



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:11 PM UTC

PDB ID : 1FOE / pdb\_00001foe  
Title : CRYSTAL STRUCTURE OF RAC1 IN COMPLEX WITH THE GUANINE NUCLEOTIDE EXCHANGE REGION OF TIAM1  
Authors : Worthylake, D.K.; Rossman, K.L.; Sondek, J.  
Deposited on : 2000-08-27  
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                     |
| Xtriage (Phenix)               | : | NOT EXECUTED                                                     |
| EDS                            | : | NOT EXECUTED                                                     |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

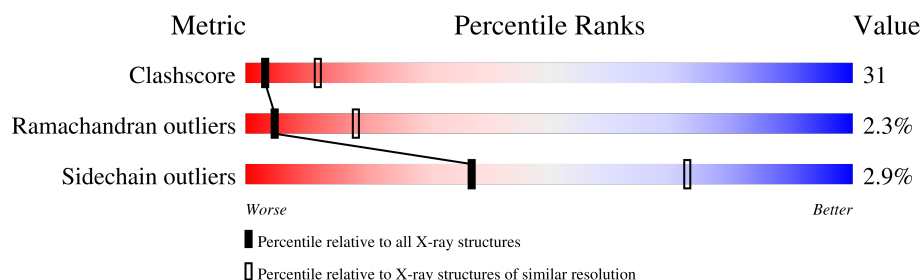
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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            | 190562                      | 4276 (2.80-2.80)                                      |
| Ramachandran outliers | 187476                      | 4196 (2.80-2.80)                                      |
| Sidechain outliers    | 187428                      | 4198 (2.80-2.80)                                      |

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

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 377    | 52% 41% . .      |
| 1   | C     | 377    | 54% 38% 5% .     |
| 1   | E     | 377    | 53% 39% 5% .     |
| 1   | G     | 377    | 52% 40% 5% .     |
| 2   | B     | 177    | 53% 42% 5%       |
| 2   | D     | 177    | 53% 43% 5%       |
| 2   | F     | 177    | 53% 44% .        |
| 2   | H     | 177    | 51% 44% 5%       |

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17570 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 T-LYMPHOMA INVASION AND METASTASIS INDUCING PROTEIN 1.

| Mol | Chain | Residues | Atoms |      |     |     |   |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|----|---------|---------|-------|
| 1   | A     | 368      | Total | C    | N   | O   | S | Se | 369     | 0       | 0     |
|     |       |          | 2989  | 1918 | 509 | 550 | 6 | 6  |         |         |       |
| 1   | C     | 366      | Total | C    | N   | O   | S | Se | 309     | 0       | 0     |
|     |       |          | 2972  | 1907 | 506 | 547 | 6 | 6  |         |         |       |
| 1   | E     | 367      | Total | C    | N   | O   | S | Se | 369     | 0       | 0     |
|     |       |          | 2980  | 1913 | 507 | 548 | 6 | 6  |         |         |       |
| 1   | G     | 367      | Total | C    | N   | O   | S | Se | 307     | 0       | 0     |
|     |       |          | 2980  | 1913 | 507 | 548 | 6 | 6  |         |         |       |

There are 32 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment          | Reference  |
|-------|---------|----------|--------|------------------|------------|
| A     | 1031    | MSE      | THR    | modified residue | UNP Q60610 |
| A     | 1032    | GLY      | THR    | cloning artifact | UNP Q60610 |
| A     | 1063    | MSE      | MET    | modified residue | UNP Q60610 |
| A     | 1091    | MSE      | MET    | modified residue | UNP Q60610 |
| A     | 1224    | MSE      | MET    | modified residue | UNP Q60610 |
| A     | 1234    | MSE      | MET    | modified residue | UNP Q60610 |
| A     | 1264    | MSE      | MET    | modified residue | UNP Q60610 |
| A     | 1334    | MSE      | MET    | modified residue | UNP Q60610 |
| C     | 1031    | MSE      | THR    | modified residue | UNP Q60610 |
| C     | 1032    | GLY      | THR    | cloning artifact | UNP Q60610 |
| C     | 1063    | MSE      | MET    | modified residue | UNP Q60610 |
| C     | 1091    | MSE      | MET    | modified residue | UNP Q60610 |
| C     | 1224    | MSE      | MET    | modified residue | UNP Q60610 |
| C     | 1234    | MSE      | MET    | modified residue | UNP Q60610 |
| C     | 1264    | MSE      | MET    | modified residue | UNP Q60610 |
| C     | 1334    | MSE      | MET    | modified residue | UNP Q60610 |
| E     | 1031    | MSE      | THR    | modified residue | UNP Q60610 |
| E     | 1032    | GLY      | THR    | cloning artifact | UNP Q60610 |
| E     | 1063    | MSE      | MET    | modified residue | UNP Q60610 |
| E     | 1091    | MSE      | MET    | modified residue | UNP Q60610 |

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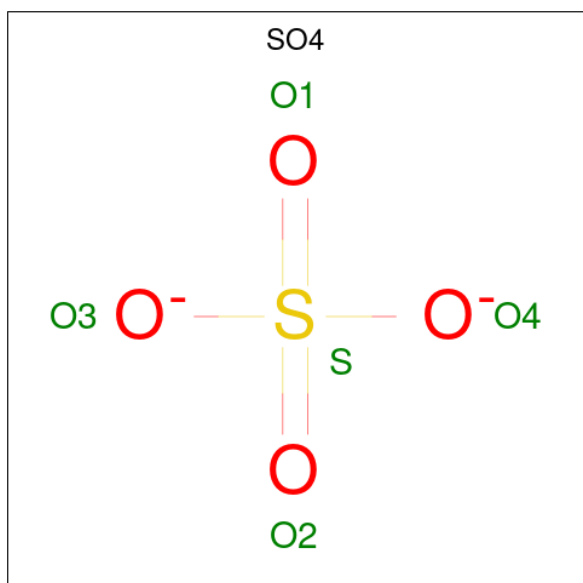
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| Chain | Residue | Modelled | Actual | Comment          | Reference  |
|-------|---------|----------|--------|------------------|------------|
| E     | 1224    | MSE      | MET    | modified residue | UNP Q60610 |
| E     | 1234    | MSE      | MET    | modified residue | UNP Q60610 |
| E     | 1264    | MSE      | MET    | modified residue | UNP Q60610 |
| E     | 1334    | MSE      | MET    | modified residue | UNP Q60610 |
| G     | 1031    | MSE      | THR    | modified residue | UNP Q60610 |
| G     | 1032    | GLY      | THR    | cloning artifact | UNP Q60610 |
| G     | 1063    | MSE      | MET    | modified residue | UNP Q60610 |
| G     | 1091    | MSE      | MET    | modified residue | UNP Q60610 |
| G     | 1224    | MSE      | MET    | modified residue | UNP Q60610 |
| G     | 1234    | MSE      | MET    | modified residue | UNP Q60610 |
| G     | 1264    | MSE      | MET    | modified residue | UNP Q60610 |
| G     | 1334    | MSE      | MET    | modified residue | UNP Q60610 |

- Molecule 2 is a protein called RAS-RELATED C3 BOTULINUM TOXIN SUBSTRATE.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2   | B     | 177      | Total | C   | N   | O   | S | 14      | 0       | 0     |
|     |       |          | 1384  | 889 | 228 | 259 | 8 |         |         |       |
| 2   | D     | 177      | Total | C   | N   | O   | S | 14      | 0       | 0     |
|     |       |          | 1384  | 889 | 228 | 259 | 8 |         |         |       |
| 2   | F     | 177      | Total | C   | N   | O   | S | 14      | 0       | 0     |
|     |       |          | 1384  | 889 | 228 | 259 | 8 |         |         |       |
| 2   | H     | 177      | Total | C   | N   | O   | S | 14      | 0       | 0     |
|     |       |          | 1384  | 889 | 228 | 259 | 8 |         |         |       |

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



| Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 3   | B     | 1        | Total O S<br>5 4 1 | 0       | 0       |
| 3   | D     | 1        | Total O S<br>5 4 1 | 0       | 0       |
| 3   | F     | 1        | Total O S<br>5 4 1 | 0       | 0       |
| 3   | H     | 1        | Total O S<br>5 4 1 | 0       | 0       |

- Molecule 4 is water.

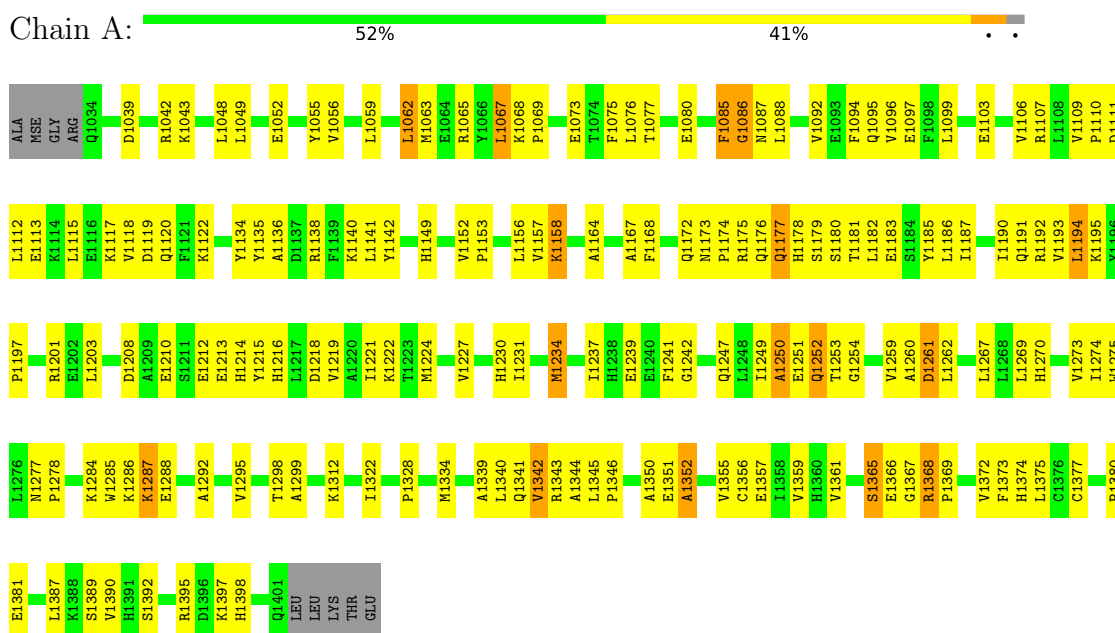
| Mol | Chain | Residues | Atoms            | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 4   | A     | 14       | Total O<br>14 14 | 0       | 0       |
| 4   | B     | 6        | Total O<br>6 6   | 0       | 0       |
| 4   | C     | 8        | Total O<br>8 8   | 0       | 0       |
| 4   | D     | 6        | Total O<br>6 6   | 0       | 0       |
| 4   | E     | 7        | Total O<br>7 7   | 0       | 0       |
| 4   | F     | 7        | Total O<br>7 7   | 0       | 0       |
| 4   | G     | 19       | Total O<br>19 19 | 0       | 0       |
| 4   | H     | 26       | Total O<br>26 26 | 0       | 0       |

### 3 Residue-property plots

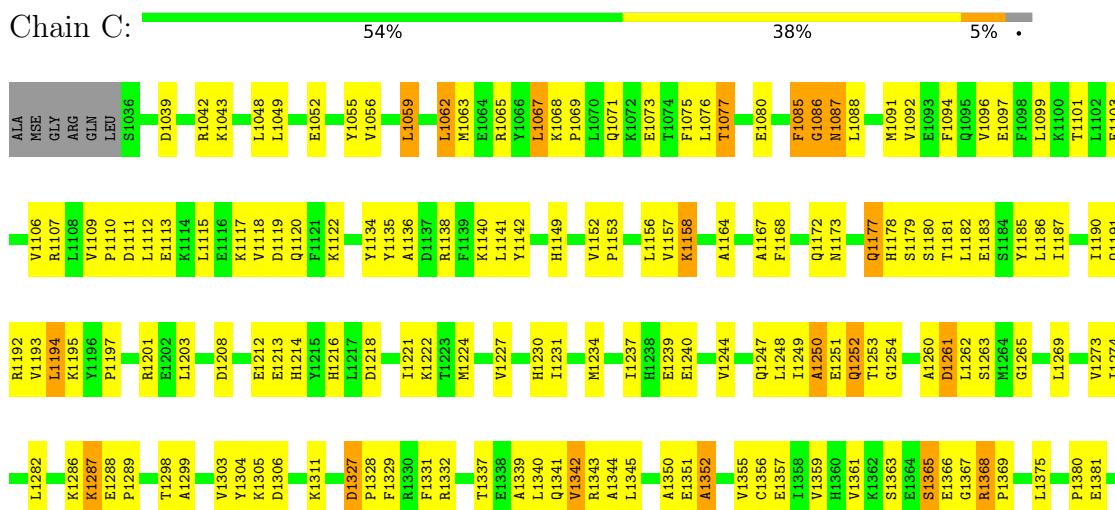
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

#### • Molecule 1: T-LYMPHOMA INVASION AND METASTASIS INDUCING PROTEIN 1



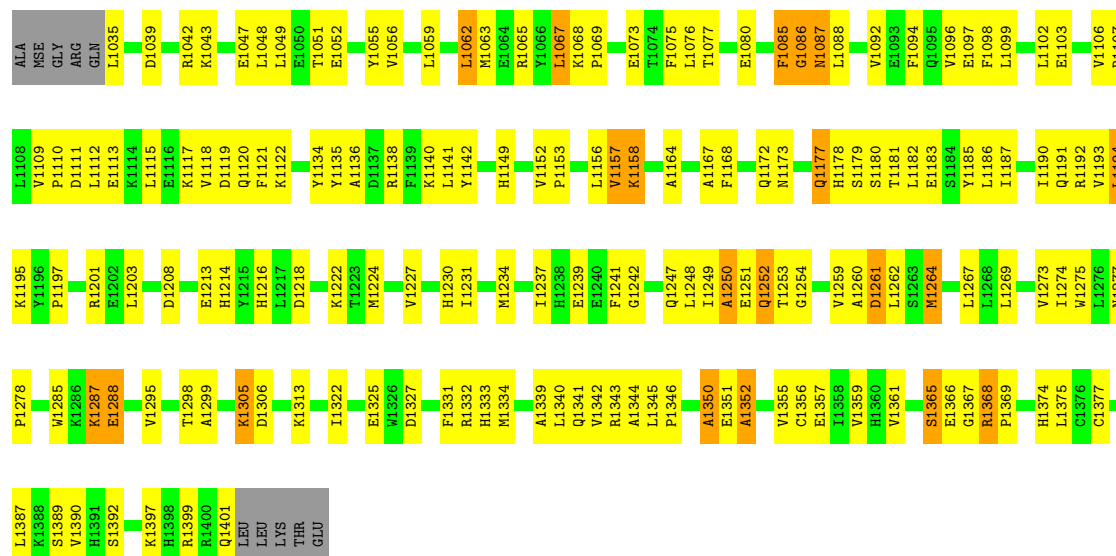
#### • Molecule 1: T-LYMPHOMA INVASION AND METASTASIS INDUCING PROTEIN 1





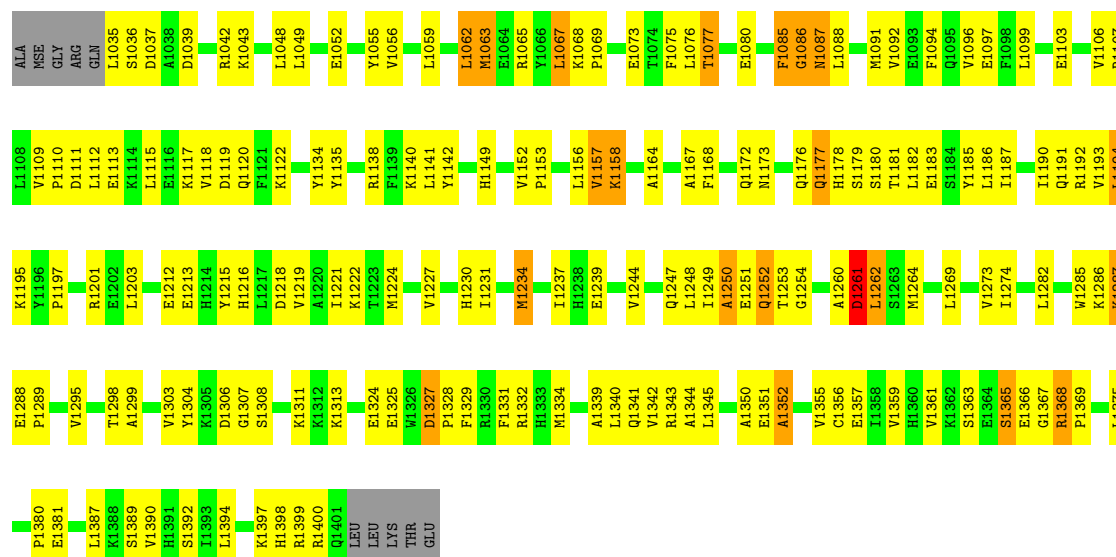
• Molecule 1: T-LYMPHOMA INVASION AND METASTASIS INDUCING PROTEIN 1

Chain E:  53% 39% 5%



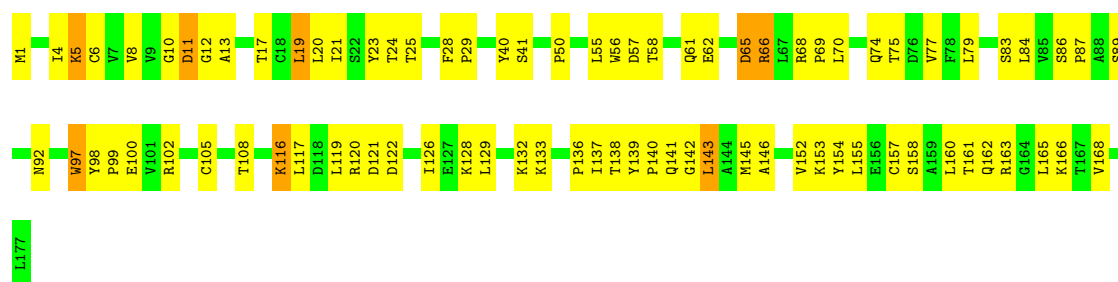
• Molecule 1: T-LYMPHOMA INVASION AND METASTASIS INDUCING PROTEIN 1

Chain G:  52% 40% 5%



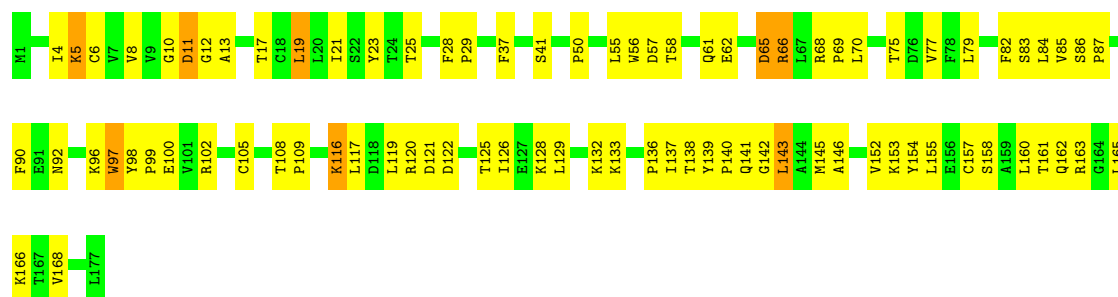
• Molecule 2: RAS-RELATED C3 BOTULINUM TOXIN SUBSTRATE

Chain B:  53% 42% 5%



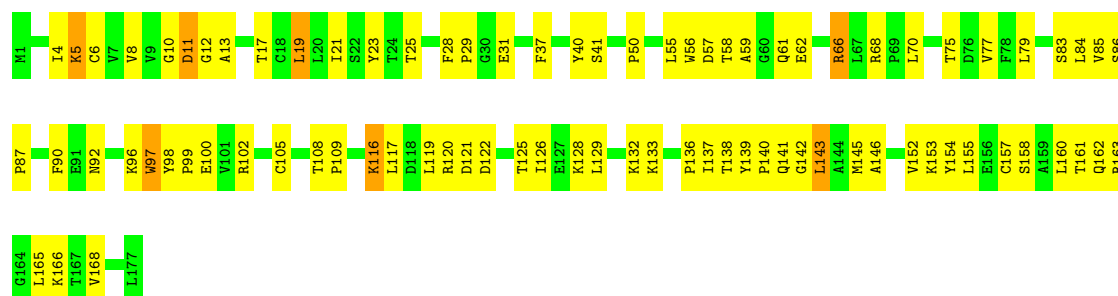
• Molecule 2: RAS-RELATED C3 BOTULINUM TOXIN SUBSTRATE

Chain D: 53% 43% 5%



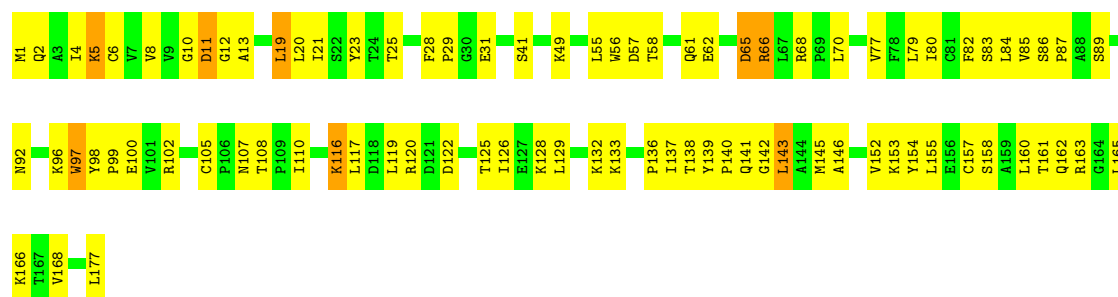
• Molecule 2: RAS-RELATED C3 BOTULINUM TOXIN SUBSTRATE

Chain F: 53% 44% .



• Molecule 2: RAS-RELATED C3 BOTULINUM TOXIN SUBSTRATE

Chain H: 51% 44% 5%





## 4 Data and refinement statistics

Xtriage (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, $\alpha$ , $\beta$ , $\gamma$ | 186.95Å 149.27Å 149.21Å<br>90.00° 121.00° 90.00° | Depositor |
| Resolution (Å)                                           | 15.00 – 2.80                                     | Depositor |
| % Data completeness<br>(in resolution range)             | 93.8 (15.00-2.80)                                | Depositor |
| $R_{merge}$                                              | 0.07                                             | Depositor |
| $R_{sym}$                                                | (Not available)                                  | Depositor |
| Refinement program                                       | CNS 0.3                                          | Depositor |
| R, $R_{free}$                                            | 0.262 , 0.293                                    | Depositor |
| Estimated twinning fraction                              | No twinning to report.                           | Xtriage   |
| Total number of atoms                                    | 17570                                            | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 60.0                                             | 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: SO4

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

| Mol | Chain | Bond lengths |                 | Bond angles |                 |
|-----|-------|--------------|-----------------|-------------|-----------------|
|     |       | RMSZ         | # $ Z  > 5$     | RMSZ        | # $ Z  > 5$     |
| 1   | A     | 0.54         | 4/3045 (0.1%)   | 0.96        | 11/4095 (0.3%)  |
| 1   | C     | 0.52         | 2/3028 (0.1%)   | 0.97        | 13/4072 (0.3%)  |
| 1   | E     | 0.51         | 3/3036 (0.1%)   | 0.96        | 12/4083 (0.3%)  |
| 1   | G     | 0.59         | 8/3036 (0.3%)   | 0.98        | 15/4083 (0.4%)  |
| 2   | B     | 0.51         | 0/1414          | 1.12        | 7/1922 (0.4%)   |
| 2   | D     | 0.49         | 0/1414          | 1.12        | 7/1922 (0.4%)   |
| 2   | F     | 0.46         | 0/1414          | 1.13        | 7/1922 (0.4%)   |
| 2   | H     | 0.65         | 0/1414          | 1.15        | 8/1922 (0.4%)   |
| All | All   | 0.54         | 17/17801 (0.1%) | 1.02        | 80/24021 (0.3%) |

All (17) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1   | G     | 1234 | MSE  | SE-CE | -6.97 | 1.74        | 1.95     |
| 1   | C     | 1224 | MSE  | SE-CE | -6.12 | 1.77        | 1.95     |
| 1   | G     | 1264 | MSE  | SE-CE | -5.83 | 1.77        | 1.95     |
| 1   | G     | 1334 | MSE  | SE-CE | -5.82 | 1.78        | 1.95     |
| 1   | G     | 1264 | MSE  | CG-SE | -5.78 | 1.78        | 1.95     |
| 1   | G     | 1091 | MSE  | SE-CE | -5.60 | 1.78        | 1.95     |
| 1   | A     | 1234 | MSE  | SE-CE | -5.41 | 1.79        | 1.95     |
| 1   | A     | 1224 | MSE  | SE-CE | -5.33 | 1.79        | 1.95     |
| 1   | C     | 1091 | MSE  | SE-CE | -5.33 | 1.79        | 1.95     |
| 1   | E     | 1334 | MSE  | CG-SE | -5.30 | 1.79        | 1.95     |
| 1   | G     | 1224 | MSE  | SE-CE | -5.18 | 1.79        | 1.95     |
| 1   | G     | 1063 | MSE  | SE-CE | -5.15 | 1.80        | 1.95     |
| 1   | E     | 1264 | MSE  | SE-CE | -5.14 | 1.80        | 1.95     |
| 1   | A     | 1334 | MSE  | SE-CE | -5.12 | 1.80        | 1.95     |
| 1   | E     | 1224 | MSE  | SE-CE | -5.11 | 1.80        | 1.95     |
| 1   | A     | 1334 | MSE  | CG-SE | -5.10 | 1.80        | 1.95     |
| 1   | G     | 1063 | MSE  | CG-SE | -5.04 | 1.80        | 1.95     |

All (80) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 2   | B     | 5    | LYS  | N-CA-CB | -15.86 | 85.67       | 110.57   |
| 2   | H     | 5    | LYS  | N-CA-CB | -15.27 | 86.58       | 110.55   |
| 2   | D     | 5    | LYS  | N-CA-CB | -15.26 | 86.59       | 110.55   |
| 2   | F     | 5    | LYS  | N-CA-CB | -15.13 | 86.79       | 110.55   |
| 2   | F     | 4    | ILE  | N-CA-C  | -10.62 | 92.82       | 108.12   |
| 2   | H     | 4    | ILE  | N-CA-C  | -10.28 | 93.32       | 108.12   |
| 2   | D     | 4    | ILE  | N-CA-C  | -10.25 | 93.36       | 108.12   |
| 2   | D     | 4    | ILE  | CB-CA-C | -10.08 | 95.61       | 110.33   |
| 2   | B     | 4    | ILE  | CB-CA-C | -10.03 | 95.69       | 110.33   |
| 2   | H     | 4    | ILE  | CB-CA-C | -9.89  | 95.89       | 110.33   |
| 2   | B     | 4    | ILE  | N-CA-C  | -9.86  | 93.92       | 108.12   |
| 2   | F     | 4    | ILE  | CB-CA-C | -9.82  | 95.99       | 110.33   |
| 2   | F     | 97   | TRP  | N-CA-C  | 7.92   | 120.62      | 111.11   |
| 2   | B     | 97   | TRP  | N-CA-C  | 7.83   | 120.51      | 111.11   |
| 2   | H     | 97   | TRP  | N-CA-C  | 7.74   | 120.40      | 111.11   |
| 2   | D     | 97   | TRP  | N-CA-C  | 7.58   | 120.21      | 111.11   |
| 1   | A     | 1067 | LEU  | N-CA-C  | 6.83   | 118.41      | 110.97   |
| 1   | G     | 1067 | LEU  | N-CA-C  | 6.82   | 118.40      | 110.97   |
| 1   | E     | 1368 | ARG  | CA-C-N  | 6.77   | 126.73      | 120.03   |
| 1   | E     | 1368 | ARG  | C-N-CA  | 6.77   | 126.73      | 120.03   |
| 1   | E     | 1067 | LEU  | N-CA-C  | 6.69   | 118.26      | 110.97   |
| 1   | A     | 1368 | ARG  | CA-C-N  | 6.56   | 126.53      | 120.03   |
| 1   | A     | 1368 | ARG  | C-N-CA  | 6.56   | 126.53      | 120.03   |
| 1   | A     | 1365 | SER  | N-CA-C  | -6.55  | 102.36      | 110.41   |
| 1   | E     | 1365 | SER  | N-CA-C  | -6.52  | 102.39      | 110.41   |
| 1   | C     | 1368 | ARG  | CA-C-N  | 6.46   | 126.43      | 120.03   |
| 1   | C     | 1368 | ARG  | C-N-CA  | 6.46   | 126.43      | 120.03   |
| 1   | C     | 1067 | LEU  | N-CA-C  | 6.45   | 118.00      | 110.97   |
| 1   | G     | 1261 | ASP  | CA-C-N  | -6.42  | 114.34      | 123.20   |
| 1   | G     | 1261 | ASP  | C-N-CA  | -6.42  | 114.34      | 123.20   |
| 1   | G     | 1365 | SER  | N-CA-C  | -6.40  | 102.54      | 110.41   |
| 1   | G     | 1368 | ARG  | CA-C-N  | 6.36   | 126.33      | 120.03   |
| 1   | G     | 1368 | ARG  | C-N-CA  | 6.36   | 126.33      | 120.03   |
| 1   | A     | 1342 | VAL  | N-CA-C  | 6.32   | 117.19      | 107.78   |
| 1   | C     | 1365 | SER  | N-CA-C  | -6.31  | 102.65      | 110.41   |
| 2   | F     | 105  | CYS  | CA-C-N  | 6.30   | 126.51      | 119.32   |
| 2   | F     | 105  | CYS  | C-N-CA  | 6.30   | 126.51      | 119.32   |
| 2   | D     | 105  | CYS  | CA-C-N  | 6.27   | 126.00      | 119.05   |
| 2   | D     | 105  | CYS  | C-N-CA  | 6.27   | 126.00      | 119.05   |
| 1   | E     | 1259 | VAL  | CB-CA-C | -6.09  | 106.53      | 111.71   |
| 1   | G     | 1342 | VAL  | N-CA-C  | 6.08   | 116.84      | 107.78   |
| 2   | H     | 105  | CYS  | CA-C-N  | 6.08   | 126.25      | 119.32   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2   | H     | 105  | CYS  | C-N-CA  | 6.08  | 126.25      | 119.32   |
| 1   | A     | 1259 | VAL  | CB-CA-C | -6.05 | 106.57      | 111.71   |
| 2   | B     | 105  | CYS  | CA-C-N  | 6.01  | 126.17      | 119.32   |
| 2   | B     | 105  | CYS  | C-N-CA  | 6.01  | 126.17      | 119.32   |
| 1   | C     | 1327 | ASP  | CA-C-N  | 5.80  | 125.48      | 119.56   |
| 1   | C     | 1327 | ASP  | C-N-CA  | 5.80  | 125.48      | 119.56   |
| 2   | F     | 5    | LYS  | N-CA-C  | -5.78 | 99.09       | 108.52   |
| 1   | E     | 1342 | VAL  | N-CA-C  | 5.78  | 116.39      | 107.78   |
| 1   | A     | 1250 | ALA  | N-CA-C  | -5.74 | 100.83      | 109.79   |
| 1   | C     | 1342 | VAL  | N-CA-C  | 5.74  | 116.33      | 107.78   |
| 1   | G     | 1250 | ALA  | N-CA-C  | -5.73 | 100.86      | 109.79   |
| 2   | B     | 5    | LYS  | N-CA-C  | -5.71 | 99.89       | 109.07   |
| 1   | C     | 1250 | ALA  | N-CA-C  | -5.65 | 100.97      | 109.79   |
| 1   | G     | 1203 | LEU  | N-CA-C  | -5.65 | 105.12      | 111.28   |
| 1   | A     | 1292 | ALA  | N-CA-C  | -5.58 | 100.15      | 109.24   |
| 1   | E     | 1250 | ALA  | N-CA-C  | -5.57 | 101.10      | 109.79   |
| 1   | E     | 1158 | LYS  | N-CA-C  | -5.53 | 106.69      | 113.50   |
| 1   | A     | 1203 | LEU  | N-CA-C  | -5.50 | 105.29      | 111.28   |
| 2   | D     | 5    | LYS  | N-CA-C  | -5.49 | 99.58       | 108.52   |
| 1   | A     | 1158 | LYS  | N-CA-C  | -5.48 | 106.76      | 113.50   |
| 1   | C     | 1158 | LYS  | N-CA-C  | -5.48 | 106.76      | 113.50   |
| 1   | G     | 1352 | ALA  | N-CA-C  | -5.36 | 107.75      | 114.56   |
| 1   | E     | 1352 | ALA  | N-CA-C  | -5.35 | 107.77      | 114.56   |
| 1   | E     | 1203 | LEU  | N-CA-C  | -5.33 | 105.47      | 111.28   |
| 1   | C     | 1203 | LEU  | N-CA-C  | -5.26 | 105.55      | 111.28   |
| 1   | A     | 1352 | ALA  | N-CA-C  | -5.24 | 107.90      | 114.56   |
| 1   | G     | 1158 | LYS  | N-CA-C  | -5.21 | 107.09      | 113.50   |
| 2   | H     | 65   | ASP  | N-CA-C  | 5.19  | 119.09      | 112.34   |
| 1   | G     | 1077 | THR  | N-CA-C  | -5.12 | 103.29      | 110.35   |
| 1   | C     | 1077 | THR  | N-CA-C  | -5.11 | 103.30      | 110.35   |
| 1   | C     | 1352 | ALA  | N-CA-C  | -5.11 | 108.07      | 114.56   |
| 1   | G     | 1327 | ASP  | CA-C-N  | 5.11  | 124.90      | 119.28   |
| 1   | G     | 1327 | ASP  | C-N-CA  | 5.11  | 124.90      | 119.28   |
| 1   | C     | 1071 | GLN  | N-CA-C  | -5.10 | 105.62      | 111.07   |
| 2   | H     | 5    | LYS  | N-CA-C  | -5.07 | 100.25      | 108.52   |
| 1   | E     | 1288 | GLU  | CA-C-N  | 5.05  | 124.98      | 119.78   |
| 1   | E     | 1288 | GLU  | C-N-CA  | 5.05  | 124.98      | 119.78   |
| 1   | G     | 1262 | LEU  | N-CA-C  | -5.02 | 101.47      | 108.54   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 2989  | 0        | 3035     | 179     | 0            |
| 1   | C     | 2972  | 0        | 3016     | 185     | 0            |
| 1   | E     | 2980  | 0        | 3027     | 182     | 0            |
| 1   | G     | 2980  | 0        | 3027     | 179     | 0            |
| 2   | B     | 1384  | 0        | 1405     | 86      | 0            |
| 2   | D     | 1384  | 0        | 1405     | 88      | 0            |
| 2   | F     | 1384  | 0        | 1405     | 84      | 1            |
| 2   | H     | 1384  | 0        | 1405     | 90      | 1            |
| 3   | B     | 5     | 0        | 0        | 0       | 0            |
| 3   | D     | 5     | 0        | 0        | 0       | 0            |
| 3   | F     | 5     | 0        | 0        | 0       | 0            |
| 3   | H     | 5     | 0        | 0        | 0       | 0            |
| 4   | A     | 14    | 0        | 0        | 0       | 0            |
| 4   | B     | 6     | 0        | 0        | 0       | 0            |
| 4   | C     | 8     | 0        | 0        | 0       | 0            |
| 4   | D     | 6     | 0        | 0        | 0       | 0            |
| 4   | E     | 7     | 0        | 0        | 0       | 0            |
| 4   | F     | 7     | 0        | 0        | 0       | 0            |
| 4   | G     | 19    | 0        | 0        | 0       | 0            |
| 4   | H     | 26    | 0        | 0        | 0       | 0            |
| All | All   | 17570 | 0        | 17725    | 995     | 1            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 31.

All (995) 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:1285:TRP:HH2  | 2:D:102:ARG:HG2  | 1.01                     | 1.09              |
| 1:A:1285:TRP:CH2  | 2:D:102:ARG:HG2  | 1.88                     | 1.08              |
| 2:B:138:THR:H     | 2:B:141:GLN:HE21 | 1.09                     | 1.00              |
| 1:C:1248:LEU:HD21 | 1:C:1332:ARG:HG3 | 1.46                     | 0.97              |
| 1:E:1249:ILE:HD12 | 1:E:1261:ASP:H   | 1.29                     | 0.96              |
| 2:H:138:THR:H     | 2:H:141:GLN:HE21 | 0.99                     | 0.95              |
| 2:F:138:THR:H     | 2:F:141:GLN:HE21 | 1.07                     | 0.94              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:138:THR:H     | 2:D:141:GLN:HE21  | 1.08                     | 0.93              |
| 1:C:1249:ILE:HD11 | 1:C:1262:LEU:HG   | 1.52                     | 0.91              |
| 1:A:1249:ILE:HD11 | 1:A:1262:LEU:HG   | 1.53                     | 0.89              |
| 1:C:1056:VAL:HG21 | 1:C:1099:LEU:HD22 | 1.55                     | 0.89              |
| 1:G:1287:LYS:HG2  | 1:G:1288:GLU:HG2  | 1.53                     | 0.89              |
| 1:E:1343:ARG:HD3  | 1:E:1357:GLU:HG3  | 1.54                     | 0.88              |
| 1:C:1287:LYS:HG2  | 1:C:1288:GLU:HG2  | 1.56                     | 0.87              |
| 1:C:1193:VAL:HG23 | 1:C:1194:LEU:HD13 | 1.57                     | 0.87              |
| 1:A:1343:ARG:HD3  | 1:A:1357:GLU:HG3  | 1.55                     | 0.87              |
| 1:C:1343:ARG:HD3  | 1:C:1357:GLU:HG3  | 1.57                     | 0.87              |
| 1:G:1190:ILE:HD13 | 2:H:70:LEU:HD13   | 1.55                     | 0.86              |
| 1:E:1193:VAL:HG23 | 1:E:1194:LEU:HD13 | 1.57                     | 0.86              |
| 1:E:1039:ASP:HA   | 1:E:1042:ARG:HH12 | 1.40                     | 0.86              |
| 1:A:1190:ILE:HD13 | 2:B:70:LEU:HD13   | 1.55                     | 0.86              |
| 1:E:1287:LYS:HG2  | 1:E:1288:GLU:HG2  | 1.57                     | 0.85              |
| 1:G:1343:ARG:HD3  | 1:G:1357:GLU:HG3  | 1.56                     | 0.85              |
| 1:A:1287:LYS:HG2  | 1:A:1288:GLU:HG2  | 1.58                     | 0.85              |
| 1:A:1039:ASP:HA   | 1:A:1042:ARG:HH12 | 1.42                     | 0.85              |
| 1:A:1239:GLU:OE2  | 2:B:66:ARG:HG3    | 1.77                     | 0.84              |
| 1:G:1193:VAL:HG23 | 1:G:1194:LEU:HD13 | 1.59                     | 0.84              |
| 2:B:138:THR:OG1   | 2:B:141:GLN:HG3   | 1.78                     | 0.84              |
| 2:B:145:MET:HA    | 2:B:145:MET:HE3   | 1.60                     | 0.84              |
| 1:E:1190:ILE:HD13 | 2:F:70:LEU:HD13   | 1.59                     | 0.83              |
| 1:A:1056:VAL:HG21 | 1:A:1099:LEU:HD22 | 1.58                     | 0.83              |
| 1:E:1260:ALA:O    | 1:E:1261:ASP:HB2  | 1.75                     | 0.83              |
| 2:H:138:THR:OG1   | 2:H:141:GLN:HG3   | 1.78                     | 0.83              |
| 1:E:1062:LEU:HD11 | 1:E:1186:LEU:HD23 | 1.60                     | 0.83              |
| 1:G:1035:LEU:HD12 | 2:H:31:GLU:HB2    | 1.61                     | 0.83              |
| 2:F:145:MET:HE3   | 2:F:145:MET:HA    | 1.60                     | 0.82              |
| 1:C:1039:ASP:HA   | 1:C:1042:ARG:HH12 | 1.42                     | 0.82              |
| 1:E:1248:LEU:HD21 | 1:E:1332:ARG:HG2  | 1.61                     | 0.82              |
| 1:A:1039:ASP:O    | 1:A:1043:LYS:HG2  | 1.78                     | 0.82              |
| 1:A:1284:LYS:HB3  | 2:D:99:PRO:HB3    | 1.62                     | 0.82              |
| 1:E:1368:ARG:HG3  | 1:E:1368:ARG:HH11 | 1.44                     | 0.82              |
| 1:E:1056:VAL:HG21 | 1:E:1099:LEU:HD22 | 1.60                     | 0.82              |
| 1:G:1039:ASP:HA   | 1:G:1042:ARG:HH12 | 1.43                     | 0.82              |
| 1:G:1249:ILE:HD11 | 1:G:1262:LEU:HG   | 1.61                     | 0.82              |
| 1:E:1039:ASP:O    | 1:E:1043:LYS:HG2  | 1.80                     | 0.81              |
| 2:H:145:MET:HE3   | 2:H:145:MET:HA    | 1.61                     | 0.81              |
| 1:G:1039:ASP:O    | 1:G:1043:LYS:HG2  | 1.79                     | 0.81              |
| 1:A:1193:VAL:HG23 | 1:A:1194:LEU:HD13 | 1.59                     | 0.81              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1039:ASP:O    | 1:C:1043:LYS:HG2  | 1.81                     | 0.81              |
| 1:E:1234:MSE:HE2  | 1:E:1234:MSE:HA   | 1.62                     | 0.81              |
| 1:G:1234:MSE:HA   | 1:G:1234:MSE:HE2  | 1.64                     | 0.80              |
| 1:C:1368:ARG:HG3  | 1:C:1368:ARG:HH11 | 1.47                     | 0.79              |
| 1:E:1249:ILE:HD11 | 1:E:1262:LEU:HG   | 1.62                     | 0.79              |
| 1:A:1249:ILE:HD12 | 1:A:1261:ASP:H    | 1.47                     | 0.79              |
| 1:G:1056:VAL:HG21 | 1:G:1099:LEU:HD22 | 1.65                     | 0.79              |
| 1:A:1062:LEU:HD11 | 1:A:1186:LEU:HD23 | 1.63                     | 0.78              |
| 2:D:145:MET:HE3   | 2:D:145:MET:HA    | 1.62                     | 0.78              |
| 1:G:1368:ARG:HG3  | 1:G:1368:ARG:HH11 | 1.47                     | 0.78              |
| 2:D:138:THR:OG1   | 2:D:141:GLN:HG3   | 1.83                     | 0.78              |
| 1:C:1234:MSE:HE2  | 1:C:1234:MSE:HA   | 1.64                     | 0.78              |
| 1:G:1248:LEU:HD21 | 1:G:1332:ARG:HG3  | 1.67                     | 0.77              |
| 1:A:1368:ARG:HG3  | 1:A:1368:ARG:HH11 | 1.50                     | 0.77              |
| 1:C:1249:ILE:HD12 | 1:C:1261:ASP:H    | 1.49                     | 0.77              |
| 1:G:1062:LEU:HD11 | 1:G:1186:LEU:HD23 | 1.67                     | 0.76              |
| 2:F:138:THR:OG1   | 2:F:141:GLN:HG3   | 1.85                     | 0.76              |
| 1:C:1062:LEU:HD11 | 1:C:1186:LEU:HD23 | 1.65                     | 0.76              |
| 1:A:1234:MSE:HE2  | 1:A:1234:MSE:HA   | 1.66                     | 0.76              |
| 1:G:1304:TYR:HB3  | 1:G:1331:PHE:HB3  | 1.68                     | 0.76              |
| 1:E:1285:TRP:HZ2  | 2:H:98:TYR:CE2    | 2.05                     | 0.74              |
| 2:H:128:LYS:HE2   | 2:H:132:LYS:HZ1   | 1.52                     | 0.74              |
| 1:C:1190:ILE:HD13 | 2:D:70:LEU:HD13   | 1.70                     | 0.74              |
| 1:G:1249:ILE:HG23 | 1:G:1260:ALA:HA   | 1.70                     | 0.73              |
| 1:C:1287:LYS:HD2  | 1:G:1306:ASP:OD2  | 1.89                     | 0.73              |
| 1:E:1287:LYS:HD3  | 1:E:1287:LYS:N    | 2.03                     | 0.73              |
| 1:C:1075:PHE:HE1  | 1:C:1168:PHE:HB2  | 1.53                     | 0.73              |
| 1:E:1039:ASP:HA   | 1:E:1042:ARG:NH1  | 2.04                     | 0.72              |
| 2:D:66:ARG:HG3    | 2:D:66:ARG:HH11   | 1.54                     | 0.72              |
| 1:A:1287:LYS:HD3  | 1:A:1287:LYS:N    | 2.04                     | 0.72              |
| 2:F:21:ILE:O      | 2:F:25:THR:HG22   | 1.90                     | 0.71              |
| 2:F:128:LYS:HE2   | 2:F:132:LYS:HZ1   | 1.52                     | 0.71              |
| 1:A:1039:ASP:HA   | 1:A:1042:ARG:NH1  | 2.05                     | 0.71              |
| 1:C:1039:ASP:HA   | 1:C:1042:ARG:NH1  | 2.05                     | 0.71              |
| 1:C:1287:LYS:HD3  | 1:C:1287:LYS:N    | 2.06                     | 0.71              |
| 2:B:128:LYS:HE2   | 2:B:132:LYS:HZ1   | 1.56                     | 0.71              |
| 1:A:1075:PHE:HE1  | 1:A:1168:PHE:HB2  | 1.55                     | 0.70              |
| 1:E:1251:GLU:O    | 1:E:1251:GLU:HG2  | 1.90                     | 0.70              |
| 1:A:1092:VAL:O    | 1:A:1096:VAL:HG23 | 1.91                     | 0.70              |
| 1:E:1075:PHE:HE1  | 1:E:1168:PHE:HB2  | 1.55                     | 0.70              |
| 1:G:1092:VAL:O    | 1:G:1096:VAL:HG23 | 1.91                     | 0.70              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1240:GLU:OE2  | 1:C:1305:LYS:NZ   | 2.24                     | 0.70              |
| 1:G:1039:ASP:HA   | 1:G:1042:ARG:NH1  | 2.05                     | 0.69              |
| 2:H:21:ILE:O      | 2:H:25:THR:HG22   | 1.91                     | 0.69              |
| 1:G:1249:ILE:HD12 | 1:G:1261:ASP:H    | 1.57                     | 0.69              |
| 1:A:1251:GLU:O    | 1:A:1251:GLU:HG2  | 1.91                     | 0.69              |
| 2:F:66:ARG:HG3    | 2:F:66:ARG:HH11   | 1.56                     | 0.69              |
| 1:G:1273:VAL:HG21 | 1:G:1375:LEU:HB3  | 1.73                     | 0.69              |
| 1:A:1249:ILE:HG23 | 1:A:1260:ALA:HA   | 1.73                     | 0.69              |
| 1:A:1157:VAL:O    | 1:A:1157:VAL:HG12 | 1.92                     | 0.69              |
| 2:H:122:ASP:O     | 2:H:126:ILE:HG13  | 1.93                     | 0.69              |
| 1:E:1249:ILE:HG23 | 1:E:1260:ALA:HA   | 1.74                     | 0.69              |
| 1:E:1092:VAL:O    | 1:E:1096:VAL:HG23 | 1.92                     | 0.68              |
| 1:G:1062:LEU:HD13 | 1:G:1088:LEU:HD11 | 1.74                     | 0.68              |
| 2:D:128:LYS:HE2   | 2:D:132:LYS:HZ1   | 1.59                     | 0.68              |
| 1:C:1249:ILE:HG23 | 1:C:1260:ALA:HA   | 1.74                     | 0.68              |
| 1:E:1157:VAL:HG12 | 1:E:1157:VAL:O    | 1.93                     | 0.68              |
| 1:A:1062:LEU:HD13 | 1:A:1088:LEU:HD11 | 1.74                     | 0.68              |
| 1:A:1260:ALA:O    | 1:A:1261:ASP:HB2  | 1.93                     | 0.68              |
| 1:G:1251:GLU:HG2  | 1:G:1251:GLU:O    | 1.93                     | 0.68              |
| 1:G:1287:LYS:HD3  | 1:G:1287:LYS:N    | 2.08                     | 0.67              |
| 1:C:1157:VAL:HG12 | 1:C:1157:VAL:O    | 1.94                     | 0.67              |
| 1:G:1157:VAL:HG12 | 1:G:1157:VAL:O    | 1.94                     | 0.67              |
| 1:E:1194:LEU:HD23 | 2:F:61:GLN:HB3    | 1.76                     | 0.67              |
| 2:D:21:ILE:O      | 2:D:25:THR:HG22   | 1.95                     | 0.67              |
| 1:C:1092:VAL:O    | 1:C:1096:VAL:HG23 | 1.95                     | 0.67              |
| 1:G:1075:PHE:HE1  | 1:G:1168:PHE:HB2  | 1.59                     | 0.67              |
| 2:H:66:ARG:HG3    | 2:H:66:ARG:HH11   | 1.59                     | 0.66              |
| 1:A:1239:GLU:OE1  | 2:B:66:ARG:NH1    | 2.28                     | 0.66              |
| 2:B:66:ARG:HG3    | 2:B:66:ARG:HH11   | 1.58                     | 0.66              |
| 1:C:1156:LEU:HD13 | 1:C:1183:GLU:HG3  | 1.76                     | 0.66              |
| 1:C:1251:GLU:O    | 1:C:1251:GLU:HG2  | 1.96                     | 0.66              |
| 1:E:1156:LEU:HD13 | 1:E:1183:GLU:HG3  | 1.78                     | 0.66              |
| 2:F:139:TYR:HE2   | 2:F:143:LEU:HD12  | 1.61                     | 0.66              |
| 2:F:161:THR:HG21  | 2:F:163:ARG:HD2   | 1.78                     | 0.66              |
| 1:A:1218:ASP:O    | 1:A:1222:LYS:HD3  | 1.96                     | 0.66              |
| 2:B:21:ILE:O      | 2:B:25:THR:HG22   | 1.96                     | 0.66              |
| 1:E:1234:MSE:HE1  | 1:E:1267:LEU:HD23 | 1.77                     | 0.66              |
| 2:D:116:LYS:HG3   | 2:D:119:LEU:HD23  | 1.77                     | 0.66              |
| 2:B:116:LYS:HG3   | 2:B:119:LEU:HD23  | 1.77                     | 0.65              |
| 2:F:138:THR:H     | 2:F:141:GLN:NE2   | 1.89                     | 0.65              |
| 2:F:102:ARG:NH2   | 2:F:108:THR:O     | 2.28                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:F:6:CYS:HB3     | 2:F:55:LEU:HD23   | 1.78                     | 0.65              |
| 2:D:102:ARG:NH2   | 2:D:108:THR:O     | 2.29                     | 0.65              |
| 2:H:102:ARG:NH2   | 2:H:108:THR:O     | 2.28                     | 0.65              |
| 1:C:1260:ALA:O    | 1:C:1261:ASP:HB2  | 1.95                     | 0.65              |
| 1:C:1156:LEU:CD1  | 1:C:1183:GLU:HG3  | 2.26                     | 0.65              |
| 2:D:120:ARG:NH2   | 2:D:139:TYR:N     | 2.45                     | 0.64              |
| 2:F:116:LYS:HG3   | 2:F:119:LEU:HD23  | 1.78                     | 0.64              |
| 2:B:120:ARG:NH2   | 2:B:139:TYR:N     | 2.45                     | 0.64              |
| 1:C:1062:LEU:HD13 | 1:C:1088:LEU:HD11 | 1.77                     | 0.64              |
| 1:A:1346:PRO:HG3  | 1:E:1374:HIS:ND1  | 2.12                     | 0.64              |
| 2:B:122:ASP:O     | 2:B:126:ILE:HG13  | 1.97                     | 0.64              |
| 1:E:1239:GLU:OE2  | 2:F:66:ARG:HG3    | 1.97                     | 0.64              |
| 1:E:1365:SER:C    | 1:E:1367:GLY:H    | 2.05                     | 0.64              |
| 2:F:120:ARG:NH2   | 2:F:139:TYR:N     | 2.45                     | 0.64              |
| 1:G:1156:LEU:HD13 | 1:G:1183:GLU:HG3  | 1.79                     | 0.64              |
| 2:D:161:THR:HG21  | 2:D:163:ARG:HD2   | 1.79                     | 0.64              |
| 2:F:154:TYR:C     | 2:F:155:LEU:HD12  | 2.23                     | 0.64              |
| 1:G:1176:GLN:NE2  | 2:H:1:MET:N       | 2.45                     | 0.64              |
| 2:D:154:TYR:C     | 2:D:155:LEU:HD12  | 2.23                     | 0.64              |
| 1:C:1140:LYS:HD2  | 1:C:1230:HIS:CD2  | 2.33                     | 0.64              |
| 2:B:157:CYS:HB2   | 2:B:165:LEU:HD12  | 1.80                     | 0.64              |
| 1:A:1365:SER:C    | 1:A:1367:GLY:H    | 2.06                     | 0.63              |
| 1:E:1179:SER:H    | 2:F:41:SER:HB2    | 1.63                     | 0.63              |
| 2:B:102:ARG:NH2   | 2:B:108:THR:O     | 2.31                     | 0.63              |
| 1:C:1273:VAL:HG21 | 1:C:1375:LEU:HB3  | 1.81                     | 0.63              |
| 2:D:138:THR:H     | 2:D:141:GLN:NE2   | 1.90                     | 0.63              |
| 1:E:1218:ASP:O    | 1:E:1222:LYS:HD3  | 1.98                     | 0.63              |
| 1:E:1248:LEU:HD21 | 1:E:1332:ARG:CG   | 2.28                     | 0.63              |
| 1:C:1056:VAL:HG21 | 1:C:1099:LEU:CD2  | 2.27                     | 0.63              |
| 1:E:1062:LEU:HD13 | 1:E:1088:LEU:HD11 | 1.79                     | 0.63              |
| 1:G:1086:GLY:O    | 1:G:1088:LEU:N    | 2.32                     | 0.63              |
| 2:F:84:LEU:HD12   | 2:F:117:LEU:HA    | 1.81                     | 0.63              |
| 1:E:1331:PHE:CZ   | 1:E:1333:HIS:HB2  | 2.34                     | 0.63              |
| 2:B:84:LEU:HD12   | 2:B:117:LEU:HA    | 1.81                     | 0.63              |
| 1:A:1212:GLU:CD   | 1:G:1097:GLU:HG2  | 2.23                     | 0.63              |
| 2:B:161:THR:HG21  | 2:B:163:ARG:HD2   | 1.81                     | 0.63              |
| 1:C:1365:SER:C    | 1:C:1367:GLY:H    | 2.06                     | 0.63              |
| 1:E:1156:LEU:CD1  | 1:E:1183:GLU:HG3  | 2.28                     | 0.62              |
| 1:E:1260:ALA:O    | 1:E:1261:ASP:CB   | 2.45                     | 0.62              |
| 1:G:1365:SER:C    | 1:G:1367:GLY:H    | 2.07                     | 0.62              |
| 1:G:1218:ASP:O    | 1:G:1222:LYS:HD3  | 1.99                     | 0.62              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:E:1088:LEU:O   | 1:E:1092:VAL:HG23 | 2.00                     | 0.62              |
| 1:C:1287:LYS:HG2 | 1:C:1288:GLU:N    | 2.15                     | 0.62              |
| 2:D:84:LEU:HD12  | 2:D:117:LEU:HA    | 1.82                     | 0.62              |
| 2:F:139:TYR:CE2  | 2:F:143:LEU:HD12  | 2.34                     | 0.62              |
| 1:G:1178:HIS:HA  | 1:G:1181:THR:HG23 | 1.82                     | 0.62              |
| 1:G:1287:LYS:HG2 | 1:G:1288:GLU:N    | 2.14                     | 0.62              |
| 2:H:116:LYS:HG3  | 2:H:119:LEU:HD23  | 1.80                     | 0.62              |
| 1:A:1086:GLY:O   | 1:A:1088:LEU:N    | 2.33                     | 0.61              |
| 2:B:154:TYR:C    | 2:B:155:LEU:HD12  | 2.25                     | 0.61              |
| 1:C:1178:HIS:HA  | 1:C:1181:THR:HG23 | 1.82                     | 0.61              |
| 2:D:122:ASP:O    | 2:D:126:ILE:HG13  | 1.99                     | 0.61              |
| 1:G:1156:LEU:CD1 | 1:G:1183:GLU:HG3  | 2.29                     | 0.61              |
| 1:C:1088:LEU:O   | 1:C:1092:VAL:HG23 | 1.99                     | 0.61              |
| 1:C:1218:ASP:O   | 1:C:1222:LYS:HD3  | 2.00                     | 0.61              |
| 2:D:139:TYR:HE2  | 2:D:143:LEU:HD12  | 1.65                     | 0.61              |
| 1:G:1365:SER:O   | 1:G:1366:GLU:HB3  | 2.01                     | 0.61              |
| 1:A:1178:HIS:HA  | 1:A:1181:THR:HG23 | 1.83                     | 0.61              |
| 1:E:1140:LYS:HD2 | 1:E:1230:HIS:CD2  | 2.36                     | 0.61              |
| 1:C:1112:LEU:HA  | 1:C:1115:LEU:HD13 | 1.83                     | 0.61              |
| 1:G:1112:LEU:HA  | 1:G:1115:LEU:HD13 | 1.83                     | 0.61              |
| 1:C:1304:TYR:HB3 | 1:C:1331:PHE:HB3  | 1.81                     | 0.60              |
| 2:F:122:ASP:O    | 2:F:126:ILE:HG13  | 2.00                     | 0.60              |
| 1:G:1140:LYS:HD2 | 1:G:1230:HIS:CD2  | 2.36                     | 0.60              |
| 2:H:161:THR:HG21 | 2:H:163:ARG:HD2   | 1.82                     | 0.60              |
| 1:C:1247:GLN:HB3 | 1:C:1332:ARG:NH1  | 2.16                     | 0.60              |
| 2:D:157:CYS:HB2  | 2:D:165:LEU:HD12  | 1.83                     | 0.60              |
| 2:H:6:CYS:HB3    | 2:H:55:LEU:HD23   | 1.83                     | 0.60              |
| 2:B:138:THR:H    | 2:B:141:GLN:NE2   | 1.89                     | 0.60              |
| 2:H:120:ARG:NH2  | 2:H:139:TYR:N     | 2.49                     | 0.60              |
| 1:E:1365:SER:O   | 1:E:1366:GLU:HB3  | 2.02                     | 0.60              |
| 2:B:6:CYS:HB3    | 2:B:55:LEU:HD23   | 1.83                     | 0.60              |
| 1:E:1076:LEU:HB3 | 1:E:1080:GLU:HB2  | 1.84                     | 0.60              |
| 1:G:1088:LEU:O   | 1:G:1092:VAL:HG23 | 2.02                     | 0.60              |
| 1:A:1076:LEU:HB3 | 1:A:1080:GLU:HB2  | 1.82                     | 0.60              |
| 1:C:1075:PHE:HE1 | 1:C:1168:PHE:CB   | 2.15                     | 0.60              |
| 1:C:1287:LYS:HD2 | 1:G:1306:ASP:CG   | 2.27                     | 0.60              |
| 1:C:1365:SER:O   | 1:C:1366:GLU:HB3  | 2.02                     | 0.60              |
| 2:F:157:CYS:HB2  | 2:F:165:LEU:HD12  | 1.82                     | 0.60              |
| 2:H:138:THR:H    | 2:H:141:GLN:NE2   | 1.84                     | 0.60              |
| 1:C:1179:SER:H   | 2:D:41:SER:HB2    | 1.67                     | 0.60              |
| 1:E:1086:GLY:O   | 1:E:1088:LEU:N    | 2.35                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1140:LYS:HD2  | 1:A:1230:HIS:CD2  | 2.37                     | 0.59              |
| 1:A:1194:LEU:HD23 | 2:B:61:GLN:HB3    | 1.84                     | 0.59              |
| 1:C:1076:LEU:HB3  | 1:C:1080:GLU:HB2  | 1.83                     | 0.59              |
| 1:G:1343:ARG:HD2  | 1:G:1343:ARG:N    | 2.17                     | 0.59              |
| 1:E:1343:ARG:HD3  | 1:E:1357:GLU:CG   | 2.29                     | 0.59              |
| 1:C:1103:GLU:O    | 1:C:1106:VAL:HG12 | 2.02                     | 0.59              |
| 1:E:1042:ARG:HE   | 1:E:1113:GLU:HA   | 1.67                     | 0.59              |
| 1:E:1112:LEU:HA   | 1:E:1115:LEU:HD13 | 1.84                     | 0.59              |
| 2:H:84:LEU:HD12   | 2:H:117:LEU:HA    | 1.83                     | 0.59              |
| 2:F:83:SER:HB3    | 2:F:86:SER:HB3    | 1.84                     | 0.59              |
| 1:G:1343:ARG:HD3  | 1:G:1357:GLU:CG   | 2.32                     | 0.59              |
| 2:H:154:TYR:C     | 2:H:155:LEU:HD12  | 2.27                     | 0.59              |
| 1:C:1042:ARG:HE   | 1:C:1113:GLU:HA   | 1.68                     | 0.59              |
| 1:C:1343:ARG:HD2  | 1:C:1343:ARG:N    | 2.17                     | 0.59              |
| 1:E:1274:ILE:HG21 | 1:E:1288:GLU:HB2  | 1.85                     | 0.59              |
| 1:G:1076:LEU:HB3  | 1:G:1080:GLU:HB2  | 1.85                     | 0.59              |
| 1:A:1365:SER:O    | 1:A:1366:GLU:HB3  | 2.03                     | 0.58              |
| 1:C:1149:HIS:HA   | 1:C:1152:VAL:HG23 | 1.85                     | 0.58              |
| 1:E:1117:LYS:HB2  | 1:E:1120:GLN:HG3  | 1.84                     | 0.58              |
| 2:H:157:CYS:HB2   | 2:H:165:LEU:HD12  | 1.85                     | 0.58              |
| 1:A:1274:ILE:HG21 | 1:A:1288:GLU:HB2  | 1.85                     | 0.58              |
| 2:D:139:TYR:CE2   | 2:D:143:LEU:HD12  | 2.39                     | 0.58              |
| 1:E:1063:MSE:CE   | 1:E:1088:LEU:HD22 | 2.34                     | 0.58              |
| 1:E:1178:HIS:HA   | 1:E:1181:THR:HG23 | 1.83                     | 0.58              |
| 1:A:1042:ARG:HE   | 1:A:1113:GLU:HA   | 1.68                     | 0.58              |
| 2:H:128:LYS:HE2   | 2:H:132:LYS:NZ    | 2.18                     | 0.58              |
| 1:A:1343:ARG:CD   | 1:A:1357:GLU:HG3  | 2.32                     | 0.58              |
| 2:D:6:CYS:HB3     | 2:D:55:LEU:HD23   | 1.85                     | 0.58              |
| 1:C:1075:PHE:CE1  | 1:C:1168:PHE:HB2  | 2.36                     | 0.58              |
| 2:H:83:SER:HB3    | 2:H:86:SER:HB3    | 1.86                     | 0.58              |
| 1:A:1149:HIS:HA   | 1:A:1152:VAL:HG23 | 1.84                     | 0.57              |
| 1:E:1343:ARG:HD2  | 1:E:1343:ARG:N    | 2.19                     | 0.57              |
| 2:F:128:LYS:HE2   | 2:F:132:LYS:NZ    | 2.18                     | 0.57              |
| 1:A:1112:LEU:HA   | 1:A:1115:LEU:HD13 | 1.86                     | 0.57              |
| 1:A:1287:LYS:HG2  | 1:A:1288:GLU:N    | 2.19                     | 0.57              |
| 1:G:1176:GLN:HE22 | 2:H:1:MET:N       | 2.02                     | 0.57              |
| 1:A:1117:LYS:HB2  | 1:A:1120:GLN:HG3  | 1.87                     | 0.57              |
| 2:D:138:THR:N     | 2:D:141:GLN:HE21  | 1.91                     | 0.57              |
| 1:E:1075:PHE:HE1  | 1:E:1168:PHE:CB   | 2.17                     | 0.57              |
| 1:A:1103:GLU:O    | 1:A:1106:VAL:HG12 | 2.04                     | 0.57              |
| 1:E:1149:HIS:HA   | 1:E:1152:VAL:HG23 | 1.86                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:E:1287:LYS:HG2  | 1:E:1288:GLU:N    | 2.19                     | 0.57              |
| 1:E:1287:LYS:HZ2  | 1:E:1288:GLU:H    | 1.53                     | 0.57              |
| 1:A:1239:GLU:CD   | 2:B:66:ARG:NH1    | 2.63                     | 0.57              |
| 1:C:1086:GLY:O    | 1:C:1088:LEU:N    | 2.38                     | 0.57              |
| 1:C:1117:LYS:HB2  | 1:C:1120:GLN:HG3  | 1.87                     | 0.57              |
| 1:C:1274:ILE:CG2  | 1:C:1288:GLU:HB2  | 2.35                     | 0.57              |
| 1:E:1274:ILE:CG2  | 1:E:1288:GLU:HB2  | 2.34                     | 0.57              |
| 1:A:1067:LEU:HB3  | 1:A:1085:PHE:CZ   | 2.40                     | 0.57              |
| 1:A:1075:PHE:HE1  | 1:A:1168:PHE:CB   | 2.17                     | 0.57              |
| 1:A:1274:ILE:CG2  | 1:A:1288:GLU:HB2  | 2.35                     | 0.57              |
| 1:A:1343:ARG:HD2  | 1:A:1343:ARG:N    | 2.20                     | 0.57              |
| 1:C:1274:ILE:HG21 | 1:C:1288:GLU:HB2  | 1.86                     | 0.57              |
| 1:A:1056:VAL:HG21 | 1:A:1099:LEU:CD2  | 2.32                     | 0.57              |
| 1:E:1343:ARG:CD   | 1:E:1357:GLU:HG3  | 2.31                     | 0.57              |
| 1:C:1343:ARG:HD3  | 1:C:1357:GLU:CG   | 2.32                     | 0.57              |
| 1:E:1177:GLN:HG3  | 2:F:41:SER:HB3    | 1.86                     | 0.57              |
| 2:D:83:SER:HB3    | 2:D:86:SER:HB3    | 1.86                     | 0.56              |
| 1:A:1088:LEU:O    | 1:A:1092:VAL:HG23 | 2.05                     | 0.56              |
| 1:C:1056:VAL:CG2  | 1:C:1099:LEU:HD22 | 2.32                     | 0.56              |
| 1:G:1042:ARG:HE   | 1:G:1113:GLU:HA   | 1.69                     | 0.56              |
| 2:H:87:PRO:HA     | 2:H:137:ILE:HD11  | 1.88                     | 0.56              |
| 2:H:139:TYR:HE2   | 2:H:143:LEU:HD12  | 1.70                     | 0.56              |
| 2:D:87:PRO:HA     | 2:D:137:ILE:HD11  | 1.87                     | 0.56              |
| 2:B:139:TYR:HE2   | 2:B:143:LEU:HD12  | 1.70                     | 0.56              |
| 1:C:1287:LYS:CD   | 1:G:1306:ASP:OD2  | 2.54                     | 0.56              |
| 1:G:1063:MSE:CE   | 1:G:1088:LEU:HD22 | 2.35                     | 0.56              |
| 2:H:138:THR:N     | 2:H:141:GLN:HE21  | 1.84                     | 0.56              |
| 1:C:1343:ARG:HD2  | 1:C:1343:ARG:H    | 1.71                     | 0.56              |
| 1:E:1067:LEU:HB3  | 1:E:1085:PHE:CZ   | 2.41                     | 0.56              |
| 1:G:1103:GLU:O    | 1:G:1106:VAL:HG12 | 2.06                     | 0.56              |
| 1:A:1343:ARG:HD3  | 1:A:1357:GLU:CG   | 2.30                     | 0.56              |
| 2:B:128:LYS:HE2   | 2:B:132:LYS:NZ    | 2.19                     | 0.56              |
| 1:C:1247:GLN:O    | 1:C:1251:GLU:HB3  | 2.05                     | 0.56              |
| 1:G:1345:LEU:HD12 | 1:G:1355:VAL:HG12 | 1.88                     | 0.56              |
| 1:E:1075:PHE:CE1  | 1:E:1168:PHE:HB2  | 2.39                     | 0.55              |
| 1:A:1190:ILE:HD13 | 2:B:70:LEU:CD1    | 2.35                     | 0.55              |
| 2:B:87:PRO:HA     | 2:B:137:ILE:HD11  | 1.87                     | 0.55              |
| 2:B:139:TYR:CE2   | 2:B:143:LEU:HD12  | 2.41                     | 0.55              |
| 1:G:1260:ALA:O    | 1:G:1261:ASP:HB2  | 2.05                     | 0.55              |
| 1:G:1343:ARG:HD2  | 1:G:1343:ARG:H    | 1.70                     | 0.55              |
| 2:D:128:LYS:HE2   | 2:D:132:LYS:NZ    | 2.20                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1295:VAL:HG11 | 1:A:1389:SER:OG   | 2.06                     | 0.55              |
| 2:B:83:SER:HB3    | 2:B:86:SER:HB3    | 1.87                     | 0.55              |
| 1:C:1248:LEU:HD21 | 1:C:1332:ARG:CG   | 2.31                     | 0.55              |
| 1:G:1111:ASP:OD2  | 1:G:1113:GLU:HB2  | 2.06                     | 0.55              |
| 2:F:139:TYR:HB3   | 2:F:140:PRO:HD3   | 1.88                     | 0.55              |
| 1:A:1173:ASN:HD21 | 1:A:1180:SER:HB2  | 1.72                     | 0.55              |
| 1:A:1183:GLU:CD   | 2:B:74:GLN:NE2    | 2.64                     | 0.55              |
| 1:A:1239:GLU:CD   | 2:B:66:ARG:HH11   | 2.15                     | 0.55              |
| 1:E:1109:VAL:HG13 | 1:E:1110:PRO:HD2  | 1.89                     | 0.55              |
| 1:G:1398:HIS:C    | 1:G:1400:ARG:H    | 2.14                     | 0.55              |
| 2:H:98:TYR:HB3    | 2:H:99:PRO:HD3    | 1.89                     | 0.55              |
| 1:A:1215:TYR:OH   | 1:G:1138:ARG:HG3  | 2.07                     | 0.55              |
| 2:B:98:TYR:OH     | 2:B:102:ARG:HD2   | 2.07                     | 0.55              |
| 1:C:1063:MSE:CE   | 1:C:1088:LEU:HD22 | 2.37                     | 0.55              |
| 1:C:1288:GLU:OE1  | 1:G:1308:SER:HB2  | 2.07                     | 0.55              |
| 2:F:87:PRO:HA     | 2:F:137:ILE:HD11  | 1.88                     | 0.55              |
| 1:G:1067:LEU:HB3  | 1:G:1085:PHE:CZ   | 2.42                     | 0.55              |
| 1:A:1119:ASP:O    | 1:A:1122:LYS:HG3  | 2.07                     | 0.55              |
| 1:C:1218:ASP:OD1  | 1:C:1222:LYS:HE3  | 2.06                     | 0.55              |
| 1:C:1306:ASP:OD2  | 1:G:1287:LYS:N    | 2.31                     | 0.55              |
| 2:H:19:LEU:C      | 2:H:19:LEU:HD23   | 2.32                     | 0.55              |
| 1:A:1287:LYS:HZ2  | 1:A:1288:GLU:H    | 1.54                     | 0.54              |
| 1:A:1345:LEU:HD12 | 1:A:1355:VAL:HG12 | 1.89                     | 0.54              |
| 1:C:1173:ASN:HD21 | 1:C:1180:SER:HB2  | 1.71                     | 0.54              |
| 1:C:1227:VAL:O    | 1:C:1231:ILE:HG12 | 2.06                     | 0.54              |
| 1:E:1035:LEU:HB2  | 1:E:1039:ASP:HB2  | 1.88                     | 0.54              |
| 1:E:1343:ARG:HD2  | 1:E:1343:ARG:H    | 1.72                     | 0.54              |
| 1:G:1179:SER:H    | 2:H:41:SER:HB2    | 1.71                     | 0.54              |
| 2:H:139:TYR:CE2   | 2:H:143:LEU:HD12  | 2.42                     | 0.54              |
| 2:B:138:THR:N     | 2:B:141:GLN:HE21  | 1.92                     | 0.54              |
| 1:C:1216:HIS:HB3  | 1:E:1134:TYR:CE2  | 2.42                     | 0.54              |
| 1:E:1247:GLN:O    | 1:E:1251:GLU:HB3  | 2.06                     | 0.54              |
| 1:E:1103:GLU:O    | 1:E:1106:VAL:HG12 | 2.07                     | 0.54              |
| 2:F:19:LEU:C      | 2:F:19:LEU:HD23   | 2.33                     | 0.54              |
| 1:G:1176:GLN:NE2  | 2:H:1:MET:H3      | 2.03                     | 0.54              |
| 2:B:139:TYR:HB3   | 2:B:140:PRO:HD3   | 1.89                     | 0.54              |
| 1:C:1067:LEU:HB3  | 1:C:1085:PHE:CZ   | 2.41                     | 0.54              |
| 1:E:1094:PHE:HE1  | 1:E:1135:TYR:HD2  | 1.55                     | 0.54              |
| 1:G:1035:LEU:HD12 | 2:H:31:GLU:CB     | 2.35                     | 0.54              |
| 1:G:1075:PHE:CE1  | 1:G:1168:PHE:HB2  | 2.43                     | 0.54              |
| 1:G:1274:ILE:HG21 | 1:G:1288:GLU:HB2  | 1.88                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1234:MSE:HE1  | 1:A:1267:LEU:HD23 | 1.90                     | 0.54              |
| 1:A:1343:ARG:HD2  | 1:A:1343:ARG:H    | 1.72                     | 0.54              |
| 1:A:1247:GLN:O    | 1:A:1251:GLU:HB3  | 2.08                     | 0.54              |
| 2:F:98:TYR:HB3    | 2:F:99:PRO:HD3    | 1.90                     | 0.54              |
| 1:A:1075:PHE:CE1  | 1:A:1168:PHE:HB2  | 2.38                     | 0.54              |
| 1:E:1115:LEU:HD12 | 1:E:1115:LEU:N    | 2.23                     | 0.54              |
| 1:A:1063:MSE:CE   | 1:A:1088:LEU:HD22 | 2.37                     | 0.53              |
| 1:A:1218:ASP:OD1  | 1:A:1222:LYS:HE3  | 2.09                     | 0.53              |
| 1:G:1117:LYS:HB2  | 1:G:1120:GLN:HG3  | 1.89                     | 0.53              |
| 1:A:1135:TYR:CE2  | 1:A:1138:ARG:NH2  | 2.75                     | 0.53              |
| 1:G:1094:PHE:HE1  | 1:G:1135:TYR:HD2  | 1.56                     | 0.53              |
| 1:G:1343:ARG:CD   | 1:G:1357:GLU:HG3  | 2.33                     | 0.53              |
| 1:A:1135:TYR:HE2  | 1:A:1138:ARG:NH2  | 2.05                     | 0.53              |
| 1:A:1395:ARG:O    | 1:A:1398:HIS:HB3  | 2.07                     | 0.53              |
| 2:F:8:VAL:HG22    | 2:F:79:LEU:HD12   | 1.90                     | 0.53              |
| 2:H:138:THR:HG1   | 2:H:141:GLN:HG3   | 1.70                     | 0.53              |
| 1:A:1111:ASP:OD2  | 1:A:1113:GLU:HB2  | 2.09                     | 0.53              |
| 1:A:1260:ALA:O    | 1:A:1261:ASP:CB   | 2.55                     | 0.53              |
| 1:C:1156:LEU:HD21 | 1:C:1182:LEU:HD23 | 1.91                     | 0.53              |
| 1:G:1274:ILE:CG2  | 1:G:1288:GLU:HB2  | 2.38                     | 0.53              |
| 1:A:1056:VAL:CG2  | 1:A:1099:LEU:HD22 | 2.36                     | 0.53              |
| 1:E:1285:TRP:HH2  | 2:H:102:ARG:HG2   | 1.74                     | 0.53              |
| 1:C:1368:ARG:HH11 | 1:C:1368:ARG:CG   | 2.19                     | 0.53              |
| 1:E:1187:ILE:O    | 1:E:1191:GLN:HG3  | 2.09                     | 0.53              |
| 1:A:1109:VAL:HG13 | 1:A:1110:PRO:HD2  | 1.89                     | 0.53              |
| 1:G:1156:LEU:C    | 1:G:1158:LYS:H    | 2.16                     | 0.53              |
| 1:E:1135:TYR:CE2  | 1:E:1138:ARG:NH2  | 2.77                     | 0.53              |
| 1:G:1247:GLN:O    | 1:G:1251:GLU:HB3  | 2.09                     | 0.53              |
| 1:C:1345:LEU:HD12 | 1:C:1355:VAL:HG12 | 1.90                     | 0.53              |
| 1:C:1140:LYS:HD2  | 1:C:1230:HIS:HD2  | 1.74                     | 0.53              |
| 1:C:1179:SER:H    | 2:D:41:SER:CB     | 2.22                     | 0.53              |
| 1:G:1075:PHE:HE1  | 1:G:1168:PHE:CB   | 2.20                     | 0.53              |
| 1:G:1140:LYS:HE2  | 1:G:1227:VAL:HA   | 1.89                     | 0.53              |
| 1:A:1094:PHE:HE1  | 1:A:1135:TYR:HD2  | 1.58                     | 0.52              |
| 1:A:1115:LEU:N    | 1:A:1115:LEU:HD12 | 2.24                     | 0.52              |
| 2:B:57:ASP:OD1    | 2:B:58:THR:N      | 2.41                     | 0.52              |
| 1:C:1115:LEU:HD12 | 1:C:1115:LEU:N    | 2.23                     | 0.52              |
| 2:D:19:LEU:HD23   | 2:D:19:LEU:C      | 2.34                     | 0.52              |
| 2:D:139:TYR:HB3   | 2:D:140:PRO:HD3   | 1.90                     | 0.52              |
| 1:E:1035:LEU:HB2  | 1:E:1039:ASP:CB   | 2.39                     | 0.52              |
| 1:G:1115:LEU:HD12 | 1:G:1115:LEU:N    | 2.23                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1282:LEU:HG   | 1:C:1289:PRO:HG2  | 1.91                     | 0.52              |
| 2:H:155:LEU:CD2   | 2:H:168:VAL:HA    | 2.39                     | 0.52              |
| 1:A:1346:PRO:HG3  | 1:E:1374:HIS:CG   | 2.44                     | 0.52              |
| 1:E:1298:THR:O    | 1:E:1299:ALA:HB2  | 2.08                     | 0.52              |
| 1:C:1306:ASP:OD2  | 1:G:1286:LYS:HA   | 2.10                     | 0.52              |
| 1:E:1249:ILE:HD12 | 1:E:1261:ASP:N    | 2.12                     | 0.52              |
| 1:G:1287:LYS:HG2  | 1:G:1288:GLU:H    | 1.72                     | 0.52              |
| 1:C:1287:LYS:HG2  | 1:C:1288:GLU:H    | 1.74                     | 0.52              |
| 1:C:1345:LEU:HD12 | 1:C:1355:VAL:CG1  | 2.40                     | 0.52              |
| 1:G:1149:HIS:HA   | 1:G:1152:VAL:HG23 | 1.92                     | 0.52              |
| 1:A:1177:GLN:HG3  | 2:B:41:SER:HB3    | 1.90                     | 0.52              |
| 2:B:68:ARG:NH1    | 2:B:100:GLU:OE1   | 2.43                     | 0.52              |
| 2:B:19:LEU:C      | 2:B:19:LEU:HD23   | 2.35                     | 0.52              |
| 1:C:1140:LYS:HE2  | 1:C:1227:VAL:HA   | 1.92                     | 0.52              |
| 1:C:1343:ARG:CD   | 1:C:1357:GLU:HG3  | 2.33                     | 0.52              |
| 1:G:1287:LYS:HZ2  | 1:G:1288:GLU:H    | 1.55                     | 0.52              |
| 1:A:1346:PRO:HG3  | 1:E:1374:HIS:CE1  | 2.45                     | 0.52              |
| 1:C:1062:LEU:HG   | 1:C:1185:TYR:HB3  | 1.92                     | 0.52              |
| 1:C:1109:VAL:HG13 | 1:C:1110:PRO:HD2  | 1.92                     | 0.52              |
| 1:C:1234:MSE:HE2  | 1:C:1237:ILE:HD12 | 1.91                     | 0.52              |
| 1:E:1056:VAL:HG21 | 1:E:1099:LEU:CD2  | 2.35                     | 0.52              |
| 1:E:1285:TRP:CZ2  | 2:H:98:TYR:CE2    | 2.92                     | 0.52              |
| 1:C:1094:PHE:HE1  | 1:C:1135:TYR:HD2  | 1.58                     | 0.51              |
| 1:C:1287:LYS:HZ2  | 1:C:1288:GLU:H    | 1.58                     | 0.51              |
| 1:E:1273:VAL:HG21 | 1:E:1375:LEU:HB3  | 1.92                     | 0.51              |
| 1:C:1156:LEU:C    | 1:C:1158:LYS:H    | 2.18                     | 0.51              |
| 2:F:5:LYS:HE3     | 2:F:56:TRP:CE3    | 2.46                     | 0.51              |
| 2:H:139:TYR:HB3   | 2:H:140:PRO:HD3   | 1.91                     | 0.51              |
| 2:B:152:VAL:HG12  | 2:B:153:LYS:HG2   | 1.91                     | 0.51              |
| 2:D:96:LYS:O      | 2:D:99:PRO:HD2    | 2.10                     | 0.51              |
| 1:A:1187:ILE:O    | 1:A:1191:GLN:HG3  | 2.09                     | 0.51              |
| 2:B:128:LYS:C     | 2:B:128:LYS:HD3   | 2.36                     | 0.51              |
| 1:C:1191:GLN:O    | 1:C:1195:LYS:HG2  | 2.11                     | 0.51              |
| 1:C:1194:LEU:HD23 | 2:D:61:GLN:HB3    | 1.93                     | 0.51              |
| 1:C:1260:ALA:O    | 1:C:1261:ASP:CB   | 2.57                     | 0.51              |
| 2:D:68:ARG:NH1    | 2:D:100:GLU:OE1   | 2.44                     | 0.51              |
| 1:G:1109:VAL:HG13 | 1:G:1110:PRO:HD2  | 1.91                     | 0.51              |
| 1:A:1345:LEU:HD12 | 1:A:1355:VAL:CG1  | 2.40                     | 0.51              |
| 1:C:1111:ASP:OD2  | 1:C:1113:GLU:HB2  | 2.10                     | 0.51              |
| 1:E:1140:LYS:HE2  | 1:E:1227:VAL:HA   | 1.91                     | 0.51              |
| 1:G:1339:ALA:HB1  | 1:G:1361:VAL:HG22 | 1.92                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1339:ALA:HB1  | 1:A:1361:VAL:HG22 | 1.92                     | 0.51              |
| 1:E:1339:ALA:HB1  | 1:E:1361:VAL:HG22 | 1.93                     | 0.51              |
| 2:B:8:VAL:HG22    | 2:B:79:LEU:HD12   | 1.93                     | 0.51              |
| 2:B:58:THR:O      | 2:B:61:GLN:HG2    | 2.11                     | 0.51              |
| 1:C:1119:ASP:O    | 1:C:1122:LYS:HG3  | 2.11                     | 0.51              |
| 1:E:1218:ASP:OD1  | 1:E:1222:LYS:HE3  | 2.10                     | 0.51              |
| 1:G:1194:LEU:HD23 | 2:H:61:GLN:HB3    | 1.93                     | 0.51              |
| 2:D:128:LYS:HD3   | 2:D:128:LYS:C     | 2.36                     | 0.51              |
| 1:E:1368:ARG:HG3  | 1:E:1368:ARG:NH1  | 2.20                     | 0.51              |
| 2:F:12:GLY:O      | 2:F:13:ALA:HB3    | 2.10                     | 0.51              |
| 1:A:1173:ASN:ND2  | 1:A:1180:SER:HB2  | 2.26                     | 0.50              |
| 2:B:142:GLY:HA3   | 2:B:154:TYR:CZ    | 2.46                     | 0.50              |
| 2:F:138:THR:OG1   | 2:F:140:PRO:HD2   | 2.12                     | 0.50              |
| 1:G:1282:LEU:HG   | 1:G:1289:PRO:HG2  | 1.93                     | 0.50              |
| 1:A:1234:MSE:SE   | 1:A:1267:LEU:HD23 | 2.61                     | 0.50              |
| 1:C:1339:ALA:HB1  | 1:C:1361:VAL:HG22 | 1.93                     | 0.50              |
| 1:C:1341:GLN:HB3  | 1:C:1359:VAL:HB   | 1.93                     | 0.50              |
| 1:E:1345:LEU:HD12 | 1:E:1355:VAL:HG12 | 1.93                     | 0.50              |
| 1:G:1119:ASP:O    | 1:G:1122:LYS:HG3  | 2.11                     | 0.50              |
| 1:C:1328:PRO:HG2  | 1:C:1329:PHE:CD1  | 2.46                     | 0.50              |
| 1:G:1282:LEU:HD21 | 1:G:1289:PRO:HB3  | 1.94                     | 0.50              |
| 2:B:138:THR:HG23  | 2:B:141:GLN:HE21  | 1.76                     | 0.50              |
| 1:C:1282:LEU:HB2  | 1:G:1285:TRP:CE2  | 2.47                     | 0.50              |
| 1:E:1135:TYR:HE2  | 1:E:1138:ARG:NH2  | 2.10                     | 0.50              |
| 1:E:1142:TYR:CE2  | 1:E:1193:VAL:HG13 | 2.46                     | 0.50              |
| 1:G:1187:ILE:O    | 1:G:1191:GLN:HG3  | 2.11                     | 0.50              |
| 1:A:1140:LYS:HE2  | 1:A:1227:VAL:HA   | 1.94                     | 0.50              |
| 2:D:66:ARG:HH11   | 2:D:66:ARG:CG     | 2.23                     | 0.50              |
| 1:C:1177:GLN:HG3  | 2:D:41:SER:HB3    | 1.94                     | 0.50              |
| 2:F:142:GLY:HA3   | 2:F:154:TYR:CZ    | 2.47                     | 0.50              |
| 2:F:153:LYS:HB3   | 2:F:155:LEU:CD1   | 2.41                     | 0.50              |
| 1:E:1062:LEU:HG   | 1:E:1185:TYR:HB3  | 1.94                     | 0.50              |
| 1:E:1179:SER:H    | 2:F:41:SER:CB     | 2.24                     | 0.50              |
| 1:E:1397:LYS:O    | 1:E:1401:GLN:HB2  | 2.12                     | 0.50              |
| 1:G:1345:LEU:HD12 | 1:G:1355:VAL:CG1  | 2.40                     | 0.50              |
| 2:H:10:GLY:HA2    | 2:H:97:TRP:CE2    | 2.47                     | 0.50              |
| 2:D:138:THR:OG1   | 2:D:140:PRO:HD2   | 2.11                     | 0.50              |
| 1:E:1368:ARG:HH11 | 1:E:1368:ARG:CG   | 2.17                     | 0.50              |
| 1:G:1135:TYR:CE2  | 1:G:1138:ARG:NH2  | 2.79                     | 0.50              |
| 2:H:28:PHE:CD1    | 2:H:29:PRO:HD2    | 2.46                     | 0.50              |
| 2:H:152:VAL:HG12  | 2:H:153:LYS:HG2   | 1.94                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1173:ASN:ND2  | 1:C:1180:SER:HB2  | 2.26                     | 0.49              |
| 1:A:1273:VAL:HG21 | 1:A:1375:LEU:HB3  | 1.94                     | 0.49              |
| 1:C:1287:LYS:CG   | 1:C:1288:GLU:N    | 2.75                     | 0.49              |
| 1:C:1306:ASP:OD2  | 1:G:1287:LYS:HD2  | 2.13                     | 0.49              |
| 2:D:155:LEU:CD2   | 2:D:168:VAL:HA    | 2.41                     | 0.49              |
| 2:F:128:LYS:HD3   | 2:F:128:LYS:C     | 2.36                     | 0.49              |
| 2:F:153:LYS:HB3   | 2:F:155:LEU:HD11  | 1.94                     | 0.49              |
| 1:A:1156:LEU:C    | 1:A:1158:LYS:H    | 2.19                     | 0.49              |
| 1:A:1212:GLU:OE1  | 1:G:1138:ARG:NH2  | 2.45                     | 0.49              |
| 1:C:1212:GLU:CD   | 1:E:1097:GLU:HG2  | 2.37                     | 0.49              |
| 2:H:146:ALA:CB    | 2:H:154:TYR:HB2   | 2.42                     | 0.49              |
| 1:C:1049:LEU:HD11 | 1:C:1106:VAL:HB   | 1.94                     | 0.49              |
| 2:D:28:PHE:CD1    | 2:D:29:PRO:HD2    | 2.47                     | 0.49              |
| 1:E:1049:LEU:HD11 | 1:E:1106:VAL:HB   | 1.94                     | 0.49              |
| 2:F:155:LEU:HD12  | 2:F:155:LEU:N     | 2.27                     | 0.49              |
| 1:A:1134:TYR:CE2  | 1:G:1216:HIS:HB3  | 2.47                     | 0.49              |
| 2:B:28:PHE:CD1    | 2:B:29:PRO:HD2    | 2.47                     | 0.49              |
| 2:D:153:LYS:HB3   | 2:D:155:LEU:CD1   | 2.43                     | 0.49              |
| 2:D:153:LYS:HB3   | 2:D:155:LEU:HD11  | 1.94                     | 0.49              |
| 1:E:1153:PRO:O    | 1:E:1157:VAL:HG23 | 2.13                     | 0.49              |
| 2:H:12:GLY:O      | 2:H:13:ALA:HB3    | 2.13                     | 0.49              |
| 2:B:98:TYR:HB3    | 2:B:99:PRO:HD3    | 1.94                     | 0.49              |
| 1:C:1350:ALA:O    | 1:C:1351:GLU:HB3  | 2.12                     | 0.49              |
| 1:E:1111:ASP:OD2  | 1:E:1113:GLU:HB2  | 2.11                     | 0.49              |
| 2:F:138:THR:N     | 2:F:141:GLN:HE21  | 1.91                     | 0.49              |
| 2:H:153:LYS:HB3   | 2:H:155:LEU:CD1   | 2.42                     | 0.49              |
| 1:A:1062:LEU:HG   | 1:A:1185:TYR:HB3  | 1.95                     | 0.49              |
| 1:A:1340:LEU:HD11 | 1:A:1390:VAL:CG1  | 2.42                     | 0.49              |
| 1:E:1156:LEU:C    | 1:E:1158:LYS:H    | 2.19                     | 0.49              |
| 1:E:1195:LYS:NZ   | 2:F:59:ALA:HB3    | 2.28                     | 0.49              |
| 2:F:155:LEU:CD2   | 2:F:168:VAL:HA    | 2.42                     | 0.49              |
| 1:A:1183:GLU:CD   | 2:B:74:GLN:HE21   | 2.21                     | 0.49              |
| 1:C:1282:LEU:HD21 | 1:C:1289:PRO:HB3  | 1.94                     | 0.49              |
| 1:C:1340:LEU:HD11 | 1:C:1390:VAL:CG1  | 2.43                     | 0.49              |
| 1:E:1227:VAL:O    | 1:E:1231:ILE:HG12 | 2.12                     | 0.49              |
| 2:F:133:LYS:HD3   | 2:F:133:LYS:N     | 2.28                     | 0.49              |
| 1:G:1173:ASN:ND2  | 1:G:1180:SER:HB2  | 2.28                     | 0.49              |
| 1:A:1213:GLU:CD   | 1:A:1213:GLU:H    | 2.20                     | 0.49              |
| 1:A:1368:ARG:HH11 | 1:A:1368:ARG:CG   | 2.21                     | 0.49              |
| 1:E:1273:VAL:HG23 | 1:E:1377:CYS:HA   | 1.95                     | 0.49              |
| 2:F:146:ALA:CB    | 2:F:154:TYR:HB2   | 2.42                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:G:1173:ASN:HD21 | 1:G:1180:SER:HB2  | 1.77                     | 0.49              |
| 1:G:1287:LYS:CG   | 1:G:1288:GLU:N    | 2.76                     | 0.49              |
| 1:G:1341:GLN:HB3  | 1:G:1359:VAL:HB   | 1.94                     | 0.49              |
| 1:G:1350:ALA:O    | 1:G:1351:GLU:HB3  | 2.13                     | 0.49              |
| 1:C:1149:HIS:CE1  | 1:C:1186:LEU:O    | 2.66                     | 0.49              |
| 1:C:1298:THR:O    | 1:C:1299:ALA:HB2  | 2.13                     | 0.49              |
| 1:G:1049:LEU:HD11 | 1:G:1106:VAL:HB   | 1.93                     | 0.49              |
| 1:G:1298:THR:O    | 1:G:1299:ALA:HB2  | 2.12                     | 0.49              |
| 1:E:1156:LEU:HD21 | 1:E:1182:LEU:HD23 | 1.94                     | 0.48              |
| 1:E:1191:GLN:O    | 1:E:1195:LYS:HG2  | 2.13                     | 0.48              |
| 1:A:1368:ARG:HG3  | 1:A:1368:ARG:NH1  | 2.25                     | 0.48              |
| 1:C:1248:LEU:CD2  | 1:C:1332:ARG:HG3  | 2.32                     | 0.48              |
| 2:F:66:ARG:HH11   | 2:F:66:ARG:CG     | 2.25                     | 0.48              |
| 2:D:8:VAL:HG22    | 2:D:79:LEU:HD12   | 1.94                     | 0.48              |
| 2:D:142:GLY:HA3   | 2:D:154:TYR:CZ    | 2.47                     | 0.48              |
| 1:G:1328:PRO:HG2  | 1:G:1329:PHE:CD1  | 2.49                     | 0.48              |
| 2:B:155:LEU:CD2   | 2:B:168:VAL:HA    | 2.43                     | 0.48              |
| 2:D:161:THR:HB    | 2:D:163:ARG:HG2   | 1.94                     | 0.48              |
| 1:C:1156:LEU:CD2  | 1:C:1182:LEU:HD23 | 2.44                     | 0.48              |
| 1:G:1135:TYR:HE2  | 1:G:1138:ARG:NH2  | 2.11                     | 0.48              |
| 1:G:1218:ASP:OD1  | 1:G:1222:LYS:HE3  | 2.13                     | 0.48              |
| 1:C:1213:GLU:CD   | 1:C:1213:GLU:H    | 2.22                     | 0.48              |
| 1:C:1287:LYS:CG   | 1:C:1288:GLU:H    | 2.27                     | 0.48              |
| 1:E:1035:LEU:HG   | 2:F:31:GLU:OE1    | 2.14                     | 0.48              |
| 1:E:1340:LEU:HD11 | 1:E:1390:VAL:CG1  | 2.44                     | 0.48              |
| 2:F:28:PHE:CD1    | 2:F:29:PRO:HD2    | 2.49                     | 0.48              |
| 2:F:68:ARG:NH1    | 2:F:100:GLU:OE1   | 2.46                     | 0.48              |
| 2:H:128:LYS:HD3   | 2:H:128:LYS:C     | 2.38                     | 0.48              |
| 2:H:142:GLY:HA3   | 2:H:154:TYR:CZ    | 2.48                     | 0.48              |
| 2:H:153:LYS:HB3   | 2:H:155:LEU:HD11  | 1.96                     | 0.48              |
| 1:A:1052:GLU:OE2  | 1:A:1095:GLN:NE2  | 2.43                     | 0.48              |
| 2:B:153:LYS:HB3   | 2:B:155:LEU:HD11  | 1.96                     | 0.48              |
| 1:C:1135:TYR:CE2  | 1:C:1138:ARG:NH2  | 2.81                     | 0.48              |
| 2:D:152:VAL:HG12  | 2:D:153:LYS:HG2   | 1.94                     | 0.48              |
| 1:E:1341:GLN:HB3  | 1:E:1359:VAL:HB   | 1.96                     | 0.48              |
| 1:G:1056:VAL:HG21 | 1:G:1099:LEU:CD2  | 2.40                     | 0.48              |
| 1:C:1134:TYR:CE2  | 1:E:1216:HIS:HB3  | 2.48                     | 0.48              |
| 2:D:146:ALA:CB    | 2:D:154:TYR:HB2   | 2.43                     | 0.48              |
| 1:E:1119:ASP:O    | 1:E:1122:LYS:HG3  | 2.13                     | 0.48              |
| 1:G:1164:ALA:O    | 1:G:1167:ALA:HB3  | 2.14                     | 0.48              |
| 1:G:1176:GLN:HE22 | 2:H:1:MET:H3      | 1.61                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:10:GLY:HA2    | 2:B:97:TRP:CE2    | 2.49                     | 0.48              |
| 1:E:1213:GLU:CD   | 1:E:1213:GLU:H    | 2.22                     | 0.48              |
| 1:A:1191:GLN:O    | 1:A:1195:LYS:HG2  | 2.14                     | 0.47              |
| 1:A:1227:VAL:O    | 1:A:1231:ILE:HG12 | 2.14                     | 0.47              |
| 1:A:1298:THR:O    | 1:A:1299:ALA:HB2  | 2.12                     | 0.47              |
| 2:B:146:ALA:CB    | 2:B:154:TYR:HB2   | 2.44                     | 0.47              |
| 1:C:1368:ARG:HG3  | 1:C:1368:ARG:NH1  | 2.23                     | 0.47              |
| 1:G:1179:SER:HB3  | 2:H:41:SER:HB2    | 1.96                     | 0.47              |
| 2:H:5:LYS:HE3     | 2:H:56:TRP:CE3    | 2.49                     | 0.47              |
| 2:H:96:LYS:O      | 2:H:99:PRO:HD2    | 2.14                     | 0.47              |
| 1:A:1077:THR:OG1  | 1:A:1080:GLU:HG3  | 2.14                     | 0.47              |
| 2:B:138:THR:HG23  | 2:B:141:GLN:NE2   | 2.29                     | 0.47              |
| 2:B:153:LYS:HB3   | 2:B:155:LEU:CD1   | 2.43                     | 0.47              |
| 1:E:1055:TYR:CD2  | 1:E:1192:ARG:HG2  | 2.49                     | 0.47              |
| 1:E:1350:ALA:O    | 1:E:1351:GLU:HB3  | 2.13                     | 0.47              |
| 2:B:161:THR:HB    | 2:B:163:ARG:HG2   | 1.96                     | 0.47              |
| 2:D:58:THR:O      | 2:D:61:GLN:HG2    | 2.14                     | 0.47              |
| 2:D:160:LEU:C     | 2:D:160:LEU:HD13  | 2.40                     | 0.47              |
| 2:H:6:CYS:HB3     | 2:H:55:LEU:CD2    | 2.45                     | 0.47              |
| 1:A:1142:TYR:CE2  | 1:A:1193:VAL:HG13 | 2.49                     | 0.47              |
| 1:A:1216:HIS:HB3  | 1:G:1134:TYR:CE2  | 2.49                     | 0.47              |
| 2:B:12:GLY:O      | 2:B:13:ALA:HB3    | 2.13                     | 0.47              |
| 1:G:1153:PRO:O    | 1:G:1157:VAL:HG23 | 2.14                     | 0.47              |
| 1:G:1227:VAL:O    | 1:G:1231:ILE:HG12 | 2.14                     | 0.47              |
| 2:H:68:ARG:HD2    | 2:H:100:GLU:OE2   | 2.14                     | 0.47              |
| 2:H:133:LYS:N     | 2:H:133:LYS:HD3   | 2.30                     | 0.47              |
| 1:A:1055:TYR:CD2  | 1:A:1192:ARG:HG2  | 2.50                     | 0.47              |
| 2:B:138:THR:OG1   | 2:B:140:PRO:HD2   | 2.14                     | 0.47              |
| 1:C:1152:VAL:HB   | 1:C:1153:PRO:HD3  | 1.95                     | 0.47              |
| 2:D:98:TYR:HB3    | 2:D:99:PRO:HD3    | 1.97                     | 0.47              |
| 1:E:1052:GLU:O    | 1:E:1056:VAL:HG23 | 2.15                     | 0.47              |
| 1:E:1287:LYS:N    | 1:E:1287:LYS:CD   | 2.76                     | 0.47              |
| 1:A:1389:SER:O    | 1:A:1392:SER:HB3  | 2.14                     | 0.47              |
| 2:B:66:ARG:HH11   | 2:B:66:ARG:CG     | 2.27                     | 0.47              |
| 2:B:133:LYS:HD3   | 2:B:133:LYS:N     | 2.30                     | 0.47              |
| 2:D:10:GLY:HA2    | 2:D:97:TRP:CE2    | 2.49                     | 0.47              |
| 2:F:152:VAL:HG12  | 2:F:153:LYS:HG2   | 1.96                     | 0.47              |
| 1:A:1049:LEU:HD11 | 1:A:1106:VAL:HB   | 1.96                     | 0.47              |
| 1:A:1241:PHE:O    | 1:A:1242:GLY:C    | 2.57                     | 0.47              |
| 1:A:1350:ALA:O    | 1:A:1351:GLU:HB3  | 2.14                     | 0.47              |
| 2:B:6:CYS:HB3     | 2:B:55:LEU:CD2    | 2.45                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1077:THR:OG1  | 1:C:1080:GLU:HG3  | 2.14                     | 0.47              |
| 2:D:133:LYS:HD3   | 2:D:133:LYS:N     | 2.30                     | 0.47              |
| 2:D:155:LEU:HD12  | 2:D:155:LEU:N     | 2.30                     | 0.47              |
| 1:E:1067:LEU:CD1  | 1:E:1088:LEU:HD13 | 2.45                     | 0.47              |
| 1:E:1164:ALA:O    | 1:E:1167:ALA:HB3  | 2.15                     | 0.47              |
| 1:E:1287:LYS:HG2  | 1:E:1288:GLU:H    | 1.79                     | 0.47              |
| 1:E:1345:LEU:HD12 | 1:E:1355:VAL:CG1  | 2.45                     | 0.47              |
| 2:F:161:THR:HB    | 2:F:163:ARG:HG2   | 1.97                     | 0.47              |
| 1:G:1287:LYS:CG   | 1:G:1288:GLU:H    | 2.27                     | 0.47              |
| 2:H:8:VAL:HG22    | 2:H:79:LEU:HD12   | 1.97                     | 0.47              |
| 2:H:68:ARG:NH1    | 2:H:100:GLU:OE1   | 2.47                     | 0.47              |
| 1:C:1287:LYS:N    | 1:C:1287:LYS:CD   | 2.77                     | 0.47              |
| 1:C:1337:THR:HG21 | 1:C:1397:LYS:HB2  | 1.97                     | 0.47              |
| 1:E:1178:HIS:C    | 1:E:1180:SER:H    | 2.23                     | 0.47              |
| 2:F:10:GLY:HA2    | 2:F:97:TRP:CE2    | 2.49                     | 0.47              |
| 1:G:1239:GLU:OE2  | 2:H:66:ARG:HG3    | 2.15                     | 0.47              |
| 2:B:11:ASP:OD1    | 2:B:89:SER:HA     | 2.15                     | 0.47              |
| 1:C:1055:TYR:CD2  | 1:C:1192:ARG:HG2  | 2.50                     | 0.47              |
| 1:G:1138:ARG:O    | 1:G:1141:LEU:HG   | 2.15                     | 0.47              |
| 1:A:1107:ARG:C    | 1:A:1109:VAL:H    | 2.23                     | 0.47              |
| 1:E:1107:ARG:C    | 1:E:1109:VAL:H    | 2.23                     | 0.47              |
| 1:E:1197:PRO:HB2  | 1:E:1201:ARG:HH12 | 1.80                     | 0.47              |
| 1:A:1273:VAL:HG23 | 1:A:1377:CYS:HA   | 1.97                     | 0.46              |
| 1:C:1234:MSE:CE   | 1:C:1237:ILE:HD12 | 2.45                     | 0.46              |
| 1:C:1368:ARG:CG   | 1:C:1368:ARG:NH1  | 2.78                     | 0.46              |
| 1:A:1157:VAL:O    | 1:A:1157:VAL:CG1  | 2.63                     | 0.46              |
| 2:B:155:LEU:HD12  | 2:B:155:LEU:N     | 2.30                     | 0.46              |
| 2:D:158:SER:O     | 2:D:162:GLN:N     | 2.47                     | 0.46              |
| 1:E:1149:HIS:CE1  | 1:E:1186:LEU:O    | 2.68                     | 0.46              |
| 1:G:1107:ARG:C    | 1:G:1109:VAL:H    | 2.23                     | 0.46              |
| 2:D:137:ILE:HD12  | 2:D:137:ILE:N     | 2.31                     | 0.46              |
| 2:F:58:THR:O      | 2:F:61:GLN:HG2    | 2.15                     | 0.46              |
| 1:A:1179:SER:H    | 2:B:41:SER:HB2    | 1.80                     | 0.46              |
| 1:A:1368:ARG:HD2  | 1:A:1369:PRO:O    | 2.15                     | 0.46              |
| 1:C:1178:HIS:C    | 1:C:1180:SER:H    | 2.22                     | 0.46              |
| 1:G:1303:VAL:HG11 | 1:G:1329:PHE:HD2  | 1.81                     | 0.46              |
| 1:G:1340:LEU:HD11 | 1:G:1390:VAL:CG1  | 2.45                     | 0.46              |
| 2:D:57:ASP:OD1    | 2:D:58:THR:N      | 2.48                     | 0.46              |
| 1:E:1234:MSE:HE2  | 1:E:1237:ILE:HD12 | 1.97                     | 0.46              |
| 2:H:11:ASP:OD1    | 2:H:89:SER:HA     | 2.16                     | 0.46              |
| 2:B:158:SER:O     | 2:B:162:GLN:N     | 2.49                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1067:LEU:CD1  | 1:C:1088:LEU:HD13 | 2.44                     | 0.46              |
| 2:D:129:LEU:HD12  | 2:D:136:PRO:HG3   | 1.97                     | 0.46              |
| 2:D:155:LEU:CD1   | 2:D:155:LEU:N     | 2.79                     | 0.46              |
| 2:F:137:ILE:N     | 2:F:137:ILE:HD12  | 2.31                     | 0.46              |
| 1:G:1250:ALA:C    | 1:G:1252:GLN:H    | 2.22                     | 0.46              |
| 1:A:1042:ARG:NE   | 1:A:1113:GLU:HA   | 2.31                     | 0.46              |
| 1:A:1164:ALA:O    | 1:A:1167:ALA:HB3  | 2.15                     | 0.46              |
| 1:A:1341:GLN:HB3  | 1:A:1359:VAL:HB   | 1.96                     | 0.46              |
| 1:C:1115:LEU:HA   | 1:C:1120:GLN:NE2  | 2.30                     | 0.46              |
| 1:C:1135:TYR:HE2  | 1:C:1138:ARG:NH2  | 2.13                     | 0.46              |
| 1:E:1173:ASN:HD21 | 1:E:1180:SER:HB2  | 1.79                     | 0.46              |
| 1:G:1179:SER:H    | 2:H:41:SER:CB     | 2.28                     | 0.46              |
| 1:A:1067:LEU:CD1  | 1:A:1088:LEU:HD13 | 2.45                     | 0.46              |
| 1:E:1168:PHE:O    | 1:E:1172:GLN:HG2  | 2.16                     | 0.46              |
| 1:E:1399:ARG:C    | 1:E:1401:GLN:H    | 2.22                     | 0.46              |
| 1:E:1063:MSE:HE2  | 1:E:1088:LEU:HD22 | 1.98                     | 0.46              |
| 1:E:1287:LYS:CG   | 1:E:1288:GLU:N    | 2.79                     | 0.46              |
| 1:A:1287:LYS:CG   | 1:A:1288:GLU:N    | 2.79                     | 0.46              |
| 1:C:1052:GLU:HG3  | 1:C:1099:LEU:HD13 | 1.97                     | 0.46              |
| 1:C:1063:MSE:HE2  | 1:C:1088:LEU:HD22 | 1.97                     | 0.46              |
| 1:E:1056:VAL:CG2  | 1:E:1099:LEU:HD22 | 2.38                     | 0.46              |
| 1:E:1138:ARG:O    | 1:E:1141:LEU:HG   | 2.16                     | 0.46              |
| 1:G:1152:VAL:HB   | 1:G:1153:PRO:HD3  | 1.97                     | 0.46              |
| 1:A:1287:LYS:HG2  | 1:A:1288:GLU:H    | 1.81                     | 0.45              |
| 1:C:1306:ASP:OD2  | 1:G:1287:LYS:CD   | 2.64                     | 0.45              |
| 2:D:120:ARG:HH21  | 2:D:139:TYR:N     | 2.13                     | 0.45              |
| 1:E:1077:THR:OG1  | 1:E:1080:GLU:HG3  | 2.16                     | 0.45              |
| 1:E:1365:SER:C    | 1:E:1367:GLY:N    | 2.70                     | 0.45              |
| 1:G:1213:GLU:H    | 1:G:1213:GLU:CD   | 2.23                     | 0.45              |
| 2:B:121:ASP:HA    | 2:B:126:ILE:HD11  | 1.98                     | 0.45              |
| 1:C:1164:ALA:O    | 1:C:1167:ALA:HB3  | 2.15                     | 0.45              |
| 1:G:1062:LEU:HG   | 1:G:1185:TYR:HB3  | 1.98                     | 0.45              |
| 1:A:1052:GLU:O    | 1:A:1056:VAL:HG23 | 2.16                     | 0.45              |
| 1:C:1107:ARG:C    | 1:C:1109:VAL:H    | 2.23                     | 0.45              |
| 2:F:121:ASP:HA    | 2:F:126:ILE:HD11  | 1.98                     | 0.45              |
| 1:G:1248:LEU:HD21 | 1:G:1332:ARG:CG   | 2.42                     | 0.45              |
| 1:C:1250:ALA:C    | 1:C:1252:GLN:H    | 2.23                     | 0.45              |
| 2:D:23:TYR:HE1    | 2:D:166:LYS:HD3   | 1.81                     | 0.45              |
| 1:E:1086:GLY:C    | 1:E:1088:LEU:N    | 2.74                     | 0.45              |
| 1:G:1086:GLY:C    | 1:G:1088:LEU:N    | 2.74                     | 0.45              |
| 1:G:1191:GLN:O    | 1:G:1195:LYS:HG2  | 2.16                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:155:LEU:CD1   | 2:B:155:LEU:N     | 2.80                     | 0.45              |
| 1:C:1138:ARG:O    | 1:C:1141:LEU:HG   | 2.16                     | 0.45              |
| 1:E:1156:LEU:CD2  | 1:E:1182:LEU:HD23 | 2.47                     | 0.45              |
| 1:G:1178:HIS:C    | 1:G:1180:SER:H    | 2.24                     | 0.45              |
| 1:G:1190:ILE:HD13 | 2:H:70:LEU:CD1    | 2.38                     | 0.45              |
| 1:A:1340:LEU:HD11 | 1:A:1390:VAL:HG13 | 1.99                     | 0.45              |
| 2:H:80:ILE:HD12   | 2:H:110:ILE:HG21  | 1.98                     | 0.45              |
| 2:H:137:ILE:N     | 2:H:137:ILE:HD12  | 2.31                     | 0.45              |
| 1:A:1063:MSE:HE2  | 1:A:1088:LEU:HD22 | 1.98                     | 0.45              |
| 1:A:1153:PRO:O    | 1:A:1157:VAL:HG23 | 2.17                     | 0.45              |
| 1:A:1190:ILE:CD1  | 2:B:70:LEU:HD13   | 2.38                     | 0.45              |
| 1:A:1212:GLU:HG3  | 1:G:1097:GLU:HG3  | 1.99                     | 0.45              |
| 2:B:23:TYR:HE1    | 2:B:166:LYS:HD3   | 1.81                     | 0.45              |
| 1:C:1086:GLY:O    | 1:C:1087:ASN:OD1  | 2.35                     | 0.45              |
| 1:G:1067:LEU:CD1  | 1:G:1088:LEU:HD13 | 2.46                     | 0.45              |
| 1:A:1178:HIS:C    | 1:A:1180:SER:H    | 2.24                     | 0.45              |
| 2:D:66:ARG:HG3    | 2:D:66:ARG:NH1    | 2.29                     | 0.45              |
| 1:E:1035:LEU:HD12 | 1:E:1035:LEU:O    | 2.17                     | 0.45              |
| 1:E:1173:ASN:ND2  | 1:E:1180:SER:HB2  | 2.32                     | 0.45              |
| 1:E:1365:SER:O    | 1:E:1367:GLY:N    | 2.50                     | 0.45              |
| 2:F:11:ASP:OD1    | 2:F:92:ASN:ND2    | 2.45                     | 0.45              |
| 2:F:155:LEU:CD1   | 2:F:155:LEU:N     | 2.79                     | 0.45              |
| 2:F:160:LEU:HD13  | 2:F:160:LEU:C     | 2.41                     | 0.45              |
| 1:G:1157:VAL:O    | 1:G:1157:VAL:CG1  | 2.64                     | 0.45              |
| 1:A:1086:GLY:C    | 1:A:1088:LEU:N    | 2.74                     | 0.45              |
| 1:C:1340:LEU:HD11 | 1:C:1390:VAL:HG13 | 1.99                     | 0.45              |
| 2:D:121:ASP:HA    | 2:D:126:ILE:HD11  | 1.99                     | 0.45              |
| 1:E:1115:LEU:HA   | 1:E:1120:GLN:NE2  | 2.31                     | 0.45              |
| 1:E:1350:ALA:C    | 1:E:1352:ALA:H    | 2.25                     | 0.45              |
| 2:F:6:CYS:HB3     | 2:F:55:LEU:CD2    | 2.43                     | 0.45              |
| 2:F:120:ARG:HH21  | 2:F:139:TYR:N     | 2.13                     | 0.45              |
| 2:F:138:THR:HG23  | 2:F:141:GLN:NE2   | 2.31                     | 0.45              |
| 2:H:58:THR:O      | 2:H:61:GLN:HG2    | 2.16                     | 0.45              |
| 2:B:137:ILE:HD12  | 2:B:137:ILE:N     | 2.32                     | 0.45              |
| 1:C:1073:GLU:HG2  | 1:C:1075:PHE:CD1  | 2.52                     | 0.45              |
| 1:C:1142:TYR:CE2  | 1:C:1193:VAL:HG13 | 2.51                     | 0.45              |
| 1:G:1063:MSE:HE2  | 1:G:1088:LEU:HD22 | 1.98                     | 0.45              |
| 1:G:1142:TYR:CE2  | 1:G:1193:VAL:HG13 | 2.52                     | 0.45              |
| 1:G:1177:GLN:HG3  | 2:H:41:SER:HB3    | 1.98                     | 0.45              |
| 1:G:1368:ARG:HG3  | 1:G:1368:ARG:NH1  | 2.23                     | 0.45              |
| 2:D:5:LYS:HE3     | 2:D:56:TRP:CE3    | 2.52                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:6:CYS:HB3     | 2:D:55:LEU:CD2    | 2.46                     | 0.44              |
| 2:D:138:THR:HG23  | 2:D:141:GLN:NE2   | 2.32                     | 0.44              |
| 1:E:1183:GLU:H    | 1:E:1183:GLU:CD   | 2.24                     | 0.44              |
| 2:F:158:SER:O     | 2:F:162:GLN:N     | 2.50                     | 0.44              |
| 1:A:1250:ALA:C    | 1:A:1252:GLN:N    | 2.75                     | 0.44              |
| 1:A:1344:ALA:HB2  | 1:A:1387:LEU:CD1  | 2.47                     | 0.44              |
| 1:C:1103:GLU:O    | 1:C:1107:ARG:HG3  | 2.17                     | 0.44              |
| 1:C:1350:ALA:C    | 1:C:1352:ALA:H    | 2.25                     | 0.44              |
| 2:D:138:THR:HG23  | 2:D:141:GLN:HE21  | 1.82                     | 0.44              |
| 2:F:139:TYR:C     | 2:F:139:TYR:CD2   | 2.95                     | 0.44              |
| 1:G:1042:ARG:NE   | 1:G:1113:GLU:HA   | 2.32                     | 0.44              |
| 1:G:1250:ALA:C    | 1:G:1252:GLN:N    | 2.73                     | 0.44              |
| 1:C:1287:LYS:HE2  | 1:G:1307:GLY:O    | 2.17                     | 0.44              |
| 1:E:1068:LYS:N    | 1:E:1069:PRO:HD2  | 2.33                     | 0.44              |
| 1:E:1152:VAL:HB   | 1:E:1153:PRO:HD3  | 2.00                     | 0.44              |
| 1:E:1340:LEU:HD11 | 1:E:1390:VAL:HG13 | 1.99                     | 0.44              |
| 2:F:23:TYR:HE1    | 2:F:166:LYS:HD3   | 1.82                     | 0.44              |
| 2:H:138:THR:OG1   | 2:H:140:PRO:HD2   | 2.18                     | 0.44              |
| 1:A:1052:GLU:HG3  | 1:A:1099:LEU:HD13 | 2.00                     | 0.44              |
| 1:A:1285:TRP:HZ2  | 2:D:98:TYR:CE2    | 2.36                     | 0.44              |
| 1:A:1374:HIS:ND1  | 1:E:1346:PRO:HG3  | 2.32                     | 0.44              |
| 1:C:1086:GLY:C    | 1:C:1088:LEU:N    | 2.76                     | 0.44              |
| 1:C:1306:ASP:CG   | 1:G:1287:LYS:HD2  | 2.42                     | 0.44              |
| 2:D:68:ARG:HD2    | 2:D:100:GLU:OE2   | 2.18                     | 0.44              |
| 1:E:1135:TYR:O    | 1:E:1136:ALA:C    | 2.60                     | 0.44              |
| 1:E:1368:ARG:HD2  | 1:E:1369:PRO:O    | 2.17                     | 0.44              |
| 2:H:162:GLN:HG3   | 2:H:165:LEU:HD22  | 1.99                     | 0.44              |
| 1:A:1115:LEU:HA   | 1:A:1120:GLN:NE2  | 2.33                     | 0.44              |
| 1:A:1138:ARG:O    | 1:A:1141:LEU:HG   | 2.17                     | 0.44              |
| 1:A:1215:TYR:O    | 1:A:1219:VAL:HG23 | 2.18                     | 0.44              |
| 1:A:1368:ARG:CG   | 1:A:1368:ARG:NH1  | 2.80                     | 0.44              |
| 1:E:1073:GLU:HG2  | 1:E:1075:PHE:CD1  | 2.52                     | 0.44              |
| 2:H:1:MET:HG2     | 2:H:2:GLN:N       | 2.33                     | 0.44              |
| 2:H:155:LEU:HD12  | 2:H:155:LEU:N     | 2.32                     | 0.44              |
| 1:E:1140:LYS:HD2  | 1:E:1230:HIS:HD2  | 1.82                     | 0.44              |
| 1:E:1234:MSE:CE   | 1:E:1237:ILE:HD12 | 2.47                     | 0.44              |
| 1:E:1389:SER:O    | 1:E:1392:SER:HB3  | 2.17                     | 0.44              |
| 1:G:1350:ALA:C    | 1:G:1352:ALA:H    | 2.25                     | 0.44              |
| 1:G:1368:ARG:NH1  | 1:G:1368:ARG:CG   | 2.78                     | 0.44              |
| 1:A:1073:GLU:HG2  | 1:A:1075:PHE:CD1  | 2.52                     | 0.44              |
| 1:C:1183:GLU:CD   | 1:C:1183:GLU:H    | 2.26                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1250:ALA:C    | 1:C:1252:GLN:N    | 2.75                     | 0.44              |
| 2:D:66:ARG:CG     | 2:D:66:ARG:NH1    | 2.80                     | 0.44              |
| 1:E:1250:ALA:C    | 1:E:1252:GLN:N    | 2.75                     | 0.44              |
| 1:G:1149:HIS:CE1  | 1:G:1186:LEU:O    | 2.71                     | 0.44              |
| 2:H:158:SER:O     | 2:H:162:GLN:N     | 2.50                     | 0.44              |
| 1:E:1344:ALA:HB2  | 1:E:1387:LEU:CD1  | 2.48                     | 0.44              |
| 2:H:23:TYR:HE1    | 2:H:166:LYS:HD3   | 1.83                     | 0.44              |
| 2:H:66:ARG:HG3    | 2:H:66:ARG:NH1    | 2.31                     | 0.44              |
| 1:A:1208:ASP:O    | 1:A:1214:HIS:HB2  | 2.17                     | 0.44              |
| 1:A:1277:ASN:OD1  | 1:A:1374:HIS:HB2  | 2.18                     | 0.44              |
| 1:C:1153:PRO:O    | 1:C:1157:VAL:HG23 | 2.18                     | 0.44              |
| 1:C:1168:PHE:O    | 1:C:1172:GLN:HG2  | 2.18                     | 0.44              |
| 1:E:1052:GLU:HG3  | 1:E:1099:LEU:HD13 | 2.00                     | 0.44              |
| 2:F:96:LYS:O      | 2:F:99:PRO:HD2    | 2.17                     | 0.44              |
| 1:G:1398:HIS:C    | 1:G:1400:ARG:N    | 2.74                     | 0.44              |
| 2:H:129:LEU:HD12  | 2:H:136:PRO:HG3   | 2.00                     | 0.44              |
| 1:A:1068:LYS:N    | 1:A:1069:PRO:HD2  | 2.33                     | 0.43              |
| 1:A:1149:HIS:CE1  | 1:A:1186:LEU:O    | 2.71                     | 0.43              |
| 1:A:1201:ARG:HG2  | 1:A:1221:ILE:HD13 | 2.00                     | 0.43              |
| 1:A:1250:ALA:C    | 1:A:1252:GLN:H    | 2.24                     | 0.43              |
| 1:C:1247:GLN:HB3  | 1:C:1332:ARG:HH11 | 1.83                     | 0.43              |
| 1:A:1042:ARG:HH11 | 1:A:1042:ARG:HB3  | 1.83                     | 0.43              |
| 1:C:1042:ARG:NE   | 1:C:1113:GLU:HA   | 2.31                     | 0.43              |
| 1:C:1327:ASP:HA   | 1:C:1328:PRO:HD2  | 1.85                     | 0.43              |
| 1:C:1368:ARG:HD2  | 1:C:1369:PRO:O    | 2.18                     | 0.43              |
| 2:H:161:THR:HB    | 2:H:163:ARG:HG2   | 2.00                     | 0.43              |
| 1:A:1287:LYS:N    | 1:A:1287:LYS:CD   | 2.76                     | 0.43              |
| 2:F:17:THR:O      | 2:F:21:ILE:HG13   | 2.18                     | 0.43              |
| 1:G:1201:ARG:HG2  | 1:G:1221:ILE:HD13 | 2.00                     | 0.43              |
| 1:C:1187:ILE:O    | 1:C:1191:GLN:HG3  | 2.19                     | 0.43              |
| 1:C:1239:GLU:OE2  | 2:D:66:ARG:HG3    | 2.18                     | 0.43              |
| 2:D:162:GLN:HG3   | 2:D:165:LEU:HD22  | 1.99                     | 0.43              |
| 1:E:1042:ARG:HH11 | 1:E:1042:ARG:HB3  | 1.82                     | 0.43              |
| 1:E:1234:MSE:CE   | 1:E:1267:LEU:HD23 | 2.47                     | 0.43              |
| 1:E:1344:ALA:HB2  | 1:E:1387:LEU:HD13 | 2.00                     | 0.43              |
| 1:G:1368:ARG:HD2  | 1:G:1369:PRO:O    | 2.18                     | 0.43              |
| 2:H:155:LEU:CD1   | 2:H:155:LEU:N     | 2.82                     | 0.43              |
| 1:A:1152:VAL:HB   | 1:A:1153:PRO:HD3  | 1.99                     | 0.43              |
| 2:B:11:ASP:OD1    | 2:B:92:ASN:ND2    | 2.47                     | 0.43              |
| 1:C:1355:VAL:HG12 | 1:C:1356:CYS:N    | 2.32                     | 0.43              |
| 2:F:85:VAL:HG11   | 2:F:125:THR:HG21  | 2.00                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:G:1156:LEU:HD21 | 1:G:1182:LEU:HD23 | 2.00                     | 0.43              |
| 1:A:1197:PRO:HB2  | 1:A:1201:ARG:HH12 | 1.84                     | 0.43              |
| 1:A:1344:ALA:HB2  | 1:A:1387:LEU:HD13 | 1.99                     | 0.43              |
| 1:C:1052:GLU:O    | 1:C:1056:VAL:HG23 | 2.19                     | 0.43              |
| 1:C:1363:SER:N    | 1:C:1368:ARG:O    | 2.49                     | 0.43              |
| 1:E:1157:VAL:O    | 1:E:1157:VAL:CG1  | 2.64                     | 0.43              |
| 2:F:161:THR:HG22  | 2:F:163:ARG:HB3   | 2.00                     | 0.43              |
| 1:G:1073:GLU:HG2  | 1:G:1075:PHE:CD1  | 2.54                     | 0.43              |
| 1:G:1077:THR:OG1  | 1:G:1080:GLU:HG3  | 2.19                     | 0.43              |
| 1:G:1086:GLY:O    | 1:G:1087:ASN:OD1  | 2.37                     | 0.43              |
| 1:A:1380:PRO:HG2  | 1:A:1381:GLU:OE2  | 2.19                     | 0.43              |
| 2:F:68:ARG:HD2    | 2:F:100:GLU:OE2   | 2.19                     | 0.43              |
| 1:C:1286:LYS:HB3  | 1:C:1289:PRO:HG3  | 2.01                     | 0.43              |
| 1:A:1176:GLN:NE2  | 2:B:1:MET:N       | 2.67                     | 0.43              |
| 2:B:8:VAL:HG21    | 2:B:20:LEU:HD21   | 2.01                     | 0.43              |
| 2:D:137:ILE:HG23  | 2:D:141:GLN:HB2   | 2.00                     | 0.43              |
| 1:E:1103:GLU:O    | 1:E:1107:ARG:HG3  | 2.18                     | 0.43              |
| 1:G:1115:LEU:HA   | 1:G:1120:GLN:NE2  | 2.34                     | 0.43              |
| 1:G:1118:VAL:HG23 | 1:G:1119:ASP:N    | 2.33                     | 0.43              |
| 1:G:1260:ALA:O    | 1:G:1261:ASP:CB   | 2.66                     | 0.43              |
| 1:G:1368:ARG:HA   | 1:G:1369:PRO:HD3  | 1.75                     | 0.43              |
| 1:E:1118:VAL:HG23 | 1:E:1119:ASP:N    | 2.34                     | 0.42              |
| 1:E:1250:ALA:C    | 1:E:1252:GLN:H    | 2.27                     | 0.42              |
| 2:F:66:ARG:HG3    | 2:F:66:ARG:NH1    | 2.30                     | 0.42              |
| 1:A:1365:SER:O    | 1:A:1367:GLY:N    | 2.52                     | 0.42              |
| 1:C:1263:SER:C    | 1:C:1265:GLY:H    | 2.27                     | 0.42              |
| 1:C:1282:LEU:HD21 | 1:C:1289:PRO:CB   | 2.48                     | 0.42              |
| 1:C:1381:GLU:H    | 1:C:1381:GLU:CD   | 2.26                     | 0.42              |
| 2:F:129:LEU:HD12  | 2:F:136:PRO:HG3   | 2.01                     | 0.42              |
| 1:G:1055:TYR:CD2  | 1:G:1192:ARG:HG2  | 2.54                     | 0.42              |
| 1:G:1365:SER:C    | 1:G:1367:GLY:N    | 2.72                     | 0.42              |
| 2:H:66:ARG:HH11   | 2:H:66:ARG:CG     | 2.28                     | 0.42              |
| 1:A:1097:GLU:HG2  | 1:G:1212:GLU:CD   | 2.44                     | 0.42              |
| 1:A:1275:TRP:O    | 1:A:1278:PRO:HD3  | 2.19                     | 0.42              |
| 2:B:120:ARG:HH21  | 2:B:139:TYR:N     | 2.15                     | 0.42              |
| 1:G:1168:PHE:O    | 1:G:1172:GLN:HG2  | 2.19                     | 0.42              |
| 1:G:1234:MSE:HE2  | 1:G:1237:ILE:HD12 | 2.00                     | 0.42              |
| 1:G:1389:SER:O    | 1:G:1392:SER:HB3  | 2.20                     | 0.42              |
| 2:H:49:LYS:HD3    | 2:H:177:LEU:HD13  | 2.01                     | 0.42              |
| 2:H:85:VAL:HG11   | 2:H:125:THR:HG21  | 2.01                     | 0.42              |
| 1:A:1342:VAL:HG13 | 1:A:1342:VAL:O    | 2.20                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1350:ALA:C    | 1:A:1352:ALA:H    | 2.26                     | 0.42              |
| 1:C:1344:ALA:HB2  | 1:C:1387:LEU:CD1  | 2.49                     | 0.42              |
| 1:C:1365:SER:O    | 1:C:1367:GLY:N    | 2.50                     | 0.42              |
| 1:C:1389:SER:O    | 1:C:1392:SER:HB3  | 2.19                     | 0.42              |
| 1:E:1042:ARG:NE   | 1:E:1113:GLU:HA   | 2.30                     | 0.42              |
| 1:E:1065:ARG:HG2  | 1:E:1065:ARG:HH11 | 1.84                     | 0.42              |
| 1:E:1094:PHE:CE1  | 1:E:1135:TYR:HD2  | 2.36                     | 0.42              |
| 1:E:1241:PHE:O    | 1:E:1242:GLY:C    | 2.61                     | 0.42              |
| 1:G:1380:PRO:HG2  | 1:G:1381:GLU:OE2  | 2.19                     | 0.42              |
| 2:H:137:ILE:HG23  | 2:H:141:GLN:HB2   | 2.00                     | 0.42              |
| 1:A:1118:VAL:HG23 | 1:A:1119:ASP:N    | 2.33                     | 0.42              |
| 1:A:1135:TYR:O    | 1:A:1136:ALA:C    | 2.63                     | 0.42              |
| 2:B:17:THR:O      | 2:B:21:ILE:HG13   | 2.20                     | 0.42              |
| 2:D:65:ASP:CG     | 2:D:66:ARG:HD3    | 2.44                     | 0.42              |
| 2:D:120:ARG:NH2   | 2:D:139:TYR:H     | 2.16                     | 0.42              |
| 1:E:1368:ARG:NH1  | 1:E:1368:ARG:CG   | 2.76                     | 0.42              |
| 1:G:1036:SER:O    | 1:G:1039:ASP:N    | 2.53                     | 0.42              |
| 2:H:160:LEU:HD13  | 2:H:160:LEU:C     | 2.44                     | 0.42              |
| 1:A:1355:VAL:HG12 | 1:A:1356:CYS:N    | 2.34                     | 0.42              |
| 2:B:5:LYS:HE3     | 2:B:56:TRP:CE3    | 2.53                     | 0.42              |
| 1:C:1244:VAL:HG21 | 1:C:1329:PHE:CD2  | 2.55                     | 0.42              |
| 1:E:1121:PHE:O    | 1:E:1122:LYS:C    | 2.63                     | 0.42              |
| 1:E:1234:MSE:O    | 1:E:1264:MSE:HE2  | 2.19                     | 0.42              |
| 2:F:138:THR:HG23  | 2:F:141:GLN:HE21  | 1.84                     | 0.42              |
| 1:E:1086:GLY:O    | 1:E:1087:ASN:OD1  | 2.38                     | 0.42              |
| 1:G:1215:TYR:O    | 1:G:1219:VAL:HG23 | 2.20                     | 0.42              |
| 1:C:1097:GLU:O    | 1:C:1101:THR:HG23 | 2.19                     | 0.42              |
| 1:E:1239:GLU:OE1  | 2:F:66:ARG:NH1    | 2.53                     | 0.42              |
| 1:E:1269:LEU:C    | 1:E:1269:LEU:HD23 | 2.44                     | 0.42              |
| 2:F:146:ALA:HB2   | 2:F:154:TYR:HB2   | 2.02                     | 0.42              |
| 1:G:1115:LEU:N    | 1:G:1115:LEU:CD1  | 2.83                     | 0.42              |
| 1:G:1244:VAL:HG21 | 1:G:1329:PHE:CD2  | 2.54                     | 0.42              |
| 2:H:57:ASP:OD1    | 2:H:58:THR:N      | 2.53                     | 0.42              |
| 2:H:82:PHE:CD1    | 2:H:82:PHE:C      | 2.98                     | 0.42              |
| 1:A:1178:HIS:HA   | 1:A:1181:THR:CG2  | 2.50                     | 0.42              |
| 1:A:1178:HIS:C    | 1:A:1180:SER:N    | 2.77                     | 0.42              |
| 2:B:5:LYS:HG3     | 2:B:75:THR:HA     | 2.00                     | 0.42              |
| 1:C:1178:HIS:C    | 1:C:1180:SER:N    | 2.76                     | 0.42              |
| 1:C:1282:LEU:HD22 | 1:G:1285:TRP:CZ3  | 2.55                     | 0.42              |
| 2:D:5:LYS:HG3     | 2:D:75:THR:HA     | 2.00                     | 0.42              |
| 2:D:68:ARG:N      | 2:D:69:PRO:HD2    | 2.34                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:108:THR:HA    | 2:D:109:PRO:HD2   | 1.90                     | 0.42              |
| 1:E:1287:LYS:CG   | 1:E:1288:GLU:H    | 2.32                     | 0.42              |
| 2:F:108:THR:HA    | 2:F:109:PRO:HD2   | 1.92                     | 0.42              |
| 1:G:1042:ARG:HB3  | 1:G:1042:ARG:HH11 | 1.85                     | 0.42              |
| 1:G:1065:ARG:HG2  | 1:G:1065:ARG:HH11 | 1.84                     | 0.42              |
| 1:G:1269:LEU:HD23 | 1:G:1269:LEU:C    | 2.44                     | 0.42              |
| 1:G:1295:VAL:HG11 | 1:G:1389:SER:OG   | 2.20                     | 0.42              |
| 1:G:1363:SER:N    | 1:G:1368:ARG:O    | 2.48                     | 0.42              |
| 2:H:65:ASP:CG     | 2:H:66:ARG:HD3    | 2.44                     | 0.42              |
| 1:A:1115:LEU:N    | 1:A:1115:LEU:CD1  | 2.83                     | 0.42              |
| 1:A:1168:PHE:O    | 1:A:1172:GLN:HG2  | 2.20                     | 0.42              |
| 2:B:24:THR:HG22   | 2:B:40:TYR:CE2    | 2.55                     | 0.42              |
| 1:C:1042:ARG:HH11 | 1:C:1042:ARG:HB3  | 1.85                     | 0.42              |
| 1:C:1065:ARG:HG2  | 1:C:1065:ARG:HH11 | 1.85                     | 0.42              |
| 1:C:1201:ARG:HG2  | 1:C:1221:ILE:HD13 | 2.02                     | 0.42              |
| 2:D:87:PRO:O      | 2:D:90:PHE:HB3    | 2.20                     | 0.42              |
| 2:D:161:THR:O     | 2:D:161:THR:HG22  | 2.20                     | 0.42              |
| 1:E:1275:TRP:O    | 1:E:1278:PRO:HD3  | 2.20                     | 0.42              |
| 1:E:1295:VAL:HG11 | 1:E:1389:SER:OG   | 2.19                     | 0.42              |
| 2:H:8:VAL:HG21    | 2:H:20:LEU:HD21   | 2.02                     | 0.42              |
| 2:H:120:ARG:HH21  | 2:H:139:TYR:N     | 2.17                     | 0.42              |
| 2:H:139:TYR:CD2   | 2:H:139:TYR:C     | 2.98                     | 0.42              |
| 1:A:1373:PHE:HB3  | 1:A:1375:LEU:HD21 | 2.02                     | 0.41              |
| 2:B:129:LEU:HD12  | 2:B:136:PRO:HG3   | 2.01                     | 0.41              |
| 1:C:1197:PRO:HB2  | 1:C:1201:ARG:HH12 | 1.85                     | 0.41              |
| 1:C:1263:SER:C    | 1:C:1265:GLY:N    | 2.78                     | 0.41              |
| 1:E:1115:LEU:N    | 1:E:1115:LEU:CD1  | 2.83                     | 0.41              |
| 1:E:1115:LEU:H    | 1:E:1115:LEU:CD1  | 2.34                     | 0.41              |
| 1:E:1277:ASN:OD1  | 1:E:1374:HIS:HB2  | 2.20                     | 0.41              |
| 2:F:57:ASP:OD1    | 2:F:58:THR:N      | 2.51                     | 0.41              |
| 2:H:146:ALA:HB2   | 2:H:154:TYR:HB2   | 2.02                     | 0.41              |
| 2:D:68:ARG:HB3    | 2:D:69:PRO:HD3    | 2.02                     | 0.41              |
| 1:E:1063:MSE:HG3  | 1:E:1068:LYS:HE3  | 2.03                     | 0.41              |
| 2:F:5:LYS:HG3     | 2:F:75:THR:HA     | 2.03                     | 0.41              |
| 2:F:66:ARG:CG     | 2:F:66:ARG:NH1    | 2.82                     | 0.41              |
| 2:B:146:ALA:HB2   | 2:B:154:TYR:HB2   | 2.02                     | 0.41              |
| 1:C:1240:GLU:CG   | 1:C:1305:LYS:NZ   | 2.82                     | 0.41              |
| 1:C:1269:LEU:C    | 1:C:1269:LEU:HD23 | 2.45                     | 0.41              |
| 2:D:17:THR:O      | 2:D:21:ILE:HG13   | 2.20                     | 0.41              |
| 1:E:1094:PHE:HE1  | 1:E:1135:TYR:CD2  | 2.37                     | 0.41              |
| 1:G:1086:GLY:C    | 1:G:1088:LEU:H    | 2.28                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:G:1197:PRO:HB2  | 1:G:1201:ARG:HH12 | 1.84                     | 0.41              |
| 1:G:1304:TYR:CB   | 1:G:1331:PHE:HB3  | 2.43                     | 0.41              |
| 1:A:1287:LYS:CG   | 1:A:1288:GLU:H    | 2.33                     | 0.41              |
| 1:A:1359:VAL:HG22 | 1:A:1372:VAL:HG22 | 2.03                     | 0.41              |
| 2:B:160:LEU:C     | 2:B:160:LEU:HD13  | 2.45                     | 0.41              |
| 1:C:1059:LEU:HD12 | 1:C:1059:LEU:HA   | 1.94                     | 0.41              |
| 2:D:12:GLY:O      | 2:D:13:ALA:HB3    | 2.21                     | 0.41              |
| 2:D:85:VAL:HG11   | 2:D:125:THR:HG21  | 2.03                     | 0.41              |
| 1:E:1368:ARG:HA   | 1:E:1369:PRO:HD3  | 1.76                     | 0.41              |
| 1:G:1052:GLU:O    | 1:G:1056:VAL:HG23 | 2.21                     | 0.41              |
| 1:G:1252:GLN:HE21 | 1:G:1252:GLN:HB2  | 1.66                     | 0.41              |
| 2:B:162:GLN:HE21  | 2:B:162:GLN:HB2   | 1.66                     | 0.41              |
| 2:B:161:THR:O     | 2:B:161:THR:HG22  | 2.20                     | 0.41              |
| 2:F:158:SER:HB3   | 2:F:161:THR:HB    | 2.03                     | 0.41              |
| 1:G:1178:HIS:C    | 1:G:1180:SER:N    | 2.78                     | 0.41              |
| 1:G:1327:ASP:HA   | 1:G:1328:PRO:HD2  | 1.86                     | 0.41              |
| 1:A:1076:LEU:HA   | 1:A:1080:GLU:OE1  | 2.21                     | 0.41              |
| 1:A:1174:PRO:HG2  | 1:A:1175:ARG:H    | 1.86                     | 0.41              |
| 1:A:1177:GLN:HG3  | 2:B:41:SER:CB     | 2.50                     | 0.41              |
| 1:A:1234:MSE:HE2  | 1:A:1237:ILE:HD12 | 2.02                     | 0.41              |
| 1:C:1068:LYS:N    | 1:C:1069:PRO:HD2  | 2.35                     | 0.41              |
| 2:D:11:ASP:OD1    | 2:D:92:ASN:ND2    | 2.51                     | 0.41              |
| 2:F:87:PRO:O      | 2:F:90:PHE:HB3    | 2.20                     | 0.41              |
| 1:G:1052:GLU:HG3  | 1:G:1099:LEU:HD13 | 2.03                     | 0.41              |
| 1:A:1107:ARG:C    | 1:A:1109:VAL:N    | 2.79                     | 0.41              |
| 1:A:1115:LEU:CD1  | 1:A:1115:LEU:H    | 2.34                     | 0.41              |
| 2:F:37:PHE:HD2    | 2:F:57:ASP:HB2    | 1.86                     | 0.41              |
| 2:F:137:ILE:HG23  | 2:F:141:GLN:HB2   | 2.02                     | 0.41              |
| 2:H:66:ARG:NH1    | 2:H:66:ARG:CG     | 2.84                     | 0.41              |
| 2:H:161:THR:O     | 2:H:161:THR:HG22  | 2.21                     | 0.41              |
| 1:A:1065:ARG:HG2  | 1:A:1065:ARG:HH11 | 1.85                     | 0.41              |
| 2:B:65:ASP:CG     | 2:B:66:ARG:HD3    | 2.46                     | 0.41              |
| 2:B:66:ARG:NH1    | 2:B:66:ARG:CG     | 2.84                     | 0.41              |
| 2:B:68:ARG:HB3    | 2:B:69:PRO:HD3    | 2.03                     | 0.41              |
| 2:B:161:THR:C     | 2:B:163:ARG:H     | 2.29                     | 0.41              |
| 1:C:1115:LEU:N    | 1:C:1115:LEU:CD1  | 2.84                     | 0.41              |
| 1:C:1115:LEU:H    | 1:C:1115:LEU:CD1  | 2.33                     | 0.41              |
| 1:C:1208:ASP:O    | 1:C:1214:HIS:HB2  | 2.21                     | 0.41              |
| 1:C:1380:PRO:HG2  | 1:C:1381:GLU:OE2  | 2.20                     | 0.41              |
| 2:D:10:GLY:O      | 2:D:11:ASP:C      | 2.64                     | 0.41              |
| 2:D:146:ALA:HB2   | 2:D:154:TYR:HB2   | 2.03                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:E:1047:GLU:O    | 1:E:1051:THR:HG23 | 2.21                     | 0.41              |
| 1:E:1106:VAL:CG2  | 1:E:1112:LEU:HD11 | 2.51                     | 0.41              |
| 2:F:161:THR:HG22  | 2:F:161:THR:O     | 2.20                     | 0.41              |
| 1:G:1355:VAL:HG12 | 1:G:1356:CYS:N    | 2.36                     | 0.41              |
| 1:A:1103:GLU:O    | 1:A:1107:ARG:HG3  | 2.21                     | 0.41              |
| 1:A:1210:GLU:OE1  | 1:A:1210:GLU:HA   | 2.21                     | 0.41              |
| 1:A:1286:LYS:O    | 1:A:1287:LYS:C    | 2.64                     | 0.41              |
| 1:C:1118:VAL:HG23 | 1:C:1119:ASP:N    | 2.34                     | 0.41              |
| 1:C:1135:TYR:O    | 1:C:1136:ALA:C    | 2.63                     | 0.41              |
| 1:C:1252:GLN:HE21 | 1:C:1252:GLN:HB2  | 1.64                     | 0.41              |
| 1:C:1345:LEU:H    | 1:C:1356:CYS:HA   | 1.86                     | 0.41              |
| 2:D:145:MET:HA    | 2:D:145:MET:CE    | 2.43                     | 0.41              |
| 1:E:1250:ALA:O    | 1:E:1251:GLU:HB3  | 2.20                     | 0.41              |
| 1:E:1355:VAL:HG12 | 1:E:1356:CYS:N    | 2.36                     | 0.41              |
| 1:G:1340:LEU:HD12 | 1:G:1394:LEU:HD21 | 2.03                     | 0.41              |
| 2:H:11:ASP:OD1    | 2:H:92:ASN:ND2    | 2.47                     | 0.41              |
| 1:C:1344:ALA:HB2  | 1:C:1387:LEU:HD13 | 2.01                     | 0.40              |
| 2:D:37:PHE:HD2    | 2:D:57:ASP:HB2    | 1.87                     | 0.40              |
| 1:E:1098:PHE:CE2  | 1:E:1102:LEU:HD11 | 2.56                     | 0.40              |
| 1:E:1107:ARG:C    | 1:E:1109:VAL:N    | 2.79                     | 0.40              |
| 1:E:1208:ASP:O    | 1:E:1214:HIS:HB2  | 2.21                     | 0.40              |
| 1:G:1287:LYS:N    | 1:G:1287:LYS:CD   | 2.80                     | 0.40              |
| 1:G:1365:SER:O    | 1:G:1367:GLY:N    | 2.55                     | 0.40              |
| 1:A:1346:PRO:HG2  | 1:E:1345:LEU:CD1  | 2.52                     | 0.40              |
| 1:C:1303:VAL:CG1  | 1:C:1329:PHE:HD2  | 2.35                     | 0.40              |
| 1:C:1342:VAL:HG13 | 1:C:1342:VAL:O    | 2.21                     | 0.40              |
| 1:A:1269:LEU:C    | 1:A:1269:LEU:HD23 | 2.47                     | 0.40              |
| 2:B:137:ILE:HG23  | 2:B:141:GLN:HB2   | 2.03                     | 0.40              |
| 1:C:1106:VAL:CG2  | 1:C:1112:LEU:HD11 | 2.51                     | 0.40              |
| 1:E:1249:ILE:CD1  | 1:E:1261:ASP:H    | 2.14                     | 0.40              |
| 2:F:161:THR:C     | 2:F:163:ARG:H     | 2.29                     | 0.40              |
| 1:G:1344:ALA:HB2  | 1:G:1387:LEU:CD1  | 2.51                     | 0.40              |
| 1:A:1237:ILE:HD11 | 1:A:1270:HIS:CD2  | 2.56                     | 0.40              |
| 1:C:1273:VAL:CG2  | 1:C:1375:LEU:HB3  | 2.51                     | 0.40              |
| 2:D:82:PHE:CD1    | 2:D:82:PHE:C      | 2.98                     | 0.40              |
| 1:E:1085:PHE:O    | 1:E:1088:LEU:HB2  | 2.20                     | 0.40              |
| 2:F:40:TYR:HB3    | 2:F:55:LEU:HB2    | 2.04                     | 0.40              |
| 1:G:1340:LEU:HD11 | 1:G:1390:VAL:HG13 | 2.03                     | 0.40              |
| 2:H:98:TYR:OH     | 2:H:102:ARG:HD2   | 2.21                     | 0.40              |
| 1:A:1156:LEU:HD21 | 1:A:1182:LEU:HD23 | 2.03                     | 0.40              |
| 1:A:1179:SER:HB3  | 2:B:41:SER:HB2    | 2.03                     | 0.40              |

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| Atom-1          | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-------------------|--------------------------|-------------------|
| 1:C:1234:MSE:HA | 1:C:1234:MSE:CE   | 2.44                     | 0.40              |
| 1:C:1386:PHE:O  | 1:C:1390:VAL:HG23 | 2.21                     | 0.40              |
| 1:G:1036:SER:O  | 1:G:1037:ASP:C    | 2.63                     | 0.40              |
| 1:G:1068:LYS:N  | 1:G:1069:PRO:HD2  | 2.35                     | 0.40              |

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

| Atom-1         | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|------------------------|--------------------------|-------------------|
| 2:F:139:TYR:OH | 2:H:107:ASN:OD1[2_657] | 2.06                     | 0.14              |

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|----------|-------------|----|
| 1   | A     | 366/377 (97%)   | 313 (86%)  | 43 (12%) | 10 (3%)  | 4           | 15 |
| 1   | C     | 364/377 (97%)   | 315 (86%)  | 41 (11%) | 8 (2%)   | 5           | 19 |
| 1   | E     | 365/377 (97%)   | 322 (88%)  | 30 (8%)  | 13 (4%)  | 2           | 10 |
| 1   | G     | 365/377 (97%)   | 322 (88%)  | 31 (8%)  | 12 (3%)  | 3           | 11 |
| 2   | B     | 175/177 (99%)   | 164 (94%)  | 9 (5%)   | 2 (1%)   | 11          | 36 |
| 2   | D     | 175/177 (99%)   | 164 (94%)  | 9 (5%)   | 2 (1%)   | 11          | 36 |
| 2   | F     | 175/177 (99%)   | 162 (93%)  | 12 (7%)  | 1 (1%)   | 21          | 51 |
| 2   | H     | 175/177 (99%)   | 163 (93%)  | 11 (6%)  | 1 (1%)   | 21          | 51 |
| All | All   | 2160/2216 (98%) | 1925 (89%) | 186 (9%) | 49 (2%)  | 5           | 18 |

All (49) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1087 | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1253 | THR  |
| 1   | A     | 1261 | ASP  |
| 1   | C     | 1087 | ASN  |
| 1   | C     | 1253 | THR  |
| 1   | C     | 1261 | ASP  |
| 1   | E     | 1087 | ASN  |
| 1   | E     | 1253 | THR  |
| 1   | E     | 1261 | ASP  |
| 1   | G     | 1087 | ASN  |
| 1   | G     | 1253 | THR  |
| 1   | G     | 1261 | ASP  |
| 1   | A     | 1086 | GLY  |
| 1   | A     | 1252 | GLN  |
| 2   | B     | 11   | ASP  |
| 1   | C     | 1086 | GLY  |
| 1   | C     | 1252 | GLN  |
| 2   | D     | 11   | ASP  |
| 1   | E     | 1086 | GLY  |
| 1   | E     | 1305 | LYS  |
| 1   | E     | 1306 | ASP  |
| 2   | F     | 11   | ASP  |
| 1   | G     | 1086 | GLY  |
| 1   | G     | 1252 | GLN  |
| 1   | G     | 1325 | GLU  |
| 1   | A     | 1085 | PHE  |
| 1   | A     | 1312 | LYS  |
| 1   | A     | 1322 | ILE  |
| 1   | C     | 1085 | PHE  |
| 1   | E     | 1085 | PHE  |
| 1   | E     | 1252 | GLN  |
| 1   | G     | 1085 | PHE  |
| 2   | H     | 11   | ASP  |
| 1   | C     | 1311 | LYS  |
| 1   | E     | 1325 | GLU  |
| 1   | A     | 1254 | GLY  |
| 1   | A     | 1328 | PRO  |
| 1   | C     | 1254 | GLY  |
| 2   | D     | 65   | ASP  |
| 1   | E     | 1254 | GLY  |
| 1   | G     | 1254 | GLY  |
| 1   | G     | 1324 | GLU  |
| 1   | G     | 1399 | ARG  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 65   | ASP  |
| 1   | E     | 1350 | ALA  |
| 1   | G     | 1311 | LYS  |
| 1   | E     | 1327 | ASP  |
| 1   | G     | 1157 | VAL  |
| 1   | E     | 1157 | VAL  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed         | Rotameric  | Outliers | Percentiles |    |
|-----|-------|------------------|------------|----------|-------------|----|
| 1   | A     | 332/332 (100%)   | 325 (98%)  | 7 (2%)   | 47          | 79 |
| 1   | C     | 330/332 (99%)    | 324 (98%)  | 6 (2%)   | 51          | 82 |
| 1   | E     | 331/332 (100%)   | 322 (97%)  | 9 (3%)   | 39          | 74 |
| 1   | G     | 331/332 (100%)   | 323 (98%)  | 8 (2%)   | 43          | 77 |
| 2   | B     | 153/153 (100%)   | 146 (95%)  | 7 (5%)   | 24          | 58 |
| 2   | D     | 153/153 (100%)   | 146 (95%)  | 7 (5%)   | 24          | 58 |
| 2   | F     | 153/153 (100%)   | 146 (95%)  | 7 (5%)   | 24          | 58 |
| 2   | H     | 153/153 (100%)   | 147 (96%)  | 6 (4%)   | 28          | 64 |
| All | All   | 1936/1940 (100%) | 1879 (97%) | 57 (3%)  | 37          | 73 |

All (57) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1048 | LEU  |
| 1   | A     | 1059 | LEU  |
| 1   | A     | 1062 | LEU  |
| 1   | A     | 1177 | GLN  |
| 1   | A     | 1194 | LEU  |
| 1   | A     | 1287 | LYS  |
| 1   | A     | 1397 | LYS  |
| 2   | B     | 19   | LEU  |
| 2   | B     | 50   | PRO  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 62   | GLU  |
| 2   | B     | 66   | ARG  |
| 2   | B     | 77   | VAL  |
| 2   | B     | 116  | LYS  |
| 2   | B     | 143  | LEU  |
| 1   | C     | 1048 | LEU  |
| 1   | C     | 1059 | LEU  |
| 1   | C     | 1062 | LEU  |
| 1   | C     | 1177 | GLN  |
| 1   | C     | 1194 | LEU  |
| 1   | C     | 1287 | LYS  |
| 2   | D     | 19   | LEU  |
| 2   | D     | 50   | PRO  |
| 2   | D     | 62   | GLU  |
| 2   | D     | 66   | ARG  |
| 2   | D     | 77   | VAL  |
| 2   | D     | 116  | LYS  |
| 2   | D     | 143  | LEU  |
| 1   | E     | 1048 | LEU  |
| 1   | E     | 1059 | LEU  |
| 1   | E     | 1062 | LEU  |
| 1   | E     | 1177 | GLN  |
| 1   | E     | 1194 | LEU  |
| 1   | E     | 1287 | LYS  |
| 1   | E     | 1305 | LYS  |
| 1   | E     | 1313 | LYS  |
| 1   | E     | 1322 | ILE  |
| 2   | F     | 19   | LEU  |
| 2   | F     | 50   | PRO  |
| 2   | F     | 62   | GLU  |
| 2   | F     | 66   | ARG  |
| 2   | F     | 77   | VAL  |
| 2   | F     | 116  | LYS  |
| 2   | F     | 143  | LEU  |
| 1   | G     | 1048 | LEU  |
| 1   | G     | 1059 | LEU  |
| 1   | G     | 1062 | LEU  |
| 1   | G     | 1177 | GLN  |
| 1   | G     | 1194 | LEU  |
| 1   | G     | 1287 | LYS  |
| 1   | G     | 1313 | LYS  |
| 1   | G     | 1397 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | H     | 19  | LEU  |
| 2   | H     | 62  | GLU  |
| 2   | H     | 66  | ARG  |
| 2   | H     | 77  | VAL  |
| 2   | H     | 116 | LYS  |
| 2   | H     | 143 | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1071 | GLN  |
| 1   | A     | 1120 | GLN  |
| 1   | A     | 1149 | HIS  |
| 1   | A     | 1173 | ASN  |
| 1   | A     | 1176 | GLN  |
| 1   | A     | 1230 | HIS  |
| 1   | A     | 1235 | GLN  |
| 1   | A     | 1238 | HIS  |
| 1   | A     | 1360 | HIS  |
| 1   | A     | 1374 | HIS  |
| 2   | B     | 2    | GLN  |
| 2   | B     | 26   | ASN  |
| 2   | B     | 74   | GLN  |
| 2   | B     | 141  | GLN  |
| 1   | C     | 1071 | GLN  |
| 1   | C     | 1120 | GLN  |
| 1   | C     | 1149 | HIS  |
| 1   | C     | 1173 | ASN  |
| 1   | C     | 1177 | GLN  |
| 1   | C     | 1178 | HIS  |
| 1   | C     | 1230 | HIS  |
| 1   | C     | 1235 | GLN  |
| 1   | C     | 1238 | HIS  |
| 1   | C     | 1247 | GLN  |
| 1   | C     | 1374 | HIS  |
| 2   | D     | 2    | GLN  |
| 2   | D     | 26   | ASN  |
| 2   | D     | 52   | ASN  |
| 2   | D     | 74   | GLN  |
| 2   | D     | 141  | GLN  |
| 1   | E     | 1071 | GLN  |
| 1   | E     | 1120 | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | E     | 1149 | HIS  |
| 1   | E     | 1173 | ASN  |
| 1   | E     | 1176 | GLN  |
| 1   | E     | 1230 | HIS  |
| 1   | E     | 1235 | GLN  |
| 1   | E     | 1238 | HIS  |
| 1   | E     | 1374 | HIS  |
| 2   | F     | 2    | GLN  |
| 2   | F     | 26   | ASN  |
| 2   | F     | 52   | ASN  |
| 2   | F     | 74   | GLN  |
| 2   | F     | 141  | GLN  |
| 1   | G     | 1071 | GLN  |
| 1   | G     | 1120 | GLN  |
| 1   | G     | 1149 | HIS  |
| 1   | G     | 1173 | ASN  |
| 1   | G     | 1176 | GLN  |
| 1   | G     | 1230 | HIS  |
| 1   | G     | 1235 | GLN  |
| 1   | G     | 1238 | HIS  |
| 1   | G     | 1374 | HIS  |
| 2   | H     | 2    | GLN  |
| 2   | H     | 26   | ASN  |
| 2   | H     | 74   | GLN  |
| 2   | H     | 141  | GLN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 3   | SO4  | F     | 4003 | -    | 4,4,4        | 0.34 | 0           | 6,6,6       | 0.15 | 0           |
| 3   | SO4  | H     | 4004 | -    | 4,4,4        | 0.42 | 0           | 6,6,6       | 0.29 | 0           |
| 3   | SO4  | B     | 4001 | -    | 4,4,4        | 0.41 | 0           | 6,6,6       | 0.11 | 0           |
| 3   | SO4  | D     | 4002 | -    | 4,4,4        | 0.39 | 0           | 6,6,6       | 0.24 | 0           |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 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.