



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 09:14 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)

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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>.

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

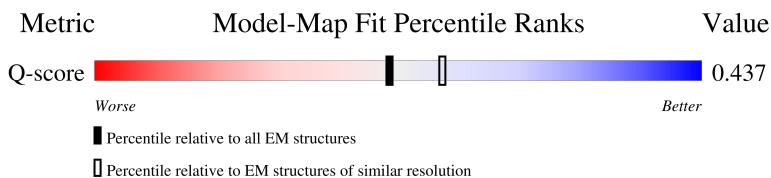
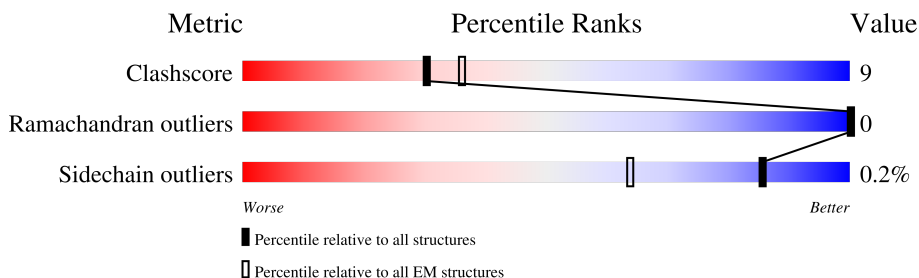
1 Overall quality at a glance

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 (#Entries)	EM structures (#Entries)	Similar EM resolution (#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 ≥ 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	 60% 15% 25%
1	B	799	 61% 15% 25%
1	C	799	 60% 15% 25%
1	D	799	 60% 15% 25%

2 Entry composition

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:

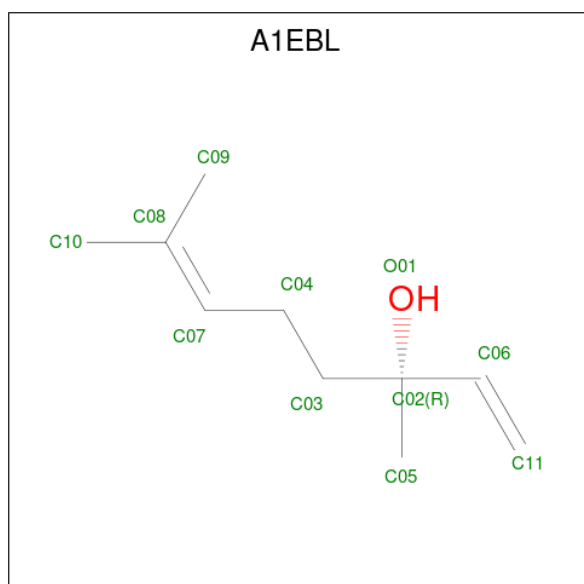
Chain	Residue	Modelled	Actual	Comment	Reference
A	25	VAL	ILE	variant	UNP Q8NET8
A	791	SER	-	expression tag	UNP Q8NET8
A	792	ASN	-	expression tag	UNP Q8NET8
A	793	SER	-	expression tag	UNP Q8NET8
A	794	LEU	-	expression tag	UNP Q8NET8
A	795	GLU	-	expression tag	UNP Q8NET8
A	796	VAL	-	expression tag	UNP 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: C₁₀H₁₈O) (labeled as "Ligand of Interest" by depositor).



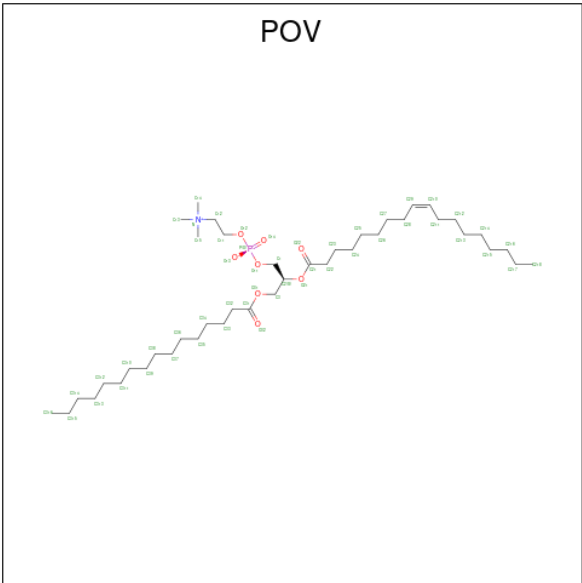
Mol	Chain	Residues	Atoms			AltConf
2	A	1	Total	C	O	0
			11	10	1	

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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: C₄₂H₈₂NO₈P).



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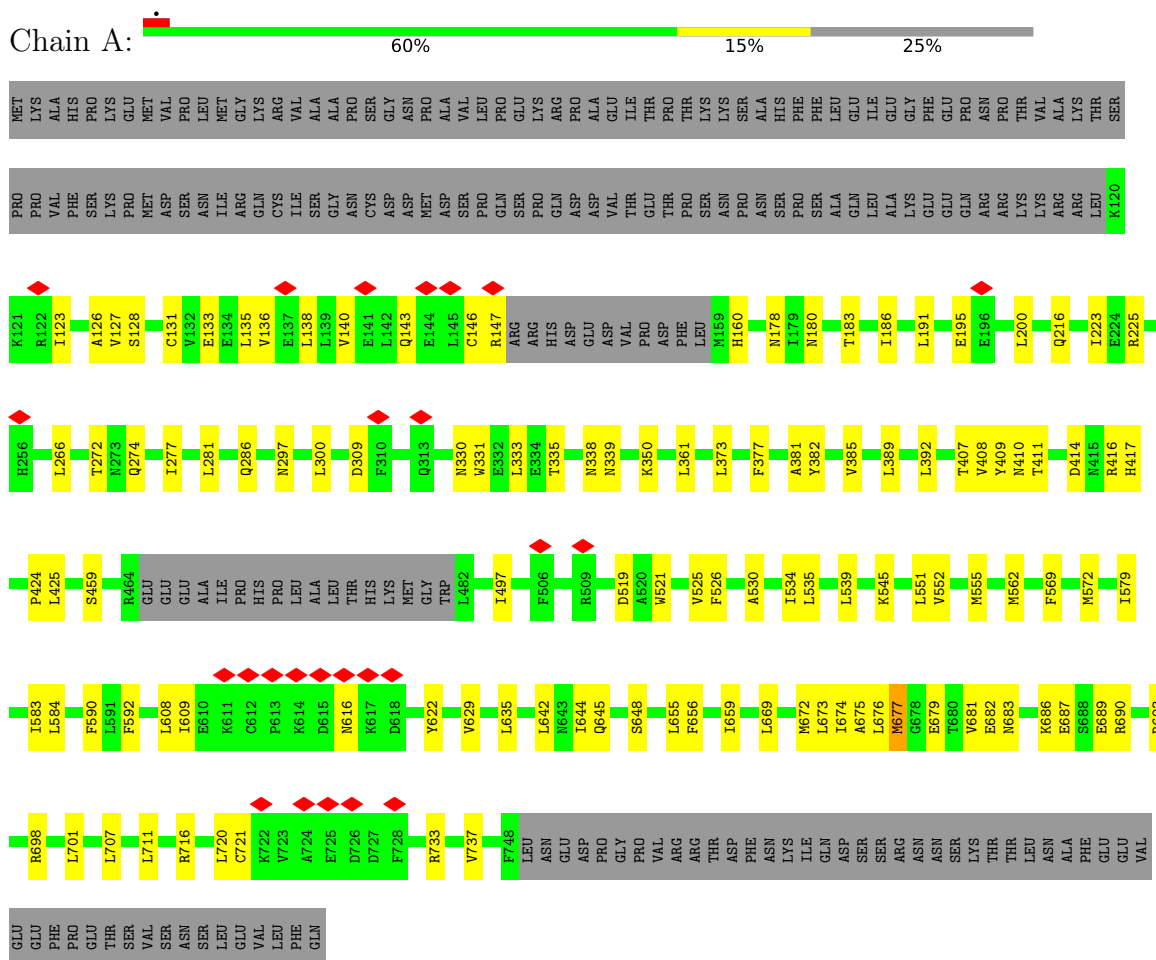
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Mol	Chain	Residues	Atoms					AltConf
3	B	1	Total	C	N	O	P	0
			45	35	1	8	1	
3	B	1	Total	C	N	O	P	0
			39	29	1	8	1	
3	C	1	Total	C	N	O	P	0
			44	34	1	8	1	
3	C	1	Total	C	N	O	P	0
			33	23	1	8	1	
3	C	1	Total	C	N	O	P	0
			38	28	1	8	1	
3	C	1	Total	C	N	O	P	0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

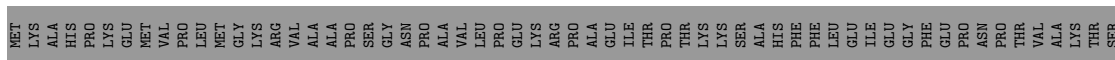
3 Residue-property plots

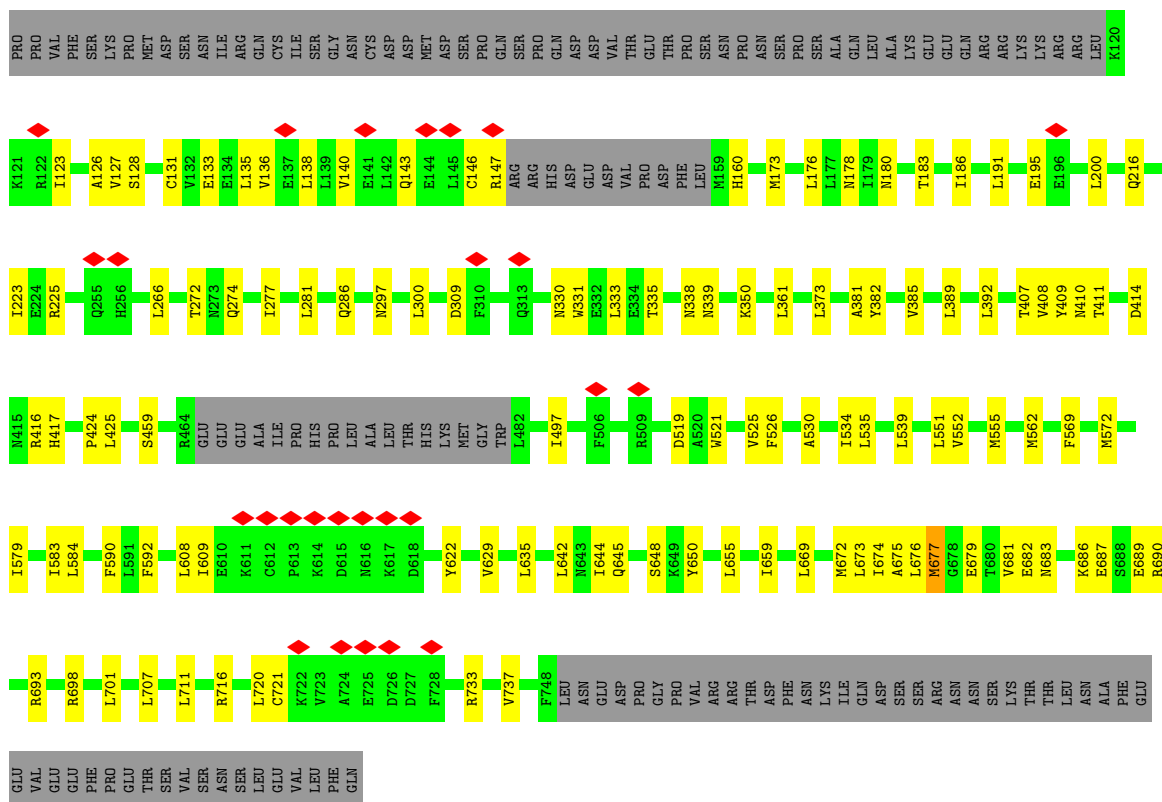
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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



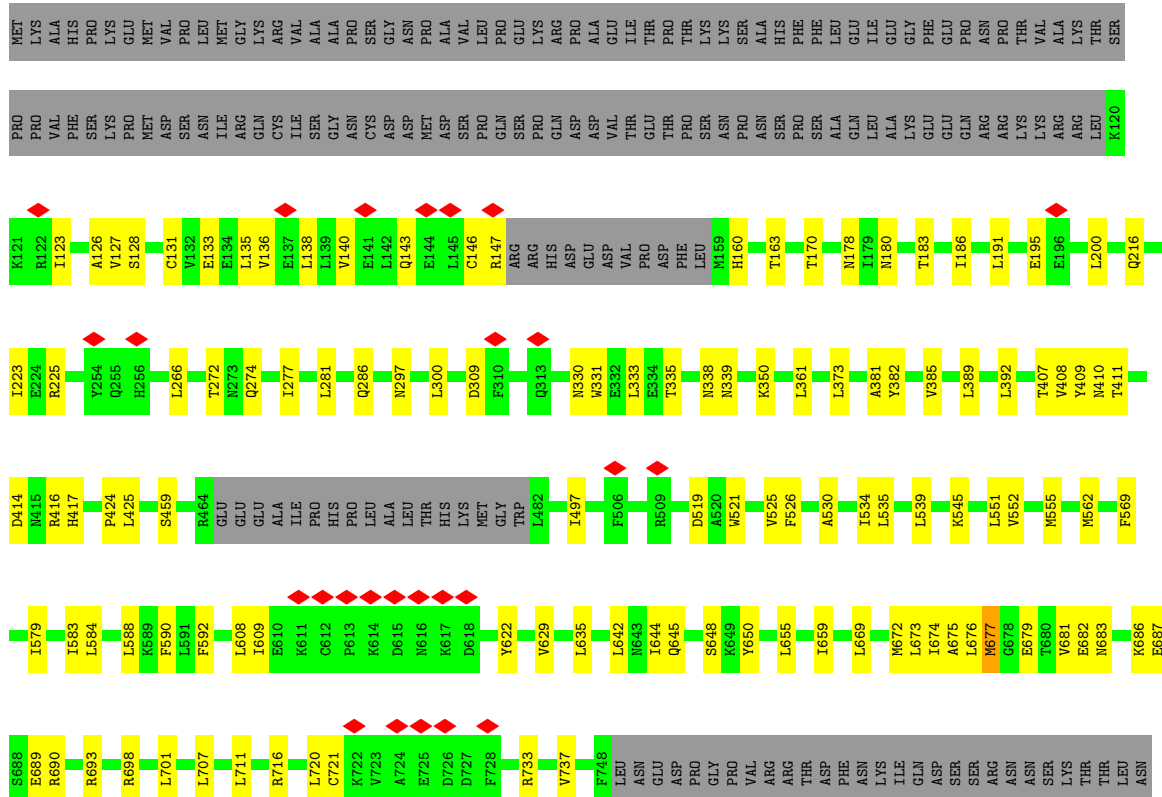
- Molecule 1: Transient receptor potential cation channel subfamily V member 3





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

Chain C: 60% 15% 25%



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
MET
ASN
LEU
GLY
VAL
SER
ALA
PRO
SER
GLY
ASN
MET
PRO
ALA
SER
VAL
LEU
PRO
SER
ALA
HIS
PHE
PHE
LEU
GLU
ILE
GLY
PHE
GLU
PRO
ASN
PRO
THR
LYS
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SER
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ASN
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
GLY
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
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
V661
F669
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
Q678
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
PRO
VAL
ARG
THR
ASP
PHE
ASN
LYS
ILE
GLN
ASP
SER
SER
ARG
ASN
ASN
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LYS
THR
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ALA
PHE
GLU
GLU
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PHE
PRO
GLU
THR
SER
VAL
SER
ASN
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.

The worst 5 of 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

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 ⓘ

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. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	256	HIS
1	D	417	HIS
1	B	256	HIS
1	B	227	GLN
1	D	646	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [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
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	-
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

The worst 5 of 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

There are no chirality outliers.

5 of 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

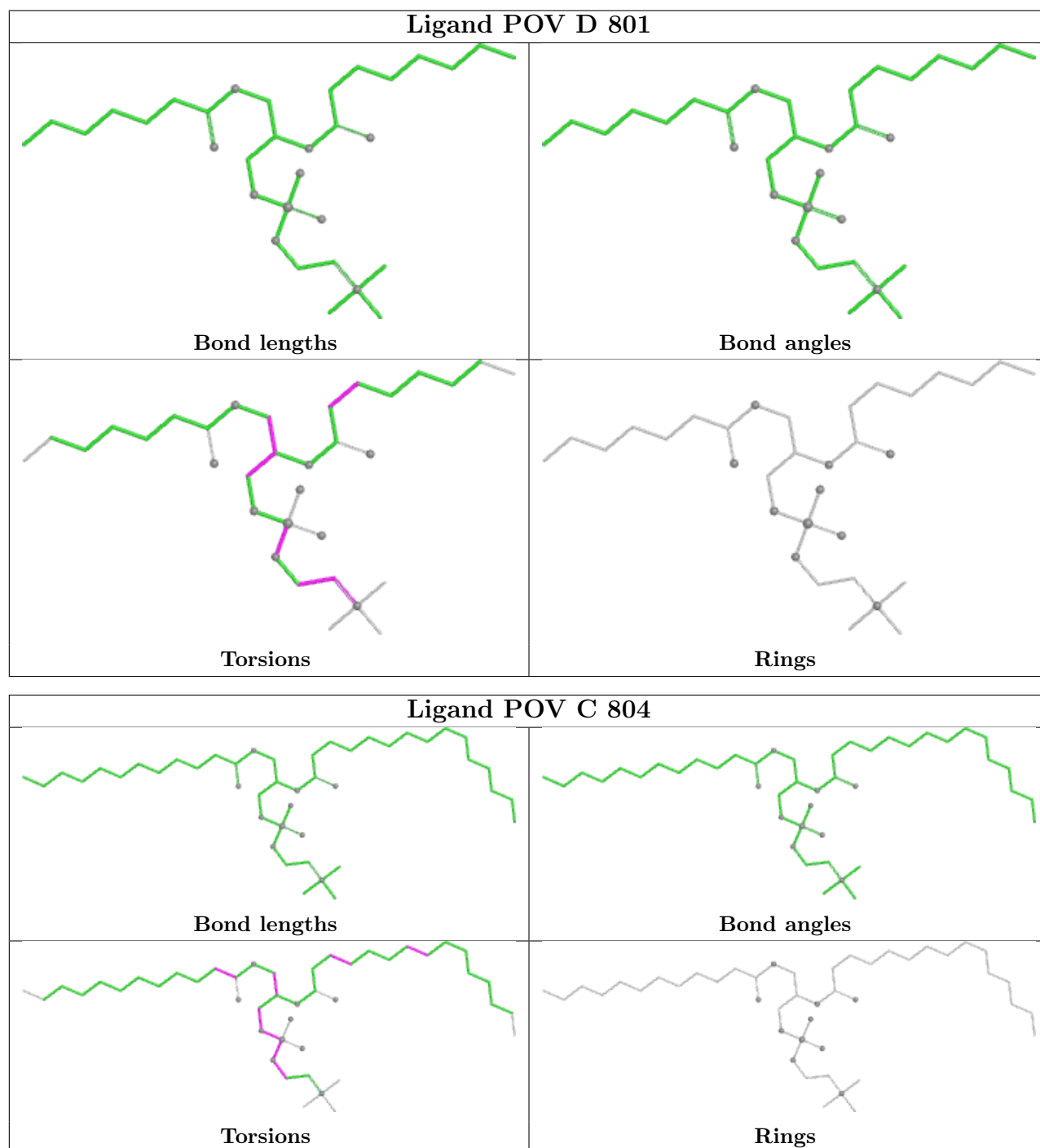
There are no ring outliers.

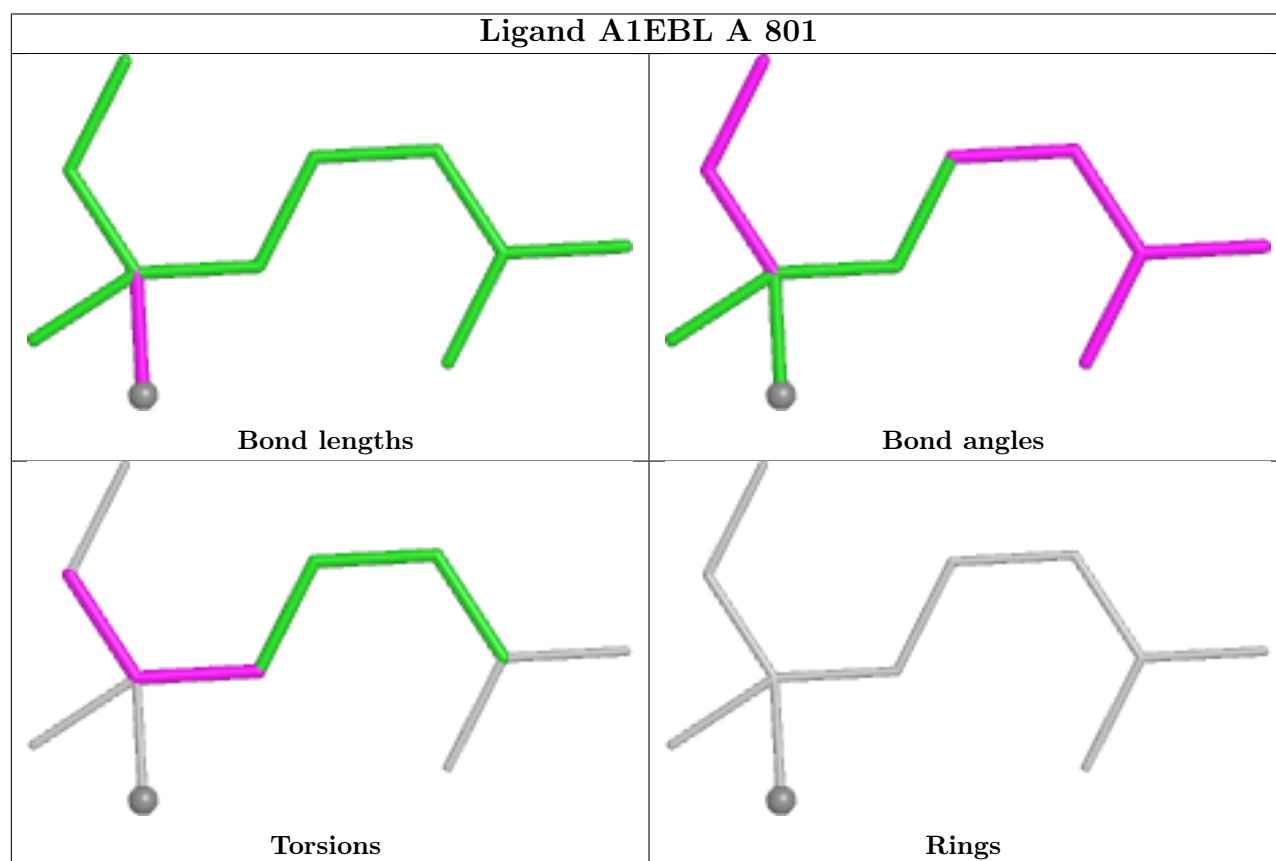
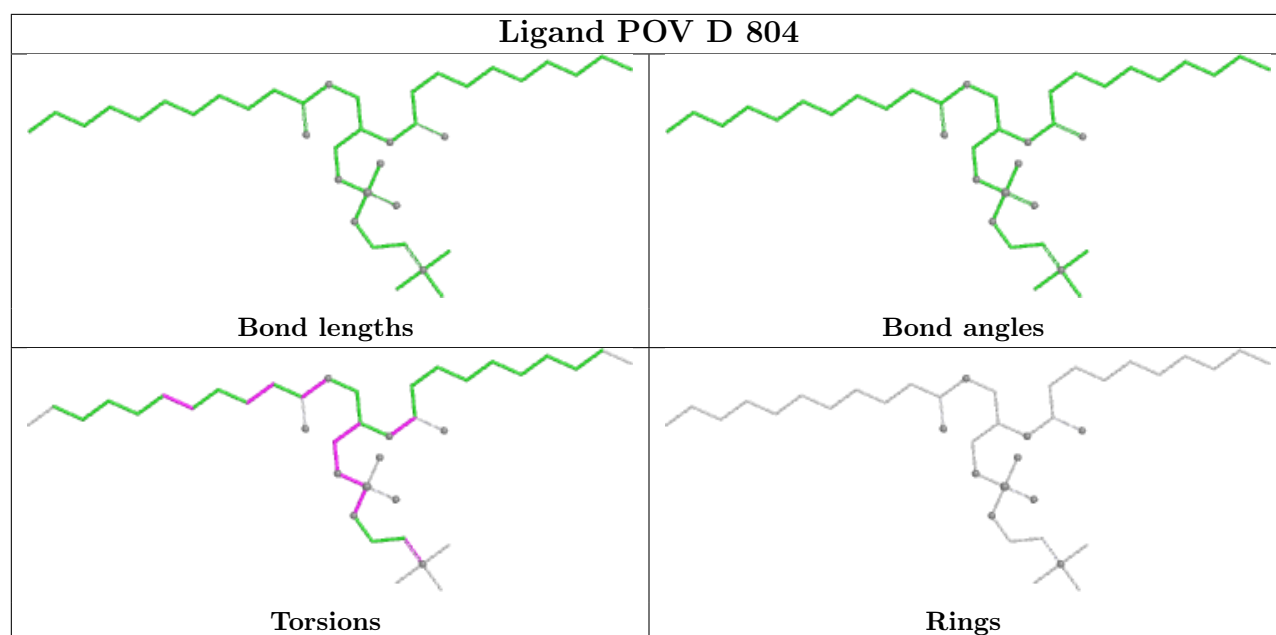
16 monomers are involved in 25 short contacts:

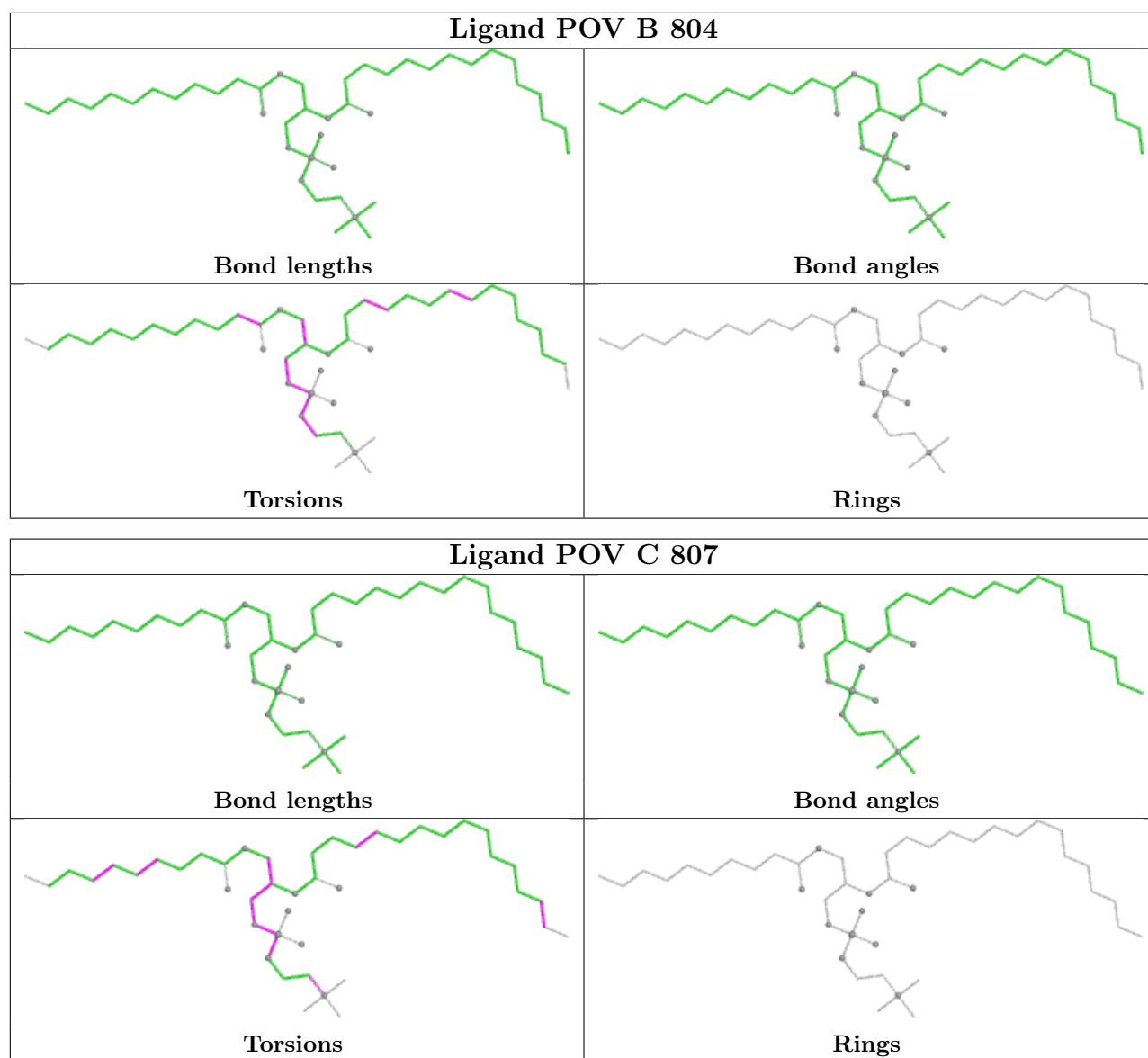
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	804	POV	1	0
3	D	804	POV	1	0
3	B	804	POV	1	0
3	C	807	POV	2	0
3	A	804	POV	2	0
3	A	802	POV	2	0
3	B	805	POV	1	0
3	D	803	POV	1	0
3	B	801	POV	3	0
3	D	802	POV	2	0
3	A	806	POV	1	0
3	A	805	POV	1	0
3	C	805	POV	1	0
3	B	803	POV	2	0
3	C	803	POV	2	0
3	C	801	POV	2	0

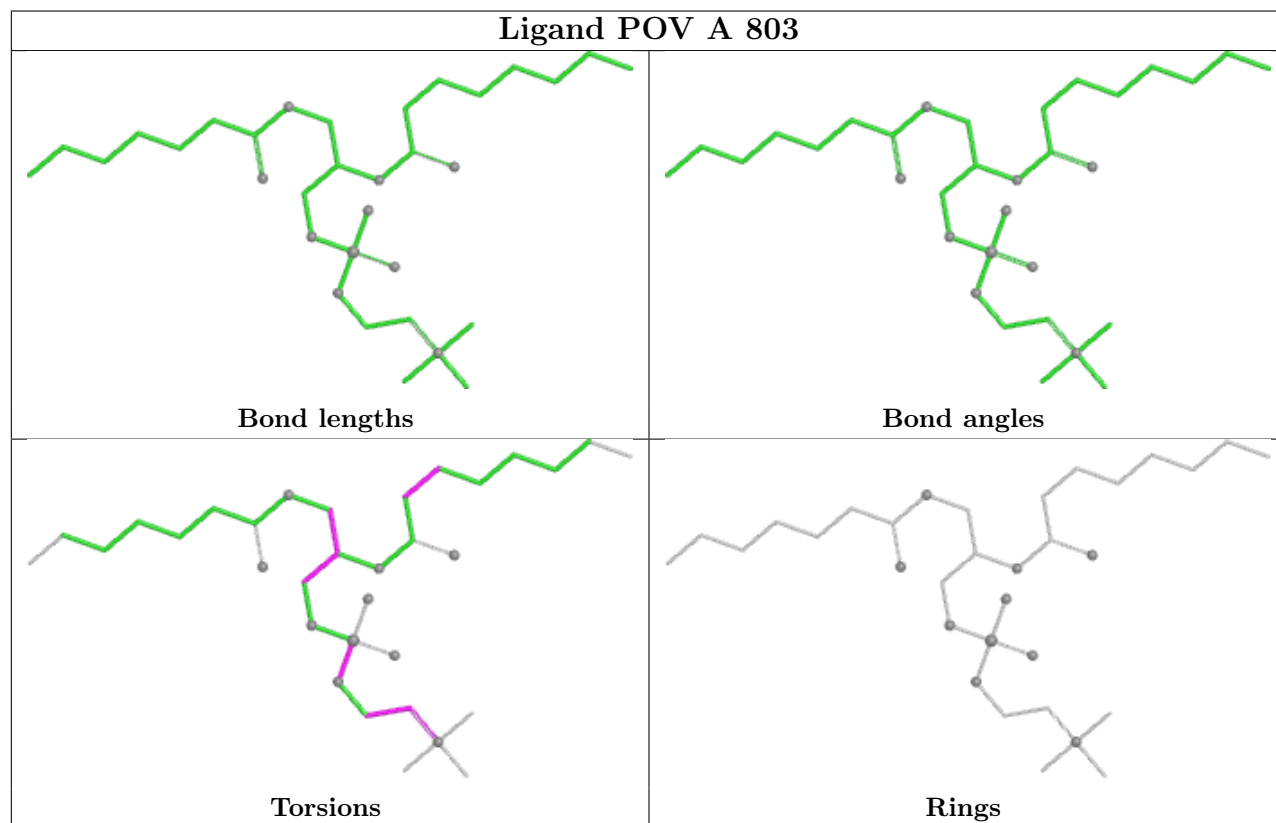
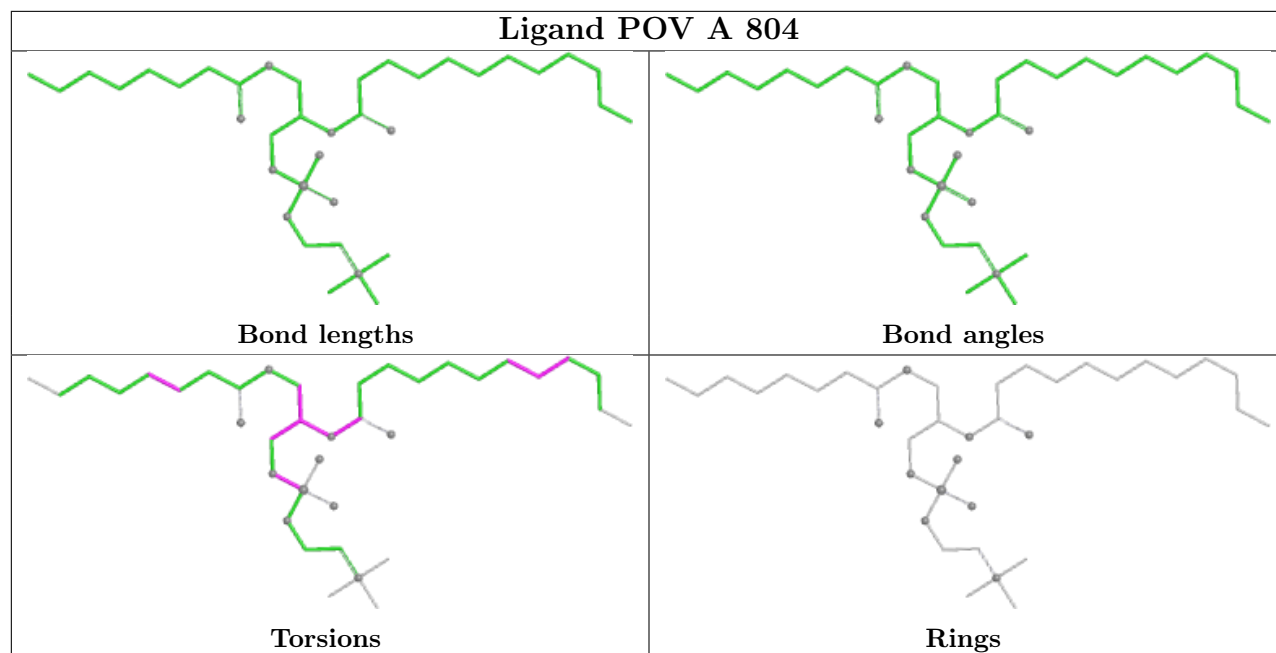
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

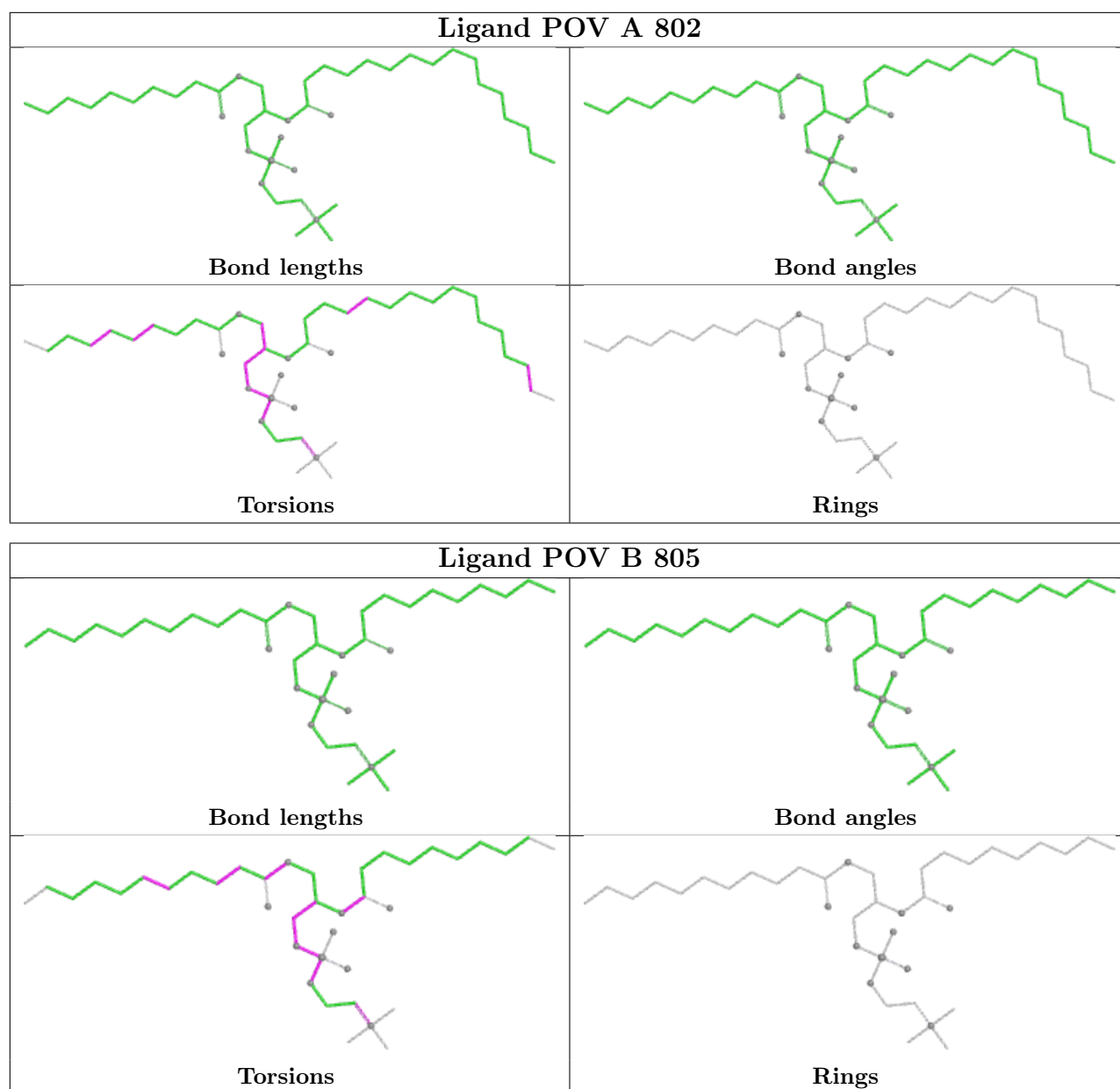
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

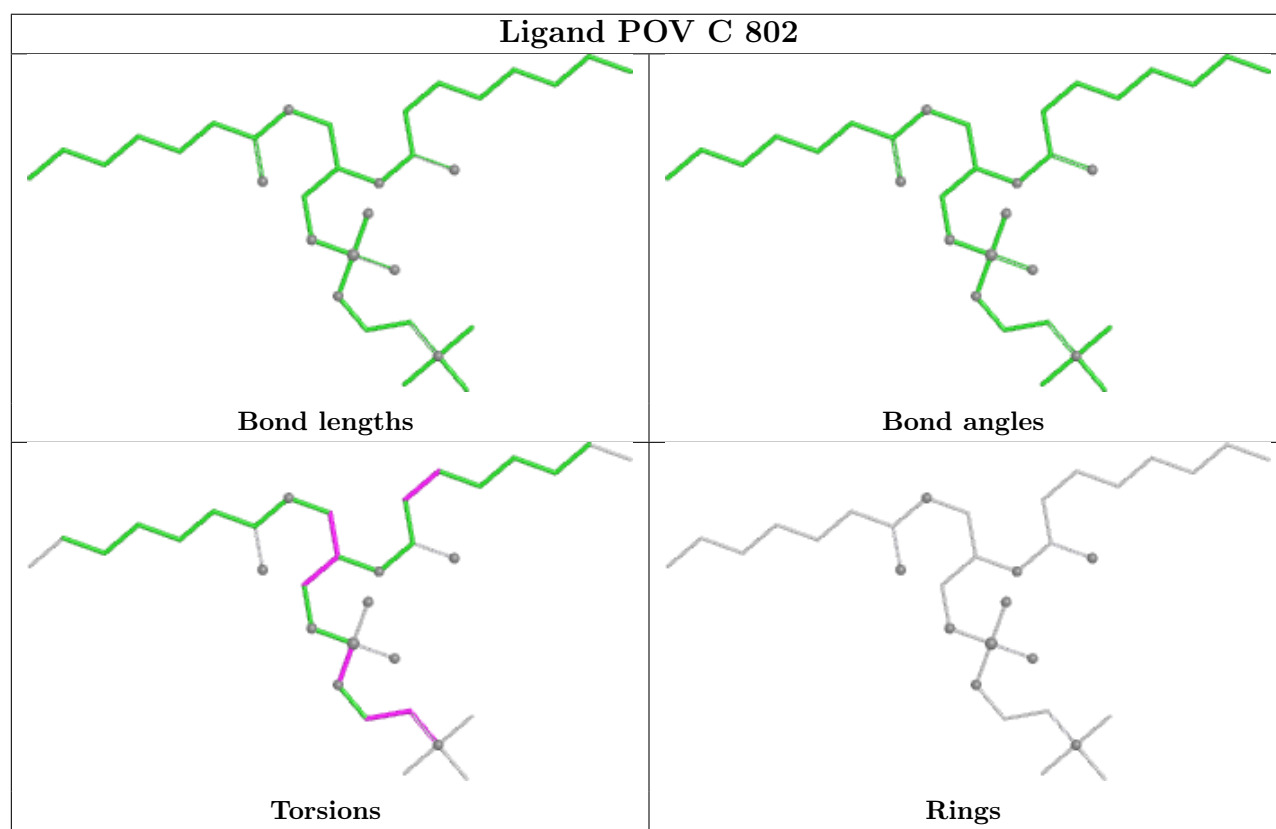
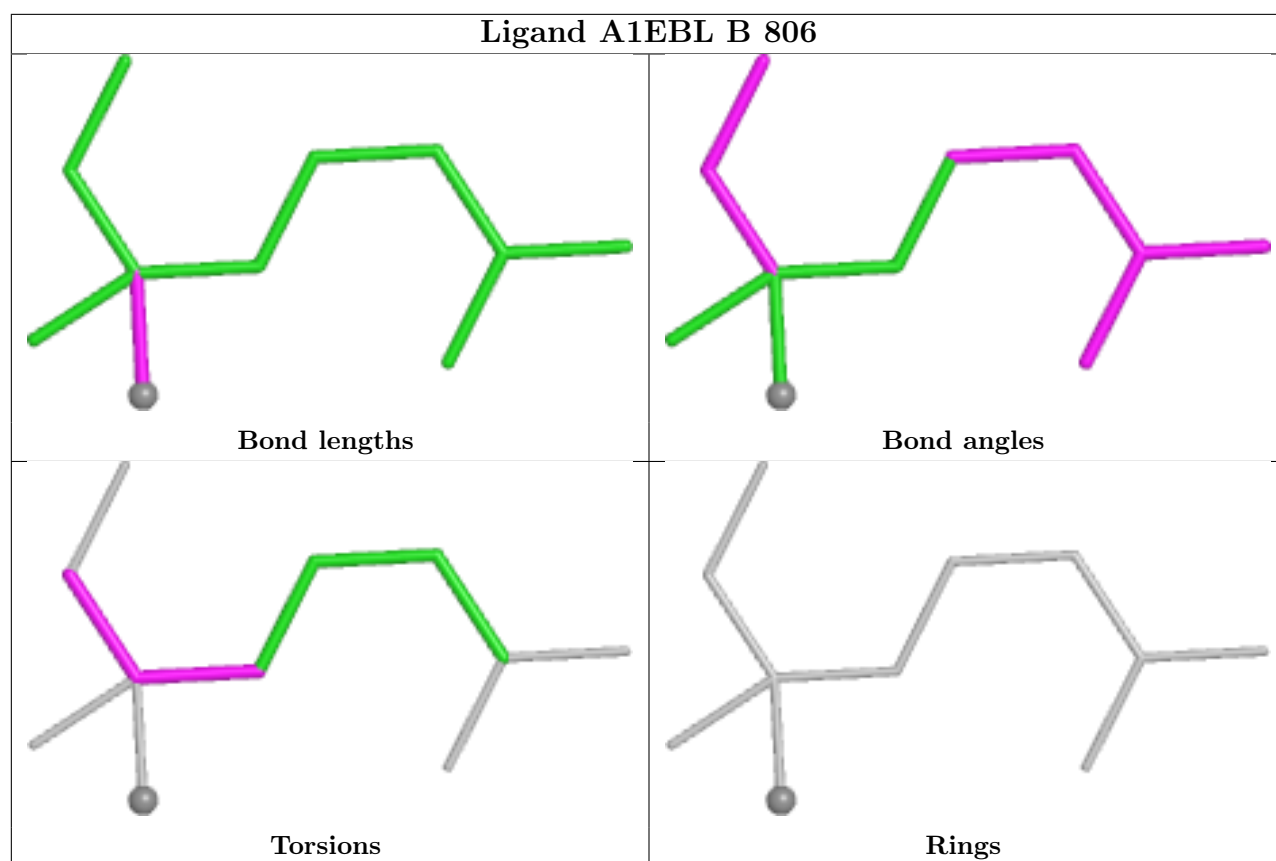


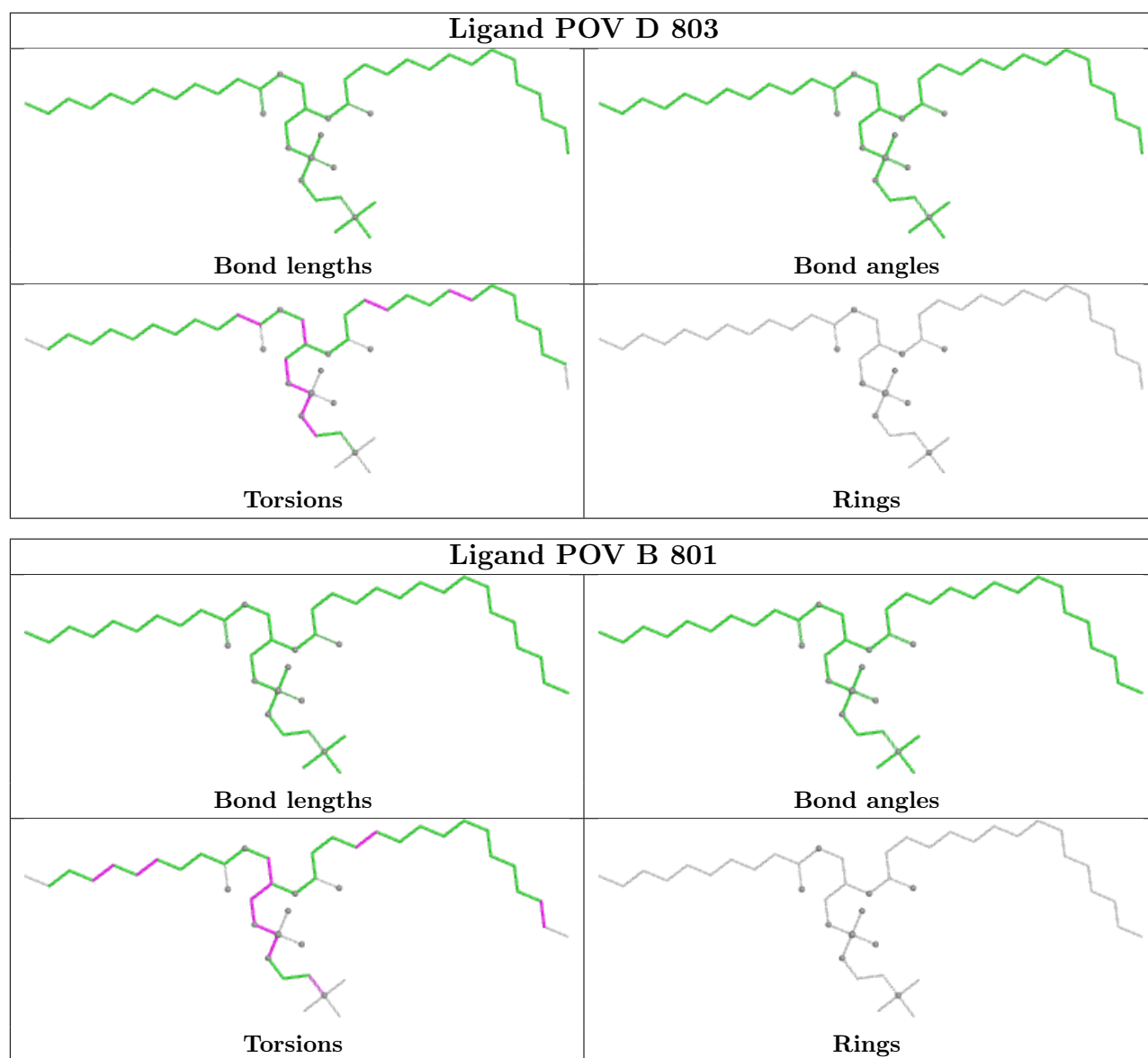


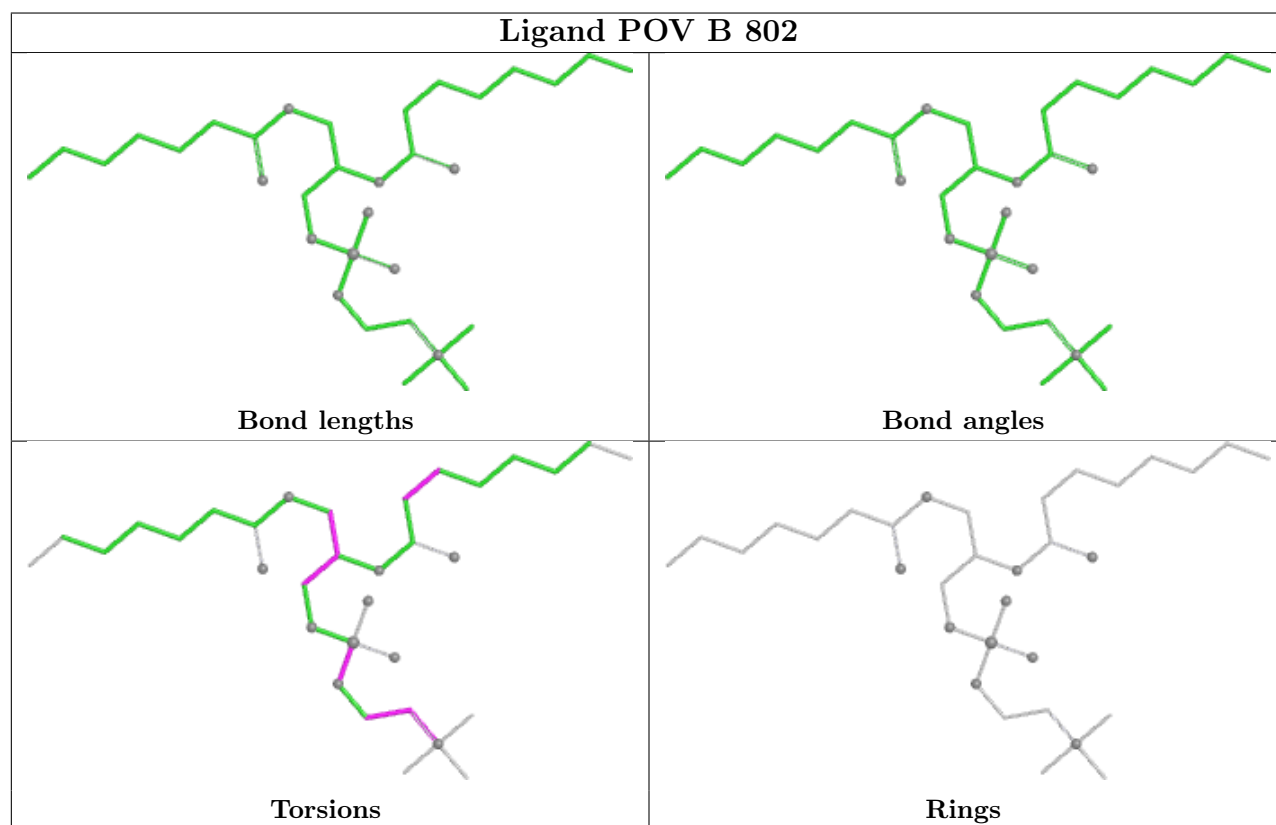
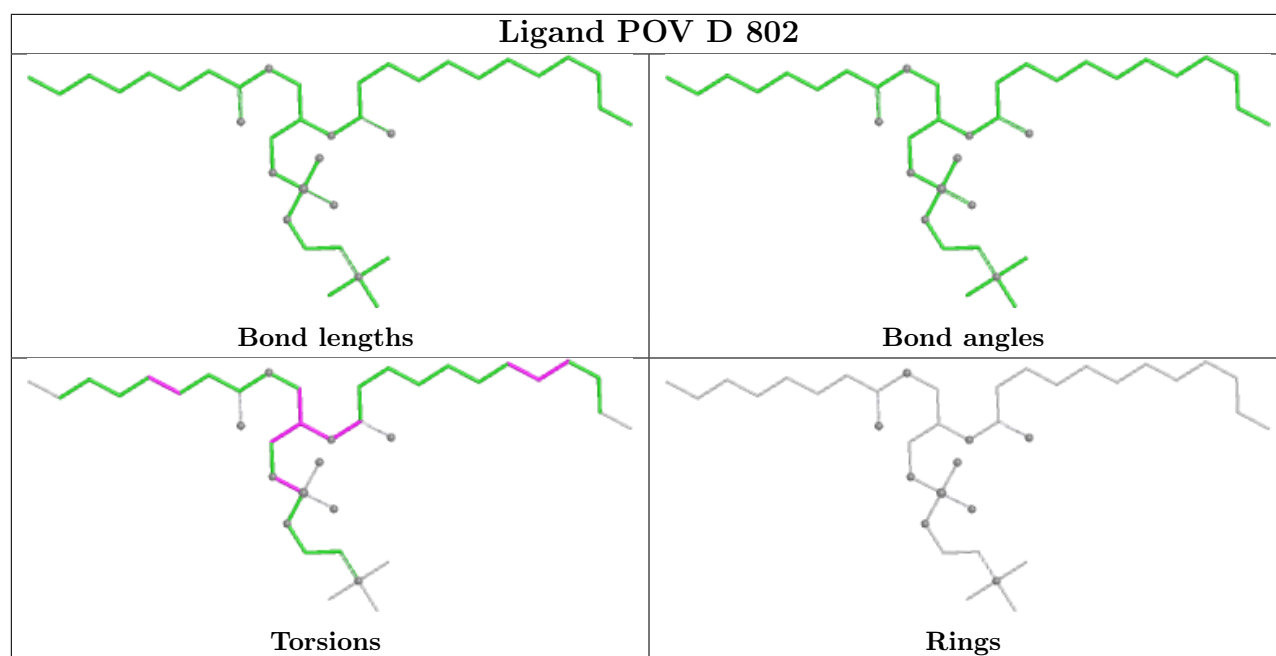


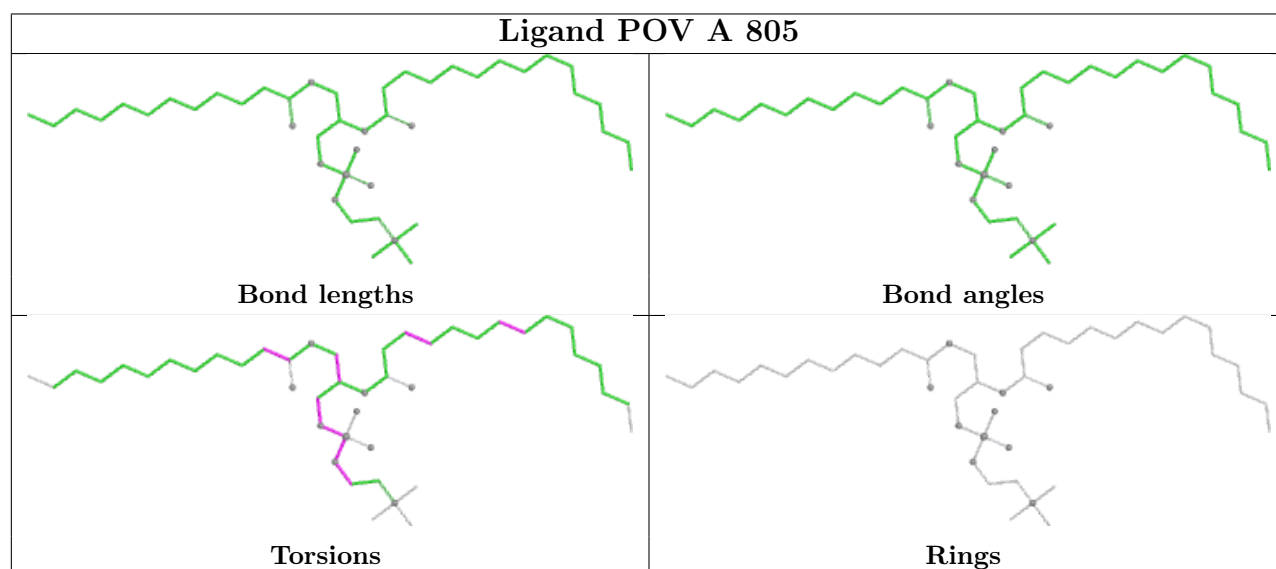
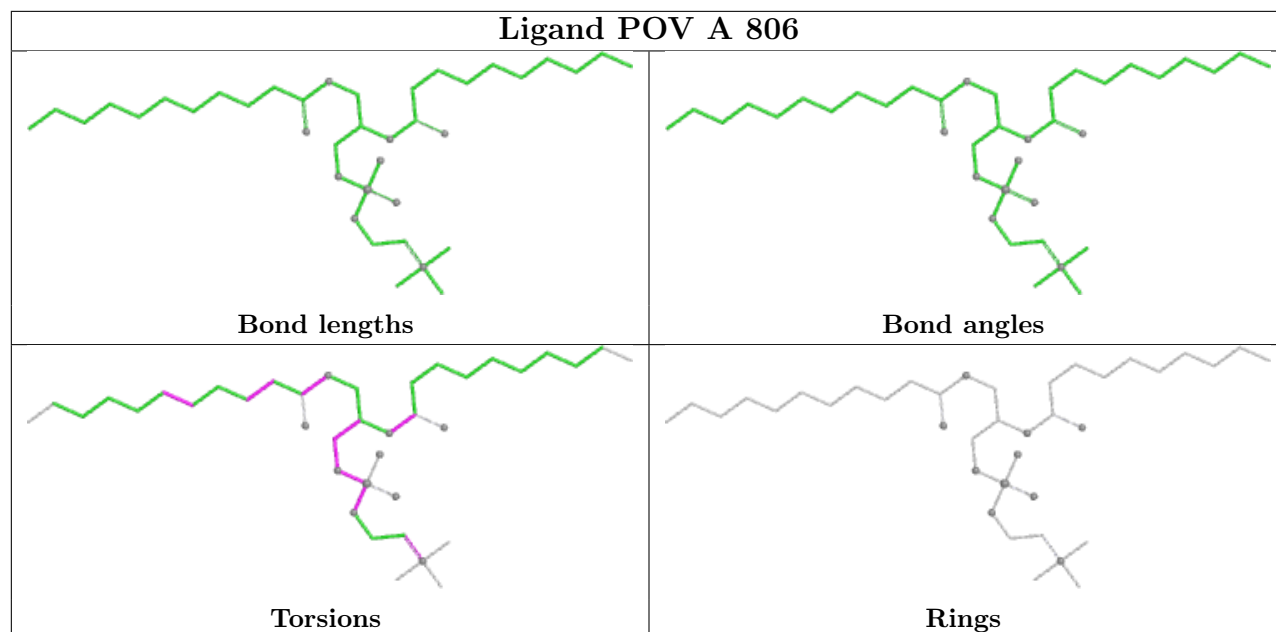


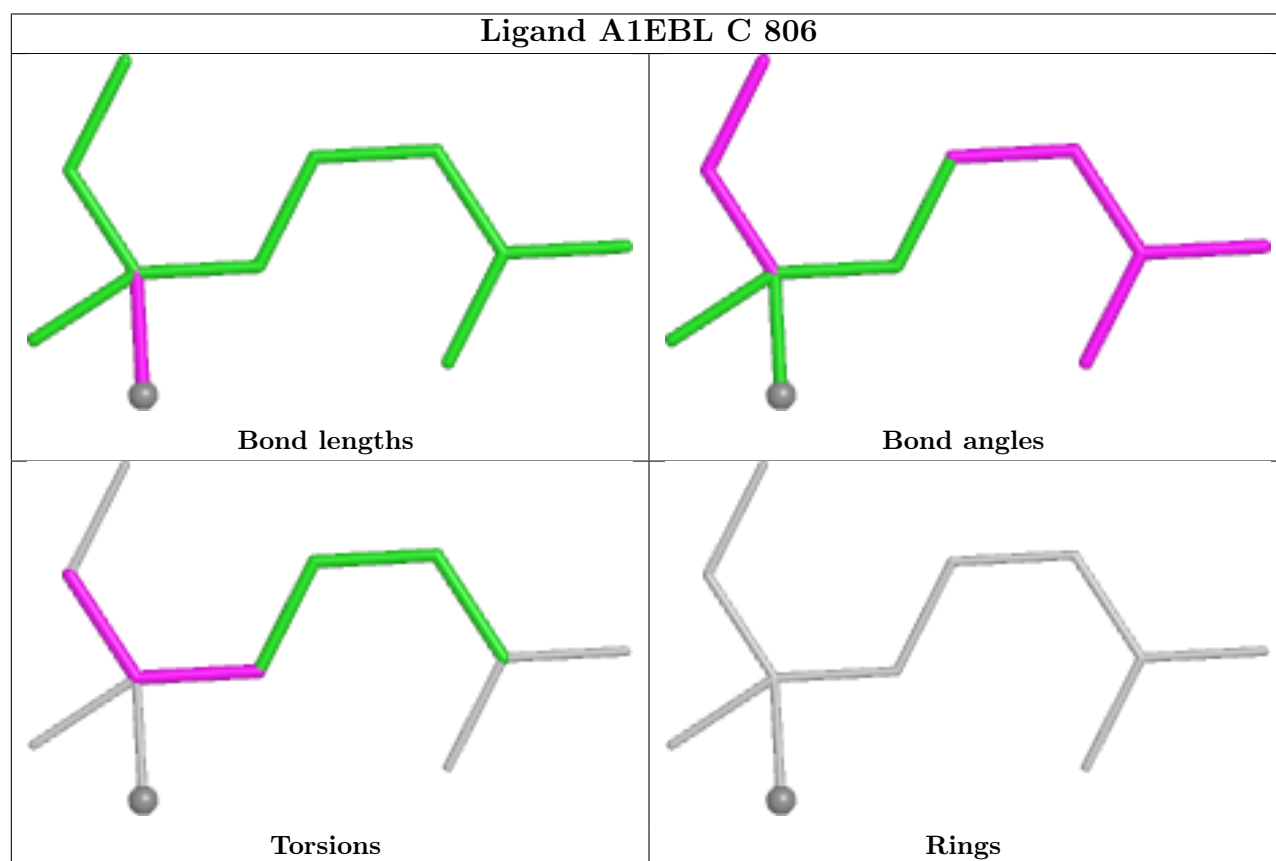
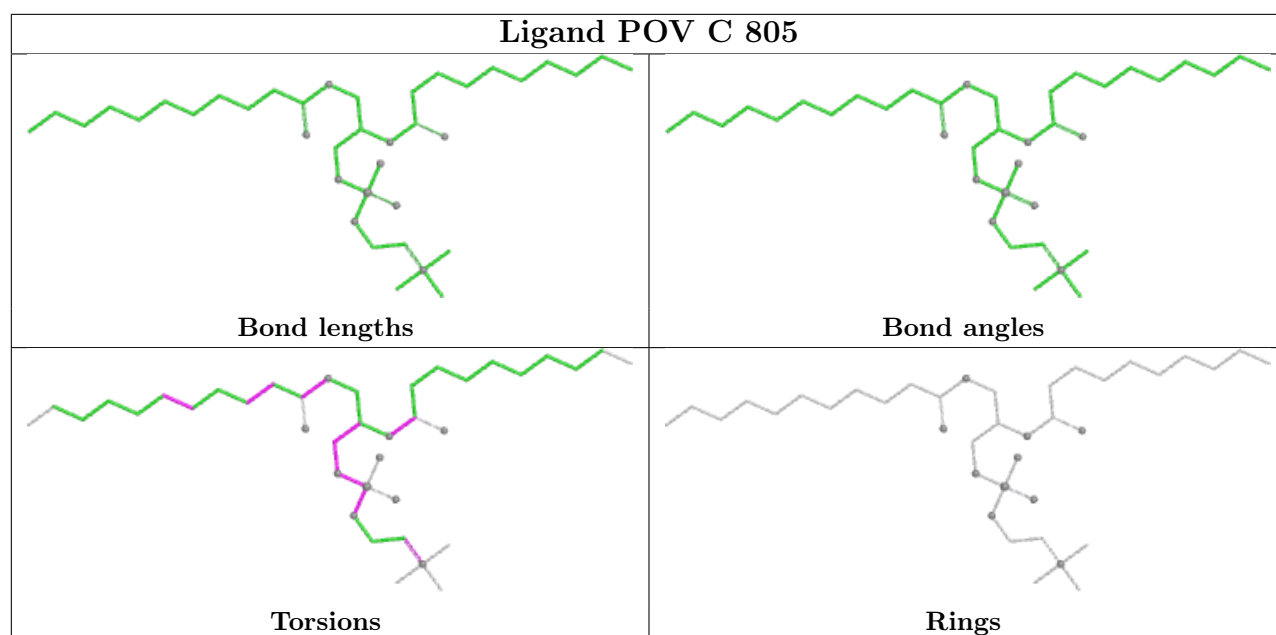


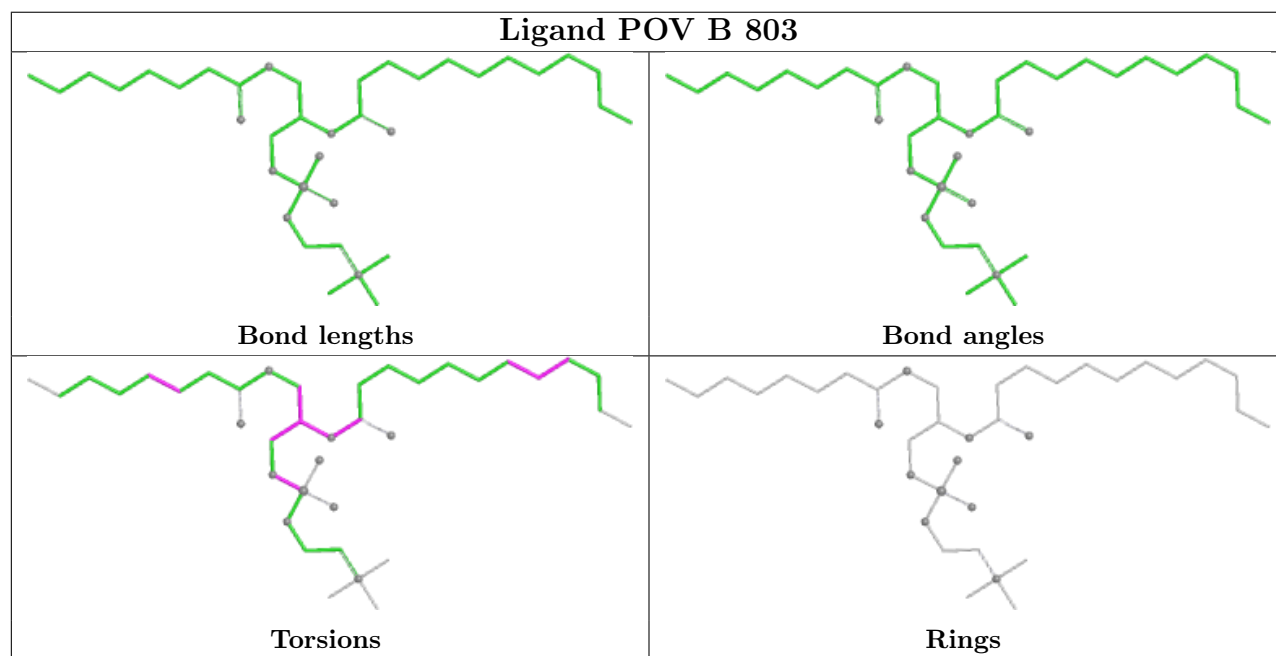
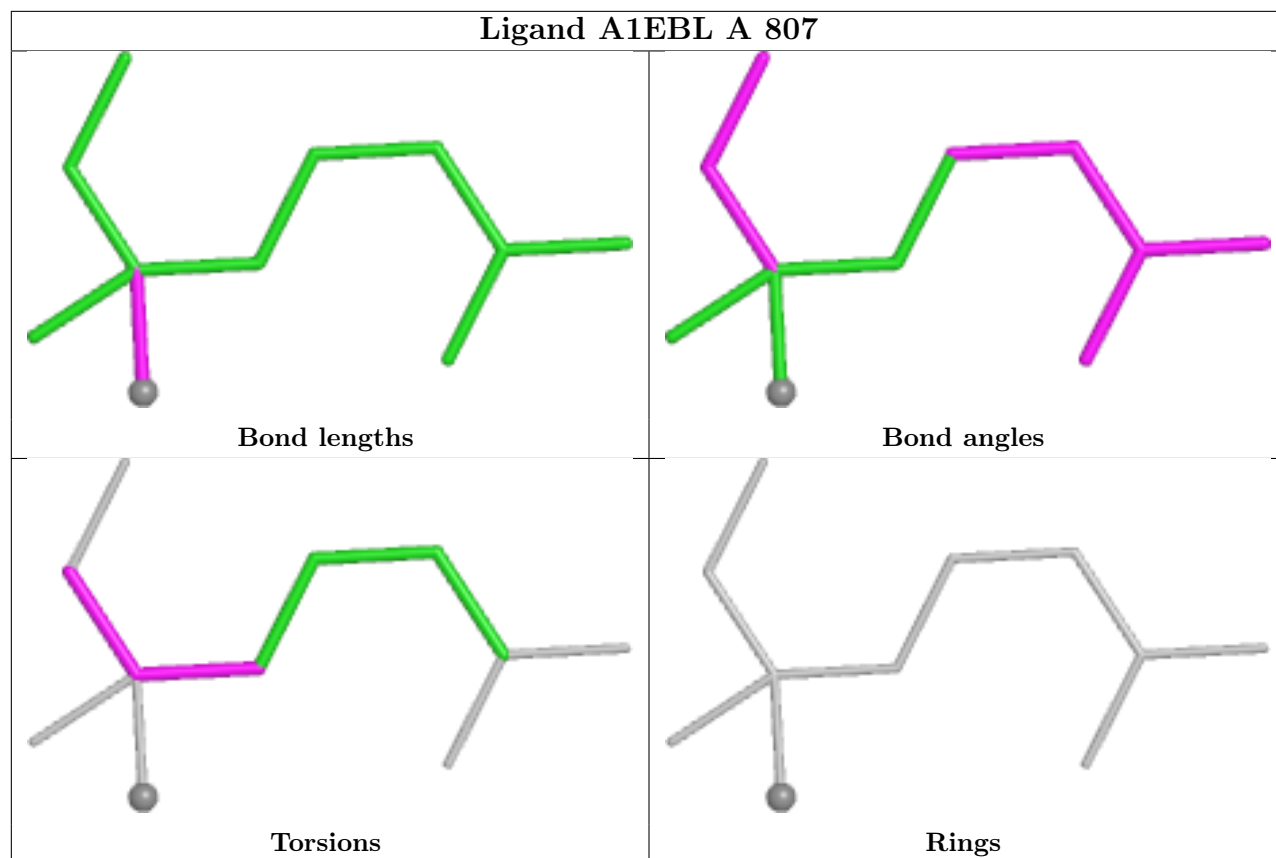


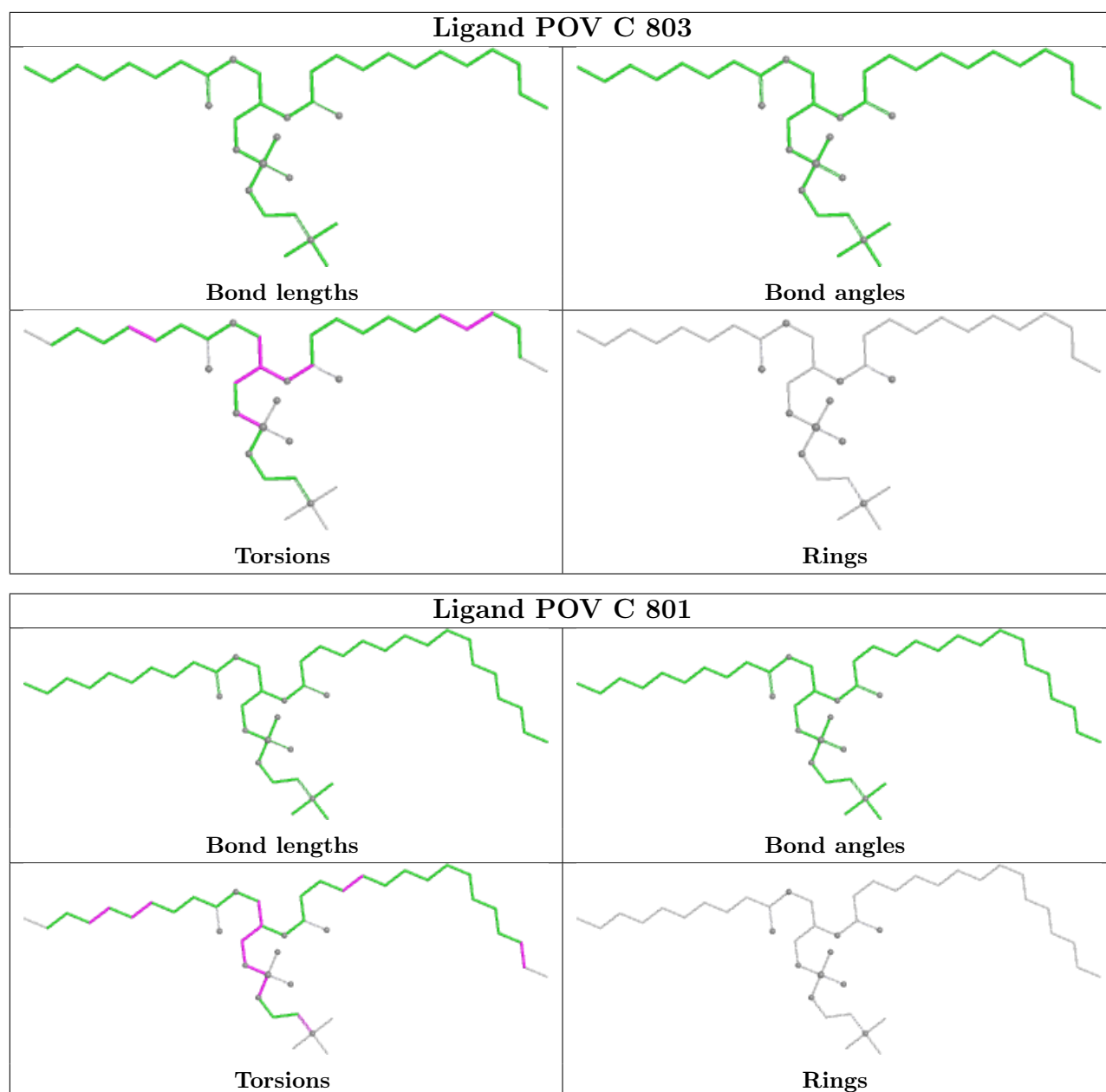












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

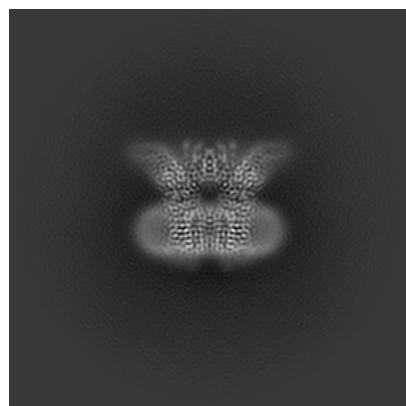
6 Map visualisation [i](#)

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.

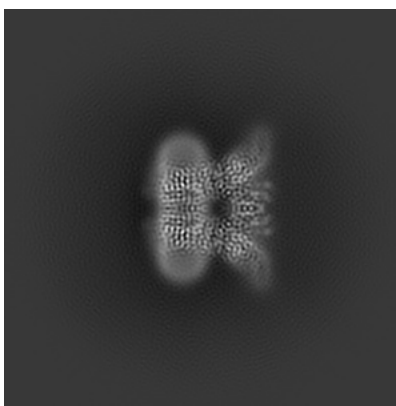
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

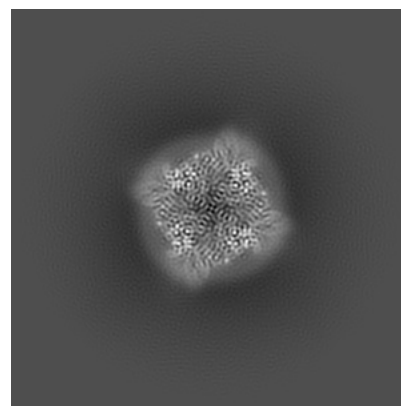
6.1.1 Primary map



X

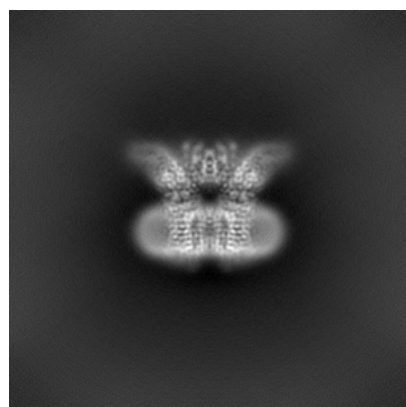


Y

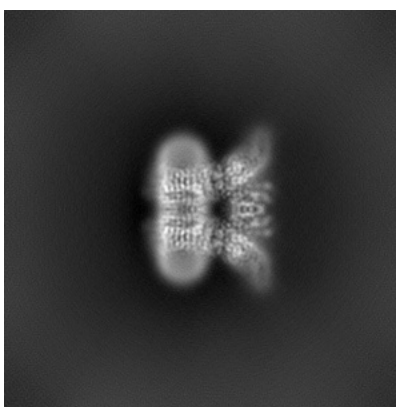


Z

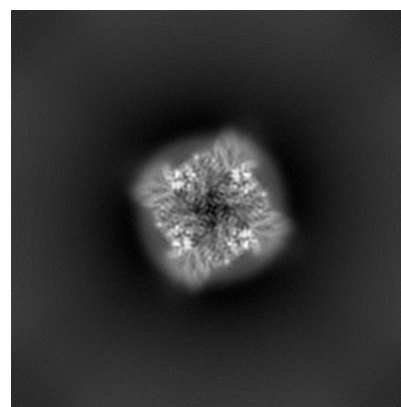
6.1.2 Raw map



X



Y

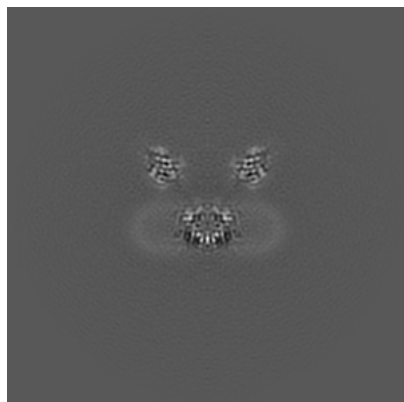


Z

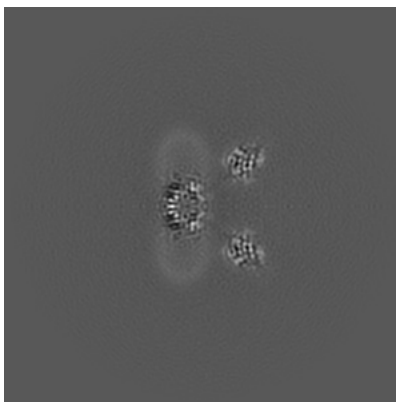
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

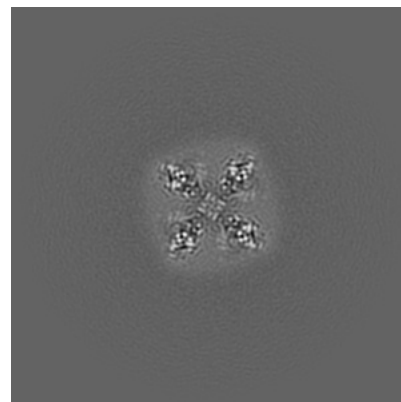
6.2.1 Primary map



X Index: 160

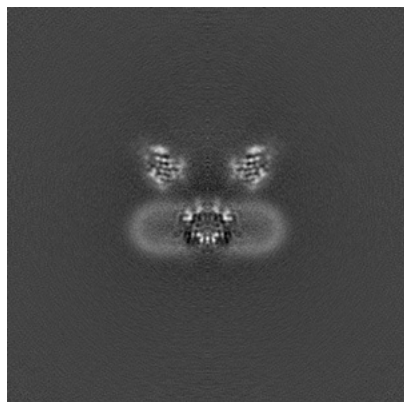


Y Index: 160

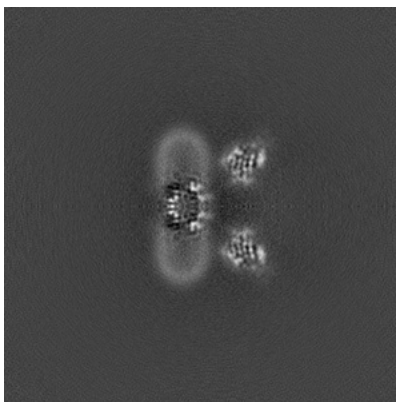


Z Index: 160

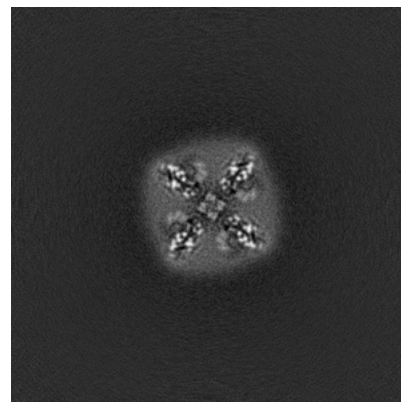
6.2.2 Raw map



X Index: 160



Y Index: 160

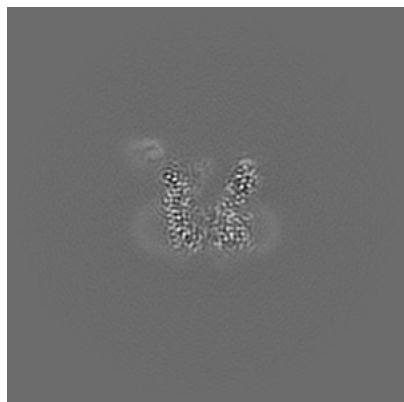


Z Index: 160

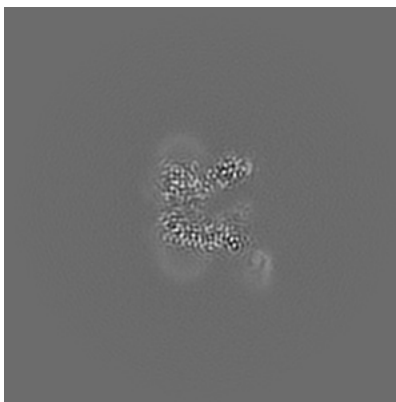
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

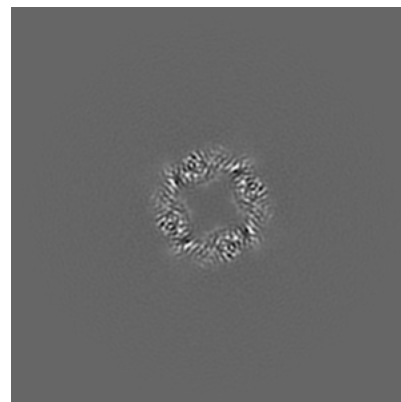
6.3.1 Primary map



X Index: 141

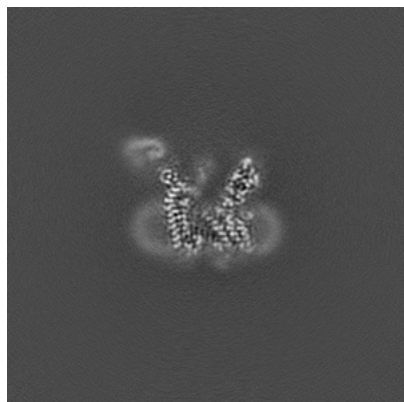


Y Index: 179

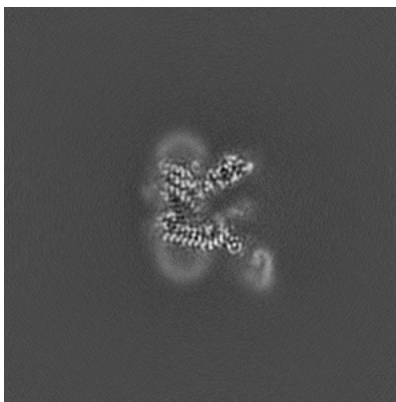


Z Index: 184

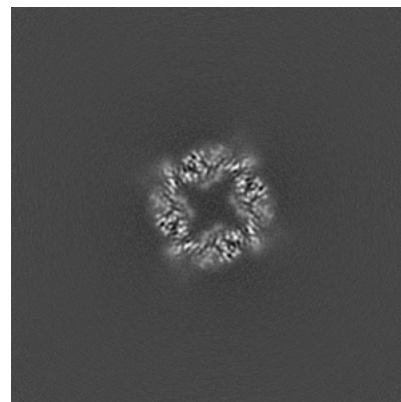
6.3.2 Raw map



X Index: 142



Y Index: 178

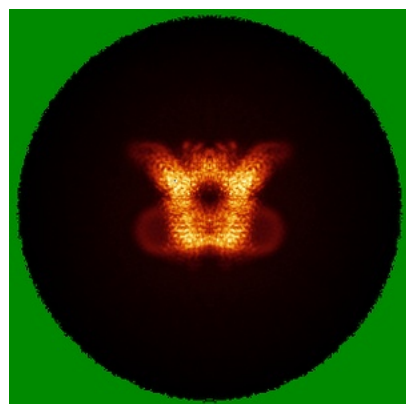


Z Index: 184

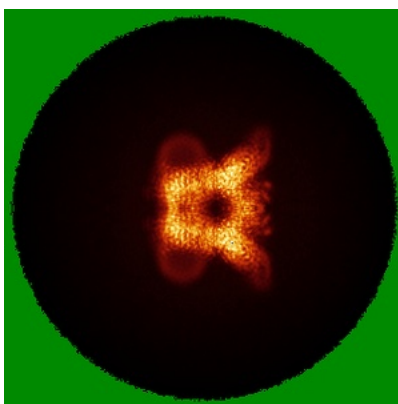
The images above show the largest variance slices of the map in three orthogonal directions.

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

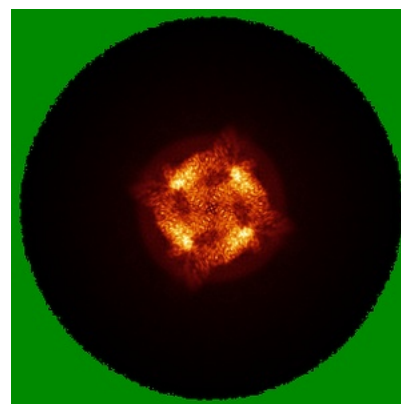
6.4.1 Primary map



X

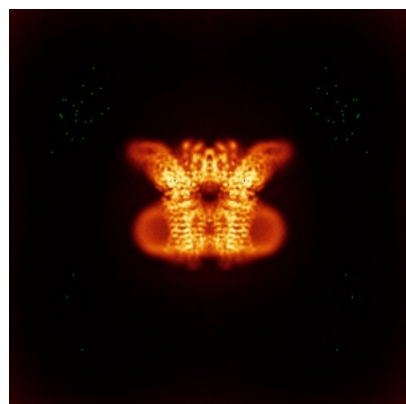


Y

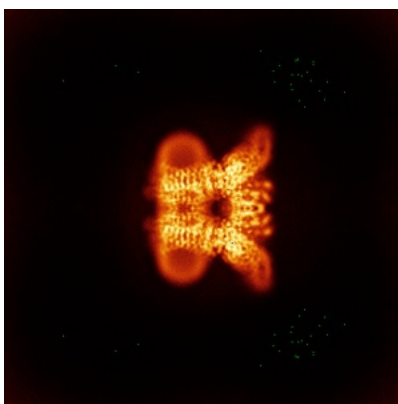


Z

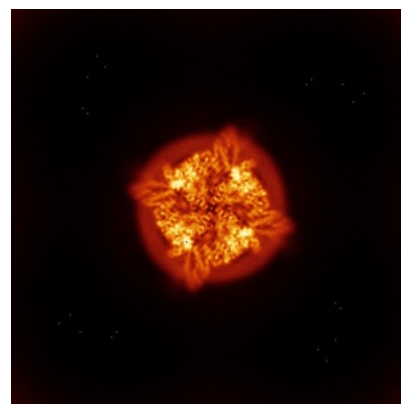
6.4.2 Raw map



X



Y

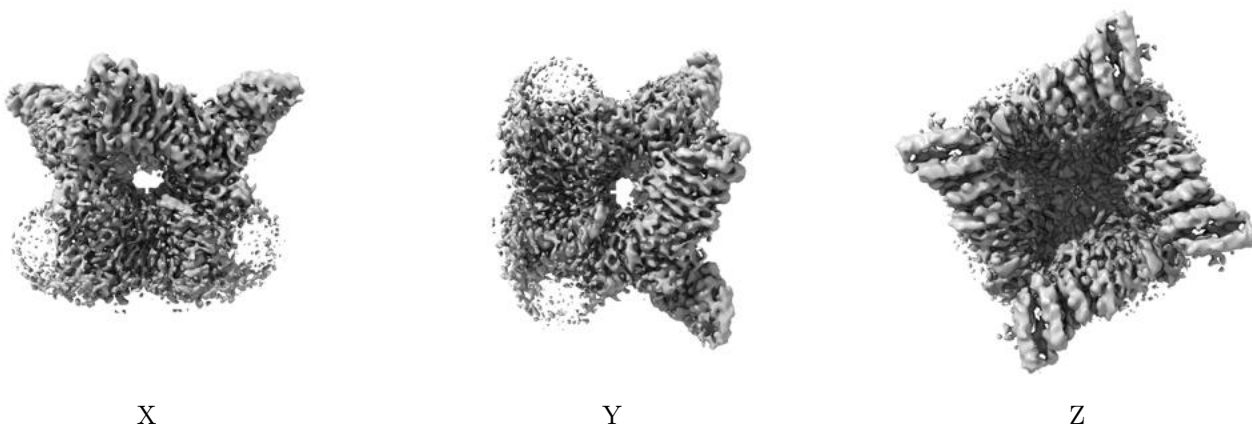


Z

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.

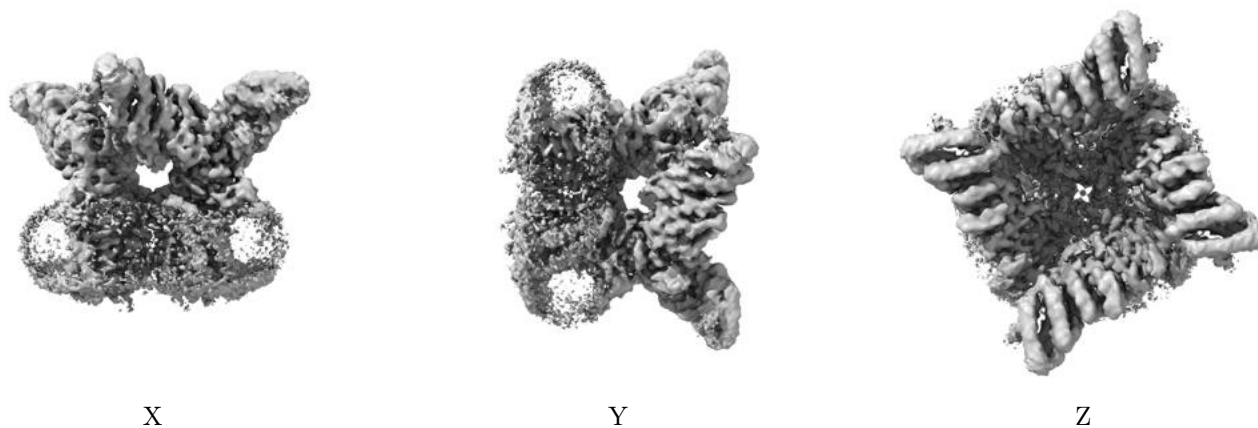
6.5 Orthogonal surface views [i](#)

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.

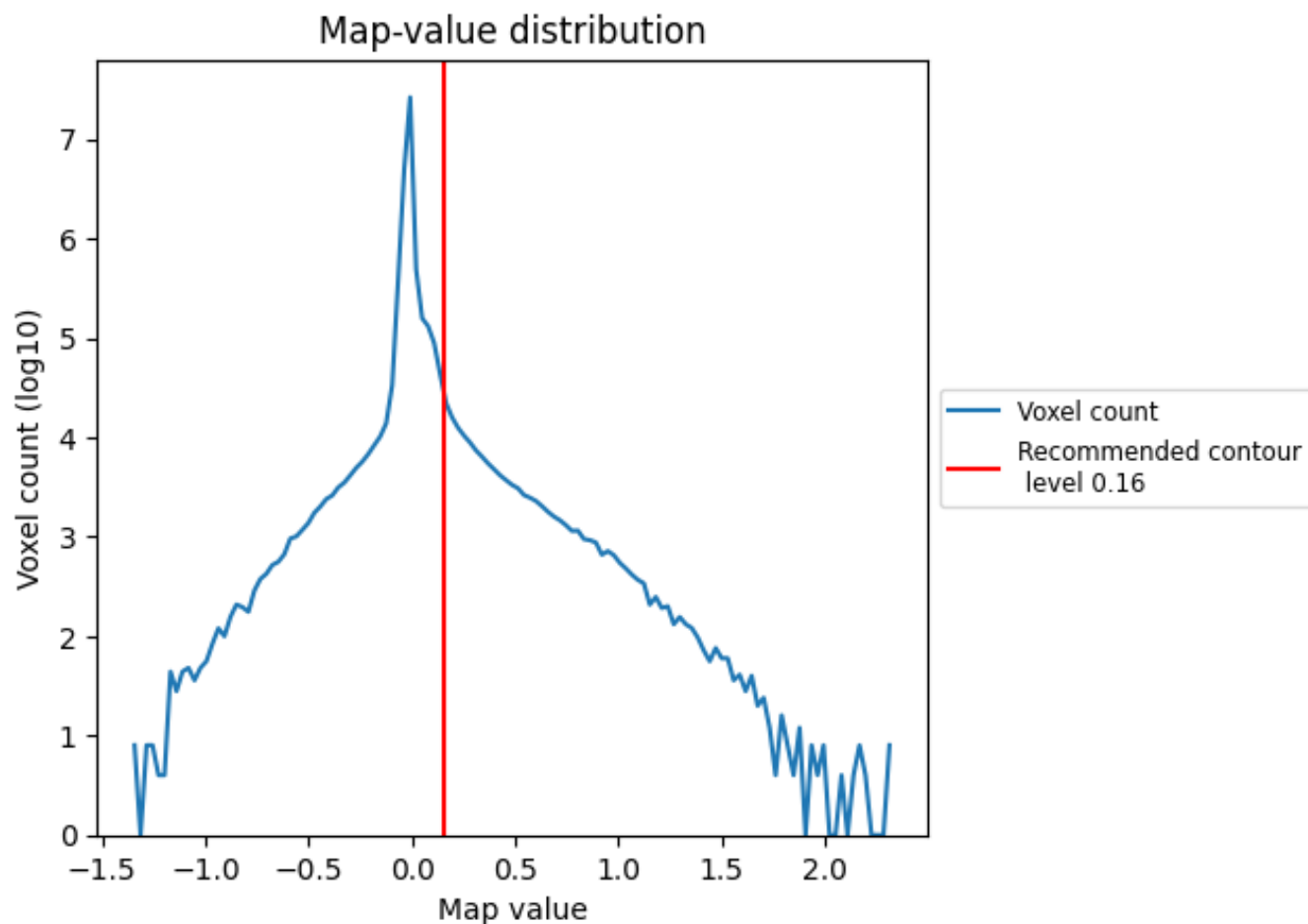
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

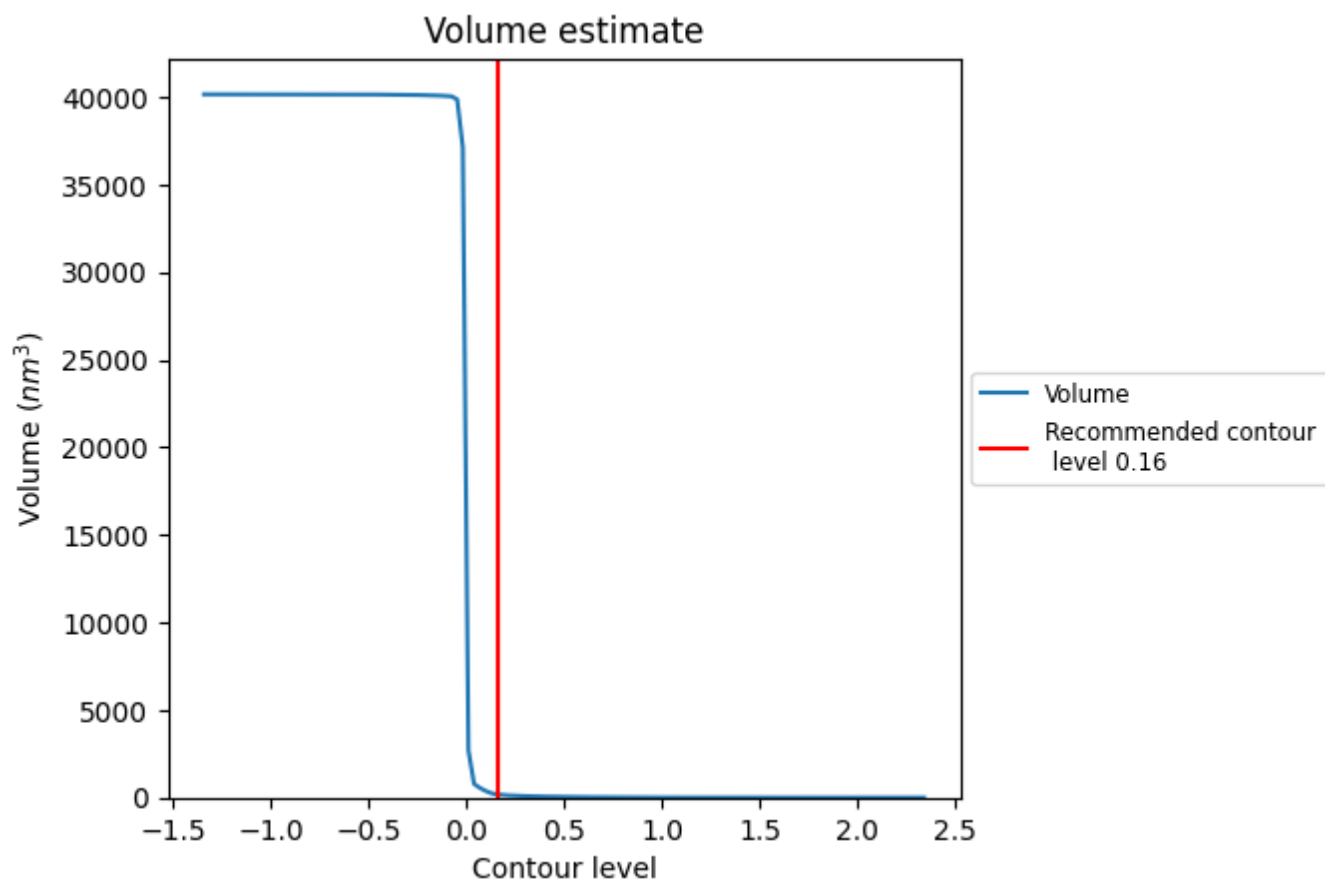
This section contains the results of statistical analysis of the map.

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.

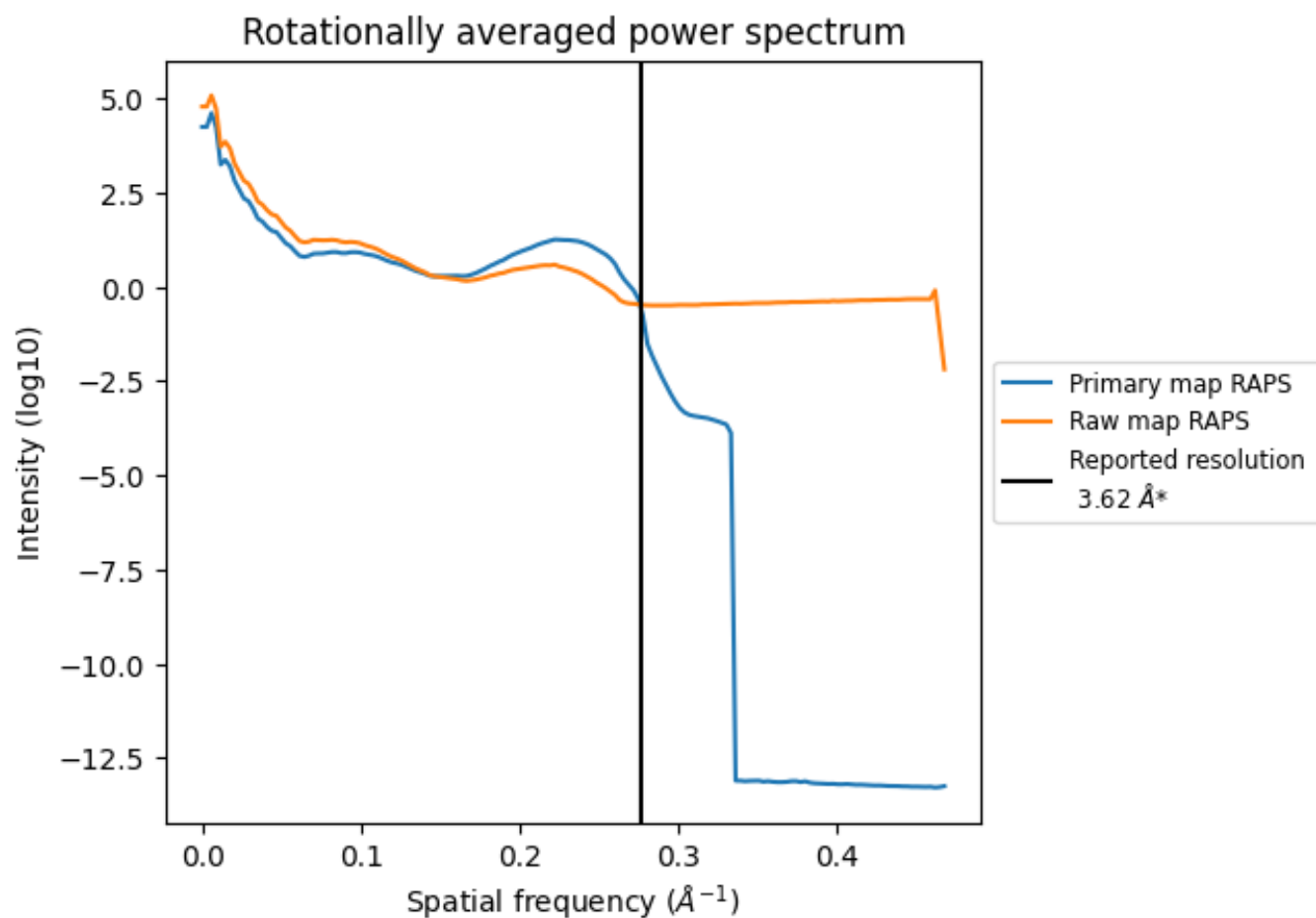
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 175 nm³; 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 ⓘ

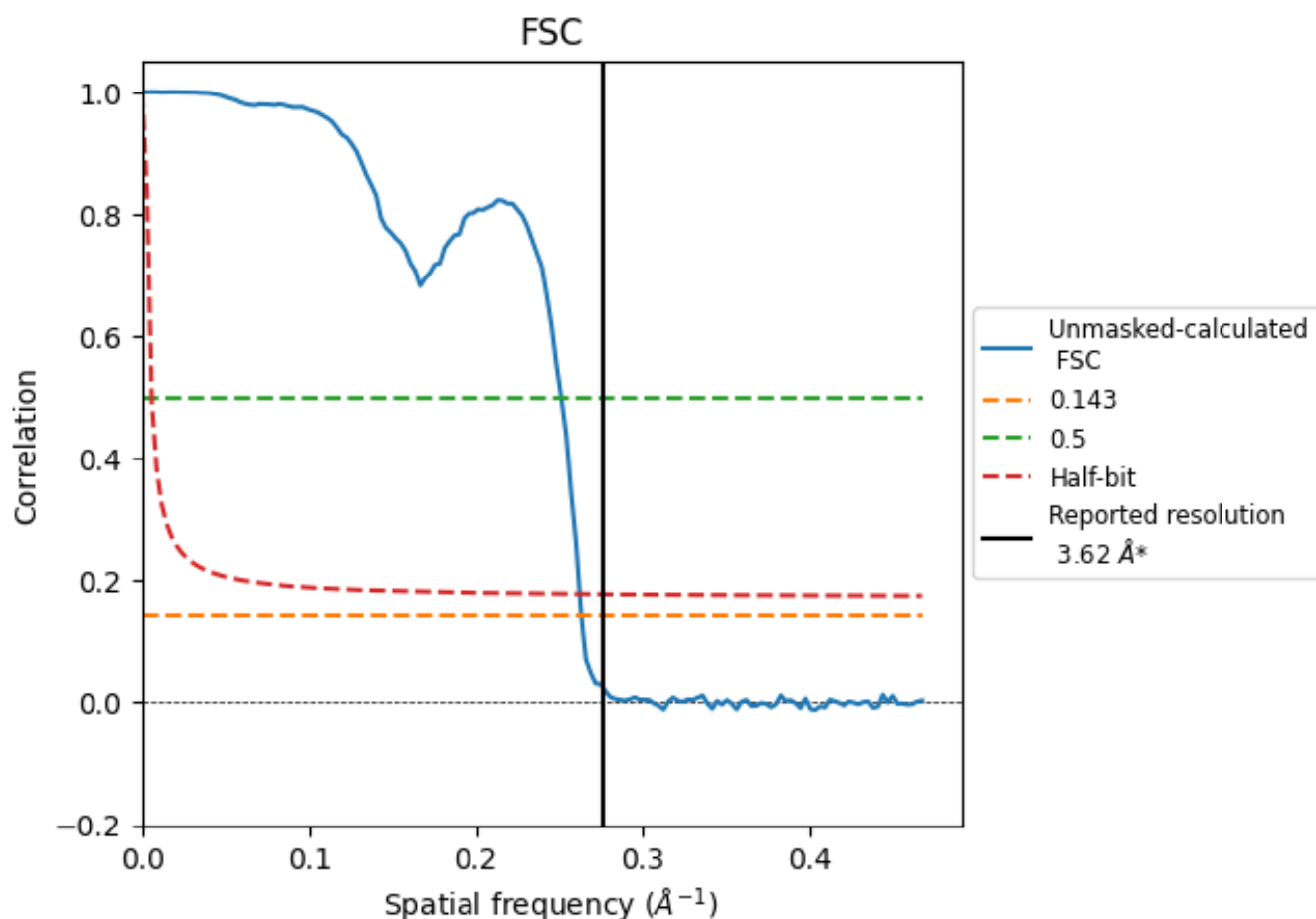


*Reported resolution corresponds to spatial frequency of 0.276 Å⁻¹

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 Å⁻¹

8.2 Resolution estimates [i](#)

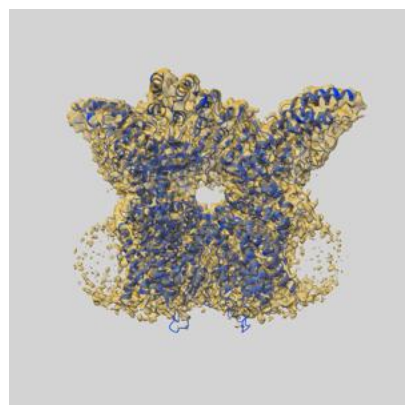
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.62	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.80	3.98	3.82

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

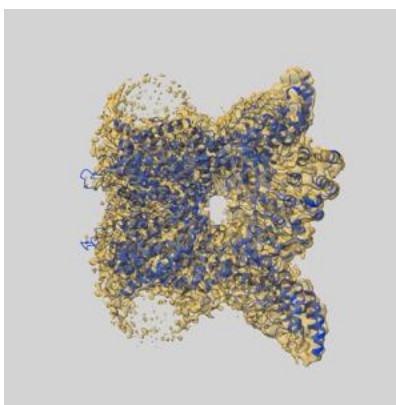
9 Map-model fit [i](#)

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](#).

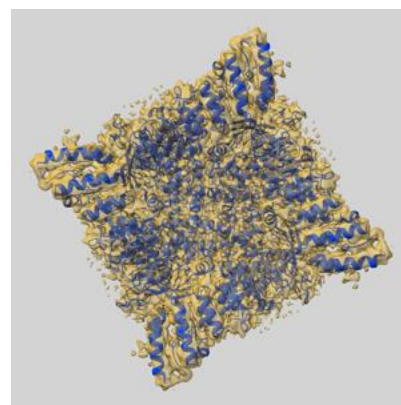
9.1 Map-model overlay [i](#)



X



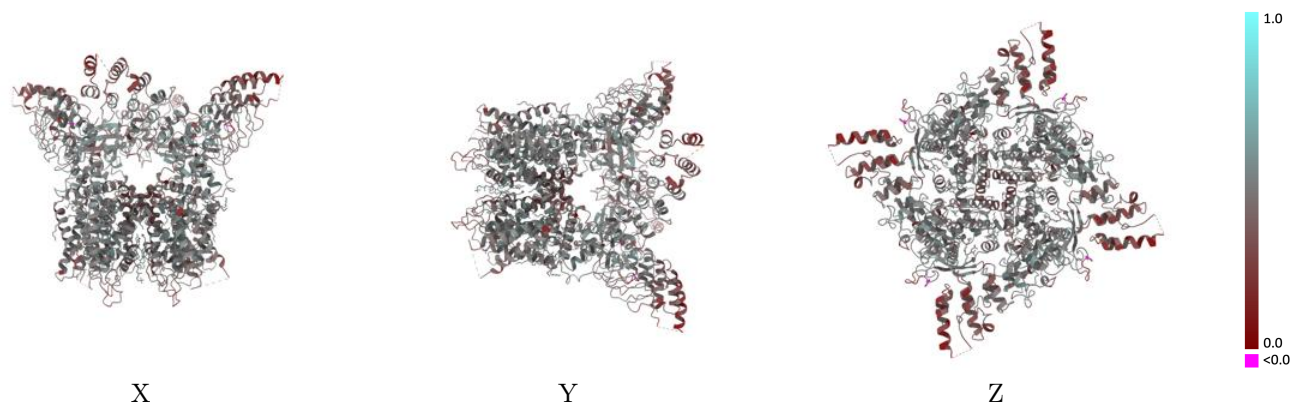
Y



Z

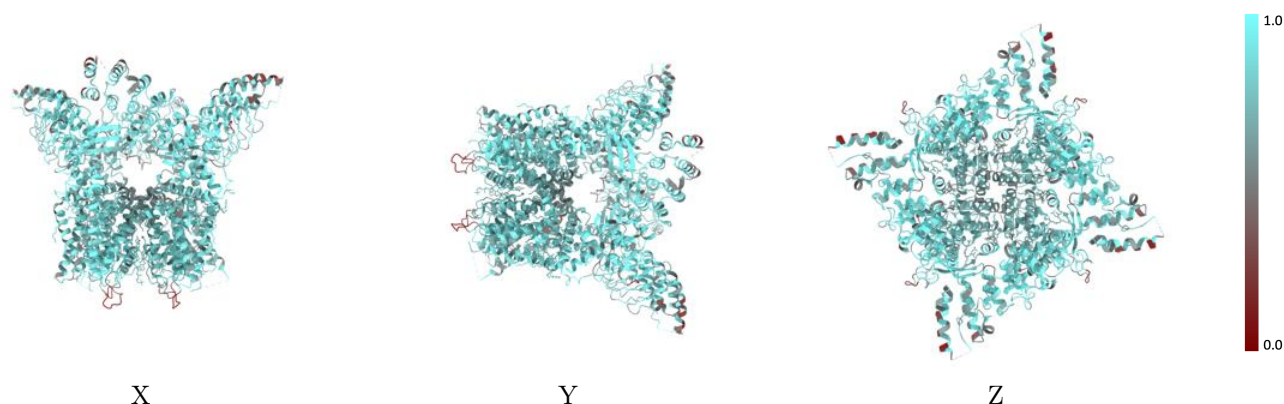
The images above show the 3D surface view of the map at the recommended contour level 0.16 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



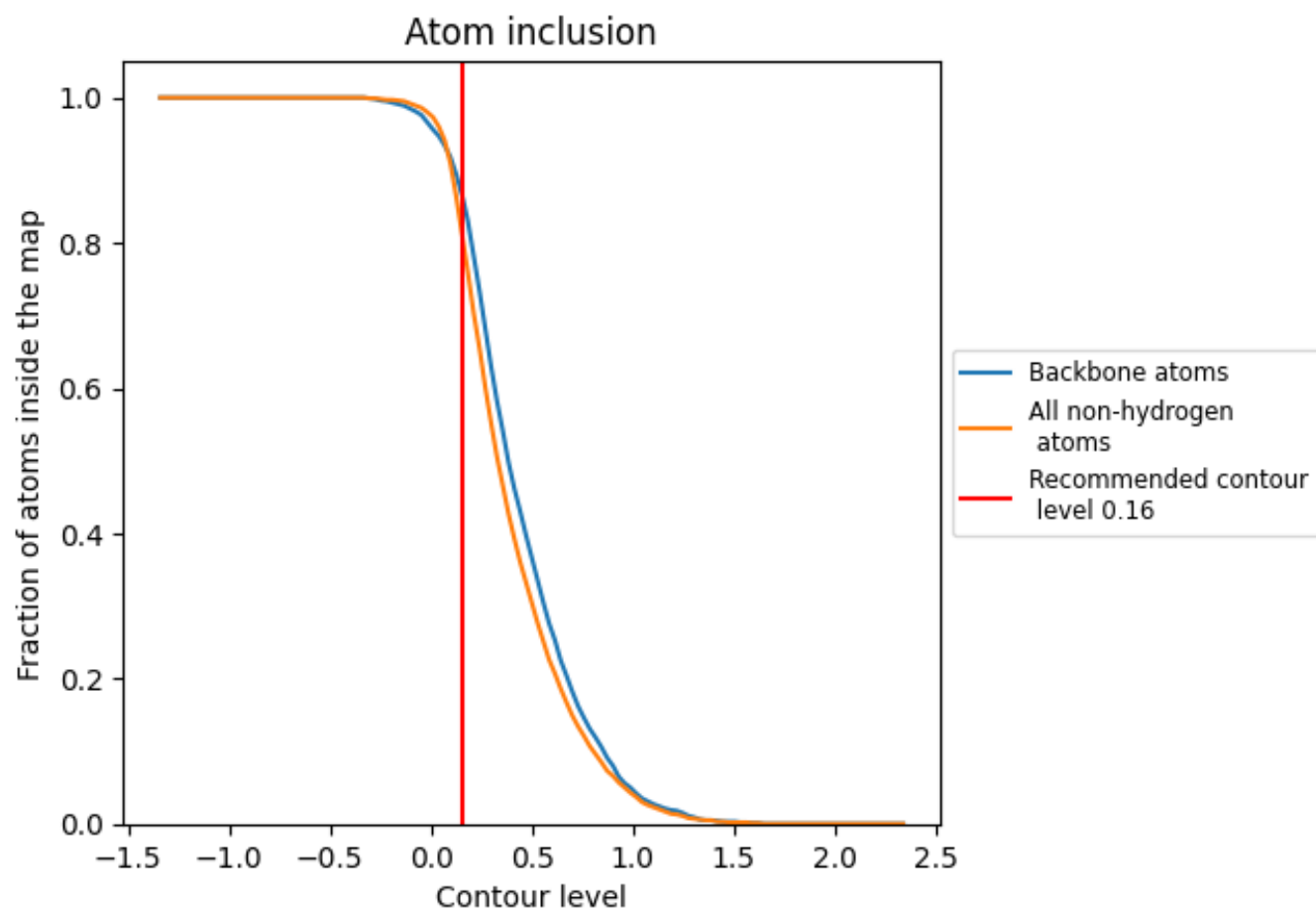
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	0.8010	0.4370
A	0.8010	0.4380
B	0.8000	0.4360
C	0.8000	0.4370
D	0.8010	0.4360

