



## Full wwPDB EM Validation Report ⓘ

Sep 29, 2026 – 05:12 PM EDT

PDB ID : 9OL4 / pdb\_00009ol4  
EMDB ID : EMD-70589  
Title : Rabbit Ryanodine Receptor 1: Atorvastatin Bound Open Conformation  
Authors : Molinarolo, S.M.; Van Petegem, F.  
Deposited on : 2025-05-12  
Resolution : 3.37 Å(reported)  
Based on initial model : 7TZC

This is a Full wwPDB EM 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/EMValidationReportHelp>  
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:

EMDB validation analysis : 0.0.1.dev133  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.2  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.51

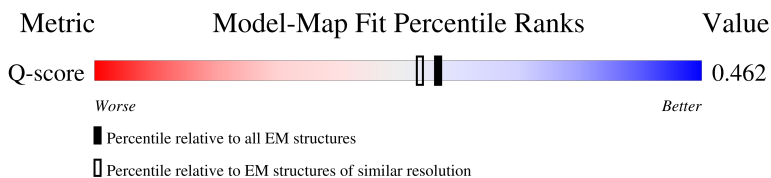
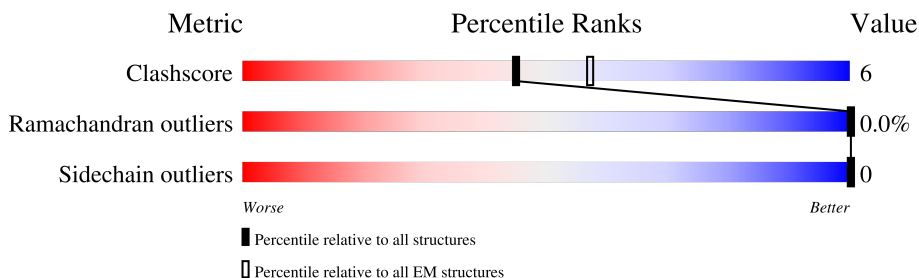
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.37 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) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 14287 ( 2.87 - 3.87 )                                    |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--------------------|
| 1   | A     | 5037   | <br>8% 70% 11% 19% |
| 1   | G     | 5037   | <br>8% 70% 11% 19% |
| 1   | M     | 5037   | <br>8% 70% 11% 19% |
| 1   | S     | 5037   | <br>8% 70% 11% 19% |

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| Mol | Chain | Length | Quality of chain                                                                           |
|-----|-------|--------|--------------------------------------------------------------------------------------------|
| 2   | B     | 111    |  86%11%• |
| 2   | H     | 111    |  86%11%• |
| 2   | N     | 111    |  86%11%• |
| 2   | T     | 111    |  86%11%• |

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 131292 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Ryanodine receptor 1.

| Mol | Chain | Residues | Atoms |       |      |      |     | AltConf | Trace |
|-----|-------|----------|-------|-------|------|------|-----|---------|-------|
| 1   | A     | 4064     | Total | C     | N    | O    | S   | 0       | 0     |
|     |       |          | 31873 | 20385 | 5494 | 5773 | 221 |         |       |
| 1   | G     | 4064     | Total | C     | N    | O    | S   | 0       | 0     |
|     |       |          | 31873 | 20385 | 5494 | 5773 | 221 |         |       |
| 1   | M     | 4064     | Total | C     | N    | O    | S   | 0       | 0     |
|     |       |          | 31873 | 20385 | 5494 | 5773 | 221 |         |       |
| 1   | S     | 4064     | Total | C     | N    | O    | S   | 0       | 0     |
|     |       |          | 31873 | 20385 | 5494 | 5773 | 221 |         |       |

- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 2   | B     | 107      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 811   | 510 | 143 | 154 | 4 |         |       |
| 2   | H     | 107      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 811   | 510 | 143 | 154 | 4 |         |       |
| 2   | N     | 107      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 811   | 510 | 143 | 154 | 4 |         |       |
| 2   | T     | 107      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 811   | 510 | 143 | 154 | 4 |         |       |

There are 12 discrepancies between the modelled and reference sequences:

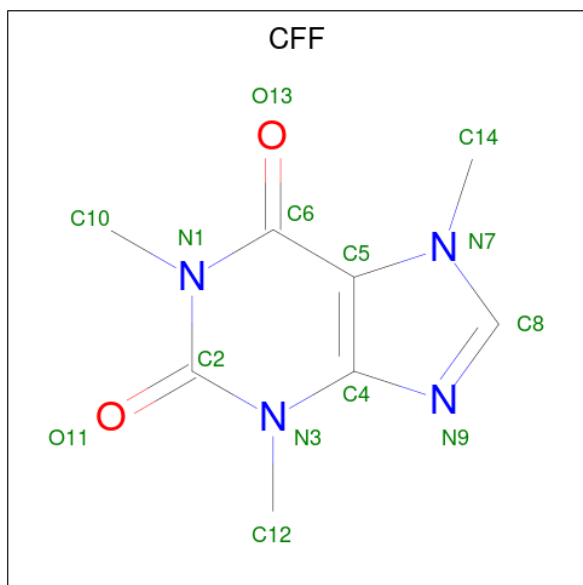
| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| B     | -2      | SER      | -      | expression tag | UNP P68106 |
| B     | -1      | ASN      | -      | expression tag | UNP P68106 |
| B     | 0       | ALA      | -      | expression tag | UNP P68106 |
| H     | -2      | SER      | -      | expression tag | UNP P68106 |
| H     | -1      | ASN      | -      | expression tag | UNP P68106 |
| H     | 0       | ALA      | -      | expression tag | UNP P68106 |
| N     | -2      | SER      | -      | expression tag | UNP P68106 |
| N     | -1      | ASN      | -      | expression tag | UNP P68106 |
| N     | 0       | ALA      | -      | expression tag | UNP P68106 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| T     | -2      | SER      | -      | expression tag | UNP P68106 |
| T     | -1      | ASN      | -      | expression tag | UNP P68106 |
| T     | 0       | ALA      | -      | expression tag | UNP P68106 |

- Molecule 3 is CAFFEINE (CCD ID: CFF) (formula:  $C_8H_{10}N_4O_2$ ).

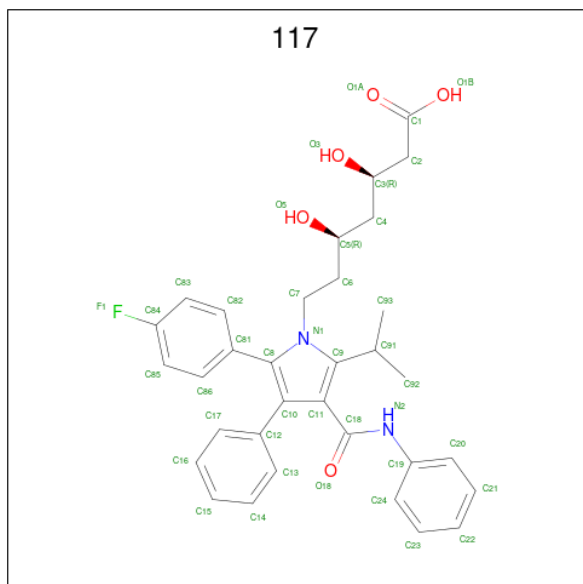


| Mol | Chain | Residues | Atoms |   |   |   | AltConf |
|-----|-------|----------|-------|---|---|---|---------|
| 3   | A     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 4 | 2 |         |
| 3   | G     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 4 | 2 |         |
| 3   | M     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 4 | 2 |         |
| 3   | S     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 4 | 2 |         |

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

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 4   | A     | 1        | Total | Ca | 0       |
|     |       |          | 1     | 1  |         |
| 4   | G     | 1        | Total | Ca | 0       |
|     |       |          | 1     | 1  |         |
| 4   | M     | 1        | Total | Ca | 0       |
|     |       |          | 1     | 1  |         |
| 4   | S     | 1        | Total | Ca | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 5 is 7-[2-(4-FLUORO-PHENYL)-5-ISOPROPYL-3-PHENYL-4-PHENYLCARBAMOYL-PYRROL-1-YL]- 3,5-DIHYDROXY-HEPTANOIC ACID (CCD ID: 117) (formula:  $C_{33}H_{35}FN_2O_5$ ) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 5   | A     | 1        | Total | C  | F | N | O | 0       |
|     |       |          | 41    | 33 | 1 | 2 | 5 |         |
| 5   | A     | 1        | Total | C  | F | N | O | 0       |
|     |       |          | 41    | 33 | 1 | 2 | 5 |         |
| 5   | A     | 1        | Total | C  | F | N | O | 0       |
|     |       |          | 41    | 33 | 1 | 2 | 5 |         |
| 5   | G     | 1        | Total | C  | F | N | O | 0       |
|     |       |          | 41    | 33 | 1 | 2 | 5 |         |
| 5   | G     | 1        | Total | C  | F | N | O | 0       |
|     |       |          | 41    | 33 | 1 | 2 | 5 |         |
| 5   | G     | 1        | Total | C  | F | N | O | 0       |
|     |       |          | 41    | 33 | 1 | 2 | 5 |         |
| 5   | M     | 1        | Total | C  | F | N | O | 0       |
|     |       |          | 41    | 33 | 1 | 2 | 5 |         |
| 5   | M     | 1        | Total | C  | F | N | O | 0       |
|     |       |          | 41    | 33 | 1 | 2 | 5 |         |
| 5   | M     | 1        | Total | C  | F | N | O | 0       |
|     |       |          | 41    | 33 | 1 | 2 | 5 |         |
| 5   | S     | 1        | Total | C  | F | N | O | 0       |
|     |       |          | 41    | 33 | 1 | 2 | 5 |         |
| 5   | S     | 1        | Total | C  | F | N | O | 0       |
|     |       |          | 41    | 33 | 1 | 2 | 5 |         |
| 5   | S     | 1        | Total | C  | F | N | O | 0       |
|     |       |          | 41    | 33 | 1 | 2 | 5 |         |

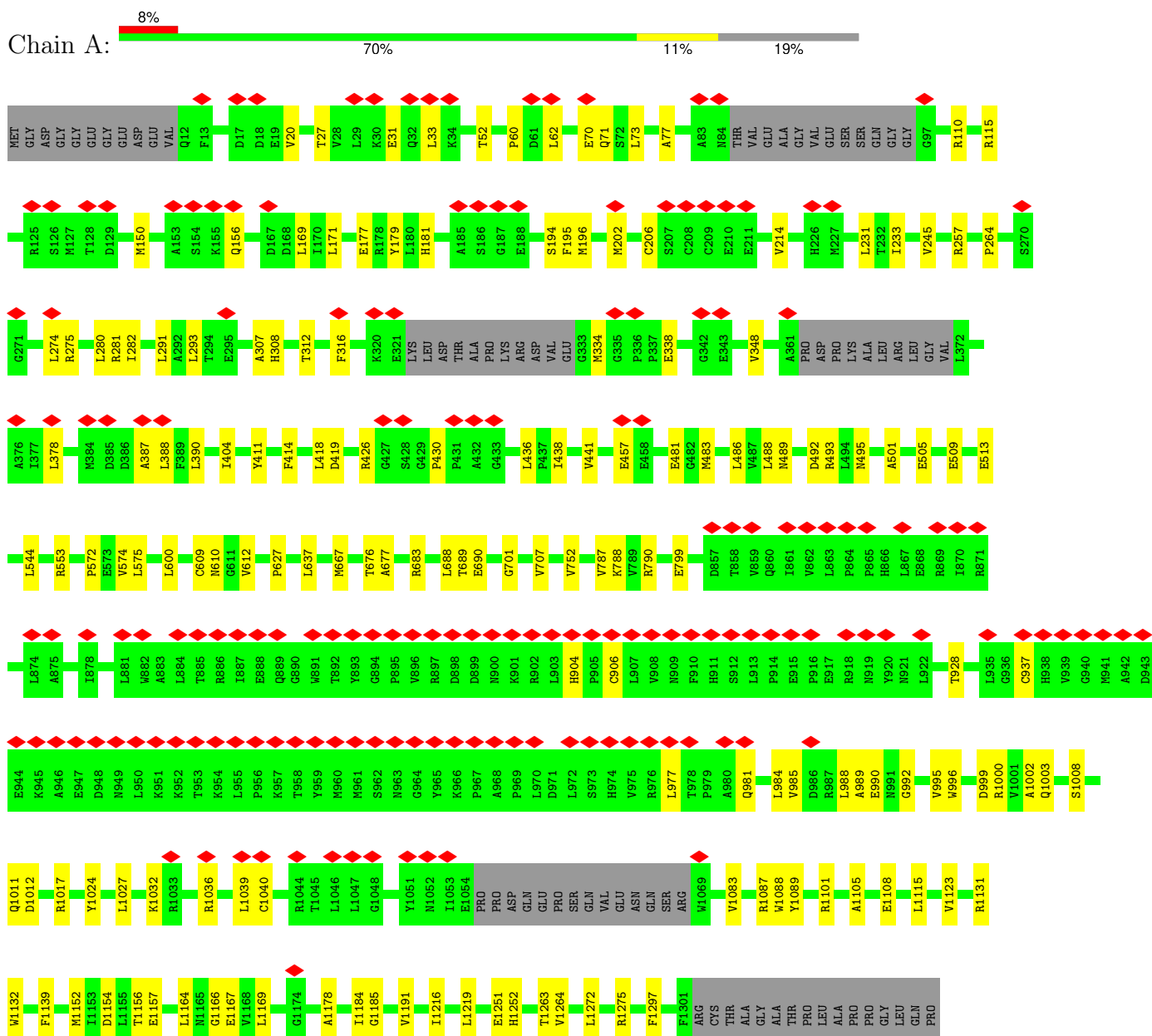
- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms      |         | AltConf |
|-----|-------|----------|------------|---------|---------|
| 6   | A     | 1        | Total<br>1 | Zn<br>1 | 0       |
| 6   | G     | 1        | Total<br>1 | Zn<br>1 | 0       |
| 6   | M     | 1        | Total<br>1 | Zn<br>1 | 0       |
| 6   | S     | 1        | Total<br>1 | Zn<br>1 | 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 and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

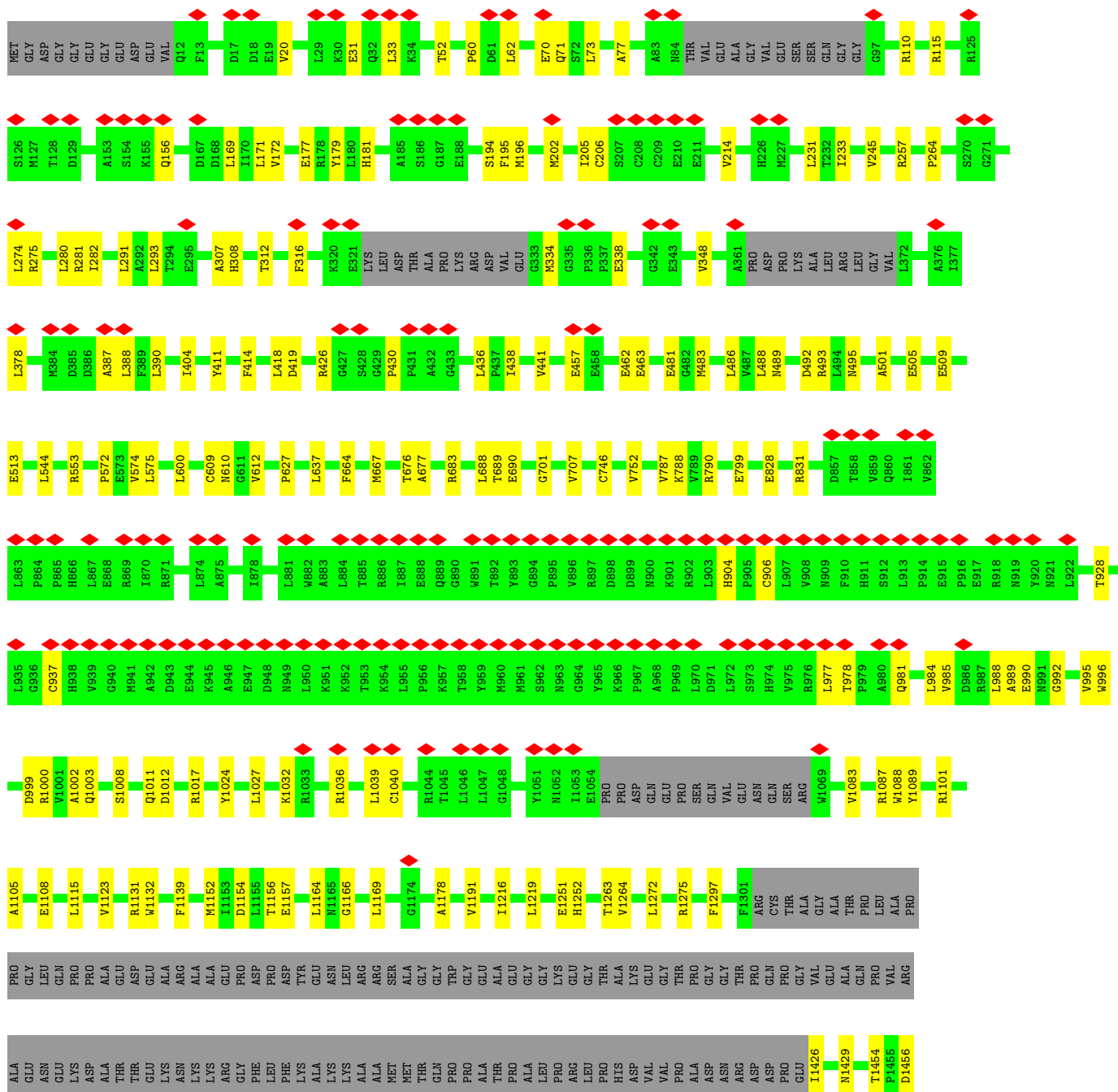
#### • Molecule 1: Ryanodine receptor 1



|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |    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| GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | 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GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU</ |
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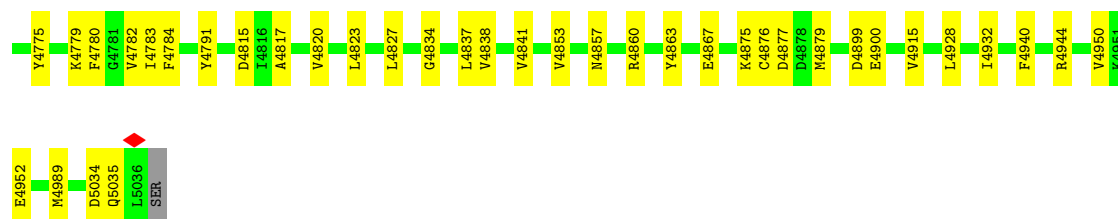


- Molecule 1: Ryanodine receptor 1

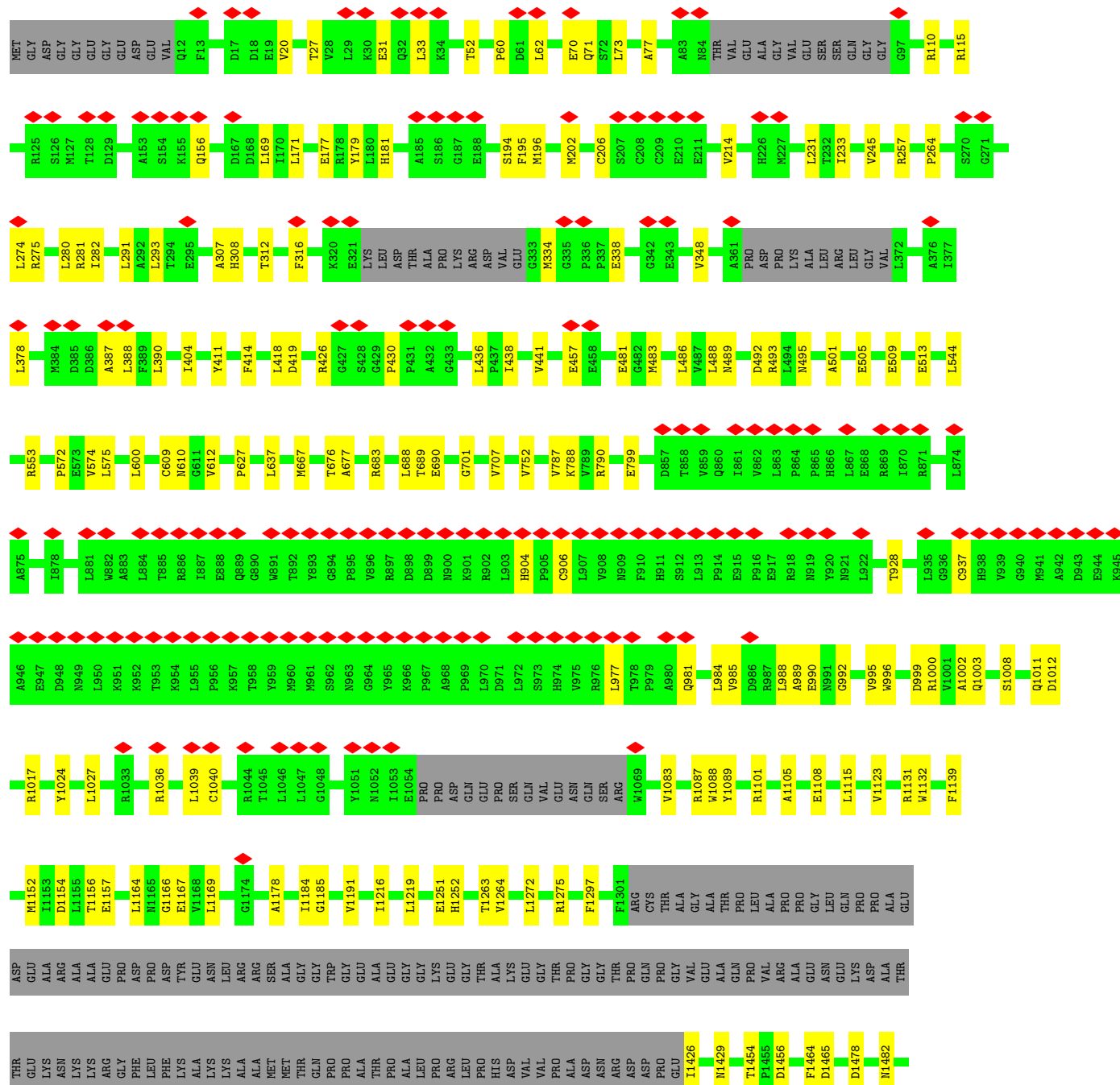


|       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| P3004 | L3005 | T3006 | N3007 | F3010 | T3011 | F3017 | T3020 | P3021 | K3036 | E3037 | M3038 | L3046 | V3050 | R3051 | H3052 | F3057 | D3060 | A3061 | P3062 | N3066 | A3077 | R3078 | T3079 | V3080 | G3084 | P3085 | V3088 | M3106 | N3109 | L3110 | R3111 | LEU   | GLY   | LYS   | VAL   | F2973 | F2974 | E2978 | ALA   | ARG   | THR   | GLN   | VAL   | VAL   | SER   | LYS   | GLY   | VAL   | PRO   | LYS   | L3003 |       |       |       |       |       |       |       |       |       |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| D2919 | R2920 | E2921 | K2922 | Q2923 | Q2924 | E2925 | L2926 | L2927 | K2928 | F2929 | L2930 | Q2931 | M2932 | N2933 | Q2934 | Y2935 | A2936 | V2937 | T2938 | E2939 | GLY   | LEU   | LYS   | ASP   | MET   | GLU   | LEU   | ASP   | THR   | G2887 | R2888 | K2889 | K2890 | K2891 | Q2892 | E2893 | L2894 | E2895 | A2896 | K2897 | G2898 | G2899 | Q2900 | T2901 | H2902 | P2903 | L2904 | L2905 | V2906 | P2907 | Y2908 | D2909 | T2910 | T2912 | A2913 | K2914 | E2915 | K2916 | A2917 | R2918 |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| E2799 | K2800 | D2801 | K2802 | E2803 | L2804 | V2805 | K2806 | W2807 | P2808 | T2809 | K2810 | E2811 | S2812 | L2813 | K2814 | A2815 | W2816 | L2817 | A2818 | W2819 | E2820 | W2821 | T2822 | L2823 | E2824 | K2825 | A2826 | R2827 | E2828 | Q2829 | E2830 | GLU   | GLU   | ARG   | THR   | LYS   | LYS   | LYS   | THR   | ARG   | LYS   | ILE   | SER   | GLN   | THR   | ALA   | GLN   | THR   | GLY   | THR   | TVR   | ASP   | PRO   | ARG   | GLU   | GLY   | Y2855 | N2856 | P2857 | Q2858 |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| P2739 | V2740 | E2741 | T2742 | L2743 | N2744 | V2745 | L2746 | L2747 | P2748 | E2749 | K2750 | L2751 | D2752 | S2753 | F2754 | L2755 | N2756 | K2757 | F2758 | A2759 | E2760 | Y2761 | T2762 | H2763 | E2764 | K2765 | W2766 | A2767 | F2768 | D2769 | K2770 | L2771 | Q2772 | N2773 | N2774 | W2775 | S2776 | Y2777 | G2778 | E2779 | N2780 | V2781 | D2782 | E2783 | E2784 | L2785 | K2786 | T2787 | H2788 | P2789 | M2790 | L2791 | R2792 | P2793 | Y2794 | K2795 | T2796 | F2797 | S2798 |       |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| R2575 | A2598 | Q2599 | V2602 | I2603 | Q2620 | R2624 | R2625 | L2626 | F2627 | V2628 | V2630 | P2631 | E2635 | M2639 | P2640 | L2643 | L2644 | R2650 | C2651 | E2670 | L2678 | R2697 | D2716 | ALA   | SER   | TVR   | SER   | LYS   | ALA   | GLU   | LYS   | LYS   | LYS   | ALA   | VAL   | ASP   | ALA   | GLU   | GLY   | ASN   | PHE   | ASP   | P2737 | R2738 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| D2389 | P2395 | GLY   | VAL   | ARG   | ASP   | ARG   | ARG   | ARG   | GLU   | HIS   | PHE   | GLY   | GLU   | PRO   | PRO   | GLU   | W2414 | E2449 | R2452 | T2478 | LEU   | GLY   | LYS   | ASP   | GLY   | ALA   | L2485 | K2499 | V2503 | Q2515 | L2519 | H2520 | D2523 | V2524 | G2525 | F2526 | L2527 | P2528 | D2529 | M2530 | F2541 | T2544 | A2547 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| THR   | LYS   | GLU   | L2223 | M2228 | F2251 | Y2256 | L2257 | L2258 | G2262 | ILE   | GLY   | LEU   | GLY   | MET   | GLN   | G2269 | S2270 | T2271 | D2274 | V2275 | A2276 | V2280 | L2286 | E2292 | Q2293 | D2294 | L2295 | E2296 | K2297 | V2298 | V2299 | N2324 | P2325 | C2326 | R2330 | D2333 | F2334 | E2348 | N2349 | A2350 | N2351 | V2352 | V2353 | V2354 | R2355 | L2368 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| GLU   | GLU   | LYS   | P2091 | V2098 | M2101 | D2109 | S2113 | L2116 | V2117 | M2120 | F2121 | S2122 | L2123 | L2124 | R2126 | Q2127 | Y2128 | D2151 | T2152 | M2153 | L2159 | G2160 | Q2161 | I2162 | R2163 | S2164 | L2165 | P2172 | E2175 | N2176 | L2177 | M2178 | K2189 | M2196 | R2199 | M2203 | V2212 | G2216 | GLY   | GLY   | GLY   | GLY   | GLY   | GLY   | GLY   | GLY   | GLY   | GLY   | GLY   | GLY   | GLY   | GLY   |       |       |       |       |       |       |       |       |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| LYS   | GLU   | ASP   | GLU   | GLU   | GLU   | LYS   | ASP   | GLY   | GLU   | ALA   | GLU   | LYS   | GLU   | PRO   | GLY   | GLY   | LYS   | GLU   | ASP   | LEU   | GLU   | E1924 | G1925 | L1926 | L1927 | Q1928 | V1935 | M1939 | L1943 | L1969 | L1980 | MET   | ARG   | ALA   | PHE   | THR   | MET   | SER   | ALA   | LYS   | THR   | ALA   | ARG   | R1994 | S2000 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| GLY   | ASN   | ALA   | R1758 | L1762 | V1765 | P1773 | L1786 | PRO   | ALA   | ALA   | GLY   | ILE   | SER   | GLN   | GLN   | THR   | D1513 | V1542 | E1543 | P1544 | T1557 | V1561 | I1562 | R1623 | Q1629 | A1638 | C1647 | L1669 | L1694 | L1698 | R1727 | L1731 | V1736 | P1740 | R1743 | P1749 | PRO   | GLY   | ARG   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   |       |       |       |       |       |       |       |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| Q2003 | L2009 | K2013 | ASP   | GLU   | ALA   | ASP   | GLU   | ASP   | C2021 | P2022 | L2023 | T2044 | GLN   | LEU   | GLU   | GLY   | GLU   | GLU   | PRO   | GLU   | GLU   | GLU   | THR   | SER   | LEU   | SER   | SER   | ARG   | LEU   | SER   | LEU   | GLU   | THR   | VAL   | ARG   | LEU   | VAL   | LYS   | LYS   | PRO   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU |





• Molecule 1: Ryanodine receptor 1



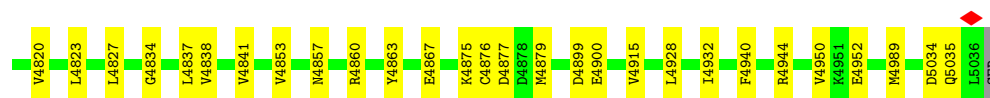
|       |       |       |     |       |       |       |       |       |       |       |       |       |       |
|-------|-------|-------|-----|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| V1501 | SER   | V1765 | GLU | K2013 | V2098 | M2228 | VAL   | I2603 | N2744 | I2804 | G2864 | Q2924 | F3010 |
| PRO   | GLY   | P1773 | GLU | ASP   | M2101 | F2251 | ARG   | Q2620 | V2745 | Y2805 | V2865 | E2925 | T3011 |
| GLN   | GLY   | L1786 | GLU | ALA   | D2109 | Y2256 | ASP   | R2624 | I2746 | R2806 | T2866 | L2926 | F3017 |
| GLY   | GLY   | L1786 | LYS | ASP   | D2109 | L2257 | ARG   | R2625 | I2747 | N2807 | L2867 | L2927 | T3020 |
| ARG   | GLY   | ALA   | ASP | GLU   | S2113 | L2258 | ARG   | L2626 | E2748 | P2808 | S2868 | K2928 | P3021 |
| ILE   | VAL   | ALA   | ALA | ASP   | L2116 | G2262 | GLU   | V2627 | K2750 | L2809 | R2869 | L2929 | K3036 |
| SER   | VAL   | GLY   | ALA | C2021 | L2117 | ILE   | HIS   | D2629 | L2751 | E2811 | L2871 | E2930 | M3038 |
| HIS   | ALA   | ALA   | LYS | L2023 | V2127 | GLY   | PHE   | P2630 | D2752 | S2812 | Q2872 | Q2931 | M3038 |
| THR   | GLU   | GLU   | GLY | L2044 | W2120 | LEU   | GLU   | P2631 | L2753 | L2813 | A2873 | M2932 | L3046 |
| D1513 | ALA   | ALA   | GLU | GLN   | F2121 | GLY   | PRO   | E2635 | F2754 | K2814 | M2874 | G2934 | L3046 |
| V1542 | P1795 | P1795 | GLU | LEU   | S2122 | GLY   | PRO   | K2638 | I2755 | A2815 | A2875 | A2935 | V3050 |
| E1543 | E1805 | E1805 | ALA | GLU   | L2123 | G2269 | GLU   | M2639 | L2756 | M2816 | E2876 | R3051 | R3051 |
| P1544 | R1808 | R1808 | GLY | GLY   | L2124 | S2270 | GLU   | P2640 | K2757 | L2817 | Q2877 | A2936 | H3052 |
| T1567 | L1815 | L1815 | GLY | GLU   | H2125 | T2271 | L2414 | L2643 | F2758 | A2818 | L2878 | T2937 | F3057 |
| V1561 | L1815 | L1815 | LYS | GLU   | D2126 | D2274 | E2449 | L2644 | A2759 | W2819 | A2879 | T2938 | F3057 |
| I1562 | V1819 | V1819 | GLU | GLU   | Q2127 | A2276 | R2452 | R2650 | E2760 | E2820 | E2880 | R2939 | D3060 |
| R1623 | V1841 | V1841 | LEU | PRO   | Y2128 | V2280 | LEU   | C2651 | Y2761 | W2821 | N2881 | GLY   | A3061 |
| Q1629 | V1845 | V1845 | GLU | GLU   | D2151 | L2286 | GLY   | E2670 | T2762 | T2822 | Y2882 | LEU   | P3062 |
| A1638 | S1846 | S1846 | THR | THR   | D2152 | L2286 | LYS   | L2678 | H2763 | L2823 | H2883 | ASP   | N3066 |
| C1647 | V1850 | V1850 | SER | SER   | L2159 | E2292 | ASP   | L2678 | E2764 | E2824 | N2884 | LYS   | C3067 |
| L1669 | E1867 | E1867 | ARG | ARG   | Q2161 | Q2293 | GLY   | K2697 | K2765 | K2825 | T2885 | GLU   | L3068 |
| L1694 | T1872 | T1872 | LEU | LEU   | L2162 | D2294 | ALA   | M2698 | W2766 | A2826 | W2886 | THR   | A3077 |
| L1698 | L1939 | L1939 | ARG | ARG   | R2163 | E2296 | L2485 | D2716 | A2767 | R2827 | Q2887 | SER   | R3078 |
| R1727 | L1943 | L1943 | LEU | LEU   | S2164 | K2297 | K2499 | ALA   | F2768 | E2828 | R2888 | S2950 | T3079 |
| L1731 | L1943 | L1943 | GLU | GLU   | L2165 | V2298 | V2503 | SER   | K2770 | Q2829 | K2889 | L2960 | G3084 |
| V1736 | L1969 | L1969 | GLU | VAL   | E2175 | N2324 | Q2515 | THR   | I2771 | GLU   | K2890 | L2965 | P3085 |
| P1740 | L1980 | L1980 | THR | THR   | L2176 | P2395 | L2519 | ARG   | Q2772 | ARG   | K2891 | W2966 | V3088 |
| R1743 | PRO   | PRO   | MET | MET   | L2177 | C2326 | H2520 | VAL   | N2773 | THR   | E2892 | VAL   | M3106 |
| P1749 | GLY   | GLY   | GLY | GLY   | M2178 | R2330 | D2523 | ALA   | N2774 | GLU   | E2893 | VAL   | N3109 |
| ARG   | GLY   | GLY   | GLY | GLY   | K2189 | F2334 | V2524 | GLY   | W2775 | LYS   | L2894 | VAL   | L3110 |
| LYS   | ASP   | ASP   | THR | THR   | N2196 | E2348 | V2524 | ASP   | S2776 | LYS   | E2895 | ALA   | R3111 |
| GLY   | GLY   | GLY   | ARG | ARG   | G2216 | N2349 | M2530 | GLY   | Q2777 | THR   | K2896 | GLY   | L3111 |
| LYS   | GLY   | GLY   | LYS | LYS   | GLY   | A2350 | F2541 | THR   | G2778 | ARG   | G2898 | GLY   | LEU   |
| ASN   | LYS   | LYS   | LYS | LYS   | R1994 | V2352 | T2544 | VAL   | E2779 | LYS   | G2899 | VAL   | LYS   |
| ALA   | GLY   | GLY   | GLY | GLY   | S2000 | V2353 | A2547 | ASP   | N2780 | ILE   | G2900 | VAL   | LYS   |
| R1758 | GLU   | GLU   | GLU | GLU   | L2009 | R2355 | R2575 | GLY   | V2781 | SER   | T2901 | VAL   | VAL   |
| L1762 | ASP   | ASP   | ASP | ASP   | G2216 | R2355 | A2598 | ASP   | D2782 | GLN   | H2902 | SER   | GLN   |
|       |       |       |     |       | GLY   | R2355 | Q2599 | ASP   | E2784 | THR   | P2903 | ARG   | THR   |
|       |       |       |     |       | GLY   | R2355 | Q2599 | ASP   | L2785 | TYR   | L2904 | GLY   | ARG   |
|       |       |       |     |       | GLY   | R2355 | Q2599 | ASP   | K2786 | ASP   | L2905 | VAL   | VAL   |
|       |       |       |     |       | GLY   | R2355 | Q2599 | ASP   | T2787 | PRO   | V2906 | VAL   | LYS   |
|       |       |       |     |       | GLY   | R2355 | Q2599 | ASP   | H2788 | ARG   | P2907 | LYS   | GLY   |
|       |       |       |     |       | GLY   | R2355 | Q2599 | ASP   | T2788 | GLY   | Y2908 | LYS   | GLY   |
|       |       |       |     |       | GLY   | R2355 | Q2599 | ASP   | T2789 | GLY   | D2909 | LYS   | GLY   |
|       |       |       |     |       | GLY   | R2355 | Q2599 | ASP   | M2790 | GLY   | T2910 | LYS   | GLY   |
|       |       |       |     |       | GLY   | R2355 | Q2599 | ASP   | L2791 | GLY   | L2911 | LYS   | GLY   |
|       |       |       |     |       | GLY   | R2355 | Q2599 | ASP   | A2792 | GLY   | T2912 | LYS   | GLY   |
|       |       |       |     |       | GLY   | R2355 | Q2599 | ASP   | K2793 | GLY   | A2913 | LYS   | GLY   |
|       |       |       |     |       | GLY   | R2355 | Q2599 | ASP   | Y2794 | GLY   | K2914 | LYS   | GLY   |
|       |       |       |     |       | GLY   | R2355 | Q2599 | ASP   | K2795 | GLY   | E2915 | LYS   | GLY   |
|       |       |       |     |       | GLY   | R2355 | Q2599 | ASP   | T2796 | GLY   | K2916 | LYS   | GLY   |
|       |       |       |     |       | GLY   | R2355 | Q2599 | ASP   | T2797 | GLY   | A2917 | LYS   | GLY   |
|       |       |       |     |       | GLY   | R2355 | Q2599 | ASP   | S2798 | GLY   | R2918 | LYS   | GLY   |
|       |       |       |     |       | GLY   | R2355 | Q2599 | ASP   | E2799 | GLY   | D2919 | LYS   | GLY   |
|       |       |       |     |       | GLY   | R2355 | Q2599 | ASP   | K2800 | GLY   | R2920 | LYS   | GLY   |
|       |       |       |     |       | GLY   | R2355 | Q2599 | ASP   | L2801 | GLY   | E2921 | LYS   | GLY   |
|       |       |       |     |       | GLY   | R2355 | Q2599 | ASP   | K2802 | GLY   | A2922 | LYS   | GLY   |
|       |       |       |     |       | GLY   | R2355 | Q2599 | ASP   | E2803 | GLY   | A2923 | LYS   | GLY   |











- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain B: 86% 11% .



- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H: 86% 11% .



- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain N: 86% 11% .



- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain T: 86% 11% .



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 694588                                  | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | TFS KRIOS                               | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 50                                      | Depositor |
| Minimum defocus (nm)                 | 500                                     | Depositor |
| Maximum defocus (nm)                 | 2500                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | FEI FALCON IV (4k x 4k)                 | Depositor |
| Maximum map value                    | 0.866                                   | Depositor |
| Minimum map value                    | 0.000                                   | Depositor |
| Average map value                    | 0.003                                   | Depositor |
| Map value standard deviation         | 0.022                                   | Depositor |
| Recommended contour level            | 0.123                                   | Depositor |
| Map size (Å)                         | 491.52, 491.52, 491.52                  | wwPDB     |
| Map dimensions                       | 512, 512, 512                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 0.96, 0.96, 0.96                        | Depositor |

## 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: 117, CA, CFF, ZN

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     | 0.37         | 2/32589 (0.0%)  | 0.55        | 7/44174 (0.0%)   |
| 1   | G     | 0.37         | 2/32589 (0.0%)  | 0.55        | 7/44174 (0.0%)   |
| 1   | M     | 0.37         | 2/32589 (0.0%)  | 0.55        | 7/44174 (0.0%)   |
| 1   | S     | 0.37         | 2/32589 (0.0%)  | 0.55        | 7/44174 (0.0%)   |
| 2   | B     | 0.18         | 0/827           | 0.38        | 0/1111           |
| 2   | H     | 0.18         | 0/827           | 0.38        | 0/1111           |
| 2   | N     | 0.18         | 0/827           | 0.38        | 0/1111           |
| 2   | T     | 0.18         | 0/827           | 0.38        | 0/1111           |
| All | All   | 0.36         | 8/133664 (0.0%) | 0.54        | 28/181140 (0.0%) |

All (8) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1   | A     | 4915 | VAL  | C-O   | -5.97 | 1.17        | 1.24     |
| 1   | G     | 4915 | VAL  | C-O   | -5.97 | 1.17        | 1.24     |
| 1   | M     | 4915 | VAL  | C-O   | -5.97 | 1.17        | 1.24     |
| 1   | S     | 4915 | VAL  | C-O   | -5.97 | 1.17        | 1.24     |
| 1   | A     | 4640 | GLU  | N-CA  | 5.53  | 1.50        | 1.46     |
| 1   | G     | 4640 | GLU  | N-CA  | 5.53  | 1.50        | 1.46     |
| 1   | M     | 4640 | GLU  | N-CA  | 5.53  | 1.50        | 1.46     |
| 1   | S     | 4640 | GLU  | N-CA  | 5.53  | 1.50        | 1.46     |

All (28) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 1   | A     | 4697 | VAL  | N-CA-C | -7.50 | 104.00      | 113.22   |
| 1   | G     | 4697 | VAL  | N-CA-C | -7.50 | 104.00      | 113.22   |
| 1   | M     | 4697 | VAL  | N-CA-C | -7.50 | 104.00      | 113.22   |
| 1   | S     | 4697 | VAL  | N-CA-C | -7.50 | 104.00      | 113.22   |
| 1   | A     | 4164 | LEU  | N-CA-C | -5.56 | 105.23      | 112.23   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 1   | G     | 4164 | LEU  | N-CA-C | -5.56 | 105.23      | 112.23   |
| 1   | M     | 4164 | LEU  | N-CA-C | -5.56 | 105.23      | 112.23   |
| 1   | S     | 4164 | LEU  | N-CA-C | -5.56 | 105.23      | 112.23   |
| 1   | A     | 1012 | ASP  | CA-C-N | 5.48  | 123.69      | 120.24   |
| 1   | A     | 1012 | ASP  | C-N-CA | 5.48  | 123.69      | 120.24   |
| 1   | G     | 1012 | ASP  | CA-C-N | 5.48  | 123.69      | 120.24   |
| 1   | G     | 1012 | ASP  | C-N-CA | 5.48  | 123.69      | 120.24   |
| 1   | M     | 1012 | ASP  | CA-C-N | 5.48  | 123.69      | 120.24   |
| 1   | M     | 1012 | ASP  | C-N-CA | 5.48  | 123.69      | 120.24   |
| 1   | S     | 1012 | ASP  | CA-C-N | 5.48  | 123.69      | 120.24   |
| 1   | S     | 1012 | ASP  | C-N-CA | 5.48  | 123.69      | 120.24   |
| 1   | A     | 4867 | GLU  | N-CA-C | -5.23 | 107.03      | 113.41   |
| 1   | G     | 4867 | GLU  | N-CA-C | -5.23 | 107.03      | 113.41   |
| 1   | M     | 4867 | GLU  | N-CA-C | -5.23 | 107.03      | 113.41   |
| 1   | S     | 4867 | GLU  | N-CA-C | -5.23 | 107.03      | 113.41   |
| 1   | A     | 1011 | GLN  | N-CA-C | 5.21  | 117.65      | 110.35   |
| 1   | G     | 1011 | GLN  | N-CA-C | 5.21  | 117.65      | 110.35   |
| 1   | M     | 1011 | GLN  | N-CA-C | 5.21  | 117.65      | 110.35   |
| 1   | S     | 1011 | GLN  | N-CA-C | 5.21  | 117.65      | 110.35   |
| 1   | A     | 4877 | ASP  | N-CA-C | -5.14 | 107.00      | 113.28   |
| 1   | G     | 4877 | ASP  | N-CA-C | -5.14 | 107.00      | 113.28   |
| 1   | M     | 4877 | ASP  | N-CA-C | -5.14 | 107.00      | 113.28   |
| 1   | S     | 4877 | ASP  | N-CA-C | -5.14 | 107.00      | 113.28   |

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     | 31873 | 0        | 31185    | 400     | 0            |
| 1   | G     | 31873 | 0        | 31185    | 408     | 0            |
| 1   | M     | 31873 | 0        | 31185    | 403     | 0            |
| 1   | S     | 31873 | 0        | 31185    | 406     | 0            |
| 2   | B     | 811   | 0        | 806      | 8       | 0            |
| 2   | H     | 811   | 0        | 806      | 8       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 2   | N     | 811    | 0        | 806      | 8       | 0            |
| 2   | T     | 811    | 0        | 806      | 8       | 0            |
| 3   | A     | 14     | 0        | 10       | 1       | 0            |
| 3   | G     | 14     | 0        | 10       | 1       | 0            |
| 3   | M     | 14     | 0        | 10       | 1       | 0            |
| 3   | S     | 14     | 0        | 10       | 1       | 0            |
| 4   | A     | 1      | 0        | 0        | 0       | 0            |
| 4   | G     | 1      | 0        | 0        | 0       | 0            |
| 4   | M     | 1      | 0        | 0        | 0       | 0            |
| 4   | S     | 1      | 0        | 0        | 0       | 0            |
| 5   | A     | 123    | 0        | 102      | 8       | 0            |
| 5   | G     | 123    | 0        | 102      | 10      | 0            |
| 5   | M     | 123    | 0        | 102      | 10      | 0            |
| 5   | S     | 123    | 0        | 102      | 9       | 0            |
| 6   | A     | 1      | 0        | 0        | 0       | 0            |
| 6   | G     | 1      | 0        | 0        | 0       | 0            |
| 6   | M     | 1      | 0        | 0        | 0       | 0            |
| 6   | S     | 1      | 0        | 0        | 0       | 0            |
| All | All   | 131292 | 0        | 128412   | 1642    | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (1642) 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:4629:TYR:OH   | 1:S:4860:ARG:NH1 | 1.94                     | 1.00              |
| 1:M:4860:ARG:NH1  | 1:S:4629:TYR:OH  | 1.94                     | 0.99              |
| 1:G:4860:ARG:NH1  | 1:M:4629:TYR:OH  | 1.94                     | 0.98              |
| 1:A:4860:ARG:NH1  | 1:G:4629:TYR:OH  | 1.94                     | 0.98              |
| 1:A:2626:LEU:HD22 | 1:A:2640:PRO:HB3 | 1.47                     | 0.96              |
| 1:M:2626:LEU:HD22 | 1:M:2640:PRO:HB3 | 1.47                     | 0.96              |
| 1:G:2626:LEU:HD22 | 1:G:2640:PRO:HB3 | 1.47                     | 0.96              |
| 1:S:2626:LEU:HD22 | 1:S:2640:PRO:HB3 | 1.47                     | 0.96              |
| 1:A:4205:TRP:CZ3  | 1:A:4989:MET:HE1 | 2.05                     | 0.91              |
| 1:S:4205:TRP:CZ3  | 1:S:4989:MET:HE1 | 2.05                     | 0.91              |
| 1:G:2324:ASN:OD1  | 1:G:2326:CYS:SG  | 2.29                     | 0.90              |
| 1:M:2324:ASN:OD1  | 1:M:2326:CYS:SG  | 2.29                     | 0.90              |
| 1:G:4205:TRP:CZ3  | 1:G:4989:MET:HE1 | 2.05                     | 0.90              |
| 1:A:1638:ALA:HB1  | 1:A:1647:CYS:SG  | 2.12                     | 0.90              |
| 1:S:2324:ASN:OD1  | 1:S:2326:CYS:SG  | 2.29                     | 0.90              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:M:4205:TRP:CZ3  | 1:M:4989:MET:HE1  | 2.05                     | 0.89              |
| 1:A:2324:ASN:OD1  | 1:A:2326:CYS:SG   | 2.29                     | 0.89              |
| 1:G:1638:ALA:HB1  | 1:G:1647:CYS:SG   | 2.12                     | 0.89              |
| 1:M:1638:ALA:HB1  | 1:M:1647:CYS:SG   | 2.12                     | 0.89              |
| 1:S:1638:ALA:HB1  | 1:S:1647:CYS:SG   | 2.12                     | 0.88              |
| 1:G:206:CYS:SG    | 1:G:334:MET:HE1   | 2.17                     | 0.85              |
| 1:M:206:CYS:SG    | 1:M:334:MET:HE1   | 2.17                     | 0.85              |
| 1:S:206:CYS:SG    | 1:S:334:MET:HE1   | 2.17                     | 0.84              |
| 1:A:206:CYS:SG    | 1:A:334:MET:HE1   | 2.17                     | 0.83              |
| 1:G:989:ALA:HB2   | 1:G:1039:LEU:HD12 | 1.60                     | 0.83              |
| 1:G:1426:ILE:CG2  | 1:G:1429:ASN:HB2  | 2.09                     | 0.83              |
| 1:M:989:ALA:HB2   | 1:M:1039:LEU:HD12 | 1.60                     | 0.83              |
| 1:A:989:ALA:HB2   | 1:A:1039:LEU:HD12 | 1.60                     | 0.83              |
| 1:A:1426:ILE:CG2  | 1:A:1429:ASN:HB2  | 2.09                     | 0.83              |
| 1:M:1426:ILE:CG2  | 1:M:1429:ASN:HB2  | 2.09                     | 0.83              |
| 1:S:1426:ILE:CG2  | 1:S:1429:ASN:HB2  | 2.09                     | 0.82              |
| 1:S:989:ALA:HB2   | 1:S:1039:LEU:HD12 | 1.60                     | 0.82              |
| 1:S:3324:VAL:HG21 | 1:S:3361:THR:HG22 | 1.61                     | 0.82              |
| 1:A:3324:VAL:HG21 | 1:A:3361:THR:HG22 | 1.61                     | 0.82              |
| 1:G:2670:GLU:OE2  | 1:G:2916:LYS:HE3  | 1.81                     | 0.81              |
| 1:G:3324:VAL:HG21 | 1:G:3361:THR:HG22 | 1.61                     | 0.81              |
| 1:A:2670:GLU:OE2  | 1:A:2916:LYS:HE3  | 1.81                     | 0.81              |
| 1:G:1156:THR:OG1  | 1:G:1157:GLU:OE1  | 1.99                     | 0.81              |
| 1:M:3324:VAL:HG21 | 1:M:3361:THR:HG22 | 1.61                     | 0.81              |
| 1:S:1156:THR:OG1  | 1:S:1157:GLU:OE1  | 1.99                     | 0.81              |
| 1:A:3575:LEU:HD13 | 1:S:1219:LEU:CD1  | 2.11                     | 0.81              |
| 1:A:1219:LEU:CD1  | 1:G:3575:LEU:HD13 | 2.11                     | 0.80              |
| 1:M:1219:LEU:CD1  | 1:S:3575:LEU:HD13 | 2.11                     | 0.80              |
| 1:M:2670:GLU:OE2  | 1:M:2916:LYS:HE3  | 1.81                     | 0.80              |
| 1:S:2670:GLU:OE2  | 1:S:2916:LYS:HE3  | 1.81                     | 0.80              |
| 1:G:1219:LEU:CD1  | 1:M:3575:LEU:HD13 | 2.11                     | 0.80              |
| 1:G:4205:TRP:CH2  | 1:G:4989:MET:HE1  | 2.17                     | 0.80              |
| 1:M:4205:TRP:CH2  | 1:M:4989:MET:HE1  | 2.17                     | 0.79              |
| 1:S:4205:TRP:CH2  | 1:S:4989:MET:HE1  | 2.17                     | 0.79              |
| 1:A:1156:THR:OG1  | 1:A:1157:GLU:OE1  | 1.99                     | 0.79              |
| 1:M:1156:THR:OG1  | 1:M:1157:GLU:OE1  | 1.99                     | 0.79              |
| 1:M:1272:LEU:HD23 | 1:M:1561:VAL:HG21 | 1.65                     | 0.79              |
| 1:A:4205:TRP:CH2  | 1:A:4989:MET:HE1  | 2.17                     | 0.79              |
| 1:G:1272:LEU:HD23 | 1:G:1561:VAL:HG21 | 1.65                     | 0.78              |
| 1:S:1272:LEU:HD23 | 1:S:1561:VAL:HG21 | 1.65                     | 0.78              |
| 1:A:1272:LEU:HD23 | 1:A:1561:VAL:HG21 | 1.65                     | 0.76              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:G:181:HIS:ND1  | 1:G:196:MET:HB2   | 2.01                     | 0.76              |
| 1:M:667:MET:SD   | 1:M:790:ARG:NH2   | 2.59                     | 0.76              |
| 1:A:181:HIS:ND1  | 1:A:196:MET:HB2   | 2.01                     | 0.76              |
| 1:G:667:MET:SD   | 1:G:790:ARG:NH2   | 2.59                     | 0.76              |
| 1:A:667:MET:SD   | 1:A:790:ARG:NH2   | 2.59                     | 0.76              |
| 1:S:181:HIS:ND1  | 1:S:196:MET:HB2   | 2.01                     | 0.76              |
| 1:S:667:MET:SD   | 1:S:790:ARG:NH2   | 2.59                     | 0.75              |
| 1:A:2172:PRO:O   | 1:A:2176:ASN:ND2  | 2.20                     | 0.75              |
| 1:M:2172:PRO:O   | 1:M:2176:ASN:ND2  | 2.20                     | 0.75              |
| 1:M:2196:ASN:OD1 | 1:M:2199:ARG:NH2  | 2.20                     | 0.75              |
| 1:M:181:HIS:ND1  | 1:M:196:MET:HB2   | 2.01                     | 0.75              |
| 1:A:110:ARG:NH2  | 1:A:115:ARG:NH2   | 2.36                     | 0.74              |
| 1:G:2172:PRO:O   | 1:G:2176:ASN:ND2  | 2.20                     | 0.74              |
| 1:G:2196:ASN:OD1 | 1:G:2199:ARG:NH2  | 2.20                     | 0.74              |
| 1:A:788:LYS:HG2  | 1:A:1629:GLN:HG3  | 1.70                     | 0.74              |
| 1:A:2196:ASN:OD1 | 1:A:2199:ARG:NH2  | 2.20                     | 0.74              |
| 1:G:110:ARG:NH2  | 1:G:115:ARG:NH2   | 2.36                     | 0.74              |
| 1:S:2196:ASN:OD1 | 1:S:2199:ARG:NH2  | 2.20                     | 0.74              |
| 1:M:414:PHE:CE2  | 1:M:418:LEU:HD11  | 2.23                     | 0.74              |
| 1:G:414:PHE:CE2  | 1:G:418:LEU:HD11  | 2.23                     | 0.74              |
| 1:G:2523:ASP:OD2 | 1:G:2575:ARG:NH2  | 2.21                     | 0.74              |
| 1:S:788:LYS:HG2  | 1:S:1629:GLN:HG3  | 1.70                     | 0.74              |
| 1:S:2172:PRO:O   | 1:S:2176:ASN:ND2  | 2.20                     | 0.74              |
| 1:S:3329:ILE:O   | 1:S:3403:ARG:NH2  | 2.21                     | 0.74              |
| 1:M:110:ARG:NH2  | 1:M:115:ARG:NH2   | 2.36                     | 0.73              |
| 1:S:414:PHE:CE2  | 1:S:418:LEU:HD11  | 2.23                     | 0.73              |
| 1:G:3329:ILE:O   | 1:G:3403:ARG:NH2  | 2.21                     | 0.73              |
| 1:S:110:ARG:NH2  | 1:S:115:ARG:NH2   | 2.36                     | 0.73              |
| 5:S:5104:117:H83 | 5:S:5105:117:H931 | 1.70                     | 0.73              |
| 5:G:5104:117:H83 | 5:G:5105:117:H931 | 1.70                     | 0.73              |
| 1:M:2523:ASP:OD2 | 1:M:2575:ARG:NH2  | 2.21                     | 0.73              |
| 5:M:5104:117:H83 | 5:M:5105:117:H931 | 1.70                     | 0.73              |
| 1:S:2523:ASP:OD2 | 1:S:2575:ARG:NH2  | 2.21                     | 0.73              |
| 1:A:2523:ASP:OD2 | 1:A:2575:ARG:NH2  | 2.21                     | 0.73              |
| 1:A:3329:ILE:O   | 1:A:3403:ARG:NH2  | 2.21                     | 0.73              |
| 5:A:5104:117:H83 | 5:A:5105:117:H931 | 1.70                     | 0.73              |
| 1:M:3329:ILE:O   | 1:M:3403:ARG:NH2  | 2.21                     | 0.73              |
| 1:G:4670:ILE:HB  | 1:G:4714:ASN:HD21 | 1.54                     | 0.73              |
| 1:A:3182:TYR:O   | 1:A:3186:LEU:HD23 | 1.89                     | 0.73              |
| 1:G:788:LYS:HG2  | 1:G:1629:GLN:HG3  | 1.70                     | 0.72              |
| 1:M:788:LYS:HG2  | 1:M:1629:GLN:HG3  | 1.70                     | 0.72              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:414:PHE:CE2   | 1:A:418:LEU:HD11  | 2.23                     | 0.72              |
| 1:S:4205:TRP:CZ3  | 1:S:4989:MET:CE   | 2.73                     | 0.72              |
| 1:A:1108:GLU:N    | 1:A:1108:GLU:OE1  | 2.23                     | 0.72              |
| 1:M:4670:ILE:HB   | 1:M:4714:ASN:HD21 | 1.54                     | 0.72              |
| 1:S:4670:ILE:HB   | 1:S:4714:ASN:HD21 | 1.54                     | 0.72              |
| 1:G:4205:TRP:CZ3  | 1:G:4989:MET:CE   | 2.73                     | 0.72              |
| 1:S:1108:GLU:OE1  | 1:S:1108:GLU:N    | 2.23                     | 0.72              |
| 1:A:4205:TRP:CZ3  | 1:A:4989:MET:CE   | 2.73                     | 0.72              |
| 1:S:3182:TYR:O    | 1:S:3186:LEU:HD23 | 1.89                     | 0.71              |
| 1:G:3182:TYR:O    | 1:G:3186:LEU:HD23 | 1.89                     | 0.71              |
| 1:G:1108:GLU:N    | 1:G:1108:GLU:OE1  | 2.23                     | 0.71              |
| 1:M:3182:TYR:O    | 1:M:3186:LEU:HD23 | 1.89                     | 0.71              |
| 1:A:4670:ILE:HB   | 1:A:4714:ASN:ND2  | 2.06                     | 0.71              |
| 1:M:20:VAL:HG21   | 1:M:202:MET:HG3   | 1.73                     | 0.71              |
| 1:M:4205:TRP:CZ3  | 1:M:4989:MET:CE   | 2.73                     | 0.71              |
| 1:A:20:VAL:HG21   | 1:A:202:MET:HG3   | 1.73                     | 0.71              |
| 1:S:20:VAL:HG21   | 1:S:202:MET:HG3   | 1.73                     | 0.71              |
| 1:G:20:VAL:HG21   | 1:G:202:MET:HG3   | 1.73                     | 0.71              |
| 1:G:4670:ILE:HB   | 1:G:4714:ASN:ND2  | 2.06                     | 0.71              |
| 1:A:4670:ILE:HB   | 1:A:4714:ASN:HD21 | 1.54                     | 0.71              |
| 1:M:1108:GLU:OE1  | 1:M:1108:GLU:N    | 2.23                     | 0.70              |
| 1:M:3017:PHE:O    | 1:M:3036:LYS:NZ   | 2.24                     | 0.70              |
| 1:S:3017:PHE:O    | 1:S:3036:LYS:NZ   | 2.24                     | 0.70              |
| 1:S:4670:ILE:HB   | 1:S:4714:ASN:ND2  | 2.06                     | 0.70              |
| 1:G:3017:PHE:O    | 1:G:3036:LYS:NZ   | 2.24                     | 0.70              |
| 1:M:3534:MET:HA   | 1:M:3534:MET:HE3  | 1.72                     | 0.70              |
| 1:M:52:THR:O      | 1:M:52:THR:HG22   | 1.91                     | 0.70              |
| 1:M:4670:ILE:HB   | 1:M:4714:ASN:ND2  | 2.06                     | 0.70              |
| 1:A:52:THR:HG22   | 1:A:52:THR:O      | 1.91                     | 0.70              |
| 1:S:52:THR:HG22   | 1:S:52:THR:O      | 1.91                     | 0.69              |
| 1:S:3534:MET:HA   | 1:S:3534:MET:HE3  | 1.72                     | 0.69              |
| 1:A:3534:MET:HA   | 1:A:3534:MET:HE3  | 1.72                     | 0.69              |
| 1:G:52:THR:O      | 1:G:52:THR:HG22   | 1.91                     | 0.69              |
| 1:A:4205:TRP:CZ3  | 1:A:4989:MET:SD   | 2.86                     | 0.69              |
| 1:G:4205:TRP:CZ3  | 1:G:4989:MET:SD   | 2.86                     | 0.69              |
| 1:M:4205:TRP:CZ3  | 1:M:4989:MET:SD   | 2.86                     | 0.69              |
| 1:A:3017:PHE:O    | 1:A:3036:LYS:NZ   | 2.24                     | 0.69              |
| 1:G:3534:MET:HA   | 1:G:3534:MET:HE3  | 1.72                     | 0.69              |
| 1:S:3144:PHE:CE2  | 1:S:3197:LEU:HD12 | 2.28                     | 0.69              |
| 1:S:4205:TRP:CZ3  | 1:S:4989:MET:SD   | 2.86                     | 0.69              |
| 1:M:4820:VAL:HG23 | 5:M:5103:117:C83  | 2.23                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:S:4820:VAL:HG23 | 5:S:5103:117:C83  | 2.23                     | 0.68              |
| 2:T:106:ASN:OD1   | 2:T:107:LEU:N     | 2.27                     | 0.68              |
| 1:M:4863:TYR:CD2  | 1:M:4876:CYS:SG   | 2.87                     | 0.68              |
| 1:S:4581:LYS:HD2  | 1:S:4632:LEU:HD22 | 1.76                     | 0.68              |
| 1:A:4863:TYR:CD2  | 1:A:4876:CYS:SG   | 2.87                     | 0.68              |
| 1:M:4581:LYS:HD2  | 1:M:4632:LEU:HD22 | 1.76                     | 0.68              |
| 1:S:4863:TYR:CD2  | 1:S:4876:CYS:SG   | 2.87                     | 0.68              |
| 1:A:3144:PHE:CE2  | 1:A:3197:LEU:HD12 | 2.28                     | 0.68              |
| 1:G:3144:PHE:CE2  | 1:G:3197:LEU:HD12 | 2.28                     | 0.68              |
| 1:A:4581:LYS:HD2  | 1:A:4632:LEU:HD22 | 1.76                     | 0.67              |
| 1:G:4581:LYS:HD2  | 1:G:4632:LEU:HD22 | 1.76                     | 0.67              |
| 1:G:4820:VAL:HG23 | 5:G:5103:117:C83  | 2.23                     | 0.67              |
| 1:M:3144:PHE:CE2  | 1:M:3197:LEU:HD12 | 2.28                     | 0.67              |
| 1:A:4231:MET:HA   | 1:A:4231:MET:HE3  | 1.76                     | 0.67              |
| 1:A:4820:VAL:HG23 | 5:A:5103:117:C83  | 2.23                     | 0.67              |
| 2:H:106:ASN:OD1   | 2:H:107:LEU:N     | 2.27                     | 0.67              |
| 1:G:4863:TYR:CD2  | 1:G:4876:CYS:SG   | 2.87                     | 0.67              |
| 2:B:106:ASN:OD1   | 2:B:107:LEU:N     | 2.27                     | 0.67              |
| 1:G:2212:VAL:HG22 | 1:G:2256:TYR:CE2  | 2.30                     | 0.67              |
| 1:G:4231:MET:HA   | 1:G:4231:MET:HE3  | 1.76                     | 0.67              |
| 1:S:4231:MET:HA   | 1:S:4231:MET:HE3  | 1.76                     | 0.67              |
| 1:A:2212:VAL:HG22 | 1:A:2256:TYR:CE2  | 2.30                     | 0.67              |
| 1:M:4231:MET:HA   | 1:M:4231:MET:HE3  | 1.76                     | 0.67              |
| 2:N:106:ASN:OD1   | 2:N:107:LEU:N     | 2.27                     | 0.67              |
| 1:A:2449:GLU:OE1  | 1:A:2452:ARG:NH2  | 2.29                     | 0.67              |
| 1:M:2212:VAL:HG22 | 1:M:2256:TYR:CE2  | 2.30                     | 0.67              |
| 1:M:3062:PRO:O    | 1:M:3066:ASN:ND2  | 2.28                     | 0.66              |
| 1:A:3062:PRO:O    | 1:A:3066:ASN:ND2  | 2.28                     | 0.66              |
| 1:S:2212:VAL:HG22 | 1:S:2256:TYR:CE2  | 2.30                     | 0.66              |
| 1:G:3062:PRO:O    | 1:G:3066:ASN:ND2  | 2.28                     | 0.66              |
| 1:S:3062:PRO:O    | 1:S:3066:ASN:ND2  | 2.28                     | 0.66              |
| 1:M:2449:GLU:OE1  | 1:M:2452:ARG:NH2  | 2.29                     | 0.66              |
| 1:G:2449:GLU:OE1  | 1:G:2452:ARG:NH2  | 2.29                     | 0.66              |
| 1:G:2620:GLN:NE2  | 1:G:2912:THR:HG22 | 2.11                     | 0.65              |
| 1:S:2620:GLN:NE2  | 1:S:2912:THR:HG22 | 2.11                     | 0.65              |
| 1:S:2449:GLU:OE1  | 1:S:2452:ARG:NH2  | 2.29                     | 0.65              |
| 1:G:1105:ALA:HB3  | 1:G:1191:VAL:HG11 | 1.78                     | 0.65              |
| 1:S:1105:ALA:HB3  | 1:S:1191:VAL:HG11 | 1.78                     | 0.64              |
| 1:M:1105:ALA:HB3  | 1:M:1191:VAL:HG11 | 1.78                     | 0.64              |
| 1:A:1105:ALA:HB3  | 1:A:1191:VAL:HG11 | 1.78                     | 0.64              |
| 1:M:2620:GLN:NE2  | 1:M:2912:THR:HG22 | 2.11                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2620:GLN:NE2  | 1:A:2912:THR:HG22 | 2.11                     | 0.64              |
| 1:G:988:LEU:HD23  | 1:G:1039:LEU:HD22 | 1.80                     | 0.64              |
| 1:A:1426:ILE:HG23 | 1:A:1429:ASN:HB2  | 1.79                     | 0.64              |
| 1:M:3969:ILE:HG21 | 1:M:3980:LEU:HD12 | 1.80                     | 0.64              |
| 1:S:988:LEU:HD23  | 1:S:1039:LEU:HD22 | 1.80                     | 0.64              |
| 1:G:2967:MET:HA   | 1:G:2967:MET:HE3  | 1.80                     | 0.64              |
| 1:M:1263:THR:HG22 | 1:M:1264:VAL:H    | 1.63                     | 0.64              |
| 1:M:988:LEU:HD23  | 1:M:1039:LEU:HD22 | 1.80                     | 0.64              |
| 1:S:977:LEU:HD22  | 1:S:981:GLN:HB3   | 1.80                     | 0.64              |
| 1:S:1263:THR:HG22 | 1:S:1264:VAL:H    | 1.63                     | 0.64              |
| 1:A:977:LEU:HA    | 1:A:981:GLN:OE1   | 1.98                     | 0.64              |
| 1:M:977:LEU:HA    | 1:M:981:GLN:OE1   | 1.98                     | 0.64              |
| 1:S:937:CYS:SG    | 1:S:984:LEU:HD13  | 2.38                     | 0.64              |
| 1:S:3969:ILE:HG21 | 1:S:3980:LEU:HD12 | 1.80                     | 0.64              |
| 1:A:988:LEU:HD23  | 1:A:1039:LEU:HD22 | 1.80                     | 0.63              |
| 1:M:4215:ARG:HG2  | 1:M:4219:PHE:CZ   | 2.33                     | 0.63              |
| 1:S:4205:TRP:HZ3  | 1:S:4989:MET:HE1  | 1.62                     | 0.63              |
| 1:M:1426:ILE:HG23 | 1:M:1429:ASN:HB2  | 1.79                     | 0.63              |
| 1:A:4586:PRO:HA   | 1:A:4628:VAL:HG11 | 1.80                     | 0.63              |
| 1:G:4215:ARG:HG2  | 1:G:4219:PHE:CZ   | 2.33                     | 0.63              |
| 1:A:977:LEU:HD22  | 1:A:981:GLN:HB3   | 1.80                     | 0.63              |
| 1:A:2967:MET:HE3  | 1:A:2967:MET:HA   | 1.80                     | 0.63              |
| 1:S:1426:ILE:HG23 | 1:S:1429:ASN:HB2  | 1.79                     | 0.63              |
| 1:G:308:HIS:O     | 1:G:312:THR:HG22  | 1.98                     | 0.63              |
| 1:S:308:HIS:O     | 1:S:312:THR:HG22  | 1.98                     | 0.63              |
| 1:S:4586:PRO:HA   | 1:S:4628:VAL:HG11 | 1.80                     | 0.63              |
| 1:A:3969:ILE:HG21 | 1:A:3980:LEU:HD12 | 1.80                     | 0.63              |
| 1:A:937:CYS:SG    | 1:A:984:LEU:HD13  | 2.38                     | 0.63              |
| 1:G:3969:ILE:HG21 | 1:G:3980:LEU:HD12 | 1.80                     | 0.63              |
| 1:M:977:LEU:HD22  | 1:M:981:GLN:HB3   | 1.80                     | 0.63              |
| 1:M:2967:MET:HA   | 1:M:2967:MET:HE3  | 1.80                     | 0.63              |
| 1:A:1131:ARG:NH1  | 1:A:1178:ALA:O    | 2.32                     | 0.63              |
| 1:A:4222:VAL:HG12 | 1:A:4950:VAL:CG1  | 2.29                     | 0.63              |
| 1:G:179:TYR:N     | 1:G:194:SER:O     | 2.32                     | 0.63              |
| 1:M:937:CYS:SG    | 1:M:984:LEU:HD13  | 2.38                     | 0.63              |
| 1:A:1263:THR:HG22 | 1:A:1264:VAL:H    | 1.63                     | 0.63              |
| 1:M:4586:PRO:HA   | 1:M:4628:VAL:HG11 | 1.80                     | 0.63              |
| 1:S:4215:ARG:HG2  | 1:S:4219:PHE:CZ   | 2.33                     | 0.63              |
| 1:S:4222:VAL:HG12 | 1:S:4950:VAL:CG1  | 2.29                     | 0.63              |
| 1:A:20:VAL:HG11   | 1:A:202:MET:SD    | 2.39                     | 0.62              |
| 1:A:2520:HIS:O    | 1:A:2524:VAL:HG22 | 1.99                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2527:LEU:HD12 | 1:A:2530:MET:HE3  | 1.81                     | 0.62              |
| 1:G:1131:ARG:NH1  | 1:G:1178:ALA:O    | 2.32                     | 0.62              |
| 1:G:2527:LEU:HD12 | 1:G:2530:MET:HE3  | 1.81                     | 0.62              |
| 1:G:4222:VAL:HG12 | 1:G:4950:VAL:CG1  | 2.29                     | 0.62              |
| 1:M:20:VAL:HG11   | 1:M:202:MET:SD    | 2.39                     | 0.62              |
| 1:M:4222:VAL:HG12 | 1:M:4950:VAL:CG1  | 2.29                     | 0.62              |
| 1:A:308:HIS:O     | 1:A:312:THR:HG22  | 1.98                     | 0.62              |
| 1:G:2520:HIS:O    | 1:G:2524:VAL:HG22 | 1.99                     | 0.62              |
| 1:S:2967:MET:HA   | 1:S:2967:MET:HE3  | 1.80                     | 0.62              |
| 1:G:20:VAL:HG11   | 1:G:202:MET:SD    | 2.39                     | 0.62              |
| 1:G:937:CYS:SG    | 1:G:984:LEU:HD13  | 2.38                     | 0.62              |
| 1:S:977:LEU:HA    | 1:S:981:GLN:OE1   | 1.98                     | 0.62              |
| 1:A:179:TYR:N     | 1:A:194:SER:O     | 2.32                     | 0.62              |
| 1:A:701:GLY:O     | 1:A:1647:CYS:HB2  | 2.00                     | 0.62              |
| 1:G:1426:ILE:HG23 | 1:G:1429:ASN:HB2  | 1.79                     | 0.62              |
| 1:G:977:LEU:HD22  | 1:G:981:GLN:HB3   | 1.80                     | 0.62              |
| 1:G:977:LEU:HA    | 1:G:981:GLN:OE1   | 1.98                     | 0.62              |
| 1:M:2520:HIS:O    | 1:M:2524:VAL:HG22 | 1.99                     | 0.62              |
| 1:S:2520:HIS:O    | 1:S:2524:VAL:HG22 | 1.99                     | 0.62              |
| 1:M:308:HIS:O     | 1:M:312:THR:HG22  | 1.98                     | 0.62              |
| 1:M:1131:ARG:NH1  | 1:M:1178:ALA:O    | 2.32                     | 0.62              |
| 1:S:20:VAL:HG11   | 1:S:202:MET:SD    | 2.39                     | 0.62              |
| 1:S:1131:ARG:NH1  | 1:S:1178:ALA:O    | 2.32                     | 0.62              |
| 1:A:4215:ARG:HG2  | 1:A:4219:PHE:CZ   | 2.33                     | 0.62              |
| 1:G:1263:THR:HG22 | 1:G:1264:VAL:H    | 1.63                     | 0.62              |
| 1:G:2862:LEU:CD1  | 1:G:2932:MET:HE1  | 2.30                     | 0.62              |
| 1:M:179:TYR:N     | 1:M:194:SER:O     | 2.32                     | 0.61              |
| 1:A:2862:LEU:CD1  | 1:A:2932:MET:HE1  | 2.30                     | 0.61              |
| 1:G:701:GLY:O     | 1:G:1647:CYS:HB2  | 2.00                     | 0.61              |
| 1:M:3110:LEU:O    | 1:M:3110:LEU:HD23 | 2.00                     | 0.61              |
| 1:S:179:TYR:N     | 1:S:194:SER:O     | 2.32                     | 0.61              |
| 1:S:676:THR:HG22  | 1:S:677:ALA:H     | 1.65                     | 0.61              |
| 1:M:2626:LEU:CD2  | 1:M:2640:PRO:HB3  | 2.27                     | 0.61              |
| 1:S:206:CYS:SG    | 1:S:334:MET:CE    | 2.88                     | 0.61              |
| 1:S:701:GLY:O     | 1:S:1647:CYS:HB2  | 2.00                     | 0.61              |
| 1:S:2527:LEU:HD12 | 1:S:2530:MET:HE3  | 1.81                     | 0.61              |
| 1:A:676:THR:HG22  | 1:A:677:ALA:H     | 1.65                     | 0.61              |
| 1:G:3110:LEU:O    | 1:G:3110:LEU:HD23 | 2.00                     | 0.61              |
| 1:G:4586:PRO:HA   | 1:G:4628:VAL:HG11 | 1.80                     | 0.61              |
| 1:G:4820:VAL:HG23 | 5:G:5103:117:H83  | 1.83                     | 0.61              |
| 1:S:2626:LEU:CD2  | 1:S:2640:PRO:HB3  | 2.27                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2485:LEU:HD22 | 1:A:2541:PHE:HE1  | 1.65                     | 0.61              |
| 1:M:206:CYS:SG    | 1:M:334:MET:CE    | 2.88                     | 0.61              |
| 1:M:2527:LEU:HD12 | 1:M:2530:MET:HE3  | 1.81                     | 0.61              |
| 1:G:676:THR:HG22  | 1:G:677:ALA:H     | 1.65                     | 0.61              |
| 1:G:2161:GLN:O    | 1:G:2165:LEU:HD22 | 2.01                     | 0.61              |
| 1:G:2485:LEU:HD22 | 1:G:2541:PHE:HE1  | 1.65                     | 0.61              |
| 1:M:701:GLY:O     | 1:M:1647:CYS:HB2  | 2.00                     | 0.61              |
| 1:A:4820:VAL:HG23 | 5:A:5103:117:H83  | 1.83                     | 0.61              |
| 1:G:206:CYS:SG    | 1:G:334:MET:CE    | 2.88                     | 0.61              |
| 1:A:206:CYS:SG    | 1:A:334:MET:CE    | 2.88                     | 0.60              |
| 1:G:989:ALA:HB2   | 1:G:1039:LEU:CD1  | 2.31                     | 0.60              |
| 1:M:2862:LEU:CD1  | 1:M:2932:MET:HE1  | 2.30                     | 0.60              |
| 1:M:4059:LEU:HD22 | 1:M:4170:ILE:CD1  | 2.31                     | 0.60              |
| 1:S:4059:LEU:HD22 | 1:S:4170:ILE:CD1  | 2.31                     | 0.60              |
| 1:A:2626:LEU:CD2  | 1:A:2640:PRO:HB3  | 2.27                     | 0.60              |
| 1:M:676:THR:HG22  | 1:M:677:ALA:H     | 1.65                     | 0.60              |
| 1:M:4820:VAL:HG23 | 5:M:5103:117:H83  | 1.83                     | 0.60              |
| 1:A:989:ALA:HB2   | 1:A:1039:LEU:CD1  | 2.31                     | 0.60              |
| 1:M:2485:LEU:HD22 | 1:M:2541:PHE:HE1  | 1.65                     | 0.60              |
| 1:S:2485:LEU:HD22 | 1:S:2541:PHE:HE1  | 1.65                     | 0.60              |
| 1:A:2116:LEU:O    | 1:A:2120:MET:HG2  | 2.02                     | 0.60              |
| 1:G:2175:GLU:HA   | 1:G:2228:MET:HE1  | 1.83                     | 0.60              |
| 1:S:2862:LEU:CD1  | 1:S:2932:MET:HE1  | 2.30                     | 0.60              |
| 1:S:4820:VAL:HG23 | 5:S:5103:117:H83  | 1.83                     | 0.60              |
| 1:A:799:GLU:OE1   | 1:A:1623:ARG:NH1  | 2.35                     | 0.60              |
| 1:A:4059:LEU:HD22 | 1:A:4170:ILE:CD1  | 2.31                     | 0.60              |
| 1:G:1272:LEU:HD23 | 1:G:1561:VAL:CG2  | 2.32                     | 0.60              |
| 1:S:2161:GLN:O    | 1:S:2165:LEU:HD22 | 2.01                     | 0.60              |
| 1:A:2161:GLN:O    | 1:A:2165:LEU:HD22 | 2.01                     | 0.60              |
| 1:A:3110:LEU:HD23 | 1:A:3110:LEU:O    | 2.00                     | 0.60              |
| 1:G:2116:LEU:O    | 1:G:2120:MET:HG2  | 2.02                     | 0.60              |
| 1:G:4059:LEU:HD22 | 1:G:4170:ILE:CD1  | 2.31                     | 0.60              |
| 1:M:2161:GLN:O    | 1:M:2165:LEU:HD22 | 2.01                     | 0.60              |
| 1:S:3110:LEU:O    | 1:S:3110:LEU:HD23 | 2.00                     | 0.60              |
| 1:M:2175:GLU:HA   | 1:M:2228:MET:HE1  | 1.83                     | 0.59              |
| 1:A:2175:GLU:HA   | 1:A:2228:MET:HE1  | 1.83                     | 0.59              |
| 1:S:2116:LEU:O    | 1:S:2120:MET:HG2  | 2.02                     | 0.59              |
| 1:A:457:GLU:OE1   | 1:A:457:GLU:N     | 2.35                     | 0.59              |
| 1:G:457:GLU:OE1   | 1:G:457:GLU:N     | 2.35                     | 0.59              |
| 1:G:2598:ALA:O    | 1:G:2602:VAL:HG23 | 2.03                     | 0.59              |
| 1:M:937:CYS:SG    | 1:M:984:LEU:CD1   | 2.91                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1272:LEU:HD23 | 1:A:1561:VAL:CG2  | 2.32                     | 0.59              |
| 1:A:4215:ARG:O    | 1:A:4218:ILE:HG22 | 2.03                     | 0.59              |
| 1:S:457:GLU:N     | 1:S:457:GLU:OE1   | 2.35                     | 0.59              |
| 1:G:4083:ASP:OD2  | 1:G:4085:ARG:NH2  | 2.36                     | 0.59              |
| 1:M:4083:ASP:OD2  | 1:M:4085:ARG:NH2  | 2.36                     | 0.59              |
| 1:M:4205:TRP:HZ3  | 1:M:4989:MET:HE1  | 1.62                     | 0.59              |
| 1:S:156:GLN:OE1   | 1:S:156:GLN:N     | 2.36                     | 0.59              |
| 1:S:937:CYS:SG    | 1:S:984:LEU:CD1   | 2.91                     | 0.59              |
| 1:S:2175:GLU:HA   | 1:S:2228:MET:HE1  | 1.83                     | 0.59              |
| 1:G:4205:TRP:HZ3  | 1:G:4989:MET:HE1  | 1.62                     | 0.59              |
| 1:G:4215:ARG:O    | 1:G:4218:ILE:HG22 | 2.03                     | 0.59              |
| 1:S:4059:LEU:HD22 | 1:S:4170:ILE:HD12 | 1.85                     | 0.59              |
| 1:G:156:GLN:OE1   | 1:G:156:GLN:N     | 2.36                     | 0.59              |
| 1:M:156:GLN:N     | 1:M:156:GLN:OE1   | 2.36                     | 0.59              |
| 1:M:2598:ALA:O    | 1:M:2602:VAL:HG23 | 2.03                     | 0.59              |
| 1:G:281:ARG:NH2   | 1:G:307:ALA:O     | 2.36                     | 0.58              |
| 1:G:799:GLU:OE1   | 1:G:1623:ARG:NH1  | 2.35                     | 0.58              |
| 1:G:937:CYS:SG    | 1:G:984:LEU:CD1   | 2.91                     | 0.58              |
| 1:M:281:ARG:NH2   | 1:M:307:ALA:O     | 2.36                     | 0.58              |
| 1:M:2116:LEU:O    | 1:M:2120:MET:HG2  | 2.02                     | 0.58              |
| 1:S:281:ARG:NH2   | 1:S:307:ALA:O     | 2.36                     | 0.58              |
| 1:S:799:GLU:OE1   | 1:S:1623:ARG:NH1  | 2.35                     | 0.58              |
| 1:S:3020:THR:HG22 | 1:S:3021:PRO:HD2  | 1.85                     | 0.58              |
| 1:A:281:ARG:NH2   | 1:A:307:ALA:O     | 2.36                     | 0.58              |
| 1:A:937:CYS:SG    | 1:A:984:LEU:CD1   | 2.91                     | 0.58              |
| 1:A:4083:ASP:OD2  | 1:A:4085:ARG:NH2  | 2.36                     | 0.58              |
| 1:M:457:GLU:OE1   | 1:M:457:GLU:N     | 2.35                     | 0.58              |
| 1:M:989:ALA:HB2   | 1:M:1039:LEU:CD1  | 2.31                     | 0.58              |
| 1:M:2544:THR:HG23 | 1:M:2547:ALA:H    | 1.68                     | 0.58              |
| 1:S:195:PHE:C     | 1:S:196:MET:HE2   | 2.29                     | 0.58              |
| 1:A:156:GLN:OE1   | 1:A:156:GLN:N     | 2.36                     | 0.58              |
| 1:M:1272:LEU:HD23 | 1:M:1561:VAL:CG2  | 2.32                     | 0.58              |
| 1:M:4059:LEU:HD22 | 1:M:4170:ILE:HD12 | 1.85                     | 0.58              |
| 1:S:4215:ARG:O    | 1:S:4218:ILE:HG22 | 2.03                     | 0.58              |
| 1:S:4820:VAL:CG2  | 5:S:5103:117:C83  | 2.81                     | 0.58              |
| 1:A:2598:ALA:O    | 1:A:2602:VAL:HG23 | 2.03                     | 0.58              |
| 1:G:4059:LEU:HD22 | 1:G:4170:ILE:HD12 | 1.85                     | 0.58              |
| 1:S:2544:THR:HG23 | 1:S:2547:ALA:H    | 1.68                     | 0.58              |
| 1:A:3944:GLU:OE1  | 1:A:3944:GLU:N    | 2.37                     | 0.58              |
| 1:A:169:LEU:HD23  | 1:A:169:LEU:H     | 1.69                     | 0.58              |
| 1:A:3020:THR:HG22 | 1:A:3021:PRO:HD2  | 1.85                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:4820:VAL:CG2  | 5:A:5103:117:C83  | 2.81                     | 0.58              |
| 1:G:2165:LEU:HB2  | 1:G:2178:MET:HE2  | 1.86                     | 0.58              |
| 1:M:195:PHE:C     | 1:M:196:MET:HE2   | 2.29                     | 0.58              |
| 1:M:3944:GLU:OE1  | 1:M:3944:GLU:N    | 2.37                     | 0.58              |
| 1:G:2544:THR:HG23 | 1:G:2547:ALA:H    | 1.68                     | 0.58              |
| 1:M:799:GLU:OE1   | 1:M:1623:ARG:NH1  | 2.35                     | 0.58              |
| 1:M:4215:ARG:O    | 1:M:4218:ILE:HG22 | 2.03                     | 0.58              |
| 1:S:989:ALA:HB2   | 1:S:1039:LEU:CD1  | 2.31                     | 0.58              |
| 1:G:195:PHE:C     | 1:G:196:MET:HE2   | 2.29                     | 0.58              |
| 1:G:3201:MET:HE3  | 1:G:3203:VAL:HG12 | 1.86                     | 0.58              |
| 1:A:2544:THR:HG23 | 1:A:2547:ALA:H    | 1.68                     | 0.58              |
| 1:G:3944:GLU:N    | 1:G:3944:GLU:OE1  | 2.37                     | 0.58              |
| 1:M:4820:VAL:CG2  | 5:M:5103:117:C83  | 2.81                     | 0.58              |
| 1:A:181:HIS:CE1   | 1:A:196:MET:HB2   | 2.39                     | 0.57              |
| 1:A:195:PHE:C     | 1:A:196:MET:HE2   | 2.29                     | 0.57              |
| 1:G:169:LEU:HD23  | 1:G:169:LEU:H     | 1.69                     | 0.57              |
| 1:S:2598:ALA:O    | 1:S:2602:VAL:HG23 | 2.03                     | 0.57              |
| 1:S:4573:ILE:HG23 | 1:S:4643:LEU:HD11 | 1.86                     | 0.57              |
| 1:G:4820:VAL:CG2  | 5:G:5103:117:C83  | 2.81                     | 0.57              |
| 1:S:4083:ASP:OD2  | 1:S:4085:ARG:NH2  | 2.36                     | 0.57              |
| 1:A:2165:LEU:HB2  | 1:A:2178:MET:HE2  | 1.86                     | 0.57              |
| 1:A:2635:GLU:OE1  | 1:A:2635:GLU:N    | 2.37                     | 0.57              |
| 1:M:3169:LEU:HD13 | 1:M:3194:LEU:HD11 | 1.87                     | 0.57              |
| 1:M:4573:ILE:HG23 | 1:M:4643:LEU:HD11 | 1.86                     | 0.57              |
| 1:S:4217:PHE:CE1  | 1:S:4237:PHE:HB2  | 2.40                     | 0.57              |
| 1:A:4059:LEU:HD22 | 1:A:4170:ILE:HD12 | 1.85                     | 0.57              |
| 1:G:1157:GLU:OE1  | 1:G:1157:GLU:N    | 2.37                     | 0.57              |
| 1:G:4576:ILE:HG23 | 1:G:4639:MET:HE2  | 1.86                     | 0.57              |
| 1:M:3020:THR:HG22 | 1:M:3021:PRO:HD2  | 1.85                     | 0.57              |
| 1:M:3201:MET:HE3  | 1:M:3203:VAL:HG12 | 1.86                     | 0.57              |
| 1:G:2635:GLU:OE1  | 1:G:2635:GLU:N    | 2.37                     | 0.57              |
| 1:M:1219:LEU:HD13 | 1:S:3575:LEU:HD13 | 1.86                     | 0.57              |
| 1:S:169:LEU:HD23  | 1:S:169:LEU:H     | 1.69                     | 0.57              |
| 1:S:3169:LEU:HD13 | 1:S:3194:LEU:HD11 | 1.87                     | 0.57              |
| 1:S:3944:GLU:OE1  | 1:S:3944:GLU:N    | 2.37                     | 0.57              |
| 1:G:414:PHE:CD1   | 1:G:436:LEU:HD22  | 2.40                     | 0.57              |
| 1:M:2635:GLU:N    | 1:M:2635:GLU:OE1  | 2.37                     | 0.57              |
| 1:M:4217:PHE:CE1  | 1:M:4237:PHE:HB2  | 2.40                     | 0.57              |
| 1:M:181:HIS:CE1   | 1:M:196:MET:HB2   | 2.39                     | 0.57              |
| 1:S:4576:ILE:HG23 | 1:S:4639:MET:HE2  | 1.86                     | 0.57              |
| 1:A:1157:GLU:OE1  | 1:A:1157:GLU:N    | 2.37                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:3201:MET:HE3  | 1:A:3203:VAL:HG12 | 1.86                     | 0.57              |
| 1:G:3020:THR:HG22 | 1:G:3021:PRO:HD2  | 1.85                     | 0.57              |
| 1:M:414:PHE:CD1   | 1:M:436:LEU:HD22  | 2.40                     | 0.57              |
| 1:A:4217:PHE:CE1  | 1:A:4237:PHE:HB2  | 2.40                     | 0.57              |
| 1:A:4576:ILE:HG23 | 1:A:4639:MET:HE2  | 1.86                     | 0.57              |
| 1:M:1157:GLU:OE1  | 1:M:1157:GLU:N    | 2.37                     | 0.57              |
| 1:S:1157:GLU:OE1  | 1:S:1157:GLU:N    | 2.37                     | 0.57              |
| 1:S:2165:LEU:HB2  | 1:S:2178:MET:HE2  | 1.86                     | 0.57              |
| 1:G:2626:LEU:CD2  | 1:G:2640:PRO:HB3  | 2.27                     | 0.56              |
| 1:S:1272:LEU:HD23 | 1:S:1561:VAL:CG2  | 2.32                     | 0.56              |
| 1:M:2165:LEU:HB2  | 1:M:2178:MET:HE2  | 1.86                     | 0.56              |
| 1:S:181:HIS:CE1   | 1:S:196:MET:HB2   | 2.39                     | 0.56              |
| 1:S:3201:MET:HE3  | 1:S:3203:VAL:HG12 | 1.86                     | 0.56              |
| 1:A:414:PHE:CD1   | 1:A:436:LEU:HD22  | 2.40                     | 0.56              |
| 1:G:181:HIS:CE1   | 1:G:196:MET:HB2   | 2.39                     | 0.56              |
| 1:M:4670:ILE:CG2  | 1:M:4714:ASN:ND2  | 2.69                     | 0.56              |
| 1:S:414:PHE:CD1   | 1:S:436:LEU:HD22  | 2.40                     | 0.56              |
| 1:A:3575:LEU:HD13 | 1:S:1219:LEU:HD13 | 1.86                     | 0.56              |
| 1:G:3169:LEU:HD13 | 1:G:3194:LEU:HD11 | 1.87                     | 0.56              |
| 1:G:4217:PHE:CE1  | 1:G:4237:PHE:HB2  | 2.40                     | 0.56              |
| 1:A:3057:PHE:O    | 1:A:3060:ASP:OD1  | 2.24                     | 0.56              |
| 1:M:3057:PHE:O    | 1:M:3060:ASP:OD1  | 2.24                     | 0.56              |
| 1:A:4573:ILE:HG23 | 1:A:4643:LEU:HD11 | 1.86                     | 0.56              |
| 1:G:2807:TRP:HB3  | 1:G:2808:PRO:HD3  | 1.88                     | 0.56              |
| 1:G:4670:ILE:CG2  | 1:G:4714:ASN:ND2  | 2.69                     | 0.56              |
| 1:M:4101:LYS:O    | 1:M:4101:LYS:HG2  | 2.06                     | 0.56              |
| 1:S:2635:GLU:OE1  | 1:S:2635:GLU:N    | 2.37                     | 0.56              |
| 1:S:3057:PHE:O    | 1:S:3060:ASP:OD1  | 2.24                     | 0.56              |
| 1:A:4101:LYS:HG2  | 1:A:4101:LYS:O    | 2.06                     | 0.56              |
| 1:A:4670:ILE:CG2  | 1:A:4714:ASN:ND2  | 2.69                     | 0.56              |
| 1:G:4205:TRP:CH2  | 1:G:4989:MET:CE   | 2.89                     | 0.56              |
| 1:M:169:LEU:H     | 1:M:169:LEU:HD23  | 1.69                     | 0.56              |
| 1:S:3007:ASN:O    | 1:S:3011:THR:OG1  | 2.16                     | 0.56              |
| 1:M:4576:ILE:HG23 | 1:M:4639:MET:HE2  | 1.86                     | 0.56              |
| 1:A:3169:LEU:HD13 | 1:A:3194:LEU:HD11 | 1.87                     | 0.56              |
| 1:M:3007:ASN:O    | 1:M:3011:THR:OG1  | 2.16                     | 0.56              |
| 1:S:2807:TRP:HB3  | 1:S:2808:PRO:HD3  | 1.88                     | 0.55              |
| 1:S:4101:LYS:O    | 1:S:4101:LYS:HG2  | 2.06                     | 0.55              |
| 1:S:4670:ILE:CG2  | 1:S:4714:ASN:ND2  | 2.69                     | 0.55              |
| 1:G:3057:PHE:O    | 1:G:3060:ASP:OD1  | 2.24                     | 0.55              |
| 1:M:2807:TRP:HB3  | 1:M:2808:PRO:HD3  | 1.88                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:S:4670:ILE:CB   | 1:S:4714:ASN:ND2  | 2.70                     | 0.55              |
| 1:G:4101:LYS:O    | 1:G:4101:LYS:HG2  | 2.06                     | 0.55              |
| 1:A:1943:LEU:HD13 | 1:A:2098:VAL:HG22 | 1.88                     | 0.55              |
| 1:A:4837:LEU:HD11 | 1:A:4932:ILE:HG23 | 1.88                     | 0.55              |
| 1:G:4573:ILE:HG23 | 1:G:4643:LEU:HD11 | 1.86                     | 0.55              |
| 1:G:4670:ILE:CB   | 1:G:4714:ASN:ND2  | 2.70                     | 0.55              |
| 1:M:2778:GLY:HA3  | 1:M:2787:THR:HB   | 1.89                     | 0.55              |
| 1:M:20:VAL:HG21   | 1:M:202:MET:SD    | 2.47                     | 0.55              |
| 1:A:293:LEU:HD12  | 1:A:378:LEU:HD12  | 1.89                     | 0.55              |
| 1:G:20:VAL:HG21   | 1:G:202:MET:SD    | 2.47                     | 0.55              |
| 1:G:989:ALA:CB    | 1:G:1039:LEU:HD12 | 2.35                     | 0.55              |
| 1:G:1219:LEU:HD13 | 1:M:3575:LEU:HD13 | 1.86                     | 0.55              |
| 1:G:1943:LEU:HD13 | 1:G:2098:VAL:HG22 | 1.88                     | 0.55              |
| 1:S:293:LEU:HD12  | 1:S:378:LEU:HD12  | 1.89                     | 0.55              |
| 1:A:2212:VAL:HG22 | 1:A:2256:TYR:HE2  | 1.72                     | 0.55              |
| 1:A:4670:ILE:CB   | 1:A:4714:ASN:ND2  | 2.70                     | 0.55              |
| 1:G:177:GLU:O     | 1:G:177:GLU:HG2   | 2.07                     | 0.55              |
| 1:G:3078:ARG:NH1  | 1:G:3155:ASP:OD2  | 2.40                     | 0.55              |
| 1:M:4940:PHE:O    | 1:M:4944:ARG:HG3  | 2.07                     | 0.55              |
| 1:S:4837:LEU:HD11 | 1:S:4932:ILE:HG23 | 1.88                     | 0.55              |
| 1:S:4940:PHE:O    | 1:S:4944:ARG:HG3  | 2.07                     | 0.55              |
| 1:A:20:VAL:HG21   | 1:A:202:MET:SD    | 2.47                     | 0.55              |
| 1:A:4217:PHE:CD1  | 1:A:4237:PHE:HB2  | 2.42                     | 0.55              |
| 1:M:4217:PHE:CD1  | 1:M:4237:PHE:HB2  | 2.42                     | 0.55              |
| 1:M:4670:ILE:CB   | 1:M:4714:ASN:ND2  | 2.70                     | 0.55              |
| 1:M:2212:VAL:HG22 | 1:M:2256:TYR:HE2  | 1.72                     | 0.54              |
| 1:S:110:ARG:HH22  | 1:S:115:ARG:HH21  | 1.55                     | 0.54              |
| 1:S:2212:VAL:HG22 | 1:S:2256:TYR:HE2  | 1.72                     | 0.54              |
| 2:B:80:ASP:OD1    | 2:B:81:VAL:N      | 2.41                     | 0.54              |
| 1:M:177:GLU:O     | 1:M:177:GLU:HG2   | 2.07                     | 0.54              |
| 1:S:177:GLU:O     | 1:S:177:GLU:HG2   | 2.07                     | 0.54              |
| 1:S:4205:TRP:CH2  | 1:S:4989:MET:CE   | 2.89                     | 0.54              |
| 1:G:3607:GLU:HA   | 1:G:3610:GLU:HG3  | 1.89                     | 0.54              |
| 1:G:4940:PHE:O    | 1:G:4944:ARG:HG3  | 2.07                     | 0.54              |
| 1:M:110:ARG:HH22  | 1:M:115:ARG:HH21  | 1.55                     | 0.54              |
| 1:M:2280:VAL:HG22 | 1:M:2280:VAL:O    | 2.08                     | 0.54              |
| 2:N:80:ASP:OD1    | 2:N:81:VAL:N      | 2.41                     | 0.54              |
| 1:A:316:PHE:CE1   | 1:A:348:VAL:HG22  | 2.43                     | 0.54              |
| 1:A:989:ALA:CB    | 1:A:1039:LEU:HD12 | 2.35                     | 0.54              |
| 1:A:4205:TRP:HZ3  | 1:A:4989:MET:HE1  | 1.62                     | 0.54              |
| 1:M:1943:LEU:HD13 | 1:M:2098:VAL:HG22 | 1.88                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:S:2280:VAL:O    | 1:S:2280:VAL:HG22 | 2.08                     | 0.54              |
| 1:A:2807:TRP:HB3  | 1:A:2808:PRO:HD3  | 1.88                     | 0.54              |
| 1:G:2778:GLY:HA3  | 1:G:2787:THR:HB   | 1.89                     | 0.54              |
| 1:M:3078:ARG:NH1  | 1:M:3155:ASP:OD2  | 2.40                     | 0.54              |
| 1:M:3607:GLU:HA   | 1:M:3610:GLU:HG3  | 1.89                     | 0.54              |
| 1:S:20:VAL:HG21   | 1:S:202:MET:SD    | 2.47                     | 0.54              |
| 1:S:2778:GLY:HA3  | 1:S:2787:THR:HB   | 1.89                     | 0.54              |
| 1:S:4217:PHE:CD1  | 1:S:4237:PHE:HB2  | 2.42                     | 0.54              |
| 1:A:2280:VAL:O    | 1:A:2280:VAL:HG22 | 2.08                     | 0.54              |
| 1:A:4940:PHE:O    | 1:A:4944:ARG:HG3  | 2.07                     | 0.54              |
| 1:G:1736:VAL:HG23 | 1:G:1736:VAL:O    | 2.08                     | 0.54              |
| 1:G:4837:LEU:HD11 | 1:G:4932:ILE:HG23 | 1.88                     | 0.54              |
| 1:S:4899:ASP:OD1  | 1:S:4900:GLU:HG3  | 2.08                     | 0.54              |
| 1:A:1219:LEU:HD13 | 1:G:3575:LEU:HD13 | 1.86                     | 0.54              |
| 1:A:2670:GLU:OE2  | 1:A:2916:LYS:CE   | 2.55                     | 0.54              |
| 1:G:316:PHE:CE1   | 1:G:348:VAL:HG22  | 2.43                     | 0.54              |
| 1:G:4217:PHE:CD1  | 1:G:4237:PHE:HB2  | 2.42                     | 0.54              |
| 1:M:4899:ASP:OD1  | 1:M:4900:GLU:HG3  | 2.08                     | 0.54              |
| 1:S:20:VAL:HG21   | 1:S:202:MET:CG    | 2.38                     | 0.54              |
| 1:S:1943:LEU:HD13 | 1:S:2098:VAL:HG22 | 1.88                     | 0.54              |
| 1:S:3078:ARG:NH1  | 1:S:3155:ASP:OD2  | 2.40                     | 0.54              |
| 1:G:4682:GLU:OE1  | 1:G:4683:PHE:CD1  | 2.61                     | 0.54              |
| 1:S:1736:VAL:O    | 1:S:1736:VAL:HG23 | 2.08                     | 0.54              |
| 1:A:3607:GLU:HA   | 1:A:3610:GLU:HG3  | 1.89                     | 0.54              |
| 1:M:20:VAL:HG21   | 1:M:202:MET:CG    | 2.38                     | 0.54              |
| 1:M:4837:LEU:HD11 | 1:M:4932:ILE:HG23 | 1.88                     | 0.54              |
| 1:A:177:GLU:HG2   | 1:A:177:GLU:O     | 2.07                     | 0.54              |
| 1:G:4670:ILE:HG22 | 1:G:4714:ASN:ND2  | 2.23                     | 0.54              |
| 1:M:60:PRO:HG2    | 1:M:62:LEU:HD11   | 1.90                     | 0.54              |
| 1:S:1454:THR:OG1  | 1:S:1456:ASP:OD1  | 2.24                     | 0.54              |
| 1:G:3130:THR:HA   | 1:G:3133:THR:HG22 | 1.90                     | 0.53              |
| 1:G:4837:LEU:CD1  | 1:G:4932:ILE:HG23 | 2.38                     | 0.53              |
| 1:M:293:LEU:HD12  | 1:M:378:LEU:HD12  | 1.89                     | 0.53              |
| 1:M:4837:LEU:CD1  | 1:M:4932:ILE:HG23 | 2.38                     | 0.53              |
| 1:S:60:PRO:HG2    | 1:S:62:LEU:HD11   | 1.90                     | 0.53              |
| 1:A:4579:PHE:CD2  | 1:A:4639:MET:HE1  | 2.44                     | 0.53              |
| 1:A:4682:GLU:OE1  | 1:A:4683:PHE:CD1  | 2.61                     | 0.53              |
| 1:G:293:LEU:HD12  | 1:G:378:LEU:HD12  | 1.89                     | 0.53              |
| 1:G:4899:ASP:OD1  | 1:G:4900:GLU:HG3  | 2.08                     | 0.53              |
| 5:M:5104:117:H83  | 5:M:5105:117:C93  | 2.39                     | 0.53              |
| 1:S:4682:GLU:OE1  | 1:S:4683:PHE:CD1  | 2.61                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:M:110:ARG:HH22  | 1:M:115:ARG:NH2   | 2.05                     | 0.53              |
| 1:M:3130:THR:HA   | 1:M:3133:THR:HG22 | 1.90                     | 0.53              |
| 1:M:4670:ILE:HG22 | 1:M:4714:ASN:ND2  | 2.23                     | 0.53              |
| 2:T:80:ASP:OD1    | 2:T:81:VAL:N      | 2.41                     | 0.53              |
| 1:A:1561:VAL:HG23 | 1:A:1562:ILE:H    | 1.74                     | 0.53              |
| 1:A:4670:ILE:HG22 | 1:A:4714:ASN:ND2  | 2.23                     | 0.53              |
| 1:G:2280:VAL:HG22 | 1:G:2280:VAL:O    | 2.08                     | 0.53              |
| 1:G:4579:PHE:CD2  | 1:G:4639:MET:HE1  | 2.44                     | 0.53              |
| 2:H:80:ASP:OD1    | 2:H:81:VAL:N      | 2.41                     | 0.53              |
| 1:S:4093:PHE:CZ   | 1:S:4097:MET:HE2  | 2.44                     | 0.53              |
| 1:G:110:ARG:HH22  | 1:G:115:ARG:HH21  | 1.55                     | 0.53              |
| 1:G:483:MET:HE2   | 1:G:483:MET:HA    | 1.90                     | 0.53              |
| 1:G:3996:PHE:HD1  | 1:G:4016:LEU:HD11 | 1.73                     | 0.53              |
| 1:M:4682:GLU:OE1  | 1:M:4683:PHE:CD1  | 2.61                     | 0.53              |
| 1:S:2670:GLU:OE2  | 1:S:2916:LYS:CE   | 2.55                     | 0.53              |
| 1:S:3607:GLU:HA   | 1:S:3610:GLU:HG3  | 1.89                     | 0.53              |
| 1:A:1164:LEU:HB2  | 1:A:1169:LEU:HD21 | 1.91                     | 0.53              |
| 1:G:1561:VAL:HG23 | 1:G:1562:ILE:H    | 1.74                     | 0.53              |
| 1:M:1736:VAL:HG23 | 1:M:1736:VAL:O    | 2.08                     | 0.53              |
| 1:S:3996:PHE:HD1  | 1:S:4016:LEU:HD11 | 1.73                     | 0.53              |
| 1:A:20:VAL:HG21   | 1:A:202:MET:CG    | 2.38                     | 0.53              |
| 1:A:2778:GLY:HA3  | 1:A:2787:THR:HB   | 1.89                     | 0.53              |
| 1:A:3130:THR:HA   | 1:A:3133:THR:HG22 | 1.90                     | 0.53              |
| 1:G:419:ASP:OD1   | 1:G:419:ASP:O     | 2.27                     | 0.53              |
| 1:M:316:PHE:CE1   | 1:M:348:VAL:HG22  | 2.43                     | 0.53              |
| 1:S:4579:PHE:CD2  | 1:S:4639:MET:HE1  | 2.44                     | 0.53              |
| 1:S:4670:ILE:HG22 | 1:S:4714:ASN:ND2  | 2.23                     | 0.53              |
| 1:G:110:ARG:HH22  | 1:G:115:ARG:NH2   | 2.05                     | 0.53              |
| 1:M:4093:PHE:CZ   | 1:M:4097:MET:HE2  | 2.44                     | 0.53              |
| 1:A:52:THR:O      | 1:A:52:THR:CG2    | 2.57                     | 0.53              |
| 1:A:627:PRO:HG3   | 2:B:90:GLY:HA2    | 1.91                     | 0.53              |
| 1:M:52:THR:O      | 1:M:52:THR:CG2    | 2.57                     | 0.53              |
| 1:M:4205:TRP:CH2  | 1:M:4989:MET:CE   | 2.89                     | 0.53              |
| 1:M:4579:PHE:CD2  | 1:M:4639:MET:HE1  | 2.44                     | 0.53              |
| 1:G:627:PRO:HG3   | 2:H:90:GLY:HA2    | 1.91                     | 0.53              |
| 1:G:1164:LEU:HB2  | 1:G:1169:LEU:HD21 | 1.91                     | 0.53              |
| 1:M:483:MET:HE2   | 1:M:483:MET:HA    | 1.90                     | 0.53              |
| 1:M:1008:SER:HB3  | 1:M:1017:ARG:HB3  | 1.91                     | 0.53              |
| 1:M:3996:PHE:HD1  | 1:M:4016:LEU:HD11 | 1.73                     | 0.53              |
| 1:S:316:PHE:CE1   | 1:S:348:VAL:HG22  | 2.43                     | 0.53              |
| 1:S:1164:LEU:HB2  | 1:S:1169:LEU:HD21 | 1.91                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:4207:MET:HA   | 1:A:4207:MET:HE2  | 1.91                     | 0.52              |
| 1:A:4899:ASP:OD1  | 1:A:4900:GLU:HG3  | 2.08                     | 0.52              |
| 1:G:60:PRO:HG2    | 1:G:62:LEU:HD11   | 1.90                     | 0.52              |
| 1:G:989:ALA:HA    | 1:G:1039:LEU:CD1  | 2.39                     | 0.52              |
| 1:G:4093:PHE:CZ   | 1:G:4097:MET:HE2  | 2.44                     | 0.52              |
| 1:M:627:PRO:HG3   | 2:N:90:GLY:HA2    | 1.91                     | 0.52              |
| 1:M:1815:LEU:HD22 | 1:M:1845:VAL:HG21 | 1.91                     | 0.52              |
| 1:S:627:PRO:HG3   | 2:T:90:GLY:HA2    | 1.91                     | 0.52              |
| 1:S:1561:VAL:HG23 | 1:S:1562:ILE:H    | 1.74                     | 0.52              |
| 5:S:5104:117:H83  | 5:S:5105:117:C93  | 2.39                     | 0.52              |
| 1:A:110:ARG:HH22  | 1:A:115:ARG:HH21  | 1.55                     | 0.52              |
| 1:A:989:ALA:HA    | 1:A:1039:LEU:CD1  | 2.39                     | 0.52              |
| 1:A:1736:VAL:HG23 | 1:A:1736:VAL:O    | 2.08                     | 0.52              |
| 1:A:3996:PHE:HD1  | 1:A:4016:LEU:HD11 | 1.73                     | 0.52              |
| 1:M:169:LEU:HD12  | 1:M:171:LEU:HD11  | 1.92                     | 0.52              |
| 1:S:1815:LEU:HD22 | 1:S:1845:VAL:HG21 | 1.91                     | 0.52              |
| 1:A:60:PRO:HG2    | 1:A:62:LEU:HD11   | 1.90                     | 0.52              |
| 1:A:1454:THR:OG1  | 1:A:1456:ASP:OD1  | 2.24                     | 0.52              |
| 1:G:52:THR:O      | 1:G:52:THR:CG2    | 2.57                     | 0.52              |
| 1:G:110:ARG:NH2   | 1:G:115:ARG:CZ    | 2.73                     | 0.52              |
| 1:S:419:ASP:OD1   | 1:S:419:ASP:O     | 2.27                     | 0.52              |
| 1:S:483:MET:HA    | 1:S:483:MET:HE2   | 1.90                     | 0.52              |
| 1:S:1008:SER:HB3  | 1:S:1017:ARG:HB3  | 1.91                     | 0.52              |
| 1:A:169:LEU:HD12  | 1:A:171:LEU:HD11  | 1.92                     | 0.52              |
| 1:A:233:ILE:O     | 1:A:257:ARG:NH1   | 2.42                     | 0.52              |
| 1:G:2628:PHE:HZ   | 1:G:2907:PRO:HD3  | 1.74                     | 0.52              |
| 1:G:4207:MET:HE2  | 1:G:4207:MET:HA   | 1.91                     | 0.52              |
| 1:M:1561:VAL:HG23 | 1:M:1562:ILE:H    | 1.74                     | 0.52              |
| 1:S:3130:THR:HA   | 1:S:3133:THR:HG22 | 1.90                     | 0.52              |
| 1:A:110:ARG:NH2   | 1:A:115:ARG:CZ    | 2.73                     | 0.52              |
| 1:G:1008:SER:HB3  | 1:G:1017:ARG:HB3  | 1.91                     | 0.52              |
| 1:G:1561:VAL:HG23 | 1:G:1562:ILE:N    | 2.25                     | 0.52              |
| 1:M:2628:PHE:HZ   | 1:M:2907:PRO:HD3  | 1.74                     | 0.52              |
| 1:S:233:ILE:O     | 1:S:257:ARG:NH1   | 2.42                     | 0.52              |
| 1:S:989:ALA:HA    | 1:S:1039:LEU:CD1  | 2.39                     | 0.52              |
| 1:S:1561:VAL:HG23 | 1:S:1562:ILE:N    | 2.25                     | 0.52              |
| 1:S:4837:LEU:CD1  | 1:S:4932:ILE:HG23 | 2.38                     | 0.52              |
| 1:A:419:ASP:O     | 1:A:419:ASP:OD1   | 2.27                     | 0.52              |
| 1:A:483:MET:HE2   | 1:A:483:MET:HA    | 1.90                     | 0.52              |
| 1:A:4093:PHE:CZ   | 1:A:4097:MET:HE2  | 2.44                     | 0.52              |
| 1:A:4837:LEU:CD1  | 1:A:4932:ILE:HG23 | 2.38                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:M:3545:THR:O    | 1:M:3549:VAL:HG22 | 2.10                     | 0.52              |
| 1:S:52:THR:O      | 1:S:52:THR:CG2    | 2.57                     | 0.52              |
| 1:A:4205:TRP:CH2  | 1:A:4989:MET:CE   | 2.89                     | 0.52              |
| 1:G:169:LEU:HD12  | 1:G:171:LEU:HD11  | 1.92                     | 0.52              |
| 1:G:2670:GLU:OE2  | 1:G:2916:LYS:CE   | 2.55                     | 0.52              |
| 1:G:4791:TYR:OH   | 1:G:4815:ASP:OD1  | 2.28                     | 0.52              |
| 1:S:3545:THR:O    | 1:S:3549:VAL:HG22 | 2.10                     | 0.52              |
| 1:A:1561:VAL:HG23 | 1:A:1562:ILE:N    | 2.25                     | 0.52              |
| 1:M:1024:TYR:HA   | 1:M:1027:LEU:HD12 | 1.92                     | 0.52              |
| 1:S:1024:TYR:HA   | 1:S:1027:LEU:HD12 | 1.92                     | 0.52              |
| 1:G:4207:MET:O    | 1:G:4210:VAL:HG22 | 2.10                     | 0.52              |
| 1:M:989:ALA:CB    | 1:M:1039:LEU:HD12 | 2.35                     | 0.52              |
| 1:A:275:ARG:NH1   | 1:A:338:GLU:OE1   | 2.43                     | 0.52              |
| 1:A:1008:SER:HB3  | 1:A:1017:ARG:HB3  | 1.91                     | 0.52              |
| 1:A:1024:TYR:HA   | 1:A:1027:LEU:HD12 | 1.92                     | 0.52              |
| 1:A:3545:THR:O    | 1:A:3549:VAL:HG22 | 2.10                     | 0.52              |
| 1:G:1024:TYR:HA   | 1:G:1027:LEU:HD12 | 1.92                     | 0.52              |
| 1:S:110:ARG:NH2   | 1:S:115:ARG:CZ    | 2.73                     | 0.52              |
| 1:S:2628:PHE:HZ   | 1:S:2907:PRO:HD3  | 1.74                     | 0.52              |
| 1:S:4220:ASP:C    | 1:S:4220:ASP:OD2  | 2.53                     | 0.52              |
| 1:A:110:ARG:HH22  | 1:A:115:ARG:NH2   | 2.05                     | 0.51              |
| 1:A:4834:GLY:O    | 1:A:4838:VAL:HG23 | 2.10                     | 0.51              |
| 1:G:20:VAL:HG21   | 1:G:202:MET:CG    | 2.38                     | 0.51              |
| 1:G:1815:LEU:HD22 | 1:G:1845:VAL:HG21 | 1.91                     | 0.51              |
| 1:G:4220:ASP:OD2  | 1:G:4220:ASP:C    | 2.53                     | 0.51              |
| 1:A:390:LEU:HD23  | 1:A:390:LEU:H     | 1.75                     | 0.51              |
| 1:A:4207:MET:O    | 1:A:4210:VAL:HG22 | 2.10                     | 0.51              |
| 1:G:1928:GLN:HG3  | 1:G:1928:GLN:O    | 2.10                     | 0.51              |
| 1:G:2970:SER:HA   | 1:G:2973:PHE:CE2  | 2.46                     | 0.51              |
| 1:M:390:LEU:HD23  | 1:M:390:LEU:H     | 1.75                     | 0.51              |
| 1:M:419:ASP:OD1   | 1:M:419:ASP:O     | 2.27                     | 0.51              |
| 1:M:1557:THR:O    | 1:M:1557:THR:HG22 | 2.11                     | 0.51              |
| 1:M:1561:VAL:HG23 | 1:M:1562:ILE:N    | 2.25                     | 0.51              |
| 1:M:3992:PHE:HB3  | 1:M:4023:MET:HE1  | 1.92                     | 0.51              |
| 1:S:4834:GLY:O    | 1:S:4838:VAL:HG23 | 2.10                     | 0.51              |
| 1:A:1815:LEU:HD22 | 1:A:1845:VAL:HG21 | 1.91                     | 0.51              |
| 1:A:2970:SER:HA   | 1:A:2973:PHE:CE2  | 2.46                     | 0.51              |
| 1:M:1164:LEU:HB2  | 1:M:1169:LEU:HD21 | 1.91                     | 0.51              |
| 1:M:4207:MET:HE2  | 1:M:4207:MET:HA   | 1.91                     | 0.51              |
| 1:S:169:LEU:HD12  | 1:S:171:LEU:HD11  | 1.92                     | 0.51              |
| 1:A:2628:PHE:HZ   | 1:A:2907:PRO:HD3  | 1.74                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:G:275:ARG:NH1   | 1:G:338:GLU:OE1   | 2.43                     | 0.51              |
| 1:G:390:LEU:HD23  | 1:G:390:LEU:H     | 1.75                     | 0.51              |
| 1:G:999:ASP:O     | 1:G:1002:ALA:HB3  | 2.11                     | 0.51              |
| 1:M:110:ARG:NH2   | 1:M:115:ARG:CZ    | 2.73                     | 0.51              |
| 1:M:999:ASP:O     | 1:M:1002:ALA:HB3  | 2.11                     | 0.51              |
| 1:M:1426:ILE:HG21 | 1:M:1429:ASN:HD22 | 1.76                     | 0.51              |
| 1:M:1928:GLN:O    | 1:M:1928:GLN:HG3  | 2.10                     | 0.51              |
| 1:M:4791:TYR:OH   | 1:M:4815:ASP:OD1  | 2.28                     | 0.51              |
| 1:S:3052:HIS:O    | 1:S:3127:GLN:NE2  | 2.44                     | 0.51              |
| 1:A:1928:GLN:HG3  | 1:A:1928:GLN:O    | 2.10                     | 0.51              |
| 1:A:3916:ILE:O    | 1:A:3920:VAL:HG23 | 2.11                     | 0.51              |
| 1:M:989:ALA:HA    | 1:M:1039:LEU:CD1  | 2.39                     | 0.51              |
| 1:S:989:ALA:CB    | 1:S:1039:LEU:HD12 | 2.35                     | 0.51              |
| 1:A:1557:THR:O    | 1:A:1557:THR:HG22 | 2.11                     | 0.51              |
| 1:G:233:ILE:O     | 1:G:257:ARG:NH1   | 2.42                     | 0.51              |
| 1:G:1454:THR:OG1  | 1:G:1456:ASP:OD1  | 2.24                     | 0.51              |
| 1:G:1557:THR:HG22 | 1:G:1557:THR:O    | 2.11                     | 0.51              |
| 5:G:5104:117:H83  | 5:G:5105:117:C93  | 2.39                     | 0.51              |
| 1:M:1773:PRO:HA   | 1:M:2153:MET:HE1  | 1.93                     | 0.51              |
| 1:M:4834:GLY:O    | 1:M:4838:VAL:HG23 | 2.10                     | 0.51              |
| 1:S:1557:THR:O    | 1:S:1557:THR:HG22 | 2.11                     | 0.51              |
| 1:S:1773:PRO:HA   | 1:S:2153:MET:HE1  | 1.93                     | 0.51              |
| 1:A:1426:ILE:HG21 | 1:A:1429:ASN:HD22 | 1.76                     | 0.51              |
| 1:M:3916:ILE:O    | 1:M:3920:VAL:HG23 | 2.11                     | 0.51              |
| 1:S:3916:ILE:O    | 1:S:3920:VAL:HG23 | 2.11                     | 0.51              |
| 1:A:3052:HIS:O    | 1:A:3127:GLN:NE2  | 2.44                     | 0.51              |
| 1:A:3078:ARG:NH1  | 1:A:3155:ASP:OD2  | 2.40                     | 0.51              |
| 1:G:3545:THR:O    | 1:G:3549:VAL:HG22 | 2.10                     | 0.51              |
| 1:G:3916:ILE:O    | 1:G:3920:VAL:HG23 | 2.11                     | 0.51              |
| 2:H:106:ASN:OD1   | 2:H:106:ASN:C     | 2.54                     | 0.51              |
| 1:M:3052:HIS:O    | 1:M:3127:GLN:NE2  | 2.44                     | 0.51              |
| 1:S:275:ARG:NH1   | 1:S:338:GLU:OE1   | 2.43                     | 0.51              |
| 1:A:3992:PHE:HB3  | 1:A:4023:MET:HE1  | 1.92                     | 0.51              |
| 1:G:3951:PHE:O    | 1:G:3955:MET:HG3  | 2.11                     | 0.51              |
| 1:M:985:VAL:HG12  | 1:M:1036:ARG:HG3  | 1.93                     | 0.51              |
| 1:S:985:VAL:HG12  | 1:S:1036:ARG:HG3  | 1.93                     | 0.51              |
| 1:A:2355:ARG:NH2  | 1:A:2449:GLU:OE2  | 2.44                     | 0.51              |
| 1:A:4940:PHE:CE2  | 1:A:4944:ARG:HD2  | 2.46                     | 0.51              |
| 1:G:4834:GLY:O    | 1:G:4838:VAL:HG23 | 2.10                     | 0.51              |
| 1:M:233:ILE:O     | 1:M:257:ARG:NH1   | 2.42                     | 0.51              |
| 1:M:275:ARG:NH1   | 1:M:338:GLU:OE1   | 2.43                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:M:3245:VAL:HG12 | 1:M:3246:LEU:N    | 2.26                     | 0.51              |
| 1:S:4207:MET:HE2  | 1:S:4207:MET:HA   | 1.91                     | 0.51              |
| 1:S:4207:MET:O    | 1:S:4210:VAL:HG22 | 2.10                     | 0.51              |
| 1:A:999:ASP:O     | 1:A:1002:ALA:HB3  | 2.11                     | 0.50              |
| 1:S:1928:GLN:HG3  | 1:S:1928:GLN:O    | 2.10                     | 0.50              |
| 2:T:106:ASN:OD1   | 2:T:106:ASN:C     | 2.54                     | 0.50              |
| 1:G:985:VAL:HG12  | 1:G:1036:ARG:HG3  | 1.93                     | 0.50              |
| 1:G:3052:HIS:O    | 1:G:3127:GLN:NE2  | 2.44                     | 0.50              |
| 1:G:3992:PHE:HB3  | 1:G:4023:MET:HE1  | 1.92                     | 0.50              |
| 1:M:2970:SER:HA   | 1:M:2973:PHE:CE2  | 2.46                     | 0.50              |
| 1:A:4160:LEU:O    | 1:A:4164:LEU:HD23 | 2.12                     | 0.50              |
| 1:M:3951:PHE:O    | 1:M:3955:MET:HG3  | 2.11                     | 0.50              |
| 2:N:106:ASN:OD1   | 2:N:106:ASN:C     | 2.54                     | 0.50              |
| 1:S:390:LEU:HD23  | 1:S:390:LEU:H     | 1.75                     | 0.50              |
| 1:S:2970:SER:HA   | 1:S:2973:PHE:CE2  | 2.46                     | 0.50              |
| 1:S:4940:PHE:CE2  | 1:S:4944:ARG:HD2  | 2.46                     | 0.50              |
| 1:S:214:VAL:HG21  | 1:S:390:LEU:HD11  | 1.93                     | 0.50              |
| 1:S:404:ILE:HG21  | 1:S:481:GLU:HG2   | 1.93                     | 0.50              |
| 1:S:3245:VAL:HG12 | 1:S:3246:LEU:N    | 2.26                     | 0.50              |
| 2:B:106:ASN:OD1   | 2:B:106:ASN:C     | 2.54                     | 0.50              |
| 1:G:4160:LEU:O    | 1:G:4164:LEU:HD23 | 2.12                     | 0.50              |
| 1:G:4217:PHE:CE1  | 1:G:4237:PHE:CB   | 2.95                     | 0.50              |
| 1:M:2670:GLU:OE2  | 1:M:2916:LYS:CE   | 2.55                     | 0.50              |
| 1:M:4217:PHE:CE1  | 1:M:4237:PHE:CB   | 2.95                     | 0.50              |
| 1:S:999:ASP:O     | 1:S:1002:ALA:HB3  | 2.11                     | 0.50              |
| 1:A:985:VAL:HG12  | 1:A:1036:ARG:HG3  | 1.93                     | 0.50              |
| 1:A:4791:TYR:OH   | 1:A:4815:ASP:OD1  | 2.28                     | 0.50              |
| 5:A:5104:117:H83  | 5:A:5105:117:C93  | 2.39                     | 0.50              |
| 1:M:31:GLU:O      | 1:M:33:LEU:HD12   | 2.12                     | 0.50              |
| 1:M:4207:MET:O    | 1:M:4210:VAL:HG22 | 2.10                     | 0.50              |
| 1:S:3992:PHE:HB3  | 1:S:4023:MET:HE1  | 1.92                     | 0.50              |
| 1:A:3951:PHE:O    | 1:A:3955:MET:HG3  | 2.11                     | 0.50              |
| 1:A:3077:ALA:HA   | 1:A:3080:VAL:HG12 | 1.94                     | 0.50              |
| 1:A:3245:VAL:HG12 | 1:A:3246:LEU:N    | 2.26                     | 0.50              |
| 1:G:4940:PHE:CE2  | 1:G:4944:ARG:HD2  | 2.46                     | 0.50              |
| 1:M:404:ILE:HG21  | 1:M:481:GLU:HG2   | 1.93                     | 0.50              |
| 1:M:1166:GLY:HA3  | 1:M:1216:ILE:HG21 | 1.94                     | 0.50              |
| 1:A:1773:PRO:HA   | 1:A:2153:MET:HE1  | 1.93                     | 0.50              |
| 1:A:4220:ASP:C    | 1:A:4220:ASP:OD2  | 2.53                     | 0.50              |
| 1:G:989:ALA:CA    | 1:G:1039:LEU:CD1  | 2.90                     | 0.50              |
| 1:G:3007:ASN:O    | 1:G:3011:THR:OG1  | 2.16                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:G:3245:VAL:HG12 | 1:G:3246:LEU:N    | 2.26                     | 0.50              |
| 1:M:4160:LEU:O    | 1:M:4164:LEU:HD23 | 2.12                     | 0.50              |
| 1:M:4940:PHE:CE2  | 1:M:4944:ARG:HD2  | 2.46                     | 0.50              |
| 1:S:509:GLU:O     | 1:S:513:GLU:OE1   | 2.30                     | 0.50              |
| 1:S:1166:GLY:HA3  | 1:S:1216:ILE:HG21 | 1.94                     | 0.50              |
| 1:G:1426:ILE:HG21 | 1:G:1429:ASN:HD22 | 1.76                     | 0.49              |
| 1:S:1426:ILE:HG21 | 1:S:1429:ASN:HD22 | 1.76                     | 0.49              |
| 1:A:404:ILE:HG21  | 1:A:481:GLU:HG2   | 1.93                     | 0.49              |
| 1:A:989:ALA:CA    | 1:A:1039:LEU:CD1  | 2.90                     | 0.49              |
| 1:A:2350:ALA:O    | 1:A:2354:VAL:HG23 | 2.13                     | 0.49              |
| 1:G:1773:PRO:HA   | 1:G:2153:MET:HE1  | 1.93                     | 0.49              |
| 1:G:2355:ARG:NH2  | 1:G:2449:GLU:OE2  | 2.44                     | 0.49              |
| 1:M:214:VAL:HG21  | 1:M:390:LEU:HD11  | 1.93                     | 0.49              |
| 1:M:2355:ARG:NH2  | 1:M:2449:GLU:OE2  | 2.44                     | 0.49              |
| 1:M:4220:ASP:OD2  | 1:M:4220:ASP:C    | 2.53                     | 0.49              |
| 1:A:1166:GLY:HA3  | 1:A:1216:ILE:HG21 | 1.94                     | 0.49              |
| 1:G:2212:VAL:HG22 | 1:G:2256:TYR:HE2  | 1.72                     | 0.49              |
| 1:M:989:ALA:CA    | 1:M:1039:LEU:CD1  | 2.90                     | 0.49              |
| 1:M:1740:PRO:HA   | 1:M:1743:ARG:HG2  | 1.95                     | 0.49              |
| 1:M:4204:GLN:HB3  | 1:M:4245:MET:HE2  | 1.94                     | 0.49              |
| 1:S:4791:TYR:OH   | 1:S:4815:ASP:OD1  | 2.28                     | 0.49              |
| 1:G:3708:THR:O    | 1:G:3711:THR:HG22 | 2.13                     | 0.49              |
| 1:S:3951:PHE:O    | 1:S:3955:MET:HG3  | 2.11                     | 0.49              |
| 1:A:509:GLU:O     | 1:A:513:GLU:OE1   | 2.30                     | 0.49              |
| 1:G:1166:GLY:HA3  | 1:G:1216:ILE:HG21 | 1.94                     | 0.49              |
| 1:G:2123:LEU:O    | 1:G:2127:GLN:HG2  | 2.13                     | 0.49              |
| 1:M:3708:THR:O    | 1:M:3711:THR:HG22 | 2.13                     | 0.49              |
| 1:S:4217:PHE:CE1  | 1:S:4237:PHE:CB   | 2.95                     | 0.49              |
| 1:A:3708:THR:O    | 1:A:3711:THR:HG22 | 2.13                     | 0.49              |
| 1:M:1454:THR:OG1  | 1:M:1456:ASP:OD1  | 2.24                     | 0.49              |
| 1:M:2159:LEU:HD21 | 1:M:2163:ARG:CZ   | 2.43                     | 0.49              |
| 1:G:404:ILE:HG21  | 1:G:481:GLU:HG2   | 1.93                     | 0.49              |
| 1:G:4823:LEU:O    | 1:G:4827:LEU:HD13 | 2.13                     | 0.49              |
| 1:S:31:GLU:O      | 1:S:33:LEU:HD12   | 2.12                     | 0.49              |
| 1:A:214:VAL:HG21  | 1:A:390:LEU:HD11  | 1.93                     | 0.49              |
| 1:A:1105:ALA:HB2  | 1:A:1191:VAL:HG21 | 1.95                     | 0.49              |
| 1:A:4217:PHE:CE1  | 1:A:4237:PHE:CB   | 2.95                     | 0.49              |
| 1:G:3077:ALA:HA   | 1:G:3080:VAL:HG12 | 1.94                     | 0.49              |
| 1:M:509:GLU:O     | 1:M:513:GLU:OE1   | 2.30                     | 0.49              |
| 1:M:2123:LEU:O    | 1:M:2127:GLN:HG2  | 2.13                     | 0.49              |
| 1:M:3322:ILE:O    | 1:M:3326:ASN:ND2  | 2.44                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:M:5105:117:H922 | 5:M:5105:117:N2   | 2.28                     | 0.49              |
| 1:S:989:ALA:CA    | 1:S:1039:LEU:CD1  | 2.90                     | 0.49              |
| 1:S:1105:ALA:HB2  | 1:S:1191:VAL:HG21 | 1.95                     | 0.49              |
| 1:S:2355:ARG:NH2  | 1:S:2449:GLU:OE2  | 2.44                     | 0.49              |
| 1:G:1740:PRO:HA   | 1:G:1743:ARG:HG2  | 1.95                     | 0.49              |
| 1:G:2350:ALA:O    | 1:G:2354:VAL:HG23 | 2.13                     | 0.49              |
| 5:G:5105:117:N2   | 5:G:5105:117:H922 | 2.28                     | 0.49              |
| 1:M:2292:GLU:O    | 1:M:2296:GLU:HG3  | 2.13                     | 0.49              |
| 1:M:2628:PHE:CZ   | 1:M:2907:PRO:HD3  | 2.48                     | 0.49              |
| 1:S:110:ARG:HH22  | 1:S:115:ARG:NH2   | 2.05                     | 0.49              |
| 1:S:3077:ALA:HA   | 1:S:3080:VAL:HG12 | 1.94                     | 0.49              |
| 1:S:4160:LEU:O    | 1:S:4164:LEU:HD23 | 2.12                     | 0.49              |
| 1:G:214:VAL:HG21  | 1:G:390:LEU:HD11  | 1.93                     | 0.49              |
| 1:G:4204:GLN:HB3  | 1:G:4245:MET:HE2  | 1.94                     | 0.49              |
| 1:S:2350:ALA:O    | 1:S:2354:VAL:HG23 | 2.13                     | 0.49              |
| 1:S:4204:GLN:HB3  | 1:S:4245:MET:HE2  | 1.94                     | 0.49              |
| 1:A:31:GLU:O      | 1:A:33:LEU:HD12   | 2.12                     | 0.48              |
| 1:A:2159:LEU:HD21 | 1:A:2163:ARG:CZ   | 2.43                     | 0.48              |
| 1:G:282:ILE:HD11  | 1:G:291:LEU:HD23  | 1.95                     | 0.48              |
| 1:M:990:GLU:HA    | 1:M:1024:TYR:CD1  | 2.48                     | 0.48              |
| 1:S:2159:LEU:HD21 | 1:S:2163:ARG:CZ   | 2.43                     | 0.48              |
| 1:S:3708:THR:O    | 1:S:3711:THR:HG22 | 2.13                     | 0.48              |
| 2:T:53:LYS:C      | 2:T:54:GLN:OE1    | 2.56                     | 0.48              |
| 1:A:495:ASN:OD1   | 1:A:553:ARG:CZ    | 2.61                     | 0.48              |
| 1:A:2292:GLU:O    | 1:A:2296:GLU:HG3  | 2.13                     | 0.48              |
| 1:G:31:GLU:O      | 1:G:33:LEU:HD12   | 2.12                     | 0.48              |
| 1:G:509:GLU:O     | 1:G:513:GLU:OE1   | 2.30                     | 0.48              |
| 1:G:2292:GLU:O    | 1:G:2296:GLU:HG3  | 2.13                     | 0.48              |
| 2:H:53:LYS:C      | 2:H:54:GLN:OE1    | 2.56                     | 0.48              |
| 1:M:1101:ARG:NH1  | 1:M:1115:LEU:O    | 2.46                     | 0.48              |
| 1:M:2350:ALA:O    | 1:M:2354:VAL:HG23 | 2.13                     | 0.48              |
| 1:M:4823:LEU:O    | 1:M:4827:LEU:HD13 | 2.13                     | 0.48              |
| 5:S:5105:117:H922 | 5:S:5105:117:N2   | 2.28                     | 0.48              |
| 1:A:274:LEU:HD22  | 1:A:280:LEU:HD11  | 1.96                     | 0.48              |
| 1:A:4204:GLN:HB3  | 1:A:4245:MET:HE2  | 1.94                     | 0.48              |
| 5:A:5105:117:H922 | 5:A:5105:117:N2   | 2.28                     | 0.48              |
| 2:B:53:LYS:C      | 2:B:54:GLN:OE1    | 2.56                     | 0.48              |
| 1:M:1105:ALA:HB2  | 1:M:1191:VAL:HG21 | 1.95                     | 0.48              |
| 1:S:2628:PHE:CZ   | 1:S:2907:PRO:HD3  | 2.48                     | 0.48              |
| 1:A:2124:LEU:HD11 | 1:A:2128:TYR:HE1  | 1.79                     | 0.48              |
| 1:G:688:LEU:HD23  | 1:G:690:GLU:H     | 1.79                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:G:1252:HIS:O    | 1:G:1275:ARG:NH1  | 2.47                     | 0.48              |
| 1:G:3249:LEU:O    | 1:G:3253:ILE:HD12 | 2.14                     | 0.48              |
| 1:G:3456:GLN:O    | 1:G:3460:VAL:HG22 | 2.14                     | 0.48              |
| 1:M:2124:LEU:HD11 | 1:M:2128:TYR:HE1  | 1.79                     | 0.48              |
| 1:M:3768:SER:HA   | 1:M:3771:HIS:CD2  | 2.49                     | 0.48              |
| 1:S:495:ASN:OD1   | 1:S:553:ARG:CZ    | 2.61                     | 0.48              |
| 1:S:990:GLU:HA    | 1:S:1024:TYR:CD1  | 2.48                     | 0.48              |
| 1:S:2292:GLU:O    | 1:S:2296:GLU:HG3  | 2.13                     | 0.48              |
| 1:G:274:LEU:HD22  | 1:G:280:LEU:HD11  | 1.96                     | 0.48              |
| 1:G:3768:SER:HA   | 1:G:3771:HIS:CD2  | 2.49                     | 0.48              |
| 2:B:6:GLU:N       | 2:B:6:GLU:OE2     | 2.47                     | 0.48              |
| 1:G:2159:LEU:HD21 | 1:G:2163:ARG:CZ   | 2.43                     | 0.48              |
| 1:M:3249:LEU:O    | 1:M:3253:ILE:HD12 | 2.14                     | 0.48              |
| 1:M:3456:GLN:O    | 1:M:3460:VAL:HG22 | 2.14                     | 0.48              |
| 1:M:4860:ARG:HH12 | 1:S:4629:TYR:HH   | 1.54                     | 0.48              |
| 1:A:264:PRO:HA    | 1:A:280:LEU:HD23  | 1.96                     | 0.48              |
| 1:A:282:ILE:HD11  | 1:A:291:LEU:HD23  | 1.95                     | 0.48              |
| 1:A:2628:PHE:CZ   | 1:A:2907:PRO:HD3  | 2.48                     | 0.48              |
| 1:A:3336:LYS:O    | 1:A:3340:VAL:HG13 | 2.13                     | 0.48              |
| 1:G:264:PRO:HA    | 1:G:280:LEU:HD23  | 1.96                     | 0.48              |
| 1:G:495:ASN:OD1   | 1:G:553:ARG:CZ    | 2.61                     | 0.48              |
| 1:G:990:GLU:HA    | 1:G:1024:TYR:CD1  | 2.48                     | 0.48              |
| 1:G:3336:LYS:O    | 1:G:3340:VAL:HG13 | 2.13                     | 0.48              |
| 1:M:3077:ALA:HA   | 1:M:3080:VAL:HG12 | 1.94                     | 0.48              |
| 1:S:2123:LEU:O    | 1:S:2127:GLN:HG2  | 2.13                     | 0.48              |
| 1:A:2123:LEU:O    | 1:A:2127:GLN:HG2  | 2.13                     | 0.48              |
| 2:N:6:GLU:N       | 2:N:6:GLU:OE2     | 2.47                     | 0.48              |
| 2:N:53:LYS:C      | 2:N:54:GLN:OE1    | 2.56                     | 0.48              |
| 1:S:3183:VAL:O    | 1:S:3187:ARG:HG3  | 2.14                     | 0.48              |
| 1:S:3249:LEU:O    | 1:S:3253:ILE:HD12 | 2.14                     | 0.48              |
| 1:A:1740:PRO:HA   | 1:A:1743:ARG:HG2  | 1.95                     | 0.48              |
| 1:A:3183:VAL:O    | 1:A:3187:ARG:HG3  | 2.14                     | 0.48              |
| 1:A:3456:GLN:O    | 1:A:3460:VAL:HG22 | 2.14                     | 0.48              |
| 1:M:1252:HIS:O    | 1:M:1275:ARG:NH1  | 2.47                     | 0.48              |
| 1:S:4823:LEU:O    | 1:S:4827:LEU:HD13 | 2.13                     | 0.48              |
| 1:A:990:GLU:HA    | 1:A:1024:TYR:CD1  | 2.48                     | 0.48              |
| 2:H:6:GLU:N       | 2:H:6:GLU:OE2     | 2.47                     | 0.48              |
| 1:S:3546:ASP:O    | 1:S:3597:GLN:NE2  | 2.47                     | 0.48              |
| 1:S:3768:SER:HA   | 1:S:3771:HIS:CD2  | 2.49                     | 0.48              |
| 1:A:1251:GLU:N    | 1:A:1251:GLU:OE1  | 2.46                     | 0.47              |
| 1:A:3768:SER:HA   | 1:A:3771:HIS:CD2  | 2.49                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:4823:LEU:O    | 1:A:4827:LEU:HD13 | 2.13                     | 0.47              |
| 1:G:3546:ASP:O    | 1:G:3597:GLN:NE2  | 2.47                     | 0.47              |
| 1:M:282:ILE:HD11  | 1:M:291:LEU:HD23  | 1.95                     | 0.47              |
| 1:M:1219:LEU:HD11 | 1:S:3575:LEU:HD13 | 1.96                     | 0.47              |
| 1:M:3183:VAL:O    | 1:M:3187:ARG:HG3  | 2.14                     | 0.47              |
| 1:A:688:LEU:HD23  | 1:A:690:GLU:H     | 1.79                     | 0.47              |
| 1:G:1105:ALA:HB2  | 1:G:1191:VAL:HG21 | 1.95                     | 0.47              |
| 1:G:1263:THR:HG22 | 1:G:1264:VAL:N    | 2.30                     | 0.47              |
| 1:G:3440:GLU:HA   | 1:G:3443:ILE:HG12 | 1.96                     | 0.47              |
| 1:M:495:ASN:OD1   | 1:M:553:ARG:CZ    | 2.61                     | 0.47              |
| 1:M:688:LEU:HD23  | 1:M:690:GLU:H     | 1.79                     | 0.47              |
| 1:S:274:LEU:HD22  | 1:S:280:LEU:HD11  | 1.96                     | 0.47              |
| 1:S:3440:GLU:HA   | 1:S:3443:ILE:HG12 | 1.96                     | 0.47              |
| 2:T:6:GLU:N       | 2:T:6:GLU:OE2     | 2.47                     | 0.47              |
| 1:A:1727:ARG:NH2  | 1:A:1773:PRO:O    | 2.47                     | 0.47              |
| 1:A:2294:ASP:O    | 1:A:2298:VAL:HG23 | 2.15                     | 0.47              |
| 1:G:1251:GLU:OE1  | 1:G:1251:GLU:N    | 2.46                     | 0.47              |
| 1:G:2628:PHE:CZ   | 1:G:2907:PRO:HD3  | 2.48                     | 0.47              |
| 1:M:1251:GLU:OE1  | 1:M:1251:GLU:N    | 2.46                     | 0.47              |
| 1:M:3440:GLU:HA   | 1:M:3443:ILE:HG12 | 1.96                     | 0.47              |
| 1:S:688:LEU:HD23  | 1:S:690:GLU:H     | 1.79                     | 0.47              |
| 1:G:977:LEU:HD11  | 1:G:1040:CYS:SG   | 2.55                     | 0.47              |
| 1:M:2294:ASP:O    | 1:M:2298:VAL:HG23 | 2.15                     | 0.47              |
| 1:M:3336:LYS:O    | 1:M:3340:VAL:HG13 | 2.13                     | 0.47              |
| 1:S:1251:GLU:OE1  | 1:S:1251:GLU:N    | 2.46                     | 0.47              |
| 1:S:2650:ARG:NH1  | 1:S:2651:CYS:SG   | 2.88                     | 0.47              |
| 1:A:1252:HIS:O    | 1:A:1275:ARG:NH1  | 2.47                     | 0.47              |
| 1:A:3440:GLU:HA   | 1:A:3443:ILE:HG12 | 1.96                     | 0.47              |
| 1:G:2650:ARG:NH1  | 1:G:2651:CYS:SG   | 2.88                     | 0.47              |
| 1:S:282:ILE:HD11  | 1:S:291:LEU:HD23  | 1.95                     | 0.47              |
| 1:S:3336:LYS:O    | 1:S:3340:VAL:HG13 | 2.13                     | 0.47              |
| 1:S:4740:LEU:HD23 | 1:S:4741:LEU:HD23 | 1.96                     | 0.47              |
| 1:A:1727:ARG:O    | 1:A:1731:LEU:HG   | 2.15                     | 0.47              |
| 1:A:3322:ILE:O    | 1:A:3326:ASN:ND2  | 2.44                     | 0.47              |
| 1:G:1727:ARG:NH2  | 1:G:1773:PRO:O    | 2.47                     | 0.47              |
| 1:G:2124:LEU:HD11 | 1:G:2128:TYR:HE1  | 1.79                     | 0.47              |
| 1:M:274:LEU:HD22  | 1:M:280:LEU:HD11  | 1.96                     | 0.47              |
| 1:M:977:LEU:HD11  | 1:M:1040:CYS:SG   | 2.55                     | 0.47              |
| 1:M:2650:ARG:NH1  | 1:M:2651:CYS:SG   | 2.88                     | 0.47              |
| 1:M:3169:LEU:HD21 | 1:M:3197:LEU:CD2  | 2.45                     | 0.47              |
| 1:M:3546:ASP:O    | 1:M:3597:GLN:NE2  | 2.47                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:S:1740:PRO:HA   | 1:S:1743:ARG:HG2  | 1.95                     | 0.47              |
| 1:S:2294:ASP:O    | 1:S:2298:VAL:HG23 | 2.15                     | 0.47              |
| 1:S:3106:MET:HA   | 1:S:3109:ASN:ND2  | 2.30                     | 0.47              |
| 1:A:2650:ARG:NH1  | 1:A:2651:CYS:SG   | 2.88                     | 0.47              |
| 1:A:3249:LEU:O    | 1:A:3253:ILE:HD12 | 2.14                     | 0.47              |
| 1:A:3546:ASP:O    | 1:A:3597:GLN:NE2  | 2.47                     | 0.47              |
| 1:G:1969:LEU:C    | 1:G:1969:LEU:HD23 | 2.40                     | 0.47              |
| 1:G:3183:VAL:O    | 1:G:3187:ARG:HG3  | 2.14                     | 0.47              |
| 1:G:3322:ILE:O    | 1:G:3326:ASN:ND2  | 2.44                     | 0.47              |
| 1:M:264:PRO:HA    | 1:M:280:LEU:HD23  | 1.96                     | 0.47              |
| 1:M:488:LEU:O     | 1:M:492:ASP:OD2   | 2.33                     | 0.47              |
| 1:M:600:LEU:CD2   | 1:M:1669:LEU:HD22 | 2.45                     | 0.47              |
| 1:M:1727:ARG:O    | 1:M:1731:LEU:HG   | 2.15                     | 0.47              |
| 1:M:4740:LEU:HD23 | 1:M:4741:LEU:HD23 | 1.96                     | 0.47              |
| 1:S:1252:HIS:O    | 1:S:1275:ARG:NH1  | 2.47                     | 0.47              |
| 1:A:1263:THR:HG22 | 1:A:1264:VAL:N    | 2.30                     | 0.47              |
| 1:A:2644:LEU:HD13 | 1:A:2678:LEU:HD21 | 1.96                     | 0.47              |
| 1:A:3106:MET:HA   | 1:A:3109:ASN:ND2  | 2.30                     | 0.47              |
| 1:G:488:LEU:O     | 1:G:492:ASP:OD2   | 2.33                     | 0.47              |
| 1:S:600:LEU:CD2   | 1:S:1669:LEU:HD22 | 2.45                     | 0.47              |
| 1:S:3456:GLN:O    | 1:S:3460:VAL:HG22 | 2.14                     | 0.47              |
| 1:A:977:LEU:HD11  | 1:A:1040:CYS:SG   | 2.55                     | 0.47              |
| 1:A:2251:PHE:CG   | 1:A:2286:LEU:HD23 | 2.50                     | 0.47              |
| 1:G:3169:LEU:HD21 | 1:G:3197:LEU:CD2  | 2.45                     | 0.47              |
| 1:M:1164:LEU:CB   | 1:M:1169:LEU:HD21 | 2.45                     | 0.47              |
| 1:M:2644:LEU:HD13 | 1:M:2678:LEU:HD21 | 1.96                     | 0.47              |
| 1:M:609:CYS:O     | 1:M:612:VAL:HG22  | 2.15                     | 0.47              |
| 1:M:2862:LEU:HD11 | 1:M:2932:MET:HE1  | 1.97                     | 0.47              |
| 1:S:264:PRO:HA    | 1:S:280:LEU:HD23  | 1.96                     | 0.47              |
| 1:S:488:LEU:O     | 1:S:492:ASP:OD2   | 2.33                     | 0.47              |
| 1:S:1727:ARG:O    | 1:S:1731:LEU:HG   | 2.15                     | 0.47              |
| 1:S:2124:LEU:HD11 | 1:S:2128:TYR:HE1  | 1.79                     | 0.47              |
| 1:A:1969:LEU:HD23 | 1:A:1969:LEU:C    | 2.40                     | 0.46              |
| 1:A:2624:ARG:NH1  | 1:A:2906:VAL:HG11 | 2.31                     | 0.46              |
| 1:G:609:CYS:O     | 1:G:612:VAL:HG22  | 2.15                     | 0.46              |
| 1:G:1101:ARG:NH1  | 1:G:1115:LEU:O    | 2.46                     | 0.46              |
| 1:G:1164:LEU:CB   | 1:G:1169:LEU:HD21 | 2.45                     | 0.46              |
| 1:G:3106:MET:HA   | 1:G:3109:ASN:ND2  | 2.30                     | 0.46              |
| 1:M:3106:MET:HA   | 1:M:3109:ASN:ND2  | 2.30                     | 0.46              |
| 1:S:2644:LEU:HD13 | 1:S:2678:LEU:HD21 | 1.96                     | 0.46              |
| 1:A:609:CYS:O     | 1:A:612:VAL:HG22  | 2.15                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:M:2624:ARG:NH1  | 1:M:2906:VAL:HG11 | 2.31                     | 0.46              |
| 1:M:3256:LEU:HB3  | 1:M:3266:MET:SD   | 2.56                     | 0.46              |
| 1:S:489:ASN:O     | 1:S:493:ARG:HG2   | 2.15                     | 0.46              |
| 1:S:3256:LEU:HB3  | 1:S:3266:MET:SD   | 2.56                     | 0.46              |
| 1:S:3322:ILE:O    | 1:S:3326:ASN:ND2  | 2.44                     | 0.46              |
| 1:A:3169:LEU:HD21 | 1:A:3197:LEU:CD2  | 2.45                     | 0.46              |
| 1:A:3521:GLY:HA2  | 1:A:3524:MET:HE2  | 1.97                     | 0.46              |
| 1:G:2251:PHE:CG   | 1:G:2286:LEU:HD23 | 2.50                     | 0.46              |
| 1:G:2644:LEU:HD13 | 1:G:2678:LEU:HD21 | 1.96                     | 0.46              |
| 1:S:1164:LEU:CB   | 1:S:1169:LEU:HD21 | 2.45                     | 0.46              |
| 1:S:1969:LEU:HD23 | 1:S:1969:LEU:C    | 2.40                     | 0.46              |
| 1:S:2251:PHE:CG   | 1:S:2286:LEU:HD23 | 2.50                     | 0.46              |
| 1:A:1101:ARG:NH1  | 1:A:1115:LEU:O    | 2.46                     | 0.46              |
| 1:A:4740:LEU:HD23 | 1:A:4741:LEU:HD23 | 1.96                     | 0.46              |
| 1:M:1727:ARG:NH2  | 1:M:1773:PRO:O    | 2.47                     | 0.46              |
| 1:M:2897:LYS:O    | 1:M:2897:LYS:HG2  | 2.16                     | 0.46              |
| 1:S:609:CYS:O     | 1:S:612:VAL:HG22  | 2.15                     | 0.46              |
| 1:S:992:GLY:O     | 1:S:995:VAL:HG12  | 2.16                     | 0.46              |
| 1:S:3169:LEU:HD21 | 1:S:3197:LEU:CD2  | 2.45                     | 0.46              |
| 1:A:3521:GLY:O    | 1:A:3524:MET:HG2  | 2.16                     | 0.46              |
| 1:S:2624:ARG:NH1  | 1:S:2906:VAL:HG11 | 2.31                     | 0.46              |
| 1:A:488:LEU:O     | 1:A:492:ASP:OD2   | 2.33                     | 0.46              |
| 1:G:2330:ARG:O    | 1:G:2333:ASP:OD1  | 2.34                     | 0.46              |
| 1:G:2624:ARG:NH1  | 1:G:2906:VAL:HG11 | 2.31                     | 0.46              |
| 1:G:4838:VAL:O    | 5:M:5103:117:H20  | 2.16                     | 0.46              |
| 1:M:489:ASN:O     | 1:M:493:ARG:HG2   | 2.15                     | 0.46              |
| 1:M:683:ARG:NE    | 1:M:707:VAL:O     | 2.48                     | 0.46              |
| 1:S:977:LEU:HD11  | 1:S:1040:CYS:SG   | 2.55                     | 0.46              |
| 1:A:600:LEU:CD2   | 1:A:1669:LEU:HD22 | 2.45                     | 0.46              |
| 1:A:992:GLY:O     | 1:A:995:VAL:HG12  | 2.16                     | 0.46              |
| 1:A:1464:PHE:O    | 1:A:1465:ASP:OD1  | 2.34                     | 0.46              |
| 1:A:2348:GLU:O    | 1:A:2352:VAL:HG23 | 2.16                     | 0.46              |
| 1:A:2825:LYS:HE3  | 1:A:2827:ARG:O    | 2.16                     | 0.46              |
| 1:A:3256:LEU:HB3  | 1:A:3266:MET:SD   | 2.56                     | 0.46              |
| 1:A:4217:PHE:CZ   | 1:A:4234:PHE:HA   | 2.51                     | 0.46              |
| 1:G:489:ASN:O     | 1:G:493:ARG:HG2   | 2.15                     | 0.46              |
| 1:G:600:LEU:CD2   | 1:G:1669:LEU:HD22 | 2.45                     | 0.46              |
| 1:G:2897:LYS:O    | 1:G:2897:LYS:HG2  | 2.16                     | 0.46              |
| 1:M:3521:GLY:O    | 1:M:3524:MET:HG2  | 2.16                     | 0.46              |
| 1:S:1727:ARG:NH2  | 1:S:1773:PRO:O    | 2.47                     | 0.46              |
| 1:S:2330:ARG:O    | 1:S:2333:ASP:OD1  | 2.34                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:489:ASN:O     | 1:A:493:ARG:HG2   | 2.15                     | 0.46              |
| 1:G:1464:PHE:O    | 1:G:1465:ASP:OD1  | 2.34                     | 0.46              |
| 1:G:2294:ASP:O    | 1:G:2298:VAL:HG23 | 2.15                     | 0.46              |
| 1:G:3256:LEU:HB3  | 1:G:3266:MET:SD   | 2.56                     | 0.46              |
| 1:G:4740:LEU:HD23 | 1:G:4741:LEU:HD23 | 1.96                     | 0.46              |
| 1:A:387:ALA:C     | 1:A:388:LEU:HD22  | 2.41                     | 0.46              |
| 1:A:1164:LEU:CB   | 1:A:1169:LEU:HD21 | 2.45                     | 0.46              |
| 1:A:4952:GLU:OE1  | 1:A:4952:GLU:HA   | 2.16                     | 0.46              |
| 5:A:5103:117:H20  | 1:S:4838:VAL:O    | 2.16                     | 0.46              |
| 1:G:1727:ARG:O    | 1:G:1731:LEU:HG   | 2.15                     | 0.46              |
| 1:G:4222:VAL:HG12 | 1:G:4950:VAL:HG11 | 1.98                     | 0.46              |
| 1:M:2330:ARG:O    | 1:M:2333:ASP:OD1  | 2.34                     | 0.46              |
| 1:A:150:MET:SD    | 1:A:150:MET:N     | 2.81                     | 0.46              |
| 1:A:4567:LEU:HD22 | 5:A:5104:117:C85  | 2.46                     | 0.46              |
| 1:G:387:ALA:C     | 1:G:388:LEU:HD22  | 2.41                     | 0.46              |
| 1:G:1087:ARG:HG2  | 1:G:1154:ASP:CG   | 2.41                     | 0.46              |
| 1:G:2862:LEU:HD11 | 1:G:2932:MET:HE1  | 1.97                     | 0.46              |
| 1:M:3521:GLY:HA2  | 1:M:3524:MET:HE2  | 1.97                     | 0.46              |
| 1:M:4838:VAL:O    | 5:S:5103:117:H20  | 2.16                     | 0.46              |
| 1:G:992:GLY:O     | 1:G:995:VAL:HG12  | 2.16                     | 0.45              |
| 1:M:2825:LYS:HE3  | 1:M:2827:ARG:O    | 2.16                     | 0.45              |
| 1:M:4217:PHE:CZ   | 1:M:4234:PHE:HA   | 2.51                     | 0.45              |
| 1:M:4222:VAL:HG12 | 1:M:4950:VAL:HG11 | 1.98                     | 0.45              |
| 1:S:62:LEU:HD12   | 1:S:62:LEU:N      | 2.31                     | 0.45              |
| 1:S:4217:PHE:CZ   | 1:S:4234:PHE:HA   | 2.51                     | 0.45              |
| 1:S:4567:LEU:HD22 | 5:S:5104:117:C85  | 2.46                     | 0.45              |
| 1:S:4952:GLU:OE1  | 1:S:4952:GLU:HA   | 2.16                     | 0.45              |
| 1:A:1087:ARG:HG2  | 1:A:1154:ASP:CG   | 2.41                     | 0.45              |
| 1:A:4780:PHE:O    | 1:A:4784:PHE:HD1  | 1.99                     | 0.45              |
| 1:G:4780:PHE:O    | 1:G:4784:PHE:HD1  | 1.99                     | 0.45              |
| 1:M:62:LEU:N      | 1:M:62:LEU:HD12   | 2.31                     | 0.45              |
| 1:M:387:ALA:C     | 1:M:388:LEU:HD22  | 2.41                     | 0.45              |
| 1:M:1464:PHE:O    | 1:M:1465:ASP:OD1  | 2.34                     | 0.45              |
| 1:S:387:ALA:C     | 1:S:388:LEU:HD22  | 2.41                     | 0.45              |
| 1:S:989:ALA:HA    | 1:S:1039:LEU:HD11 | 1.99                     | 0.45              |
| 1:S:1263:THR:HG22 | 1:S:1264:VAL:N    | 2.30                     | 0.45              |
| 1:A:2330:ARG:O    | 1:A:2333:ASP:OD1  | 2.34                     | 0.45              |
| 1:M:989:ALA:HA    | 1:M:1039:LEU:HD11 | 1.99                     | 0.45              |
| 1:M:992:GLY:O     | 1:M:995:VAL:HG12  | 2.16                     | 0.45              |
| 1:M:1087:ARG:HG2  | 1:M:1154:ASP:CG   | 2.41                     | 0.45              |
| 1:M:1969:LEU:HD23 | 1:M:1969:LEU:C    | 2.40                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:62:LEU:HD12   | 1:A:62:LEU:N      | 2.31                     | 0.45              |
| 1:A:989:ALA:HA    | 1:A:1039:LEU:HD11 | 1.99                     | 0.45              |
| 1:A:2822:THR:OG1  | 1:A:2938:THR:OG1  | 2.35                     | 0.45              |
| 1:G:572:PRO:HA    | 1:G:575:LEU:HD13  | 1.98                     | 0.45              |
| 1:G:2348:GLU:O    | 1:G:2352:VAL:HG23 | 2.16                     | 0.45              |
| 1:M:2251:PHE:CG   | 1:M:2286:LEU:HD23 | 2.50                     | 0.45              |
| 1:M:2348:GLU:O    | 1:M:2352:VAL:HG23 | 2.16                     | 0.45              |
| 1:M:2822:THR:OG1  | 1:M:2938:THR:OG1  | 2.35                     | 0.45              |
| 1:G:4817:ALA:O    | 1:G:4823:LEU:HB3  | 2.17                     | 0.45              |
| 1:M:2271:THR:OG1  | 1:M:2274:ASP:OD2  | 2.34                     | 0.45              |
| 1:M:2624:ARG:HH11 | 1:M:2906:VAL:HG11 | 1.82                     | 0.45              |
| 1:M:4952:GLU:OE1  | 1:M:4952:GLU:HA   | 2.16                     | 0.45              |
| 1:S:414:PHE:CE1   | 1:S:436:LEU:HD22  | 2.52                     | 0.45              |
| 1:S:1087:ARG:HG2  | 1:S:1154:ASP:CG   | 2.41                     | 0.45              |
| 1:S:3957:VAL:O    | 1:S:3961:VAL:HG23 | 2.17                     | 0.45              |
| 1:A:414:PHE:CE1   | 1:A:436:LEU:HD22  | 2.52                     | 0.45              |
| 1:A:3957:VAL:O    | 1:A:3961:VAL:HG23 | 2.17                     | 0.45              |
| 1:A:4134:GLU:HB2  | 1:A:4135:PRO:HD3  | 1.99                     | 0.45              |
| 1:A:4716:TRP:CH2  | 3:A:5101:CFF:H142 | 2.52                     | 0.45              |
| 1:G:414:PHE:CE1   | 1:G:436:LEU:HD22  | 2.52                     | 0.45              |
| 1:G:4134:GLU:HB2  | 1:G:4135:PRO:HD3  | 1.99                     | 0.45              |
| 1:G:4217:PHE:CZ   | 1:G:4234:PHE:HA   | 2.51                     | 0.45              |
| 1:M:414:PHE:CE1   | 1:M:436:LEU:HD22  | 2.52                     | 0.45              |
| 1:M:2009:LEU:HG   | 1:M:2023:LEU:HD21 | 1.99                     | 0.45              |
| 1:M:2159:LEU:HD12 | 1:M:2203:MET:HE2  | 1.99                     | 0.45              |
| 1:M:3080:VAL:O    | 1:M:3084:GLY:HA3  | 2.17                     | 0.45              |
| 1:S:1464:PHE:O    | 1:S:1465:ASP:OD1  | 2.34                     | 0.45              |
| 1:S:1819:VAL:HG22 | 1:S:1926:LEU:HD13 | 1.98                     | 0.45              |
| 1:S:2271:THR:OG1  | 1:S:2274:ASP:OD2  | 2.34                     | 0.45              |
| 1:A:928:THR:HG23  | 1:A:988:LEU:HD21  | 1.98                     | 0.45              |
| 1:A:4838:VAL:O    | 5:G:5103:117:H20  | 2.16                     | 0.45              |
| 1:G:1478:ASP:OD1  | 1:G:1482:ASN:N    | 2.50                     | 0.45              |
| 1:G:3521:GLY:HA2  | 1:G:3524:MET:HE2  | 1.97                     | 0.45              |
| 1:G:3521:GLY:O    | 1:G:3524:MET:HG2  | 2.16                     | 0.45              |
| 1:M:4716:TRP:CH2  | 3:M:5101:CFF:H142 | 2.52                     | 0.45              |
| 1:S:231:LEU:HD11  | 1:S:245:VAL:HG12  | 1.99                     | 0.45              |
| 1:S:2009:LEU:HG   | 1:S:2023:LEU:HD21 | 1.99                     | 0.45              |
| 1:S:2159:LEU:HD12 | 1:S:2203:MET:HE2  | 1.99                     | 0.45              |
| 1:S:2348:GLU:O    | 1:S:2352:VAL:HG23 | 2.16                     | 0.45              |
| 1:S:2825:LYS:HE3  | 1:S:2827:ARG:O    | 2.16                     | 0.45              |
| 1:S:2897:LYS:O    | 1:S:2897:LYS:HG2  | 2.16                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:S:3521:GLY:O    | 1:S:3524:MET:HG2  | 2.16                     | 0.45              |
| 1:A:2897:LYS:HG2  | 1:A:2897:LYS:O    | 2.16                     | 0.45              |
| 1:G:62:LEU:N      | 1:G:62:LEU:HD12   | 2.31                     | 0.45              |
| 1:M:2151:ASP:OD2  | 1:M:2189:LYS:NZ   | 2.41                     | 0.45              |
| 1:M:2630:VAL:N    | 1:M:2631:PRO:HD2  | 2.32                     | 0.45              |
| 1:M:4567:LEU:HD22 | 5:M:5104:117:C85  | 2.46                     | 0.45              |
| 1:M:4817:ALA:O    | 1:M:4823:LEU:HB3  | 2.17                     | 0.45              |
| 1:S:2624:ARG:HH11 | 1:S:2906:VAL:HG11 | 1.82                     | 0.45              |
| 1:S:2862:LEU:HD11 | 1:S:2932:MET:HE1  | 1.97                     | 0.45              |
| 1:S:3085:PRO:HD2  | 1:S:3088:VAL:HG21 | 1.99                     | 0.45              |
| 1:S:3569:LEU:HD22 | 1:S:3569:LEU:H    | 1.82                     | 0.45              |
| 1:S:4716:TRP:CH2  | 3:S:5101:CFF:H142 | 2.52                     | 0.45              |
| 1:A:990:GLU:HA    | 1:A:1024:TYR:CG   | 2.52                     | 0.45              |
| 1:A:2630:VAL:N    | 1:A:2631:PRO:HD2  | 2.32                     | 0.45              |
| 1:A:2862:LEU:HD11 | 1:A:2932:MET:HE1  | 1.97                     | 0.45              |
| 1:G:1943:LEU:HB2  | 1:G:2123:LEU:HD21 | 1.99                     | 0.45              |
| 1:G:2825:LYS:HE3  | 1:G:2827:ARG:O    | 2.16                     | 0.45              |
| 1:G:4853:VAL:O    | 1:G:4857:ASN:ND2  | 2.50                     | 0.45              |
| 1:M:169:LEU:HD23  | 1:M:169:LEU:N     | 2.32                     | 0.45              |
| 1:M:2971:GLN:HA   | 1:M:2974:ILE:HG22 | 1.99                     | 0.45              |
| 1:M:3085:PRO:HD2  | 1:M:3088:VAL:HG21 | 1.99                     | 0.45              |
| 1:M:3569:LEU:HD22 | 1:M:3569:LEU:H    | 1.82                     | 0.45              |
| 1:S:928:THR:HG23  | 1:S:988:LEU:HD21  | 1.98                     | 0.45              |
| 1:S:1101:ARG:NH1  | 1:S:1115:LEU:O    | 2.46                     | 0.45              |
| 1:S:1123:VAL:HG12 | 1:S:1132:TRP:HB2  | 1.99                     | 0.45              |
| 1:S:2971:GLN:HA   | 1:S:2974:ILE:HG22 | 1.99                     | 0.45              |
| 1:S:4569:LEU:CD2  | 1:S:4646:LEU:HD22 | 2.47                     | 0.45              |
| 1:S:4780:PHE:O    | 1:S:4784:PHE:HD1  | 1.99                     | 0.45              |
| 1:A:438:ILE:O     | 1:A:441:VAL:HG12  | 2.17                     | 0.45              |
| 1:A:572:PRO:HA    | 1:A:575:LEU:HD13  | 1.98                     | 0.45              |
| 1:A:2009:LEU:HG   | 1:A:2023:LEU:HD21 | 1.99                     | 0.45              |
| 1:A:2971:GLN:HA   | 1:A:2974:ILE:HG22 | 1.99                     | 0.45              |
| 1:G:990:GLU:HA    | 1:G:1024:TYR:CG   | 2.52                     | 0.45              |
| 1:G:2009:LEU:HG   | 1:G:2023:LEU:HD21 | 1.99                     | 0.45              |
| 1:G:4567:LEU:HD22 | 5:G:5104:117:C85  | 2.46                     | 0.45              |
| 1:M:70:GLU:HG3    | 1:M:71:GLN:HG2    | 1.99                     | 0.45              |
| 1:S:3521:GLY:HA2  | 1:S:3524:MET:HE2  | 1.97                     | 0.45              |
| 1:S:3959:LYS:NZ   | 1:S:4022:ASP:OD2  | 2.50                     | 0.45              |
| 1:S:4853:VAL:O    | 1:S:4857:ASN:ND2  | 2.50                     | 0.45              |
| 1:A:3969:ILE:HD13 | 1:A:4030:LEU:HD23 | 2.00                     | 0.44              |
| 1:M:3957:VAL:O    | 1:M:3961:VAL:HG23 | 2.17                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:S:70:GLU:HG3    | 1:S:71:GLN:HG2    | 1.99                     | 0.44              |
| 1:S:169:LEU:HD23  | 1:S:169:LEU:N     | 2.32                     | 0.44              |
| 1:S:990:GLU:HA    | 1:S:1024:TYR:CG   | 2.52                     | 0.44              |
| 1:S:1083:VAL:HG11 | 1:S:1088:TRP:CD1  | 2.52                     | 0.44              |
| 1:A:989:ALA:CB    | 1:A:1039:LEU:CD1  | 2.95                     | 0.44              |
| 1:A:2624:ARG:HH11 | 1:A:2906:VAL:HG11 | 1.82                     | 0.44              |
| 1:A:2763:HIS:HE1  | 1:A:2790:MET:O    | 2.01                     | 0.44              |
| 1:G:2624:ARG:HH11 | 1:G:2906:VAL:HG11 | 1.82                     | 0.44              |
| 1:G:2768:PHE:O    | 1:G:2772:GLN:HG2  | 2.18                     | 0.44              |
| 1:G:3957:VAL:O    | 1:G:3961:VAL:HG23 | 2.17                     | 0.44              |
| 1:G:4952:GLU:HA   | 1:G:4952:GLU:OE1  | 2.16                     | 0.44              |
| 1:M:572:PRO:HA    | 1:M:575:LEU:HD13  | 1.98                     | 0.44              |
| 1:M:600:LEU:HD22  | 1:M:1669:LEU:HD22 | 2.00                     | 0.44              |
| 1:M:928:THR:HG23  | 1:M:988:LEU:HD21  | 1.98                     | 0.44              |
| 1:M:1478:ASP:OD1  | 1:M:1482:ASN:N    | 2.50                     | 0.44              |
| 1:M:1943:LEU:HB2  | 1:M:2123:LEU:HD21 | 1.99                     | 0.44              |
| 1:M:2768:PHE:O    | 1:M:2772:GLN:HG2  | 2.18                     | 0.44              |
| 1:M:3571:TRP:CE3  | 1:M:3575:LEU:HD12 | 2.53                     | 0.44              |
| 1:A:1123:VAL:HG12 | 1:A:1132:TRP:HB2  | 1.99                     | 0.44              |
| 1:A:1478:ASP:OD1  | 1:A:1482:ASN:N    | 2.50                     | 0.44              |
| 1:A:3080:VAL:O    | 1:A:3084:GLY:HA3  | 2.17                     | 0.44              |
| 1:A:4207:MET:HE2  | 1:A:4207:MET:CA   | 2.48                     | 0.44              |
| 1:G:2763:HIS:HE1  | 1:G:2790:MET:O    | 2.01                     | 0.44              |
| 1:G:4716:TRP:CH2  | 3:G:5101:CFF:H142 | 2.52                     | 0.44              |
| 1:M:231:LEU:HD11  | 1:M:245:VAL:HG12  | 1.99                     | 0.44              |
| 1:S:438:ILE:O     | 1:S:441:VAL:HG12  | 2.17                     | 0.44              |
| 1:A:73:LEU:HG     | 1:A:77:ALA:HB3    | 2.00                     | 0.44              |
| 1:A:231:LEU:HD11  | 1:A:245:VAL:HG12  | 1.99                     | 0.44              |
| 1:A:1083:VAL:HG11 | 1:A:1088:TRP:CD1  | 2.52                     | 0.44              |
| 1:A:1819:VAL:HG22 | 1:A:1926:LEU:HD13 | 1.98                     | 0.44              |
| 1:A:2159:LEU:HD12 | 1:A:2203:MET:HE2  | 1.99                     | 0.44              |
| 1:A:3571:TRP:CE3  | 1:A:3575:LEU:HD12 | 2.53                     | 0.44              |
| 1:A:4569:LEU:CD2  | 1:A:4646:LEU:HD22 | 2.47                     | 0.44              |
| 1:A:4817:ALA:O    | 1:A:4823:LEU:HB3  | 2.17                     | 0.44              |
| 1:G:1123:VAL:HG12 | 1:G:1132:TRP:HB2  | 1.99                     | 0.44              |
| 1:G:4207:MET:HE2  | 1:G:4207:MET:CA   | 2.48                     | 0.44              |
| 1:G:4860:ARG:HH12 | 1:M:4629:TYR:HH   | 1.51                     | 0.44              |
| 1:M:1123:VAL:HG12 | 1:M:1132:TRP:HB2  | 1.99                     | 0.44              |
| 1:M:1263:THR:HG22 | 1:M:1264:VAL:N    | 2.30                     | 0.44              |
| 1:M:4134:GLU:HB2  | 1:M:4135:PRO:HD3  | 1.99                     | 0.44              |
| 1:M:4780:PHE:O    | 1:M:4784:PHE:HD1  | 1.99                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:S:600:LEU:HD22  | 1:S:1669:LEU:HD22 | 2.00                     | 0.44              |
| 1:S:683:ARG:NE    | 1:S:707:VAL:O     | 2.48                     | 0.44              |
| 1:S:4207:MET:HE2  | 1:S:4207:MET:CA   | 2.48                     | 0.44              |
| 1:A:2768:PHE:O    | 1:A:2772:GLN:HG2  | 2.18                     | 0.44              |
| 1:G:169:LEU:HD23  | 1:G:169:LEU:N     | 2.32                     | 0.44              |
| 1:G:438:ILE:O     | 1:G:441:VAL:HG12  | 2.17                     | 0.44              |
| 1:G:2630:VAL:N    | 1:G:2631:PRO:HD2  | 2.32                     | 0.44              |
| 1:M:3969:ILE:HD13 | 1:M:4030:LEU:HD23 | 2.00                     | 0.44              |
| 1:S:1478:ASP:OD1  | 1:S:1482:ASN:N    | 2.50                     | 0.44              |
| 1:S:1943:LEU:HB2  | 1:S:2123:LEU:HD21 | 1.99                     | 0.44              |
| 1:S:3080:VAL:O    | 1:S:3084:GLY:HA3  | 2.17                     | 0.44              |
| 1:S:4134:GLU:HB2  | 1:S:4135:PRO:HD3  | 1.99                     | 0.44              |
| 1:A:4708:THR:HG21 | 1:A:4775:TYR:HB2  | 2.00                     | 0.44              |
| 1:G:70:GLU:HG3    | 1:G:71:GLN:HG2    | 1.99                     | 0.44              |
| 1:G:73:LEU:HG     | 1:G:77:ALA:HB3    | 2.00                     | 0.44              |
| 1:G:231:LEU:HD11  | 1:G:245:VAL:HG12  | 1.99                     | 0.44              |
| 1:M:1819:VAL:HG22 | 1:M:1926:LEU:HD13 | 1.98                     | 0.44              |
| 1:S:2763:HIS:HE1  | 1:S:2790:MET:O    | 2.01                     | 0.44              |
| 1:S:4640:GLU:HB3  | 1:S:4641:PRO:CD   | 2.48                     | 0.44              |
| 1:A:70:GLU:HG3    | 1:A:71:GLN:HG2    | 1.99                     | 0.44              |
| 1:A:688:LEU:HD23  | 1:A:689:THR:N     | 2.33                     | 0.44              |
| 1:G:1002:ALA:O    | 1:G:1003:GLN:C    | 2.61                     | 0.44              |
| 1:G:1819:VAL:HG22 | 1:G:1926:LEU:HD13 | 1.98                     | 0.44              |
| 1:G:2159:LEU:HD12 | 1:G:2203:MET:HE2  | 1.99                     | 0.44              |
| 1:G:4569:LEU:CD2  | 1:G:4646:LEU:HD22 | 2.47                     | 0.44              |
| 1:G:4670:ILE:C    | 1:G:4714:ASN:HD22 | 2.26                     | 0.44              |
| 1:M:990:GLU:HA    | 1:M:1024:TYR:CG   | 2.52                     | 0.44              |
| 1:M:3571:TRP:HE3  | 1:M:3575:LEU:HD12 | 1.83                     | 0.44              |
| 1:M:4207:MET:HE2  | 1:M:4207:MET:CA   | 2.48                     | 0.44              |
| 1:S:2822:THR:OG1  | 1:S:2938:THR:OG1  | 2.35                     | 0.44              |
| 1:A:683:ARG:NE    | 1:A:707:VAL:O     | 2.48                     | 0.44              |
| 1:A:752:VAL:O     | 1:A:752:VAL:HG13  | 2.18                     | 0.44              |
| 1:G:2295:LEU:O    | 1:G:2299:VAL:HG23 | 2.18                     | 0.44              |
| 1:G:2822:THR:OG1  | 1:G:2938:THR:OG1  | 2.35                     | 0.44              |
| 1:G:2874:MET:HE1  | 1:G:2937:VAL:HG12 | 2.00                     | 0.44              |
| 1:G:2971:GLN:HA   | 1:G:2974:ILE:HG22 | 1.99                     | 0.44              |
| 1:G:4875:LYS:C    | 1:G:4876:CYS:SG   | 3.01                     | 0.44              |
| 1:M:438:ILE:O     | 1:M:441:VAL:HG12  | 2.17                     | 0.44              |
| 1:M:1083:VAL:HG11 | 1:M:1088:TRP:CD1  | 2.52                     | 0.44              |
| 1:S:4817:ALA:O    | 1:S:4823:LEU:HB3  | 2.17                     | 0.44              |
| 1:A:2295:LEU:O    | 1:A:2299:VAL:HG23 | 2.18                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:4853:VAL:O    | 1:A:4857:ASN:ND2  | 2.50                     | 0.44              |
| 1:G:609:CYS:O     | 1:G:610:ASN:OD1   | 2.36                     | 0.44              |
| 1:G:928:THR:HG23  | 1:G:988:LEU:HD21  | 1.98                     | 0.44              |
| 1:G:2212:VAL:HG13 | 1:G:2256:TYR:OH   | 2.17                     | 0.44              |
| 1:G:3080:VAL:O    | 1:G:3084:GLY:HA3  | 2.17                     | 0.44              |
| 1:M:688:LEU:HD23  | 1:M:689:THR:N     | 2.33                     | 0.44              |
| 1:M:2295:LEU:O    | 1:M:2299:VAL:HG23 | 2.18                     | 0.44              |
| 1:M:4875:LYS:C    | 1:M:4876:CYS:SG   | 3.01                     | 0.44              |
| 1:S:2630:VAL:N    | 1:S:2631:PRO:HD2  | 2.32                     | 0.44              |
| 1:A:2258:LEU:CD1  | 1:A:2294:ASP:HB3  | 2.48                     | 0.43              |
| 1:A:3007:ASN:O    | 1:A:3011:THR:OG1  | 2.16                     | 0.43              |
| 1:A:3569:LEU:H    | 1:A:3569:LEU:HD22 | 1.82                     | 0.43              |
| 1:G:3569:LEU:H    | 1:G:3569:LEU:HD22 | 1.82                     | 0.43              |
| 1:M:609:CYS:O     | 1:M:610:ASN:OD1   | 2.36                     | 0.43              |
| 1:M:4569:LEU:CD2  | 1:M:4646:LEU:HD22 | 2.47                     | 0.43              |
| 1:M:4853:VAL:O    | 1:M:4857:ASN:ND2  | 2.50                     | 0.43              |
| 1:M:4879:MET:HG2  | 1:S:4578:LEU:HA   | 2.00                     | 0.43              |
| 1:S:73:LEU:HG     | 1:S:77:ALA:HB3    | 2.00                     | 0.43              |
| 1:S:181:HIS:HD1   | 1:S:196:MET:HB2   | 1.80                     | 0.43              |
| 1:S:688:LEU:HD23  | 1:S:689:THR:N     | 2.33                     | 0.43              |
| 1:A:609:CYS:O     | 1:A:610:ASN:OD1   | 2.36                     | 0.43              |
| 1:A:787:VAL:O     | 1:A:788:LYS:HG3   | 2.18                     | 0.43              |
| 1:A:2271:THR:OG1  | 1:A:2274:ASP:OD2  | 2.34                     | 0.43              |
| 1:A:3110:LEU:HD21 | 1:A:3183:VAL:HG22 | 2.01                     | 0.43              |
| 1:A:3959:LYS:NZ   | 1:A:4022:ASP:OD2  | 2.50                     | 0.43              |
| 1:A:4640:GLU:HB3  | 1:A:4641:PRO:CD   | 2.48                     | 0.43              |
| 1:A:4875:LYS:C    | 1:A:4876:CYS:SG   | 3.01                     | 0.43              |
| 1:G:600:LEU:HD22  | 1:G:1669:LEU:HD22 | 2.00                     | 0.43              |
| 1:G:989:ALA:HA    | 1:G:1039:LEU:HD11 | 1.99                     | 0.43              |
| 1:G:2151:ASP:OD2  | 1:G:2189:LYS:NZ   | 2.41                     | 0.43              |
| 1:G:4879:MET:HG2  | 1:M:4578:LEU:HA   | 2.00                     | 0.43              |
| 1:M:73:LEU:HG     | 1:M:77:ALA:HB3    | 2.00                     | 0.43              |
| 1:M:752:VAL:HG13  | 1:M:752:VAL:O     | 2.18                     | 0.43              |
| 1:M:2258:LEU:CD1  | 1:M:2294:ASP:HB3  | 2.48                     | 0.43              |
| 1:M:4636:THR:C    | 1:M:4638:TYR:H    | 2.27                     | 0.43              |
| 1:M:4640:GLU:HB3  | 1:M:4641:PRO:CD   | 2.48                     | 0.43              |
| 1:M:4670:ILE:C    | 1:M:4714:ASN:HD22 | 2.26                     | 0.43              |
| 2:N:38:ASP:OD1    | 2:N:39:SER:N      | 2.51                     | 0.43              |
| 1:S:572:PRO:HA    | 1:S:575:LEU:HD13  | 1.98                     | 0.43              |
| 1:S:3133:THR:HG23 | 1:S:3134:VAL:HG23 | 2.01                     | 0.43              |
| 1:A:3874:VAL:HG13 | 1:A:3874:VAL:O    | 2.18                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:4138:ASP:O    | 1:A:4142:ASN:ND2  | 2.44                     | 0.43              |
| 1:A:4222:VAL:HG12 | 1:A:4950:VAL:HG11 | 1.98                     | 0.43              |
| 1:A:4838:VAL:O    | 1:A:4841:VAL:HG22 | 2.18                     | 0.43              |
| 2:B:38:ASP:OD1    | 2:B:39:SER:N      | 2.51                     | 0.43              |
| 1:G:752:VAL:O     | 1:G:752:VAL:HG13  | 2.18                     | 0.43              |
| 1:G:1083:VAL:HG11 | 1:G:1088:TRP:CD1  | 2.52                     | 0.43              |
| 1:G:2965:ARG:HA   | 1:G:2968:ASP:OD2  | 2.19                     | 0.43              |
| 1:G:3571:TRP:CE3  | 1:G:3575:LEU:HD12 | 2.53                     | 0.43              |
| 1:G:4640:GLU:HB3  | 1:G:4641:PRO:CD   | 2.48                     | 0.43              |
| 1:G:4708:THR:HG21 | 1:G:4775:TYR:HB2  | 2.00                     | 0.43              |
| 1:M:787:VAL:O     | 1:M:788:LYS:HG3   | 2.18                     | 0.43              |
| 1:M:2212:VAL:HG13 | 1:M:2256:TYR:OH   | 2.17                     | 0.43              |
| 1:M:3874:VAL:O    | 1:M:3874:VAL:HG13 | 2.18                     | 0.43              |
| 1:S:2295:LEU:O    | 1:S:2299:VAL:HG23 | 2.18                     | 0.43              |
| 1:S:3110:LEU:HD21 | 1:S:3183:VAL:HG22 | 2.01                     | 0.43              |
| 1:S:3571:TRP:CE3  | 1:S:3575:LEU:HD12 | 2.53                     | 0.43              |
| 1:S:4222:VAL:HG12 | 1:S:4950:VAL:HG11 | 1.98                     | 0.43              |
| 2:T:38:ASP:OD1    | 2:T:39:SER:N      | 2.51                     | 0.43              |
| 1:A:1943:LEU:HB2  | 1:A:2123:LEU:HD21 | 1.99                     | 0.43              |
| 1:A:3400:VAL:HG13 | 1:A:3403:ARG:HH21 | 1.83                     | 0.43              |
| 1:A:3779:VAL:HG13 | 1:A:3797:THR:HG22 | 2.00                     | 0.43              |
| 1:A:4636:THR:C    | 1:A:4638:TYR:H    | 2.27                     | 0.43              |
| 1:G:688:LEU:HD23  | 1:G:689:THR:N     | 2.33                     | 0.43              |
| 1:G:787:VAL:O     | 1:G:788:LYS:HG3   | 2.18                     | 0.43              |
| 1:G:2258:LEU:CD1  | 1:G:2294:ASP:HB3  | 2.48                     | 0.43              |
| 1:G:2599:GLN:O    | 1:G:2603:ILE:HG13 | 2.19                     | 0.43              |
| 1:G:3874:VAL:O    | 1:G:3874:VAL:HG13 | 2.18                     | 0.43              |
| 1:G:4838:VAL:O    | 1:G:4841:VAL:HG22 | 2.18                     | 0.43              |
| 1:M:1002:ALA:O    | 1:M:1003:GLN:C    | 2.61                     | 0.43              |
| 1:M:2965:ARG:HA   | 1:M:2968:ASP:OD2  | 2.19                     | 0.43              |
| 1:M:3110:LEU:HD21 | 1:M:3183:VAL:HG22 | 2.01                     | 0.43              |
| 1:M:3133:THR:HG23 | 1:M:3134:VAL:HG23 | 2.01                     | 0.43              |
| 1:S:2368:LEU:HD23 | 1:S:2368:LEU:O    | 2.19                     | 0.43              |
| 1:S:3400:VAL:HG13 | 1:S:3403:ARG:HH21 | 1.83                     | 0.43              |
| 1:S:3969:ILE:HD13 | 1:S:4030:LEU:HD23 | 2.00                     | 0.43              |
| 1:S:4636:THR:C    | 1:S:4638:TYR:H    | 2.27                     | 0.43              |
| 1:S:4838:VAL:O    | 1:S:4841:VAL:HG22 | 2.18                     | 0.43              |
| 1:A:2368:LEU:HD23 | 1:A:2368:LEU:O    | 2.19                     | 0.43              |
| 1:A:2599:GLN:O    | 1:A:2603:ILE:HG13 | 2.19                     | 0.43              |
| 1:A:3060:ASP:OD1  | 1:A:3060:ASP:N    | 2.43                     | 0.43              |
| 1:A:4041:ALA:O    | 1:A:4045:VAL:HG23 | 2.19                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:G:3110:LEU:HD21 | 1:G:3183:VAL:HG22 | 2.01                     | 0.43              |
| 1:G:3571:TRP:HE3  | 1:G:3575:LEU:HD12 | 1.83                     | 0.43              |
| 1:S:2768:PHE:O    | 1:S:2772:GLN:HG2  | 2.18                     | 0.43              |
| 1:S:4875:LYS:C    | 1:S:4876:CYS:SG   | 3.01                     | 0.43              |
| 1:A:2122:SER:O    | 1:A:2126:ARG:HG3  | 2.19                     | 0.43              |
| 1:A:2151:ASP:OD2  | 1:A:2189:LYS:NZ   | 2.41                     | 0.43              |
| 1:A:2212:VAL:HG13 | 1:A:2256:TYR:OH   | 2.17                     | 0.43              |
| 1:A:3085:PRO:HD2  | 1:A:3088:VAL:HG21 | 1.99                     | 0.43              |
| 1:A:3758:MET:SD   | 1:A:3758:MET:C    | 3.02                     | 0.43              |
| 1:G:2515:GLN:O    | 1:G:2519:LEU:HG   | 2.19                     | 0.43              |
| 1:G:3085:PRO:HD2  | 1:G:3088:VAL:HG21 | 1.99                     | 0.43              |
| 1:G:3969:ILE:HD13 | 1:G:4030:LEU:HD23 | 2.00                     | 0.43              |
| 1:M:989:ALA:CB    | 1:M:1039:LEU:CD1  | 2.95                     | 0.43              |
| 1:M:3400:VAL:HG13 | 1:M:3403:ARG:HH21 | 1.83                     | 0.43              |
| 1:M:3838:THR:HG22 | 1:M:3838:THR:O    | 2.19                     | 0.43              |
| 1:S:2109:ASP:N    | 1:S:2109:ASP:OD1  | 2.52                     | 0.43              |
| 1:S:2122:SER:O    | 1:S:2126:ARG:HG3  | 2.19                     | 0.43              |
| 1:S:3758:MET:SD   | 1:S:3758:MET:C    | 3.02                     | 0.43              |
| 1:A:600:LEU:HD22  | 1:A:1669:LEU:HD22 | 2.00                     | 0.43              |
| 1:A:2874:MET:HE1  | 1:A:2937:VAL:HG12 | 2.00                     | 0.43              |
| 1:A:4670:ILE:C    | 1:A:4714:ASN:HD22 | 2.26                     | 0.43              |
| 1:G:2109:ASP:OD1  | 1:G:2109:ASP:N    | 2.52                     | 0.43              |
| 1:G:2368:LEU:O    | 1:G:2368:LEU:HD23 | 2.19                     | 0.43              |
| 1:G:3363:GLY:O    | 1:G:3367:LYS:HG2  | 2.19                     | 0.43              |
| 1:G:3838:THR:O    | 1:G:3838:THR:HG22 | 2.19                     | 0.43              |
| 1:M:2599:GLN:O    | 1:M:2603:ILE:HG13 | 2.19                     | 0.43              |
| 1:M:3261:ALA:HB3  | 1:M:3266:MET:SD   | 2.59                     | 0.43              |
| 1:M:3959:LYS:NZ   | 1:M:4022:ASP:OD2  | 2.50                     | 0.43              |
| 1:A:3133:THR:HG23 | 1:A:3134:VAL:HG23 | 2.01                     | 0.43              |
| 1:A:3363:GLY:O    | 1:A:3367:LYS:HG2  | 2.19                     | 0.43              |
| 1:G:544:LEU:HD22  | 1:G:574:VAL:HG13  | 2.01                     | 0.43              |
| 1:G:3400:VAL:HG13 | 1:G:3403:ARG:HH21 | 1.83                     | 0.43              |
| 1:G:4041:ALA:O    | 1:G:4045:VAL:HG23 | 2.19                     | 0.43              |
| 1:M:2763:HIS:HE1  | 1:M:2790:MET:O    | 2.01                     | 0.43              |
| 1:M:3779:VAL:HG13 | 1:M:3797:THR:HG22 | 2.00                     | 0.43              |
| 1:S:2212:VAL:HG13 | 1:S:2256:TYR:OH   | 2.17                     | 0.43              |
| 1:S:2258:LEU:CD1  | 1:S:2294:ASP:HB3  | 2.48                     | 0.43              |
| 1:S:2965:ARG:HA   | 1:S:2968:ASP:OD2  | 2.19                     | 0.43              |
| 1:S:3261:ALA:HB3  | 1:S:3266:MET:SD   | 2.59                     | 0.43              |
| 1:S:4006:ASP:HB2  | 1:S:4009:GLN:OE1  | 2.19                     | 0.43              |
| 1:S:4041:ALA:O    | 1:S:4045:VAL:HG23 | 2.19                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:S:4708:THR:HG21 | 1:S:4775:TYR:HB2  | 2.00                     | 0.43              |
| 1:A:544:LEU:HD22  | 1:A:574:VAL:HG13  | 2.01                     | 0.43              |
| 1:A:1219:LEU:HD11 | 1:G:3575:LEU:HD13 | 1.96                     | 0.43              |
| 1:A:3085:PRO:O    | 1:A:3088:VAL:HG22 | 2.19                     | 0.43              |
| 1:A:4006:ASP:HB2  | 1:A:4009:GLN:OE1  | 2.19                     | 0.43              |
| 1:G:989:ALA:CB    | 1:G:1039:LEU:CD1  | 2.95                     | 0.43              |
| 1:G:3085:PRO:O    | 1:G:3088:VAL:HG22 | 2.19                     | 0.43              |
| 1:G:3959:LYS:NZ   | 1:G:4022:ASP:OD2  | 2.50                     | 0.43              |
| 1:M:996:TRP:CE2   | 1:M:1000:ARG:HG3  | 2.54                     | 0.43              |
| 1:S:1089:TYR:HD2  | 1:S:1152:MET:HG2  | 1.84                     | 0.43              |
| 1:S:4670:ILE:C    | 1:S:4714:ASN:HD22 | 2.26                     | 0.43              |
| 1:A:3550:ARG:CB   | 1:A:3597:GLN:OE1  | 2.67                     | 0.43              |
| 1:A:4576:ILE:CG2  | 1:A:4643:LEU:HD13 | 2.49                     | 0.43              |
| 2:H:38:ASP:OD1    | 2:H:39:SER:N      | 2.51                     | 0.43              |
| 1:M:544:LEU:HD22  | 1:M:574:VAL:HG13  | 2.01                     | 0.43              |
| 1:M:2515:GLN:O    | 1:M:2519:LEU:HG   | 2.19                     | 0.43              |
| 1:M:3363:GLY:O    | 1:M:3367:LYS:HG2  | 2.19                     | 0.43              |
| 1:M:4726:ASP:C    | 1:M:4726:ASP:OD1  | 2.62                     | 0.43              |
| 1:S:752:VAL:O     | 1:S:752:VAL:HG13  | 2.18                     | 0.43              |
| 1:S:3874:VAL:O    | 1:S:3874:VAL:HG13 | 2.18                     | 0.43              |
| 1:A:501:ALA:O     | 1:A:505:GLU:HG3   | 2.19                     | 0.42              |
| 1:A:1089:TYR:HD2  | 1:A:1152:MET:HG2  | 1.84                     | 0.42              |
| 1:A:1164:LEU:O    | 1:A:1167:GLU:N    | 2.50                     | 0.42              |
| 1:A:2499:LYS:O    | 1:A:2503:VAL:HG23 | 2.19                     | 0.42              |
| 1:A:2750:LYS:HG2  | 1:A:2750:LYS:O    | 2.20                     | 0.42              |
| 1:A:4091:LYS:O    | 1:A:4095:LYS:NZ   | 2.52                     | 0.42              |
| 1:A:4879:MET:HG2  | 1:G:4578:LEU:HA   | 2.00                     | 0.42              |
| 1:G:501:ALA:O     | 1:G:505:GLU:HG3   | 2.19                     | 0.42              |
| 1:G:3261:ALA:HB3  | 1:G:3266:MET:SD   | 2.59                     | 0.42              |
| 1:G:4636:THR:C    | 1:G:4638:TYR:H    | 2.27                     | 0.42              |
| 1:M:575:LEU:HD12  | 1:M:575:LEU:N     | 2.35                     | 0.42              |
| 1:M:2109:ASP:OD1  | 1:M:2109:ASP:N    | 2.52                     | 0.42              |
| 1:M:2122:SER:O    | 1:M:2126:ARG:HG3  | 2.19                     | 0.42              |
| 1:M:3550:ARG:CB   | 1:M:3597:GLN:OE1  | 2.67                     | 0.42              |
| 1:M:3991:GLY:O    | 1:M:3995:VAL:HG23 | 2.19                     | 0.42              |
| 1:M:4006:ASP:HB2  | 1:M:4009:GLN:OE1  | 2.19                     | 0.42              |
| 1:M:4576:ILE:CG2  | 1:M:4643:LEU:HD13 | 2.49                     | 0.42              |
| 1:S:2499:LYS:O    | 1:S:2503:VAL:HG23 | 2.19                     | 0.42              |
| 1:S:3363:GLY:O    | 1:S:3367:LYS:HG2  | 2.19                     | 0.42              |
| 1:A:2515:GLN:O    | 1:A:2519:LEU:HG   | 2.19                     | 0.42              |
| 1:A:3838:THR:O    | 1:A:3838:THR:HG22 | 2.19                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:3991:GLY:O    | 1:A:3995:VAL:HG23 | 2.19                     | 0.42              |
| 1:G:411:TYR:HB2   | 1:G:486:LEU:HD21  | 2.01                     | 0.42              |
| 1:G:2499:LYS:O    | 1:G:2503:VAL:HG23 | 2.19                     | 0.42              |
| 1:G:3133:THR:HG23 | 1:G:3134:VAL:HG23 | 2.01                     | 0.42              |
| 1:G:3758:MET:SD   | 1:G:3758:MET:C    | 3.02                     | 0.42              |
| 1:M:2161:GLN:O    | 1:M:2165:LEU:CD2  | 2.67                     | 0.42              |
| 1:M:3758:MET:SD   | 1:M:3758:MET:C    | 3.02                     | 0.42              |
| 1:S:996:TRP:CE2   | 1:S:1000:ARG:HG3  | 2.54                     | 0.42              |
| 1:S:1164:LEU:O    | 1:S:1167:GLU:N    | 2.50                     | 0.42              |
| 1:S:2874:MET:HE1  | 1:S:2937:VAL:HG12 | 2.00                     | 0.42              |
| 1:S:3991:GLY:O    | 1:S:3995:VAL:HG23 | 2.19                     | 0.42              |
| 1:A:169:LEU:HD23  | 1:A:169:LEU:N     | 2.32                     | 0.42              |
| 1:A:411:TYR:HB2   | 1:A:486:LEU:HD21  | 2.01                     | 0.42              |
| 1:A:2965:ARG:HA   | 1:A:2968:ASP:OD2  | 2.19                     | 0.42              |
| 1:A:3391:GLU:HA   | 1:A:3394:VAL:HG22 | 2.01                     | 0.42              |
| 1:G:3550:ARG:CB   | 1:G:3597:GLN:OE1  | 2.67                     | 0.42              |
| 1:M:2499:LYS:O    | 1:M:2503:VAL:HG23 | 2.19                     | 0.42              |
| 1:M:2639:MET:HB3  | 1:M:2640:PRO:HD3  | 2.01                     | 0.42              |
| 1:M:3391:GLU:HA   | 1:M:3394:VAL:HG22 | 2.01                     | 0.42              |
| 1:S:637:LEU:HD12  | 1:S:637:LEU:N     | 2.35                     | 0.42              |
| 1:S:787:VAL:O     | 1:S:788:LYS:HG3   | 2.18                     | 0.42              |
| 1:S:2515:GLN:O    | 1:S:2519:LEU:HG   | 2.19                     | 0.42              |
| 1:S:3571:TRP:HE3  | 1:S:3575:LEU:HD12 | 1.83                     | 0.42              |
| 1:S:4576:ILE:CG2  | 1:S:4643:LEU:HD13 | 2.49                     | 0.42              |
| 1:A:2624:ARG:NH1  | 1:A:2906:VAL:HG21 | 2.35                     | 0.42              |
| 1:G:3046:LEU:O    | 1:G:3050:VAL:HG23 | 2.19                     | 0.42              |
| 1:G:4576:ILE:CG2  | 1:G:4643:LEU:HD13 | 2.49                     | 0.42              |
| 1:M:2874:MET:HE1  | 1:M:2937:VAL:HG12 | 2.00                     | 0.42              |
| 1:M:4682:GLU:OE1  | 1:M:4682:GLU:C    | 2.63                     | 0.42              |
| 1:M:4708:THR:HG21 | 1:M:4775:TYR:HB2  | 2.00                     | 0.42              |
| 1:S:501:ALA:O     | 1:S:505:GLU:HG3   | 2.19                     | 0.42              |
| 1:S:609:CYS:O     | 1:S:610:ASN:OD1   | 2.36                     | 0.42              |
| 1:S:989:ALA:CB    | 1:S:1039:LEU:CD1  | 2.95                     | 0.42              |
| 1:S:1935:VAL:O    | 1:S:1939:MET:HG2  | 2.20                     | 0.42              |
| 1:S:3550:ARG:CB   | 1:S:3597:GLN:OE1  | 2.67                     | 0.42              |
| 1:A:1297:PHE:CZ   | 1:A:1542:VAL:HG21 | 2.55                     | 0.42              |
| 1:A:1805:GLU:HA   | 1:A:1808:ARG:NE   | 2.35                     | 0.42              |
| 1:A:3261:ALA:HB3  | 1:A:3266:MET:SD   | 2.59                     | 0.42              |
| 1:G:1935:VAL:O    | 1:G:1939:MET:HG2  | 2.20                     | 0.42              |
| 1:G:2750:LYS:O    | 1:G:2750:LYS:HG2  | 2.20                     | 0.42              |
| 1:M:3085:PRO:O    | 1:M:3088:VAL:HG22 | 2.19                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:M:4041:ALA:O   | 1:M:4045:VAL:HG23 | 2.19                     | 0.42              |
| 1:S:1272:LEU:CD2 | 1:S:1561:VAL:HG21 | 2.44                     | 0.42              |
| 1:A:2113:SER:O   | 1:A:2117:VAL:HG23 | 2.20                     | 0.42              |
| 1:A:2639:MET:HB3 | 1:A:2640:PRO:HD3  | 2.01                     | 0.42              |
| 1:A:3003:LEU:HB2 | 1:A:3004:PRO:HD3  | 2.01                     | 0.42              |
| 1:A:4578:LEU:HA  | 1:S:4879:MET:HG2  | 2.00                     | 0.42              |
| 1:A:4726:ASP:C   | 1:A:4726:ASP:OD1  | 2.62                     | 0.42              |
| 1:G:1297:PHE:CZ  | 1:G:1542:VAL:HG21 | 2.55                     | 0.42              |
| 1:G:2122:SER:O   | 1:G:2126:ARG:HG3  | 2.19                     | 0.42              |
| 1:G:2271:THR:OG1 | 1:G:2274:ASP:OD2  | 2.34                     | 0.42              |
| 1:G:3536:ALA:HB3 | 1:G:3600:SER:CB   | 2.50                     | 0.42              |
| 1:G:3991:GLY:O   | 1:G:3995:VAL:HG23 | 2.19                     | 0.42              |
| 1:M:4838:VAL:O   | 1:M:4841:VAL:HG22 | 2.18                     | 0.42              |
| 1:M:4928:LEU:O   | 1:M:4932:ILE:HG13 | 2.20                     | 0.42              |
| 1:S:1297:PHE:CZ  | 1:S:1542:VAL:HG21 | 2.55                     | 0.42              |
| 1:S:2599:GLN:O   | 1:S:2603:ILE:HG13 | 2.19                     | 0.42              |
| 1:A:3046:LEU:O   | 1:A:3050:VAL:HG23 | 2.19                     | 0.42              |
| 1:G:3391:GLU:HA  | 1:G:3394:VAL:HG22 | 2.01                     | 0.42              |
| 1:G:4006:ASP:HB2 | 1:G:4009:GLN:OE1  | 2.19                     | 0.42              |
| 1:M:3536:ALA:HB3 | 1:M:3600:SER:CB   | 2.50                     | 0.42              |
| 1:M:3698:LEU:O   | 1:M:3702:VAL:HG23 | 2.20                     | 0.42              |
| 1:M:3946:GLN:HA  | 1:M:3949:ARG:HG2  | 2.02                     | 0.42              |
| 1:S:3085:PRO:O   | 1:S:3088:VAL:HG22 | 2.19                     | 0.42              |
| 1:S:3391:GLU:HA  | 1:S:3394:VAL:HG22 | 2.01                     | 0.42              |
| 1:S:4180:ARG:HD3 | 1:S:4192:ARG:HD3  | 2.01                     | 0.42              |
| 1:S:4726:ASP:C   | 1:S:4726:ASP:OD1  | 2.62                     | 0.42              |
| 1:A:610:ASN:OD1  | 1:A:610:ASN:C     | 2.63                     | 0.42              |
| 1:A:3536:ALA:HB3 | 1:A:3600:SER:CB   | 2.50                     | 0.42              |
| 1:G:2624:ARG:NH1 | 1:G:2906:VAL:HG21 | 2.35                     | 0.42              |
| 1:G:2639:MET:HB3 | 1:G:2640:PRO:HD3  | 2.01                     | 0.42              |
| 1:G:4138:ASP:O   | 1:G:4142:ASN:ND2  | 2.44                     | 0.42              |
| 5:G:5105:117:H71 | 5:G:5105:117:H91  | 1.93                     | 0.42              |
| 1:M:1089:TYR:HD2 | 1:M:1152:MET:HG2  | 1.84                     | 0.42              |
| 1:M:2368:LEU:O   | 1:M:2368:LEU:HD23 | 2.19                     | 0.42              |
| 1:S:3060:ASP:OD1 | 1:S:3060:ASP:N    | 2.43                     | 0.42              |
| 1:A:1002:ALA:O   | 1:A:1003:GLN:C    | 2.61                     | 0.42              |
| 1:A:4180:ARG:HD3 | 1:A:4192:ARG:HD3  | 2.01                     | 0.42              |
| 1:G:996:TRP:CE2  | 1:G:1000:ARG:HG3  | 2.54                     | 0.42              |
| 1:G:1805:GLU:HA  | 1:G:1808:ARG:NE   | 2.35                     | 0.42              |
| 1:M:1935:VAL:O   | 1:M:1939:MET:HG2  | 2.20                     | 0.42              |
| 1:S:575:LEU:N    | 1:S:575:LEU:HD12  | 2.35                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:S:2643:LEU:HD23 | 1:S:2643:LEU:C    | 2.45                     | 0.42              |
| 1:S:3779:VAL:HG13 | 1:S:3797:THR:HG22 | 2.00                     | 0.42              |
| 1:S:4682:GLU:OE1  | 1:S:4682:GLU:C    | 2.63                     | 0.42              |
| 1:A:637:LEU:HD12  | 1:A:637:LEU:N     | 2.35                     | 0.42              |
| 1:A:3571:TRP:HE3  | 1:A:3575:LEU:HD12 | 1.83                     | 0.42              |
| 1:A:3946:GLN:HA   | 1:A:3949:ARG:HG2  | 2.02                     | 0.42              |
| 1:G:610:ASN:OD1   | 1:G:610:ASN:C     | 2.63                     | 0.42              |
| 1:G:2113:SER:O    | 1:G:2117:VAL:HG23 | 2.20                     | 0.42              |
| 1:G:2643:LEU:HD23 | 1:G:2643:LEU:C    | 2.45                     | 0.42              |
| 1:G:3006:ILE:HG23 | 1:G:3010:PHE:CE2  | 2.55                     | 0.42              |
| 1:G:4726:ASP:C    | 1:G:4726:ASP:OD1  | 2.62                     | 0.42              |
| 1:M:2113:SER:O    | 1:M:2117:VAL:HG23 | 2.20                     | 0.42              |
| 1:M:2960:LEU:HB3  | 1:M:3038:MET:HE2  | 2.02                     | 0.42              |
| 1:M:4708:THR:HG22 | 1:M:4710:SER:H    | 1.85                     | 0.42              |
| 1:S:411:TYR:HB2   | 1:S:486:LEU:HD21  | 2.01                     | 0.42              |
| 1:S:544:LEU:HD22  | 1:S:574:VAL:HG13  | 2.01                     | 0.42              |
| 1:S:1805:GLU:HA   | 1:S:1808:ARG:NE   | 2.35                     | 0.42              |
| 1:S:1805:GLU:HA   | 1:S:1808:ARG:HE   | 1.85                     | 0.42              |
| 1:S:2750:LYS:O    | 1:S:2750:LYS:HG2  | 2.20                     | 0.42              |
| 1:A:1935:VAL:O    | 1:A:1939:MET:HG2  | 2.20                     | 0.41              |
| 1:A:3281:LEU:HB2  | 1:A:3282:PRO:HD3  | 2.02                     | 0.41              |
| 1:A:4708:THR:HG22 | 1:A:4710:SER:H    | 1.85                     | 0.41              |
| 1:G:978:THR:N     | 1:G:981:GLN:OE1   | 2.50                     | 0.41              |
| 1:G:3281:LEU:HB2  | 1:G:3282:PRO:HD3  | 2.02                     | 0.41              |
| 1:G:4222:VAL:CG1  | 1:G:4950:VAL:CG1  | 2.98                     | 0.41              |
| 1:G:4928:LEU:O    | 1:G:4932:ILE:HG13 | 2.20                     | 0.41              |
| 1:M:637:LEU:HD12  | 1:M:637:LEU:N     | 2.35                     | 0.41              |
| 1:M:1805:GLU:HA   | 1:M:1808:ARG:HE   | 1.85                     | 0.41              |
| 1:M:2643:LEU:HD23 | 1:M:2643:LEU:C    | 2.45                     | 0.41              |
| 1:S:2624:ARG:NH1  | 1:S:2906:VAL:HG21 | 2.35                     | 0.41              |
| 1:S:3536:ALA:HB3  | 1:S:3600:SER:CB   | 2.50                     | 0.41              |
| 1:A:996:TRP:CE2   | 1:A:1000:ARG:HG3  | 2.54                     | 0.41              |
| 1:A:2276:ALA:O    | 1:A:2280:VAL:HG12 | 2.20                     | 0.41              |
| 1:G:390:LEU:H     | 1:G:390:LEU:CD2   | 2.32                     | 0.41              |
| 1:G:3698:LEU:O    | 1:G:3702:VAL:HG23 | 2.20                     | 0.41              |
| 1:G:3779:VAL:HG13 | 1:G:3797:THR:HG22 | 2.00                     | 0.41              |
| 1:M:610:ASN:OD1   | 1:M:610:ASN:C     | 2.63                     | 0.41              |
| 1:M:2276:ALA:O    | 1:M:2280:VAL:HG12 | 2.20                     | 0.41              |
| 1:S:1002:ALA:O    | 1:S:1003:GLN:C    | 2.61                     | 0.41              |
| 1:S:2960:LEU:HB3  | 1:S:3038:MET:HE2  | 2.02                     | 0.41              |
| 1:S:3006:ILE:HG23 | 1:S:3010:PHE:CE2  | 2.55                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:S:3838:THR:O    | 1:S:3838:THR:HG22 | 2.19                     | 0.41              |
| 1:A:390:LEU:H     | 1:A:390:LEU:CD2   | 2.32                     | 0.41              |
| 1:A:575:LEU:HD12  | 1:A:575:LEU:N     | 2.35                     | 0.41              |
| 1:A:2109:ASP:N    | 1:A:2109:ASP:OD1  | 2.52                     | 0.41              |
| 1:A:4682:GLU:OE1  | 1:A:4682:GLU:C    | 2.63                     | 0.41              |
| 1:G:683:ARG:NE    | 1:G:707:VAL:O     | 2.48                     | 0.41              |
| 1:G:2333:ASP:OD1  | 1:G:2334:PHE:N    | 2.54                     | 0.41              |
| 1:G:4682:GLU:OE1  | 1:G:4682:GLU:C    | 2.63                     | 0.41              |
| 1:M:3003:LEU:HB2  | 1:M:3004:PRO:HD3  | 2.01                     | 0.41              |
| 1:S:2639:MET:HB3  | 1:S:2640:PRO:HD3  | 2.01                     | 0.41              |
| 1:S:3046:LEU:O    | 1:S:3050:VAL:HG23 | 2.19                     | 0.41              |
| 1:G:1089:TYR:HD2  | 1:G:1152:MET:HG2  | 1.84                     | 0.41              |
| 1:G:1805:GLU:HA   | 1:G:1808:ARG:HE   | 1.85                     | 0.41              |
| 1:G:2276:ALA:O    | 1:G:2280:VAL:HG12 | 2.20                     | 0.41              |
| 1:M:501:ALA:O     | 1:M:505:GLU:HG3   | 2.19                     | 0.41              |
| 1:M:1297:PHE:CZ   | 1:M:1542:VAL:HG21 | 2.55                     | 0.41              |
| 1:M:1805:GLU:HA   | 1:M:1808:ARG:NE   | 2.35                     | 0.41              |
| 1:M:3046:LEU:O    | 1:M:3050:VAL:HG23 | 2.19                     | 0.41              |
| 1:S:610:ASN:OD1   | 1:S:610:ASN:C     | 2.63                     | 0.41              |
| 1:A:27:THR:HA     | 1:A:31:GLU:O      | 2.21                     | 0.41              |
| 1:A:2101:MET:HA   | 1:A:2101:MET:HE3  | 2.02                     | 0.41              |
| 1:A:3316:LEU:HD23 | 1:A:3353:LEU:CD2  | 2.51                     | 0.41              |
| 1:A:3593:VAL:HA   | 1:A:3596:VAL:HG22 | 2.03                     | 0.41              |
| 1:G:575:LEU:HD12  | 1:G:575:LEU:N     | 2.35                     | 0.41              |
| 1:G:1867:GLU:HB2  | 1:G:1927:LEU:HD12 | 2.03                     | 0.41              |
| 1:G:2161:GLN:O    | 1:G:2165:LEU:CD2  | 2.67                     | 0.41              |
| 1:G:4020:GLN:O    | 1:G:4024:VAL:HG23 | 2.21                     | 0.41              |
| 1:M:390:LEU:H     | 1:M:390:LEU:CD2   | 2.32                     | 0.41              |
| 1:M:411:TYR:HB2   | 1:M:486:LEU:HD21  | 2.01                     | 0.41              |
| 1:S:1694:LEU:O    | 1:S:1698:LEU:HG   | 2.20                     | 0.41              |
| 1:S:3003:LEU:HB2  | 1:S:3004:PRO:HD3  | 2.01                     | 0.41              |
| 1:S:4779:LYS:O    | 1:S:4783:ILE:HG13 | 2.21                     | 0.41              |
| 1:S:5034:ASP:O    | 1:S:5035:GLN:HB2  | 2.21                     | 0.41              |
| 1:A:3006:ILE:HG23 | 1:A:3010:PHE:CE2  | 2.55                     | 0.41              |
| 1:G:637:LEU:HD12  | 1:G:637:LEU:N     | 2.35                     | 0.41              |
| 1:G:828:GLU:OE2   | 1:G:831:ARG:NH1   | 2.51                     | 0.41              |
| 1:G:4708:THR:HG22 | 1:G:4710:SER:H    | 1.85                     | 0.41              |
| 1:G:5034:ASP:O    | 1:G:5035:GLN:HB2  | 2.21                     | 0.41              |
| 1:M:27:THR:HA     | 1:M:31:GLU:O      | 2.21                     | 0.41              |
| 1:M:1139:PHE:HZ   | 1:M:1169:LEU:O    | 2.04                     | 0.41              |
| 1:M:4180:ARG:HD3  | 1:M:4192:ARG:HD3  | 2.01                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:S:27:THR:HA     | 1:S:31:GLU:O      | 2.21                     | 0.41              |
| 1:S:390:LEU:H     | 1:S:390:LEU:CD2   | 2.32                     | 0.41              |
| 1:S:2333:ASP:OD1  | 1:S:2334:PHE:N    | 2.54                     | 0.41              |
| 1:S:3316:LEU:HD23 | 1:S:3353:LEU:CD2  | 2.51                     | 0.41              |
| 1:S:3698:LEU:O    | 1:S:3702:VAL:HG23 | 2.20                     | 0.41              |
| 1:S:3946:GLN:HA   | 1:S:3949:ARG:HG2  | 2.02                     | 0.41              |
| 1:S:4928:LEU:O    | 1:S:4932:ILE:HG13 | 2.20                     | 0.41              |
| 1:A:1805:GLU:HA   | 1:A:1808:ARG:HE   | 1.85                     | 0.41              |
| 1:A:2333:ASP:OD1  | 1:A:2334:PHE:N    | 2.54                     | 0.41              |
| 1:A:2992:GLU:O    | 1:A:2995:ILE:HG22 | 2.21                     | 0.41              |
| 1:G:4772:ASP:OD1  | 1:G:4775:TYR:N    | 2.46                     | 0.41              |
| 2:H:24:VAL:HG22   | 2:H:48:LYS:HG2    | 2.02                     | 0.41              |
| 1:M:495:ASN:OD1   | 1:M:553:ARG:NH1   | 2.54                     | 0.41              |
| 1:M:1426:ILE:HG23 | 1:M:1429:ASN:H    | 1.85                     | 0.41              |
| 1:M:2624:ARG:NH1  | 1:M:2906:VAL:HG21 | 2.35                     | 0.41              |
| 1:S:1184:ILE:HG23 | 1:S:1185:GLY:N    | 2.36                     | 0.41              |
| 1:A:1426:ILE:HG23 | 1:A:1429:ASN:H    | 1.85                     | 0.41              |
| 1:A:2643:LEU:HD23 | 1:A:2643:LEU:C    | 2.45                     | 0.41              |
| 1:A:3698:LEU:O    | 1:A:3702:VAL:HG23 | 2.20                     | 0.41              |
| 1:G:3593:VAL:HA   | 1:G:3596:VAL:HG22 | 2.03                     | 0.41              |
| 1:M:1867:GLU:HB2  | 1:M:1927:LEU:HD12 | 2.03                     | 0.41              |
| 1:M:2750:LYS:O    | 1:M:2750:LYS:HG2  | 2.20                     | 0.41              |
| 1:M:3281:LEU:HB2  | 1:M:3282:PRO:HD3  | 2.02                     | 0.41              |
| 1:M:3409:TYR:N    | 1:M:3410:PRO:HD2  | 2.36                     | 0.41              |
| 1:M:4020:GLN:O    | 1:M:4024:VAL:HG23 | 2.21                     | 0.41              |
| 5:M:5105:117:H91  | 5:M:5105:117:H71  | 1.93                     | 0.41              |
| 1:S:828:GLU:OE2   | 1:S:831:ARG:NH1   | 2.51                     | 0.41              |
| 1:S:1762:LEU:O    | 1:S:1765:VAL:HG22 | 2.21                     | 0.41              |
| 1:S:1773:PRO:CA   | 1:S:2153:MET:HE1  | 2.51                     | 0.41              |
| 1:S:3593:VAL:HA   | 1:S:3596:VAL:HG22 | 2.03                     | 0.41              |
| 1:S:4708:THR:HG22 | 1:S:4710:SER:H    | 1.85                     | 0.41              |
| 1:A:426:ARG:HB3   | 1:A:430:PRO:HA    | 2.03                     | 0.41              |
| 1:A:1543:GLU:HG2  | 1:A:1544:PRO:HD2  | 2.03                     | 0.41              |
| 1:A:1694:LEU:O    | 1:A:1698:LEU:HG   | 2.20                     | 0.41              |
| 1:A:3530:GLN:O    | 1:A:3534:MET:HG2  | 2.21                     | 0.41              |
| 1:A:4671:PHE:N    | 1:A:4714:ASN:HD22 | 2.19                     | 0.41              |
| 1:G:205:ILE:HG23  | 1:G:206:CYS:N     | 2.36                     | 0.41              |
| 1:G:904:HIS:HE1   | 1:G:906:CYS:SG    | 2.43                     | 0.41              |
| 1:G:1543:GLU:HG2  | 1:G:1544:PRO:HD2  | 2.03                     | 0.41              |
| 1:G:2960:LEU:HB3  | 1:G:3038:MET:HE2  | 2.02                     | 0.41              |
| 1:G:3003:LEU:HB2  | 1:G:3004:PRO:HD3  | 2.01                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:G:3530:GLN:O    | 1:G:3534:MET:HG2  | 2.21                     | 0.41              |
| 1:G:3946:GLN:HA   | 1:G:3949:ARG:HG2  | 2.02                     | 0.41              |
| 1:G:4091:LYS:O    | 1:G:4095:LYS:NZ   | 2.52                     | 0.41              |
| 1:G:4779:LYS:O    | 1:G:4782:VAL:HG12 | 2.21                     | 0.41              |
| 1:M:196:MET:HE2   | 1:M:196:MET:N     | 2.36                     | 0.41              |
| 1:M:426:ARG:HB3   | 1:M:430:PRO:HA    | 2.03                     | 0.41              |
| 1:M:1164:LEU:O    | 1:M:1167:GLU:N    | 2.50                     | 0.41              |
| 1:M:1773:PRO:CA   | 1:M:2153:MET:HE1  | 2.51                     | 0.41              |
| 1:M:3006:ILE:HG23 | 1:M:3010:PHE:CE2  | 2.55                     | 0.41              |
| 1:M:3593:VAL:HA   | 1:M:3596:VAL:HG22 | 2.03                     | 0.41              |
| 1:S:664:PHE:CE1   | 1:S:746:CYS:HB2   | 2.56                     | 0.41              |
| 1:S:2101:MET:HA   | 1:S:2101:MET:HE3  | 2.02                     | 0.41              |
| 1:S:2113:SER:O    | 1:S:2117:VAL:HG23 | 2.20                     | 0.41              |
| 1:S:3281:LEU:HB2  | 1:S:3282:PRO:HD3  | 2.02                     | 0.41              |
| 1:S:3409:TYR:N    | 1:S:3410:PRO:HD2  | 2.36                     | 0.41              |
| 1:S:4231:MET:O    | 1:S:4235:VAL:HG23 | 2.21                     | 0.41              |
| 1:A:1024:TYR:CZ   | 1:A:1032:LYS:HG2  | 2.56                     | 0.41              |
| 1:A:1184:ILE:HG23 | 1:A:1185:GLY:N    | 2.36                     | 0.41              |
| 1:A:3409:TYR:N    | 1:A:3410:PRO:HD2  | 2.36                     | 0.41              |
| 1:A:5034:ASP:O    | 1:A:5035:GLN:HB2  | 2.21                     | 0.41              |
| 1:G:664:PHE:CE1   | 1:G:746:CYS:HB2   | 2.56                     | 0.41              |
| 1:G:1828:ASP:N    | 1:G:1828:ASP:OD1  | 2.54                     | 0.41              |
| 1:G:2101:MET:HA   | 1:G:2101:MET:HE3  | 2.02                     | 0.41              |
| 1:G:3201:MET:HA   | 1:G:3202:PRO:HD3  | 1.98                     | 0.41              |
| 1:M:1184:ILE:HG23 | 1:M:1185:GLY:N    | 2.36                     | 0.41              |
| 1:M:1694:LEU:O    | 1:M:1698:LEU:HG   | 2.20                     | 0.41              |
| 1:M:3812:VAL:O    | 1:M:3816:MET:HG3  | 2.21                     | 0.41              |
| 2:N:24:VAL:HG22   | 2:N:48:LYS:HG2    | 2.02                     | 0.41              |
| 1:S:196:MET:HE2   | 1:S:196:MET:N     | 2.36                     | 0.41              |
| 1:S:1024:TYR:CZ   | 1:S:1032:LYS:HG2  | 2.56                     | 0.41              |
| 1:S:1867:GLU:HB2  | 1:S:1927:LEU:HD12 | 2.03                     | 0.41              |
| 2:T:24:VAL:HG22   | 2:T:48:LYS:HG2    | 2.02                     | 0.41              |
| 1:A:495:ASN:OD1   | 1:A:553:ARG:NH1   | 2.54                     | 0.40              |
| 1:A:1154:ASP:OD1  | 1:A:1156:THR:OG1  | 2.39                     | 0.40              |
| 1:A:4020:GLN:O    | 1:A:4024:VAL:HG23 | 2.21                     | 0.40              |
| 1:G:202:MET:HE2   | 1:G:202:MET:HB2   | 1.99                     | 0.40              |
| 1:G:3409:TYR:N    | 1:G:3410:PRO:HD2  | 2.36                     | 0.40              |
| 1:G:4662:ASN:O    | 1:G:4662:ASN:OD1  | 2.40                     | 0.40              |
| 1:G:4671:PHE:N    | 1:G:4714:ASN:HD22 | 2.19                     | 0.40              |
| 1:M:1272:LEU:CD2  | 1:M:1561:VAL:HG21 | 2.44                     | 0.40              |
| 1:M:1762:LEU:O    | 1:M:1765:VAL:HG22 | 2.21                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:M:2101:MET:HE3  | 1:M:2101:MET:HA   | 2.02                     | 0.40              |
| 1:M:4231:MET:O    | 1:M:4235:VAL:HG23 | 2.21                     | 0.40              |
| 1:S:495:ASN:OD1   | 1:S:553:ARG:NH1   | 2.54                     | 0.40              |
| 1:S:904:HIS:HE1   | 1:S:906:CYS:SG    | 2.43                     | 0.40              |
| 1:S:1154:ASP:OD1  | 1:S:1156:THR:OG1  | 2.39                     | 0.40              |
| 1:S:2276:ALA:O    | 1:S:2280:VAL:HG12 | 2.20                     | 0.40              |
| 1:S:3916:ILE:CG2  | 1:S:3980:LEU:HD21 | 2.51                     | 0.40              |
| 1:S:4671:PHE:N    | 1:S:4714:ASN:HD22 | 2.19                     | 0.40              |
| 1:S:4779:LYS:O    | 1:S:4782:VAL:HG12 | 2.21                     | 0.40              |
| 1:A:904:HIS:HE1   | 1:A:906:CYS:SG    | 2.43                     | 0.40              |
| 1:G:462:GLU:HG2   | 1:G:463:GLU:N     | 2.37                     | 0.40              |
| 1:G:495:ASN:OD1   | 1:G:553:ARG:NH1   | 2.54                     | 0.40              |
| 1:G:3316:LEU:HD23 | 1:G:3353:LEU:CD2  | 2.51                     | 0.40              |
| 1:G:3812:VAL:O    | 1:G:3816:MET:HG3  | 2.21                     | 0.40              |
| 1:G:3916:ILE:CG2  | 1:G:3980:LEU:HD21 | 2.51                     | 0.40              |
| 1:M:904:HIS:HE1   | 1:M:906:CYS:SG    | 2.43                     | 0.40              |
| 1:M:1154:ASP:OD1  | 1:M:1156:THR:OG1  | 2.39                     | 0.40              |
| 1:M:3530:GLN:O    | 1:M:3534:MET:HG2  | 2.21                     | 0.40              |
| 1:M:4779:LYS:O    | 1:M:4782:VAL:HG12 | 2.21                     | 0.40              |
| 1:M:4779:LYS:O    | 1:M:4783:ILE:HG13 | 2.21                     | 0.40              |
| 1:S:1841:VAL:O    | 1:S:1845:VAL:HG23 | 2.22                     | 0.40              |
| 1:A:1272:LEU:CD2  | 1:A:1561:VAL:HG21 | 2.44                     | 0.40              |
| 1:A:1846:SER:O    | 1:A:1850:VAL:HG23 | 2.22                     | 0.40              |
| 1:A:2865:VAL:HG21 | 1:A:2932:MET:HE2  | 2.04                     | 0.40              |
| 1:A:4779:LYS:O    | 1:A:4782:VAL:HG12 | 2.21                     | 0.40              |
| 1:G:196:MET:HE2   | 1:G:196:MET:N     | 2.36                     | 0.40              |
| 1:G:1024:TYR:CZ   | 1:G:1032:LYS:HG2  | 2.56                     | 0.40              |
| 1:G:4180:ARG:HD3  | 1:G:4192:ARG:HD3  | 2.01                     | 0.40              |
| 1:G:4779:LYS:O    | 1:G:4783:ILE:HG13 | 2.21                     | 0.40              |
| 1:M:1543:GLU:HG2  | 1:M:1544:PRO:HD2  | 2.03                     | 0.40              |
| 1:M:1846:SER:O    | 1:M:1850:VAL:HG23 | 2.22                     | 0.40              |
| 1:M:2333:ASP:OD1  | 1:M:2334:PHE:N    | 2.54                     | 0.40              |
| 1:M:3050:VAL:HG21 | 1:M:3068:LEU:HD11 | 2.03                     | 0.40              |
| 1:M:3316:LEU:HD23 | 1:M:3353:LEU:CD2  | 2.51                     | 0.40              |
| 1:S:2203:MET:HE2  | 1:S:2203:MET:HB3  | 1.97                     | 0.40              |
| 1:S:2992:GLU:O    | 1:S:2995:ILE:HG22 | 2.21                     | 0.40              |
| 1:S:3812:VAL:O    | 1:S:3816:MET:HG3  | 2.21                     | 0.40              |
| 1:A:1139:PHE:HZ   | 1:A:1169:LEU:O    | 2.04                     | 0.40              |
| 1:A:1867:GLU:HB2  | 1:A:1927:LEU:HD12 | 2.03                     | 0.40              |
| 1:A:2527:LEU:HD12 | 1:A:2530:MET:CE   | 2.50                     | 0.40              |
| 1:A:2960:LEU:HB3  | 1:A:3038:MET:HE2  | 2.02                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:3812:VAL:O    | 1:A:3816:MET:HG3  | 2.21                     | 0.40              |
| 1:G:1154:ASP:OD1  | 1:G:1156:THR:OG1  | 2.39                     | 0.40              |
| 1:G:1694:LEU:O    | 1:G:1698:LEU:HG   | 2.20                     | 0.40              |
| 5:G:5105:117:H62  | 5:G:5105:117:C81  | 2.52                     | 0.40              |
| 1:M:5034:ASP:O    | 1:M:5035:GLN:HB2  | 2.21                     | 0.40              |
| 5:M:5105:117:H62  | 5:M:5105:117:C81  | 2.52                     | 0.40              |
| 1:S:1426:ILE:HG23 | 1:S:1429:ASN:H    | 1.85                     | 0.40              |
| 1:S:1846:SER:O    | 1:S:1850:VAL:HG23 | 2.22                     | 0.40              |
| 1:S:4222:VAL:CG1  | 1:S:4950:VAL:CG1  | 2.98                     | 0.40              |
| 1:A:2161:GLN:O    | 1:A:2165:LEU:CD2  | 2.67                     | 0.40              |
| 1:A:3916:ILE:CG2  | 1:A:3980:LEU:HD21 | 2.51                     | 0.40              |
| 2:B:24:VAL:HG22   | 2:B:48:LYS:HG2    | 2.02                     | 0.40              |
| 1:G:172:VAL:HG22  | 1:G:179:TYR:CD1   | 2.57                     | 0.40              |
| 1:G:426:ARG:HB3   | 1:G:430:PRO:HA    | 2.03                     | 0.40              |
| 1:G:1139:PHE:HZ   | 1:G:1169:LEU:O    | 2.04                     | 0.40              |
| 1:G:1426:ILE:HG23 | 1:G:1429:ASN:H    | 1.85                     | 0.40              |
| 1:G:1762:LEU:O    | 1:G:1765:VAL:HG22 | 2.21                     | 0.40              |
| 1:G:2525:GLY:O    | 1:G:2528:PRO:HD2  | 2.22                     | 0.40              |
| 1:M:1841:VAL:O    | 1:M:1845:VAL:HG23 | 2.22                     | 0.40              |
| 1:M:2638:LYS:HD2  | 1:M:2698:MET:SD   | 2.62                     | 0.40              |
| 1:M:3388:GLU:O    | 1:M:3392:LEU:CD2  | 2.70                     | 0.40              |
| 1:M:4662:ASN:O    | 1:M:4662:ASN:OD1  | 2.40                     | 0.40              |
| 1:S:752:VAL:O     | 1:S:752:VAL:CG1   | 2.69                     | 0.40              |
| 1:S:1139:PHE:HZ   | 1:S:1169:LEU:O    | 2.04                     | 0.40              |
| 1:S:2161:GLN:O    | 1:S:2165:LEU:CD2  | 2.67                     | 0.40              |
| 1:S:2914:LYS:HA   | 1:S:2914:LYS:HD2  | 1.94                     | 0.40              |
| 1:S:3530:GLN:O    | 1:S:3534:MET:HG2  | 2.21                     | 0.40              |
| 5:S:5105:117:C81  | 5:S:5105:117:H62  | 2.52                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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     | 3992/5037 (79%)   | 3897 (98%)  | 94 (2%)  | 1 (0%)   | 100         | 100 |
| 1   | G     | 3992/5037 (79%)   | 3897 (98%)  | 94 (2%)  | 1 (0%)   | 100         | 100 |
| 1   | M     | 3992/5037 (79%)   | 3897 (98%)  | 94 (2%)  | 1 (0%)   | 100         | 100 |
| 1   | S     | 3992/5037 (79%)   | 3897 (98%)  | 94 (2%)  | 1 (0%)   | 100         | 100 |
| 2   | B     | 105/111 (95%)     | 100 (95%)   | 5 (5%)   | 0        | 100         | 100 |
| 2   | H     | 105/111 (95%)     | 100 (95%)   | 5 (5%)   | 0        | 100         | 100 |
| 2   | N     | 105/111 (95%)     | 100 (95%)   | 5 (5%)   | 0        | 100         | 100 |
| 2   | T     | 105/111 (95%)     | 100 (95%)   | 5 (5%)   | 0        | 100         | 100 |
| All | All   | 16388/20592 (80%) | 15988 (98%) | 396 (2%) | 4 (0%)   | 100         | 100 |

All (4) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 3971 | GLY  |
| 1   | G     | 3971 | GLY  |
| 1   | M     | 3971 | GLY  |
| 1   | S     | 3971 | GLY  |

### 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 PDB entries followed by that with respect to all EM entries.

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     | 3379/4276 (79%)   | 3379 (100%)  | 0        | 100         | 100 |
| 1   | G     | 3379/4276 (79%)   | 3379 (100%)  | 0        | 100         | 100 |
| 1   | M     | 3379/4276 (79%)   | 3379 (100%)  | 0        | 100         | 100 |
| 1   | S     | 3379/4276 (79%)   | 3379 (100%)  | 0        | 100         | 100 |
| 2   | B     | 86/91 (94%)       | 86 (100%)    | 0        | 100         | 100 |
| 2   | H     | 86/91 (94%)       | 86 (100%)    | 0        | 100         | 100 |
| 2   | N     | 86/91 (94%)       | 86 (100%)    | 0        | 100         | 100 |
| 2   | T     | 86/91 (94%)       | 86 (100%)    | 0        | 100         | 100 |
| All | All   | 13860/17468 (79%) | 13860 (100%) | 0        | 100         | 100 |

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (152) such sidechains are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 113  | HIS  |
| 1   | A     | 201  | ASN  |
| 1   | A     | 465  | GLN  |
| 1   | A     | 797  | HIS  |
| 1   | A     | 909  | ASN  |
| 1   | A     | 911  | HIS  |
| 1   | A     | 1429 | ASN  |
| 1   | A     | 1598 | GLN  |
| 1   | A     | 1629 | GLN  |
| 1   | A     | 1640 | HIS  |
| 1   | A     | 1660 | GLN  |
| 1   | A     | 1702 | HIS  |
| 1   | A     | 1928 | GLN  |
| 1   | A     | 1953 | HIS  |
| 1   | A     | 2035 | HIS  |
| 1   | A     | 2100 | HIS  |
| 1   | A     | 2125 | HIS  |
| 1   | A     | 2441 | HIS  |
| 1   | A     | 2515 | GLN  |
| 1   | A     | 2620 | GLN  |
| 1   | A     | 2773 | ASN  |
| 1   | A     | 2780 | ASN  |
| 1   | A     | 2877 | GLN  |
| 1   | A     | 2931 | GLN  |
| 1   | A     | 3146 | HIS  |
| 1   | A     | 3313 | ASN  |
| 1   | A     | 3523 | ASN  |
| 1   | A     | 3608 | GLN  |
| 1   | A     | 3667 | HIS  |
| 1   | A     | 3970 | GLN  |
| 1   | A     | 3976 | ASN  |
| 1   | A     | 4204 | GLN  |
| 1   | A     | 4574 | ASN  |
| 1   | A     | 4714 | ASN  |
| 1   | A     | 4776 | GLN  |
| 1   | A     | 4812 | HIS  |
| 1   | A     | 4947 | GLN  |
| 1   | A     | 4983 | HIS  |
| 1   | G     | 113  | HIS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | G     | 201  | ASN  |
| 1   | G     | 379  | HIS  |
| 1   | G     | 465  | GLN  |
| 1   | G     | 797  | HIS  |
| 1   | G     | 909  | ASN  |
| 1   | G     | 911  | HIS  |
| 1   | G     | 1429 | ASN  |
| 1   | G     | 1598 | GLN  |
| 1   | G     | 1629 | GLN  |
| 1   | G     | 1640 | HIS  |
| 1   | G     | 1660 | GLN  |
| 1   | G     | 1702 | HIS  |
| 1   | G     | 1928 | GLN  |
| 1   | G     | 1953 | HIS  |
| 1   | G     | 2035 | HIS  |
| 1   | G     | 2100 | HIS  |
| 1   | G     | 2441 | HIS  |
| 1   | G     | 2515 | GLN  |
| 1   | G     | 2620 | GLN  |
| 1   | G     | 2773 | ASN  |
| 1   | G     | 2780 | ASN  |
| 1   | G     | 2856 | ASN  |
| 1   | G     | 2858 | GLN  |
| 1   | G     | 2877 | GLN  |
| 1   | G     | 2931 | GLN  |
| 1   | G     | 3146 | HIS  |
| 1   | G     | 3313 | ASN  |
| 1   | G     | 3523 | ASN  |
| 1   | G     | 3608 | GLN  |
| 1   | G     | 3667 | HIS  |
| 1   | G     | 3970 | GLN  |
| 1   | G     | 3976 | ASN  |
| 1   | G     | 4204 | GLN  |
| 1   | G     | 4209 | GLN  |
| 1   | G     | 4574 | ASN  |
| 1   | G     | 4714 | ASN  |
| 1   | G     | 4776 | GLN  |
| 1   | G     | 4812 | HIS  |
| 1   | G     | 4983 | HIS  |
| 1   | M     | 113  | HIS  |
| 1   | M     | 201  | ASN  |
| 1   | M     | 379  | HIS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | M     | 465  | GLN  |
| 1   | M     | 797  | HIS  |
| 1   | M     | 909  | ASN  |
| 1   | M     | 911  | HIS  |
| 1   | M     | 1429 | ASN  |
| 1   | M     | 1598 | GLN  |
| 1   | M     | 1629 | GLN  |
| 1   | M     | 1640 | HIS  |
| 1   | M     | 1660 | GLN  |
| 1   | M     | 1702 | HIS  |
| 1   | M     | 1928 | GLN  |
| 1   | M     | 1953 | HIS  |
| 1   | M     | 2035 | HIS  |
| 1   | M     | 2100 | HIS  |
| 1   | M     | 2441 | HIS  |
| 1   | M     | 2515 | GLN  |
| 1   | M     | 2620 | GLN  |
| 1   | M     | 2773 | ASN  |
| 1   | M     | 2780 | ASN  |
| 1   | M     | 2877 | GLN  |
| 1   | M     | 3109 | ASN  |
| 1   | M     | 3146 | HIS  |
| 1   | M     | 3313 | ASN  |
| 1   | M     | 3523 | ASN  |
| 1   | M     | 3608 | GLN  |
| 1   | M     | 3667 | HIS  |
| 1   | M     | 3970 | GLN  |
| 1   | M     | 4204 | GLN  |
| 1   | M     | 4209 | GLN  |
| 1   | M     | 4714 | ASN  |
| 1   | M     | 4776 | GLN  |
| 1   | M     | 4812 | HIS  |
| 1   | S     | 113  | HIS  |
| 1   | S     | 201  | ASN  |
| 1   | S     | 465  | GLN  |
| 1   | S     | 797  | HIS  |
| 1   | S     | 909  | ASN  |
| 1   | S     | 911  | HIS  |
| 1   | S     | 1429 | ASN  |
| 1   | S     | 1598 | GLN  |
| 1   | S     | 1629 | GLN  |
| 1   | S     | 1640 | HIS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | S     | 1660 | GLN  |
| 1   | S     | 1702 | HIS  |
| 1   | S     | 1928 | GLN  |
| 1   | S     | 1953 | HIS  |
| 1   | S     | 2035 | HIS  |
| 1   | S     | 2100 | HIS  |
| 1   | S     | 2125 | HIS  |
| 1   | S     | 2441 | HIS  |
| 1   | S     | 2515 | GLN  |
| 1   | S     | 2620 | GLN  |
| 1   | S     | 2773 | ASN  |
| 1   | S     | 2780 | ASN  |
| 1   | S     | 2877 | GLN  |
| 1   | S     | 2931 | GLN  |
| 1   | S     | 3109 | ASN  |
| 1   | S     | 3146 | HIS  |
| 1   | S     | 3313 | ASN  |
| 1   | S     | 3422 | HIS  |
| 1   | S     | 3523 | ASN  |
| 1   | S     | 3608 | GLN  |
| 1   | S     | 3667 | HIS  |
| 1   | S     | 3970 | GLN  |
| 1   | S     | 3976 | ASN  |
| 1   | S     | 4204 | GLN  |
| 1   | S     | 4209 | GLN  |
| 1   | S     | 4714 | ASN  |
| 1   | S     | 4776 | GLN  |
| 1   | S     | 4812 | HIS  |
| 1   | S     | 4947 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 24 ligands modelled in this entry, 8 are monoatomic - leaving 16 for Mogul analysis.

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | CFF  | G     | 5101 | -    | 15,15,15     | 1.07 | 3 (20%)  | 23,23,23    | 2.22 | 9 (39%)  |
| 5   | 117  | G     | 5103 | -    | 44,44,44     | 0.78 | 1 (2%)   | 55,61,61    | 1.31 | 5 (9%)   |
| 5   | 117  | M     | 5104 | -    | 44,44,44     | 0.79 | 1 (2%)   | 55,61,61    | 0.90 | 2 (3%)   |
| 5   | 117  | A     | 5103 | -    | 44,44,44     | 0.78 | 1 (2%)   | 55,61,61    | 1.31 | 5 (9%)   |
| 5   | 117  | S     | 5105 | -    | 44,44,44     | 0.78 | 0        | 55,61,61    | 0.95 | 2 (3%)   |
| 5   | 117  | S     | 5104 | -    | 44,44,44     | 0.79 | 1 (2%)   | 55,61,61    | 0.90 | 2 (3%)   |
| 3   | CFF  | A     | 5101 | -    | 15,15,15     | 1.07 | 3 (20%)  | 23,23,23    | 2.22 | 9 (39%)  |
| 5   | 117  | M     | 5105 | -    | 44,44,44     | 0.78 | 0        | 55,61,61    | 0.95 | 2 (3%)   |
| 3   | CFF  | M     | 5101 | -    | 15,15,15     | 1.07 | 3 (20%)  | 23,23,23    | 2.22 | 9 (39%)  |
| 5   | 117  | G     | 5104 | -    | 44,44,44     | 0.79 | 1 (2%)   | 55,61,61    | 0.90 | 2 (3%)   |
| 5   | 117  | M     | 5103 | -    | 44,44,44     | 0.78 | 1 (2%)   | 55,61,61    | 1.31 | 5 (9%)   |
| 5   | 117  | G     | 5105 | -    | 44,44,44     | 0.78 | 0        | 55,61,61    | 0.95 | 2 (3%)   |
| 5   | 117  | A     | 5105 | -    | 44,44,44     | 0.78 | 0        | 55,61,61    | 0.95 | 2 (3%)   |
| 5   | 117  | S     | 5103 | -    | 44,44,44     | 0.78 | 1 (2%)   | 55,61,61    | 1.31 | 5 (9%)   |
| 5   | 117  | A     | 5104 | -    | 44,44,44     | 0.79 | 1 (2%)   | 55,61,61    | 0.90 | 2 (3%)   |
| 3   | CFF  | S     | 5101 | -    | 15,15,15     | 1.07 | 3 (20%)  | 23,23,23    | 2.22 | 9 (39%)  |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 3   | CFF  | G     | 5101 | -    | -       | -          | 0/2/2/2 |
| 5   | 117  | G     | 5103 | -    | -       | 6/33/33/33 | 0/4/4/4 |
| 5   | 117  | M     | 5104 | -    | -       | 0/33/33/33 | 0/4/4/4 |
| 5   | 117  | A     | 5103 | -    | -       | 6/33/33/33 | 0/4/4/4 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 5   | 117  | S     | 5105 | -    | -       | 9/33/33/33 | 0/4/4/4 |
| 5   | 117  | S     | 5104 | -    | -       | 0/33/33/33 | 0/4/4/4 |
| 3   | CFF  | A     | 5101 | -    | -       | -          | 0/2/2/2 |
| 5   | 117  | M     | 5105 | -    | -       | 9/33/33/33 | 0/4/4/4 |
| 5   | 117  | M     | 5103 | -    | -       | 6/33/33/33 | 0/4/4/4 |
| 5   | 117  | G     | 5104 | -    | -       | 0/33/33/33 | 0/4/4/4 |
| 3   | CFF  | M     | 5101 | -    | -       | -          | 0/2/2/2 |
| 5   | 117  | G     | 5105 | -    | -       | 9/33/33/33 | 0/4/4/4 |
| 3   | CFF  | S     | 5101 | -    | -       | -          | 0/2/2/2 |
| 5   | 117  | A     | 5105 | -    | -       | 9/33/33/33 | 0/4/4/4 |
| 5   | 117  | S     | 5103 | -    | -       | 6/33/33/33 | 0/4/4/4 |
| 5   | 117  | A     | 5104 | -    | -       | 0/33/33/33 | 0/4/4/4 |

All (20) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | A     | 5101 | CFF  | C6-N1   | -2.43 | 1.35        | 1.40     |
| 3   | G     | 5101 | CFF  | C6-N1   | -2.43 | 1.35        | 1.40     |
| 3   | M     | 5101 | CFF  | C6-N1   | -2.43 | 1.35        | 1.40     |
| 3   | S     | 5101 | CFF  | C6-N1   | -2.43 | 1.35        | 1.40     |
| 5   | A     | 5103 | 117  | C12-C10 | -2.21 | 1.45        | 1.49     |
| 5   | G     | 5103 | 117  | C12-C10 | -2.21 | 1.45        | 1.49     |
| 5   | M     | 5103 | 117  | C12-C10 | -2.21 | 1.45        | 1.49     |
| 5   | S     | 5103 | 117  | C12-C10 | -2.21 | 1.45        | 1.49     |
| 3   | A     | 5101 | CFF  | C2-N1   | -2.19 | 1.34        | 1.39     |
| 3   | G     | 5101 | CFF  | C2-N1   | -2.19 | 1.34        | 1.39     |
| 3   | M     | 5101 | CFF  | C2-N1   | -2.19 | 1.34        | 1.39     |
| 3   | S     | 5101 | CFF  | C2-N1   | -2.19 | 1.34        | 1.39     |
| 5   | A     | 5104 | 117  | C12-C10 | -2.12 | 1.45        | 1.49     |
| 5   | G     | 5104 | 117  | C12-C10 | -2.12 | 1.45        | 1.49     |
| 5   | M     | 5104 | 117  | C12-C10 | -2.12 | 1.45        | 1.49     |
| 5   | S     | 5104 | 117  | C12-C10 | -2.12 | 1.45        | 1.49     |
| 3   | A     | 5101 | CFF  | C2-N3   | -2.06 | 1.35        | 1.39     |
| 3   | G     | 5101 | CFF  | C2-N3   | -2.06 | 1.35        | 1.39     |
| 3   | M     | 5101 | CFF  | C2-N3   | -2.06 | 1.35        | 1.39     |
| 3   | S     | 5101 | CFF  | C2-N3   | -2.06 | 1.35        | 1.39     |

All (72) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 5   | A     | 5103 | 117  | C19-N2-C18 | -6.06 | 116.69      | 127.45   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 5   | G     | 5103 | 117  | C19-N2-C18 | -6.06 | 116.69      | 127.45   |
| 5   | M     | 5103 | 117  | C19-N2-C18 | -6.06 | 116.69      | 127.45   |
| 5   | S     | 5103 | 117  | C19-N2-C18 | -6.06 | 116.69      | 127.45   |
| 3   | A     | 5101 | CFF  | N3-C4-N9   | 4.84  | 133.88      | 126.27   |
| 3   | G     | 5101 | CFF  | N3-C4-N9   | 4.84  | 133.88      | 126.27   |
| 3   | M     | 5101 | CFF  | N3-C4-N9   | 4.84  | 133.88      | 126.27   |
| 3   | S     | 5101 | CFF  | N3-C4-N9   | 4.84  | 133.88      | 126.27   |
| 3   | A     | 5101 | CFF  | C5-C6-N1   | 3.88  | 119.16      | 112.06   |
| 3   | G     | 5101 | CFF  | C5-C6-N1   | 3.88  | 119.16      | 112.06   |
| 3   | M     | 5101 | CFF  | C5-C6-N1   | 3.88  | 119.16      | 112.06   |
| 3   | S     | 5101 | CFF  | C5-C6-N1   | 3.88  | 119.16      | 112.06   |
| 3   | A     | 5101 | CFF  | N3-C2-N1   | 3.65  | 121.70      | 117.14   |
| 3   | G     | 5101 | CFF  | N3-C2-N1   | 3.65  | 121.70      | 117.14   |
| 3   | M     | 5101 | CFF  | N3-C2-N1   | 3.65  | 121.70      | 117.14   |
| 3   | S     | 5101 | CFF  | N3-C2-N1   | 3.65  | 121.70      | 117.14   |
| 5   | A     | 5105 | 117  | C6-C7-N1   | 3.30  | 117.93      | 112.16   |
| 5   | G     | 5105 | 117  | C6-C7-N1   | 3.30  | 117.93      | 112.16   |
| 5   | M     | 5105 | 117  | C6-C7-N1   | 3.30  | 117.93      | 112.16   |
| 5   | S     | 5105 | 117  | C6-C7-N1   | 3.30  | 117.93      | 112.16   |
| 5   | A     | 5104 | 117  | C11-C10-C8 | 3.10  | 109.34      | 106.82   |
| 5   | G     | 5104 | 117  | C11-C10-C8 | 3.10  | 109.34      | 106.82   |
| 5   | M     | 5104 | 117  | C11-C10-C8 | 3.10  | 109.34      | 106.82   |
| 5   | S     | 5104 | 117  | C11-C10-C8 | 3.10  | 109.34      | 106.82   |
| 3   | A     | 5101 | CFF  | C6-C5-C4   | -2.98 | 119.16      | 122.92   |
| 3   | G     | 5101 | CFF  | C6-C5-C4   | -2.98 | 119.16      | 122.92   |
| 3   | M     | 5101 | CFF  | C6-C5-C4   | -2.98 | 119.16      | 122.92   |
| 3   | S     | 5101 | CFF  | C6-C5-C4   | -2.98 | 119.16      | 122.92   |
| 3   | A     | 5101 | CFF  | O13-C6-C5  | -2.89 | 120.46      | 126.38   |
| 3   | G     | 5101 | CFF  | O13-C6-C5  | -2.89 | 120.46      | 126.38   |
| 3   | M     | 5101 | CFF  | O13-C6-C5  | -2.89 | 120.46      | 126.38   |
| 3   | S     | 5101 | CFF  | O13-C6-C5  | -2.89 | 120.46      | 126.38   |
| 3   | A     | 5101 | CFF  | C6-N1-C2   | -2.86 | 121.01      | 125.66   |
| 3   | G     | 5101 | CFF  | C6-N1-C2   | -2.86 | 121.01      | 125.66   |
| 3   | M     | 5101 | CFF  | C6-N1-C2   | -2.86 | 121.01      | 125.66   |
| 3   | S     | 5101 | CFF  | C6-N1-C2   | -2.86 | 121.01      | 125.66   |
| 3   | A     | 5101 | CFF  | C8-N9-C4   | 2.85  | 109.82      | 102.98   |
| 3   | G     | 5101 | CFF  | C8-N9-C4   | 2.85  | 109.82      | 102.98   |
| 3   | M     | 5101 | CFF  | C8-N9-C4   | 2.85  | 109.82      | 102.98   |
| 3   | S     | 5101 | CFF  | C8-N9-C4   | 2.85  | 109.82      | 102.98   |
| 5   | A     | 5104 | 117  | C12-C10-C8 | -2.78 | 121.61      | 127.01   |
| 5   | G     | 5104 | 117  | C12-C10-C8 | -2.78 | 121.61      | 127.01   |
| 5   | M     | 5104 | 117  | C12-C10-C8 | -2.78 | 121.61      | 127.01   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 5   | S     | 5104 | 117  | C12-C10-C8  | -2.78 | 121.61      | 127.01   |
| 5   | A     | 5103 | 117  | C5-C4-C3    | 2.62  | 118.43      | 114.28   |
| 5   | G     | 5103 | 117  | C5-C4-C3    | 2.62  | 118.43      | 114.28   |
| 5   | M     | 5103 | 117  | C5-C4-C3    | 2.62  | 118.43      | 114.28   |
| 5   | S     | 5103 | 117  | C5-C4-C3    | 2.62  | 118.43      | 114.28   |
| 5   | A     | 5105 | 117  | C5-C4-C3    | 2.49  | 118.22      | 114.28   |
| 5   | G     | 5105 | 117  | C5-C4-C3    | 2.49  | 118.22      | 114.28   |
| 5   | M     | 5105 | 117  | C5-C4-C3    | 2.49  | 118.22      | 114.28   |
| 5   | S     | 5105 | 117  | C5-C4-C3    | 2.49  | 118.22      | 114.28   |
| 3   | A     | 5101 | CFF  | C5-C4-N9    | -2.46 | 107.22      | 112.10   |
| 3   | G     | 5101 | CFF  | C5-C4-N9    | -2.46 | 107.22      | 112.10   |
| 3   | M     | 5101 | CFF  | C5-C4-N9    | -2.46 | 107.22      | 112.10   |
| 3   | S     | 5101 | CFF  | C5-C4-N9    | -2.46 | 107.22      | 112.10   |
| 5   | A     | 5103 | 117  | C4-C5-C6    | -2.27 | 107.62      | 112.42   |
| 5   | G     | 5103 | 117  | C4-C5-C6    | -2.27 | 107.62      | 112.42   |
| 5   | M     | 5103 | 117  | C4-C5-C6    | -2.27 | 107.62      | 112.42   |
| 5   | S     | 5103 | 117  | C4-C5-C6    | -2.27 | 107.62      | 112.42   |
| 3   | A     | 5101 | CFF  | N7-C8-N9    | -2.08 | 109.71      | 113.48   |
| 3   | G     | 5101 | CFF  | N7-C8-N9    | -2.08 | 109.71      | 113.48   |
| 3   | M     | 5101 | CFF  | N7-C8-N9    | -2.08 | 109.71      | 113.48   |
| 3   | S     | 5101 | CFF  | N7-C8-N9    | -2.08 | 109.71      | 113.48   |
| 5   | A     | 5103 | 117  | O18-C18-C11 | -2.06 | 118.45      | 121.53   |
| 5   | G     | 5103 | 117  | O18-C18-C11 | -2.06 | 118.45      | 121.53   |
| 5   | M     | 5103 | 117  | O18-C18-C11 | -2.06 | 118.45      | 121.53   |
| 5   | S     | 5103 | 117  | O18-C18-C11 | -2.06 | 118.45      | 121.53   |
| 5   | A     | 5103 | 117  | O3-C3-C4    | -2.05 | 104.71      | 109.25   |
| 5   | G     | 5103 | 117  | O3-C3-C4    | -2.05 | 104.71      | 109.25   |
| 5   | M     | 5103 | 117  | O3-C3-C4    | -2.05 | 104.71      | 109.25   |
| 5   | S     | 5103 | 117  | O3-C3-C4    | -2.05 | 104.71      | 109.25   |

There are no chirality outliers.

All (60) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms          |
|-----|-------|------|------|----------------|
| 5   | A     | 5103 | 117  | C9-C11-C18-O18 |
| 5   | A     | 5105 | 117  | O5-C5-C6-C7    |
| 5   | A     | 5105 | 117  | C9-C11-C18-N2  |
| 5   | G     | 5103 | 117  | C9-C11-C18-O18 |
| 5   | G     | 5105 | 117  | O5-C5-C6-C7    |
| 5   | G     | 5105 | 117  | C9-C11-C18-N2  |
| 5   | M     | 5103 | 117  | C9-C11-C18-O18 |
| 5   | M     | 5105 | 117  | O5-C5-C6-C7    |

*Continued on next page...*

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 5   | M     | 5105 | 117  | C9-C11-C18-N2   |
| 5   | S     | 5103 | 117  | C9-C11-C18-O18  |
| 5   | S     | 5105 | 117  | O5-C5-C6-C7     |
| 5   | S     | 5105 | 117  | C9-C11-C18-N2   |
| 5   | A     | 5103 | 117  | C20-C19-N2-C18  |
| 5   | G     | 5103 | 117  | C20-C19-N2-C18  |
| 5   | M     | 5103 | 117  | C20-C19-N2-C18  |
| 5   | S     | 5103 | 117  | C20-C19-N2-C18  |
| 5   | A     | 5103 | 117  | C24-C19-N2-C18  |
| 5   | G     | 5103 | 117  | C24-C19-N2-C18  |
| 5   | M     | 5103 | 117  | C24-C19-N2-C18  |
| 5   | S     | 5103 | 117  | C24-C19-N2-C18  |
| 5   | A     | 5105 | 117  | C4-C5-C6-C7     |
| 5   | G     | 5105 | 117  | C4-C5-C6-C7     |
| 5   | M     | 5105 | 117  | C4-C5-C6-C7     |
| 5   | S     | 5105 | 117  | C4-C5-C6-C7     |
| 5   | A     | 5103 | 117  | C10-C11-C18-N2  |
| 5   | A     | 5103 | 117  | C10-C11-C18-O18 |
| 5   | A     | 5105 | 117  | C10-C11-C18-N2  |
| 5   | A     | 5105 | 117  | C10-C11-C18-O18 |
| 5   | G     | 5103 | 117  | C10-C11-C18-N2  |
| 5   | G     | 5103 | 117  | C10-C11-C18-O18 |
| 5   | G     | 5105 | 117  | C10-C11-C18-N2  |
| 5   | G     | 5105 | 117  | C10-C11-C18-O18 |
| 5   | M     | 5103 | 117  | C10-C11-C18-N2  |
| 5   | M     | 5103 | 117  | C10-C11-C18-O18 |
| 5   | M     | 5105 | 117  | C10-C11-C18-N2  |
| 5   | M     | 5105 | 117  | C10-C11-C18-O18 |
| 5   | S     | 5103 | 117  | C10-C11-C18-N2  |
| 5   | S     | 5103 | 117  | C10-C11-C18-O18 |
| 5   | S     | 5105 | 117  | C10-C11-C18-N2  |
| 5   | S     | 5105 | 117  | C10-C11-C18-O18 |
| 5   | A     | 5105 | 117  | C6-C7-N1-C9     |
| 5   | G     | 5105 | 117  | C6-C7-N1-C9     |
| 5   | M     | 5105 | 117  | C6-C7-N1-C9     |
| 5   | S     | 5105 | 117  | C6-C7-N1-C9     |
| 5   | A     | 5105 | 117  | C9-C11-C18-O18  |
| 5   | G     | 5105 | 117  | C9-C11-C18-O18  |
| 5   | M     | 5105 | 117  | C9-C11-C18-O18  |
| 5   | S     | 5105 | 117  | C9-C11-C18-O18  |
| 5   | A     | 5103 | 117  | C9-C11-C18-N2   |
| 5   | G     | 5103 | 117  | C9-C11-C18-N2   |

*Continued on next page...*

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| Mol | Chain | Res  | Type | Atoms         |
|-----|-------|------|------|---------------|
| 5   | M     | 5103 | 117  | C9-C11-C18-N2 |
| 5   | S     | 5103 | 117  | C9-C11-C18-N2 |
| 5   | A     | 5105 | 117  | C6-C7-N1-C8   |
| 5   | G     | 5105 | 117  | C6-C7-N1-C8   |
| 5   | M     | 5105 | 117  | C6-C7-N1-C8   |
| 5   | S     | 5105 | 117  | C6-C7-N1-C8   |
| 5   | A     | 5105 | 117  | O1A-C1-C2-C3  |
| 5   | G     | 5105 | 117  | O1A-C1-C2-C3  |
| 5   | M     | 5105 | 117  | O1A-C1-C2-C3  |
| 5   | S     | 5105 | 117  | O1A-C1-C2-C3  |

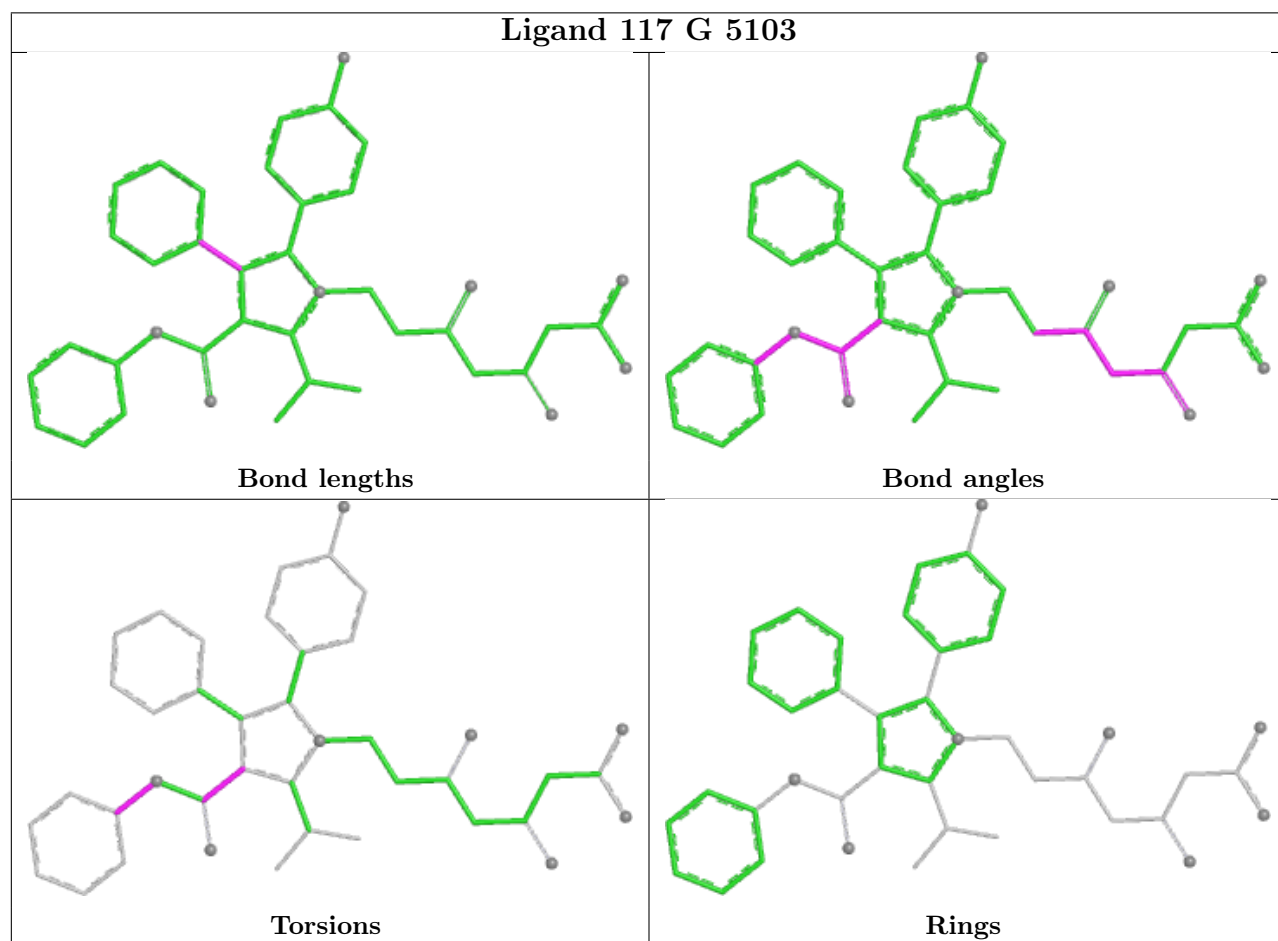
There are no ring outliers.

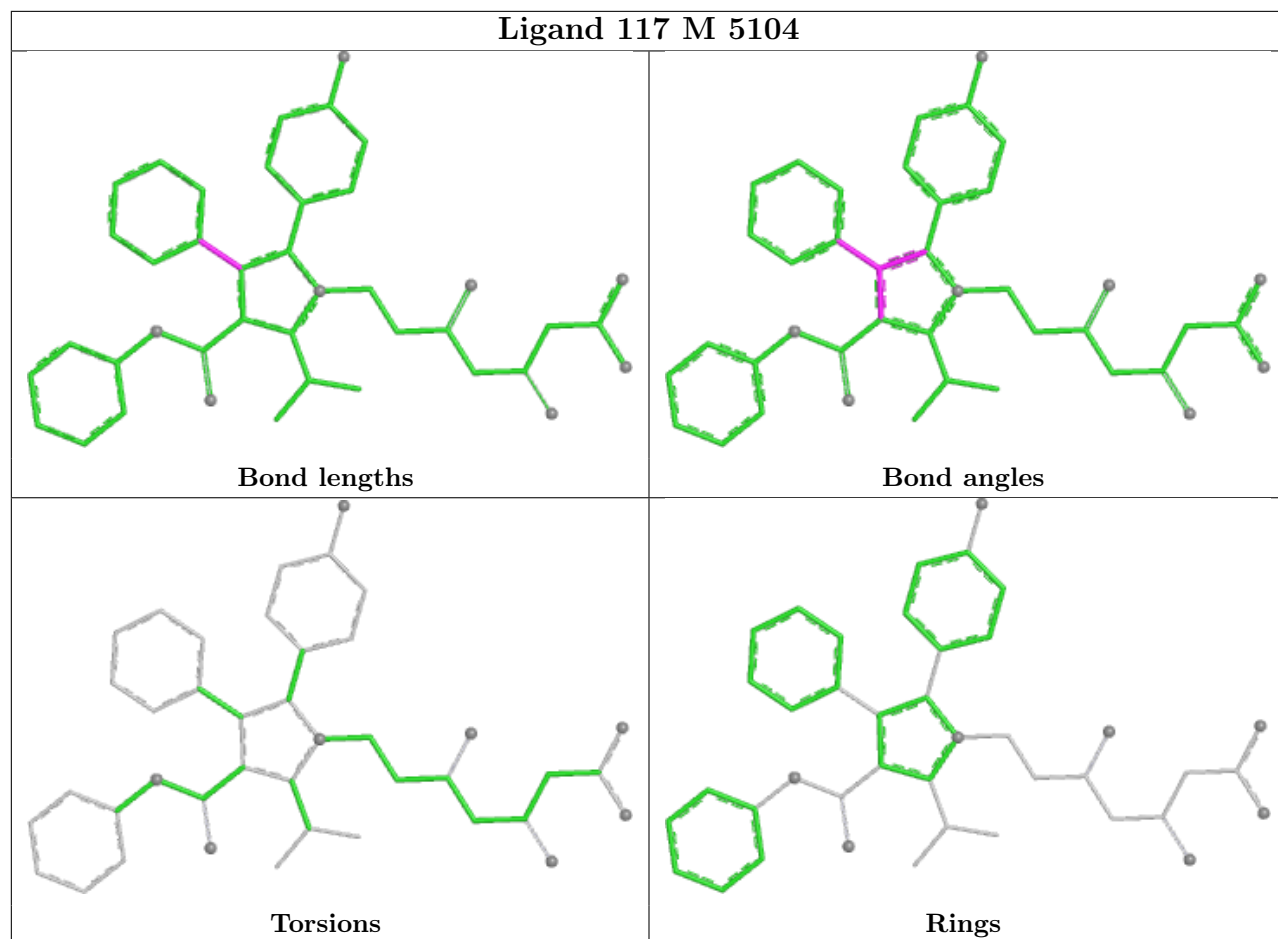
16 monomers are involved in 41 short contacts:

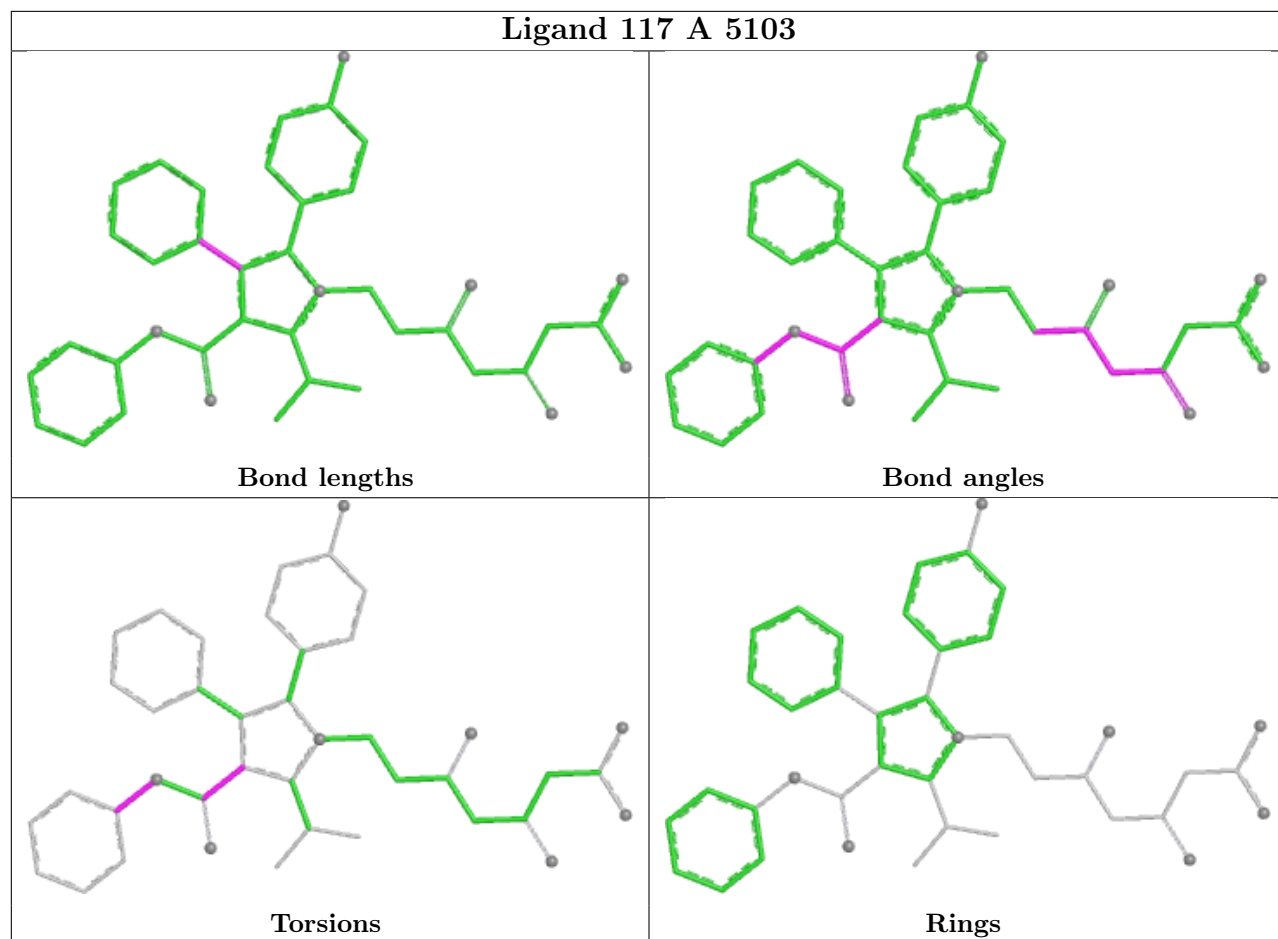
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 3   | G     | 5101 | CFF  | 1       | 0            |
| 5   | G     | 5103 | 117  | 4       | 0            |
| 5   | M     | 5104 | 117  | 3       | 0            |
| 5   | A     | 5103 | 117  | 4       | 0            |
| 5   | S     | 5105 | 117  | 4       | 0            |
| 5   | S     | 5104 | 117  | 3       | 0            |
| 3   | A     | 5101 | CFF  | 1       | 0            |
| 5   | M     | 5105 | 117  | 5       | 0            |
| 3   | M     | 5101 | CFF  | 1       | 0            |
| 5   | G     | 5104 | 117  | 3       | 0            |
| 5   | M     | 5103 | 117  | 4       | 0            |
| 5   | G     | 5105 | 117  | 5       | 0            |
| 5   | A     | 5105 | 117  | 3       | 0            |
| 5   | S     | 5103 | 117  | 4       | 0            |
| 5   | A     | 5104 | 117  | 3       | 0            |
| 3   | S     | 5101 | CFF  | 1       | 0            |

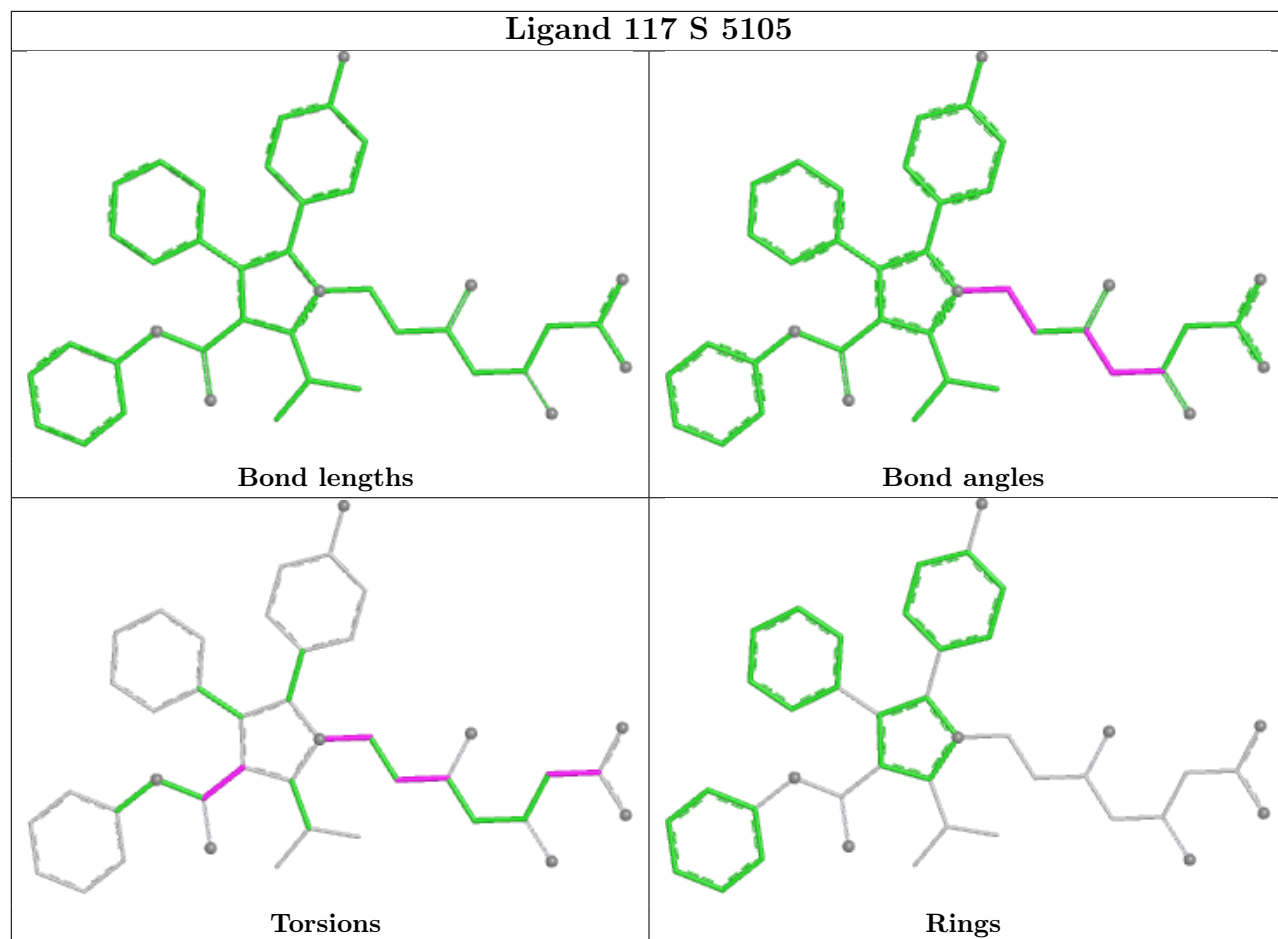
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

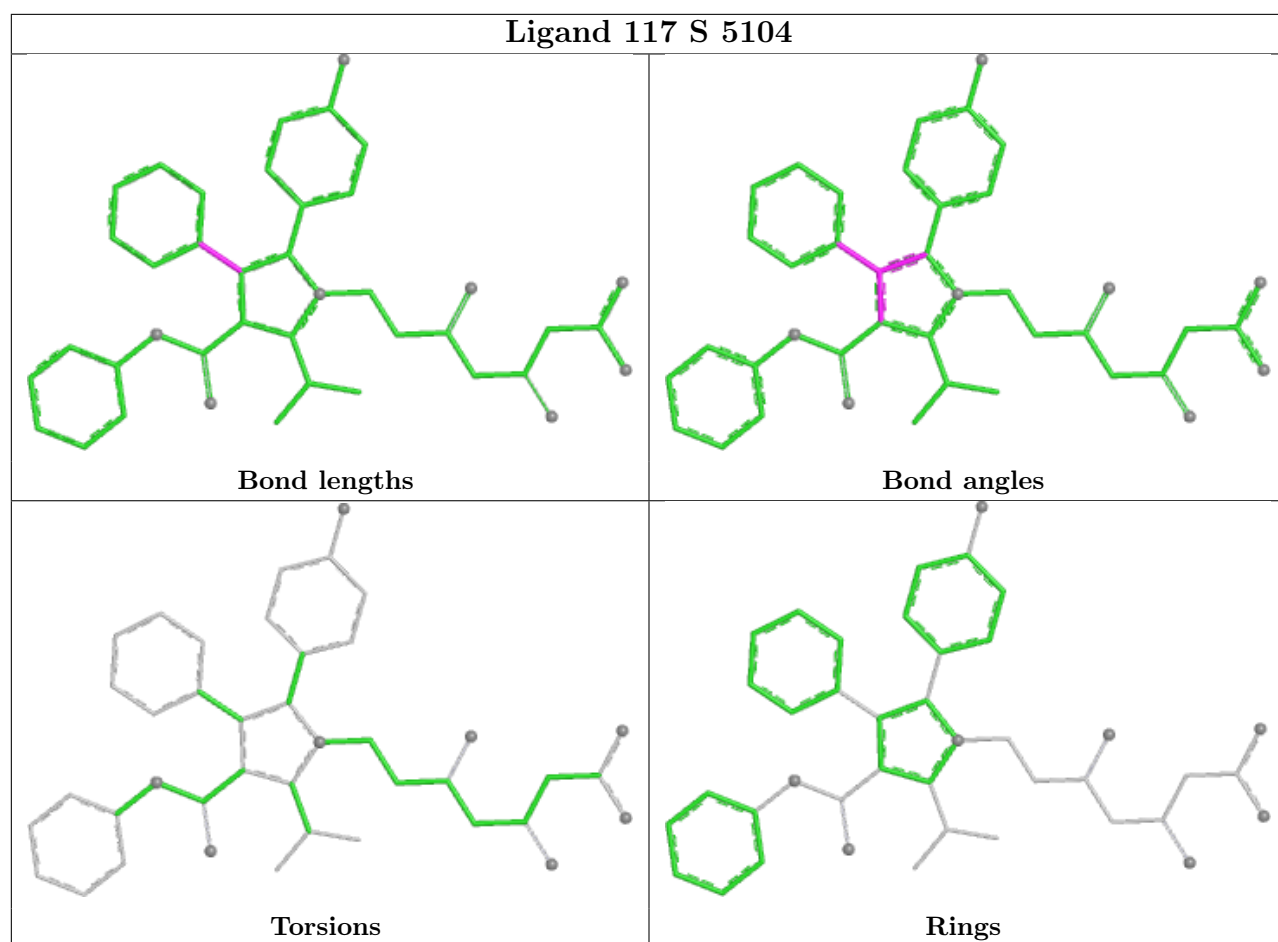
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

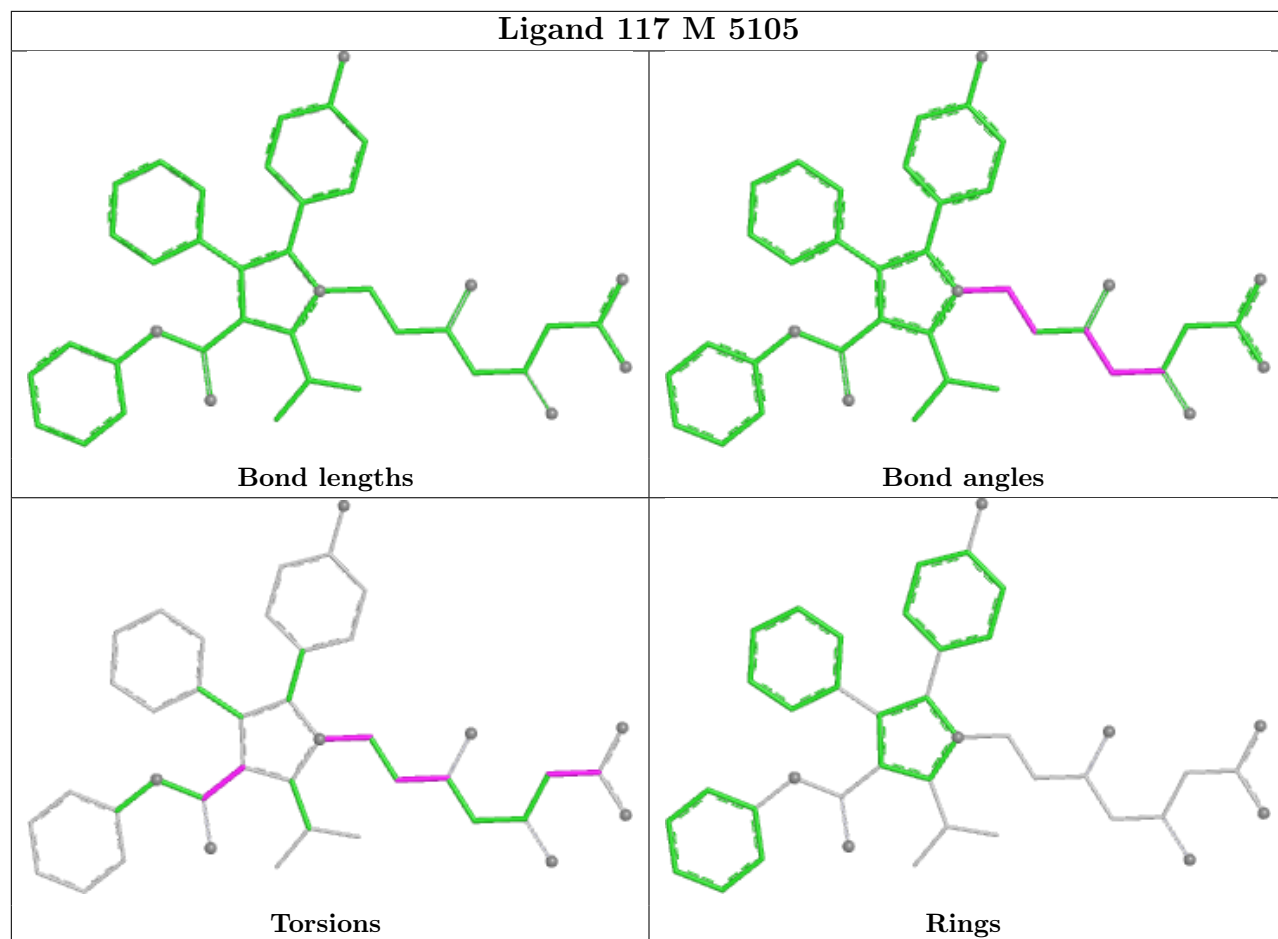


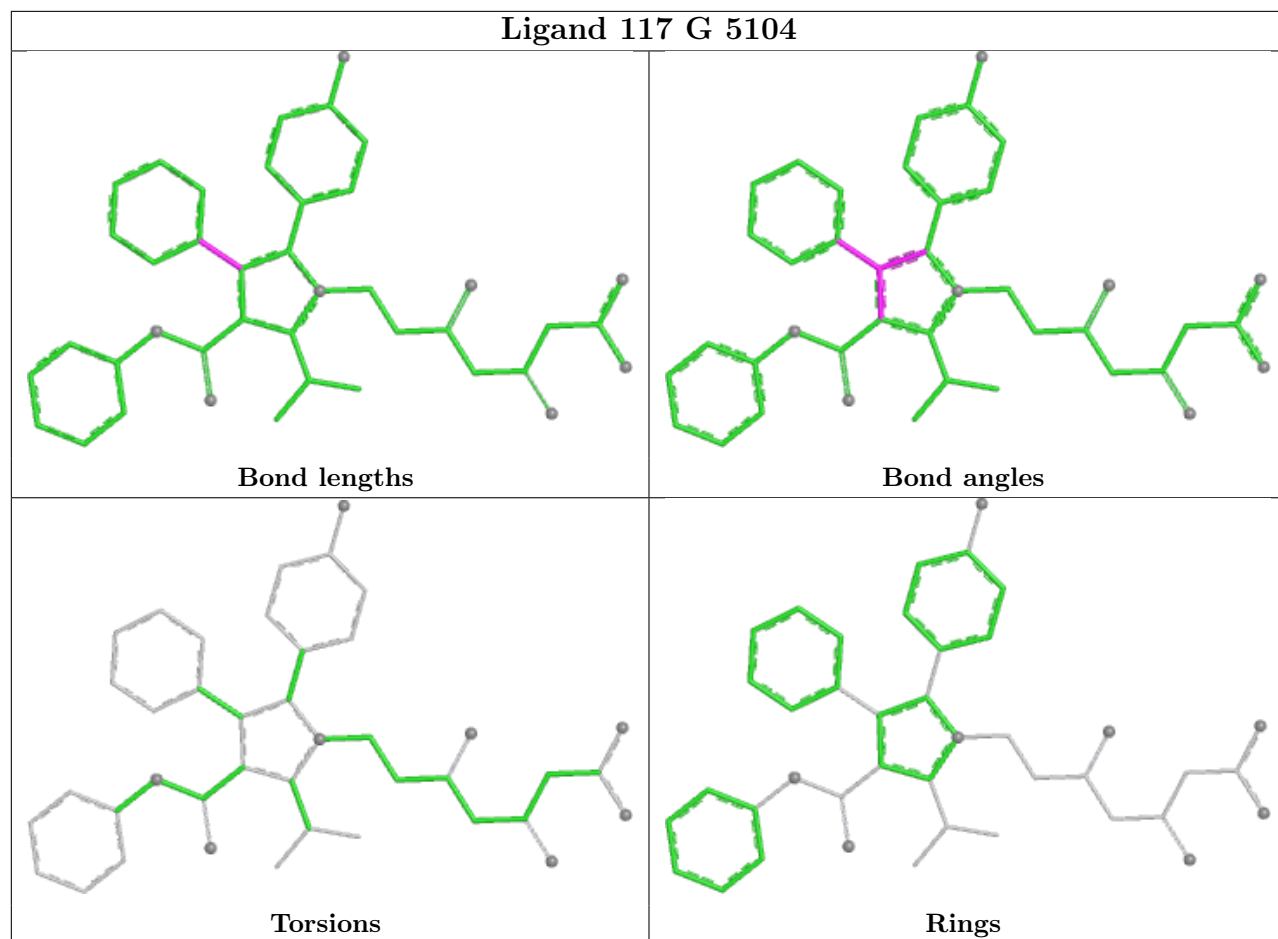


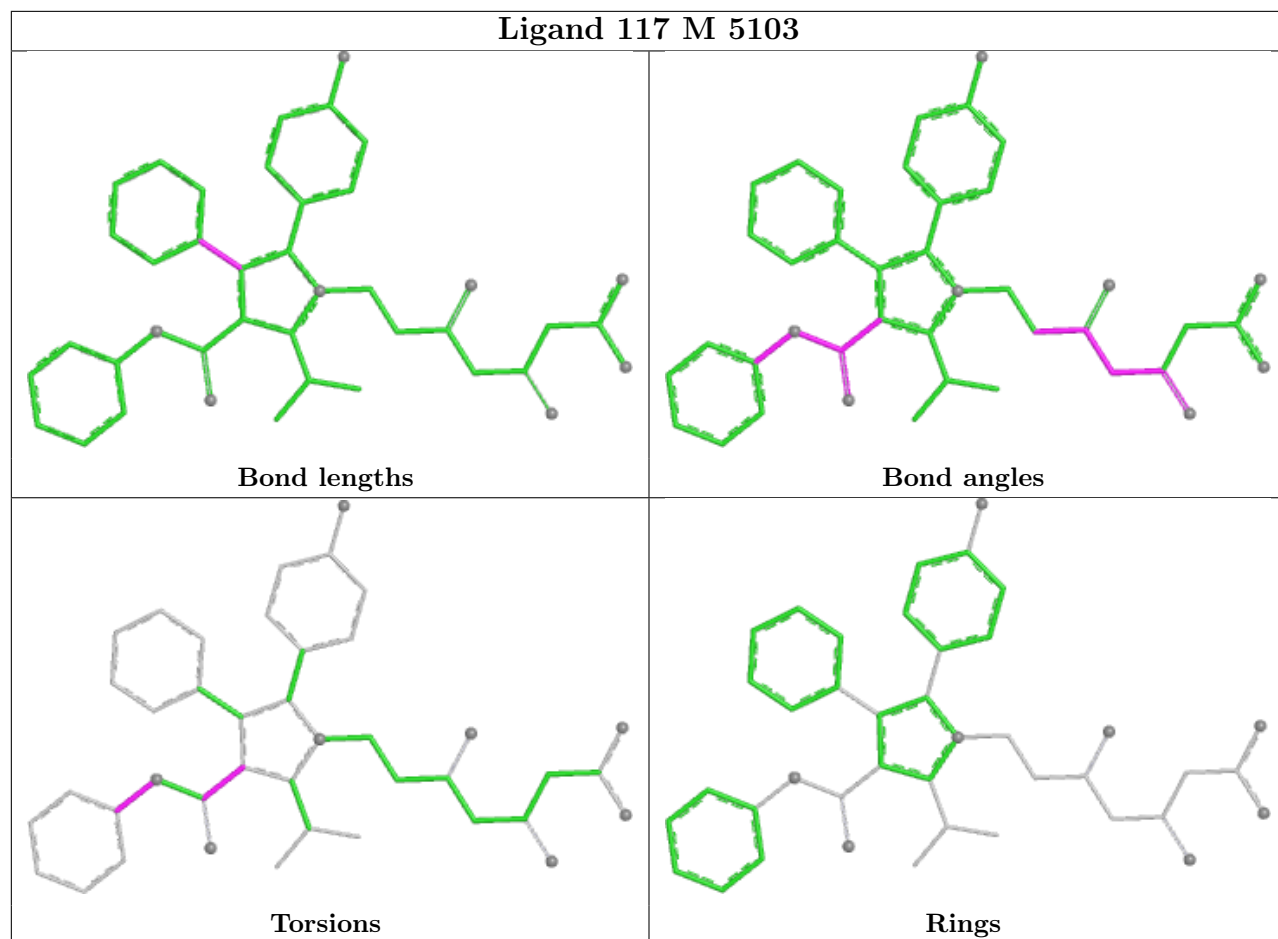


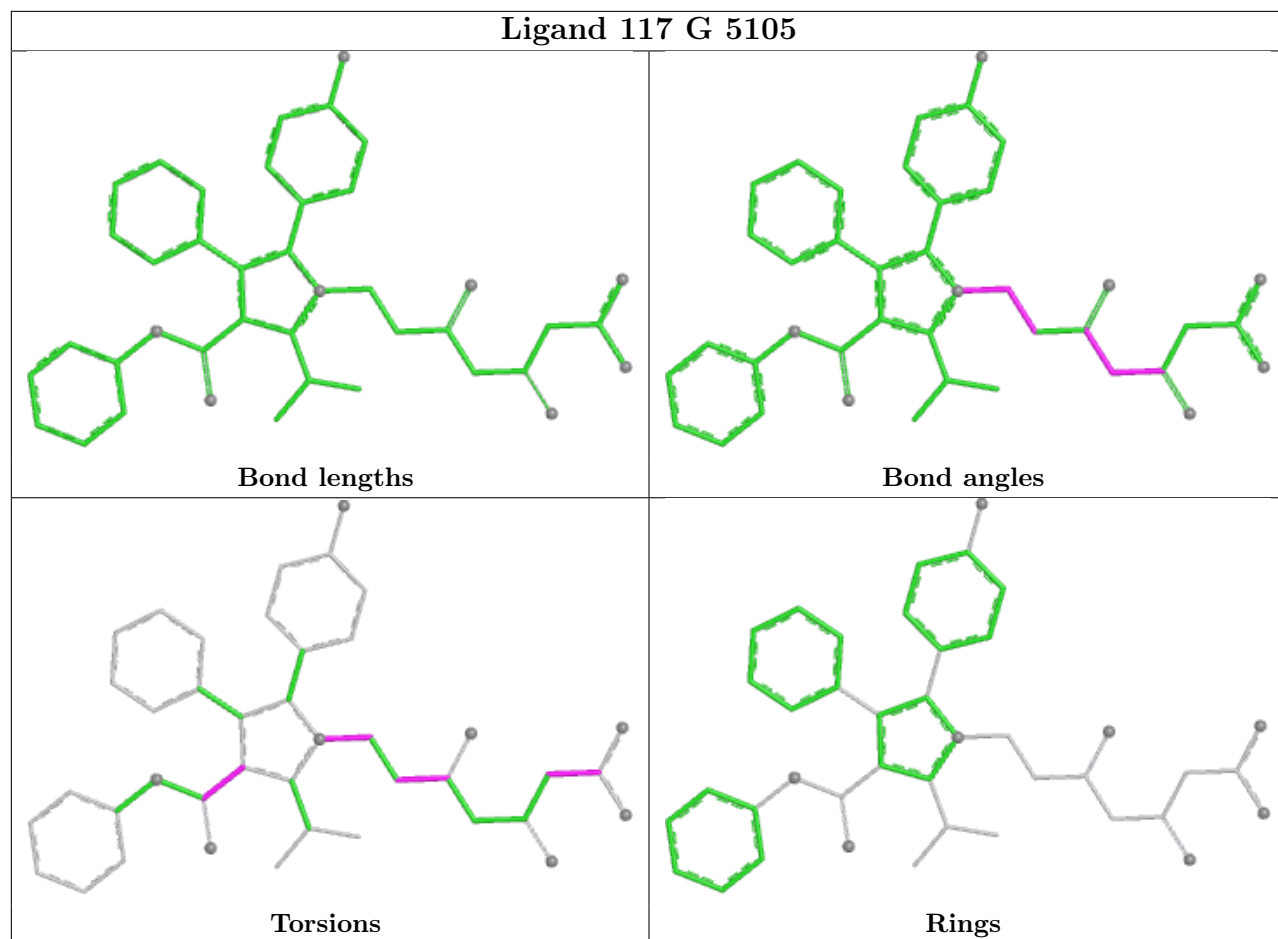


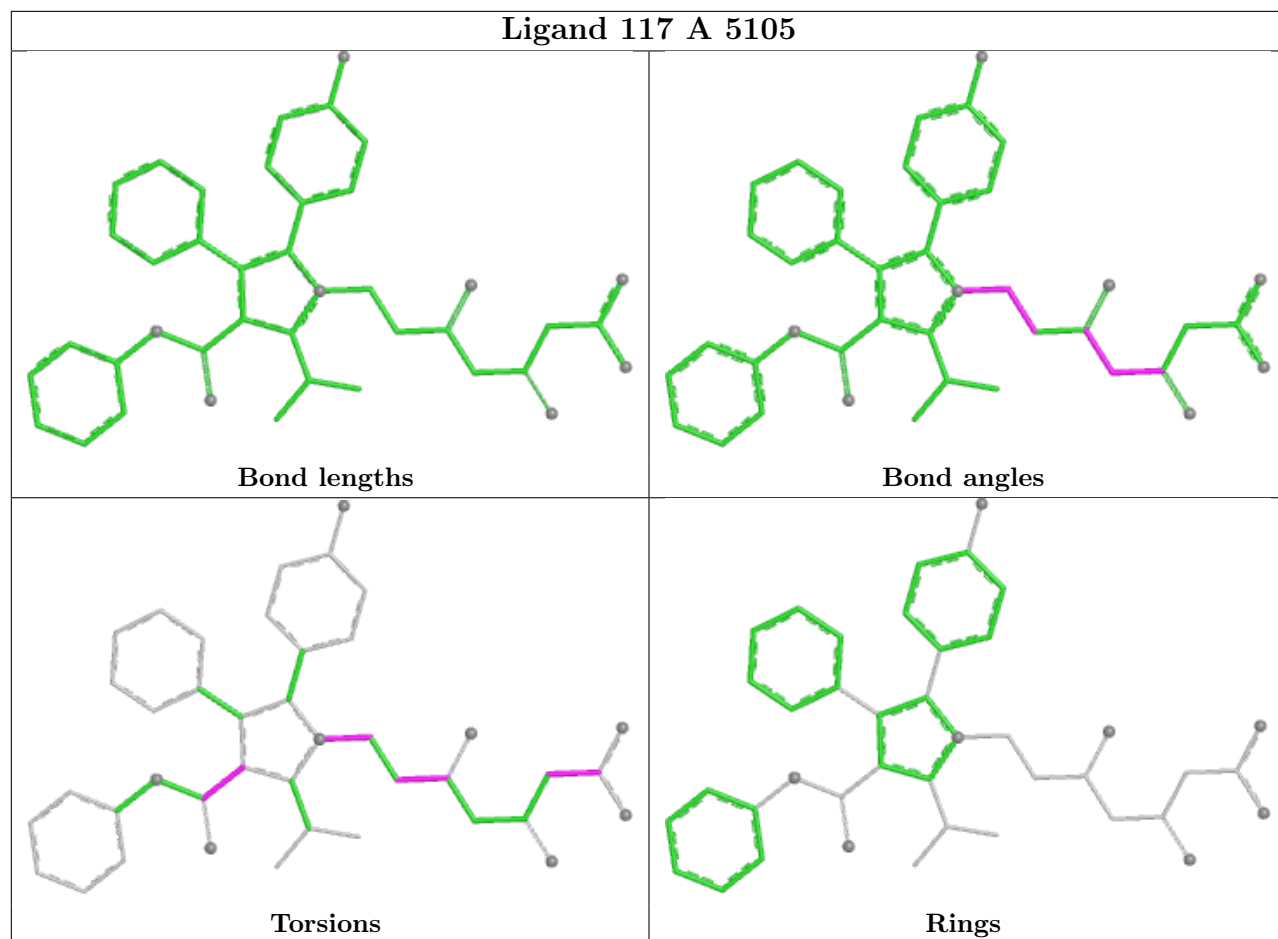


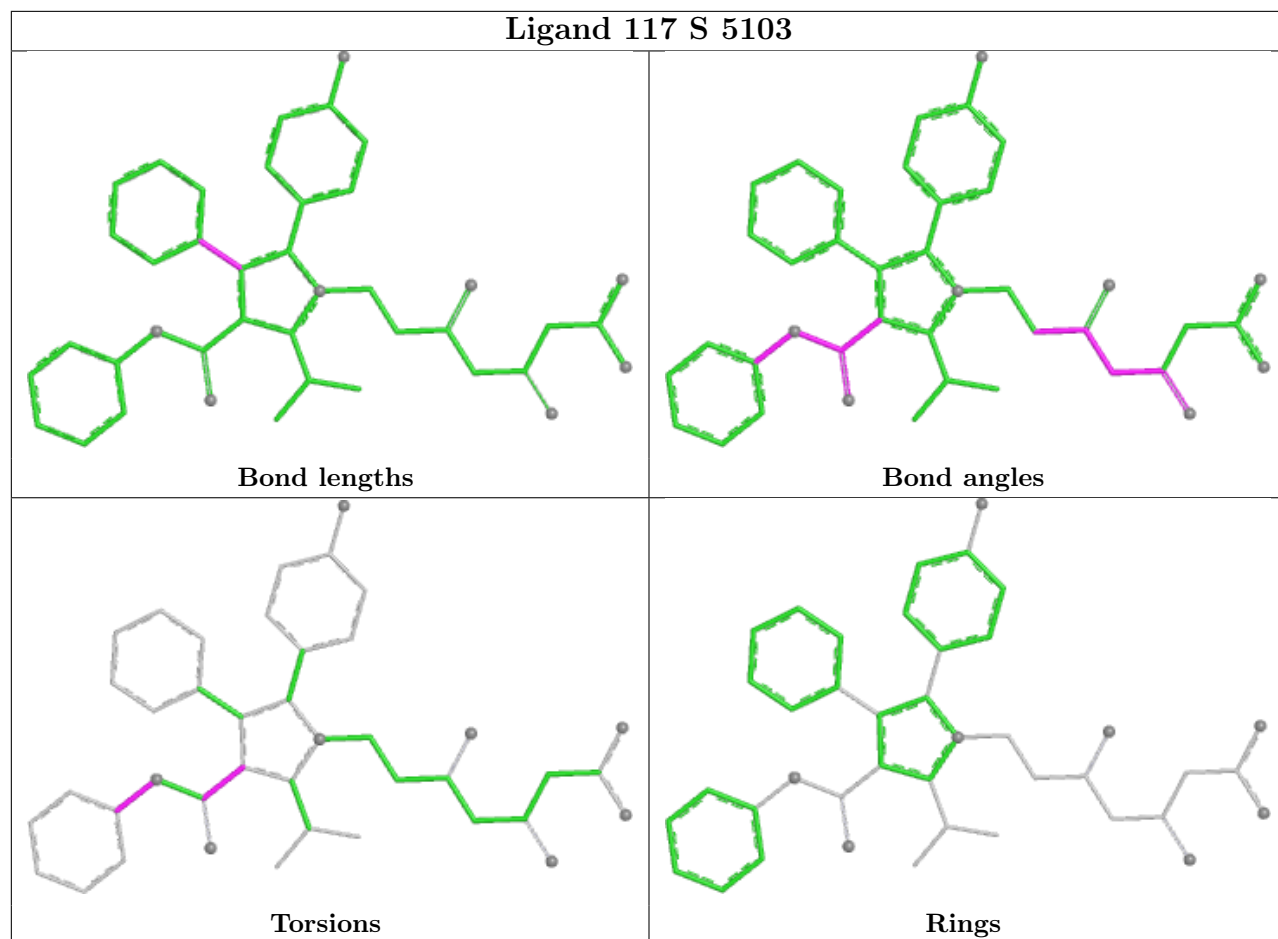


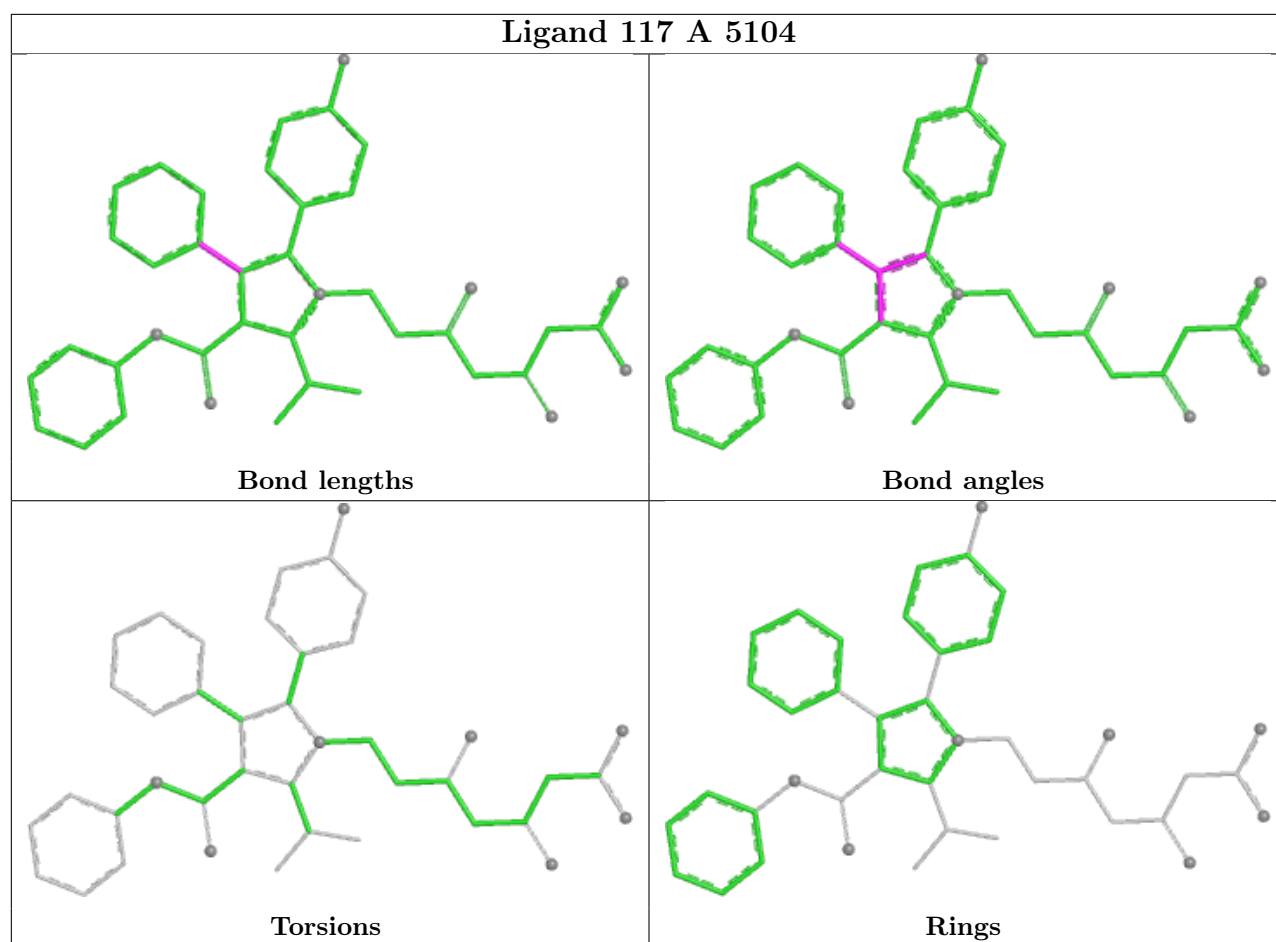












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

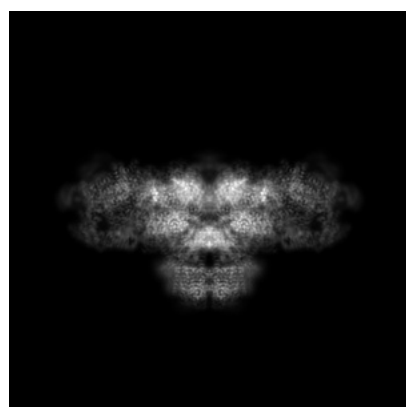
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-70589. These allow visual inspection of the internal detail of the map and identification of artifacts.

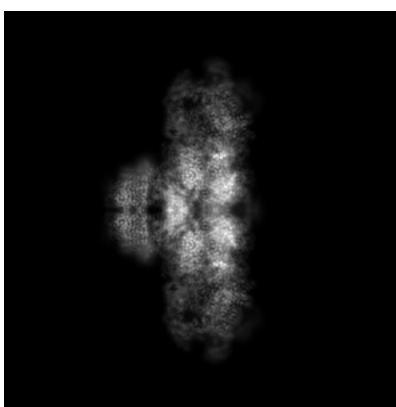
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

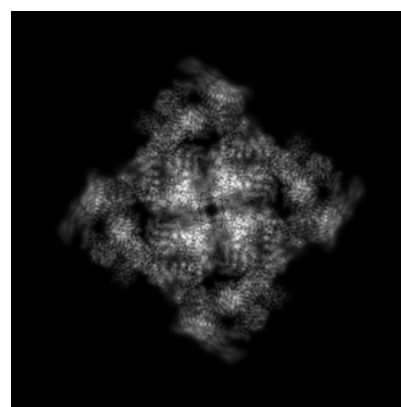
#### 6.1.1 Primary map



X



Y

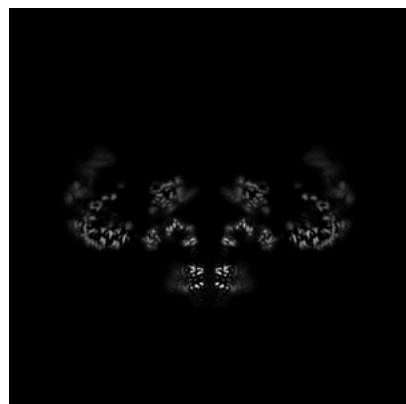


Z

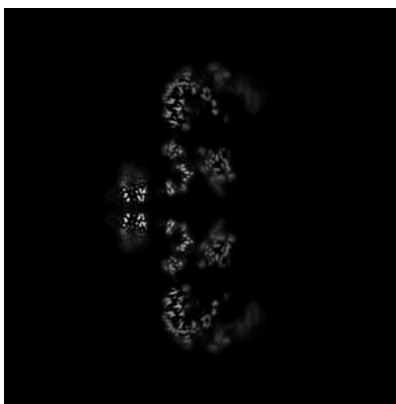
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

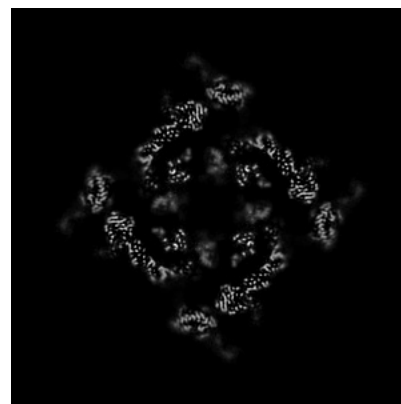
#### 6.2.1 Primary map



X Index: 256



Y Index: 256



Z Index: 256

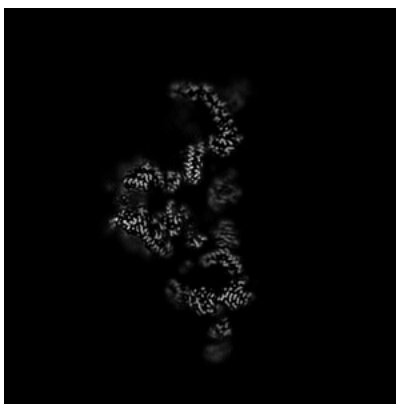
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

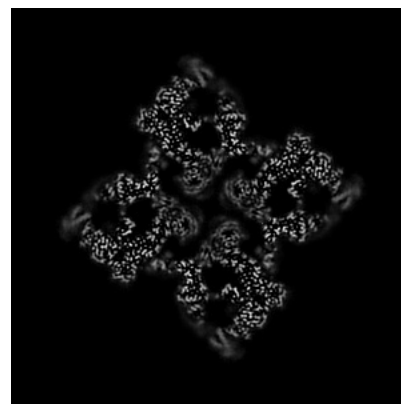
### 6.3.1 Primary map



X Index: 227



Y Index: 227

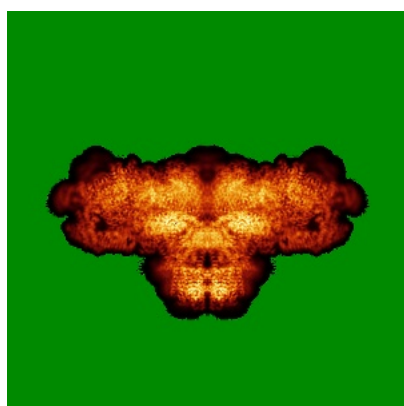


Z Index: 282

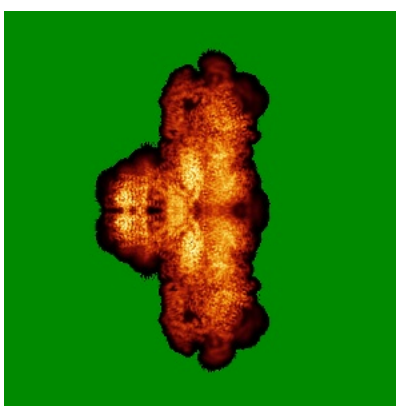
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

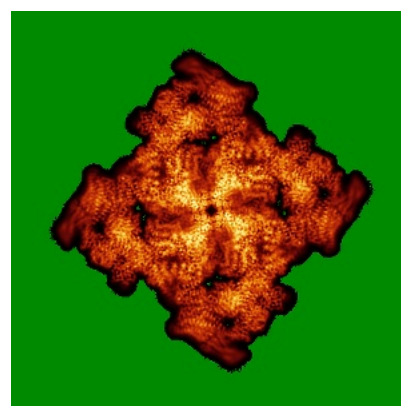
### 6.4.1 Primary map



X



Y

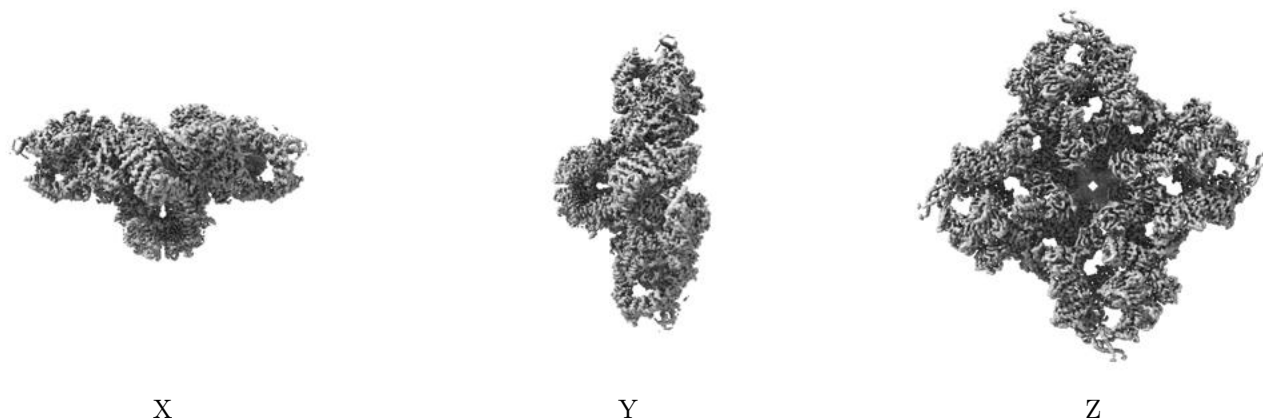


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.123. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

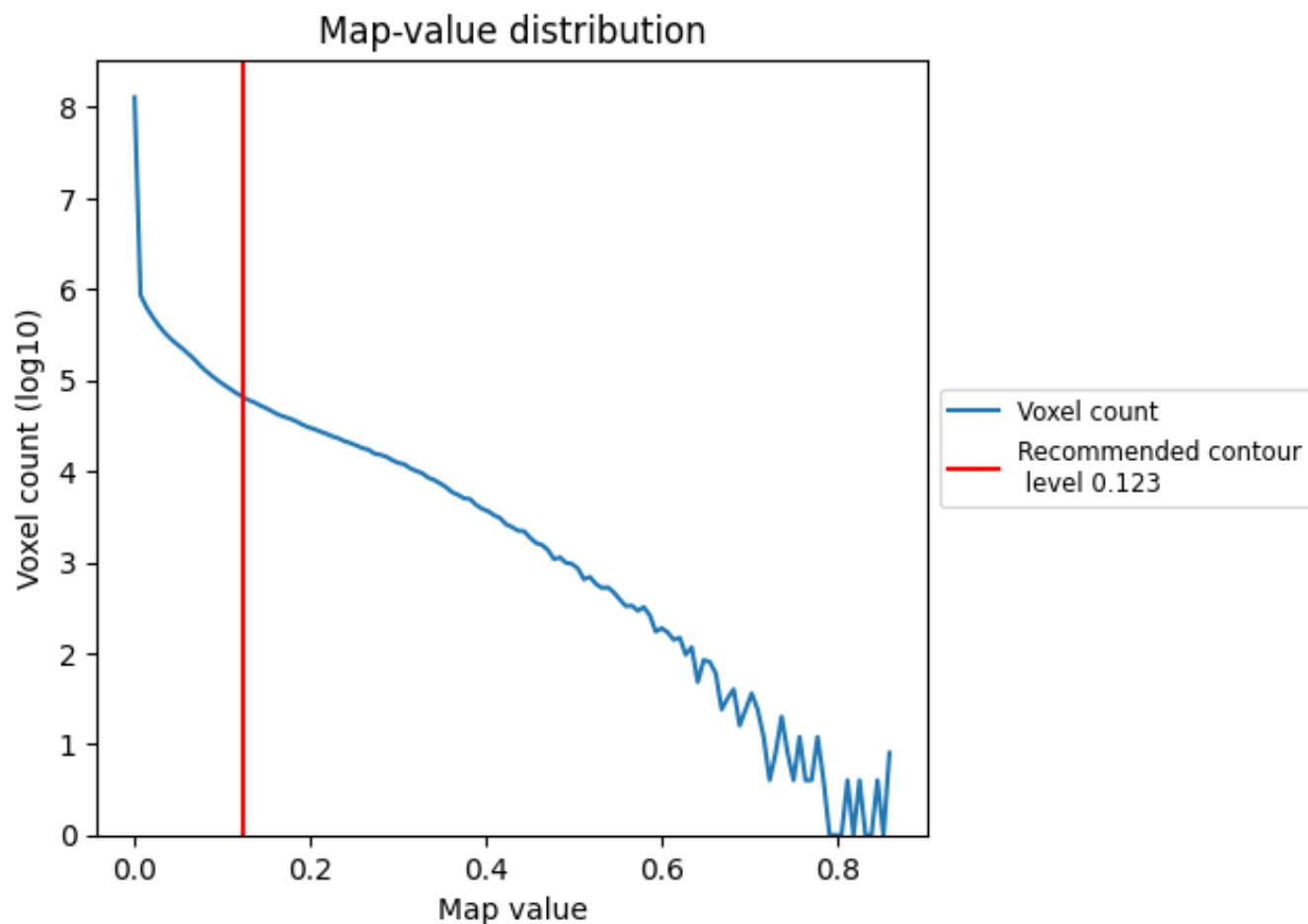
## 6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

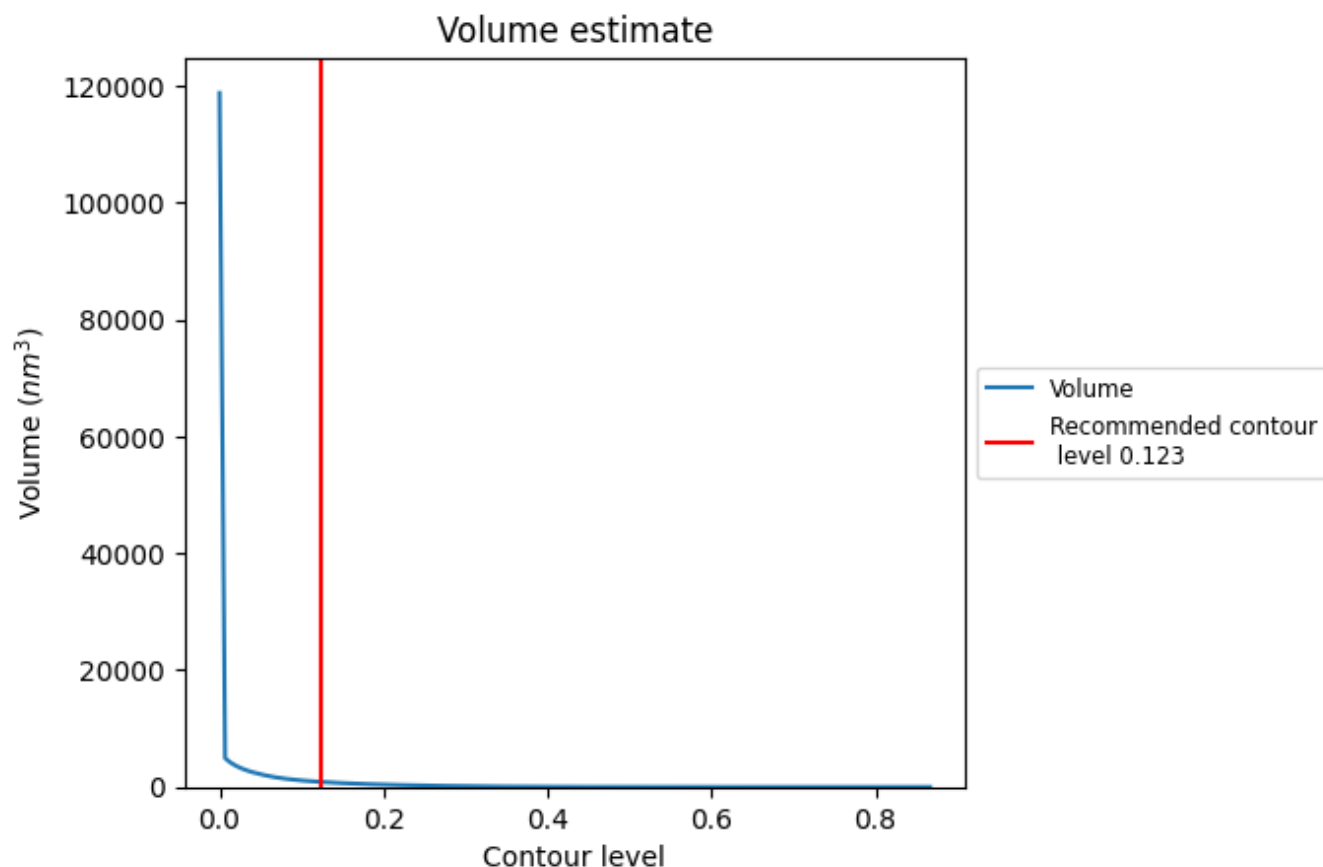
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

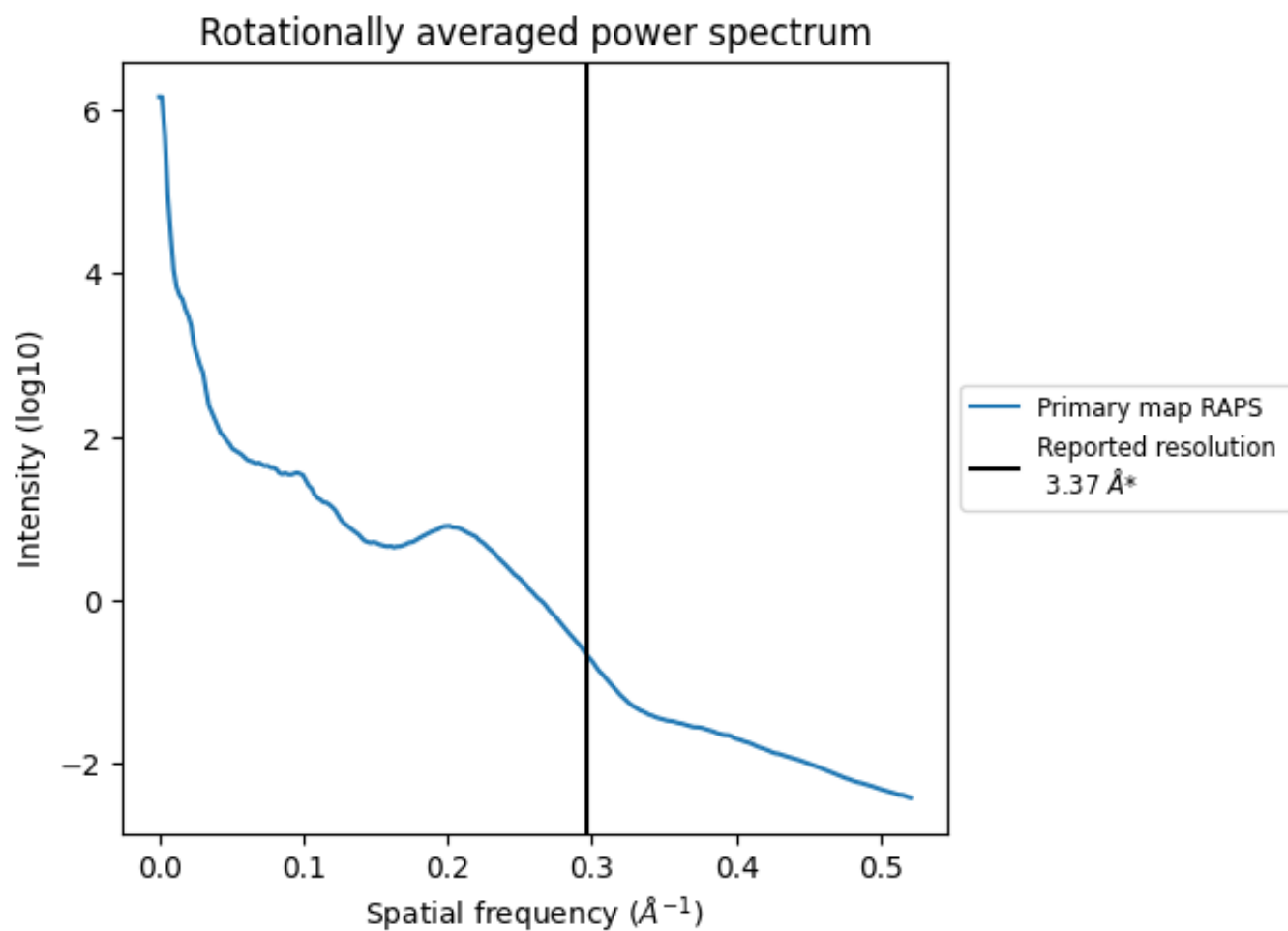
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is  $869 \text{ nm}^3$ ; this corresponds to an approximate mass of 785 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ



\*Reported resolution corresponds to spatial frequency of 0.297 Å<sup>-1</sup>

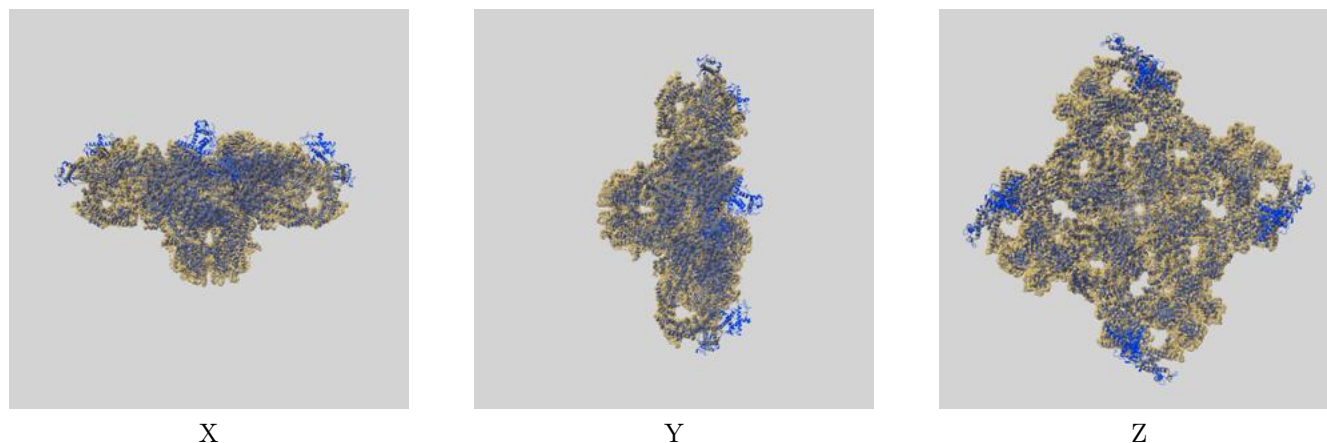
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

## 9 Map-model fit [i](#)

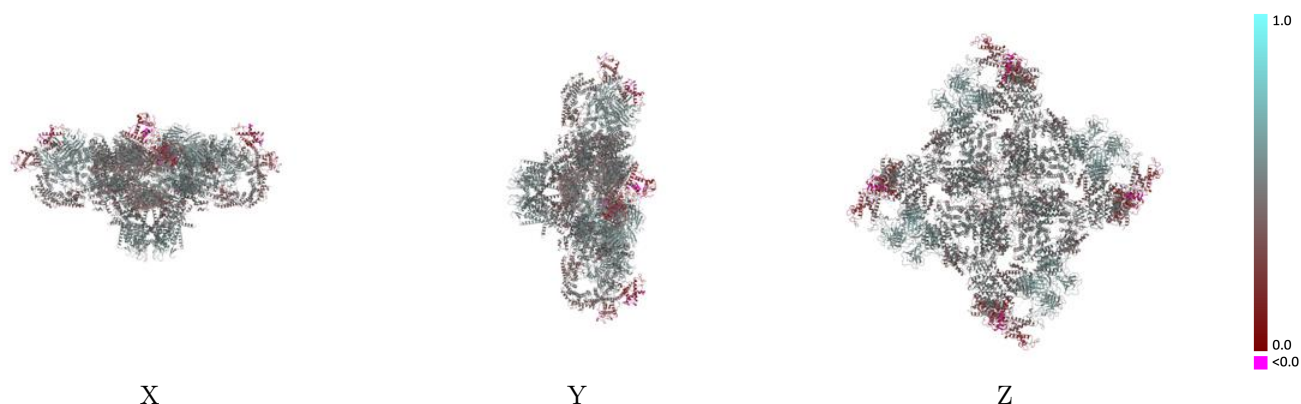
This section contains information regarding the fit between EMDB map EMD-70589 and PDB model 9OL4. Per-residue inclusion information can be found in section [3](#) on page [8](#).

### 9.1 Map-model overlay [i](#)



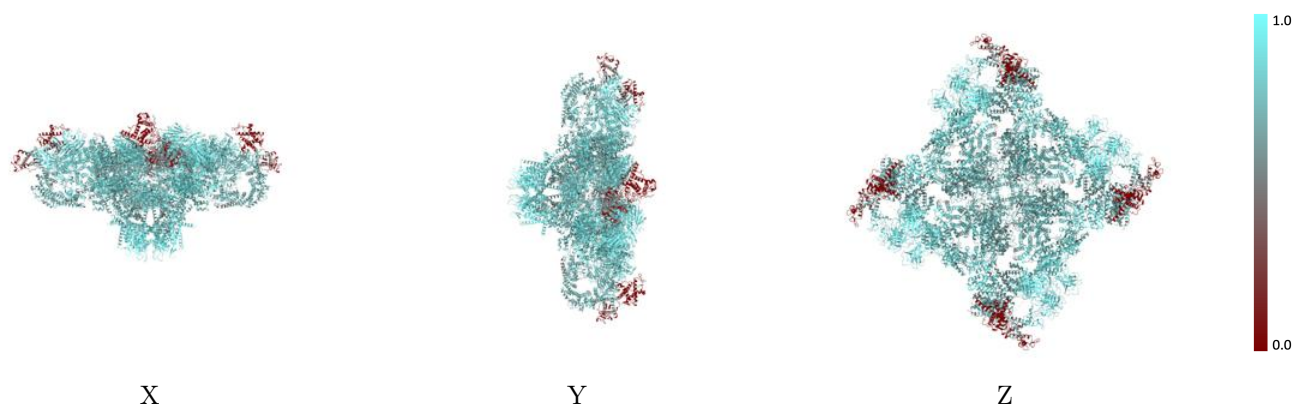
The images above show the 3D surface view of the map at the recommended contour level 0.123 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



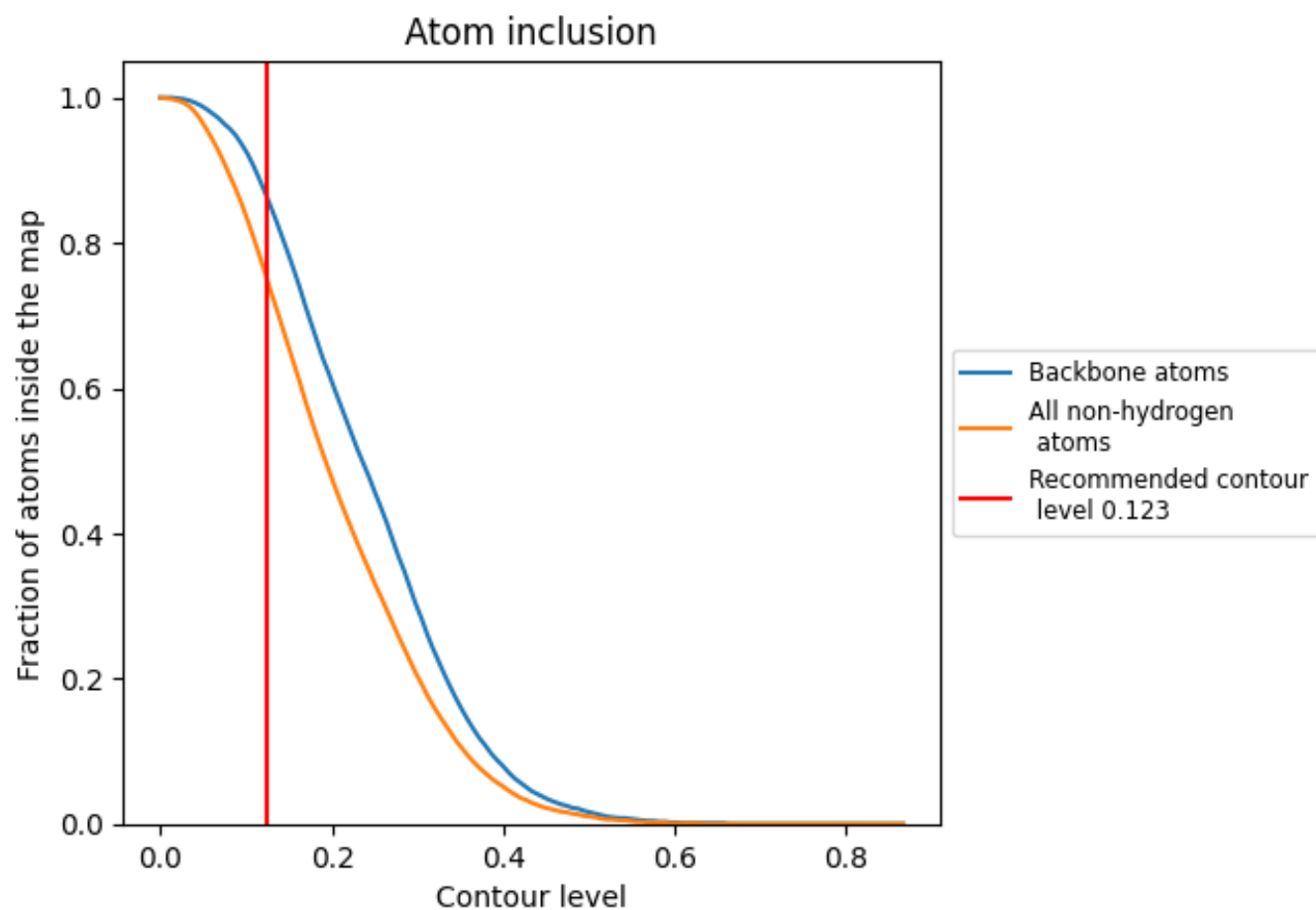
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.123).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.123) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                | Q-score                       |
|-------|-------------------------------|-------------------------------|
| All   | <div><div></div></div> 0.7560 | <div><div></div></div> 0.4620 |
| A     | <div><div></div></div> 0.7530 | <div><div></div></div> 0.4600 |
| B     | <div><div></div></div> 0.8570 | <div><div></div></div> 0.5390 |
| G     | <div><div></div></div> 0.7530 | <div><div></div></div> 0.4600 |
| H     | <div><div></div></div> 0.8570 | <div><div></div></div> 0.5390 |
| M     | <div><div></div></div> 0.7530 | <div><div></div></div> 0.4600 |
| N     | <div><div></div></div> 0.8570 | <div><div></div></div> 0.5410 |
| S     | <div><div></div></div> 0.7530 | <div><div></div></div> 0.4610 |
| T     | <div><div></div></div> 0.8570 | <div><div></div></div> 0.5400 |

1.0

0.0

<0.0