



## Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 09:15 PM UTC

PDB ID : 9JEF / pdb\_00009jef  
EMDB ID : EMD-61415  
Title : Cryo-EM structure of human TRPV3 in complex with linalool determined in MSP2N2 nanodisc  
Authors : Lu, X.; Yao, J.  
Deposited on : 2024-09-03  
Resolution : 3.62 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.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

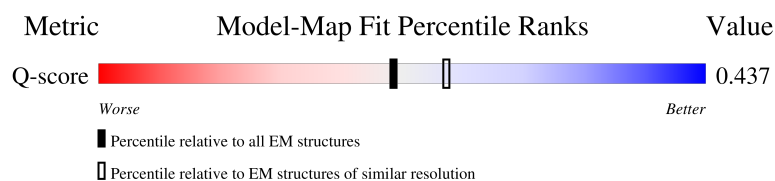
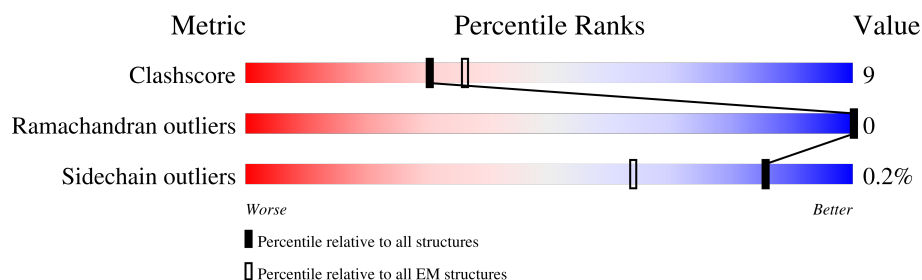
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.62 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 11773 ( 3.12 - 4.12 )                                    |

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     | 799    | <br>60% 15% 25%  |
| 1   | B     | 799    | <br>61% 15% 25%  |
| 1   | C     | 799    | <br>60% 15% 25%  |
| 1   | D     | 799    | <br>60% 15% 25%  |

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 20380 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 Transient receptor potential cation channel subfamily V member 3.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | A     | 601      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4885  | 3183 | 804 | 867 | 31 |         |       |
| 1   | B     | 601      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4885  | 3183 | 804 | 867 | 31 |         |       |
| 1   | C     | 601      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4885  | 3183 | 804 | 867 | 31 |         |       |
| 1   | D     | 601      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4885  | 3183 | 804 | 867 | 31 |         |       |

There are 40 discrepancies between the modelled and reference sequences:

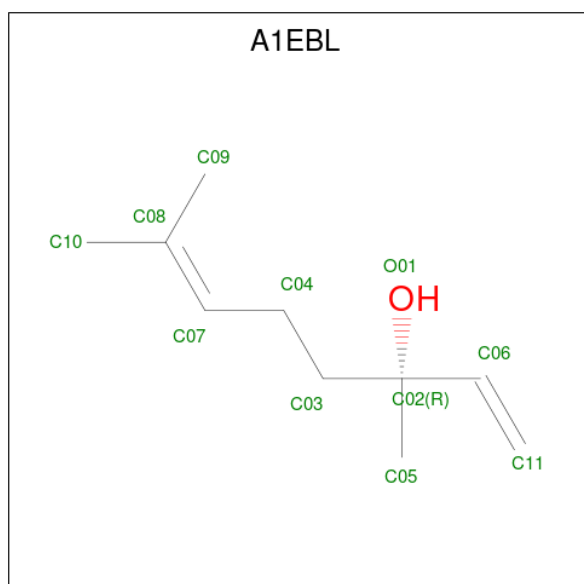
| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 25      | VAL      | ILE    | variant        | UNP Q8NET8 |
| A     | 791     | SER      | -      | expression tag | UNP Q8NET8 |
| A     | 792     | ASN      | -      | expression tag | UNP Q8NET8 |
| A     | 793     | SER      | -      | expression tag | UNP Q8NET8 |
| A     | 794     | LEU      | -      | expression tag | UNP Q8NET8 |
| A     | 795     | GLU      | -      | expression tag | UNP Q8NET8 |
| A     | 796     | VAL      | -      | expression tag | UNP Q8NET8 |
| A     | 797     | LEU      | -      | expression tag | UNP Q8NET8 |
| A     | 798     | PHE      | -      | expression tag | UNP Q8NET8 |
| A     | 799     | GLN      | -      | expression tag | UNP Q8NET8 |
| B     | 25      | VAL      | ILE    | variant        | UNP Q8NET8 |
| B     | 791     | SER      | -      | expression tag | UNP Q8NET8 |
| B     | 792     | ASN      | -      | expression tag | UNP Q8NET8 |
| B     | 793     | SER      | -      | expression tag | UNP Q8NET8 |
| B     | 794     | LEU      | -      | expression tag | UNP Q8NET8 |
| B     | 795     | GLU      | -      | expression tag | UNP Q8NET8 |
| B     | 796     | VAL      | -      | expression tag | UNP Q8NET8 |
| B     | 797     | LEU      | -      | expression tag | UNP Q8NET8 |
| B     | 798     | PHE      | -      | expression tag | UNP Q8NET8 |
| B     | 799     | GLN      | -      | expression tag | UNP Q8NET8 |
| C     | 25      | VAL      | ILE    | variant        | UNP Q8NET8 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| C     | 791     | SER      | -      | expression tag | UNP Q8NET8 |
| C     | 792     | ASN      | -      | expression tag | UNP Q8NET8 |
| C     | 793     | SER      | -      | expression tag | UNP Q8NET8 |
| C     | 794     | LEU      | -      | expression tag | UNP Q8NET8 |
| C     | 795     | GLU      | -      | expression tag | UNP Q8NET8 |
| C     | 796     | VAL      | -      | expression tag | UNP Q8NET8 |
| C     | 797     | LEU      | -      | expression tag | UNP Q8NET8 |
| C     | 798     | PHE      | -      | expression tag | UNP Q8NET8 |
| C     | 799     | GLN      | -      | expression tag | UNP Q8NET8 |
| D     | 25      | VAL      | ILE    | variant        | UNP Q8NET8 |
| D     | 791     | SER      | -      | expression tag | UNP Q8NET8 |
| D     | 792     | ASN      | -      | expression tag | UNP Q8NET8 |
| D     | 793     | SER      | -      | expression tag | UNP Q8NET8 |
| D     | 794     | LEU      | -      | expression tag | UNP Q8NET8 |
| D     | 795     | GLU      | -      | expression tag | UNP Q8NET8 |
| D     | 796     | VAL      | -      | expression tag | UNP Q8NET8 |
| D     | 797     | LEU      | -      | expression tag | UNP Q8NET8 |
| D     | 798     | PHE      | -      | expression tag | UNP Q8NET8 |
| D     | 799     | GLN      | -      | expression tag | UNP Q8NET8 |

- Molecule 2 is (3 {R})-3,7-dimethylocta-1,6-dien-3-ol (CCD ID: A1EBL) (formula: C<sub>10</sub>H<sub>18</sub>O) (labeled as "Ligand of Interest" by depositor).



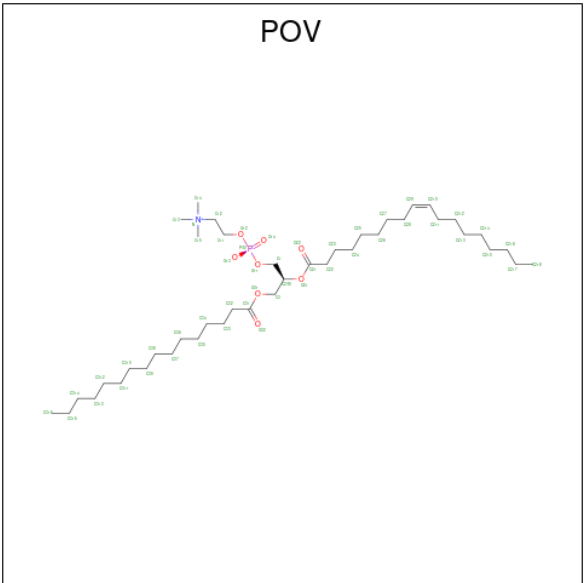
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 2   | A     | 1        | Total | C  | O | 0       |
|     |       |          | 11    | 10 | 1 |         |

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| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 2   | A     | 1        | Total | C  | O | 0       |
|     |       |          | 11    | 10 | 1 |         |
| 2   | B     | 1        | Total | C  | O | 0       |
|     |       |          | 11    | 10 | 1 |         |
| 2   | C     | 1        | Total | C  | O | 0       |
|     |       |          | 11    | 10 | 1 |         |

- Molecule 3 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylamm onio)ethyl phosphate (CCD ID: POV) (formula: C<sub>42</sub>H<sub>82</sub>NO<sub>8</sub>P).



| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 3   | A     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 44    | 34 | 1 | 8 | 1 |         |
| 3   | A     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 33    | 23 | 1 | 8 | 1 |         |
| 3   | A     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 38    | 28 | 1 | 8 | 1 |         |
| 3   | A     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 45    | 35 | 1 | 8 | 1 |         |
| 3   | A     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 39    | 29 | 1 | 8 | 1 |         |
| 3   | B     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 44    | 34 | 1 | 8 | 1 |         |
| 3   | B     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 33    | 23 | 1 | 8 | 1 |         |
| 3   | B     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 38    | 28 | 1 | 8 | 1 |         |

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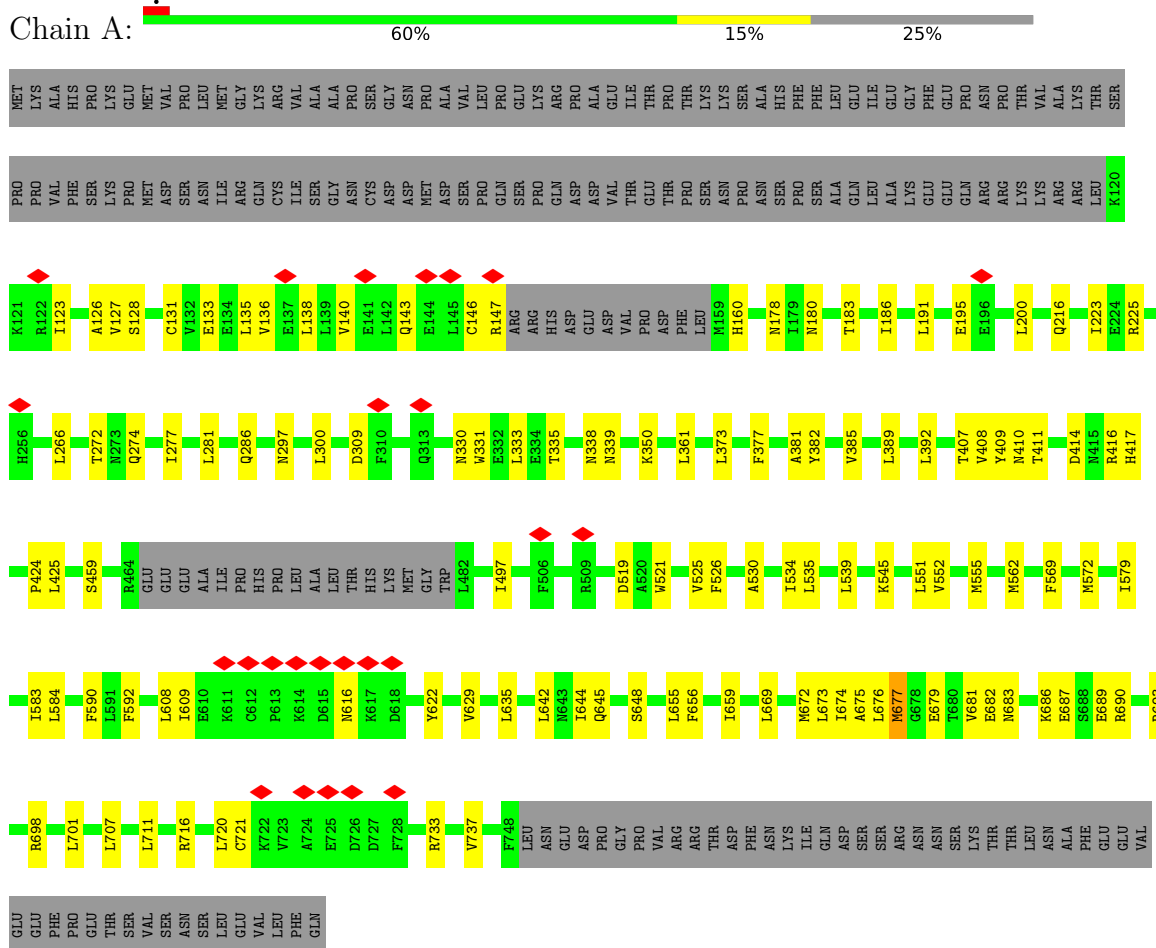
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| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 3   | B     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 45    | 35 | 1 | 8 | 1 |         |
| 3   | B     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 39    | 29 | 1 | 8 | 1 |         |
| 3   | C     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 44    | 34 | 1 | 8 | 1 |         |
| 3   | C     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 33    | 23 | 1 | 8 | 1 |         |
| 3   | C     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 38    | 28 | 1 | 8 | 1 |         |
| 3   | C     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 45    | 35 | 1 | 8 | 1 |         |
| 3   | C     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 39    | 29 | 1 | 8 | 1 |         |
| 3   | C     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 44    | 34 | 1 | 8 | 1 |         |
| 3   | D     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 33    | 23 | 1 | 8 | 1 |         |
| 3   | D     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 38    | 28 | 1 | 8 | 1 |         |
| 3   | D     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 45    | 35 | 1 | 8 | 1 |         |
| 3   | D     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 39    | 29 | 1 | 8 | 1 |         |

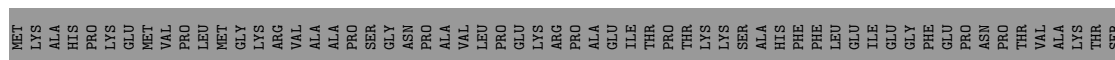
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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: Transient receptor potential cation channel subfamily V member 3



- Molecule 1: Transient receptor potential cation channel subfamily V member 3







ALA  
PHE  
GLU  
GLU  
VAL  
GLU  
GLU  
PHE  
PRO  
THR  
SER  
VAL  
SER  
ASN  
SER  
GLU  
GLU  
VAL  
LEU  
PHE  
GLN

- Molecule 1: Transient receptor potential cation channel subfamily V member 3

Chain D:



MET  
LYS  
ALA  
HIS  
PRO  
LYS  
GLU  
MET  
VAL  
SER  
PRO  
ASN  
MET  
GLY  
LYS  
ARG  
VAL  
ALA  
ALA  
PRO  
SER  
GLY  
ASN  
MET  
PRO  
ALA  
VAL  
LEU  
PRO  
GLN  
GLU  
LYS  
ARG  
PRO  
ALA  
ALA  
GLU  
ILE  
THR  
PRO  
THR  
LYS  
LYS  
SER  
PRO  
ALA  
HIS  
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PHE  
PHE  
LEU  
GLU  
ILE  
LEU  
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PRO  
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PRO  
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ASP  
SER  
ASN  
TLE  
ARG  
GLN  
CYS  
TLE  
SER  
GLY  
ASN  
CYS  
ASP  
ASP  
MET  
ASP  
SER  
PRO  
GLN  
SER  
GLU  
PRO  
GLN  
ASP  
ASP  
VAL  
ASP  
THR  
GLU  
THR  
PRO  
SER  
ASN  
PRO  
ASN  
SER  
PRO  
SER  
ALA  
GLN  
ALA  
LYS  
GLU  
GLU  
GLN  
ARG  
ARG  
LYS  
ARG  
ARG  
K120

K121  
R122  
I123  
A126  
V127  
S128  
C131  
V132  
E133  
E134  
L135  
V136  
E137  
L138  
E141  
E144  
L145  
C146  
R147  
ARG  
HIS  
ASP  
GLU  
ASP  
VAL  
PRO  
ASP  
PHE  
LEU  
M159  
H160  
M173  
L176  
M178  
M179  
M180  
T183  
I186  
L191  
E195  
E196  
L200  
Q216  
I223  
E224

R225  
R256  
L266  
T272  
Q274  
L277  
L281  
Q286  
N297  
L300  
D309  
F310  
Q313  
N330  
W331  
F332  
L333  
E334  
T335  
N338  
N339  
K350  
L361  
L373  
F377  
A381  
Y382  
V385  
L389  
L392  
T407  
V408  
Y409  
M410  
T411  
D414  
R415

R416  
H417  
P424  
L425  
S459  
R464  
GLU  
GLU  
ALA  
ILE  
PRO  
HIS  
PRO  
LEU  
ALA  
LEU  
THR  
HIS  
LYS  
MET  
GLY  
TRP  
L492  
L497  
F506  
R509  
D519  
A520  
W521  
V525  
F526  
A530  
I534  
L535  
L539  
K545  
L551  
V552  
M555  
M562  
F569  
M572

I579  
I583  
L584  
L588  
R589  
F590  
L591  
F592  
L608  
I609  
E610  
K611  
C612  
P613  
K614  
D615  
M616  
K617  
D618  
Y622  
V629  
L635  
L642  
I644  
Q645  
S648  
K649  
Y650  
L655  
T659  
L669  
M672  
L673  
I674  
A675  
L676  
M677  
G678  
E679  
T680  
V681  
E682  
M683  
K686  
E687

S688  
E689  
R690  
R693  
R698  
L701  
M706  
L707  
L711  
R716  
L720  
C721  
K722  
V723  
A724  
E725  
D726  
D727  
F728  
R733  
V737  
F748  
LEU  
ASN  
GLU  
ASP  
PRO  
GLY  
VAL  
ARG  
THR  
ASP  
PHE  
ASN  
LYS  
ILE  
GLN  
ASP  
SER  
SER  
ARG  
ASN  
ASN  
SER  
LYS  
THR  
THR  
LEU

ASN  
ALA  
PHE  
GLU  
GLU  
VAL  
GLU  
GLU  
PHE  
PRO  
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SER  
VAL  
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SER  
LEU  
GLU  
VAL  
LEU  
PHE  
GLN

## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 169275                                  | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | TFS KRIOS                               | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 50                                      | Depositor |
| Minimum defocus (nm)                 | -1400                                   | Depositor |
| Maximum defocus (nm)                 | -2400                                   | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K3 (6k x 4k)                      | Depositor |
| Maximum map value                    | 2.340                                   | Depositor |
| Minimum map value                    | -1.341                                  | Depositor |
| Average map value                    | -0.000                                  | Depositor |
| Map value standard deviation         | 0.037                                   | Depositor |
| Recommended contour level            | 0.16                                    | Depositor |
| Map size ( $\text{\AA}$ )            | 342.40002, 342.40002, 342.40002         | wwPDB     |
| Map dimensions                       | 320, 320, 320                           | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.07, 1.07, 1.07                        | Depositor |

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: A1EBL, POV

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     | 0.14         | 0/4988      | 0.36        | 0/6742      |
| 1   | B     | 0.14         | 0/4988      | 0.36        | 0/6742      |
| 1   | C     | 0.14         | 0/4988      | 0.36        | 0/6742      |
| 1   | D     | 0.14         | 0/4988      | 0.36        | 0/6742      |
| All | All   | 0.14         | 0/19952     | 0.36        | 0/26968     |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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     | 4885  | 0        | 4964     | 99      | 0            |
| 1   | B     | 4885  | 0        | 4964     | 95      | 0            |
| 1   | C     | 4885  | 0        | 4964     | 100     | 0            |
| 1   | D     | 4885  | 0        | 4964     | 102     | 0            |
| 2   | A     | 22    | 0        | 0        | 0       | 0            |
| 2   | B     | 11    | 0        | 0        | 0       | 0            |
| 2   | C     | 11    | 0        | 0        | 0       | 0            |
| 3   | A     | 199   | 0        | 261      | 6       | 0            |
| 3   | B     | 199   | 0        | 261      | 7       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3   | C     | 243   | 0        | 321      | 8       | 0            |
| 3   | D     | 155   | 0        | 201      | 4       | 0            |
| All | All   | 20380 | 0        | 20900    | 370     | 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 9.

All (370) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:551:LEU:HD23 | 1:B:555:MET:CE   | 1.89                     | 1.03              |
| 1:A:551:LEU:HD23 | 1:A:555:MET:CE   | 1.89                     | 1.03              |
| 1:D:551:LEU:HD23 | 1:D:555:MET:CE   | 1.89                     | 1.02              |
| 1:C:551:LEU:HD23 | 1:C:555:MET:CE   | 1.89                     | 1.02              |
| 1:A:551:LEU:HD23 | 1:A:555:MET:HE2  | 1.45                     | 0.97              |
| 1:B:551:LEU:HD23 | 1:B:555:MET:HE2  | 1.45                     | 0.97              |
| 1:D:551:LEU:HD23 | 1:D:555:MET:HE2  | 1.45                     | 0.96              |
| 1:D:178:ASN:OD1  | 1:D:178:ASN:O    | 1.85                     | 0.95              |
| 1:A:178:ASN:OD1  | 1:A:178:ASN:O    | 1.85                     | 0.95              |
| 1:B:178:ASN:OD1  | 1:B:178:ASN:O    | 1.85                     | 0.94              |
| 1:C:551:LEU:HD23 | 1:C:555:MET:HE2  | 1.45                     | 0.94              |
| 1:C:178:ASN:OD1  | 1:C:178:ASN:O    | 1.85                     | 0.94              |
| 1:B:146:CYS:SG   | 1:B:160:HIS:HE1  | 1.94                     | 0.91              |
| 1:C:146:CYS:SG   | 1:C:160:HIS:HE1  | 1.94                     | 0.91              |
| 1:A:146:CYS:SG   | 1:A:160:HIS:HE1  | 1.94                     | 0.91              |
| 1:D:146:CYS:SG   | 1:D:160:HIS:HE1  | 1.94                     | 0.91              |
| 1:A:146:CYS:SG   | 1:A:160:HIS:CE1  | 2.76                     | 0.79              |
| 1:A:675:ALA:HB1  | 1:B:681:VAL:HG21 | 1.65                     | 0.79              |
| 1:D:146:CYS:SG   | 1:D:160:HIS:CE1  | 2.76                     | 0.79              |
| 1:C:146:CYS:SG   | 1:C:160:HIS:CE1  | 2.76                     | 0.78              |
| 1:B:146:CYS:SG   | 1:B:160:HIS:CE1  | 2.76                     | 0.78              |
| 1:C:675:ALA:HB1  | 1:D:681:VAL:HG21 | 1.69                     | 0.75              |
| 1:A:681:VAL:HG21 | 1:D:675:ALA:HB1  | 1.70                     | 0.72              |
| 1:B:675:ALA:HB1  | 1:C:681:VAL:HG21 | 1.71                     | 0.71              |
| 1:A:642:LEU:O    | 1:A:642:LEU:HD23 | 1.94                     | 0.68              |
| 1:B:551:LEU:CD2  | 1:B:555:MET:CE   | 2.71                     | 0.68              |
| 1:D:642:LEU:HD23 | 1:D:642:LEU:O    | 1.94                     | 0.68              |
| 1:C:642:LEU:O    | 1:C:642:LEU:HD23 | 1.94                     | 0.67              |
| 1:C:551:LEU:CD2  | 1:C:555:MET:CE   | 2.71                     | 0.67              |
| 1:A:551:LEU:CD2  | 1:A:555:MET:CE   | 2.71                     | 0.67              |
| 1:D:551:LEU:CD2  | 1:D:555:MET:CE   | 2.71                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:642:LEU:HD23 | 1:B:642:LEU:O    | 1.94                     | 0.67              |
| 1:A:655:LEU:HD11 | 3:B:801:POV:H25A | 1.77                     | 0.66              |
| 1:B:191:LEU:HD22 | 1:B:200:LEU:HD11 | 1.78                     | 0.65              |
| 1:B:519:ASP:OD2  | 1:B:698:ARG:HD2  | 1.97                     | 0.65              |
| 1:A:191:LEU:HD22 | 1:A:200:LEU:HD11 | 1.78                     | 0.65              |
| 1:A:459:SER:CB   | 1:A:555:MET:HE1  | 2.27                     | 0.65              |
| 1:C:519:ASP:OD2  | 1:C:698:ARG:HD2  | 1.97                     | 0.65              |
| 1:D:519:ASP:OD2  | 1:D:698:ARG:HD2  | 1.97                     | 0.65              |
| 1:C:191:LEU:HD22 | 1:C:200:LEU:HD11 | 1.78                     | 0.65              |
| 1:C:459:SER:CB   | 1:C:555:MET:HE1  | 2.27                     | 0.65              |
| 1:D:191:LEU:HD22 | 1:D:200:LEU:HD11 | 1.78                     | 0.65              |
| 1:D:459:SER:CB   | 1:D:555:MET:HE1  | 2.27                     | 0.65              |
| 1:B:459:SER:CB   | 1:B:555:MET:HE1  | 2.27                     | 0.64              |
| 1:A:519:ASP:OD2  | 1:A:698:ARG:HD2  | 1.97                     | 0.64              |
| 1:A:411:THR:HG1  | 1:A:698:ARG:HH22 | 1.45                     | 0.64              |
| 1:C:655:LEU:HD11 | 3:C:807:POV:H25A | 1.81                     | 0.63              |
| 1:C:672:MET:HE1  | 1:D:579:ILE:HG13 | 1.81                     | 0.62              |
| 3:A:802:POV:H25A | 1:D:655:LEU:HD11 | 1.80                     | 0.62              |
| 1:A:562:MET:HG2  | 3:A:804:POV:H210 | 1.82                     | 0.62              |
| 1:B:672:MET:HE1  | 1:C:579:ILE:HG13 | 1.82                     | 0.61              |
| 1:B:562:MET:HG2  | 3:B:803:POV:H210 | 1.82                     | 0.61              |
| 1:D:562:MET:HG2  | 3:D:802:POV:H210 | 1.82                     | 0.61              |
| 1:A:608:LEU:HG   | 1:B:552:VAL:HG11 | 1.83                     | 0.60              |
| 1:A:579:ILE:HG13 | 1:D:672:MET:HE1  | 1.83                     | 0.60              |
| 1:B:655:LEU:HD11 | 3:C:801:POV:H25A | 1.82                     | 0.60              |
| 1:A:180:ASN:O    | 1:A:183:THR:OG1  | 2.20                     | 0.60              |
| 1:B:180:ASN:O    | 1:B:183:THR:OG1  | 2.20                     | 0.60              |
| 1:B:687:GLU:OE2  | 1:B:690:ARG:NH1  | 2.35                     | 0.60              |
| 1:C:562:MET:HG2  | 3:C:803:POV:H210 | 1.82                     | 0.60              |
| 1:A:687:GLU:OE2  | 1:A:690:ARG:NH1  | 2.35                     | 0.59              |
| 1:C:180:ASN:O    | 1:C:183:THR:OG1  | 2.20                     | 0.59              |
| 1:D:180:ASN:O    | 1:D:183:THR:OG1  | 2.20                     | 0.59              |
| 1:D:644:ILE:HG13 | 1:D:645:GLN:HG2  | 1.85                     | 0.59              |
| 1:A:644:ILE:HG13 | 1:A:645:GLN:HG2  | 1.85                     | 0.59              |
| 1:D:551:LEU:CD2  | 1:D:555:MET:HE2  | 2.28                     | 0.59              |
| 1:D:687:GLU:OE2  | 1:D:690:ARG:NH1  | 2.35                     | 0.59              |
| 1:C:687:GLU:OE2  | 1:C:690:ARG:NH1  | 2.35                     | 0.59              |
| 1:B:191:LEU:HD22 | 1:B:200:LEU:CD1  | 2.33                     | 0.59              |
| 1:C:644:ILE:HG13 | 1:C:645:GLN:HG2  | 1.85                     | 0.58              |
| 1:B:644:ILE:HG13 | 1:B:645:GLN:HG2  | 1.85                     | 0.58              |
| 1:A:551:LEU:CD2  | 1:A:555:MET:HE2  | 2.28                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:191:LEU:HD22 | 1:C:200:LEU:CD1  | 2.33                     | 0.58              |
| 1:A:672:MET:HE1  | 1:B:579:ILE:HG13 | 1.86                     | 0.57              |
| 1:A:411:THR:OG1  | 1:A:698:ARG:NH2  | 2.35                     | 0.57              |
| 1:A:682:GLU:O    | 1:A:686:LYS:NZ   | 2.38                     | 0.57              |
| 1:D:682:GLU:O    | 1:D:686:LYS:NZ   | 2.38                     | 0.57              |
| 1:A:191:LEU:HD22 | 1:A:200:LEU:CD1  | 2.33                     | 0.57              |
| 1:D:191:LEU:HD22 | 1:D:200:LEU:CD1  | 2.33                     | 0.57              |
| 1:B:682:GLU:O    | 1:B:686:LYS:NZ   | 2.38                     | 0.57              |
| 1:B:551:LEU:CD2  | 1:B:555:MET:HE2  | 2.28                     | 0.56              |
| 1:D:389:LEU:HD13 | 1:D:733:ARG:HE   | 1.70                     | 0.56              |
| 1:D:689:GLU:OE2  | 1:D:693:ARG:NH2  | 2.39                     | 0.56              |
| 1:C:389:LEU:HD13 | 1:C:733:ARG:HE   | 1.70                     | 0.56              |
| 1:C:682:GLU:O    | 1:C:686:LYS:NZ   | 2.38                     | 0.56              |
| 1:C:689:GLU:OE2  | 1:C:693:ARG:NH2  | 2.39                     | 0.56              |
| 1:C:608:LEU:HG   | 1:D:552:VAL:HG11 | 1.87                     | 0.56              |
| 1:B:389:LEU:HD13 | 1:B:733:ARG:HE   | 1.70                     | 0.56              |
| 3:B:804:POV:H22A | 3:B:804:POV:H33A | 1.88                     | 0.56              |
| 3:C:804:POV:H22A | 3:C:804:POV:H33A | 1.88                     | 0.56              |
| 3:D:803:POV:H22A | 3:D:803:POV:H33A | 1.88                     | 0.56              |
| 1:A:552:VAL:HG11 | 1:D:608:LEU:HG   | 1.87                     | 0.56              |
| 1:A:389:LEU:HD13 | 1:A:733:ARG:HE   | 1.70                     | 0.55              |
| 3:A:805:POV:H22A | 3:A:805:POV:H33A | 1.88                     | 0.55              |
| 1:D:330:ASN:OD1  | 1:D:330:ASN:N    | 2.39                     | 0.55              |
| 1:A:689:GLU:OE2  | 1:A:693:ARG:NH2  | 2.39                     | 0.55              |
| 1:B:286:GLN:OE1  | 1:B:286:GLN:N    | 2.36                     | 0.55              |
| 1:B:608:LEU:HG   | 1:C:552:VAL:HG11 | 1.87                     | 0.55              |
| 1:C:127:VAL:HG12 | 1:C:186:ILE:HD11 | 1.88                     | 0.55              |
| 1:A:674:ILE:HA   | 1:A:677:MET:SD   | 2.47                     | 0.55              |
| 1:B:689:GLU:OE2  | 1:B:693:ARG:NH2  | 2.39                     | 0.55              |
| 1:D:592:PHE:HB2  | 3:D:804:POV:H36A | 1.89                     | 0.55              |
| 1:B:330:ASN:OD1  | 1:B:330:ASN:N    | 2.39                     | 0.54              |
| 1:D:389:LEU:CD1  | 1:D:733:ARG:HE   | 2.20                     | 0.54              |
| 1:B:674:ILE:HA   | 1:B:677:MET:SD   | 2.47                     | 0.54              |
| 1:C:411:THR:OG1  | 1:C:698:ARG:NH2  | 2.35                     | 0.54              |
| 1:C:592:PHE:HB2  | 3:C:805:POV:H36A | 1.89                     | 0.54              |
| 1:C:674:ILE:HA   | 1:C:677:MET:SD   | 2.47                     | 0.54              |
| 1:A:389:LEU:CD1  | 1:A:733:ARG:HE   | 2.20                     | 0.54              |
| 1:D:127:VAL:HG12 | 1:D:186:ILE:HD11 | 1.88                     | 0.54              |
| 1:D:411:THR:OG1  | 1:D:698:ARG:NH2  | 2.35                     | 0.54              |
| 1:C:389:LEU:CD1  | 1:C:733:ARG:HE   | 2.20                     | 0.54              |
| 1:D:674:ILE:HA   | 1:D:677:MET:SD   | 2.47                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:389:LEU:CD1  | 1:B:733:ARG:HE   | 2.20                     | 0.54              |
| 1:A:592:PHE:HB2  | 3:A:806:POV:H36A | 1.89                     | 0.54              |
| 1:B:127:VAL:HG12 | 1:B:186:ILE:HD11 | 1.88                     | 0.54              |
| 1:B:592:PHE:HB2  | 3:B:805:POV:H36A | 1.89                     | 0.54              |
| 1:A:331:TRP:O    | 1:A:335:THR:OG1  | 2.22                     | 0.53              |
| 1:D:223:ILE:O    | 1:D:274:GLN:NE2  | 2.35                     | 0.53              |
| 1:A:127:VAL:HG12 | 1:A:186:ILE:HD11 | 1.88                     | 0.53              |
| 1:B:411:THR:OG1  | 1:B:698:ARG:NH2  | 2.35                     | 0.53              |
| 1:C:331:TRP:O    | 1:C:335:THR:OG1  | 2.22                     | 0.53              |
| 1:C:223:ILE:O    | 1:C:274:GLN:NE2  | 2.35                     | 0.52              |
| 1:C:551:LEU:CD2  | 1:C:555:MET:HE2  | 2.28                     | 0.52              |
| 1:A:223:ILE:O    | 1:A:274:GLN:NE2  | 2.35                     | 0.51              |
| 1:B:552:VAL:HA   | 1:B:555:MET:HE3  | 1.92                     | 0.51              |
| 1:C:552:VAL:HA   | 1:C:555:MET:HE3  | 1.92                     | 0.51              |
| 1:C:459:SER:HB3  | 1:C:555:MET:HE1  | 1.92                     | 0.51              |
| 1:A:552:VAL:HA   | 1:A:555:MET:HE3  | 1.92                     | 0.51              |
| 1:B:459:SER:HB3  | 1:B:555:MET:HE1  | 1.93                     | 0.51              |
| 1:B:331:TRP:O    | 1:B:335:THR:OG1  | 2.22                     | 0.51              |
| 1:B:300:LEU:HD11 | 1:B:333:LEU:HG   | 1.92                     | 0.51              |
| 1:A:459:SER:HB3  | 1:A:555:MET:HE1  | 1.92                     | 0.51              |
| 1:B:679:GLU:O    | 1:B:683:ASN:ND2  | 2.44                     | 0.51              |
| 1:D:552:VAL:HA   | 1:D:555:MET:HE3  | 1.92                     | 0.51              |
| 1:A:679:GLU:O    | 1:A:683:ASN:ND2  | 2.44                     | 0.51              |
| 1:A:300:LEU:HD11 | 1:A:333:LEU:HG   | 1.92                     | 0.51              |
| 1:D:679:GLU:O    | 1:D:683:ASN:ND2  | 2.44                     | 0.51              |
| 1:B:223:ILE:O    | 1:B:274:GLN:NE2  | 2.35                     | 0.51              |
| 1:C:679:GLU:O    | 1:C:683:ASN:ND2  | 2.44                     | 0.51              |
| 1:C:274:GLN:HE21 | 1:C:277:ILE:HD13 | 1.77                     | 0.50              |
| 1:C:286:GLN:OE1  | 1:C:286:GLN:N    | 2.36                     | 0.50              |
| 1:D:146:CYS:SG   | 1:D:147:ARG:NH2  | 2.84                     | 0.50              |
| 1:D:300:LEU:HD11 | 1:D:333:LEU:HG   | 1.92                     | 0.50              |
| 1:D:707:LEU:HD22 | 1:D:711:LEU:HD23 | 1.93                     | 0.50              |
| 1:C:146:CYS:SG   | 1:C:147:ARG:NH2  | 2.84                     | 0.50              |
| 1:D:361:LEU:HB3  | 1:D:424:PRO:HG2  | 1.93                     | 0.50              |
| 1:D:459:SER:HB3  | 1:D:555:MET:HE1  | 1.93                     | 0.50              |
| 1:A:146:CYS:SG   | 1:A:147:ARG:NH2  | 2.84                     | 0.50              |
| 1:B:707:LEU:HD22 | 1:B:711:LEU:HD23 | 1.93                     | 0.50              |
| 1:A:361:LEU:HB3  | 1:A:424:PRO:HG2  | 1.93                     | 0.50              |
| 1:D:274:GLN:HE21 | 1:D:277:ILE:HD13 | 1.76                     | 0.50              |
| 1:A:274:GLN:HE21 | 1:A:277:ILE:HD13 | 1.76                     | 0.50              |
| 1:B:146:CYS:SG   | 1:B:147:ARG:NH2  | 2.84                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:361:LEU:HB3  | 1:B:424:PRO:HG2  | 1.93                     | 0.50              |
| 1:C:707:LEU:HD22 | 1:C:711:LEU:HD23 | 1.93                     | 0.49              |
| 1:A:414:ASP:HA   | 1:A:690:ARG:HH21 | 1.77                     | 0.49              |
| 1:B:195:GLU:HB3  | 1:B:200:LEU:HD22 | 1.94                     | 0.49              |
| 1:C:300:LEU:HD11 | 1:C:333:LEU:HG   | 1.92                     | 0.49              |
| 1:C:361:LEU:HB3  | 1:C:424:PRO:HG2  | 1.93                     | 0.49              |
| 1:D:195:GLU:HB3  | 1:D:200:LEU:HD22 | 1.94                     | 0.49              |
| 1:D:331:TRP:O    | 1:D:335:THR:OG1  | 2.22                     | 0.49              |
| 1:B:414:ASP:HA   | 1:B:690:ARG:HH21 | 1.77                     | 0.49              |
| 1:A:707:LEU:HD22 | 1:A:711:LEU:HD23 | 1.93                     | 0.49              |
| 1:B:225:ARG:NH2  | 1:C:381:ALA:O    | 2.43                     | 0.49              |
| 1:A:195:GLU:HB3  | 1:A:200:LEU:HD22 | 1.94                     | 0.49              |
| 1:B:274:GLN:HE21 | 1:B:277:ILE:HD13 | 1.76                     | 0.49              |
| 1:C:414:ASP:HA   | 1:C:690:ARG:HH21 | 1.78                     | 0.49              |
| 1:C:330:ASN:OD1  | 1:C:330:ASN:N    | 2.39                     | 0.49              |
| 1:D:286:GLN:OE1  | 1:D:286:GLN:N    | 2.36                     | 0.49              |
| 1:C:195:GLU:HB3  | 1:C:200:LEU:HD22 | 1.94                     | 0.48              |
| 1:D:414:ASP:HA   | 1:D:690:ARG:HH21 | 1.77                     | 0.48              |
| 1:B:338:ASN:OD1  | 1:B:339:ASN:N    | 2.47                     | 0.48              |
| 1:A:272:THR:OG1  | 1:A:274:GLN:OE1  | 2.26                     | 0.48              |
| 1:D:551:LEU:HD23 | 1:D:555:MET:HE1  | 1.91                     | 0.48              |
| 1:B:679:GLU:O    | 1:B:682:GLU:HG3  | 2.14                     | 0.48              |
| 1:C:408:VAL:HG11 | 1:C:701:LEU:HG   | 1.96                     | 0.48              |
| 1:C:679:GLU:O    | 1:C:682:GLU:HG3  | 2.14                     | 0.48              |
| 1:A:338:ASN:OD1  | 1:A:339:ASN:N    | 2.47                     | 0.48              |
| 1:A:408:VAL:HG11 | 1:A:701:LEU:HG   | 1.96                     | 0.48              |
| 1:B:272:THR:OG1  | 1:B:274:GLN:OE1  | 2.27                     | 0.48              |
| 1:C:569:PHE:HE2  | 3:C:803:POV:H27  | 1.79                     | 0.48              |
| 1:D:408:VAL:HG11 | 1:D:701:LEU:HG   | 1.96                     | 0.48              |
| 1:A:569:PHE:HE2  | 3:A:804:POV:H27  | 1.79                     | 0.47              |
| 1:A:286:GLN:OE1  | 1:A:286:GLN:N    | 2.36                     | 0.47              |
| 1:B:408:VAL:HG11 | 1:B:701:LEU:HG   | 1.96                     | 0.47              |
| 1:C:126:ALA:HA   | 1:C:131:CYS:HB2  | 1.97                     | 0.47              |
| 1:C:338:ASN:OD1  | 1:C:339:ASN:N    | 2.47                     | 0.47              |
| 1:D:338:ASN:OD1  | 1:D:339:ASN:N    | 2.47                     | 0.47              |
| 1:D:569:PHE:HE2  | 3:D:802:POV:H27  | 1.79                     | 0.47              |
| 1:C:551:LEU:CD2  | 1:C:555:MET:HE1  | 2.45                     | 0.47              |
| 1:D:126:ALA:HA   | 1:D:131:CYS:HB2  | 1.97                     | 0.47              |
| 1:D:679:GLU:O    | 1:D:682:GLU:HG3  | 2.14                     | 0.47              |
| 1:B:126:ALA:HA   | 1:B:131:CYS:HB2  | 1.97                     | 0.47              |
| 1:B:569:PHE:HE2  | 3:B:803:POV:H27  | 1.79                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:350:LYS:O    | 1:A:416:ARG:NH2  | 2.48                     | 0.47              |
| 1:D:350:LYS:O    | 1:D:416:ARG:NH2  | 2.48                     | 0.47              |
| 1:A:126:ALA:HA   | 1:A:131:CYS:HB2  | 1.97                     | 0.47              |
| 1:A:679:GLU:O    | 1:A:682:GLU:HG3  | 2.14                     | 0.47              |
| 1:B:551:LEU:CD2  | 1:B:555:MET:HE1  | 2.45                     | 0.47              |
| 1:C:272:THR:OG1  | 1:C:274:GLN:OE1  | 2.27                     | 0.47              |
| 1:C:677:MET:HE2  | 1:C:677:MET:HB2  | 1.83                     | 0.46              |
| 1:A:592:PHE:HD2  | 1:B:572:MET:HE2  | 1.81                     | 0.46              |
| 1:D:297:ASN:OD1  | 1:D:338:ASN:ND2  | 2.49                     | 0.46              |
| 1:B:297:ASN:OD1  | 1:B:338:ASN:ND2  | 2.49                     | 0.46              |
| 1:D:720:LEU:O    | 1:D:721:CYS:HB3  | 2.15                     | 0.46              |
| 1:A:297:ASN:OD1  | 1:A:338:ASN:ND2  | 2.49                     | 0.46              |
| 1:C:350:LYS:O    | 1:C:416:ARG:NH2  | 2.48                     | 0.46              |
| 1:B:350:LYS:O    | 1:B:416:ARG:NH2  | 2.48                     | 0.46              |
| 1:B:407:THR:HA   | 1:B:416:ARG:NH1  | 2.31                     | 0.46              |
| 1:B:720:LEU:O    | 1:B:721:CYS:HB3  | 2.15                     | 0.46              |
| 1:C:297:ASN:OD1  | 1:C:338:ASN:ND2  | 2.49                     | 0.46              |
| 1:D:407:THR:HA   | 1:D:416:ARG:NH1  | 2.31                     | 0.46              |
| 1:C:407:THR:HA   | 1:C:416:ARG:NH1  | 2.31                     | 0.45              |
| 1:C:720:LEU:O    | 1:C:721:CYS:HB3  | 2.15                     | 0.45              |
| 1:C:225:ARG:NH2  | 1:D:381:ALA:O    | 2.41                     | 0.45              |
| 1:A:616:ASN:OD1  | 1:A:616:ASN:N    | 2.45                     | 0.45              |
| 1:C:609:ILE:HD12 | 1:C:622:TYR:HB2  | 1.99                     | 0.45              |
| 1:C:675:ALA:HB2  | 1:D:677:MET:CE   | 2.47                     | 0.45              |
| 1:D:609:ILE:HD12 | 1:D:622:TYR:HB2  | 1.99                     | 0.45              |
| 1:A:677:MET:CE   | 1:D:675:ALA:HB2  | 2.47                     | 0.45              |
| 1:B:133:GLU:HA   | 1:B:136:VAL:HG22 | 1.99                     | 0.45              |
| 1:B:409:TYR:HE1  | 1:B:698:ARG:HG3  | 1.82                     | 0.45              |
| 1:A:720:LEU:O    | 1:A:721:CYS:HB3  | 2.15                     | 0.45              |
| 1:C:672:MET:HG2  | 1:C:676:LEU:HD23 | 1.99                     | 0.45              |
| 1:A:133:GLU:HA   | 1:A:136:VAL:HG22 | 1.99                     | 0.45              |
| 1:A:609:ILE:HD12 | 1:A:622:TYR:HB2  | 1.99                     | 0.45              |
| 1:C:385:VAL:HG12 | 1:C:737:VAL:HG12 | 1.99                     | 0.45              |
| 1:D:409:TYR:HE1  | 1:D:698:ARG:HG3  | 1.82                     | 0.45              |
| 1:A:672:MET:HG2  | 1:A:676:LEU:HD23 | 1.99                     | 0.45              |
| 1:B:392:LEU:HD12 | 1:B:716:ARG:HG3  | 1.99                     | 0.45              |
| 1:C:409:TYR:HE1  | 1:C:698:ARG:HG3  | 1.82                     | 0.45              |
| 1:D:133:GLU:HA   | 1:D:136:VAL:HG22 | 1.99                     | 0.45              |
| 1:A:407:THR:HA   | 1:A:416:ARG:NH1  | 2.31                     | 0.45              |
| 1:A:551:LEU:CD2  | 1:A:555:MET:HE1  | 2.45                     | 0.45              |
| 3:C:807:POV:H26  | 1:D:629:VAL:HG12 | 1.99                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:672:MET:HG2  | 1:D:676:LEU:HD23 | 1.99                     | 0.45              |
| 1:C:133:GLU:HA   | 1:C:136:VAL:HG22 | 1.99                     | 0.44              |
| 1:C:407:THR:HG21 | 1:C:425:LEU:HD13 | 1.99                     | 0.44              |
| 1:A:675:ALA:HB2  | 1:B:677:MET:CE   | 2.47                     | 0.44              |
| 1:B:609:ILE:HD12 | 1:B:622:TYR:HB2  | 1.99                     | 0.44              |
| 1:C:123:ILE:HG13 | 1:C:138:LEU:HD13 | 2.00                     | 0.44              |
| 1:C:216:GLN:NE2  | 1:D:382:TYR:OH   | 2.50                     | 0.44              |
| 1:B:672:MET:HG2  | 1:B:676:LEU:HD23 | 1.99                     | 0.44              |
| 1:B:675:ALA:HB2  | 1:C:677:MET:CE   | 2.48                     | 0.44              |
| 1:D:407:THR:HG21 | 1:D:425:LEU:HD13 | 1.99                     | 0.44              |
| 1:A:629:VAL:HG12 | 3:A:802:POV:H26  | 1.99                     | 0.44              |
| 1:B:407:THR:HG21 | 1:B:425:LEU:HD13 | 1.99                     | 0.44              |
| 1:D:673:LEU:O    | 1:D:677:MET:HG3  | 2.18                     | 0.44              |
| 1:D:272:THR:OG1  | 1:D:274:GLN:OE1  | 2.26                     | 0.44              |
| 1:A:381:ALA:O    | 1:D:225:ARG:NH2  | 2.42                     | 0.44              |
| 1:B:385:VAL:HG12 | 1:B:737:VAL:HG12 | 1.99                     | 0.44              |
| 1:D:392:LEU:HD12 | 1:D:716:ARG:HG3  | 1.99                     | 0.44              |
| 1:A:407:THR:HG21 | 1:A:425:LEU:HD13 | 1.99                     | 0.44              |
| 1:A:409:TYR:HE1  | 1:A:698:ARG:HG3  | 1.82                     | 0.44              |
| 1:B:216:GLN:NE2  | 1:C:382:TYR:OH   | 2.50                     | 0.44              |
| 1:D:590:PHE:HD1  | 1:D:669:LEU:HD12 | 1.83                     | 0.44              |
| 1:A:590:PHE:HD1  | 1:A:669:LEU:HD12 | 1.83                     | 0.44              |
| 1:C:673:LEU:O    | 1:C:677:MET:HG3  | 2.18                     | 0.44              |
| 1:A:382:TYR:OH   | 1:D:216:GLN:NE2  | 2.51                     | 0.43              |
| 1:A:385:VAL:HG12 | 1:A:737:VAL:HG12 | 1.99                     | 0.43              |
| 1:A:673:LEU:O    | 1:A:677:MET:HG3  | 2.18                     | 0.43              |
| 1:B:583:ILE:HG23 | 1:B:584:LEU:HG   | 1.99                     | 0.43              |
| 1:B:673:LEU:O    | 1:B:677:MET:HG3  | 2.18                     | 0.43              |
| 1:D:385:VAL:HG12 | 1:D:737:VAL:HG12 | 1.99                     | 0.43              |
| 1:A:635:LEU:HD13 | 1:A:642:LEU:HD12 | 2.00                     | 0.43              |
| 1:B:629:VAL:HG12 | 3:B:801:POV:H26  | 1.99                     | 0.43              |
| 1:C:411:THR:HG1  | 1:C:698:ARG:HH22 | 1.59                     | 0.43              |
| 1:C:629:VAL:HG12 | 3:C:801:POV:H26  | 1.99                     | 0.43              |
| 1:A:392:LEU:HD12 | 1:A:716:ARG:HG3  | 1.99                     | 0.43              |
| 1:A:583:ILE:HG23 | 1:A:584:LEU:HG   | 2.00                     | 0.43              |
| 1:C:392:LEU:HD12 | 1:C:716:ARG:HG3  | 1.99                     | 0.43              |
| 1:D:123:ILE:HG13 | 1:D:138:LEU:HD13 | 2.00                     | 0.43              |
| 1:B:590:PHE:HD1  | 1:B:669:LEU:HD12 | 1.83                     | 0.43              |
| 1:C:590:PHE:HD1  | 1:C:669:LEU:HD12 | 1.83                     | 0.43              |
| 1:D:583:ILE:HG23 | 1:D:584:LEU:HG   | 2.00                     | 0.43              |
| 1:A:123:ILE:HG13 | 1:A:138:LEU:HD13 | 2.00                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:225:ARG:NH2  | 1:B:381:ALA:O    | 2.46                     | 0.43              |
| 1:A:330:ASN:OD1  | 1:A:330:ASN:N    | 2.39                     | 0.43              |
| 1:B:635:LEU:HD13 | 1:B:642:LEU:HD12 | 2.01                     | 0.43              |
| 1:C:497:ILE:HD11 | 1:C:526:PHE:HD2  | 1.84                     | 0.43              |
| 1:B:223:ILE:HG23 | 1:B:277:ILE:HG21 | 2.01                     | 0.43              |
| 1:C:583:ILE:HG23 | 1:C:584:LEU:HG   | 1.99                     | 0.43              |
| 1:D:551:LEU:CD2  | 1:D:555:MET:HE1  | 2.45                     | 0.43              |
| 1:D:706:MET:HE3  | 1:D:706:MET:HB2  | 1.86                     | 0.43              |
| 1:B:389:LEU:HD12 | 1:B:389:LEU:HA   | 1.91                     | 0.43              |
| 1:C:650:TYR:OH   | 1:D:545:LYS:O    | 2.36                     | 0.43              |
| 1:A:309:ASP:OD1  | 1:A:309:ASP:N    | 2.52                     | 0.43              |
| 1:B:266:LEU:HD13 | 1:B:281:LEU:HB3  | 2.01                     | 0.43              |
| 1:A:377:PHE:O    | 1:A:389:LEU:N    | 2.45                     | 0.43              |
| 1:C:223:ILE:HG23 | 1:C:277:ILE:HG21 | 2.01                     | 0.43              |
| 1:D:530:ALA:O    | 1:D:534:ILE:HG12 | 2.19                     | 0.43              |
| 1:A:521:TRP:O    | 1:A:525:VAL:HG23 | 2.19                     | 0.42              |
| 1:A:530:ALA:O    | 1:A:534:ILE:HG12 | 2.19                     | 0.42              |
| 1:B:123:ILE:HG13 | 1:B:138:LEU:HD13 | 2.00                     | 0.42              |
| 1:B:530:ALA:O    | 1:B:534:ILE:HG12 | 2.19                     | 0.42              |
| 1:A:223:ILE:HG23 | 1:A:277:ILE:HG21 | 2.01                     | 0.42              |
| 1:C:530:ALA:O    | 1:C:534:ILE:HG12 | 2.19                     | 0.42              |
| 1:D:677:MET:HE2  | 1:D:677:MET:HB2  | 1.83                     | 0.42              |
| 1:A:410:ASN:HB2  | 1:A:416:ARG:NH1  | 2.34                     | 0.42              |
| 1:D:330:ASN:HA   | 1:D:373:LEU:HD11 | 2.01                     | 0.42              |
| 1:A:330:ASN:HA   | 1:A:373:LEU:HD11 | 2.01                     | 0.42              |
| 1:B:655:LEU:O    | 1:B:659:ILE:HG12 | 2.19                     | 0.42              |
| 1:C:266:LEU:HD13 | 1:C:281:LEU:HB3  | 2.01                     | 0.42              |
| 1:D:135:LEU:HD13 | 1:D:186:ILE:HG13 | 2.01                     | 0.42              |
| 1:D:410:ASN:HB2  | 1:D:416:ARG:NH1  | 2.35                     | 0.42              |
| 1:D:521:TRP:O    | 1:D:525:VAL:HG23 | 2.19                     | 0.42              |
| 1:A:135:LEU:HD13 | 1:A:186:ILE:HG13 | 2.01                     | 0.42              |
| 1:C:521:TRP:O    | 1:C:525:VAL:HG23 | 2.19                     | 0.42              |
| 1:D:655:LEU:O    | 1:D:659:ILE:HG12 | 2.20                     | 0.42              |
| 1:B:497:ILE:HD11 | 1:B:526:PHE:HD2  | 1.84                     | 0.42              |
| 1:C:609:ILE:HG12 | 1:C:648:SER:HB3  | 2.02                     | 0.42              |
| 1:D:266:LEU:HD13 | 1:D:281:LEU:HB3  | 2.01                     | 0.42              |
| 1:B:300:LEU:HD12 | 1:B:300:LEU:H    | 1.85                     | 0.42              |
| 1:B:410:ASN:HB2  | 1:B:416:ARG:NH1  | 2.34                     | 0.42              |
| 1:C:635:LEU:HD13 | 1:C:642:LEU:HD12 | 2.01                     | 0.42              |
| 1:C:655:LEU:O    | 1:C:659:ILE:HG12 | 2.19                     | 0.42              |
| 1:A:497:ILE:HD11 | 1:A:526:PHE:HD2  | 1.84                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:497:ILE:HD11 | 1:D:526:PHE:HD2  | 1.84                     | 0.42              |
| 1:A:655:LEU:O    | 1:A:659:ILE:HG12 | 2.20                     | 0.42              |
| 1:C:300:LEU:HD12 | 1:C:300:LEU:H    | 1.85                     | 0.42              |
| 1:D:223:ILE:HG23 | 1:D:277:ILE:HG21 | 2.01                     | 0.42              |
| 1:D:309:ASP:N    | 1:D:309:ASP:OD1  | 2.52                     | 0.41              |
| 1:D:635:LEU:HD13 | 1:D:642:LEU:HD12 | 2.00                     | 0.41              |
| 1:A:300:LEU:H    | 1:A:300:LEU:HD12 | 1.85                     | 0.41              |
| 1:A:656:PHE:HD1  | 3:B:801:POV:H37A | 1.84                     | 0.41              |
| 1:B:135:LEU:HD13 | 1:B:186:ILE:HG13 | 2.01                     | 0.41              |
| 1:B:330:ASN:HA   | 1:B:373:LEU:HD11 | 2.01                     | 0.41              |
| 1:B:521:TRP:O    | 1:B:525:VAL:HG23 | 2.19                     | 0.41              |
| 1:C:135:LEU:HD13 | 1:C:186:ILE:HG13 | 2.01                     | 0.41              |
| 1:C:410:ASN:HB2  | 1:C:416:ARG:NH1  | 2.35                     | 0.41              |
| 1:C:592:PHE:HD2  | 1:D:572:MET:HE2  | 1.85                     | 0.41              |
| 1:A:545:LYS:O    | 1:D:650:TYR:OH   | 2.38                     | 0.41              |
| 1:B:650:TYR:OH   | 1:C:545:LYS:O    | 2.37                     | 0.41              |
| 1:C:417:HIS:CE1  | 1:C:693:ARG:HB3  | 2.55                     | 0.41              |
| 1:D:417:HIS:CE1  | 1:D:693:ARG:HB3  | 2.55                     | 0.41              |
| 1:A:140:VAL:HA   | 1:A:143:GLN:HE22 | 1.85                     | 0.41              |
| 1:A:266:LEU:HD13 | 1:A:281:LEU:HB3  | 2.01                     | 0.41              |
| 1:B:173:MET:O    | 1:B:176:LEU:N    | 2.50                     | 0.41              |
| 1:C:677:MET:HG3  | 1:C:677:MET:H    | 1.67                     | 0.41              |
| 1:D:173:MET:O    | 1:D:176:LEU:N    | 2.50                     | 0.41              |
| 1:D:609:ILE:HG12 | 1:D:648:SER:HB3  | 2.02                     | 0.41              |
| 1:B:417:HIS:CE1  | 1:B:693:ARG:HB3  | 2.55                     | 0.41              |
| 1:C:128:SER:O    | 1:C:178:ASN:ND2  | 2.53                     | 0.41              |
| 1:C:588:LEU:HD23 | 1:C:588:LEU:HA   | 1.94                     | 0.41              |
| 1:D:128:SER:O    | 1:D:178:ASN:ND2  | 2.53                     | 0.41              |
| 1:A:417:HIS:CE1  | 1:A:693:ARG:HB3  | 2.55                     | 0.41              |
| 1:A:609:ILE:HG12 | 1:A:648:SER:HB3  | 2.02                     | 0.41              |
| 1:B:128:SER:O    | 1:B:178:ASN:ND2  | 2.53                     | 0.41              |
| 1:C:330:ASN:HA   | 1:C:373:LEU:HD11 | 2.01                     | 0.41              |
| 1:A:216:GLN:NE2  | 1:B:382:TYR:OH   | 2.53                     | 0.41              |
| 1:B:140:VAL:HA   | 1:B:143:GLN:HE22 | 1.85                     | 0.41              |
| 1:C:389:LEU:HD12 | 1:C:389:LEU:HA   | 1.91                     | 0.41              |
| 1:A:143:GLN:OE1  | 1:A:143:GLN:N    | 2.53                     | 0.41              |
| 1:A:535:LEU:O    | 1:A:539:LEU:HG   | 2.21                     | 0.41              |
| 1:B:309:ASP:N    | 1:B:309:ASP:OD1  | 2.52                     | 0.41              |
| 1:C:309:ASP:OD1  | 1:C:309:ASP:N    | 2.52                     | 0.41              |
| 1:D:588:LEU:HD23 | 1:D:588:LEU:HA   | 1.94                     | 0.41              |
| 1:D:677:MET:HG3  | 1:D:677:MET:H    | 1.68                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:572:MET:HE2  | 1:D:592:PHE:HD2  | 1.85                     | 0.41              |
| 1:B:535:LEU:O    | 1:B:539:LEU:HG   | 2.21                     | 0.41              |
| 1:C:140:VAL:HA   | 1:C:143:GLN:HE22 | 1.85                     | 0.41              |
| 1:A:128:SER:O    | 1:A:178:ASN:ND2  | 2.53                     | 0.40              |
| 1:B:609:ILE:HG12 | 1:B:648:SER:HB3  | 2.02                     | 0.40              |
| 1:C:163:THR:HG22 | 1:C:170:THR:HG23 | 2.03                     | 0.40              |
| 1:C:535:LEU:O    | 1:C:539:LEU:HG   | 2.21                     | 0.40              |
| 1:D:300:LEU:HD12 | 1:D:300:LEU:H    | 1.85                     | 0.40              |
| 1:D:389:LEU:HD12 | 1:D:389:LEU:HA   | 1.91                     | 0.40              |
| 1:D:535:LEU:O    | 1:D:539:LEU:HG   | 2.21                     | 0.40              |
| 1:D:377:PHE:O    | 1:D:389:LEU:N    | 2.45                     | 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     | 595/799 (74%)   | 557 (94%)  | 38 (6%)  | 0        | 100         | 100 |
| 1   | B     | 595/799 (74%)   | 557 (94%)  | 38 (6%)  | 0        | 100         | 100 |
| 1   | C     | 595/799 (74%)   | 557 (94%)  | 38 (6%)  | 0        | 100         | 100 |
| 1   | D     | 595/799 (74%)   | 557 (94%)  | 38 (6%)  | 0        | 100         | 100 |
| All | All   | 2380/3196 (74%) | 2228 (94%) | 152 (6%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

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

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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     | 532/712 (75%)   | 531 (100%)  | 1 (0%)   | 87          | 84 |
| 1   | B     | 532/712 (75%)   | 531 (100%)  | 1 (0%)   | 87          | 84 |
| 1   | C     | 532/712 (75%)   | 531 (100%)  | 1 (0%)   | 87          | 84 |
| 1   | D     | 532/712 (75%)   | 530 (100%)  | 2 (0%)   | 84          | 79 |
| All | All   | 2128/2848 (75%) | 2123 (100%) | 5 (0%)   | 85          | 84 |

All (5) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 677 | MET  |
| 1   | B     | 677 | MET  |
| 1   | C     | 677 | MET  |
| 1   | D     | 330 | ASN  |
| 1   | D     | 677 | MET  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 160 | HIS  |
| 1   | A     | 178 | ASN  |
| 1   | A     | 216 | GLN  |
| 1   | A     | 227 | GLN  |
| 1   | A     | 256 | HIS  |
| 1   | A     | 417 | HIS  |
| 1   | A     | 646 | GLN  |
| 1   | A     | 647 | ASN  |
| 1   | B     | 160 | HIS  |
| 1   | B     | 178 | ASN  |
| 1   | B     | 216 | GLN  |
| 1   | B     | 227 | GLN  |
| 1   | B     | 256 | HIS  |
| 1   | B     | 417 | HIS  |
| 1   | B     | 646 | GLN  |
| 1   | B     | 647 | ASN  |
| 1   | C     | 160 | HIS  |
| 1   | C     | 178 | ASN  |
| 1   | C     | 216 | GLN  |
| 1   | C     | 227 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 256 | HIS  |
| 1   | C     | 417 | HIS  |
| 1   | C     | 646 | GLN  |
| 1   | C     | 647 | ASN  |
| 1   | D     | 160 | HIS  |
| 1   | D     | 178 | ASN  |
| 1   | D     | 216 | GLN  |
| 1   | D     | 227 | GLN  |
| 1   | D     | 256 | HIS  |
| 1   | D     | 417 | HIS  |
| 1   | D     | 646 | GLN  |
| 1   | D     | 647 | ASN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

24 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 3   | POV  | D     | 801 | -    | 32,32,51     | 0.62 | 0           | 38,40,59    | 0.54 | 0           |
| 3   | POV  | C     | 804 | -    | 44,44,51     | 0.54 | 0           | 50,52,59    | 0.49 | 0           |

| Mol | Type  | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|-------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |       |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | POV   | D     | 804 | -    | 38,38,51     | 0.58 | 0        | 44,46,59    | 0.50 | 0        |
| 2   | A1EBL | A     | 801 | -    | 10,10,10     | 1.16 | 1 (10%)  | 12,13,13    | 1.51 | 3 (25%)  |
| 3   | POV   | B     | 804 | -    | 44,44,51     | 0.54 | 0        | 50,52,59    | 0.49 | 0        |
| 3   | POV   | C     | 807 | -    | 43,43,51     | 0.54 | 0        | 49,51,59    | 0.48 | 0        |
| 3   | POV   | A     | 804 | -    | 37,37,51     | 0.58 | 0        | 43,45,59    | 0.50 | 0        |
| 3   | POV   | A     | 803 | -    | 32,32,51     | 0.62 | 0        | 38,40,59    | 0.54 | 0        |
| 3   | POV   | A     | 802 | -    | 43,43,51     | 0.54 | 0        | 49,51,59    | 0.48 | 0        |
| 3   | POV   | B     | 805 | -    | 38,38,51     | 0.57 | 0        | 44,46,59    | 0.50 | 0        |
| 2   | A1EBL | B     | 806 | -    | 10,10,10     | 1.16 | 1 (10%)  | 12,13,13    | 1.50 | 3 (25%)  |
| 3   | POV   | C     | 802 | -    | 32,32,51     | 0.62 | 0        | 38,40,59    | 0.54 | 0        |
| 3   | POV   | D     | 803 | -    | 44,44,51     | 0.54 | 0        | 50,52,59    | 0.49 | 0        |
| 3   | POV   | B     | 801 | -    | 43,43,51     | 0.54 | 0        | 49,51,59    | 0.48 | 0        |
| 3   | POV   | D     | 802 | -    | 37,37,51     | 0.59 | 0        | 43,45,59    | 0.50 | 0        |
| 3   | POV   | B     | 802 | -    | 32,32,51     | 0.62 | 0        | 38,40,59    | 0.54 | 0        |
| 3   | POV   | A     | 806 | -    | 38,38,51     | 0.58 | 0        | 44,46,59    | 0.50 | 0        |
| 3   | POV   | A     | 805 | -    | 44,44,51     | 0.54 | 0        | 50,52,59    | 0.49 | 0        |
| 3   | POV   | C     | 805 | -    | 38,38,51     | 0.57 | 0        | 44,46,59    | 0.50 | 0        |
| 2   | A1EBL | C     | 806 | -    | 10,10,10     | 1.17 | 1 (10%)  | 12,13,13    | 1.51 | 3 (25%)  |
| 2   | A1EBL | A     | 807 | -    | 10,10,10     | 1.16 | 1 (10%)  | 12,13,13    | 1.50 | 3 (25%)  |
| 3   | POV   | B     | 803 | -    | 37,37,51     | 0.59 | 0        | 43,45,59    | 0.50 | 0        |
| 3   | POV   | C     | 803 | -    | 37,37,51     | 0.58 | 0        | 43,45,59    | 0.49 | 0        |
| 3   | POV   | C     | 801 | -    | 43,43,51     | 0.54 | 0        | 49,51,59    | 0.48 | 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 |
|-----|-------|-------|-----|------|---------|-------------|-------|
| 3   | POV   | D     | 801 | -    | -       | 8/36/36/55  | -     |
| 3   | POV   | C     | 804 | -    | -       | 10/48/48/55 | -     |
| 3   | POV   | D     | 804 | -    | -       | 16/42/42/55 | -     |
| 2   | A1EBL | A     | 801 | -    | -       | 5/10/10/10  | -     |
| 3   | POV   | B     | 804 | -    | -       | 10/48/48/55 | -     |
| 3   | POV   | C     | 807 | -    | -       | 16/47/47/55 | -     |
| 3   | POV   | A     | 804 | -    | -       | 12/41/41/55 | -     |
| 3   | POV   | A     | 803 | -    | -       | 8/36/36/55  | -     |
| 3   | POV   | A     | 802 | -    | -       | 16/47/47/55 | -     |
| 3   | POV   | B     | 805 | -    | -       | 16/42/42/55 | -     |

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| Mol | Type  | Chain | Res | Link | Chirals | Torsions    | Rings |
|-----|-------|-------|-----|------|---------|-------------|-------|
| 2   | A1EBL | B     | 806 | -    | -       | 5/10/10/10  | -     |
| 3   | POV   | C     | 802 | -    | -       | 8/36/36/55  | -     |
| 3   | POV   | D     | 803 | -    | -       | 10/48/48/55 | -     |
| 3   | POV   | B     | 801 | -    | -       | 16/47/47/55 | -     |
| 3   | POV   | D     | 802 | -    | -       | 12/41/41/55 | -     |
| 3   | POV   | B     | 802 | -    | -       | 8/36/36/55  | -     |
| 3   | POV   | A     | 806 | -    | -       | 16/42/42/55 | -     |
| 3   | POV   | A     | 805 | -    | -       | 10/48/48/55 | -     |
| 3   | POV   | C     | 805 | -    | -       | 16/42/42/55 | -     |
| 2   | A1EBL | C     | 806 | -    | -       | 5/10/10/10  | -     |
| 2   | A1EBL | A     | 807 | -    | -       | 5/10/10/10  | -     |
| 3   | POV   | B     | 803 | -    | -       | 12/41/41/55 | -     |
| 3   | POV   | C     | 803 | -    | -       | 12/41/41/55 | -     |
| 3   | POV   | C     | 801 | -    | -       | 16/47/47/55 | -     |

All (4) bond length outliers are listed below:

| Mol | Chain | Res | Type  | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|-------|---------|-------|-------------|----------|
| 2   | A     | 801 | A1EBL | O01-C02 | -2.52 | 1.41        | 1.44     |
| 2   | A     | 807 | A1EBL | O01-C02 | -2.52 | 1.41        | 1.44     |
| 2   | B     | 806 | A1EBL | O01-C02 | -2.52 | 1.41        | 1.44     |
| 2   | C     | 806 | A1EBL | O01-C02 | -2.52 | 1.41        | 1.44     |

All (12) bond angle outliers are listed below:

| Mol | Chain | Res | Type  | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|-------|-------------|-------|-------------|----------|
| 2   | A     | 801 | A1EBL | C02-C06-C11 | -3.16 | 111.62      | 128.34   |
| 2   | A     | 807 | A1EBL | C02-C06-C11 | -3.15 | 111.65      | 128.34   |
| 2   | B     | 806 | A1EBL | C02-C06-C11 | -3.15 | 111.65      | 128.34   |
| 2   | C     | 806 | A1EBL | C02-C06-C11 | -3.15 | 111.67      | 128.34   |
| 2   | A     | 807 | A1EBL | C09-C08-C10 | 2.48  | 120.30      | 114.59   |
| 2   | A     | 801 | A1EBL | C09-C08-C10 | 2.47  | 120.26      | 114.59   |
| 2   | B     | 806 | A1EBL | C09-C08-C10 | 2.47  | 120.26      | 114.59   |
| 2   | C     | 806 | A1EBL | C09-C08-C10 | 2.46  | 120.25      | 114.59   |
| 2   | C     | 806 | A1EBL | C04-C07-C08 | -2.39 | 119.68      | 127.64   |
| 2   | A     | 801 | A1EBL | C04-C07-C08 | -2.37 | 119.72      | 127.64   |
| 2   | A     | 807 | A1EBL | C04-C07-C08 | -2.36 | 119.76      | 127.64   |
| 2   | B     | 806 | A1EBL | C04-C07-C08 | -2.36 | 119.78      | 127.64   |

There are no chirality outliers.

All (268) torsion outliers are listed below:

| Mol | Chain | Res | Type  | Atoms           |
|-----|-------|-----|-------|-----------------|
| 2   | A     | 801 | A1EBL | C05-C02-C03-C04 |
| 2   | A     | 801 | A1EBL | C06-C02-C03-C04 |
| 2   | A     | 801 | A1EBL | O01-C02-C03-C04 |
| 2   | A     | 807 | A1EBL | C05-C02-C03-C04 |
| 2   | A     | 807 | A1EBL | C06-C02-C03-C04 |
| 2   | A     | 807 | A1EBL | O01-C02-C03-C04 |
| 2   | B     | 806 | A1EBL | C05-C02-C03-C04 |
| 2   | B     | 806 | A1EBL | C06-C02-C03-C04 |
| 2   | B     | 806 | A1EBL | O01-C02-C03-C04 |
| 2   | C     | 806 | A1EBL | C05-C02-C03-C04 |
| 2   | C     | 806 | A1EBL | C06-C02-C03-C04 |
| 2   | C     | 806 | A1EBL | O01-C02-C03-C04 |
| 3   | A     | 802 | POV   | C1-O11-P-O12    |
| 3   | A     | 802 | POV   | C1-O11-P-O13    |
| 3   | A     | 802 | POV   | C1-O11-P-O14    |
| 3   | A     | 802 | POV   | C2-C1-O11-P     |
| 3   | A     | 803 | POV   | C11-O12-P-O14   |
| 3   | A     | 803 | POV   | O12-C11-C12-N   |
| 3   | A     | 804 | POV   | C1-O11-P-O12    |
| 3   | A     | 804 | POV   | O21-C2-C3-O31   |
| 3   | A     | 805 | POV   | C11-O12-P-O11   |
| 3   | A     | 805 | POV   | C12-C11-O12-P   |
| 3   | A     | 806 | POV   | C1-O11-P-O12    |
| 3   | A     | 806 | POV   | C1-O11-P-O13    |
| 3   | A     | 806 | POV   | C1-O11-P-O14    |
| 3   | B     | 801 | POV   | C1-O11-P-O12    |
| 3   | B     | 801 | POV   | C1-O11-P-O13    |
| 3   | B     | 801 | POV   | C1-O11-P-O14    |
| 3   | B     | 801 | POV   | C2-C1-O11-P     |
| 3   | B     | 802 | POV   | C11-O12-P-O14   |
| 3   | B     | 802 | POV   | O12-C11-C12-N   |
| 3   | B     | 803 | POV   | C1-O11-P-O12    |
| 3   | B     | 803 | POV   | O21-C2-C3-O31   |
| 3   | B     | 804 | POV   | C11-O12-P-O11   |
| 3   | B     | 804 | POV   | C12-C11-O12-P   |
| 3   | B     | 805 | POV   | C1-O11-P-O12    |
| 3   | B     | 805 | POV   | C1-O11-P-O13    |
| 3   | B     | 805 | POV   | C1-O11-P-O14    |
| 3   | C     | 801 | POV   | C1-O11-P-O12    |
| 3   | C     | 801 | POV   | C1-O11-P-O13    |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 3   | C     | 801 | POV  | C1-O11-P-O14    |
| 3   | C     | 801 | POV  | C2-C1-O11-P     |
| 3   | C     | 802 | POV  | C11-O12-P-O14   |
| 3   | C     | 802 | POV  | O12-C11-C12-N   |
| 3   | C     | 803 | POV  | C1-O11-P-O12    |
| 3   | C     | 803 | POV  | O21-C2-C3-O31   |
| 3   | C     | 804 | POV  | C11-O12-P-O11   |
| 3   | C     | 804 | POV  | C12-C11-O12-P   |
| 3   | C     | 805 | POV  | C1-O11-P-O12    |
| 3   | C     | 805 | POV  | C1-O11-P-O13    |
| 3   | C     | 805 | POV  | C1-O11-P-O14    |
| 3   | C     | 807 | POV  | C1-O11-P-O12    |
| 3   | C     | 807 | POV  | C1-O11-P-O13    |
| 3   | C     | 807 | POV  | C1-O11-P-O14    |
| 3   | C     | 807 | POV  | C2-C1-O11-P     |
| 3   | D     | 801 | POV  | C11-O12-P-O14   |
| 3   | D     | 801 | POV  | O12-C11-C12-N   |
| 3   | D     | 802 | POV  | C1-O11-P-O12    |
| 3   | D     | 802 | POV  | O21-C2-C3-O31   |
| 3   | D     | 803 | POV  | C11-O12-P-O11   |
| 3   | D     | 803 | POV  | C12-C11-O12-P   |
| 3   | D     | 804 | POV  | C1-O11-P-O12    |
| 3   | D     | 804 | POV  | C1-O11-P-O13    |
| 3   | D     | 804 | POV  | C1-O11-P-O14    |
| 3   | A     | 806 | POV  | C31-C32-C33-C34 |
| 3   | B     | 805 | POV  | C31-C32-C33-C34 |
| 3   | C     | 805 | POV  | C31-C32-C33-C34 |
| 3   | D     | 804 | POV  | C31-C32-C33-C34 |
| 3   | A     | 805 | POV  | C2-C1-O11-P     |
| 3   | B     | 804 | POV  | C2-C1-O11-P     |
| 3   | C     | 804 | POV  | C2-C1-O11-P     |
| 3   | D     | 803 | POV  | C2-C1-O11-P     |
| 3   | A     | 803 | POV  | C21-C22-C23-C24 |
| 3   | B     | 802 | POV  | C21-C22-C23-C24 |
| 3   | C     | 802 | POV  | C21-C22-C23-C24 |
| 3   | D     | 801 | POV  | C21-C22-C23-C24 |
| 3   | A     | 802 | POV  | C1-C2-C3-O31    |
| 3   | A     | 803 | POV  | C1-C2-C3-O31    |
| 3   | B     | 801 | POV  | C1-C2-C3-O31    |
| 3   | B     | 802 | POV  | C1-C2-C3-O31    |
| 3   | C     | 801 | POV  | C1-C2-C3-O31    |
| 3   | C     | 802 | POV  | C1-C2-C3-O31    |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 3   | C     | 807 | POV  | C1-C2-C3-O31    |
| 3   | D     | 801 | POV  | C1-C2-C3-O31    |
| 3   | A     | 802 | POV  | C23-C24-C25-C26 |
| 3   | B     | 801 | POV  | C23-C24-C25-C26 |
| 3   | C     | 801 | POV  | C23-C24-C25-C26 |
| 3   | C     | 807 | POV  | C23-C24-C25-C26 |
| 3   | A     | 804 | POV  | C22-C21-O21-C2  |
| 3   | B     | 803 | POV  | C22-C21-O21-C2  |
| 3   | C     | 803 | POV  | C22-C21-O21-C2  |
| 3   | D     | 802 | POV  | C22-C21-O21-C2  |
| 3   | A     | 803 | POV  | O21-C2-C3-O31   |
| 3   | A     | 805 | POV  | O21-C2-C3-O31   |
| 3   | B     | 802 | POV  | O21-C2-C3-O31   |
| 3   | B     | 804 | POV  | O21-C2-C3-O31   |
| 3   | C     | 802 | POV  | O21-C2-C3-O31   |
| 3   | C     | 804 | POV  | O21-C2-C3-O31   |
| 3   | D     | 801 | POV  | O21-C2-C3-O31   |
| 3   | D     | 803 | POV  | O21-C2-C3-O31   |
| 3   | A     | 802 | POV  | C35-C36-C37-C38 |
| 3   | B     | 801 | POV  | C35-C36-C37-C38 |
| 3   | C     | 801 | POV  | C35-C36-C37-C38 |
| 3   | C     | 807 | POV  | C35-C36-C37-C38 |
| 3   | A     | 803 | POV  | O11-C1-C2-C3    |
| 3   | A     | 806 | POV  | O11-C1-C2-C3    |
| 3   | B     | 802 | POV  | O11-C1-C2-C3    |
| 3   | B     | 805 | POV  | O11-C1-C2-C3    |
| 3   | C     | 802 | POV  | O11-C1-C2-C3    |
| 3   | C     | 805 | POV  | O11-C1-C2-C3    |
| 3   | D     | 801 | POV  | O11-C1-C2-C3    |
| 3   | D     | 804 | POV  | O11-C1-C2-C3    |
| 3   | A     | 804 | POV  | O22-C21-O21-C2  |
| 3   | B     | 803 | POV  | O22-C21-O21-C2  |
| 3   | C     | 803 | POV  | O22-C21-O21-C2  |
| 3   | D     | 802 | POV  | O22-C21-O21-C2  |
| 3   | A     | 805 | POV  | C1-C2-C3-O31    |
| 3   | B     | 804 | POV  | C1-C2-C3-O31    |
| 3   | C     | 804 | POV  | C1-C2-C3-O31    |
| 3   | D     | 803 | POV  | C1-C2-C3-O31    |
| 3   | A     | 804 | POV  | O11-C1-C2-C3    |
| 3   | B     | 803 | POV  | O11-C1-C2-C3    |
| 3   | C     | 803 | POV  | O11-C1-C2-C3    |
| 3   | D     | 802 | POV  | O11-C1-C2-C3    |

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| Mol | Chain | Res | Type  | Atoms               |
|-----|-------|-----|-------|---------------------|
| 3   | A     | 806 | POV   | C22-C21-O21-C2      |
| 3   | B     | 805 | POV   | C22-C21-O21-C2      |
| 3   | C     | 805 | POV   | C22-C21-O21-C2      |
| 3   | D     | 804 | POV   | C22-C21-O21-C2      |
| 3   | A     | 804 | POV   | C1-C2-C3-O31        |
| 3   | B     | 803 | POV   | C1-C2-C3-O31        |
| 3   | C     | 803 | POV   | C1-C2-C3-O31        |
| 3   | D     | 802 | POV   | C1-C2-C3-O31        |
| 3   | A     | 802 | POV   | O11-C1-C2-O21       |
| 3   | A     | 806 | POV   | O11-C1-C2-O21       |
| 3   | B     | 801 | POV   | O11-C1-C2-O21       |
| 3   | B     | 805 | POV   | O11-C1-C2-O21       |
| 3   | C     | 801 | POV   | O11-C1-C2-O21       |
| 3   | C     | 805 | POV   | O11-C1-C2-O21       |
| 3   | C     | 807 | POV   | O11-C1-C2-O21       |
| 3   | D     | 804 | POV   | O11-C1-C2-O21       |
| 3   | A     | 802 | POV   | C33-C34-C35-C36     |
| 3   | C     | 801 | POV   | C33-C34-C35-C36     |
| 3   | C     | 807 | POV   | C33-C34-C35-C36     |
| 3   | B     | 801 | POV   | C33-C34-C35-C36     |
| 3   | A     | 806 | POV   | O22-C21-O21-C2      |
| 3   | B     | 805 | POV   | O22-C21-O21-C2      |
| 3   | C     | 805 | POV   | O22-C21-O21-C2      |
| 3   | D     | 804 | POV   | O22-C21-O21-C2      |
| 3   | A     | 804 | POV   | O11-C1-C2-O21       |
| 3   | B     | 803 | POV   | O11-C1-C2-O21       |
| 3   | C     | 803 | POV   | O11-C1-C2-O21       |
| 3   | D     | 802 | POV   | O11-C1-C2-O21       |
| 3   | A     | 802 | POV   | C213-C214-C215-C216 |
| 3   | B     | 801 | POV   | C213-C214-C215-C216 |
| 3   | C     | 801 | POV   | C213-C214-C215-C216 |
| 3   | C     | 807 | POV   | C213-C214-C215-C216 |
| 3   | A     | 802 | POV   | O21-C2-C3-O31       |
| 3   | B     | 801 | POV   | O21-C2-C3-O31       |
| 3   | C     | 801 | POV   | O21-C2-C3-O31       |
| 3   | C     | 807 | POV   | O21-C2-C3-O31       |
| 2   | A     | 801 | A1EBL | C05-C02-C06-C11     |
| 2   | A     | 807 | A1EBL | C05-C02-C06-C11     |
| 2   | B     | 806 | A1EBL | C05-C02-C06-C11     |
| 2   | C     | 806 | A1EBL | C05-C02-C06-C11     |
| 3   | B     | 805 | POV   | C34-C35-C36-C37     |
| 3   | A     | 806 | POV   | C34-C35-C36-C37     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 3   | C     | 805 | POV  | C34-C35-C36-C37 |
| 3   | D     | 804 | POV  | C34-C35-C36-C37 |
| 3   | A     | 802 | POV  | O11-C1-C2-C3    |
| 3   | B     | 801 | POV  | O11-C1-C2-C3    |
| 3   | C     | 801 | POV  | O11-C1-C2-C3    |
| 3   | C     | 807 | POV  | O11-C1-C2-C3    |
| 3   | A     | 802 | POV  | C11-O12-P-O11   |
| 3   | A     | 802 | POV  | C11-O12-P-O13   |
| 3   | A     | 802 | POV  | C11-O12-P-O14   |
| 3   | A     | 804 | POV  | C1-O11-P-O14    |
| 3   | A     | 805 | POV  | C1-O11-P-O14    |
| 3   | A     | 805 | POV  | C11-O12-P-O14   |
| 3   | A     | 806 | POV  | C11-O12-P-O11   |
| 3   | A     | 806 | POV  | C11-O12-P-O13   |
| 3   | A     | 806 | POV  | C11-O12-P-O14   |
| 3   | B     | 801 | POV  | C11-O12-P-O11   |
| 3   | B     | 801 | POV  | C11-O12-P-O13   |
| 3   | B     | 801 | POV  | C11-O12-P-O14   |
| 3   | B     | 803 | POV  | C1-O11-P-O14    |
| 3   | B     | 804 | POV  | C1-O11-P-O14    |
| 3   | B     | 804 | POV  | C11-O12-P-O14   |
| 3   | B     | 805 | POV  | C11-O12-P-O11   |
| 3   | B     | 805 | POV  | C11-O12-P-O13   |
| 3   | B     | 805 | POV  | C11-O12-P-O14   |
| 3   | C     | 801 | POV  | C11-O12-P-O11   |
| 3   | C     | 801 | POV  | C11-O12-P-O13   |
| 3   | C     | 801 | POV  | C11-O12-P-O14   |
| 3   | C     | 803 | POV  | C1-O11-P-O14    |
| 3   | C     | 804 | POV  | C1-O11-P-O14    |
| 3   | C     | 804 | POV  | C11-O12-P-O14   |
| 3   | C     | 805 | POV  | C11-O12-P-O11   |
| 3   | C     | 805 | POV  | C11-O12-P-O13   |
| 3   | C     | 805 | POV  | C11-O12-P-O14   |
| 3   | C     | 807 | POV  | C11-O12-P-O11   |
| 3   | C     | 807 | POV  | C11-O12-P-O13   |
| 3   | C     | 807 | POV  | C11-O12-P-O14   |
| 3   | D     | 802 | POV  | C1-O11-P-O14    |
| 3   | D     | 803 | POV  | C1-O11-P-O14    |
| 3   | D     | 803 | POV  | C11-O12-P-O14   |
| 3   | D     | 804 | POV  | C11-O12-P-O11   |
| 3   | D     | 804 | POV  | C11-O12-P-O13   |
| 3   | D     | 804 | POV  | C11-O12-P-O14   |

*Continued on next page...*

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| Mol | Chain | Res | Type  | Atoms            |
|-----|-------|-----|-------|------------------|
| 3   | A     | 805 | POV   | C22-C23-C24-C25  |
| 3   | B     | 804 | POV   | C22-C23-C24-C25  |
| 3   | D     | 803 | POV   | C22-C23-C24-C25  |
| 3   | C     | 804 | POV   | C22-C23-C24-C25  |
| 3   | A     | 803 | POV   | O11-C1-C2-O21    |
| 3   | B     | 802 | POV   | O11-C1-C2-O21    |
| 3   | C     | 802 | POV   | O11-C1-C2-O21    |
| 3   | D     | 801 | POV   | O11-C1-C2-O21    |
| 3   | A     | 806 | POV   | C32-C31-O31-C3   |
| 3   | B     | 805 | POV   | C32-C31-O31-C3   |
| 3   | C     | 805 | POV   | C32-C31-O31-C3   |
| 3   | D     | 804 | POV   | C32-C31-O31-C3   |
| 3   | A     | 806 | POV   | O32-C31-O31-C3   |
| 3   | B     | 805 | POV   | O32-C31-O31-C3   |
| 3   | C     | 805 | POV   | O32-C31-O31-C3   |
| 3   | D     | 804 | POV   | O32-C31-O31-C3   |
| 3   | B     | 803 | POV   | C32-C33-C34-C35  |
| 3   | A     | 804 | POV   | C27-C28-C29-C210 |
| 3   | B     | 803 | POV   | C27-C28-C29-C210 |
| 3   | C     | 803 | POV   | C27-C28-C29-C210 |
| 3   | D     | 802 | POV   | C27-C28-C29-C210 |
| 3   | A     | 804 | POV   | C32-C33-C34-C35  |
| 3   | D     | 802 | POV   | C32-C33-C34-C35  |
| 3   | C     | 803 | POV   | C32-C33-C34-C35  |
| 3   | A     | 806 | POV   | C11-C12-N-C15    |
| 3   | B     | 805 | POV   | C11-C12-N-C15    |
| 3   | C     | 805 | POV   | C11-C12-N-C15    |
| 3   | D     | 804 | POV   | C11-C12-N-C15    |
| 3   | C     | 805 | POV   | C2-C1-O11-P      |
| 3   | A     | 806 | POV   | C2-C1-O11-P      |
| 3   | B     | 805 | POV   | C2-C1-O11-P      |
| 3   | D     | 804 | POV   | C2-C1-O11-P      |
| 3   | A     | 802 | POV   | C11-C12-N-C13    |
| 3   | B     | 801 | POV   | C11-C12-N-C13    |
| 3   | C     | 801 | POV   | C11-C12-N-C13    |
| 3   | C     | 807 | POV   | C11-C12-N-C13    |
| 2   | A     | 801 | A1EBL | C03-C02-C06-C11  |
| 2   | A     | 807 | A1EBL | C03-C02-C06-C11  |
| 2   | B     | 806 | A1EBL | C03-C02-C06-C11  |
| 2   | C     | 806 | A1EBL | C03-C02-C06-C11  |
| 3   | A     | 803 | POV   | C11-C12-N-C15    |
| 3   | B     | 802 | POV   | C11-C12-N-C15    |

*Continued on next page...*

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 3   | C     | 802 | POV  | C11-C12-N-C15   |
| 3   | D     | 801 | POV  | C11-C12-N-C15   |
| 3   | A     | 805 | POV  | C26-C27-C28-C29 |
| 3   | B     | 804 | POV  | C26-C27-C28-C29 |
| 3   | C     | 804 | POV  | C26-C27-C28-C29 |
| 3   | D     | 803 | POV  | C26-C27-C28-C29 |
| 3   | A     | 804 | POV  | C1-C2-O21-C21   |
| 3   | B     | 803 | POV  | C1-C2-O21-C21   |
| 3   | C     | 803 | POV  | C1-C2-O21-C21   |
| 3   | D     | 802 | POV  | C1-C2-O21-C21   |
| 3   | A     | 804 | POV  | C26-C27-C28-C29 |
| 3   | C     | 803 | POV  | C26-C27-C28-C29 |
| 3   | B     | 804 | POV  | O31-C31-C32-C33 |
| 3   | C     | 804 | POV  | O31-C31-C32-C33 |
| 3   | A     | 805 | POV  | O31-C31-C32-C33 |
| 3   | D     | 803 | POV  | O31-C31-C32-C33 |
| 3   | B     | 803 | POV  | C26-C27-C28-C29 |
| 3   | D     | 802 | POV  | C26-C27-C28-C29 |

There are no ring outliers.

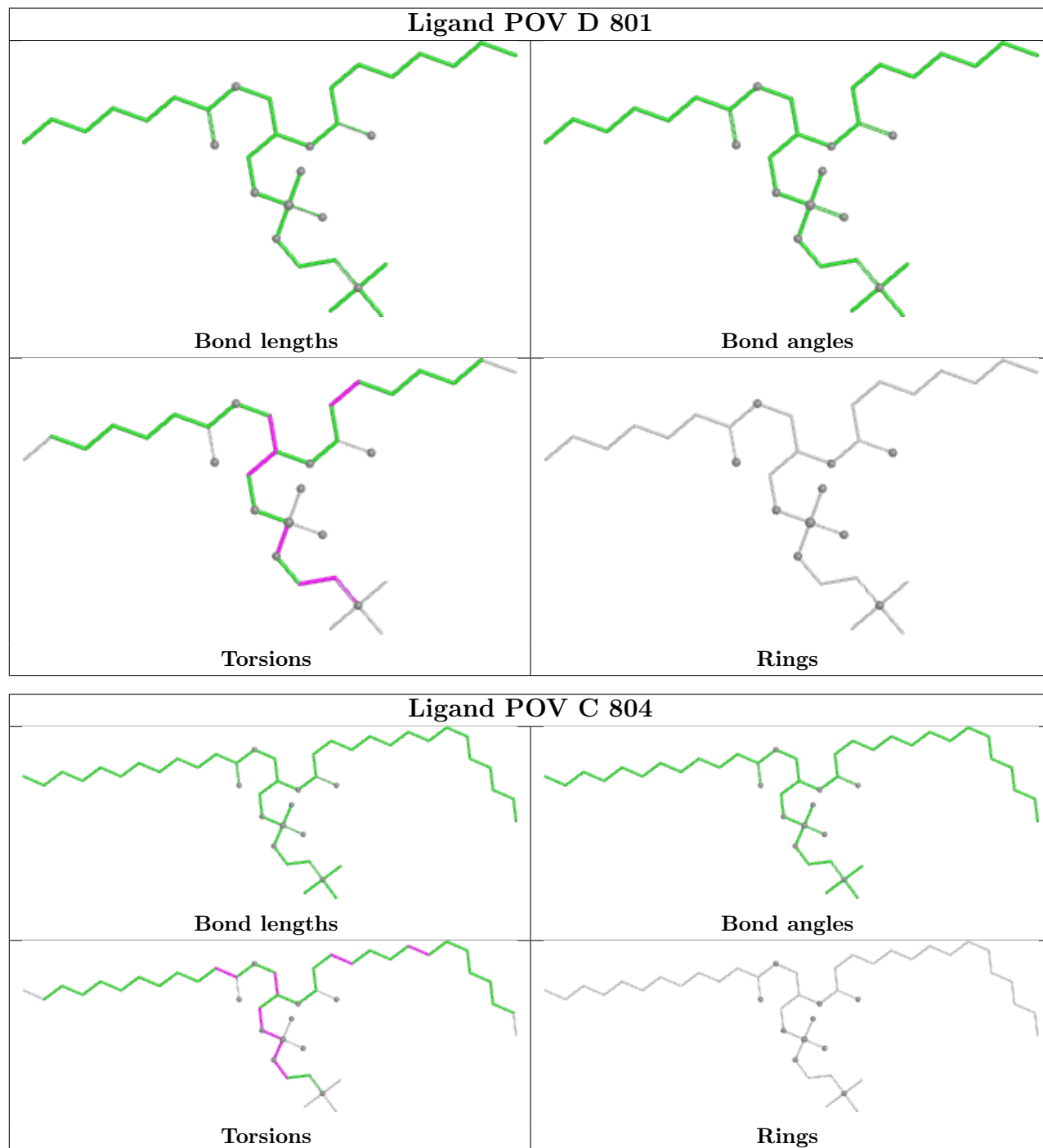
16 monomers are involved in 25 short contacts:

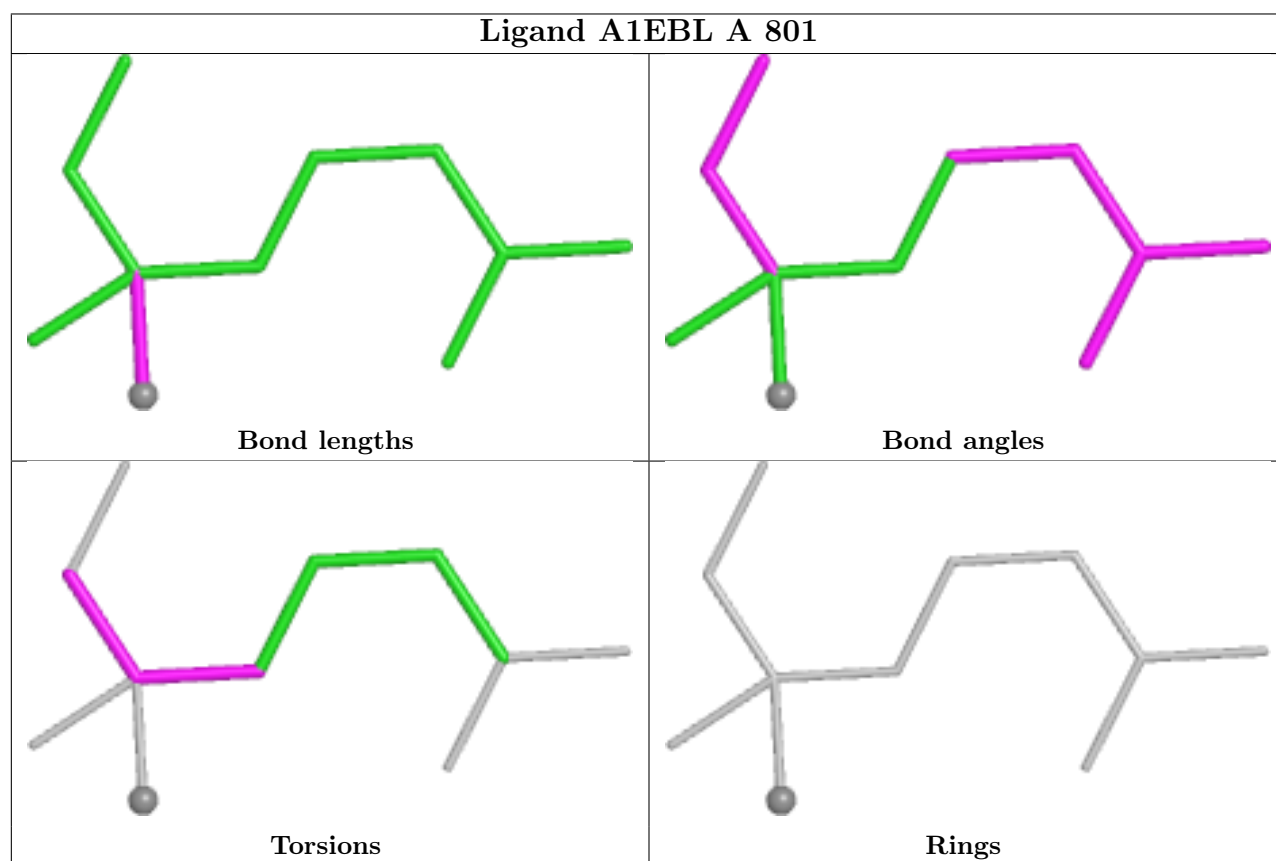
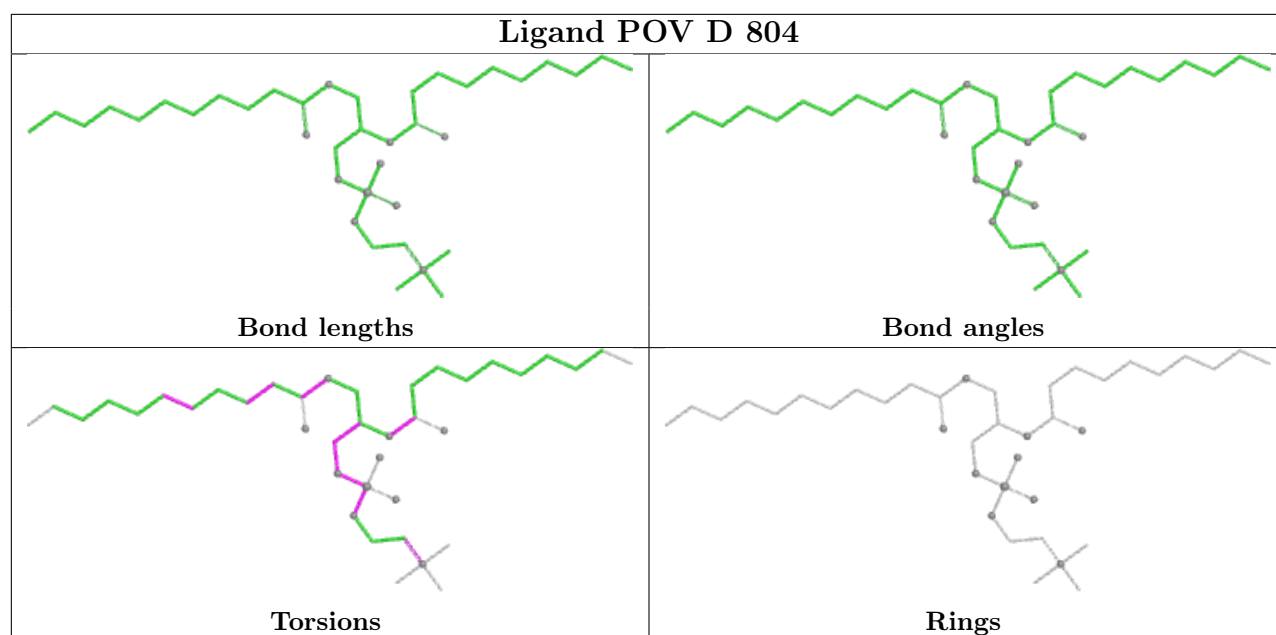
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | C     | 804 | POV  | 1       | 0            |
| 3   | D     | 804 | POV  | 1       | 0            |
| 3   | B     | 804 | POV  | 1       | 0            |
| 3   | C     | 807 | POV  | 2       | 0            |
| 3   | A     | 804 | POV  | 2       | 0            |
| 3   | A     | 802 | POV  | 2       | 0            |
| 3   | B     | 805 | POV  | 1       | 0            |
| 3   | D     | 803 | POV  | 1       | 0            |
| 3   | B     | 801 | POV  | 3       | 0            |
| 3   | D     | 802 | POV  | 2       | 0            |
| 3   | A     | 806 | POV  | 1       | 0            |
| 3   | A     | 805 | POV  | 1       | 0            |
| 3   | C     | 805 | POV  | 1       | 0            |
| 3   | B     | 803 | POV  | 2       | 0            |
| 3   | C     | 803 | POV  | 2       | 0            |
| 3   | C     | 801 | POV  | 2       | 0            |

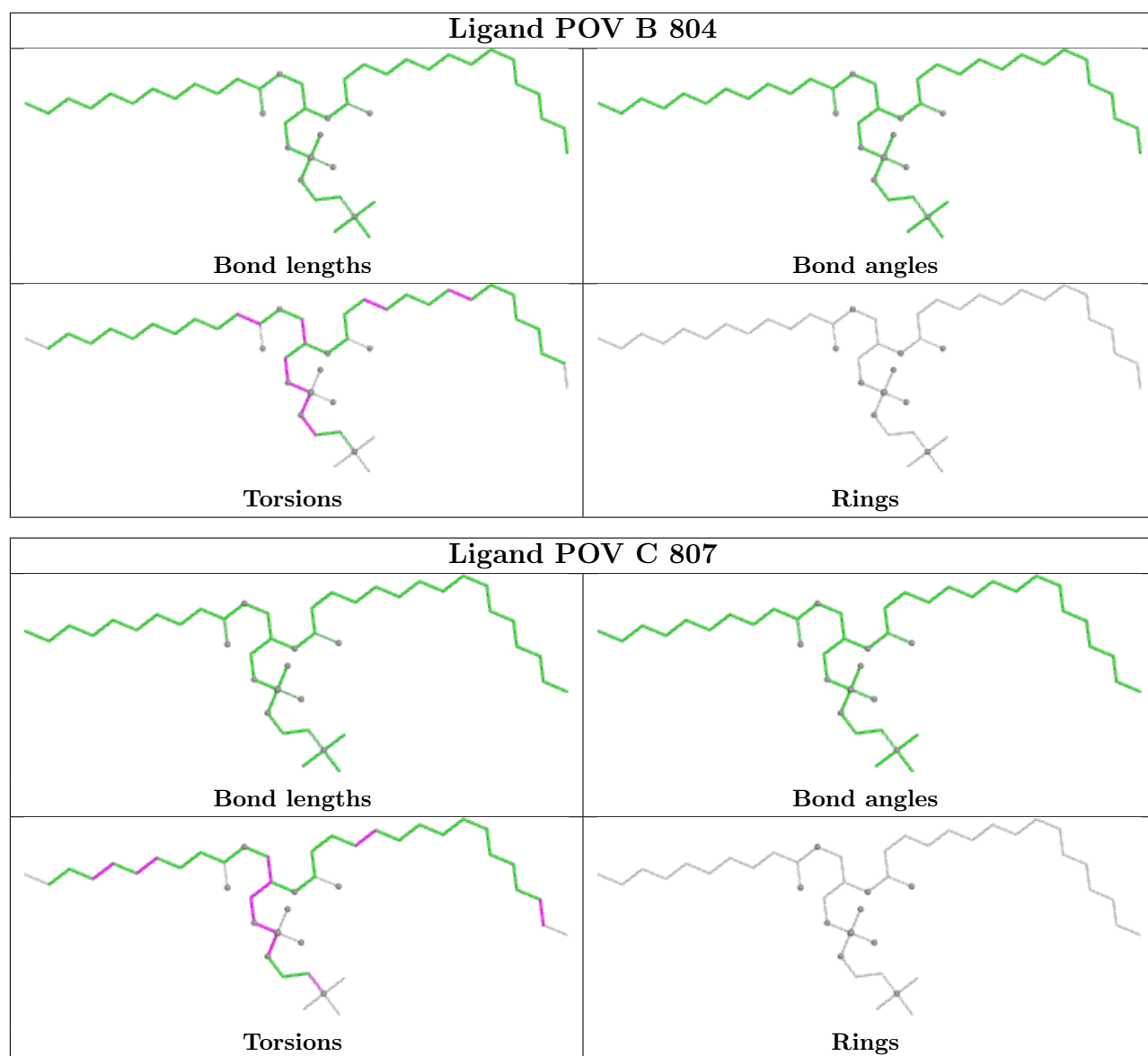
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

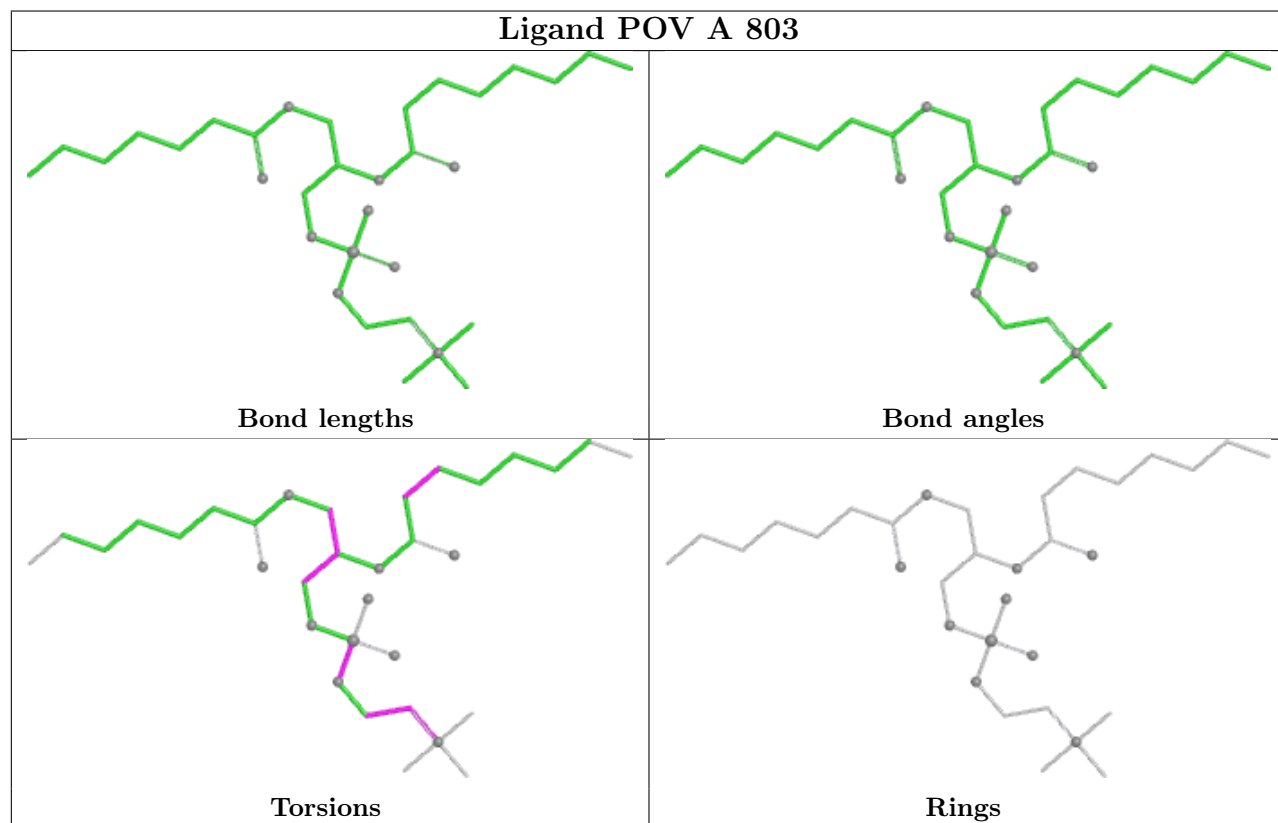
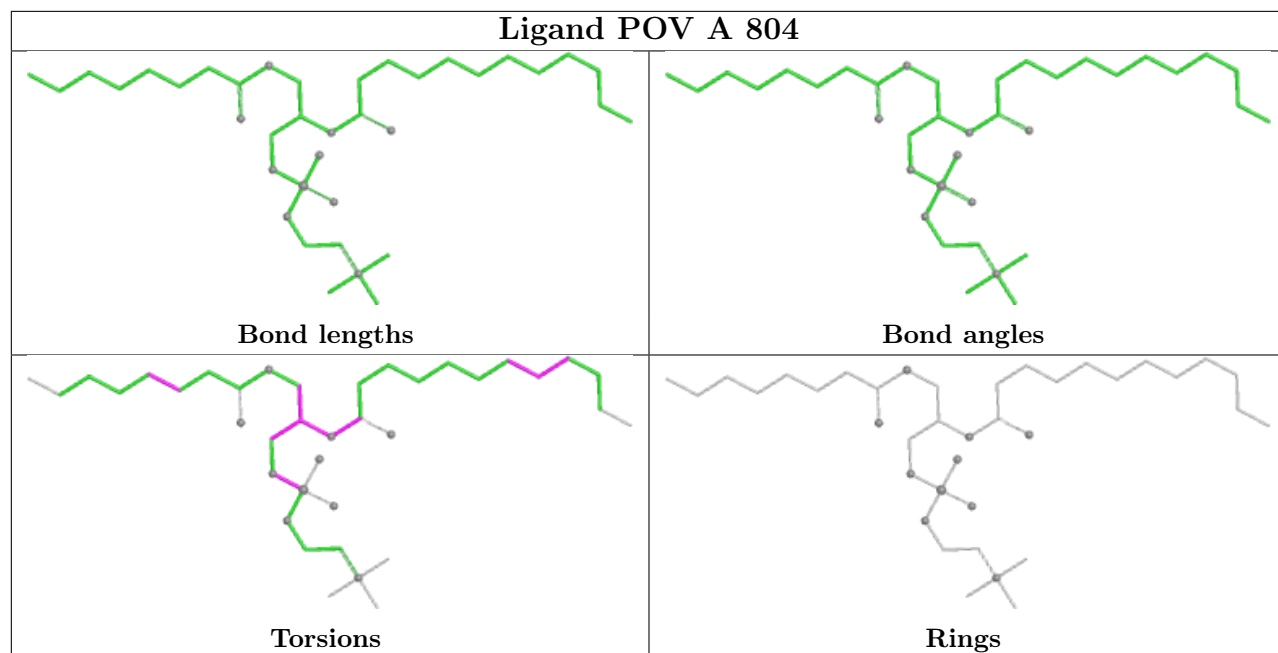


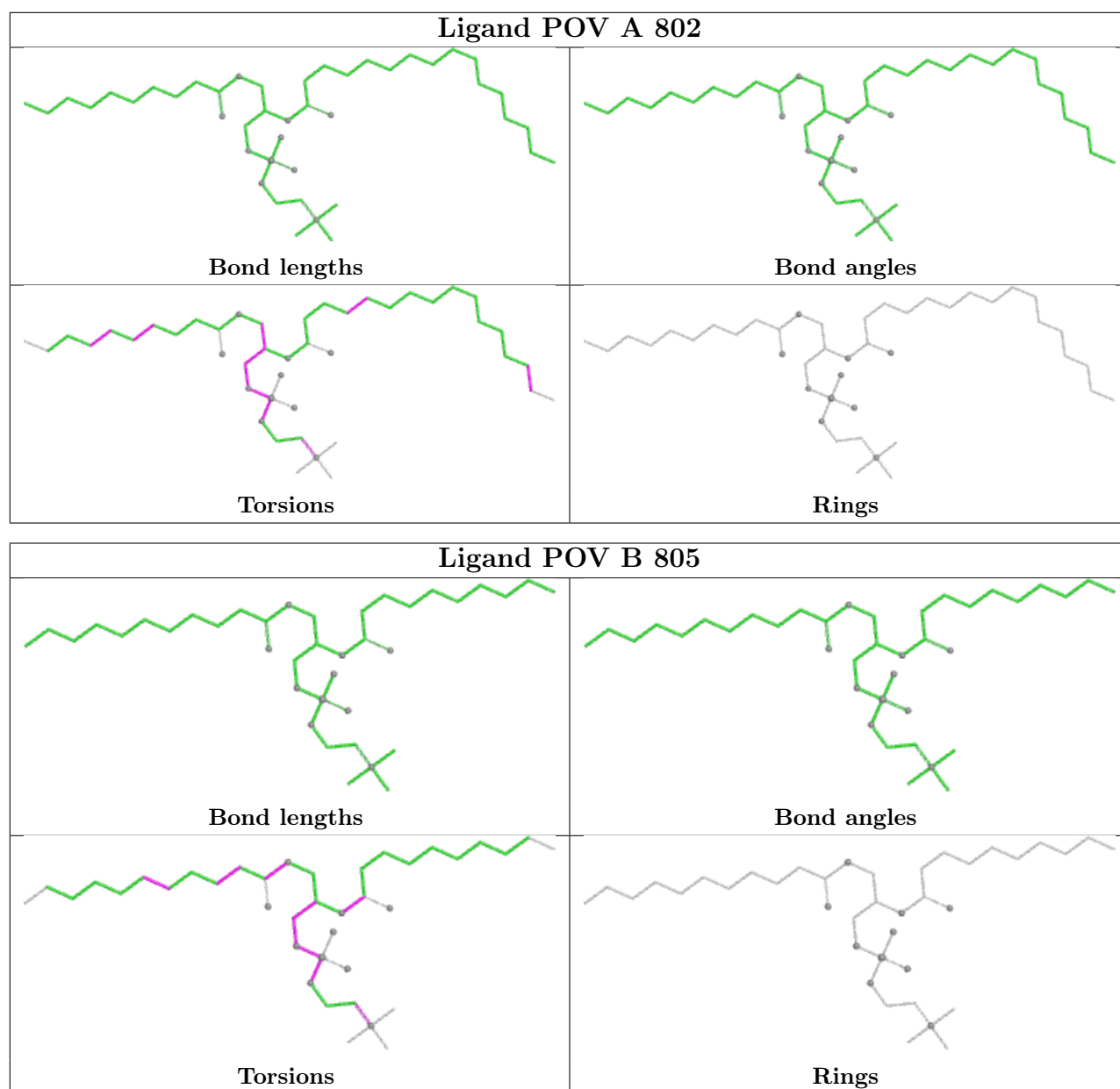
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.



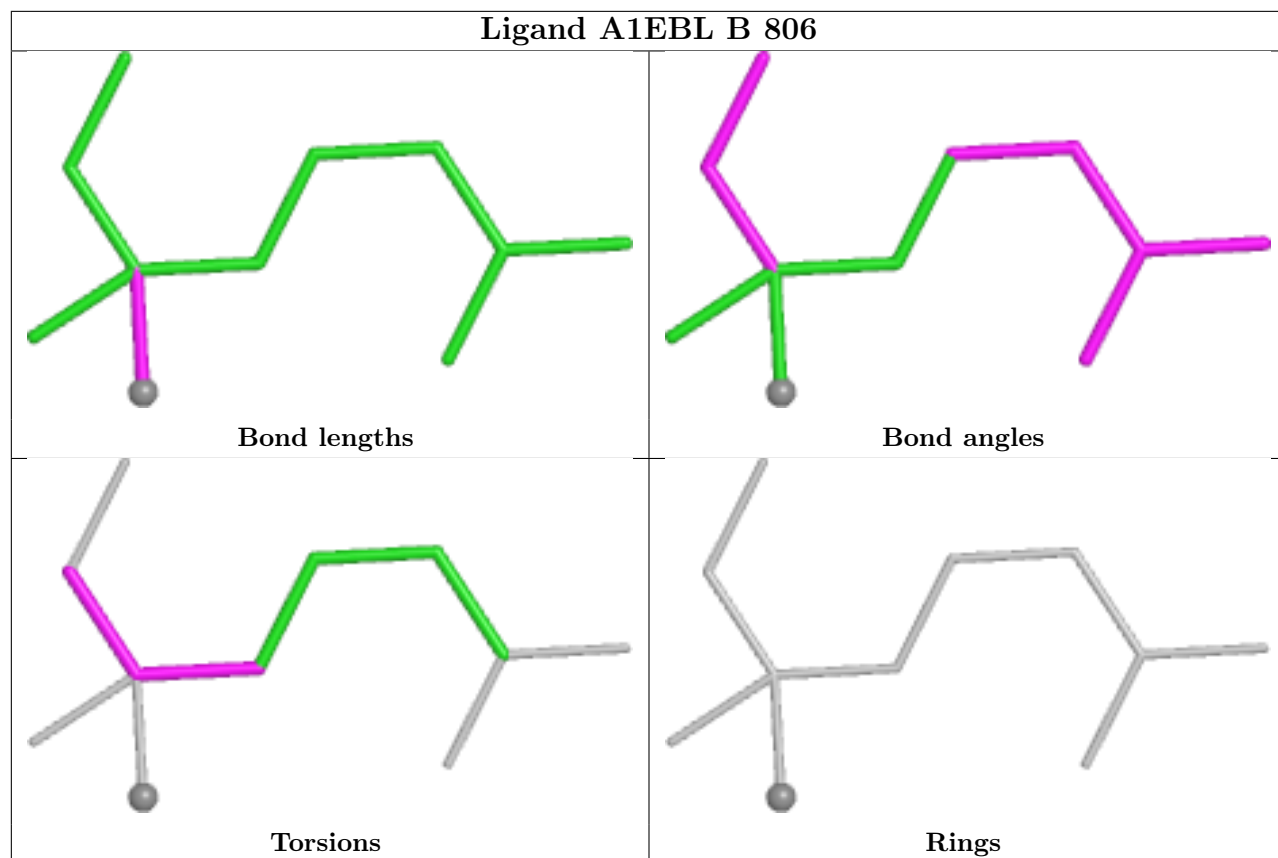




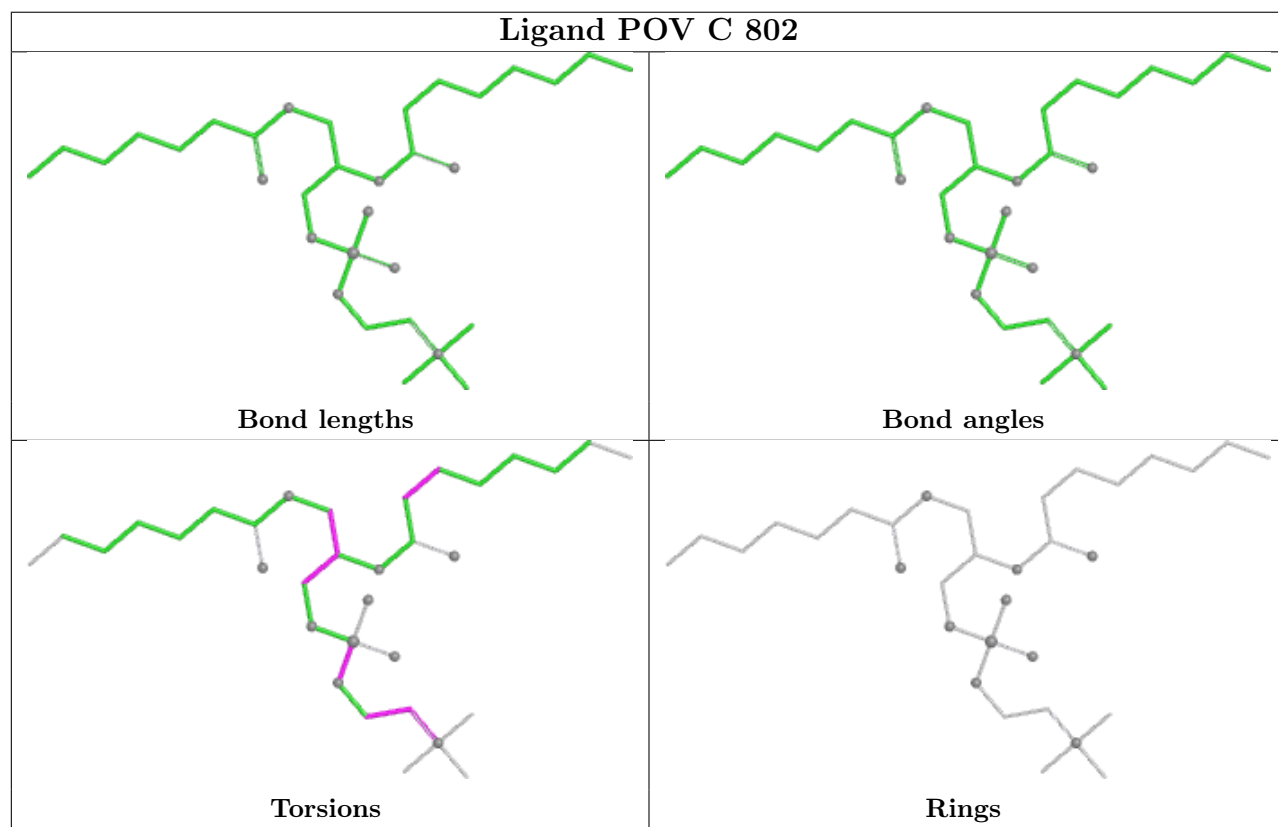


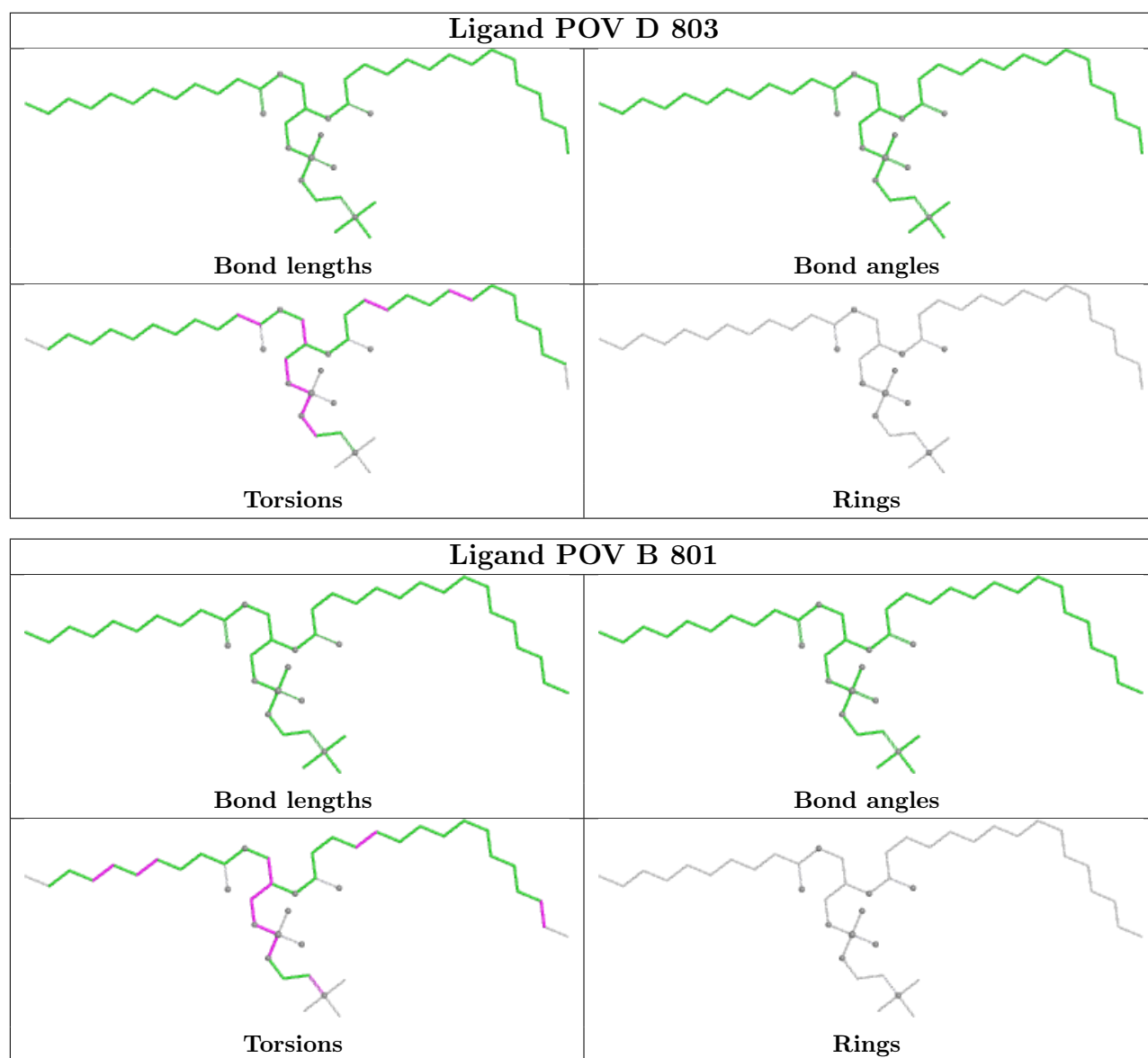


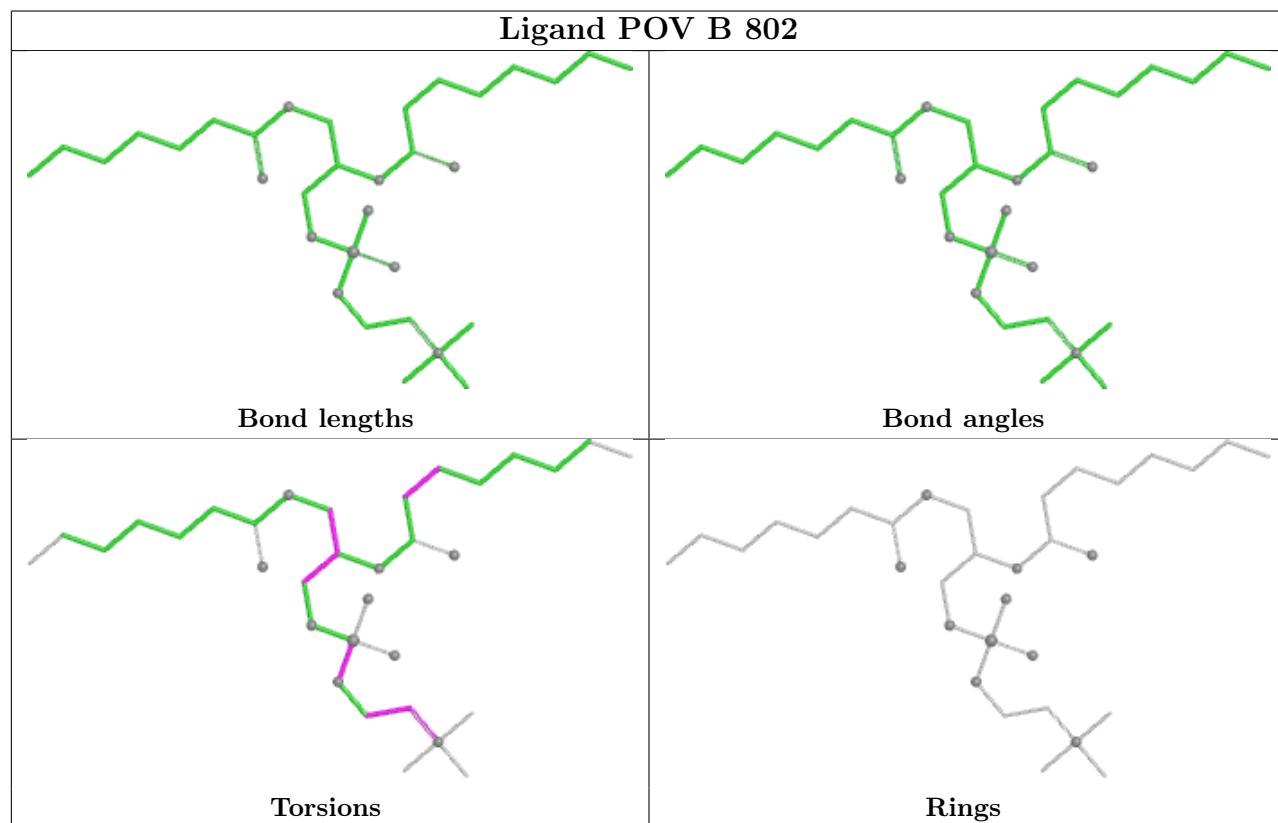
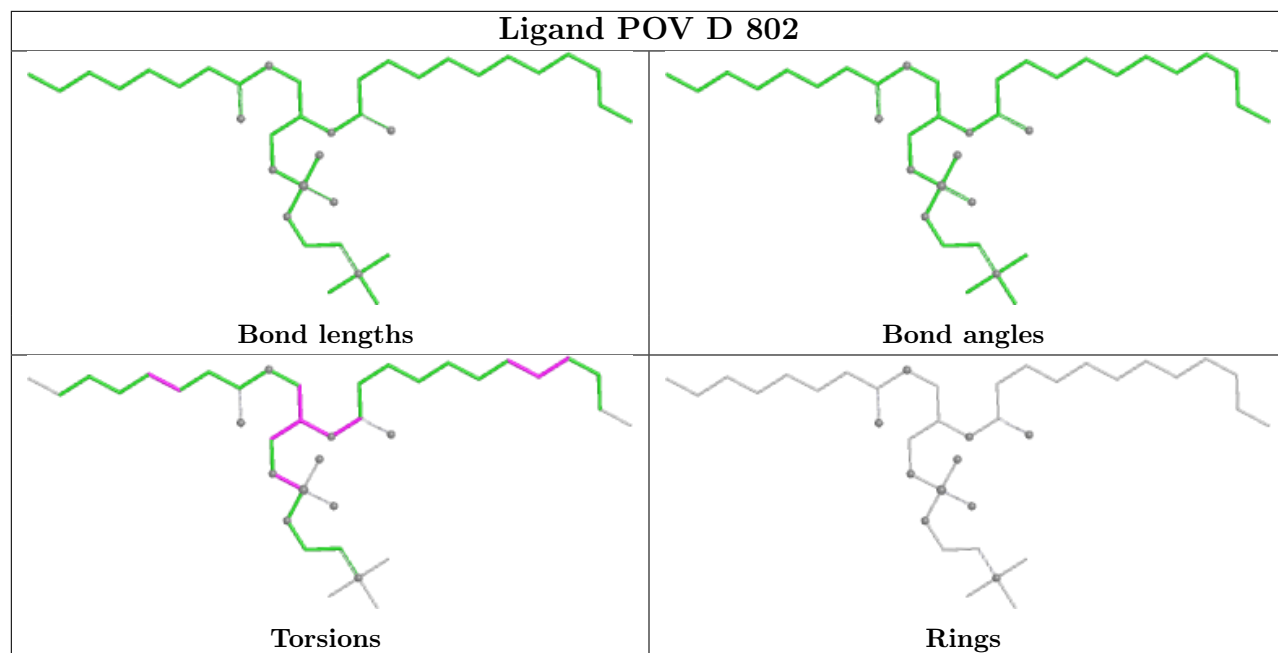
## Ligand A1EBL B 806



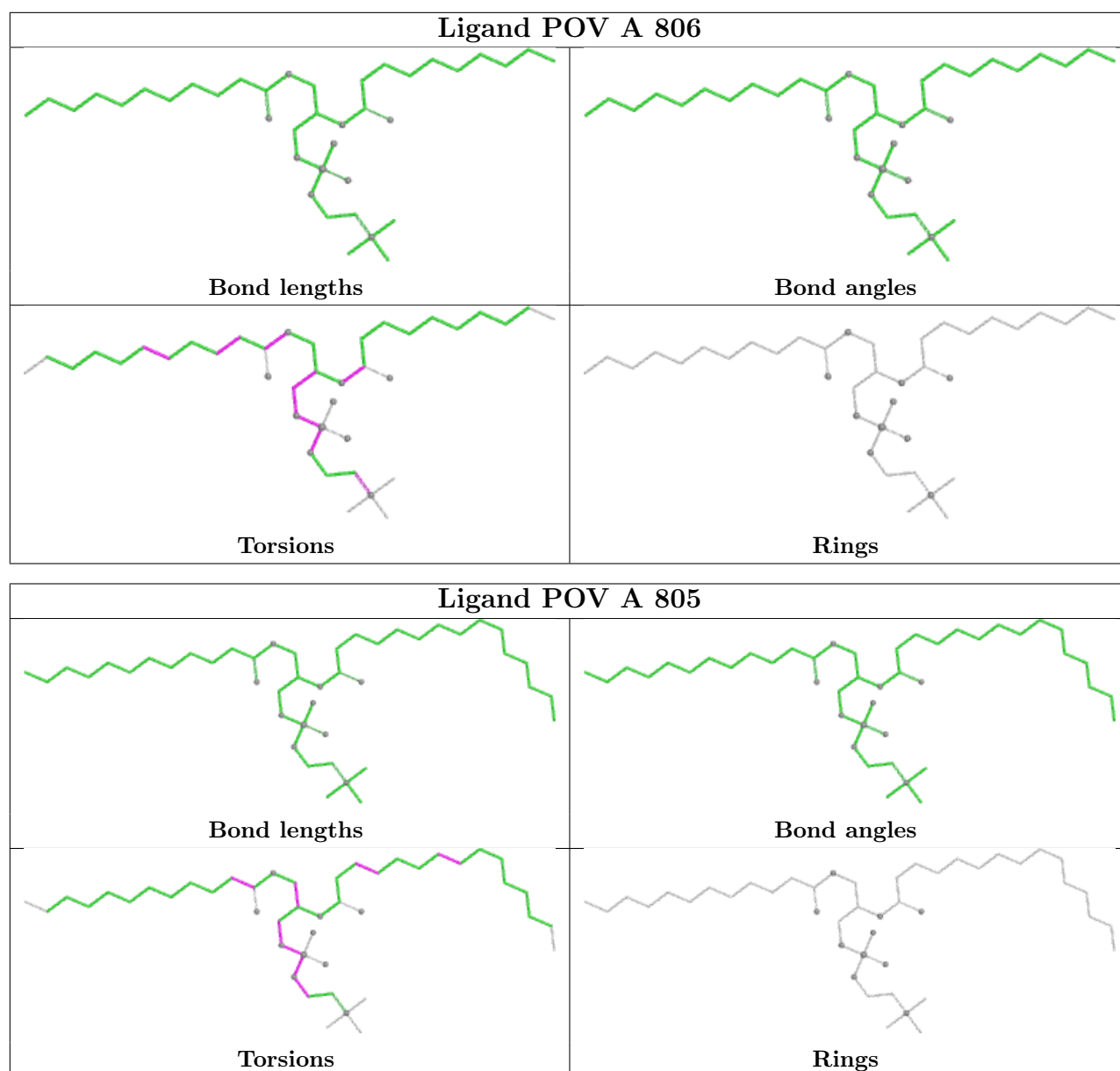
## Ligand POV C 802

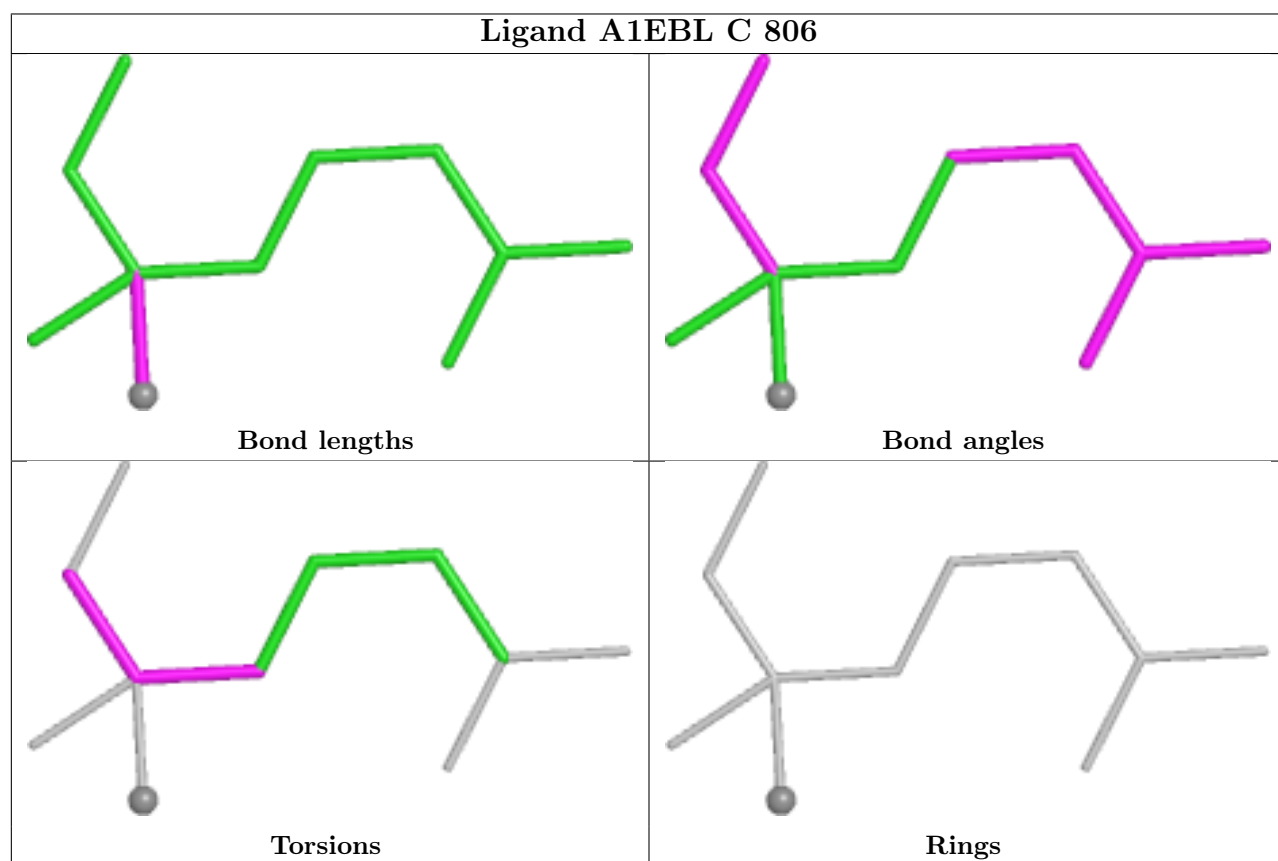
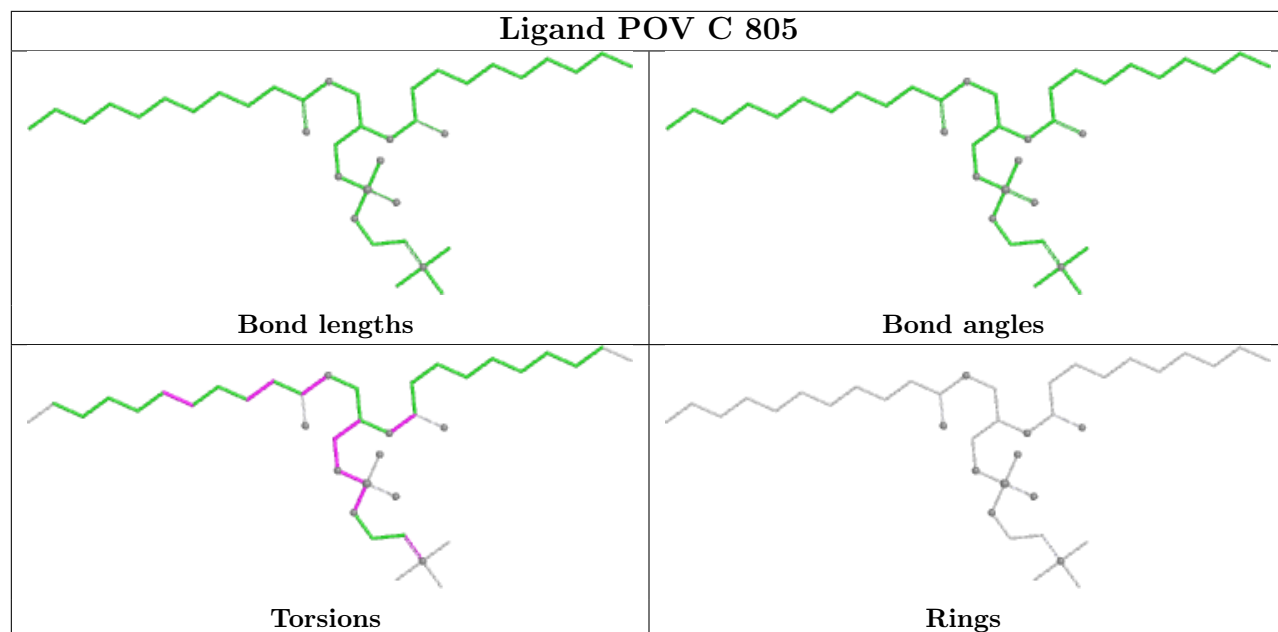


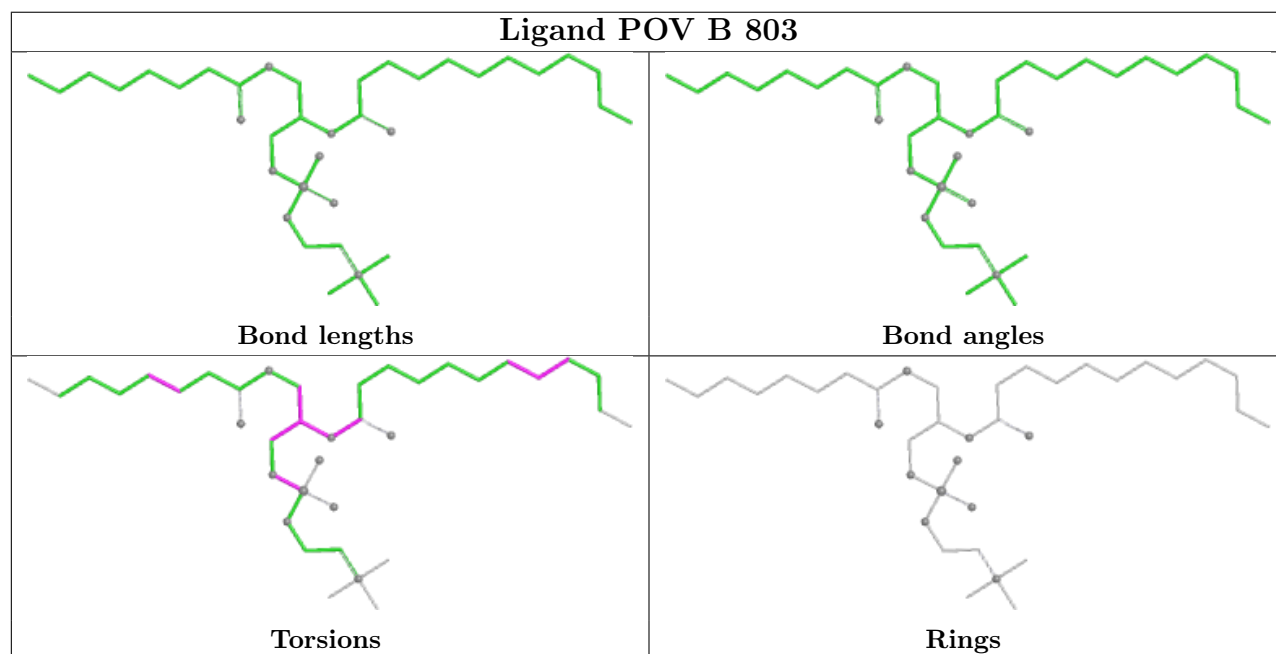
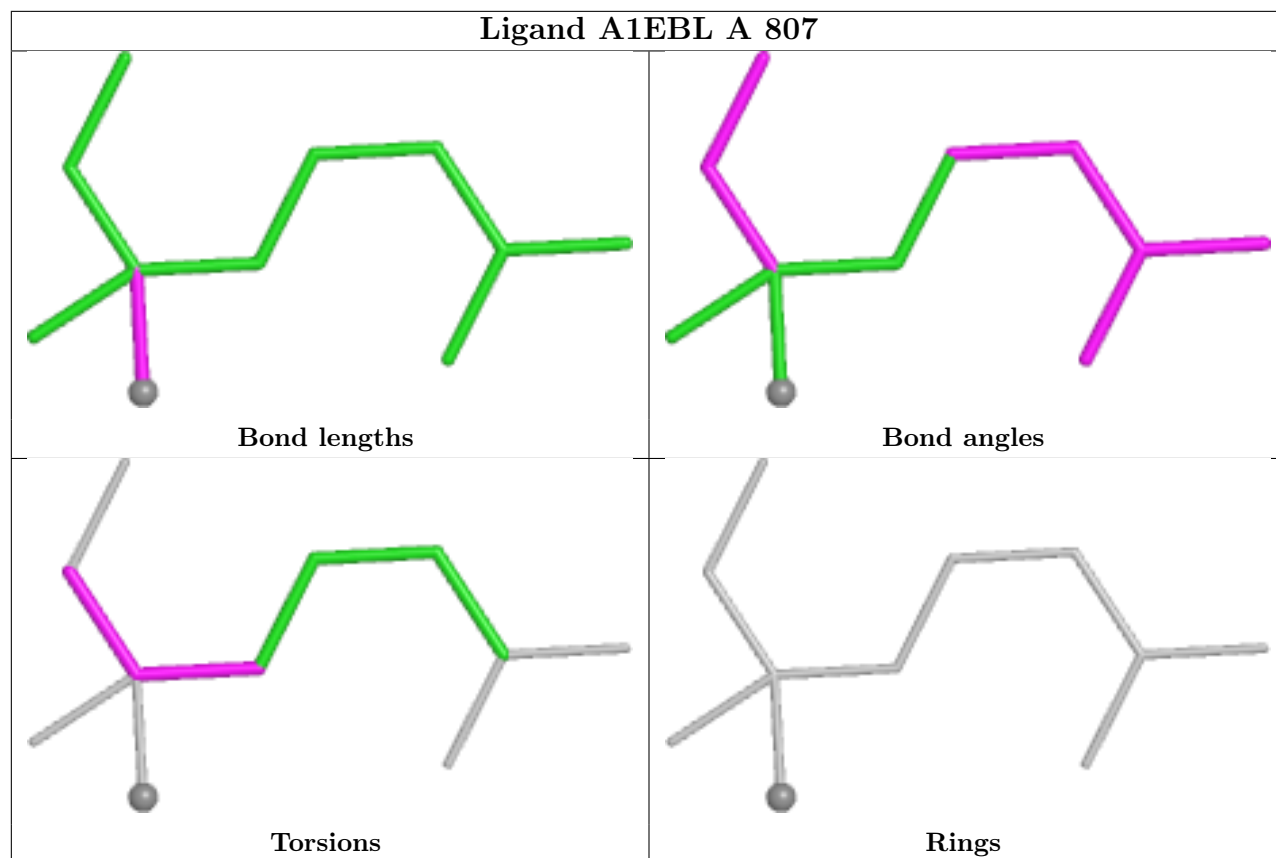


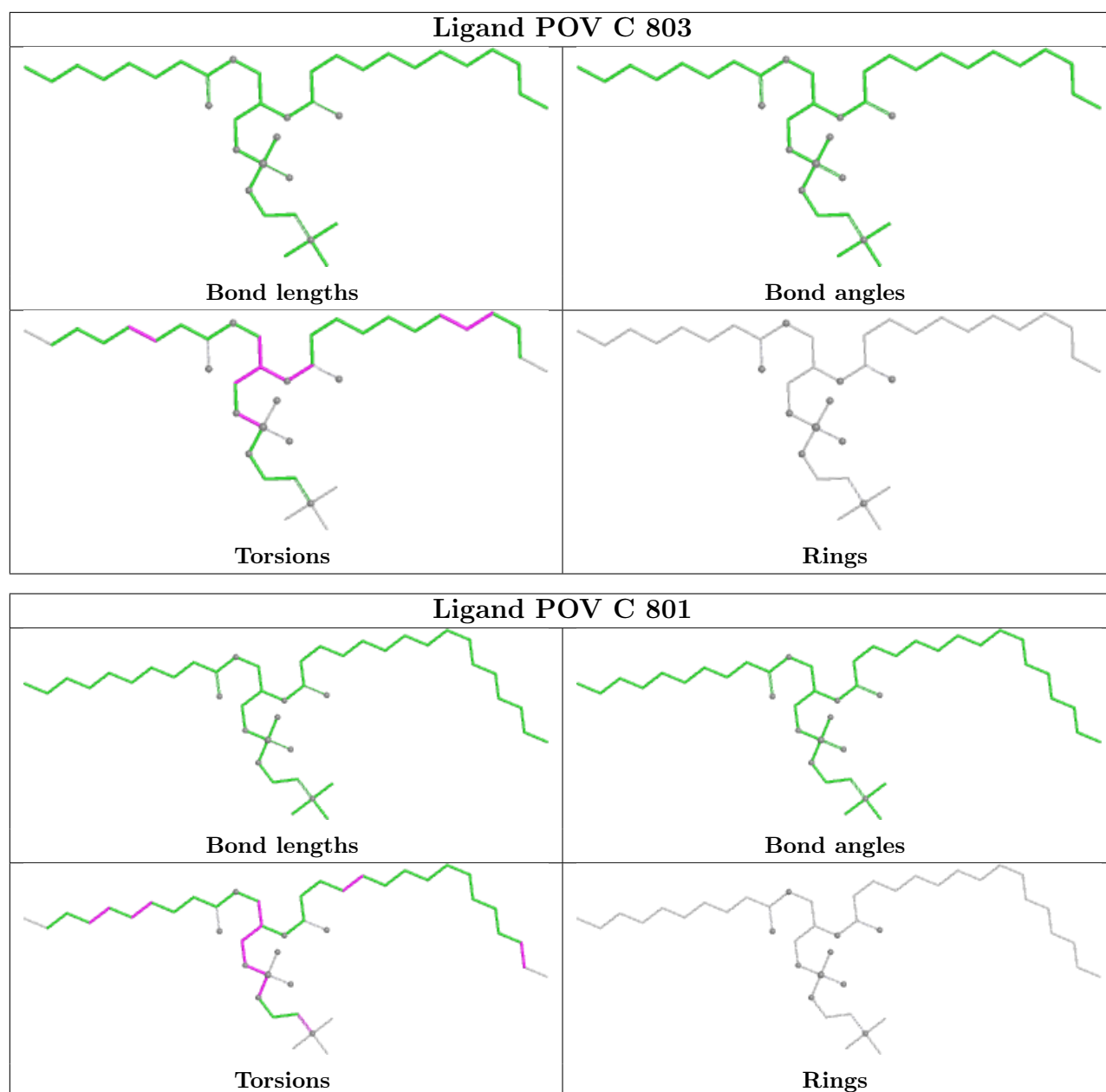












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

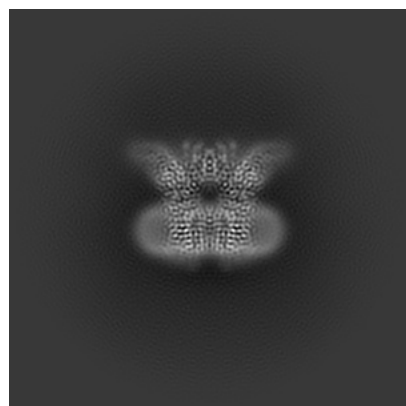
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-61415. These allow visual inspection of the internal detail of the map and identification of artifacts.

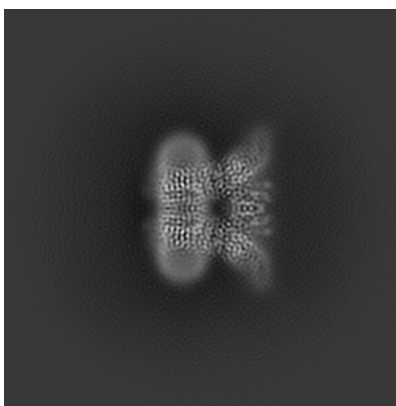
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

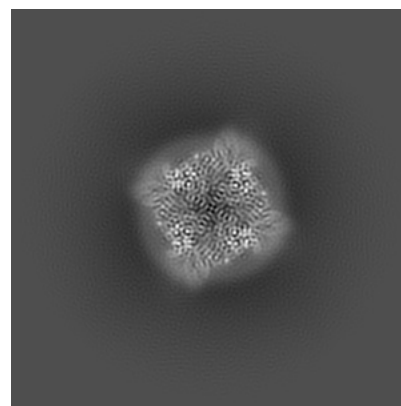
#### 6.1.1 Primary map



X

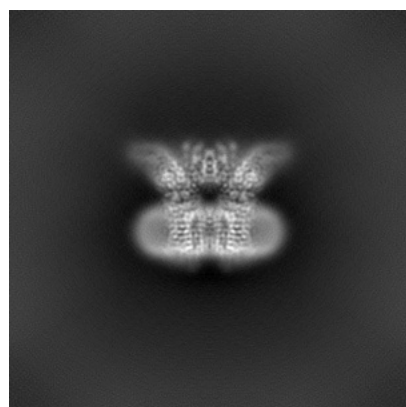


Y

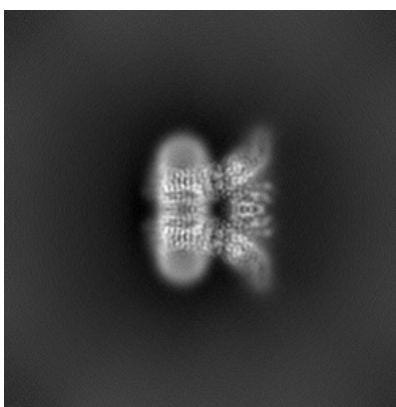


Z

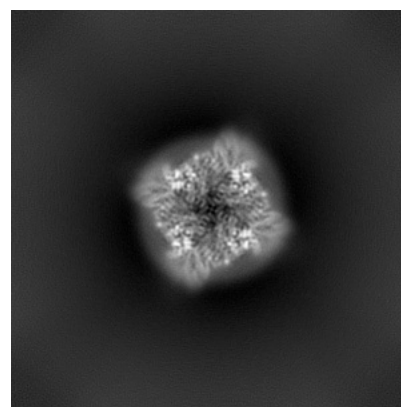
#### 6.1.2 Raw map



X



Y

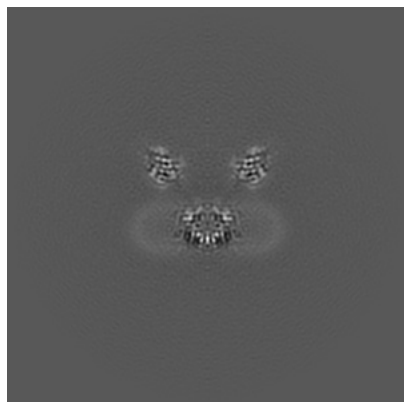


Z

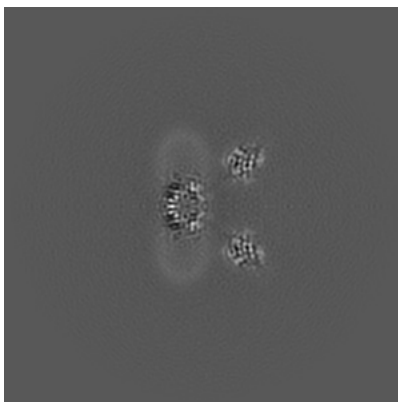
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

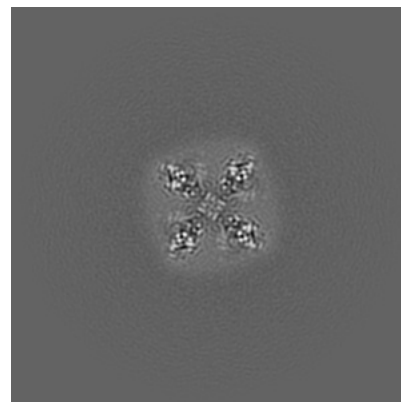
### 6.2.1 Primary map



X Index: 160

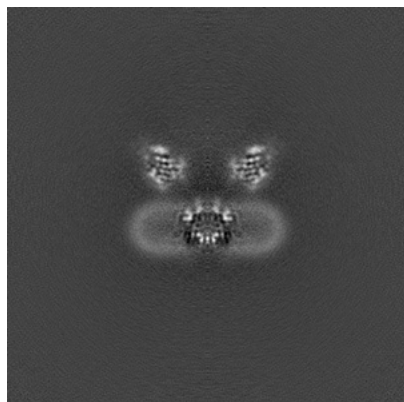


Y Index: 160

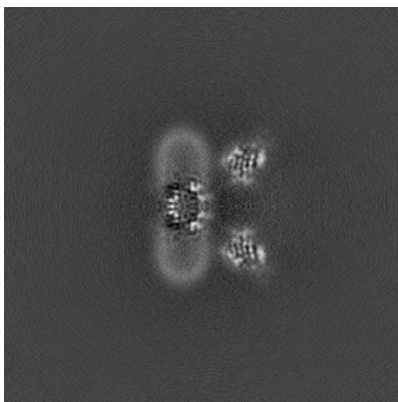


Z Index: 160

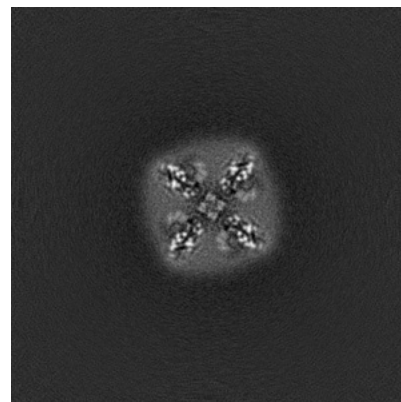
### 6.2.2 Raw map



X Index: 160



Y Index: 160

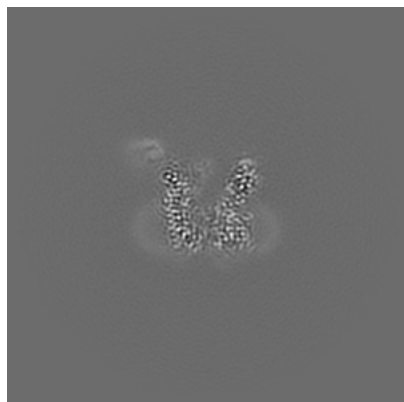


Z Index: 160

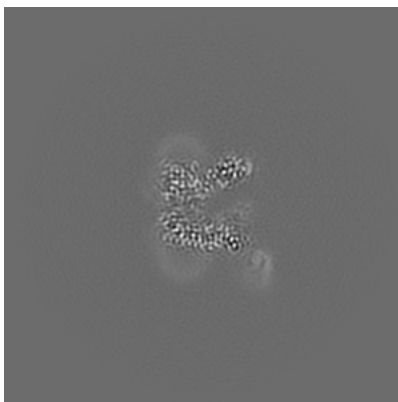
The images above show central slices of the map in three orthogonal directions.

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

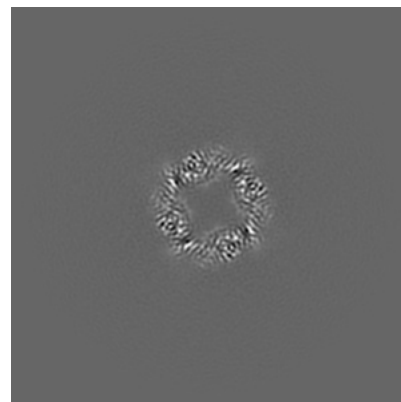
### 6.3.1 Primary map



X Index: 141

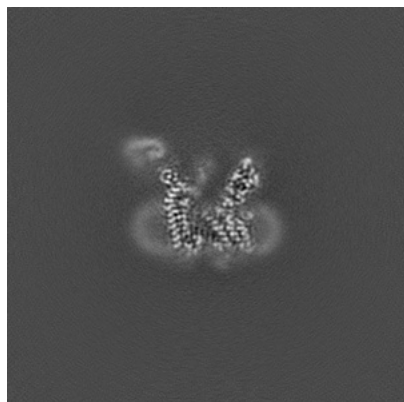


Y Index: 179

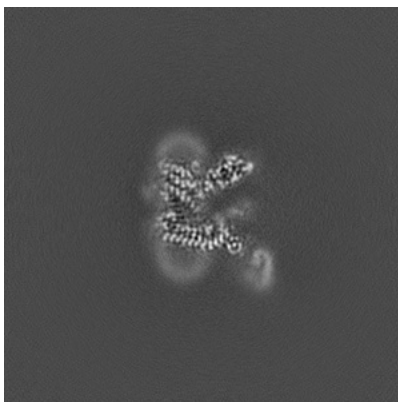


Z Index: 184

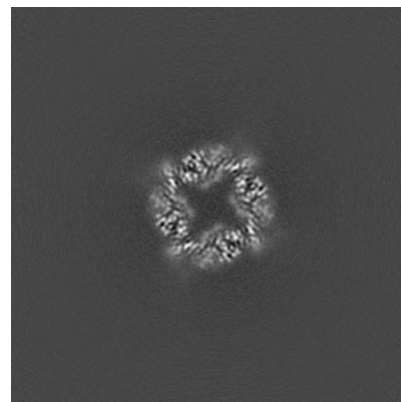
### 6.3.2 Raw map



X Index: 142



Y Index: 178

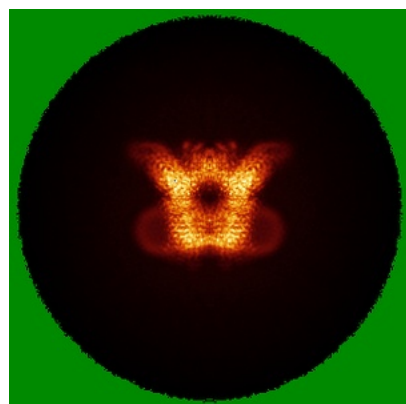


Z Index: 184

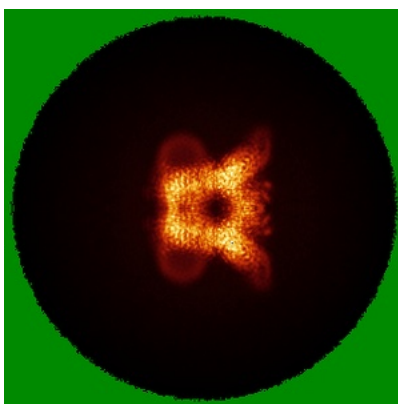
The images above show the largest variance slices of the map in three orthogonal directions.

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

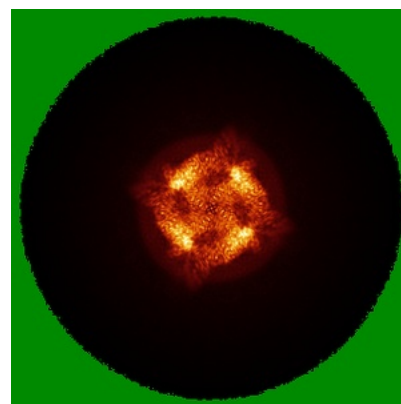
### 6.4.1 Primary map



X

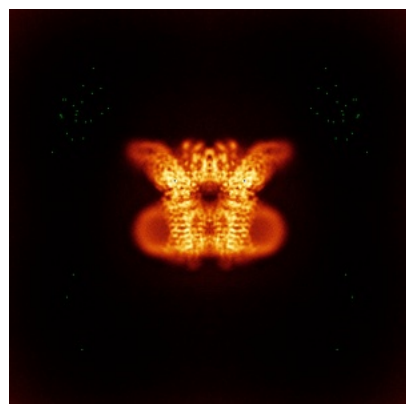


Y

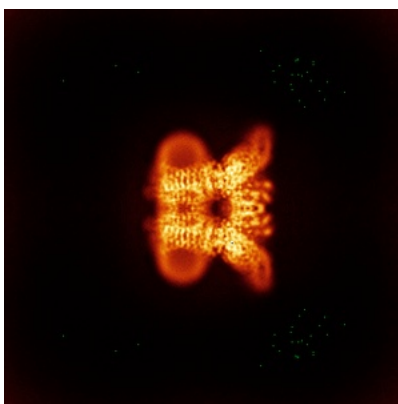


Z

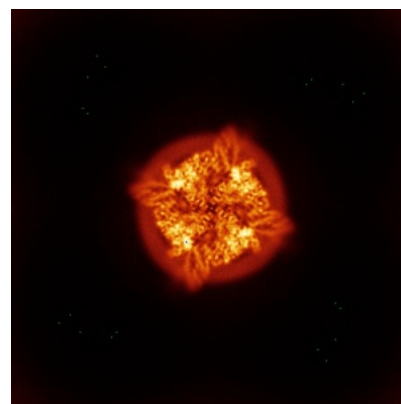
### 6.4.2 Raw map



X



Y



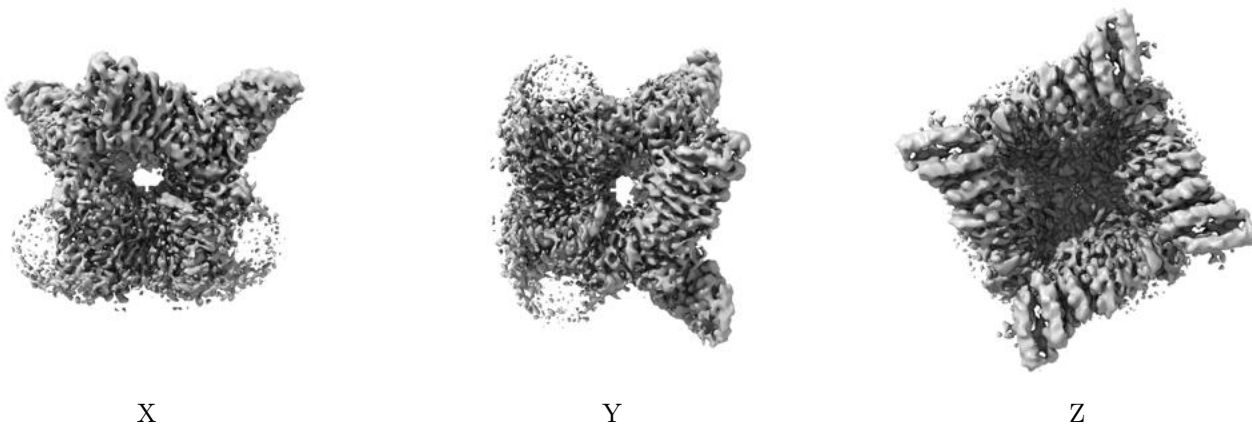
Z

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.



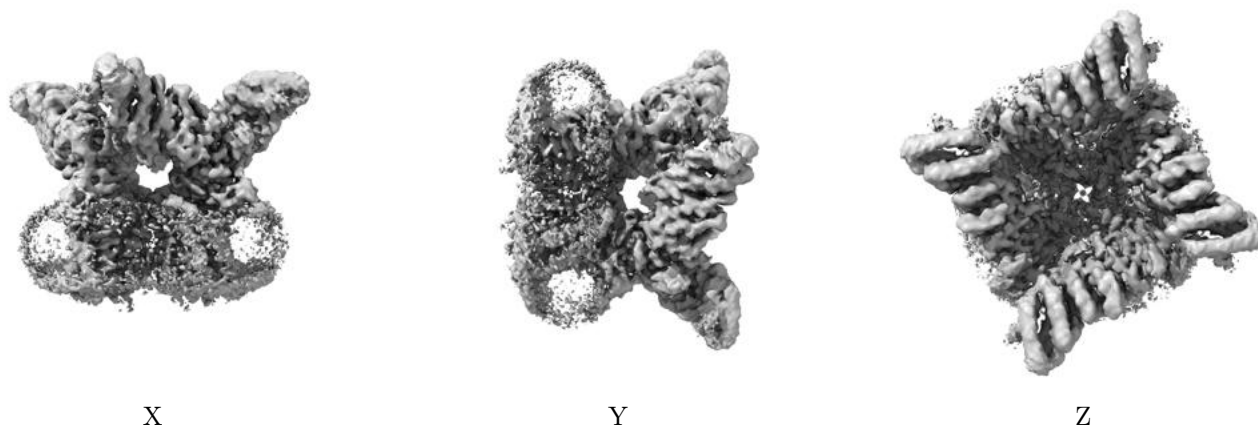
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.16. 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.

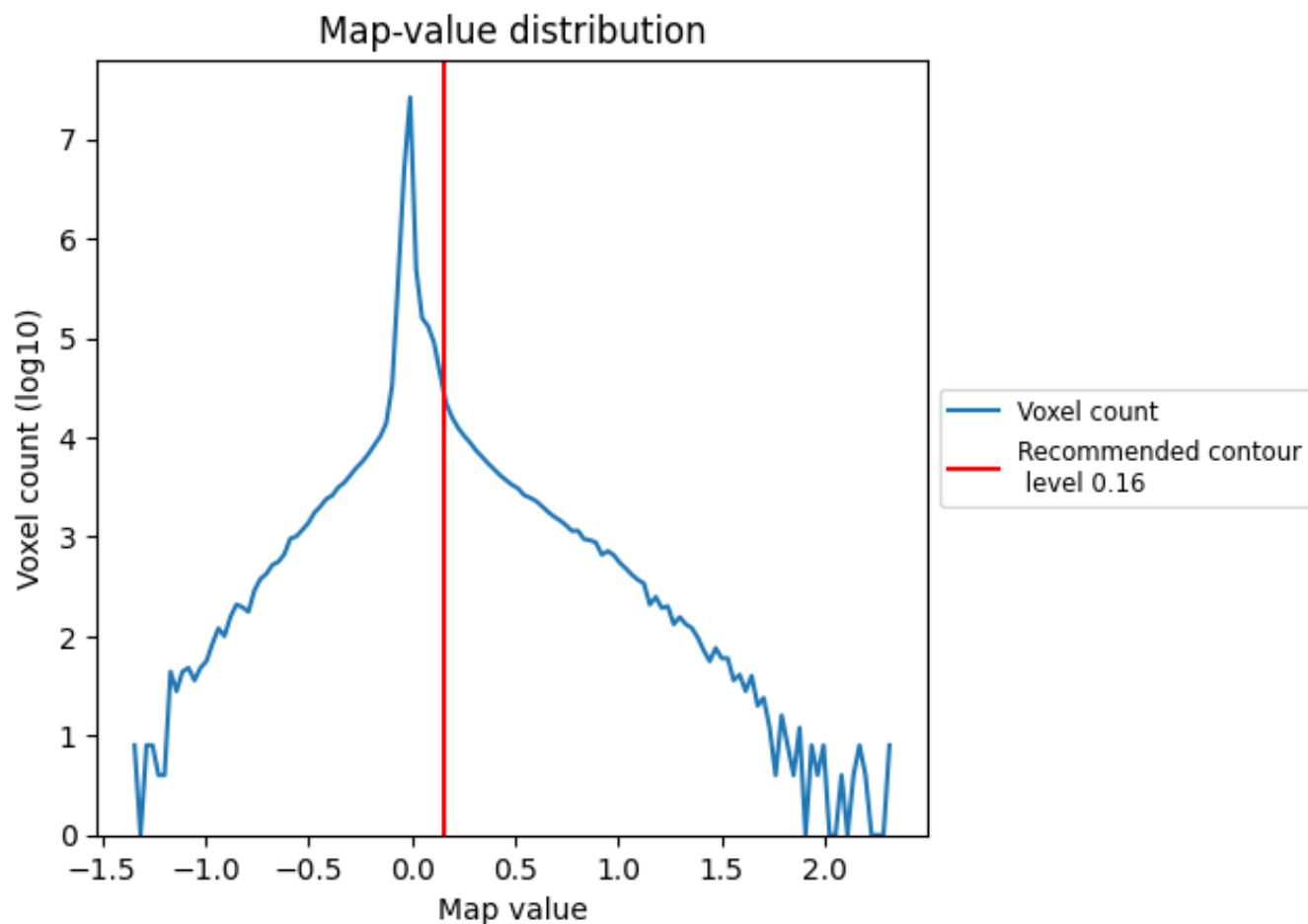
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

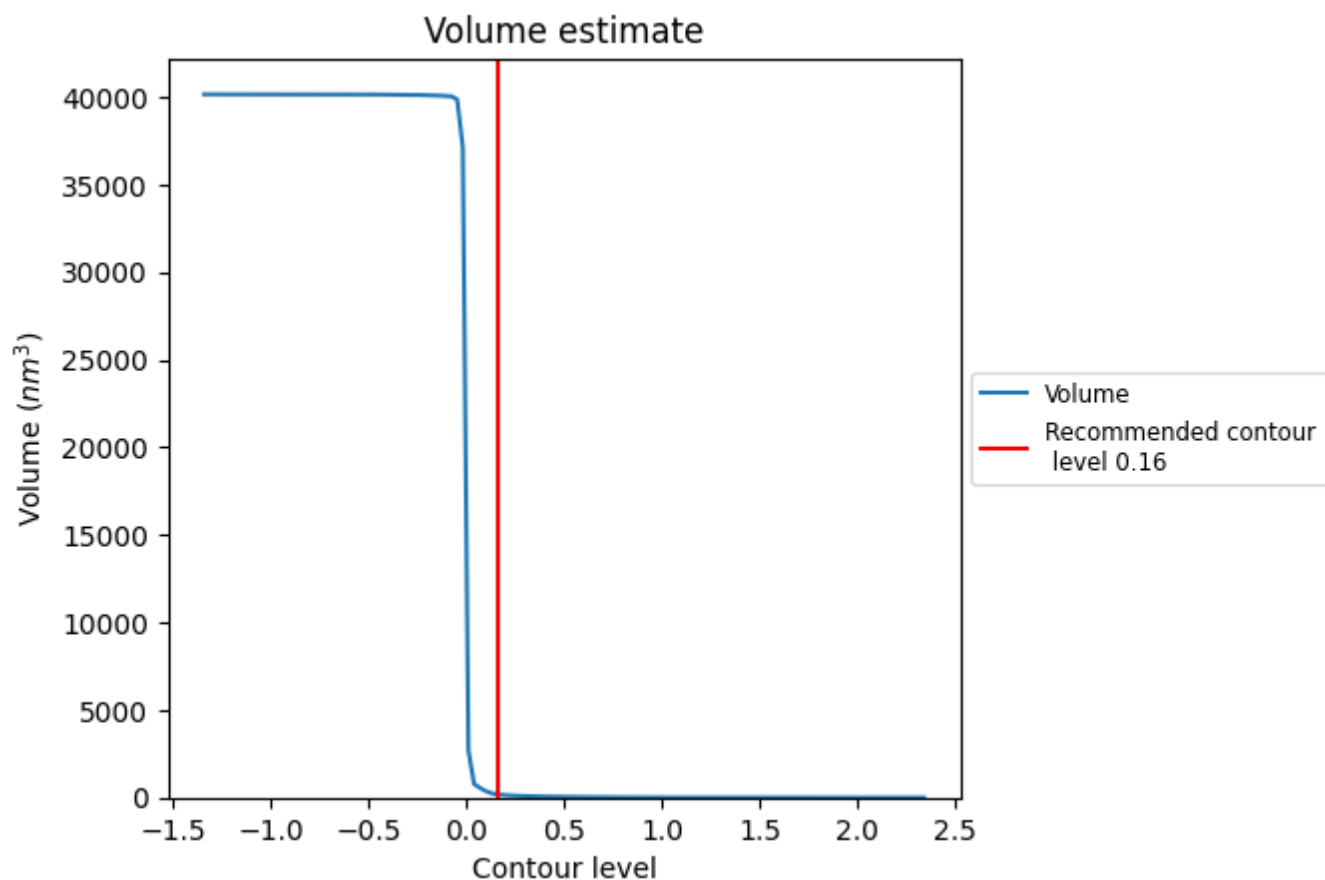
This section contains the results of statistical analysis of the map.

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



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

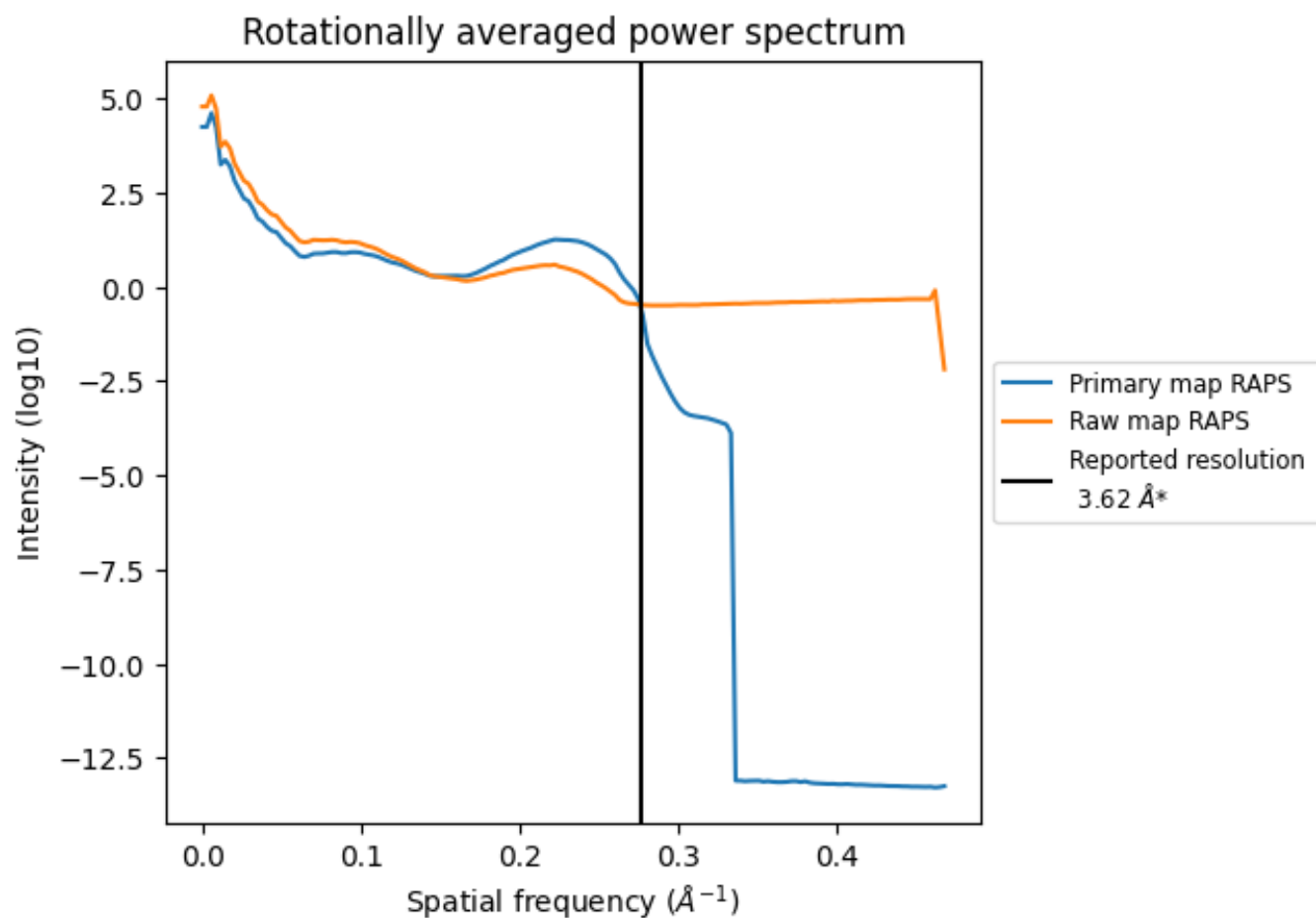
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 175  $\text{nm}^3$ ; this corresponds to an approximate mass of 158 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 ⓘ

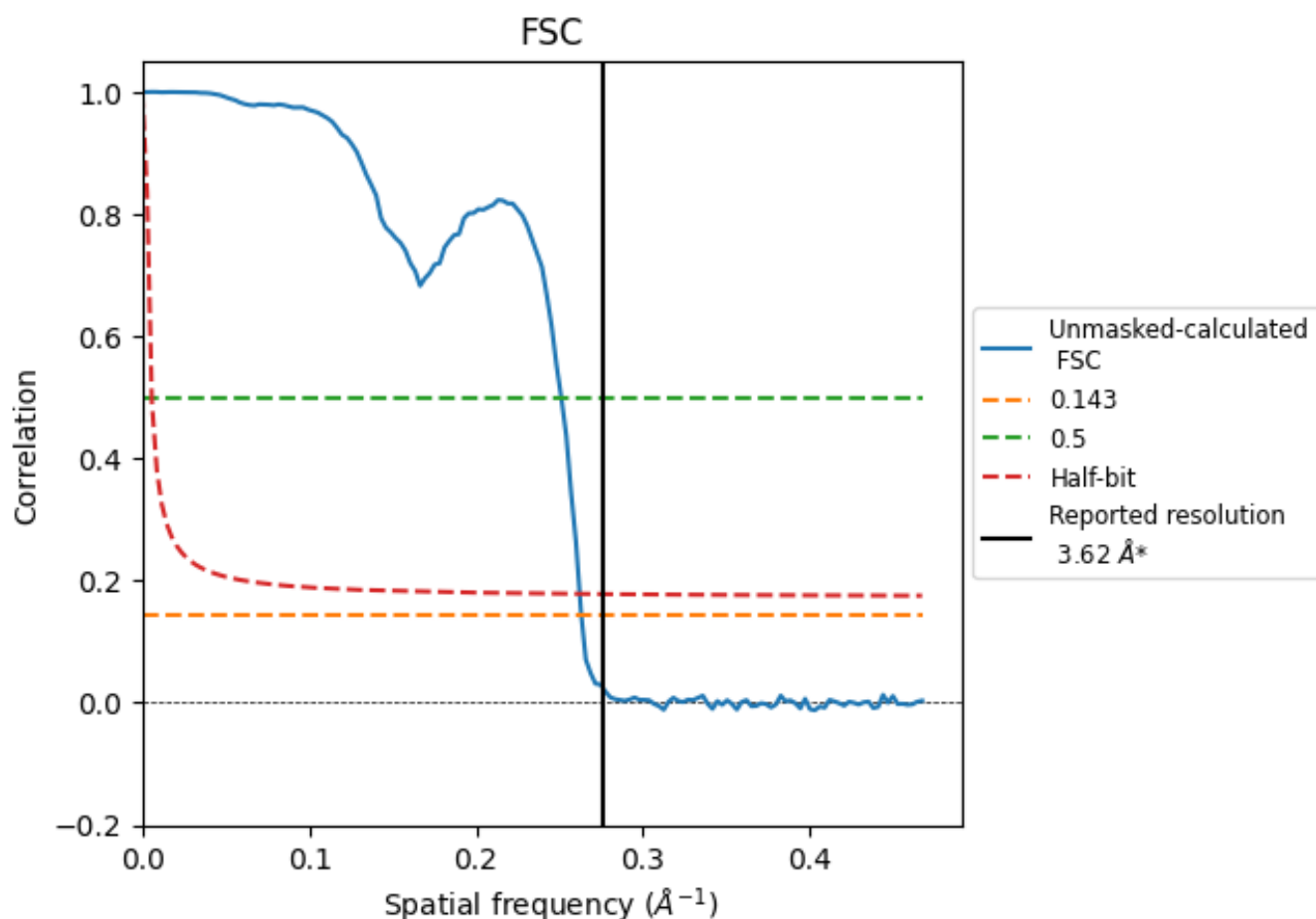


\*Reported resolution corresponds to spatial frequency of 0.276 Å<sup>-1</sup>

## 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  $0.276 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

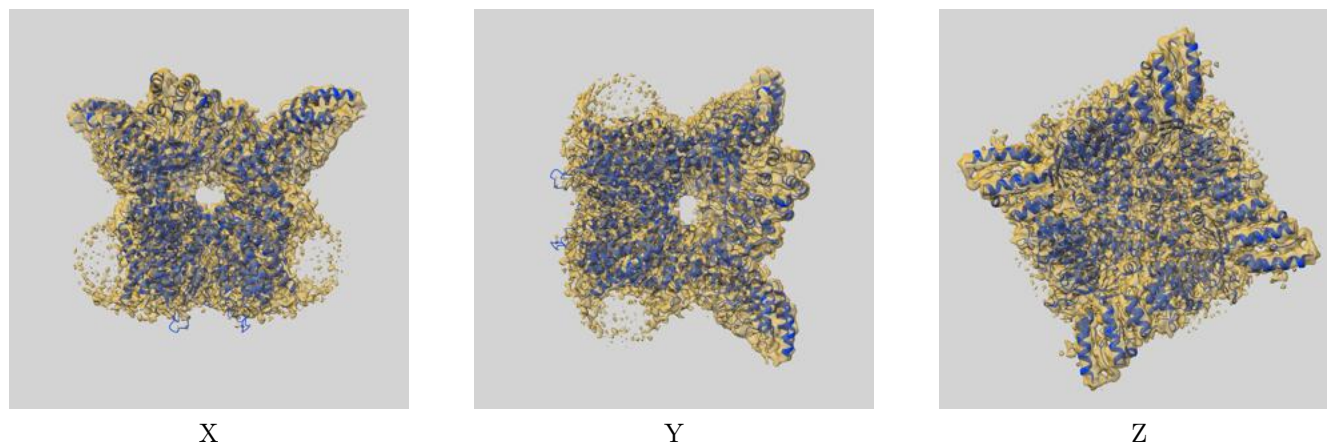
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 3.62                               | -    | -        |
| Author-provided FSC curve | -                                  | -    | -        |
| Unmasked-calculated*      | 3.80                               | 3.98 | 3.82     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

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

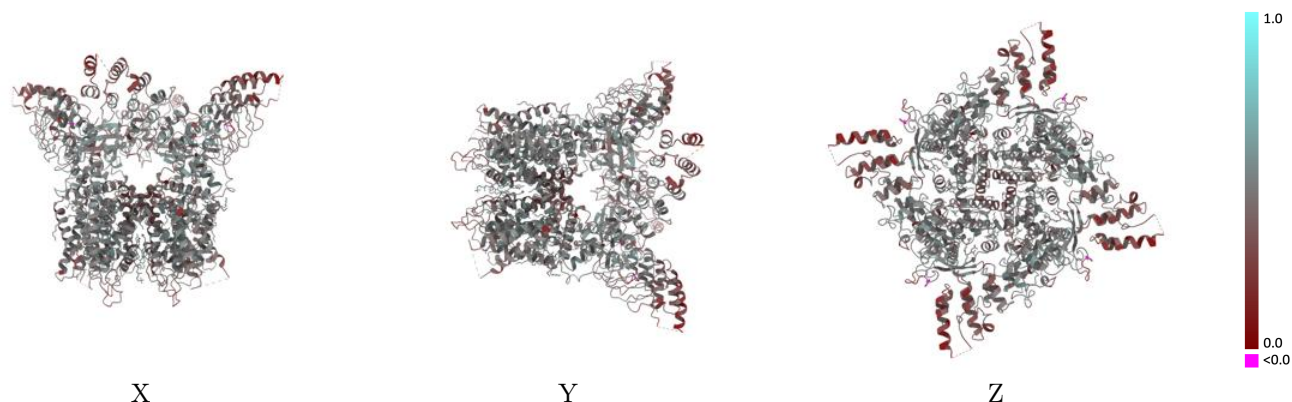
This section contains information regarding the fit between EMDB map EMD-61415 and PDB model 9JEF. Per-residue inclusion information can be found in section [3](#) on page [7](#).

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



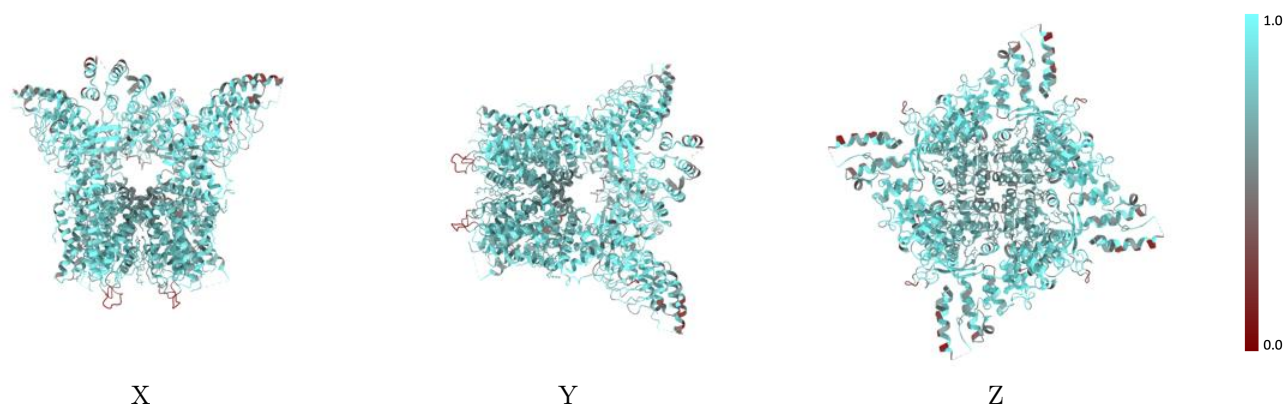
The images above show the 3D surface view of the map at the recommended contour level 0.16 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

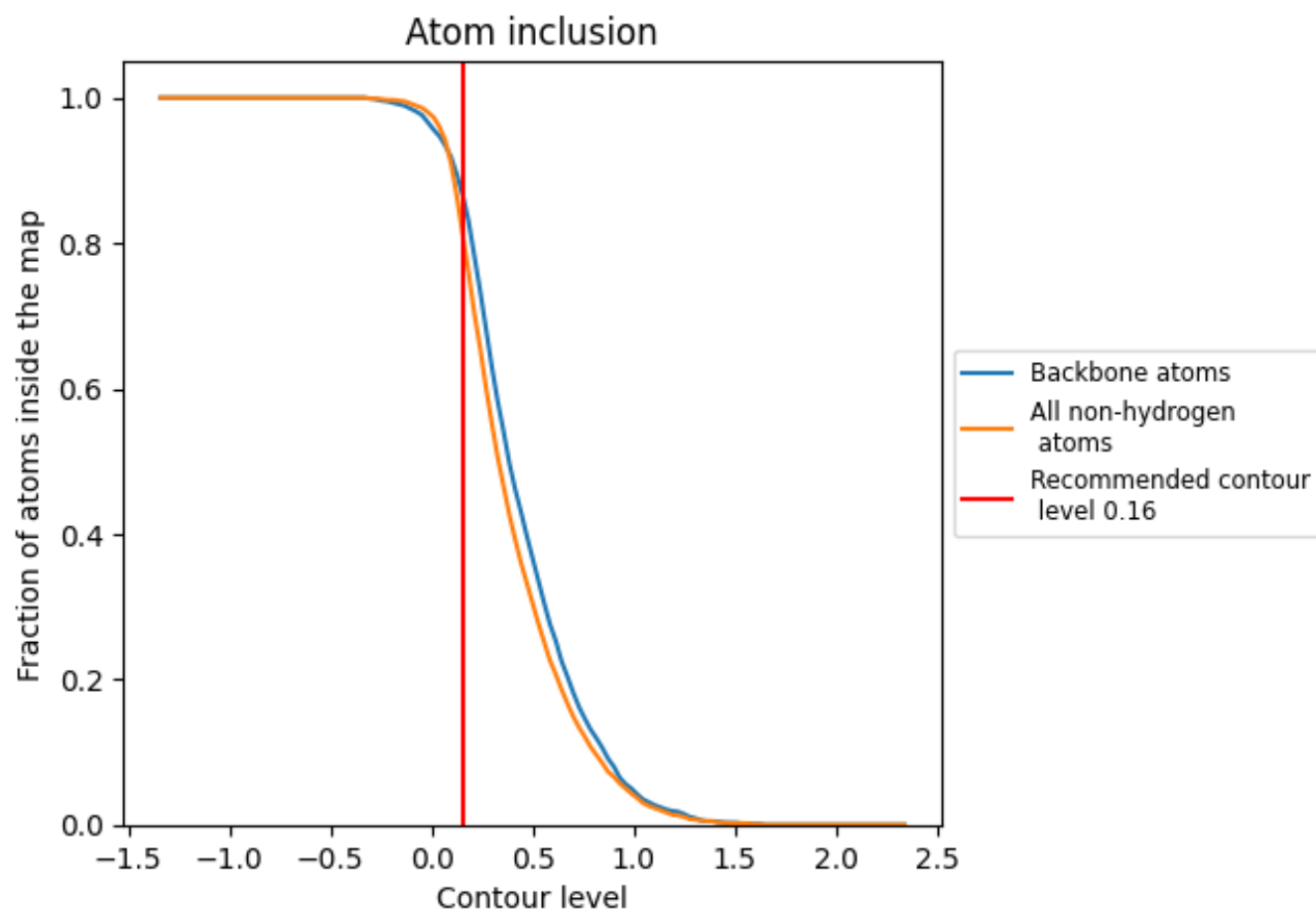
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.16).



## 9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 80% 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 (0.16) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion     | Q-score            |
|-------|--------------------|--------------------|
| All   | <div></div> 0.8010 | <div></div> 0.4370 |
| A     | <div></div> 0.8010 | <div></div> 0.4380 |
| B     | <div></div> 0.8000 | <div></div> 0.4360 |
| C     | <div></div> 0.8000 | <div></div> 0.4370 |
| D     | <div></div> 0.8010 | <div></div> 0.4360 |

