



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:49 AM UTC

PDB ID : 3AVU / pdb\_00003avu  
Title : Structure of viral RNA polymerase complex 2  
Authors : Takeshita, D.; Tomita, K.  
Deposited on : 2011-03-08  
Resolution : 2.91 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

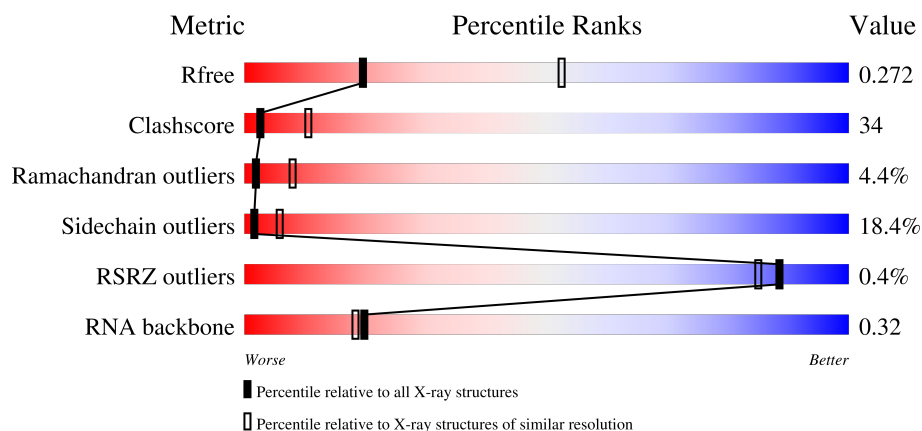
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.91 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                      | 2481 (2.90-2.90)                                      |
| Clashscore            | 190562                      | 2690 (2.90-2.90)                                      |
| Ramachandran outliers | 187476                      | 2623 (2.90-2.90)                                      |
| Sidechain outliers    | 187428                      | 2625 (2.90-2.90)                                      |
| RSRZ outliers         | 180081                      | 2481 (2.90-2.90)                                      |
| RNA backbone          | 3983                        | 1120 (3.10-2.70)                                      |

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

| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 1   | A     | 1289   |  |
| 2   | G     | 7      |  |
| 3   | T     | 12     |  |

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9635 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Elongation factor Ts, Elongation factor Tu, LINKER, Q beta replicase.

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 1   | A     | 1203     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 9287  | 5865 | 1605 | 1772 | 45 |         |         |       |

There are 7 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 284     | HIS      | -      | linker         | UNP P0A6P3 |
| A     | 1284    | HIS      | -      | expression tag | UNP Q8LTE0 |
| A     | 1285    | HIS      | -      | expression tag | UNP Q8LTE0 |
| A     | 1286    | HIS      | -      | expression tag | UNP Q8LTE0 |
| A     | 1287    | HIS      | -      | expression tag | UNP Q8LTE0 |
| A     | 1288    | HIS      | -      | expression tag | UNP Q8LTE0 |
| A     | 1289    | HIS      | -      | expression tag | UNP Q8LTE0 |

- Molecule 2 is a RNA chain called RNA (5'-R(\*GP\*GP\*GP\*UP\*CP\*CP\*A)-3').

| Mol | Chain | Residues | Atoms |    |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|---------|-------|
| 2   | G     | 7        | Total | C  | N  | O  | P | 0       | 0       | 0     |
|     |       |          | 148   | 67 | 28 | 47 | 6 |         |         |       |

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

| Mol | Chain | Residues | Atoms |    |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|---------|-------|
| 3   | T     | 9        | Total | C  | N  | O  | P | 8       | 0       | 0     |
|     |       |          | 193   | 86 | 36 | 62 | 9 |         |         |       |

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 4   | A     | 2        | Total | Ca | 0       | 0       |
|     |       |          | 2     | 2  |         |         |

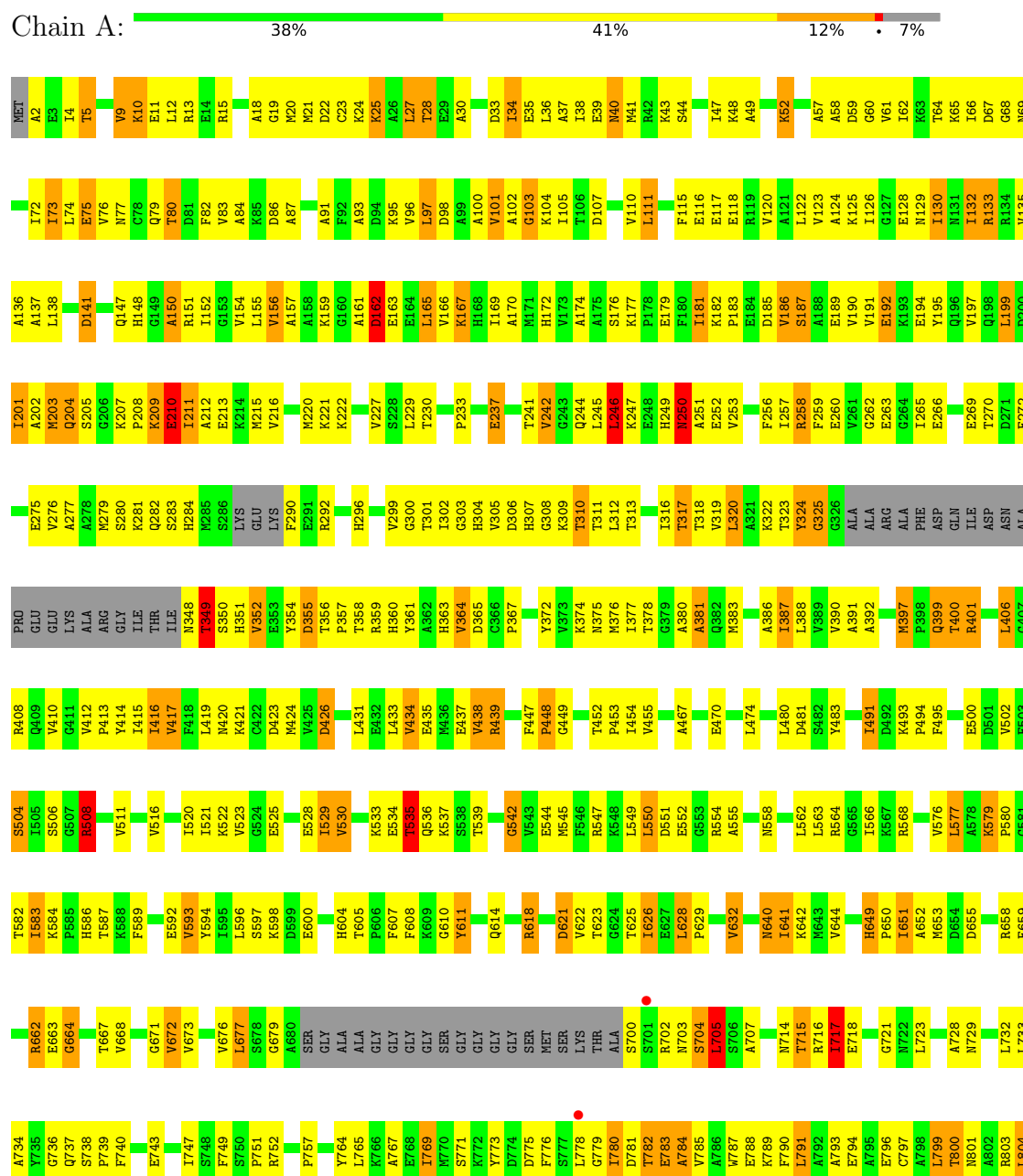
- Molecule 5 is water.

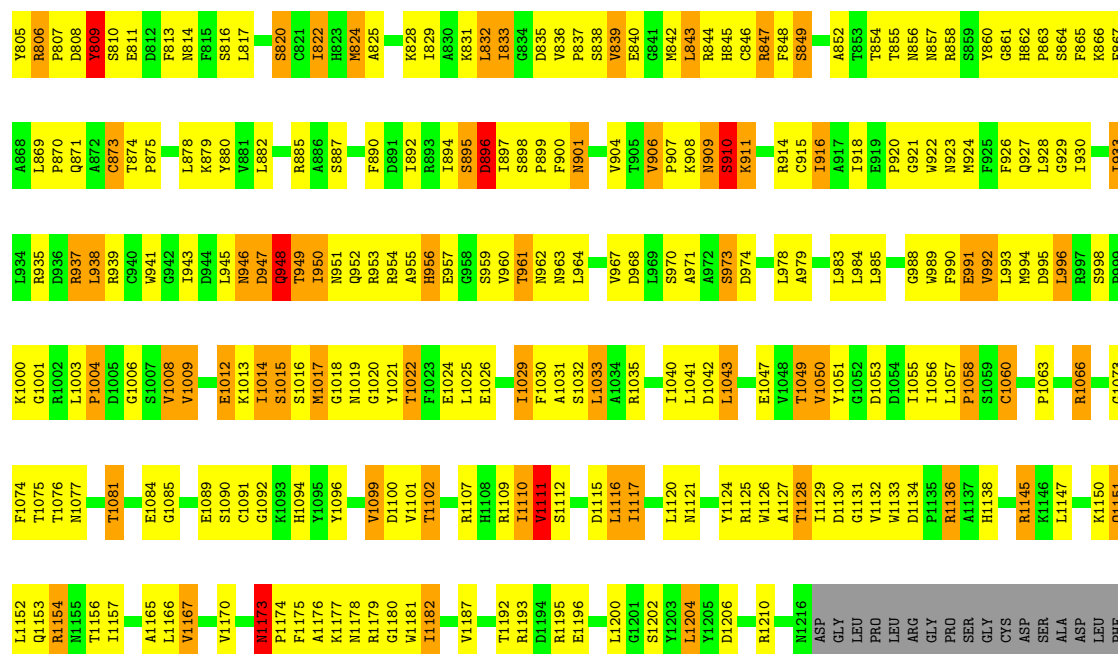
| Mol | Chain | Residues | Atoms |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 5   | A     | 4        | Total | O | 0       | 0       |
|     |       |          | 4     | 4 |         |         |
| 5   | T     | 1        | Total | O | 0       | 0       |
|     |       |          | 1     | 1 |         |         |

### 3 Residue-property plots

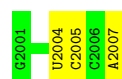
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Elongation factor Ts, Elongation factor Tu, LINKER, Q beta replicase

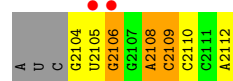




- Molecule 2: RNA (5'-R(\*GP\*GP\*GP\*UP\*CP\*CP\*A)-3')



- Molecule 3: RNA (5'-R(\*AP\*UP\*CP\*GP\*UP\*GP\*GP\*AP\*CP\*CP\*CP\*A)-3')



## 4 Data and refinement statistics

| Property                                                                | Value                                                                         | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------------------------|------------------|
| Space group                                                             | C 2 2 21                                                                      | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 139.00Å 255.47Å 101.11Å<br>90.00° 90.00° 90.00°                               | Depositor        |
| Resolution (Å)                                                          | 19.97 – 2.91<br>19.97 – 2.91                                                  | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 93.8 (19.97-2.91)<br>98.0 (19.97-2.91)                                        | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                                               | Depositor        |
| $R_{sym}$                                                               | (Not available)                                                               | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.93 (at 2.91Å)                                                               | Xtriage          |
| Refinement program                                                      | PHENIX (phenix.refine: 1.6.4_486)                                             | Depositor        |
| R, $R_{free}$                                                           | 0.219 , 0.280<br>0.213 , 0.272                                                | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 1971 reflections (4.93%)                                                      | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 67.9                                                                          | Xtriage          |
| Anisotropy                                                              | 0.301                                                                         | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.29 , 36.6                                                                   | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$                   | Xtriage          |
| Estimated twinning fraction                                             | 0.028 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l<br>0.030 for 1/2*h+1/2*k,3/2*h-1/2*k,-l | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.94                                                                          | EDS              |
| Total number of atoms                                                   | 9635                                                                          | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 82.0                                                                          | 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 i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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

| Mol | Chain | Bond lengths |               | Bond angles |                 |
|-----|-------|--------------|---------------|-------------|-----------------|
|     |       | RMSZ         | $\# Z  > 5$   | RMSZ        | $\# Z  > 5$     |
| 1   | A     | 0.65         | 1/9456 (0.0%) | 1.02        | 32/12787 (0.3%) |
| 2   | G     | 0.45         | 0/165         | 0.42        | 0/256           |
| 3   | T     | 0.37         | 0/215         | 0.41        | 0/333           |
| All | All   | 0.64         | 1/9836 (0.0%) | 1.00        | 32/13376 (0.2%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 1                   |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 1   | A     | 717 | ILE  | CA-CB | 6.25 | 1.61        | 1.54     |

All (32) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 1   | A     | 1173 | ASN  | CA-C-N | 9.90  | 131.44      | 120.45   |
| 1   | A     | 1173 | ASN  | C-N-CA | 9.90  | 131.44      | 120.45   |
| 1   | A     | 1243 | ASN  | N-CA-C | 8.32  | 121.56      | 110.08   |
| 1   | A     | 948  | GLN  | N-CA-C | -8.30 | 103.15      | 113.20   |
| 1   | A     | 941  | TRP  | N-CA-C | -7.87 | 103.00      | 112.59   |
| 1   | A     | 649  | HIS  | CA-C-N | 6.72  | 128.24      | 119.84   |
| 1   | A     | 649  | HIS  | C-N-CA | 6.72  | 128.24      | 119.84   |
| 1   | A     | 9    | VAL  | N-CA-C | -6.68 | 106.49      | 111.90   |
| 1   | A     | 910  | SER  | N-CA-C | -6.16 | 104.37      | 113.61   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | A     | 1243 | ASN  | CA-C-N  | 5.99  | 125.75      | 119.76   |
| 1   | A     | 1243 | ASN  | C-N-CA  | 5.99  | 125.75      | 119.76   |
| 1   | A     | 211  | ILE  | N-CA-C  | -5.91 | 106.06      | 111.67   |
| 1   | A     | 998  | SER  | CA-C-N  | 5.85  | 127.15      | 119.84   |
| 1   | A     | 998  | SER  | C-N-CA  | 5.85  | 127.15      | 119.84   |
| 1   | A     | 279  | MET  | N-CA-C  | -5.77 | 106.36      | 113.41   |
| 1   | A     | 27   | LEU  | N-CA-C  | -5.70 | 106.31      | 113.72   |
| 1   | A     | 417  | VAL  | N-CA-C  | 5.62  | 115.98      | 108.11   |
| 1   | A     | 1004 | PRO  | N-CA-C  | -5.62 | 106.21      | 113.57   |
| 1   | A     | 542  | GLY  | N-CA-C  | 5.60  | 118.67      | 110.38   |
| 1   | A     | 769  | ILE  | N-CA-C  | 5.57  | 116.30      | 110.62   |
| 1   | A     | 783  | GLU  | N-CA-C  | -5.40 | 104.97      | 113.02   |
| 1   | A     | 1050 | VAL  | N-CA-C  | 5.33  | 116.34      | 108.45   |
| 1   | A     | 721  | GLY  | N-CA-C  | 5.27  | 119.91      | 110.95   |
| 1   | A     | 1204 | LEU  | N-CA-C  | -5.20 | 105.52      | 111.14   |
| 1   | A     | 150  | ALA  | N-CA-C  | -5.17 | 106.50      | 114.16   |
| 1   | A     | 1057 | LEU  | CA-C-N  | 5.16  | 126.29      | 119.84   |
| 1   | A     | 1057 | LEU  | C-N-CA  | 5.16  | 126.29      | 119.84   |
| 1   | A     | 705  | LEU  | N-CA-C  | -5.15 | 106.33      | 113.18   |
| 1   | A     | 508  | ARG  | N-CA-C  | -5.08 | 105.11      | 113.50   |
| 1   | A     | 946  | ASN  | CB-CA-C | -5.04 | 104.90      | 111.40   |
| 1   | A     | 167  | LYS  | N-CA-C  | -5.03 | 105.49      | 110.97   |
| 1   | A     | 784  | ALA  | N-CA-C  | -5.01 | 105.92      | 112.23   |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group   |
|-----|-------|------|------|---------|
| 1   | A     | 1085 | GLY  | Peptide |

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 9287  | 0        | 9273     | 645     | 0            |
| 2   | G     | 148   | 0        | 78       | 7       | 0            |
| 3   | T     | 193   | 0        | 99       | 13      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4   | A     | 2     | 0        | 0        | 0       | 0            |
| 5   | A     | 4     | 0        | 0        | 0       | 0            |
| 5   | T     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 9635  | 0        | 9450     | 649     | 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 34.

All (649) 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) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:949:THR:HG23 | 1:A:953:ARG:NH1   | 1.58                     | 1.17              |
| 1:A:1017:MET:HB3 | 2:G:2007:A:C2     | 1.83                     | 1.14              |
| 1:A:949:THR:HG23 | 1:A:953:ARG:HH12  | 0.92                     | 1.04              |
| 1:A:847:ARG:HH22 | 1:A:849:SER:HB2   | 1.24                     | 1.02              |
| 1:A:949:THR:CG2  | 1:A:953:ARG:HH12  | 1.72                     | 1.01              |
| 1:A:467:ALA:HA   | 1:A:470:GLU:HB2   | 1.42                     | 1.01              |
| 1:A:1077:ASN:O   | 1:A:1081:THR:HG23 | 1.61                     | 1.00              |
| 1:A:906:VAL:HG23 | 3:T:2104:G:H21    | 1.22                     | 0.99              |
| 1:A:800:THR:HG22 | 1:A:803:ARG:HH11  | 1.24                     | 0.97              |
| 1:A:212:ALA:O    | 1:A:216:VAL:HG23  | 1.67                     | 0.94              |
| 1:A:356:THR:HG22 | 1:A:358:THR:H     | 1.30                     | 0.94              |
| 1:A:12:LEU:HD22  | 1:A:27:LEU:HD13   | 1.49                     | 0.93              |
| 1:A:968:ASP:H    | 1:A:1081:THR:HG22 | 1.33                     | 0.93              |
| 1:A:304:HIS:HD2  | 1:A:397:MET:HG2   | 1.34                     | 0.92              |
| 1:A:849:SER:HA   | 1:A:863:PRO:HG3   | 1.52                     | 0.89              |
| 1:A:1017:MET:HB3 | 2:G:2007:A:H2     | 1.30                     | 0.89              |
| 1:A:93:ALA:HA    | 1:A:96:VAL:HG12   | 1.56                     | 0.87              |
| 1:A:717:ILE:HD13 | 1:A:717:ILE:C     | 2.01                     | 0.85              |
| 1:A:15:ARG:HH22  | 1:A:38:ILE:HD13   | 1.43                     | 0.84              |
| 1:A:916:ILE:HD11 | 1:A:1017:MET:HB2  | 1.59                     | 0.84              |
| 1:A:800:THR:HG22 | 1:A:803:ARG:NH1   | 1.91                     | 0.83              |
| 1:A:10:LYS:HB3   | 1:A:433:LEU:HD21  | 1.59                     | 0.83              |
| 1:A:356:THR:HG21 | 1:A:481:ASP:OD1   | 1.78                     | 0.83              |
| 1:A:1047:GLU:HB3 | 1:A:1058:PRO:HD3  | 1.61                     | 0.82              |
| 1:A:161:ALA:HB1  | 1:A:165:LEU:HB3   | 1.61                     | 0.82              |
| 1:A:59:ASP:O     | 1:A:77:ASN:HB2    | 1.79                     | 0.82              |
| 1:A:1003:LEU:HB3 | 1:A:1004:PRO:HD2  | 1.62                     | 0.82              |
| 1:A:386:ALA:HB3  | 1:A:415:ILE:HG12  | 1.63                     | 0.81              |
| 1:A:839:VAL:HG12 | 1:A:843:LEU:HD23  | 1.62                     | 0.81              |
| 1:A:103:GLY:O    | 1:A:105:ILE:HG13  | 1.81                     | 0.81              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1100:ASP:OD1  | 1:A:1102:THR:CG2  | 2.29                     | 0.80              |
| 1:A:49:ALA:HB2    | 1:A:123:VAL:HG11  | 1.63                     | 0.80              |
| 1:A:789:LYS:HE2   | 1:A:789:LYS:HA    | 1.65                     | 0.78              |
| 1:A:592:GLU:HG2   | 1:A:642:LYS:HG2   | 1.65                     | 0.77              |
| 1:A:955:ALA:HB2   | 1:A:1090:SER:HB3  | 1.67                     | 0.77              |
| 1:A:1050:VAL:HG22 | 1:A:1055:ILE:HA   | 1.67                     | 0.77              |
| 1:A:930:ILE:HA    | 1:A:933:ILE:HG23  | 1.67                     | 0.76              |
| 1:A:948:GLN:O     | 1:A:952:GLN:HG2   | 1.84                     | 0.76              |
| 1:A:199:LEU:O     | 1:A:203:MET:HG3   | 1.85                     | 0.75              |
| 1:A:1092:GLY:HA3  | 2:G:2005:C:H5"    | 1.67                     | 0.75              |
| 1:A:604:HIS:HE1   | 1:A:1262:SER:HB3  | 1.52                     | 0.74              |
| 1:A:847:ARG:NH2   | 1:A:849:SER:HB2   | 2.00                     | 0.74              |
| 1:A:1019:ASN:HB3  | 1:A:1022:THR:HG22 | 1.68                     | 0.74              |
| 1:A:148:HIS:HB3   | 1:A:152:ILE:CG2   | 2.18                     | 0.74              |
| 1:A:805:TYR:O     | 1:A:806:ARG:HB2   | 1.85                     | 0.74              |
| 1:A:304:HIS:CD2   | 1:A:397:MET:HG2   | 2.23                     | 0.74              |
| 1:A:181:ILE:HG23  | 1:A:185:ASP:OD1   | 1.88                     | 0.73              |
| 1:A:1003:LEU:HD12 | 1:A:1003:LEU:N    | 2.03                     | 0.73              |
| 1:A:779:GLY:C     | 1:A:781:ASP:H     | 1.94                     | 0.73              |
| 1:A:1017:MET:CB   | 2:G:2007:A:C2     | 2.66                     | 0.73              |
| 1:A:1173:ASN:HD22 | 1:A:1175:PHE:H    | 1.36                     | 0.73              |
| 1:A:12:LEU:HG     | 1:A:23:CYS:SG     | 2.28                     | 0.73              |
| 1:A:388:LEU:HB3   | 1:A:417:VAL:HG22  | 1.70                     | 0.73              |
| 1:A:930:ILE:HD11  | 1:A:1021:TYR:CG   | 2.24                     | 0.72              |
| 1:A:378:THR:HG23  | 1:A:380:ALA:H     | 1.54                     | 0.72              |
| 1:A:930:ILE:HD11  | 1:A:1021:TYR:CB   | 2.19                     | 0.72              |
| 1:A:596:LEU:HD12  | 1:A:600:GLU:HB2   | 1.71                     | 0.72              |
| 1:A:504:SER:HB2   | 1:A:568:ARG:HG2   | 1.71                     | 0.71              |
| 1:A:211:ILE:O     | 1:A:215:MET:HG3   | 1.91                     | 0.71              |
| 1:A:1096:TYR:O    | 1:A:1099:VAL:HG13 | 1.91                     | 0.71              |
| 1:A:1100:ASP:OD1  | 1:A:1102:THR:HG22 | 1.89                     | 0.70              |
| 1:A:1151:GLN:HE21 | 1:A:1151:GLN:H    | 1.37                     | 0.70              |
| 1:A:375:ASN:HA    | 1:A:378:THR:HG22  | 1.73                     | 0.70              |
| 1:A:20:MET:HE3    | 1:A:20:MET:HA     | 1.73                     | 0.69              |
| 1:A:1025:LEU:HG   | 1:A:1029:ILE:HD13 | 1.75                     | 0.69              |
| 1:A:906:VAL:HG13  | 1:A:914:ARG:HB3   | 1.75                     | 0.69              |
| 1:A:806:ARG:H     | 1:A:807:PRO:HD3   | 1.57                     | 0.69              |
| 1:A:1031:ALA:O    | 1:A:1035:ARG:HG3  | 1.92                     | 0.69              |
| 1:A:618:ARG:HG2   | 1:A:618:ARG:HH21  | 1.57                     | 0.69              |
| 1:A:874:THR:CG2   | 1:A:923:ASN:HD21  | 2.05                     | 0.69              |
| 1:A:237:GLU:OE2   | 1:A:237:GLU:HA    | 1.91                     | 0.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:906:VAL:HG23  | 3:T:2104:G:N2     | 2.04                     | 0.68              |
| 1:A:1100:ASP:OD1  | 1:A:1102:THR:HG23 | 1.93                     | 0.68              |
| 1:A:419:LEU:HD11  | 1:A:434:VAL:HG11  | 1.76                     | 0.68              |
| 1:A:148:HIS:HB3   | 1:A:152:ILE:HG22  | 1.76                     | 0.67              |
| 1:A:365:ASP:O     | 1:A:367:PRO:HD3   | 1.93                     | 0.67              |
| 1:A:833:ILE:HG23  | 1:A:989:TRP:CE2   | 2.30                     | 0.67              |
| 1:A:380:ALA:O     | 1:A:381:ALA:HB2   | 1.95                     | 0.67              |
| 1:A:276:VAL:HG11  | 1:A:352:VAL:HG11  | 1.75                     | 0.67              |
| 1:A:229:LEU:HG    | 1:A:242:VAL:HG11  | 1.75                     | 0.67              |
| 1:A:861:GLY:O     | 1:A:866:LYS:HE3   | 1.95                     | 0.66              |
| 1:A:614:GLN:HE22  | 1:A:664:GLY:H     | 1.41                     | 0.66              |
| 1:A:290:PHE:N     | 1:A:292:ARG:HH11  | 1.93                     | 0.66              |
| 1:A:968:ASP:N     | 1:A:1081:THR:HG22 | 2.10                     | 0.66              |
| 1:A:837:PRO:HG2   | 1:A:992:VAL:HG21  | 1.76                     | 0.66              |
| 1:A:406:LEU:O     | 1:A:410:VAL:HG12  | 1.96                     | 0.66              |
| 1:A:392:ALA:HB2   | 1:A:419:LEU:HD12  | 1.78                     | 0.65              |
| 1:A:663:GLU:HG2   | 1:A:1182:ILE:HD12 | 1.76                     | 0.65              |
| 1:A:1173:ASN:ND2  | 1:A:1175:PHE:H    | 1.95                     | 0.65              |
| 1:A:808:ASP:O     | 1:A:809:TYR:C     | 2.39                     | 0.65              |
| 1:A:187:SER:O     | 1:A:190:VAL:HG12  | 1.96                     | 0.65              |
| 1:A:1180:GLY:O    | 1:A:1181:TRP:HB2  | 1.96                     | 0.65              |
| 1:A:1003:LEU:HD11 | 1:A:1009:VAL:HG23 | 1.80                     | 0.64              |
| 1:A:923:ASN:O     | 1:A:927:GLN:HG3   | 1.97                     | 0.64              |
| 1:A:898:SER:OG    | 1:A:899:PRO:HD2   | 1.97                     | 0.64              |
| 1:A:439:ARG:HG2   | 1:A:449:GLY:O     | 1.96                     | 0.64              |
| 1:A:797:CYS:HB2   | 1:A:1012:GLU:HB3  | 1.79                     | 0.63              |
| 1:A:874:THR:HA    | 1:A:898:SER:O     | 1.98                     | 0.63              |
| 1:A:30:ALA:O      | 1:A:33:ASP:HB2    | 1.98                     | 0.63              |
| 1:A:895:SER:OG    | 1:A:896:ASP:N     | 2.30                     | 0.63              |
| 1:A:1195:ARG:HG2  | 1:A:1196:GLU:N    | 2.14                     | 0.63              |
| 1:A:961:THR:HG22  | 1:A:963:ASN:H     | 1.63                     | 0.62              |
| 1:A:1014:ILE:HG23 | 1:A:1015:SER:HB3  | 1.80                     | 0.62              |
| 1:A:221:LYS:HD3   | 1:A:222:LYS:N     | 2.15                     | 0.62              |
| 1:A:604:HIS:CE1   | 1:A:1262:SER:HB3  | 2.32                     | 0.62              |
| 1:A:729:ASN:HD21  | 1:A:740:PHE:H     | 1.47                     | 0.62              |
| 1:A:1117:ILE:HD13 | 1:A:1166:LEU:HG   | 1.82                     | 0.62              |
| 1:A:133:ARG:NH2   | 1:A:263:GLU:O     | 2.32                     | 0.62              |
| 1:A:208:PRO:HG2   | 1:A:211:ILE:HG13  | 1.81                     | 0.62              |
| 1:A:296:HIS:CD2   | 1:A:360:HIS:HD2   | 2.17                     | 0.62              |
| 1:A:1173:ASN:HD22 | 1:A:1173:ASN:C    | 2.07                     | 0.62              |
| 1:A:732:LEU:HD12  | 1:A:739:PRO:HA    | 1.82                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:747:ILE:HG22  | 1:A:771:SER:HA    | 1.82                     | 0.61              |
| 1:A:749:PHE:HD1   | 1:A:767:ALA:HB2   | 1.65                     | 0.61              |
| 1:A:202:ALA:HB1   | 1:A:207:LYS:HD2   | 1.82                     | 0.61              |
| 1:A:558:ASN:HB3   | 1:A:1210:ARG:HB3  | 1.82                     | 0.61              |
| 1:A:302:ILE:O     | 1:A:388:LEU:HD12  | 2.01                     | 0.61              |
| 1:A:304:HIS:CE1   | 1:A:305:VAL:HG12  | 2.35                     | 0.61              |
| 1:A:662:ARG:HD2   | 1:A:667:THR:HG22  | 1.83                     | 0.61              |
| 1:A:991:GLU:O     | 1:A:994:MET:N     | 2.34                     | 0.61              |
| 1:A:191:VAL:HG13  | 1:A:220:MET:HE2   | 1.82                     | 0.61              |
| 1:A:96:VAL:HG21   | 1:A:132:ILE:CD1   | 2.31                     | 0.61              |
| 1:A:65:LYS:HB2    | 1:A:97:LEU:CD1    | 2.31                     | 0.60              |
| 1:A:828:LYS:HE2   | 1:A:1035:ARG:HB2  | 1.82                     | 0.60              |
| 1:A:19:GLY:O      | 1:A:23:CYS:HB2    | 2.00                     | 0.60              |
| 1:A:500:GLU:CD    | 1:A:1210:ARG:HH22 | 2.09                     | 0.60              |
| 1:A:351:HIS:CG    | 1:A:351:HIS:O     | 2.55                     | 0.60              |
| 1:A:892:ILE:HG23  | 1:A:922:TRP:CZ2   | 2.35                     | 0.60              |
| 1:A:73:ILE:HD13   | 1:A:259:PHE:CD1   | 2.37                     | 0.60              |
| 1:A:968:ASP:H     | 1:A:1081:THR:CG2  | 2.11                     | 0.60              |
| 1:A:658:ARG:HG2   | 1:A:658:ARG:HH11  | 1.67                     | 0.60              |
| 1:A:37:ALA:O      | 1:A:41:MET:HG3    | 2.02                     | 0.60              |
| 1:A:871:GLN:HE21  | 1:A:921:GLY:HA3   | 1.67                     | 0.59              |
| 1:A:1047:GLU:HB3  | 1:A:1058:PRO:CD   | 2.30                     | 0.59              |
| 1:A:516:VAL:HG13  | 1:A:555:ALA:HA    | 1.84                     | 0.59              |
| 1:A:874:THR:HG22  | 1:A:923:ASN:HD21  | 1.67                     | 0.59              |
| 1:A:80:THR:HG23   | 1:A:82:PHE:H      | 1.66                     | 0.59              |
| 1:A:545:MET:HE2   | 1:A:550:LEU:HD11  | 1.84                     | 0.59              |
| 1:A:589:PHE:HA    | 1:A:677:LEU:H     | 1.68                     | 0.59              |
| 1:A:83:VAL:HG21   | 1:A:128:GLU:OE2   | 2.02                     | 0.59              |
| 1:A:1019:ASN:HB3  | 1:A:1022:THR:CG2  | 2.32                     | 0.59              |
| 1:A:128:GLU:O     | 1:A:130:ILE:HG23  | 2.02                     | 0.59              |
| 1:A:839:VAL:HG12  | 1:A:843:LEU:CD2   | 2.31                     | 0.59              |
| 1:A:530:VAL:HG22  | 1:A:652:ALA:HB2   | 1.84                     | 0.59              |
| 1:A:182:LYS:HA    | 1:A:230:THR:OG1   | 2.02                     | 0.58              |
| 1:A:611:TYR:N     | 1:A:1181:TRP:HD1  | 2.01                     | 0.58              |
| 1:A:1110:ILE:HD12 | 1:A:1111:VAL:N    | 2.18                     | 0.58              |
| 1:A:300:GLY:HA3   | 1:A:383:MET:SD    | 2.43                     | 0.58              |
| 1:A:846:CYS:SG    | 1:A:929:GLY:HA3   | 2.44                     | 0.58              |
| 1:A:952:GLN:O     | 1:A:955:ALA:HB3   | 2.03                     | 0.58              |
| 1:A:628:LEU:HD12  | 1:A:641:ILE:HD11  | 1.84                     | 0.58              |
| 1:A:717:ILE:HD13  | 1:A:718:GLU:N     | 2.18                     | 0.58              |
| 1:A:773:TYR:CE2   | 1:A:775:ASP:HB3   | 2.38                     | 0.58              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:951:ASN:OD1  | 1:A:1049:THR:HG23 | 2.02                     | 0.58              |
| 1:A:956:HIS:O    | 1:A:959:SER:HB3   | 2.04                     | 0.58              |
| 1:A:423:ASP:OD2  | 1:A:424:MET:HG3   | 2.03                     | 0.58              |
| 1:A:72:ILE:HD11  | 1:A:135:VAL:HG22  | 1.85                     | 0.58              |
| 1:A:399:GLN:H    | 1:A:399:GLN:HE21  | 1.52                     | 0.58              |
| 1:A:801:ASN:HD22 | 1:A:1012:GLU:HG3  | 1.69                     | 0.58              |
| 1:A:111:LEU:HD23 | 1:A:111:LEU:H     | 1.68                     | 0.58              |
| 1:A:743:GLU:HB3  | 1:A:776:PHE:CD2   | 2.39                     | 0.58              |
| 1:A:920:PRO:O    | 1:A:923:ASN:HB2   | 2.02                     | 0.58              |
| 1:A:152:ILE:HD11 | 1:A:258:ARG:CZ    | 2.34                     | 0.58              |
| 1:A:262:GLY:HA2  | 1:A:265:ILE:HD12  | 1.85                     | 0.58              |
| 1:A:467:ALA:HA   | 1:A:470:GLU:CB    | 2.28                     | 0.58              |
| 1:A:626:ILE:HD13 | 1:A:626:ILE:H     | 1.69                     | 0.58              |
| 1:A:299:VAL:O    | 1:A:364:VAL:HG23  | 2.04                     | 0.58              |
| 1:A:939:ARG:HB3  | 1:A:939:ARG:NH1   | 2.19                     | 0.58              |
| 1:A:947:ASP:C    | 1:A:949:THR:H     | 2.10                     | 0.58              |
| 1:A:80:THR:HG22  | 1:A:83:VAL:HG23   | 1.86                     | 0.58              |
| 1:A:155:LEU:O    | 1:A:256:PHE:HA    | 2.04                     | 0.57              |
| 1:A:210:GLU:OE2  | 1:A:210:GLU:N     | 2.37                     | 0.57              |
| 1:A:1121:ASN:ND2 | 1:A:1167:VAL:HG23 | 2.19                     | 0.57              |
| 1:A:181:ILE:CD1  | 1:A:253:VAL:HG23  | 2.34                     | 0.57              |
| 1:A:359:ARG:NH2  | 1:A:480:LEU:O     | 2.38                     | 0.57              |
| 1:A:824:MET:O    | 1:A:828:LYS:HG3   | 2.04                     | 0.57              |
| 1:A:801:ASN:HA   | 1:A:979:ALA:HB2   | 1.87                     | 0.57              |
| 1:A:49:ALA:HB2   | 1:A:123:VAL:CG1   | 2.32                     | 0.57              |
| 1:A:65:LYS:HB2   | 1:A:97:LEU:HD11   | 1.87                     | 0.57              |
| 1:A:152:ILE:HG13 | 1:A:260:GLU:HG3   | 1.86                     | 0.57              |
| 1:A:177:LYS:HB3  | 1:A:258:ARG:CZ    | 2.35                     | 0.57              |
| 1:A:939:ARG:HB3  | 1:A:939:ARG:HH11  | 1.69                     | 0.57              |
| 1:A:846:CYS:SG   | 1:A:926:PHE:HA    | 2.44                     | 0.57              |
| 1:A:930:ILE:HD11 | 1:A:1021:TYR:HB2  | 1.87                     | 0.57              |
| 1:A:115:PHE:O    | 1:A:117:GLU:N     | 2.37                     | 0.57              |
| 1:A:522:LYS:HB2  | 1:A:525:GLU:OE1   | 2.05                     | 0.57              |
| 1:A:837:PRO:HD3  | 1:A:989:TRP:CD2   | 2.40                     | 0.57              |
| 1:A:840:GLU:O    | 1:A:844:ARG:HD3   | 2.04                     | 0.57              |
| 1:A:301:THR:HB   | 1:A:363:HIS:NE2   | 2.20                     | 0.56              |
| 1:A:80:THR:HG22  | 1:A:83:VAL:H      | 1.70                     | 0.56              |
| 1:A:500:GLU:OE1  | 1:A:1241:ARG:HD3  | 2.05                     | 0.56              |
| 1:A:117:GLU:O    | 1:A:120:VAL:HG22  | 2.05                     | 0.56              |
| 1:A:304:HIS:ND1  | 1:A:305:VAL:N     | 2.53                     | 0.56              |
| 1:A:528:GLU:HG3  | 1:A:580:PRO:HA    | 1.87                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:528:GLU:O     | 1:A:577:LEU:HA    | 2.06                     | 0.56              |
| 1:A:49:ALA:CB     | 1:A:123:VAL:HG11  | 2.34                     | 0.56              |
| 1:A:154:VAL:HG21  | 1:A:170:ALA:O     | 2.05                     | 0.56              |
| 1:A:1195:ARG:HH21 | 1:A:1249:ARG:HB2  | 1.71                     | 0.56              |
| 1:A:316:ILE:O     | 1:A:320:LEU:HB2   | 2.04                     | 0.56              |
| 1:A:583:ILE:HD13  | 1:A:584:LYS:H     | 1.70                     | 0.56              |
| 1:A:900:PHE:CE2   | 1:A:1008:VAL:HG12 | 2.41                     | 0.56              |
| 1:A:1112:SER:HB3  | 1:A:1115:ASP:OD1  | 2.05                     | 0.56              |
| 1:A:44:SER:O      | 1:A:47:ILE:HG22   | 2.05                     | 0.56              |
| 1:A:189:GLU:HA    | 1:A:192:GLU:HB2   | 1.88                     | 0.56              |
| 1:A:250:ASN:HD22  | 1:A:251:ALA:H     | 1.54                     | 0.56              |
| 1:A:324:TYR:CD1   | 1:A:357:PRO:HD3   | 2.40                     | 0.56              |
| 1:A:658:ARG:NH1   | 1:A:672:VAL:HB    | 2.20                     | 0.56              |
| 1:A:1053:ASP:OD1  | 2:G:2007:A:H4'    | 2.05                     | 0.56              |
| 1:A:250:ASN:HD22  | 1:A:250:ASN:N     | 2.04                     | 0.56              |
| 1:A:794:GLU:OE1   | 1:A:1013:LYS:HE2  | 2.05                     | 0.56              |
| 1:A:208:PRO:HG2   | 1:A:211:ILE:CG1   | 2.36                     | 0.56              |
| 1:A:521:ILE:O     | 1:A:552:GLU:HA    | 2.07                     | 0.55              |
| 1:A:846:CYS:HG    | 1:A:926:PHE:HD1   | 1.54                     | 0.55              |
| 1:A:1110:ILE:HD11 | 1:A:1116:LEU:HB2  | 1.88                     | 0.55              |
| 1:A:61:VAL:CG1    | 1:A:84:ALA:HB1    | 2.36                     | 0.55              |
| 1:A:947:ASP:C     | 1:A:949:THR:N     | 2.65                     | 0.55              |
| 1:A:990:PHE:O     | 1:A:994:MET:HG2   | 2.06                     | 0.55              |
| 1:A:611:TYR:HB3   | 1:A:626:ILE:CD1   | 2.36                     | 0.55              |
| 1:A:205:SER:HA    | 1:A:757:PRO:HG2   | 1.89                     | 0.55              |
| 1:A:900:PHE:HE2   | 1:A:1008:VAL:HG12 | 1.72                     | 0.55              |
| 1:A:194:GLU:HA    | 1:A:197:VAL:HG12  | 1.89                     | 0.55              |
| 1:A:650:PRO:O     | 1:A:651:ILE:HD12  | 2.07                     | 0.55              |
| 1:A:703:ASN:C     | 1:A:705:LEU:H     | 2.14                     | 0.55              |
| 1:A:280:SER:O     | 1:A:284:HIS:N     | 2.40                     | 0.55              |
| 1:A:312:LEU:O     | 1:A:316:ILE:HG13  | 2.07                     | 0.55              |
| 1:A:1151:GLN:H    | 1:A:1151:GLN:NE2  | 2.04                     | 0.55              |
| 1:A:39:GLU:O      | 1:A:43:LYS:HG2    | 2.07                     | 0.55              |
| 1:A:130:ILE:O     | 1:A:130:ILE:HG13  | 2.05                     | 0.55              |
| 1:A:204:GLN:HA    | 1:A:204:GLN:HE21  | 1.71                     | 0.55              |
| 1:A:306:ASP:C     | 1:A:308:GLY:H     | 2.15                     | 0.55              |
| 1:A:614:GLN:HE22  | 1:A:664:GLY:N     | 2.05                     | 0.55              |
| 1:A:374:LYS:HD2   | 1:A:594:TYR:CE1   | 2.42                     | 0.54              |
| 1:A:52:LYS:HB3    | 1:A:129:ASN:OD1   | 2.07                     | 0.54              |
| 1:A:773:TYR:O     | 1:A:910:SER:HB3   | 2.07                     | 0.54              |
| 1:A:837:PRO:HD3   | 1:A:989:TRP:CE2   | 2.42                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:930:ILE:HA    | 1:A:933:ILE:CG2   | 2.37                     | 0.54              |
| 1:A:60:GLY:HA3    | 1:A:77:ASN:HA     | 1.89                     | 0.54              |
| 1:A:356:THR:HG23  | 1:A:357:PRO:HD2   | 1.88                     | 0.54              |
| 1:A:836:VAL:CG2   | 1:A:837:PRO:HD2   | 2.37                     | 0.54              |
| 1:A:1049:THR:HG22 | 1:A:1056:ILE:HB   | 1.89                     | 0.54              |
| 1:A:1121:ASN:CG   | 1:A:1167:VAL:HG23 | 2.33                     | 0.54              |
| 1:A:375:ASN:HA    | 1:A:378:THR:CG2   | 2.37                     | 0.54              |
| 1:A:380:ALA:O     | 1:A:381:ALA:CB    | 2.55                     | 0.54              |
| 1:A:663:GLU:O     | 1:A:664:GLY:C     | 2.50                     | 0.54              |
| 1:A:951:ASN:OD1   | 1:A:1049:THR:CG2  | 2.55                     | 0.54              |
| 1:A:871:GLN:HB2   | 1:A:922:TRP:CD1   | 2.42                     | 0.54              |
| 1:A:1040:ILE:HG22 | 1:A:1040:ILE:O    | 2.06                     | 0.54              |
| 1:A:62:ILE:HG12   | 1:A:75:GLU:HG3    | 1.91                     | 0.53              |
| 1:A:351:HIS:O     | 1:A:351:HIS:CD2   | 2.62                     | 0.53              |
| 1:A:985:LEU:HD13  | 1:A:993:LEU:HD22  | 1.89                     | 0.53              |
| 1:A:250:ASN:N     | 1:A:250:ASN:ND2   | 2.57                     | 0.53              |
| 1:A:544:GLU:HB3   | 1:A:549:LEU:HG    | 1.90                     | 0.53              |
| 1:A:831:LYS:HD2   | 1:A:831:LYS:C     | 2.34                     | 0.53              |
| 1:A:1151:GLN:O    | 1:A:1175:PHE:HE1  | 1.91                     | 0.53              |
| 1:A:806:ARG:H     | 1:A:807:PRO:CD    | 2.20                     | 0.53              |
| 1:A:67:ASP:O      | 1:A:69:ASN:N      | 2.41                     | 0.53              |
| 1:A:529:ILE:O     | 1:A:529:ILE:HG12  | 2.06                     | 0.53              |
| 1:A:967:VAL:HA    | 1:A:1081:THR:HB   | 1.89                     | 0.53              |
| 1:A:5:THR:O       | 1:A:9:VAL:HG23    | 2.08                     | 0.53              |
| 1:A:98:ASP:HA     | 1:A:101:VAL:HG23  | 1.91                     | 0.53              |
| 1:A:181:ILE:HD13  | 1:A:253:VAL:HG23  | 1.91                     | 0.53              |
| 1:A:420:ASN:HD22  | 1:A:421:LYS:HD3   | 1.74                     | 0.53              |
| 1:A:1015:SER:OG   | 1:A:1022:THR:HB   | 2.09                     | 0.53              |
| 1:A:155:LEU:N     | 1:A:257:ILE:O     | 2.41                     | 0.53              |
| 1:A:957:GLU:C     | 1:A:959:SER:H     | 2.16                     | 0.53              |
| 1:A:1025:LEU:HG   | 1:A:1029:ILE:CD1  | 2.38                     | 0.53              |
| 1:A:1170:VAL:O    | 1:A:1170:VAL:HG22 | 2.09                     | 0.53              |
| 1:A:282:GLN:HG2   | 1:A:282:GLN:O     | 2.08                     | 0.53              |
| 1:A:30:ALA:HB1    | 1:A:33:ASP:HB3    | 1.91                     | 0.53              |
| 1:A:174:ALA:O     | 1:A:258:ARG:NH1   | 2.42                     | 0.52              |
| 1:A:523:VAL:HG13  | 1:A:551:ASP:HA    | 1.92                     | 0.52              |
| 1:A:508:ARG:HD3   | 1:A:562:LEU:HD21  | 1.90                     | 0.52              |
| 1:A:608:PHE:HD2   | 1:A:1181:TRP:CZ2  | 2.27                     | 0.52              |
| 1:A:21:MET:HE2    | 1:A:424:MET:O     | 2.09                     | 0.52              |
| 1:A:723:LEU:HD23  | 1:A:1110:ILE:HG13 | 1.91                     | 0.52              |
| 1:A:773:TYR:HA    | 1:A:1107:ARG:O    | 2.09                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:904:VAL:CG2   | 1:A:916:ILE:HG22  | 2.39                     | 0.52              |
| 1:A:69:ASN:HB2    | 1:A:141:ASP:O     | 2.10                     | 0.52              |
| 1:A:152:ILE:CG1   | 1:A:260:GLU:HG3   | 2.40                     | 0.52              |
| 1:A:899:PRO:HG2   | 1:A:900:PHE:CD1   | 2.44                     | 0.52              |
| 1:A:1116:LEU:HD22 | 1:A:1120:LEU:HG   | 1.90                     | 0.52              |
| 1:A:100:ALA:O     | 1:A:104:LYS:HA    | 2.09                     | 0.52              |
| 1:A:658:ARG:HG2   | 1:A:658:ARG:NH1   | 2.24                     | 0.52              |
| 1:A:836:VAL:HA    | 1:A:989:TRP:CD1   | 2.45                     | 0.52              |
| 1:A:397:MET:O     | 1:A:400:THR:HB    | 2.10                     | 0.52              |
| 1:A:48:LYS:NZ     | 1:A:124:ALA:HA    | 2.24                     | 0.52              |
| 1:A:858:ARG:CG    | 3:T:2104:G:H5''   | 2.40                     | 0.52              |
| 1:A:874:THR:OG1   | 1:A:875:PRO:HD2   | 2.10                     | 0.52              |
| 1:A:195:TYR:HE1   | 1:A:199:LEU:HD12  | 1.74                     | 0.51              |
| 1:A:491:ILE:N     | 1:A:491:ILE:HD13  | 2.24                     | 0.51              |
| 1:A:663:GLU:O     | 1:A:664:GLY:O     | 2.27                     | 0.51              |
| 1:A:49:ALA:O      | 1:A:52:LYS:HB2    | 2.10                     | 0.51              |
| 1:A:190:VAL:HG13  | 1:A:191:VAL:HG23  | 1.90                     | 0.51              |
| 1:A:714:ASN:HD21  | 1:A:1254:PHE:H    | 1.57                     | 0.51              |
| 1:A:764:TYR:HE2   | 1:A:1094:HIS:CD2  | 2.26                     | 0.51              |
| 1:A:197:VAL:O     | 1:A:201:ILE:HG13  | 2.11                     | 0.51              |
| 1:A:598:LYS:CD    | 1:A:604:HIS:HB2   | 2.40                     | 0.51              |
| 1:A:971:ALA:HB1   | 1:A:974:ASP:HB2   | 1.91                     | 0.51              |
| 1:A:1195:ARG:HD2  | 1:A:1247:ILE:HG21 | 1.93                     | 0.51              |
| 1:A:377:ILE:HG23  | 1:A:671:GLY:HA2   | 1.91                     | 0.51              |
| 1:A:534:GLU:O     | 1:A:535:THR:C     | 2.53                     | 0.51              |
| 1:A:607:PHE:CD1   | 1:A:611:TYR:HB2   | 2.46                     | 0.51              |
| 1:A:1176:ALA:O    | 1:A:1178:ASN:N    | 2.43                     | 0.51              |
| 1:A:1181:TRP:HA   | 1:A:1181:TRP:CE3  | 2.44                     | 0.51              |
| 1:A:354:TYR:CE2   | 1:A:361:TYR:HB2   | 2.45                     | 0.51              |
| 1:A:1157:ILE:HG12 | 1:A:1165:ALA:HB3  | 1.91                     | 0.51              |
| 1:A:1173:ASN:HD21 | 1:A:1175:PHE:HB2  | 1.76                     | 0.51              |
| 1:A:57:ALA:HA     | 1:A:79:GLN:HB3    | 1.93                     | 0.51              |
| 1:A:704:SER:HA    | 1:A:707:ALA:HB3   | 1.93                     | 0.51              |
| 3:T:2112:A:N3     | 3:T:2112:A:H2'    | 2.25                     | 0.51              |
| 1:A:230:THR:HA    | 1:A:242:VAL:HG12  | 1.93                     | 0.51              |
| 1:A:74:LEU:HD21   | 1:A:96:VAL:HG13   | 1.93                     | 0.51              |
| 1:A:276:VAL:HG13  | 1:A:277:ALA:N     | 2.25                     | 0.51              |
| 1:A:195:TYR:OH    | 1:A:213:GLU:HG3   | 2.10                     | 0.51              |
| 1:A:649:HIS:HB2   | 1:A:650:PRO:HD2   | 1.93                     | 0.51              |
| 1:A:700:SER:O     | 1:A:1179:ARG:HD2  | 2.11                     | 0.51              |
| 1:A:828:LYS:O     | 1:A:831:LYS:HG3   | 2.11                     | 0.51              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:908:LYS:HG2  | 1:A:909:ASN:N     | 2.25                     | 0.50              |
| 1:A:728:ALA:O    | 1:A:732:LEU:HG    | 2.11                     | 0.50              |
| 1:A:836:VAL:HG23 | 1:A:988:GLY:C     | 2.37                     | 0.50              |
| 1:A:901:ASN:HD22 | 1:A:901:ASN:H     | 1.58                     | 0.50              |
| 1:A:1206:ASP:O   | 1:A:1210:ARG:HG3  | 2.11                     | 0.50              |
| 1:A:387:ILE:HA   | 1:A:416:ILE:O     | 2.11                     | 0.50              |
| 1:A:797:CYS:CB   | 1:A:1012:GLU:HB3  | 2.42                     | 0.50              |
| 1:A:829:ILE:HD11 | 1:A:1032:SER:CB   | 2.42                     | 0.50              |
| 1:A:1173:ASN:ND2 | 1:A:1174:PRO:HD2  | 2.26                     | 0.50              |
| 1:A:195:TYR:CE1  | 1:A:199:LEU:HD12  | 2.47                     | 0.50              |
| 1:A:1003:LEU:N   | 1:A:1003:LEU:CD1  | 2.74                     | 0.50              |
| 1:A:310:THR:O    | 1:A:313:THR:HG22  | 2.11                     | 0.50              |
| 1:A:191:VAL:HG12 | 1:A:191:VAL:O     | 2.10                     | 0.50              |
| 1:A:610:GLY:H    | 1:A:1181:TRP:HE1  | 1.59                     | 0.50              |
| 1:A:1004:PRO:C   | 1:A:1006:GLY:H    | 2.18                     | 0.50              |
| 1:A:138:LEU:HD21 | 1:A:157:ALA:N     | 2.27                     | 0.50              |
| 1:A:784:ALA:O    | 1:A:788:GLU:HG3   | 2.12                     | 0.50              |
| 1:A:864:SER:HB2  | 1:A:1202:SER:HA   | 1.94                     | 0.50              |
| 1:A:86:ASP:CG    | 1:A:87:ALA:N      | 2.70                     | 0.49              |
| 1:A:629:PRO:HD2  | 1:A:632:VAL:HG11  | 1.94                     | 0.49              |
| 1:A:749:PHE:CD1  | 1:A:767:ALA:HB2   | 2.47                     | 0.49              |
| 1:A:1032:SER:OG  | 1:A:1033:LEU:N    | 2.44                     | 0.49              |
| 1:A:435:GLU:O    | 1:A:439:ARG:HB2   | 2.11                     | 0.49              |
| 1:A:1026:GLU:HB2 | 1:A:1030:PHE:CE1  | 2.47                     | 0.49              |
| 1:A:416:ILE:HD11 | 1:A:483:TYR:HD2   | 1.77                     | 0.49              |
| 1:A:820:SER:O    | 1:A:824:MET:HE3   | 2.13                     | 0.49              |
| 1:A:860:TYR:HA   | 1:A:865:PHE:CD1   | 2.47                     | 0.49              |
| 1:A:946:ASN:HB3  | 3:T:2109:C:OP1    | 2.13                     | 0.49              |
| 1:A:618:ARG:NH1  | 1:A:652:ALA:O     | 2.35                     | 0.49              |
| 1:A:621:ASP:OD2  | 1:A:662:ARG:NH2   | 2.46                     | 0.49              |
| 1:A:662:ARG:NH2  | 1:A:662:ARG:HG2   | 2.28                     | 0.49              |
| 1:A:662:ARG:HG2  | 1:A:662:ARG:HH21  | 1.77                     | 0.49              |
| 1:A:717:ILE:C    | 1:A:717:ILE:CD1   | 2.78                     | 0.49              |
| 1:A:869:LEU:HD12 | 1:A:869:LEU:N     | 2.27                     | 0.49              |
| 1:A:787:TRP:O    | 1:A:790:PHE:HB3   | 2.13                     | 0.49              |
| 1:A:800:THR:HG21 | 1:A:1073:GLY:HA2  | 1.94                     | 0.49              |
| 1:A:1156:THR:HA  | 1:A:1166:LEU:O    | 2.13                     | 0.49              |
| 1:A:111:LEU:H    | 1:A:111:LEU:CD2   | 2.25                     | 0.49              |
| 1:A:376:MET:HG3  | 1:A:410:VAL:CG2   | 2.43                     | 0.49              |
| 1:A:799:LEU:HD13 | 1:A:799:LEU:N     | 2.28                     | 0.49              |
| 1:A:1016:SER:O   | 1:A:1022:THR:HG21 | 2.12                     | 0.49              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:1130:ASP:O   | 1:A:1132:VAL:HG23 | 2.13                     | 0.49              |
| 1:A:324:TYR:O    | 1:A:325:GLY:O     | 2.30                     | 0.49              |
| 1:A:542:GLY:N    | 1:A:562:LEU:HB2   | 2.28                     | 0.49              |
| 1:A:865:PHE:CZ   | 1:A:1247:ILE:HD13 | 2.48                     | 0.49              |
| 1:A:848:PHE:HD2  | 1:A:867:PHE:CE1   | 2.31                     | 0.49              |
| 1:A:873:CYS:HB2  | 1:A:922:TRP:HB2   | 1.94                     | 0.49              |
| 1:A:1237:GLN:O   | 1:A:1237:GLN:HG2  | 2.12                     | 0.49              |
| 1:A:372:TYR:HE1  | 1:A:410:VAL:HG21  | 1.76                     | 0.48              |
| 1:A:413:PRO:HB2  | 1:A:414:TYR:HD1   | 1.78                     | 0.48              |
| 1:A:871:GLN:NE2  | 1:A:921:GLY:HA3   | 2.27                     | 0.48              |
| 1:A:937:ARG:HH21 | 1:A:937:ARG:HG3   | 1.78                     | 0.48              |
| 1:A:991:GLU:O    | 1:A:992:VAL:C     | 2.53                     | 0.48              |
| 1:A:534:GLU:O    | 1:A:536:GLN:HG3   | 2.13                     | 0.48              |
| 1:A:152:ILE:HD11 | 1:A:258:ARG:NH1   | 2.28                     | 0.48              |
| 1:A:659:PHE:O    | 1:A:659:PHE:CD2   | 2.67                     | 0.48              |
| 1:A:878:LEU:HD11 | 1:A:882:LEU:HD21  | 1.96                     | 0.48              |
| 1:A:281:LYS:C    | 1:A:283:SER:H     | 2.20                     | 0.48              |
| 1:A:431:LEU:C    | 1:A:433:LEU:N     | 2.71                     | 0.48              |
| 1:A:906:VAL:HG22 | 1:A:907:PRO:O     | 2.13                     | 0.48              |
| 1:A:1000:LYS:HA  | 1:A:1009:VAL:O    | 2.13                     | 0.48              |
| 1:A:86:ASP:CG    | 1:A:87:ALA:H      | 2.21                     | 0.48              |
| 1:A:550:LEU:H    | 1:A:550:LEU:HD22  | 1.78                     | 0.48              |
| 1:A:1001:GLY:N   | 1:A:1009:VAL:O    | 2.42                     | 0.48              |
| 1:A:179:GLU:HB2  | 1:A:227:VAL:CG2   | 2.42                     | 0.48              |
| 1:A:848:PHE:O    | 1:A:849:SER:C     | 2.56                     | 0.48              |
| 1:A:858:ARG:HB2  | 3:T:2104:G:OP2    | 2.13                     | 0.48              |
| 1:A:323:THR:O    | 1:A:324:TYR:O     | 2.31                     | 0.48              |
| 1:A:598:LYS:HD2  | 1:A:604:HIS:HB2   | 1.94                     | 0.48              |
| 1:A:250:ASN:HD22 | 1:A:251:ALA:N     | 2.11                     | 0.48              |
| 1:A:794:GLU:OE1  | 1:A:794:GLU:HA    | 2.12                     | 0.48              |
| 1:A:1195:ARG:HG2 | 1:A:1196:GLU:H    | 1.77                     | 0.48              |
| 1:A:547:ARG:HG2  | 1:A:887:SER:O     | 2.14                     | 0.48              |
| 1:A:1092:GLY:CA  | 2:G:2005:C:H5"    | 2.42                     | 0.48              |
| 1:A:1133:TRP:CE3 | 1:A:1138:HIS:HA   | 2.49                     | 0.48              |
| 1:A:204:GLN:HA   | 1:A:204:GLN:NE2   | 2.28                     | 0.47              |
| 1:A:495:PHE:HB3  | 1:A:579:LYS:HE3   | 1.94                     | 0.47              |
| 1:A:12:LEU:HD23  | 1:A:23:CYS:O      | 2.14                     | 0.47              |
| 1:A:61:VAL:HG13  | 1:A:84:ALA:HB1    | 1.96                     | 0.47              |
| 1:A:97:LEU:O     | 1:A:101:VAL:HG23  | 2.14                     | 0.47              |
| 1:A:470:GLU:O    | 1:A:474:LEU:HG    | 2.13                     | 0.47              |
| 1:A:516:VAL:HG13 | 1:A:516:VAL:O     | 2.14                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:897:ILE:O     | 1:A:897:ILE:HG23  | 2.13                     | 0.47              |
| 1:A:1043:LEU:HA   | 1:A:1043:LEU:HD13 | 1.26                     | 0.47              |
| 1:A:416:ILE:HG13  | 1:A:453:PRO:HG2   | 1.96                     | 0.47              |
| 1:A:448:PRO:O     | 1:A:452:THR:HB    | 2.15                     | 0.47              |
| 1:A:649:HIS:CB    | 1:A:650:PRO:HD2   | 2.44                     | 0.47              |
| 1:A:40:ASN:N      | 1:A:40:ASN:ND2    | 2.60                     | 0.47              |
| 1:A:22:ASP:O      | 1:A:41:MET:HE3    | 2.13                     | 0.47              |
| 1:A:183:PRO:HD3   | 1:A:230:THR:OG1   | 2.15                     | 0.47              |
| 1:A:356:THR:HG21  | 1:A:481:ASP:CG    | 2.39                     | 0.47              |
| 1:A:1021:TYR:CD1  | 1:A:1021:TYR:C    | 2.91                     | 0.47              |
| 1:A:1121:ASN:HD21 | 1:A:1167:VAL:H    | 1.62                     | 0.47              |
| 1:A:18:ALA:HB1    | 1:A:41:MET:HE1    | 1.96                     | 0.47              |
| 1:A:83:VAL:HG21   | 1:A:128:GLU:CD    | 2.39                     | 0.47              |
| 1:A:838:SER:O     | 1:A:842:MET:HB2   | 2.15                     | 0.47              |
| 1:A:885:ARG:HG2   | 1:A:885:ARG:O     | 2.14                     | 0.47              |
| 1:A:973:SER:CB    | 1:A:1017:MET:HG3  | 2.45                     | 0.47              |
| 1:A:1195:ARG:HB3  | 1:A:1247:ILE:HG22 | 1.96                     | 0.47              |
| 1:A:93:ALA:O      | 1:A:97:LEU:HB2    | 2.14                     | 0.47              |
| 1:A:320:LEU:HD12  | 1:A:355:ASP:O     | 2.15                     | 0.47              |
| 1:A:628:LEU:HB3   | 1:A:632:VAL:HG13  | 1.97                     | 0.47              |
| 1:A:764:TYR:CE2   | 1:A:1094:HIS:CD2  | 3.02                     | 0.47              |
| 1:A:904:VAL:HG22  | 1:A:916:ILE:HG22  | 1.96                     | 0.47              |
| 1:A:626:ILE:H     | 1:A:626:ILE:CD1   | 2.28                     | 0.47              |
| 1:A:937:ARG:HG3   | 1:A:937:ARG:NH2   | 2.30                     | 0.47              |
| 1:A:107:ASP:HB3   | 1:A:110:VAL:HG23  | 1.97                     | 0.46              |
| 1:A:130:ILE:O     | 1:A:130:ILE:CG1   | 2.63                     | 0.46              |
| 1:A:511:VAL:HB    | 1:A:562:LEU:HD23  | 1.95                     | 0.46              |
| 1:A:447:PHE:O     | 1:A:449:GLY:N     | 2.48                     | 0.46              |
| 1:A:376:MET:HG3   | 1:A:410:VAL:HG23  | 1.98                     | 0.46              |
| 1:A:493:LYS:HB3   | 1:A:494:PRO:HD2   | 1.97                     | 0.46              |
| 1:A:825:ALA:O     | 1:A:829:ILE:HG12  | 2.15                     | 0.46              |
| 1:A:829:ILE:HD11  | 1:A:1032:SER:HB3  | 1.97                     | 0.46              |
| 1:A:586:HIS:O     | 1:A:653:MET:HE3   | 2.15                     | 0.46              |
| 1:A:775:ASP:OD2   | 1:A:1109:ARG:HD3  | 2.15                     | 0.46              |
| 1:A:779:GLY:C     | 1:A:781:ASP:N     | 2.62                     | 0.46              |
| 1:A:579:LYS:O     | 1:A:582:THR:HB    | 2.16                     | 0.46              |
| 1:A:629:PRO:HD3   | 1:A:642:LYS:O     | 2.15                     | 0.46              |
| 1:A:1235:ILE:HD13 | 1:A:1235:ILE:N    | 2.30                     | 0.46              |
| 1:A:734:ALA:O     | 1:A:1136:ARG:HB3  | 2.16                     | 0.46              |
| 1:A:810:SER:C     | 1:A:811:GLU:HG2   | 2.40                     | 0.46              |
| 1:A:1047:GLU:HB3  | 1:A:1058:PRO:CG   | 2.46                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:579:LYS:HE3   | 1:A:579:LYS:HB2   | 1.68                     | 0.46              |
| 1:A:852:ALA:N     | 3:T:2105:U:H5"    | 2.30                     | 0.46              |
| 1:A:1173:ASN:HD22 | 1:A:1174:PRO:N    | 2.13                     | 0.46              |
| 1:A:34:ILE:HG22   | 1:A:35:GLU:N      | 2.31                     | 0.46              |
| 1:A:520:ILE:HG12  | 1:A:554:ARG:HA    | 1.98                     | 0.46              |
| 1:A:408:ARG:O     | 1:A:408:ARG:HD3   | 2.16                     | 0.46              |
| 1:A:700:SER:O     | 1:A:1179:ARG:CD   | 2.64                     | 0.46              |
| 1:A:804:LEU:HB3   | 1:A:983:LEU:HD11  | 1.98                     | 0.46              |
| 1:A:73:ILE:HG23   | 1:A:259:PHE:CE1   | 2.51                     | 0.45              |
| 1:A:117:GLU:OE1   | 1:A:117:GLU:HA    | 2.15                     | 0.45              |
| 1:A:736:GLY:C     | 1:A:737:GLN:HG2   | 2.40                     | 0.45              |
| 1:A:796:GLU:O     | 1:A:800:THR:HG23  | 2.15                     | 0.45              |
| 1:A:911:LYS:HB3   | 1:A:911:LYS:HE3   | 1.55                     | 0.45              |
| 1:A:1041:LEU:C    | 1:A:1043:LEU:H    | 2.23                     | 0.45              |
| 1:A:281:LYS:C     | 1:A:283:SER:N     | 2.74                     | 0.45              |
| 1:A:528:GLU:HG3   | 1:A:580:PRO:CA    | 2.47                     | 0.45              |
| 1:A:839:VAL:HA    | 1:A:842:MET:HB3   | 1.97                     | 0.45              |
| 1:A:147:GLN:HE21  | 1:A:150:ALA:HA    | 1.81                     | 0.45              |
| 1:A:611:TYR:HB3   | 1:A:626:ILE:HD12  | 1.99                     | 0.45              |
| 1:A:790:PHE:HD1   | 1:A:791:LEU:HD13  | 1.81                     | 0.45              |
| 1:A:1165:ALA:HB2  | 1:A:1187:VAL:HG12 | 1.98                     | 0.45              |
| 1:A:310:THR:C     | 1:A:313:THR:HG22  | 2.41                     | 0.45              |
| 1:A:1100:ASP:OD1  | 1:A:1100:ASP:C    | 2.59                     | 0.45              |
| 1:A:233:PRO:HA    | 1:A:241:THR:HA    | 1.99                     | 0.45              |
| 1:A:272:PHE:O     | 1:A:275:GLU:HB3   | 2.16                     | 0.45              |
| 1:A:611:TYR:HB3   | 1:A:626:ILE:HD11  | 1.98                     | 0.45              |
| 1:A:789:LYS:HA    | 1:A:789:LYS:CE    | 2.38                     | 0.45              |
| 1:A:822:ILE:HB    | 1:A:984:LEU:HD11  | 1.98                     | 0.45              |
| 1:A:862:HIS:CD2   | 1:A:864:SER:H     | 2.34                     | 0.45              |
| 1:A:990:PHE:O     | 1:A:990:PHE:CG    | 2.69                     | 0.45              |
| 1:A:1129:ILE:O    | 1:A:1129:ILE:HG22 | 2.16                     | 0.45              |
| 1:A:1195:ARG:HD2  | 1:A:1247:ILE:CG2  | 2.46                     | 0.45              |
| 1:A:25:LYS:O      | 1:A:28:THR:HG22   | 2.16                     | 0.45              |
| 1:A:73:ILE:HB     | 1:A:155:LEU:HD22  | 1.98                     | 0.45              |
| 1:A:618:ARG:HH21  | 1:A:618:ARG:CG    | 2.28                     | 0.45              |
| 1:A:1090:SER:O    | 1:A:1091:CYS:HB2  | 2.16                     | 0.45              |
| 1:A:96:VAL:HG23   | 1:A:115:PHE:CE1   | 2.51                     | 0.45              |
| 1:A:161:ALA:HB1   | 1:A:165:LEU:CB    | 2.41                     | 0.45              |
| 1:A:210:GLU:HA    | 1:A:213:GLU:HB3   | 1.99                     | 0.45              |
| 1:A:640:ASN:O     | 1:A:641:ILE:HB    | 2.17                     | 0.45              |
| 1:A:1157:ILE:O    | 1:A:1167:VAL:HA   | 2.16                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:714:ASN:C    | 1:A:715:THR:O     | 2.56                     | 0.45              |
| 1:A:843:LEU:HD13 | 1:A:843:LEU:HA    | 1.85                     | 0.45              |
| 1:A:1025:LEU:HA  | 1:A:1025:LEU:HD12 | 1.59                     | 0.45              |
| 2:G:2004:U:H2'   | 2:G:2005:C:H5'    | 1.99                     | 0.45              |
| 1:A:316:ILE:O    | 1:A:316:ILE:HG22  | 2.17                     | 0.45              |
| 1:A:361:TYR:CZ   | 1:A:480:LEU:HB3   | 2.52                     | 0.45              |
| 1:A:1145:ARG:CD  | 1:A:1153:GLN:HG2  | 2.47                     | 0.45              |
| 1:A:195:TYR:O    | 1:A:199:LEU:HB2   | 2.17                     | 0.45              |
| 1:A:304:HIS:HB3  | 1:A:307:HIS:CG    | 2.51                     | 0.45              |
| 1:A:824:MET:HE3  | 1:A:824:MET:HB2   | 1.63                     | 0.45              |
| 1:A:176:SER:O    | 1:A:177:LYS:C     | 2.61                     | 0.44              |
| 1:A:348:ASN:O    | 1:A:349:THR:O     | 2.35                     | 0.44              |
| 1:A:817:LEU:HD12 | 1:A:817:LEU:O     | 2.18                     | 0.44              |
| 1:A:413:PRO:HB2  | 1:A:414:TYR:CD1   | 2.52                     | 0.44              |
| 1:A:927:GLN:HB2  | 1:A:1020:GLY:HA3  | 1.98                     | 0.44              |
| 3:T:2108:A:H3'   | 3:T:2109:C:C6     | 2.52                     | 0.44              |
| 1:A:48:LYS:HZ2   | 1:A:124:ALA:HA    | 1.81                     | 0.44              |
| 1:A:655:ASP:HA   | 1:A:673:VAL:HG23  | 1.99                     | 0.44              |
| 1:A:782:THR:OG1  | 1:A:783:GLU:N     | 2.47                     | 0.44              |
| 1:A:836:VAL:HG22 | 1:A:837:PRO:HD2   | 2.00                     | 0.44              |
| 1:A:890:PHE:CG   | 1:A:1204:LEU:HD21 | 2.53                     | 0.44              |
| 1:A:947:ASP:OD2  | 1:A:950:ILE:HG23  | 2.18                     | 0.44              |
| 1:A:957:GLU:C    | 1:A:959:SER:N     | 2.74                     | 0.44              |
| 1:A:1060:CYS:O   | 1:A:1063:PRO:HD2  | 2.18                     | 0.44              |
| 1:A:96:VAL:HG21  | 1:A:132:ILE:HD11  | 1.99                     | 0.44              |
| 1:A:167:LYS:O    | 1:A:170:ALA:HB3   | 2.18                     | 0.44              |
| 1:A:209:LYS:C    | 1:A:211:ILE:H     | 2.25                     | 0.44              |
| 1:A:593:VAL:HG22 | 1:A:641:ILE:HG23  | 1.98                     | 0.44              |
| 1:A:862:HIS:HD2  | 1:A:864:SER:H     | 1.64                     | 0.44              |
| 1:A:13:ARG:NH2   | 1:A:437:GLU:OE2   | 2.51                     | 0.44              |
| 1:A:610:GLY:O    | 1:A:611:TYR:C     | 2.60                     | 0.44              |
| 1:A:880:TYR:OH   | 1:A:995:ASP:OD1   | 2.31                     | 0.44              |
| 1:A:945:LEU:O    | 1:A:1051:TYR:HE1  | 2.00                     | 0.44              |
| 1:A:1116:LEU:O   | 1:A:1117:ILE:C    | 2.59                     | 0.44              |
| 1:A:1145:ARG:HD2 | 1:A:1153:GLN:HG2  | 1.99                     | 0.44              |
| 1:A:377:ILE:CG2  | 1:A:671:GLY:HA2   | 2.47                     | 0.44              |
| 1:A:412:VAL:HG13 | 1:A:412:VAL:O     | 2.18                     | 0.44              |
| 1:A:28:THR:O     | 1:A:28:THR:HG23   | 2.16                     | 0.44              |
| 1:A:72:ILE:HD12  | 1:A:136:ALA:O     | 2.17                     | 0.44              |
| 1:A:316:ILE:HG21 | 1:A:354:TYR:CZ    | 2.53                     | 0.44              |
| 1:A:629:PRO:HG2  | 1:A:632:VAL:CG1   | 2.47                     | 0.44              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:909:ASN:HB3   | 1:A:910:SER:H    | 1.63                     | 0.44              |
| 1:A:9:VAL:HG12    | 1:A:20:MET:HE2   | 1.98                     | 0.43              |
| 1:A:122:LEU:HD22  | 1:A:130:ILE:HD13 | 1.98                     | 0.43              |
| 1:A:749:PHE:HD1   | 1:A:767:ALA:CB   | 2.30                     | 0.43              |
| 1:A:901:ASN:HD22  | 1:A:901:ASN:N    | 2.15                     | 0.43              |
| 1:A:608:PHE:CD2   | 1:A:1181:TRP:CZ2 | 3.07                     | 0.43              |
| 1:A:833:ILE:HD13  | 1:A:833:ILE:HA   | 1.56                     | 0.43              |
| 1:A:194:GLU:HG3   | 1:A:220:MET:HE3  | 2.01                     | 0.43              |
| 1:A:1243:ASN:HA   | 1:A:1244:PRO:HD3 | 1.88                     | 0.43              |
| 1:A:74:LEU:HB3    | 1:A:97:LEU:HD23  | 2.01                     | 0.43              |
| 1:A:246:LEU:O     | 1:A:247:LYS:C    | 2.61                     | 0.43              |
| 1:A:318:THR:O     | 1:A:322:LYS:HB2  | 2.18                     | 0.43              |
| 1:A:319:VAL:HG12  | 1:A:474:LEU:HD21 | 2.01                     | 0.43              |
| 1:A:846:CYS:HG    | 1:A:926:PHE:HA   | 1.82                     | 0.43              |
| 1:A:954:ARG:NH1   | 1:A:1049:THR:HB  | 2.34                     | 0.43              |
| 1:A:1018:GLY:HA2  | 3:T:2105:U:H2'   | 1.99                     | 0.43              |
| 1:A:48:LYS:HD3    | 1:A:124:ALA:HA   | 2.01                     | 0.43              |
| 1:A:96:VAL:HG22   | 1:A:111:LEU:HD12 | 2.01                     | 0.43              |
| 1:A:162:ASP:HB2   | 1:A:163:GLU:H    | 1.62                     | 0.43              |
| 1:A:203:MET:HE2   | 1:A:203:MET:HB3  | 1.73                     | 0.43              |
| 1:A:831:LYS:HD2   | 1:A:832:LEU:N    | 2.33                     | 0.43              |
| 1:A:874:THR:HG22  | 1:A:923:ASN:ND2  | 2.32                     | 0.43              |
| 1:A:80:THR:HG23   | 1:A:82:PHE:N     | 2.31                     | 0.43              |
| 1:A:96:VAL:HG22   | 1:A:96:VAL:O     | 2.17                     | 0.43              |
| 1:A:194:GLU:HA    | 1:A:197:VAL:CG1  | 2.49                     | 0.43              |
| 1:A:793:ALA:HB1   | 1:A:974:ASP:O    | 2.19                     | 0.43              |
| 1:A:924:MET:HE2   | 3:T:2106:G:OP1   | 2.18                     | 0.43              |
| 1:A:15:ARG:NH2    | 1:A:38:ILE:HG21  | 2.33                     | 0.43              |
| 1:A:33:ASP:HB3    | 1:A:36:LEU:HB3   | 2.01                     | 0.43              |
| 1:A:303:GLY:H     | 1:A:309:LYS:NZ   | 2.16                     | 0.43              |
| 1:A:539:THR:CG2   | 1:A:564:ARG:HD2  | 2.49                     | 0.43              |
| 1:A:156:VAL:HG12  | 1:A:156:VAL:O    | 2.17                     | 0.43              |
| 1:A:642:LYS:HE3   | 1:A:642:LYS:HB3  | 1.75                     | 0.43              |
| 1:A:1003:LEU:HB3  | 1:A:1004:PRO:CD  | 2.40                     | 0.43              |
| 1:A:806:ARG:N     | 1:A:807:PRO:CD   | 2.82                     | 0.42              |
| 1:A:1134:ASP:OD1  | 1:A:1136:ARG:HG3 | 2.19                     | 0.42              |
| 1:A:438:VAL:O     | 1:A:438:VAL:HG22 | 2.19                     | 0.42              |
| 1:A:1154:ARG:HH11 | 1:A:1154:ARG:CB  | 2.32                     | 0.42              |
| 1:A:58:ALA:HB2    | 1:A:265:ILE:HG21 | 2.01                     | 0.42              |
| 1:A:62:ILE:O      | 1:A:147:GLN:NE2  | 2.52                     | 0.42              |
| 1:A:72:ILE:CD1    | 1:A:137:ALA:HB2  | 2.50                     | 0.42              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:186:VAL:O     | 1:A:187:SER:C    | 2.63                     | 0.42              |
| 1:A:191:VAL:HG13  | 1:A:220:MET:CE   | 2.48                     | 0.42              |
| 1:A:246:LEU:HD12  | 1:A:246:LEU:HA   | 1.80                     | 0.42              |
| 1:A:715:THR:HG23  | 1:A:716:ARG:N    | 2.33                     | 0.42              |
| 1:A:1003:LEU:HD11 | 1:A:1009:VAL:CG2 | 2.49                     | 0.42              |
| 1:A:1192:THR:HG22 | 1:A:1250:SER:HA  | 2.02                     | 0.42              |
| 1:A:312:LEU:O     | 1:A:312:LEU:HG   | 2.19                     | 0.42              |
| 1:A:611:TYR:O     | 1:A:626:ILE:HD12 | 2.19                     | 0.42              |
| 1:A:723:LEU:HD23  | 1:A:1110:ILE:CG1 | 2.48                     | 0.42              |
| 1:A:1040:ILE:O    | 1:A:1040:ILE:CG2 | 2.68                     | 0.42              |
| 1:A:1124:TYR:O    | 1:A:1128:THR:HB  | 2.20                     | 0.42              |
| 1:A:252:GLU:OE2   | 1:A:253:VAL:O    | 2.37                     | 0.42              |
| 1:A:924:MET:O     | 1:A:928:LEU:HG   | 2.19                     | 0.42              |
| 1:A:996:LEU:HA    | 1:A:996:LEU:HD12 | 1.78                     | 0.42              |
| 1:A:1033:LEU:HD12 | 1:A:1033:LEU:HA  | 1.76                     | 0.42              |
| 1:A:1206:ASP:OD1  | 1:A:1206:ASP:C   | 2.62                     | 0.42              |
| 1:A:249:HIS:C     | 1:A:250:ASN:ND2  | 2.77                     | 0.42              |
| 1:A:265:ILE:O     | 1:A:266:GLU:C    | 2.62                     | 0.42              |
| 1:A:269:GLU:HG3   | 1:A:270:THR:N    | 2.35                     | 0.42              |
| 1:A:307:HIS:CD2   | 1:A:391:ALA:H    | 2.37                     | 0.42              |
| 1:A:596:LEU:HB2   | 1:A:668:VAL:O    | 2.20                     | 0.42              |
| 1:A:857:ASN:O     | 1:A:858:ARG:C    | 2.63                     | 0.42              |
| 1:A:9:VAL:C       | 1:A:11:GLU:N     | 2.76                     | 0.42              |
| 1:A:40:ASN:N      | 1:A:40:ASN:HD22  | 2.17                     | 0.42              |
| 1:A:618:ARG:HG2   | 1:A:618:ARG:NH2  | 2.29                     | 0.42              |
| 1:A:118:GLU:O     | 1:A:122:LEU:HB2  | 2.19                     | 0.41              |
| 1:A:187:SER:HB3   | 1:A:190:VAL:HG12 | 2.02                     | 0.41              |
| 1:A:419:LEU:HD11  | 1:A:434:VAL:CG1  | 2.46                     | 0.41              |
| 1:A:930:ILE:C     | 1:A:930:ILE:HD12 | 2.45                     | 0.41              |
| 1:A:985:LEU:CD1   | 1:A:993:LEU:HD22 | 2.50                     | 0.41              |
| 1:A:1066:ARG:HH21 | 1:A:1066:ARG:CG  | 2.33                     | 0.41              |
| 1:A:172:HIS:CD2   | 1:A:172:HIS:C    | 2.98                     | 0.41              |
| 1:A:249:HIS:O     | 1:A:250:ASN:CB   | 2.68                     | 0.41              |
| 1:A:452:THR:HG23  | 1:A:452:THR:O    | 2.19                     | 0.41              |
| 1:A:626:ILE:HA    | 1:A:644:VAL:O    | 2.20                     | 0.41              |
| 1:A:857:ASN:O     | 1:A:860:TYR:N    | 2.53                     | 0.41              |
| 1:A:927:GLN:OE1   | 1:A:1020:GLY:N   | 2.47                     | 0.41              |
| 1:A:1126:TRP:CE3  | 1:A:1127:ALA:HB2 | 2.56                     | 0.41              |
| 3:T:2108:A:H5'    | 3:T:2109:C:OP2   | 2.20                     | 0.41              |
| 1:A:120:VAL:HA    | 1:A:123:VAL:HG12 | 2.01                     | 0.41              |
| 1:A:401:ARG:HE    | 1:A:401:ARG:HB3  | 1.50                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:790:PHE:CD1   | 1:A:791:LEU:HD13  | 2.54                     | 0.41              |
| 1:A:1047:GLU:CB   | 1:A:1058:PRO:CG   | 2.99                     | 0.41              |
| 1:A:1099:VAL:O    | 1:A:1101:VAL:HG13 | 2.20                     | 0.41              |
| 1:A:1154:ARG:HB2  | 1:A:1154:ARG:NH1  | 2.35                     | 0.41              |
| 1:A:1193:ARG:HD2  | 1:A:1249:ARG:HH12 | 1.85                     | 0.41              |
| 1:A:122:LEU:O     | 1:A:125:LYS:N     | 2.53                     | 0.41              |
| 1:A:2:ALA:N       | 1:A:426:ASP:O     | 2.53                     | 0.41              |
| 1:A:626:ILE:HD13  | 1:A:626:ILE:O     | 2.20                     | 0.41              |
| 1:A:935:ARG:NH2   | 1:A:1024:GLU:OE2  | 2.53                     | 0.41              |
| 1:A:1151:GLN:HE21 | 1:A:1151:GLN:N    | 2.12                     | 0.41              |
| 1:A:91:ALA:O      | 1:A:95:LYS:HB2    | 2.20                     | 0.41              |
| 1:A:155:LEU:O     | 1:A:257:ILE:N     | 2.51                     | 0.41              |
| 1:A:194:GLU:C     | 1:A:197:VAL:HG12  | 2.46                     | 0.41              |
| 1:A:378:THR:CG2   | 1:A:380:ALA:H     | 2.27                     | 0.41              |
| 1:A:937:ARG:C     | 1:A:939:ARG:H     | 2.28                     | 0.41              |
| 1:A:1018:GLY:HA2  | 3:T:2105:U:C2'    | 2.51                     | 0.41              |
| 1:A:870:PRO:C     | 1:A:895:SER:HB3   | 2.46                     | 0.41              |
| 1:A:24:LYS:C      | 1:A:24:LYS:HD3    | 2.46                     | 0.41              |
| 1:A:64:THR:HA     | 1:A:72:ILE:O      | 2.21                     | 0.41              |
| 1:A:126:ILE:HG23  | 1:A:399:GLN:HE22  | 1.86                     | 0.41              |
| 1:A:229:LEU:HD11  | 1:A:242:VAL:HG21  | 2.02                     | 0.41              |
| 1:A:677:LEU:HA    | 1:A:677:LEU:HD23  | 1.79                     | 0.41              |
| 1:A:845:HIS:C     | 1:A:929:GLY:HA2   | 2.46                     | 0.41              |
| 1:A:1254:PHE:CD1  | 1:A:1254:PHE:N    | 2.89                     | 0.41              |
| 1:A:301:THR:HG23  | 1:A:365:ASP:OD2   | 2.20                     | 0.41              |
| 1:A:751:PRO:HG3   | 1:A:767:ALA:CB    | 2.50                     | 0.41              |
| 1:A:790:PHE:HB2   | 1:A:915:CYS:SG    | 2.61                     | 0.41              |
| 1:A:916:ILE:HG12  | 3:T:2105:U:C2     | 2.55                     | 0.41              |
| 1:A:930:ILE:CD1   | 1:A:1021:TYR:HB2  | 2.51                     | 0.41              |
| 1:A:961:THR:CG2   | 1:A:963:ASN:H     | 2.29                     | 0.41              |
| 1:A:4:ILE:HG22    | 1:A:5:THR:N       | 2.34                     | 0.40              |
| 1:A:310:THR:HA    | 1:A:313:THR:HG22  | 2.02                     | 0.40              |
| 1:A:930:ILE:CD1   | 1:A:1021:TYR:CB   | 2.94                     | 0.40              |
| 1:A:126:ILE:HG23  | 1:A:399:GLN:NE2   | 2.37                     | 0.40              |
| 1:A:431:LEU:C     | 1:A:433:LEU:H     | 2.27                     | 0.40              |
| 1:A:765:LEU:O     | 1:A:769:ILE:HG22  | 2.22                     | 0.40              |
| 1:A:856:ASN:ND2   | 1:A:866:LYS:HD3   | 2.36                     | 0.40              |
| 1:A:938:LEU:HD12  | 1:A:938:LEU:HA    | 1.75                     | 0.40              |
| 1:A:18:ALA:CB     | 1:A:41:MET:HE1    | 2.51                     | 0.40              |
| 1:A:317:THR:HG22  | 1:A:354:TYR:HB3   | 2.03                     | 0.40              |
| 1:A:323:THR:HG22  | 1:A:324:TYR:N     | 2.36                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:348:ASN:O     | 1:A:349:THR:C     | 2.64                     | 0.40              |
| 1:A:1204:LEU:HA   | 1:A:1204:LEU:HD23 | 1.72                     | 0.40              |
| 1:A:1110:ILE:HD12 | 1:A:1111:VAL:H    | 1.87                     | 0.40              |
| 1:A:1121:ASN:O    | 1:A:1125:ARG:HG3  | 2.22                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed        | Favoured  | Allowed   | Outliers | Percentiles       |
|-----|-------|-----------------|-----------|-----------|----------|-------------------|
| 1   | A     | 1193/1289 (93%) | 987 (83%) | 154 (13%) | 52 (4%)  | <b>2</b> <b>8</b> |

All (52) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 34   | ILE  |
| 1   | A     | 101  | VAL  |
| 1   | A     | 116  | GLU  |
| 1   | A     | 141  | ASP  |
| 1   | A     | 209  | LYS  |
| 1   | A     | 250  | ASN  |
| 1   | A     | 324  | TYR  |
| 1   | A     | 325  | GLY  |
| 1   | A     | 349  | THR  |
| 1   | A     | 381  | ALA  |
| 1   | A     | 778  | LEU  |
| 1   | A     | 806  | ARG  |
| 1   | A     | 809  | TYR  |
| 1   | A     | 896  | ASP  |
| 1   | A     | 970  | SER  |
| 1   | A     | 1177 | LYS  |
| 1   | A     | 68   | GLY  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 102  | ALA  |
| 1   | A     | 159  | LYS  |
| 1   | A     | 210  | GLU  |
| 1   | A     | 664  | GLY  |
| 1   | A     | 677  | LEU  |
| 1   | A     | 813  | PHE  |
| 1   | A     | 849  | SER  |
| 1   | A     | 895  | SER  |
| 1   | A     | 947  | ASP  |
| 1   | A     | 1015 | SER  |
| 1   | A     | 1074 | PHE  |
| 1   | A     | 162  | ASP  |
| 1   | A     | 577  | LEU  |
| 1   | A     | 679  | GLY  |
| 1   | A     | 1084 | GLU  |
| 1   | A     | 1241 | ARG  |
| 1   | A     | 187  | SER  |
| 1   | A     | 246  | LEU  |
| 1   | A     | 350  | SER  |
| 1   | A     | 506  | SER  |
| 1   | A     | 535  | THR  |
| 1   | A     | 611  | TYR  |
| 1   | A     | 641  | ILE  |
| 1   | A     | 702  | ARG  |
| 1   | A     | 909  | ASN  |
| 1   | A     | 448  | PRO  |
| 1   | A     | 780  | ILE  |
| 1   | A     | 576  | VAL  |
| 1   | A     | 1131 | GLY  |
| 1   | A     | 103  | GLY  |
| 1   | A     | 201  | ILE  |
| 1   | A     | 566  | ILE  |
| 1   | A     | 1239 | ILE  |
| 1   | A     | 1058 | PRO  |
| 1   | A     | 1111 | VAL  |

### 5.3.2 Protein sidechains ⓘ

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

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

analysed, and the total number of residues.

| Mol | Chain | Analysed       | Rotameric | Outliers  | Percentiles       |
|-----|-------|----------------|-----------|-----------|-------------------|
| 1   | A     | 995/1060 (94%) | 812 (82%) | 183 (18%) | <b>1</b> <b>6</b> |

All (183) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 5   | THR  |
| 1   | A     | 10  | LYS  |
| 1   | A     | 25  | LYS  |
| 1   | A     | 28  | THR  |
| 1   | A     | 40  | ASN  |
| 1   | A     | 52  | LYS  |
| 1   | A     | 66  | ILE  |
| 1   | A     | 73  | ILE  |
| 1   | A     | 75  | GLU  |
| 1   | A     | 76  | VAL  |
| 1   | A     | 80  | THR  |
| 1   | A     | 97  | LEU  |
| 1   | A     | 111 | LEU  |
| 1   | A     | 130 | ILE  |
| 1   | A     | 132 | ILE  |
| 1   | A     | 133 | ARG  |
| 1   | A     | 151 | ARG  |
| 1   | A     | 156 | VAL  |
| 1   | A     | 162 | ASP  |
| 1   | A     | 165 | LEU  |
| 1   | A     | 166 | VAL  |
| 1   | A     | 169 | ILE  |
| 1   | A     | 181 | ILE  |
| 1   | A     | 186 | VAL  |
| 1   | A     | 192 | GLU  |
| 1   | A     | 199 | LEU  |
| 1   | A     | 203 | MET  |
| 1   | A     | 204 | GLN  |
| 1   | A     | 210 | GLU  |
| 1   | A     | 237 | GLU  |
| 1   | A     | 242 | VAL  |
| 1   | A     | 244 | GLN  |
| 1   | A     | 245 | LEU  |
| 1   | A     | 246 | LEU  |
| 1   | A     | 250 | ASN  |
| 1   | A     | 258 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 310 | THR  |
| 1   | A     | 311 | THR  |
| 1   | A     | 317 | THR  |
| 1   | A     | 320 | LEU  |
| 1   | A     | 349 | THR  |
| 1   | A     | 352 | VAL  |
| 1   | A     | 355 | ASP  |
| 1   | A     | 364 | VAL  |
| 1   | A     | 387 | ILE  |
| 1   | A     | 390 | VAL  |
| 1   | A     | 397 | MET  |
| 1   | A     | 399 | GLN  |
| 1   | A     | 400 | THR  |
| 1   | A     | 401 | ARG  |
| 1   | A     | 406 | LEU  |
| 1   | A     | 416 | ILE  |
| 1   | A     | 426 | ASP  |
| 1   | A     | 434 | VAL  |
| 1   | A     | 438 | VAL  |
| 1   | A     | 439 | ARG  |
| 1   | A     | 454 | ILE  |
| 1   | A     | 455 | VAL  |
| 1   | A     | 491 | ILE  |
| 1   | A     | 502 | VAL  |
| 1   | A     | 504 | SER  |
| 1   | A     | 508 | ARG  |
| 1   | A     | 529 | ILE  |
| 1   | A     | 530 | VAL  |
| 1   | A     | 533 | LYS  |
| 1   | A     | 535 | THR  |
| 1   | A     | 537 | LYS  |
| 1   | A     | 550 | LEU  |
| 1   | A     | 563 | LEU  |
| 1   | A     | 579 | LYS  |
| 1   | A     | 583 | ILE  |
| 1   | A     | 587 | THR  |
| 1   | A     | 593 | VAL  |
| 1   | A     | 597 | SER  |
| 1   | A     | 605 | THR  |
| 1   | A     | 618 | ARG  |
| 1   | A     | 621 | ASP  |
| 1   | A     | 622 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 623 | THR  |
| 1   | A     | 625 | THR  |
| 1   | A     | 626 | ILE  |
| 1   | A     | 628 | LEU  |
| 1   | A     | 632 | VAL  |
| 1   | A     | 640 | ASN  |
| 1   | A     | 651 | ILE  |
| 1   | A     | 662 | ARG  |
| 1   | A     | 672 | VAL  |
| 1   | A     | 676 | VAL  |
| 1   | A     | 704 | SER  |
| 1   | A     | 705 | LEU  |
| 1   | A     | 715 | THR  |
| 1   | A     | 717 | ILE  |
| 1   | A     | 733 | LEU  |
| 1   | A     | 738 | SER  |
| 1   | A     | 752 | ARG  |
| 1   | A     | 780 | ILE  |
| 1   | A     | 782 | THR  |
| 1   | A     | 785 | VAL  |
| 1   | A     | 791 | LEU  |
| 1   | A     | 799 | LEU  |
| 1   | A     | 800 | THR  |
| 1   | A     | 804 | LEU  |
| 1   | A     | 809 | TYR  |
| 1   | A     | 814 | ASN  |
| 1   | A     | 816 | SER  |
| 1   | A     | 820 | SER  |
| 1   | A     | 822 | ILE  |
| 1   | A     | 824 | MET  |
| 1   | A     | 832 | LEU  |
| 1   | A     | 833 | ILE  |
| 1   | A     | 835 | ASP  |
| 1   | A     | 839 | VAL  |
| 1   | A     | 843 | LEU  |
| 1   | A     | 847 | ARG  |
| 1   | A     | 854 | THR  |
| 1   | A     | 855 | THR  |
| 1   | A     | 873 | CYS  |
| 1   | A     | 879 | LYS  |
| 1   | A     | 894 | ILE  |
| 1   | A     | 896 | ASP  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 901  | ASN  |
| 1   | A     | 906  | VAL  |
| 1   | A     | 910  | SER  |
| 1   | A     | 911  | LYS  |
| 1   | A     | 916  | ILE  |
| 1   | A     | 918  | ILE  |
| 1   | A     | 933  | ILE  |
| 1   | A     | 937  | ARG  |
| 1   | A     | 938  | LEU  |
| 1   | A     | 943  | ILE  |
| 1   | A     | 948  | GLN  |
| 1   | A     | 949  | THR  |
| 1   | A     | 950  | ILE  |
| 1   | A     | 956  | HIS  |
| 1   | A     | 960  | VAL  |
| 1   | A     | 961  | THR  |
| 1   | A     | 962  | ASN  |
| 1   | A     | 964  | LEU  |
| 1   | A     | 973  | SER  |
| 1   | A     | 978  | LEU  |
| 1   | A     | 991  | GLU  |
| 1   | A     | 992  | VAL  |
| 1   | A     | 996  | LEU  |
| 1   | A     | 1008 | VAL  |
| 1   | A     | 1009 | VAL  |
| 1   | A     | 1012 | GLU  |
| 1   | A     | 1014 | ILE  |
| 1   | A     | 1017 | MET  |
| 1   | A     | 1022 | THR  |
| 1   | A     | 1029 | ILE  |
| 1   | A     | 1033 | LEU  |
| 1   | A     | 1042 | ASP  |
| 1   | A     | 1043 | LEU  |
| 1   | A     | 1049 | THR  |
| 1   | A     | 1060 | CYS  |
| 1   | A     | 1066 | ARG  |
| 1   | A     | 1075 | THR  |
| 1   | A     | 1076 | THR  |
| 1   | A     | 1081 | THR  |
| 1   | A     | 1089 | GLU  |
| 1   | A     | 1099 | VAL  |
| 1   | A     | 1102 | THR  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1110 | ILE  |
| 1   | A     | 1111 | VAL  |
| 1   | A     | 1116 | LEU  |
| 1   | A     | 1117 | ILE  |
| 1   | A     | 1128 | THR  |
| 1   | A     | 1136 | ARG  |
| 1   | A     | 1145 | ARG  |
| 1   | A     | 1147 | LEU  |
| 1   | A     | 1150 | LYS  |
| 1   | A     | 1151 | GLN  |
| 1   | A     | 1152 | LEU  |
| 1   | A     | 1154 | ARG  |
| 1   | A     | 1167 | VAL  |
| 1   | A     | 1173 | ASN  |
| 1   | A     | 1182 | ILE  |
| 1   | A     | 1200 | LEU  |
| 1   | A     | 1235 | ILE  |
| 1   | A     | 1239 | ILE  |
| 1   | A     | 1249 | ARG  |
| 1   | A     | 1251 | THR  |
| 1   | A     | 1257 | GLN  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 40  | ASN  |
| 1   | A     | 114 | GLN  |
| 1   | A     | 147 | GLN  |
| 1   | A     | 168 | HIS  |
| 1   | A     | 204 | GLN  |
| 1   | A     | 250 | ASN  |
| 1   | A     | 296 | HIS  |
| 1   | A     | 307 | HIS  |
| 1   | A     | 351 | HIS  |
| 1   | A     | 360 | HIS  |
| 1   | A     | 382 | GLN  |
| 1   | A     | 399 | GLN  |
| 1   | A     | 409 | GLN  |
| 1   | A     | 420 | ASN  |
| 1   | A     | 614 | GLN  |
| 1   | A     | 714 | ASN  |
| 1   | A     | 729 | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 741  | ASN  |
| 1   | A     | 763  | ASN  |
| 1   | A     | 845  | HIS  |
| 1   | A     | 856  | ASN  |
| 1   | A     | 857  | ASN  |
| 1   | A     | 871  | GLN  |
| 1   | A     | 901  | ASN  |
| 1   | A     | 946  | ASN  |
| 1   | A     | 962  | ASN  |
| 1   | A     | 1077 | ASN  |
| 1   | A     | 1094 | HIS  |
| 1   | A     | 1121 | ASN  |
| 1   | A     | 1122 | ASN  |
| 1   | A     | 1151 | GLN  |
| 1   | A     | 1155 | ASN  |
| 1   | A     | 1173 | ASN  |
| 1   | A     | 1237 | GLN  |
| 1   | A     | 1257 | GLN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed    | Backbone Outliers | Pucker Outliers |
|-----|-------|-------------|-------------------|-----------------|
| 2   | G     | 6/7 (85%)   | 0                 | 0               |
| 3   | T     | 8/12 (66%)  | 4 (50%)           | 0               |
| All | All   | 14/19 (73%) | 4 (28%)           | 0               |

All (4) RNA backbone outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | T     | 2106 | G    |
| 3   | T     | 2108 | A    |
| 3   | T     | 2109 | C    |
| 3   | T     | 2110 | C    |

There are no RNA pucker outliers to report.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

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

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

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2      | OWAB(Å <sup>2</sup> ) | Q<0.9   |
|-----|-------|-----------------|--------|--------------|-----------------------|---------|
| 1   | A     | 1203/1289 (93%) | -0.56  | 3 (0%) 91 89 | 31, 80, 128, 147      | 0       |
| 2   | G     | 7/7 (100%)      | 0.81   | 0 100 100    | 116, 131, 163, 165    | 0       |
| 3   | T     | 9/12 (75%)      | 0.81   | 2 (22%) 2 2  | 63, 126, 154, 160     | 1 (11%) |
| All | All   | 1219/1308 (93%) | -0.54  | 5 (0%) 88 85 | 31, 80, 129, 165      | 1 (0%)  |

All (5) RSRZ outliers are listed below:

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | A     | 701  | SER  | 3.0  |
| 3   | T     | 2106 | G    | 2.8  |
| 1   | A     | 1263 | SER  | 2.7  |
| 1   | A     | 778  | LEU  | 2.6  |
| 3   | T     | 2105 | U    | 2.1  |

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

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

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 4   | CA   | A     | 3001 | 1/1   | 0.90 | 0.07 | 82,82,82,82                 | 0     |
| 4   | CA   | A     | 3002 | 1/1   | 0.96 | 0.07 | 77,77,77,77                 | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.