



## Full wwPDB EM Validation Report ⓘ

Nov 4, 2024 – 12:45 am GMT

PDB ID : 8A1D  
EMDB ID : EMD-15072  
Title : Structure of murine perforin-2 (Mpeg1) pore in ring form  
Authors : Yu, X.; Ni, T.; Zhang, P.; Gilbert, R.  
Deposited on : 2022-06-01  
Resolution : 3.00 Å(reported)

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.dev113  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39



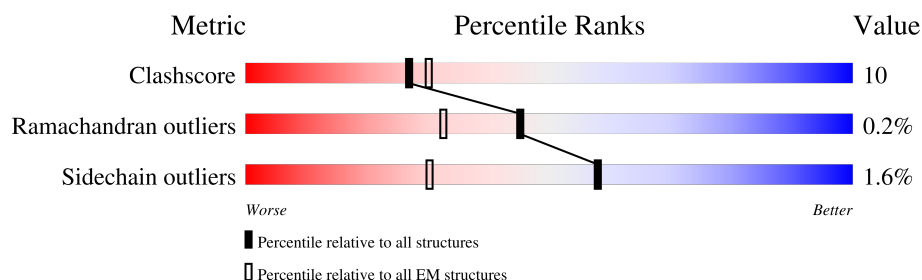
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.00 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) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore            | 210492                      | 15764                       |
| Ramachandran outliers | 207382                      | 16835                       |
| Sidechain outliers    | 206894                      | 16415                       |

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     | 648    | <div> <div>5%</div> <div>61%</div> <div>20%</div> <div>18%</div> </div>  |
| 1   | B     | 648    | <div> <div>6%</div> <div>63%</div> <div>19%</div> <div>18%</div> </div>  |
| 1   | C     | 648    | <div> <div>8%</div> <div>62%</div> <div>20%</div> <div>18%</div> </div>  |
| 1   | D     | 648    | <div> <div>12%</div> <div>63%</div> <div>19%</div> <div>18%</div> </div> |
| 1   | E     | 648    | <div> <div>20%</div> <div>62%</div> <div>20%</div> <div>18%</div> </div> |
| 1   | F     | 648    | <div> <div>25%</div> <div>65%</div> <div>17%</div> <div>18%</div> </div> |
| 1   | G     | 648    | <div> <div>17%</div> <div>61%</div> <div>21%</div> <div>18%</div> </div> |
| 1   | H     | 648    | <div> <div>6%</div> <div>61%</div> <div>20%</div> <div>18%</div> </div>  |

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| Mol | Chain | Length | Quality of chain    |
|-----|-------|--------|---------------------|
| 1   | I     | 648    | <br>6% 64% 17% 18%  |
| 1   | J     | 648    | <br>6% 61% 20% 18%  |
| 1   | K     | 648    | <br>8% 62% 19% 18%  |
| 1   | L     | 648    | <br>13% 62% 20% 18% |
| 1   | M     | 648    | <br>20% 62% 19% 18% |
| 1   | N     | 648    | <br>26% 62% 19% 18% |
| 1   | O     | 648    | <br>17% 62% 19% 18% |
| 1   | P     | 648    | <br>6% 63% 19% 18%  |



## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 67152 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 Macrophage-expressed gene 1 protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | A     | 533      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4148  | 2650 | 687 | 784 | 27 |         |       |
| 1   | B     | 533      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4148  | 2650 | 687 | 784 | 27 |         |       |
| 1   | C     | 533      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4148  | 2650 | 687 | 784 | 27 |         |       |
| 1   | D     | 533      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4148  | 2650 | 687 | 784 | 27 |         |       |
| 1   | E     | 533      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4148  | 2650 | 687 | 784 | 27 |         |       |
| 1   | F     | 533      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4148  | 2650 | 687 | 784 | 27 |         |       |
| 1   | G     | 533      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4148  | 2650 | 687 | 784 | 27 |         |       |
| 1   | H     | 533      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4148  | 2650 | 687 | 784 | 27 |         |       |
| 1   | I     | 533      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4148  | 2650 | 687 | 784 | 27 |         |       |
| 1   | J     | 533      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4148  | 2650 | 687 | 784 | 27 |         |       |
| 1   | K     | 533      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4148  | 2650 | 687 | 784 | 27 |         |       |
| 1   | L     | 533      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4148  | 2650 | 687 | 784 | 27 |         |       |
| 1   | M     | 533      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4148  | 2650 | 687 | 784 | 27 |         |       |
| 1   | N     | 533      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4148  | 2650 | 687 | 784 | 27 |         |       |
| 1   | O     | 533      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4148  | 2650 | 687 | 784 | 27 |         |       |
| 1   | P     | 533      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4148  | 2650 | 687 | 784 | 27 |         |       |

There are 240 discrepancies between the modelled and reference sequences:



| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 17      | GLU      | -      | expression tag | UNP A1L314 |
| A     | 18      | THR      | -      | expression tag | UNP A1L314 |
| A     | 19      | GLY      | -      | expression tag | UNP A1L314 |
| A     | 653     | GLY      | -      | expression tag | UNP A1L314 |
| A     | 654     | THR      | -      | expression tag | UNP A1L314 |
| A     | 655     | LYS      | -      | expression tag | UNP A1L314 |
| A     | 656     | THR      | -      | expression tag | UNP A1L314 |
| A     | 657     | GLU      | -      | expression tag | UNP A1L314 |
| A     | 658     | THR      | -      | expression tag | UNP A1L314 |
| A     | 659     | SER      | -      | expression tag | UNP A1L314 |
| A     | 660     | GLN      | -      | expression tag | UNP A1L314 |
| A     | 661     | VAL      | -      | expression tag | UNP A1L314 |
| A     | 662     | ALA      | -      | expression tag | UNP A1L314 |
| A     | 663     | PRO      | -      | expression tag | UNP A1L314 |
| A     | 664     | ALA      | -      | expression tag | UNP A1L314 |
| B     | 17      | GLU      | -      | expression tag | UNP A1L314 |
| B     | 18      | THR      | -      | expression tag | UNP A1L314 |
| B     | 19      | GLY      | -      | expression tag | UNP A1L314 |
| B     | 653     | GLY      | -      | expression tag | UNP A1L314 |
| B     | 654     | THR      | -      | expression tag | UNP A1L314 |
| B     | 655     | LYS      | -      | expression tag | UNP A1L314 |
| B     | 656     | THR      | -      | expression tag | UNP A1L314 |
| B     | 657     | GLU      | -      | expression tag | UNP A1L314 |
| B     | 658     | THR      | -      | expression tag | UNP A1L314 |
| B     | 659     | SER      | -      | expression tag | UNP A1L314 |
| B     | 660     | GLN      | -      | expression tag | UNP A1L314 |
| B     | 661     | VAL      | -      | expression tag | UNP A1L314 |
| B     | 662     | ALA      | -      | expression tag | UNP A1L314 |
| B     | 663     | PRO      | -      | expression tag | UNP A1L314 |
| B     | 664     | ALA      | -      | expression tag | UNP A1L314 |
| C     | 17      | GLU      | -      | expression tag | UNP A1L314 |
| C     | 18      | THR      | -      | expression tag | UNP A1L314 |
| C     | 19      | GLY      | -      | expression tag | UNP A1L314 |
| C     | 653     | GLY      | -      | expression tag | UNP A1L314 |
| C     | 654     | THR      | -      | expression tag | UNP A1L314 |
| C     | 655     | LYS      | -      | expression tag | UNP A1L314 |
| C     | 656     | THR      | -      | expression tag | UNP A1L314 |
| C     | 657     | GLU      | -      | expression tag | UNP A1L314 |
| C     | 658     | THR      | -      | expression tag | UNP A1L314 |
| C     | 659     | SER      | -      | expression tag | UNP A1L314 |
| C     | 660     | GLN      | -      | expression tag | UNP A1L314 |
| C     | 661     | VAL      | -      | expression tag | UNP A1L314 |
| C     | 662     | ALA      | -      | expression tag | UNP A1L314 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| C     | 663     | PRO      | -      | expression tag | UNP A1L314 |
| C     | 664     | ALA      | -      | expression tag | UNP A1L314 |
| D     | 17      | GLU      | -      | expression tag | UNP A1L314 |
| D     | 18      | THR      | -      | expression tag | UNP A1L314 |
| D     | 19      | GLY      | -      | expression tag | UNP A1L314 |
| D     | 653     | GLY      | -      | expression tag | UNP A1L314 |
| D     | 654     | THR      | -      | expression tag | UNP A1L314 |
| D     | 655     | LYS      | -      | expression tag | UNP A1L314 |
| D     | 656     | THR      | -      | expression tag | UNP A1L314 |
| D     | 657     | GLU      | -      | expression tag | UNP A1L314 |
| D     | 658     | THR      | -      | expression tag | UNP A1L314 |
| D     | 659     | SER      | -      | expression tag | UNP A1L314 |
| D     | 660     | GLN      | -      | expression tag | UNP A1L314 |
| D     | 661     | VAL      | -      | expression tag | UNP A1L314 |
| D     | 662     | ALA      | -      | expression tag | UNP A1L314 |
| D     | 663     | PRO      | -      | expression tag | UNP A1L314 |
| D     | 664     | ALA      | -      | expression tag | UNP A1L314 |
| E     | 17      | GLU      | -      | expression tag | UNP A1L314 |
| E     | 18      | THR      | -      | expression tag | UNP A1L314 |
| E     | 19      | GLY      | -      | expression tag | UNP A1L314 |
| E     | 653     | GLY      | -      | expression tag | UNP A1L314 |
| E     | 654     | THR      | -      | expression tag | UNP A1L314 |
| E     | 655     | LYS      | -      | expression tag | UNP A1L314 |
| E     | 656     | THR      | -      | expression tag | UNP A1L314 |
| E     | 657     | GLU      | -      | expression tag | UNP A1L314 |
| E     | 658     | THR      | -      | expression tag | UNP A1L314 |
| E     | 659     | SER      | -      | expression tag | UNP A1L314 |
| E     | 660     | GLN      | -      | expression tag | UNP A1L314 |
| E     | 661     | VAL      | -      | expression tag | UNP A1L314 |
| E     | 662     | ALA      | -      | expression tag | UNP A1L314 |
| E     | 663     | PRO      | -      | expression tag | UNP A1L314 |
| E     | 664     | ALA      | -      | expression tag | UNP A1L314 |
| F     | 17      | GLU      | -      | expression tag | UNP A1L314 |
| F     | 18      | THR      | -      | expression tag | UNP A1L314 |
| F     | 19      | GLY      | -      | expression tag | UNP A1L314 |
| F     | 653     | GLY      | -      | expression tag | UNP A1L314 |
| F     | 654     | THR      | -      | expression tag | UNP A1L314 |
| F     | 655     | LYS      | -      | expression tag | UNP A1L314 |
| F     | 656     | THR      | -      | expression tag | UNP A1L314 |
| F     | 657     | GLU      | -      | expression tag | UNP A1L314 |
| F     | 658     | THR      | -      | expression tag | UNP A1L314 |
| F     | 659     | SER      | -      | expression tag | UNP A1L314 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| F     | 660     | GLN      | -      | expression tag | UNP A1L314 |
| F     | 661     | VAL      | -      | expression tag | UNP A1L314 |
| F     | 662     | ALA      | -      | expression tag | UNP A1L314 |
| F     | 663     | PRO      | -      | expression tag | UNP A1L314 |
| F     | 664     | ALA      | -      | expression tag | UNP A1L314 |
| G     | 17      | GLU      | -      | expression tag | UNP A1L314 |
| G     | 18      | THR      | -      | expression tag | UNP A1L314 |
| G     | 19      | GLY      | -      | expression tag | UNP A1L314 |
| G     | 653     | GLY      | -      | expression tag | UNP A1L314 |
| G     | 654     | THR      | -      | expression tag | UNP A1L314 |
| G     | 655     | LYS      | -      | expression tag | UNP A1L314 |
| G     | 656     | THR      | -      | expression tag | UNP A1L314 |
| G     | 657     | GLU      | -      | expression tag | UNP A1L314 |
| G     | 658     | THR      | -      | expression tag | UNP A1L314 |
| G     | 659     | SER      | -      | expression tag | UNP A1L314 |
| G     | 660     | GLN      | -      | expression tag | UNP A1L314 |
| G     | 661     | VAL      | -      | expression tag | UNP A1L314 |
| G     | 662     | ALA      | -      | expression tag | UNP A1L314 |
| G     | 663     | PRO      | -      | expression tag | UNP A1L314 |
| G     | 664     | ALA      | -      | expression tag | UNP A1L314 |
| H     | 17      | GLU      | -      | expression tag | UNP A1L314 |
| H     | 18      | THR      | -      | expression tag | UNP A1L314 |
| H     | 19      | GLY      | -      | expression tag | UNP A1L314 |
| H     | 653     | GLY      | -      | expression tag | UNP A1L314 |
| H     | 654     | THR      | -      | expression tag | UNP A1L314 |
| H     | 655     | LYS      | -      | expression tag | UNP A1L314 |
| H     | 656     | THR      | -      | expression tag | UNP A1L314 |
| H     | 657     | GLU      | -      | expression tag | UNP A1L314 |
| H     | 658     | THR      | -      | expression tag | UNP A1L314 |
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| H     | 661     | VAL      | -      | expression tag | UNP A1L314 |
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| H     | 663     | PRO      | -      | expression tag | UNP A1L314 |
| H     | 664     | ALA      | -      | expression tag | UNP A1L314 |
| I     | 17      | GLU      | -      | expression tag | UNP A1L314 |
| I     | 18      | THR      | -      | expression tag | UNP A1L314 |
| I     | 19      | GLY      | -      | expression tag | UNP A1L314 |
| I     | 653     | GLY      | -      | expression tag | UNP A1L314 |
| I     | 654     | THR      | -      | expression tag | UNP A1L314 |
| I     | 655     | LYS      | -      | expression tag | UNP A1L314 |
| I     | 656     | THR      | -      | expression tag | UNP A1L314 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| I     | 657     | GLU      | -      | expression tag | UNP A1L314 |
| I     | 658     | THR      | -      | expression tag | UNP A1L314 |
| I     | 659     | SER      | -      | expression tag | UNP A1L314 |
| I     | 660     | GLN      | -      | expression tag | UNP A1L314 |
| I     | 661     | VAL      | -      | expression tag | UNP A1L314 |
| I     | 662     | ALA      | -      | expression tag | UNP A1L314 |
| I     | 663     | PRO      | -      | expression tag | UNP A1L314 |
| I     | 664     | ALA      | -      | expression tag | UNP A1L314 |
| J     | 17      | GLU      | -      | expression tag | UNP A1L314 |
| J     | 18      | THR      | -      | expression tag | UNP A1L314 |
| J     | 19      | GLY      | -      | expression tag | UNP A1L314 |
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| J     | 654     | THR      | -      | expression tag | UNP A1L314 |
| J     | 655     | LYS      | -      | expression tag | UNP A1L314 |
| J     | 656     | THR      | -      | expression tag | UNP A1L314 |
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| J     | 661     | VAL      | -      | expression tag | UNP A1L314 |
| J     | 662     | ALA      | -      | expression tag | UNP A1L314 |
| J     | 663     | PRO      | -      | expression tag | UNP A1L314 |
| J     | 664     | ALA      | -      | expression tag | UNP A1L314 |
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| K     | 18      | THR      | -      | expression tag | UNP A1L314 |
| K     | 19      | GLY      | -      | expression tag | UNP A1L314 |
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| K     | 654     | THR      | -      | expression tag | UNP A1L314 |
| K     | 655     | LYS      | -      | expression tag | UNP A1L314 |
| K     | 656     | THR      | -      | expression tag | UNP A1L314 |
| K     | 657     | GLU      | -      | expression tag | UNP A1L314 |
| K     | 658     | THR      | -      | expression tag | UNP A1L314 |
| K     | 659     | SER      | -      | expression tag | UNP A1L314 |
| K     | 660     | GLN      | -      | expression tag | UNP A1L314 |
| K     | 661     | VAL      | -      | expression tag | UNP A1L314 |
| K     | 662     | ALA      | -      | expression tag | UNP A1L314 |
| K     | 663     | PRO      | -      | expression tag | UNP A1L314 |
| K     | 664     | ALA      | -      | expression tag | UNP A1L314 |
| L     | 17      | GLU      | -      | expression tag | UNP A1L314 |
| L     | 18      | THR      | -      | expression tag | UNP A1L314 |
| L     | 19      | GLY      | -      | expression tag | UNP A1L314 |
| L     | 653     | GLY      | -      | expression tag | UNP A1L314 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| L     | 654     | THR      | -      | expression tag | UNP A1L314 |
| L     | 655     | LYS      | -      | expression tag | UNP A1L314 |
| L     | 656     | THR      | -      | expression tag | UNP A1L314 |
| L     | 657     | GLU      | -      | expression tag | UNP A1L314 |
| L     | 658     | THR      | -      | expression tag | UNP A1L314 |
| L     | 659     | SER      | -      | expression tag | UNP A1L314 |
| L     | 660     | GLN      | -      | expression tag | UNP A1L314 |
| L     | 661     | VAL      | -      | expression tag | UNP A1L314 |
| L     | 662     | ALA      | -      | expression tag | UNP A1L314 |
| L     | 663     | PRO      | -      | expression tag | UNP A1L314 |
| L     | 664     | ALA      | -      | expression tag | UNP A1L314 |
| M     | 17      | GLU      | -      | expression tag | UNP A1L314 |
| M     | 18      | THR      | -      | expression tag | UNP A1L314 |
| M     | 19      | GLY      | -      | expression tag | UNP A1L314 |
| M     | 653     | GLY      | -      | expression tag | UNP A1L314 |
| M     | 654     | THR      | -      | expression tag | UNP A1L314 |
| M     | 655     | LYS      | -      | expression tag | UNP A1L314 |
| M     | 656     | THR      | -      | expression tag | UNP A1L314 |
| M     | 657     | GLU      | -      | expression tag | UNP A1L314 |
| M     | 658     | THR      | -      | expression tag | UNP A1L314 |
| M     | 659     | SER      | -      | expression tag | UNP A1L314 |
| M     | 660     | GLN      | -      | expression tag | UNP A1L314 |
| M     | 661     | VAL      | -      | expression tag | UNP A1L314 |
| M     | 662     | ALA      | -      | expression tag | UNP A1L314 |
| M     | 663     | PRO      | -      | expression tag | UNP A1L314 |
| M     | 664     | ALA      | -      | expression tag | UNP A1L314 |
| N     | 17      | GLU      | -      | expression tag | UNP A1L314 |
| N     | 18      | THR      | -      | expression tag | UNP A1L314 |
| N     | 19      | GLY      | -      | expression tag | UNP A1L314 |
| N     | 653     | GLY      | -      | expression tag | UNP A1L314 |
| N     | 654     | THR      | -      | expression tag | UNP A1L314 |
| N     | 655     | LYS      | -      | expression tag | UNP A1L314 |
| N     | 656     | THR      | -      | expression tag | UNP A1L314 |
| N     | 657     | GLU      | -      | expression tag | UNP A1L314 |
| N     | 658     | THR      | -      | expression tag | UNP A1L314 |
| N     | 659     | SER      | -      | expression tag | UNP A1L314 |
| N     | 660     | GLN      | -      | expression tag | UNP A1L314 |
| N     | 661     | VAL      | -      | expression tag | UNP A1L314 |
| N     | 662     | ALA      | -      | expression tag | UNP A1L314 |
| N     | 663     | PRO      | -      | expression tag | UNP A1L314 |
| N     | 664     | ALA      | -      | expression tag | UNP A1L314 |
| O     | 17      | GLU      | -      | expression tag | UNP A1L314 |

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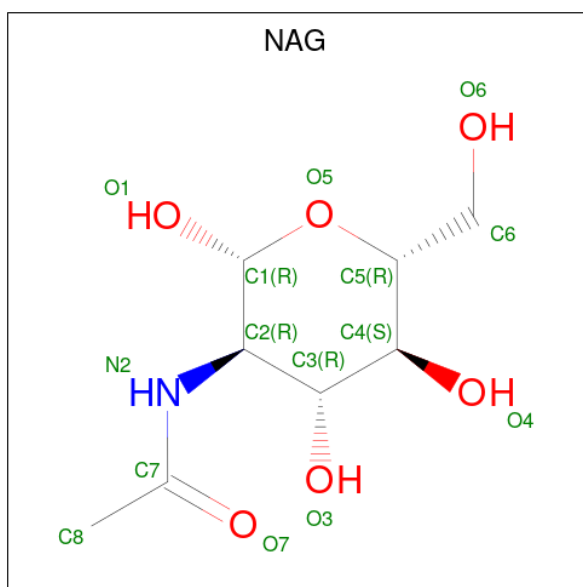


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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| O     | 18      | THR      | -      | expression tag | UNP A1L314 |
| O     | 19      | GLY      | -      | expression tag | UNP A1L314 |
| O     | 653     | GLY      | -      | expression tag | UNP A1L314 |
| O     | 654     | THR      | -      | expression tag | UNP A1L314 |
| O     | 655     | LYS      | -      | expression tag | UNP A1L314 |
| O     | 656     | THR      | -      | expression tag | UNP A1L314 |
| O     | 657     | GLU      | -      | expression tag | UNP A1L314 |
| O     | 658     | THR      | -      | expression tag | UNP A1L314 |
| O     | 659     | SER      | -      | expression tag | UNP A1L314 |
| O     | 660     | GLN      | -      | expression tag | UNP A1L314 |
| O     | 661     | VAL      | -      | expression tag | UNP A1L314 |
| O     | 662     | ALA      | -      | expression tag | UNP A1L314 |
| O     | 663     | PRO      | -      | expression tag | UNP A1L314 |
| O     | 664     | ALA      | -      | expression tag | UNP A1L314 |
| P     | 17      | GLU      | -      | expression tag | UNP A1L314 |
| P     | 18      | THR      | -      | expression tag | UNP A1L314 |
| P     | 19      | GLY      | -      | expression tag | UNP A1L314 |
| P     | 653     | GLY      | -      | expression tag | UNP A1L314 |
| P     | 654     | THR      | -      | expression tag | UNP A1L314 |
| P     | 655     | LYS      | -      | expression tag | UNP A1L314 |
| P     | 656     | THR      | -      | expression tag | UNP A1L314 |
| P     | 657     | GLU      | -      | expression tag | UNP A1L314 |
| P     | 658     | THR      | -      | expression tag | UNP A1L314 |
| P     | 659     | SER      | -      | expression tag | UNP A1L314 |
| P     | 660     | GLN      | -      | expression tag | UNP A1L314 |
| P     | 661     | VAL      | -      | expression tag | UNP A1L314 |
| P     | 662     | ALA      | -      | expression tag | UNP A1L314 |
| P     | 663     | PRO      | -      | expression tag | UNP A1L314 |
| P     | 664     | ALA      | -      | expression tag | UNP A1L314 |

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ) (labeled as "Ligand of Interest" by depositor).





| Mol | Chain | Residues | Atoms |   |   |   | AltConf |
|-----|-------|----------|-------|---|---|---|---------|
| 2   | A     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 2   | B     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 2   | C     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 2   | D     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 2   | E     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 2   | F     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 2   | G     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 2   | H     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 2   | I     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 2   | J     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 2   | K     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 2   | L     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 2   | M     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 2   | N     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |

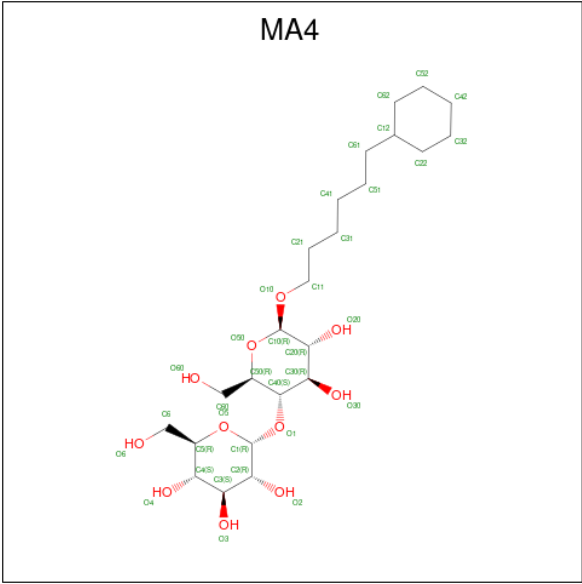
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| Mol | Chain | Residues | Atoms |   |   |   | AltConf |
|-----|-------|----------|-------|---|---|---|---------|
| 2   | O     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 2   | P     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |

- Molecule 3 is CYCLOHEXYL-HEXYL-BETA-D-MALTOSIDE (three-letter code: MA4) (formula: C<sub>24</sub>H<sub>44</sub>O<sub>11</sub>) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 3   | A     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 3   | B     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 3   | C     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 3   | D     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 3   | E     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 3   | F     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 3   | G     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 3   | H     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 3   | I     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |

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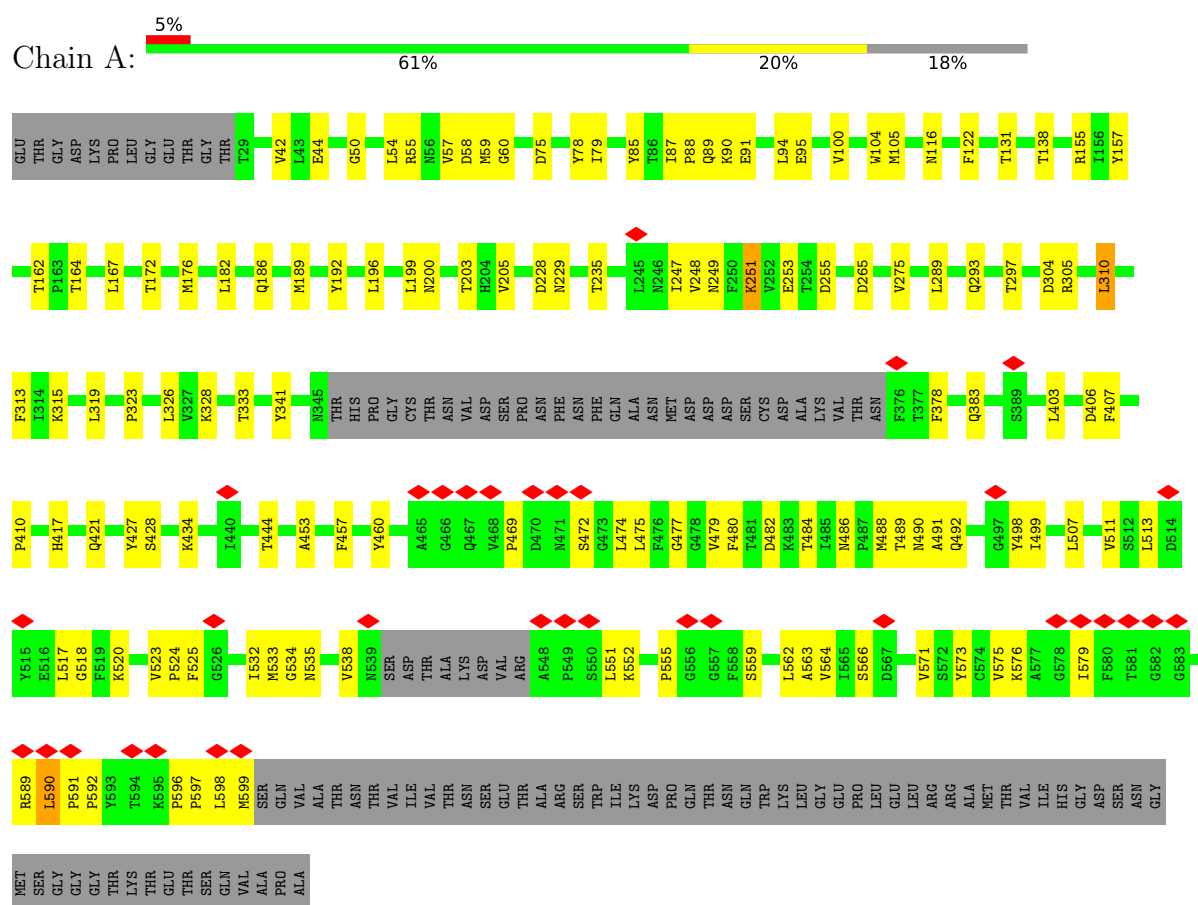
| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 3   | J     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 3   | K     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 3   | L     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 3   | M     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 3   | N     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 3   | O     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 3   | P     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |



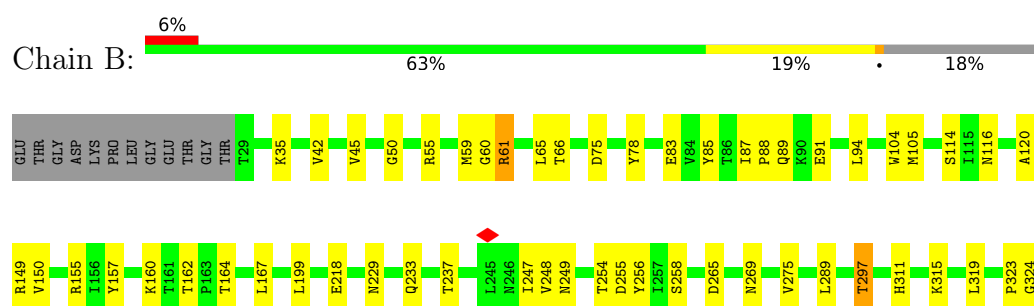
### 3 Residue-property plots [i](#)

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: Macrophage-expressed gene 1 protein

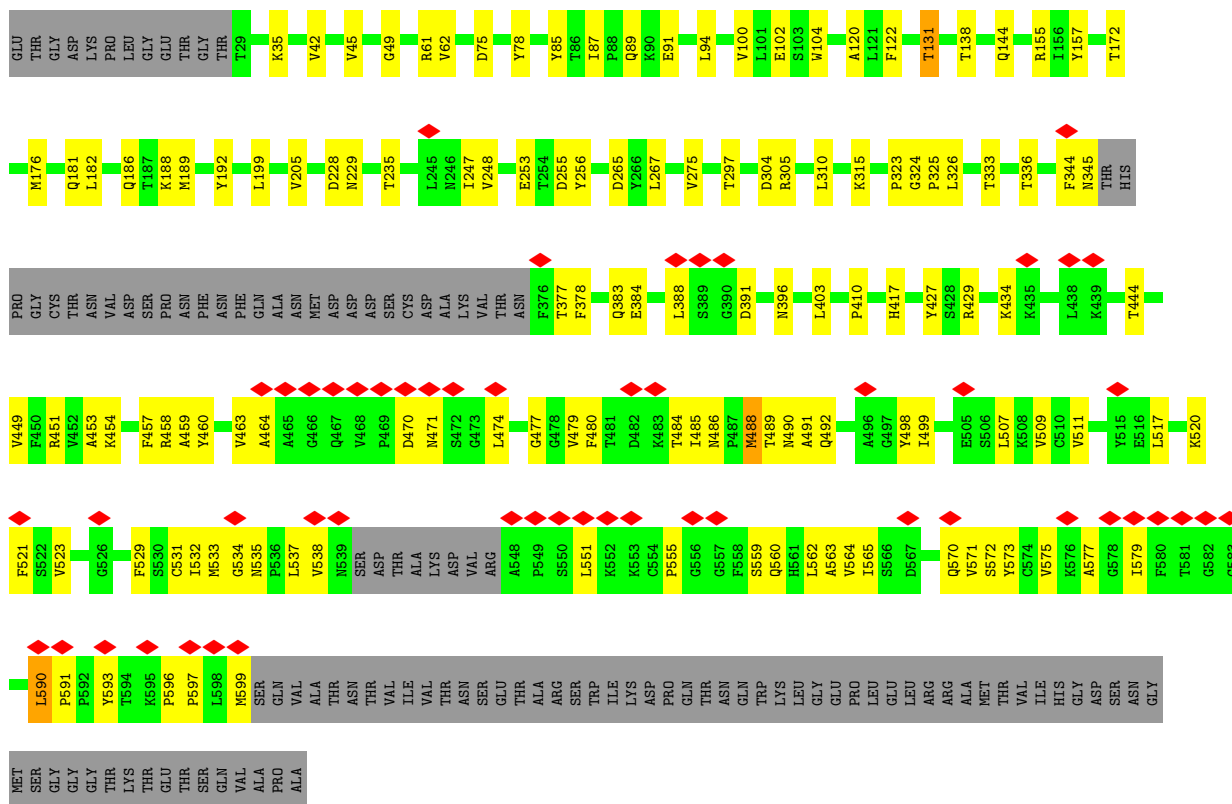


#### • Molecule 1: Macrophage-expressed gene 1 protein





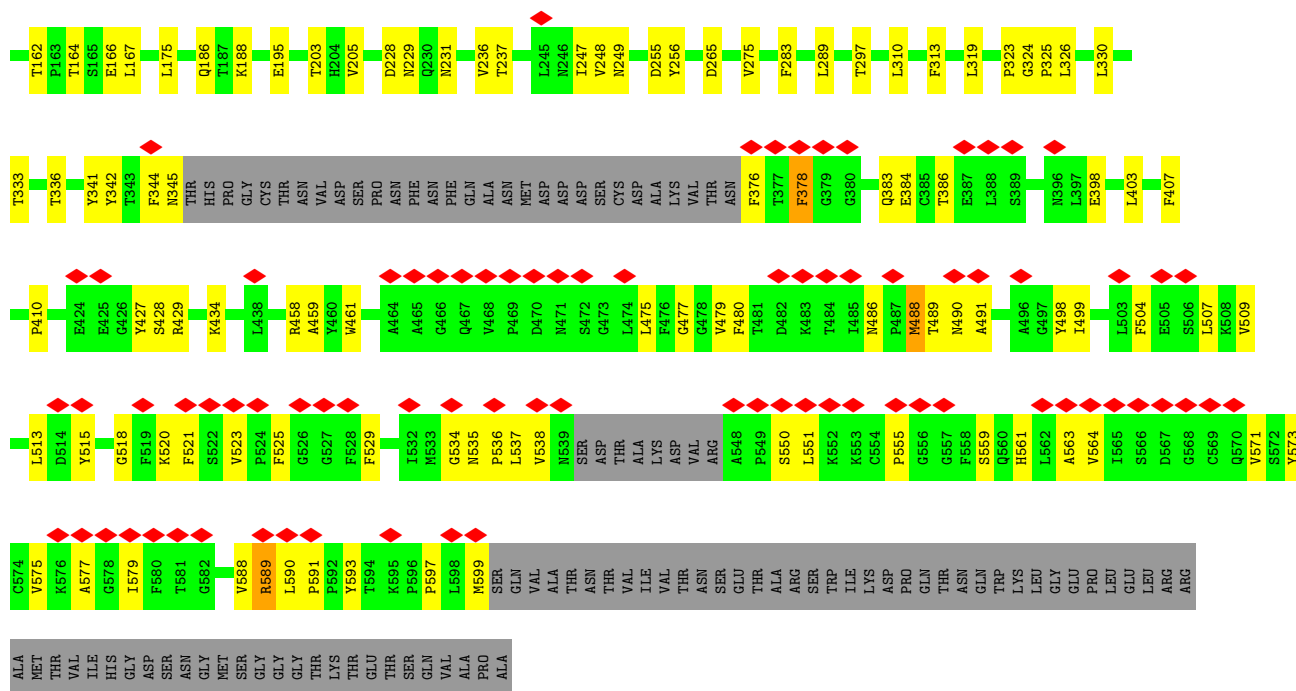
- Molecule 1: Macrophage-expressed gene 1 protein



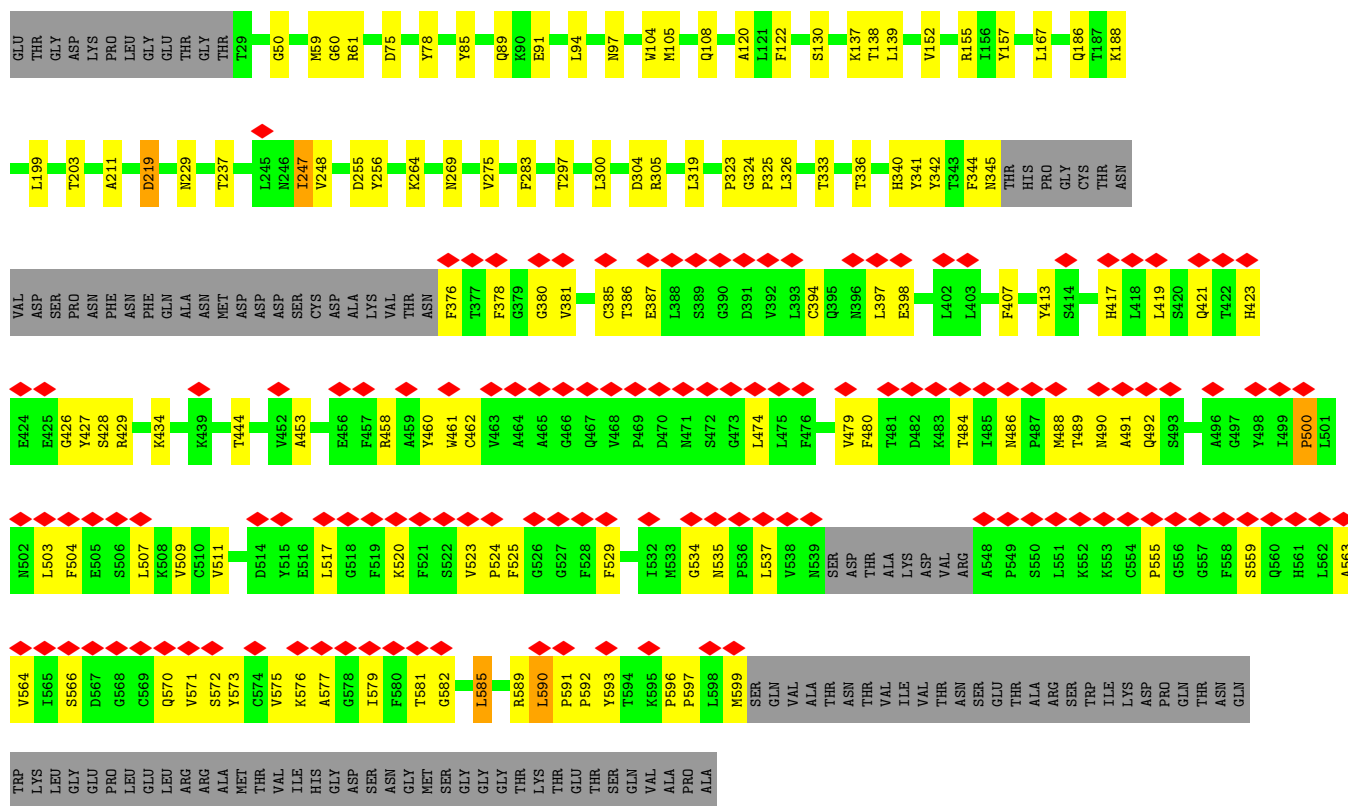
- Molecule 1: Macrophage-expressed gene 1 protein





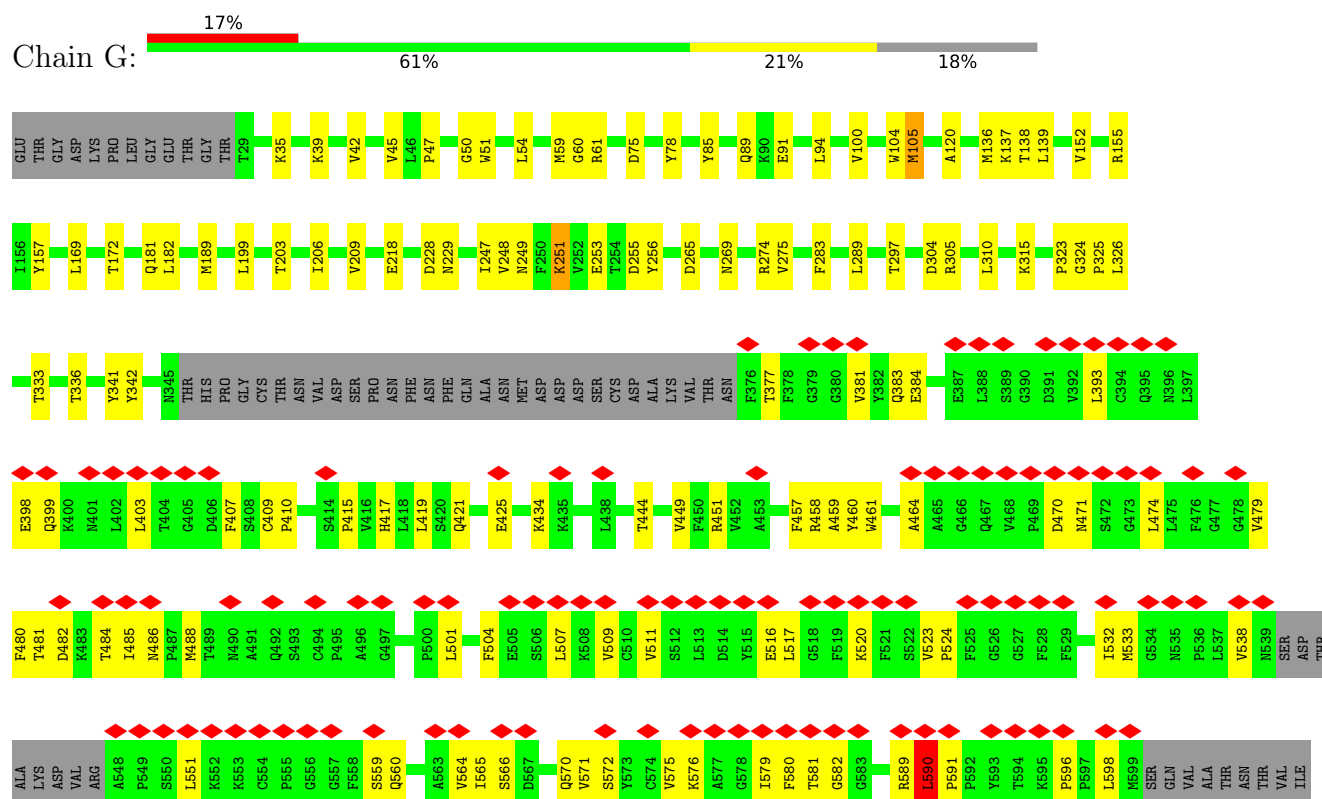


• Molecule 1: Macrophage-expressed gene 1 protein



• Molecule 1: Macrophage-expressed gene 1 protein



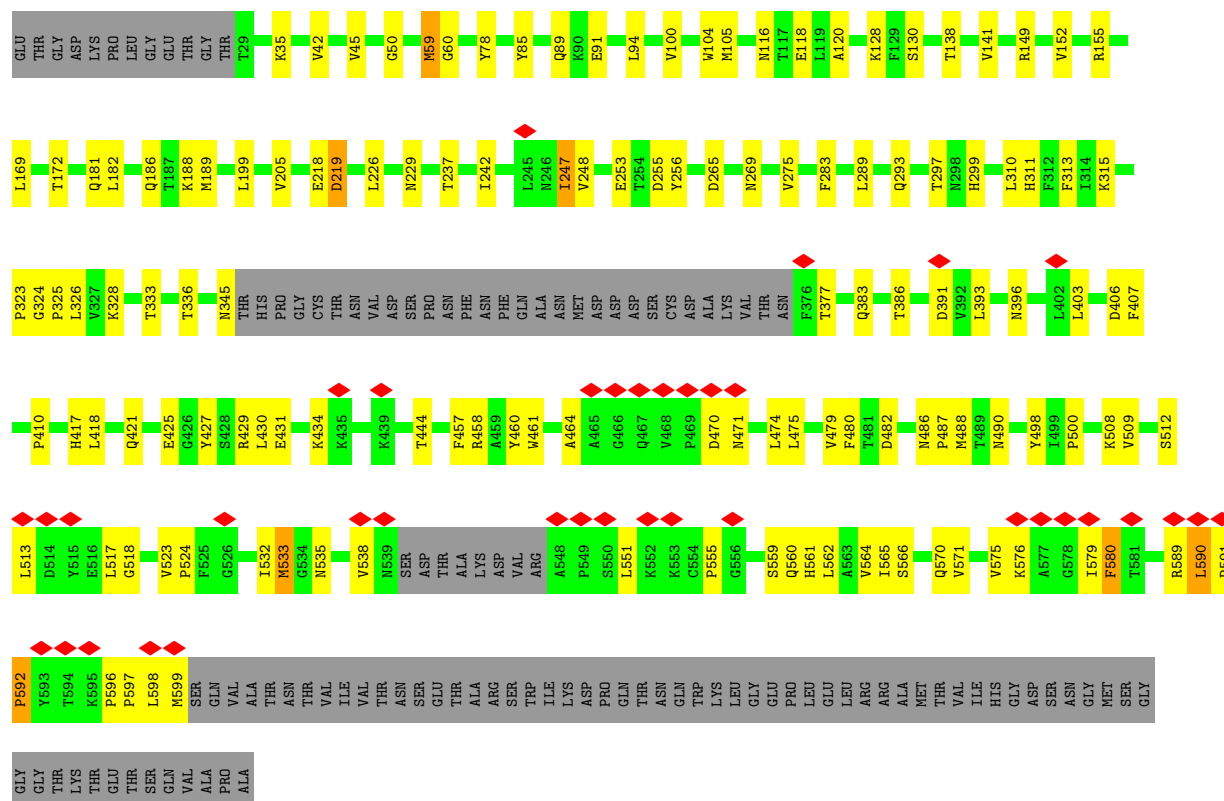




VAL THR ASN SER GLU THR THR ARG SER GLU THR ILE LYS ASP PRO GLN THR GLN THR LYS LEU GLU ARG ARG ALA MET THR VAL ILE HIS GLY GLY THR LYS THR THR SER GLN VAL ALA PRO ALA

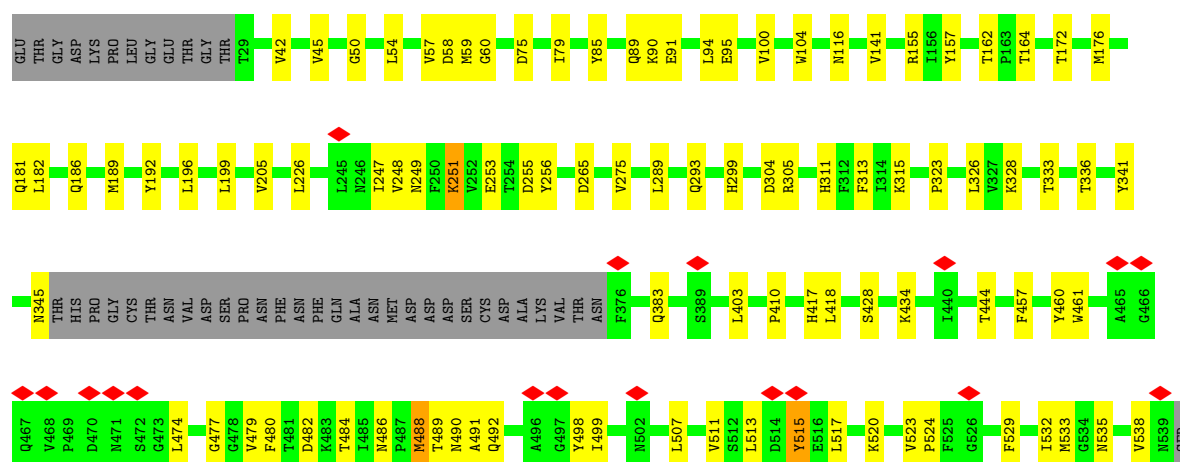
• Molecule 1: Macrophage-expressed gene 1 protein

Chain H: 6% 61% 20% 18%



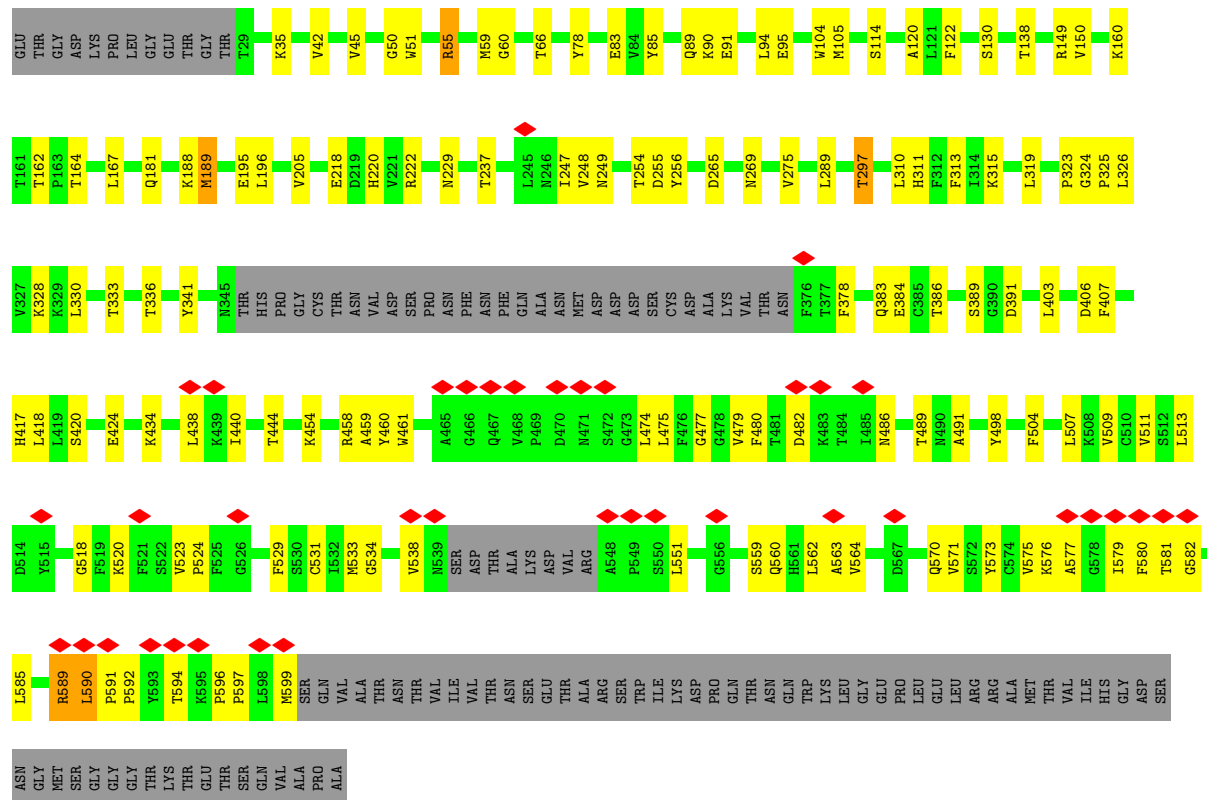
• Molecule 1: Macrophage-expressed gene 1 protein

Chain I: 6% 64% 17% 18%

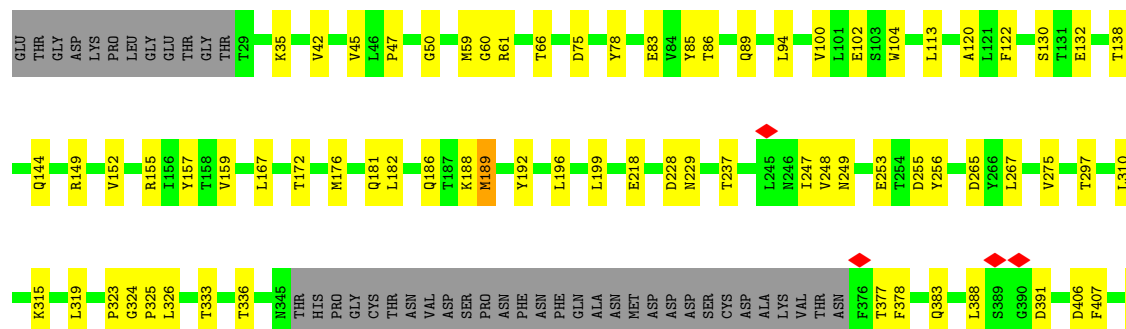




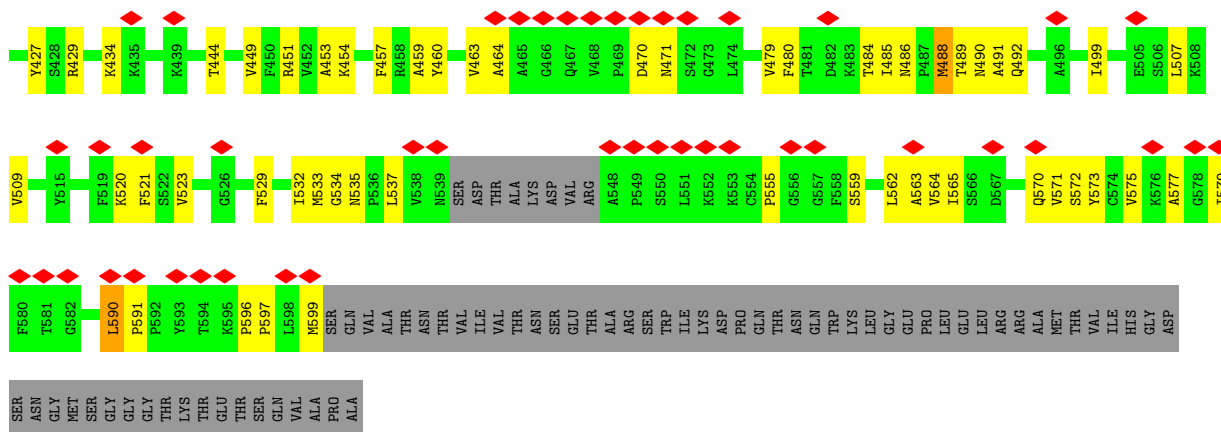
- Molecule 1: Macrophage-expressed gene 1 protein



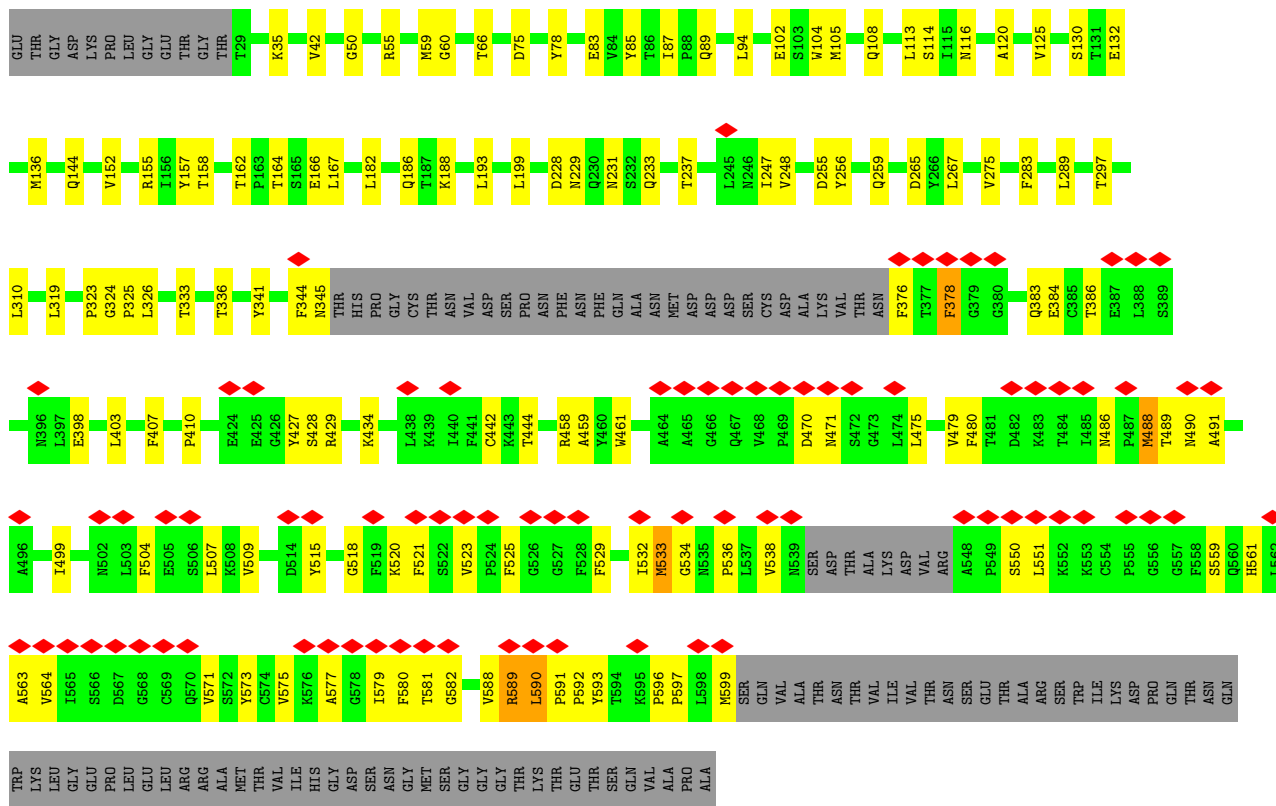
- Molecule 1: Macrophage-expressed gene 1 protein







- Molecule 1: Macrophage-expressed gene 1 protein



- Molecule 1: Macrophage-expressed gene 1 protein





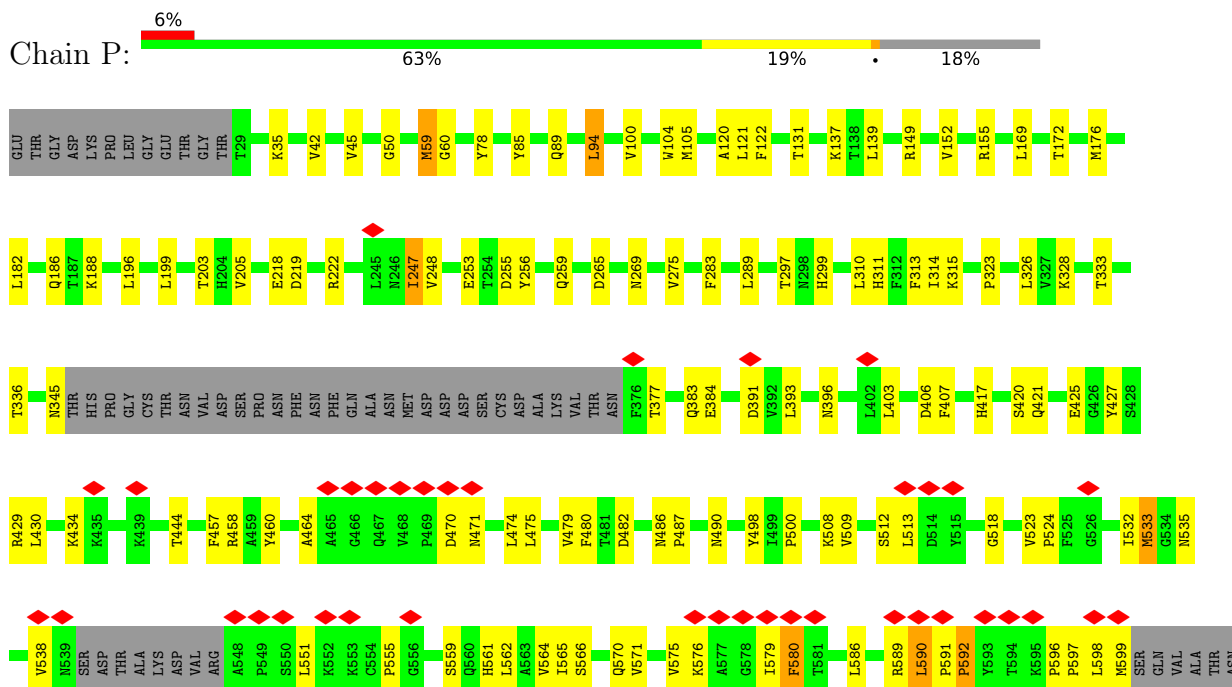




## Chain 0:



Chain P:





|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| THR | VAL | ILE | VAL | THR | ASN | SER | GLU | THR | ALA | ARG | SER | TRP | ILE | LYS | ASP | PRO | GLN | THR | ASN | GLN | TRP | LYS | LEU | GLY | GLU | PRO | LEU | GLU | LEU | ARG | ARG | ALA | MET | THR | VAL | ILE | HIS | GLY | ASP | SER | ASN | GLY | MET | SER | GLY | GLY | GLY | THR | LYS | THR | GLU | THR | SER | GLN | VAL | ALA | PRO | ALA |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|---|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, C2                               | Depositor |
| Number of particles used             | 519614                                  | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 40                                      | Depositor |
| Minimum defocus (nm)                 | 1000                                    | Depositor |
| Maximum defocus (nm)                 | 2400                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K2 QUANTUM (4k x 4k)              | Depositor |
| Maximum map value                    | 0.316                                   | Depositor |
| Minimum map value                    | -0.178                                  | Depositor |
| Average map value                    | 0.000                                   | Depositor |
| Map value standard deviation         | 0.007                                   | Depositor |
| Recommended contour level            | 0.0225                                  | Depositor |
| Map size (Å)                         | 376.92, 376.92, 376.92                  | wwPDB     |
| Map dimensions                       | 360, 360, 360                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.047, 1.047, 1.047                     | Depositor |



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, MA4

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     | 0.42         | 0/4238  | 0.53        | 0/5752         |
| 1   | B     | 0.41         | 0/4238  | 0.53        | 0/5752         |
| 1   | C     | 0.41         | 0/4238  | 0.52        | 0/5752         |
| 1   | D     | 0.41         | 0/4238  | 0.52        | 0/5752         |
| 1   | E     | 0.41         | 0/4238  | 0.54        | 1/5752 (0.0%)  |
| 1   | F     | 0.40         | 0/4238  | 0.53        | 0/5752         |
| 1   | G     | 0.41         | 0/4238  | 0.52        | 1/5752 (0.0%)  |
| 1   | H     | 0.42         | 0/4238  | 0.53        | 1/5752 (0.0%)  |
| 1   | I     | 0.42         | 0/4238  | 0.53        | 0/5752         |
| 1   | J     | 0.41         | 0/4238  | 0.53        | 0/5752         |
| 1   | K     | 0.41         | 0/4238  | 0.52        | 0/5752         |
| 1   | L     | 0.41         | 0/4238  | 0.53        | 0/5752         |
| 1   | M     | 0.41         | 0/4238  | 0.53        | 1/5752 (0.0%)  |
| 1   | N     | 0.40         | 0/4238  | 0.52        | 0/5752         |
| 1   | O     | 0.41         | 0/4238  | 0.52        | 0/5752         |
| 1   | P     | 0.42         | 0/4238  | 0.53        | 1/5752 (0.0%)  |
| All | All   | 0.41         | 0/67808 | 0.53        | 5/92032 (0.0%) |

There are no bond length outliers.

All (5) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | E     | 500 | PRO  | CA-N-CD  | -7.91 | 100.43      | 111.50   |
| 1   | M     | 500 | PRO  | CA-N-CD  | -7.69 | 100.73      | 111.50   |
| 1   | P     | 592 | PRO  | CA-N-CD  | -5.95 | 103.16      | 111.50   |
| 1   | H     | 592 | PRO  | CA-N-CD  | -5.94 | 103.18      | 111.50   |
| 1   | G     | 590 | LEU  | CA-CB-CG | 5.52  | 128.00      | 115.30   |

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     | 4148  | 0        | 4124     | 94      | 0            |
| 1   | B     | 4148  | 0        | 4124     | 85      | 0            |
| 1   | C     | 4148  | 0        | 4124     | 92      | 0            |
| 1   | D     | 4148  | 0        | 4124     | 86      | 0            |
| 1   | E     | 4148  | 0        | 4124     | 91      | 0            |
| 1   | F     | 4148  | 0        | 4124     | 77      | 0            |
| 1   | G     | 4148  | 0        | 4124     | 94      | 0            |
| 1   | H     | 4148  | 0        | 4124     | 100     | 0            |
| 1   | I     | 4148  | 0        | 4124     | 89      | 0            |
| 1   | J     | 4148  | 0        | 4124     | 88      | 0            |
| 1   | K     | 4148  | 0        | 4124     | 83      | 0            |
| 1   | L     | 4148  | 0        | 4124     | 94      | 0            |
| 1   | M     | 4148  | 0        | 4124     | 93      | 0            |
| 1   | N     | 4148  | 0        | 4124     | 92      | 0            |
| 1   | O     | 4148  | 0        | 4124     | 89      | 0            |
| 1   | P     | 4148  | 0        | 4124     | 90      | 0            |
| 2   | A     | 14    | 0        | 13       | 0       | 0            |
| 2   | B     | 14    | 0        | 13       | 0       | 0            |
| 2   | C     | 14    | 0        | 13       | 0       | 0            |
| 2   | D     | 14    | 0        | 13       | 0       | 0            |
| 2   | E     | 14    | 0        | 13       | 0       | 0            |
| 2   | F     | 14    | 0        | 13       | 0       | 0            |
| 2   | G     | 14    | 0        | 13       | 0       | 0            |
| 2   | H     | 14    | 0        | 13       | 0       | 0            |
| 2   | I     | 14    | 0        | 13       | 0       | 0            |
| 2   | J     | 14    | 0        | 13       | 0       | 0            |
| 2   | K     | 14    | 0        | 13       | 0       | 0            |
| 2   | L     | 14    | 0        | 13       | 0       | 0            |
| 2   | M     | 14    | 0        | 13       | 0       | 0            |
| 2   | N     | 14    | 0        | 13       | 0       | 0            |
| 2   | O     | 14    | 0        | 13       | 0       | 0            |
| 2   | P     | 14    | 0        | 13       | 0       | 0            |
| 3   | A     | 35    | 0        | 44       | 2       | 0            |
| 3   | B     | 35    | 0        | 44       | 1       | 0            |
| 3   | C     | 35    | 0        | 44       | 2       | 0            |
| 3   | D     | 35    | 0        | 44       | 3       | 0            |
| 3   | E     | 35    | 0        | 44       | 5       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3   | F     | 35    | 0        | 44       | 1       | 0            |
| 3   | G     | 35    | 0        | 44       | 0       | 0            |
| 3   | H     | 35    | 0        | 44       | 1       | 0            |
| 3   | I     | 35    | 0        | 44       | 1       | 0            |
| 3   | J     | 35    | 0        | 44       | 0       | 0            |
| 3   | K     | 35    | 0        | 44       | 1       | 0            |
| 3   | L     | 35    | 0        | 44       | 5       | 0            |
| 3   | M     | 35    | 0        | 44       | 4       | 0            |
| 3   | N     | 35    | 0        | 44       | 2       | 0            |
| 3   | O     | 35    | 0        | 44       | 1       | 0            |
| 3   | P     | 35    | 0        | 44       | 1       | 0            |
| All | All   | 67152 | 0        | 66896    | 1303    | 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 10.

All (1303) 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) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:702:MA4:HO6  | 3:C:702:MA4:HO60 | 1.17                     | 0.91              |
| 1:K:186:GLN:NE2  | 1:K:599:MET:SD   | 2.44                     | 0.89              |
| 1:H:186:GLN:NE2  | 1:H:599:MET:SD   | 2.48                     | 0.85              |
| 1:C:199:LEU:HB2  | 1:C:591:PRO:HG2  | 1.58                     | 0.84              |
| 1:G:596:PRO:HG3  | 1:H:315:LYS:HE3  | 1.61                     | 0.82              |
| 1:K:199:LEU:HB2  | 1:K:591:PRO:HG2  | 1.61                     | 0.81              |
| 1:C:186:GLN:NE2  | 1:C:599:MET:SD   | 2.53                     | 0.80              |
| 1:K:149:ARG:NH1  | 1:K:218:GLU:OE2  | 2.14                     | 0.80              |
| 1:M:345:ASN:OD1  | 1:M:593:TYR:OH   | 1.99                     | 0.79              |
| 1:O:55:ARG:HD3   | 1:O:590:LEU:HD11 | 1.65                     | 0.78              |
| 1:P:199:LEU:HB2  | 1:P:591:PRO:HG2  | 1.64                     | 0.78              |
| 1:A:59:MET:O     | 1:B:85:TYR:OH    | 2.00                     | 0.78              |
| 1:A:85:TYR:OH    | 1:P:59:MET:O     | 2.02                     | 0.78              |
| 1:M:186:GLN:NE2  | 1:M:599:MET:SD   | 2.53                     | 0.78              |
| 1:E:345:ASN:OD1  | 1:E:593:TYR:OH   | 2.00                     | 0.77              |
| 1:O:59:MET:O     | 1:P:85:TYR:OH    | 2.02                     | 0.77              |
| 1:C:181:GLN:HE21 | 1:C:189:MET:HB3  | 1.49                     | 0.77              |
| 1:H:59:MET:O     | 1:I:85:TYR:OH    | 2.01                     | 0.77              |
| 1:N:59:MET:O     | 1:O:85:TYR:OH    | 2.01                     | 0.77              |
| 1:J:59:MET:O     | 1:K:85:TYR:OH    | 2.01                     | 0.77              |
| 1:G:59:MET:O     | 1:H:85:TYR:OH    | 2.03                     | 0.77              |
| 1:P:417:HIS:ND1  | 1:P:533:MET:SD   | 2.56                     | 0.76              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:59:MET:O     | 1:F:85:TYR:OH    | 2.03                     | 0.76              |
| 1:I:59:MET:O     | 1:J:85:TYR:OH    | 2.02                     | 0.76              |
| 1:P:247:ILE:HG13 | 1:P:248:VAL:HG23 | 1.66                     | 0.76              |
| 1:D:136:MET:HG3  | 1:D:231:ASN:HB2  | 1.68                     | 0.76              |
| 1:B:59:MET:O     | 1:C:85:TYR:OH    | 2.04                     | 0.76              |
| 1:H:417:HIS:ND1  | 1:H:533:MET:SD   | 2.56                     | 0.76              |
| 1:M:199:LEU:HB2  | 1:M:591:PRO:HG2  | 1.67                     | 0.76              |
| 1:N:199:LEU:HB2  | 1:N:591:PRO:HG2  | 1.67                     | 0.75              |
| 1:E:199:LEU:HB2  | 1:E:591:PRO:HG2  | 1.68                     | 0.75              |
| 1:F:59:MET:O     | 1:G:85:TYR:OH    | 2.05                     | 0.75              |
| 1:F:386:THR:OG1  | 1:F:458:ARG:NH1  | 2.21                     | 0.74              |
| 1:H:199:LEU:HB2  | 1:H:591:PRO:HG2  | 1.68                     | 0.74              |
| 1:K:59:MET:O     | 1:L:85:TYR:OH    | 2.04                     | 0.74              |
| 1:F:323:PRO:HD2  | 1:F:326:LEU:HD12 | 1.69                     | 0.74              |
| 1:A:186:GLN:NE2  | 1:A:599:MET:SD   | 2.60                     | 0.74              |
| 1:F:247:ILE:HG12 | 1:F:248:VAL:HG23 | 1.68                     | 0.74              |
| 1:D:195:GLU:HB3  | 1:D:591:PRO:HB2  | 1.68                     | 0.74              |
| 1:H:247:ILE:HG13 | 1:H:248:VAL:HG23 | 1.69                     | 0.74              |
| 1:M:590:LEU:HB2  | 1:M:591:PRO:CD   | 2.18                     | 0.74              |
| 1:D:59:MET:O     | 1:E:85:TYR:OH    | 2.05                     | 0.74              |
| 1:M:434:LYS:HG2  | 1:M:444:THR:HG22 | 1.69                     | 0.73              |
| 1:P:186:GLN:NE2  | 1:P:599:MET:SD   | 2.56                     | 0.73              |
| 1:E:247:ILE:HG13 | 1:E:248:VAL:HG23 | 1.68                     | 0.73              |
| 1:L:247:ILE:HG12 | 1:L:248:VAL:HG23 | 1.70                     | 0.73              |
| 1:E:590:LEU:HB2  | 1:E:591:PRO:CD   | 2.18                     | 0.73              |
| 1:H:562:LEU:HD22 | 1:I:499:ILE:HD11 | 1.70                     | 0.73              |
| 1:E:434:LYS:HG2  | 1:E:444:THR:HG22 | 1.69                     | 0.73              |
| 1:G:323:PRO:HD2  | 1:G:326:LEU:HD12 | 1.69                     | 0.73              |
| 1:E:590:LEU:HB2  | 1:E:591:PRO:HD3  | 1.70                     | 0.73              |
| 1:O:323:PRO:HD2  | 1:O:326:LEU:HD12 | 1.70                     | 0.73              |
| 1:A:417:HIS:ND1  | 1:A:533:MET:SD   | 2.60                     | 0.72              |
| 1:B:589:ARG:NH2  | 1:B:590:LEU:O    | 2.22                     | 0.72              |
| 1:M:590:LEU:HB2  | 1:M:591:PRO:HD3  | 1.71                     | 0.72              |
| 1:A:499:ILE:HD11 | 1:P:562:LEU:HD22 | 1.71                     | 0.72              |
| 1:H:323:PRO:HD2  | 1:H:326:LEU:HD12 | 1.72                     | 0.72              |
| 1:N:149:ARG:NH1  | 1:N:218:GLU:OE2  | 2.23                     | 0.72              |
| 1:M:480:PHE:HB3  | 1:M:486:ASN:HB2  | 1.72                     | 0.72              |
| 1:L:479:VAL:HB   | 1:L:507:LEU:HD11 | 1.72                     | 0.72              |
| 1:D:479:VAL:HB   | 1:D:507:LEU:HD11 | 1.72                     | 0.71              |
| 1:N:323:PRO:HD2  | 1:N:326:LEU:HD12 | 1.70                     | 0.71              |
| 1:F:149:ARG:NH1  | 1:F:218:GLU:OE2  | 2.24                     | 0.71              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:59:MET:O     | 1:N:85:TYR:OH    | 2.04                     | 0.71              |
| 1:C:49:GLY:HA2   | 1:C:61:ARG:HA    | 1.70                     | 0.71              |
| 1:G:598:LEU:HD22 | 1:H:328:LYS:HD3  | 1.71                     | 0.71              |
| 1:I:186:GLN:NE2  | 1:I:599:MET:SD   | 2.62                     | 0.71              |
| 1:L:59:MET:O     | 1:M:85:TYR:OH    | 2.04                     | 0.70              |
| 1:K:247:ILE:HG12 | 1:K:248:VAL:HG23 | 1.73                     | 0.70              |
| 1:O:598:LEU:HD22 | 1:P:328:LYS:HD3  | 1.71                     | 0.70              |
| 1:A:78:TYR:OH    | 1:A:297:THR:O    | 2.07                     | 0.70              |
| 1:I:199:LEU:HB2  | 1:I:591:PRO:HG2  | 1.73                     | 0.70              |
| 1:M:323:PRO:HD2  | 1:M:326:LEU:HD12 | 1.74                     | 0.70              |
| 1:D:247:ILE:HG12 | 1:D:248:VAL:HG23 | 1.72                     | 0.70              |
| 1:E:479:VAL:HG12 | 1:E:509:VAL:HG22 | 1.74                     | 0.70              |
| 1:P:323:PRO:HD2  | 1:P:326:LEU:HD12 | 1.73                     | 0.70              |
| 1:N:247:ILE:HG12 | 1:N:248:VAL:HG23 | 1.73                     | 0.70              |
| 1:H:598:LEU:HD22 | 1:I:328:LYS:HD3  | 1.74                     | 0.70              |
| 1:J:589:ARG:NH2  | 1:J:590:LEU:O    | 2.25                     | 0.70              |
| 1:N:479:VAL:HB   | 1:N:507:LEU:HD11 | 1.73                     | 0.70              |
| 1:E:480:PHE:HB3  | 1:E:486:ASN:HB2  | 1.72                     | 0.70              |
| 1:G:78:TYR:OH    | 1:G:297:THR:O    | 2.07                     | 0.70              |
| 1:N:386:THR:OG1  | 1:N:458:ARG:NH1  | 2.24                     | 0.70              |
| 1:I:417:HIS:ND1  | 1:I:533:MET:SD   | 2.65                     | 0.69              |
| 1:D:344:PHE:HB3  | 1:D:593:TYR:HE1  | 1.57                     | 0.69              |
| 1:D:186:GLN:NE2  | 1:D:599:MET:SD   | 2.63                     | 0.69              |
| 1:E:428:SER:H    | 3:E:702:MA4:H601 | 1.57                     | 0.69              |
| 1:L:186:GLN:NE2  | 1:L:599:MET:SD   | 2.62                     | 0.69              |
| 1:C:247:ILE:HG12 | 1:C:248:VAL:HG23 | 1.72                     | 0.69              |
| 1:L:89:GLN:OE1   | 1:L:155:ARG:NH1  | 2.26                     | 0.69              |
| 1:E:323:PRO:HD2  | 1:E:326:LEU:HD12 | 1.74                     | 0.68              |
| 1:L:323:PRO:HD2  | 1:L:326:LEU:HD12 | 1.75                     | 0.68              |
| 1:A:328:LYS:HD3  | 1:P:598:LEU:HD22 | 1.74                     | 0.68              |
| 1:D:323:PRO:HD2  | 1:D:326:LEU:HD12 | 1.75                     | 0.68              |
| 1:L:199:LEU:HB2  | 1:L:591:PRO:HG2  | 1.74                     | 0.68              |
| 1:I:532:ILE:HG13 | 1:I:533:MET:HG3  | 1.75                     | 0.68              |
| 1:M:479:VAL:HG12 | 1:M:509:VAL:HG22 | 1.74                     | 0.68              |
| 1:I:323:PRO:HD2  | 1:I:326:LEU:HD12 | 1.76                     | 0.68              |
| 1:M:592:PRO:HD3  | 1:N:312:PHE:HE1  | 1.59                     | 0.68              |
| 1:A:517:LEU:HA   | 1:A:520:LYS:HZ2  | 1.58                     | 0.67              |
| 1:O:589:ARG:NH2  | 1:O:592:PRO:O    | 2.26                     | 0.67              |
| 1:E:344:PHE:HB3  | 1:E:593:TYR:CZ   | 2.29                     | 0.67              |
| 1:N:517:LEU:HD23 | 1:N:520:LYS:HE3  | 1.77                     | 0.67              |
| 1:O:78:TYR:OH    | 1:O:297:THR:O    | 2.06                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:377:THR:HB   | 1:O:464:ALA:HB2  | 1.77                     | 0.67              |
| 1:M:344:PHE:HB3  | 1:M:593:TYR:CZ   | 2.30                     | 0.67              |
| 1:N:89:GLN:OE1   | 1:N:155:ARG:NH1  | 2.28                     | 0.67              |
| 1:I:559:SER:N    | 1:I:575:VAL:O    | 2.22                     | 0.67              |
| 1:M:386:THR:OG1  | 1:M:458:ARG:NH1  | 2.27                     | 0.66              |
| 1:H:523:VAL:HG23 | 1:H:579:ILE:HD12 | 1.76                     | 0.66              |
| 1:I:517:LEU:HA   | 1:I:520:LYS:HZ2  | 1.58                     | 0.66              |
| 1:L:592:PRO:HD3  | 1:M:312:PHE:HE1  | 1.61                     | 0.66              |
| 1:A:323:PRO:HD2  | 1:A:326:LEU:HD12 | 1.76                     | 0.66              |
| 1:B:89:GLN:OE1   | 1:B:155:ARG:NH1  | 2.28                     | 0.66              |
| 1:B:559:SER:N    | 1:B:575:VAL:O    | 2.25                     | 0.66              |
| 1:L:523:VAL:HG23 | 1:L:579:ILE:HD12 | 1.78                     | 0.66              |
| 1:B:247:ILE:HG22 | 1:B:248:VAL:HG23 | 1.77                     | 0.65              |
| 1:L:480:PHE:HB3  | 1:L:486:ASN:HB2  | 1.78                     | 0.65              |
| 1:N:523:VAL:HG23 | 1:N:579:ILE:HD12 | 1.77                     | 0.65              |
| 1:C:523:VAL:HG23 | 1:C:579:ILE:HD12 | 1.78                     | 0.65              |
| 1:E:89:GLN:OE1   | 1:E:155:ARG:NH1  | 2.29                     | 0.65              |
| 1:F:186:GLN:NE2  | 1:F:599:MET:SD   | 2.60                     | 0.65              |
| 1:M:249:ASN:HB3  | 1:N:120:ALA:HB3  | 1.79                     | 0.65              |
| 1:D:480:PHE:HB3  | 1:D:486:ASN:HB2  | 1.77                     | 0.65              |
| 1:J:323:PRO:HD2  | 1:J:326:LEU:HD12 | 1.79                     | 0.65              |
| 1:P:523:VAL:HG23 | 1:P:579:ILE:HD12 | 1.78                     | 0.65              |
| 1:G:377:THR:HB   | 1:G:464:ALA:HB2  | 1.77                     | 0.65              |
| 1:B:323:PRO:HD2  | 1:B:326:LEU:HD12 | 1.79                     | 0.64              |
| 1:H:589:ARG:NH2  | 1:H:592:PRO:O    | 2.29                     | 0.64              |
| 1:L:589:ARG:NH2  | 1:L:590:LEU:O    | 2.29                     | 0.64              |
| 1:F:418:LEU:HA   | 1:F:533:MET:HE1  | 1.79                     | 0.64              |
| 1:J:480:PHE:HB3  | 1:J:486:ASN:HB2  | 1.80                     | 0.64              |
| 1:P:188:LYS:HB3  | 1:P:597:PRO:HB2  | 1.80                     | 0.64              |
| 1:O:94:LEU:HD13  | 1:O:152:VAL:HG22 | 1.79                     | 0.64              |
| 1:B:149:ARG:NH1  | 1:B:218:GLU:OE1  | 2.31                     | 0.64              |
| 1:H:434:LYS:HG2  | 1:H:444:THR:HG22 | 1.80                     | 0.64              |
| 1:H:89:GLN:OE1   | 1:H:155:ARG:NH1  | 2.30                     | 0.64              |
| 1:C:255:ASP:HB3  | 1:D:114:SER:HB2  | 1.80                     | 0.64              |
| 1:E:479:VAL:HB   | 1:E:507:LEU:HD11 | 1.80                     | 0.64              |
| 1:G:590:LEU:HB3  | 1:G:591:PRO:HD3  | 1.79                     | 0.63              |
| 1:E:386:THR:OG1  | 1:E:458:ARG:NH1  | 2.26                     | 0.63              |
| 1:J:149:ARG:NH1  | 1:J:218:GLU:OE2  | 2.31                     | 0.63              |
| 1:P:434:LYS:HG2  | 1:P:444:THR:HG22 | 1.80                     | 0.63              |
| 1:I:89:GLN:OE1   | 1:I:155:ARG:NH1  | 2.31                     | 0.63              |
| 1:K:130:SER:HG   | 1:K:237:THR:HG1  | 1.34                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:479:VAL:HB   | 1:M:507:LEU:HD11 | 1.81                     | 0.63              |
| 1:N:304:ASP:OD1  | 1:N:305:ARG:N    | 2.31                     | 0.63              |
| 1:P:89:GLN:OE1   | 1:P:155:ARG:NH1  | 2.31                     | 0.63              |
| 1:A:89:GLN:OE1   | 1:A:155:ARG:NH1  | 2.31                     | 0.63              |
| 1:M:89:GLN:OE1   | 1:M:155:ARG:NH1  | 2.32                     | 0.63              |
| 1:N:186:GLN:NE2  | 1:N:599:MET:SD   | 2.61                     | 0.63              |
| 1:B:529:PHE:HB2  | 1:B:534:GLY:HA2  | 1.81                     | 0.63              |
| 1:J:434:LYS:HG2  | 1:J:444:THR:HG22 | 1.81                     | 0.63              |
| 1:B:523:VAL:HG23 | 1:B:579:ILE:HD12 | 1.79                     | 0.63              |
| 1:K:434:LYS:HG2  | 1:K:444:THR:HG22 | 1.81                     | 0.63              |
| 1:M:426:GLY:O    | 3:M:702:MA4:O4   | 2.16                     | 0.63              |
| 1:H:188:LYS:HB3  | 1:H:597:PRO:HB2  | 1.81                     | 0.62              |
| 1:N:589:ARG:NH2  | 1:N:590:LEU:O    | 2.32                     | 0.62              |
| 1:G:89:GLN:OE1   | 1:G:155:ARG:NH1  | 2.32                     | 0.62              |
| 1:J:559:SER:N    | 1:J:575:VAL:O    | 2.24                     | 0.62              |
| 1:L:87:ILE:HG13  | 1:L:158:THR:HB   | 1.82                     | 0.62              |
| 1:G:523:VAL:HG23 | 1:G:579:ILE:HD12 | 1.82                     | 0.62              |
| 1:J:529:PHE:HB2  | 1:J:534:GLY:HA2  | 1.81                     | 0.62              |
| 1:L:275:VAL:HB   | 1:M:94:LEU:HB2   | 1.82                     | 0.62              |
| 1:D:564:VAL:HG12 | 1:D:571:VAL:HB   | 1.82                     | 0.62              |
| 1:C:434:LYS:HG2  | 1:C:444:THR:HG22 | 1.81                     | 0.62              |
| 1:L:341:TYR:HE1  | 1:L:590:LEU:HB3  | 1.65                     | 0.62              |
| 1:E:426:GLY:O    | 3:E:702:MA4:O4   | 2.17                     | 0.62              |
| 1:E:186:GLN:NE2  | 1:E:599:MET:SD   | 2.67                     | 0.61              |
| 1:L:428:SER:H    | 3:L:702:MA4:H601 | 1.65                     | 0.61              |
| 1:M:428:SER:H    | 3:M:702:MA4:H601 | 1.65                     | 0.61              |
| 1:N:502:ASN:OD1  | 1:N:508:LYS:NZ   | 2.29                     | 0.61              |
| 1:A:304:ASP:OD1  | 1:A:305:ARG:N    | 2.33                     | 0.61              |
| 1:A:559:SER:N    | 1:A:575:VAL:O    | 2.26                     | 0.61              |
| 1:I:247:ILE:HG12 | 1:I:248:VAL:HG23 | 1.81                     | 0.61              |
| 1:P:427:TYR:OH   | 1:P:429:ARG:NH2  | 2.33                     | 0.61              |
| 1:B:480:PHE:HB3  | 1:B:486:ASN:HB2  | 1.82                     | 0.61              |
| 1:C:345:ASN:OD1  | 1:C:593:TYR:OH   | 2.16                     | 0.61              |
| 1:L:564:VAL:HG12 | 1:L:571:VAL:HB   | 1.83                     | 0.61              |
| 1:A:315:LYS:HE3  | 1:P:596:PRO:HG3  | 1.82                     | 0.61              |
| 1:I:564:VAL:HG12 | 1:I:571:VAL:HB   | 1.81                     | 0.61              |
| 1:D:188:LYS:HD3  | 1:D:597:PRO:HB2  | 1.83                     | 0.61              |
| 1:A:247:ILE:HG12 | 1:A:248:VAL:HG23 | 1.83                     | 0.61              |
| 1:B:434:LYS:HG2  | 1:B:444:THR:HG22 | 1.83                     | 0.61              |
| 1:B:199:LEU:HD13 | 1:B:591:PRO:HD2  | 1.83                     | 0.61              |
| 1:C:304:ASP:OD2  | 1:C:305:ARG:N    | 2.33                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:434:LYS:HG2  | 1:F:444:THR:HG22 | 1.83                     | 0.61              |
| 1:L:166:GLU:OE1  | 1:L:166:GLU:N    | 2.34                     | 0.61              |
| 1:A:564:VAL:HG12 | 1:A:571:VAL:HB   | 1.83                     | 0.60              |
| 1:I:434:LYS:HG2  | 1:I:444:THR:HG22 | 1.80                     | 0.60              |
| 1:K:253:GLU:HG3  | 1:L:116:ASN:HB2  | 1.82                     | 0.60              |
| 1:L:589:ARG:NH2  | 1:L:592:PRO:O    | 2.30                     | 0.60              |
| 1:N:434:LYS:HG2  | 1:N:444:THR:HG22 | 1.83                     | 0.60              |
| 1:A:434:LYS:HG2  | 1:A:444:THR:HG22 | 1.82                     | 0.60              |
| 1:M:78:TYR:OH    | 1:M:297:THR:O    | 2.10                     | 0.60              |
| 1:M:523:VAL:HG23 | 1:M:579:ILE:HD12 | 1.83                     | 0.60              |
| 1:E:523:VAL:HG23 | 1:E:579:ILE:HD12 | 1.83                     | 0.60              |
| 1:G:247:ILE:HG22 | 1:G:248:VAL:HG23 | 1.83                     | 0.60              |
| 1:K:590:LEU:HB2  | 1:K:591:PRO:HD3  | 1.83                     | 0.60              |
| 1:A:523:VAL:HG23 | 1:A:579:ILE:HD12 | 1.82                     | 0.60              |
| 1:H:427:TYR:OH   | 1:H:429:ARG:NH2  | 2.34                     | 0.60              |
| 1:K:532:ILE:HG13 | 1:K:533:MET:HG2  | 1.84                     | 0.60              |
| 1:H:560:GLN:OE1  | 1:I:515:TYR:OH   | 2.13                     | 0.60              |
| 1:P:94:LEU:HD13  | 1:P:152:VAL:HG22 | 1.84                     | 0.60              |
| 1:A:275:VAL:HB   | 1:B:94:LEU:HB2   | 1.84                     | 0.60              |
| 1:F:55:ARG:HE    | 1:F:590:LEU:HD21 | 1.67                     | 0.60              |
| 1:P:589:ARG:NH2  | 1:P:592:PRO:O    | 2.35                     | 0.60              |
| 1:D:75:ASP:OD2   | 1:D:157:TYR:OH   | 2.17                     | 0.59              |
| 1:J:523:VAL:HG23 | 1:J:579:ILE:HD12 | 1.82                     | 0.59              |
| 1:C:89:GLN:OE1   | 1:C:155:ARG:NH1  | 2.35                     | 0.59              |
| 1:N:345:ASN:OD1  | 1:N:593:TYR:OH   | 2.20                     | 0.59              |
| 1:K:89:GLN:OE1   | 1:K:155:ARG:NH1  | 2.35                     | 0.59              |
| 1:C:427:TYR:OH   | 1:C:429:ARG:NH2  | 2.36                     | 0.59              |
| 1:D:166:GLU:OE2  | 1:D:166:GLU:N    | 2.35                     | 0.59              |
| 1:G:589:ARG:NH2  | 1:G:590:LEU:O    | 2.25                     | 0.59              |
| 1:K:427:TYR:OH   | 1:K:429:ARG:NH2  | 2.36                     | 0.59              |
| 1:N:401:ASN:HD21 | 1:N:410:PRO:HG3  | 1.68                     | 0.59              |
| 1:O:247:ILE:HG22 | 1:O:248:VAL:HG23 | 1.83                     | 0.59              |
| 1:D:275:VAL:HB   | 1:E:94:LEU:HB2   | 1.83                     | 0.59              |
| 1:K:47:PRO:O     | 1:K:61:ARG:NH1   | 2.35                     | 0.59              |
| 1:E:559:SER:N    | 1:E:575:VAL:O    | 2.35                     | 0.59              |
| 1:O:523:VAL:HG23 | 1:O:579:ILE:HD12 | 1.83                     | 0.58              |
| 1:F:401:ASN:HD21 | 1:F:410:PRO:HG3  | 1.67                     | 0.58              |
| 1:A:535:ASN:ND2  | 1:A:555:PRO:HD3  | 2.18                     | 0.58              |
| 1:A:598:LEU:HD22 | 1:B:328:LYS:HD3  | 1.86                     | 0.58              |
| 1:E:78:TYR:OH    | 1:E:297:THR:O    | 2.09                     | 0.58              |
| 1:K:488:MET:HE1  | 1:K:489:THR:HB   | 1.85                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:50:GLY:N     | 1:E:60:GLY:O     | 2.25                     | 0.58              |
| 1:K:590:LEU:HB2  | 1:K:591:PRO:CD   | 2.33                     | 0.58              |
| 1:O:131:THR:HG22 | 1:O:236:VAL:HG22 | 1.85                     | 0.58              |
| 1:D:427:TYR:OH   | 1:D:429:ARG:NH2  | 2.36                     | 0.58              |
| 1:L:504:PHE:HB2  | 1:L:507:LEU:HB3  | 1.86                     | 0.58              |
| 1:A:513:LEU:HD12 | 1:P:562:LEU:HB2  | 1.86                     | 0.58              |
| 1:F:89:GLN:OE1   | 1:F:155:ARG:NH1  | 2.37                     | 0.58              |
| 1:G:479:VAL:HB   | 1:G:507:LEU:HD11 | 1.84                     | 0.58              |
| 1:O:249:ASN:HB3  | 1:P:120:ALA:HB3  | 1.86                     | 0.58              |
| 1:C:75:ASP:OD2   | 1:C:157:TYR:OH   | 2.21                     | 0.58              |
| 1:I:524:PRO:HG2  | 1:I:576:LYS:HD2  | 1.85                     | 0.58              |
| 1:J:386:THR:OG1  | 1:J:458:ARG:NH1  | 2.30                     | 0.58              |
| 1:O:479:VAL:HB   | 1:O:507:LEU:HD11 | 1.85                     | 0.58              |
| 1:A:562:LEU:HB2  | 1:B:513:LEU:HD12 | 1.85                     | 0.58              |
| 1:B:275:VAL:HB   | 1:C:94:LEU:HB2   | 1.85                     | 0.58              |
| 1:I:535:ASN:ND2  | 1:I:555:PRO:HD3  | 2.18                     | 0.58              |
| 1:C:480:PHE:HB3  | 1:C:486:ASN:HB2  | 1.86                     | 0.58              |
| 1:I:75:ASP:OD2   | 1:I:157:TYR:OH   | 2.22                     | 0.58              |
| 1:F:275:VAL:HB   | 1:G:94:LEU:HB2   | 1.86                     | 0.58              |
| 1:F:523:VAL:HG23 | 1:F:579:ILE:HD12 | 1.83                     | 0.58              |
| 1:L:538:VAL:HG11 | 1:L:551:LEU:HB2  | 1.86                     | 0.58              |
| 1:M:138:THR:HB   | 1:M:229:ASN:HB3  | 1.85                     | 0.58              |
| 1:F:564:VAL:HG12 | 1:F:571:VAL:HB   | 1.86                     | 0.57              |
| 1:I:275:VAL:HB   | 1:J:94:LEU:HB2   | 1.86                     | 0.57              |
| 1:N:384:GLU:OE1  | 1:N:458:ARG:NH2  | 2.30                     | 0.57              |
| 1:P:78:TYR:OH    | 1:P:297:THR:O    | 2.17                     | 0.57              |
| 1:A:532:ILE:HG13 | 1:A:533:MET:HG3  | 1.86                     | 0.57              |
| 1:N:421:GLN:OE1  | 1:N:566:SER:OG   | 2.17                     | 0.57              |
| 1:N:589:ARG:NH2  | 1:N:592:PRO:O    | 2.25                     | 0.57              |
| 1:B:403:LEU:HD21 | 1:B:474:LEU:HD21 | 1.87                     | 0.57              |
| 1:M:247:ILE:HG13 | 1:M:248:VAL:HG23 | 1.85                     | 0.57              |
| 1:A:589:ARG:NH2  | 1:A:592:PRO:O    | 2.30                     | 0.57              |
| 1:O:570:GLN:NE2  | 1:O:572:SER:OG   | 2.37                     | 0.57              |
| 1:K:480:PHE:HB3  | 1:K:486:ASN:HB2  | 1.86                     | 0.57              |
| 1:K:486:ASN:O    | 1:K:490:ASN:N    | 2.37                     | 0.57              |
| 1:L:344:PHE:HB3  | 1:L:593:TYR:HE1  | 1.69                     | 0.57              |
| 1:L:427:TYR:OH   | 1:L:429:ARG:NH2  | 2.37                     | 0.57              |
| 1:L:529:PHE:HB2  | 1:L:534:GLY:HA2  | 1.87                     | 0.57              |
| 1:B:311:HIS:O    | 1:B:315:LYS:NZ   | 2.38                     | 0.57              |
| 1:I:598:LEU:HD22 | 1:J:328:LYS:HD3  | 1.85                     | 0.57              |
| 1:D:403:LEU:HD12 | 1:D:410:PRO:HB3  | 1.85                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:590:LEU:HB3  | 1:F:591:PRO:HD3  | 1.87                     | 0.57              |
| 1:C:486:ASN:O    | 1:C:490:ASN:N    | 2.38                     | 0.56              |
| 1:F:596:PRO:HG2  | 1:G:315:LYS:HE3  | 1.86                     | 0.56              |
| 1:P:377:THR:HB   | 1:P:464:ALA:HB2  | 1.87                     | 0.56              |
| 1:B:50:GLY:N     | 1:B:60:GLY:O     | 2.28                     | 0.56              |
| 1:C:590:LEU:HB2  | 1:C:591:PRO:HD3  | 1.86                     | 0.56              |
| 1:D:529:PHE:HB2  | 1:D:534:GLY:HA2  | 1.88                     | 0.56              |
| 1:G:181:GLN:NE2  | 1:G:189:MET:HB3  | 2.21                     | 0.56              |
| 1:G:559:SER:N    | 1:G:575:VAL:O    | 2.32                     | 0.56              |
| 1:H:559:SER:N    | 1:H:575:VAL:O    | 2.32                     | 0.56              |
| 1:L:403:LEU:HD12 | 1:L:410:PRO:HB3  | 1.87                     | 0.56              |
| 1:P:559:SER:N    | 1:P:575:VAL:O    | 2.31                     | 0.56              |
| 1:H:562:LEU:HB2  | 1:I:513:LEU:HD12 | 1.87                     | 0.56              |
| 1:M:559:SER:N    | 1:M:575:VAL:O    | 2.35                     | 0.56              |
| 1:D:89:GLN:OE1   | 1:D:155:ARG:NH1  | 2.39                     | 0.56              |
| 1:G:532:ILE:HG13 | 1:G:533:MET:HG2  | 1.88                     | 0.56              |
| 1:K:275:VAL:HB   | 1:L:94:LEU:HB2   | 1.88                     | 0.56              |
| 1:A:524:PRO:HG2  | 1:A:576:LYS:HD2  | 1.86                     | 0.56              |
| 1:B:78:TYR:OH    | 1:B:297:THR:O    | 2.15                     | 0.56              |
| 1:D:538:VAL:HG11 | 1:D:551:LEU:HB2  | 1.87                     | 0.56              |
| 1:L:344:PHE:CB   | 1:L:593:TYR:HE1  | 2.19                     | 0.56              |
| 1:M:186:GLN:HG3  | 1:M:188:LYS:HE2  | 1.88                     | 0.56              |
| 1:I:523:VAL:HG23 | 1:I:579:ILE:HD12 | 1.86                     | 0.56              |
| 1:N:502:ASN:ND2  | 1:N:504:PHE:O    | 2.38                     | 0.56              |
| 1:G:479:VAL:HG12 | 1:G:509:VAL:HG22 | 1.87                     | 0.56              |
| 1:J:275:VAL:HB   | 1:K:94:LEU:HB2   | 1.86                     | 0.56              |
| 1:J:311:HIS:O    | 1:J:315:LYS:NZ   | 2.38                     | 0.56              |
| 1:M:304:ASP:OD2  | 1:M:305:ARG:N    | 2.38                     | 0.56              |
| 1:N:517:LEU:HA   | 1:N:520:LYS:HE2  | 1.88                     | 0.56              |
| 1:J:89:GLN:O     | 1:J:91:GLU:HG3   | 2.05                     | 0.56              |
| 1:O:590:LEU:HB2  | 1:O:591:PRO:CD   | 2.36                     | 0.56              |
| 1:I:480:PHE:HB3  | 1:I:486:ASN:HB2  | 1.87                     | 0.56              |
| 1:K:75:ASP:OD2   | 1:K:157:TYR:OH   | 2.24                     | 0.55              |
| 1:N:596:PRO:HG2  | 1:O:315:LYS:HE3  | 1.87                     | 0.55              |
| 1:O:589:ARG:NH2  | 1:O:590:LEU:O    | 2.39                     | 0.55              |
| 1:A:480:PHE:HB3  | 1:A:486:ASN:HB2  | 1.87                     | 0.55              |
| 1:I:484:THR:O    | 1:I:492:GLN:NE2  | 2.39                     | 0.55              |
| 1:N:479:VAL:HG12 | 1:N:509:VAL:HG22 | 1.88                     | 0.55              |
| 1:A:94:LEU:HB2   | 1:P:275:VAL:HB   | 1.87                     | 0.55              |
| 1:O:434:LYS:HG2  | 1:O:444:THR:HG22 | 1.88                     | 0.55              |
| 1:C:265:ASP:HB2  | 1:D:104:TRP:HB3  | 1.88                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:377:THR:HB   | 1:K:464:ALA:HB2  | 1.88                     | 0.55              |
| 1:K:479:VAL:HG12 | 1:K:509:VAL:HA   | 1.89                     | 0.55              |
| 1:L:488:MET:HE1  | 1:L:489:THR:HB   | 1.88                     | 0.55              |
| 1:O:501:LEU:HB3  | 1:O:509:VAL:HG23 | 1.89                     | 0.55              |
| 1:O:538:VAL:HG11 | 1:O:551:LEU:HB2  | 1.87                     | 0.55              |
| 1:F:413:TYR:HB3  | 1:F:462:CYS:HB3  | 1.89                     | 0.55              |
| 1:G:564:VAL:HG12 | 1:G:571:VAL:HB   | 1.89                     | 0.55              |
| 1:H:377:THR:HB   | 1:H:464:ALA:HB2  | 1.87                     | 0.55              |
| 1:O:564:VAL:HG12 | 1:O:571:VAL:HB   | 1.87                     | 0.55              |
| 1:B:389:SER:OG   | 1:B:454:LYS:N    | 2.32                     | 0.55              |
| 1:B:564:VAL:HG12 | 1:B:571:VAL:HB   | 1.87                     | 0.55              |
| 1:C:532:ILE:HG13 | 1:C:533:MET:HG2  | 1.87                     | 0.55              |
| 1:E:304:ASP:OD1  | 1:E:305:ARG:N    | 2.40                     | 0.55              |
| 1:E:517:LEU:HD23 | 1:E:520:LYS:HD3  | 1.89                     | 0.55              |
| 1:C:275:VAL:HB   | 1:D:94:LEU:HB2   | 1.88                     | 0.55              |
| 1:C:488:MET:HE1  | 1:C:489:THR:HB   | 1.89                     | 0.55              |
| 1:N:199:LEU:HD13 | 1:N:591:PRO:HD2  | 1.88                     | 0.55              |
| 1:O:381:VAL:HG12 | 1:O:461:TRP:HA   | 1.89                     | 0.55              |
| 1:P:564:VAL:HG12 | 1:P:571:VAL:HB   | 1.89                     | 0.55              |
| 1:H:498:TYR:CZ   | 1:H:512:SER:HB2  | 2.41                     | 0.55              |
| 1:O:383:GLN:HE21 | 1:O:457:PHE:HB2  | 1.72                     | 0.55              |
| 1:O:479:VAL:HG12 | 1:O:509:VAL:HG12 | 1.88                     | 0.55              |
| 1:I:596:PRO:HG2  | 1:J:315:LYS:HE3  | 1.89                     | 0.55              |
| 1:M:255:ASP:HB3  | 1:N:114:SER:HB2  | 1.88                     | 0.55              |
| 1:M:564:VAL:HG12 | 1:M:571:VAL:HB   | 1.89                     | 0.55              |
| 1:A:75:ASP:OD2   | 1:A:157:TYR:OH   | 2.22                     | 0.54              |
| 1:G:51:TRP:HB2   | 1:G:206:ILE:HD13 | 1.88                     | 0.54              |
| 1:G:249:ASN:HB3  | 1:H:120:ALA:HB3  | 1.89                     | 0.54              |
| 1:K:529:PHE:HB2  | 1:K:534:GLY:HA2  | 1.89                     | 0.54              |
| 1:B:35:LYS:HE3   | 1:B:42:VAL:HG23  | 1.88                     | 0.54              |
| 1:D:504:PHE:HB2  | 1:D:507:LEU:HB3  | 1.89                     | 0.54              |
| 1:L:386:THR:OG1  | 1:L:458:ARG:NH1  | 2.37                     | 0.54              |
| 1:P:345:ASN:HD21 | 1:P:590:LEU:HD12 | 1.73                     | 0.54              |
| 1:C:529:PHE:HB2  | 1:C:534:GLY:HA2  | 1.90                     | 0.54              |
| 1:E:564:VAL:HG12 | 1:E:571:VAL:HB   | 1.89                     | 0.54              |
| 1:J:220:HIS:HD2  | 1:J:222:ARG:HH12 | 1.55                     | 0.54              |
| 1:L:188:LYS:HD3  | 1:L:597:PRO:HB2  | 1.89                     | 0.54              |
| 1:N:564:VAL:HG12 | 1:N:571:VAL:HB   | 1.88                     | 0.54              |
| 1:P:498:TYR:CZ   | 1:P:512:SER:HB2  | 2.43                     | 0.54              |
| 1:G:434:LYS:HG2  | 1:G:444:THR:HG22 | 1.88                     | 0.54              |
| 1:H:564:VAL:HG12 | 1:H:571:VAL:HB   | 1.89                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:136:MET:HG2  | 1:L:231:ASN:HB2  | 1.89                     | 0.54              |
| 1:H:89:GLN:O     | 1:H:91:GLU:N     | 2.40                     | 0.54              |
| 1:N:78:TYR:OH    | 1:N:297:THR:O    | 2.11                     | 0.54              |
| 1:A:228:ASP:OD1  | 1:A:229:ASN:N    | 2.40                     | 0.53              |
| 1:C:377:THR:HB   | 1:C:464:ALA:HB2  | 1.90                     | 0.53              |
| 1:E:380:GLY:HA2  | 1:E:474:LEU:HD21 | 1.90                     | 0.53              |
| 1:G:383:GLN:HE21 | 1:G:457:PHE:HB2  | 1.73                     | 0.53              |
| 1:G:570:GLN:NE2  | 1:G:572:SER:OG   | 2.40                     | 0.53              |
| 1:G:590:LEU:HB3  | 1:G:591:PRO:CD   | 2.38                     | 0.53              |
| 1:G:89:GLN:O     | 1:G:91:GLU:N     | 2.42                     | 0.53              |
| 1:A:484:THR:O    | 1:A:492:GLN:NE2  | 2.40                     | 0.53              |
| 1:C:323:PRO:HD2  | 1:C:326:LEU:HD12 | 1.90                     | 0.53              |
| 1:J:596:PRO:HG2  | 1:K:315:LYS:HE3  | 1.90                     | 0.53              |
| 1:B:75:ASP:OD2   | 1:B:157:TYR:OH   | 2.21                     | 0.53              |
| 1:E:563:ALA:HB2  | 1:E:573:TYR:HD2  | 1.73                     | 0.53              |
| 1:J:504:PHE:HB2  | 1:J:507:LEU:HB3  | 1.89                     | 0.53              |
| 1:P:396:ASN:OD1  | 1:P:396:ASN:N    | 2.41                     | 0.53              |
| 1:K:113:LEU:O    | 1:K:132:GLU:HA   | 2.09                     | 0.53              |
| 1:C:479:VAL:HG12 | 1:C:509:VAL:HA   | 1.91                     | 0.53              |
| 1:H:199:LEU:HD13 | 1:H:591:PRO:HD2  | 1.90                     | 0.53              |
| 1:H:396:ASN:N    | 1:H:396:ASN:OD1  | 2.41                     | 0.53              |
| 1:J:564:VAL:HG12 | 1:J:571:VAL:HB   | 1.89                     | 0.53              |
| 1:K:323:PRO:HD2  | 1:K:326:LEU:HD12 | 1.91                     | 0.53              |
| 1:K:570:GLN:NE2  | 1:K:572:SER:OG   | 2.41                     | 0.53              |
| 1:A:255:ASP:HB3  | 1:B:114:SER:HB2  | 1.91                     | 0.53              |
| 1:E:398:GLU:HB2  | 1:E:407:PHE:HZ   | 1.74                     | 0.53              |
| 1:I:89:GLN:O     | 1:I:91:GLU:HG3   | 2.09                     | 0.53              |
| 1:C:590:LEU:HB2  | 1:C:591:PRO:CD   | 2.38                     | 0.53              |
| 1:E:344:PHE:HB3  | 1:E:593:TYR:OH   | 2.08                     | 0.53              |
| 1:F:421:GLN:OE1  | 1:F:566:SER:OG   | 2.18                     | 0.53              |
| 1:I:589:ARG:NH2  | 1:I:592:PRO:O    | 2.31                     | 0.53              |
| 1:L:130:SER:HB2  | 1:L:237:THR:OG1  | 2.08                     | 0.53              |
| 1:O:75:ASP:OD2   | 1:O:157:TYR:OH   | 2.25                     | 0.53              |
| 1:G:50:GLY:N     | 1:G:60:GLY:O     | 2.27                     | 0.53              |
| 1:H:486:ASN:O    | 1:H:490:ASN:N    | 2.42                     | 0.53              |
| 1:C:228:ASP:OD2  | 1:C:229:ASN:N    | 2.41                     | 0.52              |
| 1:G:484:THR:OG1  | 1:G:485:ILE:N    | 2.42                     | 0.52              |
| 1:A:42:VAL:HG22  | 1:A:79:ILE:HB    | 1.90                     | 0.52              |
| 1:C:479:VAL:HB   | 1:C:507:LEU:HD11 | 1.90                     | 0.52              |
| 1:D:590:LEU:HB3  | 1:D:591:PRO:HD3  | 1.91                     | 0.52              |
| 1:F:479:VAL:HB   | 1:F:507:LEU:HD11 | 1.90                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:58:ASP:O     | 1:J:160:LYS:NZ   | 2.43                     | 0.52              |
| 1:J:249:ASN:HB3  | 1:K:120:ALA:HB3  | 1.90                     | 0.52              |
| 1:P:417:HIS:HA   | 1:P:460:TYR:CD2  | 2.45                     | 0.52              |
| 1:I:563:ALA:HB2  | 1:I:573:TYR:HD1  | 1.74                     | 0.52              |
| 1:I:590:LEU:HB2  | 1:I:591:PRO:CD   | 2.40                     | 0.52              |
| 1:J:389:SER:OG   | 1:J:454:LYS:N    | 2.34                     | 0.52              |
| 1:A:50:GLY:N     | 1:A:60:GLY:O     | 2.38                     | 0.52              |
| 1:A:596:PRO:HG2  | 1:B:315:LYS:HE3  | 1.89                     | 0.52              |
| 1:C:559:SER:N    | 1:C:575:VAL:O    | 2.27                     | 0.52              |
| 1:H:417:HIS:HA   | 1:H:460:TYR:CD2  | 2.45                     | 0.52              |
| 1:K:228:ASP:OD1  | 1:K:229:ASN:N    | 2.42                     | 0.52              |
| 1:M:344:PHE:HB3  | 1:M:593:TYR:OH   | 2.09                     | 0.52              |
| 1:N:486:ASN:O    | 1:N:490:ASN:N    | 2.42                     | 0.52              |
| 1:E:427:TYR:OH   | 1:E:429:ARG:NH2  | 2.43                     | 0.52              |
| 1:G:393:LEU:HD21 | 1:G:425:GLU:HB3  | 1.91                     | 0.52              |
| 1:A:89:GLN:O     | 1:A:91:GLU:HG3   | 2.09                     | 0.52              |
| 1:A:138:THR:HB   | 1:A:229:ASN:HB3  | 1.92                     | 0.52              |
| 1:C:255:ASP:N    | 1:D:114:SER:O    | 2.37                     | 0.52              |
| 1:C:559:SER:HB3  | 1:C:577:ALA:HB2  | 1.92                     | 0.52              |
| 1:H:275:VAL:HB   | 1:I:94:LEU:HB2   | 1.90                     | 0.52              |
| 1:M:50:GLY:N     | 1:M:60:GLY:O     | 2.28                     | 0.52              |
| 1:F:304:ASP:OD1  | 1:F:305:ARG:N    | 2.42                     | 0.52              |
| 1:G:75:ASP:OD2   | 1:G:157:TYR:OH   | 2.26                     | 0.52              |
| 1:K:102:GLU:HG2  | 1:K:144:GLN:HG2  | 1.92                     | 0.52              |
| 1:F:384:GLU:OE1  | 1:F:458:ARG:NH2  | 2.35                     | 0.52              |
| 1:I:50:GLY:N     | 1:I:60:GLY:O     | 2.27                     | 0.52              |
| 1:L:75:ASP:OD2   | 1:L:157:TYR:OH   | 2.27                     | 0.52              |
| 1:L:559:SER:N    | 1:L:575:VAL:O    | 2.40                     | 0.52              |
| 1:M:275:VAL:HB   | 1:N:94:LEU:HB2   | 1.92                     | 0.52              |
| 1:O:524:PRO:HG2  | 1:O:576:LYS:HD2  | 1.91                     | 0.52              |
| 1:A:383:GLN:HE21 | 1:A:457:PHE:HB2  | 1.75                     | 0.52              |
| 1:C:188:LYS:HB3  | 1:C:597:PRO:HB2  | 1.91                     | 0.52              |
| 1:H:78:TYR:OH    | 1:H:297:THR:O    | 2.18                     | 0.52              |
| 1:K:35:LYS:HE3   | 1:K:42:VAL:HG23  | 1.92                     | 0.52              |
| 1:A:203:THR:O    | 1:A:310:LEU:HD22 | 2.09                     | 0.52              |
| 1:F:479:VAL:HG12 | 1:F:509:VAL:HG22 | 1.92                     | 0.52              |
| 1:G:524:PRO:HG2  | 1:G:576:LYS:HD2  | 1.91                     | 0.52              |
| 1:H:596:PRO:HG3  | 1:I:315:LYS:HE3  | 1.92                     | 0.52              |
| 1:I:383:GLN:HE21 | 1:I:457:PHE:HB2  | 1.75                     | 0.52              |
| 1:K:479:VAL:HB   | 1:K:507:LEU:HD11 | 1.92                     | 0.52              |
| 1:M:341:TYR:HA   | 1:M:593:TYR:HE2  | 1.75                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:563:ALA:HB2  | 1:M:573:TYR:HD2  | 1.75                     | 0.52              |
| 1:A:563:ALA:HB2  | 1:A:573:TYR:HD1  | 1.75                     | 0.51              |
| 1:D:102:GLU:HG2  | 1:D:144:GLN:HG2  | 1.92                     | 0.51              |
| 1:G:275:VAL:HB   | 1:H:94:LEU:HB2   | 1.92                     | 0.51              |
| 1:G:560:GLN:HG2  | 1:H:513:LEU:HD11 | 1.91                     | 0.51              |
| 1:J:50:GLY:N     | 1:J:60:GLY:O     | 2.28                     | 0.51              |
| 1:J:195:GLU:HB3  | 1:J:591:PRO:HB2  | 1.91                     | 0.51              |
| 1:J:247:ILE:HG22 | 1:J:248:VAL:HG23 | 1.93                     | 0.51              |
| 1:A:403:LEU:HD21 | 1:A:474:LEU:HD21 | 1.92                     | 0.51              |
| 1:B:538:VAL:HG11 | 1:B:551:LEU:HB2  | 1.92                     | 0.51              |
| 1:I:311:HIS:O    | 1:I:315:LYS:NZ   | 2.43                     | 0.51              |
| 1:J:35:LYS:HE3   | 1:J:42:VAL:HG23  | 1.93                     | 0.51              |
| 1:K:265:ASP:HB2  | 1:L:104:TRP:HB3  | 1.93                     | 0.51              |
| 1:C:35:LYS:HE3   | 1:C:42:VAL:HG23  | 1.92                     | 0.51              |
| 1:F:480:PHE:HB3  | 1:F:486:ASN:HB2  | 1.92                     | 0.51              |
| 1:G:580:PHE:HZ   | 1:H:517:LEU:HD11 | 1.75                     | 0.51              |
| 1:L:344:PHE:HB3  | 1:L:593:TYR:CE1  | 2.44                     | 0.51              |
| 1:L:434:LYS:HE3  | 1:L:442:CYS:HB3  | 1.91                     | 0.51              |
| 1:M:417:HIS:HA   | 1:M:460:TYR:CD2  | 2.46                     | 0.51              |
| 1:N:480:PHE:HB3  | 1:N:486:ASN:HB2  | 1.91                     | 0.51              |
| 1:F:570:GLN:NE2  | 1:F:572:SER:OG   | 2.44                     | 0.51              |
| 1:M:421:GLN:OE1  | 1:M:566:SER:OG   | 2.20                     | 0.51              |
| 1:N:249:ASN:HB3  | 1:O:120:ALA:HB3  | 1.92                     | 0.51              |
| 1:N:450:PHE:HE1  | 3:N:702:MA4:H62  | 1.76                     | 0.51              |
| 1:O:54:LEU:HD23  | 1:O:341:TYR:HE2  | 1.75                     | 0.51              |
| 1:P:199:LEU:HD13 | 1:P:591:PRO:HD2  | 1.93                     | 0.51              |
| 1:H:532:ILE:HG13 | 1:H:533:MET:HG3  | 1.93                     | 0.51              |
| 3:L:702:MA4:O60  | 3:L:702:MA4:O6   | 2.24                     | 0.51              |
| 1:P:532:ILE:HG13 | 1:P:533:MET:HG3  | 1.93                     | 0.51              |
| 1:D:398:GLU:HB2  | 1:D:407:PHE:CZ   | 2.46                     | 0.51              |
| 1:E:417:HIS:HA   | 1:E:460:TYR:CD2  | 2.45                     | 0.51              |
| 1:H:35:LYS:HE3   | 1:H:42:VAL:HG23  | 1.93                     | 0.51              |
| 3:M:702:MA4:O6   | 3:M:702:MA4:O60  | 2.26                     | 0.51              |
| 1:O:560:GLN:HG2  | 1:P:513:LEU:HD11 | 1.92                     | 0.51              |
| 1:E:275:VAL:HB   | 1:F:94:LEU:HB2   | 1.92                     | 0.51              |
| 1:H:283:PHE:O    | 1:I:293:GLN:NE2  | 2.29                     | 0.51              |
| 1:K:267:LEU:HB3  | 1:L:102:GLU:HB2  | 1.93                     | 0.51              |
| 1:C:102:GLU:HG2  | 1:C:144:GLN:HG2  | 1.92                     | 0.51              |
| 1:C:138:THR:HB   | 1:C:229:ASN:HB3  | 1.93                     | 0.51              |
| 3:L:702:MA4:H602 | 3:L:702:MA4:O10  | 2.10                     | 0.51              |
| 1:N:311:HIS:O    | 1:N:315:LYS:NZ   | 2.44                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:535:ASN:ND2  | 1:H:555:PRO:HD3  | 2.26                     | 0.51              |
| 1:M:517:LEU:HD23 | 1:M:520:LYS:HD3  | 1.93                     | 0.51              |
| 1:P:535:ASN:ND2  | 1:P:555:PRO:HD3  | 2.26                     | 0.51              |
| 1:E:75:ASP:OD2   | 1:E:157:TYR:OH   | 2.29                     | 0.51              |
| 1:I:589:ARG:O    | 1:I:590:LEU:HD23 | 2.10                     | 0.51              |
| 1:P:538:VAL:HG21 | 1:P:551:LEU:H    | 1.75                     | 0.51              |
| 1:H:182:LEU:HD11 | 1:H:333:THR:HG21 | 1.93                     | 0.50              |
| 1:L:398:GLU:HB2  | 1:L:407:PHE:CZ   | 2.46                     | 0.50              |
| 1:M:525:PHE:HE1  | 1:M:573:TYR:HB2  | 1.76                     | 0.50              |
| 1:O:403:LEU:HD12 | 1:O:410:PRO:HG2  | 1.93                     | 0.50              |
| 1:A:428:SER:N    | 3:A:702:MA4:O60  | 2.44                     | 0.50              |
| 1:D:175:LEU:HD12 | 1:D:330:LEU:HD21 | 1.91                     | 0.50              |
| 1:F:89:GLN:O     | 1:F:91:GLU:HG3   | 2.11                     | 0.50              |
| 1:O:89:GLN:OE1   | 1:O:155:ARG:NH1  | 2.44                     | 0.50              |
| 1:P:590:LEU:HB2  | 1:P:591:PRO:HD3  | 1.92                     | 0.50              |
| 1:G:89:GLN:O     | 1:G:91:GLU:HG3   | 2.11                     | 0.50              |
| 1:H:265:ASP:HB2  | 1:I:104:TRP:HB3  | 1.93                     | 0.50              |
| 1:H:345:ASN:HD21 | 1:H:590:LEU:HD12 | 1.76                     | 0.50              |
| 1:P:149:ARG:NH1  | 1:P:218:GLU:OE2  | 2.44                     | 0.50              |
| 1:E:340:HIS:HD1  | 1:E:593:TYR:HD2  | 1.58                     | 0.50              |
| 1:J:130:SER:HB2  | 1:J:237:THR:OG1  | 2.11                     | 0.50              |
| 1:K:463:VAL:HG21 | 1:K:537:LEU:HD11 | 1.93                     | 0.50              |
| 1:O:565:ILE:HD13 | 1:O:570:GLN:HA   | 1.93                     | 0.50              |
| 1:D:78:TYR:OH    | 1:D:297:THR:O    | 2.19                     | 0.50              |
| 1:D:428:SER:H    | 3:D:702:MA4:C60  | 2.24                     | 0.50              |
| 1:J:188:LYS:HB3  | 1:J:597:PRO:HB2  | 1.92                     | 0.50              |
| 1:N:418:LEU:HA   | 1:N:533:MET:HE1  | 1.94                     | 0.50              |
| 1:O:393:LEU:HD21 | 1:O:425:GLU:HB3  | 1.93                     | 0.50              |
| 1:C:570:GLN:NE2  | 1:C:572:SER:OG   | 2.42                     | 0.50              |
| 1:E:500:PRO:HD2  | 1:E:500:PRO:O    | 2.12                     | 0.50              |
| 1:J:417:HIS:NE2  | 1:J:420:SER:OG   | 2.30                     | 0.50              |
| 1:M:340:HIS:HD1  | 1:M:593:TYR:HD2  | 1.58                     | 0.50              |
| 1:O:480:PHE:HB3  | 1:O:486:ASN:HB2  | 1.94                     | 0.50              |
| 1:A:104:TRP:HB3  | 1:P:265:ASP:HB2  | 1.93                     | 0.50              |
| 1:C:564:VAL:HG12 | 1:C:571:VAL:HB   | 1.94                     | 0.50              |
| 1:D:386:THR:OG1  | 1:D:458:ARG:NH1  | 2.38                     | 0.50              |
| 1:G:381:VAL:HG12 | 1:G:461:TRP:HA   | 1.93                     | 0.50              |
| 1:G:538:VAL:HG11 | 1:G:551:LEU:HB2  | 1.92                     | 0.50              |
| 1:J:181:GLN:HE21 | 1:J:189:MET:HB3  | 1.77                     | 0.50              |
| 1:K:564:VAL:HG12 | 1:K:571:VAL:HB   | 1.94                     | 0.50              |
| 1:H:421:GLN:OE1  | 1:H:566:SER:OG   | 2.27                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:78:TYR:OH    | 1:K:297:THR:O    | 2.18                     | 0.50              |
| 1:A:417:HIS:HA   | 1:A:460:TYR:CD2  | 2.48                     | 0.49              |
| 1:C:417:HIS:HA   | 1:C:460:TYR:CD2  | 2.47                     | 0.49              |
| 1:F:249:ASN:HB3  | 1:G:120:ALA:HB3  | 1.94                     | 0.49              |
| 1:G:565:ILE:HD13 | 1:G:570:GLN:HA   | 1.92                     | 0.49              |
| 1:K:255:ASP:HB3  | 1:L:114:SER:HB2  | 1.94                     | 0.49              |
| 1:J:403:LEU:HD21 | 1:J:474:LEU:HD21 | 1.94                     | 0.49              |
| 1:C:87:ILE:HG22  | 1:C:89:GLN:HG3   | 1.94                     | 0.49              |
| 1:D:523:VAL:HG23 | 1:D:579:ILE:HD12 | 1.94                     | 0.49              |
| 1:E:89:GLN:O     | 1:E:91:GLU:HG3   | 2.12                     | 0.49              |
| 1:E:255:ASP:OD1  | 1:E:256:TYR:N    | 2.45                     | 0.49              |
| 1:F:486:ASN:O    | 1:F:490:ASN:N    | 2.42                     | 0.49              |
| 1:G:421:GLN:OE1  | 1:G:566:SER:OG   | 2.25                     | 0.49              |
| 1:B:388:LEU:HB2  | 1:B:454:LYS:HG3  | 1.94                     | 0.49              |
| 1:E:525:PHE:HE1  | 1:E:573:TYR:HB2  | 1.77                     | 0.49              |
| 1:E:596:PRO:HG2  | 1:F:315:LYS:HE3  | 1.95                     | 0.49              |
| 1:F:55:ARG:HD3   | 1:F:590:LEU:HD11 | 1.94                     | 0.49              |
| 1:I:199:LEU:HD13 | 1:I:591:PRO:HD2  | 1.94                     | 0.49              |
| 1:I:479:VAL:HB   | 1:I:507:LEU:HD11 | 1.95                     | 0.49              |
| 1:J:247:ILE:O    | 1:K:122:PHE:N    | 2.43                     | 0.49              |
| 1:L:102:GLU:HG2  | 1:L:144:GLN:HG2  | 1.94                     | 0.49              |
| 1:M:89:GLN:O     | 1:M:91:GLU:HG3   | 2.12                     | 0.49              |
| 1:G:384:GLU:N    | 1:G:458:ARG:O    | 2.45                     | 0.49              |
| 1:H:311:HIS:O    | 1:H:315:LYS:NZ   | 2.46                     | 0.49              |
| 1:K:138:THR:HB   | 1:K:229:ASN:HB3  | 1.94                     | 0.49              |
| 1:N:598:LEU:HD22 | 1:O:328:LYS:HD3  | 1.95                     | 0.49              |
| 1:P:486:ASN:O    | 1:P:490:ASN:N    | 2.44                     | 0.49              |
| 1:I:486:ASN:O    | 1:I:490:ASN:N    | 2.45                     | 0.49              |
| 1:L:78:TYR:OH    | 1:L:297:THR:O    | 2.20                     | 0.49              |
| 1:M:570:GLN:NE2  | 1:M:572:SER:OG   | 2.46                     | 0.49              |
| 1:D:188:LYS:HB3  | 1:D:597:PRO:HG2  | 1.94                     | 0.49              |
| 1:G:398:GLU:HB2  | 1:G:407:PHE:CZ   | 2.48                     | 0.49              |
| 1:B:563:ALA:HB2  | 1:B:573:TYR:HD1  | 1.77                     | 0.49              |
| 1:G:137:LYS:HE2  | 1:G:139:LEU:HD11 | 1.95                     | 0.49              |
| 1:K:417:HIS:HA   | 1:K:460:TYR:CD2  | 2.48                     | 0.49              |
| 1:M:427:TYR:OH   | 1:M:429:ARG:NH2  | 2.46                     | 0.49              |
| 1:N:75:ASP:OD2   | 1:N:157:TYR:OH   | 2.23                     | 0.49              |
| 1:D:398:GLU:HB2  | 1:D:407:PHE:HZ   | 1.78                     | 0.49              |
| 1:D:488:MET:HE1  | 1:D:489:THR:HB   | 1.95                     | 0.49              |
| 1:F:75:ASP:OD2   | 1:F:157:TYR:OH   | 2.23                     | 0.49              |
| 1:L:188:LYS:HB3  | 1:L:597:PRO:HB2  | 1.94                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:275:VAL:HB   | 1:O:94:LEU:HB2   | 1.95                     | 0.49              |
| 1:H:255:ASP:OD1  | 1:H:256:TYR:N    | 2.46                     | 0.49              |
| 1:K:181:GLN:HE22 | 1:K:189:MET:HG2  | 1.78                     | 0.49              |
| 1:L:559:SER:HB3  | 1:L:577:ALA:HB2  | 1.95                     | 0.49              |
| 1:O:517:LEU:HA   | 1:O:520:LYS:HZ2  | 1.77                     | 0.49              |
| 1:D:341:TYR:O    | 1:D:345:ASN:ND2  | 2.45                     | 0.48              |
| 1:D:563:ALA:HB2  | 1:D:573:TYR:HD2  | 1.77                     | 0.48              |
| 1:I:403:LEU:HD21 | 1:I:474:LEU:HD21 | 1.95                     | 0.48              |
| 1:B:255:ASP:OD1  | 1:B:256:TYR:N    | 2.46                     | 0.48              |
| 1:C:383:GLN:HE21 | 1:C:457:PHE:HB2  | 1.78                     | 0.48              |
| 1:F:417:HIS:HA   | 1:F:460:TYR:CD2  | 2.47                     | 0.48              |
| 1:L:486:ASN:O    | 1:L:490:ASN:N    | 2.47                     | 0.48              |
| 1:P:311:HIS:O    | 1:P:315:LYS:NZ   | 2.42                     | 0.48              |
| 1:B:89:GLN:O     | 1:B:91:GLU:HG3   | 2.14                     | 0.48              |
| 1:B:269:ASN:HB2  | 1:C:100:VAL:HB   | 1.96                     | 0.48              |
| 1:D:249:ASN:HB3  | 1:E:120:ALA:HB3  | 1.95                     | 0.48              |
| 1:H:524:PRO:HG2  | 1:H:576:LYS:HD2  | 1.94                     | 0.48              |
| 1:H:538:VAL:HG21 | 1:H:551:LEU:H    | 1.78                     | 0.48              |
| 1:I:249:ASN:HB3  | 1:J:120:ALA:HB3  | 1.96                     | 0.48              |
| 1:J:269:ASN:HB2  | 1:K:100:VAL:HB   | 1.95                     | 0.48              |
| 1:J:538:VAL:HG11 | 1:J:551:LEU:HB2  | 1.95                     | 0.48              |
| 1:C:463:VAL:HG21 | 1:C:537:LEU:HD11 | 1.95                     | 0.48              |
| 1:J:386:THR:HG1  | 1:J:458:ARG:HH12 | 1.55                     | 0.48              |
| 1:M:398:GLU:HB2  | 1:M:407:PHE:HZ   | 1.78                     | 0.48              |
| 1:N:565:ILE:HD13 | 1:N:570:GLN:HA   | 1.96                     | 0.48              |
| 1:O:275:VAL:HB   | 1:P:94:LEU:HB2   | 1.96                     | 0.48              |
| 1:O:559:SER:N    | 1:O:575:VAL:O    | 2.33                     | 0.48              |
| 1:A:293:GLN:NE2  | 1:P:283:PHE:O    | 2.29                     | 0.48              |
| 1:F:199:LEU:HD13 | 1:F:591:PRO:HD2  | 1.95                     | 0.48              |
| 1:G:383:GLN:HA   | 1:G:459:ALA:HA   | 1.94                     | 0.48              |
| 1:G:516:GLU:HB2  | 1:G:520:LYS:HZ1  | 1.79                     | 0.48              |
| 1:H:89:GLN:O     | 1:H:91:GLU:HG3   | 2.13                     | 0.48              |
| 1:J:417:HIS:HA   | 1:J:460:TYR:CD2  | 2.48                     | 0.48              |
| 1:L:398:GLU:HB2  | 1:L:407:PHE:HZ   | 1.78                     | 0.48              |
| 1:N:417:HIS:HA   | 1:N:460:TYR:HD2  | 1.78                     | 0.48              |
| 1:O:398:GLU:HB2  | 1:O:407:PHE:CZ   | 2.48                     | 0.48              |
| 1:B:386:THR:HG1  | 1:B:458:ARG:HH12 | 1.56                     | 0.48              |
| 1:E:333:THR:O    | 1:E:336:THR:HG22 | 2.13                     | 0.48              |
| 1:E:474:LEU:HD22 | 1:E:511:VAL:HG11 | 1.95                     | 0.48              |
| 1:J:563:ALA:HB2  | 1:J:573:TYR:HD1  | 1.77                     | 0.48              |
| 1:A:479:VAL:HB   | 1:A:507:LEU:HD11 | 1.95                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:485:ILE:HD12 | 1:C:492:GLN:HG3  | 1.96                     | 0.48              |
| 1:E:188:LYS:HB3  | 1:E:597:PRO:HB2  | 1.96                     | 0.48              |
| 1:F:517:LEU:HD23 | 1:F:520:LYS:HD3  | 1.95                     | 0.48              |
| 1:G:517:LEU:HA   | 1:G:520:LYS:HZ2  | 1.78                     | 0.48              |
| 1:O:421:GLN:OE1  | 1:O:566:SER:OG   | 2.25                     | 0.48              |
| 1:P:524:PRO:HG2  | 1:P:576:LYS:HD2  | 1.94                     | 0.48              |
| 1:A:406:ASP:OD1  | 1:A:407:PHE:N    | 2.44                     | 0.48              |
| 1:E:341:TYR:HA   | 1:E:593:TYR:HE2  | 1.78                     | 0.48              |
| 1:G:35:LYS:HE3   | 1:G:42:VAL:HG23  | 1.95                     | 0.48              |
| 1:G:403:LEU:HD12 | 1:G:410:PRO:HG2  | 1.94                     | 0.48              |
| 1:H:500:PRO:HA   | 1:H:509:VAL:O    | 2.12                     | 0.48              |
| 1:M:596:PRO:HG2  | 1:N:315:LYS:HE3  | 1.96                     | 0.48              |
| 1:P:182:LEU:HD11 | 1:P:333:THR:HG21 | 1.96                     | 0.48              |
| 1:J:424:GLU:HG2  | 1:J:454:LYS:HG3  | 1.96                     | 0.48              |
| 1:M:563:ALA:HB2  | 1:M:573:TYR:CD2  | 2.48                     | 0.48              |
| 1:O:311:HIS:O    | 1:O:315:LYS:NZ   | 2.47                     | 0.48              |
| 1:B:233:GLN:HA   | 1:B:258:SER:O    | 2.14                     | 0.48              |
| 1:B:417:HIS:HA   | 1:B:460:TYR:CD2  | 2.49                     | 0.48              |
| 1:E:563:ALA:HB2  | 1:E:573:TYR:CD2  | 2.49                     | 0.48              |
| 1:L:536:PRO:HA   | 1:L:550:SER:HA   | 1.96                     | 0.48              |
| 1:M:333:THR:O    | 1:M:336:THR:HG22 | 2.13                     | 0.48              |
| 1:B:590:LEU:HB2  | 1:B:591:PRO:CD   | 2.43                     | 0.47              |
| 1:G:480:PHE:HB3  | 1:G:486:ASN:HB2  | 1.96                     | 0.47              |
| 1:M:269:ASN:HB2  | 1:N:100:VAL:HB   | 1.96                     | 0.47              |
| 1:M:484:THR:O    | 1:M:492:GLN:NE2  | 2.46                     | 0.47              |
| 1:M:500:PRO:HD2  | 1:M:500:PRO:O    | 2.13                     | 0.47              |
| 1:O:199:LEU:HD13 | 1:O:591:PRO:HD2  | 1.96                     | 0.47              |
| 1:A:255:ASP:N    | 1:B:114:SER:O    | 2.37                     | 0.47              |
| 1:B:418:LEU:HD12 | 1:B:461:TRP:CD1  | 2.49                     | 0.47              |
| 1:C:192:TYR:CE1  | 1:C:596:PRO:HG3  | 2.50                     | 0.47              |
| 1:I:417:HIS:HA   | 1:I:460:TYR:CD2  | 2.49                     | 0.47              |
| 1:K:172:THR:O    | 1:K:176:MET:HG3  | 2.13                     | 0.47              |
| 1:O:403:LEU:HD11 | 1:O:474:LEU:HG   | 1.95                     | 0.47              |
| 1:O:403:LEU:HD21 | 1:O:474:LEU:HD21 | 1.96                     | 0.47              |
| 1:E:484:THR:O    | 1:E:492:GLN:NE2  | 2.47                     | 0.47              |
| 1:J:66:THR:OG1   | 1:J:83:GLU:OE2   | 2.22                     | 0.47              |
| 1:O:35:LYS:HE3   | 1:O:42:VAL:HG23  | 1.95                     | 0.47              |
| 1:C:396:ASN:N    | 1:C:396:ASN:OD1  | 2.46                     | 0.47              |
| 1:D:486:ASN:O    | 1:D:490:ASN:N    | 2.47                     | 0.47              |
| 1:D:559:SER:HB3  | 1:D:577:ALA:HB2  | 1.96                     | 0.47              |
| 1:E:559:SER:HB3  | 1:E:577:ALA:HB2  | 1.96                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:589:ARG:NH2  | 1:J:592:PRO:O    | 2.47                     | 0.47              |
| 1:M:75:ASP:OD2   | 1:M:157:TYR:OH   | 2.28                     | 0.47              |
| 1:O:137:LYS:HE2  | 1:O:139:LEU:HD11 | 1.96                     | 0.47              |
| 1:P:421:GLN:OE1  | 1:P:566:SER:OG   | 2.26                     | 0.47              |
| 1:A:589:ARG:O    | 1:A:590:LEU:HD23 | 2.15                     | 0.47              |
| 1:C:172:THR:O    | 1:C:176:MET:HG3  | 2.14                     | 0.47              |
| 1:F:535:ASN:HD22 | 1:F:555:PRO:HD3  | 1.80                     | 0.47              |
| 1:J:562:LEU:HD22 | 1:K:499:ILE:HD11 | 1.96                     | 0.47              |
| 1:N:138:THR:HB   | 1:N:229:ASN:HB3  | 1.96                     | 0.47              |
| 1:N:534:GLY:HA3  | 1:N:550:SER:C    | 2.35                     | 0.47              |
| 1:O:484:THR:OG1  | 1:O:485:ILE:N    | 2.47                     | 0.47              |
| 1:P:500:PRO:HA   | 1:P:509:VAL:O    | 2.15                     | 0.47              |
| 1:A:122:PHE:N    | 1:P:247:ILE:O    | 2.38                     | 0.47              |
| 1:L:162:THR:HG22 | 1:L:164:THR:H    | 1.80                     | 0.47              |
| 1:N:590:LEU:HB2  | 1:N:591:PRO:CD   | 2.44                     | 0.47              |
| 1:O:218:GLU:OE1  | 1:O:274:ARG:NH2  | 2.39                     | 0.47              |
| 1:O:517:LEU:HD23 | 1:O:520:LYS:NZ   | 2.29                     | 0.47              |
| 1:B:130:SER:HB2  | 1:B:237:THR:OG1  | 2.15                     | 0.47              |
| 1:D:162:THR:HG22 | 1:D:164:THR:H    | 1.80                     | 0.47              |
| 1:E:75:ASP:OD1   | 1:E:75:ASP:N     | 2.46                     | 0.47              |
| 1:E:186:GLN:NE2  | 1:E:599:MET:HA   | 2.30                     | 0.47              |
| 3:E:702:MA4:O6   | 3:E:702:MA4:O60  | 2.27                     | 0.47              |
| 1:F:565:ILE:HD13 | 1:F:570:GLN:HA   | 1.96                     | 0.47              |
| 1:G:47:PRO:O     | 1:G:61:ARG:NH1   | 2.46                     | 0.47              |
| 1:I:265:ASP:HB2  | 1:J:104:TRP:HB3  | 1.97                     | 0.47              |
| 1:J:78:TYR:OH    | 1:J:297:THR:O    | 2.17                     | 0.47              |
| 1:J:255:ASP:OD1  | 1:J:256:TYR:N    | 2.46                     | 0.47              |
| 1:K:559:SER:HB3  | 1:K:577:ALA:HB2  | 1.95                     | 0.47              |
| 1:L:35:LYS:HE3   | 1:L:42:VAL:HG23  | 1.97                     | 0.47              |
| 1:P:314:ILE:O    | 1:P:315:LYS:HD3  | 2.14                     | 0.47              |
| 1:P:590:LEU:HB2  | 1:P:591:PRO:CD   | 2.44                     | 0.47              |
| 1:B:138:THR:HB   | 1:B:229:ASN:HB3  | 1.97                     | 0.47              |
| 1:B:406:ASP:OD1  | 1:B:407:PHE:N    | 2.44                     | 0.47              |
| 1:L:233:GLN:HG3  | 1:L:259:GLN:HG2  | 1.97                     | 0.47              |
| 1:L:563:ALA:HB2  | 1:L:573:TYR:HD2  | 1.80                     | 0.47              |
| 1:M:529:PHE:HB2  | 1:M:534:GLY:HA2  | 1.97                     | 0.47              |
| 1:O:75:ASP:OD1   | 1:O:75:ASP:N     | 2.48                     | 0.47              |
| 1:O:590:LEU:HB2  | 1:O:591:PRO:HD3  | 1.96                     | 0.47              |
| 1:C:383:GLN:HA   | 1:C:459:ALA:HA   | 1.97                     | 0.47              |
| 1:E:94:LEU:HD13  | 1:E:152:VAL:HG22 | 1.97                     | 0.47              |
| 1:H:487:PRO:HB2  | 1:H:580:PHE:CE1  | 2.50                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:428:SER:N    | 3:I:702:MA4:O60  | 2.48                     | 0.47              |
| 1:I:517:LEU:HD23 | 1:I:520:LYS:NZ   | 2.30                     | 0.47              |
| 1:J:418:LEU:HD12 | 1:J:461:TRP:CD1  | 2.49                     | 0.47              |
| 1:P:255:ASP:OD1  | 1:P:256:TYR:N    | 2.47                     | 0.47              |
| 1:P:393:LEU:HD21 | 1:P:425:GLU:HB3  | 1.97                     | 0.47              |
| 1:K:255:ASP:OD1  | 1:K:256:TYR:N    | 2.48                     | 0.47              |
| 1:L:475:LEU:HD12 | 1:L:518:GLY:HA3  | 1.96                     | 0.47              |
| 1:B:333:THR:O    | 1:B:336:THR:HG22 | 2.15                     | 0.46              |
| 1:C:427:TYR:HA   | 3:C:702:MA4:H501 | 1.97                     | 0.46              |
| 1:D:265:ASP:HB2  | 1:E:104:TRP:HB3  | 1.97                     | 0.46              |
| 1:O:47:PRO:O     | 1:O:61:ARG:NH1   | 2.45                     | 0.46              |
| 1:A:315:LYS:HE3  | 1:P:596:PRO:CG   | 2.45                     | 0.46              |
| 1:G:403:LEU:HD21 | 1:G:474:LEU:HD21 | 1.97                     | 0.46              |
| 1:G:481:THR:OG1  | 1:G:484:THR:HG22 | 2.14                     | 0.46              |
| 1:G:516:GLU:O    | 1:G:520:LYS:HG2  | 2.15                     | 0.46              |
| 1:L:345:ASN:OD1  | 1:L:593:TYR:OH   | 2.33                     | 0.46              |
| 1:M:341:TYR:HA   | 1:M:593:TYR:CE2  | 2.50                     | 0.46              |
| 1:H:289:LEU:HD23 | 1:H:289:LEU:HA   | 1.77                     | 0.46              |
| 1:O:169:LEU:O    | 1:O:172:THR:OG1  | 2.31                     | 0.46              |
| 1:O:516:GLU:HB2  | 1:O:520:LYS:HZ1  | 1.80                     | 0.46              |
| 1:P:35:LYS:HE3   | 1:P:42:VAL:HG23  | 1.97                     | 0.46              |
| 1:B:61:ARG:HD3   | 1:B:65:LEU:HG    | 1.97                     | 0.46              |
| 1:B:596:PRO:HG2  | 1:C:315:LYS:HE3  | 1.97                     | 0.46              |
| 1:C:565:ILE:HD13 | 1:C:570:GLN:HA   | 1.97                     | 0.46              |
| 1:F:333:THR:O    | 1:F:336:THR:HG22 | 2.16                     | 0.46              |
| 1:H:149:ARG:NH1  | 1:H:218:GLU:OE2  | 2.47                     | 0.46              |
| 1:J:333:THR:O    | 1:J:336:THR:HG22 | 2.15                     | 0.46              |
| 1:J:531:CYS:HB3  | 1:J:570:GLN:H    | 1.80                     | 0.46              |
| 1:K:485:ILE:HD12 | 1:K:492:GLN:HG3  | 1.97                     | 0.46              |
| 1:N:417:HIS:HA   | 1:N:460:TYR:CD2  | 2.50                     | 0.46              |
| 1:P:487:PRO:HB2  | 1:P:580:PHE:CE1  | 2.50                     | 0.46              |
| 1:A:486:ASN:O    | 1:A:490:ASN:N    | 2.45                     | 0.46              |
| 1:D:341:TYR:CE1  | 1:D:591:PRO:HD3  | 2.51                     | 0.46              |
| 1:E:589:ARG:HD2  | 1:E:589:ARG:HA   | 1.60                     | 0.46              |
| 3:E:702:MA4:H602 | 3:E:702:MA4:O10  | 2.14                     | 0.46              |
| 1:F:403:LEU:HD12 | 1:F:410:PRO:HG2  | 1.96                     | 0.46              |
| 1:K:50:GLY:N     | 1:K:60:GLY:O     | 2.31                     | 0.46              |
| 1:K:559:SER:N    | 1:K:575:VAL:O    | 2.27                     | 0.46              |
| 1:L:113:LEU:O    | 1:L:132:GLU:HA   | 2.15                     | 0.46              |
| 1:L:333:THR:O    | 1:L:336:THR:HG22 | 2.15                     | 0.46              |
| 1:N:333:THR:O    | 1:N:336:THR:HG22 | 2.15                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:413:TYR:HB3  | 1:N:462:CYS:HB3  | 1.97                     | 0.46              |
| 1:A:253:GLU:HG3  | 1:B:116:ASN:HB2  | 1.98                     | 0.46              |
| 1:G:517:LEU:HD23 | 1:G:520:LYS:HZ2  | 1.81                     | 0.46              |
| 1:K:523:VAL:HG23 | 1:K:579:ILE:HD12 | 1.96                     | 0.46              |
| 1:M:264:LYS:HE3  | 1:N:105:MET:HE2  | 1.97                     | 0.46              |
| 1:N:516:GLU:O    | 1:N:520:LYS:HG2  | 2.15                     | 0.46              |
| 1:D:475:LEU:HD12 | 1:D:518:GLY:HA3  | 1.97                     | 0.46              |
| 1:D:536:PRO:HA   | 1:D:550:SER:HA   | 1.97                     | 0.46              |
| 1:F:387:GLU:HG2  | 1:F:394:CYS:SG   | 2.56                     | 0.46              |
| 1:F:534:GLY:HA3  | 1:F:550:SER:C    | 2.36                     | 0.46              |
| 1:H:498:TYR:CE2  | 1:H:512:SER:HB2  | 2.51                     | 0.46              |
| 1:H:538:VAL:HG11 | 1:H:551:LEU:HB2  | 1.98                     | 0.46              |
| 1:L:376:PHE:HB2  | 1:L:525:PHE:O    | 2.15                     | 0.46              |
| 1:M:131:THR:HG23 | 1:M:236:VAL:HG22 | 1.98                     | 0.46              |
| 1:O:104:TRP:HD1  | 1:O:105:MET:N    | 2.14                     | 0.46              |
| 1:D:35:LYS:HE3   | 1:D:42:VAL:HG23  | 1.97                     | 0.46              |
| 1:D:188:LYS:HB3  | 1:D:597:PRO:HB2  | 1.98                     | 0.46              |
| 1:E:138:THR:HB   | 1:E:229:ASN:HB3  | 1.97                     | 0.46              |
| 1:E:570:GLN:NE2  | 1:E:572:SER:OG   | 2.48                     | 0.46              |
| 1:F:341:TYR:HE1  | 1:F:590:LEU:HB3  | 1.80                     | 0.46              |
| 1:J:406:ASP:OD1  | 1:J:407:PHE:N    | 2.44                     | 0.46              |
| 1:K:383:GLN:HA   | 1:K:459:ALA:HA   | 1.97                     | 0.46              |
| 1:L:120:ALA:HA   | 1:L:125:VAL:O    | 2.16                     | 0.46              |
| 1:O:383:GLN:HA   | 1:O:459:ALA:HA   | 1.97                     | 0.46              |
| 1:P:289:LEU:HD23 | 1:P:289:LEU:HA   | 1.77                     | 0.46              |
| 1:P:538:VAL:HG11 | 1:P:551:LEU:HB2  | 1.98                     | 0.46              |
| 1:D:131:THR:HG22 | 1:D:236:VAL:HG22 | 1.96                     | 0.46              |
| 1:D:333:THR:O    | 1:D:336:THR:HG22 | 2.16                     | 0.46              |
| 1:H:104:TRP:HD1  | 1:H:105:MET:N    | 2.14                     | 0.46              |
| 1:H:393:LEU:HD21 | 1:H:425:GLU:HB3  | 1.97                     | 0.46              |
| 1:M:503:LEU:HD23 | 1:M:507:LEU:HD23 | 1.97                     | 0.46              |
| 1:N:570:GLN:NE2  | 1:N:572:SER:OG   | 2.48                     | 0.46              |
| 1:P:498:TYR:CE2  | 1:P:512:SER:HB2  | 2.51                     | 0.46              |
| 1:A:182:LEU:HD11 | 1:A:333:THR:HG21 | 1.98                     | 0.46              |
| 1:A:538:VAL:HG11 | 1:A:551:LEU:HB2  | 1.98                     | 0.46              |
| 1:E:421:GLN:OE1  | 1:E:566:SER:OG   | 2.22                     | 0.46              |
| 1:E:486:ASN:HB3  | 1:E:491:ALA:O    | 2.16                     | 0.46              |
| 1:E:535:ASN:HD22 | 1:E:555:PRO:HD3  | 1.80                     | 0.46              |
| 1:F:389:SER:OG   | 1:F:453:ALA:HA   | 2.16                     | 0.46              |
| 1:G:403:LEU:HD11 | 1:G:474:LEU:HG   | 1.96                     | 0.46              |
| 1:G:517:LEU:HD23 | 1:G:520:LYS:NZ   | 2.30                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:383:GLN:HE21 | 1:K:457:PHE:HB2  | 1.80                     | 0.46              |
| 1:K:427:TYR:HA   | 3:K:702:MA4:H501 | 1.99                     | 0.46              |
| 1:B:504:PHE:HB2  | 1:B:507:LEU:HB3  | 1.97                     | 0.45              |
| 1:C:265:ASP:N    | 1:D:104:TRP:O    | 2.45                     | 0.45              |
| 1:D:255:ASP:OD1  | 1:D:256:TYR:N    | 2.48                     | 0.45              |
| 1:F:377:THR:HB   | 1:F:464:ALA:HB2  | 1.98                     | 0.45              |
| 1:M:228:ASP:OD1  | 1:M:229:ASN:N    | 2.49                     | 0.45              |
| 1:B:531:CYS:HB3  | 1:B:570:GLN:H    | 1.81                     | 0.45              |
| 1:F:104:TRP:HD1  | 1:F:105:MET:N    | 2.15                     | 0.45              |
| 1:F:417:HIS:HA   | 1:F:460:TYR:HD2  | 1.81                     | 0.45              |
| 1:F:418:LEU:HD12 | 1:F:461:TRP:CD1  | 2.51                     | 0.45              |
| 1:I:57:VAL:HG22  | 1:J:160:LYS:HZ1  | 1.82                     | 0.45              |
| 1:J:138:THR:HB   | 1:J:229:ASN:HB3  | 1.97                     | 0.45              |
| 1:M:385:CYS:SG   | 1:M:397:LEU:HD22 | 2.56                     | 0.45              |
| 1:N:47:PRO:O     | 1:N:61:ARG:NH1   | 2.50                     | 0.45              |
| 1:N:590:LEU:HB2  | 1:N:591:PRO:HD3  | 1.99                     | 0.45              |
| 1:A:100:VAL:HB   | 1:P:269:ASN:HB2  | 1.98                     | 0.45              |
| 1:I:538:VAL:HG11 | 1:I:551:LEU:HB2  | 1.98                     | 0.45              |
| 1:L:188:LYS:HB3  | 1:L:597:PRO:HG2  | 1.98                     | 0.45              |
| 1:L:434:LYS:HD3  | 1:L:444:THR:HG22 | 1.98                     | 0.45              |
| 1:M:535:ASN:HD22 | 1:M:555:PRO:HD3  | 1.82                     | 0.45              |
| 1:A:44:GLU:HB2   | 1:B:88:PRO:HG2   | 1.99                     | 0.45              |
| 1:A:251:LYS:NZ   | 1:A:253:GLU:HG2  | 2.31                     | 0.45              |
| 1:E:529:PHE:HB2  | 1:E:534:GLY:HA2  | 1.98                     | 0.45              |
| 1:H:253:GLU:HG3  | 1:I:116:ASN:HB2  | 1.98                     | 0.45              |
| 1:I:182:LEU:HD11 | 1:I:333:THR:HG21 | 1.98                     | 0.45              |
| 1:P:104:TRP:HD1  | 1:P:105:MET:N    | 2.15                     | 0.45              |
| 1:A:517:LEU:HD23 | 1:A:520:LYS:NZ   | 2.31                     | 0.45              |
| 1:C:489:THR:HG23 | 1:C:491:ALA:H    | 1.82                     | 0.45              |
| 1:D:378:PHE:CE2  | 1:D:461:TRP:HE3  | 2.34                     | 0.45              |
| 1:E:385:CYS:SG   | 1:E:397:LEU:HD22 | 2.57                     | 0.45              |
| 3:F:702:MA4:H612 | 3:F:702:MA4:H312 | 1.61                     | 0.45              |
| 1:G:209:VAL:HG12 | 1:G:305:ARG:HB3  | 1.99                     | 0.45              |
| 1:K:565:ILE:HD13 | 1:K:570:GLN:HA   | 1.97                     | 0.45              |
| 1:L:378:PHE:CE2  | 1:L:461:TRP:HE3  | 2.34                     | 0.45              |
| 1:O:203:THR:O    | 1:O:310:LEU:HB2  | 2.16                     | 0.45              |
| 1:B:167:LEU:HD12 | 1:B:319:LEU:HD21 | 1.97                     | 0.45              |
| 1:H:475:LEU:HD12 | 1:H:518:GLY:HA3  | 1.99                     | 0.45              |
| 1:I:403:LEU:HD12 | 1:I:410:PRO:HG2  | 1.99                     | 0.45              |
| 1:O:588:VAL:HG12 | 1:O:588:VAL:O    | 2.17                     | 0.45              |
| 1:C:78:TYR:OH    | 1:C:297:THR:O    | 2.16                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:399:GLN:H    | 1:G:407:PHE:HE1  | 1.65                     | 0.45              |
| 1:G:474:LEU:HD13 | 1:G:511:VAL:HG11 | 1.99                     | 0.45              |
| 1:I:599:MET:SD   | 1:I:599:MET:N    | 2.89                     | 0.45              |
| 1:N:530:SER:H    | 1:N:533:MET:HB3  | 1.82                     | 0.45              |
| 1:B:562:LEU:HD22 | 1:C:499:ILE:HD11 | 1.97                     | 0.45              |
| 1:E:211:ALA:HB1  | 1:E:300:LEU:HD13 | 1.99                     | 0.45              |
| 1:G:75:ASP:OD1   | 1:G:75:ASP:N     | 2.49                     | 0.45              |
| 1:G:104:TRP:HD1  | 1:G:105:MET:N    | 2.15                     | 0.45              |
| 1:H:188:LYS:HB3  | 1:H:597:PRO:CB   | 2.47                     | 0.45              |
| 1:M:94:LEU:HD13  | 1:M:152:VAL:HG22 | 1.99                     | 0.45              |
| 1:M:589:ARG:HD2  | 1:M:589:ARG:HA   | 1.59                     | 0.45              |
| 1:C:590:LEU:CB   | 1:C:591:PRO:HD3  | 2.46                     | 0.45              |
| 1:I:94:LEU:C     | 1:I:95:GLU:OE1   | 2.55                     | 0.45              |
| 1:I:304:ASP:OD1  | 1:I:305:ARG:N    | 2.50                     | 0.45              |
| 1:J:486:ASN:HB3  | 1:J:491:ALA:O    | 2.17                     | 0.45              |
| 1:O:516:GLU:O    | 1:O:520:LYS:HG2  | 2.16                     | 0.45              |
| 1:P:475:LEU:HD12 | 1:P:518:GLY:HA3  | 1.98                     | 0.45              |
| 1:A:167:LEU:HD12 | 1:A:319:LEU:HD21 | 1.99                     | 0.45              |
| 1:B:199:LEU:HB2  | 1:B:591:PRO:HG2  | 1.98                     | 0.45              |
| 1:G:449:VAL:HG11 | 1:G:451:ARG:HE   | 1.82                     | 0.45              |
| 1:K:485:ILE:HD11 | 1:K:491:ALA:HA   | 1.99                     | 0.45              |
| 1:M:559:SER:HB3  | 1:M:577:ALA:HB2  | 1.97                     | 0.45              |
| 1:N:387:GLU:HG2  | 1:N:394:CYS:SG   | 2.57                     | 0.45              |
| 1:P:565:ILE:HD13 | 1:P:570:GLN:HA   | 1.99                     | 0.45              |
| 1:A:403:LEU:HD12 | 1:A:410:PRO:HG2  | 1.98                     | 0.44              |
| 1:G:470:ASP:HA   | 1:G:471:ASN:HA   | 1.68                     | 0.44              |
| 1:H:596:PRO:CG   | 1:I:315:LYS:HE3  | 2.47                     | 0.44              |
| 1:K:188:LYS:HB3  | 1:K:597:PRO:HB2  | 1.98                     | 0.44              |
| 1:N:172:THR:O    | 1:N:176:MET:HG2  | 2.17                     | 0.44              |
| 1:P:406:ASP:OD1  | 1:P:407:PHE:N    | 2.49                     | 0.44              |
| 1:A:131:THR:HA   | 1:A:235:THR:O    | 2.16                     | 0.44              |
| 1:D:588:VAL:HB   | 1:D:590:LEU:HD23 | 1.99                     | 0.44              |
| 1:E:488:MET:HE1  | 1:E:489:THR:HB   | 1.99                     | 0.44              |
| 1:H:169:LEU:O    | 1:H:172:THR:OG1  | 2.31                     | 0.44              |
| 1:J:592:PRO:HB2  | 1:J:594:THR:O    | 2.17                     | 0.44              |
| 1:L:434:LYS:HD2  | 1:L:434:LYS:HA   | 1.73                     | 0.44              |
| 1:P:480:PHE:HB3  | 1:P:486:ASN:HB2  | 1.98                     | 0.44              |
| 1:B:383:GLN:HA   | 1:B:459:ALA:HA   | 1.98                     | 0.44              |
| 1:B:391:ASP:OD1  | 1:B:391:ASP:N    | 2.50                     | 0.44              |
| 1:F:381:VAL:HG12 | 1:F:461:TRP:HA   | 1.99                     | 0.44              |
| 1:L:265:ASP:HB2  | 1:M:104:TRP:HB3  | 1.99                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:417:HIS:HA   | 1:O:460:TYR:CD2  | 2.52                     | 0.44              |
| 1:P:203:THR:O    | 1:P:310:LEU:HB2  | 2.16                     | 0.44              |
| 1:B:486:ASN:HB3  | 1:B:491:ALA:O    | 2.18                     | 0.44              |
| 1:G:218:GLU:OE1  | 1:G:274:ARG:NH2  | 2.38                     | 0.44              |
| 1:H:299:HIS:HB3  | 1:I:90:LYS:HD2   | 1.99                     | 0.44              |
| 1:I:205:VAL:HB   | 1:I:313:PHE:CE2  | 2.53                     | 0.44              |
| 1:J:167:LEU:HD12 | 1:J:319:LEU:HD21 | 1.99                     | 0.44              |
| 1:K:333:THR:O    | 1:K:336:THR:HG22 | 2.17                     | 0.44              |
| 1:M:486:ASN:HB3  | 1:M:491:ALA:O    | 2.17                     | 0.44              |
| 1:N:381:VAL:HG12 | 1:N:461:TRP:HA   | 1.99                     | 0.44              |
| 1:B:55:ARG:HE    | 1:B:590:LEU:HD11 | 1.82                     | 0.44              |
| 1:E:130:SER:HB2  | 1:E:237:THR:OG1  | 2.17                     | 0.44              |
| 1:E:376:PHE:CE1  | 1:E:537:LEU:HD13 | 2.53                     | 0.44              |
| 1:I:289:LEU:HA   | 1:I:289:LEU:HD23 | 1.71                     | 0.44              |
| 1:J:581:THR:OG1  | 1:J:582:GLY:N    | 2.50                     | 0.44              |
| 1:O:182:LEU:HD11 | 1:O:333:THR:HG21 | 1.97                     | 0.44              |
| 1:B:66:THR:OG1   | 1:B:83:GLU:OE2   | 2.24                     | 0.44              |
| 1:F:269:ASN:HB2  | 1:G:100:VAL:HB   | 1.99                     | 0.44              |
| 1:H:269:ASN:HB2  | 1:I:100:VAL:HB   | 2.00                     | 0.44              |
| 1:J:205:VAL:HB   | 1:J:313:PHE:CE2  | 2.53                     | 0.44              |
| 1:L:520:LYS:HG3  | 1:L:521:PHE:CD2  | 2.52                     | 0.44              |
| 1:L:581:THR:OG1  | 1:L:582:GLY:N    | 2.51                     | 0.44              |
| 1:A:162:THR:HG22 | 1:A:164:THR:H    | 1.83                     | 0.44              |
| 1:A:421:GLN:OE1  | 1:A:566:SER:OG   | 2.30                     | 0.44              |
| 1:C:255:ASP:OD1  | 1:C:256:TYR:N    | 2.49                     | 0.44              |
| 1:C:535:ASN:HD22 | 1:C:555:PRO:HD3  | 1.82                     | 0.44              |
| 1:E:324:GLY:N    | 1:E:325:PRO:HD2  | 2.33                     | 0.44              |
| 1:F:78:TYR:OH    | 1:F:297:THR:O    | 2.23                     | 0.44              |
| 1:G:417:HIS:HA   | 1:G:460:TYR:CD2  | 2.52                     | 0.44              |
| 1:G:581:THR:OG1  | 1:G:582:GLY:N    | 2.50                     | 0.44              |
| 1:H:333:THR:O    | 1:H:336:THR:HG22 | 2.18                     | 0.44              |
| 1:H:383:GLN:HE21 | 1:H:457:PHE:HB2  | 1.82                     | 0.44              |
| 1:H:479:VAL:HG12 | 1:H:509:VAL:HA   | 1.98                     | 0.44              |
| 1:E:585:LEU:HD13 | 1:F:51:TRP:CD1   | 2.53                     | 0.44              |
| 1:H:480:PHE:HB3  | 1:H:486:ASN:HB2  | 1.99                     | 0.44              |
| 1:H:565:ILE:HD13 | 1:H:570:GLN:HA   | 2.00                     | 0.44              |
| 1:J:384:GLU:N    | 1:J:458:ARG:O    | 2.49                     | 0.44              |
| 1:N:104:TRP:HD1  | 1:N:105:MET:N    | 2.15                     | 0.44              |
| 1:N:389:SER:OG   | 1:N:453:ALA:HA   | 2.18                     | 0.44              |
| 1:O:419:LEU:HD23 | 1:O:504:PHE:HE1  | 1.81                     | 0.44              |
| 1:P:403:LEU:HD21 | 1:P:474:LEU:HD21 | 2.00                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:95:GLU:N     | 1:A:95:GLU:OE1   | 2.51                     | 0.44              |
| 1:A:205:VAL:HB   | 1:A:313:PHE:CE2  | 2.52                     | 0.44              |
| 1:A:249:ASN:HB3  | 1:B:120:ALA:HB3  | 2.00                     | 0.44              |
| 1:A:477:GLY:HA3  | 1:A:498:TYR:CE2  | 2.53                     | 0.44              |
| 1:A:482:ASP:OD1  | 1:A:482:ASP:N    | 2.49                     | 0.44              |
| 1:B:524:PRO:HG2  | 1:B:576:LYS:HD2  | 2.00                     | 0.44              |
| 1:C:333:THR:O    | 1:C:336:THR:HG22 | 2.18                     | 0.44              |
| 1:E:592:PRO:HD3  | 1:F:312:PHE:HE1  | 1.83                     | 0.44              |
| 1:H:487:PRO:HB2  | 1:H:580:PHE:HE1  | 1.83                     | 0.44              |
| 1:I:590:LEU:HB2  | 1:I:591:PRO:HD3  | 1.99                     | 0.44              |
| 1:J:538:VAL:HG21 | 1:J:551:LEU:H    | 1.83                     | 0.44              |
| 1:K:489:THR:HG23 | 1:K:491:ALA:H    | 1.82                     | 0.44              |
| 1:K:590:LEU:CB   | 1:K:591:PRO:HD3  | 2.48                     | 0.44              |
| 1:L:383:GLN:HA   | 1:L:459:ALA:HA   | 2.00                     | 0.44              |
| 3:M:702:MA4:H602 | 3:M:702:MA4:O10  | 2.18                     | 0.44              |
| 1:O:449:VAL:HG11 | 1:O:451:ARG:HE   | 1.82                     | 0.44              |
| 1:A:599:MET:SD   | 1:A:599:MET:N    | 2.91                     | 0.43              |
| 1:B:474:LEU:HD13 | 1:B:511:VAL:HG11 | 2.00                     | 0.43              |
| 1:D:130:SER:HB2  | 1:D:237:THR:OG1  | 2.17                     | 0.43              |
| 1:D:247:ILE:O    | 1:E:122:PHE:N    | 2.45                     | 0.43              |
| 1:I:247:ILE:O    | 1:J:122:PHE:N    | 2.42                     | 0.43              |
| 1:I:255:ASP:HB3  | 1:J:114:SER:HB2  | 1.99                     | 0.43              |
| 1:K:449:VAL:HG11 | 1:K:451:ARG:HE   | 1.83                     | 0.43              |
| 1:L:267:LEU:HB3  | 1:M:102:GLU:HB3  | 2.00                     | 0.43              |
| 1:M:203:THR:HG21 | 1:M:342:TYR:HE2  | 1.83                     | 0.43              |
| 1:O:399:GLN:H    | 1:O:407:PHE:HE1  | 1.65                     | 0.43              |
| 1:D:383:GLN:HA   | 1:D:459:ALA:HA   | 2.00                     | 0.43              |
| 1:E:503:LEU:HD23 | 1:E:507:LEU:HD23 | 2.00                     | 0.43              |
| 1:F:195:GLU:HB3  | 1:F:591:PRO:HB2  | 1.99                     | 0.43              |
| 1:H:138:THR:HB   | 1:H:229:ASN:HB3  | 2.00                     | 0.43              |
| 1:H:406:ASP:OD1  | 1:H:407:PHE:N    | 2.48                     | 0.43              |
| 1:J:265:ASP:HB2  | 1:K:104:TRP:HB3  | 2.01                     | 0.43              |
| 1:J:383:GLN:HA   | 1:J:459:ALA:HA   | 1.99                     | 0.43              |
| 1:L:596:PRO:HG2  | 1:M:315:LYS:HE3  | 2.00                     | 0.43              |
| 1:M:186:GLN:HA   | 1:M:188:LYS:NZ   | 2.33                     | 0.43              |
| 1:O:304:ASP:OD2  | 1:O:305:ARG:N    | 2.52                     | 0.43              |
| 1:P:417:HIS:HA   | 1:P:460:TYR:HD2  | 1.83                     | 0.43              |
| 1:C:391:ASP:N    | 1:C:391:ASP:OD1  | 2.52                     | 0.43              |
| 1:C:562:LEU:HD22 | 1:D:499:ILE:HD11 | 2.00                     | 0.43              |
| 1:F:105:MET:HE2  | 1:F:105:MET:HB2  | 1.86                     | 0.43              |
| 1:F:517:LEU:HA   | 1:F:520:LYS:HG2  | 1.99                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:563:ALA:HB2  | 1:I:573:TYR:CD1  | 2.53                     | 0.43              |
| 1:K:599:MET:SD   | 1:K:599:MET:N    | 2.92                     | 0.43              |
| 1:N:427:TYR:OH   | 1:N:429:ARG:NH2  | 2.51                     | 0.43              |
| 1:A:116:ASN:HB2  | 1:P:253:GLU:HG3  | 2.00                     | 0.43              |
| 1:D:376:PHE:HB2  | 1:D:525:PHE:O    | 2.18                     | 0.43              |
| 1:E:341:TYR:HA   | 1:E:593:TYR:CE2  | 2.53                     | 0.43              |
| 1:E:387:GLU:HG2  | 1:E:394:CYS:SG   | 2.59                     | 0.43              |
| 1:F:383:GLN:HA   | 1:F:459:ALA:HA   | 2.00                     | 0.43              |
| 1:H:417:HIS:HA   | 1:H:460:TYR:HD2  | 1.83                     | 0.43              |
| 1:J:477:GLY:HA3  | 1:J:498:TYR:CE2  | 2.54                     | 0.43              |
| 1:K:94:LEU:HD13  | 1:K:152:VAL:HG22 | 1.99                     | 0.43              |
| 1:K:192:TYR:CZ   | 1:K:596:PRO:HG3  | 2.54                     | 0.43              |
| 1:M:58:ASP:HB2   | 1:N:87:ILE:HG12  | 2.00                     | 0.43              |
| 1:N:255:ASP:OD1  | 1:N:256:TYR:N    | 2.52                     | 0.43              |
| 1:P:333:THR:O    | 1:P:336:THR:HG22 | 2.17                     | 0.43              |
| 1:B:324:GLY:N    | 1:B:325:PRO:HD2  | 2.33                     | 0.43              |
| 1:D:520:LYS:HG3  | 1:D:521:PHE:CD2  | 2.53                     | 0.43              |
| 1:D:559:SER:N    | 1:D:575:VAL:O    | 2.42                     | 0.43              |
| 1:E:219:ASP:OD2  | 1:E:219:ASP:N    | 2.51                     | 0.43              |
| 1:I:162:THR:HG22 | 1:I:164:THR:H    | 1.84                     | 0.43              |
| 1:K:192:TYR:CE1  | 1:K:596:PRO:HG3  | 2.52                     | 0.43              |
| 1:L:75:ASP:OD1   | 1:L:75:ASP:N     | 2.49                     | 0.43              |
| 1:P:590:LEU:CB   | 1:P:591:PRO:HD3  | 2.47                     | 0.43              |
| 1:A:469:PRO:O    | 1:A:472:SER:OG   | 2.27                     | 0.43              |
| 1:B:265:ASP:HB2  | 1:C:104:TRP:HB3  | 1.99                     | 0.43              |
| 1:B:475:LEU:HD12 | 1:B:518:GLY:HA3  | 2.00                     | 0.43              |
| 1:E:524:PRO:HG2  | 1:E:576:LYS:HD2  | 2.01                     | 0.43              |
| 1:J:330:LEU:HD12 | 1:J:330:LEU:HA   | 1.84                     | 0.43              |
| 1:J:341:TYR:CE1  | 1:J:591:PRO:HD3  | 2.53                     | 0.43              |
| 1:L:324:GLY:N    | 1:L:325:PRO:HD2  | 2.33                     | 0.43              |
| 1:M:536:PRO:HA   | 1:M:550:SER:HA   | 2.00                     | 0.43              |
| 1:N:94:LEU:HD13  | 1:N:152:VAL:HG22 | 1.99                     | 0.43              |
| 1:N:403:LEU:HD12 | 1:N:410:PRO:HG2  | 2.01                     | 0.43              |
| 1:P:589:ARG:O    | 1:P:590:LEU:HD13 | 2.17                     | 0.43              |
| 1:A:192:TYR:CZ   | 1:A:596:PRO:HG3  | 2.54                     | 0.43              |
| 1:E:167:LEU:HD12 | 1:E:319:LEU:HD21 | 2.01                     | 0.43              |
| 1:G:269:ASN:HB2  | 1:H:100:VAL:HB   | 2.00                     | 0.43              |
| 1:H:597:PRO:O    | 1:H:599:MET:HE1  | 2.18                     | 0.43              |
| 1:I:255:ASP:OD1  | 1:I:256:TYR:N    | 2.52                     | 0.43              |
| 1:I:482:ASP:OD1  | 1:I:482:ASP:N    | 2.49                     | 0.43              |
| 1:J:391:ASP:OD1  | 1:J:391:ASP:N    | 2.52                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:105:MET:HE2  | 1:M:105:MET:HB2  | 1.83                     | 0.43              |
| 1:M:376:PHE:CE1  | 1:M:537:LEU:HD13 | 2.53                     | 0.43              |
| 1:M:470:ASP:HA   | 1:M:471:ASN:HA   | 1.70                     | 0.43              |
| 1:N:269:ASN:HB2  | 1:O:100:VAL:HB   | 2.01                     | 0.43              |
| 1:O:52:ASP:OD2   | 1:O:55:ARG:HG3   | 2.19                     | 0.43              |
| 1:O:324:GLY:N    | 1:O:325:PRO:HD2  | 2.34                     | 0.43              |
| 1:G:333:THR:O    | 1:G:336:THR:HG22 | 2.19                     | 0.43              |
| 1:H:403:LEU:HB2  | 1:H:410:PRO:HG3  | 2.01                     | 0.43              |
| 1:I:474:LEU:HD13 | 1:I:511:VAL:HG11 | 2.00                     | 0.43              |
| 1:M:387:GLU:HG2  | 1:M:394:CYS:SG   | 2.58                     | 0.43              |
| 1:A:265:ASP:HB2  | 1:B:104:TRP:HB3  | 2.00                     | 0.43              |
| 1:D:275:VAL:HG11 | 1:D:283:PHE:CD1  | 2.54                     | 0.43              |
| 1:G:324:GLY:N    | 1:G:325:PRO:HD2  | 2.34                     | 0.43              |
| 1:J:524:PRO:HG2  | 1:J:576:LYS:HD2  | 2.01                     | 0.43              |
| 1:L:94:LEU:HD13  | 1:L:152:VAL:HG22 | 2.01                     | 0.43              |
| 1:O:333:THR:O    | 1:O:336:THR:HG22 | 2.18                     | 0.43              |
| 1:A:58:ASP:O     | 1:B:160:LYS:HE3  | 2.19                     | 0.43              |
| 1:A:489:THR:HG23 | 1:A:491:ALA:H    | 1.83                     | 0.43              |
| 1:C:427:TYR:HE1  | 1:C:453:ALA:HB2  | 1.84                     | 0.43              |
| 1:C:531:CYS:SG   | 1:C:532:ILE:HG23 | 2.59                     | 0.43              |
| 1:C:563:ALA:HB2  | 1:C:573:TYR:HD2  | 1.83                     | 0.43              |
| 1:H:590:LEU:CB   | 1:H:591:PRO:HD3  | 2.49                     | 0.43              |
| 1:I:251:LYS:NZ   | 1:I:253:GLU:HG2  | 2.34                     | 0.43              |
| 1:K:391:ASP:OD1  | 1:K:391:ASP:N    | 2.51                     | 0.43              |
| 1:L:384:GLU:N    | 1:L:458:ARG:O    | 2.51                     | 0.43              |
| 1:L:479:VAL:HG12 | 1:L:509:VAL:HG22 | 2.01                     | 0.43              |
| 1:M:423:HIS:ND1  | 1:M:505:GLU:OE2  | 2.52                     | 0.43              |
| 1:N:344:PHE:HD2  | 1:N:593:TYR:HH   | 1.66                     | 0.43              |
| 1:O:406:ASP:OD1  | 1:O:407:PHE:N    | 2.51                     | 0.43              |
| 1:P:383:GLN:HE21 | 1:P:457:PHE:HB2  | 1.84                     | 0.43              |
| 1:P:470:ASP:HA   | 1:P:471:ASN:HA   | 1.73                     | 0.43              |
| 1:G:409:CYS:HB2  | 1:G:415:PRO:HG3  | 2.00                     | 0.42              |
| 1:M:427:TYR:HE1  | 1:M:453:ALA:HB2  | 1.84                     | 0.42              |
| 1:N:418:LEU:HB3  | 1:N:459:ALA:O    | 2.19                     | 0.42              |
| 1:N:590:LEU:CB   | 1:N:591:PRO:HD3  | 2.48                     | 0.42              |
| 1:P:391:ASP:OD1  | 1:P:391:ASP:N    | 2.52                     | 0.42              |
| 1:C:474:LEU:HD13 | 1:C:511:VAL:HG11 | 2.01                     | 0.42              |
| 1:D:167:LEU:HD12 | 1:D:319:LEU:HD21 | 2.02                     | 0.42              |
| 1:D:324:GLY:N    | 1:D:325:PRO:HD2  | 2.34                     | 0.42              |
| 1:D:333:THR:HA   | 1:D:336:THR:HG22 | 2.01                     | 0.42              |
| 1:E:427:TYR:HE1  | 1:E:453:ALA:HB2  | 1.84                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:228:ASP:OD1  | 1:G:229:ASN:N    | 2.51                     | 0.42              |
| 1:M:324:GLY:N    | 1:M:325:PRO:HD2  | 2.33                     | 0.42              |
| 1:M:345:ASN:OD1  | 1:M:345:ASN:N    | 2.52                     | 0.42              |
| 1:B:150:VAL:HG11 | 1:B:289:LEU:HD11 | 2.01                     | 0.42              |
| 1:B:427:TYR:HA   | 3:B:702:MA4:H501 | 2.00                     | 0.42              |
| 1:F:47:PRO:O     | 1:F:61:ARG:NH1   | 2.52                     | 0.42              |
| 1:G:381:VAL:HG23 | 1:G:501:LEU:HD22 | 2.01                     | 0.42              |
| 1:H:391:ASP:N    | 1:H:391:ASP:OD1  | 2.52                     | 0.42              |
| 1:H:430:LEU:HD12 | 3:H:702:MA4:H322 | 2.02                     | 0.42              |
| 1:H:589:ARG:O    | 1:H:590:LEU:HD13 | 2.19                     | 0.42              |
| 1:I:489:THR:HG23 | 1:I:491:ALA:H    | 1.85                     | 0.42              |
| 1:I:560:GLN:NE2  | 1:J:513:LEU:HD11 | 2.34                     | 0.42              |
| 1:M:89:GLN:O     | 1:M:91:GLU:N     | 2.53                     | 0.42              |
| 1:N:409:CYS:HB2  | 1:N:415:PRO:HG3  | 2.02                     | 0.42              |
| 1:D:205:VAL:HB   | 1:D:313:PHE:CE2  | 2.55                     | 0.42              |
| 1:F:340:HIS:HE1  | 1:F:593:TYR:HD1  | 1.65                     | 0.42              |
| 1:G:54:LEU:HD23  | 1:G:341:TYR:HE2  | 1.84                     | 0.42              |
| 1:L:275:VAL:HG11 | 1:L:283:PHE:CD1  | 2.54                     | 0.42              |
| 1:M:289:LEU:HD23 | 1:M:289:LEU:HA   | 1.83                     | 0.42              |
| 1:A:199:LEU:HB2  | 1:A:591:PRO:HG2  | 2.00                     | 0.42              |
| 1:B:249:ASN:HB3  | 1:C:120:ALA:HB3  | 2.00                     | 0.42              |
| 1:C:131:THR:HA   | 1:C:235:THR:O    | 2.19                     | 0.42              |
| 1:E:255:ASP:HB3  | 1:F:114:SER:HB2  | 2.02                     | 0.42              |
| 1:G:54:LEU:HD13  | 1:G:54:LEU:HA    | 1.90                     | 0.42              |
| 1:H:403:LEU:HD21 | 1:H:474:LEU:HD21 | 2.01                     | 0.42              |
| 1:L:105:MET:HE1  | 3:L:702:MA4:H322 | 2.01                     | 0.42              |
| 1:P:384:GLU:OE1  | 1:P:458:ARG:NH2  | 2.40                     | 0.42              |
| 1:P:535:ASN:HD22 | 1:P:555:PRO:HD3  | 1.84                     | 0.42              |
| 1:C:485:ILE:HD11 | 1:C:491:ALA:HA   | 2.00                     | 0.42              |
| 1:D:66:THR:OG1   | 1:D:83:GLU:OE2   | 2.24                     | 0.42              |
| 1:E:105:MET:HE2  | 1:E:105:MET:HB2  | 1.87                     | 0.42              |
| 1:G:169:LEU:O    | 1:G:172:THR:OG1  | 2.32                     | 0.42              |
| 1:G:419:LEU:HD23 | 1:G:504:PHE:HE1  | 1.84                     | 0.42              |
| 1:K:388:LEU:HD12 | 1:K:454:LYS:HG2  | 2.02                     | 0.42              |
| 1:L:532:ILE:HG13 | 1:L:533:MET:HG3  | 2.01                     | 0.42              |
| 1:L:589:ARG:O    | 1:L:590:LEU:HD13 | 2.20                     | 0.42              |
| 1:N:535:ASN:HD22 | 1:N:555:PRO:HD3  | 1.84                     | 0.42              |
| 1:O:209:VAL:HG12 | 1:O:305:ARG:HB3  | 2.01                     | 0.42              |
| 1:C:470:ASP:HA   | 1:C:471:ASN:HA   | 1.76                     | 0.42              |
| 1:F:55:ARG:NE    | 1:F:590:LEU:HD21 | 2.34                     | 0.42              |
| 1:F:188:LYS:HB3  | 1:F:597:PRO:HB2  | 2.01                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:535:ASN:HD22 | 1:H:555:PRO:HD3  | 1.83                     | 0.42              |
| 1:I:192:TYR:CZ   | 1:I:596:PRO:HG3  | 2.55                     | 0.42              |
| 1:I:418:LEU:HB2  | 1:I:461:TRP:HD1  | 1.84                     | 0.42              |
| 1:I:477:GLY:HA3  | 1:I:498:TYR:CE2  | 2.55                     | 0.42              |
| 1:N:87:ILE:HG22  | 1:N:89:GLN:HG3   | 2.02                     | 0.42              |
| 1:O:269:ASN:HB2  | 1:P:100:VAL:HB   | 2.01                     | 0.42              |
| 1:P:188:LYS:HB3  | 1:P:597:PRO:CB   | 2.47                     | 0.42              |
| 1:A:341:TYR:OH   | 1:A:590:LEU:HD13 | 2.18                     | 0.42              |
| 1:A:428:SER:H    | 3:A:702:MA4:C60  | 2.32                     | 0.42              |
| 1:F:172:THR:O    | 1:F:176:MET:HG2  | 2.20                     | 0.42              |
| 1:G:94:LEU:HD13  | 1:G:152:VAL:HG22 | 2.01                     | 0.42              |
| 1:H:50:GLY:N     | 1:H:60:GLY:O     | 2.27                     | 0.42              |
| 1:I:529:PHE:HZ   | 1:I:560:GLN:HG3  | 1.85                     | 0.42              |
| 1:J:289:LEU:HD23 | 1:J:289:LEU:HA   | 1.75                     | 0.42              |
| 1:K:406:ASP:OD1  | 1:K:407:PHE:N    | 2.47                     | 0.42              |
| 1:K:563:ALA:HB2  | 1:K:573:TYR:HD1  | 1.84                     | 0.42              |
| 1:M:167:LEU:HD12 | 1:M:319:LEU:HD21 | 2.01                     | 0.42              |
| 1:P:430:LEU:HD12 | 3:P:702:MA4:H322 | 2.02                     | 0.42              |
| 1:A:474:LEU:HD13 | 1:A:511:VAL:HG11 | 2.01                     | 0.42              |
| 1:B:55:ARG:NE    | 1:B:590:LEU:HD11 | 2.35                     | 0.42              |
| 1:B:581:THR:OG1  | 1:B:582:GLY:N    | 2.51                     | 0.42              |
| 1:C:267:LEU:HB3  | 1:D:102:GLU:HB3  | 2.02                     | 0.42              |
| 1:C:384:GLU:N    | 1:C:458:ARG:O    | 2.49                     | 0.42              |
| 1:C:403:LEU:HD12 | 1:C:410:PRO:HG2  | 2.01                     | 0.42              |
| 1:E:381:VAL:HG12 | 1:E:461:TRP:HA   | 2.01                     | 0.42              |
| 1:F:255:ASP:OD1  | 1:F:256:TYR:N    | 2.52                     | 0.42              |
| 1:G:304:ASP:OD2  | 1:G:305:ARG:N    | 2.53                     | 0.42              |
| 1:G:398:GLU:HB2  | 1:G:407:PHE:HZ   | 1.84                     | 0.42              |
| 1:H:324:GLY:N    | 1:H:325:PRO:HD2  | 2.35                     | 0.42              |
| 1:H:470:ASP:HA   | 1:H:471:ASN:HA   | 1.73                     | 0.42              |
| 1:I:590:LEU:CB   | 1:I:591:PRO:HD3  | 2.50                     | 0.42              |
| 1:L:588:VAL:O    | 1:L:588:VAL:HG23 | 2.20                     | 0.42              |
| 1:N:171:PHE:CE1  | 1:N:197:LEU:HD11 | 2.55                     | 0.42              |
| 3:N:702:MA4:O10  | 3:N:702:MA4:H602 | 2.20                     | 0.42              |
| 1:O:142:LYS:HB3  | 1:O:225:PHE:HB3  | 2.02                     | 0.42              |
| 1:A:104:TRP:HD1  | 1:A:105:MET:N    | 2.18                     | 0.42              |
| 1:B:162:THR:HG22 | 1:B:164:THR:H    | 1.85                     | 0.42              |
| 1:D:117:THR:HB   | 1:D:129:PHE:HB3  | 2.02                     | 0.42              |
| 1:D:434:LYS:HD2  | 1:D:434:LYS:HA   | 1.89                     | 0.42              |
| 1:F:563:ALA:HB2  | 1:F:573:TYR:CD2  | 2.55                     | 0.42              |
| 1:J:55:ARG:NE    | 1:J:590:LEU:HD11 | 2.35                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:324:GLY:N    | 1:J:325:PRO:HD2  | 2.35                     | 0.42              |
| 1:J:438:LEU:O    | 1:J:440:ILE:HG22 | 2.20                     | 0.42              |
| 1:L:427:TYR:HA   | 3:L:702:MA4:H501 | 2.01                     | 0.42              |
| 1:M:277:SER:O    | 1:N:91:GLU:HA    | 2.20                     | 0.42              |
| 1:M:406:ASP:OD1  | 1:M:407:PHE:N    | 2.53                     | 0.42              |
| 1:N:54:LEU:HD13  | 1:N:54:LEU:HA    | 1.89                     | 0.42              |
| 1:N:324:GLY:N    | 1:N:325:PRO:HD2  | 2.35                     | 0.42              |
| 1:N:340:HIS:CE1  | 1:N:593:TYR:HD1  | 2.37                     | 0.42              |
| 1:P:169:LEU:O    | 1:P:172:THR:OG1  | 2.32                     | 0.42              |
| 1:P:172:THR:O    | 1:P:176:MET:HG3  | 2.19                     | 0.42              |
| 1:D:228:ASP:OD1  | 1:D:229:ASN:N    | 2.52                     | 0.41              |
| 1:F:340:HIS:CE1  | 1:F:593:TYR:HD1  | 2.38                     | 0.41              |
| 1:F:418:LEU:HB3  | 1:F:459:ALA:O    | 2.20                     | 0.41              |
| 1:H:430:LEU:HD22 | 1:H:431:GLU:N    | 2.35                     | 0.41              |
| 1:I:333:THR:O    | 1:I:336:THR:HG22 | 2.20                     | 0.41              |
| 1:M:186:GLN:NE2  | 1:M:599:MET:HA   | 2.35                     | 0.41              |
| 1:M:517:LEU:HA   | 1:M:520:LYS:HG2  | 2.02                     | 0.41              |
| 1:N:182:LEU:HD11 | 1:N:333:THR:HG21 | 2.02                     | 0.41              |
| 1:N:430:LEU:HD22 | 1:N:431:GLU:N    | 2.35                     | 0.41              |
| 1:O:481:THR:OG1  | 1:O:484:THR:HG22 | 2.19                     | 0.41              |
| 1:A:534:GLY:HA2  | 1:A:552:LYS:HG2  | 2.02                     | 0.41              |
| 1:C:449:VAL:HG11 | 1:C:451:ARG:HE   | 1.85                     | 0.41              |
| 1:F:324:GLY:N    | 1:F:325:PRO:HD2  | 2.35                     | 0.41              |
| 1:G:138:THR:HB   | 1:G:229:ASN:HB3  | 2.02                     | 0.41              |
| 1:J:220:HIS:CD2  | 1:J:222:ARG:HH12 | 2.37                     | 0.41              |
| 1:K:86:THR:HG22  | 1:K:159:VAL:HG22 | 2.02                     | 0.41              |
| 1:K:535:ASN:HD22 | 1:K:555:PRO:HD3  | 1.84                     | 0.41              |
| 1:O:199:LEU:HB2  | 1:O:591:PRO:HG2  | 2.01                     | 0.41              |
| 1:O:384:GLU:N    | 1:O:458:ARG:O    | 2.48                     | 0.41              |
| 1:O:409:CYS:HB2  | 1:O:415:PRO:HG3  | 2.02                     | 0.41              |
| 1:O:428:SER:O    | 3:O:702:MA4:H212 | 2.20                     | 0.41              |
| 1:A:55:ARG:HE    | 1:A:590:LEU:HD21 | 1.85                     | 0.41              |
| 1:B:589:ARG:O    | 1:B:590:LEU:HD23 | 2.20                     | 0.41              |
| 1:C:520:LYS:HG3  | 1:C:521:PHE:CD2  | 2.55                     | 0.41              |
| 1:D:479:VAL:HG12 | 1:D:509:VAL:HG22 | 2.02                     | 0.41              |
| 1:E:137:LYS:HE2  | 1:E:139:LEU:HD11 | 2.02                     | 0.41              |
| 1:E:203:THR:HG21 | 1:E:342:TYR:HE2  | 1.85                     | 0.41              |
| 1:F:54:LEU:HD23  | 1:F:341:TYR:HE2  | 1.85                     | 0.41              |
| 1:G:251:LYS:HG2  | 1:H:118:GLU:HB2  | 2.03                     | 0.41              |
| 1:G:265:ASP:HB2  | 1:H:104:TRP:HB3  | 2.02                     | 0.41              |
| 1:H:130:SER:HB2  | 1:H:237:THR:OG1  | 2.21                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:482:ASP:OD1  | 1:H:482:ASP:N    | 2.52                     | 0.41              |
| 1:I:95:GLU:OE1   | 1:I:95:GLU:N     | 2.53                     | 0.41              |
| 1:I:488:MET:HE1  | 1:I:489:THR:HB   | 2.02                     | 0.41              |
| 1:K:66:THR:OG1   | 1:K:83:GLU:OE2   | 2.26                     | 0.41              |
| 1:M:381:VAL:HG12 | 1:M:461:TRP:HA   | 2.02                     | 0.41              |
| 1:N:470:ASP:HA   | 1:N:471:ASN:HA   | 1.76                     | 0.41              |
| 1:A:172:THR:O    | 1:A:176:MET:HG2  | 2.20                     | 0.41              |
| 1:C:344:PHE:CD2  | 1:C:593:TYR:CE2  | 3.08                     | 0.41              |
| 1:C:388:LEU:HD12 | 1:C:454:LYS:HG2  | 2.02                     | 0.41              |
| 1:C:417:HIS:HA   | 1:C:460:TYR:HD2  | 1.84                     | 0.41              |
| 1:C:484:THR:O    | 1:C:492:GLN:NE2  | 2.53                     | 0.41              |
| 1:D:535:ASN:HD21 | 1:D:537:LEU:HB2  | 1.86                     | 0.41              |
| 1:D:535:ASN:HD22 | 1:D:555:PRO:HD3  | 1.86                     | 0.41              |
| 1:F:289:LEU:HD23 | 1:F:289:LEU:HA   | 1.77                     | 0.41              |
| 1:G:199:LEU:HD13 | 1:G:591:PRO:HD2  | 2.03                     | 0.41              |
| 1:H:403:LEU:HD11 | 1:H:474:LEU:HG   | 2.02                     | 0.41              |
| 1:J:475:LEU:HD12 | 1:J:518:GLY:HA3  | 2.03                     | 0.41              |
| 1:B:289:LEU:HA   | 1:B:289:LEU:HD23 | 1.75                     | 0.41              |
| 1:C:89:GLN:O     | 1:C:91:GLU:HG3   | 2.21                     | 0.41              |
| 1:C:253:GLU:HG3  | 1:D:116:ASN:HB2  | 2.01                     | 0.41              |
| 1:D:589:ARG:HD2  | 1:D:589:ARG:HA   | 1.74                     | 0.41              |
| 1:D:590:LEU:HB3  | 1:D:591:PRO:CD   | 2.50                     | 0.41              |
| 1:E:386:THR:HG1  | 1:E:458:ARG:HH12 | 1.61                     | 0.41              |
| 1:G:136:MET:HE3  | 1:G:136:MET:HB3  | 1.96                     | 0.41              |
| 1:I:54:LEU:HD23  | 1:I:341:TYR:HE2  | 1.85                     | 0.41              |
| 1:J:482:ASP:N    | 1:J:482:ASP:OD1  | 2.53                     | 0.41              |
| 1:L:247:ILE:O    | 1:M:122:PHE:N    | 2.51                     | 0.41              |
| 1:N:209:VAL:HG12 | 1:N:305:ARG:HB3  | 2.01                     | 0.41              |
| 1:P:137:LYS:HE2  | 1:P:139:LEU:HD11 | 2.01                     | 0.41              |
| 1:P:479:VAL:HG12 | 1:P:509:VAL:HA   | 2.01                     | 0.41              |
| 1:P:482:ASP:N    | 1:P:482:ASP:OD1  | 2.52                     | 0.41              |
| 1:A:90:LYS:HD2   | 1:P:299:HIS:HB3  | 2.02                     | 0.41              |
| 1:C:62:VAL:HG21  | 1:C:205:VAL:HG22 | 2.02                     | 0.41              |
| 1:C:324:GLY:N    | 1:C:325:PRO:HD2  | 2.35                     | 0.41              |
| 1:D:94:LEU:HD13  | 1:D:152:VAL:HG22 | 2.00                     | 0.41              |
| 1:D:489:THR:HG23 | 1:D:491:ALA:H    | 1.85                     | 0.41              |
| 1:G:482:ASP:OD1  | 1:G:482:ASP:N    | 2.54                     | 0.41              |
| 1:I:172:THR:O    | 1:I:176:MET:HG2  | 2.21                     | 0.41              |
| 1:K:427:TYR:HE1  | 1:K:453:ALA:HB2  | 1.84                     | 0.41              |
| 1:K:520:LYS:HG3  | 1:K:521:PHE:CD2  | 2.56                     | 0.41              |
| 1:N:219:ASP:N    | 1:N:219:ASP:OD1  | 2.53                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:507:LEU:HD22 | 1:O:564:VAL:HB   | 2.03                     | 0.41              |
| 1:B:589:ARG:NH2  | 1:B:592:PRO:O    | 2.40                     | 0.41              |
| 1:D:477:GLY:HA3  | 1:D:498:TYR:CE2  | 2.56                     | 0.41              |
| 3:D:702:MA4:H112 | 3:D:702:MA4:H201 | 1.88                     | 0.41              |
| 1:E:413:TYR:HB3  | 1:E:462:CYS:HB3  | 2.03                     | 0.41              |
| 1:G:105:MET:HE2  | 1:G:105:MET:HB2  | 1.89                     | 0.41              |
| 1:G:182:LEU:HD11 | 1:G:333:THR:HG21 | 2.02                     | 0.41              |
| 1:I:255:ASP:N    | 1:J:114:SER:O    | 2.45                     | 0.41              |
| 1:J:479:VAL:HG12 | 1:J:509:VAL:HA   | 2.03                     | 0.41              |
| 1:K:562:LEU:HD22 | 1:L:499:ILE:HD11 | 2.03                     | 0.41              |
| 1:L:228:ASP:OD1  | 1:L:229:ASN:N    | 2.53                     | 0.41              |
| 1:L:489:THR:HG23 | 1:L:491:ALA:H    | 1.85                     | 0.41              |
| 1:M:486:ASN:O    | 1:M:490:ASN:N    | 2.54                     | 0.41              |
| 1:N:560:GLN:O    | 1:N:561:HIS:ND1  | 2.53                     | 0.41              |
| 1:A:59:MET:HG3   | 1:A:200:ASN:O    | 2.21                     | 0.41              |
| 1:A:189:MET:HG2  | 1:A:597:PRO:HG2  | 2.03                     | 0.41              |
| 1:D:138:THR:HB   | 1:D:229:ASN:HB3  | 2.03                     | 0.41              |
| 1:E:264:LYS:HE3  | 1:F:105:MET:HE2  | 2.02                     | 0.41              |
| 1:E:419:LEU:HD23 | 1:E:504:PHE:HE1  | 1.86                     | 0.41              |
| 1:F:228:ASP:N    | 1:F:228:ASP:OD1  | 2.54                     | 0.41              |
| 1:G:203:THR:HG21 | 1:G:342:TYR:HE2  | 1.86                     | 0.41              |
| 1:I:299:HIS:HB3  | 1:J:90:LYS:HD2   | 2.02                     | 0.41              |
| 1:J:162:THR:HG22 | 1:J:164:THR:H    | 1.86                     | 0.41              |
| 1:K:182:LEU:HA   | 1:K:182:LEU:HD23 | 1.75                     | 0.41              |
| 1:L:193:LEU:HD12 | 1:L:193:LEU:HA   | 1.94                     | 0.41              |
| 1:O:381:VAL:HG23 | 1:O:501:LEU:HD22 | 2.03                     | 0.41              |
| 1:O:563:ALA:HB2  | 1:O:573:TYR:HD2  | 1.84                     | 0.41              |
| 1:P:487:PRO:HB2  | 1:P:580:PHE:HE1  | 1.86                     | 0.41              |
| 1:A:87:ILE:HA    | 1:A:88:PRO:HD3   | 1.90                     | 0.41              |
| 1:A:475:LEU:HD12 | 1:A:518:GLY:HA3  | 2.03                     | 0.41              |
| 1:B:87:ILE:HA    | 1:B:88:PRO:HD3   | 1.92                     | 0.41              |
| 1:B:384:GLU:N    | 1:B:458:ARG:O    | 2.53                     | 0.41              |
| 1:B:463:VAL:HG21 | 1:B:537:LEU:HD11 | 2.03                     | 0.41              |
| 1:B:531:CYS:SG   | 1:B:532:ILE:HG23 | 2.60                     | 0.41              |
| 1:B:596:PRO:CG   | 1:C:315:LYS:HE3  | 2.51                     | 0.41              |
| 1:C:538:VAL:HG11 | 1:C:551:LEU:HB2  | 2.02                     | 0.41              |
| 1:D:289:LEU:HA   | 1:D:289:LEU:HD23 | 1.77                     | 0.41              |
| 1:D:384:GLU:N    | 1:D:458:ARG:O    | 2.53                     | 0.41              |
| 1:E:486:ASN:O    | 1:E:490:ASN:N    | 2.53                     | 0.41              |
| 1:F:175:LEU:HD23 | 1:F:175:LEU:HA   | 1.91                     | 0.41              |
| 1:H:94:LEU:HD13  | 1:H:152:VAL:HG22 | 2.02                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:386:THR:OG1  | 1:H:458:ARG:NH1  | 2.34                     | 0.41              |
| 1:H:418:LEU:HD12 | 1:H:461:TRP:CD1  | 2.56                     | 0.41              |
| 1:I:345:ASN:N    | 1:I:345:ASN:OD1  | 2.54                     | 0.41              |
| 1:I:585:LEU:HD13 | 1:J:51:TRP:CD1   | 2.56                     | 0.41              |
| 1:J:590:LEU:CB   | 1:J:591:PRO:CD   | 2.99                     | 0.41              |
| 1:K:249:ASN:HB3  | 1:L:120:ALA:HB3  | 2.03                     | 0.41              |
| 1:K:324:GLY:N    | 1:K:325:PRO:HD2  | 2.35                     | 0.41              |
| 1:L:66:THR:OG1   | 1:L:83:GLU:OE2   | 2.23                     | 0.41              |
| 1:M:275:VAL:HG11 | 1:M:283:PHE:CD1  | 2.56                     | 0.41              |
| 1:N:345:ASN:OD1  | 1:N:345:ASN:N    | 2.54                     | 0.41              |
| 1:O:162:THR:HG22 | 1:O:164:THR:H    | 1.86                     | 0.41              |
| 1:O:470:ASP:HA   | 1:O:471:ASN:HA   | 1.66                     | 0.41              |
| 1:P:121:LEU:HB3  | 1:P:122:PHE:CD2  | 2.56                     | 0.41              |
| 1:P:403:LEU:HD11 | 1:P:474:LEU:HG   | 2.03                     | 0.41              |
| 1:P:417:HIS:NE2  | 1:P:420:SER:OG   | 2.44                     | 0.41              |
| 1:A:54:LEU:HD23  | 1:A:341:TYR:HE2  | 1.86                     | 0.41              |
| 1:A:427:TYR:CE1  | 1:A:453:ALA:HB2  | 2.56                     | 0.41              |
| 1:D:203:THR:HG21 | 1:D:342:TYR:HE1  | 1.85                     | 0.41              |
| 1:F:219:ASP:N    | 1:F:219:ASP:OD1  | 2.54                     | 0.41              |
| 1:H:219:ASP:N    | 1:H:219:ASP:OD1  | 2.54                     | 0.41              |
| 1:L:182:LEU:HD11 | 1:L:333:THR:HG21 | 2.02                     | 0.41              |
| 1:B:247:ILE:O    | 1:C:122:PHE:N    | 2.46                     | 0.40              |
| 1:C:477:GLY:HA3  | 1:C:498:TYR:CE2  | 2.56                     | 0.40              |
| 1:E:97:ASN:N     | 1:E:97:ASN:OD1   | 2.54                     | 0.40              |
| 1:E:345:ASN:OD1  | 1:E:345:ASN:N    | 2.54                     | 0.40              |
| 1:F:75:ASP:N     | 1:F:75:ASP:OD1   | 2.52                     | 0.40              |
| 1:F:115:ILE:O    | 1:F:130:SER:HA   | 2.21                     | 0.40              |
| 1:G:283:PHE:O    | 1:H:293:GLN:NE2  | 2.33                     | 0.40              |
| 1:H:141:VAL:HG22 | 1:H:226:LEU:HD13 | 2.04                     | 0.40              |
| 1:I:141:VAL:HG22 | 1:I:226:LEU:HD13 | 2.03                     | 0.40              |
| 1:K:470:ASP:HB3  | 1:K:471:ASN:OD1  | 2.21                     | 0.40              |
| 1:L:50:GLY:N     | 1:L:60:GLY:O     | 2.32                     | 0.40              |
| 1:L:55:ARG:HD3   | 1:L:590:LEU:HD21 | 2.03                     | 0.40              |
| 1:L:289:LEU:HA   | 1:L:289:LEU:HD23 | 1.78                     | 0.40              |
| 1:L:470:ASP:HA   | 1:L:471:ASN:HA   | 1.77                     | 0.40              |
| 1:N:533:MET:HG2  | 1:N:534:GLY:O    | 2.22                     | 0.40              |
| 1:N:589:ARG:O    | 1:N:590:LEU:HD13 | 2.22                     | 0.40              |
| 1:O:384:GLU:OE1  | 1:O:458:ARG:NH2  | 2.39                     | 0.40              |
| 1:O:420:SER:HB3  | 1:O:458:ARG:HG2  | 2.03                     | 0.40              |
| 1:P:50:GLY:N     | 1:P:60:GLY:O     | 2.28                     | 0.40              |
| 1:P:222:ARG:HE   | 1:P:222:ARG:HB3  | 1.70                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:479:VAL:HG12 | 1:B:509:VAL:HA   | 2.03                     | 0.40              |
| 1:C:517:LEU:HA   | 1:C:520:LYS:HG2  | 2.03                     | 0.40              |
| 1:D:55:ARG:HD3   | 1:D:590:LEU:HD21 | 2.03                     | 0.40              |
| 1:G:253:GLU:HG3  | 1:H:116:ASN:HB2  | 2.04                     | 0.40              |
| 1:H:118:GLU:HG2  | 1:H:128:LYS:HG2  | 2.04                     | 0.40              |
| 1:H:181:GLN:HE21 | 1:H:189:MET:CB   | 2.34                     | 0.40              |
| 1:J:150:VAL:HG11 | 1:J:289:LEU:HD11 | 2.01                     | 0.40              |
| 1:J:474:LEU:HD13 | 1:J:511:VAL:HG11 | 2.03                     | 0.40              |
| 1:J:486:ASN:ND2  | 1:J:489:THR:HG22 | 2.36                     | 0.40              |
| 1:M:384:GLU:OE1  | 1:M:458:ARG:NH2  | 2.42                     | 0.40              |
| 1:M:520:LYS:HG3  | 1:M:521:PHE:CD2  | 2.57                     | 0.40              |
| 1:A:289:LEU:HD23 | 1:A:289:LEU:HA   | 1.71                     | 0.40              |
| 1:B:377:THR:HB   | 1:B:464:ALA:HB2  | 2.03                     | 0.40              |
| 1:C:344:PHE:CD2  | 1:C:593:TYR:HE2  | 2.39                     | 0.40              |
| 1:C:560:GLN:HG2  | 1:D:513:LEU:HD11 | 2.03                     | 0.40              |
| 1:E:269:ASN:HB2  | 1:F:100:VAL:HB   | 2.02                     | 0.40              |
| 1:E:427:TYR:HA   | 3:E:702:MA4:H501 | 2.03                     | 0.40              |
| 1:G:255:ASP:OD1  | 1:G:256:TYR:N    | 2.54                     | 0.40              |
| 1:G:289:LEU:HA   | 1:G:289:LEU:HD23 | 1.80                     | 0.40              |
| 1:H:205:VAL:HB   | 1:H:313:PHE:CE2  | 2.56                     | 0.40              |
| 1:K:167:LEU:HD12 | 1:K:319:LEU:HD21 | 2.03                     | 0.40              |
| 1:L:167:LEU:HD12 | 1:L:319:LEU:HD21 | 2.04                     | 0.40              |
| 1:L:563:ALA:HB2  | 1:L:573:TYR:CD2  | 2.55                     | 0.40              |
| 1:M:419:LEU:HD23 | 1:M:504:PHE:HE2  | 1.86                     | 0.40              |
| 1:N:378:PHE:HB2  | 1:N:525:PHE:HD2  | 1.86                     | 0.40              |
| 1:O:482:ASP:N    | 1:O:482:ASP:OD1  | 2.53                     | 0.40              |
| 1:P:205:VAL:HB   | 1:P:313:PHE:CE2  | 2.56                     | 0.40              |
| 1:B:503:LEU:HD13 | 1:B:503:LEU:O    | 2.22                     | 0.40              |
| 1:B:529:PHE:HZ   | 1:B:560:GLN:HG3  | 1.86                     | 0.40              |
| 1:D:345:ASN:ND2  | 1:D:593:TYR:OH   | 2.52                     | 0.40              |
| 1:E:581:THR:OG1  | 1:E:582:GLY:N    | 2.55                     | 0.40              |
| 1:F:171:PHE:CE1  | 1:F:197:LEU:HD11 | 2.56                     | 0.40              |
| 1:I:42:VAL:HG22  | 1:I:79:ILE:HB    | 2.03                     | 0.40              |
| 1:K:484:THR:O    | 1:K:492:GLN:NE2  | 2.55                     | 0.40              |
| 1:L:255:ASP:OD1  | 1:L:256:TYR:N    | 2.54                     | 0.40              |
| 1:N:54:LEU:HD23  | 1:N:341:TYR:HE2  | 1.87                     | 0.40              |
| 1:O:398:GLU:HB2  | 1:O:407:PHE:HZ   | 1.86                     | 0.40              |
| 1:A:57:VAL:HG13  | 1:A:59:MET:CE    | 2.52                     | 0.40              |
| 1:A:378:PHE:HB2  | 1:A:525:PHE:HD2  | 1.87                     | 0.40              |
| 1:A:590:LEU:CB   | 1:A:591:PRO:CD   | 3.00                     | 0.40              |
| 1:B:538:VAL:HG21 | 1:B:551:LEU:H    | 1.86                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:182:LEU:HD23 | 1:C:182:LEU:HA   | 1.75                     | 0.40              |
| 1:C:470:ASP:HB3  | 1:C:471:ASN:OD1  | 2.21                     | 0.40              |
| 3:D:702:MA4:H612 | 3:D:702:MA4:H312 | 1.90                     | 0.40              |
| 1:E:275:VAL:HG11 | 1:E:283:PHE:CD1  | 2.56                     | 0.40              |
| 1:I:181:GLN:OE1  | 1:I:189:MET:HB2  | 2.21                     | 0.40              |
| 1:J:529:PHE:HZ   | 1:J:560:GLN:HG3  | 1.85                     | 0.40              |
| 1:J:559:SER:HB3  | 1:J:577:ALA:HB2  | 2.04                     | 0.40              |
| 1:M:524:PRO:HG2  | 1:M:576:LYS:HD2  | 2.03                     | 0.40              |
| 1:N:488:MET:HE3  | 1:N:489:THR:HB   | 2.03                     | 0.40              |
| 1:N:581:THR:OG1  | 1:N:582:GLY:N    | 2.54                     | 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     | 527/648 (81%) | 508 (96%) | 18 (3%) | 1 (0%)   | 44          | 77  |
| 1   | B     | 527/648 (81%) | 505 (96%) | 21 (4%) | 1 (0%)   | 44          | 77  |
| 1   | C     | 527/648 (81%) | 505 (96%) | 21 (4%) | 1 (0%)   | 44          | 77  |
| 1   | D     | 527/648 (81%) | 512 (97%) | 15 (3%) | 0        | 100         | 100 |
| 1   | E     | 527/648 (81%) | 504 (96%) | 22 (4%) | 1 (0%)   | 44          | 77  |
| 1   | F     | 527/648 (81%) | 501 (95%) | 25 (5%) | 1 (0%)   | 44          | 77  |
| 1   | G     | 527/648 (81%) | 506 (96%) | 20 (4%) | 1 (0%)   | 44          | 77  |
| 1   | H     | 527/648 (81%) | 502 (95%) | 24 (5%) | 1 (0%)   | 44          | 77  |
| 1   | I     | 527/648 (81%) | 507 (96%) | 19 (4%) | 1 (0%)   | 44          | 77  |
| 1   | J     | 527/648 (81%) | 505 (96%) | 21 (4%) | 1 (0%)   | 44          | 77  |
| 1   | K     | 527/648 (81%) | 502 (95%) | 24 (5%) | 1 (0%)   | 44          | 77  |
| 1   | L     | 527/648 (81%) | 511 (97%) | 15 (3%) | 1 (0%)   | 44          | 77  |

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| Mol | Chain | Analysed         | Favoured   | Allowed  | Outliers | Percentiles |    |
|-----|-------|------------------|------------|----------|----------|-------------|----|
| 1   | M     | 527/648 (81%)    | 507 (96%)  | 19 (4%)  | 1 (0%)   | 44          | 77 |
| 1   | N     | 527/648 (81%)    | 505 (96%)  | 21 (4%)  | 1 (0%)   | 44          | 77 |
| 1   | O     | 527/648 (81%)    | 507 (96%)  | 19 (4%)  | 1 (0%)   | 44          | 77 |
| 1   | P     | 527/648 (81%)    | 504 (96%)  | 22 (4%)  | 1 (0%)   | 44          | 77 |
| All | All   | 8432/10368 (81%) | 8091 (96%) | 326 (4%) | 15 (0%)  | 45          | 77 |

All (15) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 590 | LEU  |
| 1   | B     | 590 | LEU  |
| 1   | C     | 590 | LEU  |
| 1   | E     | 590 | LEU  |
| 1   | F     | 590 | LEU  |
| 1   | G     | 590 | LEU  |
| 1   | H     | 590 | LEU  |
| 1   | I     | 590 | LEU  |
| 1   | J     | 590 | LEU  |
| 1   | K     | 590 | LEU  |
| 1   | L     | 590 | LEU  |
| 1   | M     | 590 | LEU  |
| 1   | N     | 590 | LEU  |
| 1   | O     | 590 | LEU  |
| 1   | P     | 590 | LEU  |

### 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     | 469/566 (83%) | 465 (99%) | 4 (1%)   | 75          | 89 |
| 1   | B     | 469/566 (83%) | 460 (98%) | 9 (2%)   | 52          | 79 |
| 1   | C     | 469/566 (83%) | 464 (99%) | 5 (1%)   | 70          | 87 |
| 1   | D     | 469/566 (83%) | 462 (98%) | 7 (2%)   | 60          | 83 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1   | E     | 469/566 (83%)   | 462 (98%)  | 7 (2%)   | 60          | 83 |
| 1   | F     | 469/566 (83%)   | 461 (98%)  | 8 (2%)   | 56          | 81 |
| 1   | G     | 469/566 (83%)   | 463 (99%)  | 6 (1%)   | 65          | 85 |
| 1   | H     | 469/566 (83%)   | 458 (98%)  | 11 (2%)  | 45          | 75 |
| 1   | I     | 469/566 (83%)   | 464 (99%)  | 5 (1%)   | 70          | 87 |
| 1   | J     | 469/566 (83%)   | 453 (97%)  | 16 (3%)  | 32          | 66 |
| 1   | K     | 469/566 (83%)   | 463 (99%)  | 6 (1%)   | 65          | 85 |
| 1   | L     | 469/566 (83%)   | 460 (98%)  | 9 (2%)   | 52          | 79 |
| 1   | M     | 469/566 (83%)   | 465 (99%)  | 4 (1%)   | 75          | 89 |
| 1   | N     | 469/566 (83%)   | 462 (98%)  | 7 (2%)   | 60          | 83 |
| 1   | O     | 469/566 (83%)   | 464 (99%)  | 5 (1%)   | 70          | 87 |
| 1   | P     | 469/566 (83%)   | 456 (97%)  | 13 (3%)  | 38          | 70 |
| All | All   | 7504/9056 (83%) | 7382 (98%) | 122 (2%) | 58          | 82 |

All (122) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 196 | LEU  |
| 1   | A     | 251 | LYS  |
| 1   | A     | 310 | LEU  |
| 1   | A     | 488 | MET  |
| 1   | B     | 45  | VAL  |
| 1   | B     | 61  | ARG  |
| 1   | B     | 105 | MET  |
| 1   | B     | 254 | THR  |
| 1   | B     | 297 | THR  |
| 1   | B     | 378 | PHE  |
| 1   | B     | 454 | LYS  |
| 1   | B     | 520 | LYS  |
| 1   | B     | 533 | MET  |
| 1   | C     | 45  | VAL  |
| 1   | C     | 131 | THR  |
| 1   | C     | 310 | LEU  |
| 1   | C     | 378 | PHE  |
| 1   | C     | 488 | MET  |
| 1   | D     | 108 | GLN  |
| 1   | D     | 310 | LEU  |
| 1   | D     | 378 | PHE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 488 | MET  |
| 1   | D     | 515 | TYR  |
| 1   | D     | 561 | HIS  |
| 1   | D     | 589 | ARG  |
| 1   | E     | 61  | ARG  |
| 1   | E     | 108 | GLN  |
| 1   | E     | 219 | ASP  |
| 1   | E     | 247 | ILE  |
| 1   | E     | 378 | PHE  |
| 1   | E     | 423 | HIS  |
| 1   | E     | 585 | LEU  |
| 1   | F     | 45  | VAL  |
| 1   | F     | 105 | MET  |
| 1   | F     | 189 | MET  |
| 1   | F     | 219 | ASP  |
| 1   | F     | 310 | LEU  |
| 1   | F     | 378 | PHE  |
| 1   | F     | 521 | PHE  |
| 1   | F     | 593 | TYR  |
| 1   | G     | 39  | LYS  |
| 1   | G     | 45  | VAL  |
| 1   | G     | 105 | MET  |
| 1   | G     | 251 | LYS  |
| 1   | G     | 310 | LEU  |
| 1   | G     | 488 | MET  |
| 1   | H     | 45  | VAL  |
| 1   | H     | 59  | MET  |
| 1   | H     | 219 | ASP  |
| 1   | H     | 242 | ILE  |
| 1   | H     | 247 | ILE  |
| 1   | H     | 310 | LEU  |
| 1   | H     | 488 | MET  |
| 1   | H     | 508 | LYS  |
| 1   | H     | 533 | MET  |
| 1   | H     | 561 | HIS  |
| 1   | H     | 580 | PHE  |
| 1   | I     | 45  | VAL  |
| 1   | I     | 196 | LEU  |
| 1   | I     | 251 | LYS  |
| 1   | I     | 488 | MET  |
| 1   | I     | 515 | TYR  |
| 1   | J     | 45  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | J     | 55  | ARG  |
| 1   | J     | 95  | GLU  |
| 1   | J     | 105 | MET  |
| 1   | J     | 189 | MET  |
| 1   | J     | 196 | LEU  |
| 1   | J     | 254 | THR  |
| 1   | J     | 297 | THR  |
| 1   | J     | 310 | LEU  |
| 1   | J     | 378 | PHE  |
| 1   | J     | 520 | LYS  |
| 1   | J     | 533 | MET  |
| 1   | J     | 580 | PHE  |
| 1   | J     | 585 | LEU  |
| 1   | J     | 589 | ARG  |
| 1   | J     | 599 | MET  |
| 1   | K     | 45  | VAL  |
| 1   | K     | 189 | MET  |
| 1   | K     | 196 | LEU  |
| 1   | K     | 310 | LEU  |
| 1   | K     | 378 | PHE  |
| 1   | K     | 488 | MET  |
| 1   | L     | 108 | GLN  |
| 1   | L     | 310 | LEU  |
| 1   | L     | 378 | PHE  |
| 1   | L     | 488 | MET  |
| 1   | L     | 515 | TYR  |
| 1   | L     | 533 | MET  |
| 1   | L     | 561 | HIS  |
| 1   | L     | 580 | PHE  |
| 1   | L     | 589 | ARG  |
| 1   | M     | 105 | MET  |
| 1   | M     | 310 | LEU  |
| 1   | M     | 378 | PHE  |
| 1   | M     | 423 | HIS  |
| 1   | N     | 45  | VAL  |
| 1   | N     | 94  | LEU  |
| 1   | N     | 219 | ASP  |
| 1   | N     | 247 | ILE  |
| 1   | N     | 259 | GLN  |
| 1   | N     | 520 | LYS  |
| 1   | N     | 521 | PHE  |
| 1   | O     | 45  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | O     | 105 | MET  |
| 1   | O     | 251 | LYS  |
| 1   | O     | 488 | MET  |
| 1   | O     | 561 | HIS  |
| 1   | P     | 45  | VAL  |
| 1   | P     | 59  | MET  |
| 1   | P     | 94  | LEU  |
| 1   | P     | 131 | THR  |
| 1   | P     | 196 | LEU  |
| 1   | P     | 219 | ASP  |
| 1   | P     | 247 | ILE  |
| 1   | P     | 259 | GLN  |
| 1   | P     | 508 | LYS  |
| 1   | P     | 533 | MET  |
| 1   | P     | 561 | HIS  |
| 1   | P     | 580 | PHE  |
| 1   | P     | 586 | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (102) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 32  | GLN  |
| 1   | A     | 134 | GLN  |
| 1   | A     | 234 | ASN  |
| 1   | A     | 259 | GLN  |
| 1   | A     | 276 | GLN  |
| 1   | A     | 340 | HIS  |
| 1   | A     | 383 | GLN  |
| 1   | A     | 467 | GLN  |
| 1   | B     | 32  | GLN  |
| 1   | B     | 467 | GLN  |
| 1   | C     | 32  | GLN  |
| 1   | C     | 181 | GLN  |
| 1   | C     | 276 | GLN  |
| 1   | C     | 311 | HIS  |
| 1   | C     | 467 | GLN  |
| 1   | D     | 32  | GLN  |
| 1   | D     | 181 | GLN  |
| 1   | D     | 276 | GLN  |
| 1   | D     | 311 | HIS  |
| 1   | D     | 401 | ASN  |
| 1   | D     | 467 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 570 | GLN  |
| 1   | E     | 32  | GLN  |
| 1   | E     | 234 | ASN  |
| 1   | E     | 276 | GLN  |
| 1   | E     | 401 | ASN  |
| 1   | E     | 467 | GLN  |
| 1   | E     | 570 | GLN  |
| 1   | F     | 32  | GLN  |
| 1   | F     | 234 | ASN  |
| 1   | F     | 259 | GLN  |
| 1   | F     | 276 | GLN  |
| 1   | F     | 311 | HIS  |
| 1   | F     | 340 | HIS  |
| 1   | F     | 401 | ASN  |
| 1   | F     | 467 | GLN  |
| 1   | F     | 486 | ASN  |
| 1   | F     | 570 | GLN  |
| 1   | G     | 32  | GLN  |
| 1   | G     | 234 | ASN  |
| 1   | G     | 276 | GLN  |
| 1   | G     | 340 | HIS  |
| 1   | G     | 383 | GLN  |
| 1   | G     | 401 | ASN  |
| 1   | G     | 467 | GLN  |
| 1   | G     | 570 | GLN  |
| 1   | H     | 134 | GLN  |
| 1   | H     | 181 | GLN  |
| 1   | H     | 234 | ASN  |
| 1   | H     | 276 | GLN  |
| 1   | H     | 311 | HIS  |
| 1   | H     | 340 | HIS  |
| 1   | H     | 467 | GLN  |
| 1   | I     | 234 | ASN  |
| 1   | I     | 276 | GLN  |
| 1   | I     | 340 | HIS  |
| 1   | I     | 383 | GLN  |
| 1   | I     | 467 | GLN  |
| 1   | J     | 32  | GLN  |
| 1   | J     | 89  | GLN  |
| 1   | J     | 181 | GLN  |
| 1   | J     | 220 | HIS  |
| 1   | J     | 467 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K     | 32  | GLN  |
| 1   | K     | 276 | GLN  |
| 1   | K     | 311 | HIS  |
| 1   | K     | 467 | GLN  |
| 1   | K     | 570 | GLN  |
| 1   | L     | 32  | GLN  |
| 1   | L     | 181 | GLN  |
| 1   | L     | 276 | GLN  |
| 1   | L     | 311 | HIS  |
| 1   | L     | 401 | ASN  |
| 1   | L     | 467 | GLN  |
| 1   | L     | 570 | GLN  |
| 1   | M     | 32  | GLN  |
| 1   | M     | 234 | ASN  |
| 1   | M     | 276 | GLN  |
| 1   | M     | 311 | HIS  |
| 1   | M     | 401 | ASN  |
| 1   | M     | 467 | GLN  |
| 1   | M     | 570 | GLN  |
| 1   | N     | 32  | GLN  |
| 1   | N     | 234 | ASN  |
| 1   | N     | 276 | GLN  |
| 1   | N     | 401 | ASN  |
| 1   | N     | 467 | GLN  |
| 1   | N     | 570 | GLN  |
| 1   | O     | 32  | GLN  |
| 1   | O     | 234 | ASN  |
| 1   | O     | 276 | GLN  |
| 1   | O     | 340 | HIS  |
| 1   | O     | 383 | GLN  |
| 1   | O     | 401 | ASN  |
| 1   | O     | 467 | GLN  |
| 1   | O     | 570 | GLN  |
| 1   | P     | 32  | GLN  |
| 1   | P     | 77  | GLN  |
| 1   | P     | 234 | ASN  |
| 1   | P     | 276 | GLN  |
| 1   | P     | 340 | HIS  |
| 1   | P     | 467 | 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 ⓘ

32 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 2   | NAG  | H     | 701 | 1    | 14,14,15     | 0.54 | 0           | 17,19,21    | 0.42 | 0           |
| 3   | MA4  | B     | 702 | -    | 37,37,37     | 0.14 | 0           | 50,50,50    | 0.36 | 0           |
| 2   | NAG  | P     | 701 | 1    | 14,14,15     | 0.54 | 0           | 17,19,21    | 0.42 | 0           |
| 2   | NAG  | D     | 701 | 1    | 14,14,15     | 0.55 | 0           | 17,19,21    | 0.42 | 0           |
| 3   | MA4  | D     | 702 | -    | 37,37,37     | 0.15 | 0           | 50,50,50    | 0.40 | 0           |
| 2   | NAG  | B     | 701 | 1    | 14,14,15     | 0.51 | 0           | 17,19,21    | 0.42 | 0           |
| 3   | MA4  | F     | 702 | -    | 37,37,37     | 0.16 | 0           | 50,50,50    | 0.37 | 0           |
| 3   | MA4  | G     | 702 | -    | 37,37,37     | 0.12 | 0           | 50,50,50    | 0.17 | 0           |
| 3   | MA4  | K     | 702 | -    | 37,37,37     | 0.15 | 0           | 50,50,50    | 0.38 | 0           |
| 3   | MA4  | A     | 702 | -    | 37,37,37     | 0.15 | 0           | 50,50,50    | 0.33 | 0           |
| 2   | NAG  | F     | 701 | 1    | 14,14,15     | 0.57 | 0           | 17,19,21    | 0.43 | 0           |
| 2   | NAG  | G     | 701 | 1    | 14,14,15     | 0.51 | 0           | 17,19,21    | 0.41 | 0           |
| 2   | NAG  | K     | 701 | 1    | 14,14,15     | 0.57 | 0           | 17,19,21    | 0.44 | 0           |
| 3   | MA4  | C     | 702 | -    | 37,37,37     | 0.15 | 0           | 50,50,50    | 0.37 | 0           |
| 2   | NAG  | J     | 701 | 1    | 14,14,15     | 0.53 | 0           | 17,19,21    | 0.42 | 0           |
| 3   | MA4  | J     | 702 | -    | 37,37,37     | 0.15 | 0           | 50,50,50    | 0.36 | 0           |
| 2   | NAG  | M     | 701 | 1    | 14,14,15     | 0.68 | 1 (7%)      | 17,19,21    | 0.44 | 0           |



| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | MA4  | M     | 702 | -    | 37,37,37     | 0.15 | 0        | 50,50,50    | 0.36 | 0        |
| 2   | NAG  | E     | 701 | 1    | 14,14,15     | 0.64 | 1 (7%)   | 17,19,21    | 0.43 | 0        |
| 2   | NAG  | C     | 701 | 1    | 14,14,15     | 0.60 | 1 (7%)   | 17,19,21    | 0.44 | 0        |
| 3   | MA4  | E     | 702 | -    | 37,37,37     | 0.15 | 0        | 50,50,50    | 0.36 | 0        |
| 3   | MA4  | P     | 702 | -    | 37,37,37     | 0.16 | 0        | 50,50,50    | 0.37 | 0        |
| 3   | MA4  | I     | 702 | -    | 37,37,37     | 0.12 | 0        | 50,50,50    | 0.18 | 0        |
| 3   | MA4  | O     | 702 | -    | 37,37,37     | 0.12 | 0        | 50,50,50    | 0.17 | 0        |
| 3   | MA4  | N     | 702 | -    | 37,37,37     | 0.16 | 0        | 50,50,50    | 0.38 | 0        |
| 2   | NAG  | A     | 701 | 1    | 14,14,15     | 0.48 | 0        | 17,19,21    | 0.42 | 0        |
| 2   | NAG  | I     | 701 | 1    | 14,14,15     | 0.51 | 0        | 17,19,21    | 0.43 | 0        |
| 3   | MA4  | L     | 702 | -    | 37,37,37     | 0.15 | 0        | 50,50,50    | 0.37 | 0        |
| 2   | NAG  | O     | 701 | 1    | 14,14,15     | 0.51 | 0        | 17,19,21    | 0.41 | 0        |
| 3   | MA4  | H     | 702 | -    | 37,37,37     | 0.15 | 0        | 50,50,50    | 0.37 | 0        |
| 2   | NAG  | N     | 701 | 1    | 14,14,15     | 0.55 | 0        | 17,19,21    | 0.42 | 0        |
| 2   | NAG  | L     | 701 | 1    | 14,14,15     | 0.56 | 0        | 17,19,21    | 0.42 | 0        |

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   |
|-----|------|-------|-----|------|---------|-------------|---------|
| 2   | NAG  | H     | 701 | 1    | -       | 1/6/23/26   | 0/1/1/1 |
| 3   | MA4  | B     | 702 | -    | -       | 8/18/66/66  | 0/3/3/3 |
| 2   | NAG  | P     | 701 | 1    | -       | 2/6/23/26   | 0/1/1/1 |
| 2   | NAG  | D     | 701 | 1    | -       | 1/6/23/26   | 0/1/1/1 |
| 3   | MA4  | D     | 702 | -    | -       | 11/18/66/66 | 0/3/3/3 |
| 2   | NAG  | B     | 701 | 1    | -       | 2/6/23/26   | 0/1/1/1 |
| 3   | MA4  | F     | 702 | -    | -       | 10/18/66/66 | 0/3/3/3 |
| 3   | MA4  | G     | 702 | -    | -       | 8/18/66/66  | 0/3/3/3 |
| 3   | MA4  | K     | 702 | -    | -       | 10/18/66/66 | 0/3/3/3 |
| 3   | MA4  | A     | 702 | -    | -       | 12/18/66/66 | 0/3/3/3 |
| 2   | NAG  | F     | 701 | 1    | -       | 2/6/23/26   | 0/1/1/1 |
| 2   | NAG  | G     | 701 | 1    | -       | 1/6/23/26   | 0/1/1/1 |
| 2   | NAG  | K     | 701 | 1    | -       | 2/6/23/26   | 0/1/1/1 |
| 3   | MA4  | C     | 702 | -    | -       | 10/18/66/66 | 0/3/3/3 |
| 2   | NAG  | J     | 701 | 1    | -       | 2/6/23/26   | 0/1/1/1 |
| 3   | MA4  | J     | 702 | -    | -       | 8/18/66/66  | 0/3/3/3 |
| 2   | NAG  | M     | 701 | 1    | -       | 1/6/23/26   | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions    | Rings   |
|-----|------|-------|-----|------|---------|-------------|---------|
| 3   | MA4  | M     | 702 | -    | -       | 9/18/66/66  | 0/3/3/3 |
| 2   | NAG  | E     | 701 | 1    | -       | 1/6/23/26   | 0/1/1/1 |
| 2   | NAG  | C     | 701 | 1    | -       | 2/6/23/26   | 0/1/1/1 |
| 3   | MA4  | E     | 702 | -    | -       | 9/18/66/66  | 0/3/3/3 |
| 3   | MA4  | P     | 702 | -    | -       | 10/18/66/66 | 0/3/3/3 |
| 3   | MA4  | I     | 702 | -    | -       | 7/18/66/66  | 0/3/3/3 |
| 3   | MA4  | O     | 702 | -    | -       | 8/18/66/66  | 0/3/3/3 |
| 3   | MA4  | N     | 702 | -    | -       | 11/18/66/66 | 0/3/3/3 |
| 2   | NAG  | A     | 701 | 1    | -       | 2/6/23/26   | 0/1/1/1 |
| 2   | NAG  | I     | 701 | 1    | -       | 2/6/23/26   | 0/1/1/1 |
| 3   | MA4  | L     | 702 | -    | -       | 12/18/66/66 | 0/3/3/3 |
| 2   | NAG  | O     | 701 | 1    | -       | 2/6/23/26   | 0/1/1/1 |
| 3   | MA4  | H     | 702 | -    | -       | 12/18/66/66 | 0/3/3/3 |
| 2   | NAG  | N     | 701 | 1    | -       | 1/6/23/26   | 0/1/1/1 |
| 2   | NAG  | L     | 701 | 1    | -       | 1/6/23/26   | 0/1/1/1 |

All (3) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 2   | M     | 701 | NAG  | O5-C1 | -2.24 | 1.40        | 1.43     |
| 2   | E     | 701 | NAG  | O5-C1 | -2.17 | 1.40        | 1.43     |
| 2   | C     | 701 | NAG  | O5-C1 | -2.01 | 1.40        | 1.43     |

There are no bond angle outliers.

There are no chirality outliers.

All (180) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 3   | A     | 702 | MA4  | C20-C10-O10-C11 |
| 3   | A     | 702 | MA4  | O50-C10-O10-C11 |
| 3   | B     | 702 | MA4  | C20-C10-O10-C11 |
| 3   | B     | 702 | MA4  | O50-C10-O10-C11 |
| 3   | C     | 702 | MA4  | O50-C10-O10-C11 |
| 3   | C     | 702 | MA4  | C21-C11-O10-C10 |
| 3   | D     | 702 | MA4  | C20-C10-O10-C11 |
| 3   | D     | 702 | MA4  | O50-C10-O10-C11 |
| 3   | E     | 702 | MA4  | O50-C10-O10-C11 |
| 3   | F     | 702 | MA4  | O50-C10-O10-C11 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 3   | G     | 702 | MA4  | O50-C10-O10-C11 |
| 3   | G     | 702 | MA4  | C21-C11-O10-C10 |
| 3   | H     | 702 | MA4  | O50-C10-O10-C11 |
| 3   | I     | 702 | MA4  | O50-C10-O10-C11 |
| 3   | I     | 702 | MA4  | C21-C11-O10-C10 |
| 3   | J     | 702 | MA4  | C20-C10-O10-C11 |
| 3   | J     | 702 | MA4  | O50-C10-O10-C11 |
| 3   | K     | 702 | MA4  | O50-C10-O10-C11 |
| 3   | K     | 702 | MA4  | C21-C11-O10-C10 |
| 3   | L     | 702 | MA4  | O50-C10-O10-C11 |
| 3   | L     | 702 | MA4  | C21-C11-O10-C10 |
| 3   | M     | 702 | MA4  | O50-C10-O10-C11 |
| 3   | N     | 702 | MA4  | C20-C10-O10-C11 |
| 3   | N     | 702 | MA4  | O50-C10-O10-C11 |
| 3   | O     | 702 | MA4  | O50-C10-O10-C11 |
| 3   | O     | 702 | MA4  | C21-C11-O10-C10 |
| 3   | P     | 702 | MA4  | C20-C10-O10-C11 |
| 3   | P     | 702 | MA4  | O50-C10-O10-C11 |
| 3   | A     | 702 | MA4  | O50-C50-C60-O60 |
| 3   | B     | 702 | MA4  | O50-C50-C60-O60 |
| 3   | F     | 702 | MA4  | O50-C50-C60-O60 |
| 3   | N     | 702 | MA4  | C40-C50-C60-O60 |
| 3   | J     | 702 | MA4  | O50-C50-C60-O60 |
| 3   | L     | 702 | MA4  | C40-C50-C60-O60 |
| 3   | H     | 702 | MA4  | O5-C5-C6-O6     |
| 3   | H     | 702 | MA4  | C4-C5-C6-O6     |
| 3   | H     | 702 | MA4  | C40-C50-C60-O60 |
| 3   | J     | 702 | MA4  | C40-C50-C60-O60 |
| 3   | G     | 702 | MA4  | O50-C50-C60-O60 |
| 3   | L     | 702 | MA4  | O50-C50-C60-O60 |
| 3   | O     | 702 | MA4  | O50-C50-C60-O60 |
| 3   | A     | 702 | MA4  | C40-C50-C60-O60 |
| 3   | D     | 702 | MA4  | O50-C50-C60-O60 |
| 3   | I     | 702 | MA4  | O50-C50-C60-O60 |
| 3   | B     | 702 | MA4  | C40-C50-C60-O60 |
| 3   | C     | 702 | MA4  | O50-C50-C60-O60 |
| 3   | K     | 702 | MA4  | O50-C50-C60-O60 |
| 3   | N     | 702 | MA4  | O50-C50-C60-O60 |
| 3   | F     | 702 | MA4  | C40-C50-C60-O60 |
| 3   | I     | 702 | MA4  | C40-C50-C60-O60 |
| 3   | K     | 702 | MA4  | C40-C50-C60-O60 |
| 3   | D     | 702 | MA4  | C40-C50-C60-O60 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 3   | H     | 702 | MA4  | C20-C10-O10-C11 |
| 3   | M     | 702 | MA4  | C20-C10-O10-C11 |
| 3   | P     | 702 | MA4  | C41-C51-C61-C12 |
| 3   | C     | 702 | MA4  | C40-C50-C60-O60 |
| 3   | F     | 702 | MA4  | C31-C41-C51-C61 |
| 3   | A     | 702 | MA4  | O5-C5-C6-O6     |
| 3   | H     | 702 | MA4  | O50-C50-C60-O60 |
| 3   | G     | 702 | MA4  | C40-C50-C60-O60 |
| 3   | O     | 702 | MA4  | C40-C50-C60-O60 |
| 3   | H     | 702 | MA4  | C41-C51-C61-C12 |
| 3   | M     | 702 | MA4  | C41-C51-C61-C12 |
| 3   | F     | 702 | MA4  | C41-C51-C61-C12 |
| 3   | B     | 702 | MA4  | O10-C11-C21-C31 |
| 3   | M     | 702 | MA4  | O10-C11-C21-C31 |
| 3   | A     | 702 | MA4  | O10-C11-C21-C31 |
| 3   | P     | 702 | MA4  | C11-C21-C31-C41 |
| 3   | J     | 702 | MA4  | O10-C11-C21-C31 |
| 3   | H     | 702 | MA4  | O10-C11-C21-C31 |
| 3   | E     | 702 | MA4  | O10-C11-C21-C31 |
| 3   | F     | 702 | MA4  | O10-C11-C21-C31 |
| 3   | O     | 702 | MA4  | C4-C5-C6-O6     |
| 3   | H     | 702 | MA4  | C11-C21-C31-C41 |
| 3   | N     | 702 | MA4  | O10-C11-C21-C31 |
| 3   | G     | 702 | MA4  | C20-C10-O10-C11 |
| 3   | I     | 702 | MA4  | C20-C10-O10-C11 |
| 3   | O     | 702 | MA4  | C20-C10-O10-C11 |
| 3   | F     | 702 | MA4  | C11-C21-C31-C41 |
| 3   | C     | 702 | MA4  | C22-C12-C61-C51 |
| 3   | F     | 702 | MA4  | C22-C12-C61-C51 |
| 3   | M     | 702 | MA4  | C22-C12-C61-C51 |
| 3   | M     | 702 | MA4  | C62-C12-C61-C51 |
| 3   | N     | 702 | MA4  | C62-C12-C61-C51 |
| 3   | C     | 702 | MA4  | C11-C21-C31-C41 |
| 3   | D     | 702 | MA4  | C11-C21-C31-C41 |
| 3   | E     | 702 | MA4  | C41-C51-C61-C12 |
| 3   | N     | 702 | MA4  | C41-C51-C61-C12 |
| 3   | E     | 702 | MA4  | C62-C12-C61-C51 |
| 3   | H     | 702 | MA4  | C22-C12-C61-C51 |
| 3   | K     | 702 | MA4  | C22-C12-C61-C51 |
| 3   | N     | 702 | MA4  | C22-C12-C61-C51 |
| 3   | P     | 702 | MA4  | C62-C12-C61-C51 |
| 3   | C     | 702 | MA4  | C20-C10-O10-C11 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 3   | F     | 702 | MA4  | C20-C10-O10-C11 |
| 3   | L     | 702 | MA4  | C20-C10-O10-C11 |
| 3   | A     | 702 | MA4  | C22-C12-C61-C51 |
| 3   | E     | 702 | MA4  | O50-C50-C60-O60 |
| 3   | K     | 702 | MA4  | C11-C21-C31-C41 |
| 3   | P     | 702 | MA4  | O50-C50-C60-O60 |
| 3   | M     | 702 | MA4  | C11-C21-C31-C41 |
| 3   | A     | 702 | MA4  | C4-C5-C6-O6     |
| 3   | E     | 702 | MA4  | C21-C31-C41-C51 |
| 3   | O     | 702 | MA4  | O5-C5-C6-O6     |
| 3   | C     | 702 | MA4  | C62-C12-C61-C51 |
| 3   | D     | 702 | MA4  | C22-C12-C61-C51 |
| 3   | D     | 702 | MA4  | C62-C12-C61-C51 |
| 3   | E     | 702 | MA4  | C22-C12-C61-C51 |
| 3   | H     | 702 | MA4  | C62-C12-C61-C51 |
| 3   | P     | 702 | MA4  | C22-C12-C61-C51 |
| 3   | L     | 702 | MA4  | C21-C31-C41-C51 |
| 3   | G     | 702 | MA4  | C4-C5-C6-O6     |
| 3   | P     | 702 | MA4  | C40-C50-C60-O60 |
| 3   | I     | 702 | MA4  | O10-C11-C21-C31 |
| 3   | F     | 702 | MA4  | C62-C12-C61-C51 |
| 3   | K     | 702 | MA4  | C62-C12-C61-C51 |
| 3   | M     | 702 | MA4  | O50-C50-C60-O60 |
| 3   | E     | 702 | MA4  | C20-C10-O10-C11 |
| 3   | K     | 702 | MA4  | C20-C10-O10-C11 |
| 3   | B     | 702 | MA4  | C22-C12-C61-C51 |
| 3   | D     | 702 | MA4  | O5-C1-O1-C40    |
| 3   | A     | 702 | MA4  | C62-C12-C61-C51 |
| 3   | B     | 702 | MA4  | C62-C12-C61-C51 |
| 3   | A     | 702 | MA4  | C21-C11-O10-C10 |
| 3   | B     | 702 | MA4  | C21-C11-O10-C10 |
| 3   | J     | 702 | MA4  | C21-C11-O10-C10 |
| 3   | J     | 702 | MA4  | C62-C12-C61-C51 |
| 3   | L     | 702 | MA4  | C62-C12-C61-C51 |
| 3   | P     | 702 | MA4  | O10-C11-C21-C31 |
| 3   | K     | 702 | MA4  | O10-C11-C21-C31 |
| 3   | M     | 702 | MA4  | C31-C41-C51-C61 |
| 3   | L     | 702 | MA4  | C22-C12-C61-C51 |
| 3   | E     | 702 | MA4  | C31-C41-C51-C61 |
| 3   | J     | 702 | MA4  | C22-C12-C61-C51 |
| 3   | O     | 702 | MA4  | C41-C51-C61-C12 |
| 3   | L     | 702 | MA4  | C11-C21-C31-C41 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 3   | G     | 702 | MA4  | C41-C51-C61-C12 |
| 3   | C     | 702 | MA4  | C31-C41-C51-C61 |
| 3   | H     | 702 | MA4  | C31-C41-C51-C61 |
| 3   | G     | 702 | MA4  | O5-C5-C6-O6     |
| 3   | D     | 702 | MA4  | C31-C41-C51-C61 |
| 2   | H     | 701 | NAG  | C3-C2-N2-C7     |
| 2   | O     | 701 | NAG  | C4-C5-C6-O6     |
| 3   | D     | 702 | MA4  | C2-C1-O1-C40    |
| 3   | N     | 702 | MA4  | C31-C41-C51-C61 |
| 3   | N     | 702 | MA4  | O5-C5-C6-O6     |
| 3   | A     | 702 | MA4  | O5-C1-O1-C40    |
| 3   | L     | 702 | MA4  | O5-C1-O1-C40    |
| 3   | C     | 702 | MA4  | O10-C11-C21-C31 |
| 3   | N     | 702 | MA4  | C11-C21-C31-C41 |
| 3   | I     | 702 | MA4  | C62-C12-C61-C51 |
| 3   | A     | 702 | MA4  | C2-C1-O1-C40    |
| 3   | K     | 702 | MA4  | C31-C41-C51-C61 |
| 2   | A     | 701 | NAG  | C3-C2-N2-C7     |
| 2   | B     | 701 | NAG  | C3-C2-N2-C7     |
| 2   | C     | 701 | NAG  | C3-C2-N2-C7     |
| 2   | D     | 701 | NAG  | C3-C2-N2-C7     |
| 2   | E     | 701 | NAG  | C3-C2-N2-C7     |
| 2   | F     | 701 | NAG  | C3-C2-N2-C7     |
| 2   | G     | 701 | NAG  | C3-C2-N2-C7     |
| 2   | I     | 701 | NAG  | C3-C2-N2-C7     |
| 2   | J     | 701 | NAG  | C3-C2-N2-C7     |
| 2   | K     | 701 | NAG  | C3-C2-N2-C7     |
| 2   | L     | 701 | NAG  | C3-C2-N2-C7     |
| 2   | M     | 701 | NAG  | C3-C2-N2-C7     |
| 2   | N     | 701 | NAG  | C3-C2-N2-C7     |
| 2   | O     | 701 | NAG  | C3-C2-N2-C7     |
| 2   | P     | 701 | NAG  | C3-C2-N2-C7     |
| 3   | L     | 702 | MA4  | C2-C1-O1-C40    |
| 3   | D     | 702 | MA4  | C21-C31-C41-C51 |
| 2   | C     | 701 | NAG  | C1-C2-N2-C7     |
| 2   | F     | 701 | NAG  | C1-C2-N2-C7     |
| 3   | L     | 702 | MA4  | O5-C5-C6-O6     |
| 3   | P     | 702 | MA4  | C21-C31-C41-C51 |
| 2   | A     | 701 | NAG  | C1-C2-N2-C7     |
| 2   | B     | 701 | NAG  | C1-C2-N2-C7     |
| 2   | I     | 701 | NAG  | C1-C2-N2-C7     |
| 2   | J     | 701 | NAG  | C1-C2-N2-C7     |

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| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 2   | K     | 701 | NAG  | C1-C2-N2-C7 |
| 2   | P     | 701 | NAG  | C1-C2-N2-C7 |

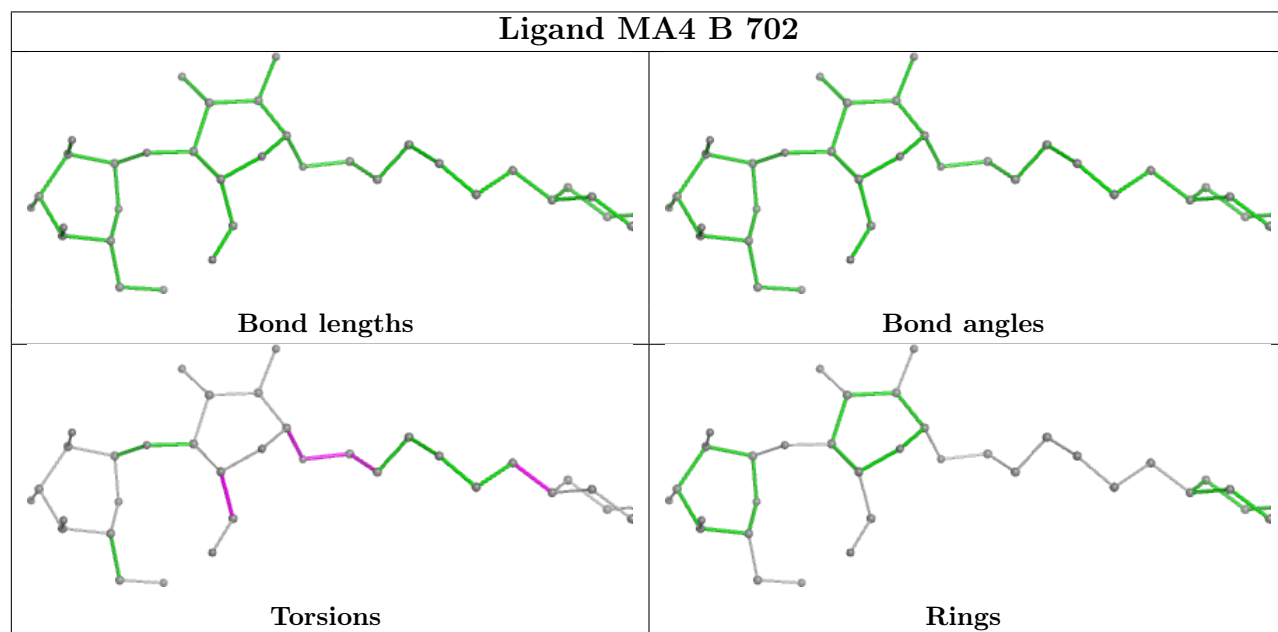
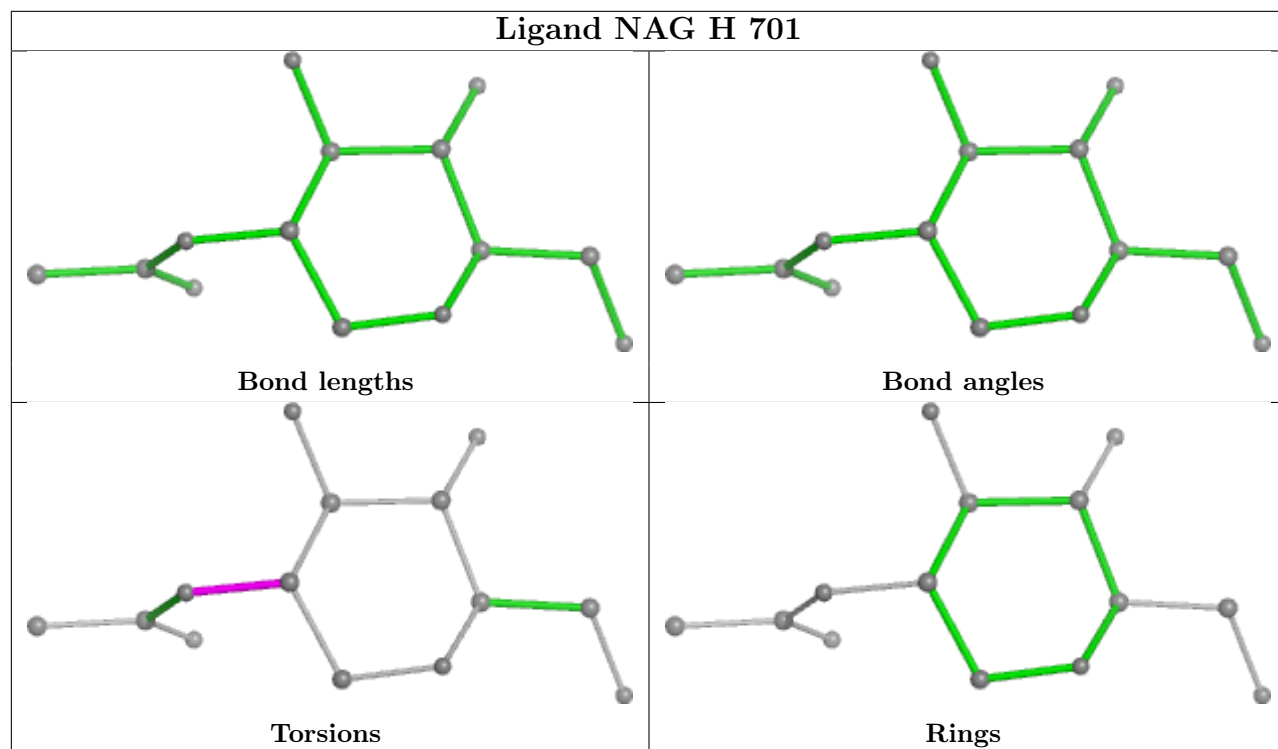
There are no ring outliers.

14 monomers are involved in 30 short contacts:

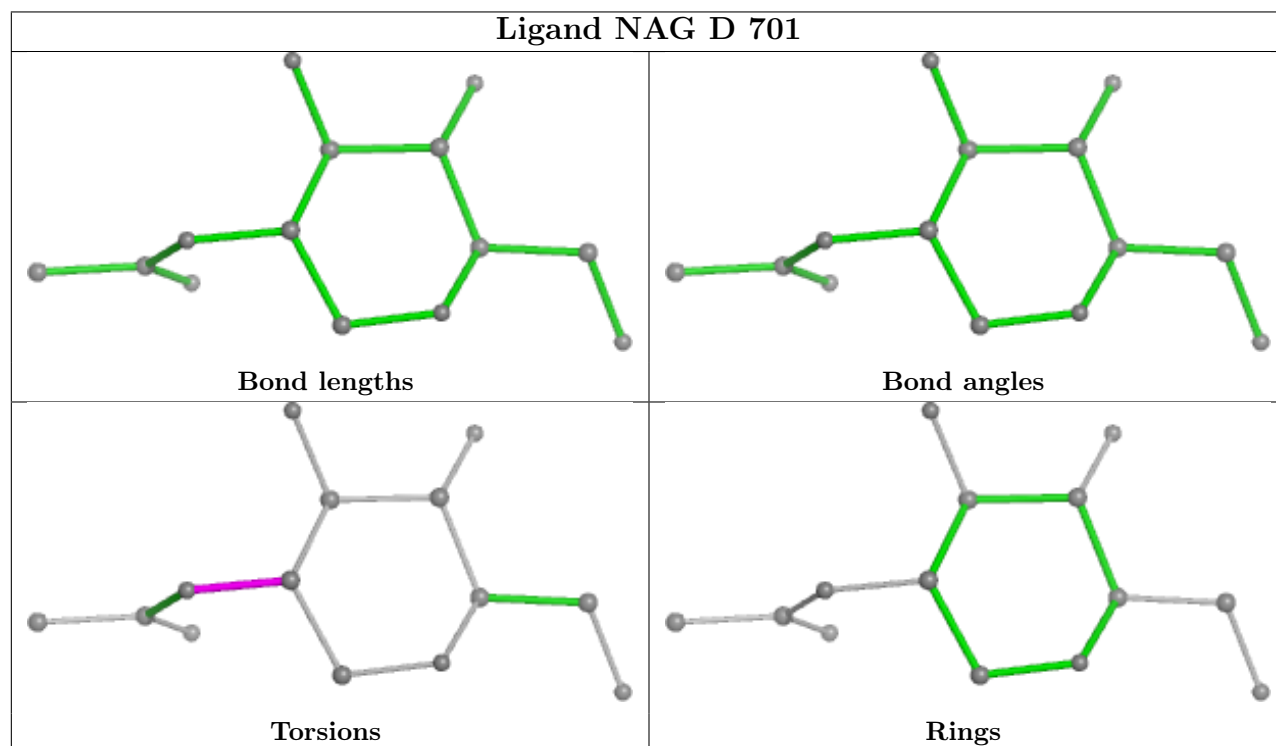
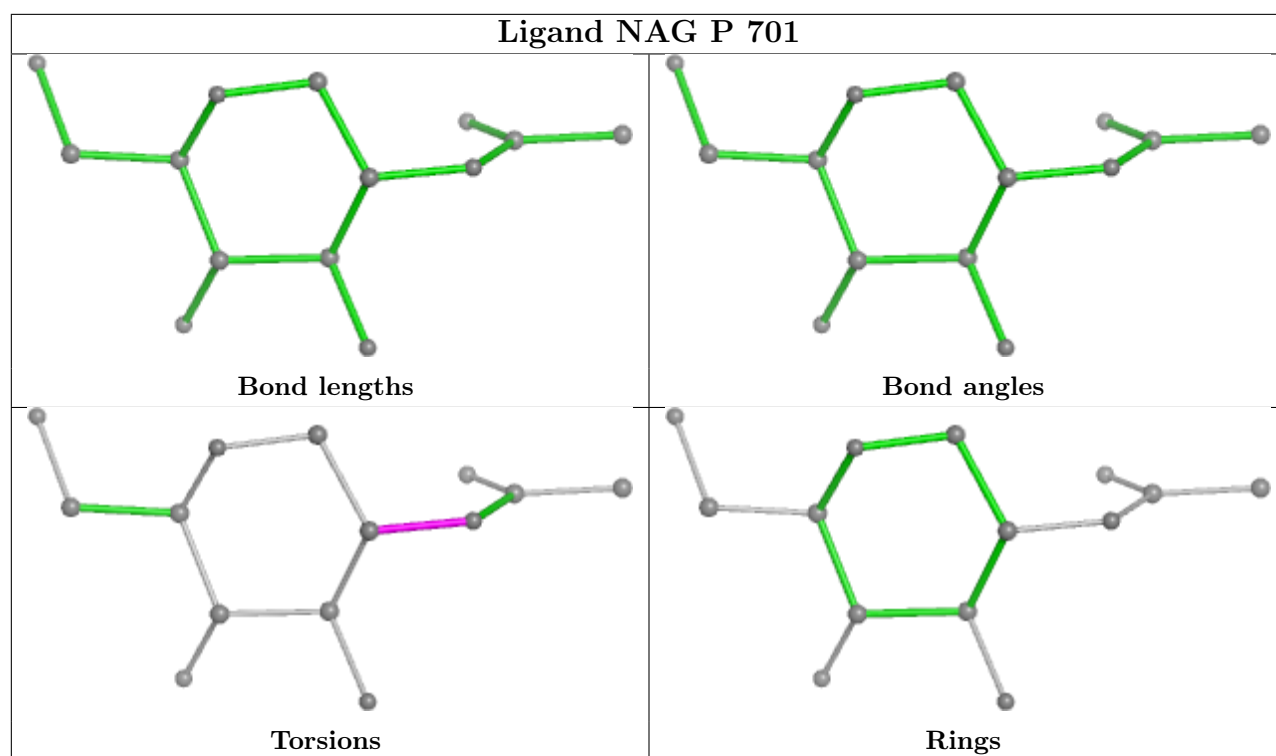
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | B     | 702 | MA4  | 1       | 0            |
| 3   | D     | 702 | MA4  | 3       | 0            |
| 3   | F     | 702 | MA4  | 1       | 0            |
| 3   | K     | 702 | MA4  | 1       | 0            |
| 3   | A     | 702 | MA4  | 2       | 0            |
| 3   | C     | 702 | MA4  | 2       | 0            |
| 3   | M     | 702 | MA4  | 4       | 0            |
| 3   | E     | 702 | MA4  | 5       | 0            |
| 3   | P     | 702 | MA4  | 1       | 0            |
| 3   | I     | 702 | MA4  | 1       | 0            |
| 3   | O     | 702 | MA4  | 1       | 0            |
| 3   | N     | 702 | MA4  | 2       | 0            |
| 3   | L     | 702 | MA4  | 5       | 0            |
| 3   | H     | 702 | MA4  | 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.

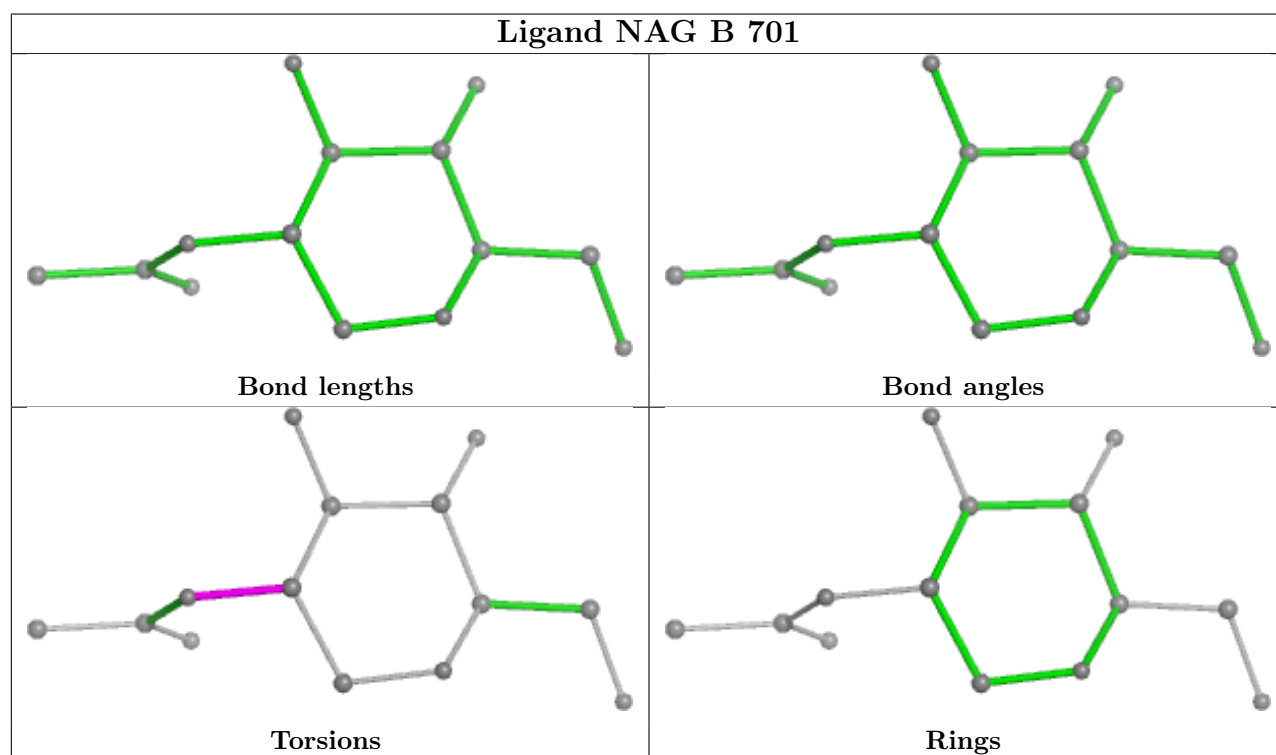
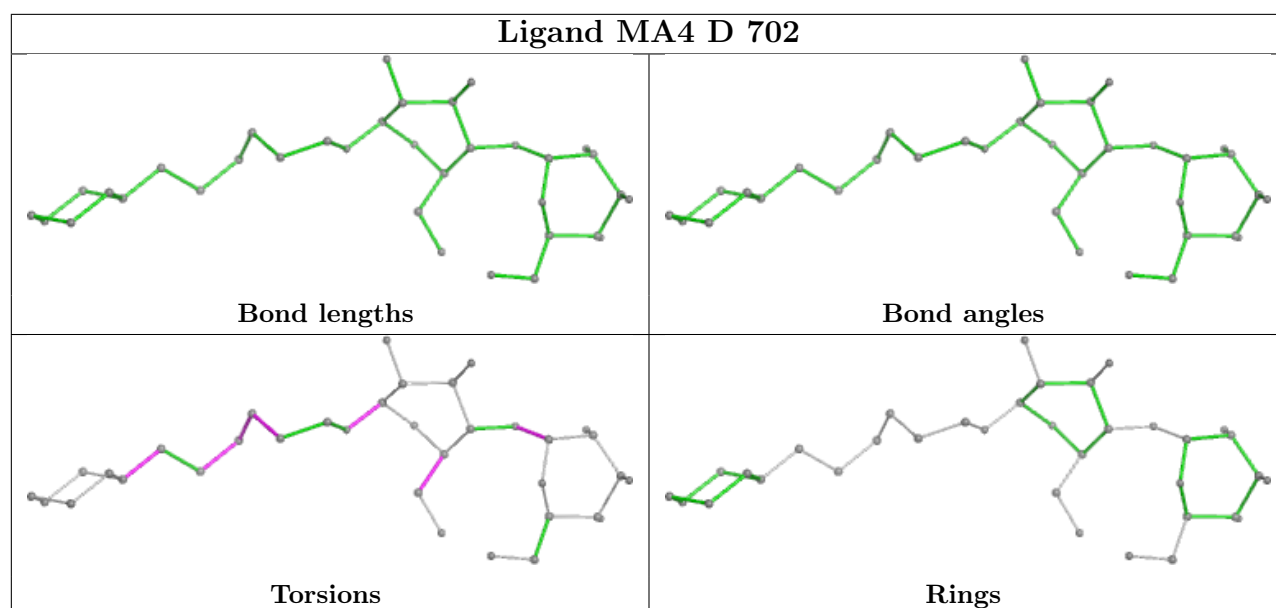




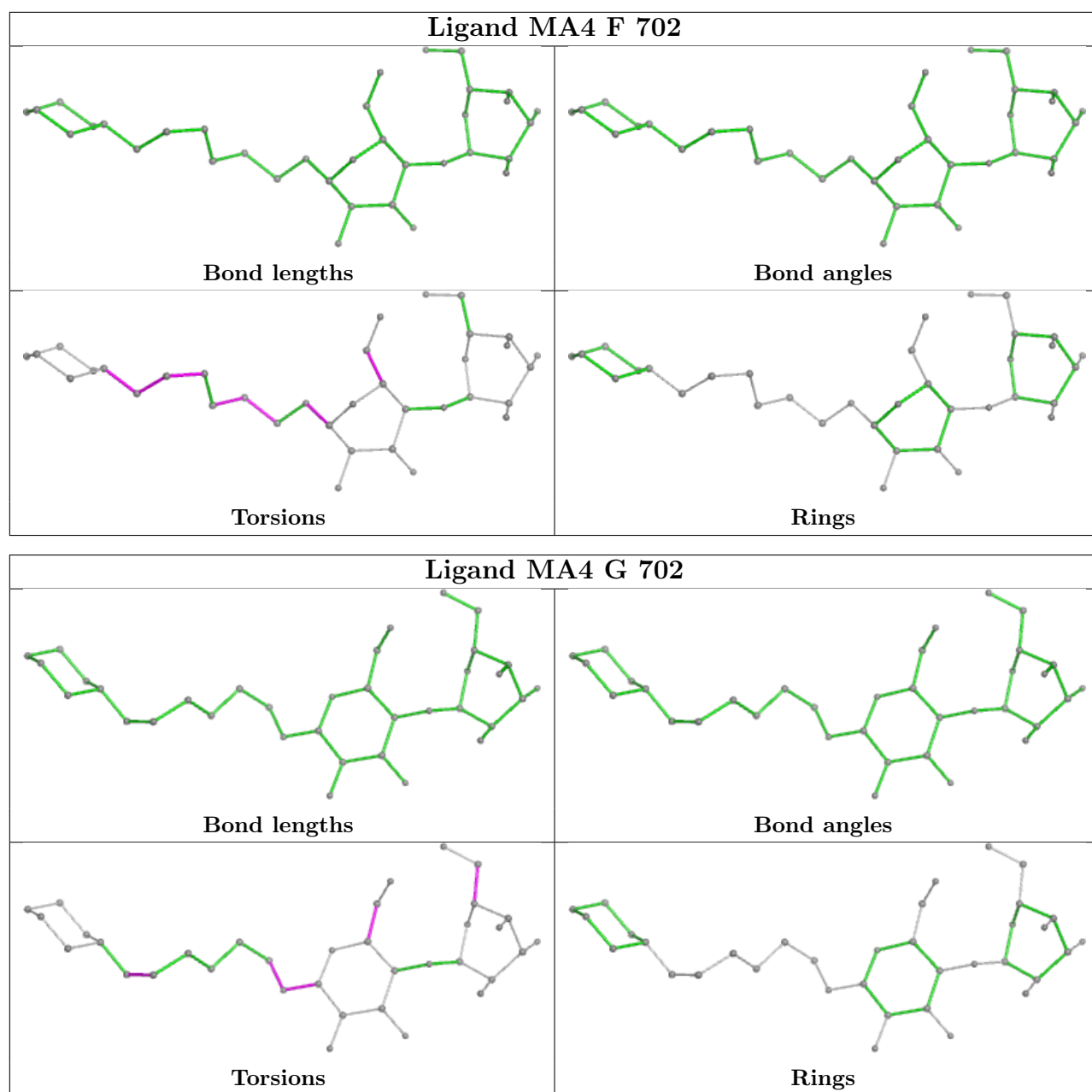




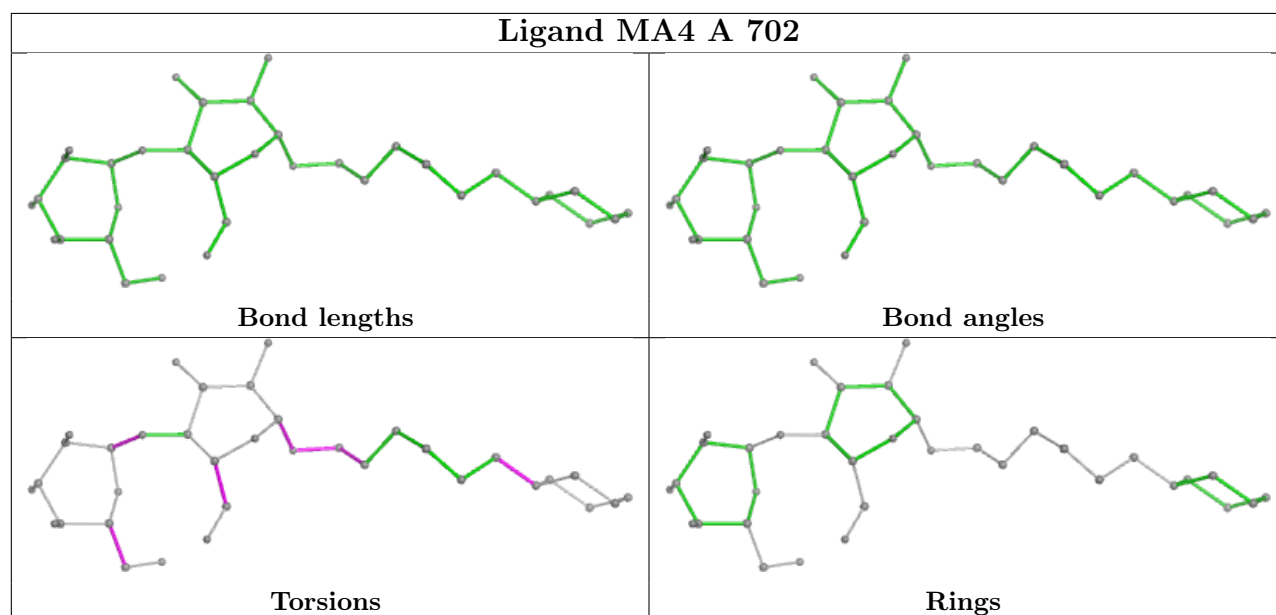
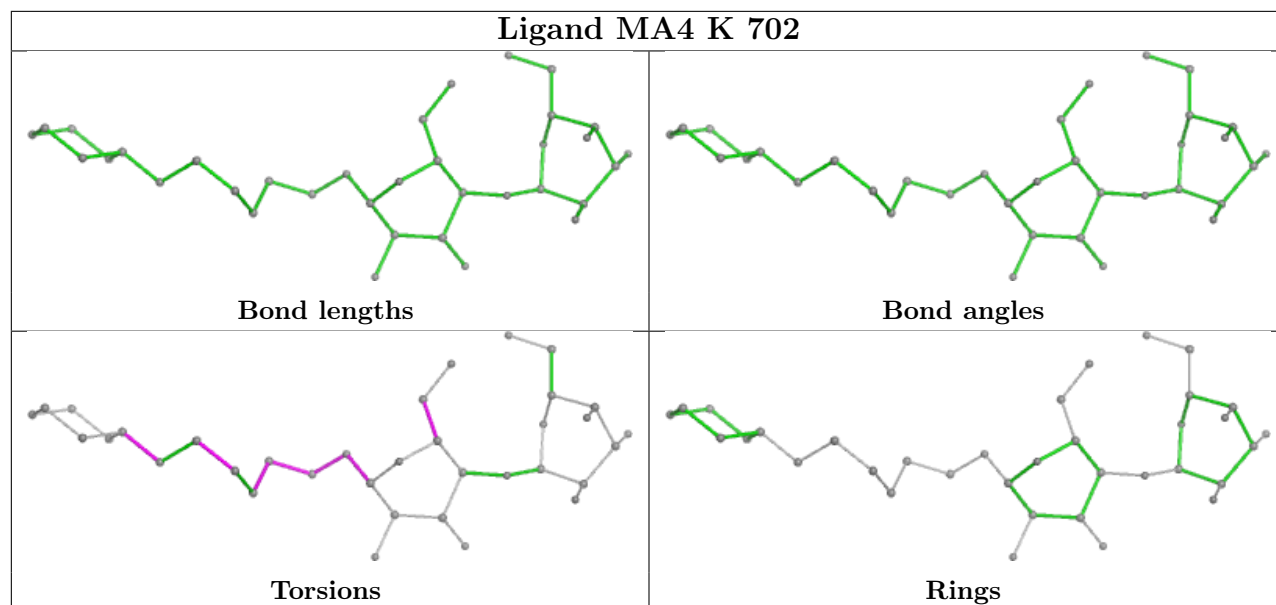




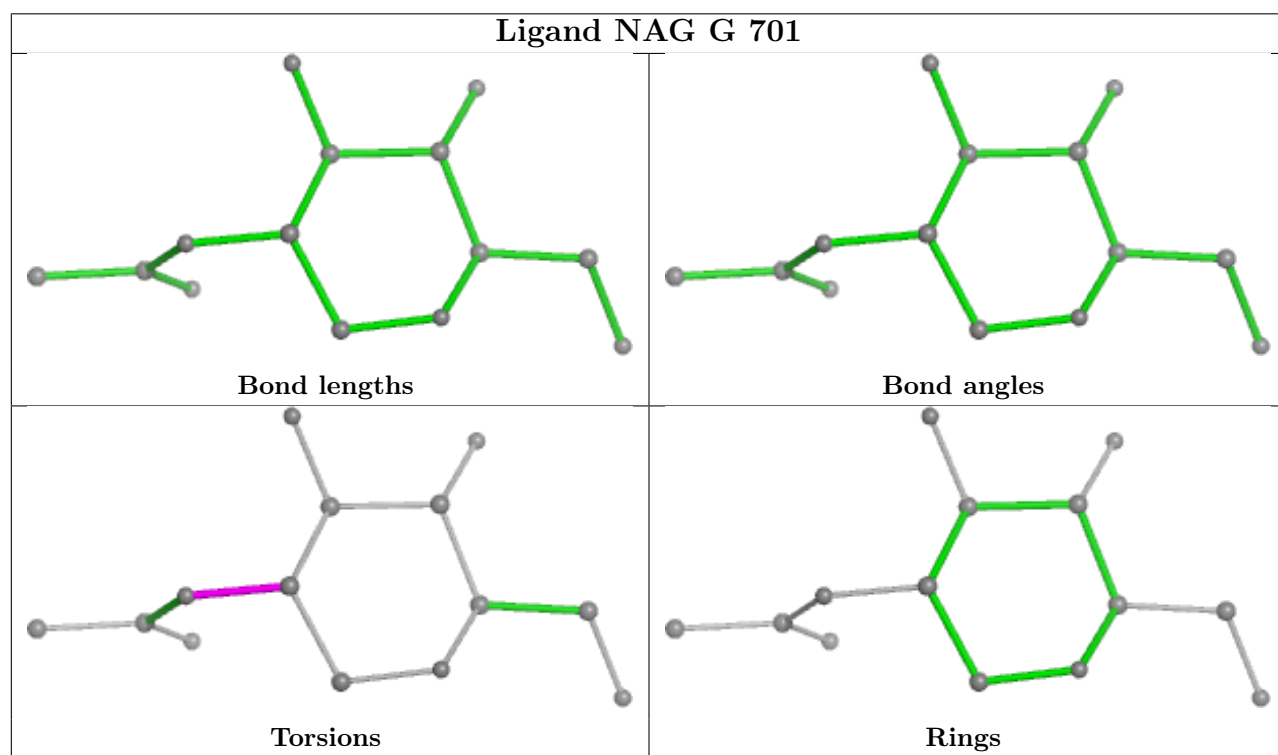
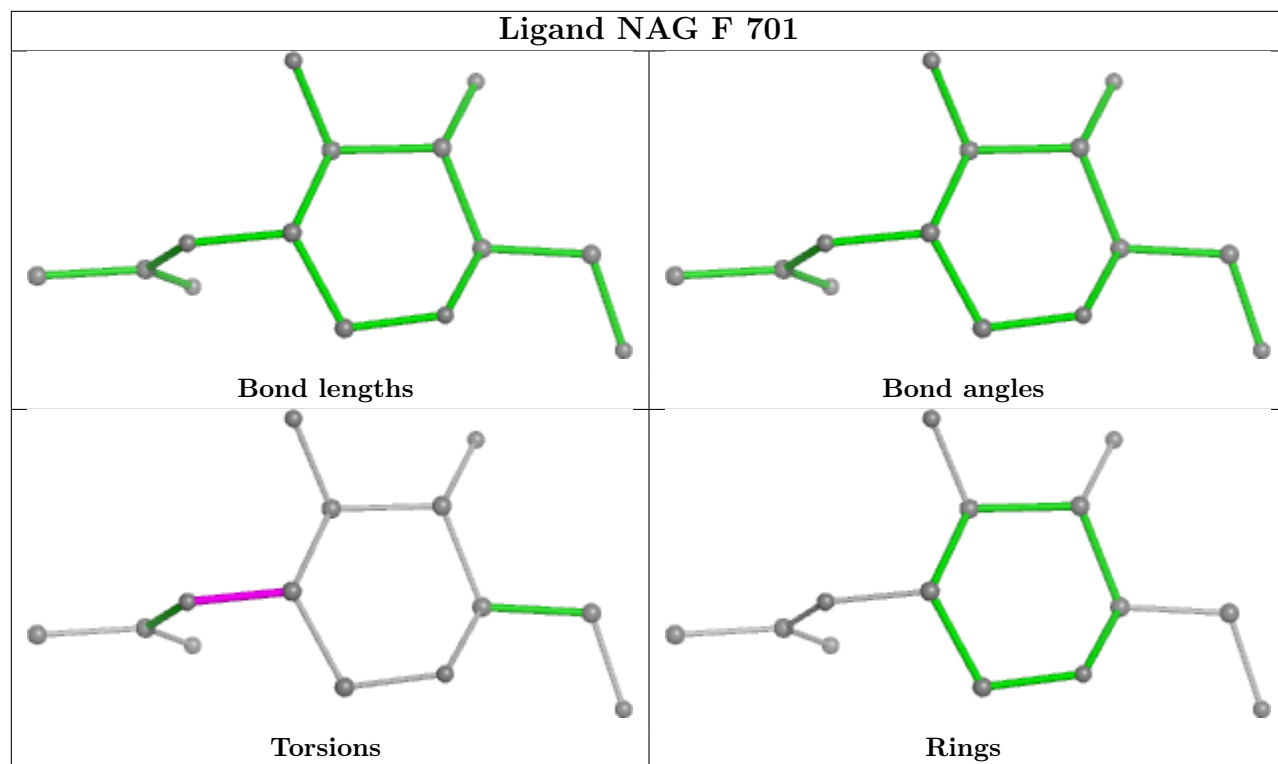




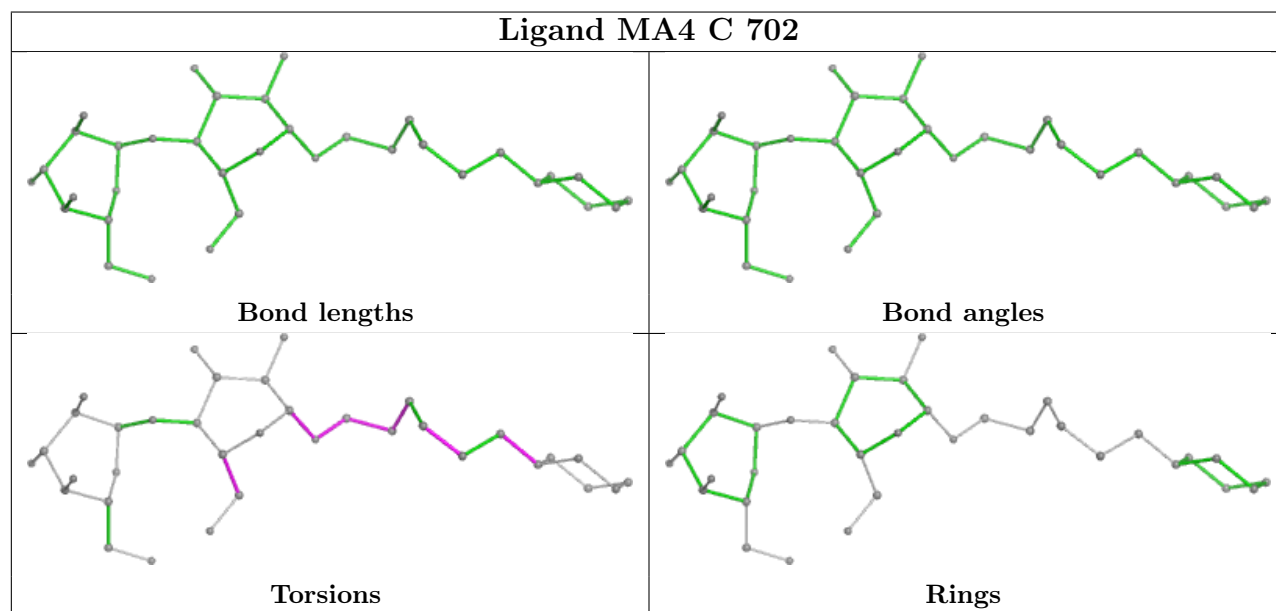
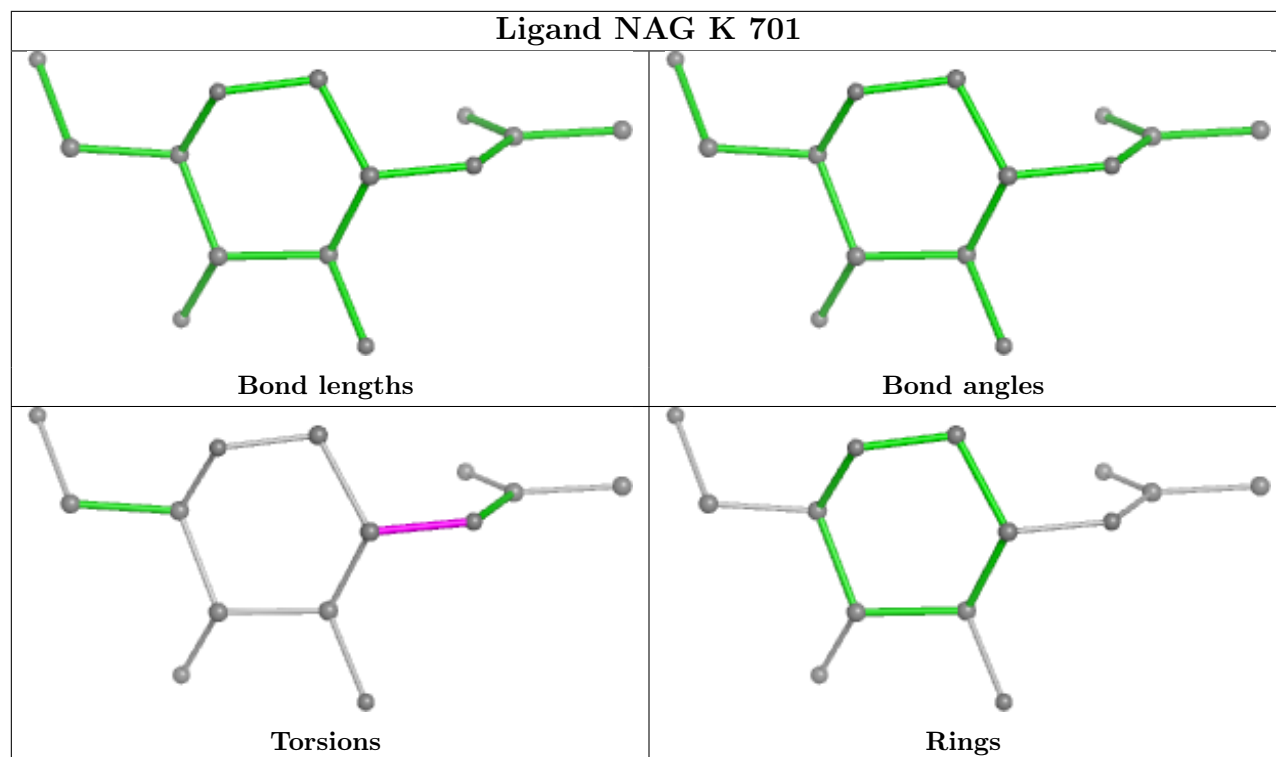




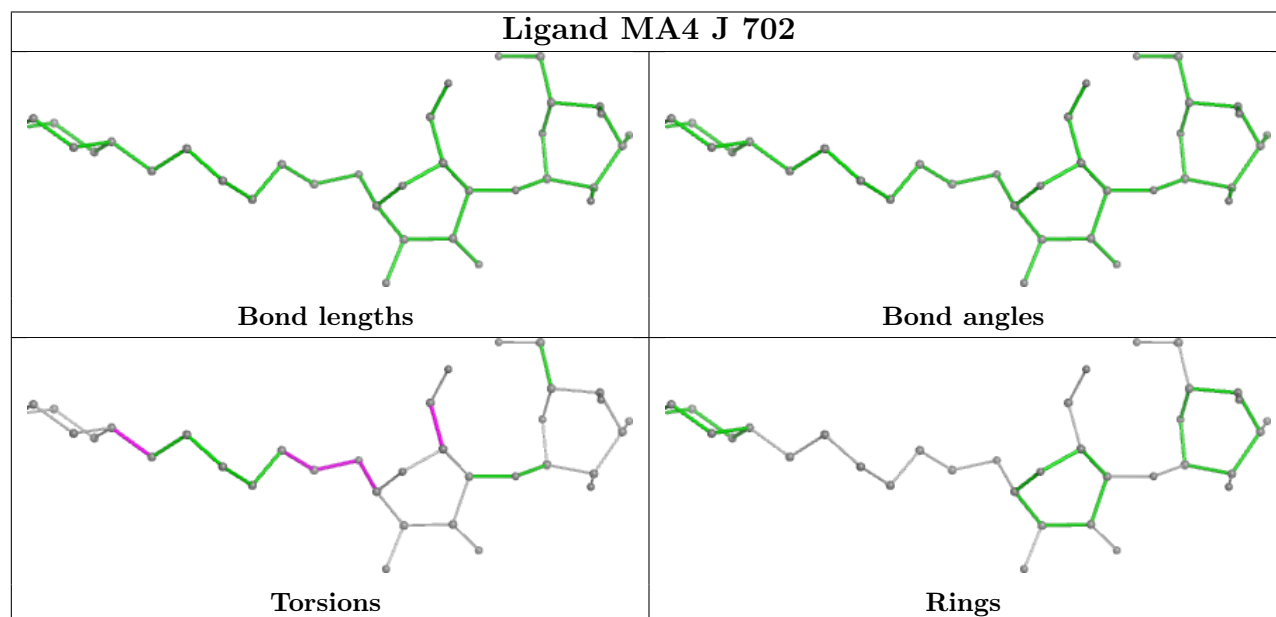
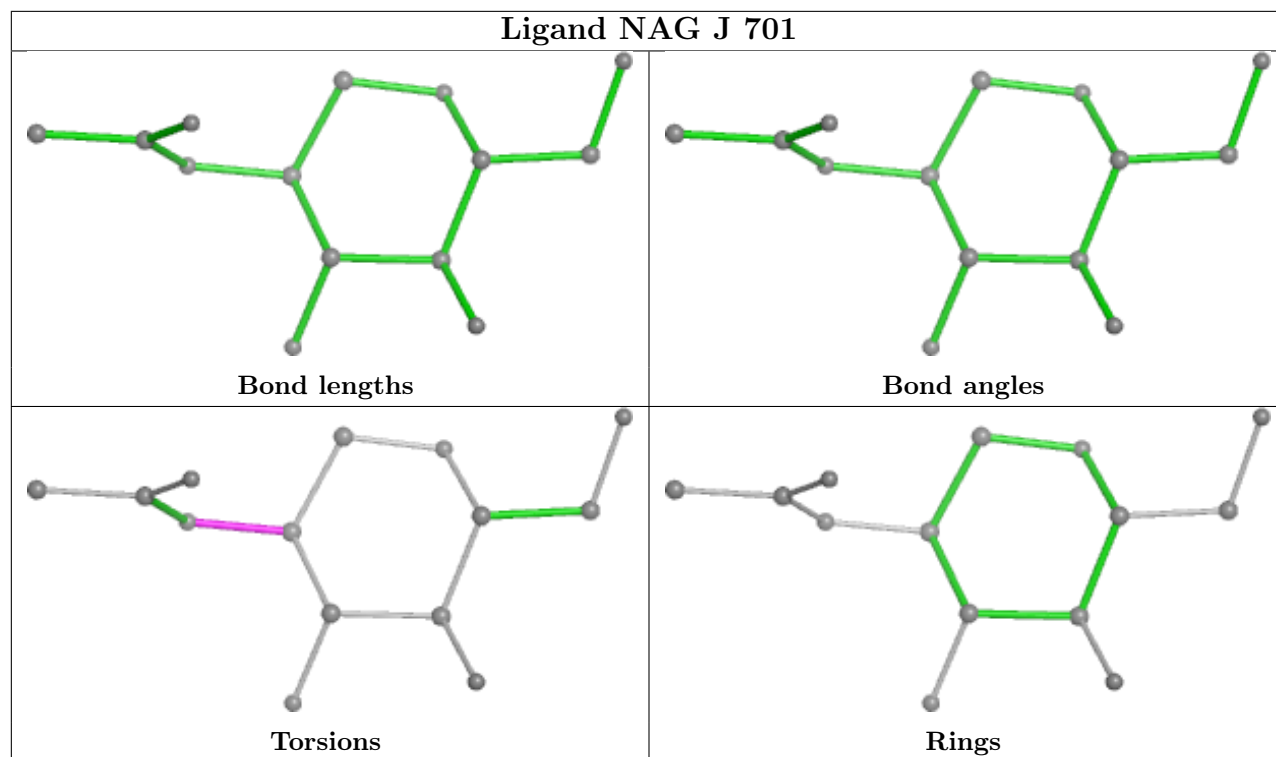




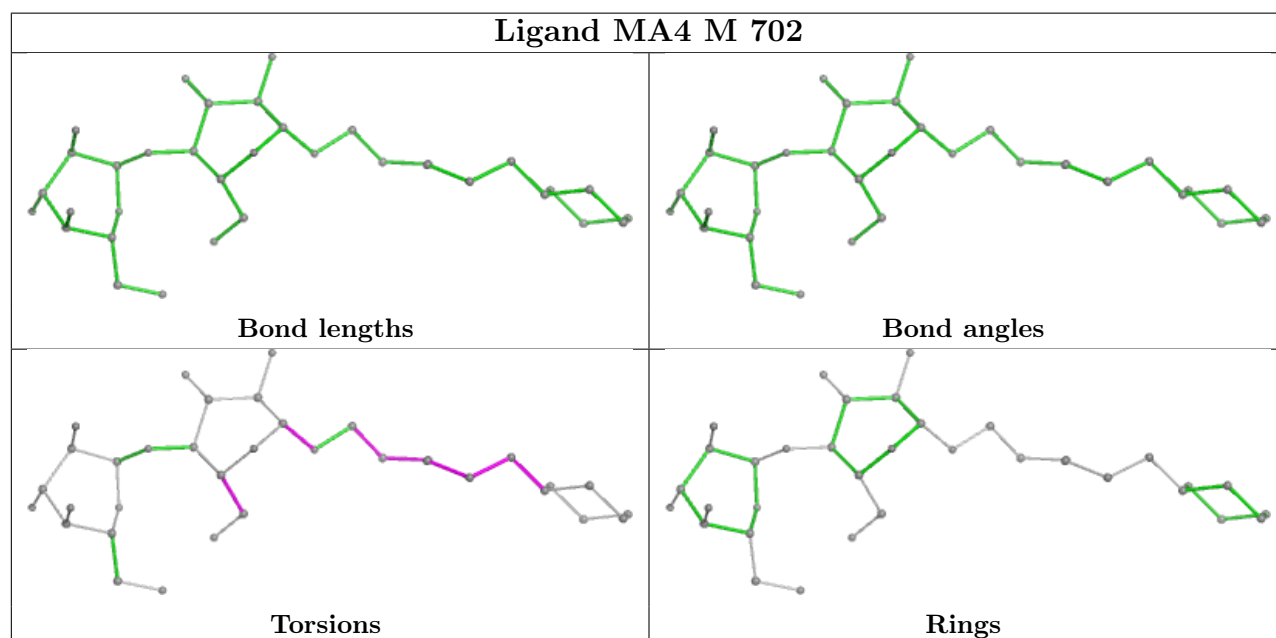
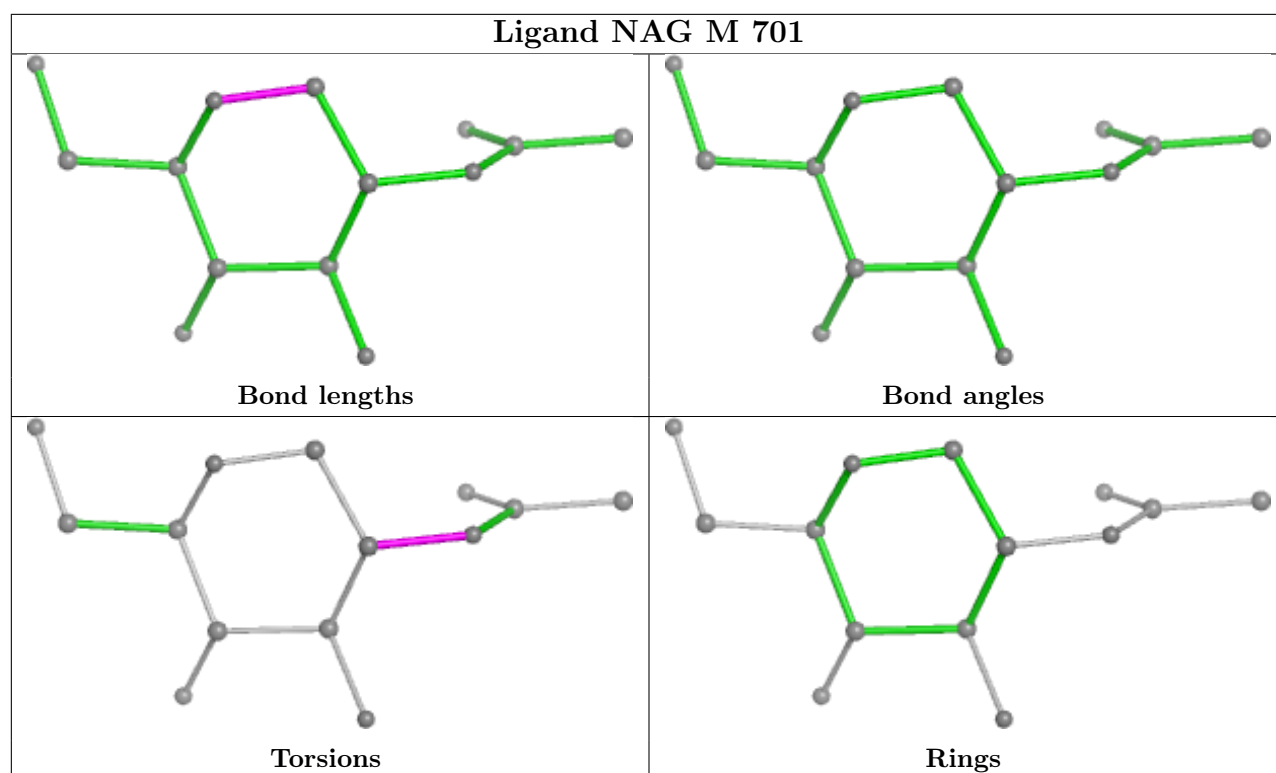




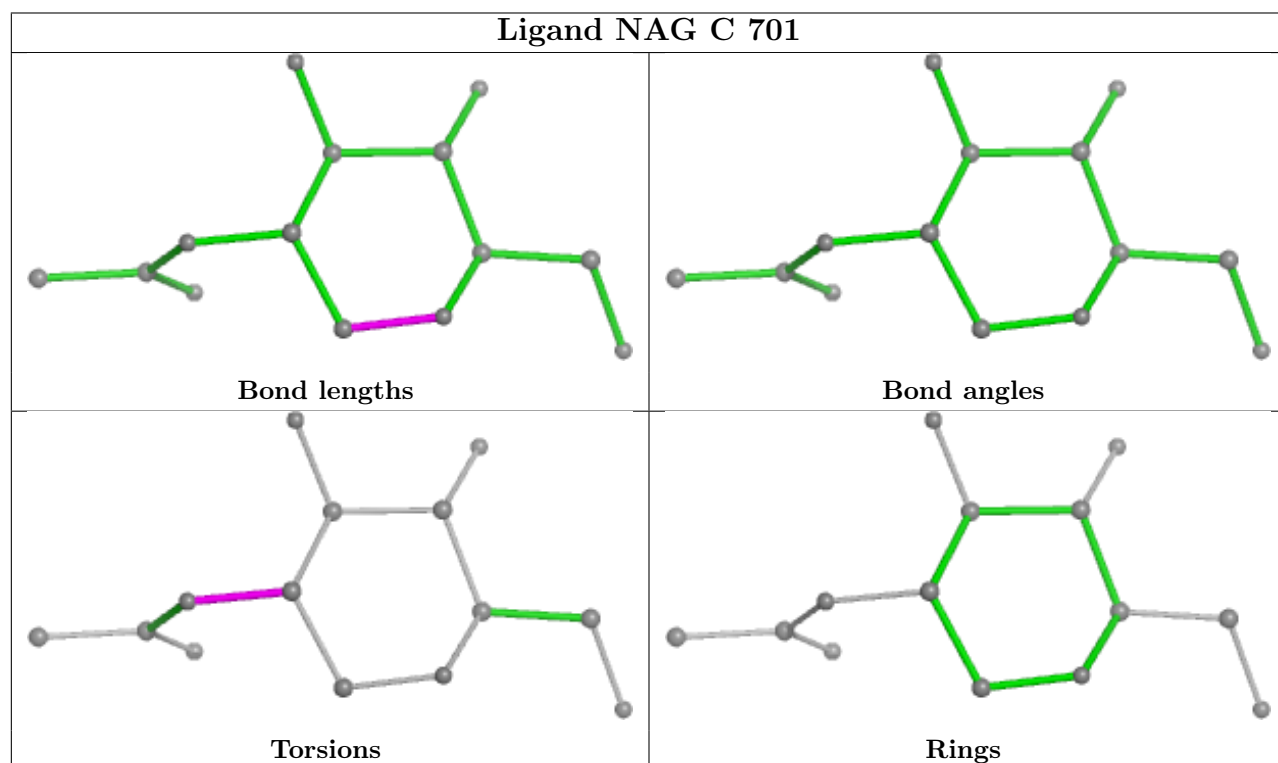
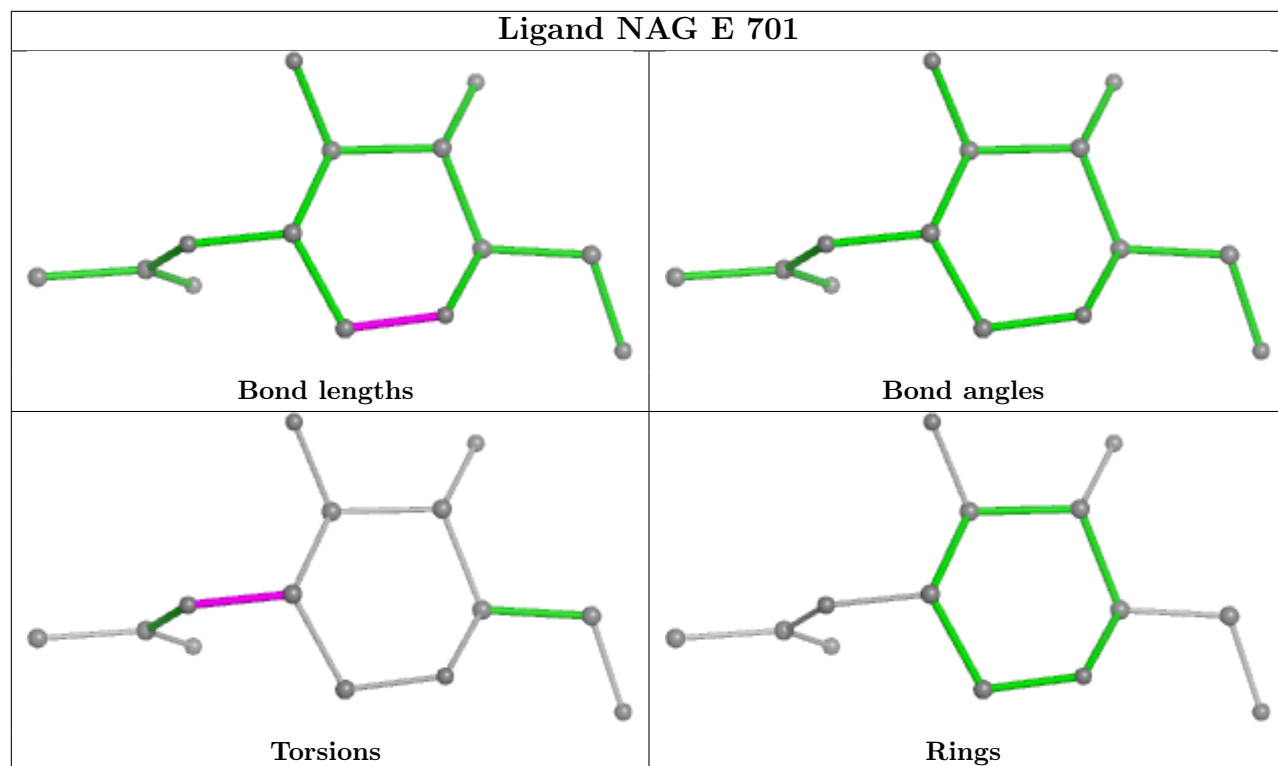




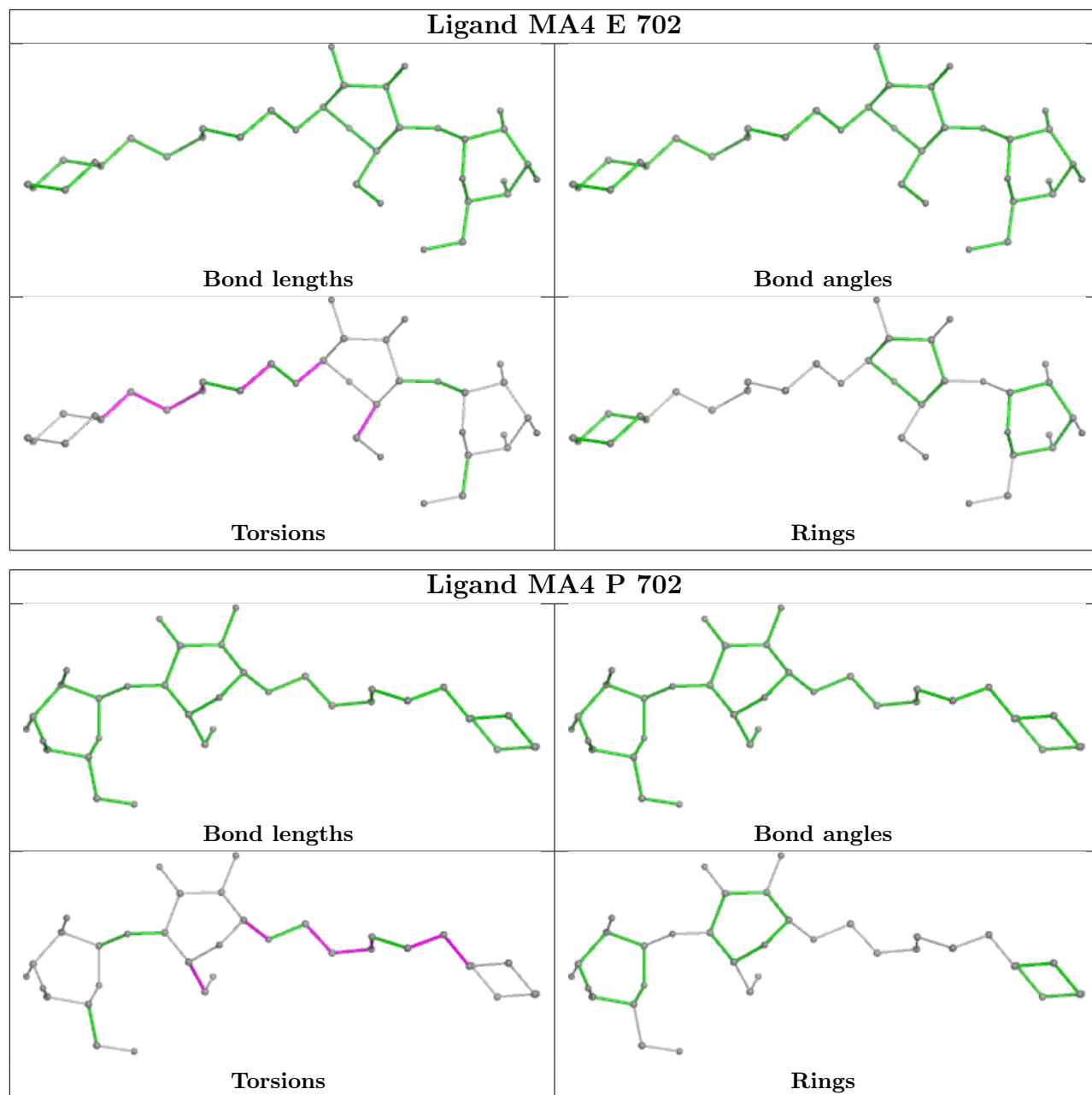




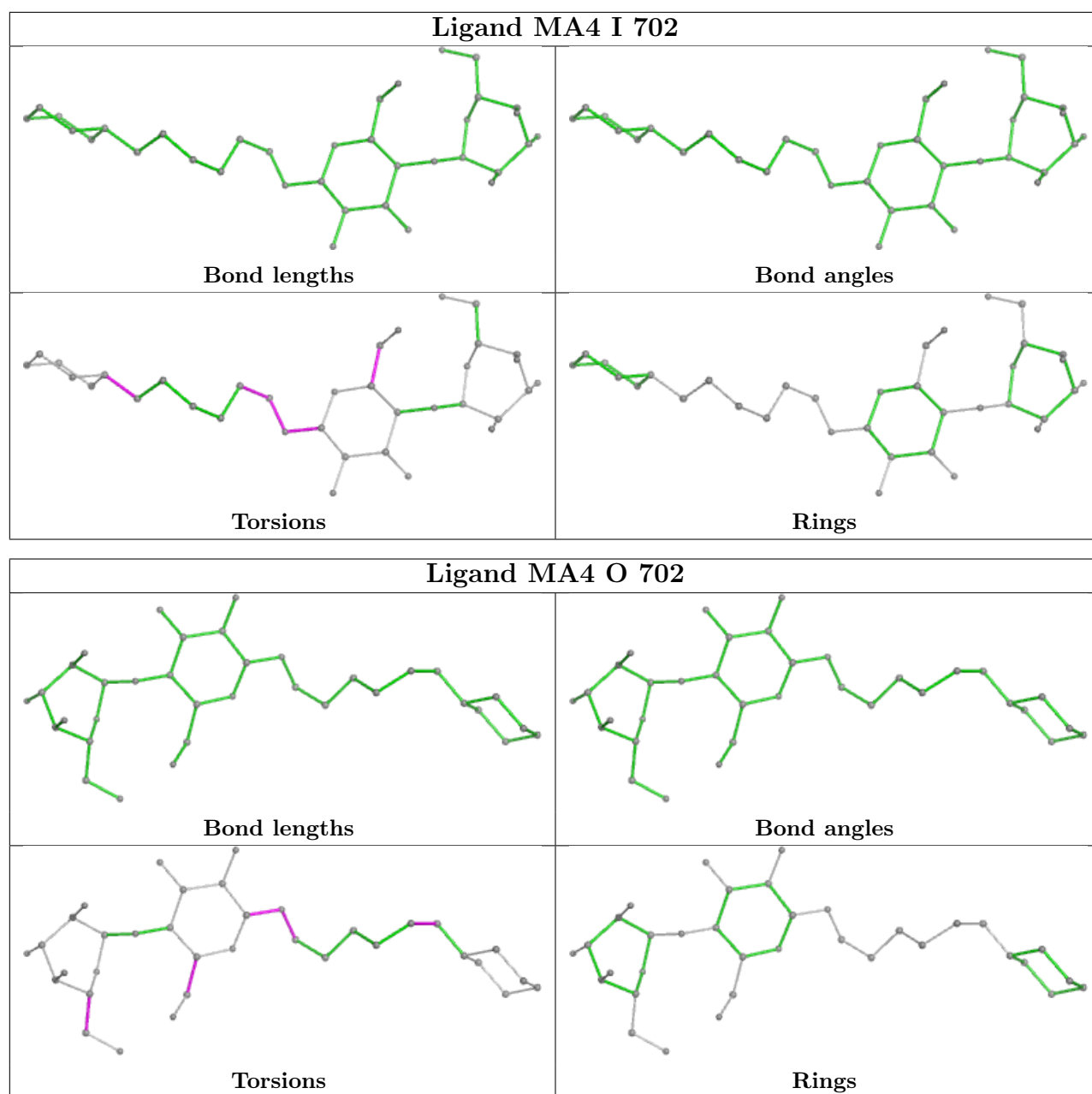




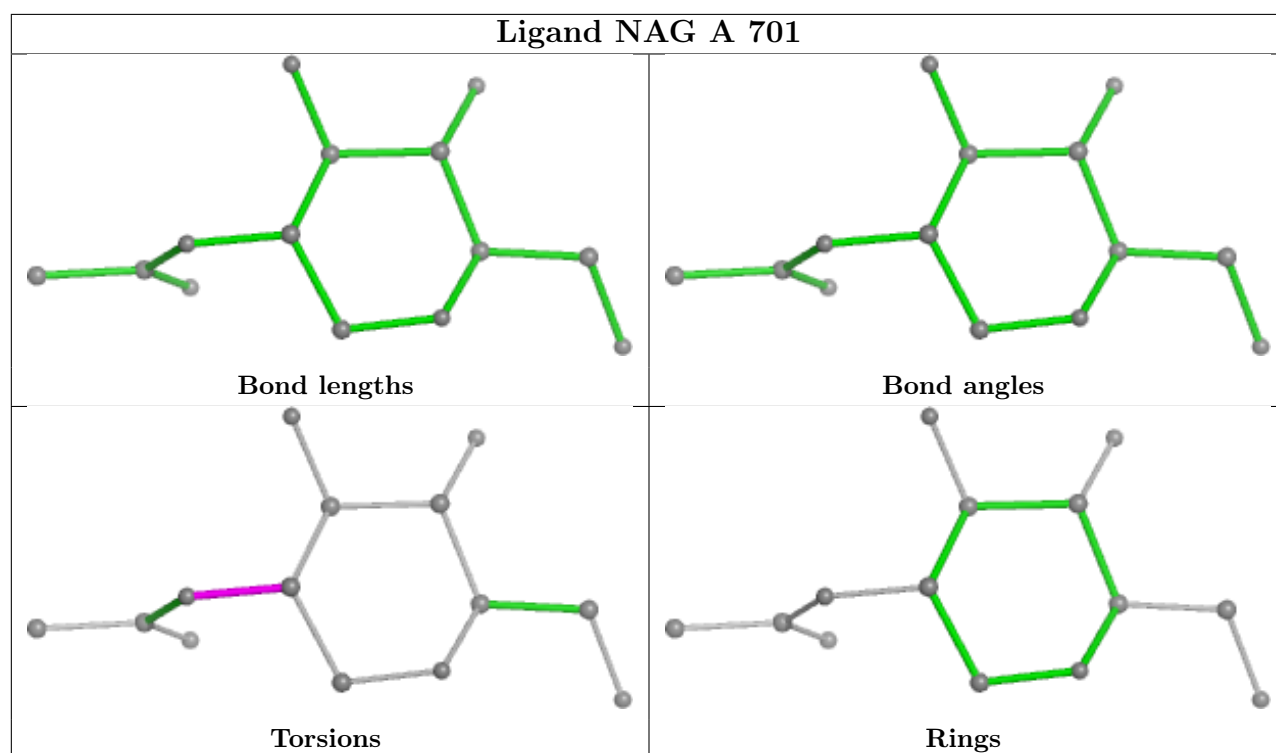
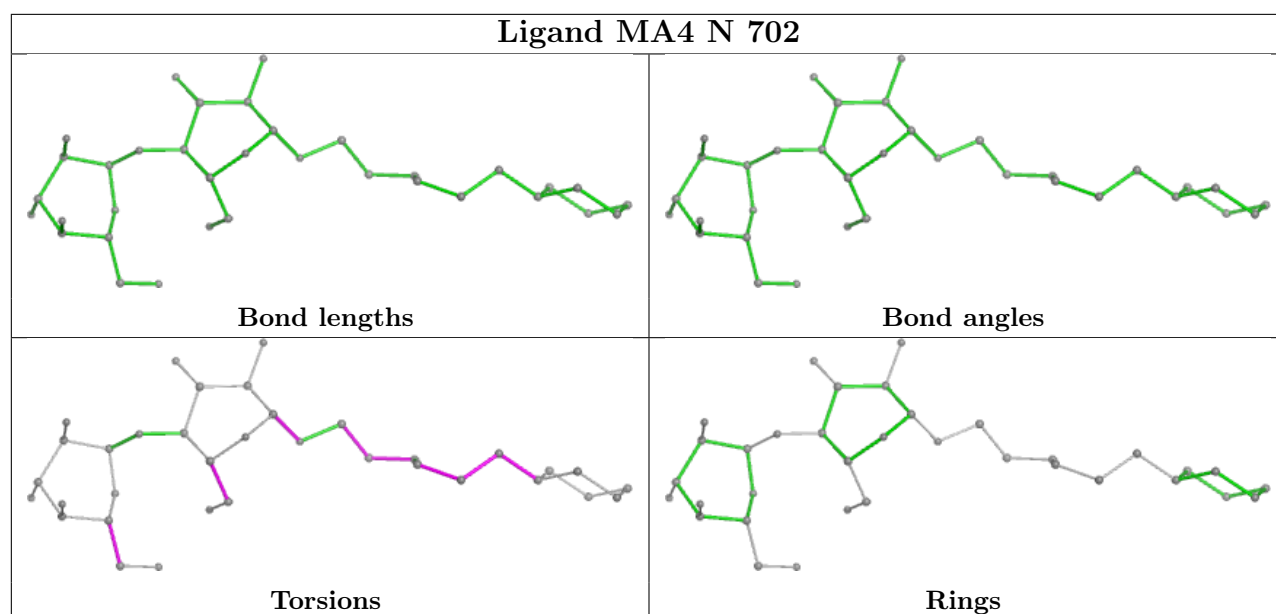




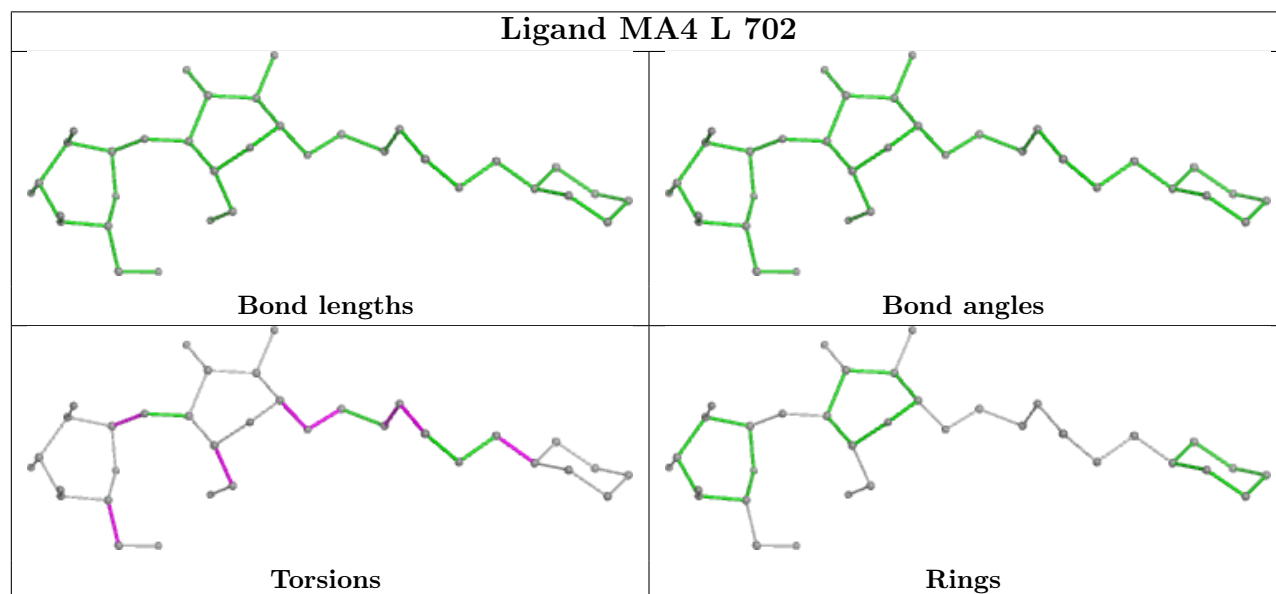
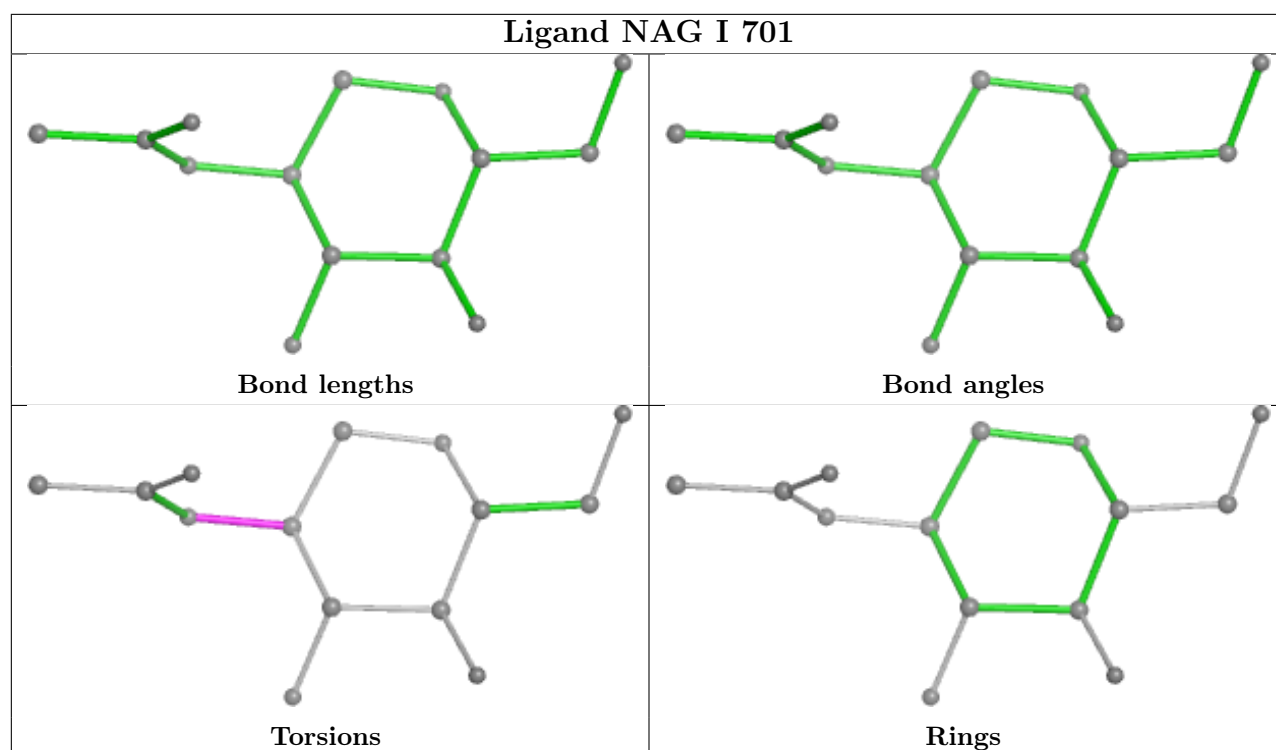




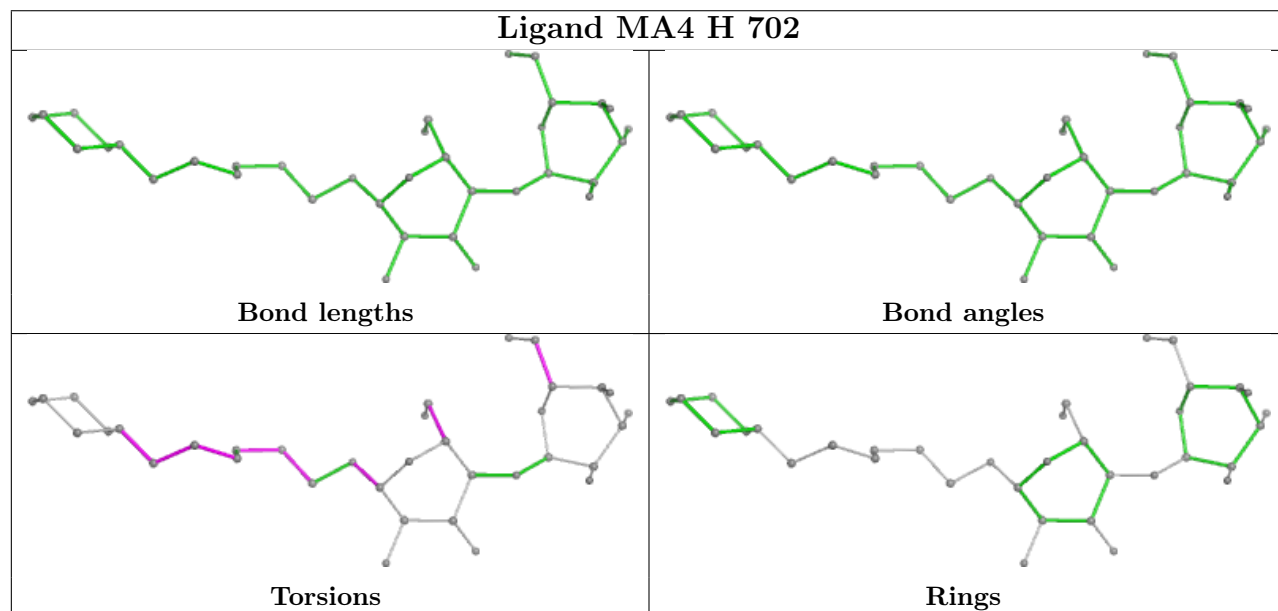
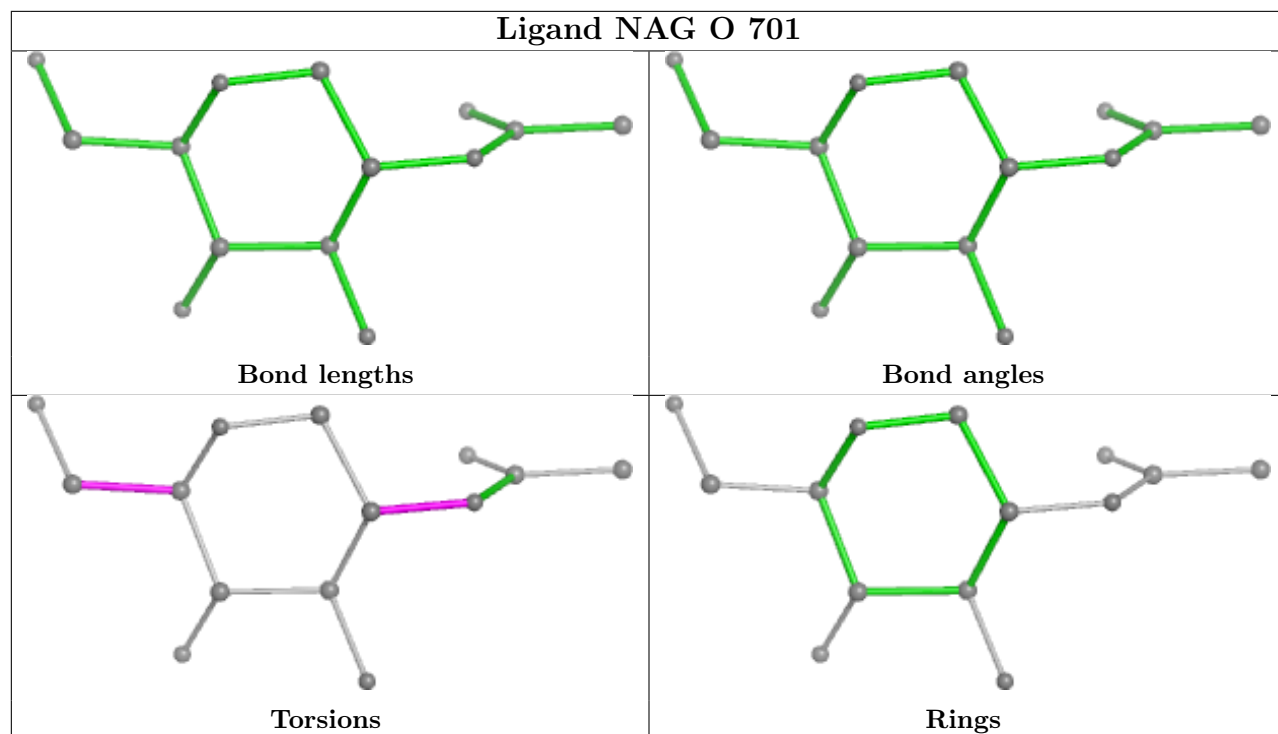




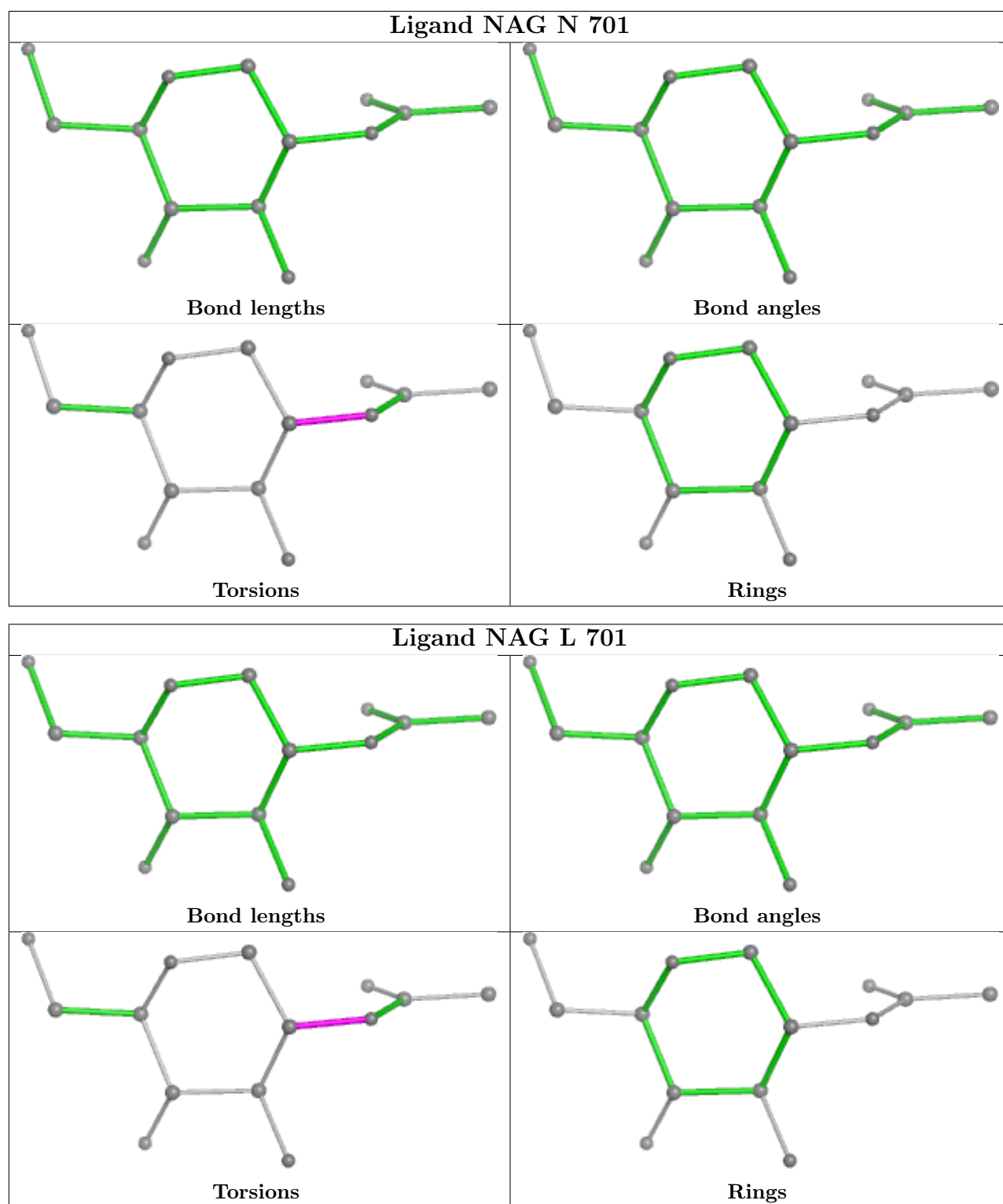












## 5.7 Other polymers ⓘ

There are no such residues in this entry.



## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.



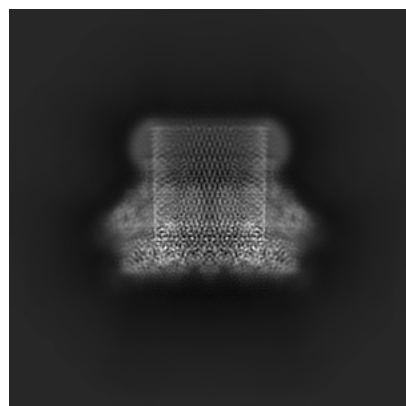
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15072. These allow visual inspection of the internal detail of the map and identification of artifacts.

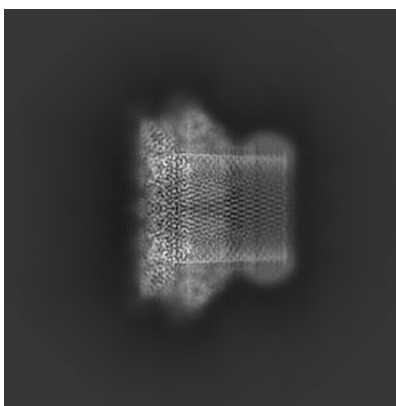
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

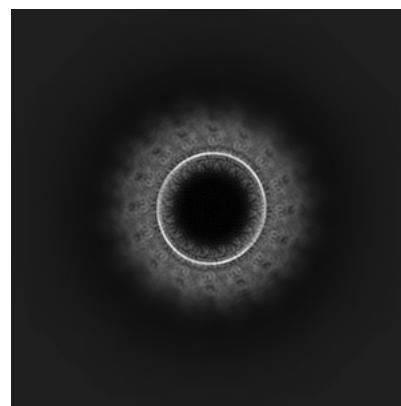
#### 6.1.1 Primary map



X

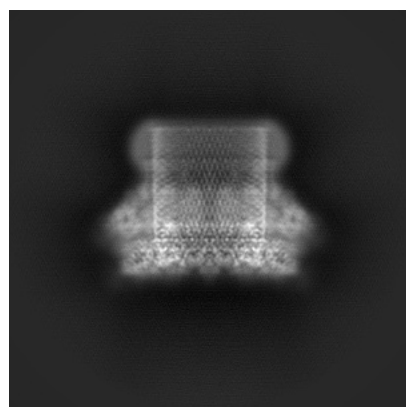


Y

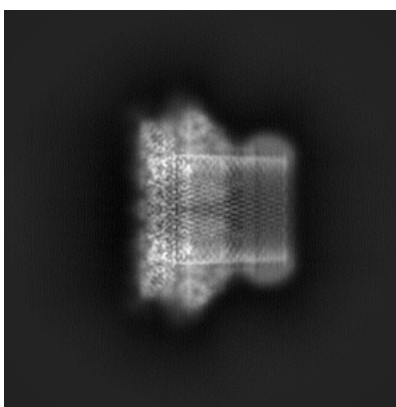


Z

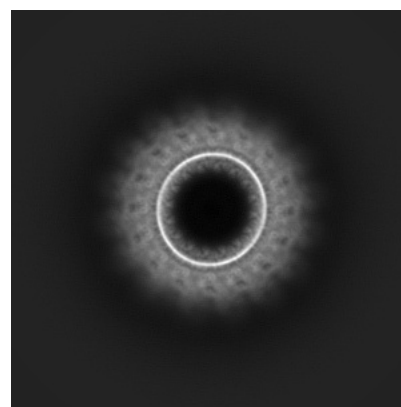
#### 6.1.2 Raw map



X



Y



Z

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

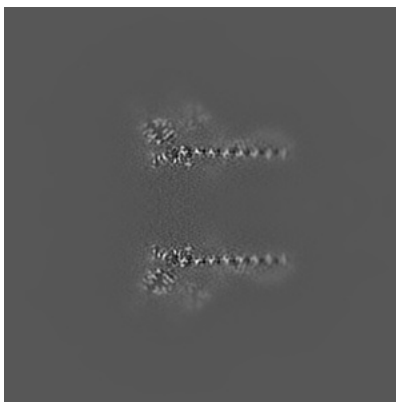


## 6.2 Central slices [i](#)

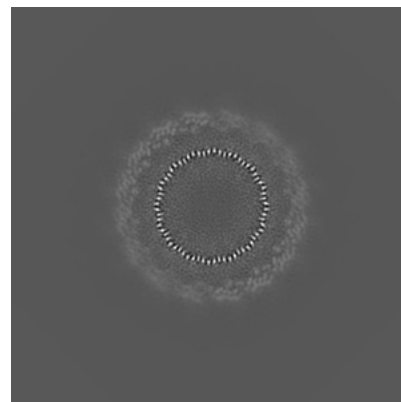
### 6.2.1 Primary map



X Index: 180

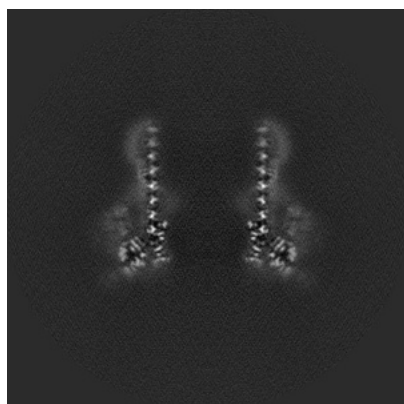


Y Index: 180

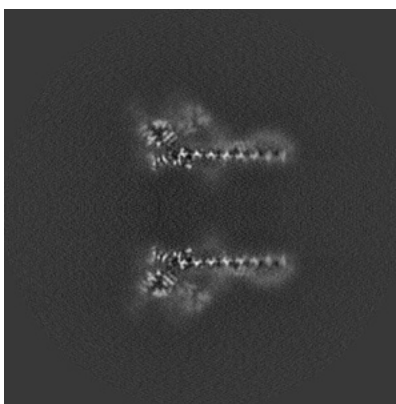


Z Index: 180

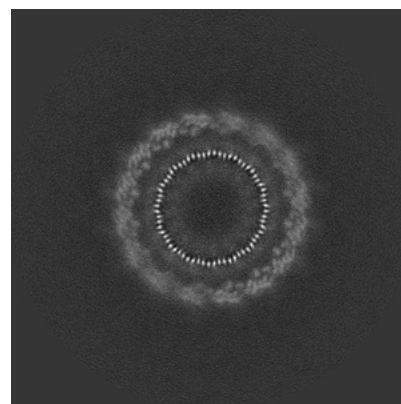
### 6.2.2 Raw map



X Index: 180



Y Index: 180



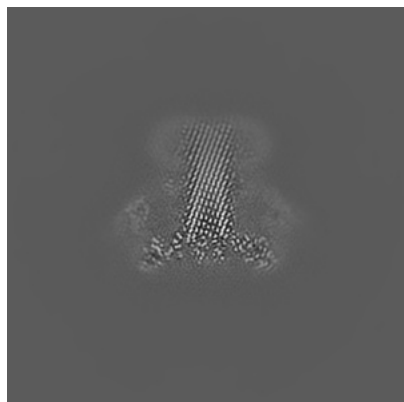
Z Index: 180

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

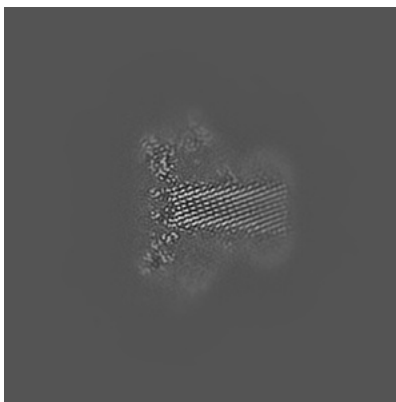


## 6.3 Largest variance slices [i](#)

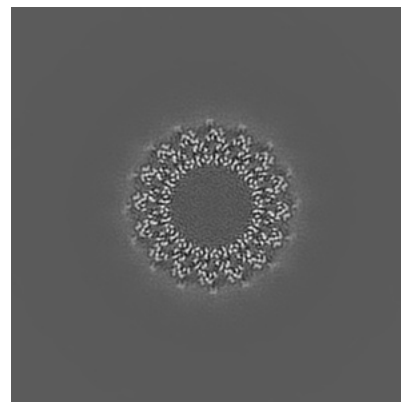
### 6.3.1 Primary map



X Index: 227

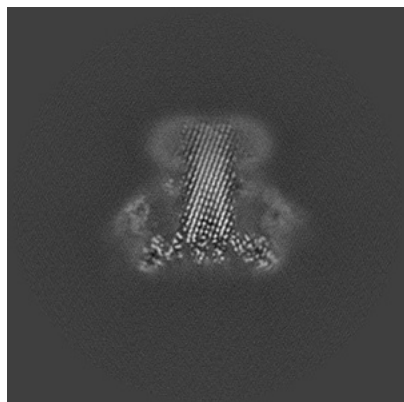


Y Index: 132

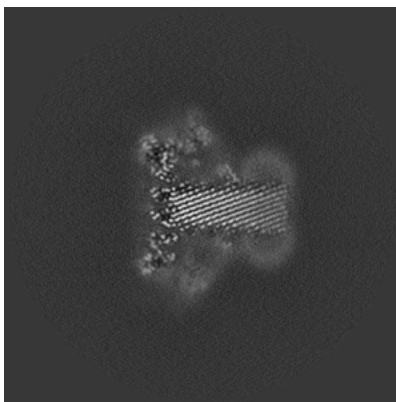


Z Index: 144

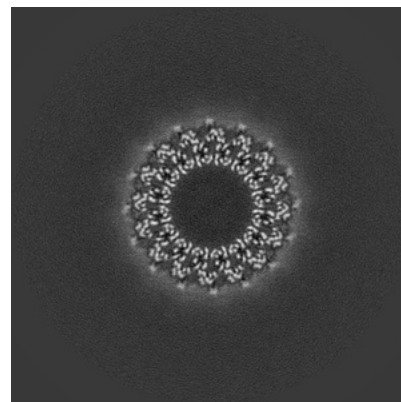
### 6.3.2 Raw map



X Index: 227



Y Index: 131



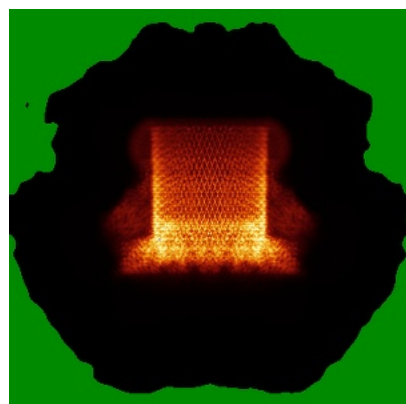
Z Index: 144

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

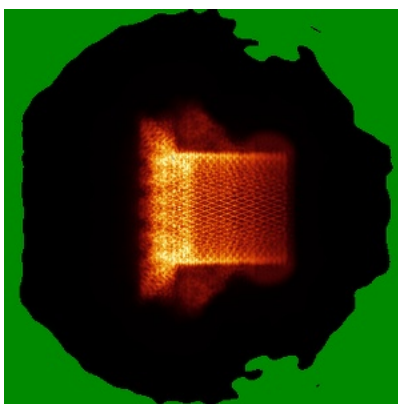


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

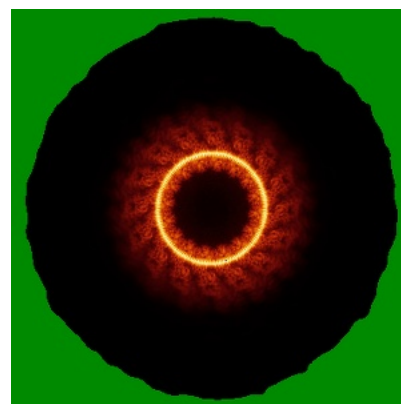
### 6.4.1 Primary map



X

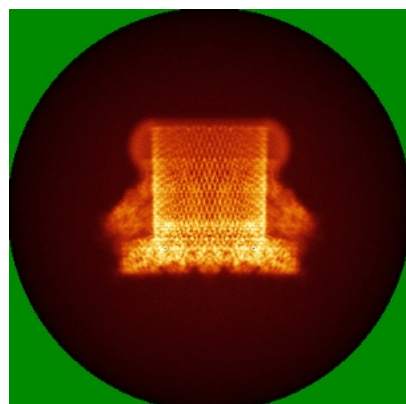


Y

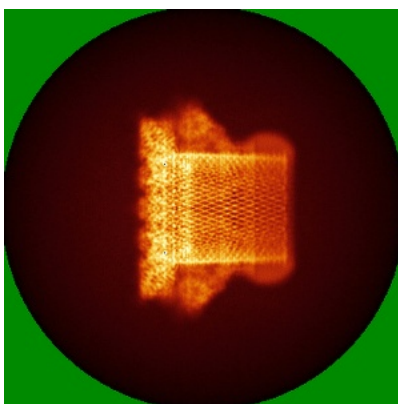


Z

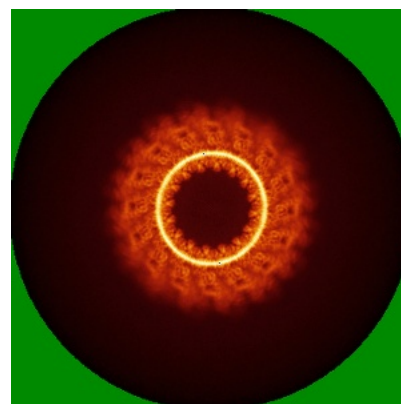
### 6.4.2 Raw map



X



Y



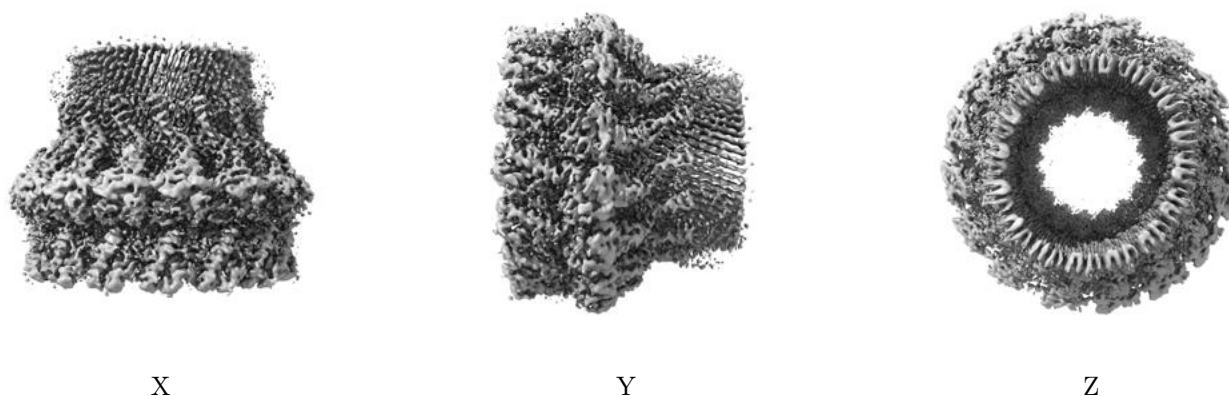
Z

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.



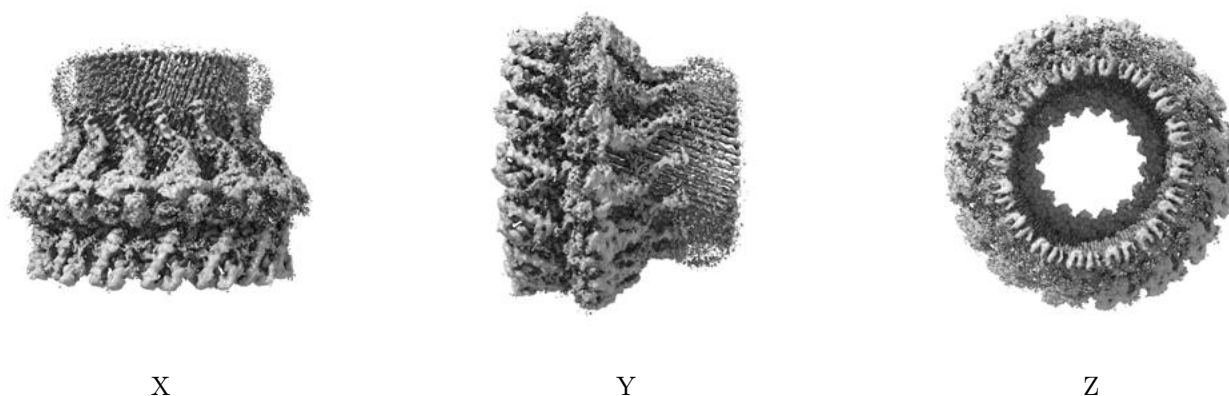
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0225. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.



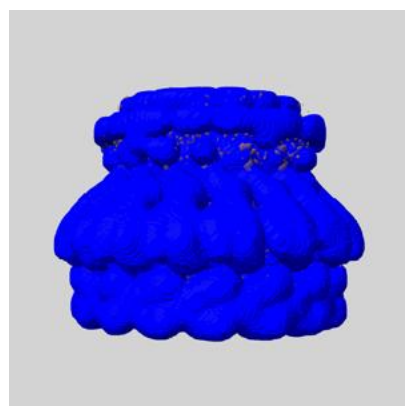
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

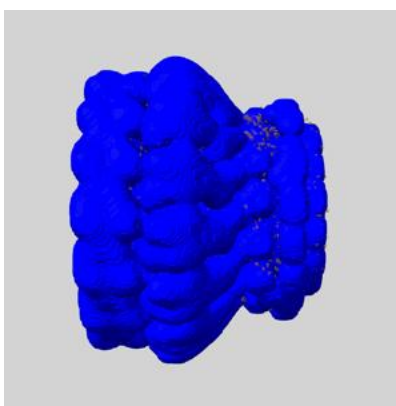
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

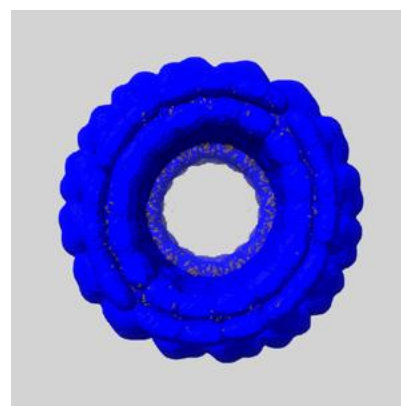
### 6.6.1 emd\_15072\_msk\_1.map [i](#)



X



Y



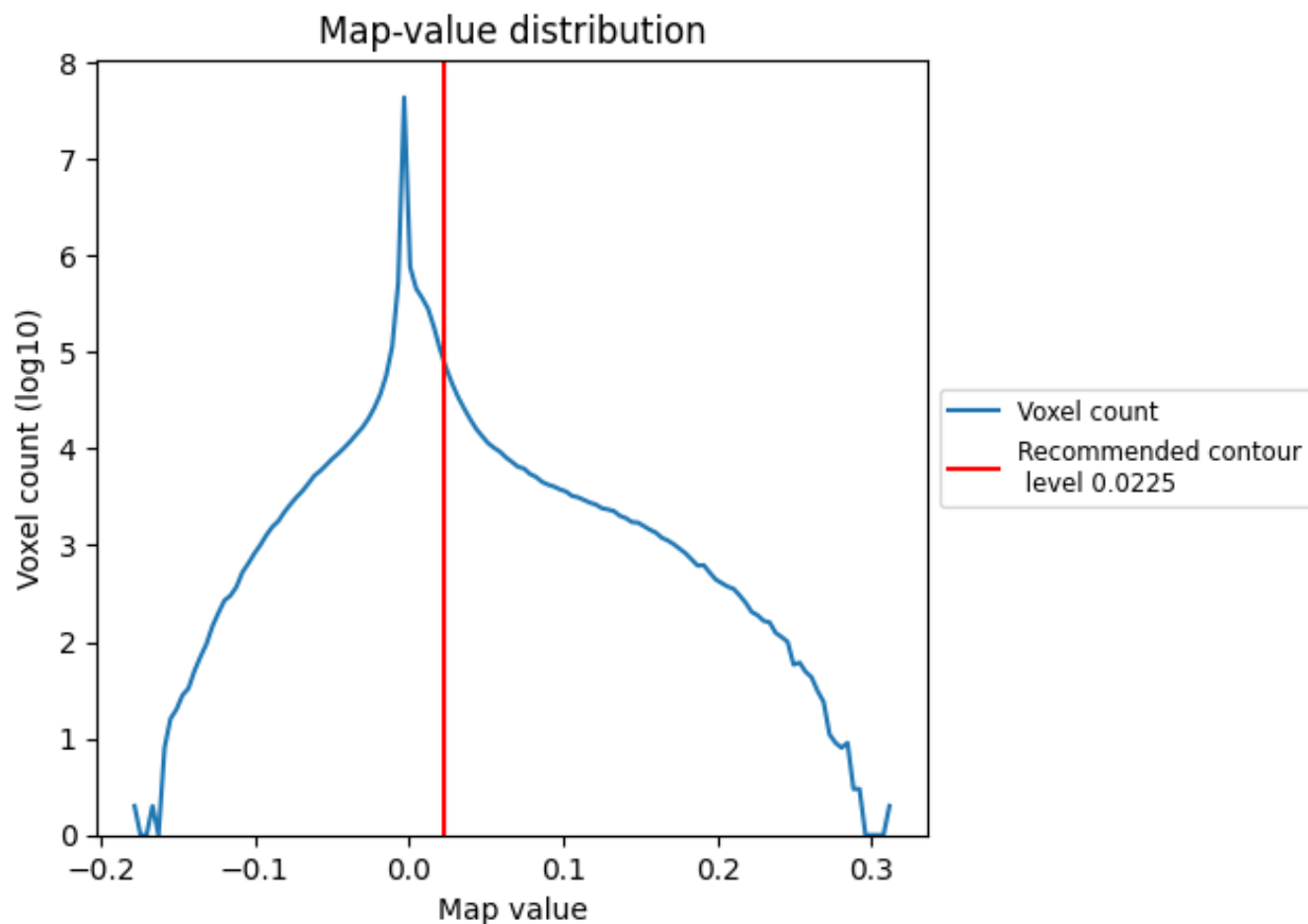
Z



## 7 Map analysis [i](#)

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

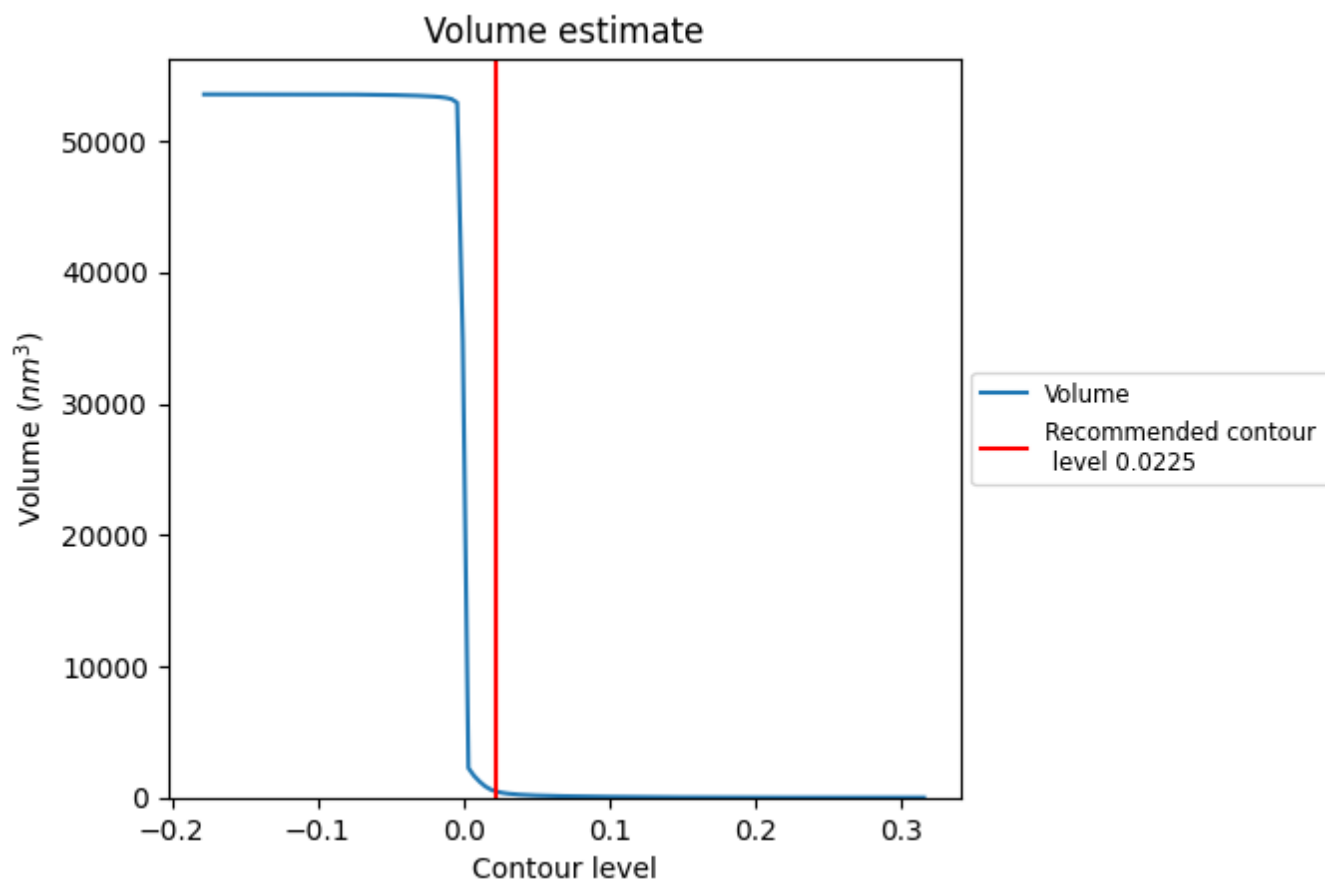
### 7.1 Map-value distribution [i](#)



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](#)

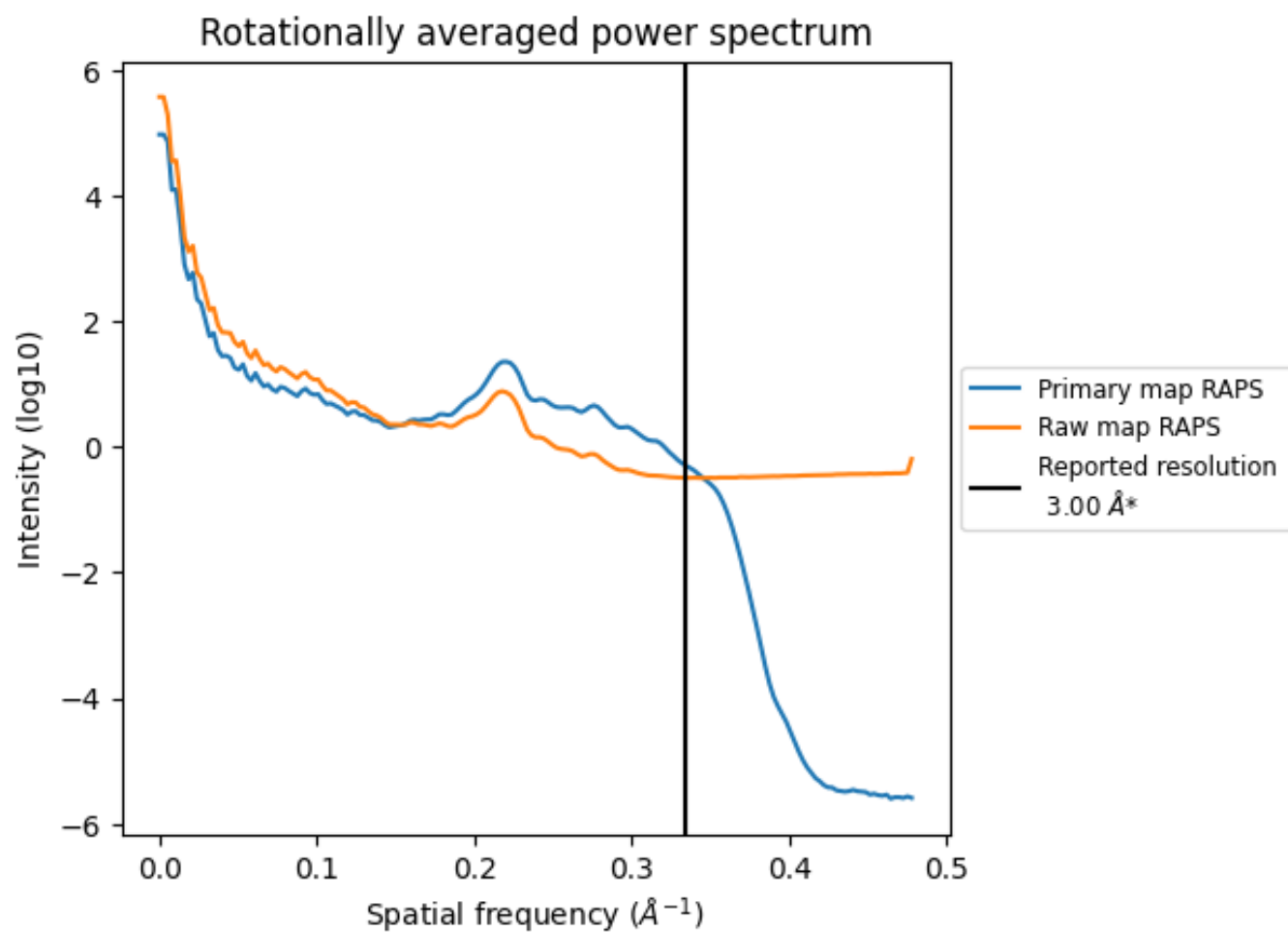


The volume at the recommended contour level is 461  $\text{nm}^3$ ; this corresponds to an approximate mass of 417 kDa.

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 ⓘ



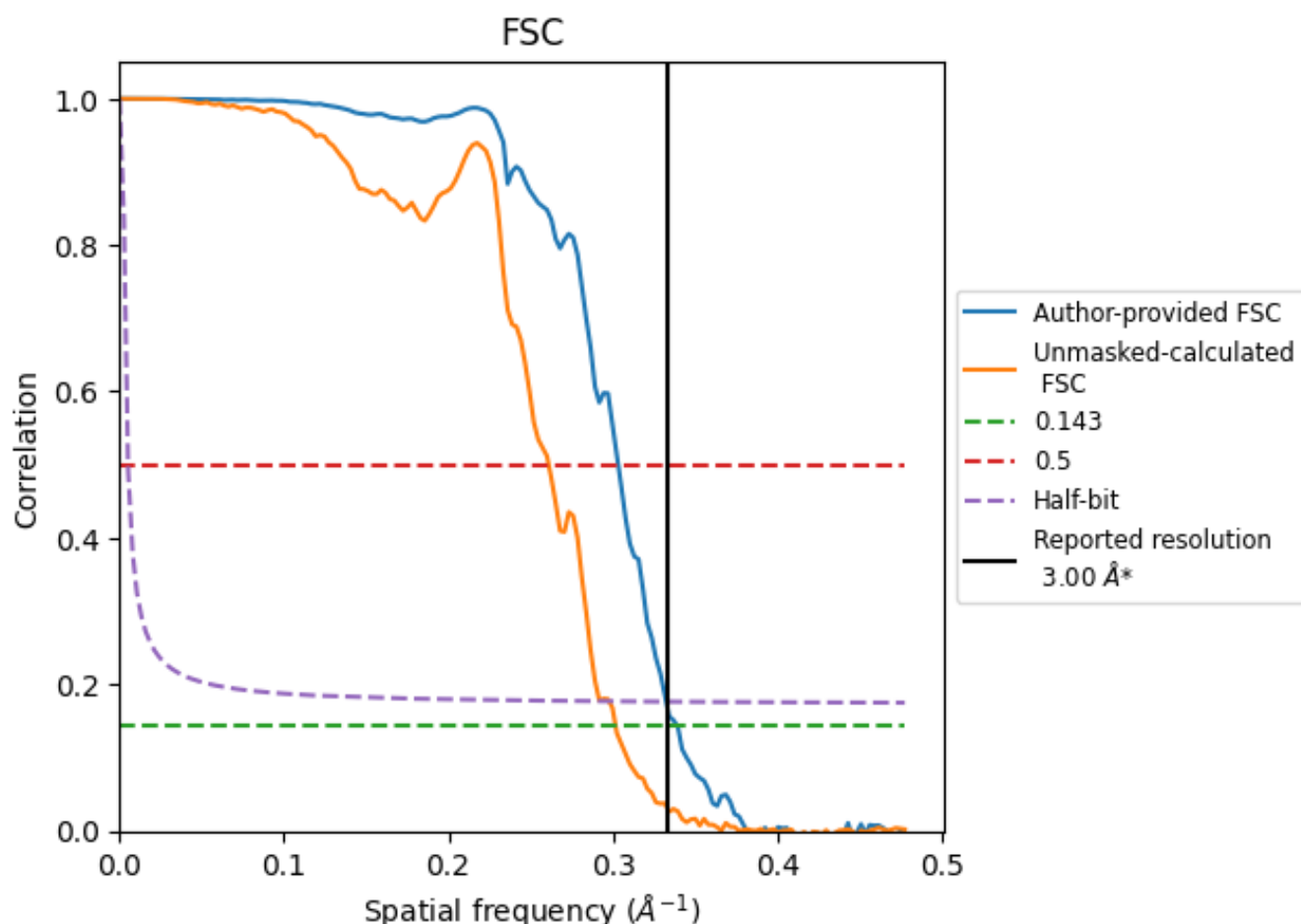
\*Reported resolution corresponds to spatial frequency of 0.333 Å<sup>-1</sup>



## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.333 Å<sup>-1</sup>



## 8.2 Resolution estimates [i](#)

| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 3.00                               | -    | -        |
| Author-provided FSC curve | 2.95                               | 3.30 | 3.01     |
| Unmasked-calculated*      | 3.31                               | 3.83 | 3.36     |

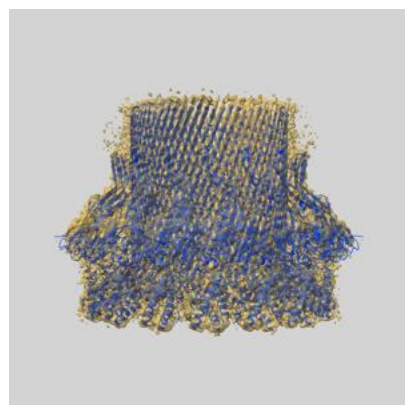
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.31 differs from the reported value 3.0 by more than 10 %



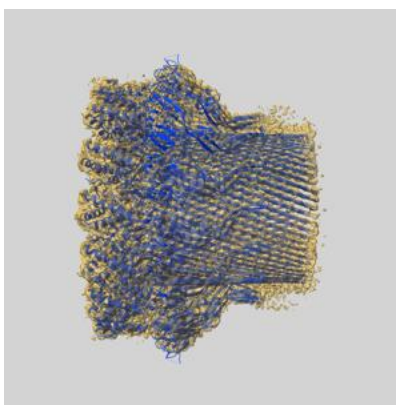
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-15072 and PDB model 8A1D. Per-residue inclusion information can be found in section [3](#) on page [14](#).

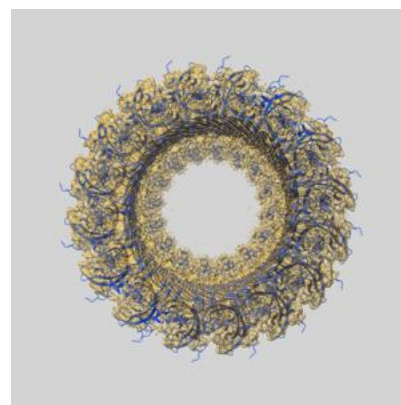
### 9.1 Map-model overlay [i](#)



X



Y

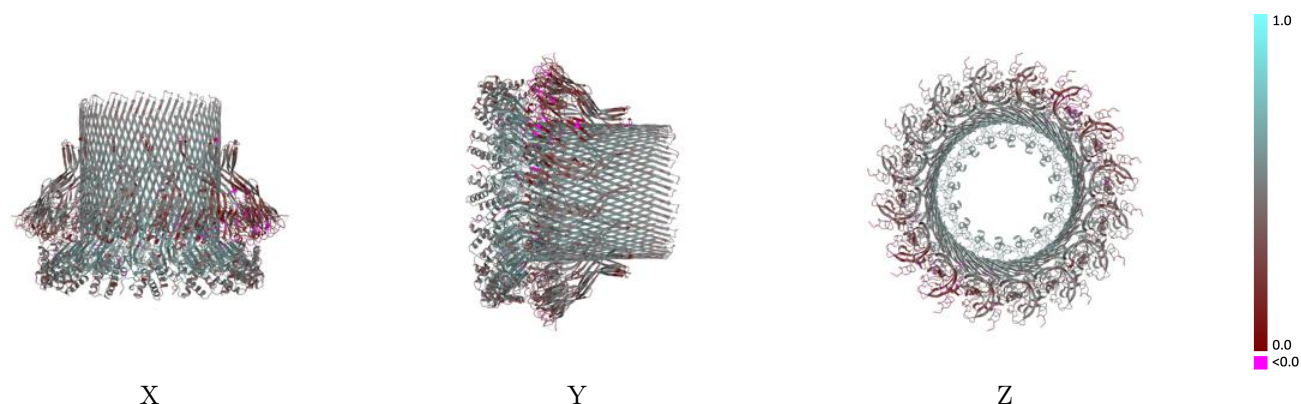


Z

The images above show the 3D surface view of the map at the recommended contour level 0.0225 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.

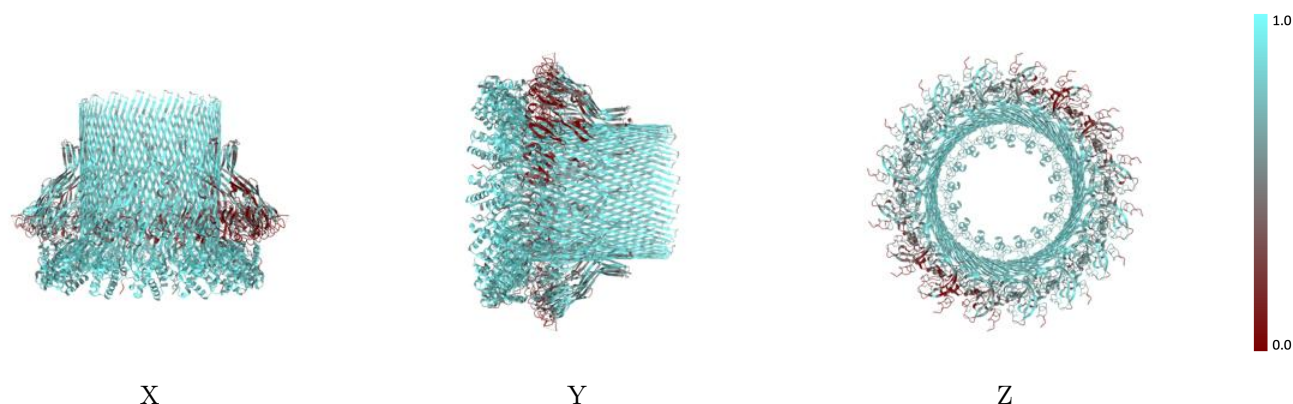


## 9.2 Q-score mapped to coordinate model [i](#)



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.

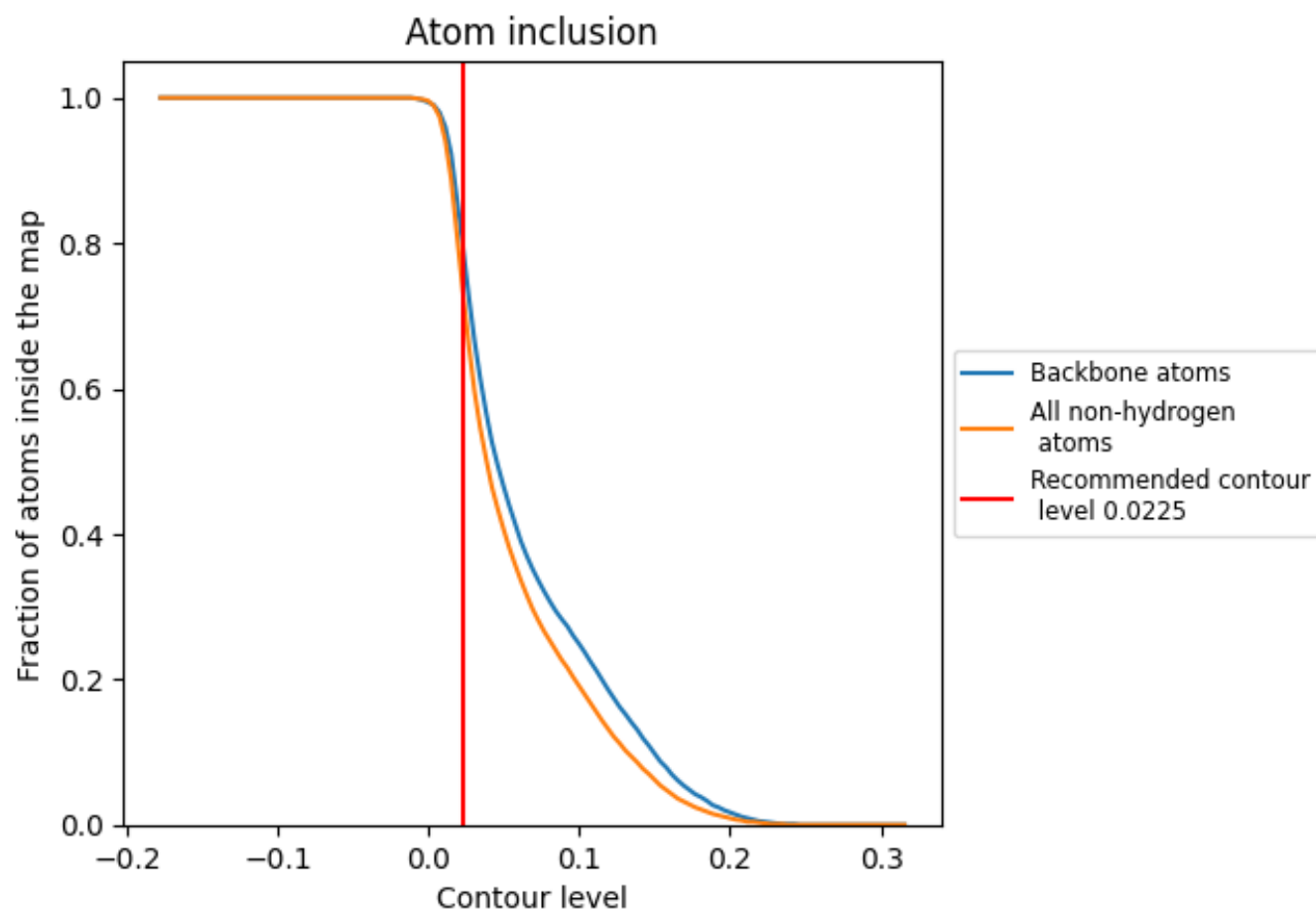
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.0225).



## 9.4 Atom inclusion [i](#)





































At the recommended contour level, 80% of all backbone atoms, 74% 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 (0.0225) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion   | Q-score  |
|-------|--|--|
| All   |  0.7380   |  0.4580   |
| A     |  0.8040   |  0.4940   |
| B     |  0.7970   |  0.4880   |
| C     |  0.7700   |  0.4740   |
| D     |  0.7350   |  0.4500   |
| E     |  0.6780   |  0.4220   |
| F     |  0.6350   |  0.4020   |
| G     |  0.6980   |  0.4480   |
| H     |  0.7840   |  0.4820   |
| I     |  0.8040   |  0.4930   |
| J     |  0.7970   |  0.4860   |
| K     |  0.7700   |  0.4740   |
| L     |  0.7340   |  0.4510   |
| M     |  0.6780   |  0.4260   |
| N     |  0.6360  |  0.4050  |
| O     |  0.6980 |  0.4490 |
| P     |  0.7860 |  0.4840 |

