



# Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 09:27 am BST

PDB ID : 7ADH  
Title : THREE-DIMENSIONAL STRUCTURE OF ISONICOTINIMIDYLATED  
LIVER ALCOHOL DEHYDROGENASE  
Authors : Plapp, B.; Eklund, H.  
Deposited on : 1984-01-16  
Resolution : 3.20 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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

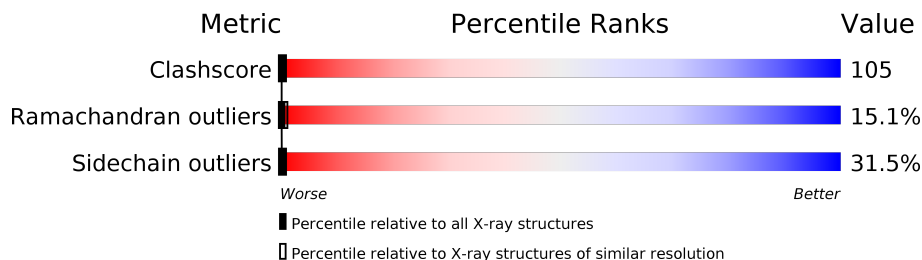
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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)) |
|-----------------------|-----------------------------|---|
| Clashscore            | 141614                      | 1253 (3.20-3.20)                                      |
| Ramachandran outliers | 138981                      | 1234 (3.20-3.20)                                      |
| Sidechain outliers    | 138945                      | 1233 (3.20-3.20)                                      |

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 on 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  $\leq 5\%$

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 374    |                  |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 3   | NTN  | A     | 377 | -         | -        | X       | -                |
| 3   | NTN  | A     | 378 | -         | -        | X       | -                |
| 3   | NTN  | A     | 379 | -         | -        | X       | -                |
| 3   | NTN  | A     | 382 | -         | -        | X       | -                |
| 3   | NTN  | A     | 383 | -         | -        | X       | -                |
| 3   | NTN  | A     | 385 | -         | -        | X       | -                |

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| <b>Mol</b> | <b>Type</b> | <b>Chain</b> | <b>Res</b> | <b>Chirality</b> | <b>Geometry</b> | <b>Clashes</b> | <b>Electron density</b> |
|------------|-------------|--------------|------------|------------------|-----------------|----------------|-------------------------|
| 3          | NTN         | A            | 386        | -                | -               | X              | -                       |
| 3          | NTN         | A            | 390        | -                | -               | X              | -                       |
| 3          | NTN         | A            | 391        | -                | -               | X              | -                       |
| 3          | NTN         | A            | 397        | -                | -               | X              | -                       |

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2970 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.

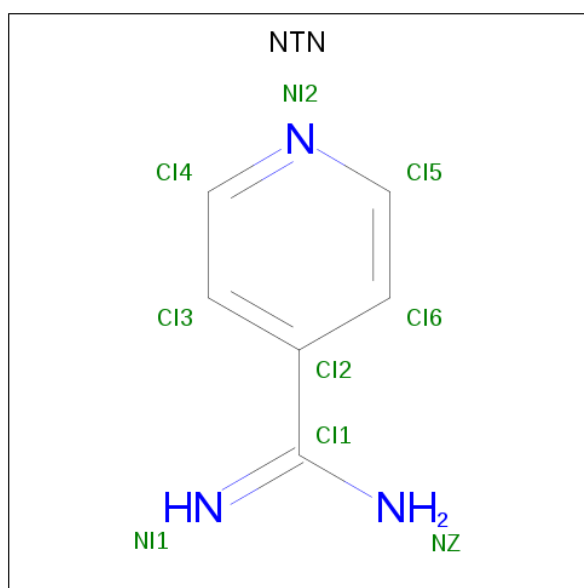
- Molecule 1 is a protein called ISONICOTINIMIDYLATED LIVER ALCOHOL DEHYDROGENASE.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
|     |       |          | Total | C    | N   | O   | S  |         |         |       |
| 1   | A     | 374      | 2784  | 1769 | 472 | 520 | 23 | 32      | 0       | 0     |

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is ISONICOTINAMIDINE (three-letter code: NTN) (formula: C<sub>6</sub>H<sub>7</sub>N<sub>3</sub>).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 3   | A     | 1        | Total | C | N | 0       | 0       |
|     |       |          | 8     | 6 | 2 |         |         |
| 3   | A     | 1        | Total | C | N | 0       | 0       |
|     |       |          | 8     | 6 | 2 |         |         |

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| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 3   | A     | 1        | Total | C | N | 0       | 0       |
|     |       |          | 8     | 6 | 2 |         |         |
| 3   | A     | 1        | Total | C | N | 0       | 0       |
|     |       |          | 8     | 6 | 2 |         |         |
| 3   | A     | 1        | Total | C | N | 0       | 0       |
|     |       |          | 8     | 6 | 2 |         |         |
| 3   | A     | 1        | Total | C | N | 0       | 0       |
|     |       |          | 8     | 6 | 2 |         |         |
| 3   | A     | 1        | Total | C | N | 0       | 0       |
|     |       |          | 8     | 6 | 2 |         |         |
| 3   | A     | 1        | Total | C | N | 0       | 0       |
|     |       |          | 8     | 6 | 2 |         |         |
| 3   | A     | 1        | Total | C | N | 0       | 0       |
|     |       |          | 8     | 6 | 2 |         |         |
| 3   | A     | 1        | Total | C | N | 0       | 0       |
|     |       |          | 8     | 6 | 2 |         |         |
| 3   | A     | 1        | Total | C | N | 0       | 0       |
|     |       |          | 8     | 6 | 2 |         |         |
| 3   | A     | 1        | Total | C | N | 0       | 0       |
|     |       |          | 8     | 6 | 2 |         |         |
| 3   | A     | 1        | Total | C | N | 0       | 0       |
|     |       |          | 8     | 6 | 2 |         |         |
| 3   | A     | 1        | Total | C | N | 0       | 0       |
|     |       |          | 8     | 6 | 2 |         |         |
| 3   | A     | 1        | Total | C | N | 0       | 0       |
|     |       |          | 8     | 6 | 2 |         |         |
| 3   | A     | 1        | Total | C | N | 0       | 0       |
|     |       |          | 8     | 6 | 2 |         |         |
| 3   | A     | 1        | Total | C | N | 0       | 0       |
|     |       |          | 8     | 6 | 2 |         |         |



## 4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

| Property   | Value  | Source    |
|--|--|-----------|
| Space group  | C 1 2 1  | Depositor |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$ | 177.80Å 61.20Å 56.50Å<br>90.00° 104.00° 90.00° | Depositor |
| Resolution (Å)   | (Not available) – 3.20                         | Depositor |
| % Data completeness<br>(in resolution range)             | (Not available) ((Not available)-3.20)         | Depositor |
| $R_{merge}$  | (Not available)                                | Depositor |
| $R_{sym}$  | (Not available)                                | Depositor |
| Refinement program                                       | CORELS   | Depositor |
| R, $R_{free}$  | 0.290 , (Not available)                        | Depositor |
| Estimated twinning fraction                              | No twinning to report.                         | Xtrriage  |
| Total number of atoms                                    | 2970   | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 20.0   | wwPDB-VP  |

## 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: ZN, NTN

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     | 1.68         | 20/2836 (0.7%) | 2.78        | 264/3834 (6.9%) |

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                   | 4                   |

All (20) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 1   | A     | 96  | GLN  | CA-CB  | -23.87 | 1.01        | 1.53     |
| 1   | A     | 96  | GLN  | N-CA   | 11.88  | 1.70        | 1.46     |
| 1   | A     | 364 | SER  | CB-OG  | 8.78   | 1.53        | 1.42     |
| 1   | A     | 35  | GLU  | CG-CD  | -6.34  | 1.42        | 1.51     |
| 1   | A     | 192 | GLY  | N-CA   | 6.29   | 1.55        | 1.46     |
| 1   | A     | 16  | GLU  | CB-CG  | 5.98   | 1.63        | 1.52     |
| 1   | A     | 144 | SER  | CA-CB  | -5.86  | 1.44        | 1.52     |
| 1   | A     | 366 | GLU  | C-O    | 5.84   | 1.34        | 1.23     |
| 1   | A     | 357 | GLU  | CD-OE2 | 5.75   | 1.31        | 1.25     |
| 1   | A     | 107 | GLU  | CD-OE2 | 5.74   | 1.31        | 1.25     |
| 1   | A     | 212 | LYS  | CE-NZ  | -5.70  | 1.34        | 1.49     |
| 1   | A     | 298 | SER  | CA-CB  | 5.65   | 1.61        | 1.52     |
| 1   | A     | 236 | GLY  | N-CA   | 5.59   | 1.54        | 1.46     |
| 1   | A     | 281 | CYS  | CB-SG  | -5.52  | 1.72        | 1.81     |
| 1   | A     | 184 | VAL  | C-O    | 5.50   | 1.33        | 1.23     |
| 1   | A     | 215 | GLY  | C-O    | 5.43   | 1.32        | 1.23     |
| 1   | A     | 215 | GLY  | N-CA   | 5.23   | 1.53        | 1.46     |
| 1   | A     | 167 | GLU  | CD-OE2 | 5.21   | 1.31        | 1.25     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | A     | 129 | ARG  | CG-CD | -5.19 | 1.39        | 1.51     |
| 1   | A     | 354 | LYS  | N-CA  | 5.03  | 1.56        | 1.46     |

All (264) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 1   | A     | 37  | ARG  | NE-CZ-NH2  | -21.26 | 109.67      | 120.30   |
| 1   | A     | 120 | ARG  | NE-CZ-NH2  | -17.88 | 111.36      | 120.30   |
| 1   | A     | 363 | ARG  | NE-CZ-NH2  | -14.40 | 113.10      | 120.30   |
| 1   | A     | 117 | SER  | N-CA-CB    | 13.27  | 130.41      | 110.50   |
| 1   | A     | 239 | GLU  | OE1-CD-OE2 | 13.20  | 139.14      | 123.30   |
| 1   | A     | 334 | ASP  | CB-CG-OD1  | 13.20  | 130.18      | 118.30   |
| 1   | A     | 216 | ALA  | O-C-N      | 12.47  | 142.65      | 122.70   |
| 1   | A     | 107 | GLU  | N-CA-CB    | 11.96  | 132.12      | 110.60   |
| 1   | A     | 363 | ARG  | NE-CZ-NH1  | 11.92  | 126.26      | 120.30   |
| 1   | A     | 149 | TYR  | CB-CG-CD1  | 11.21  | 127.72      | 121.00   |
| 1   | A     | 120 | ARG  | NE-CZ-NH1  | 11.14  | 125.87      | 120.30   |
| 1   | A     | 252 | GLU  | CA-CB-CG   | 11.01  | 137.63      | 113.40   |
| 1   | A     | 149 | TYR  | CB-CG-CD2  | -10.70 | 114.58      | 121.00   |
| 1   | A     | 267 | GLU  | CA-CB-CG   | 10.31  | 136.07      | 113.40   |
| 1   | A     | 275 | MET  | CA-CB-CG   | 10.22  | 130.67      | 113.30   |
| 1   | A     | 343 | ASP  | CB-CG-OD2  | 10.16  | 127.45      | 118.30   |
| 1   | A     | 254 | LEU  | CA-CB-CG   | 9.70   | 137.62      | 115.30   |
| 1   | A     | 27  | GLU  | OE1-CD-OE2 | 9.56   | 134.77      | 123.30   |
| 1   | A     | 37  | ARG  | NE-CZ-NH1  | 9.55   | 125.07      | 120.30   |
| 1   | A     | 27  | GLU  | CA-CB-CG   | 9.51   | 134.32      | 113.40   |
| 1   | A     | 16  | GLU  | C-N-CA     | 9.50   | 145.45      | 121.70   |
| 1   | A     | 353 | GLU  | OE1-CD-OE2 | 9.45   | 134.64      | 123.30   |
| 1   | A     | 125 | ASP  | CB-CG-OD1  | 9.39   | 126.75      | 118.30   |
| 1   | A     | 35  | GLU  | CB-CG-CD   | 9.30   | 139.31      | 114.20   |
| 1   | A     | 129 | ARG  | CB-CG-CD   | 9.29   | 135.76      | 111.60   |
| 1   | A     | 343 | ASP  | CB-CG-OD1  | -9.21  | 110.01      | 118.30   |
| 1   | A     | 263 | ASP  | C-N-CA     | 9.16   | 144.61      | 121.70   |
| 1   | A     | 267 | GLU  | OE1-CD-OE2 | 9.04   | 134.15      | 123.30   |
| 1   | A     | 141 | LEU  | CB-CA-C    | 9.00   | 127.30      | 110.20   |
| 1   | A     | 132 | CYS  | O-C-N      | 8.94   | 137.01      | 122.70   |
| 1   | A     | 311 | GLY  | C-N-CA     | 8.65   | 143.31      | 121.70   |
| 1   | A     | 50  | ASP  | O-C-N      | 8.60   | 136.46      | 122.70   |
| 1   | A     | 112 | LEU  | CA-CB-CG   | 8.54   | 134.94      | 115.30   |
| 1   | A     | 338 | LYS  | N-CA-CB    | 8.52   | 125.93      | 110.60   |
| 1   | A     | 262 | VAL  | C-N-CA     | 8.52   | 142.99      | 121.70   |
| 1   | A     | 285 | ALA  | C-N-CA     | 8.42   | 142.75      | 121.70   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 315 | LYS  | C-N-CA     | 8.41  | 139.97      | 122.30   |
| 1   | A     | 89  | VAL  | N-CA-CB    | -8.35 | 93.13       | 111.50   |
| 1   | A     | 245 | ASP  | C-N-CA     | 8.33  | 142.52      | 121.70   |
| 1   | A     | 145 | THR  | CA-CB-CG2  | 8.29  | 124.00      | 112.40   |
| 1   | A     | 216 | ALA  | CA-C-N     | -8.19 | 99.17       | 117.20   |
| 1   | A     | 227 | ASP  | CB-CG-OD1  | 8.18  | 125.66      | 118.30   |
| 1   | A     | 96  | GLN  | N-CA-CB    | 8.14  | 125.26      | 110.60   |
| 1   | A     | 271 | ARG  | NE-CZ-NH1  | -8.12 | 116.24      | 120.30   |
| 1   | A     | 59  | THR  | N-CA-CB    | 8.10  | 125.69      | 110.30   |
| 1   | A     | 215 | GLY  | CA-C-O     | -7.98 | 106.24      | 120.60   |
| 1   | A     | 286 | TYR  | CB-CG-CD2  | 7.98  | 125.79      | 121.00   |
| 1   | A     | 332 | VAL  | CA-C-N     | -7.95 | 99.71       | 117.20   |
| 1   | A     | 3   | ALA  | O-C-N      | 7.76  | 136.39      | 123.20   |
| 1   | A     | 282 | CYS  | N-CA-CB    | -7.74 | 96.68       | 110.60   |
| 1   | A     | 109 | ASN  | CB-CG-OD1  | -7.73 | 106.15      | 121.60   |
| 1   | A     | 161 | ASP  | CB-CG-OD1  | -7.72 | 111.35      | 118.30   |
| 1   | A     | 354 | LYS  | CB-CA-C    | 7.71  | 125.82      | 110.40   |
| 1   | A     | 110 | PHE  | O-C-N      | 7.70  | 135.01      | 122.70   |
| 1   | A     | 176 | PHE  | CA-C-N     | 7.66  | 134.05      | 117.20   |
| 1   | A     | 233 | LYS  | CB-CA-C    | 7.60  | 125.59      | 110.40   |
| 1   | A     | 116 | LEU  | CA-CB-CG   | 7.56  | 132.69      | 115.30   |
| 1   | A     | 47  | ARG  | NE-CZ-NH2  | 7.52  | 124.06      | 120.30   |
| 1   | A     | 141 | LEU  | N-CA-C     | -7.49 | 90.78       | 111.00   |
| 1   | A     | 218 | ARG  | NE-CZ-NH2  | 7.49  | 124.04      | 120.30   |
| 1   | A     | 16  | GLU  | CB-CA-C    | 7.42  | 125.25      | 110.40   |
| 1   | A     | 153 | ASP  | CB-CG-OD2  | -7.39 | 111.65      | 118.30   |
| 1   | A     | 89  | VAL  | CB-CA-C    | 7.39  | 125.44      | 111.40   |
| 1   | A     | 301 | LEU  | CA-CB-CG   | 7.38  | 132.28      | 115.30   |
| 1   | A     | 343 | ASP  | CB-CA-C    | 7.36  | 125.13      | 110.40   |
| 1   | A     | 52  | VAL  | CB-CA-C    | 7.30  | 125.27      | 111.40   |
| 1   | A     | 281 | CYS  | CA-CB-SG   | 7.26  | 127.06      | 114.00   |
| 1   | A     | 35  | GLU  | CA-CB-CG   | 7.25  | 129.36      | 113.40   |
| 1   | A     | 334 | ASP  | CB-CG-OD2  | -7.25 | 111.78      | 118.30   |
| 1   | A     | 324 | SER  | N-CA-C     | 7.24  | 130.55      | 111.00   |
| 1   | A     | 234 | GLU  | O-C-N      | 7.20  | 134.21      | 122.70   |
| 1   | A     | 142 | GLY  | O-C-N      | 7.19  | 134.21      | 122.70   |
| 1   | A     | 168 | LYS  | CB-CA-C    | -7.14 | 96.12       | 110.40   |
| 1   | A     | 1   | SER  | O-C-N      | 7.13  | 134.10      | 122.70   |
| 1   | A     | 279 | LEU  | N-CA-C     | -7.11 | 91.80       | 111.00   |
| 1   | A     | 167 | GLU  | C-N-CA     | 7.09  | 139.43      | 121.70   |
| 1   | A     | 189 | VAL  | C-N-CA     | 7.08  | 139.40      | 121.70   |
| 1   | A     | 76  | ILE  | CB-CG1-CD1 | 7.07  | 133.71      | 113.90   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 112 | LEU  | CB-CG-CD2  | -7.06 | 98.99       | 111.00   |
| 1   | A     | 35  | GLU  | OE1-CD-OE2 | -7.03 | 114.86      | 123.30   |
| 1   | A     | 42  | ALA  | CB-CA-C    | -7.03 | 99.56       | 110.10   |
| 1   | A     | 65  | ALA  | C-N-CA     | 7.02  | 137.04      | 122.30   |
| 1   | A     | 194 | THR  | O-C-N      | 7.01  | 133.91      | 122.70   |
| 1   | A     | 101 | ARG  | NE-CZ-NH2  | 7.00  | 123.80      | 120.30   |
| 1   | A     | 304 | ASN  | CA-CB-CG   | -7.00 | 98.00       | 113.40   |
| 1   | A     | 353 | GLU  | N-CA-CB    | -7.00 | 98.01       | 110.60   |
| 1   | A     | 216 | ALA  | N-CA-CB    | -6.99 | 100.31      | 110.10   |
| 1   | A     | 158 | ALA  | CB-CA-C    | -6.97 | 99.65       | 110.10   |
| 1   | A     | 152 | VAL  | CA-C-N     | 6.95  | 132.48      | 117.20   |
| 1   | A     | 78  | GLU  | CB-CG-CD   | 6.94  | 132.95      | 114.20   |
| 1   | A     | 271 | ARG  | NE-CZ-NH2  | 6.93  | 123.76      | 120.30   |
| 1   | A     | 179 | GLY  | N-CA-C     | -6.89 | 95.87       | 113.10   |
| 1   | A     | 54  | SER  | CA-C-N     | 6.85  | 129.91      | 116.20   |
| 1   | A     | 139 | HIS  | N-CA-CB    | 6.85  | 122.93      | 110.60   |
| 1   | A     | 132 | CYS  | CA-C-N     | -6.85 | 102.13      | 117.20   |
| 1   | A     | 48  | SER  | C-N-CA     | 6.83  | 138.78      | 121.70   |
| 1   | A     | 211 | CYS  | CA-C-N     | -6.83 | 102.17      | 117.20   |
| 1   | A     | 273 | ASP  | CB-CG-OD1  | -6.83 | 112.15      | 118.30   |
| 1   | A     | 289 | SER  | N-CA-CB    | 6.82  | 120.73      | 110.50   |
| 1   | A     | 239 | GLU  | N-CA-CB    | -6.78 | 98.41       | 110.60   |
| 1   | A     | 3   | ALA  | CA-C-N     | -6.75 | 102.71      | 116.20   |
| 1   | A     | 162 | ALA  | CA-C-N     | 6.74  | 132.03      | 117.20   |
| 1   | A     | 207 | VAL  | C-N-CA     | 6.73  | 138.53      | 121.70   |
| 1   | A     | 211 | CYS  | CA-C-O     | 6.71  | 134.20      | 120.10   |
| 1   | A     | 302 | SER  | C-N-CA     | -6.71 | 104.91      | 121.70   |
| 1   | A     | 75  | SER  | CB-CA-C    | 6.71  | 122.84      | 110.10   |
| 1   | A     | 152 | VAL  | CA-C-O     | -6.68 | 106.08      | 120.10   |
| 1   | A     | 350 | LEU  | CA-CB-CG   | 6.63  | 130.56      | 115.30   |
| 1   | A     | 214 | ALA  | C-N-CA     | -6.57 | 108.51      | 122.30   |
| 1   | A     | 155 | ILE  | CA-CB-CG1  | 6.57  | 123.47      | 111.00   |
| 1   | A     | 28  | VAL  | CG1-CB-CG2 | 6.52  | 121.33      | 110.90   |
| 1   | A     | 234 | GLU  | CG-CD-OE2  | -6.42 | 105.45      | 118.30   |
| 1   | A     | 350 | LEU  | N-CA-C     | 6.42  | 128.34      | 111.00   |
| 1   | A     | 369 | ARG  | NE-CZ-NH2  | 6.42  | 123.51      | 120.30   |
| 1   | A     | 27  | GLU  | N-CA-CB    | -6.42 | 99.04       | 110.60   |
| 1   | A     | 122 | THR  | C-N-CA     | 6.41  | 137.73      | 121.70   |
| 1   | A     | 215 | GLY  | C-N-CA     | -6.40 | 105.69      | 121.70   |
| 1   | A     | 152 | VAL  | N-CA-CB    | -6.39 | 97.44       | 111.50   |
| 1   | A     | 26  | VAL  | CA-C-N     | -6.38 | 103.16      | 117.20   |
| 1   | A     | 306 | MET  | CA-CB-CG   | -6.38 | 102.46      | 113.30   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 194 | THR  | N-CA-CB    | 6.38  | 122.41      | 110.30   |
| 1   | A     | 284 | GLU  | CB-CA-C    | -6.36 | 97.67       | 110.40   |
| 1   | A     | 301 | LEU  | N-CA-CB    | 6.34  | 123.08      | 110.40   |
| 1   | A     | 311 | GLY  | N-CA-C     | 6.34  | 128.95      | 113.10   |
| 1   | A     | 144 | SER  | CB-CA-C    | 6.34  | 122.14      | 110.10   |
| 1   | A     | 28  | VAL  | CA-C-N     | 6.31  | 131.08      | 117.20   |
| 1   | A     | 356 | ASN  | CA-C-N     | 6.30  | 131.05      | 117.20   |
| 1   | A     | 325 | LYS  | N-CA-CB    | 6.29  | 121.92      | 110.60   |
| 1   | A     | 312 | ARG  | NE-CZ-NH1  | -6.28 | 117.16      | 120.30   |
| 1   | A     | 315 | LYS  | CB-CA-C    | 6.24  | 122.87      | 110.40   |
| 1   | A     | 90  | ILE  | CG1-CB-CG2 | -6.21 | 97.73       | 111.40   |
| 1   | A     | 18  | LYS  | O-C-N      | 6.19  | 132.61      | 122.70   |
| 1   | A     | 219 | ILE  | N-CA-CB    | 6.18  | 125.01      | 110.80   |
| 1   | A     | 54  | SER  | CA-C-O     | -6.17 | 107.15      | 120.10   |
| 1   | A     | 248 | LYS  | N-CA-CB    | 6.16  | 121.68      | 110.60   |
| 1   | A     | 300 | ASN  | CA-CB-CG   | -6.14 | 99.88       | 113.40   |
| 1   | A     | 304 | ASN  | OD1-CG-ND2 | 6.14  | 136.03      | 121.90   |
| 1   | A     | 3   | ALA  | CB-CA-C    | -6.14 | 100.90      | 110.10   |
| 1   | A     | 161 | ASP  | CB-CG-OD2  | 6.14  | 123.82      | 118.30   |
| 1   | A     | 14  | LEU  | N-CA-CB    | 6.12  | 122.65      | 110.40   |
| 1   | A     | 365 | GLY  | N-CA-C     | 6.12  | 128.41      | 113.10   |
| 1   | A     | 104 | LYS  | CA-C-O     | -6.12 | 107.25      | 120.10   |
| 1   | A     | 109 | ASN  | CB-CG-ND2  | 6.12  | 131.39      | 116.70   |
| 1   | A     | 193 | SER  | N-CA-CB    | -6.11 | 101.33      | 110.50   |
| 1   | A     | 184 | VAL  | N-CA-C     | 6.11  | 127.49      | 111.00   |
| 1   | A     | 59  | THR  | CA-CB-OG1  | -6.07 | 96.24       | 109.00   |
| 1   | A     | 332 | VAL  | CA-C-O     | 6.05  | 132.81      | 120.10   |
| 1   | A     | 132 | CYS  | N-CA-CB    | 6.04  | 121.47      | 110.60   |
| 1   | A     | 182 | SER  | CA-C-N     | -6.04 | 103.91      | 117.20   |
| 1   | A     | 301 | LEU  | CA-C-N     | -6.03 | 103.92      | 117.20   |
| 1   | A     | 82  | THR  | N-CA-C     | 6.02  | 127.26      | 111.00   |
| 1   | A     | 16  | GLU  | CA-C-O     | 6.01  | 132.72      | 120.10   |
| 1   | A     | 169 | VAL  | CA-CB-CG1  | 6.01  | 119.91      | 110.90   |
| 1   | A     | 194 | THR  | N-CA-C     | -5.99 | 94.82       | 111.00   |
| 1   | A     | 285 | ALA  | O-C-N      | 5.99  | 132.28      | 122.70   |
| 1   | A     | 141 | LEU  | CA-CB-CG   | 5.96  | 129.00      | 115.30   |
| 1   | A     | 6   | VAL  | N-CA-CB    | -5.95 | 98.41       | 111.50   |
| 1   | A     | 169 | VAL  | CG1-CB-CG2 | -5.94 | 101.40      | 110.90   |
| 1   | A     | 43  | THR  | CB-CA-C    | -5.92 | 95.63       | 111.60   |
| 1   | A     | 71  | GLY  | C-N-CA     | 5.91  | 136.47      | 121.70   |
| 1   | A     | 238 | THR  | O-C-N      | 5.90  | 132.14      | 122.70   |
| 1   | A     | 75  | SER  | CA-C-N     | 5.88  | 130.13      | 117.20   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | A     | 14  | LEU  | CA-C-N    | -5.87 | 104.29      | 117.20   |
| 1   | A     | 78  | GLU  | CA-CB-CG  | 5.86  | 126.30      | 113.40   |
| 1   | A     | 340 | PHE  | CA-C-O    | -5.85 | 107.82      | 120.10   |
| 1   | A     | 246 | TYR  | CB-CA-C   | -5.83 | 98.75       | 110.40   |
| 1   | A     | 145 | THR  | CB-CA-C   | 5.82  | 127.32      | 111.60   |
| 1   | A     | 272 | LEU  | CB-CA-C   | 5.80  | 121.23      | 110.20   |
| 1   | A     | 361 | LEU  | CA-CB-CG  | 5.77  | 128.57      | 115.30   |
| 1   | A     | 271 | ARG  | CG-CD-NE  | -5.76 | 99.70       | 111.80   |
| 1   | A     | 176 | PHE  | CA-C-O    | -5.75 | 108.03      | 120.10   |
| 1   | A     | 361 | LEU  | CB-CA-C   | 5.75  | 121.12      | 110.20   |
| 1   | A     | 99  | LYS  | N-CA-CB   | 5.73  | 120.91      | 110.60   |
| 1   | A     | 108 | GLY  | O-C-N     | 5.73  | 131.86      | 122.70   |
| 1   | A     | 106 | PRO  | CA-C-N    | 5.72  | 129.78      | 117.20   |
| 1   | A     | 267 | GLU  | CG-CD-OE2 | -5.71 | 106.88      | 118.30   |
| 1   | A     | 140 | PHE  | CA-C-N    | -5.70 | 104.65      | 117.20   |
| 1   | A     | 315 | LYS  | N-CA-CB   | -5.70 | 100.34      | 110.60   |
| 1   | A     | 133 | ARG  | NE-CZ-NH2 | 5.69  | 123.14      | 120.30   |
| 1   | A     | 308 | LEU  | CA-C-O    | -5.68 | 108.17      | 120.10   |
| 1   | A     | 108 | GLY  | N-CA-C    | -5.67 | 98.91       | 113.10   |
| 1   | A     | 116 | LEU  | O-C-N     | 5.65  | 131.75      | 122.70   |
| 1   | A     | 117 | SER  | CA-C-O    | -5.65 | 108.24      | 120.10   |
| 1   | A     | 167 | GLU  | CB-CG-CD  | 5.65  | 129.44      | 114.20   |
| 1   | A     | 84  | ARG  | NE-CZ-NH2 | 5.64  | 123.12      | 120.30   |
| 1   | A     | 138 | HIS  | CB-CA-C   | -5.64 | 99.11       | 110.40   |
| 1   | A     | 91  | PRO  | CA-C-N    | 5.63  | 129.58      | 117.20   |
| 1   | A     | 212 | LYS  | CA-CB-CG  | 5.62  | 125.76      | 113.40   |
| 1   | A     | 215 | GLY  | N-CA-C    | -5.61 | 99.08       | 113.10   |
| 1   | A     | 1   | SER  | CA-C-N    | -5.59 | 104.91      | 117.20   |
| 1   | A     | 293 | GLY  | CA-C-N    | -5.58 | 104.92      | 117.20   |
| 1   | A     | 193 | SER  | CA-C-O    | 5.58  | 131.81      | 120.10   |
| 1   | A     | 16  | GLU  | CA-CB-CG  | -5.57 | 101.14      | 113.40   |
| 1   | A     | 370 | THR  | O-C-N     | 5.56  | 131.60      | 122.70   |
| 1   | A     | 155 | ILE  | CB-CA-C   | 5.56  | 122.72      | 111.60   |
| 1   | A     | 78  | GLU  | N-CA-C    | -5.54 | 96.04       | 111.00   |
| 1   | A     | 150 | THR  | CA-CB-CG2 | 5.54  | 120.16      | 112.40   |
| 1   | A     | 328 | VAL  | CA-CB-CG2 | 5.53  | 119.20      | 110.90   |
| 1   | A     | 113 | LYS  | CB-CA-C   | -5.53 | 99.35       | 110.40   |
| 1   | A     | 295 | PRO  | O-C-N     | 5.51  | 131.57      | 121.10   |
| 1   | A     | 27  | GLU  | CG-CD-OE2 | -5.50 | 107.31      | 118.30   |
| 1   | A     | 264 | PHE  | CB-CG-CD2 | -5.49 | 116.96      | 120.80   |
| 1   | A     | 337 | ALA  | C-N-CA    | 5.49  | 135.42      | 121.70   |
| 1   | A     | 153 | ASP  | N-CA-CB   | 5.49  | 120.48      | 110.60   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 140 | PHE  | O-C-N      | 5.46  | 131.44      | 122.70   |
| 1   | A     | 75  | SER  | CA-C-O     | -5.46 | 108.63      | 120.10   |
| 1   | A     | 249 | PRO  | O-C-N      | 5.46  | 131.43      | 122.70   |
| 1   | A     | 124 | GLN  | CA-CB-CG   | 5.45  | 125.38      | 113.40   |
| 1   | A     | 28  | VAL  | N-CA-CB    | -5.43 | 99.56       | 111.50   |
| 1   | A     | 3   | ALA  | C-N-CA     | 5.41  | 133.66      | 122.30   |
| 1   | A     | 323 | LYS  | CD-CE-NZ   | 5.39  | 124.10      | 111.70   |
| 1   | A     | 28  | VAL  | CA-C-O     | -5.39 | 108.78      | 120.10   |
| 1   | A     | 370 | THR  | CA-C-N     | -5.38 | 105.36      | 117.20   |
| 1   | A     | 89  | VAL  | CA-CB-CG1  | 5.37  | 118.96      | 110.90   |
| 1   | A     | 194 | THR  | CA-CB-CG2  | 5.37  | 119.92      | 112.40   |
| 1   | A     | 80  | VAL  | CA-CB-CG2  | 5.37  | 118.95      | 110.90   |
| 1   | A     | 50  | ASP  | CB-CG-OD2  | -5.36 | 113.48      | 118.30   |
| 1   | A     | 264 | PHE  | CB-CA-C    | -5.36 | 99.68       | 110.40   |
| 1   | A     | 300 | ASN  | C-N-CA     | 5.35  | 135.08      | 121.70   |
| 1   | A     | 144 | SER  | N-CA-C     | -5.35 | 96.55       | 111.00   |
| 1   | A     | 286 | TYR  | O-C-N      | -5.34 | 114.12      | 123.20   |
| 1   | A     | 363 | ARG  | CB-CG-CD   | 5.34  | 125.49      | 111.60   |
| 1   | A     | 290 | VAL  | O-C-N      | 5.33  | 131.24      | 122.70   |
| 1   | A     | 216 | ALA  | C-N-CA     | 5.32  | 134.99      | 121.70   |
| 1   | A     | 259 | ASN  | O-C-N      | 5.32  | 132.24      | 123.20   |
| 1   | A     | 223 | ASP  | CB-CG-OD1  | -5.30 | 113.53      | 118.30   |
| 1   | A     | 212 | LYS  | CB-CG-CD   | -5.28 | 97.87       | 111.60   |
| 1   | A     | 292 | VAL  | CA-C-O     | 5.28  | 131.18      | 120.10   |
| 1   | A     | 202 | GLY  | CA-C-O     | -5.27 | 111.12      | 120.60   |
| 1   | A     | 99  | LYS  | CB-CA-C    | -5.27 | 99.87       | 110.40   |
| 1   | A     | 296 | PRO  | O-C-N      | 5.26  | 131.12      | 122.70   |
| 1   | A     | 54  | SER  | N-CA-C     | 5.26  | 125.20      | 111.00   |
| 1   | A     | 127 | THR  | N-CA-CB    | -5.26 | 100.31      | 110.30   |
| 1   | A     | 220 | ILE  | N-CA-C     | -5.25 | 96.81       | 111.00   |
| 1   | A     | 50  | ASP  | CB-CA-C    | -5.23 | 99.94       | 110.40   |
| 1   | A     | 37  | ARG  | NH1-CZ-NH2 | 5.23  | 125.15      | 119.40   |
| 1   | A     | 234 | GLU  | CA-C-O     | -5.22 | 109.13      | 120.10   |
| 1   | A     | 279 | LEU  | N-CA-CB    | 5.22  | 120.84      | 110.40   |
| 1   | A     | 326 | ASP  | CA-C-O     | -5.22 | 109.14      | 120.10   |
| 1   | A     | 37  | ARG  | CB-CA-C    | 5.21  | 120.83      | 110.40   |
| 1   | A     | 239 | GLU  | CB-CA-C    | -5.21 | 99.97       | 110.40   |
| 1   | A     | 370 | THR  | CA-CB-OG1  | -5.20 | 98.07       | 109.00   |
| 1   | A     | 295 | PRO  | CA-CB-CG   | -5.20 | 94.12       | 104.00   |
| 1   | A     | 125 | ASP  | OD1-CG-OD2 | -5.18 | 113.47      | 123.30   |
| 1   | A     | 200 | LEU  | CB-CA-C    | 5.17  | 120.02      | 110.20   |
| 1   | A     | 278 | ALA  | N-CA-CB    | 5.16  | 117.32      | 110.10   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | A     | 182 | SER  | O-C-N     | 5.15  | 130.94      | 122.70   |
| 1   | A     | 112 | LEU  | CB-CG-CD1 | 5.15  | 119.75      | 111.00   |
| 1   | A     | 140 | PHE  | CA-CB-CG  | 5.14  | 126.24      | 113.90   |
| 1   | A     | 142 | GLY  | N-CA-C    | -5.13 | 100.26      | 113.10   |
| 1   | A     | 143 | THR  | CB-CA-C   | 5.13  | 125.46      | 111.60   |
| 1   | A     | 342 | LEU  | N-CA-CB   | -5.13 | 100.15      | 110.40   |
| 1   | A     | 360 | ASP  | CB-CG-OD1 | -5.11 | 113.70      | 118.30   |
| 1   | A     | 332 | VAL  | C-N-CA    | 5.10  | 134.46      | 121.70   |
| 1   | A     | 63  | VAL  | CA-CB-CG2 | 5.09  | 118.53      | 110.90   |
| 1   | A     | 100 | CYS  | O-C-N     | -5.09 | 114.56      | 122.70   |
| 1   | A     | 271 | ARG  | CD-NE-CZ  | -5.06 | 116.52      | 123.60   |
| 1   | A     | 283 | GLN  | N-CA-CB   | -5.04 | 101.53      | 110.60   |
| 1   | A     | 167 | GLU  | CG-CD-OE1 | 5.03  | 128.36      | 118.30   |
| 1   | A     | 320 | GLY  | N-CA-C    | 5.03  | 125.67      | 113.10   |
| 1   | A     | 215 | GLY  | O-C-N     | 5.02  | 130.74      | 122.70   |
| 1   | A     | 107 | GLU  | N-CA-C    | -5.01 | 97.46       | 111.00   |
| 1   | A     | 213 | ALA  | CB-CA-C   | 5.01  | 117.62      | 110.10   |
| 1   | A     | 318 | ILE  | CA-CB-CG2 | 5.00  | 120.90      | 110.90   |

There are no chirality outliers.

All (4) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | A     | 129 | ARG  | Sidechain |
| 1   | A     | 271 | ARG  | Sidechain |
| 1   | A     | 363 | ARG  | Sidechain |
| 1   | A     | 37  | ARG  | Sidechain |

## 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     | 2784  | 0        | 2788     | 603     | 730          |
| 2   | A     | 2     | 0        | 0        | 0       | 1            |
| 3   | A     | 184   | 0        | 92       | 9       | 145          |
| All | All   | 2970  | 0        | 2880     | 604     | 734          |

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 105.

All (604) 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:96:GLN:N     | 1:A:96:GLN:CA    | 1.70                     | 1.55              |
| 1:A:45:ILE:HD12  | 1:A:359:PHE:CE1  | 1.69                     | 1.27              |
| 1:A:15:TRP:O     | 1:A:16:GLU:HG3   | 1.45                     | 1.16              |
| 1:A:5:LYS:O      | 1:A:6:VAL:O      | 1.62                     | 1.14              |
| 1:A:14:LEU:HB2   | 1:A:21:PHE:HE2   | 1.08                     | 1.13              |
| 1:A:15:TRP:C     | 1:A:16:GLU:HG3   | 1.66                     | 1.13              |
| 1:A:347:THR:HG21 | 1:A:368:ILE:H    | 1.11                     | 1.12              |
| 1:A:110:PHE:HE1  | 1:A:116:LEU:HD13 | 1.06                     | 1.12              |
| 1:A:76:ILE:HG13  | 1:A:80:VAL:HG22  | 1.27                     | 1.12              |
| 1:A:19:LYS:HD3   | 3:A:381:NTN:NI1  | 1.51                     | 1.11              |
| 1:A:194:THR:HG22 | 1:A:262:VAL:HG12 | 1.23                     | 1.11              |
| 1:A:125:ASP:OD1  | 1:A:127:THR:HB   | 1.49                     | 1.11              |
| 1:A:101:ARG:HH11 | 1:A:101:ARG:HG2  | 1.08                     | 1.10              |
| 1:A:272:LEU:HD22 | 1:A:301:LEU:HB3  | 1.15                     | 1.10              |
| 1:A:218:ARG:HH11 | 1:A:218:ARG:HG3  | 0.97                     | 1.10              |
| 1:A:11:ALA:HB2   | 1:A:147:SER:HB2  | 1.35                     | 1.08              |
| 1:A:224:ILE:HA   | 1:A:242:ASN:ND2  | 1.70                     | 1.07              |
| 1:A:229:PHE:O    | 1:A:232:ALA:HB3  | 1.54                     | 1.07              |
| 1:A:113:LYS:O    | 1:A:113:LYS:HG3  | 1.52                     | 1.05              |
| 1:A:194:THR:CG2  | 1:A:262:VAL:HG12 | 1.87                     | 1.03              |
| 1:A:194:THR:O    | 1:A:263:ASP:HB2  | 1.56                     | 1.03              |
| 1:A:110:PHE:CE1  | 1:A:116:LEU:HD13 | 1.93                     | 1.02              |
| 1:A:11:ALA:CB    | 1:A:147:SER:HB2  | 1.89                     | 1.02              |
| 1:A:121:GLY:O    | 1:A:139:HIS:N    | 1.93                     | 1.01              |
| 1:A:304:ASN:O    | 1:A:307:LEU:HD12 | 1.61                     | 1.01              |
| 1:A:90:ILE:HG12  | 1:A:160:ILE:HG21 | 1.41                     | 1.01              |
| 1:A:45:ILE:HD12  | 1:A:359:PHE:HE1  | 1.09                     | 1.00              |
| 1:A:26:VAL:HG12  | 1:A:131:THR:O    | 1.61                     | 1.00              |
| 1:A:200:LEU:HD11 | 1:A:208:ILE:HD11 | 1.44                     | 0.99              |
| 1:A:224:ILE:HA   | 1:A:242:ASN:HD22 | 1.20                     | 0.99              |
| 1:A:272:LEU:HD11 | 1:A:299:GLN:O    | 1.63                     | 0.99              |
| 1:A:334:ASP:HB3  | 1:A:339:LYS:HD2  | 1.45                     | 0.99              |
| 1:A:233:LYS:HA   | 1:A:237:ALA:HB3  | 1.43                     | 0.98              |
| 1:A:205:LEU:O    | 1:A:209:MET:HB2  | 1.63                     | 0.98              |
| 1:A:14:LEU:HB2   | 1:A:21:PHE:CE2   | 1.98                     | 0.98              |
| 1:A:30:PRO:HA    | 1:A:37:ARG:NH1   | 1.78                     | 0.98              |
| 1:A:269:ILE:HG23 | 1:A:271:ARG:HG3  | 1.46                     | 0.97              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:269:ILE:CG2  | 1:A:271:ARG:HG3  | 1.94                     | 0.97              |
| 1:A:272:LEU:CD2  | 1:A:301:LEU:HB3  | 1.95                     | 0.97              |
| 1:A:110:PHE:HE1  | 1:A:116:LEU:CD1  | 1.77                     | 0.97              |
| 1:A:60:PRO:C     | 1:A:61:LEU:HD23  | 1.85                     | 0.97              |
| 1:A:15:TRP:O     | 1:A:16:GLU:CG    | 2.13                     | 0.96              |
| 1:A:187:ALA:O    | 1:A:189:VAL:N    | 1.97                     | 0.96              |
| 1:A:269:ILE:HG22 | 1:A:271:ARG:H    | 1.28                     | 0.96              |
| 1:A:69:ALA:HB3   | 1:A:145:THR:CG2  | 1.95                     | 0.96              |
| 1:A:129:ARG:HG3  | 1:A:129:ARG:HH11 | 1.25                     | 0.96              |
| 1:A:64:ILE:HD12  | 1:A:130:PHE:CE1  | 2.00                     | 0.96              |
| 1:A:346:ILE:HD12 | 1:A:371:ILE:HD13 | 1.47                     | 0.95              |
| 1:A:218:ARG:NH2  | 1:A:239:GLU:OE2  | 1.99                     | 0.95              |
| 1:A:355:ILE:HG12 | 1:A:372:LEU:HD21 | 1.43                     | 0.95              |
| 1:A:288:VAL:HG23 | 1:A:313:THR:HB   | 1.49                     | 0.95              |
| 1:A:218:ARG:CG   | 1:A:218:ARG:HH11 | 1.80                     | 0.94              |
| 1:A:218:ARG:NH1  | 1:A:218:ARG:HG3  | 1.68                     | 0.94              |
| 1:A:346:ILE:HD12 | 1:A:371:ILE:CD1  | 1.97                     | 0.94              |
| 1:A:132:CYS:C    | 1:A:134:GLY:H    | 1.69                     | 0.94              |
| 1:A:200:LEU:HB2  | 1:A:223:ASP:HB2  | 1.51                     | 0.93              |
| 1:A:73:VAL:HG23  | 1:A:87:ASP:O     | 1.67                     | 0.93              |
| 1:A:15:TRP:C     | 1:A:16:GLU:CG    | 2.37                     | 0.93              |
| 1:A:3:ALA:HB1    | 1:A:5:LYS:H      | 1.33                     | 0.92              |
| 1:A:123:MET:HE1  | 1:A:151:VAL:HG12 | 1.48                     | 0.91              |
| 1:A:45:ILE:HD12  | 1:A:359:PHE:CD1  | 2.06                     | 0.91              |
| 1:A:101:ARG:NH1  | 1:A:101:ARG:HG2  | 1.82                     | 0.91              |
| 1:A:90:ILE:CG1   | 1:A:160:ILE:HG21 | 2.00                     | 0.91              |
| 1:A:272:LEU:HD21 | 1:A:300:ASN:O    | 1.71                     | 0.91              |
| 1:A:52:VAL:CG1   | 1:A:59:THR:HG22  | 2.01                     | 0.90              |
| 1:A:101:ARG:HH11 | 1:A:101:ARG:CG   | 1.83                     | 0.90              |
| 1:A:82:THR:HG22  | 1:A:83:VAL:HG22  | 1.51                     | 0.89              |
| 1:A:200:LEU:O    | 1:A:228:LYS:CG   | 2.21                     | 0.89              |
| 1:A:347:THR:HG21 | 1:A:368:ILE:N    | 1.85                     | 0.88              |
| 1:A:358:GLY:O    | 1:A:361:LEU:HD12 | 1.72                     | 0.88              |
| 1:A:200:LEU:O    | 1:A:228:LYS:HG2  | 1.73                     | 0.88              |
| 1:A:265:SER:OG   | 1:A:289:SER:OG   | 1.69                     | 0.88              |
| 1:A:95:PRO:HB3   | 1:A:155:ILE:HD13 | 1.54                     | 0.88              |
| 1:A:346:ILE:HG23 | 1:A:371:ILE:HD13 | 1.54                     | 0.87              |
| 1:A:88:LYS:O     | 1:A:89:VAL:HG23  | 1.72                     | 0.87              |
| 1:A:51:HIS:CE1   | 1:A:296:PRO:HD3  | 2.09                     | 0.87              |
| 1:A:69:ALA:HB3   | 1:A:145:THR:HG22 | 1.57                     | 0.87              |
| 1:A:231:LYS:O    | 1:A:235:VAL:HG13 | 1.76                     | 0.86              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:198:PHE:CE1  | 1:A:222:VAL:HG21 | 2.10                     | 0.86              |
| 1:A:334:ASP:CB   | 1:A:339:LYS:HD2  | 2.04                     | 0.86              |
| 1:A:74:GLU:OE2   | 1:A:75:SER:HB2   | 1.76                     | 0.85              |
| 1:A:110:PHE:CE1  | 1:A:116:LEU:CD1  | 2.57                     | 0.85              |
| 1:A:38:ILE:HD11  | 1:A:152:VAL:HG21 | 1.58                     | 0.85              |
| 1:A:284:GLU:O    | 1:A:310:SER:HB2  | 1.75                     | 0.85              |
| 1:A:42:ALA:O     | 1:A:69:ALA:HB1   | 1.77                     | 0.85              |
| 1:A:194:THR:HG22 | 1:A:262:VAL:CG1  | 2.06                     | 0.85              |
| 1:A:132:CYS:O    | 1:A:134:GLY:N    | 2.10                     | 0.85              |
| 1:A:137:ILE:N    | 1:A:137:ILE:HD13 | 1.91                     | 0.85              |
| 1:A:43:THR:CG2   | 1:A:69:ALA:HB2   | 2.06                     | 0.85              |
| 1:A:113:LYS:CG   | 1:A:113:LYS:O    | 2.20                     | 0.84              |
| 1:A:196:ALA:HB2  | 1:A:262:VAL:HG21 | 1.60                     | 0.83              |
| 1:A:129:ARG:CD   | 1:A:151:VAL:HG11 | 2.09                     | 0.83              |
| 1:A:283:GLN:HE22 | 1:A:285:ALA:CB   | 1.91                     | 0.83              |
| 1:A:348:HIS:ND1  | 1:A:361:LEU:HD22 | 1.94                     | 0.83              |
| 1:A:99:LYS:HG3   | 1:A:104:LYS:HE3  | 1.61                     | 0.83              |
| 1:A:217:ALA:O    | 1:A:238:THR:HG21 | 1.80                     | 0.82              |
| 1:A:49:ASP:O     | 1:A:52:VAL:HG23  | 1.78                     | 0.82              |
| 1:A:90:ILE:HG12  | 1:A:160:ILE:CG2  | 2.10                     | 0.81              |
| 1:A:333:ALA:O    | 1:A:337:ALA:N    | 2.13                     | 0.81              |
| 1:A:100:CYS:O    | 1:A:101:ARG:C    | 2.14                     | 0.81              |
| 1:A:21:PHE:HB2   | 1:A:356:ASN:HD21 | 1.44                     | 0.81              |
| 1:A:348:HIS:O    | 1:A:370:THR:OG1  | 1.98                     | 0.81              |
| 1:A:35:GLU:O     | 1:A:36:VAL:HG23  | 1.80                     | 0.81              |
| 1:A:197:VAL:HG21 | 1:A:208:ILE:HG12 | 1.62                     | 0.81              |
| 1:A:45:ILE:CD1   | 1:A:359:PHE:HE1  | 1.93                     | 0.81              |
| 1:A:332:VAL:O    | 1:A:335:PHE:HB3  | 1.80                     | 0.81              |
| 1:A:283:GLN:NE2  | 1:A:285:ALA:HB3  | 1.96                     | 0.81              |
| 1:A:204:GLY:O    | 1:A:207:VAL:HG12 | 1.81                     | 0.80              |
| 1:A:84:ARG:O     | 1:A:87:ASP:HB2   | 1.80                     | 0.80              |
| 1:A:35:GLU:OE1   | 1:A:129:ARG:NE   | 2.14                     | 0.80              |
| 1:A:283:GLN:HE22 | 1:A:285:ALA:HB3  | 1.46                     | 0.80              |
| 1:A:71:GLY:O     | 1:A:166:LEU:HD11 | 1.81                     | 0.80              |
| 1:A:129:ARG:HD3  | 1:A:151:VAL:HG11 | 1.64                     | 0.80              |
| 1:A:194:THR:OG1  | 1:A:218:ARG:HB3  | 1.82                     | 0.80              |
| 1:A:76:ILE:HG13  | 1:A:80:VAL:CG2   | 2.09                     | 0.80              |
| 1:A:176:PHE:CD1  | 1:A:176:PHE:O    | 2.36                     | 0.79              |
| 1:A:269:ILE:HG22 | 1:A:271:ARG:N    | 1.97                     | 0.79              |
| 1:A:51:HIS:ND1   | 1:A:296:PRO:CD   | 2.46                     | 0.79              |
| 1:A:256:GLU:O    | 1:A:259:ASN:N    | 2.16                     | 0.79              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:340:PHE:O    | 1:A:340:PHE:CD2  | 2.36                     | 0.79              |
| 1:A:171:LEU:HD22 | 1:A:346:ILE:HD11 | 1.65                     | 0.78              |
| 1:A:233:LYS:CA   | 1:A:237:ALA:HB3  | 2.13                     | 0.78              |
| 1:A:69:ALA:CB    | 1:A:145:THR:HG22 | 2.11                     | 0.78              |
| 1:A:369:ARG:HH11 | 1:A:369:ARG:HB2  | 1.46                     | 0.78              |
| 1:A:161:ASP:O    | 1:A:163:ALA:N    | 2.17                     | 0.77              |
| 1:A:11:ALA:HA    | 1:A:147:SER:HA   | 1.65                     | 0.77              |
| 1:A:64:ILE:HD11  | 1:A:130:PHE:CD1  | 2.20                     | 0.77              |
| 1:A:171:LEU:HD11 | 1:A:369:ARG:HG2  | 1.65                     | 0.77              |
| 1:A:229:PHE:HD1  | 1:A:240:CYS:HG   | 1.31                     | 0.77              |
| 1:A:132:CYS:C    | 1:A:134:GLY:N    | 2.38                     | 0.77              |
| 1:A:348:HIS:CE1  | 1:A:367:SER:HB3  | 2.20                     | 0.76              |
| 1:A:129:ARG:NH1  | 1:A:129:ARG:HG3  | 1.95                     | 0.76              |
| 1:A:304:ASN:ND2  | 1:A:305:PRO:HD2  | 1.99                     | 0.76              |
| 1:A:355:ILE:CG1  | 1:A:372:LEU:HD21 | 2.16                     | 0.75              |
| 1:A:95:PRO:C     | 1:A:96:GLN:CA    | 2.54                     | 0.75              |
| 1:A:279:LEU:HD11 | 1:A:308:LEU:HD23 | 1.68                     | 0.75              |
| 1:A:218:ARG:CZ   | 1:A:239:GLU:OE2  | 2.34                     | 0.75              |
| 1:A:51:HIS:ND1   | 1:A:296:PRO:HD3  | 2.00                     | 0.75              |
| 1:A:176:PHE:C    | 1:A:176:PHE:CD1  | 2.59                     | 0.75              |
| 1:A:64:ILE:CD1   | 1:A:130:PHE:CE1  | 2.70                     | 0.74              |
| 1:A:43:THR:HG22  | 1:A:69:ALA:HB2   | 1.68                     | 0.74              |
| 1:A:74:GLU:HG2   | 1:A:149:TYR:HE1  | 1.52                     | 0.74              |
| 1:A:349:VAL:HG13 | 1:A:371:ILE:HG22 | 1.69                     | 0.74              |
| 1:A:64:ILE:CD1   | 1:A:130:PHE:CD1  | 2.71                     | 0.73              |
| 1:A:122:THR:HG21 | 1:A:126:GLY:HA2  | 1.69                     | 0.73              |
| 1:A:274:THR:HA   | 1:A:277:THR:HB   | 1.68                     | 0.73              |
| 1:A:224:ILE:CA   | 1:A:242:ASN:ND2  | 2.50                     | 0.73              |
| 1:A:229:PHE:O    | 1:A:232:ALA:CB   | 2.36                     | 0.73              |
| 1:A:95:PRO:HB3   | 1:A:155:ILE:CD1  | 2.17                     | 0.72              |
| 1:A:304:ASN:HD22 | 1:A:305:PRO:HD2  | 1.53                     | 0.72              |
| 1:A:111:CYS:C    | 1:A:113:LYS:H    | 1.93                     | 0.72              |
| 1:A:212:LYS:HE3  | 1:A:236:GLY:HA2  | 1.70                     | 0.72              |
| 1:A:16:GLU:O     | 1:A:19:LYS:HG3   | 1.89                     | 0.72              |
| 1:A:61:LEU:HD23  | 1:A:61:LEU:N     | 1.98                     | 0.72              |
| 1:A:110:PHE:CD1  | 1:A:318:ILE:HG21 | 2.24                     | 0.72              |
| 1:A:349:VAL:HG13 | 1:A:371:ILE:CG2  | 2.20                     | 0.72              |
| 1:A:204:GLY:CA   | 1:A:268:VAL:HG21 | 2.19                     | 0.72              |
| 1:A:267:GLU:OE2  | 1:A:275:MET:HG3  | 1.90                     | 0.72              |
| 1:A:369:ARG:NH1  | 1:A:369:ARG:HB2  | 2.04                     | 0.72              |
| 1:A:19:LYS:CD    | 3:A:381:NTN:NI1  | 2.37                     | 0.72              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:85:PRO:C     | 1:A:87:ASP:H     | 1.94                     | 0.72              |
| 1:A:209:MET:HE2  | 1:A:235:VAL:HB   | 1.72                     | 0.71              |
| 1:A:21:PHE:HB2   | 1:A:356:ASN:ND2  | 2.04                     | 0.71              |
| 1:A:369:ARG:HH11 | 1:A:369:ARG:CB   | 2.03                     | 0.71              |
| 1:A:52:VAL:HG11  | 1:A:59:THR:HG22  | 1.73                     | 0.71              |
| 1:A:15:TRP:O     | 1:A:16:GLU:CB    | 2.37                     | 0.71              |
| 1:A:171:LEU:CD2  | 1:A:346:ILE:HD11 | 2.21                     | 0.71              |
| 1:A:140:PHE:CE2  | 1:A:141:LEU:HD22 | 2.26                     | 0.70              |
| 1:A:272:LEU:CD1  | 1:A:299:GLN:O    | 2.39                     | 0.70              |
| 1:A:45:ILE:HG23  | 1:A:359:PHE:CE1  | 2.26                     | 0.70              |
| 1:A:82:THR:CG2   | 1:A:82:THR:O     | 2.40                     | 0.70              |
| 1:A:229:PHE:CD1  | 1:A:240:CYS:SG   | 2.85                     | 0.70              |
| 1:A:248:LYS:HB3  | 1:A:249:PRO:HD2  | 1.73                     | 0.70              |
| 1:A:154:GLU:HA   | 1:A:157:VAL:HG12 | 1.74                     | 0.69              |
| 1:A:132:CYS:N    | 1:A:135:LYS:O    | 2.24                     | 0.69              |
| 1:A:225:ASN:O    | 1:A:227:ASP:N    | 2.25                     | 0.69              |
| 1:A:264:PHE:HD2  | 1:A:288:VAL:HG12 | 1.57                     | 0.69              |
| 1:A:30:PRO:CA    | 1:A:37:ARG:NH1   | 2.55                     | 0.69              |
| 1:A:3:ALA:CB     | 1:A:5:LYS:HD2    | 2.22                     | 0.69              |
| 1:A:52:VAL:HG11  | 1:A:59:THR:CG2   | 2.22                     | 0.69              |
| 1:A:182:SER:HA   | 1:A:186:VAL:CG2  | 2.23                     | 0.69              |
| 1:A:365:GLY:O    | 1:A:367:SER:N    | 2.26                     | 0.69              |
| 1:A:82:THR:O     | 1:A:82:THR:HG23  | 1.93                     | 0.69              |
| 1:A:347:THR:HG22 | 1:A:369:ARG:H    | 1.55                     | 0.69              |
| 1:A:243:PRO:HG3  | 1:A:250:ILE:HD13 | 1.75                     | 0.69              |
| 1:A:273:ASP:OD1  | 1:A:273:ASP:N    | 2.26                     | 0.69              |
| 1:A:67:HIS:HA    | 1:A:143:THR:OG1  | 1.93                     | 0.69              |
| 1:A:319:PHE:O    | 1:A:321:GLY:N    | 2.25                     | 0.68              |
| 1:A:56:THR:HB    | 1:A:297:ASP:HB3  | 1.75                     | 0.68              |
| 1:A:13:VAL:N     | 1:A:22:SER:O     | 2.27                     | 0.68              |
| 1:A:264:PHE:CD2  | 1:A:288:VAL:HG12 | 2.29                     | 0.68              |
| 1:A:347:THR:CG2  | 1:A:368:ILE:H    | 1.99                     | 0.68              |
| 1:A:255:THR:O    | 1:A:260:GLY:N    | 2.25                     | 0.68              |
| 1:A:272:LEU:HD22 | 1:A:301:LEU:CB   | 2.09                     | 0.68              |
| 1:A:271:ARG:O    | 1:A:275:MET:HE3  | 1.93                     | 0.67              |
| 1:A:176:PHE:CG   | 1:A:176:PHE:O    | 2.47                     | 0.67              |
| 1:A:129:ARG:HD2  | 1:A:151:VAL:HG11 | 1.77                     | 0.67              |
| 1:A:96:GLN:N     | 1:A:96:GLN:C     | 2.47                     | 0.67              |
| 1:A:328:VAL:N    | 1:A:329:PRO:CD   | 2.58                     | 0.67              |
| 1:A:105:HIS:HD2  | 1:A:107:GLU:H    | 1.44                     | 0.66              |
| 1:A:304:ASN:HD22 | 1:A:305:PRO:CD   | 2.07                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:346:ILE:HD12 | 1:A:371:ILE:HD11 | 1.77                     | 0.66              |
| 1:A:83:VAL:HG12  | 1:A:87:ASP:OD2   | 1.94                     | 0.66              |
| 1:A:279:LEU:HD11 | 1:A:308:LEU:CD2  | 2.24                     | 0.66              |
| 1:A:30:PRO:HG2   | 1:A:30:PRO:O     | 1.93                     | 0.66              |
| 1:A:347:THR:CG2  | 1:A:368:ILE:N    | 2.57                     | 0.66              |
| 1:A:113:LYS:HG2  | 1:A:155:ILE:CD1  | 2.26                     | 0.66              |
| 1:A:204:GLY:HA3  | 1:A:268:VAL:HG21 | 1.78                     | 0.65              |
| 1:A:330:LYS:O    | 1:A:333:ALA:HB3  | 1.95                     | 0.65              |
| 1:A:204:GLY:HA2  | 1:A:207:VAL:HG12 | 1.77                     | 0.65              |
| 1:A:277:THR:O    | 1:A:277:THR:CG2  | 2.43                     | 0.65              |
| 1:A:69:ALA:O     | 1:A:91:PRO:HD2   | 1.96                     | 0.65              |
| 1:A:174:CYS:O    | 1:A:178:THR:HB   | 1.95                     | 0.65              |
| 1:A:243:PRO:HG3  | 1:A:250:ILE:CD1  | 2.26                     | 0.65              |
| 1:A:182:SER:HA   | 1:A:186:VAL:HG23 | 1.79                     | 0.65              |
| 1:A:219:ILE:HD13 | 1:A:236:GLY:O    | 1.97                     | 0.65              |
| 1:A:179:GLY:CA   | 1:A:203:VAL:HG13 | 2.26                     | 0.65              |
| 1:A:288:VAL:HG23 | 1:A:313:THR:CB   | 2.27                     | 0.64              |
| 1:A:323:LYS:O    | 1:A:327:SER:OG   | 2.09                     | 0.64              |
| 1:A:147:SER:OG   | 1:A:149:TYR:O    | 2.15                     | 0.64              |
| 1:A:41:VAL:CG2   | 1:A:166:LEU:HD12 | 2.27                     | 0.64              |
| 1:A:284:GLU:HB2  | 1:A:310:SER:CB   | 2.27                     | 0.64              |
| 1:A:41:VAL:HG21  | 1:A:166:LEU:HD12 | 1.78                     | 0.64              |
| 1:A:307:LEU:O    | 1:A:312:ARG:HD2  | 1.97                     | 0.64              |
| 1:A:329:PRO:HA   | 1:A:332:VAL:HG23 | 1.80                     | 0.64              |
| 1:A:24:GLU:OE2   | 1:A:132:CYS:SG   | 2.55                     | 0.64              |
| 1:A:262:VAL:O    | 1:A:282:CYS:HA   | 1.98                     | 0.64              |
| 1:A:172:ILE:HG22 | 1:A:328:VAL:HG13 | 1.81                     | 0.63              |
| 1:A:332:VAL:O    | 1:A:335:PHE:N    | 2.31                     | 0.63              |
| 1:A:65:ALA:O     | 1:A:146:PHE:HB2  | 1.98                     | 0.63              |
| 1:A:150:THR:OG1  | 1:A:151:VAL:N    | 2.31                     | 0.63              |
| 1:A:211:CYS:O    | 1:A:214:ALA:N    | 2.32                     | 0.63              |
| 1:A:171:LEU:C    | 1:A:173:GLY:H    | 2.00                     | 0.63              |
| 1:A:347:THR:O    | 1:A:348:HIS:CD2  | 2.52                     | 0.63              |
| 1:A:331:LEU:HD12 | 1:A:340:PHE:HZ   | 1.63                     | 0.62              |
| 1:A:50:ASP:OD1   | 1:A:363:ARG:NH1  | 2.32                     | 0.62              |
| 1:A:43:THR:HG23  | 1:A:69:ALA:HB2   | 1.80                     | 0.62              |
| 1:A:102:VAL:CG1  | 1:A:112:LEU:HD23 | 2.29                     | 0.62              |
| 1:A:219:ILE:HD12 | 1:A:238:THR:HG23 | 1.82                     | 0.62              |
| 1:A:348:HIS:HB2  | 1:A:370:THR:CB   | 2.30                     | 0.62              |
| 1:A:81:THR:OG1   | 1:A:82:THR:N     | 2.33                     | 0.62              |
| 1:A:258:SER:OG   | 1:A:261:GLY:CA   | 2.48                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:333:ALA:HA   | 1:A:336:MET:HB2  | 1.81                     | 0.62              |
| 1:A:218:ARG:NH2  | 1:A:239:GLU:CD   | 2.53                     | 0.62              |
| 1:A:250:ILE:HG12 | 1:A:254:LEU:HD23 | 1.82                     | 0.62              |
| 1:A:200:LEU:O    | 1:A:228:LYS:HG3  | 1.99                     | 0.61              |
| 1:A:343:ASP:O    | 1:A:346:ILE:N    | 2.33                     | 0.61              |
| 1:A:200:LEU:HB2  | 1:A:223:ASP:CB   | 2.29                     | 0.61              |
| 1:A:252:GLU:C    | 1:A:254:LEU:H    | 2.02                     | 0.61              |
| 1:A:92:LEU:HD21  | 1:A:328:VAL:HG21 | 1.82                     | 0.61              |
| 1:A:219:ILE:N    | 1:A:238:THR:OG1  | 2.32                     | 0.61              |
| 1:A:268:VAL:HG12 | 1:A:292:VAL:HG21 | 1.83                     | 0.61              |
| 1:A:83:VAL:O     | 1:A:84:ARG:HG2   | 2.01                     | 0.60              |
| 1:A:192:GLY:O    | 1:A:217:ALA:HB3  | 2.01                     | 0.60              |
| 1:A:194:THR:HG23 | 1:A:220:ILE:CD1  | 2.31                     | 0.60              |
| 1:A:95:PRO:HB2   | 1:A:111:CYS:HB3  | 1.81                     | 0.60              |
| 1:A:258:SER:OG   | 1:A:261:GLY:HA2  | 2.00                     | 0.60              |
| 3:A:381:NTN:H5   | 3:A:387:NTN:H4   | 1.82                     | 0.60              |
| 1:A:99:LYS:HG2   | 1:A:100:CYS:N    | 2.16                     | 0.60              |
| 1:A:284:GLU:HB2  | 1:A:310:SER:HB2  | 1.84                     | 0.60              |
| 1:A:110:PHE:HD1  | 1:A:318:ILE:HG21 | 1.64                     | 0.60              |
| 1:A:111:CYS:O    | 1:A:113:LYS:N    | 2.34                     | 0.60              |
| 1:A:288:VAL:HG22 | 1:A:313:THR:HG22 | 1.83                     | 0.60              |
| 1:A:90:ILE:CG1   | 1:A:160:ILE:CG2  | 2.77                     | 0.60              |
| 1:A:102:VAL:HG21 | 1:A:110:PHE:O    | 2.02                     | 0.59              |
| 1:A:198:PHE:HB2  | 1:A:266:PHE:O    | 2.03                     | 0.59              |
| 1:A:219:ILE:CD1  | 1:A:238:THR:HG23 | 2.33                     | 0.59              |
| 1:A:348:HIS:HB2  | 1:A:370:THR:HB   | 1.83                     | 0.59              |
| 1:A:288:VAL:CG2  | 1:A:313:THR:CG2  | 2.81                     | 0.59              |
| 1:A:343:ASP:OD2  | 1:A:343:ASP:N    | 2.35                     | 0.59              |
| 1:A:249:PRO:CB   | 1:A:251:GLN:HG3  | 2.32                     | 0.59              |
| 1:A:3:ALA:HB1    | 1:A:5:LYS:N      | 2.13                     | 0.58              |
| 1:A:129:ARG:HD2  | 1:A:151:VAL:CG1  | 2.32                     | 0.58              |
| 1:A:100:CYS:SG   | 1:A:103:CYS:HB2  | 2.44                     | 0.58              |
| 1:A:252:GLU:O    | 1:A:254:LEU:N    | 2.36                     | 0.58              |
| 1:A:277:THR:HG22 | 1:A:277:THR:O    | 2.02                     | 0.58              |
| 1:A:74:GLU:OE2   | 1:A:75:SER:CB    | 2.49                     | 0.58              |
| 1:A:105:HIS:CD2  | 1:A:107:GLU:H    | 2.21                     | 0.58              |
| 1:A:283:GLN:HE22 | 1:A:285:ALA:HB2  | 1.68                     | 0.58              |
| 1:A:229:PHE:HZ   | 1:A:242:ASN:HB2  | 1.68                     | 0.58              |
| 1:A:283:GLN:NE2  | 1:A:285:ALA:CB   | 2.61                     | 0.58              |
| 1:A:352:PHE:CD2  | 1:A:374:PHE:CZ   | 2.92                     | 0.58              |
| 1:A:64:ILE:HB    | 1:A:144:SER:HB3  | 1.85                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:292:VAL:HG12 | 1:A:293:GLY:N    | 2.18                     | 0.58              |
| 1:A:211:CYS:C    | 1:A:213:ALA:N    | 2.54                     | 0.57              |
| 1:A:267:GLU:HG3  | 1:A:275:MET:HA   | 1.86                     | 0.57              |
| 1:A:69:ALA:CB    | 1:A:145:THR:CG2  | 2.72                     | 0.57              |
| 1:A:267:GLU:OE2  | 1:A:275:MET:HE3  | 2.04                     | 0.57              |
| 1:A:60:PRO:O     | 1:A:61:LEU:HD23  | 2.04                     | 0.57              |
| 1:A:74:GLU:HG2   | 1:A:149:TYR:CE1  | 2.38                     | 0.57              |
| 1:A:122:THR:OG1  | 1:A:123:MET:N    | 2.28                     | 0.57              |
| 1:A:66:GLY:N     | 1:A:146:PHE:CD1  | 2.72                     | 0.57              |
| 1:A:65:ALA:C     | 1:A:146:PHE:HD1  | 2.08                     | 0.57              |
| 1:A:161:ASP:O    | 1:A:164:SER:OG   | 2.16                     | 0.57              |
| 1:A:327:SER:C    | 1:A:329:PRO:HD2  | 2.24                     | 0.57              |
| 1:A:347:THR:HG23 | 1:A:367:SER:HB2  | 1.87                     | 0.57              |
| 1:A:96:GLN:C     | 1:A:98:GLY:H     | 2.07                     | 0.57              |
| 1:A:90:ILE:CD1   | 1:A:169:VAL:O    | 2.53                     | 0.57              |
| 1:A:92:LEU:HD21  | 1:A:328:VAL:CG2  | 2.34                     | 0.57              |
| 1:A:85:PRO:O     | 1:A:87:ASP:N     | 2.38                     | 0.57              |
| 1:A:113:LYS:HG2  | 1:A:155:ILE:HD11 | 1.85                     | 0.57              |
| 1:A:273:ASP:O    | 1:A:276:VAL:HG12 | 2.05                     | 0.56              |
| 1:A:96:GLN:N     | 1:A:96:GLN:CB    | 2.42                     | 0.56              |
| 1:A:35:GLU:O     | 1:A:36:VAL:CG2   | 2.51                     | 0.56              |
| 1:A:14:LEU:HD13  | 1:A:16:GLU:H     | 1.70                     | 0.56              |
| 1:A:70:ALA:HB1   | 1:A:166:LEU:HD22 | 1.86                     | 0.56              |
| 1:A:250:ILE:HA   | 1:A:253:VAL:HG13 | 1.87                     | 0.56              |
| 1:A:332:VAL:O    | 1:A:335:PHE:CB   | 2.53                     | 0.56              |
| 1:A:21:PHE:CB    | 1:A:356:ASN:HD21 | 2.17                     | 0.56              |
| 1:A:59:THR:HA    | 1:A:119:PRO:HB2  | 1.87                     | 0.56              |
| 1:A:113:LYS:HE2  | 1:A:124:GLN:HG2  | 1.86                     | 0.56              |
| 1:A:42:ALA:O     | 1:A:69:ALA:CB    | 2.52                     | 0.56              |
| 1:A:154:GLU:HA   | 1:A:157:VAL:CG1  | 2.36                     | 0.56              |
| 1:A:327:SER:O    | 1:A:328:VAL:C    | 2.44                     | 0.56              |
| 1:A:334:ASP:HB3  | 1:A:339:LYS:CD   | 2.28                     | 0.56              |
| 1:A:14:LEU:CD1   | 1:A:61:LEU:HD13  | 2.35                     | 0.56              |
| 1:A:10:LYS:HG2   | 1:A:24:GLU:O     | 2.05                     | 0.56              |
| 1:A:333:ALA:O    | 1:A:336:MET:N    | 2.39                     | 0.56              |
| 1:A:132:CYS:HB2  | 1:A:137:ILE:HD11 | 1.86                     | 0.56              |
| 1:A:194:THR:HG23 | 1:A:220:ILE:HD12 | 1.87                     | 0.55              |
| 1:A:59:THR:OG1   | 1:A:60:PRO:CD    | 2.54                     | 0.55              |
| 1:A:93:PHE:HE1   | 1:A:174:CYS:SG   | 2.29                     | 0.55              |
| 1:A:267:GLU:HG2  | 1:A:274:THR:O    | 2.05                     | 0.55              |
| 1:A:350:LEU:O    | 1:A:373:THR:N    | 2.39                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:7:ILE:HG22   | 1:A:8:LYS:N      | 2.21                     | 0.55              |
| 1:A:99:LYS:HG3   | 1:A:104:LYS:CE   | 2.34                     | 0.55              |
| 1:A:204:GLY:O    | 1:A:207:VAL:N    | 2.40                     | 0.55              |
| 1:A:228:LYS:O    | 1:A:232:ALA:HB2  | 2.06                     | 0.55              |
| 1:A:360:ASP:O    | 1:A:363:ARG:N    | 2.39                     | 0.55              |
| 1:A:11:ALA:HB1   | 1:A:147:SER:HB2  | 1.84                     | 0.55              |
| 1:A:223:ASP:C    | 1:A:225:ASN:H    | 2.10                     | 0.55              |
| 1:A:41:VAL:HG13  | 3:A:383:NTN:H5   | 1.87                     | 0.55              |
| 1:A:16:GLU:HA    | 1:A:61:LEU:HD12  | 1.88                     | 0.55              |
| 1:A:99:LYS:CG    | 1:A:104:LYS:HD2  | 2.37                     | 0.55              |
| 1:A:26:VAL:CG1   | 1:A:131:THR:O    | 2.47                     | 0.54              |
| 1:A:180:TYR:CA   | 1:A:206:SER:O    | 2.56                     | 0.54              |
| 1:A:14:LEU:HD12  | 1:A:61:LEU:HD13  | 1.87                     | 0.54              |
| 1:A:225:ASN:C    | 1:A:227:ASP:H    | 2.11                     | 0.54              |
| 1:A:52:VAL:C     | 1:A:54:SER:N     | 2.59                     | 0.54              |
| 1:A:74:GLU:O     | 1:A:75:SER:HB2   | 2.07                     | 0.54              |
| 1:A:171:LEU:CD2  | 1:A:346:ILE:CD1  | 2.84                     | 0.54              |
| 1:A:65:ALA:C     | 1:A:146:PHE:CD1  | 2.81                     | 0.54              |
| 1:A:124:GLN:NE2  | 1:A:155:ILE:HD11 | 2.22                     | 0.54              |
| 1:A:109:ASN:N    | 1:A:109:ASN:OD1  | 2.39                     | 0.54              |
| 1:A:218:ARG:HD3  | 1:A:220:ILE:HD11 | 1.89                     | 0.54              |
| 1:A:288:VAL:CG2  | 1:A:313:THR:HG22 | 2.38                     | 0.54              |
| 1:A:93:PHE:CE1   | 1:A:174:CYS:SG   | 3.01                     | 0.54              |
| 1:A:272:LEU:HD23 | 1:A:275:MET:SD   | 2.48                     | 0.54              |
| 1:A:276:VAL:HB   | 1:A:301:LEU:HD22 | 1.90                     | 0.54              |
| 1:A:334:ASP:O    | 1:A:339:LYS:HB2  | 2.07                     | 0.54              |
| 1:A:73:VAL:CG2   | 1:A:87:ASP:HB3   | 2.38                     | 0.54              |
| 1:A:105:HIS:CD2  | 1:A:106:PRO:HD2  | 2.43                     | 0.54              |
| 1:A:215:GLY:O    | 1:A:216:ALA:HB2  | 2.07                     | 0.53              |
| 1:A:11:ALA:HB3   | 1:A:26:VAL:HG21  | 1.90                     | 0.53              |
| 1:A:291:ILE:HD11 | 1:A:314:TRP:CE2  | 2.43                     | 0.53              |
| 1:A:46:CYS:O     | 1:A:49:ASP:HB2   | 2.08                     | 0.53              |
| 1:A:96:GLN:HE21  | 1:A:325:LYS:HB2  | 1.73                     | 0.53              |
| 1:A:182:SER:HA   | 1:A:186:VAL:HG21 | 1.91                     | 0.53              |
| 1:A:59:THR:OG1   | 1:A:60:PRO:HD2   | 2.08                     | 0.53              |
| 1:A:90:ILE:HG13  | 1:A:328:VAL:HG11 | 1.90                     | 0.53              |
| 1:A:99:LYS:HG3   | 1:A:104:LYS:HD2  | 1.89                     | 0.53              |
| 1:A:250:ILE:CG1  | 1:A:254:LEU:HD23 | 2.39                     | 0.53              |
| 1:A:11:ALA:HB3   | 1:A:26:VAL:CG2   | 2.38                     | 0.53              |
| 1:A:178:THR:HA   | 1:A:320:GLY:H    | 1.73                     | 0.53              |
| 1:A:201:GLY:O    | 1:A:205:LEU:HD13 | 2.09                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:195:CYS:HA   | 1:A:264:PHE:O    | 2.09                     | 0.52              |
| 1:A:198:PHE:HE1  | 1:A:222:VAL:HG21 | 1.71                     | 0.52              |
| 1:A:23:ILE:HD11  | 1:A:353:GLU:O    | 2.10                     | 0.52              |
| 1:A:146:PHE:CE2  | 1:A:355:ILE:HD11 | 2.44                     | 0.52              |
| 1:A:67:HIS:HA    | 1:A:143:THR:HG1  | 1.73                     | 0.52              |
| 1:A:180:TYR:HA   | 1:A:206:SER:O    | 2.10                     | 0.52              |
| 1:A:64:ILE:HD12  | 1:A:130:PHE:CZ   | 2.44                     | 0.52              |
| 1:A:198:PHE:CE1  | 1:A:222:VAL:CG2  | 2.88                     | 0.52              |
| 1:A:273:ASP:C    | 1:A:275:MET:H    | 2.13                     | 0.52              |
| 1:A:9:CYS:SG     | 1:A:28:VAL:CG2   | 2.98                     | 0.52              |
| 1:A:252:GLU:HA   | 1:A:255:THR:OG1  | 2.10                     | 0.52              |
| 1:A:349:VAL:HG12 | 1:A:373:THR:HG23 | 1.92                     | 0.52              |
| 1:A:70:ALA:O     | 1:A:166:LEU:HD13 | 2.10                     | 0.52              |
| 1:A:288:VAL:HG23 | 1:A:313:THR:CG2  | 2.40                     | 0.51              |
| 1:A:360:ASP:O    | 1:A:362:LEU:N    | 2.42                     | 0.51              |
| 1:A:284:GLU:O    | 1:A:310:SER:CB   | 2.51                     | 0.51              |
| 1:A:229:PHE:CD1  | 1:A:240:CYS:HB3  | 2.45                     | 0.51              |
| 1:A:21:PHE:HD1   | 1:A:355:ILE:HG23 | 1.76                     | 0.51              |
| 1:A:352:PHE:CE2  | 1:A:374:PHE:CZ   | 2.98                     | 0.51              |
| 1:A:351:PRO:O    | 1:A:354:LYS:HG3  | 2.10                     | 0.51              |
| 1:A:15:TRP:O     | 1:A:16:GLU:HB2   | 2.08                     | 0.51              |
| 1:A:200:LEU:C    | 1:A:228:LYS:HG2  | 2.31                     | 0.51              |
| 1:A:229:PHE:O    | 1:A:230:ALA:C    | 2.49                     | 0.51              |
| 1:A:333:ALA:O    | 1:A:336:MET:HB2  | 2.10                     | 0.51              |
| 1:A:40:MET:HE1   | 1:A:145:THR:HG23 | 1.92                     | 0.51              |
| 1:A:328:VAL:HB   | 1:A:329:PRO:HD3  | 1.91                     | 0.51              |
| 1:A:346:ILE:CG2  | 1:A:371:ILE:HD13 | 2.34                     | 0.51              |
| 1:A:100:CYS:HB2  | 1:A:112:LEU:HG   | 1.93                     | 0.51              |
| 1:A:64:ILE:HD12  | 1:A:130:PHE:CD1  | 2.41                     | 0.51              |
| 1:A:331:LEU:HD12 | 1:A:340:PHE:CZ   | 2.43                     | 0.50              |
| 1:A:335:PHE:CD2  | 1:A:342:LEU:HD12 | 2.46                     | 0.50              |
| 1:A:349:VAL:CG2  | 3:A:389:NTN:CI5  | 2.89                     | 0.50              |
| 1:A:165:PRO:O    | 1:A:169:VAL:HG22 | 2.11                     | 0.50              |
| 1:A:100:CYS:O    | 1:A:101:ARG:O    | 2.29                     | 0.50              |
| 1:A:185:LYS:O    | 1:A:185:LYS:CD   | 2.60                     | 0.50              |
| 1:A:224:ILE:HD12 | 1:A:244:GLN:NE2  | 2.27                     | 0.50              |
| 1:A:73:VAL:HG21  | 1:A:87:ASP:HB3   | 1.93                     | 0.50              |
| 1:A:300:ASN:OD1  | 1:A:300:ASN:N    | 2.24                     | 0.50              |
| 1:A:229:PHE:HD1  | 1:A:240:CYS:SG   | 2.28                     | 0.50              |
| 1:A:110:PHE:CE1  | 1:A:116:LEU:HD12 | 2.43                     | 0.50              |
| 1:A:113:LYS:HD3  | 1:A:155:ILE:HD11 | 1.93                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:187:ALA:O    | 1:A:189:VAL:HG23 | 2.11                     | 0.50              |
| 1:A:225:ASN:C    | 1:A:227:ASP:N    | 2.64                     | 0.50              |
| 1:A:161:ASP:HB3  | 1:A:164:SER:OG   | 2.10                     | 0.50              |
| 1:A:171:LEU:O    | 1:A:173:GLY:N    | 2.45                     | 0.50              |
| 1:A:200:LEU:HB3  | 1:A:228:LYS:HG2  | 1.93                     | 0.50              |
| 1:A:102:VAL:HG23 | 1:A:108:GLY:C    | 2.31                     | 0.50              |
| 1:A:113:LYS:HG2  | 1:A:155:ILE:HD13 | 1.93                     | 0.50              |
| 1:A:69:ALA:HB2   | 1:A:145:THR:HG22 | 1.93                     | 0.50              |
| 1:A:340:PHE:O    | 1:A:340:PHE:CG   | 2.59                     | 0.50              |
| 1:A:88:LYS:O     | 1:A:89:VAL:CG2   | 2.53                     | 0.50              |
| 1:A:249:PRO:HB3  | 1:A:251:GLN:HG3  | 1.95                     | 0.49              |
| 1:A:121:GLY:HA2  | 1:A:139:HIS:O    | 2.12                     | 0.49              |
| 1:A:113:LYS:HD3  | 1:A:155:ILE:CD1  | 2.42                     | 0.49              |
| 1:A:229:PHE:HB3  | 1:A:240:CYS:SG   | 2.52                     | 0.49              |
| 1:A:23:ILE:CD1   | 1:A:353:GLU:O    | 2.61                     | 0.49              |
| 1:A:82:THR:HG22  | 1:A:83:VAL:CG2   | 2.34                     | 0.49              |
| 1:A:205:LEU:H    | 1:A:205:LEU:HD12 | 1.77                     | 0.49              |
| 1:A:205:LEU:O    | 1:A:209:MET:CB   | 2.51                     | 0.49              |
| 1:A:332:VAL:O    | 1:A:336:MET:N    | 2.46                     | 0.49              |
| 1:A:355:ILE:HA   | 1:A:372:LEU:HD11 | 1.93                     | 0.49              |
| 1:A:111:CYS:C    | 1:A:113:LYS:N    | 2.65                     | 0.49              |
| 1:A:267:GLU:OE1  | 1:A:269:ILE:HB   | 2.13                     | 0.49              |
| 1:A:8:LYS:HG2    | 1:A:9:CYS:N      | 2.28                     | 0.49              |
| 1:A:171:LEU:HD22 | 1:A:346:ILE:CD1  | 2.37                     | 0.49              |
| 1:A:327:SER:C    | 1:A:329:PRO:CD   | 2.80                     | 0.49              |
| 1:A:303:MET:O    | 1:A:305:PRO:HD3  | 2.13                     | 0.49              |
| 1:A:90:ILE:HD11  | 1:A:169:VAL:O    | 2.13                     | 0.49              |
| 1:A:360:ASP:C    | 1:A:362:LEU:N    | 2.66                     | 0.48              |
| 1:A:52:VAL:C     | 1:A:54:SER:H     | 2.16                     | 0.48              |
| 1:A:13:VAL:O     | 1:A:22:SER:N     | 2.37                     | 0.48              |
| 1:A:113:LYS:CG   | 1:A:155:ILE:HD11 | 2.43                     | 0.48              |
| 1:A:302:SER:O    | 1:A:303:MET:HB2  | 2.12                     | 0.48              |
| 1:A:30:PRO:HA    | 1:A:37:ARG:CZ    | 2.41                     | 0.48              |
| 1:A:5:LYS:C      | 1:A:6:VAL:O      | 2.43                     | 0.48              |
| 1:A:229:PHE:HA   | 1:A:232:ALA:CB   | 2.43                     | 0.48              |
| 1:A:5:LYS:O      | 1:A:6:VAL:C      | 2.44                     | 0.48              |
| 1:A:40:MET:HE2   | 1:A:69:ALA:HB3   | 1.96                     | 0.48              |
| 1:A:75:SER:O     | 1:A:76:ILE:HG22  | 2.14                     | 0.48              |
| 1:A:250:ILE:C    | 1:A:252:GLU:H    | 2.16                     | 0.48              |
| 1:A:116:LEU:O    | 1:A:117:SER:O    | 2.32                     | 0.48              |
| 1:A:252:GLU:C    | 1:A:254:LEU:N    | 2.67                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:88:LYS:HD3   | 1:A:166:LEU:HG   | 1.96                     | 0.48              |
| 1:A:88:LYS:C     | 1:A:89:VAL:HG23  | 2.33                     | 0.48              |
| 1:A:49:ASP:OD2   | 1:A:140:PHE:HE1  | 1.97                     | 0.48              |
| 1:A:146:PHE:HE2  | 1:A:372:LEU:CD2  | 2.27                     | 0.48              |
| 1:A:56:THR:OG1   | 1:A:296:PRO:HD2  | 2.14                     | 0.48              |
| 1:A:169:VAL:CG1  | 1:A:332:VAL:HG13 | 2.45                     | 0.47              |
| 1:A:219:ILE:HD12 | 1:A:219:ILE:N    | 2.29                     | 0.47              |
| 1:A:309:LEU:C    | 1:A:311:GLY:H    | 2.16                     | 0.47              |
| 1:A:123:MET:HB3  | 1:A:127:THR:O    | 2.15                     | 0.47              |
| 1:A:90:ILE:HG13  | 1:A:160:ILE:HG21 | 1.90                     | 0.47              |
| 1:A:249:PRO:O    | 1:A:252:GLU:HB3  | 2.13                     | 0.47              |
| 1:A:182:SER:CA   | 1:A:186:VAL:HG23 | 2.42                     | 0.47              |
| 1:A:332:VAL:O    | 1:A:335:PHE:CA   | 2.63                     | 0.47              |
| 1:A:346:ILE:HG21 | 3:A:389:NTN:H6   | 1.96                     | 0.47              |
| 1:A:52:VAL:CG1   | 1:A:59:THR:CG2   | 2.77                     | 0.47              |
| 1:A:96:GLN:N     | 1:A:97:CYS:N     | 2.62                     | 0.47              |
| 1:A:192:GLY:O    | 1:A:217:ALA:CB   | 2.62                     | 0.47              |
| 1:A:250:ILE:C    | 1:A:252:GLU:N    | 2.68                     | 0.47              |
| 1:A:205:LEU:CD1  | 1:A:205:LEU:H    | 2.27                     | 0.47              |
| 1:A:131:THR:HG22 | 1:A:133:ARG:C    | 2.35                     | 0.47              |
| 1:A:164:SER:O    | 1:A:166:LEU:N    | 2.47                     | 0.47              |
| 1:A:171:LEU:C    | 1:A:173:GLY:N    | 2.67                     | 0.47              |
| 1:A:258:SER:OG   | 1:A:261:GLY:N    | 2.48                     | 0.47              |
| 1:A:26:VAL:CG1   | 1:A:132:CYS:HA   | 2.45                     | 0.47              |
| 1:A:357:GLU:OE2  | 3:A:399:NTN:H6   | 2.15                     | 0.47              |
| 1:A:3:ALA:HB2    | 1:A:5:LYS:HD2    | 1.96                     | 0.47              |
| 1:A:358:GLY:C    | 1:A:360:ASP:H    | 2.16                     | 0.47              |
| 1:A:180:TYR:C    | 1:A:180:TYR:CD1  | 2.88                     | 0.47              |
| 1:A:95:PRO:HB2   | 1:A:111:CYS:CB   | 2.44                     | 0.46              |
| 1:A:290:VAL:HG22 | 1:A:315:LYS:HB3  | 1.97                     | 0.46              |
| 1:A:211:CYS:O    | 1:A:212:LYS:C    | 2.53                     | 0.46              |
| 1:A:279:LEU:HD22 | 1:A:312:ARG:HD3  | 1.97                     | 0.46              |
| 1:A:186:VAL:C    | 1:A:188:LYS:H    | 2.19                     | 0.46              |
| 1:A:272:LEU:HA   | 1:A:272:LEU:HD23 | 1.83                     | 0.46              |
| 1:A:46:CYS:HB3   | 1:A:67:HIS:HE1   | 1.81                     | 0.46              |
| 1:A:69:ALA:HB3   | 1:A:145:THR:HG23 | 1.92                     | 0.46              |
| 1:A:165:PRO:O    | 1:A:167:GLU:N    | 2.49                     | 0.46              |
| 1:A:333:ALA:CA   | 1:A:336:MET:HB2  | 2.45                     | 0.46              |
| 1:A:220:ILE:CG2  | 1:A:241:VAL:CG2  | 2.94                     | 0.46              |
| 1:A:224:ILE:HD12 | 1:A:244:GLN:HE21 | 1.81                     | 0.46              |
| 1:A:118:MET:HA   | 1:A:119:PRO:HD2  | 1.79                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:160:ILE:HG13 | 1:A:161:ASP:H    | 1.80                     | 0.46              |
| 1:A:195:CYS:SG   | 1:A:264:PHE:HB2  | 2.56                     | 0.46              |
| 1:A:198:PHE:CD1  | 1:A:222:VAL:CG2  | 2.99                     | 0.46              |
| 1:A:153:ASP:HB3  | 1:A:154:GLU:H    | 1.45                     | 0.45              |
| 1:A:210:GLY:O    | 1:A:213:ALA:HB3  | 2.16                     | 0.45              |
| 1:A:224:ILE:HG22 | 1:A:243:PRO:HD2  | 1.97                     | 0.45              |
| 1:A:148:GLN:HB3  | 1:A:374:PHE:CE2  | 2.52                     | 0.45              |
| 1:A:369:ARG:HH11 | 1:A:369:ARG:HA   | 1.80                     | 0.45              |
| 1:A:11:ALA:CB    | 1:A:147:SER:CB   | 2.80                     | 0.45              |
| 1:A:220:ILE:CG2  | 1:A:241:VAL:HG23 | 2.47                     | 0.45              |
| 1:A:249:PRO:HB2  | 1:A:251:GLN:HG3  | 1.97                     | 0.45              |
| 1:A:309:LEU:C    | 1:A:311:GLY:N    | 2.70                     | 0.45              |
| 1:A:7:ILE:CG2    | 1:A:8:LYS:N      | 2.79                     | 0.45              |
| 1:A:3:ALA:CA     | 1:A:5:LYS:HD2    | 2.46                     | 0.45              |
| 1:A:224:ILE:CA   | 1:A:242:ASN:HD22 | 2.09                     | 0.45              |
| 1:A:268:VAL:O    | 1:A:268:VAL:HG23 | 2.15                     | 0.45              |
| 1:A:272:LEU:HD11 | 1:A:299:GLN:C    | 2.32                     | 0.45              |
| 1:A:160:ILE:HG13 | 1:A:164:SER:OG   | 2.15                     | 0.45              |
| 1:A:284:GLU:HB2  | 1:A:310:SER:HB3  | 1.99                     | 0.45              |
| 1:A:329:PRO:O    | 1:A:332:VAL:HG23 | 2.16                     | 0.45              |
| 1:A:357:GLU:HA   | 1:A:360:ASP:OD1  | 2.16                     | 0.45              |
| 1:A:137:ILE:HA   | 1:A:137:ILE:HD12 | 1.71                     | 0.45              |
| 1:A:171:LEU:HA   | 1:A:171:LEU:HD12 | 1.75                     | 0.45              |
| 1:A:190:THR:OG1  | 1:A:264:PHE:HE1  | 1.99                     | 0.45              |
| 1:A:204:GLY:HA2  | 1:A:207:VAL:CG1  | 2.44                     | 0.45              |
| 1:A:94:THR:O     | 1:A:95:PRO:O     | 2.35                     | 0.45              |
| 1:A:188:LYS:O    | 1:A:189:VAL:C    | 2.54                     | 0.44              |
| 1:A:338:LYS:O    | 1:A:339:LYS:C    | 2.56                     | 0.44              |
| 1:A:358:GLY:O    | 1:A:360:ASP:N    | 2.50                     | 0.44              |
| 1:A:51:HIS:ND1   | 1:A:296:PRO:CG   | 2.81                     | 0.44              |
| 1:A:194:THR:OG1  | 1:A:218:ARG:CB   | 2.59                     | 0.44              |
| 1:A:253:VAL:O    | 1:A:257:MET:HG3  | 2.18                     | 0.44              |
| 1:A:328:VAL:O    | 1:A:331:LEU:HB3  | 2.17                     | 0.44              |
| 1:A:229:PHE:C    | 1:A:232:ALA:HB3  | 2.36                     | 0.44              |
| 1:A:349:VAL:CG1  | 1:A:371:ILE:HG22 | 2.41                     | 0.44              |
| 1:A:99:LYS:HG3   | 1:A:104:LYS:CD   | 2.47                     | 0.44              |
| 1:A:267:GLU:OE2  | 1:A:275:MET:CG   | 2.63                     | 0.44              |
| 1:A:105:HIS:CD2  | 1:A:106:PRO:N    | 2.86                     | 0.44              |
| 1:A:194:THR:HG22 | 1:A:262:VAL:CB   | 2.47                     | 0.44              |
| 1:A:204:GLY:CA   | 1:A:207:VAL:HG12 | 2.44                     | 0.44              |
| 1:A:187:ALA:HB2  | 1:A:290:VAL:HG21 | 1.99                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:315:LYS:HE3  | 3:A:391:NTN:H5   | 1.98                     | 0.44              |
| 1:A:169:VAL:HG12 | 1:A:332:VAL:HG13 | 2.00                     | 0.44              |
| 1:A:348:HIS:CE1  | 1:A:367:SER:CB   | 2.97                     | 0.44              |
| 1:A:82:THR:HB    | 1:A:154:GLU:OE2  | 2.18                     | 0.44              |
| 1:A:243:PRO:HG3  | 1:A:250:ILE:HD12 | 2.00                     | 0.43              |
| 1:A:95:PRO:HB3   | 1:A:113:LYS:HG2  | 2.00                     | 0.43              |
| 1:A:166:LEU:HA   | 1:A:169:VAL:HG23 | 1.99                     | 0.43              |
| 1:A:279:LEU:CD1  | 1:A:308:LEU:HD23 | 2.43                     | 0.43              |
| 1:A:68:GLU:OE1   | 1:A:369:ARG:NE   | 2.45                     | 0.43              |
| 1:A:200:LEU:O    | 1:A:205:LEU:HD11 | 2.18                     | 0.43              |
| 1:A:205:LEU:N    | 1:A:205:LEU:HD12 | 2.33                     | 0.43              |
| 1:A:76:ILE:HG12  | 1:A:77:GLY:O     | 2.19                     | 0.43              |
| 1:A:129:ARG:NH1  | 1:A:129:ARG:CG   | 2.76                     | 0.43              |
| 1:A:232:ALA:O    | 1:A:237:ALA:HB2  | 2.18                     | 0.43              |
| 1:A:220:ILE:HD13 | 1:A:262:VAL:CG1  | 2.49                     | 0.43              |
| 1:A:39:LYS:CG    | 1:A:39:LYS:O     | 2.67                     | 0.43              |
| 1:A:109:ASN:O    | 1:A:111:CYS:N    | 2.52                     | 0.43              |
| 1:A:67:HIS:HD1   | 1:A:67:HIS:N     | 2.16                     | 0.43              |
| 1:A:64:ILE:HG12  | 1:A:137:ILE:HG21 | 2.01                     | 0.43              |
| 1:A:351:PRO:O    | 1:A:354:LYS:CG   | 2.66                     | 0.42              |
| 1:A:140:PHE:O    | 1:A:141:LEU:HB2  | 2.19                     | 0.42              |
| 1:A:154:GLU:O    | 1:A:157:VAL:HG12 | 2.19                     | 0.42              |
| 1:A:166:LEU:HA   | 1:A:166:LEU:HD22 | 1.39                     | 0.42              |
| 1:A:10:LYS:HA    | 1:A:25:GLU:HA    | 2.01                     | 0.42              |
| 1:A:30:PRO:O     | 1:A:30:PRO:CG    | 2.66                     | 0.42              |
| 1:A:39:LYS:HG3   | 1:A:40:MET:O     | 2.19                     | 0.42              |
| 1:A:74:GLU:O     | 1:A:74:GLU:OE2   | 2.37                     | 0.42              |
| 1:A:269:ILE:CG2  | 1:A:271:ARG:CG   | 2.81                     | 0.42              |
| 1:A:348:HIS:ND1  | 1:A:367:SER:CB   | 2.81                     | 0.42              |
| 1:A:368:ILE:HD13 | 1:A:368:ILE:HG21 | 1.67                     | 0.42              |
| 1:A:18:LYS:N     | 1:A:53:VAL:O     | 2.51                     | 0.42              |
| 1:A:273:ASP:C    | 1:A:275:MET:N    | 2.73                     | 0.42              |
| 1:A:307:LEU:O    | 1:A:312:ARG:CD   | 2.66                     | 0.42              |
| 1:A:279:LEU:HA   | 1:A:279:LEU:HD23 | 1.71                     | 0.42              |
| 1:A:58:VAL:O     | 1:A:58:VAL:HG12  | 2.19                     | 0.42              |
| 1:A:312:ARG:HH11 | 1:A:312:ARG:HD2  | 1.60                     | 0.42              |
| 1:A:38:ILE:HD11  | 1:A:152:VAL:CG2  | 2.39                     | 0.42              |
| 1:A:357:GLU:OE2  | 3:A:399:NTN:CI6  | 2.68                     | 0.42              |
| 1:A:26:VAL:HG12  | 1:A:132:CYS:HA   | 2.02                     | 0.41              |
| 1:A:160:ILE:HG13 | 1:A:161:ASP:N    | 2.34                     | 0.41              |
| 1:A:340:PHE:O    | 1:A:340:PHE:HD2  | 2.00                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:348:HIS:HB2  | 1:A:370:THR:OG1  | 2.20                     | 0.41              |
| 1:A:21:PHE:CD1   | 1:A:355:ILE:HG23 | 2.55                     | 0.41              |
| 1:A:220:ILE:HG23 | 1:A:241:VAL:HG23 | 2.01                     | 0.41              |
| 1:A:102:VAL:HG23 | 1:A:102:VAL:O    | 2.19                     | 0.41              |
| 1:A:211:CYS:O    | 1:A:215:GLY:N    | 2.45                     | 0.41              |
| 1:A:198:PHE:CD1  | 1:A:222:VAL:HG22 | 2.54                     | 0.41              |
| 1:A:334:ASP:HA   | 1:A:337:ALA:HB3  | 2.01                     | 0.41              |
| 1:A:346:ILE:HD12 | 1:A:346:ILE:HG23 | 1.83                     | 0.41              |
| 1:A:35:GLU:C     | 1:A:36:VAL:HG23  | 2.39                     | 0.41              |
| 1:A:309:LEU:HD12 | 1:A:309:LEU:HA   | 1.29                     | 0.41              |
| 1:A:85:PRO:C     | 1:A:87:ASP:N     | 2.65                     | 0.41              |
| 1:A:140:PHE:CD2  | 1:A:141:LEU:HD22 | 2.56                     | 0.41              |
| 1:A:178:THR:O    | 1:A:179:GLY:O    | 2.39                     | 0.41              |
| 1:A:268:VAL:HG12 | 1:A:292:VAL:HG11 | 2.03                     | 0.41              |
| 1:A:35:GLU:OE1   | 1:A:129:ARG:NH2  | 2.52                     | 0.41              |
| 1:A:51:HIS:CE1   | 1:A:296:PRO:CD   | 2.91                     | 0.41              |
| 1:A:272:LEU:HD11 | 1:A:300:ASN:C    | 2.41                     | 0.41              |
| 1:A:176:PHE:CZ   | 1:A:340:PHE:CE2  | 3.09                     | 0.41              |
| 1:A:136:PRO:C    | 1:A:137:ILE:HD13 | 2.39                     | 0.41              |
| 1:A:168:LYS:HG2  | 1:A:342:LEU:HB2  | 2.03                     | 0.41              |
| 1:A:161:ASP:C    | 1:A:164:SER:HG   | 2.18                     | 0.41              |
| 1:A:209:MET:CE   | 1:A:235:VAL:HB   | 2.46                     | 0.41              |
| 1:A:304:ASN:O    | 1:A:305:PRO:C    | 2.58                     | 0.41              |
| 1:A:338:LYS:O    | 1:A:340:PHE:N    | 2.54                     | 0.41              |
| 1:A:121:GLY:O    | 1:A:139:HIS:CA   | 2.65                     | 0.40              |
| 1:A:179:GLY:HA3  | 1:A:206:SER:HB2  | 2.03                     | 0.40              |
| 1:A:273:ASP:O    | 1:A:275:MET:N    | 2.54                     | 0.40              |
| 1:A:152:VAL:O    | 1:A:152:VAL:CG2  | 2.69                     | 0.40              |
| 1:A:179:GLY:O    | 1:A:181:GLY:N    | 2.54                     | 0.40              |
| 1:A:200:LEU:HA   | 1:A:200:LEU:HD12 | 1.71                     | 0.40              |
| 1:A:96:GLN:C     | 1:A:98:GLY:N     | 2.73                     | 0.40              |
| 1:A:250:ILE:HG12 | 1:A:254:LEU:CD2  | 2.49                     | 0.40              |
| 1:A:146:PHE:CE2  | 1:A:372:LEU:CD2  | 3.04                     | 0.40              |
| 1:A:199:GLY:HA3  | 1:A:268:VAL:HG23 | 2.03                     | 0.40              |

All (734) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1        | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------|----------------------|--------------------------|-------------------|
| 1:A:103:CYS:C | 1:A:325:LYS:N[2_556] | 0.24                     | 1.96              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:A:9:CYS:C     | 1:A:10:LYS:N[2_555]    | 0.30                     | 1.90              |
| 1:A:34:HIS:CB   | 1:A:188:LYS:NZ[2_556]  | 0.31                     | 1.89              |
| 1:A:24:GLU:CG   | 3:A:379:NTN:CI5[2_555] | 0.38                     | 1.82              |
| 1:A:123:MET:O   | 1:A:316:GLY:N[2_556]   | 0.38                     | 1.82              |
| 1:A:24:GLU:O    | 1:A:25:GLU:CA[2_555]   | 0.40                     | 1.80              |
| 1:A:34:HIS:C    | 3:A:391:NTN:CI2[2_556] | 0.41                     | 1.79              |
| 1:A:94:THR:O    | 1:A:102:VAL:CG2[2_556] | 0.45                     | 1.75              |
| 1:A:94:THR:CA   | 1:A:110:PHE:O[2_556]   | 0.46                     | 1.74              |
| 1:A:120:ARG:CZ  | 1:A:291:ILE:O[2_556]   | 0.47                     | 1.73              |
| 1:A:7:ILE:O     | 1:A:148:GLN:NE2[2_555] | 0.50                     | 1.70              |
| 1:A:1:SER:OG    | 1:A:40:MET:CA[2_555]   | 0.53                     | 1.67              |
| 1:A:125:ASP:O   | 1:A:290:VAL:N[2_556]   | 0.57                     | 1.63              |
| 1:A:105:HIS:NE2 | 1:A:157:VAL:CB[2_556]  | 0.57                     | 1.63              |
| 1:A:5:LYS:N     | 3:A:383:NTN:NI2[2_555] | 0.58                     | 1.62              |
| 1:A:1:SER:CB    | 1:A:40:MET:N[2_555]    | 0.58                     | 1.62              |
| 1:A:114:ASN:N   | 1:A:318:ILE:CG2[2_556] | 0.59                     | 1.61              |
| 1:A:34:HIS:CG   | 1:A:188:LYS:CE[2_556]  | 0.60                     | 1.60              |
| 1:A:107:GLU:N   | 1:A:154:GLU:O[2_556]   | 0.61                     | 1.59              |
| 1:A:166:LEU:O   | 3:A:377:NTN:CI4[2_555] | 0.64                     | 1.56              |
| 1:A:34:HIS:CA   | 3:A:391:NTN:CI1[2_556] | 0.65                     | 1.55              |
| 1:A:105:HIS:CG  | 1:A:157:VAL:C[2_556]   | 0.67                     | 1.53              |
| 1:A:110:PHE:CE1 | 1:A:114:ASN:ND2[2_556] | 0.67                     | 1.53              |
| 1:A:11:ALA:C    | 1:A:25:GLU:CD[2_555]   | 0.69                     | 1.51              |
| 1:A:27:GLU:CD   | 1:A:353:GLU:CG[2_555]  | 0.69                     | 1.51              |
| 1:A:35:GLU:N    | 3:A:391:NTN:CI3[2_556] | 0.69                     | 1.51              |
| 1:A:100:CYS:CB  | 1:A:319:PHE:CE2[2_556] | 0.71                     | 1.49              |
| 1:A:113:LYS:CA  | 1:A:318:ILE:O[2_556]   | 0.72                     | 1.48              |
| 1:A:97:CYS:SG   | 1:A:322:PHE:C[2_556]   | 0.73                     | 1.47              |
| 1:A:107:GLU:C   | 1:A:155:ILE:C[2_556]   | 0.73                     | 1.47              |
| 1:A:127:THR:CG2 | 1:A:314:TRP:N[2_556]   | 0.73                     | 1.47              |
| 1:A:8:LYS:N     | 1:A:148:GLN:CB[2_555]  | 0.74                     | 1.46              |
| 1:A:3:ALA:CB    | 3:A:383:NTN:CI6[2_555] | 0.74                     | 1.46              |
| 1:A:24:GLU:CD   | 3:A:379:NTN:NI2[2_555] | 0.74                     | 1.46              |
| 1:A:35:GLU:CB   | 3:A:391:NTN:NI2[2_556] | 0.75                     | 1.45              |
| 1:A:34:HIS:CD2  | 1:A:188:LYS:CD[2_556]  | 0.77                     | 1.43              |
| 1:A:103:CYS:CB  | 1:A:324:SER:N[2_556]   | 0.77                     | 1.43              |
| 1:A:99:LYS:CB   | 1:A:327:SER:CB[2_556]  | 0.77                     | 1.43              |
| 1:A:116:LEU:CD2 | 1:A:117:SER:OG[2_556]  | 0.78                     | 1.42              |
| 1:A:151:VAL:CG2 | 3:A:378:NTN:CI4[2_555] | 0.78                     | 1.42              |
| 1:A:10:LYS:CD   | 1:A:26:VAL:CB[2_555]   | 0.80                     | 1.40              |
| 1:A:99:LYS:CA   | 1:A:327:SER:CB[2_556]  | 0.80                     | 1.40              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:A:11:ALA:O    | 1:A:25:GLU:CD[2_555]   | 0.81                     | 1.39              |
| 1:A:11:ALA:C    | 1:A:25:GLU:OE2[2_555]  | 0.81                     | 1.39              |
| 1:A:110:PHE:CD1 | 1:A:114:ASN:CB[2_556]  | 0.81                     | 1.39              |
| 1:A:108:GLY:N   | 1:A:155:ILE:C[2_556]   | 0.83                     | 1.37              |
| 1:A:24:GLU:OE2  | 3:A:379:NTN:CI4[2_555] | 0.84                     | 1.36              |
| 1:A:10:LYS:CE   | 1:A:26:VAL:CG2[2_555]  | 0.84                     | 1.36              |
| 1:A:8:LYS:CA    | 1:A:148:GLN:CB[2_555]  | 0.84                     | 1.36              |
| 1:A:9:CYS:O     | 1:A:10:LYS:CA[2_555]   | 0.85                     | 1.35              |
| 1:A:1:SER:O     | 1:A:39:LYS:CA[2_555]   | 0.86                     | 1.34              |
| 1:A:108:GLY:N   | 1:A:155:ILE:O[2_556]   | 0.87                     | 1.33              |
| 1:A:134:GLY:O   | 1:A:305:PRO:CB[2_556]  | 0.88                     | 1.32              |
| 1:A:1:SER:CA    | 1:A:39:LYS:C[2_555]    | 0.88                     | 1.32              |
| 1:A:23:ILE:CG2  | 1:A:133:ARG:CG[2_555]  | 0.89                     | 1.31              |
| 1:A:105:HIS:CE1 | 1:A:157:VAL:CB[2_556]  | 0.89                     | 1.31              |
| 1:A:92:LEU:CD2  | 1:A:101:ARG:C[2_556]   | 0.90                     | 1.30              |
| 1:A:151:VAL:CB  | 3:A:378:NTN:CI4[2_555] | 0.90                     | 1.30              |
| 1:A:313:THR:N   | 3:A:382:NTN:NI1[2_556] | 0.91                     | 1.29              |
| 1:A:5:LYS:CE    | 1:A:41:VAL:CG1[2_555]  | 0.91                     | 1.29              |
| 1:A:103:CYS:CB  | 1:A:324:SER:CA[2_556]  | 0.92                     | 1.28              |
| 1:A:96:GLN:O    | 1:A:323:LYS:CG[2_556]  | 0.92                     | 1.28              |
| 1:A:328:VAL:CG1 | 3:A:385:NTN:CI5[2_556] | 0.93                     | 1.27              |
| 1:A:94:THR:CG2  | 1:A:111:CYS:N[2_556]   | 0.94                     | 1.26              |
| 1:A:8:LYS:C     | 1:A:148:GLN:CG[2_555]  | 0.94                     | 1.26              |
| 1:A:11:ALA:CA   | 1:A:25:GLU:OE2[2_555]  | 0.94                     | 1.26              |
| 1:A:1:SER:CB    | 1:A:39:LYS:C[2_555]    | 0.95                     | 1.25              |
| 1:A:10:LYS:CG   | 1:A:26:VAL:N[2_555]    | 0.95                     | 1.25              |
| 1:A:127:THR:CG2 | 1:A:313:THR:C[2_556]   | 0.95                     | 1.25              |
| 1:A:35:GLU:CA   | 3:A:391:NTN:CI4[2_556] | 0.95                     | 1.25              |
| 3:A:390:NTN:NI1 | 3:A:397:NTN:NI2[2_556] | 0.95                     | 1.25              |
| 1:A:150:THR:N   | 3:A:378:NTN:NI1[2_555] | 0.96                     | 1.24              |
| 1:A:9:CYS:O     | 1:A:10:LYS:N[2_555]    | 0.96                     | 1.24              |
| 1:A:107:GLU:C   | 1:A:156:SER:N[2_556]   | 0.97                     | 1.23              |
| 1:A:120:ARG:NH1 | 1:A:291:ILE:O[2_556]   | 0.97                     | 1.23              |
| 1:A:99:LYS:N    | 1:A:323:LYS:O[2_556]   | 0.97                     | 1.23              |
| 1:A:24:GLU:CB   | 3:A:379:NTN:CI6[2_555] | 0.98                     | 1.22              |
| 1:A:149:TYR:OH  | 1:A:149:TYR:OH[2_555]  | 0.98                     | 1.22              |
| 1:A:125:ASP:O   | 1:A:290:VAL:CA[2_556]  | 0.98                     | 1.22              |
| 1:A:123:MET:O   | 1:A:315:LYS:C[2_556]   | 0.98                     | 1.22              |
| 1:A:172:ILE:CG2 | 3:A:385:NTN:CI3[2_556] | 0.99                     | 1.21              |
| 1:A:95:PRO:CA   | 1:A:109:ASN:N[2_556]   | 1.00                     | 1.20              |
| 1:A:107:GLU:CA  | 1:A:155:ILE:N[2_556]   | 1.00                     | 1.20              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:A:5:LYS:NZ    | 1:A:41:VAL:CG1[2_555]  | 1.00                     | 1.20              |
| 1:A:120:ARG:NH2 | 1:A:292:VAL:N[2_556]   | 1.00                     | 1.20              |
| 1:A:8:LYS:CB    | 1:A:148:GLN:CA[2_555]  | 1.01                     | 1.19              |
| 1:A:96:GLN:C    | 1:A:323:LYS:CG[2_556]  | 1.01                     | 1.19              |
| 1:A:8:LYS:CE    | 1:A:149:TYR:C[2_555]   | 1.02                     | 1.18              |
| 1:A:125:ASP:C   | 1:A:290:VAL:CA[2_556]  | 1.02                     | 1.18              |
| 1:A:150:THR:CA  | 3:A:378:NTN:NI1[2_555] | 1.03                     | 1.17              |
| 1:A:1:SER:O     | 1:A:39:LYS:CB[2_555]   | 1.03                     | 1.17              |
| 1:A:105:HIS:O   | 1:A:325:LYS:CD[2_556]  | 1.04                     | 1.16              |
| 1:A:127:THR:O   | 1:A:314:TRP:O[2_556]   | 1.05                     | 1.15              |
| 1:A:35:GLU:CA   | 3:A:391:NTN:NI2[2_556] | 1.05                     | 1.15              |
| 1:A:24:GLU:C    | 1:A:25:GLU:N[2_555]    | 1.05                     | 1.15              |
| 1:A:34:HIS:CB   | 3:A:391:NTN:CI1[2_556] | 1.06                     | 1.14              |
| 1:A:104:LYS:NZ  | 1:A:329:PRO:C[2_556]   | 1.07                     | 1.13              |
| 1:A:105:HIS:CG  | 1:A:157:VAL:CA[2_556]  | 1.07                     | 1.13              |
| 1:A:107:GLU:O   | 1:A:156:SER:CA[2_556]  | 1.07                     | 1.13              |
| 1:A:129:ARG:NH2 | 1:A:313:THR:CG2[2_556] | 1.08                     | 1.12              |
| 1:A:35:GLU:N    | 3:A:391:NTN:CI4[2_556] | 1.09                     | 1.11              |
| 1:A:95:PRO:CB   | 1:A:109:ASN:OD1[2_556] | 1.09                     | 1.11              |
| 1:A:178:THR:O   | 3:A:386:NTN:NI2[2_556] | 1.10                     | 1.10              |
| 1:A:127:THR:O   | 1:A:314:TRP:C[2_556]   | 1.10                     | 1.10              |
| 1:A:101:ARG:CZ  | 1:A:173:GLY:CA[2_556]  | 1.12                     | 1.08              |
| 1:A:1:SER:C     | 1:A:39:LYS:CA[2_555]   | 1.12                     | 1.08              |
| 1:A:27:GLU:OE1  | 1:A:353:GLU:CG[2_555]  | 1.14                     | 1.06              |
| 1:A:104:LYS:CA  | 1:A:325:LYS:C[2_556]   | 1.14                     | 1.06              |
| 1:A:1:SER:CA    | 1:A:39:LYS:O[2_555]    | 1.15                     | 1.05              |
| 1:A:97:CYS:SG   | 1:A:322:PHE:O[2_556]   | 1.15                     | 1.05              |
| 1:A:331:LEU:CG  | 3:A:385:NTN:NI1[2_556] | 1.15                     | 1.05              |
| 1:A:5:LYS:CE    | 1:A:41:VAL:CB[2_555]   | 1.15                     | 1.05              |
| 1:A:34:HIS:CD2  | 1:A:188:LYS:CG[2_556]  | 1.16                     | 1.04              |
| 1:A:5:LYS:NZ    | 1:A:41:VAL:CB[2_555]   | 1.16                     | 1.04              |
| 1:A:10:LYS:CB   | 1:A:26:VAL:N[2_555]    | 1.16                     | 1.04              |
| 1:A:8:LYS:CB    | 1:A:148:GLN:C[2_555]   | 1.17                     | 1.03              |
| 1:A:95:PRO:C    | 1:A:109:ASN:N[2_556]   | 1.17                     | 1.03              |
| 1:A:166:LEU:O   | 3:A:377:NTN:CI3[2_555] | 1.17                     | 1.03              |
| 1:A:98:GLY:N    | 1:A:323:LYS:CB[2_556]  | 1.18                     | 1.02              |
| 1:A:101:ARG:NH2 | 1:A:173:GLY:C[2_556]   | 1.18                     | 1.02              |
| 1:A:104:LYS:N   | 1:A:324:SER:C[2_556]   | 1.18                     | 1.02              |
| 1:A:34:HIS:ND1  | 1:A:188:LYS:CE[2_556]  | 1.18                     | 1.02              |
| 1:A:22:SER:C    | 1:A:133:ARG:NH2[2_555] | 1.18                     | 1.02              |
| 1:A:104:LYS:N   | 1:A:324:SER:O[2_556]   | 1.18                     | 1.02              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:A:105:HIS:ND1 | 1:A:157:VAL:CA[2_556]  | 1.18                     | 1.02              |
| 1:A:8:LYS:CE    | 1:A:149:TYR:O[2_555]   | 1.19                     | 1.01              |
| 1:A:104:LYS:CA  | 1:A:325:LYS:O[2_556]   | 1.19                     | 1.01              |
| 1:A:127:THR:C   | 1:A:314:TRP:CB[2_556]  | 1.19                     | 1.01              |
| 1:A:9:CYS:C     | 1:A:9:CYS:C[2_555]     | 1.20                     | 1.00              |
| 1:A:105:HIS:NE2 | 1:A:157:VAL:CG1[2_556] | 1.20                     | 1.00              |
| 1:A:24:GLU:CB   | 3:A:379:NTN:CI5[2_555] | 1.20                     | 1.00              |
| 1:A:127:THR:CA  | 1:A:314:TRP:CA[2_556]  | 1.20                     | 1.00              |
| 1:A:127:THR:CB  | 1:A:314:TRP:CA[2_556]  | 1.20                     | 1.00              |
| 1:A:10:LYS:CD   | 1:A:26:VAL:CG2[2_555]  | 1.20                     | 1.00              |
| 1:A:112:LEU:O   | 1:A:319:PHE:N[2_556]   | 1.21                     | 0.99              |
| 1:A:34:HIS:C    | 3:A:391:NTN:CI3[2_556] | 1.21                     | 0.99              |
| 1:A:107:GLU:O   | 1:A:156:SER:N[2_556]   | 1.21                     | 0.99              |
| 1:A:107:GLU:CB  | 1:A:155:ILE:N[2_556]   | 1.22                     | 0.98              |
| 1:A:24:GLU:CG   | 3:A:379:NTN:NI2[2_555] | 1.22                     | 0.98              |
| 1:A:34:HIS:CG   | 1:A:188:LYS:NZ[2_556]  | 1.22                     | 0.98              |
| 1:A:99:LYS:N    | 1:A:327:SER:OG[2_556]  | 1.23                     | 0.97              |
| 1:A:96:GLN:N    | 1:A:109:ASN:CA[2_556]  | 1.23                     | 0.97              |
| 1:A:11:ALA:O    | 1:A:25:GLU:CG[2_555]   | 1.24                     | 0.96              |
| 1:A:103:CYS:C   | 1:A:324:SER:C[2_556]   | 1.24                     | 0.96              |
| 1:A:127:THR:CA  | 1:A:314:TRP:CB[2_556]  | 1.24                     | 0.96              |
| 1:A:34:HIS:NE2  | 1:A:188:LYS:CD[2_556]  | 1.25                     | 0.95              |
| 1:A:99:LYS:CA   | 1:A:327:SER:OG[2_556]  | 1.25                     | 0.95              |
| 1:A:99:LYS:CE   | 1:A:331:LEU:CD2[2_556] | 1.25                     | 0.95              |
| 1:A:107:GLU:CA  | 1:A:154:GLU:C[2_556]   | 1.26                     | 0.94              |
| 1:A:23:ILE:CG1  | 1:A:133:ARG:NE[2_555]  | 1.26                     | 0.94              |
| 1:A:97:CYS:CB   | 1:A:322:PHE:C[2_556]   | 1.26                     | 0.94              |
| 1:A:114:ASN:O   | 1:A:318:ILE:CD1[2_556] | 1.26                     | 0.94              |
| 1:A:95:PRO:CD   | 1:A:110:PHE:N[2_556]   | 1.26                     | 0.94              |
| 1:A:109:ASN:ND2 | 1:A:113:LYS:CB[2_556]  | 1.26                     | 0.94              |
| 1:A:110:PHE:CE1 | 1:A:114:ASN:CG[2_556]  | 1.27                     | 0.93              |
| 1:A:105:HIS:CE1 | 1:A:157:VAL:CG2[2_556] | 1.27                     | 0.93              |
| 1:A:101:ARG:NH1 | 1:A:173:GLY:CA[2_556]  | 1.27                     | 0.93              |
| 1:A:105:HIS:CD2 | 1:A:157:VAL:CA[2_556]  | 1.28                     | 0.92              |
| 1:A:34:HIS:NE2  | 1:A:188:LYS:CG[2_556]  | 1.28                     | 0.92              |
| 1:A:120:ARG:NH2 | 1:A:292:VAL:CA[2_556]  | 1.28                     | 0.92              |
| 1:A:123:MET:C   | 1:A:316:GLY:N[2_556]   | 1.28                     | 0.92              |
| 1:A:151:VAL:CG2 | 3:A:378:NTN:NI2[2_555] | 1.29                     | 0.91              |
| 1:A:8:LYS:CA    | 1:A:148:GLN:CA[2_555]  | 1.29                     | 0.91              |
| 1:A:103:CYS:O   | 1:A:325:LYS:N[2_556]   | 1.29                     | 0.91              |
| 1:A:112:LEU:CB  | 1:A:319:PHE:CG[2_556]  | 1.29                     | 0.91              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:A:120:ARG:NH2 | 1:A:291:ILE:C[2_556]   | 1.29                     | 0.91              |
| 1:A:8:LYS:CE    | 1:A:149:TYR:CA[2_555]  | 1.31                     | 0.89              |
| 1:A:97:CYS:C    | 1:A:323:LYS:N[2_556]   | 1.31                     | 0.89              |
| 1:A:24:GLU:O    | 1:A:25:GLU:N[2_555]    | 1.32                     | 0.88              |
| 1:A:120:ARG:CZ  | 1:A:291:ILE:C[2_556]   | 1.32                     | 0.88              |
| 1:A:288:VAL:CA  | 3:A:382:NTN:CI6[2_556] | 1.32                     | 0.88              |
| 1:A:103:CYS:SG  | 1:A:324:SER:N[2_556]   | 1.33                     | 0.87              |
| 1:A:1:SER:C     | 1:A:39:LYS:CB[2_555]   | 1.33                     | 0.87              |
| 1:A:9:CYS:N     | 1:A:148:GLN:CG[2_555]  | 1.33                     | 0.87              |
| 1:A:113:LYS:NZ  | 1:A:321:GLY:N[2_556]   | 1.33                     | 0.87              |
| 1:A:104:LYS:CD  | 1:A:329:PRO:CD[2_556]  | 1.34                     | 0.86              |
| 1:A:34:HIS:CA   | 3:A:391:NTN:CI2[2_556] | 1.36                     | 0.84              |
| 1:A:122:THR:CG2 | 1:A:291:ILE:CD1[2_556] | 1.36                     | 0.84              |
| 1:A:24:GLU:OE2  | 3:A:379:NTN:CI3[2_555] | 1.36                     | 0.84              |
| 1:A:104:LYS:N   | 1:A:325:LYS:N[2_556]   | 1.36                     | 0.84              |
| 1:A:95:PRO:C    | 1:A:109:ASN:CA[2_556]  | 1.37                     | 0.83              |
| 1:A:320:GLY:CA  | 3:A:386:NTN:CI6[2_556] | 1.37                     | 0.83              |
| 1:A:23:ILE:N    | 1:A:133:ARG:NH2[2_555] | 1.37                     | 0.83              |
| 1:A:34:HIS:CA   | 3:A:391:NTN:NI1[2_556] | 1.38                     | 0.82              |
| 1:A:24:GLU:O    | 1:A:25:GLU:CB[2_555]   | 1.38                     | 0.82              |
| 1:A:104:LYS:NZ  | 1:A:329:PRO:CA[2_556]  | 1.38                     | 0.82              |
| 1:A:27:GLU:OE2  | 1:A:353:GLU:CG[2_555]  | 1.38                     | 0.82              |
| 1:A:94:THR:CG2  | 1:A:110:PHE:C[2_556]   | 1.39                     | 0.81              |
| 1:A:112:LEU:CG  | 1:A:319:PHE:CD1[2_556] | 1.39                     | 0.81              |
| 1:A:35:GLU:N    | 3:A:391:NTN:CI2[2_556] | 1.39                     | 0.81              |
| 1:A:107:GLU:C   | 1:A:155:ILE:O[2_556]   | 1.40                     | 0.80              |
| 1:A:110:PHE:CD1 | 1:A:114:ASN:CG[2_556]  | 1.40                     | 0.80              |
| 1:A:113:LYS:CA  | 1:A:318:ILE:C[2_556]   | 1.40                     | 0.80              |
| 1:A:103:CYS:CA  | 1:A:325:LYS:N[2_556]   | 1.40                     | 0.80              |
| 1:A:95:PRO:CD   | 1:A:110:PHE:CA[2_556]  | 1.41                     | 0.79              |
| 1:A:103:CYS:N   | 1:A:324:SER:CB[2_556]  | 1.41                     | 0.79              |
| 1:A:128:SER:N   | 1:A:314:TRP:CB[2_556]  | 1.41                     | 0.79              |
| 1:A:105:HIS:CE1 | 1:A:157:VAL:CA[2_556]  | 1.41                     | 0.79              |
| 1:A:10:LYS:CD   | 1:A:26:VAL:CA[2_555]   | 1.41                     | 0.79              |
| 1:A:107:GLU:CA  | 1:A:155:ILE:CA[2_556]  | 1.41                     | 0.79              |
| 1:A:92:LEU:CD2  | 1:A:102:VAL:N[2_556]   | 1.42                     | 0.78              |
| 1:A:105:HIS:NE2 | 1:A:157:VAL:CA[2_556]  | 1.43                     | 0.77              |
| 1:A:112:LEU:CB  | 1:A:319:PHE:CB[2_556]  | 1.43                     | 0.77              |
| 1:A:22:SER:O    | 1:A:133:ARG:NH2[2_555] | 1.43                     | 0.77              |
| 1:A:125:ASP:CA  | 1:A:290:VAL:CG2[2_556] | 1.43                     | 0.77              |
| 1:A:94:THR:CB   | 1:A:110:PHE:O[2_556]   | 1.43                     | 0.77              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:A:113:LYS:CB  | 1:A:318:ILE:O[2_556]   | 1.44                     | 0.76              |
| 1:A:127:THR:C   | 1:A:314:TRP:CA[2_556]  | 1.44                     | 0.76              |
| 1:A:103:CYS:CA  | 1:A:324:SER:C[2_556]   | 1.44                     | 0.76              |
| 1:A:34:HIS:O    | 3:A:391:NTN:CI2[2_556] | 1.45                     | 0.75              |
| 1:A:106:PRO:C   | 1:A:154:GLU:O[2_556]   | 1.45                     | 0.75              |
| 1:A:8:LYS:CA    | 1:A:148:GLN:CG[2_555]  | 1.46                     | 0.74              |
| 1:A:97:CYS:CB   | 1:A:322:PHE:CA[2_556]  | 1.46                     | 0.74              |
| 1:A:95:PRO:N    | 1:A:110:PHE:N[2_556]   | 1.46                     | 0.74              |
| 1:A:116:LEU:CD2 | 1:A:117:SER:CB[2_556]  | 1.47                     | 0.73              |
| 1:A:105:HIS:CD2 | 1:A:157:VAL:C[2_556]   | 1.47                     | 0.73              |
| 1:A:10:LYS:CE   | 1:A:26:VAL:CB[2_555]   | 1.47                     | 0.73              |
| 1:A:11:ALA:C    | 1:A:25:GLU:OE1[2_555]  | 1.47                     | 0.73              |
| 1:A:37:ARG:NH2  | 3:A:383:NTN:NI1[2_555] | 1.47                     | 0.73              |
| 1:A:104:LYS:NZ  | 1:A:330:LYS:N[2_556]   | 1.47                     | 0.73              |
| 1:A:101:ARG:CZ  | 1:A:173:GLY:C[2_556]   | 1.47                     | 0.73              |
| 1:A:149:TYR:CZ  | 1:A:149:TYR:OH[2_555]  | 1.48                     | 0.72              |
| 1:A:23:ILE:CA   | 1:A:133:ARG:CZ[2_555]  | 1.48                     | 0.72              |
| 1:A:104:LYS:CD  | 1:A:327:SER:C[2_556]   | 1.48                     | 0.72              |
| 1:A:107:GLU:O   | 1:A:156:SER:C[2_556]   | 1.48                     | 0.72              |
| 1:A:1:SER:CB    | 1:A:40:MET:CA[2_555]   | 1.48                     | 0.72              |
| 1:A:98:GLY:C    | 1:A:323:LYS:O[2_556]   | 1.49                     | 0.71              |
| 1:A:107:GLU:N   | 1:A:154:GLU:C[2_556]   | 1.49                     | 0.71              |
| 1:A:114:ASN:N   | 1:A:318:ILE:CB[2_556]  | 1.49                     | 0.71              |
| 1:A:3:ALA:CB    | 3:A:383:NTN:CI2[2_555] | 1.49                     | 0.71              |
| 1:A:320:GLY:N   | 3:A:386:NTN:CI6[2_556] | 1.49                     | 0.71              |
| 1:A:166:LEU:CD1 | 3:A:377:NTN:NI1[2_555] | 1.49                     | 0.71              |
| 1:A:82:THR:CG2  | 1:A:106:PRO:CG[2_556]  | 1.50                     | 0.70              |
| 1:A:103:CYS:C   | 1:A:325:LYS:CA[2_556]  | 1.50                     | 0.70              |
| 1:A:1:SER:C     | 1:A:39:LYS:C[2_555]    | 1.50                     | 0.70              |
| 1:A:24:GLU:OE2  | 3:A:379:NTN:NI2[2_555] | 1.50                     | 0.70              |
| 1:A:131:THR:CG2 | 1:A:353:GLU:OE1[2_555] | 1.50                     | 0.70              |
| 1:A:24:GLU:C    | 1:A:25:GLU:CA[2_555]   | 1.51                     | 0.69              |
| 1:A:96:GLN:N    | 1:A:109:ASN:N[2_556]   | 1.51                     | 0.69              |
| 1:A:282:CYS:SG  | 3:A:382:NTN:NI2[2_556] | 1.51                     | 0.69              |
| 1:A:172:ILE:CG2 | 3:A:385:NTN:CI2[2_556] | 1.51                     | 0.69              |
| 1:A:98:GLY:C    | 1:A:327:SER:OG[2_556]  | 1.51                     | 0.69              |
| 1:A:34:HIS:CD2  | 1:A:188:LYS:CE[2_556]  | 1.51                     | 0.69              |
| 1:A:95:PRO:C    | 1:A:108:GLY:C[2_556]   | 1.52                     | 0.68              |
| 1:A:24:GLU:CD   | 3:A:379:NTN:CI4[2_555] | 1.52                     | 0.68              |
| 1:A:10:LYS:N    | 1:A:10:LYS:N[2_555]    | 1.52                     | 0.68              |
| 1:A:126:GLY:O   | 1:A:314:TRP:CD1[2_556] | 1.52                     | 0.68              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:A:94:THR:C    | 1:A:110:PHE:O[2_556]   | 1.52                     | 0.68              |
| 1:A:97:CYS:CA   | 1:A:323:LYS:N[2_556]   | 1.52                     | 0.68              |
| 1:A:95:PRO:CD   | 1:A:110:PHE:CB[2_556]  | 1.53                     | 0.67              |
| 1:A:96:GLN:O    | 1:A:323:LYS:CD[2_556]  | 1.53                     | 0.67              |
| 1:A:5:LYS:N     | 3:A:383:NTN:CI4[2_555] | 1.53                     | 0.67              |
| 1:A:135:LYS:CA  | 1:A:305:PRO:CG[2_556]  | 1.53                     | 0.67              |
| 1:A:123:MET:C   | 1:A:315:LYS:C[2_556]   | 1.53                     | 0.67              |
| 1:A:113:LYS:CD  | 1:A:321:GLY:CA[2_556]  | 1.53                     | 0.67              |
| 1:A:113:LYS:C   | 1:A:318:ILE:CG2[2_556] | 1.55                     | 0.65              |
| 1:A:1:SER:OG    | 1:A:40:MET:C[2_555]    | 1.55                     | 0.65              |
| 1:A:105:HIS:CB  | 1:A:158:ALA:N[2_556]   | 1.55                     | 0.65              |
| 1:A:35:GLU:C    | 3:A:391:NTN:CI4[2_556] | 1.55                     | 0.65              |
| 1:A:134:GLY:C   | 1:A:305:PRO:CB[2_556]  | 1.55                     | 0.65              |
| 1:A:172:ILE:CG2 | 3:A:385:NTN:CI4[2_556] | 1.55                     | 0.65              |
| 1:A:28:VAL:CG1  | 3:A:378:NTN:CI6[2_555] | 1.55                     | 0.65              |
| 1:A:24:GLU:O    | 1:A:25:GLU:C[2_555]    | 1.55                     | 0.65              |
| 1:A:133:ARG:CA  | 1:A:353:GLU:OE2[2_555] | 1.56                     | 0.64              |
| 1:A:312:ARG:C   | 3:A:382:NTN:NI1[2_556] | 1.56                     | 0.64              |
| 1:A:7:ILE:O     | 1:A:148:GLN:CD[2_555]  | 1.56                     | 0.64              |
| 1:A:97:CYS:SG   | 1:A:322:PHE:CA[2_556]  | 1.56                     | 0.64              |
| 1:A:104:LYS:N   | 1:A:325:LYS:CA[2_556]  | 1.57                     | 0.63              |
| 1:A:101:ARG:NH2 | 1:A:173:GLY:CA[2_556]  | 1.57                     | 0.63              |
| 1:A:107:GLU:OE1 | 1:A:155:ILE:CG1[2_556] | 1.57                     | 0.63              |
| 1:A:104:LYS:CG  | 1:A:329:PRO:CD[2_556]  | 1.57                     | 0.63              |
| 1:A:1:SER:OG    | 1:A:40:MET:N[2_555]    | 1.57                     | 0.63              |
| 1:A:127:THR:CG2 | 1:A:313:THR:O[2_556]   | 1.57                     | 0.63              |
| 1:A:2:THR:N     | 1:A:39:LYS:O[2_555]    | 1.57                     | 0.63              |
| 1:A:105:HIS:CB  | 1:A:157:VAL:C[2_556]   | 1.57                     | 0.63              |
| 1:A:127:THR:CG2 | 1:A:314:TRP:CA[2_556]  | 1.58                     | 0.62              |
| 1:A:132:CYS:SG  | 3:A:379:NTN:CI3[2_555] | 1.58                     | 0.62              |
| 1:A:127:THR:CA  | 1:A:314:TRP:CG[2_556]  | 1.58                     | 0.62              |
| 1:A:107:GLU:CA  | 1:A:155:ILE:C[2_556]   | 1.58                     | 0.62              |
| 1:A:11:ALA:O    | 1:A:25:GLU:OE1[2_555]  | 1.59                     | 0.61              |
| 1:A:99:LYS:CB   | 1:A:327:SER:OG[2_556]  | 1.59                     | 0.61              |
| 1:A:23:ILE:CB   | 1:A:133:ARG:NE[2_555]  | 1.59                     | 0.61              |
| 1:A:105:HIS:CG  | 1:A:158:ALA:N[2_556]   | 1.59                     | 0.61              |
| 1:A:106:PRO:CD  | 1:A:157:VAL:O[2_556]   | 1.59                     | 0.61              |
| 1:A:125:ASP:O   | 1:A:289:SER:C[2_556]   | 1.59                     | 0.61              |
| 1:A:107:GLU:OE2 | 1:A:153:ASP:CG[2_556]  | 1.59                     | 0.61              |
| 1:A:1:SER:N     | 1:A:39:LYS:N[2_555]    | 1.59                     | 0.61              |
| 1:A:104:LYS:CD  | 1:A:328:VAL:N[2_556]   | 1.60                     | 0.60              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:A:288:VAL:N   | 3:A:382:NTN:CI6[2_556] | 1.60                     | 0.60              |
| 1:A:107:GLU:CB  | 1:A:154:GLU:C[2_556]   | 1.60                     | 0.60              |
| 1:A:123:MET:O   | 1:A:316:GLY:CA[2_556]  | 1.60                     | 0.60              |
| 1:A:103:CYS:CA  | 1:A:324:SER:CA[2_556]  | 1.60                     | 0.60              |
| 1:A:25:GLU:N    | 1:A:25:GLU:N[2_555]    | 1.60                     | 0.60              |
| 1:A:8:LYS:CG    | 1:A:149:TYR:N[2_555]   | 1.60                     | 0.60              |
| 1:A:7:ILE:C     | 1:A:148:GLN:NE2[2_555] | 1.60                     | 0.60              |
| 1:A:103:CYS:O   | 1:A:325:LYS:CA[2_556]  | 1.60                     | 0.60              |
| 1:A:35:GLU:CG   | 3:A:391:NTN:CI5[2_556] | 1.61                     | 0.59              |
| 1:A:120:ARG:NH2 | 1:A:291:ILE:O[2_556]   | 1.61                     | 0.59              |
| 1:A:1:SER:C     | 1:A:39:LYS:O[2_555]    | 1.61                     | 0.59              |
| 1:A:94:THR:O    | 1:A:102:VAL:CB[2_556]  | 1.61                     | 0.59              |
| 1:A:101:ARG:NH2 | 1:A:174:CYS:N[2_556]   | 1.61                     | 0.59              |
| 1:A:107:GLU:OE2 | 1:A:153:ASP:CB[2_556]  | 1.61                     | 0.59              |
| 1:A:101:ARG:NH1 | 1:A:173:GLY:C[2_556]   | 1.61                     | 0.59              |
| 1:A:3:ALA:CB    | 3:A:383:NTN:CI5[2_555] | 1.61                     | 0.59              |
| 1:A:104:LYS:CE  | 1:A:327:SER:O[2_556]   | 1.62                     | 0.58              |
| 1:A:12:ALA:N    | 1:A:25:GLU:OE1[2_555]  | 1.62                     | 0.58              |
| 1:A:320:GLY:CA  | 3:A:386:NTN:CI2[2_556] | 1.62                     | 0.58              |
| 1:A:92:LEU:CD2  | 1:A:101:ARG:O[2_556]   | 1.62                     | 0.58              |
| 1:A:41:VAL:CB   | 3:A:377:NTN:CI1[2_555] | 1.62                     | 0.58              |
| 1:A:101:ARG:CA  | 1:A:328:VAL:CG2[2_556] | 1.62                     | 0.58              |
| 1:A:110:PHE:CZ  | 1:A:114:ASN:ND2[2_556] | 1.62                     | 0.58              |
| 1:A:9:CYS:O     | 1:A:10:LYS:CB[2_555]   | 1.63                     | 0.57              |
| 1:A:104:LYS:CD  | 1:A:329:PRO:N[2_556]   | 1.63                     | 0.57              |
| 3:A:390:NTN:CI1 | 3:A:397:NTN:NI2[2_556] | 1.63                     | 0.57              |
| 1:A:98:GLY:O    | 1:A:327:SER:OG[2_556]  | 1.63                     | 0.57              |
| 1:A:34:HIS:C    | 3:A:391:NTN:CI1[2_556] | 1.64                     | 0.56              |
| 1:A:99:LYS:CB   | 1:A:327:SER:CA[2_556]  | 1.64                     | 0.56              |
| 1:A:1:SER:O     | 1:A:39:LYS:N[2_555]    | 1.64                     | 0.56              |
| 1:A:105:HIS:CD2 | 1:A:157:VAL:O[2_556]   | 1.64                     | 0.56              |
| 1:A:151:VAL:CG2 | 3:A:378:NTN:CI3[2_555] | 1.64                     | 0.56              |
| 1:A:24:GLU:CD   | 3:A:379:NTN:CI5[2_555] | 1.65                     | 0.55              |
| 1:A:94:THR:OG1  | 1:A:112:LEU:N[2_556]   | 1.65                     | 0.55              |
| 1:A:104:LYS:CA  | 1:A:325:LYS:CA[2_556]  | 1.65                     | 0.55              |
| 1:A:34:HIS:C    | 3:A:391:NTN:CI6[2_556] | 1.65                     | 0.55              |
| 1:A:182:SER:N   | 3:A:386:NTN:CI4[2_556] | 1.65                     | 0.55              |
| 1:A:136:PRO:CG  | 1:A:303:MET:CE[2_556]  | 1.65                     | 0.55              |
| 1:A:104:LYS:NZ  | 1:A:329:PRO:N[2_556]   | 1.65                     | 0.55              |
| 1:A:94:THR:C    | 1:A:102:VAL:CG2[2_556] | 1.65                     | 0.55              |
| 1:A:100:CYS:CB  | 1:A:319:PHE:CD2[2_556] | 1.66                     | 0.54              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:A:125:ASP:N   | 1:A:315:LYS:CB[2_556]  | 1.66                     | 0.54              |
| 1:A:4:GLY:C     | 3:A:383:NTN:NI2[2_555] | 1.66                     | 0.54              |
| 1:A:94:THR:CB   | 1:A:110:PHE:C[2_556]   | 1.66                     | 0.54              |
| 1:A:287:GLY:O   | 3:A:382:NTN:CI1[2_556] | 1.66                     | 0.54              |
| 1:A:105:HIS:O   | 1:A:325:LYS:CG[2_556]  | 1.66                     | 0.54              |
| 1:A:151:VAL:N   | 3:A:378:NTN:CI3[2_555] | 1.66                     | 0.54              |
| 1:A:8:LYS:CD    | 1:A:149:TYR:N[2_555]   | 1.67                     | 0.53              |
| 1:A:306:MET:CE  | 1:A:354:LYS:CD[1_556]  | 1.67                     | 0.53              |
| 3:A:390:NTN:NI1 | 3:A:397:NTN:CI4[2_556] | 1.67                     | 0.53              |
| 1:A:322:PHE:O   | 2:A:376:ZN:ZN[2_556]   | 1.67                     | 0.53              |
| 1:A:110:PHE:CG  | 1:A:114:ASN:CB[2_556]  | 1.67                     | 0.53              |
| 1:A:27:GLU:OE2  | 1:A:353:GLU:CB[2_555]  | 1.67                     | 0.53              |
| 1:A:109:ASN:O   | 1:A:111:CYS:CB[2_556]  | 1.67                     | 0.53              |
| 1:A:127:THR:C   | 1:A:314:TRP:C[2_556]   | 1.68                     | 0.52              |
| 1:A:23:ILE:CG1  | 1:A:133:ARG:CD[2_555]  | 1.68                     | 0.52              |
| 1:A:288:VAL:C   | 3:A:382:NTN:CI6[2_556] | 1.68                     | 0.52              |
| 1:A:99:LYS:CG   | 1:A:327:SER:C[2_556]   | 1.68                     | 0.52              |
| 1:A:34:HIS:CG   | 1:A:188:LYS:CD[2_556]  | 1.69                     | 0.51              |
| 1:A:120:ARG:NE  | 1:A:291:ILE:O[2_556]   | 1.70                     | 0.50              |
| 1:A:12:ALA:N    | 1:A:25:GLU:OE2[2_555]  | 1.70                     | 0.50              |
| 1:A:8:LYS:CB    | 1:A:148:GLN:N[2_555]   | 1.70                     | 0.50              |
| 1:A:150:THR:C   | 3:A:378:NTN:NI1[2_555] | 1.70                     | 0.50              |
| 1:A:94:THR:CA   | 1:A:110:PHE:C[2_556]   | 1.70                     | 0.50              |
| 1:A:95:PRO:CB   | 1:A:109:ASN:N[2_556]   | 1.70                     | 0.50              |
| 1:A:105:HIS:ND1 | 1:A:157:VAL:C[2_556]   | 1.70                     | 0.50              |
| 1:A:112:LEU:C   | 1:A:319:PHE:CB[2_556]  | 1.70                     | 0.50              |
| 1:A:24:GLU:OE1  | 3:A:379:NTN:NI2[2_555] | 1.71                     | 0.49              |
| 1:A:103:CYS:N   | 1:A:324:SER:OG[2_556]  | 1.71                     | 0.49              |
| 1:A:134:GLY:O   | 1:A:305:PRO:CG[2_556]  | 1.71                     | 0.49              |
| 1:A:105:HIS:C   | 1:A:325:LYS:CG[2_556]  | 1.71                     | 0.49              |
| 1:A:5:LYS:CD    | 1:A:41:VAL:CG1[2_555]  | 1.71                     | 0.49              |
| 1:A:107:GLU:CA  | 1:A:154:GLU:O[2_556]   | 1.72                     | 0.48              |
| 1:A:94:THR:CG2  | 1:A:111:CYS:CA[2_556]  | 1.72                     | 0.48              |
| 1:A:112:LEU:CD1 | 1:A:319:PHE:CD1[2_556] | 1.72                     | 0.48              |
| 1:A:8:LYS:CA    | 1:A:148:GLN:N[2_555]   | 1.72                     | 0.48              |
| 1:A:331:LEU:CG  | 3:A:385:NTN:CI1[2_556] | 1.72                     | 0.48              |
| 1:A:104:LYS:CB  | 1:A:325:LYS:O[2_556]   | 1.72                     | 0.48              |
| 1:A:107:GLU:OE2 | 1:A:153:ASP:OD1[2_556] | 1.72                     | 0.48              |
| 1:A:178:THR:C   | 3:A:386:NTN:NI2[2_556] | 1.72                     | 0.48              |
| 1:A:5:LYS:CE    | 1:A:41:VAL:CG2[2_555]  | 1.73                     | 0.47              |
| 1:A:109:ASN:CB  | 1:A:111:CYS:SG[2_556]  | 1.73                     | 0.47              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:A:24:GLU:C    | 1:A:25:GLU:CB[2_555]   | 1.73                     | 0.47              |
| 1:A:105:HIS:C   | 1:A:325:LYS:CD[2_556]  | 1.73                     | 0.47              |
| 1:A:113:LYS:N   | 1:A:318:ILE:O[2_556]   | 1.73                     | 0.47              |
| 1:A:9:CYS:CA    | 1:A:9:CYS:CA[2_555]    | 1.73                     | 0.47              |
| 1:A:108:GLY:CA  | 1:A:155:ILE:O[2_556]   | 1.73                     | 0.47              |
| 1:A:1:SER:N     | 1:A:38:ILE:C[2_555]    | 1.74                     | 0.46              |
| 1:A:126:GLY:CA  | 1:A:291:ILE:N[2_556]   | 1.74                     | 0.46              |
| 1:A:23:ILE:CG2  | 1:A:133:ARG:CD[2_555]  | 1.74                     | 0.46              |
| 1:A:105:HIS:CD2 | 1:A:157:VAL:N[2_556]   | 1.74                     | 0.46              |
| 1:A:42:ALA:CB   | 3:A:377:NTN:CI5[2_555] | 1.74                     | 0.46              |
| 1:A:98:GLY:N    | 1:A:323:LYS:CA[2_556]  | 1.75                     | 0.45              |
| 1:A:96:GLN:N    | 1:A:108:GLY:C[2_556]   | 1.75                     | 0.45              |
| 1:A:34:HIS:CB   | 1:A:188:LYS:CE[2_556]  | 1.75                     | 0.45              |
| 1:A:1:SER:CB    | 1:A:39:LYS:O[2_555]    | 1.76                     | 0.44              |
| 1:A:126:GLY:N   | 1:A:290:VAL:CA[2_556]  | 1.76                     | 0.44              |
| 1:A:123:MET:N   | 1:A:315:LYS:O[2_556]   | 1.76                     | 0.44              |
| 1:A:106:PRO:N   | 1:A:157:VAL:O[2_556]   | 1.76                     | 0.44              |
| 1:A:2:THR:CG2   | 1:A:72:ILE:CG2[2_555]  | 1.76                     | 0.44              |
| 1:A:1:SER:CA    | 1:A:39:LYS:CA[2_555]   | 1.76                     | 0.44              |
| 1:A:104:LYS:CE  | 1:A:330:LYS:N[2_556]   | 1.76                     | 0.44              |
| 1:A:35:GLU:CB   | 3:A:391:NTN:CI5[2_556] | 1.77                     | 0.43              |
| 1:A:105:HIS:CG  | 1:A:157:VAL:O[2_556]   | 1.77                     | 0.43              |
| 1:A:92:LEU:CB   | 1:A:102:VAL:CA[2_556]  | 1.77                     | 0.43              |
| 1:A:11:ALA:CA   | 1:A:25:GLU:CD[2_555]   | 1.77                     | 0.43              |
| 1:A:96:GLN:CB   | 1:A:108:GLY:O[2_556]   | 1.77                     | 0.43              |
| 1:A:24:GLU:CG   | 3:A:379:NTN:CI6[2_555] | 1.78                     | 0.42              |
| 1:A:95:PRO:CG   | 1:A:110:PHE:N[2_556]   | 1.78                     | 0.42              |
| 1:A:24:GLU:C    | 1:A:24:GLU:C[2_555]    | 1.78                     | 0.42              |
| 1:A:125:ASP:C   | 1:A:290:VAL:N[2_556]   | 1.79                     | 0.41              |
| 1:A:34:HIS:CA   | 1:A:188:LYS:NZ[2_556]  | 1.79                     | 0.41              |
| 1:A:35:GLU:N    | 3:A:391:NTN:NI2[2_556] | 1.79                     | 0.41              |
| 1:A:9:CYS:CA    | 1:A:10:LYS:N[2_555]    | 1.79                     | 0.41              |
| 1:A:9:CYS:C     | 1:A:10:LYS:CA[2_555]   | 1.80                     | 0.40              |
| 1:A:166:LEU:C   | 3:A:377:NTN:CI4[2_555] | 1.80                     | 0.40              |
| 1:A:2:THR:CA    | 1:A:39:LYS:CG[2_555]   | 1.80                     | 0.40              |
| 1:A:23:ILE:CB   | 1:A:133:ARG:CG[2_555]  | 1.80                     | 0.40              |
| 1:A:112:LEU:CB  | 1:A:319:PHE:CD1[2_556] | 1.80                     | 0.40              |
| 1:A:8:LYS:CD    | 1:A:149:TYR:CB[2_555]  | 1.80                     | 0.40              |
| 1:A:110:PHE:CE1 | 1:A:114:ASN:CB[2_556]  | 1.81                     | 0.39              |
| 1:A:1:SER:C     | 1:A:39:LYS:N[2_555]    | 1.81                     | 0.39              |
| 1:A:94:THR:OG1  | 1:A:111:CYS:C[2_556]   | 1.81                     | 0.39              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:A:166:LEU:O   | 3:A:377:NTN:NI2[2_555] | 1.81                     | 0.39              |
| 1:A:8:LYS:NZ    | 1:A:149:TYR:O[2_555]   | 1.81                     | 0.39              |
| 1:A:108:GLY:N   | 1:A:156:SER:N[2_556]   | 1.81                     | 0.39              |
| 1:A:2:THR:N     | 1:A:39:LYS:CG[2_555]   | 1.81                     | 0.39              |
| 1:A:178:THR:CA  | 3:A:386:NTN:CI5[2_556] | 1.81                     | 0.39              |
| 1:A:123:MET:O   | 1:A:315:LYS:O[2_556]   | 1.82                     | 0.38              |
| 1:A:92:LEU:CD1  | 1:A:102:VAL:CA[2_556]  | 1.82                     | 0.38              |
| 1:A:92:LEU:CD1  | 1:A:102:VAL:C[2_556]   | 1.82                     | 0.38              |
| 1:A:99:LYS:CG   | 1:A:327:SER:CB[2_556]  | 1.82                     | 0.38              |
| 1:A:35:GLU:CG   | 3:A:391:NTN:NI2[2_556] | 1.82                     | 0.38              |
| 1:A:99:LYS:CD   | 1:A:331:LEU:CD2[2_556] | 1.82                     | 0.38              |
| 1:A:95:PRO:CB   | 1:A:109:ASN:CA[2_556]  | 1.82                     | 0.38              |
| 1:A:126:GLY:O   | 1:A:314:TRP:NE1[2_556] | 1.82                     | 0.38              |
| 1:A:26:VAL:CG1  | 3:A:379:NTN:NI1[2_555] | 1.82                     | 0.38              |
| 1:A:10:LYS:CG   | 1:A:25:GLU:C[2_555]    | 1.83                     | 0.37              |
| 1:A:8:LYS:CE    | 1:A:149:TYR:CB[2_555]  | 1.83                     | 0.37              |
| 1:A:113:LYS:CE  | 1:A:321:GLY:CA[2_556]  | 1.83                     | 0.37              |
| 1:A:95:PRO:CB   | 1:A:110:PHE:N[2_556]   | 1.83                     | 0.37              |
| 1:A:37:ARG:CZ   | 3:A:383:NTN:NI1[2_555] | 1.83                     | 0.37              |
| 1:A:8:LYS:CB    | 1:A:149:TYR:N[2_555]   | 1.83                     | 0.37              |
| 1:A:92:LEU:CG   | 1:A:102:VAL:CA[2_556]  | 1.83                     | 0.37              |
| 1:A:112:LEU:CA  | 1:A:319:PHE:CB[2_556]  | 1.83                     | 0.37              |
| 1:A:4:GLY:C     | 3:A:383:NTN:CI4[2_555] | 1.83                     | 0.37              |
| 1:A:105:HIS:CD2 | 1:A:157:VAL:CB[2_556]  | 1.83                     | 0.37              |
| 1:A:178:THR:O   | 3:A:386:NTN:CI5[2_556] | 1.83                     | 0.37              |
| 1:A:112:LEU:O   | 1:A:319:PHE:CA[2_556]  | 1.84                     | 0.36              |
| 1:A:11:ALA:O    | 1:A:25:GLU:OE2[2_555]  | 1.84                     | 0.36              |
| 1:A:12:ALA:N    | 1:A:25:GLU:CD[2_555]   | 1.84                     | 0.36              |
| 1:A:8:LYS:CD    | 1:A:149:TYR:CA[2_555]  | 1.84                     | 0.36              |
| 1:A:27:GLU:CD   | 1:A:353:GLU:CB[2_555]  | 1.84                     | 0.36              |
| 1:A:99:LYS:CG   | 1:A:327:SER:O[2_556]   | 1.84                     | 0.36              |
| 1:A:96:GLN:CB   | 1:A:323:LYS:NZ[2_556]  | 1.84                     | 0.36              |
| 1:A:101:ARG:NH1 | 1:A:173:GLY:O[2_556]   | 1.84                     | 0.36              |
| 1:A:11:ALA:O    | 1:A:25:GLU:CB[2_555]   | 1.84                     | 0.36              |
| 1:A:10:LYS:CG   | 1:A:26:VAL:CA[2_555]   | 1.84                     | 0.36              |
| 1:A:122:THR:CB  | 1:A:315:LYS:O[2_556]   | 1.84                     | 0.36              |
| 1:A:23:ILE:CA   | 1:A:133:ARG:NH2[2_555] | 1.84                     | 0.36              |
| 1:A:104:LYS:C   | 1:A:325:LYS:CA[2_556]  | 1.84                     | 0.36              |
| 1:A:35:GLU:O    | 3:A:391:NTN:CI4[2_556] | 1.85                     | 0.35              |
| 1:A:288:VAL:C   | 3:A:382:NTN:CI5[2_556] | 1.85                     | 0.35              |
| 1:A:135:LYS:N   | 1:A:305:PRO:CG[2_556]  | 1.85                     | 0.35              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:A:8:LYS:CB    | 1:A:148:GLN:CB[2_555]  | 1.85                     | 0.35              |
| 1:A:1:SER:CA    | 1:A:40:MET:N[2_555]    | 1.86                     | 0.34              |
| 1:A:99:LYS:C    | 1:A:327:SER:CB[2_556]  | 1.86                     | 0.34              |
| 1:A:97:CYS:CB   | 1:A:323:LYS:N[2_556]   | 1.86                     | 0.34              |
| 1:A:5:LYS:CA    | 3:A:383:NTN:NI2[2_555] | 1.86                     | 0.34              |
| 1:A:97:CYS:SG   | 1:A:323:LYS:N[2_556]   | 1.86                     | 0.34              |
| 1:A:313:THR:N   | 3:A:382:NTN:CI1[2_556] | 1.86                     | 0.34              |
| 1:A:113:LYS:CE  | 1:A:321:GLY:N[2_556]   | 1.87                     | 0.33              |
| 1:A:96:GLN:N    | 1:A:108:GLY:O[2_556]   | 1.87                     | 0.33              |
| 1:A:100:CYS:SG  | 1:A:319:PHE:CD2[2_556] | 1.87                     | 0.33              |
| 1:A:8:LYS:NZ    | 1:A:149:TYR:C[2_555]   | 1.88                     | 0.32              |
| 1:A:9:CYS:CA    | 1:A:9:CYS:CB[2_555]    | 1.88                     | 0.32              |
| 1:A:124:GLN:CG  | 1:A:317:ALA:CB[2_556]  | 1.88                     | 0.32              |
| 1:A:5:LYS:N     | 3:A:383:NTN:CI5[2_555] | 1.88                     | 0.32              |
| 1:A:104:LYS:CE  | 1:A:329:PRO:N[2_556]   | 1.88                     | 0.32              |
| 1:A:321:GLY:N   | 3:A:386:NTN:CI1[2_556] | 1.88                     | 0.32              |
| 1:A:103:CYS:O   | 1:A:326:ASP:N[2_556]   | 1.88                     | 0.32              |
| 1:A:100:CYS:CA  | 1:A:319:PHE:CE2[2_556] | 1.88                     | 0.32              |
| 1:A:7:ILE:C     | 1:A:148:GLN:CD[2_555]  | 1.88                     | 0.32              |
| 1:A:103:CYS:CB  | 1:A:323:LYS:C[2_556]   | 1.88                     | 0.32              |
| 1:A:100:CYS:CB  | 1:A:319:PHE:CZ[2_556]  | 1.88                     | 0.32              |
| 1:A:27:GLU:OE1  | 1:A:353:GLU:CB[2_555]  | 1.88                     | 0.32              |
| 1:A:11:ALA:N    | 1:A:25:GLU:CG[2_555]   | 1.88                     | 0.32              |
| 1:A:112:LEU:CG  | 1:A:319:PHE:CG[2_556]  | 1.88                     | 0.32              |
| 1:A:166:LEU:C   | 3:A:377:NTN:CI3[2_555] | 1.88                     | 0.32              |
| 1:A:105:HIS:CD2 | 1:A:157:VAL:CG1[2_556] | 1.89                     | 0.31              |
| 1:A:149:TYR:C   | 3:A:378:NTN:NI1[2_555] | 1.89                     | 0.31              |
| 1:A:99:LYS:O    | 1:A:322:PHE:CB[2_556]  | 1.89                     | 0.31              |
| 1:A:150:THR:C   | 3:A:378:NTN:CI3[2_555] | 1.89                     | 0.31              |
| 1:A:94:THR:CB   | 1:A:111:CYS:C[2_556]   | 1.89                     | 0.31              |
| 1:A:101:ARG:CZ  | 1:A:173:GLY:O[2_556]   | 1.89                     | 0.31              |
| 1:A:32:LYS:CE   | 1:A:313:THR:CB[2_556]  | 1.89                     | 0.31              |
| 1:A:35:GLU:OE2  | 1:A:315:LYS:NZ[2_556]  | 1.90                     | 0.30              |
| 1:A:95:PRO:CA   | 1:A:110:PHE:N[2_556]   | 1.90                     | 0.30              |
| 1:A:320:GLY:C   | 3:A:386:NTN:CI1[2_556] | 1.90                     | 0.30              |
| 1:A:282:CYS:SG  | 3:A:382:NTN:CI5[2_556] | 1.91                     | 0.29              |
| 1:A:95:PRO:CG   | 1:A:109:ASN:OD1[2_556] | 1.91                     | 0.29              |
| 1:A:96:GLN:CA   | 1:A:108:GLY:O[2_556]   | 1.91                     | 0.29              |
| 1:A:8:LYS:N     | 1:A:148:GLN:CG[2_555]  | 1.91                     | 0.29              |
| 1:A:10:LYS:CE   | 1:A:26:VAL:CG1[2_555]  | 1.91                     | 0.29              |
| 1:A:178:THR:C   | 3:A:386:NTN:CI5[2_556] | 1.91                     | 0.29              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:A:2:THR:N     | 1:A:39:LYS:CB[2_555]   | 1.91                     | 0.29              |
| 1:A:331:LEU:CD1 | 3:A:385:NTN:NI1[2_556] | 1.92                     | 0.28              |
| 1:A:107:GLU:O   | 1:A:157:VAL:N[2_556]   | 1.92                     | 0.28              |
| 1:A:103:CYS:N   | 1:A:324:SER:C[2_556]   | 1.92                     | 0.28              |
| 1:A:178:THR:O   | 3:A:386:NTN:CI4[2_556] | 1.92                     | 0.28              |
| 1:A:107:GLU:C   | 1:A:156:SER:CA[2_556]  | 1.92                     | 0.28              |
| 1:A:95:PRO:CA   | 1:A:109:ASN:CA[2_556]  | 1.92                     | 0.28              |
| 1:A:103:CYS:SG  | 1:A:323:LYS:C[2_556]   | 1.92                     | 0.28              |
| 1:A:105:HIS:ND1 | 1:A:158:ALA:N[2_556]   | 1.93                     | 0.27              |
| 1:A:104:LYS:N   | 1:A:325:LYS:C[2_556]   | 1.93                     | 0.27              |
| 1:A:95:PRO:CB   | 1:A:109:ASN:CG[2_556]  | 1.93                     | 0.27              |
| 1:A:103:CYS:CB  | 1:A:324:SER:C[2_556]   | 1.93                     | 0.27              |
| 1:A:92:LEU:CD2  | 1:A:101:ARG:CA[2_556]  | 1.93                     | 0.27              |
| 1:A:114:ASN:ND2 | 1:A:116:LEU:CD1[2_556] | 1.93                     | 0.27              |
| 1:A:10:LYS:CD   | 1:A:26:VAL:N[2_555]    | 1.93                     | 0.27              |
| 1:A:96:GLN:OE1  | 1:A:96:GLN:OE1[2_556]  | 1.93                     | 0.27              |
| 1:A:106:PRO:CA  | 3:A:397:NTN:NI1[2_556] | 1.93                     | 0.27              |
| 1:A:34:HIS:O    | 3:A:391:NTN:CI6[2_556] | 1.93                     | 0.27              |
| 1:A:35:GLU:CA   | 3:A:391:NTN:CI3[2_556] | 1.93                     | 0.27              |
| 1:A:23:ILE:CB   | 1:A:133:ARG:CD[2_555]  | 1.94                     | 0.26              |
| 1:A:127:THR:N   | 1:A:315:LYS:N[2_556]   | 1.94                     | 0.26              |
| 1:A:125:ASP:C   | 1:A:290:VAL:CB[2_556]  | 1.94                     | 0.26              |
| 1:A:100:CYS:SG  | 1:A:319:PHE:CE2[2_556] | 1.94                     | 0.26              |
| 1:A:113:LYS:C   | 1:A:318:ILE:CB[2_556]  | 1.94                     | 0.26              |
| 1:A:114:ASN:CA  | 1:A:318:ILE:CG2[2_556] | 1.94                     | 0.26              |
| 1:A:110:PHE:CD1 | 1:A:114:ASN:ND2[2_556] | 1.94                     | 0.26              |
| 1:A:98:GLY:N    | 1:A:323:LYS:N[2_556]   | 1.94                     | 0.26              |
| 1:A:103:CYS:CA  | 1:A:324:SER:OG[2_556]  | 1.95                     | 0.25              |
| 1:A:10:LYS:NZ   | 1:A:26:VAL:CG2[2_555]  | 1.95                     | 0.25              |
| 1:A:94:THR:N    | 1:A:110:PHE:O[2_556]   | 1.95                     | 0.25              |
| 1:A:127:THR:CB  | 1:A:314:TRP:N[2_556]   | 1.95                     | 0.25              |
| 1:A:107:GLU:O   | 1:A:155:ILE:C[2_556]   | 1.95                     | 0.25              |
| 1:A:97:CYS:CB   | 1:A:322:PHE:N[2_556]   | 1.95                     | 0.25              |
| 1:A:1:SER:CA    | 1:A:39:LYS:N[2_555]    | 1.95                     | 0.25              |
| 1:A:104:LYS:CB  | 1:A:329:PRO:CD[2_556]  | 1.95                     | 0.25              |
| 1:A:96:GLN:N    | 1:A:109:ASN:CB[2_556]  | 1.95                     | 0.25              |
| 1:A:92:LEU:CG   | 1:A:102:VAL:N[2_556]   | 1.95                     | 0.25              |
| 1:A:122:THR:OG1 | 1:A:315:LYS:O[2_556]   | 1.95                     | 0.25              |
| 1:A:41:VAL:CB   | 3:A:377:NTN:NI1[2_555] | 1.96                     | 0.24              |
| 1:A:134:GLY:C   | 1:A:305:PRO:CG[2_556]  | 1.96                     | 0.24              |
| 1:A:114:ASN:O   | 1:A:318:ILE:CB[2_556]  | 1.96                     | 0.24              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:A:95:PRO:CA   | 1:A:108:GLY:C[2_556]   | 1.96                     | 0.24              |
| 1:A:150:THR:N   | 3:A:378:NTN:CI1[2_555] | 1.97                     | 0.23              |
| 1:A:126:GLY:C   | 1:A:314:TRP:CD1[2_556] | 1.97                     | 0.23              |
| 1:A:129:ARG:CZ  | 1:A:313:THR:OG1[2_556] | 1.97                     | 0.23              |
| 1:A:94:THR:CB   | 1:A:111:CYS:N[2_556]   | 1.97                     | 0.23              |
| 1:A:8:LYS:O     | 1:A:148:GLN:CG[2_555]  | 1.98                     | 0.22              |
| 1:A:113:LYS:N   | 1:A:318:ILE:C[2_556]   | 1.98                     | 0.22              |
| 1:A:105:HIS:ND1 | 1:A:157:VAL:CB[2_556]  | 1.98                     | 0.22              |
| 1:A:97:CYS:SG   | 1:A:322:PHE:CB[2_556]  | 1.98                     | 0.22              |
| 1:A:150:THR:O   | 3:A:378:NTN:NI1[2_555] | 1.98                     | 0.22              |
| 1:A:95:PRO:CB   | 1:A:109:ASN:C[2_556]   | 1.98                     | 0.22              |
| 1:A:35:GLU:N    | 3:A:391:NTN:CI6[2_556] | 1.98                     | 0.22              |
| 1:A:150:THR:CA  | 3:A:378:NTN:CI1[2_555] | 1.98                     | 0.22              |
| 1:A:151:VAL:CB  | 3:A:378:NTN:CI3[2_555] | 1.99                     | 0.21              |
| 1:A:35:GLU:CB   | 3:A:391:NTN:CI4[2_556] | 1.99                     | 0.21              |
| 1:A:94:THR:CB   | 1:A:111:CYS:CA[2_556]  | 1.99                     | 0.21              |
| 1:A:105:HIS:NE2 | 1:A:157:VAL:CG2[2_556] | 1.99                     | 0.21              |
| 1:A:23:ILE:O    | 1:A:25:GLU:O[2_555]    | 1.99                     | 0.21              |
| 1:A:127:THR:CA  | 1:A:314:TRP:CD1[2_556] | 1.99                     | 0.21              |
| 1:A:104:LYS:CD  | 1:A:327:SER:O[2_556]   | 1.99                     | 0.21              |
| 1:A:12:ALA:CA   | 1:A:25:GLU:OE1[2_555]  | 2.00                     | 0.20              |
| 1:A:37:ARG:NH2  | 3:A:383:NTN:CI1[2_555] | 2.00                     | 0.20              |
| 1:A:124:GLN:CB  | 1:A:186:VAL:CG1[2_556] | 2.00                     | 0.20              |
| 1:A:114:ASN:O   | 1:A:318:ILE:CG1[2_556] | 2.00                     | 0.20              |
| 1:A:328:VAL:CG1 | 3:A:385:NTN:NI2[2_556] | 2.00                     | 0.20              |
| 1:A:94:THR:CG2  | 1:A:111:CYS:C[2_556]   | 2.00                     | 0.20              |
| 1:A:7:ILE:C     | 1:A:148:GLN:CB[2_555]  | 2.00                     | 0.20              |
| 1:A:34:HIS:O    | 3:A:391:NTN:CI1[2_556] | 2.00                     | 0.20              |
| 1:A:151:VAL:CA  | 3:A:378:NTN:CI4[2_555] | 2.01                     | 0.19              |
| 1:A:97:CYS:N    | 1:A:323:LYS:CG[2_556]  | 2.01                     | 0.19              |
| 1:A:129:ARG:NH2 | 1:A:313:THR:CB[2_556]  | 2.01                     | 0.19              |
| 1:A:151:VAL:CA  | 3:A:378:NTN:CI3[2_555] | 2.01                     | 0.19              |
| 1:A:103:CYS:N   | 1:A:324:SER:CA[2_556]  | 2.01                     | 0.19              |
| 1:A:34:HIS:CD2  | 1:A:188:LYS:CB[2_556]  | 2.01                     | 0.19              |
| 1:A:99:LYS:CG   | 1:A:327:SER:CA[2_556]  | 2.01                     | 0.19              |
| 1:A:108:GLY:N   | 1:A:155:ILE:CA[2_556]  | 2.01                     | 0.19              |
| 1:A:34:HIS:CE1  | 1:A:188:LYS:CE[2_556]  | 2.01                     | 0.19              |
| 1:A:95:PRO:C    | 1:A:108:GLY:O[2_556]   | 2.02                     | 0.18              |
| 1:A:112:LEU:CG  | 1:A:319:PHE:CE1[2_556] | 2.02                     | 0.18              |
| 1:A:8:LYS:N     | 1:A:148:GLN:CA[2_555]  | 2.02                     | 0.18              |
| 1:A:104:LYS:O   | 1:A:325:LYS:O[2_556]   | 2.02                     | 0.18              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:A:27:GLU:OE1  | 1:A:353:GLU:CA[2_555]  | 2.02                     | 0.18              |
| 1:A:23:ILE:CA   | 1:A:133:ARG:NE[2_555]  | 2.02                     | 0.18              |
| 1:A:172:ILE:CB  | 3:A:385:NTN:CI3[2_556] | 2.02                     | 0.18              |
| 1:A:97:CYS:O    | 1:A:323:LYS:N[2_556]   | 2.02                     | 0.18              |
| 1:A:105:HIS:N   | 1:A:325:LYS:CG[2_556]  | 2.02                     | 0.18              |
| 1:A:124:GLN:O   | 1:A:290:VAL:CG1[2_556] | 2.03                     | 0.17              |
| 1:A:35:GLU:CA   | 3:A:391:NTN:CI5[2_556] | 2.03                     | 0.17              |
| 1:A:97:CYS:N    | 1:A:323:LYS:CA[2_556]  | 2.03                     | 0.17              |
| 1:A:104:LYS:C   | 1:A:325:LYS:O[2_556]   | 2.03                     | 0.17              |
| 1:A:136:PRO:CG  | 1:A:303:MET:SD[2_556]  | 2.03                     | 0.17              |
| 1:A:1:SER:OG    | 1:A:40:MET:CB[2_555]   | 2.03                     | 0.17              |
| 1:A:112:LEU:C   | 1:A:319:PHE:N[2_556]   | 2.03                     | 0.17              |
| 1:A:4:GLY:CA    | 3:A:383:NTN:CI4[2_555] | 2.03                     | 0.17              |
| 1:A:328:VAL:CG1 | 3:A:385:NTN:CI6[2_556] | 2.03                     | 0.17              |
| 1:A:1:SER:N     | 1:A:39:LYS:C[2_555]    | 2.03                     | 0.17              |
| 1:A:96:GLN:CA   | 1:A:323:LYS:CG[2_556]  | 2.04                     | 0.16              |
| 1:A:8:LYS:C     | 1:A:148:GLN:CB[2_555]  | 2.04                     | 0.16              |
| 1:A:11:ALA:N    | 1:A:25:GLU:OE2[2_555]  | 2.04                     | 0.16              |
| 1:A:112:LEU:O   | 1:A:318:ILE:C[2_556]   | 2.04                     | 0.16              |
| 1:A:5:LYS:NZ    | 1:A:41:VAL:CA[2_555]   | 2.04                     | 0.16              |
| 1:A:27:GLU:CG   | 1:A:353:GLU:CG[2_555]  | 2.04                     | 0.16              |
| 1:A:32:LYS:NZ   | 1:A:287:GLY:O[2_556]   | 2.04                     | 0.16              |
| 1:A:8:LYS:CG    | 1:A:148:GLN:N[2_555]   | 2.04                     | 0.16              |
| 1:A:8:LYS:CE    | 1:A:149:TYR:N[2_555]   | 2.04                     | 0.16              |
| 1:A:10:LYS:CB   | 1:A:26:VAL:CA[2_555]   | 2.04                     | 0.16              |
| 1:A:101:ARG:N   | 1:A:328:VAL:CG2[2_556] | 2.04                     | 0.16              |
| 1:A:8:LYS:O     | 1:A:10:LYS:O[2_555]    | 2.04                     | 0.16              |
| 1:A:172:ILE:CB  | 3:A:385:NTN:CI4[2_556] | 2.04                     | 0.16              |
| 1:A:112:LEU:CD1 | 1:A:319:PHE:CE1[2_556] | 2.05                     | 0.15              |
| 1:A:104:LYS:CE  | 1:A:327:SER:C[2_556]   | 2.05                     | 0.15              |
| 1:A:8:LYS:C     | 1:A:148:GLN:CD[2_555]  | 2.05                     | 0.15              |
| 1:A:120:ARG:NH1 | 1:A:291:ILE:C[2_556]   | 2.05                     | 0.15              |
| 1:A:34:HIS:N    | 3:A:391:NTN:CI1[2_556] | 2.05                     | 0.15              |
| 1:A:122:THR:CG2 | 1:A:291:ILE:CG1[2_556] | 2.05                     | 0.15              |
| 1:A:151:VAL:CB  | 3:A:378:NTN:NI2[2_555] | 2.05                     | 0.15              |
| 1:A:127:THR:O   | 1:A:314:TRP:CA[2_556]  | 2.05                     | 0.15              |
| 1:A:99:LYS:N    | 1:A:323:LYS:C[2_556]   | 2.06                     | 0.14              |
| 1:A:105:HIS:CG  | 1:A:157:VAL:N[2_556]   | 2.06                     | 0.14              |
| 1:A:125:ASP:CB  | 1:A:290:VAL:CG2[2_556] | 2.06                     | 0.14              |
| 1:A:124:GLN:OE1 | 1:A:316:GLY:O[2_556]   | 2.06                     | 0.14              |
| 1:A:287:GLY:O   | 3:A:382:NTN:CI2[2_556] | 2.06                     | 0.14              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:A:124:GLN:N   | 1:A:316:GLY:N[2_556]   | 2.06                     | 0.14              |
| 1:A:92:LEU:CD1  | 1:A:102:VAL:O[2_556]   | 2.06                     | 0.14              |
| 1:A:23:ILE:CA   | 1:A:133:ARG:NH1[2_555] | 2.06                     | 0.14              |
| 1:A:99:LYS:CA   | 1:A:327:SER:CA[2_556]  | 2.06                     | 0.14              |
| 1:A:34:HIS:CE1  | 1:A:188:LYS:CD[2_556]  | 2.07                     | 0.13              |
| 1:A:113:LYS:NZ  | 1:A:320:GLY:C[2_556]   | 2.07                     | 0.13              |
| 1:A:94:THR:C    | 1:A:110:PHE:C[2_556]   | 2.07                     | 0.13              |
| 1:A:127:THR:CA  | 1:A:314:TRP:C[2_556]   | 2.07                     | 0.13              |
| 1:A:114:ASN:C   | 1:A:318:ILE:CD1[2_556] | 2.07                     | 0.13              |
| 1:A:97:CYS:CA   | 1:A:322:PHE:C[2_556]   | 2.08                     | 0.12              |
| 1:A:107:GLU:C   | 1:A:155:ILE:CA[2_556]  | 2.08                     | 0.12              |
| 1:A:99:LYS:N    | 1:A:327:SER:CB[2_556]  | 2.08                     | 0.12              |
| 1:A:10:LYS:CG   | 1:A:26:VAL:CG2[2_555]  | 2.08                     | 0.12              |
| 1:A:96:GLN:C    | 1:A:323:LYS:CB[2_556]  | 2.08                     | 0.12              |
| 1:A:113:LYS:C   | 1:A:318:ILE:O[2_556]   | 2.08                     | 0.12              |
| 1:A:23:ILE:N    | 1:A:133:ARG:CZ[2_555]  | 2.08                     | 0.12              |
| 1:A:107:GLU:CB  | 1:A:154:GLU:N[2_556]   | 2.08                     | 0.12              |
| 1:A:103:CYS:O   | 1:A:325:LYS:CB[2_556]  | 2.09                     | 0.11              |
| 1:A:1:SER:C     | 1:A:39:LYS:CG[2_555]   | 2.09                     | 0.11              |
| 1:A:104:LYS:CG  | 1:A:327:SER:N[2_556]   | 2.09                     | 0.11              |
| 1:A:125:ASP:OD1 | 1:A:315:LYS:N[2_556]   | 2.09                     | 0.11              |
| 1:A:41:VAL:CG1  | 3:A:377:NTN:CI1[2_555] | 2.09                     | 0.11              |
| 1:A:103:CYS:O   | 1:A:325:LYS:C[2_556]   | 2.09                     | 0.11              |
| 1:A:125:ASP:O   | 1:A:290:VAL:CB[2_556]  | 2.09                     | 0.11              |
| 1:A:97:CYS:CB   | 1:A:322:PHE:O[2_556]   | 2.09                     | 0.11              |
| 1:A:125:ASP:CA  | 1:A:290:VAL:CB[2_556]  | 2.09                     | 0.11              |
| 1:A:37:ARG:NE   | 3:A:383:NTN:NI1[2_555] | 2.10                     | 0.10              |
| 1:A:97:CYS:N    | 1:A:323:LYS:N[2_556]   | 2.10                     | 0.10              |
| 1:A:98:GLY:CA   | 1:A:323:LYS:CB[2_556]  | 2.10                     | 0.10              |
| 1:A:331:LEU:CB  | 3:A:385:NTN:CI1[2_556] | 2.10                     | 0.10              |
| 1:A:101:ARG:NH2 | 1:A:173:GLY:O[2_556]   | 2.10                     | 0.10              |
| 1:A:185:LYS:NZ  | 3:A:397:NTN:NI2[2_556] | 2.10                     | 0.10              |
| 1:A:4:GLY:N     | 3:A:383:NTN:NI2[2_555] | 2.10                     | 0.10              |
| 1:A:95:PRO:CA   | 1:A:109:ASN:C[2_556]   | 2.10                     | 0.10              |
| 1:A:124:GLN:CA  | 1:A:316:GLY:O[2_556]   | 2.10                     | 0.10              |
| 1:A:135:LYS:N   | 1:A:305:PRO:CB[2_556]  | 2.10                     | 0.10              |
| 1:A:106:PRO:CB  | 3:A:397:NTN:NI1[2_556] | 2.10                     | 0.10              |
| 1:A:103:CYS:CA  | 1:A:324:SER:CB[2_556]  | 2.10                     | 0.10              |
| 1:A:107:GLU:CA  | 1:A:156:SER:N[2_556]   | 2.10                     | 0.10              |
| 1:A:110:PHE:CE2 | 1:A:116:LEU:CG[2_556]  | 2.11                     | 0.09              |
| 1:A:9:CYS:CA    | 1:A:9:CYS:C[2_555]     | 2.11                     | 0.09              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:A:127:THR:OG1 | 1:A:289:SER:O[2_556]   | 2.11                     | 0.09              |
| 1:A:92:LEU:CB   | 1:A:102:VAL:CB[2_556]  | 2.11                     | 0.09              |
| 1:A:103:CYS:CB  | 1:A:324:SER:CB[2_556]  | 2.11                     | 0.09              |
| 1:A:34:HIS:CB   | 3:A:391:NTN:NI1[2_556] | 2.11                     | 0.09              |
| 1:A:104:LYS:CA  | 1:A:324:SER:O[2_556]   | 2.11                     | 0.09              |
| 1:A:312:ARG:CA  | 3:A:382:NTN:NI1[2_556] | 2.11                     | 0.09              |
| 1:A:100:CYS:SG  | 1:A:324:SER:CB[2_556]  | 2.11                     | 0.09              |
| 1:A:105:HIS:C   | 1:A:157:VAL:O[2_556]   | 2.11                     | 0.09              |
| 1:A:95:PRO:C    | 1:A:109:ASN:C[2_556]   | 2.11                     | 0.09              |
| 1:A:112:LEU:CD1 | 1:A:173:GLY:O[2_556]   | 2.12                     | 0.08              |
| 1:A:12:ALA:CA   | 1:A:133:ARG:NH1[2_555] | 2.12                     | 0.08              |
| 1:A:179:GLY:O   | 3:A:386:NTN:NI2[2_556] | 2.12                     | 0.08              |
| 1:A:4:GLY:N     | 3:A:383:NTN:CI4[2_555] | 2.12                     | 0.08              |
| 1:A:104:LYS:CD  | 1:A:328:VAL:C[2_556]   | 2.12                     | 0.08              |
| 1:A:120:ARG:CZ  | 1:A:292:VAL:N[2_556]   | 2.12                     | 0.08              |
| 1:A:5:LYS:CD    | 3:A:383:NTN:CI5[2_555] | 2.13                     | 0.07              |
| 1:A:127:THR:C   | 1:A:314:TRP:O[2_556]   | 2.13                     | 0.07              |
| 1:A:7:ILE:CD1   | 1:A:39:LYS:CE[2_555]   | 2.13                     | 0.07              |
| 1:A:109:ASN:ND2 | 1:A:113:LYS:CG[2_556]  | 2.13                     | 0.07              |
| 1:A:27:GLU:OE2  | 1:A:309:LEU:CD2[2_556] | 2.13                     | 0.07              |
| 1:A:127:THR:O   | 1:A:315:LYS:N[2_556]   | 2.13                     | 0.07              |
| 1:A:34:HIS:CG   | 3:A:391:NTN:CI1[2_556] | 2.13                     | 0.07              |
| 1:A:8:LYS:CG    | 1:A:148:GLN:C[2_555]   | 2.13                     | 0.07              |
| 1:A:105:HIS:CA  | 1:A:325:LYS:CG[2_556]  | 2.13                     | 0.07              |
| 1:A:172:ILE:CD1 | 3:A:385:NTN:CI3[2_556] | 2.13                     | 0.07              |
| 1:A:24:GLU:OE2  | 3:A:379:NTN:CI2[2_555] | 2.13                     | 0.07              |
| 1:A:35:GLU:N    | 3:A:391:NTN:CI5[2_556] | 2.13                     | 0.07              |
| 1:A:11:ALA:C    | 1:A:25:GLU:CG[2_555]   | 2.14                     | 0.06              |
| 1:A:123:MET:CA  | 1:A:315:LYS:C[2_556]   | 2.14                     | 0.06              |
| 1:A:39:LYS:CE   | 1:A:74:GLU:OE1[2_555]  | 2.14                     | 0.06              |
| 1:A:136:PRO:CB  | 1:A:303:MET:CE[2_556]  | 2.14                     | 0.06              |
| 1:A:105:HIS:N   | 1:A:325:LYS:CA[2_556]  | 2.14                     | 0.06              |
| 1:A:23:ILE:CD1  | 1:A:133:ARG:CB[2_555]  | 2.14                     | 0.06              |
| 1:A:127:THR:CB  | 1:A:289:SER:O[2_556]   | 2.14                     | 0.06              |
| 1:A:288:VAL:O   | 3:A:382:NTN:CI5[2_556] | 2.15                     | 0.05              |
| 1:A:105:HIS:NE2 | 1:A:157:VAL:N[2_556]   | 2.15                     | 0.05              |
| 1:A:35:GLU:CD   | 3:A:391:NTN:CI5[2_556] | 2.15                     | 0.05              |
| 1:A:104:LYS:NZ  | 1:A:328:VAL:C[2_556]   | 2.15                     | 0.05              |
| 1:A:132:CYS:SG  | 3:A:379:NTN:NI1[2_555] | 2.15                     | 0.05              |
| 1:A:149:TYR:C   | 3:A:378:NTN:CI1[2_555] | 2.15                     | 0.05              |
| 1:A:109:ASN:C   | 1:A:111:CYS:CB[2_556]  | 2.15                     | 0.05              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:A:5:LYS:CG    | 1:A:41:VAL:CG1[2_555]  | 2.15                     | 0.05              |
| 1:A:127:THR:CB  | 1:A:313:THR:O[2_556]   | 2.15                     | 0.05              |
| 3:A:390:NTN:NI1 | 3:A:397:NTN:CI5[2_556] | 2.15                     | 0.05              |
| 1:A:94:THR:OG1  | 1:A:112:LEU:CA[2_556]  | 2.15                     | 0.05              |
| 1:A:185:LYS:CE  | 3:A:397:NTN:NI2[2_556] | 2.15                     | 0.05              |
| 1:A:97:CYS:C    | 1:A:323:LYS:CA[2_556]  | 2.16                     | 0.04              |
| 1:A:23:ILE:CB   | 1:A:133:ARG:CB[2_555]  | 2.16                     | 0.04              |
| 1:A:27:GLU:OE1  | 1:A:353:GLU:CD[2_555]  | 2.16                     | 0.04              |
| 1:A:9:CYS:SG    | 1:A:148:GLN:OE1[2_555] | 2.16                     | 0.04              |
| 1:A:112:LEU:O   | 1:A:319:PHE:CB[2_556]  | 2.16                     | 0.04              |
| 1:A:34:HIS:NE2  | 1:A:188:LYS:CE[2_556]  | 2.16                     | 0.04              |
| 1:A:34:HIS:N    | 3:A:391:NTN:CI2[2_556] | 2.16                     | 0.04              |
| 1:A:92:LEU:CG   | 1:A:101:ARG:C[2_556]   | 2.17                     | 0.03              |
| 1:A:99:LYS:CA   | 1:A:323:LYS:O[2_556]   | 2.17                     | 0.03              |
| 1:A:320:GLY:CA  | 3:A:386:NTN:CI1[2_556] | 2.17                     | 0.03              |
| 1:A:105:HIS:ND1 | 1:A:157:VAL:CG2[2_556] | 2.17                     | 0.03              |
| 1:A:23:ILE:CB   | 1:A:133:ARG:CZ[2_555]  | 2.17                     | 0.03              |
| 1:A:10:LYS:CD   | 1:A:26:VAL:CG1[2_555]  | 2.17                     | 0.03              |
| 1:A:99:LYS:NZ   | 1:A:331:LEU:CD2[2_556] | 2.17                     | 0.03              |
| 1:A:120:ARG:NE  | 1:A:291:ILE:C[2_556]   | 2.17                     | 0.03              |
| 1:A:123:MET:C   | 1:A:315:LYS:CA[2_556]  | 2.17                     | 0.03              |
| 1:A:82:THR:CG2  | 1:A:106:PRO:CB[2_556]  | 2.17                     | 0.03              |
| 1:A:94:THR:CB   | 1:A:112:LEU:N[2_556]   | 2.18                     | 0.02              |
| 1:A:151:VAL:CG2 | 3:A:378:NTN:CI5[2_555] | 2.18                     | 0.02              |
| 1:A:106:PRO:C   | 1:A:154:GLU:C[2_556]   | 2.18                     | 0.02              |
| 1:A:127:THR:N   | 1:A:314:TRP:CD1[2_556] | 2.18                     | 0.02              |
| 1:A:124:GLN:N   | 1:A:316:GLY:O[2_556]   | 2.18                     | 0.02              |
| 1:A:94:THR:CG2  | 1:A:111:CYS:O[2_556]   | 2.18                     | 0.02              |
| 1:A:120:ARG:NH2 | 1:A:292:VAL:C[2_556]   | 2.18                     | 0.02              |
| 1:A:105:HIS:CA  | 1:A:157:VAL:O[2_556]   | 2.18                     | 0.02              |
| 1:A:133:ARG:N   | 1:A:353:GLU:OE2[2_555] | 2.19                     | 0.01              |
| 1:A:104:LYS:NZ  | 1:A:329:PRO:O[2_556]   | 2.19                     | 0.01              |
| 1:A:125:ASP:O   | 1:A:290:VAL:C[2_556]   | 2.19                     | 0.01              |
| 1:A:10:LYS:C    | 1:A:25:GLU:CG[2_555]   | 2.19                     | 0.01              |
| 1:A:98:GLY:CA   | 1:A:323:LYS:O[2_556]   | 2.19                     | 0.01              |
| 1:A:74:GLU:OE2  | 3:A:383:NTN:NI1[2_555] | 2.19                     | 0.01              |



## 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     | 372/374 (100%) | 247 (66%) | 69 (18%) | 56 (15%) | <b>0</b> <b>1</b> |

All (56) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 6   | VAL  |
| 1   | A     | 8   | LYS  |
| 1   | A     | 9   | CYS  |
| 1   | A     | 16  | GLU  |
| 1   | A     | 32  | LYS  |
| 1   | A     | 85  | PRO  |
| 1   | A     | 95  | PRO  |
| 1   | A     | 96  | GLN  |
| 1   | A     | 112 | LEU  |
| 1   | A     | 129 | ARG  |
| 1   | A     | 133 | ARG  |
| 1   | A     | 162 | ALA  |
| 1   | A     | 166 | LEU  |
| 1   | A     | 180 | TYR  |
| 1   | A     | 188 | LYS  |
| 1   | A     | 193 | SER  |
| 1   | A     | 226 | LYS  |
| 1   | A     | 301 | LEU  |
| 1   | A     | 320 | GLY  |
| 1   | A     | 338 | LYS  |
| 1   | A     | 339 | LYS  |
| 1   | A     | 365 | GLY  |
| 1   | A     | 366 | GLU  |
| 1   | A     | 17  | GLU  |
| 1   | A     | 20  | PRO  |
| 1   | A     | 86  | GLY  |
| 1   | A     | 99  | LYS  |
| 1   | A     | 117 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 153 | ASP  |
| 1   | A     | 172 | ILE  |
| 1   | A     | 253 | VAL  |
| 1   | A     | 256 | GLU  |
| 1   | A     | 257 | MET  |
| 1   | A     | 352 | PHE  |
| 1   | A     | 359 | PHE  |
| 1   | A     | 361 | LEU  |
| 1   | A     | 4   | GLY  |
| 1   | A     | 122 | THR  |
| 1   | A     | 165 | PRO  |
| 1   | A     | 217 | ALA  |
| 1   | A     | 230 | ALA  |
| 1   | A     | 274 | THR  |
| 1   | A     | 300 | ASN  |
| 1   | A     | 306 | MET  |
| 1   | A     | 36  | VAL  |
| 1   | A     | 179 | GLY  |
| 1   | A     | 189 | VAL  |
| 1   | A     | 243 | PRO  |
| 1   | A     | 160 | ILE  |
| 1   | A     | 224 | ILE  |
| 1   | A     | 346 | ILE  |
| 1   | A     | 73  | VAL  |
| 1   | A     | 202 | GLY  |
| 1   | A     | 319 | PHE  |
| 1   | A     | 175 | GLY  |
| 1   | A     | 344 | PRO  |

### 5.3.2 Protein sidechains [i](#)

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     | 308/308 (100%) | 211 (68%) | 97 (32%) | <b>0</b> <b>0</b> |

All (97) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 5   | LYS  |
| 1   | A     | 9   | CYS  |
| 1   | A     | 18  | LYS  |
| 1   | A     | 19  | LYS  |
| 1   | A     | 26  | VAL  |
| 1   | A     | 32  | LYS  |
| 1   | A     | 39  | LYS  |
| 1   | A     | 40  | MET  |
| 1   | A     | 47  | ARG  |
| 1   | A     | 50  | ASP  |
| 1   | A     | 52  | VAL  |
| 1   | A     | 56  | THR  |
| 1   | A     | 58  | VAL  |
| 1   | A     | 61  | LEU  |
| 1   | A     | 74  | GLU  |
| 1   | A     | 76  | ILE  |
| 1   | A     | 78  | GLU  |
| 1   | A     | 83  | VAL  |
| 1   | A     | 87  | ASP  |
| 1   | A     | 89  | VAL  |
| 1   | A     | 93  | PHE  |
| 1   | A     | 96  | GLN  |
| 1   | A     | 99  | LYS  |
| 1   | A     | 101 | ARG  |
| 1   | A     | 102 | VAL  |
| 1   | A     | 105 | HIS  |
| 1   | A     | 107 | GLU  |
| 1   | A     | 112 | LEU  |
| 1   | A     | 113 | LYS  |
| 1   | A     | 118 | MET  |
| 1   | A     | 124 | GLN  |
| 1   | A     | 129 | ARG  |
| 1   | A     | 132 | CYS  |
| 1   | A     | 135 | LYS  |
| 1   | A     | 137 | ILE  |
| 1   | A     | 141 | LEU  |
| 1   | A     | 143 | THR  |
| 1   | A     | 147 | SER  |
| 1   | A     | 153 | ASP  |
| 1   | A     | 160 | ILE  |
| 1   | A     | 166 | LEU  |
| 1   | A     | 167 | GLU  |
| 1   | A     | 168 | LYS  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | A            | 169        | VAL         |
| 1          | A            | 171        | LEU         |
| 1          | A            | 174        | CYS         |
| 1          | A            | 176        | PHE         |
| 1          | A            | 177        | SER         |
| 1          | A            | 178        | THR         |
| 1          | A            | 185        | LYS         |
| 1          | A            | 186        | VAL         |
| 1          | A            | 188        | LYS         |
| 1          | A            | 191        | GLN         |
| 1          | A            | 205        | LEU         |
| 1          | A            | 207        | VAL         |
| 1          | A            | 218        | ARG         |
| 1          | A            | 219        | ILE         |
| 1          | A            | 222        | VAL         |
| 1          | A            | 225        | ASN         |
| 1          | A            | 228        | LYS         |
| 1          | A            | 231        | LYS         |
| 1          | A            | 233        | LYS         |
| 1          | A            | 235        | VAL         |
| 1          | A            | 242        | ASN         |
| 1          | A            | 251        | GLN         |
| 1          | A            | 253        | VAL         |
| 1          | A            | 254        | LEU         |
| 1          | A            | 255        | THR         |
| 1          | A            | 267        | GLU         |
| 1          | A            | 269        | ILE         |
| 1          | A            | 272        | LEU         |
| 1          | A            | 273        | ASP         |
| 1          | A            | 274        | THR         |
| 1          | A            | 279        | LEU         |
| 1          | A            | 283        | GLN         |
| 1          | A            | 284        | GLU         |
| 1          | A            | 288        | VAL         |
| 1          | A            | 289        | SER         |
| 1          | A            | 295        | PRO         |
| 1          | A            | 301        | LEU         |
| 1          | A            | 304        | ASN         |
| 1          | A            | 306        | MET         |
| 1          | A            | 309        | LEU         |
| 1          | A            | 310        | SER         |
| 1          | A            | 314        | TRP         |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 315 | LYS  |
| 1   | A     | 318 | ILE  |
| 1   | A     | 331 | LEU  |
| 1   | A     | 338 | LYS  |
| 1   | A     | 343 | ASP  |
| 1   | A     | 349 | VAL  |
| 1   | A     | 352 | PHE  |
| 1   | A     | 353 | GLU  |
| 1   | A     | 354 | LYS  |
| 1   | A     | 355 | ILE  |
| 1   | A     | 361 | LEU  |
| 1   | A     | 369 | ARG  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 96  | GLN  |
| 1   | A     | 105 | HIS  |
| 1   | A     | 124 | GLN  |
| 1   | A     | 191 | GLN  |
| 1   | A     | 242 | ASN  |
| 1   | A     | 244 | GLN  |
| 1   | A     | 251 | GLN  |
| 1   | A     | 283 | GLN  |
| 1   | A     | 304 | ASN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 25 ligands modelled in this entry, 2 are monoatomic - leaving 23 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | NTN  | A     | 388 | 1    | 7,8,9        | 1.54 | 2 (28%)  | 7,9,11      | 1.54 | 2 (28%)  |
| 3   | NTN  | A     | 392 | 1    | 7,8,9        | 1.41 | 1 (14%)  | 7,9,11      | 3.68 | 4 (57%)  |
| 3   | NTN  | A     | 396 | 1    | 7,8,9        | 1.23 | 2 (28%)  | 7,9,11      | 1.83 | 3 (42%)  |
| 3   | NTN  | A     | 398 | 1    | 7,8,9        | 1.40 | 2 (28%)  | 7,9,11      | 2.02 | 3 (42%)  |
| 3   | NTN  | A     | 395 | 1    | 7,8,9        | 2.24 | 4 (57%)  | 7,9,11      | 1.39 | 1 (14%)  |
| 3   | NTN  | A     | 382 | 1    | 7,8,9        | 1.28 | 2 (28%)  | 7,9,11      | 1.46 | 2 (28%)  |
| 3   | NTN  | A     | 380 | 1    | 7,8,9        | 1.33 | 2 (28%)  | 7,9,11      | 1.45 | 1 (14%)  |
| 3   | NTN  | A     | 397 | 1    | 7,8,9        | 1.27 | 2 (28%)  | 7,9,11      | 1.63 | 2 (28%)  |
| 3   | NTN  | A     | 383 | 1    | 7,8,9        | 1.45 | 1 (14%)  | 7,9,11      | 2.89 | 3 (42%)  |
| 3   | NTN  | A     | 377 | 1    | 7,8,9        | 1.44 | 2 (28%)  | 7,9,11      | 1.38 | 2 (28%)  |
| 3   | NTN  | A     | 387 | 1    | 7,8,9        | 1.42 | 2 (28%)  | 7,9,11      | 2.03 | 3 (42%)  |
| 3   | NTN  | A     | 399 | 1    | 7,8,9        | 1.22 | 2 (28%)  | 7,9,11      | 1.65 | 2 (28%)  |
| 3   | NTN  | A     | 381 | 1    | 7,8,9        | 1.59 | 3 (42%)  | 7,9,11      | 2.02 | 3 (42%)  |
| 3   | NTN  | A     | 385 | 1    | 7,8,9        | 1.40 | 3 (42%)  | 7,9,11      | 2.45 | 2 (28%)  |
| 3   | NTN  | A     | 379 | 1    | 7,8,9        | 1.46 | 2 (28%)  | 7,9,11      | 1.40 | 2 (28%)  |
| 3   | NTN  | A     | 389 | 1    | 7,8,9        | 2.02 | 4 (57%)  | 7,9,11      | 1.36 | 1 (14%)  |
| 3   | NTN  | A     | 386 | 1    | 7,8,9        | 1.35 | 2 (28%)  | 7,9,11      | 2.19 | 4 (57%)  |
| 3   | NTN  | A     | 378 | 1    | 7,8,9        | 2.53 | 5 (71%)  | 7,9,11      | 1.83 | 2 (28%)  |
| 3   | NTN  | A     | 391 | 1    | 7,8,9        | 2.06 | 3 (42%)  | 7,9,11      | 1.78 | 2 (28%)  |
| 3   | NTN  | A     | 393 | 1    | 7,8,9        | 1.52 | 2 (28%)  | 7,9,11      | 1.40 | 2 (28%)  |
| 3   | NTN  | A     | 384 | 1    | 7,8,9        | 1.38 | 2 (28%)  | 7,9,11      | 1.40 | 2 (28%)  |
| 3   | NTN  | A     | 390 | 1    | 7,8,9        | 1.33 | 2 (28%)  | 7,9,11      | 2.00 | 2 (28%)  |
| 3   | NTN  | A     | 394 | 1    | 7,8,9        | 1.31 | 2 (28%)  | 7,9,11      | 1.78 | 2 (28%)  |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.  
'-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings   |
|-----|------|-------|-----|------|---------|----------|---------|
| 3   | NTN  | A     | 388 | 1    | -       | 0/2/2/4  | 0/1/1/1 |
| 3   | NTN  | A     | 392 | 1    | -       | 0/2/2/4  | 0/1/1/1 |
| 3   | NTN  | A     | 396 | 1    | -       | 0/2/2/4  | 0/1/1/1 |
| 3   | NTN  | A     | 398 | 1    | -       | 0/2/2/4  | 0/1/1/1 |
| 3   | NTN  | A     | 395 | 1    | -       | 0/2/2/4  | 0/1/1/1 |
| 3   | NTN  | A     | 382 | 1    | -       | 0/2/2/4  | 0/1/1/1 |
| 3   | NTN  | A     | 380 | 1    | -       | 0/2/2/4  | 0/1/1/1 |
| 3   | NTN  | A     | 397 | 1    | -       | 0/2/2/4  | 0/1/1/1 |
| 3   | NTN  | A     | 383 | 1    | -       | 0/2/2/4  | 0/1/1/1 |
| 3   | NTN  | A     | 377 | 1    | -       | 0/2/2/4  | 0/1/1/1 |
| 3   | NTN  | A     | 387 | 1    | -       | 0/2/2/4  | 0/1/1/1 |
| 3   | NTN  | A     | 399 | 1    | -       | 0/2/2/4  | 0/1/1/1 |
| 3   | NTN  | A     | 381 | 1    | -       | 0/2/2/4  | 0/1/1/1 |
| 3   | NTN  | A     | 385 | 1    | -       | 0/2/2/4  | 0/1/1/1 |
| 3   | NTN  | A     | 379 | 1    | -       | 0/2/2/4  | 0/1/1/1 |
| 3   | NTN  | A     | 389 | 1    | -       | 0/2/2/4  | 0/1/1/1 |
| 3   | NTN  | A     | 386 | 1    | -       | 0/2/2/4  | 0/1/1/1 |
| 3   | NTN  | A     | 378 | 1    | -       | 0/2/2/4  | 0/1/1/1 |
| 3   | NTN  | A     | 391 | 1    | -       | 0/2/2/4  | 0/1/1/1 |
| 3   | NTN  | A     | 393 | 1    | -       | 0/2/2/4  | 0/1/1/1 |
| 3   | NTN  | A     | 384 | 1    | -       | 0/2/2/4  | 0/1/1/1 |
| 3   | NTN  | A     | 390 | 1    | -       | 0/2/2/4  | 0/1/1/1 |
| 3   | NTN  | A     | 394 | 1    | -       | 0/2/2/4  | 0/1/1/1 |

All (54) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 3   | A     | 378 | NTN  | CI2-CI1 | 4.43 | 1.56        | 1.47     |
| 3   | A     | 395 | NTN  | CI2-CI1 | 3.53 | 1.54        | 1.47     |
| 3   | A     | 391 | NTN  | CI2-CI1 | 3.41 | 1.54        | 1.47     |
| 3   | A     | 389 | NTN  | CI2-CI1 | 3.13 | 1.53        | 1.47     |
| 3   | A     | 395 | NTN  | CI3-CI4 | 2.71 | 1.44        | 1.38     |
| 3   | A     | 378 | NTN  | CI3-CI4 | 2.50 | 1.43        | 1.38     |
| 3   | A     | 378 | NTN  | CI5-NI2 | 2.36 | 1.40        | 1.33     |
| 3   | A     | 387 | NTN  | CI5-NI2 | 2.36 | 1.40        | 1.33     |
| 3   | A     | 386 | NTN  | CI5-NI2 | 2.35 | 1.40        | 1.33     |
| 3   | A     | 391 | NTN  | CI5-NI2 | 2.34 | 1.40        | 1.33     |
| 3   | A     | 381 | NTN  | CI3-CI4 | 2.33 | 1.43        | 1.38     |
| 3   | A     | 398 | NTN  | CI4-NI2 | 2.31 | 1.40        | 1.33     |
| 3   | A     | 397 | NTN  | CI4-NI2 | 2.31 | 1.40        | 1.33     |
| 3   | A     | 394 | NTN  | CI5-NI2 | 2.31 | 1.40        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 3   | A     | 394 | NTN  | CI4-NI2 | 2.30 | 1.40        | 1.33     |
| 3   | A     | 384 | NTN  | CI4-NI2 | 2.29 | 1.40        | 1.33     |
| 3   | A     | 388 | NTN  | CI5-NI2 | 2.29 | 1.40        | 1.33     |
| 3   | A     | 386 | NTN  | CI4-NI2 | 2.29 | 1.40        | 1.33     |
| 3   | A     | 379 | NTN  | CI4-NI2 | 2.28 | 1.40        | 1.33     |
| 3   | A     | 381 | NTN  | CI4-NI2 | 2.27 | 1.40        | 1.33     |
| 3   | A     | 383 | NTN  | CI4-NI2 | 2.27 | 1.40        | 1.33     |
| 3   | A     | 387 | NTN  | CI4-NI2 | 2.27 | 1.40        | 1.33     |
| 3   | A     | 377 | NTN  | CI4-NI2 | 2.27 | 1.40        | 1.33     |
| 3   | A     | 395 | NTN  | CI5-NI2 | 2.27 | 1.40        | 1.33     |
| 3   | A     | 380 | NTN  | CI4-NI2 | 2.27 | 1.40        | 1.33     |
| 3   | A     | 399 | NTN  | CI4-NI2 | 2.26 | 1.40        | 1.33     |
| 3   | A     | 382 | NTN  | CI4-NI2 | 2.26 | 1.40        | 1.33     |
| 3   | A     | 393 | NTN  | CI4-NI2 | 2.25 | 1.40        | 1.33     |
| 3   | A     | 388 | NTN  | CI4-NI2 | 2.25 | 1.40        | 1.33     |
| 3   | A     | 391 | NTN  | CI4-NI2 | 2.25 | 1.40        | 1.33     |
| 3   | A     | 389 | NTN  | CI5-NI2 | 2.25 | 1.40        | 1.33     |
| 3   | A     | 382 | NTN  | CI5-NI2 | 2.25 | 1.40        | 1.33     |
| 3   | A     | 378 | NTN  | CI4-NI2 | 2.24 | 1.40        | 1.33     |
| 3   | A     | 389 | NTN  | CI4-NI2 | 2.24 | 1.40        | 1.33     |
| 3   | A     | 392 | NTN  | CI4-NI2 | 2.24 | 1.40        | 1.33     |
| 3   | A     | 396 | NTN  | CI4-NI2 | 2.24 | 1.40        | 1.33     |
| 3   | A     | 390 | NTN  | CI4-NI2 | 2.24 | 1.40        | 1.33     |
| 3   | A     | 385 | NTN  | CI4-NI2 | 2.23 | 1.40        | 1.33     |
| 3   | A     | 379 | NTN  | CI5-NI2 | 2.23 | 1.40        | 1.33     |
| 3   | A     | 377 | NTN  | CI5-NI2 | 2.23 | 1.40        | 1.33     |
| 3   | A     | 395 | NTN  | CI4-NI2 | 2.21 | 1.40        | 1.33     |
| 3   | A     | 384 | NTN  | CI5-NI2 | 2.21 | 1.40        | 1.33     |
| 3   | A     | 393 | NTN  | CI5-NI2 | 2.20 | 1.40        | 1.33     |
| 3   | A     | 380 | NTN  | CI5-NI2 | 2.19 | 1.40        | 1.33     |
| 3   | A     | 397 | NTN  | CI5-NI2 | 2.18 | 1.40        | 1.33     |
| 3   | A     | 378 | NTN  | CI3-CI2 | 2.17 | 1.43        | 1.39     |
| 3   | A     | 389 | NTN  | CI3-CI4 | 2.17 | 1.43        | 1.38     |
| 3   | A     | 399 | NTN  | CI5-NI2 | 2.13 | 1.40        | 1.33     |
| 3   | A     | 396 | NTN  | CI5-NI2 | 2.13 | 1.40        | 1.33     |
| 3   | A     | 381 | NTN  | CI5-NI2 | 2.10 | 1.40        | 1.33     |
| 3   | A     | 398 | NTN  | CI5-NI2 | 2.10 | 1.40        | 1.33     |
| 3   | A     | 385 | NTN  | CI3-CI4 | 2.10 | 1.42        | 1.38     |
| 3   | A     | 390 | NTN  | CI5-NI2 | 2.05 | 1.39        | 1.33     |
| 3   | A     | 385 | NTN  | CI5-NI2 | 2.02 | 1.39        | 1.33     |

All (52) bond angle outliers are listed below:



| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | A     | 392 | NTN  | CI2-CI1-NI1 | 8.40  | 138.53      | 121.66   |
| 3   | A     | 383 | NTN  | CI2-CI1-NI1 | 5.94  | 133.57      | 121.66   |
| 3   | A     | 385 | NTN  | CI2-CI1-NI1 | 4.97  | 131.63      | 121.66   |
| 3   | A     | 386 | NTN  | CI2-CI1-NI1 | -4.02 | 113.59      | 121.66   |
| 3   | A     | 381 | NTN  | CI2-CI1-NI1 | 3.78  | 129.25      | 121.66   |
| 3   | A     | 387 | NTN  | CI2-CI1-NI1 | -3.66 | 114.32      | 121.66   |
| 3   | A     | 390 | NTN  | CI2-CI1-NI1 | 3.58  | 128.85      | 121.66   |
| 3   | A     | 398 | NTN  | CI6-CI2-CI3 | 3.11  | 122.25      | 117.64   |
| 3   | A     | 383 | NTN  | CI6-CI2-CI3 | 3.01  | 122.09      | 117.64   |
| 3   | A     | 391 | NTN  | CI2-CI1-NI1 | -2.99 | 115.65      | 121.66   |
| 3   | A     | 378 | NTN  | CI2-CI1-NI1 | -2.92 | 115.80      | 121.66   |
| 3   | A     | 392 | NTN  | CI6-CI2-CI3 | 2.84  | 121.84      | 117.64   |
| 3   | A     | 397 | NTN  | CI6-CI2-CI3 | 2.73  | 121.67      | 117.64   |
| 3   | A     | 392 | NTN  | CI6-CI5-NI2 | -2.69 | 118.93      | 123.62   |
| 3   | A     | 394 | NTN  | CI6-CI2-CI3 | 2.66  | 121.57      | 117.64   |
| 3   | A     | 383 | NTN  | CI6-CI5-NI2 | -2.64 | 119.02      | 123.62   |
| 3   | A     | 398 | NTN  | CI2-CI1-NI1 | 2.64  | 126.95      | 121.66   |
| 3   | A     | 398 | NTN  | CI6-CI5-NI2 | -2.62 | 119.05      | 123.62   |
| 3   | A     | 378 | NTN  | CI3-CI4-NI2 | -2.62 | 119.06      | 123.62   |
| 3   | A     | 396 | NTN  | CI2-CI1-NI1 | 2.48  | 126.63      | 121.66   |
| 3   | A     | 397 | NTN  | CI6-CI5-NI2 | -2.46 | 119.34      | 123.62   |
| 3   | A     | 395 | NTN  | CI3-CI4-NI2 | -2.44 | 119.36      | 123.62   |
| 3   | A     | 391 | NTN  | CI3-CI4-NI2 | -2.44 | 119.38      | 123.62   |
| 3   | A     | 396 | NTN  | CI6-CI5-NI2 | -2.39 | 119.45      | 123.62   |
| 3   | A     | 396 | NTN  | CI6-CI2-CI3 | 2.39  | 121.18      | 117.64   |
| 3   | A     | 386 | NTN  | CI6-CI2-CI3 | 2.38  | 121.17      | 117.64   |
| 3   | A     | 399 | NTN  | CI6-CI5-NI2 | -2.37 | 119.49      | 123.62   |
| 3   | A     | 399 | NTN  | CI6-CI2-CI3 | 2.35  | 121.12      | 117.64   |
| 3   | A     | 394 | NTN  | CI6-CI5-NI2 | -2.32 | 119.58      | 123.62   |
| 3   | A     | 389 | NTN  | CI3-CI4-NI2 | -2.31 | 119.59      | 123.62   |
| 3   | A     | 382 | NTN  | CI6-CI5-NI2 | -2.25 | 119.70      | 123.62   |
| 3   | A     | 386 | NTN  | CI6-CI5-NI2 | -2.21 | 119.78      | 123.62   |
| 3   | A     | 392 | NTN  | CI4-CI3-CI2 | -2.20 | 117.24      | 119.62   |
| 3   | A     | 390 | NTN  | CI6-CI5-NI2 | -2.20 | 119.80      | 123.62   |
| 3   | A     | 385 | NTN  | CI6-CI5-NI2 | -2.18 | 119.83      | 123.62   |
| 3   | A     | 380 | NTN  | CI6-CI5-NI2 | -2.17 | 119.84      | 123.62   |
| 3   | A     | 387 | NTN  | CI6-CI5-NI2 | -2.14 | 119.90      | 123.62   |
| 3   | A     | 393 | NTN  | CI3-CI4-NI2 | -2.12 | 119.92      | 123.62   |
| 3   | A     | 388 | NTN  | CI3-CI4-NI2 | -2.11 | 119.94      | 123.62   |
| 3   | A     | 387 | NTN  | CI3-CI4-NI2 | -2.11 | 119.95      | 123.62   |
| 3   | A     | 384 | NTN  | CI6-CI5-NI2 | -2.10 | 119.97      | 123.62   |
| 3   | A     | 377 | NTN  | CI6-CI5-NI2 | -2.10 | 119.97      | 123.62   |
| 3   | A     | 379 | NTN  | CI3-CI4-NI2 | -2.08 | 120.00      | 123.62   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | A     | 382 | NTN  | CI6-CI2-CI3 | 2.08  | 120.71      | 117.64   |
| 3   | A     | 393 | NTN  | CI6-CI5-NI2 | -2.06 | 120.03      | 123.62   |
| 3   | A     | 379 | NTN  | CI6-CI5-NI2 | -2.06 | 120.04      | 123.62   |
| 3   | A     | 384 | NTN  | CI3-CI4-NI2 | -2.06 | 120.04      | 123.62   |
| 3   | A     | 388 | NTN  | CI6-CI5-NI2 | -2.05 | 120.05      | 123.62   |
| 3   | A     | 381 | NTN  | CI3-CI4-NI2 | -2.05 | 120.05      | 123.62   |
| 3   | A     | 386 | NTN  | CI3-CI4-NI2 | -2.02 | 120.10      | 123.62   |
| 3   | A     | 381 | NTN  | CI6-CI5-NI2 | -2.02 | 120.11      | 123.62   |
| 3   | A     | 377 | NTN  | CI3-CI4-NI2 | -2.01 | 120.11      | 123.62   |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 154 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | A     | 382 | NTN  | 0       | 13           |
| 3   | A     | 397 | NTN  | 0       | 8            |
| 3   | A     | 383 | NTN  | 1       | 18           |
| 3   | A     | 377 | NTN  | 0       | 10           |
| 3   | A     | 387 | NTN  | 1       | 0            |
| 3   | A     | 399 | NTN  | 2       | 0            |
| 3   | A     | 381 | NTN  | 3       | 0            |
| 3   | A     | 385 | NTN  | 0       | 13           |
| 3   | A     | 379 | NTN  | 0       | 16           |
| 3   | A     | 389 | NTN  | 2       | 0            |
| 3   | A     | 386 | NTN  | 0       | 14           |
| 3   | A     | 378 | NTN  | 0       | 20           |
| 3   | A     | 391 | NTN  | 1       | 33           |
| 3   | A     | 390 | NTN  | 0       | 4            |

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.