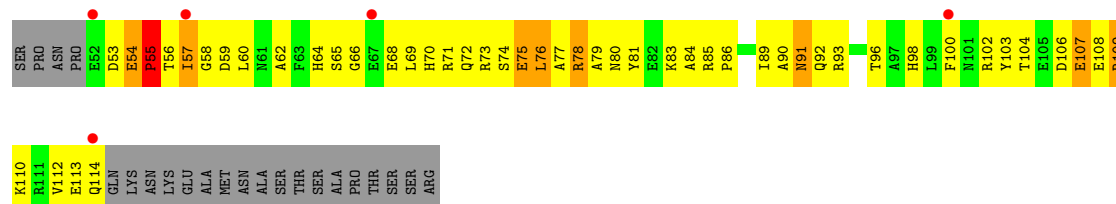
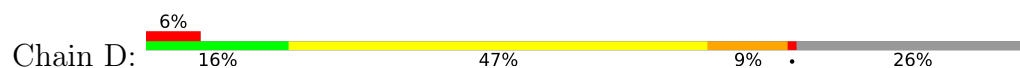
- Molecule 3: Lin-12 and glp-1 phenotype protein 1, isoform b

Chain A: 

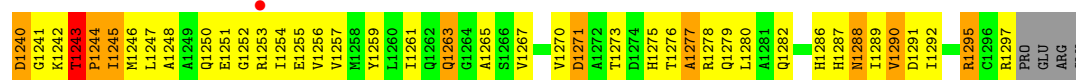
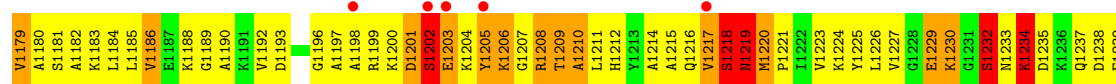
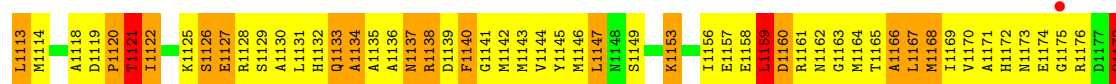
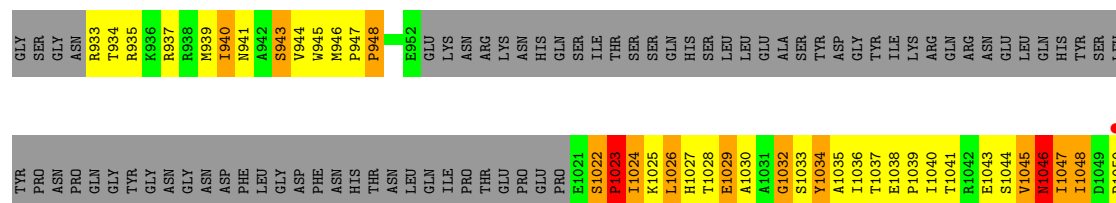
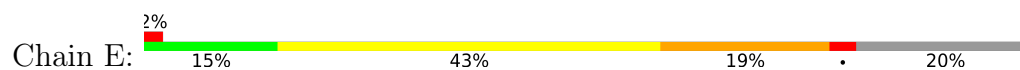




• Molecule 4: Protein lag-3



• Molecule 5: Lin-12 protein



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 21 21                                                  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 66.09Å 96.78Å 243.54Å<br>90.00° 90.00° 90.00°               | Depositor        |
| Resolution (Å)                                                          | 43.51 – 3.12<br>43.51 – 3.12                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 88.6 (43.51-3.12)<br>88.9 (43.51-3.12)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | 0.09                                                        | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.67 (at 3.12Å)                                             | Xtriage          |
| Refinement program                                                      | CNS 1.1                                                     | Depositor        |
| R, $R_{free}$                                                           | 0.273 , 0.340<br>0.276 , 0.327                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 4706 reflections (9.04%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 94.2                                                        | Xtriage          |
| Anisotropy                                                              | 0.612                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.27 , 88.4                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.92                                                        | EDS              |
| Total number of atoms                                                   | 6939                                                        | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 103.0                                                       | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% 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   | B     | 0.41         | 0/350         | 0.74        | 0/540          |
| 2   | C     | 0.39         | 0/332         | 0.85        | 0/509          |
| 3   | A     | 0.54         | 1/3573 (0.0%) | 1.07        | 21/4822 (0.4%) |
| 4   | D     | 0.45         | 0/532         | 1.21        | 9/714 (1.3%)   |
| 5   | E     | 0.55         | 0/2327        | 1.14        | 21/3113 (0.7%) |
| All | All   | 0.53         | 1/7114 (0.0%) | 1.07        | 51/9698 (0.5%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | B     | 0                   | 2                   |
| 2   | C     | 0                   | 2                   |
| All | All   | 0                   | 4                   |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 3   | A     | 386 | ILE  | CA-CB | -5.68 | 1.47        | 1.54     |

All (51) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 4   | D     | 54   | GLU  | CA-C-N | 10.07 | 132.43      | 119.84   |
| 4   | D     | 54   | GLU  | C-N-CA | 10.07 | 132.43      | 119.84   |
| 5   | E     | 1267 | VAL  | N-CA-C | -9.87 | 103.50      | 113.47   |
| 3   | A     | 419  | SER  | N-CA-C | -8.91 | 102.92      | 113.88   |
| 5   | E     | 1083 | ALA  | N-CA-C | -8.44 | 103.09      | 112.72   |
| 5   | E     | 1048 | ILE  | N-CA-C | 8.26  | 119.62      | 109.30   |
| 4   | D     | 62   | ALA  | N-CA-C | -8.00 | 99.32       | 111.56   |
| 5   | E     | 1134 | ALA  | N-CA-C | -7.98 | 101.28      | 111.02   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 3   | A     | 562  | CYS  | CA-C-N | 7.47  | 127.23      | 119.76   |
| 3   | A     | 562  | CYS  | C-N-CA | 7.47  | 127.23      | 119.76   |
| 3   | A     | 295  | ASP  | N-CA-C | -7.33 | 105.52      | 114.75   |
| 5   | E     | 1067 | GLU  | N-CA-C | -7.29 | 102.42      | 113.51   |
| 3   | A     | 505  | LEU  | N-CA-C | -7.25 | 105.61      | 114.75   |
| 5   | E     | 1181 | SER  | N-CA-C | -6.99 | 102.81      | 111.75   |
| 3   | A     | 229  | TYR  | N-CA-C | 6.75  | 120.23      | 109.24   |
| 5   | E     | 1047 | ILE  | N-CA-C | 6.66  | 118.26      | 111.00   |
| 5   | E     | 1240 | ASP  | N-CA-C | -6.59 | 103.64      | 112.94   |
| 3   | A     | 481  | LEU  | N-CA-C | 6.55  | 121.61      | 109.56   |
| 5   | E     | 1052 | HIS  | N-CA-C | -6.30 | 104.86      | 113.30   |
| 5   | E     | 946  | MSE  | CA-C-N | 6.24  | 126.81      | 120.38   |
| 5   | E     | 946  | MSE  | C-N-CA | 6.24  | 126.81      | 120.38   |
| 4   | D     | 107  | GLU  | N-CA-C | -6.13 | 106.12      | 113.97   |
| 4   | D     | 106  | ASP  | N-CA-C | -6.11 | 105.58      | 113.16   |
| 4   | D     | 71   | ARG  | N-CA-C | -6.04 | 104.76      | 111.71   |
| 4   | D     | 78   | ARG  | N-CA-C | -6.01 | 104.65      | 112.23   |
| 3   | A     | 628  | PHE  | N-CA-C | -5.76 | 106.29      | 113.38   |
| 3   | A     | 608  | SER  | N-CA-C | 5.73  | 117.83      | 108.55   |
| 5   | E     | 1205 | TYR  | N-CA-C | -5.72 | 99.68       | 109.24   |
| 3   | A     | 643  | VAL  | N-CA-C | 5.72  | 116.71      | 108.48   |
| 5   | E     | 1209 | THR  | N-CA-C | 5.61  | 117.10      | 107.28   |
| 5   | E     | 1071 | ASP  | N-CA-C | 5.58  | 119.19      | 112.38   |
| 5   | E     | 1218 | SER  | N-CA-C | 5.56  | 122.63      | 110.80   |
| 4   | D     | 102  | ARG  | N-CA-C | -5.50 | 105.30      | 112.23   |
| 3   | A     | 525  | GLU  | N-CA-C | -5.43 | 107.30      | 114.31   |
| 3   | A     | 487  | GLU  | N-CA-C | -5.37 | 105.37      | 112.94   |
| 5   | E     | 940  | ILE  | N-CA-C | 5.36  | 115.49      | 107.51   |
| 3   | A     | 606  | GLU  | N-CA-C | -5.35 | 106.79      | 113.15   |
| 3   | A     | 560  | SER  | CA-C-N | -5.33 | 113.18      | 119.84   |
| 3   | A     | 560  | SER  | C-N-CA | -5.33 | 113.18      | 119.84   |
| 4   | D     | 98   | HIS  | N-CA-C | -5.32 | 105.59      | 111.71   |
| 5   | E     | 1295 | ARG  | N-CA-C | -5.29 | 106.77      | 113.18   |
| 3   | A     | 442  | PHE  | N-CA-C | 5.27  | 116.82      | 108.96   |
| 3   | A     | 390  | THR  | N-CA-C | 5.23  | 117.57      | 110.35   |
| 3   | A     | 426  | THR  | N-CA-C | -5.18 | 102.38      | 110.10   |
| 3   | A     | 310  | ARG  | N-CA-C | 5.15  | 116.74      | 111.03   |
| 5   | E     | 1069 | SER  | N-CA-C | -5.11 | 102.75      | 110.06   |
| 5   | E     | 1243 | THR  | N-CA-C | -5.11 | 103.33      | 109.72   |
| 3   | A     | 597  | THR  | CA-C-N | 5.06  | 124.97      | 119.76   |
| 3   | A     | 597  | THR  | C-N-CA | 5.06  | 124.97      | 119.76   |
| 5   | E     | 1159 | LEU  | N-CA-C | 5.06  | 117.73      | 109.59   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 5   | E     | 1219 | ASN  | N-CA-C | -5.05 | 100.04      | 110.80   |

There are no chirality outliers.

All (4) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | B     | 12  | DA   | Sidechain |
| 1   | B     | 2   | DT   | Sidechain |
| 2   | C     | 2   | DA   | Sidechain |
| 2   | C     | 5   | DT   | Sidechain |

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | B     | 311   | 0        | 171      | 19      | 0            |
| 2   | C     | 298   | 0        | 172      | 17      | 0            |
| 3   | A     | 3497  | 0        | 3441     | 354     | 0            |
| 4   | D     | 524   | 0        | 491      | 52      | 0            |
| 5   | E     | 2309  | 0        | 2301     | 408     | 0            |
| All | All   | 6939  | 0        | 6576     | 811     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 60.

All (811) 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) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:E:1022:SER:H    | 5:E:1023:PRO:HD2  | 1.17                     | 1.08              |
| 5:E:1167:LEU:H    | 5:E:1167:LEU:HD12 | 1.14                     | 1.07              |
| 3:A:283:ALA:HB1   | 3:A:351:CYS:HB3   | 1.33                     | 1.07              |
| 5:E:935:ARG:NH1   | 5:E:1158:GLU:HG2  | 1.69                     | 1.06              |
| 2:C:8:DC:H2''     | 2:C:9:DC:H5'      | 1.33                     | 1.04              |
| 3:A:328:LYS:HD3   | 3:A:328:LYS:H     | 1.20                     | 1.04              |
| 5:E:1057:LEU:HD12 | 5:E:1057:LEU:H    | 1.19                     | 1.03              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:E:1037:THR:HG22 | 5:E:1038:GLU:H    | 1.24                     | 1.01              |
| 5:E:1063:ASN:ND2  | 5:E:1106:ARG:HD3  | 1.74                     | 1.01              |
| 5:E:1098:LEU:HD12 | 5:E:1098:LEU:O    | 1.58                     | 1.01              |
| 3:A:293:GLY:HA3   | 3:A:338:ARG:HH22  | 1.25                     | 0.99              |
| 3:A:479:VAL:HG12  | 3:A:481:LEU:HD23  | 1.39                     | 0.99              |
| 5:E:1055:THR:H    | 5:E:1058:HIS:HD2  | 1.04                     | 0.98              |
| 5:E:1055:THR:H    | 5:E:1058:HIS:CD2  | 1.83                     | 0.97              |
| 5:E:1246:MSE:HE1  | 5:E:1271:ASP:HB3  | 1.43                     | 0.97              |
| 3:A:631:ARG:H     | 3:A:631:ARG:HD2   | 1.27                     | 0.96              |
| 5:E:1129:SER:H    | 5:E:1132:HIS:HD2  | 1.12                     | 0.95              |
| 5:E:1034:TYR:HD1  | 5:E:1035:ALA:H    | 1.11                     | 0.93              |
| 1:B:1:DT:H2'      | 1:B:2:DT:H72      | 1.50                     | 0.93              |
| 5:E:1120:PRO:HG2  | 5:E:1121:THR:H    | 1.32                     | 0.93              |
| 5:E:1229:GLU:HG3  | 5:E:1230:LYS:N    | 1.81                     | 0.93              |
| 5:E:1104:ALA:O    | 5:E:1105:ARG:HG2  | 1.70                     | 0.92              |
| 5:E:1073:ILE:HD11 | 5:E:1106:ARG:CZ   | 1.98                     | 0.92              |
| 2:C:7:DT:H2''     | 2:C:8:DC:H5''     | 1.53                     | 0.91              |
| 4:D:54:GLU:HB3    | 4:D:55:PRO:HD2    | 1.51                     | 0.91              |
| 5:E:1129:SER:H    | 5:E:1132:HIS:CD2  | 1.88                     | 0.90              |
| 3:A:199:THR:HG23  | 3:A:202:ARG:HB2   | 1.51                     | 0.90              |
| 3:A:472:ARG:HD3   | 3:A:499:GLN:OE1   | 1.72                     | 0.90              |
| 3:A:328:LYS:HD3   | 3:A:328:LYS:N     | 1.88                     | 0.89              |
| 5:E:1063:ASN:HD21 | 5:E:1106:ARG:HD3  | 1.37                     | 0.89              |
| 5:E:1110:VAL:HG21 | 5:E:1142:MSE:HE1  | 1.55                     | 0.88              |
| 5:E:1165:THR:O    | 5:E:1169:ILE:HG13 | 1.71                     | 0.88              |
| 3:A:479:VAL:HG23  | 3:A:530:ILE:HD12  | 1.56                     | 0.88              |
| 5:E:1119:ASP:OD1  | 5:E:1121:THR:HB   | 1.74                     | 0.87              |
| 3:A:560:SER:HB3   | 3:A:561:PRO:HD3   | 1.56                     | 0.87              |
| 3:A:293:GLY:HA3   | 3:A:338:ARG:NH2   | 1.90                     | 0.87              |
| 5:E:933:ARG:HH12  | 5:E:1090:MSE:SE   | 2.08                     | 0.87              |
| 5:E:1276:THR:HG22 | 5:E:1279:GLN:HE21 | 1.37                     | 0.87              |
| 3:A:644:ARG:HB2   | 3:A:648:VAL:HG12  | 1.57                     | 0.86              |
| 3:A:349:TYR:CE1   | 3:A:355:ILE:HD11  | 2.10                     | 0.86              |
| 5:E:1156:ILE:HG21 | 5:E:1190:ALA:HB2  | 1.56                     | 0.86              |
| 3:A:292:ILE:C     | 3:A:294:SER:H     | 1.84                     | 0.86              |
| 3:A:573:HIS:HB2   | 5:E:1104:ALA:HA   | 1.58                     | 0.85              |
| 5:E:1167:LEU:HD12 | 5:E:1167:LEU:N    | 1.91                     | 0.84              |
| 5:E:1197:ALA:C    | 5:E:1199:ARG:H    | 1.83                     | 0.84              |
| 3:A:300:GLN:HG2   | 3:A:329:THR:OG1   | 1.78                     | 0.84              |
| 3:A:388:SER:HB3   | 5:E:1202:SER:OG   | 1.76                     | 0.84              |
| 3:A:479:VAL:HG12  | 3:A:479:VAL:O     | 1.77                     | 0.84              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:E:1205:TYR:O    | 5:E:1206:LYS:CG   | 2.26                     | 0.83              |
| 1:B:6:DG:H2'      | 1:B:7:DT:H71      | 1.60                     | 0.83              |
| 5:E:1045:VAL:HG23 | 5:E:1046:ASN:H    | 1.43                     | 0.83              |
| 5:E:1245:ILE:HD13 | 5:E:1245:ILE:H    | 1.44                     | 0.83              |
| 5:E:1114:MSE:HE2  | 5:E:1146:MSE:HG2  | 1.59                     | 0.82              |
| 3:A:644:ARG:HB3   | 3:A:646:ASP:OD1   | 1.80                     | 0.81              |
| 3:A:530:ILE:HD13  | 3:A:530:ILE:H     | 1.44                     | 0.81              |
| 5:E:1114:MSE:HE1  | 5:E:1146:MSE:HA   | 1.62                     | 0.81              |
| 3:A:355:ILE:O     | 3:A:559:ILE:HG12  | 1.82                     | 0.80              |
| 3:A:427:ILE:HG23  | 3:A:427:ILE:O     | 1.82                     | 0.79              |
| 3:A:283:ALA:CB    | 3:A:351:CYS:HB3   | 2.11                     | 0.79              |
| 5:E:1074:VAL:O    | 5:E:1078:LYS:HG3  | 1.82                     | 0.79              |
| 3:A:293:GLY:CA    | 3:A:338:ARG:HH22  | 1.96                     | 0.79              |
| 5:E:1129:SER:N    | 5:E:1132:HIS:HD2  | 1.80                     | 0.79              |
| 5:E:1099:MSE:HE1  | 5:E:1130:ALA:HA   | 1.63                     | 0.79              |
| 5:E:1051:ARG:NH2  | 5:E:1051:ARG:HB2  | 1.97                     | 0.79              |
| 5:E:1205:TYR:O    | 5:E:1206:LYS:HG3  | 1.82                     | 0.79              |
| 3:A:298:GLU:O     | 3:A:299:ARG:HB3   | 1.82                     | 0.78              |
| 5:E:1141:GLY:HA2  | 5:E:1144:VAL:HG12 | 1.65                     | 0.78              |
| 3:A:251:LEU:CD1   | 3:A:255:ARG:HD2   | 2.13                     | 0.78              |
| 3:A:631:ARG:H     | 3:A:631:ARG:CD    | 1.96                     | 0.77              |
| 5:E:1225:TYR:O    | 5:E:1229:GLU:HB3  | 1.84                     | 0.77              |
| 2:C:7:DT:C2'      | 2:C:8:DC:H5''     | 2.15                     | 0.77              |
| 5:E:1127:GLU:O    | 5:E:1160:ASP:HA   | 1.85                     | 0.77              |
| 4:D:65:SER:O      | 4:D:69:LEU:HD13   | 1.85                     | 0.77              |
| 3:A:199:THR:CG2   | 3:A:202:ARG:HB2   | 2.15                     | 0.77              |
| 5:E:1056:VAL:O    | 5:E:1060:ILE:HG12 | 1.86                     | 0.76              |
| 3:A:213:TYR:HB3   | 3:A:549:PHE:CE2   | 2.20                     | 0.76              |
| 3:A:223:LYS:HD2   | 3:A:383:TYR:HE2   | 1.51                     | 0.76              |
| 5:E:934:THR:HG22  | 5:E:935:ARG:N     | 2.01                     | 0.76              |
| 5:E:1037:THR:HG22 | 5:E:1038:GLU:N    | 2.00                     | 0.76              |
| 5:E:1229:GLU:HG3  | 5:E:1230:LYS:H    | 1.47                     | 0.76              |
| 3:A:397:ARG:C     | 3:A:398:LEU:HD22  | 2.11                     | 0.76              |
| 5:E:1237:GLN:HB3  | 5:E:1241:GLY:HA2  | 1.65                     | 0.76              |
| 5:E:1128:ARG:HG2  | 5:E:1132:HIS:CB   | 2.15                     | 0.76              |
| 5:E:1282:GLN:HG2  | 5:E:1290:VAL:HG22 | 1.67                     | 0.75              |
| 3:A:432:ASP:H     | 3:A:443:ALA:HB3   | 1.50                     | 0.75              |
| 5:E:1135:ALA:HA   | 5:E:1143:MSE:HE1  | 1.65                     | 0.75              |
| 5:E:1217:VAL:HA   | 5:E:1253:ARG:CG   | 2.16                     | 0.75              |
| 3:A:292:ILE:O     | 3:A:294:SER:N     | 2.17                     | 0.75              |
| 3:A:579:VAL:HG23  | 3:A:613:ILE:HD11  | 1.67                     | 0.75              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:E:934:THR:HG22  | 5:E:935:ARG:H     | 1.52                     | 0.75              |
| 5:E:1243:THR:HB   | 5:E:1245:ILE:HG12 | 1.68                     | 0.75              |
| 3:A:447:GLY:H     | 5:E:1202:SER:HB2  | 1.51                     | 0.74              |
| 5:E:1062:SER:C    | 5:E:1064:SER:H    | 1.92                     | 0.74              |
| 3:A:493:LEU:HD21  | 3:A:539:ILE:HD12  | 1.70                     | 0.74              |
| 3:A:392:VAL:HG12  | 3:A:540:SER:HA    | 1.68                     | 0.74              |
| 5:E:1051:ARG:HB2  | 5:E:1051:ARG:HH21 | 1.50                     | 0.74              |
| 3:A:571:ASP:HB3   | 5:E:1133:GLN:HE22 | 1.52                     | 0.73              |
| 5:E:1201:ASP:CG   | 5:E:1202:SER:H    | 1.96                     | 0.73              |
| 4:D:86:PRO:HA     | 4:D:89:ILE:HG12   | 1.70                     | 0.73              |
| 3:A:263:LEU:O     | 3:A:263:LEU:HD23  | 1.88                     | 0.73              |
| 3:A:469:LEU:HB3   | 3:A:498:PHE:HB3   | 1.68                     | 0.73              |
| 5:E:1141:GLY:HA2  | 5:E:1144:VAL:CG1  | 2.19                     | 0.73              |
| 3:A:568:LEU:C     | 3:A:568:LEU:HD23  | 2.13                     | 0.73              |
| 3:A:588:PRO:HG3   | 3:A:603:PHE:CG    | 2.24                     | 0.73              |
| 2:C:8:DC:C2'      | 2:C:9:DC:H5'      | 2.15                     | 0.73              |
| 5:E:1147:LEU:HG   | 5:E:1188:LYS:HG3  | 1.71                     | 0.73              |
| 4:D:83:LYS:HD2    | 4:D:84:ALA:N      | 2.04                     | 0.72              |
| 4:D:69:LEU:O      | 4:D:72:GLN:HB2    | 1.89                     | 0.72              |
| 3:A:216:VAL:HB    | 3:A:245:ILE:HB    | 1.72                     | 0.72              |
| 5:E:1057:LEU:H    | 5:E:1057:LEU:CD1  | 1.99                     | 0.72              |
| 5:E:1121:THR:HG22 | 5:E:1122:ILE:N    | 2.05                     | 0.71              |
| 5:E:1288:ASN:O    | 5:E:1292:ILE:HG12 | 1.89                     | 0.71              |
| 3:A:631:ARG:HD2   | 3:A:631:ARG:N     | 2.04                     | 0.71              |
| 5:E:1055:THR:O    | 5:E:1058:HIS:HB2  | 1.89                     | 0.71              |
| 4:D:89:ILE:O      | 4:D:93:ARG:HB2    | 1.88                     | 0.71              |
| 5:E:1197:ALA:O    | 5:E:1199:ARG:N    | 2.23                     | 0.71              |
| 5:E:1057:LEU:HD12 | 5:E:1057:LEU:N    | 2.00                     | 0.71              |
| 3:A:387:ALA:HB3   | 3:A:390:THR:CG2   | 2.21                     | 0.71              |
| 4:D:56:THR:HG23   | 5:E:1106:ARG:CZ   | 2.20                     | 0.71              |
| 5:E:1218:SER:H    | 5:E:1253:ARG:HG3  | 1.55                     | 0.71              |
| 3:A:569:GLU:HG2   | 5:E:1128:ARG:NH2  | 2.06                     | 0.71              |
| 5:E:1098:LEU:HD12 | 5:E:1098:LEU:C    | 2.14                     | 0.71              |
| 5:E:1024:ILE:HG22 | 5:E:1027:HIS:H    | 1.55                     | 0.70              |
| 3:A:217:ILE:HD13  | 3:A:217:ILE:C     | 2.16                     | 0.70              |
| 5:E:1072:LEU:HD12 | 5:E:1073:ILE:N    | 2.06                     | 0.70              |
| 5:E:1114:MSE:HE3  | 5:E:1145:TYR:HE2  | 1.57                     | 0.70              |
| 3:A:604:ARG:HG2   | 3:A:604:ARG:HH21  | 1.57                     | 0.70              |
| 2:C:7:DT:H2''     | 2:C:8:DC:C5'      | 2.22                     | 0.70              |
| 3:A:387:ALA:HB3   | 3:A:390:THR:HG23  | 1.74                     | 0.70              |
| 4:D:54:GLU:CB     | 4:D:55:PRO:HD2    | 2.15                     | 0.70              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:E:1098:LEU:O    | 5:E:1101:ALA:HB3  | 1.91                     | 0.70              |
| 5:E:1147:LEU:HB3  | 5:E:1188:LYS:HE3  | 1.73                     | 0.70              |
| 3:A:293:GLY:CA    | 3:A:338:ARG:HH12  | 2.05                     | 0.69              |
| 3:A:298:GLU:O     | 3:A:299:ARG:CB    | 2.41                     | 0.69              |
| 5:E:1100:LEU:HD12 | 5:E:1100:LEU:H    | 1.58                     | 0.69              |
| 3:A:637:GLU:HA    | 3:A:656:PHE:O     | 1.92                     | 0.69              |
| 3:A:197:SER:O     | 3:A:552:MET:HE2   | 1.91                     | 0.69              |
| 5:E:1070:GLU:O    | 5:E:1073:ILE:HG12 | 1.91                     | 0.69              |
| 5:E:1200:LYS:HA   | 5:E:1206:LYS:HD2  | 1.74                     | 0.69              |
| 3:A:223:LYS:HB2   | 3:A:540:SER:O     | 1.93                     | 0.69              |
| 3:A:293:GLY:HA3   | 3:A:338:ARG:HH12  | 1.56                     | 0.69              |
| 5:E:1095:ASN:OD1  | 5:E:1099:MSE:HG2  | 1.93                     | 0.69              |
| 5:E:1138:ARG:HG3  | 5:E:1178:GLN:HE22 | 1.55                     | 0.69              |
| 3:A:559:ILE:HA    | 3:A:644:ARG:HH22  | 1.56                     | 0.69              |
| 5:E:1104:ALA:C    | 5:E:1105:ARG:HG2  | 2.17                     | 0.69              |
| 5:E:1257:VAL:O    | 5:E:1261:ILE:HG12 | 1.92                     | 0.68              |
| 3:A:442:PHE:CE2   | 3:A:456:LYS:HE2   | 2.28                     | 0.68              |
| 4:D:70:HIS:CE1    | 5:E:1174:GLU:H    | 2.11                     | 0.68              |
| 5:E:1045:VAL:HG12 | 5:E:1056:VAL:HG21 | 1.74                     | 0.68              |
| 5:E:1102:VAL:HG13 | 5:E:1142:MSE:HG2  | 1.74                     | 0.68              |
| 3:A:237:CYS:HA    | 3:A:238:PRO:C     | 2.18                     | 0.68              |
| 3:A:425:PHE:HD2   | 3:A:459:ASP:HA    | 1.59                     | 0.68              |
| 5:E:1205:TYR:O    | 5:E:1206:LYS:CB   | 2.41                     | 0.68              |
| 1:B:13:DA:H1'     | 1:B:14:DG:H5''    | 1.76                     | 0.68              |
| 3:A:415:PHE:HE1   | 3:A:464:ILE:HG23  | 1.58                     | 0.68              |
| 3:A:548:PHE:HE1   | 3:A:559:ILE:HG13  | 1.59                     | 0.68              |
| 5:E:1128:ARG:HG2  | 5:E:1132:HIS:HB2  | 1.76                     | 0.68              |
| 3:A:560:SER:CB    | 3:A:561:PRO:HD3   | 2.24                     | 0.68              |
| 3:A:557:ASN:N     | 3:A:557:ASN:HD22  | 1.91                     | 0.67              |
| 5:E:1114:MSE:HE3  | 5:E:1145:TYR:CE2  | 2.29                     | 0.67              |
| 5:E:1202:SER:O    | 5:E:1203:GLU:C    | 2.37                     | 0.67              |
| 5:E:1061:ALA:O    | 5:E:1063:ASN:N    | 2.27                     | 0.67              |
| 3:A:310:ARG:HD2   | 3:A:311:HIS:H     | 1.58                     | 0.67              |
| 5:E:1217:VAL:HA   | 5:E:1253:ARG:HG3  | 1.76                     | 0.67              |
| 3:A:474:VAL:HG13  | 3:A:496:CYS:HA    | 1.77                     | 0.67              |
| 5:E:1045:VAL:HG23 | 5:E:1046:ASN:N    | 2.10                     | 0.67              |
| 5:E:1156:ILE:CG2  | 5:E:1190:ALA:HB2  | 2.24                     | 0.67              |
| 5:E:1223:VAL:O    | 5:E:1227:VAL:HG22 | 1.94                     | 0.67              |
| 5:E:1167:LEU:H    | 5:E:1167:LEU:CD1  | 1.96                     | 0.67              |
| 5:E:1220:MSE:HA   | 5:E:1223:VAL:HG22 | 1.77                     | 0.66              |
| 3:A:548:PHE:CE1   | 3:A:559:ILE:HG13  | 2.30                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:A:471:ILE:HG13  | 3:A:498:PHE:CE1   | 2.30                     | 0.66              |
| 5:E:1077:ALA:O    | 5:E:1081:ILE:HG22 | 1.94                     | 0.66              |
| 5:E:1120:PRO:CG   | 5:E:1121:THR:H    | 2.05                     | 0.66              |
| 4:D:91:ASN:N      | 4:D:91:ASN:HD22   | 1.94                     | 0.66              |
| 3:A:229:TYR:O     | 3:A:232:GLU:HG2   | 1.96                     | 0.66              |
| 5:E:1297:ARG:HH11 | 5:E:1297:ARG:HB3  | 1.61                     | 0.66              |
| 3:A:521:THR:OG1   | 3:A:529:GLN:HB2   | 1.95                     | 0.66              |
| 4:D:107:GLU:OE1   | 4:D:110:LYS:HD2   | 1.94                     | 0.65              |
| 5:E:1041:THR:H    | 5:E:1044:SER:CB   | 2.09                     | 0.65              |
| 3:A:245:ILE:N     | 3:A:245:ILE:HD12  | 2.11                     | 0.65              |
| 3:A:293:GLY:HA3   | 3:A:338:ARG:NH1   | 2.11                     | 0.65              |
| 3:A:592:VAL:HG12  | 3:A:601:THR:OG1   | 1.96                     | 0.65              |
| 5:E:1162:ASN:HB2  | 5:E:1164:MSE:HE2  | 1.78                     | 0.65              |
| 3:A:431:ASP:HB3   | 3:A:443:ALA:HB1   | 1.78                     | 0.65              |
| 4:D:76:LEU:HD11   | 5:E:1253:ARG:HH12 | 1.62                     | 0.65              |
| 5:E:1132:HIS:O    | 5:E:1136:ALA:N    | 2.25                     | 0.65              |
| 3:A:251:LEU:HD13  | 3:A:255:ARG:HD2   | 1.79                     | 0.65              |
| 3:A:510:LEU:HD23  | 3:A:533:GLY:O     | 1.95                     | 0.64              |
| 4:D:73:ARG:NH1    | 5:E:1218:SER:OG   | 2.30                     | 0.64              |
| 5:E:1055:THR:N    | 5:E:1058:HIS:HD2  | 1.86                     | 0.64              |
| 3:A:447:GLY:N     | 5:E:1202:SER:HB2  | 2.12                     | 0.64              |
| 5:E:1056:VAL:HG12 | 5:E:1060:ILE:HD11 | 1.80                     | 0.64              |
| 5:E:1209:THR:O    | 5:E:1209:THR:HG23 | 1.97                     | 0.64              |
| 3:A:459:ASP:OD1   | 3:A:462:THR:HG23  | 1.97                     | 0.64              |
| 3:A:530:ILE:HD13  | 3:A:530:ILE:N     | 2.13                     | 0.64              |
| 5:E:1234:LYS:HD3  | 5:E:1234:LYS:H    | 1.63                     | 0.64              |
| 5:E:1282:GLN:HG2  | 5:E:1290:VAL:CG2  | 2.27                     | 0.64              |
| 1:B:6:DG:H4'      | 3:A:235:PHE:HE2   | 1.61                     | 0.64              |
| 3:A:479:VAL:O     | 3:A:481:LEU:HD23  | 1.99                     | 0.63              |
| 5:E:1157:GLU:O    | 5:E:1165:THR:HG22 | 1.97                     | 0.63              |
| 3:A:509:CYS:SG    | 3:A:510:LEU:N     | 2.71                     | 0.63              |
| 1:B:7:DT:H2''     | 1:B:8:DG:C8       | 2.34                     | 0.63              |
| 5:E:1039:PRO:C    | 5:E:1040:ILE:HD12 | 2.24                     | 0.63              |
| 5:E:1143:MSE:O    | 5:E:1147:LEU:HD22 | 1.98                     | 0.63              |
| 5:E:1045:VAL:HG11 | 5:E:1080:CYS:CB   | 2.28                     | 0.63              |
| 3:A:551:ALA:HB3   | 3:A:647:GLY:O     | 1.99                     | 0.62              |
| 3:A:640:ILE:HD11  | 3:A:656:PHE:HB2   | 1.80                     | 0.62              |
| 5:E:1217:VAL:HG23 | 5:E:1251:GLU:HB3  | 1.81                     | 0.62              |
| 5:E:1241:GLY:O    | 5:E:1271:ASP:HA   | 1.99                     | 0.62              |
| 3:A:244:LEU:HB2   | 3:A:323:ASP:O     | 1.99                     | 0.62              |
| 4:D:58:GLY:O      | 4:D:60:LEU:N      | 2.32                     | 0.62              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 5:E:1064:SER:C    | 5:E:1066:ALA:H   | 2.07                     | 0.62              |
| 2:C:14:DG:H2'     | 2:C:15:DT:C7     | 2.30                     | 0.62              |
| 5:E:1139:ASP:OD2  | 5:E:1142:MSE:HB2 | 2.00                     | 0.62              |
| 3:A:408:LEU:HD21  | 3:A:415:PHE:HD2  | 1.64                     | 0.62              |
| 5:E:1243:THR:OG1  | 5:E:1246:MSE:HG3 | 1.99                     | 0.62              |
| 5:E:1022:SER:N    | 5:E:1023:PRO:HD2 | 1.97                     | 0.62              |
| 5:E:1245:ILE:HD13 | 5:E:1245:ILE:N   | 2.10                     | 0.62              |
| 5:E:1040:ILE:HD12 | 5:E:1040:ILE:N   | 2.14                     | 0.62              |
| 5:E:1091:ASP:OD2  | 5:E:1095:ASN:N   | 2.30                     | 0.62              |
| 5:E:1270:VAL:HG12 | 5:E:1276:THR:HB  | 1.82                     | 0.62              |
| 3:A:349:TYR:HE1   | 3:A:355:ILE:HD11 | 1.61                     | 0.61              |
| 5:E:1246:MSE:O    | 5:E:1247:LEU:C   | 2.43                     | 0.61              |
| 3:A:287:VAL:HB    | 3:A:348:PHE:CE1  | 2.35                     | 0.61              |
| 5:E:1287:HIS:O    | 5:E:1288:ASN:C   | 2.41                     | 0.61              |
| 3:A:560:SER:HB3   | 3:A:561:PRO:CD   | 2.30                     | 0.61              |
| 5:E:1051:ARG:HH21 | 5:E:1051:ARG:CB  | 2.12                     | 0.61              |
| 5:E:1110:VAL:HG21 | 5:E:1142:MSE:CE  | 2.27                     | 0.61              |
| 5:E:1120:PRO:HG2  | 5:E:1121:THR:N   | 2.10                     | 0.61              |
| 3:A:289:TYR:CE2   | 3:A:301:GLN:HB2  | 2.35                     | 0.61              |
| 3:A:513:ASP:O     | 3:A:514:LYS:HG2  | 2.01                     | 0.61              |
| 5:E:1078:LYS:HA   | 5:E:1081:ILE:CG2 | 2.29                     | 0.61              |
| 3:A:388:SER:HB2   | 3:A:447:GLY:O    | 2.00                     | 0.61              |
| 5:E:1220:MSE:HE3  | 5:E:1224:LYS:HG3 | 1.82                     | 0.61              |
| 5:E:1167:LEU:O    | 5:E:1168:MSE:C   | 2.43                     | 0.61              |
| 3:A:259:LEU:O     | 3:A:263:LEU:HB3  | 2.01                     | 0.61              |
| 3:A:503:ASN:O     | 3:A:505:LEU:N    | 2.25                     | 0.61              |
| 4:D:66:GLY:C      | 4:D:68:GLU:N     | 2.57                     | 0.61              |
| 5:E:1030:ALA:HB1  | 5:E:1060:ILE:CD1 | 2.31                     | 0.61              |
| 3:A:213:TYR:HB3   | 3:A:549:PHE:CD2  | 2.35                     | 0.60              |
| 3:A:506:VAL:HA    | 3:A:518:HIS:O    | 2.01                     | 0.60              |
| 4:D:70:HIS:HE1    | 5:E:1174:GLU:H   | 1.48                     | 0.60              |
| 3:A:557:ASN:HB3   | 3:A:558:PRO:HD2  | 1.83                     | 0.60              |
| 5:E:1133:GLN:HA   | 5:E:1136:ALA:HB3 | 1.83                     | 0.60              |
| 5:E:1229:GLU:O    | 5:E:1230:LYS:HB2 | 2.00                     | 0.60              |
| 1:B:3:DA:H1'      | 1:B:4:DC:H5'     | 1.83                     | 0.60              |
| 3:A:293:GLY:HA3   | 3:A:338:ARG:CZ   | 2.30                     | 0.60              |
| 3:A:548:PHE:HD2   | 3:A:548:PHE:O    | 1.85                     | 0.60              |
| 3:A:586:PHE:HB2   | 3:A:606:GLU:O    | 2.01                     | 0.60              |
| 4:D:55:PRO:O      | 5:E:1108:ARG:HB2 | 2.01                     | 0.60              |
| 3:A:251:LEU:HD11  | 3:A:255:ARG:HD2  | 1.82                     | 0.60              |
| 3:A:477:GLN:HG2   | 3:A:477:GLN:O    | 2.00                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:A:577:SER:HB3   | 3:A:613:ILE:HD13  | 1.83                     | 0.60              |
| 5:E:1141:GLY:CA   | 5:E:1144:VAL:HG12 | 2.30                     | 0.60              |
| 3:A:290:ILE:HD13  | 3:A:345:ALA:HB2   | 1.84                     | 0.60              |
| 5:E:1062:SER:C    | 5:E:1064:SER:N    | 2.56                     | 0.60              |
| 3:A:402:THR:O     | 3:A:404:SER:N     | 2.34                     | 0.60              |
| 3:A:573:HIS:NE2   | 5:E:1064:SER:N    | 2.50                     | 0.60              |
| 3:A:255:ARG:HH21  | 3:A:553:GLY:H     | 1.48                     | 0.59              |
| 5:E:944:VAL:HG22  | 5:E:945:TRP:H     | 1.67                     | 0.59              |
| 5:E:1133:GLN:NE2  | 5:E:1136:ALA:HB3  | 2.16                     | 0.59              |
| 3:A:637:GLU:HA    | 3:A:657:SER:HA    | 1.83                     | 0.59              |
| 5:E:1096:THR:HG23 | 5:E:1099:MSE:H    | 1.67                     | 0.59              |
| 3:A:552:MET:O     | 3:A:553:GLY:O     | 2.20                     | 0.59              |
| 5:E:1037:THR:CG2  | 5:E:1038:GLU:H    | 2.04                     | 0.59              |
| 5:E:1027:HIS:CE1  | 5:E:1048:ILE:HG22 | 2.37                     | 0.59              |
| 3:A:292:ILE:C     | 3:A:294:SER:N     | 2.51                     | 0.59              |
| 3:A:506:VAL:HG11  | 3:A:517:GLN:HG2   | 1.84                     | 0.59              |
| 4:D:104:THR:O     | 4:D:108:GLU:N     | 2.35                     | 0.59              |
| 5:E:1102:VAL:HA   | 5:E:1142:MSE:HE3  | 1.85                     | 0.59              |
| 3:A:586:PHE:HB2   | 3:A:606:GLU:C     | 2.28                     | 0.59              |
| 3:A:633:THR:O     | 3:A:635:ASP:N     | 2.36                     | 0.59              |
| 5:E:1081:ILE:HD13 | 5:E:1081:ILE:C    | 2.27                     | 0.58              |
| 5:E:1245:ILE:H    | 5:E:1245:ILE:CD1  | 2.06                     | 0.58              |
| 3:A:644:ARG:O     | 3:A:646:ASP:N     | 2.31                     | 0.58              |
| 4:D:66:GLY:C      | 4:D:68:GLU:H      | 2.09                     | 0.58              |
| 5:E:1140:PHE:CD1  | 5:E:1140:PHE:C    | 2.81                     | 0.58              |
| 5:E:1072:LEU:O    | 5:E:1076:GLU:N    | 2.27                     | 0.58              |
| 5:E:1078:LYS:HA   | 5:E:1081:ILE:HG23 | 1.86                     | 0.58              |
| 5:E:1133:GLN:HA   | 5:E:1133:GLN:NE2  | 2.18                     | 0.58              |
| 5:E:1182:ALA:O    | 5:E:1186:VAL:HG12 | 2.03                     | 0.58              |
| 3:A:494:HIS:O     | 3:A:537:THR:HA    | 2.04                     | 0.58              |
| 5:E:1126:SER:HA   | 5:E:1161:ARG:HD2  | 1.85                     | 0.58              |
| 5:E:944:VAL:HG22  | 5:E:945:TRP:N     | 2.18                     | 0.58              |
| 3:A:432:ASP:CG    | 3:A:433:GLU:H     | 2.11                     | 0.58              |
| 4:D:109:ARG:O     | 4:D:113:GLU:HG2   | 2.03                     | 0.58              |
| 3:A:215:CYS:HB3   | 3:A:548:PHE:HE2   | 1.68                     | 0.58              |
| 3:A:520:ALA:HB1   | 3:A:530:ILE:HA    | 1.85                     | 0.58              |
| 5:E:1126:SER:O    | 5:E:1127:GLU:C    | 2.46                     | 0.57              |
| 5:E:1199:ARG:C    | 5:E:1201:ASP:N    | 2.60                     | 0.57              |
| 3:A:427:ILE:HD13  | 3:A:449:VAL:HG21  | 1.86                     | 0.57              |
| 3:A:588:PRO:O     | 4:D:78:ARG:NH1    | 2.37                     | 0.57              |
| 5:E:1086:ASP:O    | 5:E:1088:ASN:N    | 2.38                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:E:1045:VAL:O    | 5:E:1047:ILE:N    | 2.38                     | 0.57              |
| 5:E:1086:ASP:C    | 5:E:1088:ASN:H    | 2.11                     | 0.57              |
| 3:A:252:LYS:NZ    | 3:A:554:GLN:HB2   | 2.19                     | 0.57              |
| 5:E:1030:ALA:HB1  | 5:E:1060:ILE:HD13 | 1.87                     | 0.57              |
| 5:E:1038:GLU:O    | 5:E:1040:ILE:CD1  | 2.53                     | 0.57              |
| 3:A:479:VAL:HG12  | 3:A:481:LEU:CD2   | 2.25                     | 0.57              |
| 5:E:1217:VAL:HA   | 5:E:1253:ARG:HG2  | 1.86                     | 0.57              |
| 3:A:500:MET:HE2   | 3:A:517:GLN:CD    | 2.29                     | 0.57              |
| 3:A:536:TRP:CD1   | 3:A:536:TRP:N     | 2.73                     | 0.57              |
| 5:E:1022:SER:H    | 5:E:1023:PRO:CD   | 2.05                     | 0.57              |
| 5:E:1200:LYS:O    | 5:E:1201:ASP:O    | 2.22                     | 0.57              |
| 3:A:347:PHE:O     | 3:A:355:ILE:HB    | 2.05                     | 0.57              |
| 3:A:559:ILE:HA    | 3:A:644:ARG:NH2   | 2.19                     | 0.57              |
| 3:A:579:VAL:HG23  | 3:A:613:ILE:CD1   | 2.34                     | 0.57              |
| 5:E:1270:VAL:HB   | 5:E:1275:HIS:O    | 2.05                     | 0.56              |
| 3:A:252:LYS:HG3   | 3:A:349:TYR:OH    | 2.05                     | 0.56              |
| 3:A:255:ARG:HH21  | 3:A:553:GLY:N     | 2.04                     | 0.56              |
| 4:D:60:LEU:O      | 4:D:64:HIS:ND1    | 2.30                     | 0.56              |
| 4:D:83:LYS:O      | 4:D:86:PRO:HD2    | 2.05                     | 0.56              |
| 5:E:935:ARG:CB    | 5:E:1199:ARG:HH22 | 2.19                     | 0.56              |
| 5:E:1045:VAL:HG11 | 5:E:1080:CYS:HB2  | 1.85                     | 0.56              |
| 5:E:1220:MSE:SE   | 5:E:1223:VAL:HG21 | 2.56                     | 0.56              |
| 5:E:1242:LYS:HZ2  | 5:E:1250:GLN:HE22 | 1.53                     | 0.56              |
| 3:A:495:LYS:HA    | 3:A:536:TRP:O     | 2.05                     | 0.56              |
| 3:A:542:ASP:CG    | 3:A:543:LYS:H     | 2.14                     | 0.56              |
| 5:E:1135:ALA:CA   | 5:E:1143:MSE:HE1  | 2.35                     | 0.56              |
| 3:A:203:MET:HG3   | 3:A:207:LEU:HD12  | 1.87                     | 0.56              |
| 3:A:479:VAL:O     | 3:A:479:VAL:CG1   | 2.51                     | 0.56              |
| 5:E:945:TRP:CZ3   | 5:E:947:PRO:HB3   | 2.40                     | 0.56              |
| 3:A:415:PHE:CE2   | 3:A:466:LEU:HG    | 2.40                     | 0.56              |
| 5:E:1066:ALA:O    | 5:E:1067:GLU:HB3  | 2.06                     | 0.56              |
| 5:E:1109:LEU:O    | 5:E:1113:LEU:HB2  | 2.04                     | 0.56              |
| 3:A:441:ASN:HB2   | 5:E:939:MSE:HE1   | 1.87                     | 0.56              |
| 5:E:1041:THR:O    | 5:E:1045:VAL:HG22 | 2.05                     | 0.56              |
| 5:E:1184:LEU:C    | 5:E:1184:LEU:HD13 | 2.31                     | 0.56              |
| 3:A:383:TYR:O     | 3:A:384:LEU:HD23  | 2.06                     | 0.56              |
| 3:A:408:LEU:HB3   | 3:A:425:PHE:HE1   | 1.71                     | 0.56              |
| 3:A:615:PRO:O     | 3:A:618:GLN:HG2   | 2.05                     | 0.56              |
| 5:E:1062:SER:O    | 5:E:1064:SER:N    | 2.38                     | 0.56              |
| 5:E:1214:ALA:O    | 5:E:1215:ALA:C    | 2.49                     | 0.56              |
| 5:E:934:THR:CG2   | 5:E:935:ARG:H     | 2.17                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:E:1186:VAL:HG11 | 5:E:1225:TYR:OH   | 2.05                     | 0.55              |
| 1:B:1:DT:C2'      | 1:B:2:DT:H72      | 2.30                     | 0.55              |
| 2:C:1:DA:H2''     | 2:C:2:DA:C8       | 2.41                     | 0.55              |
| 2:C:13:DA:H2''    | 2:C:14:DG:H8      | 1.72                     | 0.55              |
| 3:A:536:TRP:CD1   | 3:A:536:TRP:H     | 2.25                     | 0.55              |
| 5:E:1087:VAL:HG22 | 5:E:1118:ALA:HB2  | 1.88                     | 0.55              |
| 5:E:1109:LEU:HG   | 5:E:1113:LEU:HD23 | 1.88                     | 0.55              |
| 5:E:1129:SER:N    | 5:E:1132:HIS:CD2  | 2.63                     | 0.55              |
| 3:A:425:PHE:CD2   | 3:A:459:ASP:HA    | 2.40                     | 0.55              |
| 3:A:568:LEU:C     | 3:A:568:LEU:CD2   | 2.79                     | 0.55              |
| 3:A:644:ARG:C     | 3:A:646:ASP:H     | 2.13                     | 0.55              |
| 5:E:1045:VAL:CG2  | 5:E:1046:ASN:H    | 2.09                     | 0.55              |
| 3:A:548:PHE:O     | 3:A:548:PHE:CD2   | 2.60                     | 0.55              |
| 4:D:100:PHE:O     | 4:D:103:TYR:HB3   | 2.05                     | 0.55              |
| 3:A:228:SER:OG    | 3:A:234:ARG:HB2   | 2.06                     | 0.55              |
| 5:E:1149:SER:O    | 5:E:1153:LYS:HD3  | 2.07                     | 0.55              |
| 5:E:1197:ALA:HA   | 5:E:1200:LYS:HG3  | 1.87                     | 0.55              |
| 5:E:1224:LYS:HA   | 5:E:1259:TYR:HE1  | 1.71                     | 0.55              |
| 3:A:198:LEU:HD12  | 3:A:199:THR:H     | 1.72                     | 0.55              |
| 3:A:362:ARG:HD2   | 3:A:362:ARG:N     | 2.21                     | 0.55              |
| 4:D:76:LEU:HD13   | 4:D:77:ALA:N      | 2.22                     | 0.55              |
| 5:E:1217:VAL:O    | 5:E:1218:SER:O    | 2.24                     | 0.55              |
| 5:E:1242:LYS:NZ   | 5:E:1250:GLN:HE22 | 2.04                     | 0.55              |
| 3:A:548:PHE:HD1   | 3:A:559:ILE:HG21  | 1.72                     | 0.55              |
| 5:E:1276:THR:C    | 5:E:1280:LEU:HD23 | 2.32                     | 0.55              |
| 3:A:220:PHE:HB3   | 3:A:422:TRP:CZ2   | 2.42                     | 0.55              |
| 3:A:261:LYS:HG3   | 3:A:262:THR:N     | 2.22                     | 0.55              |
| 5:E:1114:MSE:CE   | 5:E:1146:MSE:HG2  | 2.32                     | 0.55              |
| 5:E:1211:LEU:HD12 | 5:E:1211:LEU:O    | 2.07                     | 0.55              |
| 3:A:588:PRO:HG3   | 3:A:603:PHE:CD2   | 2.42                     | 0.54              |
| 4:D:75:GLU:HA     | 4:D:75:GLU:OE1    | 2.06                     | 0.54              |
| 3:A:415:PHE:CE1   | 3:A:464:ILE:CG2   | 2.90                     | 0.54              |
| 2:C:8:DC:H5'      | 2:C:8:DC:H6       | 1.71                     | 0.54              |
| 2:C:14:DG:H4'     | 2:C:14:DG:OP1     | 2.08                     | 0.54              |
| 5:E:1022:SER:O    | 5:E:1023:PRO:C    | 2.51                     | 0.54              |
| 5:E:1128:ARG:HG2  | 5:E:1132:HIS:HB3  | 1.89                     | 0.54              |
| 5:E:1047:ILE:N    | 5:E:1047:ILE:HD12 | 2.22                     | 0.54              |
| 5:E:1099:MSE:C    | 5:E:1101:ALA:N    | 2.64                     | 0.54              |
| 3:A:259:LEU:O     | 3:A:263:LEU:CB    | 2.55                     | 0.54              |
| 3:A:402:THR:HG23  | 3:A:403:VAL:H     | 1.72                     | 0.54              |
| 3:A:599:VAL:HG12  | 3:A:600:GLU:N     | 2.22                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:6:DG:N2       | 3:A:400:SER:HB3   | 2.22                     | 0.54              |
| 4:D:92:GLN:HE21   | 4:D:96:THR:HB     | 1.73                     | 0.54              |
| 1:B:13:DA:C2'     | 1:B:14:DG:H5''    | 2.38                     | 0.54              |
| 3:A:410:VAL:HG21  | 3:A:459:ASP:OD1   | 2.08                     | 0.54              |
| 3:A:571:ASP:N     | 3:A:571:ASP:OD1   | 2.40                     | 0.54              |
| 3:A:255:ARG:NH2   | 3:A:553:GLY:H     | 2.06                     | 0.53              |
| 5:E:1086:ASP:C    | 5:E:1088:ASN:N    | 2.66                     | 0.53              |
| 5:E:1133:GLN:HA   | 5:E:1136:ALA:CB   | 2.38                     | 0.53              |
| 3:A:287:VAL:HG11  | 3:A:348:PHE:CZ    | 2.43                     | 0.53              |
| 5:E:1245:ILE:O    | 5:E:1248:ALA:HB3  | 2.07                     | 0.53              |
| 3:A:243:TYR:HB3   | 3:A:245:ILE:HD11  | 1.89                     | 0.53              |
| 3:A:415:PHE:HE1   | 3:A:464:ILE:CG2   | 2.21                     | 0.53              |
| 5:E:935:ARG:CZ    | 5:E:1158:GLU:HG2  | 2.37                     | 0.53              |
| 5:E:1201:ASP:CG   | 5:E:1202:SER:N    | 2.61                     | 0.53              |
| 5:E:1238:ASP:OD1  | 5:E:1242:LYS:N    | 2.37                     | 0.53              |
| 5:E:1096:THR:O    | 5:E:1100:LEU:HD12 | 2.08                     | 0.53              |
| 5:E:1131:LEU:HD21 | 5:E:1185:LEU:HD21 | 1.90                     | 0.53              |
| 3:A:500:MET:HE2   | 3:A:517:GLN:NE2   | 2.24                     | 0.53              |
| 3:A:572:GLY:N     | 5:E:1137:ASN:HD22 | 2.06                     | 0.53              |
| 3:A:410:VAL:HG23  | 3:A:410:VAL:O     | 2.07                     | 0.53              |
| 4:D:76:LEU:HD13   | 4:D:76:LEU:C      | 2.33                     | 0.53              |
| 5:E:934:THR:CG2   | 5:E:935:ARG:N     | 2.69                     | 0.53              |
| 5:E:1057:LEU:HA   | 5:E:1060:ILE:HG12 | 1.90                     | 0.53              |
| 5:E:1197:ALA:C    | 5:E:1199:ARG:N    | 2.48                     | 0.53              |
| 5:E:1200:LYS:HG2  | 5:E:1206:LYS:HD2  | 1.90                     | 0.53              |
| 5:E:1233:ASN:C    | 5:E:1235:ASP:H    | 2.16                     | 0.53              |
| 5:E:1219:ASN:O    | 5:E:1220:MSE:C    | 2.52                     | 0.53              |
| 3:A:613:ILE:HD12  | 3:A:613:ILE:H     | 1.73                     | 0.53              |
| 4:D:77:ALA:HA     | 4:D:80:ASN:HD22   | 1.74                     | 0.53              |
| 3:A:415:PHE:CE1   | 3:A:464:ILE:HG23  | 2.43                     | 0.52              |
| 5:E:1027:HIS:HE1  | 5:E:1048:ILE:HG22 | 1.73                     | 0.52              |
| 5:E:1048:ILE:HD12 | 5:E:1048:ILE:N    | 2.24                     | 0.52              |
| 5:E:1159:LEU:HD13 | 5:E:1159:LEU:H    | 1.73                     | 0.52              |
| 5:E:1203:GLU:HB3  | 5:E:1205:TYR:CD1  | 2.44                     | 0.52              |
| 2:C:14:DG:H2'     | 2:C:15:DT:H72     | 1.90                     | 0.52              |
| 3:A:199:THR:HG23  | 3:A:202:ARG:H     | 1.74                     | 0.52              |
| 3:A:442:PHE:CZ    | 3:A:456:LYS:HG2   | 2.45                     | 0.52              |
| 4:D:91:ASN:HD22   | 4:D:91:ASN:H      | 1.57                     | 0.52              |
| 3:A:411:GLU:O     | 3:A:412:GLY:C     | 2.50                     | 0.52              |
| 3:A:548:PHE:CD2   | 3:A:548:PHE:C     | 2.86                     | 0.52              |
| 5:E:1167:LEU:O    | 5:E:1170:VAL:N    | 2.42                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:A:262:THR:HG22  | 3:A:262:THR:O     | 2.08                     | 0.52              |
| 5:E:1196:GLY:O    | 5:E:1199:ARG:HB2  | 2.10                     | 0.52              |
| 3:A:479:VAL:HG11  | 3:A:507:TYR:OH    | 2.10                     | 0.52              |
| 5:E:1182:ALA:C    | 5:E:1184:LEU:N    | 2.67                     | 0.52              |
| 5:E:1254:ILE:HG22 | 5:E:1289:ILE:HG12 | 1.92                     | 0.52              |
| 3:A:199:THR:O     | 3:A:200:SER:C     | 2.52                     | 0.52              |
| 3:A:254:ASP:C     | 3:A:256:VAL:H     | 2.17                     | 0.52              |
| 3:A:369:PRO:HG3   | 3:A:493:LEU:HD12  | 1.92                     | 0.52              |
| 5:E:1064:SER:C    | 5:E:1066:ALA:N    | 2.67                     | 0.52              |
| 3:A:432:ASP:O     | 3:A:433:GLU:CB    | 2.57                     | 0.52              |
| 5:E:1046:ASN:HB3  | 5:E:1047:ILE:HD12 | 1.90                     | 0.52              |
| 3:A:626:TRP:O     | 3:A:627:MET:HB2   | 2.10                     | 0.52              |
| 5:E:1140:PHE:C    | 5:E:1140:PHE:HD1  | 2.17                     | 0.52              |
| 5:E:1209:THR:O    | 5:E:1211:LEU:N    | 2.43                     | 0.52              |
| 5:E:1243:THR:O    | 5:E:1244:PRO:C    | 2.53                     | 0.52              |
| 3:A:249:TRP:HA    | 3:A:249:TRP:CE3   | 2.45                     | 0.51              |
| 5:E:1045:VAL:HG11 | 5:E:1080:CYS:HB3  | 1.91                     | 0.51              |
| 3:A:590:LEU:HA    | 3:A:643:VAL:O     | 2.10                     | 0.51              |
| 5:E:945:TRP:CH2   | 5:E:947:PRO:HB3   | 2.45                     | 0.51              |
| 5:E:1038:GLU:O    | 5:E:1040:ILE:HD12 | 2.10                     | 0.51              |
| 3:A:557:ASN:N     | 3:A:557:ASN:ND2   | 2.54                     | 0.51              |
| 5:E:1131:LEU:HD21 | 5:E:1185:LEU:CD2  | 2.40                     | 0.51              |
| 3:A:509:CYS:O     | 3:A:515:ILE:HG23  | 2.11                     | 0.51              |
| 5:E:1242:LYS:HG2  | 5:E:1246:MSE:HE2  | 1.93                     | 0.51              |
| 3:A:254:ASP:C     | 3:A:256:VAL:N     | 2.69                     | 0.51              |
| 5:E:1098:LEU:HD13 | 5:E:1110:VAL:HG13 | 1.92                     | 0.51              |
| 4:D:56:THR:HG22   | 4:D:57:ILE:HD13   | 1.92                     | 0.51              |
| 5:E:1159:LEU:HD23 | 5:E:1163:GLY:HA2  | 1.93                     | 0.51              |
| 5:E:1220:MSE:O    | 5:E:1223:VAL:HG22 | 2.11                     | 0.51              |
| 5:E:1235:ASP:HA   | 5:E:1243:THR:HG22 | 1.92                     | 0.51              |
| 1:B:1:DT:H2'      | 1:B:2:DT:C7       | 2.32                     | 0.51              |
| 3:A:251:LEU:O     | 3:A:255:ARG:HG3   | 2.10                     | 0.51              |
| 3:A:427:ILE:O     | 3:A:427:ILE:CG2   | 2.54                     | 0.51              |
| 5:E:1121:THR:O    | 5:E:1122:ILE:C    | 2.53                     | 0.51              |
| 3:A:220:PHE:HB3   | 3:A:422:TRP:CH2   | 2.46                     | 0.51              |
| 3:A:387:ALA:HB3   | 3:A:390:THR:HG21  | 1.93                     | 0.51              |
| 3:A:555:VAL:HG11  | 3:A:646:ASP:OD2   | 2.10                     | 0.51              |
| 3:A:289:TYR:HB3   | 3:A:299:ARG:HG2   | 1.93                     | 0.51              |
| 5:E:1219:ASN:C    | 5:E:1221:PRO:HD2  | 2.36                     | 0.51              |
| 5:E:1297:ARG:HB3  | 5:E:1297:ARG:NH1  | 2.24                     | 0.51              |
| 3:A:568:LEU:C     | 3:A:569:GLU:OE1   | 2.54                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:A:571:ASP:OD2   | 5:E:1136:ALA:HB1  | 2.11                     | 0.50              |
| 4:D:104:THR:HA    | 4:D:107:GLU:HB3   | 1.92                     | 0.50              |
| 5:E:1029:GLU:O    | 5:E:1030:ALA:C    | 2.54                     | 0.50              |
| 5:E:1178:GLN:O    | 5:E:1180:ALA:N    | 2.44                     | 0.50              |
| 3:A:349:TYR:HB2   | 3:A:353:MET:HB3   | 1.93                     | 0.50              |
| 3:A:402:THR:HG23  | 3:A:403:VAL:N     | 2.27                     | 0.50              |
| 3:A:619:VAL:HG11  | 3:A:638:VAL:HG11  | 1.94                     | 0.50              |
| 5:E:1159:LEU:HD13 | 5:E:1159:LEU:N    | 2.27                     | 0.50              |
| 1:B:13:DA:H2''    | 1:B:14:DG:H5''    | 1.93                     | 0.50              |
| 5:E:1141:GLY:O    | 5:E:1144:VAL:HG12 | 2.11                     | 0.50              |
| 5:E:1252:GLY:HA3  | 5:E:1286:HIS:CE1  | 2.46                     | 0.50              |
| 3:A:386:ILE:HD13  | 3:A:392:VAL:HG11  | 1.94                     | 0.50              |
| 3:A:521:THR:HG1   | 3:A:529:GLN:HB2   | 1.75                     | 0.50              |
| 3:A:542:ASP:CG    | 3:A:543:LYS:N     | 2.69                     | 0.50              |
| 4:D:66:GLY:O      | 4:D:68:GLU:N      | 2.44                     | 0.50              |
| 5:E:935:ARG:HB2   | 5:E:1199:ARG:NH2  | 2.27                     | 0.50              |
| 5:E:1056:VAL:C    | 5:E:1060:ILE:HG12 | 2.36                     | 0.50              |
| 3:A:243:TYR:CB    | 3:A:245:ILE:HD11  | 2.41                     | 0.50              |
| 3:A:474:VAL:HG21  | 3:A:535:ALA:HB1   | 1.93                     | 0.50              |
| 5:E:1220:MSE:HE1  | 5:E:1259:TYR:CD1  | 2.46                     | 0.50              |
| 3:A:280:GLU:C     | 3:A:282:GLN:H     | 2.20                     | 0.50              |
| 5:E:1276:THR:HG22 | 5:E:1279:GLN:NE2  | 2.17                     | 0.50              |
| 5:E:1289:ILE:O    | 5:E:1290:VAL:C    | 2.53                     | 0.50              |
| 5:E:1063:ASN:C    | 5:E:1065:SER:H    | 2.20                     | 0.50              |
| 5:E:1184:LEU:HD13 | 5:E:1188:LYS:HG2  | 1.92                     | 0.50              |
| 3:A:568:LEU:HB2   | 3:A:654:LEU:HD23  | 1.94                     | 0.50              |
| 3:A:659:LYS:HD3   | 5:E:1052:HIS:HD2  | 1.77                     | 0.50              |
| 5:E:1028:THR:HG23 | 5:E:1029:GLU:N    | 2.27                     | 0.49              |
| 5:E:1178:GLN:C    | 5:E:1180:ALA:H    | 2.20                     | 0.49              |
| 2:C:1:DA:H1'      | 2:C:2:DA:H5'      | 1.94                     | 0.49              |
| 5:E:1138:ARG:CG   | 5:E:1178:GLN:HE22 | 2.23                     | 0.49              |
| 1:B:6:DG:H4'      | 3:A:235:PHE:CE2   | 2.45                     | 0.49              |
| 3:A:608:SER:O     | 3:A:609:LEU:HD23  | 2.12                     | 0.49              |
| 4:D:86:PRO:HA     | 4:D:89:ILE:CG1    | 2.39                     | 0.49              |
| 5:E:1026:LEU:C    | 5:E:1026:LEU:HD12 | 2.37                     | 0.49              |
| 5:E:1072:LEU:HD13 | 5:E:1076:GLU:OE2  | 2.12                     | 0.49              |
| 5:E:1099:MSE:O    | 5:E:1101:ALA:N    | 2.45                     | 0.49              |
| 3:A:319:PRO:HG2   | 3:A:321:ILE:HG13  | 1.94                     | 0.49              |
| 3:A:560:SER:O     | 3:A:562:CYS:N     | 2.46                     | 0.49              |
| 3:A:637:GLU:HG3   | 3:A:637:GLU:O     | 2.13                     | 0.49              |
| 5:E:1056:VAL:CG1  | 5:E:1060:ILE:HD11 | 2.42                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:E:1081:ILE:HD13 | 5:E:1082:ALA:N    | 2.27                     | 0.49              |
| 5:E:1244:PRO:O    | 5:E:1245:ILE:C    | 2.55                     | 0.49              |
| 5:E:1141:GLY:O    | 5:E:1142:MSE:C    | 2.55                     | 0.49              |
| 5:E:1153:LYS:HA   | 5:E:1156:ILE:HG12 | 1.94                     | 0.49              |
| 5:E:1252:GLY:HA3  | 5:E:1286:HIS:ND1  | 2.28                     | 0.49              |
| 5:E:1201:ASP:OD1  | 5:E:1202:SER:N    | 2.42                     | 0.49              |
| 3:A:394:LEU:HD11  | 3:A:457:LEU:HD13  | 1.94                     | 0.49              |
| 3:A:501:ILE:HD13  | 3:A:501:ILE:C     | 2.38                     | 0.49              |
| 3:A:388:SER:CB    | 5:E:1202:SER:OG   | 2.56                     | 0.49              |
| 3:A:506:VAL:HG13  | 3:A:518:HIS:H     | 1.76                     | 0.49              |
| 5:E:1110:VAL:CG2  | 5:E:1142:MSE:HE1  | 2.36                     | 0.49              |
| 2:C:1:DA:H1'      | 2:C:2:DA:C5'      | 2.43                     | 0.48              |
| 3:A:220:PHE:CE2   | 3:A:543:LYS:HD2   | 2.48                     | 0.48              |
| 3:A:224:VAL:HG11  | 3:A:492:GLN:HG2   | 1.94                     | 0.48              |
| 3:A:605:SER:C     | 3:A:607:GLU:H     | 2.20                     | 0.48              |
| 5:E:1114:MSE:HA   | 5:E:1118:ALA:HB3  | 1.95                     | 0.48              |
| 5:E:1253:ARG:O    | 5:E:1256:VAL:HG12 | 2.13                     | 0.48              |
| 3:A:644:ARG:C     | 3:A:646:ASP:N     | 2.71                     | 0.48              |
| 5:E:1133:GLN:NE2  | 5:E:1133:GLN:CA   | 2.74                     | 0.48              |
| 5:E:1180:ALA:C    | 5:E:1182:ALA:N    | 2.67                     | 0.48              |
| 5:E:1200:LYS:C    | 5:E:1201:ASP:O    | 2.54                     | 0.48              |
| 5:E:1220:MSE:HB2  | 5:E:1221:PRO:HD3  | 1.94                     | 0.48              |
| 3:A:215:CYS:HB2   | 3:A:548:PHE:O     | 2.13                     | 0.48              |
| 3:A:245:ILE:HG22  | 3:A:246:GLY:N     | 2.27                     | 0.48              |
| 3:A:432:ASP:O     | 3:A:433:GLU:HB2   | 2.12                     | 0.48              |
| 3:A:462:THR:OG1   | 3:A:463:GLY:N     | 2.46                     | 0.48              |
| 2:C:14:DG:H2''    | 2:C:15:DT:O5'     | 2.12                     | 0.48              |
| 3:A:516:ILE:HA    | 5:E:947:PRO:HB2   | 1.96                     | 0.48              |
| 4:D:83:LYS:CD     | 4:D:84:ALA:N      | 2.75                     | 0.48              |
| 3:A:223:LYS:HD2   | 3:A:383:TYR:CE2   | 2.40                     | 0.48              |
| 3:A:593:TRP:CE2   | 3:A:598:PRO:HB3   | 2.48                     | 0.48              |
| 5:E:1058:HIS:CE1  | 5:E:1089:ALA:O    | 2.66                     | 0.48              |
| 5:E:1201:ASP:O    | 5:E:1202:SER:O    | 2.31                     | 0.48              |
| 4:D:64:HIS:C      | 4:D:66:GLY:N      | 2.68                     | 0.48              |
| 4:D:91:ASN:H      | 4:D:91:ASN:ND2    | 2.12                     | 0.48              |
| 5:E:1099:MSE:HE1  | 5:E:1130:ALA:CA   | 2.38                     | 0.48              |
| 3:A:472:ARG:O     | 3:A:496:CYS:HB2   | 2.13                     | 0.48              |
| 5:E:1173:ASN:O    | 5:E:1178:GLN:HG2  | 2.14                     | 0.48              |
| 3:A:604:ARG:HG2   | 3:A:604:ARG:NH2   | 2.25                     | 0.48              |
| 3:A:613:ILE:HD12  | 3:A:613:ILE:N     | 2.29                     | 0.48              |
| 5:E:1253:ARG:HA   | 5:E:1253:ARG:NE   | 2.29                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:A:242:ILE:HD12  | 3:A:242:ILE:N     | 2.28                     | 0.48              |
| 3:A:250:LYS:O     | 3:A:253:LYS:HB3   | 2.14                     | 0.48              |
| 3:A:310:ARG:HG2   | 3:A:310:ARG:HH11  | 1.79                     | 0.48              |
| 5:E:935:ARG:HB2   | 5:E:1199:ARG:HH22 | 1.79                     | 0.48              |
| 3:A:300:GLN:H     | 3:A:300:GLN:HE21  | 1.62                     | 0.47              |
| 3:A:430:PHE:C     | 3:A:430:PHE:CD1   | 2.92                     | 0.47              |
| 5:E:1242:LYS:HG2  | 5:E:1246:MSE:CE   | 2.44                     | 0.47              |
| 3:A:506:VAL:HG11  | 3:A:517:GLN:HE21  | 1.80                     | 0.47              |
| 5:E:935:ARG:NH1   | 5:E:1158:GLU:CG   | 2.59                     | 0.47              |
| 5:E:1133:GLN:O    | 5:E:1134:ALA:C    | 2.55                     | 0.47              |
| 3:A:441:ASN:HA    | 5:E:941:ASN:HA    | 1.96                     | 0.47              |
| 5:E:1022:SER:N    | 5:E:1023:PRO:CD   | 2.73                     | 0.47              |
| 5:E:1040:ILE:N    | 5:E:1040:ILE:CD1  | 2.77                     | 0.47              |
| 5:E:1087:VAL:CG2  | 5:E:1118:ALA:HB2  | 2.44                     | 0.47              |
| 5:E:1167:LEU:N    | 5:E:1167:LEU:CD1  | 2.65                     | 0.47              |
| 5:E:1072:LEU:HD12 | 5:E:1072:LEU:C    | 2.39                     | 0.47              |
| 5:E:1278:ARG:O    | 5:E:1279:GLN:C    | 2.56                     | 0.47              |
| 1:B:13:DA:C1'     | 1:B:14:DG:H5''    | 2.42                     | 0.47              |
| 3:A:418:SER:HB3   | 3:A:421:LYS:O     | 2.15                     | 0.47              |
| 3:A:451:TYR:CE1   | 3:A:490:VAL:HG22  | 2.50                     | 0.47              |
| 3:A:508:LEU:HD11  | 3:A:515:ILE:CG2   | 2.45                     | 0.47              |
| 4:D:80:ASN:O      | 4:D:83:LYS:HB3    | 2.13                     | 0.47              |
| 5:E:1178:GLN:C    | 5:E:1180:ALA:N    | 2.71                     | 0.47              |
| 5:E:1252:GLY:HA2  | 5:E:1289:ILE:HD11 | 1.96                     | 0.47              |
| 3:A:251:LEU:HD13  | 3:A:251:LEU:C     | 2.40                     | 0.47              |
| 3:A:341:PHE:CD1   | 3:A:341:PHE:C     | 2.92                     | 0.47              |
| 3:A:550:GLU:HA    | 3:A:648:VAL:HG23  | 1.97                     | 0.47              |
| 1:B:13:DA:H2''    | 1:B:14:DG:C5'     | 2.45                     | 0.47              |
| 5:E:1034:TYR:HD1  | 5:E:1035:ALA:N    | 1.94                     | 0.47              |
| 5:E:1045:VAL:HG12 | 5:E:1056:VAL:CG2  | 2.41                     | 0.47              |
| 5:E:1093:ASP:HA   | 5:E:1125:LYS:HD2  | 1.97                     | 0.47              |
| 5:E:1276:THR:O    | 5:E:1278:ARG:N    | 2.48                     | 0.47              |
| 5:E:1196:GLY:O    | 5:E:1199:ARG:N    | 2.47                     | 0.47              |
| 5:E:1208:ARG:HB3  | 5:E:1212:HIS:HB2  | 1.96                     | 0.47              |
| 3:A:254:ASP:O     | 3:A:256:VAL:N     | 2.47                     | 0.47              |
| 3:A:560:SER:CB    | 3:A:561:PRO:CD    | 2.90                     | 0.47              |
| 5:E:1182:ALA:O    | 5:E:1183:LYS:C    | 2.56                     | 0.47              |
| 5:E:1210:ALA:O    | 5:E:1211:LEU:C    | 2.58                     | 0.47              |
| 4:D:76:LEU:HD22   | 4:D:76:LEU:O      | 2.14                     | 0.47              |
| 3:A:415:PHE:CZ    | 3:A:466:LEU:HG    | 2.50                     | 0.46              |
| 3:A:493:LEU:CD2   | 3:A:539:ILE:HD12  | 2.41                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:E:1073:ILE:HD11 | 5:E:1106:ARG:NH2  | 2.30                     | 0.46              |
| 5:E:1220:MSE:HE1  | 5:E:1259:TYR:HD1  | 1.80                     | 0.46              |
| 5:E:1075:HIS:C    | 5:E:1077:ALA:H    | 2.24                     | 0.46              |
| 5:E:1091:ASP:O    | 5:E:1092:CYS:C    | 2.58                     | 0.46              |
| 5:E:1099:MSE:CE   | 5:E:1130:ALA:HA   | 2.40                     | 0.46              |
| 3:A:362:ARG:HD2   | 3:A:362:ARG:H     | 1.81                     | 0.46              |
| 3:A:441:ASN:HB2   | 5:E:939:MSE:CE    | 2.46                     | 0.46              |
| 3:A:485:CYS:C     | 3:A:487:GLU:H     | 2.23                     | 0.46              |
| 3:A:510:LEU:HG    | 3:A:510:LEU:O     | 2.15                     | 0.46              |
| 3:A:569:GLU:CG    | 5:E:1128:ARG:NH2  | 2.78                     | 0.46              |
| 5:E:1199:ARG:NH1  | 5:E:1203:GLU:OE1  | 2.48                     | 0.46              |
| 5:E:1233:ASN:C    | 5:E:1235:ASP:N    | 2.71                     | 0.46              |
| 5:E:1234:LYS:HG3  | 5:E:1265:ALA:HB2  | 1.98                     | 0.46              |
| 3:A:406:ARG:CZ    | 3:A:419:SER:HB3   | 2.45                     | 0.46              |
| 3:A:508:LEU:HD11  | 3:A:515:ILE:HG21  | 1.96                     | 0.46              |
| 5:E:943:SER:OG    | 5:E:944:VAL:N     | 2.46                     | 0.46              |
| 5:E:1097:PRO:HA   | 5:E:1100:LEU:HD13 | 1.98                     | 0.46              |
| 5:E:1259:TYR:CE2  | 5:E:1263:GLN:HG3  | 2.50                     | 0.46              |
| 5:E:1107:ARG:HA   | 5:E:1142:MSE:HE1  | 1.96                     | 0.46              |
| 3:A:255:ARG:HH21  | 3:A:553:GLY:HA2   | 1.80                     | 0.46              |
| 3:A:265:ALA:O     | 3:A:266:SER:HB3   | 2.15                     | 0.46              |
| 3:A:506:VAL:CG1   | 3:A:517:GLN:HG2   | 2.46                     | 0.46              |
| 3:A:342:ASP:OD1   | 3:A:342:ASP:N     | 2.45                     | 0.46              |
| 3:A:555:VAL:HG12  | 3:A:556:ALA:N     | 2.31                     | 0.46              |
| 3:A:616:VAL:HG22  | 3:A:658:TYR:CE1   | 2.50                     | 0.46              |
| 3:A:215:CYS:HB3   | 3:A:548:PHE:CE2   | 2.50                     | 0.46              |
| 3:A:523:ILE:HG23  | 3:A:524:ASN:N     | 2.30                     | 0.46              |
| 3:A:553:GLY:O     | 3:A:554:GLN:C     | 2.58                     | 0.46              |
| 5:E:1066:ALA:O    | 5:E:1067:GLU:CB   | 2.63                     | 0.46              |
| 5:E:1193:ASP:OD1  | 5:E:1232:SER:HA   | 2.15                     | 0.46              |
| 3:A:290:ILE:CD1   | 3:A:345:ALA:HB2   | 2.45                     | 0.46              |
| 3:A:568:LEU:HD23  | 3:A:569:GLU:N     | 2.30                     | 0.46              |
| 5:E:1174:GLU:CG   | 5:E:1175:GLY:H    | 2.29                     | 0.46              |
| 3:A:258:GLN:HA    | 3:A:261:LYS:HE2   | 1.97                     | 0.46              |
| 3:A:514:LYS:HD3   | 3:A:514:LYS:HA    | 1.76                     | 0.46              |
| 3:A:563:PRO:HG3   | 3:A:650:TYR:CD2   | 2.51                     | 0.46              |
| 3:A:620:ARG:HA    | 3:A:624:THR:OG1   | 2.15                     | 0.46              |
| 5:E:1025:LYS:O    | 5:E:1029:GLU:HG3  | 2.16                     | 0.46              |
| 5:E:1113:LEU:HD13 | 5:E:1113:LEU:HA   | 1.73                     | 0.46              |
| 3:A:447:GLY:HA2   | 5:E:1201:ASP:OD1  | 2.16                     | 0.45              |
| 3:A:510:LEU:HD23  | 3:A:510:LEU:H     | 1.81                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:E:1133:GLN:O    | 5:E:1137:ASN:OD1  | 2.34                     | 0.45              |
| 1:B:7:DT:H2"      | 1:B:8:DG:H8       | 1.80                     | 0.45              |
| 3:A:348:PHE:CD1   | 3:A:348:PHE:C     | 2.93                     | 0.45              |
| 3:A:431:ASP:HB3   | 3:A:443:ALA:CB    | 2.45                     | 0.45              |
| 3:A:470:ARG:HB3   | 3:A:499:GLN:HG2   | 1.98                     | 0.45              |
| 5:E:933:ARG:NH1   | 5:E:1090:MSE:SE   | 2.88                     | 0.45              |
| 5:E:1087:VAL:CG2  | 5:E:1113:LEU:HD12 | 2.46                     | 0.45              |
| 5:E:1291:ASP:O    | 5:E:1295:ARG:HB2  | 2.16                     | 0.45              |
| 3:A:255:ARG:HH21  | 3:A:553:GLY:CA    | 2.28                     | 0.45              |
| 5:E:1075:HIS:C    | 5:E:1077:ALA:N    | 2.71                     | 0.45              |
| 5:E:1183:LYS:O    | 5:E:1186:VAL:HG13 | 2.17                     | 0.45              |
| 5:E:1218:SER:N    | 5:E:1253:ARG:HG3  | 2.27                     | 0.45              |
| 3:A:475:ASP:O     | 3:A:476:LYS:C     | 2.59                     | 0.45              |
| 3:A:499:GLN:HA    | 3:A:506:VAL:O     | 2.17                     | 0.45              |
| 5:E:1273:THR:O    | 5:E:1275:HIS:HD2  | 2.00                     | 0.45              |
| 3:A:593:TRP:NE1   | 3:A:598:PRO:HB3   | 2.32                     | 0.45              |
| 4:D:113:GLU:O     | 4:D:114:GLN:HG3   | 2.17                     | 0.45              |
| 3:A:588:PRO:HG3   | 3:A:603:PHE:CD1   | 2.52                     | 0.45              |
| 4:D:90:ALA:C      | 4:D:92:GLN:N      | 2.74                     | 0.45              |
| 5:E:1026:LEU:O    | 5:E:1029:GLU:HB2  | 2.17                     | 0.45              |
| 5:E:1174:GLU:HG2  | 5:E:1175:GLY:H    | 1.80                     | 0.45              |
| 3:A:245:ILE:N     | 3:A:245:ILE:CD1   | 2.80                     | 0.45              |
| 3:A:394:LEU:HD11  | 3:A:457:LEU:CD1   | 2.46                     | 0.45              |
| 5:E:1098:LEU:HD11 | 5:E:1146:MSE:CE   | 2.47                     | 0.45              |
| 5:E:1238:ASP:C    | 5:E:1240:ASP:H    | 2.25                     | 0.45              |
| 3:A:261:LYS:C     | 3:A:263:LEU:H     | 2.25                     | 0.45              |
| 3:A:430:PHE:HB3   | 3:A:454:VAL:HB    | 1.98                     | 0.45              |
| 3:A:503:ASN:C     | 3:A:503:ASN:HD22  | 2.25                     | 0.45              |
| 5:E:1066:ALA:C    | 5:E:1068:LYS:H    | 2.22                     | 0.45              |
| 5:E:1089:ALA:O    | 5:E:1097:PRO:HD3  | 2.16                     | 0.45              |
| 3:A:557:ASN:HB3   | 3:A:558:PRO:CD    | 2.47                     | 0.45              |
| 3:A:616:VAL:HG22  | 3:A:658:TYR:CD1   | 2.52                     | 0.45              |
| 5:E:1027:HIS:O    | 5:E:1028:THR:C    | 2.60                     | 0.45              |
| 5:E:1034:TYR:CD1  | 5:E:1035:ALA:N    | 2.75                     | 0.45              |
| 5:E:1073:ILE:HD11 | 5:E:1106:ARG:NH1  | 2.31                     | 0.45              |
| 5:E:1209:THR:N    | 5:E:1212:HIS:ND1  | 2.65                     | 0.45              |
| 5:E:1234:LYS:H    | 5:E:1234:LYS:CD   | 2.25                     | 0.44              |
| 2:C:12:DC:H2"     | 2:C:13:DA:C8      | 2.53                     | 0.44              |
| 5:E:1029:GLU:OE1  | 5:E:1037:THR:HB   | 2.17                     | 0.44              |
| 5:E:1220:MSE:O    | 5:E:1221:PRO:C    | 2.60                     | 0.44              |
| 3:A:280:GLU:C     | 3:A:282:GLN:N     | 2.74                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:E:1179:VAL:HG22 | 5:E:1179:VAL:O    | 2.17                     | 0.44              |
| 1:B:8:DG:OP1      | 3:A:397:ARG:HD3   | 2.18                     | 0.44              |
| 3:A:244:LEU:HD23  | 3:A:244:LEU:HA    | 1.83                     | 0.44              |
| 1:B:6:DG:H21      | 3:A:400:SER:HB3   | 1.82                     | 0.44              |
| 5:E:1199:ARG:O    | 5:E:1200:LYS:C    | 2.60                     | 0.44              |
| 5:E:1199:ARG:O    | 5:E:1201:ASP:N    | 2.49                     | 0.44              |
| 5:E:1276:THR:O    | 5:E:1277:ALA:C    | 2.60                     | 0.44              |
| 3:A:515:ILE:HG22  | 3:A:516:ILE:N     | 2.31                     | 0.44              |
| 3:A:244:LEU:O     | 3:A:322:TYR:HB3   | 2.18                     | 0.44              |
| 3:A:599:VAL:CG1   | 3:A:600:GLU:N     | 2.80                     | 0.44              |
| 5:E:1099:MSE:O    | 5:E:1100:LEU:C    | 2.60                     | 0.44              |
| 3:A:592:VAL:HA    | 3:A:641:SER:O     | 2.18                     | 0.44              |
| 3:A:206:PHE:CE2   | 3:A:649:VAL:HG21  | 2.53                     | 0.44              |
| 3:A:239:PRO:HA    | 3:A:240:PRO:HD3   | 1.88                     | 0.44              |
| 3:A:328:LYS:H     | 3:A:328:LYS:CD    | 2.06                     | 0.44              |
| 3:A:411:GLU:HG3   | 3:A:416:HIS:NE2   | 2.33                     | 0.44              |
| 4:D:65:SER:O      | 4:D:68:GLU:HB2    | 2.17                     | 0.44              |
| 5:E:1025:LYS:HD3  | 5:E:1038:GLU:OE1  | 2.17                     | 0.44              |
| 5:E:1099:MSE:SE   | 5:E:1133:GLN:HG3  | 2.68                     | 0.44              |
| 5:E:1207:GLY:HA2  | 5:E:1239:GLU:H    | 1.83                     | 0.44              |
| 3:A:198:LEU:HD12  | 3:A:199:THR:N     | 2.33                     | 0.43              |
| 4:D:85:ARG:N      | 4:D:86:PRO:HD2    | 2.33                     | 0.43              |
| 5:E:1036:ILE:HG12 | 5:E:1076:GLU:CD   | 2.43                     | 0.43              |
| 5:E:1134:ALA:C    | 5:E:1143:MSE:HE2  | 2.43                     | 0.43              |
| 3:A:573:HIS:O     | 3:A:575:GLU:N     | 2.51                     | 0.43              |
| 4:D:83:LYS:C      | 4:D:85:ARG:H      | 2.27                     | 0.43              |
| 3:A:398:LEU:HD22  | 3:A:398:LEU:N     | 2.32                     | 0.43              |
| 3:A:589:ASN:HD22  | 4:D:81:TYR:HE2    | 1.65                     | 0.43              |
| 3:A:203:MET:HE2   | 3:A:593:TRP:CE3   | 2.53                     | 0.43              |
| 3:A:215:CYS:CB    | 3:A:548:PHE:HE2   | 2.31                     | 0.43              |
| 3:A:416:HIS:CG    | 3:A:417:ALA:N     | 2.87                     | 0.43              |
| 3:A:633:THR:C     | 3:A:635:ASP:N     | 2.76                     | 0.43              |
| 5:E:940:ILE:O     | 5:E:940:ILE:HG22  | 2.17                     | 0.43              |
| 3:A:609:LEU:HD12  | 3:A:642:LEU:HD21  | 2.00                     | 0.43              |
| 4:D:76:LEU:O      | 4:D:79:ALA:HB3    | 2.19                     | 0.43              |
| 1:B:6:DG:H2"      | 1:B:7:DT:C6       | 2.54                     | 0.43              |
| 3:A:451:TYR:CD1   | 3:A:490:VAL:HG22  | 2.54                     | 0.43              |
| 3:A:503:ASN:C     | 3:A:505:LEU:H     | 2.20                     | 0.43              |
| 5:E:1025:LYS:O    | 5:E:1028:THR:HG22 | 2.18                     | 0.43              |
| 5:E:1033:SER:O    | 5:E:1069:SER:CB   | 2.66                     | 0.43              |
| 5:E:1243:THR:O    | 5:E:1246:MSE:N    | 2.51                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:A:235:PHE:CD1   | 3:A:329:THR:HA    | 2.53                     | 0.43              |
| 5:E:1139:ASP:O    | 5:E:1140:PHE:C    | 2.61                     | 0.43              |
| 5:E:1165:THR:OG1  | 5:E:1168:MSE:HE3  | 2.19                     | 0.43              |
| 3:A:388:SER:HB2   | 3:A:447:GLY:N     | 2.33                     | 0.43              |
| 5:E:1170:VAL:C    | 5:E:1172:HIS:N    | 2.77                     | 0.43              |
| 5:E:1243:THR:H    | 5:E:1246:MSE:SE   | 2.51                     | 0.43              |
| 5:E:1253:ARG:HB2  | 5:E:1256:VAL:HG12 | 2.01                     | 0.43              |
| 2:C:13:DA:C4      | 2:C:14:DG:N7      | 2.87                     | 0.43              |
| 3:A:302:LEU:CD2   | 3:A:327:ALA:HB2   | 2.49                     | 0.43              |
| 3:A:516:ILE:HG22  | 5:E:948:PRO:HG2   | 2.00                     | 0.43              |
| 3:A:603:PHE:CE1   | 3:A:606:GLU:HA    | 2.54                     | 0.43              |
| 5:E:1073:ILE:CD1  | 5:E:1106:ARG:CZ   | 2.86                     | 0.43              |
| 5:E:1170:VAL:O    | 5:E:1171:ALA:C    | 2.62                     | 0.43              |
| 5:E:1217:VAL:HG23 | 5:E:1251:GLU:CB   | 2.48                     | 0.43              |
| 3:A:539:ILE:O     | 3:A:539:ILE:HG23  | 2.18                     | 0.42              |
| 5:E:1219:ASN:O    | 5:E:1219:ASN:OD1  | 2.36                     | 0.42              |
| 3:A:362:ARG:H     | 3:A:362:ARG:CD    | 2.32                     | 0.42              |
| 3:A:406:ARG:HE    | 3:A:513:ASP:CG    | 2.27                     | 0.42              |
| 3:A:530:ILE:N     | 3:A:530:ILE:CD1   | 2.81                     | 0.42              |
| 5:E:1192:VAL:CG1  | 5:E:1226:LEU:HD22 | 2.50                     | 0.42              |
| 3:A:196:GLN:HB3   | 3:A:552:MET:HG3   | 2.01                     | 0.42              |
| 4:D:92:GLN:NE2    | 4:D:96:THR:HB     | 2.33                     | 0.42              |
| 5:E:1099:MSE:C    | 5:E:1101:ALA:H    | 2.26                     | 0.42              |
| 3:A:388:SER:OG    | 3:A:445:ARG:O     | 2.31                     | 0.42              |
| 3:A:586:PHE:CE2   | 3:A:642:LEU:HD11  | 2.54                     | 0.42              |
| 4:D:109:ARG:HA    | 4:D:112:VAL:HG22  | 2.01                     | 0.42              |
| 5:E:1057:LEU:HA   | 5:E:1060:ILE:CG1  | 2.49                     | 0.42              |
| 5:E:1063:ASN:HD21 | 5:E:1106:ARG:HH11 | 1.67                     | 0.42              |
| 3:A:213:TYR:CB    | 3:A:549:PHE:CE2   | 2.99                     | 0.42              |
| 3:A:215:CYS:CB    | 3:A:548:PHE:CE2   | 3.02                     | 0.42              |
| 3:A:348:PHE:HA    | 3:A:355:ILE:HG12  | 2.02                     | 0.42              |
| 3:A:427:ILE:HG13  | 3:A:457:LEU:CD2   | 2.49                     | 0.42              |
| 3:A:597:THR:HA    | 3:A:598:PRO:HD2   | 1.85                     | 0.42              |
| 5:E:1073:ILE:O    | 5:E:1074:VAL:C    | 2.62                     | 0.42              |
| 3:A:386:ILE:HD12  | 3:A:538:ILE:HD13  | 2.00                     | 0.42              |
| 3:A:388:SER:HB2   | 3:A:447:GLY:H     | 1.85                     | 0.42              |
| 3:A:481:LEU:HD12  | 3:A:481:LEU:O     | 2.19                     | 0.42              |
| 3:A:413:ASN:HA    | 3:A:464:ILE:HD12  | 2.00                     | 0.42              |
| 3:A:416:HIS:HD1   | 3:A:417:ALA:H     | 1.67                     | 0.42              |
| 5:E:1078:LYS:CA   | 5:E:1081:ILE:HG23 | 2.49                     | 0.42              |
| 5:E:1188:LYS:HA   | 5:E:1188:LYS:HD3  | 1.68                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:A:252:LYS:HA    | 3:A:252:LYS:HD2   | 1.80                     | 0.42              |
| 5:E:1043:GLU:O    | 5:E:1048:ILE:HD13 | 2.20                     | 0.42              |
| 5:E:1034:TYR:O    | 5:E:1036:ILE:HG13 | 2.20                     | 0.42              |
| 5:E:1026:LEU:HD12 | 5:E:1026:LEU:O    | 2.20                     | 0.42              |
| 5:E:1237:GLN:HB3  | 5:E:1241:GLY:CA   | 2.45                     | 0.42              |
| 5:E:1253:ARG:CB   | 5:E:1256:VAL:HG12 | 2.50                     | 0.42              |
| 3:A:407:TYR:CG    | 3:A:422:TRP:HB3   | 2.55                     | 0.41              |
| 5:E:1059:TRP:O    | 5:E:1062:SER:HB3  | 2.19                     | 0.41              |
| 5:E:1166:ALA:HB1  | 5:E:1185:LEU:CD1  | 2.50                     | 0.41              |
| 5:E:1167:LEU:HA   | 5:E:1170:VAL:HB   | 2.00                     | 0.41              |
| 5:E:1256:VAL:O    | 5:E:1257:VAL:C    | 2.63                     | 0.41              |
| 5:E:1098:LEU:C    | 5:E:1098:LEU:CD1  | 2.85                     | 0.41              |
| 5:E:1126:SER:O    | 5:E:1128:ARG:N    | 2.53                     | 0.41              |
| 5:E:1182:ALA:O    | 5:E:1184:LEU:N    | 2.53                     | 0.41              |
| 5:E:1054:ARG:HG2  | 5:E:1091:ASP:HB3  | 2.01                     | 0.41              |
| 5:E:1078:LYS:CA   | 5:E:1081:ILE:CG2  | 2.96                     | 0.41              |
| 5:E:1135:ALA:N    | 5:E:1143:MSE:HE2  | 2.35                     | 0.41              |
| 3:A:206:PHE:C     | 3:A:208:SER:N     | 2.78                     | 0.41              |
| 3:A:659:LYS:CD    | 5:E:1052:HIS:HD2  | 2.33                     | 0.41              |
| 4:D:53:ASP:OD1    | 5:E:1108:ARG:NH2  | 2.53                     | 0.41              |
| 4:D:68:GLU:O      | 4:D:69:LEU:C      | 2.61                     | 0.41              |
| 5:E:935:ARG:HB3   | 5:E:1199:ARG:HH22 | 1.84                     | 0.41              |
| 5:E:1053:ASN:O    | 5:E:1091:ASP:HA   | 2.21                     | 0.41              |
| 5:E:1077:ALA:C    | 5:E:1079:GLU:N    | 2.76                     | 0.41              |
| 3:A:249:TRP:HB3   | 3:A:322:TYR:CE1   | 2.56                     | 0.41              |
| 3:A:388:SER:HB3   | 5:E:1202:SER:CB   | 2.48                     | 0.41              |
| 5:E:1120:PRO:O    | 5:E:1121:THR:C    | 2.63                     | 0.41              |
| 3:A:408:LEU:HD22  | 3:A:425:PHE:CE1   | 2.55                     | 0.41              |
| 3:A:446:ASP:CG    | 5:E:1203:GLU:HG3  | 2.45                     | 0.41              |
| 3:A:580:GLU:C     | 3:A:581:LEU:HD23  | 2.46                     | 0.41              |
| 3:A:614:PRO:HA    | 3:A:615:PRO:HD3   | 1.91                     | 0.41              |
| 5:E:1254:ILE:HG13 | 5:E:1255:GLU:N    | 2.36                     | 0.41              |
| 3:A:217:ILE:HG23  | 3:A:217:ILE:O     | 2.21                     | 0.41              |
| 3:A:642:LEU:HD23  | 3:A:642:LEU:HA    | 1.82                     | 0.41              |
| 5:E:1233:ASN:O    | 5:E:1235:ASP:N    | 2.54                     | 0.41              |
| 3:A:249:TRP:HB3   | 3:A:322:TYR:CD1   | 2.55                     | 0.41              |
| 3:A:287:VAL:CB    | 3:A:348:PHE:CE1   | 3.04                     | 0.41              |
| 3:A:559:ILE:O     | 3:A:561:PRO:N     | 2.53                     | 0.41              |
| 5:E:1140:PHE:HD1  | 5:E:1141:GLY:N    | 2.19                     | 0.41              |
| 1:B:6:DG:H2''     | 1:B:7:DT:H6       | 1.86                     | 0.41              |
| 2:C:1:DA:H1'      | 2:C:2:DA:O5'      | 2.21                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:A:348:PHE:HB2  | 3:A:353:MET:O     | 2.21                     | 0.41              |
| 3:A:442:PHE:CZ   | 3:A:456:LYS:HE2   | 2.56                     | 0.41              |
| 3:A:446:ASP:OD2  | 5:E:1203:GLU:HG3  | 2.21                     | 0.41              |
| 5:E:1040:ILE:O   | 5:E:1040:ILE:HG22 | 2.20                     | 0.41              |
| 5:E:1253:ARG:O   | 5:E:1257:VAL:HG23 | 2.20                     | 0.41              |
| 5:E:1271:ASP:OD2 | 5:E:1275:HIS:HB2  | 2.21                     | 0.41              |
| 3:A:255:ARG:NH2  | 3:A:553:GLY:HA2   | 2.36                     | 0.41              |
| 3:A:441:ASN:HB3  | 5:E:941:ASN:HB3   | 2.02                     | 0.41              |
| 3:A:466:LEU:HB3  | 3:A:467:PRO:HD2   | 2.03                     | 0.41              |
| 3:A:654:LEU:HA   | 3:A:654:LEU:HD12  | 1.86                     | 0.41              |
| 5:E:1028:THR:O   | 5:E:1032:GLY:N    | 2.38                     | 0.41              |
| 5:E:1033:SER:O   | 5:E:1069:SER:HB3  | 2.20                     | 0.41              |
| 5:E:1048:ILE:N   | 5:E:1048:ILE:CD1  | 2.83                     | 0.41              |
| 5:E:1216:GLN:O   | 5:E:1217:VAL:O    | 2.39                     | 0.41              |
| 3:A:610:HIS:HE1  | 5:E:1173:ASN:HD21 | 1.68                     | 0.40              |
| 3:A:220:PHE:N    | 3:A:220:PHE:CD2   | 2.90                     | 0.40              |
| 3:A:343:LEU:O    | 3:A:359:VAL:HA    | 2.21                     | 0.40              |
| 3:A:399:ARG:O    | 3:A:401:GLN:N     | 2.55                     | 0.40              |
| 4:D:57:ILE:HB    | 4:D:58:GLY:H      | 1.58                     | 0.40              |
| 5:E:1061:ALA:HA  | 5:E:1109:LEU:HD21 | 2.04                     | 0.40              |
| 5:E:1199:ARG:C   | 5:E:1201:ASP:H    | 2.29                     | 0.40              |
| 3:A:340:TYR:CE2  | 3:A:383:TYR:CE1   | 3.10                     | 0.40              |
| 3:A:409:HIS:ND1  | 3:A:410:VAL:N     | 2.69                     | 0.40              |
| 3:A:602:THR:HG23 | 4:D:74:SER:HB2    | 2.02                     | 0.40              |
| 3:A:416:HIS:ND1  | 3:A:417:ALA:N     | 2.70                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles       |
|-----|-------|---------------|-----------|----------|----------|-------------------|
| 3   | A     | 429/477 (90%) | 324 (76%) | 77 (18%) | 28 (6%)  | <b>1</b> <b>6</b> |

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| Mol | Chain | Analysed      | Favoured  | Allowed   | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|-----------|----------|-------------|----|
| 4   | D     | 61/85 (72%)   | 44 (72%)  | 14 (23%)  | 3 (5%)   | 1           | 10 |
| 5   | E     | 293/373 (79%) | 170 (58%) | 76 (26%)  | 47 (16%) | 0           | 0  |
| All | All   | 783/935 (84%) | 538 (69%) | 167 (21%) | 78 (10%) | 0           | 2  |

All (78) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | A     | 299  | ARG  |
| 3   | A     | 399  | ARG  |
| 3   | A     | 400  | SER  |
| 3   | A     | 403  | VAL  |
| 3   | A     | 504  | GLU  |
| 3   | A     | 513  | ASP  |
| 3   | A     | 553  | GLY  |
| 3   | A     | 560  | SER  |
| 3   | A     | 574  | GLY  |
| 3   | A     | 627  | MET  |
| 3   | A     | 634  | GLY  |
| 4   | D     | 55   | PRO  |
| 4   | D     | 59   | ASP  |
| 5   | E     | 943  | SER  |
| 5   | E     | 1023 | PRO  |
| 5   | E     | 1032 | GLY  |
| 5   | E     | 1045 | VAL  |
| 5   | E     | 1046 | ASN  |
| 5   | E     | 1062 | SER  |
| 5   | E     | 1066 | ALA  |
| 5   | E     | 1070 | GLU  |
| 5   | E     | 1122 | ILE  |
| 5   | E     | 1198 | ALA  |
| 5   | E     | 1201 | ASP  |
| 5   | E     | 1202 | SER  |
| 5   | E     | 1204 | LYS  |
| 5   | E     | 1206 | LYS  |
| 5   | E     | 1217 | VAL  |
| 5   | E     | 1218 | SER  |
| 5   | E     | 1219 | ASN  |
| 5   | E     | 1230 | LYS  |
| 5   | E     | 1277 | ALA  |
| 3   | A     | 266  | SER  |
| 3   | A     | 300  | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | A     | 303  | ASP  |
| 3   | A     | 412  | GLY  |
| 5   | E     | 948  | PRO  |
| 5   | E     | 1022 | SER  |
| 5   | E     | 1050 | PRO  |
| 5   | E     | 1063 | ASN  |
| 5   | E     | 1087 | VAL  |
| 5   | E     | 1121 | THR  |
| 5   | E     | 1138 | ARG  |
| 5   | E     | 1203 | GLU  |
| 5   | E     | 1232 | SER  |
| 5   | E     | 1271 | ASP  |
| 3   | A     | 265  | ALA  |
| 3   | A     | 416  | HIS  |
| 3   | A     | 645  | ASP  |
| 5   | E     | 1024 | ILE  |
| 5   | E     | 1078 | LYS  |
| 5   | E     | 1140 | PHE  |
| 5   | E     | 1160 | ASP  |
| 5   | E     | 1166 | ALA  |
| 5   | E     | 1189 | GLY  |
| 5   | E     | 1210 | ALA  |
| 3   | A     | 207  | LEU  |
| 3   | A     | 214  | GLU  |
| 3   | A     | 255  | ARG  |
| 3   | A     | 479  | VAL  |
| 3   | A     | 532  | ASP  |
| 5   | E     | 1107 | ARG  |
| 5   | E     | 1127 | GLU  |
| 5   | E     | 1179 | VAL  |
| 5   | E     | 1234 | LYS  |
| 5   | E     | 1029 | GLU  |
| 5   | E     | 1068 | LYS  |
| 5   | E     | 1178 | GLN  |
| 5   | E     | 1208 | ARG  |
| 5   | E     | 1220 | MSE  |
| 3   | A     | 476  | LYS  |
| 3   | A     | 480  | ILE  |
| 5   | E     | 1120 | PRO  |
| 5   | E     | 1290 | VAL  |
| 3   | A     | 464  | ILE  |
| 3   | A     | 293  | GLY  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | A     | 558 | PRO  |
| 4   | D     | 57  | ILE  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 3   | A     | 385/416 (92%) | 337 (88%) | 48 (12%) | 4           | 18 |
| 4   | D     | 54/73 (74%)   | 49 (91%)  | 5 (9%)   | 8           | 29 |
| 5   | E     | 244/298 (82%) | 208 (85%) | 36 (15%) | 3           | 13 |
| All | All   | 683/787 (87%) | 594 (87%) | 89 (13%) | 4           | 17 |

All (89) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | A     | 199 | THR  |
| 3   | A     | 202 | ARG  |
| 3   | A     | 217 | ILE  |
| 3   | A     | 233 | LYS  |
| 3   | A     | 239 | PRO  |
| 3   | A     | 245 | ILE  |
| 3   | A     | 251 | LEU  |
| 3   | A     | 256 | VAL  |
| 3   | A     | 296 | THR  |
| 3   | A     | 300 | GLN  |
| 3   | A     | 310 | ARG  |
| 3   | A     | 328 | LYS  |
| 3   | A     | 346 | GLN  |
| 3   | A     | 362 | ARG  |
| 3   | A     | 383 | TYR  |
| 3   | A     | 408 | LEU  |
| 3   | A     | 426 | THR  |
| 3   | A     | 427 | ILE  |
| 3   | A     | 441 | ASN  |
| 3   | A     | 454 | VAL  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | A     | 464  | ILE  |
| 3   | A     | 474  | VAL  |
| 3   | A     | 481  | LEU  |
| 3   | A     | 482  | ASP  |
| 3   | A     | 485  | CYS  |
| 3   | A     | 492  | GLN  |
| 3   | A     | 501  | ILE  |
| 3   | A     | 511  | SER  |
| 3   | A     | 530  | ILE  |
| 3   | A     | 536  | TRP  |
| 3   | A     | 537  | THR  |
| 3   | A     | 548  | PHE  |
| 3   | A     | 550  | GLU  |
| 3   | A     | 552  | MET  |
| 3   | A     | 557  | ASN  |
| 3   | A     | 559  | ILE  |
| 3   | A     | 568  | LEU  |
| 3   | A     | 569  | GLU  |
| 3   | A     | 570  | VAL  |
| 3   | A     | 571  | ASP  |
| 3   | A     | 581  | LEU  |
| 3   | A     | 588  | PRO  |
| 3   | A     | 592  | VAL  |
| 3   | A     | 623  | GLN  |
| 3   | A     | 644  | ARG  |
| 3   | A     | 648  | VAL  |
| 3   | A     | 651  | SER  |
| 3   | A     | 662  | GLU  |
| 4   | D     | 55   | PRO  |
| 4   | D     | 75   | GLU  |
| 4   | D     | 76   | LEU  |
| 4   | D     | 91   | ASN  |
| 4   | D     | 109  | ARG  |
| 5   | E     | 937  | ARG  |
| 5   | E     | 1023 | PRO  |
| 5   | E     | 1026 | LEU  |
| 5   | E     | 1034 | TYR  |
| 5   | E     | 1046 | ASN  |
| 5   | E     | 1055 | THR  |
| 5   | E     | 1057 | LEU  |
| 5   | E     | 1072 | LEU  |
| 5   | E     | 1073 | ILE  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 5   | E     | 1079 | GLU  |
| 5   | E     | 1080 | CYS  |
| 5   | E     | 1081 | ILE  |
| 5   | E     | 1098 | LEU  |
| 5   | E     | 1105 | ARG  |
| 5   | E     | 1113 | LEU  |
| 5   | E     | 1121 | THR  |
| 5   | E     | 1126 | SER  |
| 5   | E     | 1133 | GLN  |
| 5   | E     | 1137 | ASN  |
| 5   | E     | 1147 | LEU  |
| 5   | E     | 1153 | LYS  |
| 5   | E     | 1159 | LEU  |
| 5   | E     | 1167 | LEU  |
| 5   | E     | 1168 | MSE  |
| 5   | E     | 1176 | ARG  |
| 5   | E     | 1178 | GLN  |
| 5   | E     | 1186 | VAL  |
| 5   | E     | 1202 | SER  |
| 5   | E     | 1229 | GLU  |
| 5   | E     | 1232 | SER  |
| 5   | E     | 1234 | LYS  |
| 5   | E     | 1243 | THR  |
| 5   | E     | 1244 | PRO  |
| 5   | E     | 1245 | ILE  |
| 5   | E     | 1263 | GLN  |
| 5   | E     | 1288 | ASN  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | A     | 221 | HIS  |
| 3   | A     | 258 | GLN  |
| 3   | A     | 320 | ASN  |
| 3   | A     | 361 | GLN  |
| 3   | A     | 401 | GLN  |
| 3   | A     | 441 | ASN  |
| 3   | A     | 478 | GLN  |
| 3   | A     | 503 | ASN  |
| 3   | A     | 517 | GLN  |
| 3   | A     | 519 | GLN  |
| 3   | A     | 524 | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | A     | 528  | HIS  |
| 3   | A     | 557  | ASN  |
| 3   | A     | 610  | HIS  |
| 3   | A     | 618  | GLN  |
| 3   | A     | 623  | GLN  |
| 3   | A     | 630  | ASN  |
| 4   | D     | 70   | HIS  |
| 4   | D     | 80   | ASN  |
| 4   | D     | 91   | ASN  |
| 4   | D     | 92   | GLN  |
| 4   | D     | 98   | HIS  |
| 5   | E     | 1027 | HIS  |
| 5   | E     | 1046 | ASN  |
| 5   | E     | 1058 | HIS  |
| 5   | E     | 1063 | ASN  |
| 5   | E     | 1075 | HIS  |
| 5   | E     | 1132 | HIS  |
| 5   | E     | 1133 | GLN  |
| 5   | E     | 1137 | ASN  |
| 5   | E     | 1162 | ASN  |
| 5   | E     | 1250 | GLN  |
| 5   | E     | 1263 | GLN  |
| 5   | E     | 1275 | HIS  |
| 5   | E     | 1279 | GLN  |
| 5   | E     | 1282 | GLN  |
| 5   | E     | 1285 | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 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   | B     | 15/15 (100%)  | 0.55   | 0         | 100 | 100 | 72, 88, 113, 115      | 0       |
| 2   | C     | 15/15 (100%)  | 0.31   | 0         | 100 | 100 | 66, 85, 113, 113      | 0       |
| 3   | A     | 439/477 (92%) | 0.14   | 15 (3%)   | 48  | 28  | 37, 97, 165, 197      | 0       |
| 4   | D     | 63/85 (74%)   | 0.34   | 5 (7%)    | 18  | 10  | 68, 123, 174, 200     | 0       |
| 5   | E     | 283/373 (75%) | 0.14   | 9 (3%)    | 50  | 30  | 52, 94, 165, 202      | 0       |
| All | All   | 815/965 (84%) | 0.17   | 29 (3%)   | 46  | 26  | 37, 98, 166, 202      | 0       |

All (29) RSRZ outliers are listed below:

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 5   | E     | 1203 | GLU  | 6.9  |
| 3   | A     | 401  | GLN  | 5.3  |
| 4   | D     | 57   | ILE  | 5.0  |
| 3   | A     | 400  | SER  | 4.4  |
| 5   | E     | 1050 | PRO  | 3.6  |
| 5   | E     | 1205 | TYR  | 3.6  |
| 3   | A     | 554  | GLN  | 3.5  |
| 4   | D     | 52   | GLU  | 3.3  |
| 5   | E     | 1202 | SER  | 3.0  |
| 4   | D     | 114  | GLN  | 2.9  |
| 3   | A     | 661  | LEU  | 2.9  |
| 3   | A     | 278  | ILE  | 2.8  |
| 3   | A     | 630  | ASN  | 2.8  |
| 5   | E     | 1198 | ALA  | 2.7  |
| 3   | A     | 409  | HIS  | 2.6  |
| 4   | D     | 67   | GLU  | 2.5  |
| 3   | A     | 222  | ALA  | 2.4  |
| 3   | A     | 454  | VAL  | 2.4  |
| 3   | A     | 480  | ILE  | 2.4  |
| 5   | E     | 1079 | GLU  | 2.4  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 3   | A     | 411  | GLU  | 2.4  |
| 3   | A     | 629  | THR  | 2.3  |
| 5   | E     | 1175 | GLY  | 2.3  |
| 3   | A     | 433  | GLU  | 2.2  |
| 5   | E     | 1253 | ARG  | 2.2  |
| 3   | A     | 580  | GLU  | 2.2  |
| 4   | D     | 100  | PHE  | 2.1  |
| 5   | E     | 1217 | VAL  | 2.0  |
| 3   | A     | 311  | HIS  | 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.