



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 11:55 AM UTC

PDB ID : 8GKA / pdb_00008gka
EMDB ID : EMD-40181
Title : Human TRPV3 tetramer structure, closed conformation
Authors : Lansky, S.; Betancourt, J.M.; Scheuring, S.
Deposited on : 2023-03-17
Resolution : 2.55 Å(reported)
Based on initial model : 6UW4

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at 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>.

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

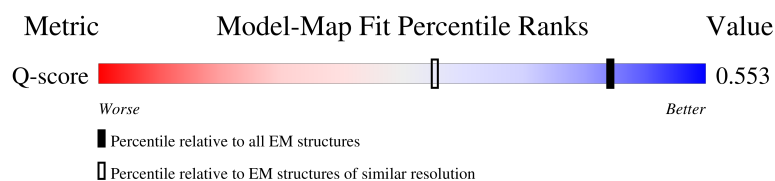
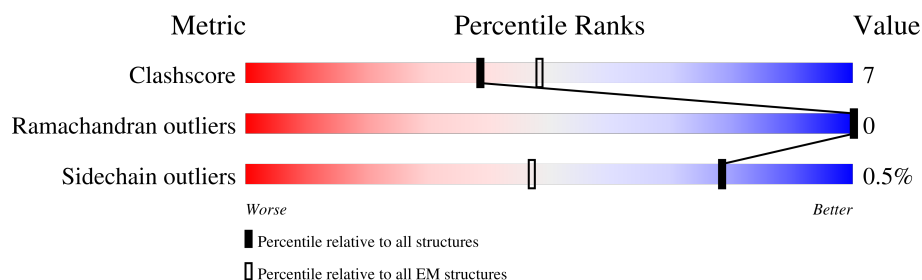
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.55 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	7475 (2.05 - 3.05)

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	790	7% 64% 15% 21%
1	B	790	7% 64% 15% 21%
1	C	790	7% 64% 15% 21%
1	D	790	7% 64% 15% 21%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 21812 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.

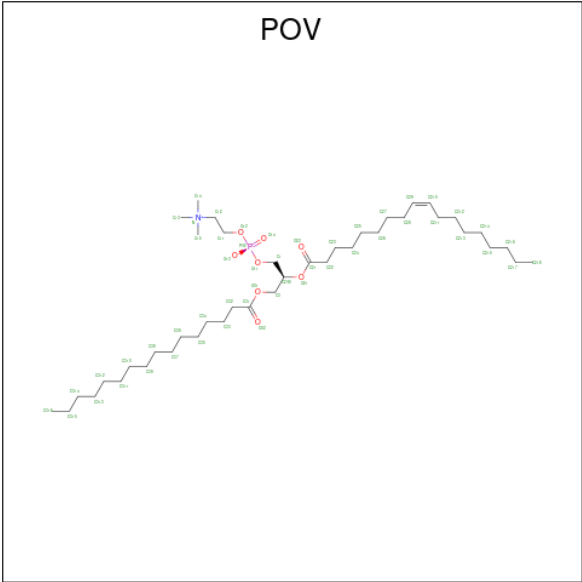
- Molecule 1 is a protein called Transient receptor potential cation channel subfamily V member 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	625	Total	C	N	O	S	0	0
			5090	3310	844	905	31		
1	B	625	Total	C	N	O	S	0	0
			5090	3310	844	905	31		
1	C	625	Total	C	N	O	S	0	0
			5090	3310	844	905	31		
1	D	625	Total	C	N	O	S	0	0
			5090	3310	844	905	31		

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total	Na	0
			1	1	

- Molecule 3 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (CCD ID: POV) (formula: C₄₂H₈₂NO₈P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	A	1	Total	C	N	O	P	0
			46	36	1	8	1	
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	A	1	Total	C	N	O	P	0
			36	26	1	8	1	
3	A	1	Total	C	N	O	P	0
			41	31	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
			46	36	1	8	1	
3	A	1	Total	C	N	O	P	0
			47	37	1	8	1	
3	B	1	Total	C	N	O	P	0
			47	37	1	8	1	
3	B	1	Total	C	N	O	P	0
			46	36	1	8	1	
3	B	1	Total	C	N	O	P	0
			45	35	1	8	1	
3	B	1	Total	C	N	O	P	0
			34	24	1	8	1	
3	B	1	Total	C	N	O	P	0
			39	29	1	8	1	
3	B	1	Total	C	N	O	P	0
			40	30	1	8	1	

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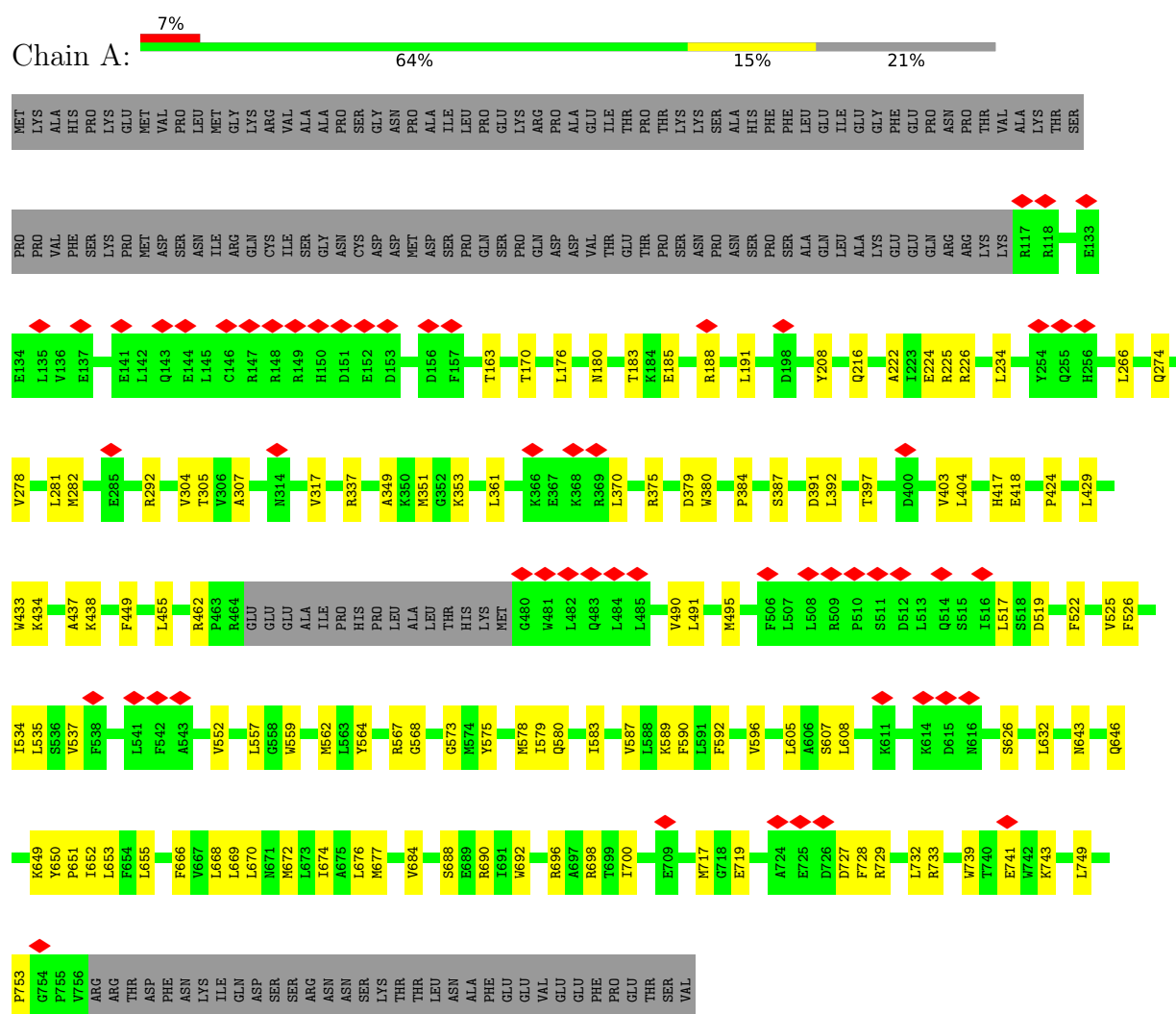
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Mol	Chain	Residues	Atoms					AltConf
3	B	1	Total	C	N	O	P	0
			46	36	1	8	1	
3	B	1	Total	C	N	O	P	0
			40	30	1	8	1	
3	B	1	Total	C	N	O	P	0
			46	36	1	8	1	
3	B	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	C	1	Total	C	N	O	P	0
			42	32	1	8	1	
3	C	1	Total	C	N	O	P	0
			37	27	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
			39	29	1	8	1	
3	C	1	Total	C	N	O	P	0
			40	30	1	8	1	
3	C	1	Total	C	N	O	P	0
			42	32	1	8	1	
3	D	1	Total	C	N	O	P	0
			48	38	1	8	1	
3	D	1	Total	C	N	O	P	0
			44	34	1	8	1	
3	D	1	Total	C	N	O	P	0
			44	34	1	8	1	
3	D	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	D	1	Total	C	N	O	P	0
			39	29	1	8	1	
3	D	1	Total	C	N	O	P	0
			41	31	1	8	1	
3	D	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	D	1	Total	C	N	O	P	0
			52	42	1	8	1	

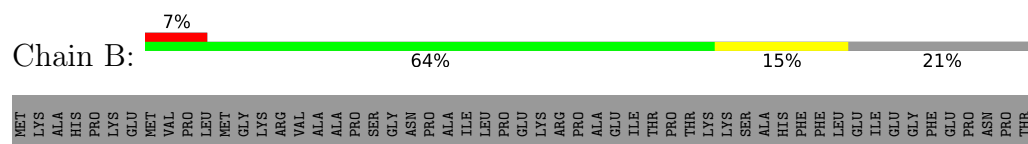
3 Residue-property plots

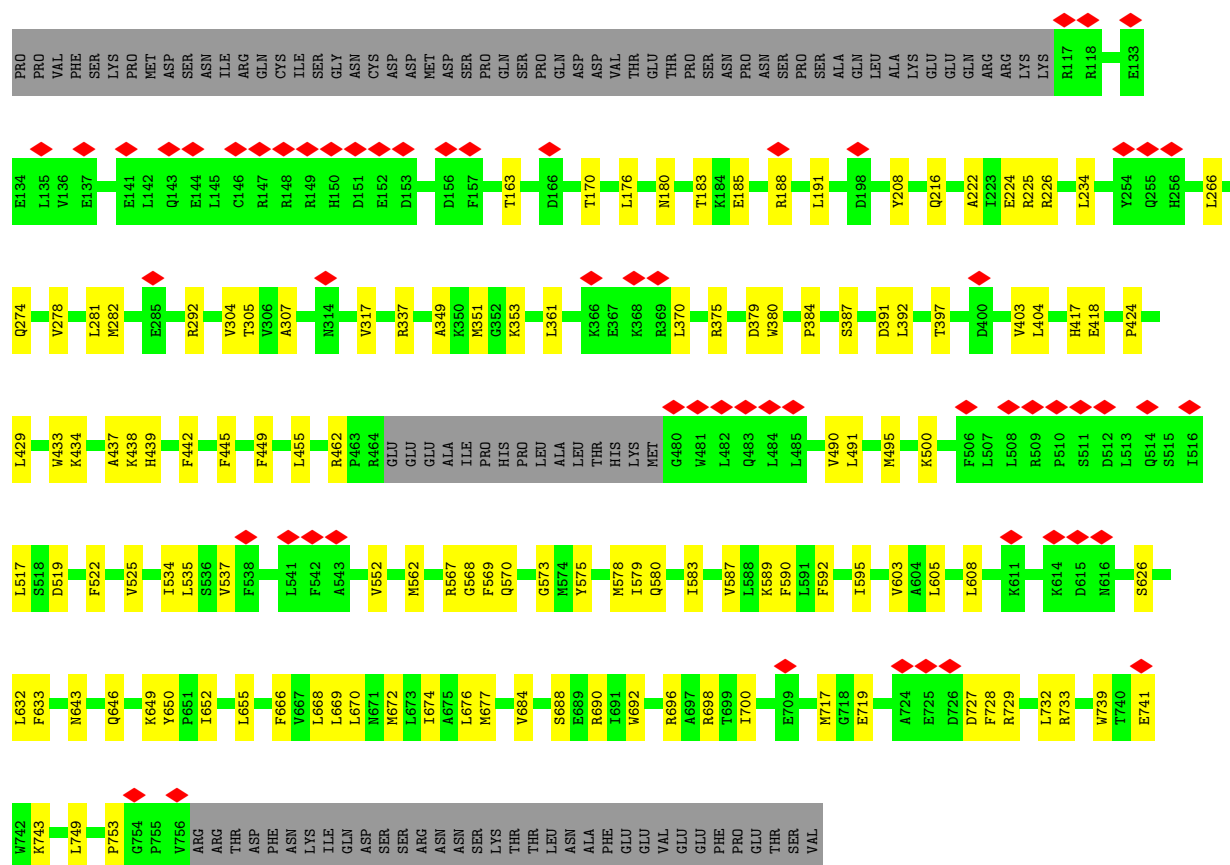
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

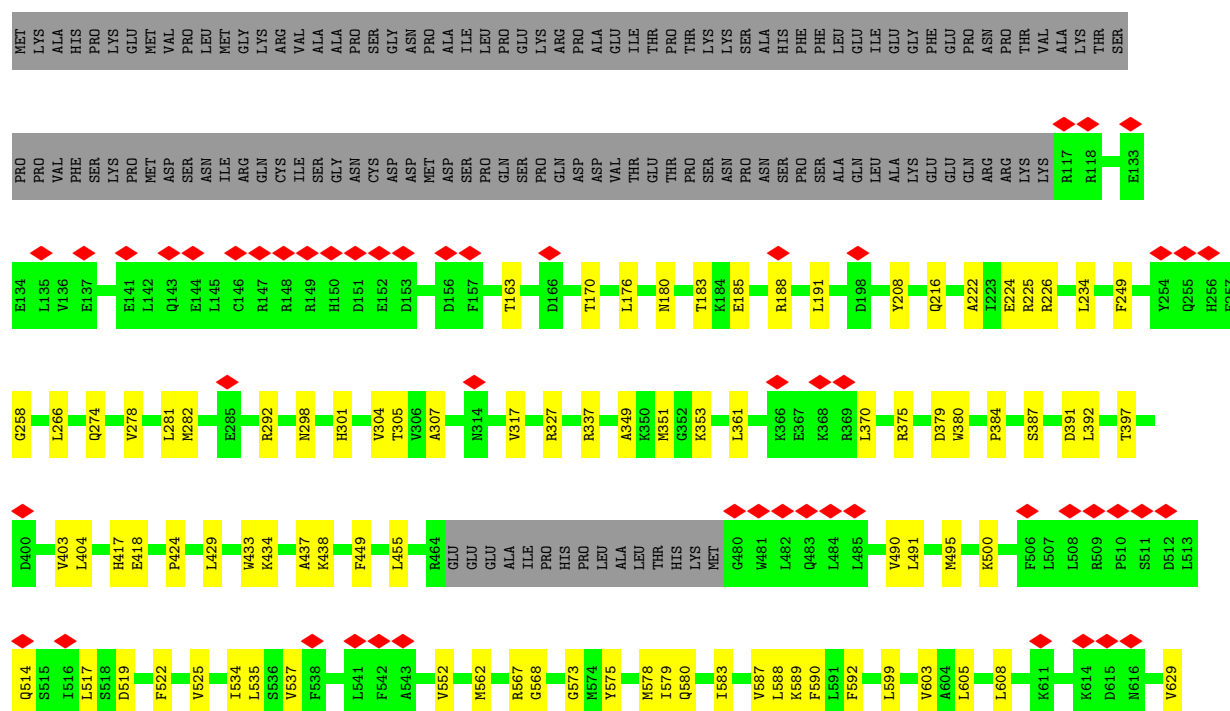


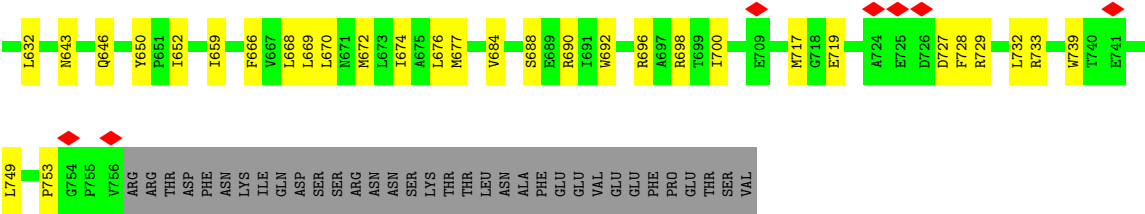
- Molecule 1: Transient receptor potential cation channel subfamily V member 3



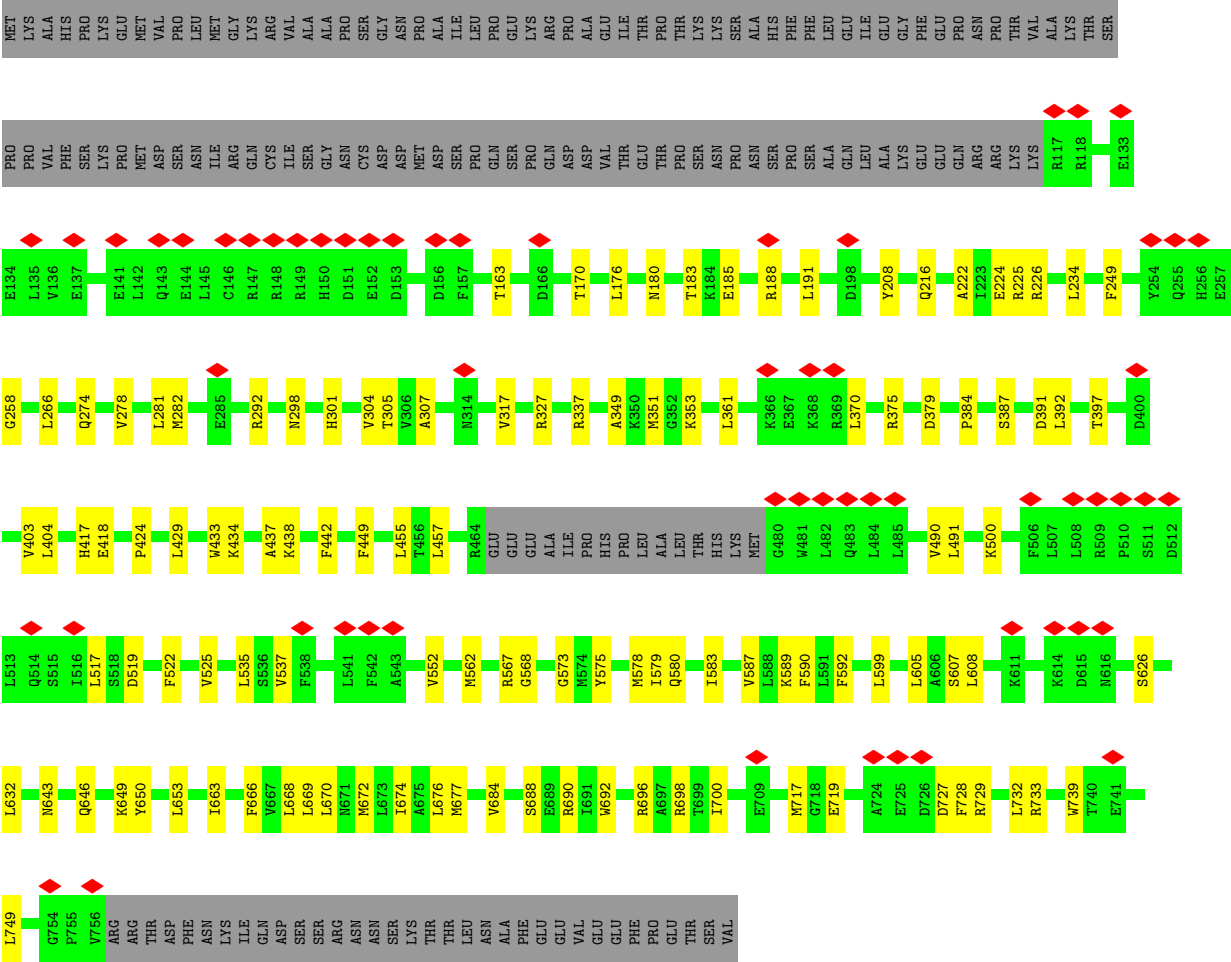


- Molecule 1: Transient receptor potential cation channel subfamily V member 3





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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	1532979	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	53.27	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	5.196	Depositor
Minimum map value	-2.731	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.128	Depositor
Recommended contour level	0.596	Depositor
Map size ($\text{\AA}$)	301.28, 301.28, 301.28	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.076, 1.076, 1.076	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: POV, NA

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	0.07	0/5201	0.21	0/7035
1	B	0.07	0/5201	0.21	0/7035
1	C	0.07	0/5201	0.21	0/7035
1	D	0.07	0/5201	0.21	0/7035
All	All	0.07	0/20804	0.21	0/28140

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	5090	0	5155	82	0
1	B	5090	0	5155	89	0
1	C	5090	0	5155	86	0
1	D	5090	0	5155	77	0
2	A	1	0	0	0	0
3	A	353	0	511	24	0
3	B	435	0	618	39	0
3	C	291	0	407	20	0
3	D	372	0	554	13	0
All	All	21812	0	22710	326	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 7.

All (326) 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:717:MET:HE1	1:B:733:ARG:HE	1.58	0.69
1:C:717:MET:HE1	1:C:733:ARG:HE	1.58	0.69
1:A:717:MET:HE1	1:A:733:ARG:HE	1.58	0.68
1:D:717:MET:HE1	1:D:733:ARG:HE	1.58	0.68
1:A:655:LEU:HD23	3:B:802:POV:H32	1.77	0.67
1:B:655:LEU:HD23	3:B:810:POV:H32	1.81	0.63
1:D:719:GLU:HB3	1:D:728:PHE:HB3	1.82	0.62
1:C:719:GLU:HB3	1:C:728:PHE:HB3	1.82	0.62
1:C:224:GLU:OE1	1:C:225:ARG:NH1	2.33	0.62
1:D:224:GLU:OE1	1:D:225:ARG:NH1	2.33	0.62
1:A:224:GLU:OE1	1:A:225:ARG:NH1	2.33	0.62
1:B:224:GLU:OE1	1:B:225:ARG:NH1	2.33	0.61
1:B:655:LEU:HD21	3:B:810:POV:H26	1.82	0.61
1:A:719:GLU:HB3	1:A:728:PHE:HB3	1.82	0.61
1:B:719:GLU:HB3	1:B:728:PHE:HB3	1.82	0.61
1:C:304:VAL:O	1:C:353:LYS:NZ	2.34	0.61
1:C:567:ARG:HH22	3:C:806:POV:H13A	1.66	0.61
1:B:567:ARG:HH22	3:B:808:POV:H13A	1.66	0.60
1:D:653:LEU:HB2	3:D:802:POV:H3	1.84	0.60
1:C:589:LYS:NZ	3:C:805:POV:O14	2.30	0.60
1:A:666:PHE:HA	1:A:670:LEU:HD12	1.84	0.59
1:B:519:ASP:OD1	1:B:698:ARG:NH2	2.36	0.59
1:C:562:MET:HB3	3:C:802:POV:H212	1.85	0.59
1:C:666:PHE:HA	1:C:670:LEU:HD12	1.84	0.59
1:D:519:ASP:OD1	1:D:698:ARG:NH2	2.36	0.59
1:C:517:LEU:O	1:C:580:GLN:NE2	2.36	0.58
1:A:517:LEU:O	1:A:580:GLN:NE2	2.36	0.58
1:A:519:ASP:OD1	1:A:698:ARG:NH2	2.36	0.58
1:D:517:LEU:O	1:D:580:GLN:NE2	2.36	0.58
1:D:666:PHE:HA	1:D:670:LEU:HD12	1.84	0.58
1:B:666:PHE:HA	1:B:670:LEU:HD12	1.84	0.58
1:B:517:LEU:O	1:B:580:GLN:NE2	2.36	0.58
1:C:519:ASP:OD1	1:C:698:ARG:NH2	2.36	0.58
1:A:626:SER:HB2	3:A:802:POV:H23	1.85	0.57
1:D:304:VAL:O	1:D:353:LYS:NZ	2.34	0.57
1:A:304:VAL:O	1:A:353:LYS:NZ	2.34	0.57
3:B:810:POV:H28	1:C:629:VAL:HG12	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:433:TRP:HA	1:D:437:ALA:HB3	1.87	0.57
1:B:433:TRP:HA	1:B:437:ALA:HB3	1.87	0.56
1:D:361:LEU:HB3	1:D:424:PRO:HG3	1.88	0.56
1:A:567:ARG:NH2	3:A:806:POV:O13	2.39	0.56
1:A:674:ILE:HA	1:A:677:MET:HE2	1.88	0.56
1:D:674:ILE:HA	1:D:677:MET:HE2	1.88	0.56
1:B:304:VAL:O	1:B:353:LYS:NZ	2.34	0.56
1:C:361:LEU:HB3	1:C:424:PRO:HG3	1.88	0.56
1:D:379:ASP:OD2	1:D:733:ARG:NH1	2.36	0.56
1:C:433:TRP:HA	1:C:437:ALA:HB3	1.87	0.56
1:B:361:LEU:HB3	1:B:424:PRO:HG3	1.88	0.55
1:A:361:LEU:HB3	1:A:424:PRO:HG3	1.88	0.55
1:A:433:TRP:HA	1:A:437:ALA:HB3	1.87	0.55
1:B:674:ILE:HA	1:B:677:MET:HE2	1.88	0.55
1:C:674:ILE:HA	1:C:677:MET:HE2	1.88	0.55
1:B:379:ASP:OD2	1:B:733:ARG:NH1	2.36	0.55
1:A:305:THR:HG23	1:A:351:MET:HE1	1.89	0.55
1:B:568:GLY:H	1:B:692:TRP:HE1	1.55	0.55
1:C:305:THR:HG23	1:C:351:MET:HE1	1.89	0.55
1:C:514:GLN:HE22	3:C:805:POV:H23	1.72	0.55
1:A:568:GLY:H	1:A:692:TRP:HE1	1.55	0.55
1:A:596:VAL:HA	3:A:803:POV:H311	1.88	0.55
1:C:379:ASP:OD2	1:C:733:ARG:NH1	2.36	0.54
1:B:590:PHE:HE1	1:B:669:LEU:HB3	1.73	0.54
1:D:590:PHE:HE1	1:D:669:LEU:HB3	1.73	0.54
1:D:568:GLY:H	1:D:692:TRP:HE1	1.55	0.54
1:C:568:GLY:H	1:C:692:TRP:HE1	1.55	0.54
1:B:305:THR:HG23	1:B:351:MET:HE1	1.89	0.54
1:B:500:LYS:NZ	3:B:806:POV:O13	2.41	0.54
1:B:307:ALA:HB2	1:B:317:VAL:HG11	1.90	0.53
1:D:305:THR:HG23	1:D:351:MET:HE1	1.89	0.53
1:A:590:PHE:HE1	1:A:669:LEU:HB3	1.73	0.53
1:C:176:LEU:HD13	1:C:222:ALA:HB2	1.91	0.53
1:C:590:PHE:HE1	1:C:669:LEU:HB3	1.73	0.53
1:C:599:LEU:HB3	3:C:803:POV:H36A	1.91	0.53
1:D:176:LEU:HD13	1:D:222:ALA:HB2	1.91	0.53
1:A:292:ARG:NH1	1:A:337:ARG:O	2.36	0.53
1:D:307:ALA:HB2	1:D:317:VAL:HG11	1.90	0.53
1:A:379:ASP:OD2	1:A:733:ARG:NH1	2.36	0.53
1:C:676:LEU:HD21	1:D:578:MET:HG2	1.91	0.53
1:D:643:ASN:O	1:D:646:GLN:NE2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:307:ALA:HB2	1:C:317:VAL:HG11	1.90	0.53
1:A:578:MET:HG2	1:D:676:LEU:HD21	1.90	0.53
1:C:643:ASN:O	1:C:646:GLN:NE2	2.41	0.53
1:A:176:LEU:HD13	1:A:222:ALA:HB2	1.91	0.52
1:A:307:ALA:HB2	1:A:317:VAL:HG11	1.90	0.52
1:B:176:LEU:HD13	1:B:222:ALA:HB2	1.91	0.52
1:D:567:ARG:HH22	3:D:806:POV:H14A	1.74	0.52
1:B:292:ARG:NH1	1:B:337:ARG:O	2.36	0.52
1:C:659:ILE:HD12	3:D:808:POV:H36	1.89	0.52
1:A:643:ASN:O	1:A:646:GLN:NE2	2.41	0.52
1:B:676:LEU:HD21	1:C:578:MET:HG2	1.90	0.52
1:D:433:TRP:HE1	3:D:803:POV:H12	1.74	0.52
1:A:676:LEU:HD21	1:B:578:MET:HG2	1.90	0.52
3:B:805:POV:H22A	3:C:801:POV:H29	1.91	0.52
1:D:583:ILE:HA	1:D:587:VAL:HB	1.92	0.52
1:A:526:PHE:CG	3:A:804:POV:H15B	2.45	0.52
1:C:349:ALA:HB2	1:C:403:VAL:HG13	1.92	0.51
1:D:292:ARG:NH1	1:D:337:ARG:O	2.36	0.51
1:B:643:ASN:O	1:B:646:GLN:NE2	2.41	0.51
1:D:349:ALA:HB2	1:D:403:VAL:HG13	1.92	0.51
1:B:583:ILE:HA	1:B:587:VAL:HB	1.92	0.51
1:C:185:GLU:OE1	1:C:188:ARG:NH2	2.44	0.51
1:D:185:GLU:OE1	1:D:188:ARG:NH2	2.44	0.51
1:B:417:HIS:HB2	1:B:690:ARG:HB3	1.92	0.51
1:D:567:ARG:NH2	3:D:806:POV:O13	2.42	0.51
1:A:455:LEU:HD13	1:A:490:VAL:HG11	1.93	0.51
1:A:449:PHE:HA	1:A:562:MET:HE1	1.91	0.51
1:B:185:GLU:OE1	1:B:188:ARG:NH2	2.44	0.51
1:D:417:HIS:HB2	1:D:690:ARG:HB3	1.92	0.51
1:D:455:LEU:HD13	1:D:490:VAL:HG11	1.93	0.51
3:D:801:POV:H21J	3:D:808:POV:H38A	1.93	0.51
1:C:500:LYS:NZ	3:C:804:POV:O13	2.44	0.51
1:B:449:PHE:HA	1:B:562:MET:HE1	1.91	0.51
1:C:449:PHE:HA	1:C:562:MET:HE1	1.91	0.51
1:A:185:GLU:OE1	1:A:188:ARG:NH2	2.44	0.51
1:D:392:LEU:HD11	1:D:732:LEU:HB2	1.94	0.50
1:D:449:PHE:HA	1:D:562:MET:HE1	1.91	0.50
1:B:455:LEU:HD13	1:B:490:VAL:HG11	1.93	0.50
1:C:583:ILE:HA	1:C:587:VAL:HB	1.92	0.50
1:A:349:ALA:HB2	1:A:403:VAL:HG13	1.92	0.50
1:A:417:HIS:HB2	1:A:690:ARG:HB3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:583:ILE:HA	1:A:587:VAL:HB	1.92	0.50
3:A:809:POV:H28	1:D:592:PHE:HE2	1.76	0.50
1:B:349:ALA:HB2	1:B:403:VAL:HG13	1.92	0.50
1:C:392:LEU:HD11	1:C:732:LEU:HB2	1.94	0.50
1:A:655:LEU:HD21	3:B:802:POV:H26	1.93	0.50
1:C:417:HIS:HB2	1:C:690:ARG:HB3	1.92	0.50
1:C:652:ILE:HB	3:C:807:POV:H1	1.94	0.50
1:B:442:PHE:HD1	3:B:803:POV:H22	1.76	0.50
1:C:455:LEU:HD13	1:C:490:VAL:HG11	1.93	0.50
1:A:522:PHE:HA	1:A:525:VAL:HG22	1.94	0.50
1:C:500:LYS:HZ2	3:C:804:POV:H1	1.76	0.50
1:A:392:LEU:HD11	1:A:732:LEU:HB2	1.94	0.49
1:A:433:TRP:HE1	3:A:809:POV:H12A	1.77	0.49
1:D:522:PHE:HA	1:D:525:VAL:HG22	1.94	0.49
1:B:442:PHE:HB2	3:B:803:POV:H3	1.95	0.49
1:B:522:PHE:HA	1:B:525:VAL:HG22	1.94	0.49
1:C:379:ASP:OD1	1:C:387:SER:OG	2.30	0.49
1:C:603:VAL:HG11	3:C:803:POV:H33A	1.94	0.49
3:B:803:POV:H13	3:B:804:POV:H13A	1.94	0.49
1:B:392:LEU:HD11	1:B:732:LEU:HB2	1.94	0.49
1:C:292:ARG:NH1	1:C:337:ARG:O	2.36	0.49
1:C:522:PHE:HA	1:C:525:VAL:HG22	1.94	0.49
1:B:379:ASP:OD1	1:B:387:SER:OG	2.30	0.48
1:B:375:ARG:NH1	1:B:391:ASP:OD2	2.47	0.48
1:B:562:MET:HB3	3:B:803:POV:H212	1.95	0.48
1:C:433:TRP:HE1	3:C:802:POV:H14B	1.78	0.48
1:B:592:PHE:HB2	3:B:807:POV:H37A	1.94	0.48
1:D:375:ARG:NH1	1:D:391:ASP:OD2	2.47	0.48
1:D:379:ASP:OD1	1:D:387:SER:OG	2.30	0.48
1:A:375:ARG:NH1	1:A:391:ASP:OD2	2.47	0.48
1:C:517:LEU:HD22	3:C:806:POV:H24A	1.96	0.48
1:C:375:ARG:NH1	1:C:391:ASP:OD2	2.47	0.47
1:C:684:VAL:HG12	1:C:688:SER:HB3	1.97	0.47
1:D:404:LEU:HD11	1:D:429:LEU:HD21	1.97	0.47
1:B:517:LEU:HD22	3:B:808:POV:H24A	1.97	0.47
1:D:684:VAL:HG12	1:D:688:SER:HB3	1.97	0.47
1:B:163:THR:HG22	1:B:170:THR:HG22	1.97	0.47
3:B:803:POV:H25A	3:B:803:POV:H22A	1.70	0.47
1:A:163:THR:HG22	1:A:170:THR:HG22	1.97	0.46
1:B:684:VAL:HG12	1:B:688:SER:HB3	1.97	0.46
1:C:580:GLN:HB2	3:C:806:POV:H1	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:626:SER:HB2	3:D:808:POV:H22	1.97	0.46
3:A:802:POV:H12	3:A:802:POV:H1A	1.96	0.46
1:B:404:LEU:HD11	1:B:429:LEU:HD21	1.97	0.46
1:C:163:THR:HG22	1:C:170:THR:HG22	1.97	0.46
1:D:442:PHE:HD1	3:D:803:POV:H22	1.81	0.46
1:C:589:LYS:HD3	1:D:575:TYR:HB2	1.98	0.46
1:A:404:LEU:HD11	1:A:429:LEU:HD21	1.97	0.46
1:B:569:PHE:CD1	3:B:804:POV:H3A	2.50	0.46
1:C:404:LEU:HD11	1:C:429:LEU:HD21	1.97	0.46
3:C:802:POV:H26A	3:C:802:POV:H29	1.66	0.46
1:B:562:MET:O	3:B:803:POV:H210	2.15	0.46
1:B:580:GLN:HB2	3:B:808:POV:H1	1.98	0.46
1:B:589:LYS:HD3	1:C:575:TYR:HB2	1.98	0.46
1:A:567:ARG:HH22	3:A:806:POV:H13A	1.80	0.46
1:B:608:LEU:HD12	1:B:650:TYR:HB2	1.98	0.46
1:D:163:THR:HG22	1:D:170:THR:HG22	1.97	0.46
1:A:684:VAL:HG12	1:A:688:SER:HB3	1.97	0.46
1:B:633:PHE:CD1	3:B:802:POV:H210	2.51	0.46
3:A:803:POV:H31H	3:B:803:POV:H215	1.98	0.45
1:B:522:PHE:HD2	3:B:808:POV:H13B	1.82	0.45
1:B:595:ILE:HD11	3:B:807:POV:H21J	1.97	0.45
1:C:522:PHE:HD2	3:C:806:POV:H13B	1.82	0.45
1:C:608:LEU:HD12	1:C:650:TYR:HB2	1.98	0.45
3:A:802:POV:H36	3:B:801:POV:H217	1.98	0.45
1:D:626:SER:HB3	3:D:801:POV:H28A	1.98	0.45
1:B:573:GLY:HA3	1:B:692:TRP:CD1	2.52	0.45
1:A:672:MET:HE1	1:B:579:ILE:HG12	1.98	0.45
1:B:672:MET:HE1	1:C:579:ILE:HG12	1.98	0.45
1:C:668:LEU:HD13	1:D:587:VAL:HG21	1.98	0.45
1:A:668:LEU:HD13	1:B:587:VAL:HG21	1.99	0.45
1:C:573:GLY:HA3	1:C:692:TRP:CD1	2.52	0.45
1:D:608:LEU:HD12	1:D:650:TYR:HB2	1.98	0.45
1:A:180:ASN:N	1:A:183:THR:OG1	2.43	0.45
1:A:587:VAL:HG21	1:D:668:LEU:HD13	1.99	0.45
1:A:573:GLY:HA3	1:A:692:TRP:CD1	2.52	0.45
1:A:575:TYR:HB2	1:D:589:LYS:HD3	1.98	0.45
3:A:802:POV:H214	1:D:663:ILE:HD11	1.99	0.45
1:A:559:TRP:CE2	3:A:808:POV:H38	2.52	0.45
3:A:803:POV:H14	3:B:801:POV:H12A	1.98	0.45
1:B:434:LYS:HA	1:B:438:LYS:HE3	1.99	0.45
1:B:439:HIS:HB3	3:B:803:POV:H38A	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:580:GLN:HB2	3:A:806:POV:H1	1.99	0.45
1:A:589:LYS:HD3	1:B:575:TYR:HB2	1.98	0.45
1:B:668:LEU:HD13	1:C:587:VAL:HG21	1.99	0.45
1:D:573:GLY:HA3	1:D:692:TRP:CD1	2.52	0.45
1:A:579:ILE:HG12	1:D:672:MET:HE1	1.98	0.44
1:A:608:LEU:HD12	1:A:650:TYR:HB2	1.98	0.44
1:B:626:SER:HB2	3:B:802:POV:H23	1.98	0.44
1:C:434:LYS:HA	1:C:438:LYS:HE3	1.99	0.44
3:B:809:POV:H31C	3:B:810:POV:H36	1.98	0.44
1:D:605:LEU:HD12	1:D:632:LEU:HD11	1.99	0.44
1:B:605:LEU:HD12	1:B:632:LEU:HD11	1.99	0.44
1:C:672:MET:HE1	1:D:579:ILE:HG12	1.99	0.44
1:A:379:ASP:OD1	1:A:387:SER:OG	2.30	0.44
1:A:434:LYS:HA	1:A:438:LYS:HE3	1.99	0.44
1:A:517:LEU:HD22	3:A:806:POV:H24A	2.00	0.44
1:B:491:LEU:HD13	1:B:537:VAL:HG21	2.00	0.44
3:A:807:POV:H35A	3:B:808:POV:H31E	2.00	0.44
1:B:570:GLN:HB2	3:B:804:POV:H15B	2.00	0.44
1:A:491:LEU:HD13	1:A:537:VAL:HG21	2.00	0.43
1:C:605:LEU:HD12	1:C:632:LEU:HD11	1.99	0.43
1:A:727:ASP:OD2	1:A:729:ARG:NH2	2.51	0.43
1:B:727:ASP:OD2	1:B:729:ARG:NH2	2.51	0.43
1:D:491:LEU:HD13	1:D:537:VAL:HG21	2.00	0.43
1:C:588:LEU:HD13	3:C:805:POV:H28A	2.00	0.43
1:D:180:ASN:N	1:D:183:THR:OG1	2.43	0.43
1:D:727:ASP:OD2	1:D:729:ARG:NH2	2.51	0.43
1:A:557:LEU:HB2	3:A:806:POV:H312	2.00	0.43
1:B:278:VAL:HG12	1:B:282:MET:HE2	2.01	0.43
1:C:696:ARG:O	1:C:700:ILE:HG12	2.19	0.43
1:C:491:LEU:HD13	1:C:537:VAL:HG21	2.00	0.43
1:D:434:LYS:HA	1:D:438:LYS:HE3	1.99	0.43
1:D:684:VAL:O	1:D:688:SER:N	2.52	0.43
1:A:607:SER:O	1:B:462:ARG:NH2	2.44	0.43
1:C:684:VAL:O	1:C:688:SER:N	2.52	0.43
1:A:208:TYR:HD2	1:A:216:GLN:HB3	1.84	0.43
1:B:226:ARG:HG2	1:B:274:GLN:NE2	2.34	0.43
1:A:605:LEU:HD12	1:A:632:LEU:HD11	1.99	0.43
1:C:727:ASP:OD2	1:C:729:ARG:NH2	2.51	0.43
1:B:442:PHE:CD2	3:B:803:POV:H35A	2.54	0.43
1:A:651:PRO:HD2	3:A:807:POV:H15A	2.01	0.43
1:A:652:ILE:HG23	3:B:802:POV:H32A	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:226:ARG:HG2	1:C:274:GLN:NE2	2.34	0.43
1:B:696:ARG:O	1:B:700:ILE:HG12	2.19	0.42
1:D:278:VAL:HG12	1:D:282:MET:HE2	2.01	0.42
1:A:684:VAL:O	1:A:688:SER:N	2.52	0.42
1:D:191:LEU:HD11	1:D:234:LEU:HD23	2.02	0.42
1:D:226:ARG:HG2	1:D:274:GLN:NE2	2.34	0.42
1:D:696:ARG:O	1:D:700:ILE:HG12	2.19	0.42
1:A:226:ARG:HG2	1:A:274:GLN:NE2	2.34	0.42
1:A:696:ARG:O	1:A:700:ILE:HG12	2.19	0.42
3:A:808:POV:H35A	3:D:801:POV:H38A	2.01	0.42
3:A:808:POV:H31B	1:D:599:LEU:HD12	2.01	0.42
1:B:208:TYR:HD2	1:B:216:GLN:HB3	1.84	0.42
1:B:684:VAL:O	1:B:688:SER:N	2.52	0.42
1:C:191:LEU:HD11	1:C:234:LEU:HD23	2.02	0.42
1:A:278:VAL:HG12	1:A:282:MET:HE2	2.01	0.42
1:B:569:PHE:HD1	3:B:804:POV:H1A	1.85	0.42
1:C:278:VAL:HG12	1:C:282:MET:HE2	2.01	0.42
1:C:384:PRO:HG3	1:C:739:TRP:CZ3	2.55	0.42
3:A:802:POV:H25	3:B:801:POV:H21A	2.02	0.42
1:C:180:ASN:N	1:C:183:THR:OG1	2.43	0.42
1:C:379:ASP:HA	1:C:749:LEU:HB2	2.02	0.42
1:C:417:HIS:CE1	1:C:418:GLU:HG3	2.55	0.42
1:A:191:LEU:HD11	1:A:234:LEU:HD23	2.02	0.42
1:A:384:PRO:HG3	1:A:739:TRP:CZ3	2.54	0.42
1:A:417:HIS:CE1	1:A:418:GLU:HG3	2.55	0.42
1:B:384:PRO:HG3	1:B:739:TRP:CZ3	2.54	0.42
1:D:384:PRO:HG3	1:D:739:TRP:CZ3	2.55	0.42
1:B:379:ASP:HA	1:B:749:LEU:HB2	2.02	0.42
1:B:603:VAL:HG11	3:B:805:POV:H33A	2.01	0.42
1:D:208:TYR:HD2	1:D:216:GLN:HB3	1.84	0.42
1:D:608:LEU:HD23	1:D:608:LEU:H	1.85	0.42
1:A:592:PHE:CE2	3:B:803:POV:H211	2.55	0.41
1:B:417:HIS:CE1	1:B:418:GLU:HG3	2.55	0.41
1:C:500:LYS:NZ	3:C:804:POV:H1	2.35	0.41
1:C:608:LEU:HD22	1:D:552:VAL:HG11	2.02	0.41
1:A:653:LEU:HB2	3:A:807:POV:H3	2.02	0.41
1:A:674:ILE:HD12	1:B:674:ILE:HD13	2.02	0.41
1:B:191:LEU:HD11	1:B:234:LEU:HD23	2.02	0.41
1:B:266:LEU:HA	1:B:281:LEU:HD13	2.02	0.41
1:B:380:TRP:HB2	1:B:753:PRO:HA	2.02	0.41
1:B:652:ILE:HG23	3:B:810:POV:H32A	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:495:MET:HE2	1:C:534:ILE:HD12	2.02	0.41
1:D:417:HIS:CE1	1:D:418:GLU:HG3	2.55	0.41
1:A:462:ARG:NH2	1:D:607:SER:O	2.42	0.41
3:A:804:POV:H21D	3:A:804:POV:H21A	1.85	0.41
1:B:180:ASN:N	1:B:183:THR:OG1	2.43	0.41
1:B:495:MET:HE2	1:B:534:ILE:HD12	2.02	0.41
1:C:266:LEU:HA	1:C:281:LEU:HD13	2.02	0.41
1:B:608:LEU:H	1:B:608:LEU:HD23	1.85	0.41
1:C:208:TYR:HD2	1:C:216:GLN:HB3	1.84	0.41
1:C:674:ILE:HD12	1:D:674:ILE:HD13	2.03	0.41
1:A:380:TRP:HB2	1:A:753:PRO:HA	2.02	0.41
1:A:564:TYR:CE1	3:A:804:POV:H14B	2.56	0.41
1:C:608:LEU:HD23	1:C:608:LEU:H	1.85	0.41
3:B:802:POV:H1	3:C:801:POV:H28A	2.02	0.41
1:D:379:ASP:HA	1:D:749:LEU:HB2	2.02	0.41
1:A:379:ASP:HA	1:A:749:LEU:HB2	2.02	0.41
1:B:445:PHE:HZ	3:B:803:POV:H216	1.85	0.41
1:C:282:MET:HB3	1:C:327:ARG:HG2	2.03	0.41
1:C:433:TRP:HE1	3:C:802:POV:H12A	1.85	0.41
1:C:592:PHE:HD1	3:C:805:POV:H39	1.85	0.41
1:D:282:MET:HB3	1:D:327:ARG:HG2	2.03	0.41
3:D:807:POV:H313	3:D:807:POV:H310	1.90	0.41
1:B:608:LEU:HD22	1:C:552:VAL:HG11	2.02	0.41
3:B:808:POV:H14B	3:B:808:POV:H11	1.86	0.41
1:A:649:LYS:HG3	1:A:650:TYR:CD2	2.56	0.40
1:B:674:ILE:HD12	1:C:674:ILE:HD13	2.03	0.40
1:D:649:LYS:HG3	1:D:650:TYR:CD2	2.56	0.40
1:A:552:VAL:HG11	1:D:608:LEU:HD22	2.02	0.40
1:A:741:GLU:HG3	1:A:743:LYS:NZ	2.37	0.40
1:B:649:LYS:HG3	1:B:650:TYR:CD2	2.56	0.40
1:A:608:LEU:HD22	1:B:552:VAL:HG11	2.01	0.40
1:D:457:LEU:HD21	3:D:807:POV:H38A	2.03	0.40
1:A:266:LEU:HA	1:A:281:LEU:HD13	2.02	0.40
1:C:249:PHE:CE1	1:C:258:GLY:HA2	2.57	0.40
1:C:380:TRP:HB2	1:C:753:PRO:HA	2.02	0.40
1:D:500:LYS:HZ2	3:D:804:POV:H1A	1.86	0.40
1:A:495:MET:HE2	1:A:534:ILE:HD12	2.02	0.40
1:B:741:GLU:HG3	1:B:743:LYS:NZ	2.37	0.40
1:C:298:ASN:OD1	1:C:301:HIS:ND1	2.55	0.40
1:C:589:LYS:HE3	1:C:589:LYS:HB2	1.93	0.40
1:D:249:PHE:CE1	1:D:258:GLY:HA2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:266:LEU:HA	1:D:281:LEU:HD13	2.02	0.40
1:D:298:ASN:OD1	1:D:301:HIS:ND1	2.55	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	621/790 (79%)	601 (97%)	20 (3%)	0	100	100
1	B	621/790 (79%)	601 (97%)	20 (3%)	0	100	100
1	C	621/790 (79%)	601 (97%)	20 (3%)	0	100	100
1	D	621/790 (79%)	601 (97%)	20 (3%)	0	100	100
All	All	2484/3160 (79%)	2404 (97%)	80 (3%)	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	554/703 (79%)	551 (100%)	3 (0%)	81	88
1	B	554/703 (79%)	551 (100%)	3 (0%)	81	88
1	C	554/703 (79%)	551 (100%)	3 (0%)	81	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	554/703 (79%)	551 (100%)	3 (0%)	81	88
All	All	2216/2812 (79%)	2204 (100%)	12 (0%)	78	88

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	370	LEU
1	A	397	THR
1	A	535	LEU
1	B	370	LEU
1	B	397	THR
1	B	535	LEU
1	C	370	LEU
1	C	397	THR
1	C	535	LEU
1	D	370	LEU
1	D	397	THR
1	D	535	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	426	HIS
1	A	585	HIS
1	A	745	HIS
1	B	244	HIS
1	B	745	HIS
1	C	244	HIS
1	C	514	GLN
1	C	745	HIS
1	D	426	HIS
1	D	439	HIS
1	D	695	GLN
1	D	745	HIS

5.3.3 RNA ⓘ

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](#)

Of 34 ligands modelled in this entry, 1 is monoatomic - leaving 33 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	POV	A	808	-	45,45,51	0.54	0	51,53,59	0.49	0
3	POV	C	801	-	51,51,51	0.50	0	57,59,59	0.46	0
3	POV	A	806	-	40,40,51	0.55	0	46,48,59	0.51	0
3	POV	C	803	-	36,36,51	0.58	0	42,44,59	0.52	0
3	POV	B	808	-	39,39,51	0.55	0	45,47,59	0.50	0
3	POV	D	808	-	51,51,51	0.50	0	57,59,59	0.45	0
3	POV	A	804	-	51,51,51	0.50	0	57,59,59	0.49	0
3	POV	D	802	-	43,43,51	0.54	0	49,51,59	0.50	0
3	POV	A	807	-	32,32,51	0.62	0	38,40,59	0.52	0
3	POV	C	807	-	41,41,51	0.55	0	47,49,59	0.50	0
3	POV	B	803	-	44,44,51	0.52	0	50,52,59	0.56	0
3	POV	B	804	-	33,33,51	0.61	0	39,41,59	0.53	0
3	POV	C	804	-	38,38,51	0.57	0	44,46,59	0.49	0
3	POV	D	804	-	51,51,51	0.49	0	57,59,59	0.50	0
3	POV	C	802	-	41,41,51	0.55	0	47,49,59	0.47	0
3	POV	D	801	-	47,47,51	0.51	0	53,55,59	0.46	0
3	POV	D	805	-	38,38,51	0.58	0	44,46,59	0.50	0
3	POV	D	806	-	40,40,51	0.56	0	46,48,59	0.52	0
3	POV	C	805	-	38,38,51	0.56	0	44,46,59	0.52	0
3	POV	A	803	-	45,45,51	0.53	0	51,53,59	0.49	0
3	POV	B	806	-	39,39,51	0.56	0	45,47,59	0.50	0
3	POV	A	802	-	51,51,51	0.50	0	57,59,59	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	POV	B	809	-	45,45,51	0.54	0	51,53,59	0.50	0
3	POV	B	801	-	46,46,51	0.52	0	52,54,59	0.46	0
3	POV	D	803	-	43,43,51	0.53	0	49,51,59	0.57	0
3	POV	B	807	-	45,45,51	0.53	0	51,53,59	0.49	0
3	POV	A	805	-	35,35,51	0.60	0	41,43,59	0.49	0
3	POV	B	802	-	45,45,51	0.53	0	51,53,59	0.48	0
3	POV	B	810	-	51,51,51	0.50	0	57,59,59	0.46	0
3	POV	D	807	-	51,51,51	0.50	0	57,59,59	0.46	0
3	POV	C	806	-	39,39,51	0.56	0	45,47,59	0.50	0
3	POV	B	805	-	38,38,51	0.58	0	44,46,59	0.52	0
3	POV	A	809	-	46,46,51	0.52	0	52,54,59	0.50	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	A	808	-	-	17/49/49/55	-
3	POV	C	801	-	-	13/55/55/55	-
3	POV	A	806	-	-	14/44/44/55	-
3	POV	C	803	-	-	6/40/40/55	-
3	POV	B	808	-	-	16/43/43/55	-
3	POV	D	808	-	-	15/55/55/55	-
3	POV	A	804	-	-	23/55/55/55	-
3	POV	D	802	-	-	26/47/47/55	-
3	POV	A	807	-	-	13/36/36/55	-
3	POV	C	807	-	-	14/45/45/55	-
3	POV	B	803	-	-	20/48/48/55	-
3	POV	B	804	-	-	12/37/37/55	-
3	POV	C	804	-	-	11/42/42/55	-
3	POV	D	804	-	-	17/55/55/55	-
3	POV	C	802	-	-	15/45/45/55	-
3	POV	D	801	-	-	17/51/51/55	-
3	POV	D	805	-	-	11/42/42/55	-
3	POV	D	806	-	-	15/44/44/55	-
3	POV	C	805	-	-	11/42/42/55	-
3	POV	A	803	-	-	22/49/49/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	POV	B	806	-	-	19/43/43/55	-
3	POV	A	802	-	-	8/55/55/55	-
3	POV	B	809	-	-	11/49/49/55	-
3	POV	B	801	-	-	13/50/50/55	-
3	POV	D	803	-	-	16/47/47/55	-
3	POV	B	807	-	-	5/49/49/55	-
3	POV	A	805	-	-	6/39/39/55	-
3	POV	B	802	-	-	13/49/49/55	-
3	POV	B	810	-	-	9/55/55/55	-
3	POV	D	807	-	-	17/55/55/55	-
3	POV	C	806	-	-	16/43/43/55	-
3	POV	B	805	-	-	12/42/42/55	-
3	POV	A	809	-	-	16/50/50/55	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (469) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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	802	POV	O11-C1-C2-O21
3	A	803	POV	C11-O12-P-O11
3	A	803	POV	C11-O12-P-O13
3	A	804	POV	C1-O11-P-O13
3	A	804	POV	C11-O12-P-O11
3	A	804	POV	C11-O12-P-O14
3	A	804	POV	C22-C21-O21-C2
3	A	804	POV	O22-C21-O21-C2
3	A	805	POV	C11-O12-P-O14
3	A	805	POV	O21-C2-C3-O31
3	A	806	POV	C1-O11-P-O14
3	A	807	POV	C1-O11-P-O14
3	A	807	POV	O12-C11-C12-N
3	A	807	POV	O22-C21-O21-C2
3	A	808	POV	C11-O12-P-O11

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Mol	Chain	Res	Type	Atoms
3	A	808	POV	C11-O12-P-O13
3	A	809	POV	C1-O11-P-O12
3	A	809	POV	C1-O11-P-O13
3	A	809	POV	C1-O11-P-O14
3	B	801	POV	C1-O11-P-O12
3	B	801	POV	C1-O11-P-O14
3	B	801	POV	C11-O12-P-O13
3	B	801	POV	C11-O12-P-O14
3	B	801	POV	O22-C21-O21-C2
3	B	802	POV	C11-O12-P-O14
3	B	803	POV	C11-O12-P-O11
3	B	803	POV	C11-O12-P-O14
3	B	803	POV	C22-C21-O21-C2
3	B	804	POV	C1-O11-P-O13
3	B	804	POV	C11-O12-P-O14
3	B	804	POV	O21-C2-C3-O31
3	B	804	POV	O12-C11-C12-N
3	B	806	POV	C11-O12-P-O11
3	B	806	POV	C11-O12-P-O13
3	B	806	POV	C12-C11-O12-P
3	B	806	POV	C22-C21-O21-C2
3	B	807	POV	C11-O12-P-O11
3	B	808	POV	C11-O12-P-O11
3	B	808	POV	C11-O12-P-O14
3	B	809	POV	C1-O11-P-O12
3	B	809	POV	C1-O11-P-O13
3	B	809	POV	O11-C1-C2-O21
3	B	809	POV	C22-C21-O21-C2
3	B	809	POV	O22-C21-O21-C2
3	B	810	POV	C11-O12-P-O14
3	C	801	POV	C1-O11-P-O12
3	C	801	POV	C1-O11-P-O13
3	C	801	POV	C11-O12-P-O14
3	C	802	POV	C1-O11-P-O13
3	C	802	POV	O12-C11-C12-N
3	C	804	POV	C11-O12-P-O11
3	C	804	POV	C11-O12-P-O13
3	C	804	POV	O12-C11-C12-N
3	C	805	POV	C22-C21-O21-C2
3	C	805	POV	O22-C21-O21-C2
3	C	806	POV	C11-O12-P-O11
3	C	806	POV	C11-O12-P-O14

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Mol	Chain	Res	Type	Atoms
3	C	807	POV	C1-O11-P-O12
3	C	807	POV	C1-O11-P-O14
3	C	807	POV	C11-O12-P-O11
3	C	807	POV	C11-O12-P-O13
3	C	807	POV	O11-C1-C2-O21
3	C	807	POV	C22-C21-O21-C2
3	D	801	POV	C1-O11-P-O12
3	D	801	POV	C1-O11-P-O13
3	D	801	POV	C11-O12-P-O11
3	D	801	POV	C11-O12-P-O13
3	D	801	POV	O22-C21-O21-C2
3	D	802	POV	C1-O11-P-O12
3	D	802	POV	C1-O11-P-O13
3	D	802	POV	C1-O11-P-O14
3	D	802	POV	C11-O12-P-O11
3	D	802	POV	C11-O12-P-O13
3	D	802	POV	O12-C11-C12-N
3	D	802	POV	C12-C11-O12-P
3	D	802	POV	O22-C21-O21-C2
3	D	803	POV	C1-O11-P-O12
3	D	803	POV	C1-O11-P-O13
3	D	803	POV	O12-C11-C12-N
3	D	803	POV	C22-C21-O21-C2
3	D	804	POV	C1-O11-P-O13
3	D	804	POV	C11-O12-P-O11
3	D	804	POV	C11-O12-P-O13
3	D	805	POV	C11-O12-P-O11
3	D	806	POV	C1-O11-P-O14
3	D	808	POV	C11-O12-P-O14
3	B	808	POV	O32-C31-O31-C3
3	C	806	POV	O32-C31-O31-C3
3	A	808	POV	O32-C31-O31-C3
3	C	807	POV	O22-C21-O21-C2
3	D	803	POV	O22-C21-O21-C2
3	D	804	POV	O22-C21-O21-C2
3	B	808	POV	C32-C31-O31-C3
3	C	806	POV	C32-C31-O31-C3
3	A	807	POV	C22-C21-O21-C2
3	B	801	POV	C22-C21-O21-C2
3	D	801	POV	C22-C21-O21-C2
3	D	802	POV	C22-C21-O21-C2
3	D	804	POV	C22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
3	A	806	POV	O32-C31-O31-C3
3	A	808	POV	C32-C31-O31-C3
3	B	803	POV	C32-C31-O31-C3
3	D	806	POV	C32-C31-O31-C3
3	A	803	POV	O32-C31-O31-C3
3	D	806	POV	O32-C31-O31-C3
3	B	803	POV	O22-C21-O21-C2
3	B	806	POV	O22-C21-O21-C2
3	A	803	POV	C32-C31-O31-C3
3	A	806	POV	C32-C31-O31-C3
3	B	803	POV	O32-C31-O31-C3
3	C	802	POV	C32-C31-O31-C3
3	B	803	POV	C31-C32-C33-C34
3	B	806	POV	C32-C31-O31-C3
3	C	805	POV	C32-C31-O31-C3
3	D	804	POV	C32-C31-O31-C3
3	B	806	POV	C11-C12-N-C13
3	B	806	POV	C11-C12-N-C14
3	B	806	POV	O32-C31-O31-C3
3	C	805	POV	O32-C31-O31-C3
3	B	804	POV	C32-C31-O31-C3
3	B	801	POV	C21-C22-C23-C24
3	C	801	POV	C21-C22-C23-C24
3	B	806	POV	C21-C22-C23-C24
3	D	804	POV	C31-C32-C33-C34
3	D	804	POV	O32-C31-O31-C3
3	D	803	POV	C32-C31-O31-C3
3	D	807	POV	C31-C32-C33-C34
3	C	802	POV	O32-C31-O31-C3
3	B	810	POV	C31-C32-C33-C34
3	D	803	POV	C21-C22-C23-C24
3	B	804	POV	O32-C31-O31-C3
3	C	802	POV	C21-C22-C23-C24
3	B	805	POV	C32-C31-O31-C3
3	A	806	POV	C11-C12-N-C13
3	A	806	POV	C11-C12-N-C14
3	A	806	POV	C11-C12-N-C15
3	D	802	POV	C11-C12-N-C13
3	D	802	POV	C11-C12-N-C14
3	D	806	POV	C11-C12-N-C13
3	D	806	POV	C11-C12-N-C14
3	D	806	POV	C11-C12-N-C15

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Mol	Chain	Res	Type	Atoms
3	B	802	POV	C212-C213-C214-C215
3	A	808	POV	C21-C22-C23-C24
3	D	803	POV	O32-C31-O31-C3
3	B	803	POV	C1-C2-O21-C21
3	D	803	POV	C1-C2-O21-C21
3	D	802	POV	C11-C12-N-C15
3	B	808	POV	C2-C3-O31-C31
3	D	802	POV	C24-C25-C26-C27
3	B	803	POV	C212-C213-C214-C215
3	C	807	POV	C22-C23-C24-C25
3	D	802	POV	C22-C23-C24-C25
3	A	806	POV	C34-C35-C36-C37
3	A	802	POV	C213-C214-C215-C216
3	A	809	POV	C23-C24-C25-C26
3	A	803	POV	C33-C34-C35-C36
3	B	810	POV	C32-C33-C34-C35
3	D	808	POV	C311-C312-C313-C314
3	A	803	POV	C39-C310-C311-C312
3	C	802	POV	C212-C213-C214-C215
3	A	807	POV	C22-C23-C24-C25
3	B	809	POV	C22-C23-C24-C25
3	C	805	POV	C23-C24-C25-C26
3	C	806	POV	C2-C3-O31-C31
3	B	805	POV	O32-C31-O31-C3
3	A	808	POV	C33-C34-C35-C36
3	D	804	POV	C33-C34-C35-C36
3	D	802	POV	C39-C310-C311-C312
3	B	806	POV	C1-C2-C3-O31
3	B	803	POV	C32-C33-C34-C35
3	D	804	POV	C32-C33-C34-C35
3	C	807	POV	C37-C38-C39-C310
3	D	808	POV	C35-C36-C37-C38
3	B	808	POV	C37-C38-C39-C310
3	C	806	POV	C37-C38-C39-C310
3	A	803	POV	C310-C311-C312-C313
3	B	810	POV	C33-C34-C35-C36
3	B	806	POV	C11-C12-N-C15
3	A	804	POV	C21-C22-C23-C24
3	A	807	POV	C31-C32-C33-C34
3	A	804	POV	C25-C26-C27-C28
3	B	804	POV	C32-C33-C34-C35
3	D	807	POV	C22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
3	D	801	POV	C2-C1-O11-P
3	C	807	POV	C33-C34-C35-C36
3	A	803	POV	C34-C35-C36-C37
3	D	801	POV	C23-C24-C25-C26
3	B	809	POV	C37-C38-C39-C310
3	C	805	POV	C24-C25-C26-C27
3	D	808	POV	C312-C313-C314-C315
3	A	809	POV	C22-C21-O21-C2
3	C	801	POV	C31-C32-C33-C34
3	A	809	POV	O22-C21-O21-C2
3	B	803	POV	C33-C34-C35-C36
3	A	804	POV	C35-C36-C37-C38
3	B	808	POV	C34-C35-C36-C37
3	A	803	POV	C24-C25-C26-C27
3	A	803	POV	C22-C23-C24-C25
3	D	807	POV	C24-C25-C26-C27
3	D	807	POV	O22-C21-O21-C2
3	B	802	POV	O11-C1-C2-O21
3	D	808	POV	O11-C1-C2-O21
3	A	809	POV	C210-C211-C212-C213
3	B	806	POV	O21-C2-C3-O31
3	A	805	POV	C32-C31-O31-C3
3	D	804	POV	C23-C24-C25-C26
3	A	804	POV	C24-C25-C26-C27
3	C	802	POV	C25-C26-C27-C28
3	A	807	POV	C32-C33-C34-C35
3	C	806	POV	C34-C35-C36-C37
3	D	805	POV	C34-C35-C36-C37
3	A	808	POV	C310-C311-C312-C313
3	B	805	POV	C22-C23-C24-C25
3	A	802	POV	C25-C26-C27-C28
3	A	804	POV	C310-C311-C312-C313
3	A	804	POV	C211-C212-C213-C214
3	B	807	POV	C32-C33-C34-C35
3	B	810	POV	C212-C213-C214-C215
3	B	806	POV	O11-C1-C2-C3
3	B	809	POV	O11-C1-C2-C3
3	C	802	POV	O11-C1-C2-C3
3	D	808	POV	O11-C1-C2-C3
3	C	801	POV	C25-C26-C27-C28
3	A	809	POV	C32-C33-C34-C35
3	B	810	POV	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
3	C	802	POV	C23-C24-C25-C26
3	A	804	POV	C1-C2-C3-O31
3	A	808	POV	C1-C2-C3-O31
3	B	804	POV	C1-C2-C3-O31
3	B	808	POV	C1-C2-C3-O31
3	C	806	POV	C1-C2-C3-O31
3	D	802	POV	C1-C2-C3-O31
3	A	804	POV	C210-C211-C212-C213
3	B	803	POV	C26-C27-C28-C29
3	B	809	POV	C33-C34-C35-C36
3	A	805	POV	O32-C31-O31-C3
3	D	808	POV	C24-C25-C26-C27
3	D	805	POV	C36-C37-C38-C39
3	C	804	POV	C21-C22-C23-C24
3	D	805	POV	O11-C1-C2-O21
3	D	807	POV	O11-C1-C2-O21
3	B	805	POV	C32-C33-C34-C35
3	D	805	POV	C23-C24-C25-C26
3	B	805	POV	C24-C25-C26-C27
3	D	801	POV	O21-C2-C3-O31
3	C	801	POV	C24-C25-C26-C27
3	B	803	POV	C24-C25-C26-C27
3	A	804	POV	C37-C38-C39-C310
3	D	802	POV	C311-C310-C39-C38
3	A	808	POV	C25-C26-C27-C28
3	B	803	POV	C34-C35-C36-C37
3	B	808	POV	C35-C36-C37-C38
3	D	802	POV	C32-C31-O31-C3
3	B	810	POV	C24-C25-C26-C27
3	A	802	POV	O11-C1-C2-C3
3	B	802	POV	O11-C1-C2-C3
3	C	805	POV	O11-C1-C2-C3
3	C	807	POV	O11-C1-C2-C3
3	D	806	POV	O11-C1-C2-C3
3	D	805	POV	C35-C36-C37-C38
3	C	806	POV	C311-C310-C39-C38
3	D	804	POV	C211-C212-C213-C214
3	A	803	POV	C1-C2-C3-O31
3	A	807	POV	C1-C2-C3-O31
3	D	806	POV	C1-C2-C3-O31
3	A	803	POV	C311-C310-C39-C38
3	C	806	POV	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
3	B	806	POV	O11-C1-C2-O21
3	D	806	POV	O11-C1-C2-O21
3	A	807	POV	O21-C2-C3-O31
3	D	803	POV	O21-C2-C3-O31
3	C	803	POV	C36-C37-C38-C39
3	D	808	POV	C212-C213-C214-C215
3	B	802	POV	C211-C212-C213-C214
3	A	803	POV	C35-C36-C37-C38
3	D	807	POV	C33-C34-C35-C36
3	B	804	POV	C33-C34-C35-C36
3	C	801	POV	C22-C23-C24-C25
3	C	804	POV	C24-C25-C26-C27
3	B	802	POV	C32-C33-C34-C35
3	D	802	POV	O32-C31-O31-C3
3	B	802	POV	C24-C25-C26-C27
3	A	803	POV	O11-C1-C2-O21
3	A	808	POV	O11-C1-C2-O21
3	C	802	POV	O11-C1-C2-O21
3	C	804	POV	O11-C1-C2-O21
3	C	805	POV	O11-C1-C2-O21
3	B	803	POV	C22-C23-C24-C25
3	A	805	POV	C1-C2-C3-O31
3	A	806	POV	C1-C2-C3-O31
3	D	801	POV	C1-C2-C3-O31
3	A	804	POV	C12-C11-O12-P
3	A	806	POV	C12-C11-O12-P
3	A	807	POV	C12-C11-O12-P
3	C	802	POV	C12-C11-O12-P
3	D	806	POV	C12-C11-O12-P
3	A	803	POV	O21-C2-C3-O31
3	A	804	POV	O21-C2-C3-O31
3	A	808	POV	O21-C2-C3-O31
3	B	808	POV	O21-C2-C3-O31
3	C	806	POV	O21-C2-C3-O31
3	D	802	POV	O21-C2-C3-O31
3	D	806	POV	O21-C2-C3-O31
3	C	807	POV	C39-C310-C311-C312
3	B	805	POV	C11-C12-N-C13
3	B	808	POV	C311-C310-C39-C38
3	B	801	POV	O12-C11-C12-N
3	D	804	POV	O12-C11-C12-N
3	C	801	POV	C213-C214-C215-C216

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Mol	Chain	Res	Type	Atoms
3	C	802	POV	C26-C27-C28-C29
3	D	807	POV	C22-C23-C24-C25
3	A	803	POV	C11-C12-N-C15
3	A	808	POV	C35-C36-C37-C38
3	D	808	POV	C211-C212-C213-C214
3	A	803	POV	O11-C1-C2-C3
3	A	806	POV	O11-C1-C2-C3
3	A	808	POV	O11-C1-C2-C3
3	A	809	POV	O11-C1-C2-C3
3	C	804	POV	O11-C1-C2-C3
3	D	801	POV	O11-C1-C2-C3
3	D	805	POV	O11-C1-C2-C3
3	A	809	POV	C33-C34-C35-C36
3	A	806	POV	O11-C1-C2-O21
3	A	809	POV	O11-C1-C2-O21
3	B	808	POV	O11-C1-C2-O21
3	C	806	POV	O11-C1-C2-O21
3	A	806	POV	O21-C2-C3-O31
3	D	801	POV	C32-C31-O31-C3
3	D	808	POV	C39-C310-C311-C312
3	A	804	POV	C1-O11-P-O12
3	A	804	POV	C1-O11-P-O14
3	A	804	POV	C11-O12-P-O13
3	A	806	POV	C11-O12-P-O11
3	B	801	POV	C1-O11-P-O13
3	B	801	POV	C11-O12-P-O11
3	B	805	POV	C11-O12-P-O14
3	B	807	POV	C11-O12-P-O14
3	B	808	POV	C11-O12-P-O13
3	C	802	POV	C11-O12-P-O14
3	C	803	POV	C11-O12-P-O14
3	C	806	POV	C11-O12-P-O13
3	D	801	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	C1-O11-P-O12
3	D	804	POV	C1-O11-P-O14
3	D	805	POV	C11-O12-P-O14
3	D	806	POV	C1-O11-P-O12
3	D	806	POV	C11-O12-P-O11
3	D	807	POV	C11-O12-P-O14
3	D	802	POV	C37-C38-C39-C310

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Mol	Chain	Res	Type	Atoms
3	A	809	POV	C2-C1-O11-P
3	B	806	POV	C2-C1-O11-P
3	D	801	POV	O32-C31-O31-C3
3	B	802	POV	C22-C23-C24-C25
3	D	801	POV	C31-C32-C33-C34
3	B	803	POV	O11-C1-C2-C3
3	C	801	POV	O11-C1-C2-C3
3	D	807	POV	O11-C1-C2-C3
3	D	807	POV	C29-C210-C211-C212
3	D	805	POV	C24-C25-C26-C27
3	C	806	POV	C39-C310-C311-C312
3	D	808	POV	C23-C24-C25-C26
3	D	806	POV	C35-C36-C37-C38
3	C	807	POV	C1-C2-C3-O31
3	D	805	POV	C37-C38-C39-C310
3	A	803	POV	C32-C33-C34-C35
3	D	807	POV	C35-C36-C37-C38
3	B	805	POV	C11-C12-N-C15
3	B	807	POV	C33-C34-C35-C36
3	C	805	POV	C32-C33-C34-C35
3	B	802	POV	C214-C215-C216-C217
3	D	804	POV	C212-C213-C214-C215
3	A	802	POV	C212-C213-C214-C215
3	D	805	POV	C22-C23-C24-C25
3	C	807	POV	C2-C1-O11-P
3	A	808	POV	C2-C3-O31-C31
3	A	809	POV	C29-C210-C211-C212
3	D	803	POV	C1-C2-C3-O31
3	B	801	POV	C35-C36-C37-C38
3	C	801	POV	C36-C37-C38-C39
3	A	809	POV	C22-C23-C24-C25
3	B	805	POV	C11-C12-N-C14
3	D	806	POV	C37-C38-C39-C310
3	C	805	POV	C33-C34-C35-C36
3	D	807	POV	C26-C27-C28-C29
3	A	806	POV	C33-C34-C35-C36
3	D	803	POV	C34-C35-C36-C37
3	B	802	POV	C33-C34-C35-C36
3	C	801	POV	C211-C212-C213-C214
3	B	801	POV	C34-C35-C36-C37
3	B	803	POV	C21-C22-C23-C24
3	C	802	POV	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
3	C	803	POV	O11-C1-C2-O21
3	D	801	POV	O11-C1-C2-O21
3	D	807	POV	C310-C311-C312-C313
3	A	803	POV	C11-C12-N-C14
3	B	808	POV	O11-C1-C2-C3
3	C	806	POV	O11-C1-C2-C3
3	D	803	POV	O11-C1-C2-C3
3	A	805	POV	C21-C22-C23-C24
3	A	809	POV	C35-C36-C37-C38
3	D	807	POV	C21-C22-C23-C24
3	A	808	POV	C36-C37-C38-C39
3	B	805	POV	C23-C24-C25-C26
3	B	802	POV	C27-C28-C29-C210
3	A	803	POV	C11-C12-N-C13
3	C	801	POV	C27-C28-C29-C210
3	C	802	POV	C210-C211-C212-C213
3	A	804	POV	C29-C210-C211-C212
3	C	804	POV	O22-C21-O21-C2
3	B	809	POV	C39-C310-C311-C312
3	A	803	POV	C31-C32-C33-C34
3	D	801	POV	C35-C36-C37-C38
3	B	802	POV	C29-C210-C211-C212
3	D	807	POV	O21-C21-C22-C23
3	A	807	POV	O21-C21-C22-C23
3	C	804	POV	O31-C31-C32-C33
3	C	804	POV	C22-C21-O21-C2
3	A	804	POV	C39-C310-C311-C312
3	B	810	POV	C27-C28-C29-C210
3	D	808	POV	O21-C21-C22-C23
3	B	810	POV	O11-C1-C2-O21
3	B	805	POV	C25-C26-C27-C28
3	A	803	POV	C36-C37-C38-C39
3	A	808	POV	C24-C25-C26-C27
3	B	804	POV	O31-C31-C32-C33
3	B	806	POV	O31-C31-C32-C33
3	D	802	POV	O21-C21-C22-C23
3	B	803	POV	C1-C2-C3-O31
3	A	809	POV	C311-C310-C39-C38
3	B	801	POV	O21-C2-C3-O31
3	B	803	POV	C29-C210-C211-C212
3	B	805	POV	C35-C36-C37-C38
3	C	803	POV	C11-C12-N-C13

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Mol	Chain	Res	Type	Atoms
3	A	807	POV	C23-C24-C25-C26
3	D	802	POV	O31-C31-C32-C33
3	D	804	POV	C35-C36-C37-C38
3	A	804	POV	C311-C312-C313-C314
3	B	804	POV	C22-C23-C24-C25
3	D	807	POV	C212-C213-C214-C215
3	A	804	POV	O11-C1-C2-O21
3	D	808	POV	C313-C314-C315-C316
3	D	808	POV	C311-C310-C39-C38
3	A	807	POV	O22-C21-C22-C23
3	C	805	POV	C36-C37-C38-C39
3	D	802	POV	C311-C312-C313-C314
3	D	802	POV	C21-C22-C23-C24
3	C	804	POV	C25-C26-C27-C28
3	C	803	POV	O32-C31-O31-C3
3	D	802	POV	O22-C21-C22-C23
3	C	803	POV	C34-C35-C36-C37
3	D	807	POV	O22-C21-C22-C23
3	B	807	POV	C24-C25-C26-C27
3	B	804	POV	O32-C31-C32-C33
3	D	808	POV	O22-C21-C22-C23
3	B	809	POV	C311-C312-C313-C314
3	B	808	POV	C39-C310-C311-C312
3	B	802	POV	C31-C32-C33-C34
3	B	806	POV	O21-C21-C22-C23
3	B	808	POV	O31-C31-C32-C33
3	B	806	POV	O32-C31-C32-C33
3	D	803	POV	C35-C36-C37-C38
3	B	803	POV	O21-C21-C22-C23
3	C	806	POV	O31-C31-C32-C33
3	A	808	POV	C31-C32-C33-C34

There are no ring outliers.

31 monomers are involved in 88 short contacts:

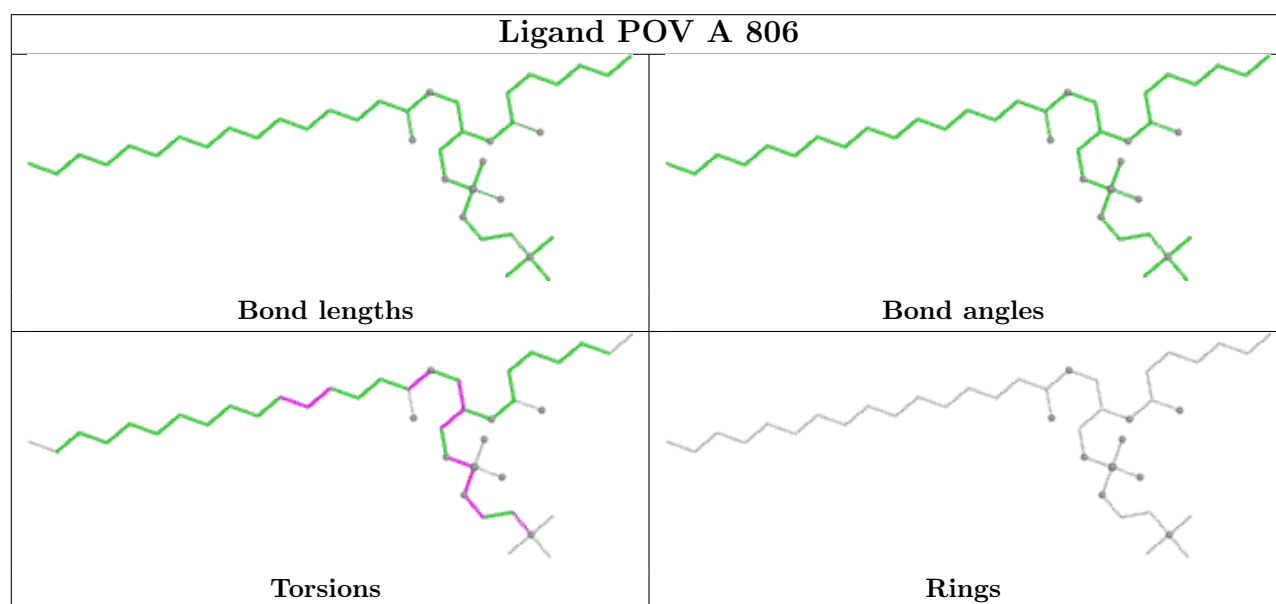
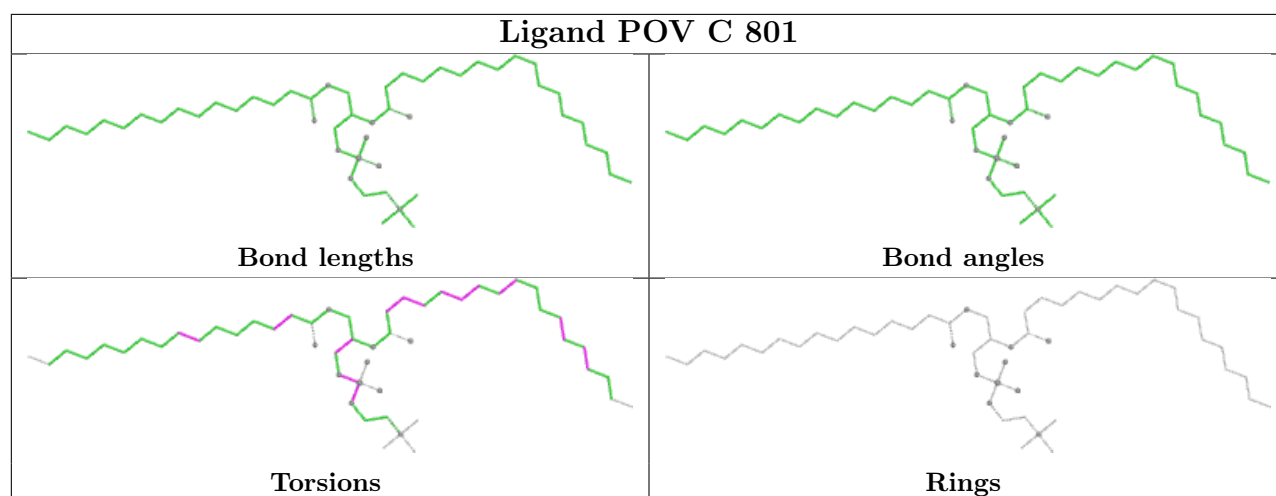
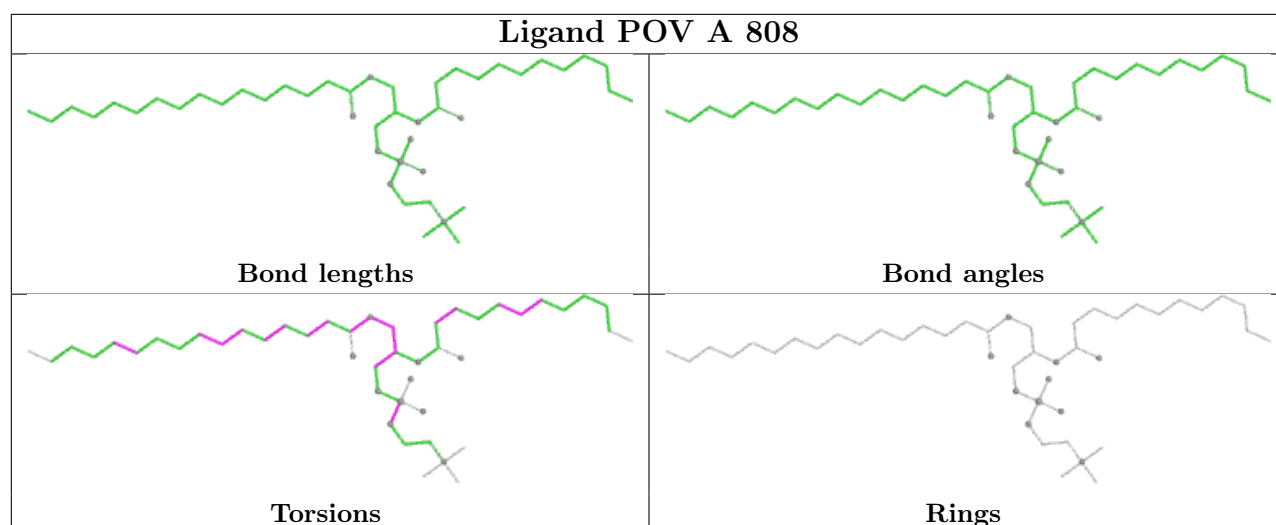
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	808	POV	3	0
3	C	801	POV	2	0
3	A	806	POV	5	0
3	C	803	POV	2	0
3	B	808	POV	6	0
3	D	808	POV	3	0

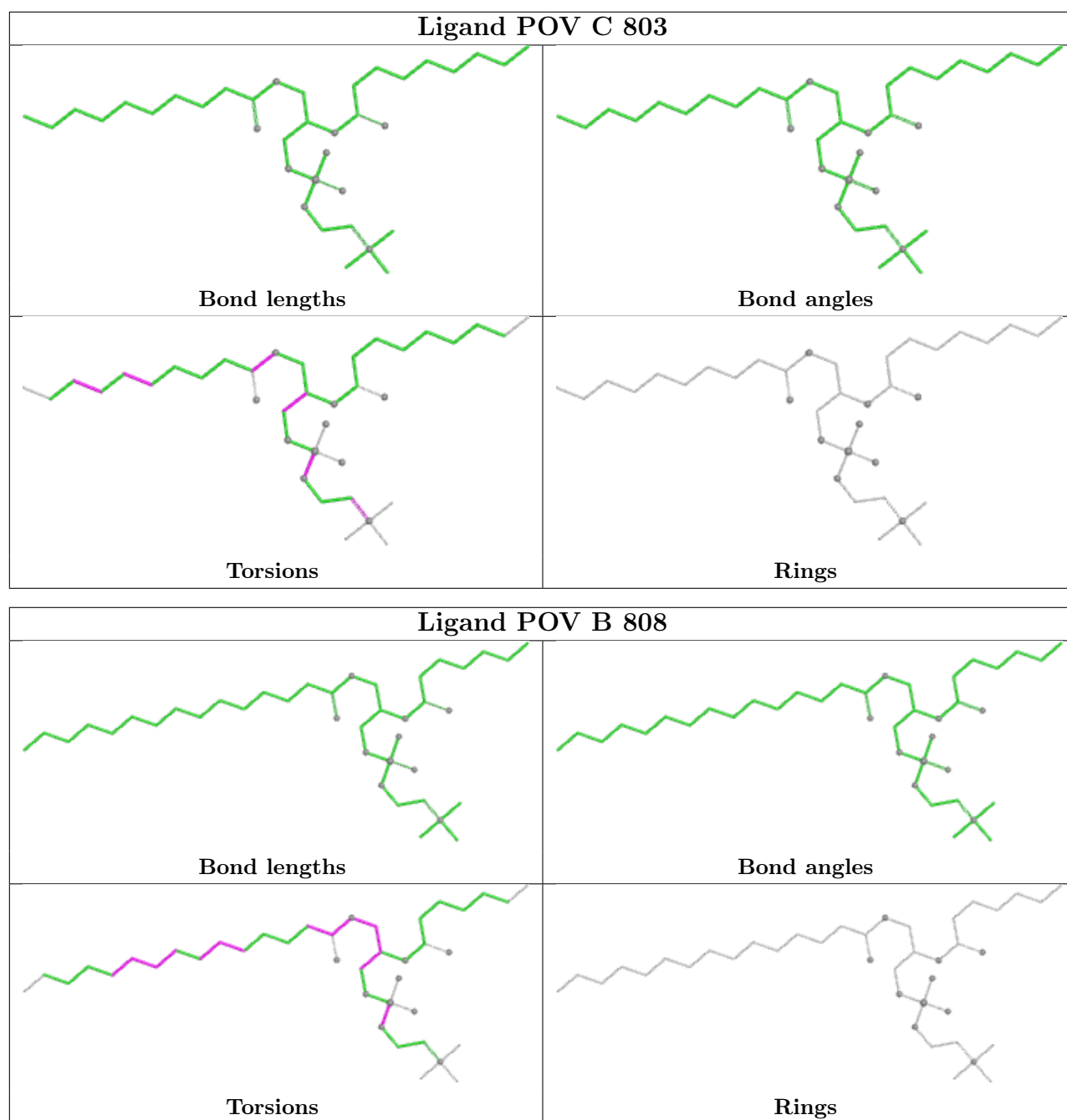
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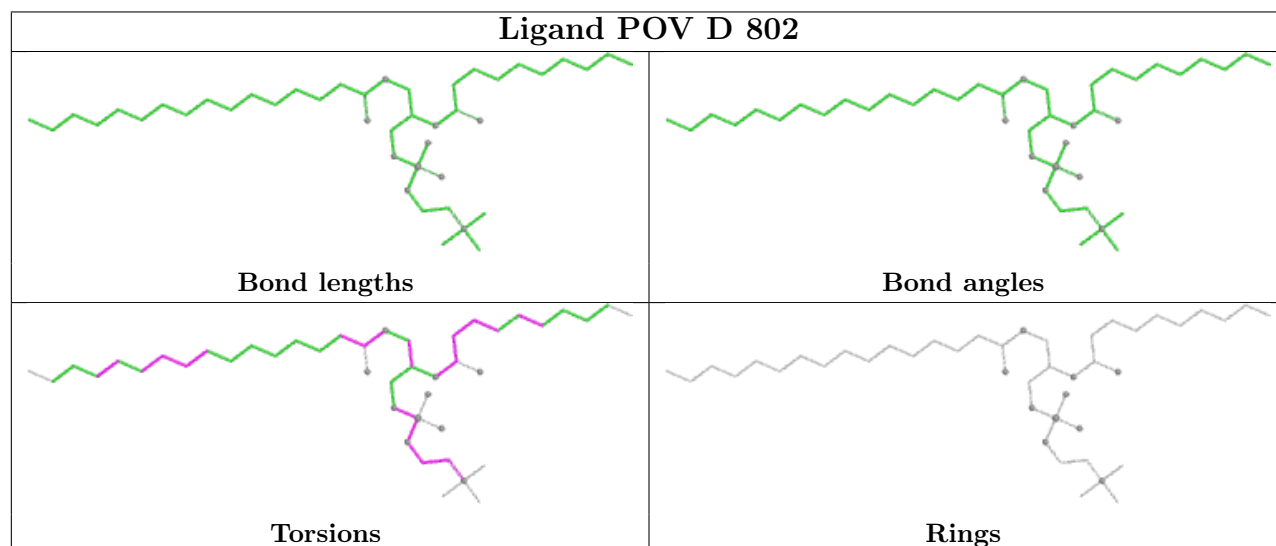
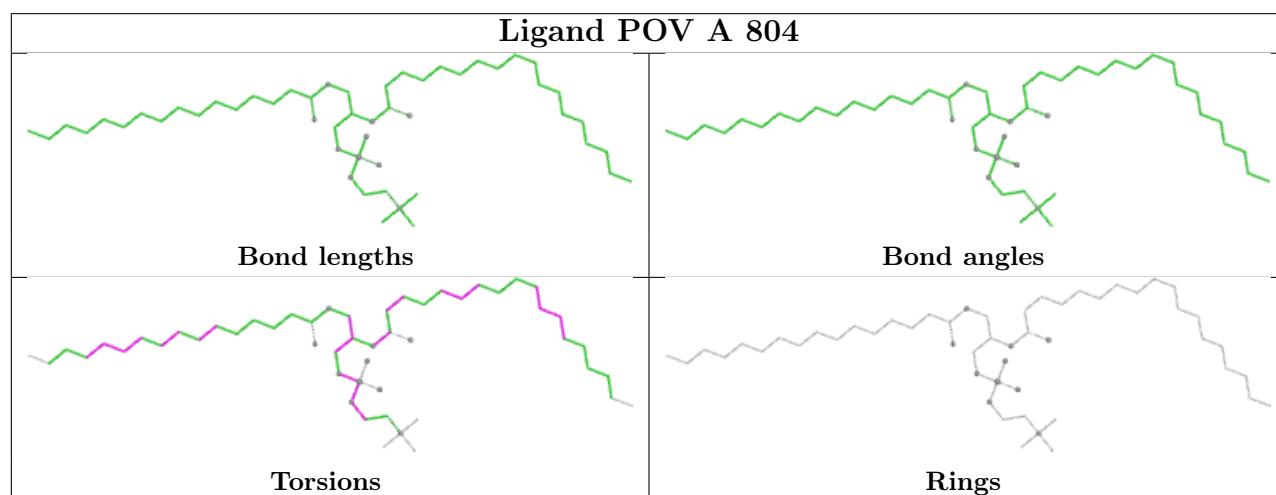
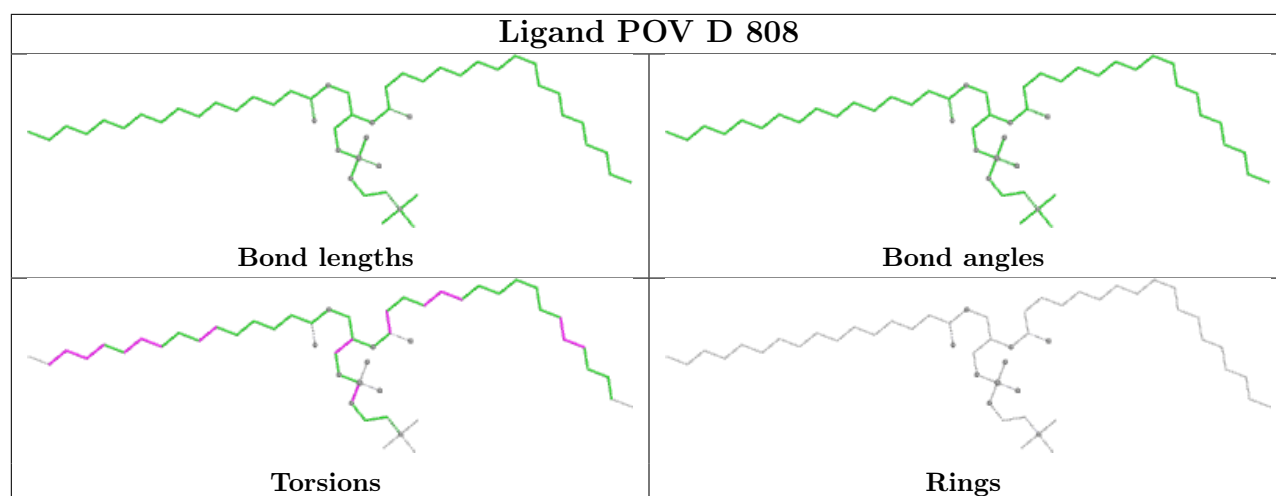
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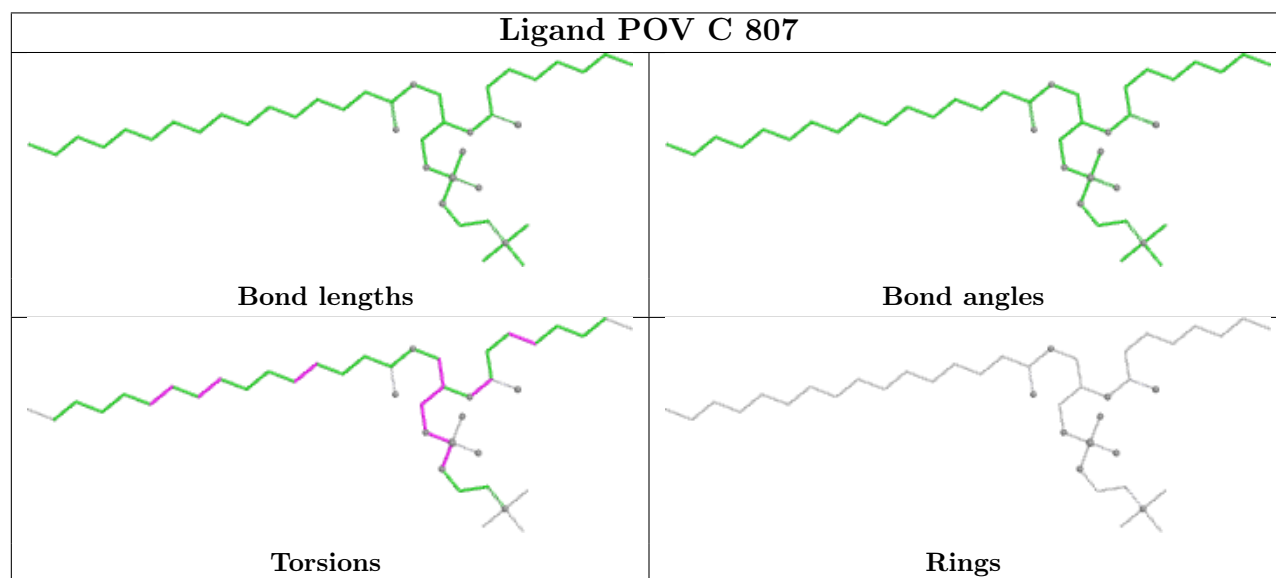
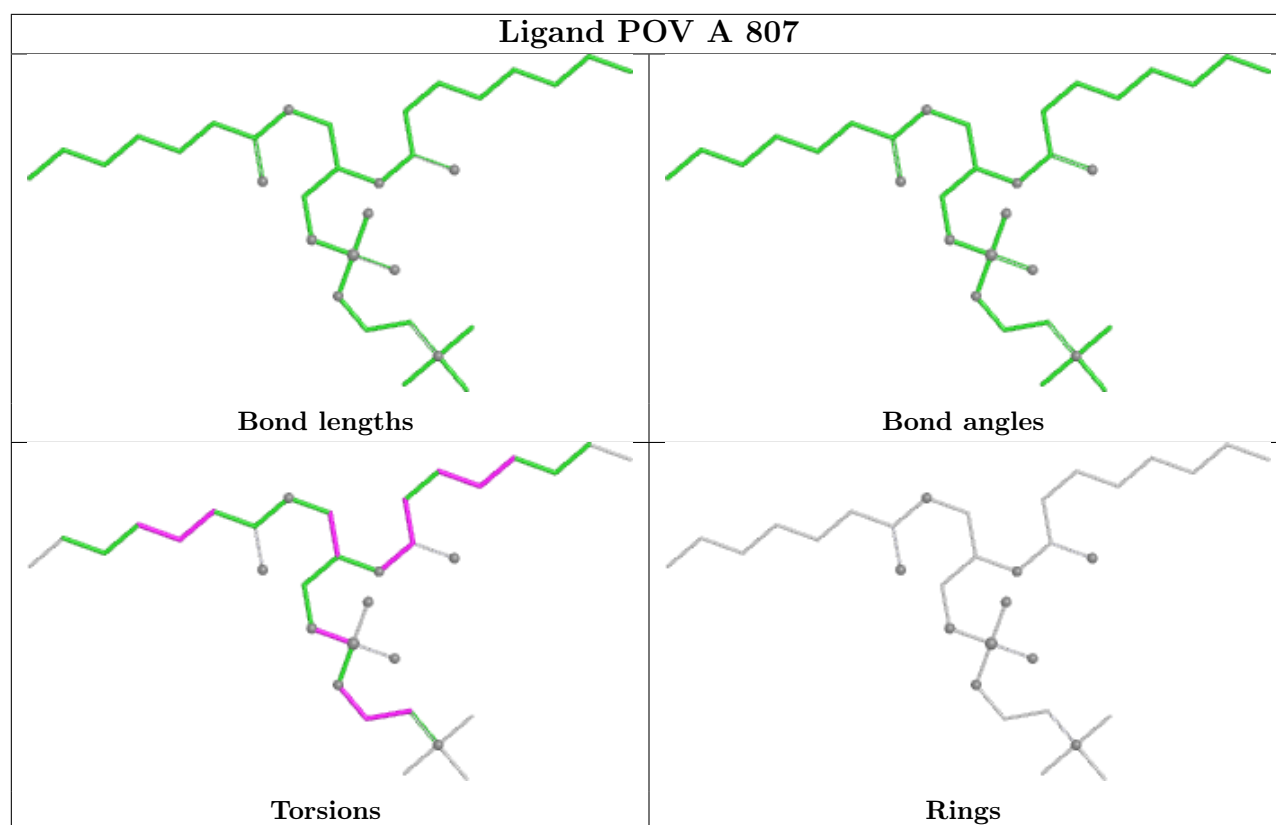
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	804	POV	3	0
3	D	802	POV	1	0
3	A	807	POV	3	0
3	C	807	POV	1	0
3	B	803	POV	11	0
3	B	804	POV	4	0
3	C	804	POV	3	0
3	D	804	POV	1	0
3	C	802	POV	4	0
3	D	801	POV	3	0
3	D	806	POV	2	0
3	C	805	POV	4	0
3	A	803	POV	3	0
3	B	806	POV	1	0
3	A	802	POV	5	0
3	B	809	POV	1	0
3	B	801	POV	3	0
3	D	803	POV	2	0
3	B	807	POV	2	0
3	B	802	POV	6	0
3	B	810	POV	5	0
3	D	807	POV	2	0
3	C	806	POV	4	0
3	B	805	POV	2	0
3	A	809	POV	2	0

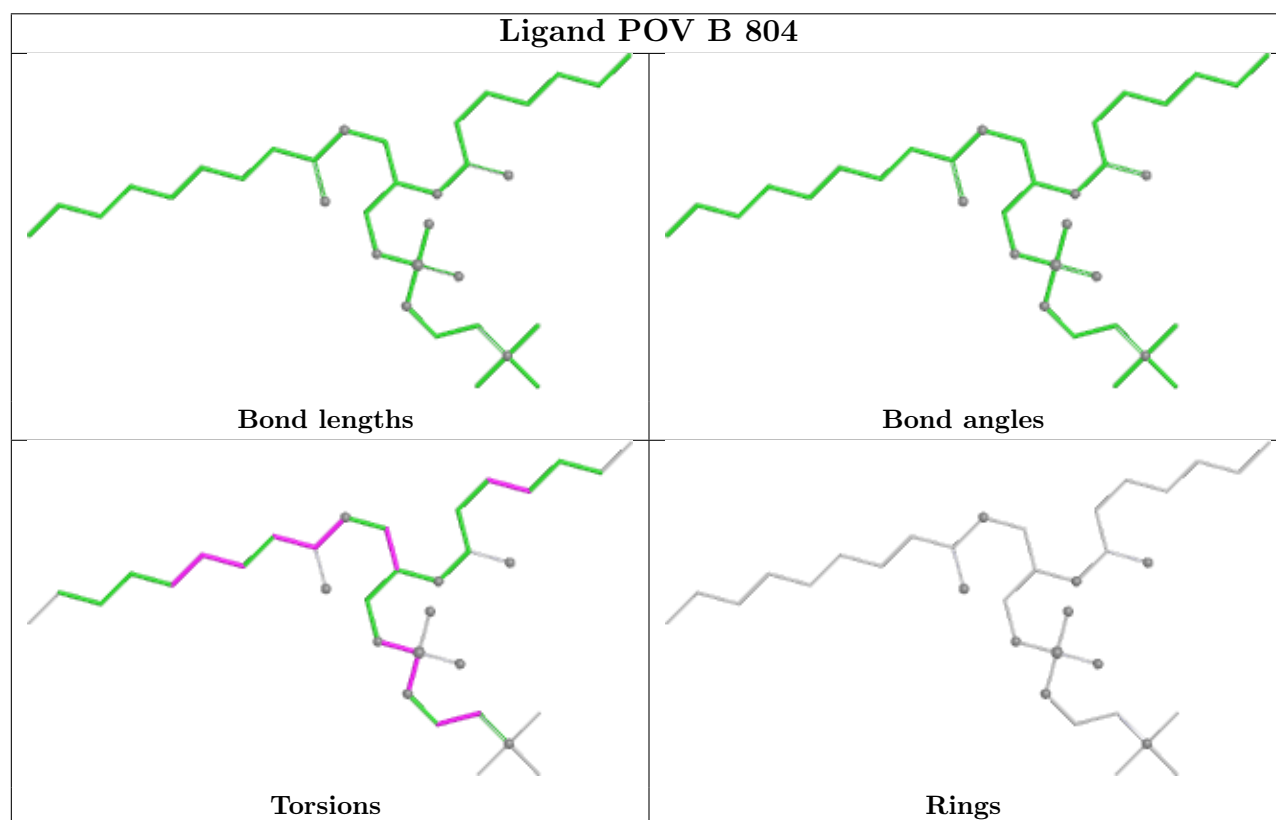
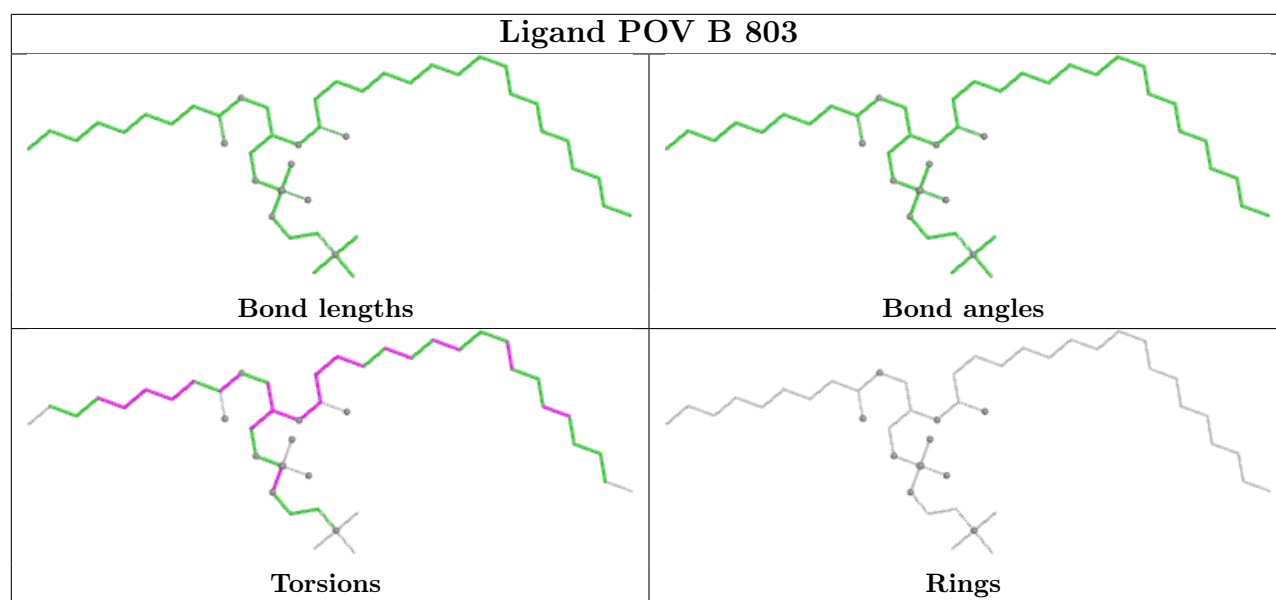
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

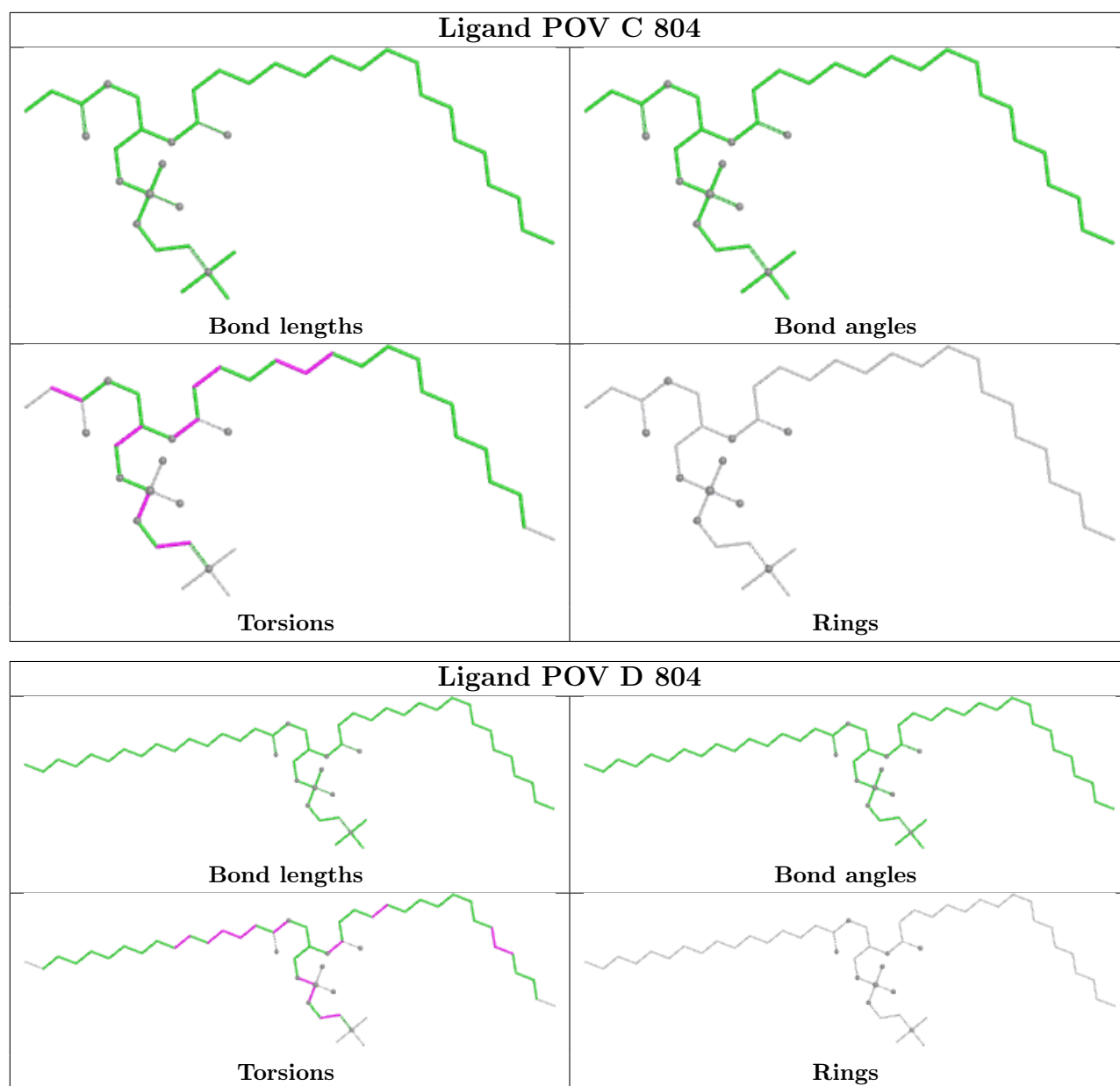


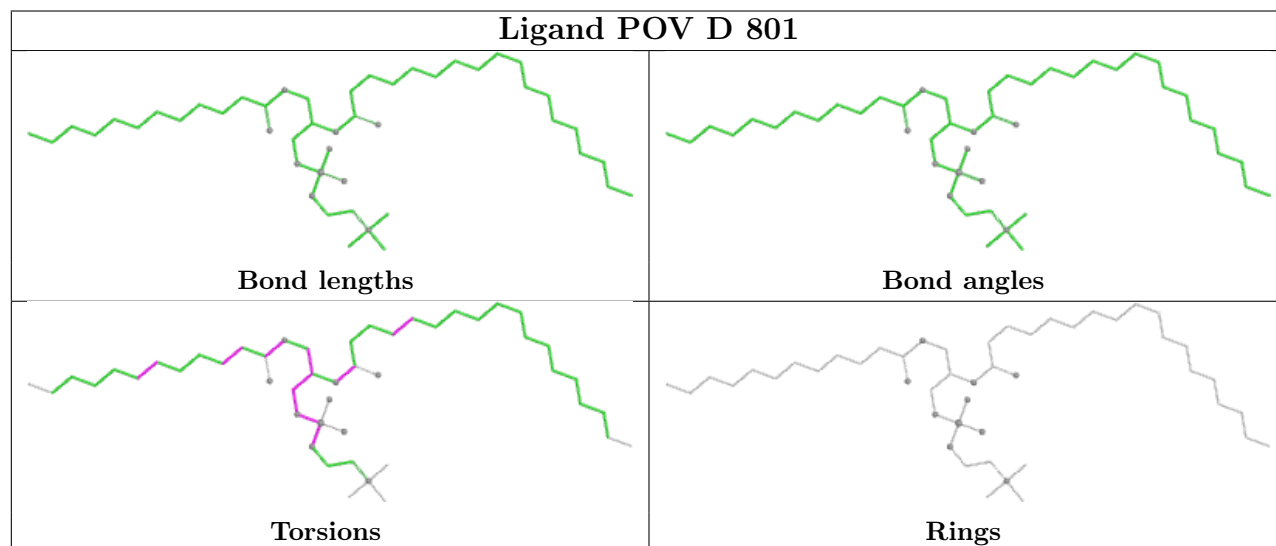
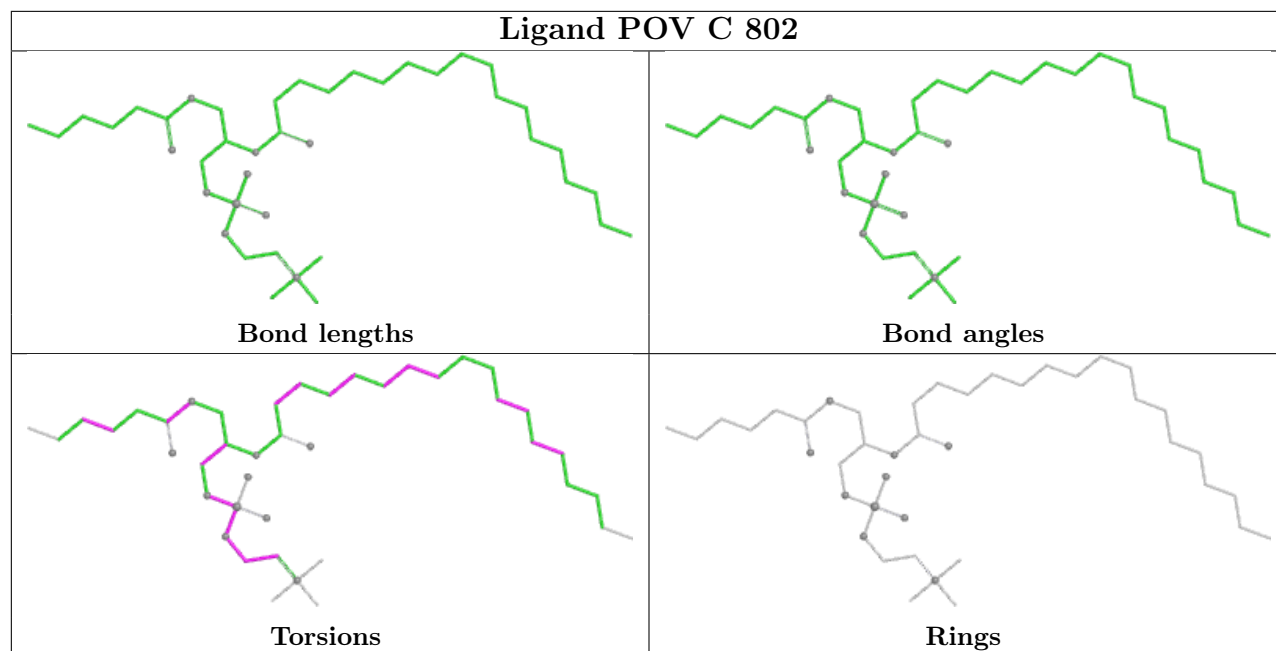


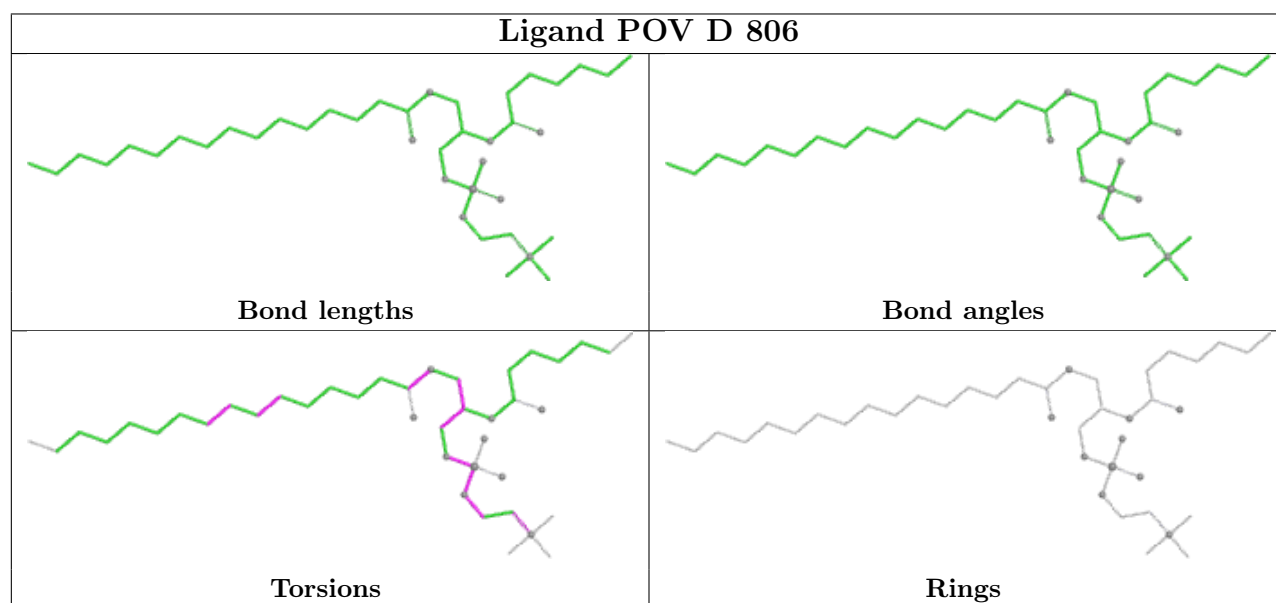
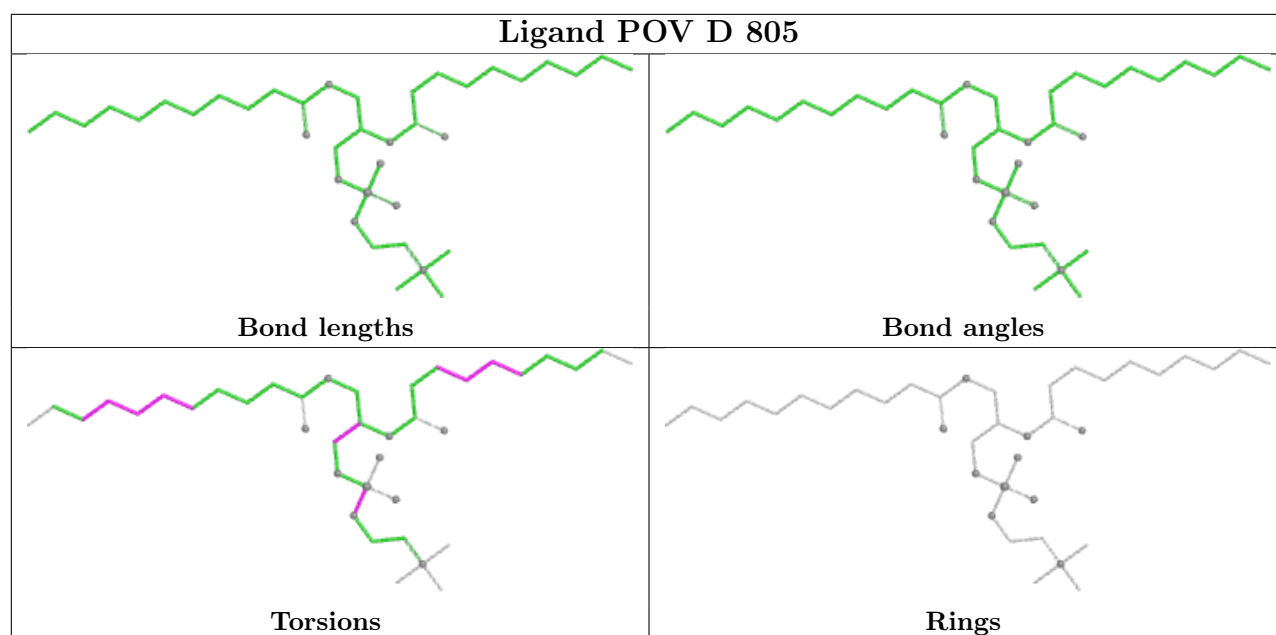


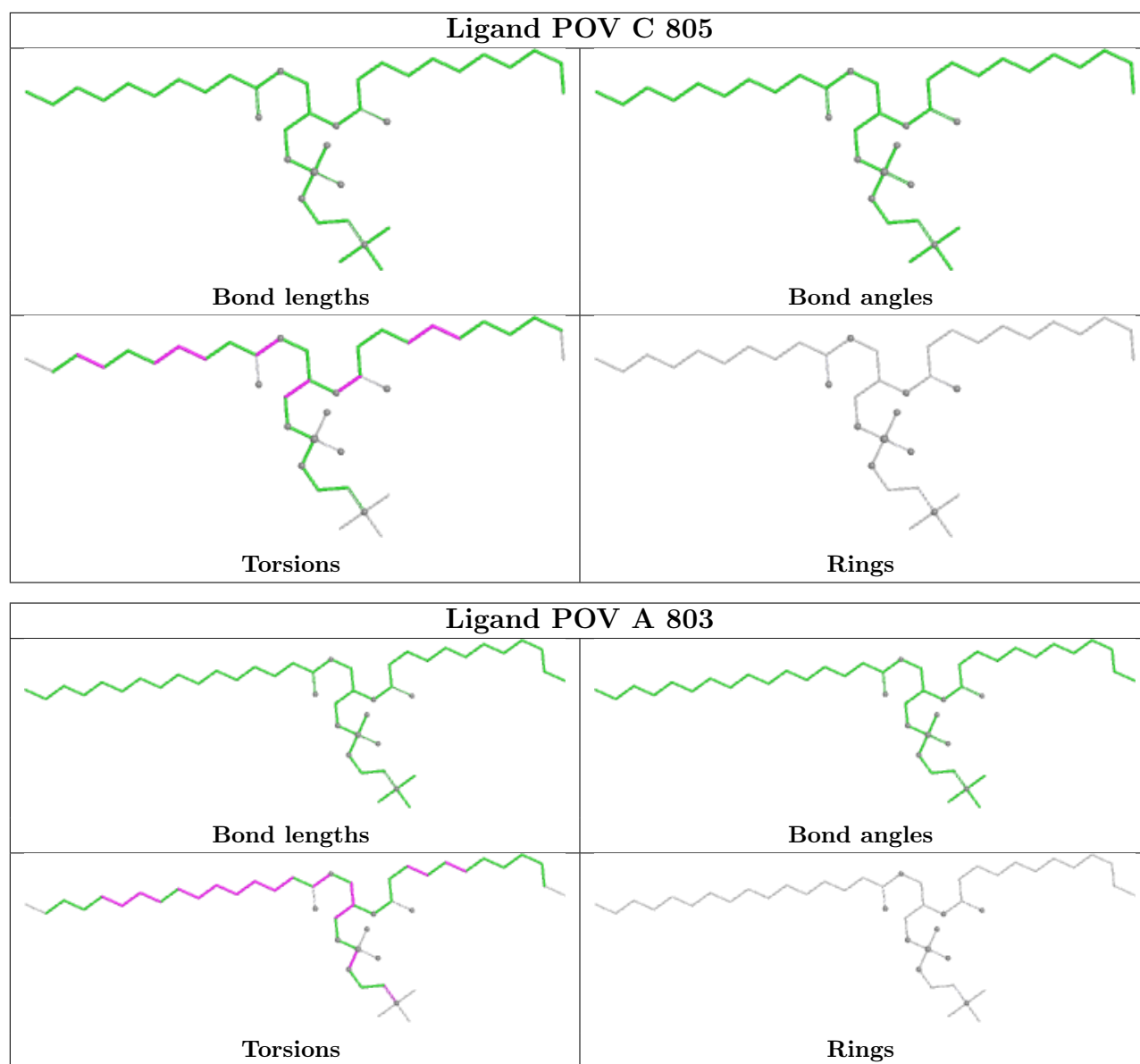


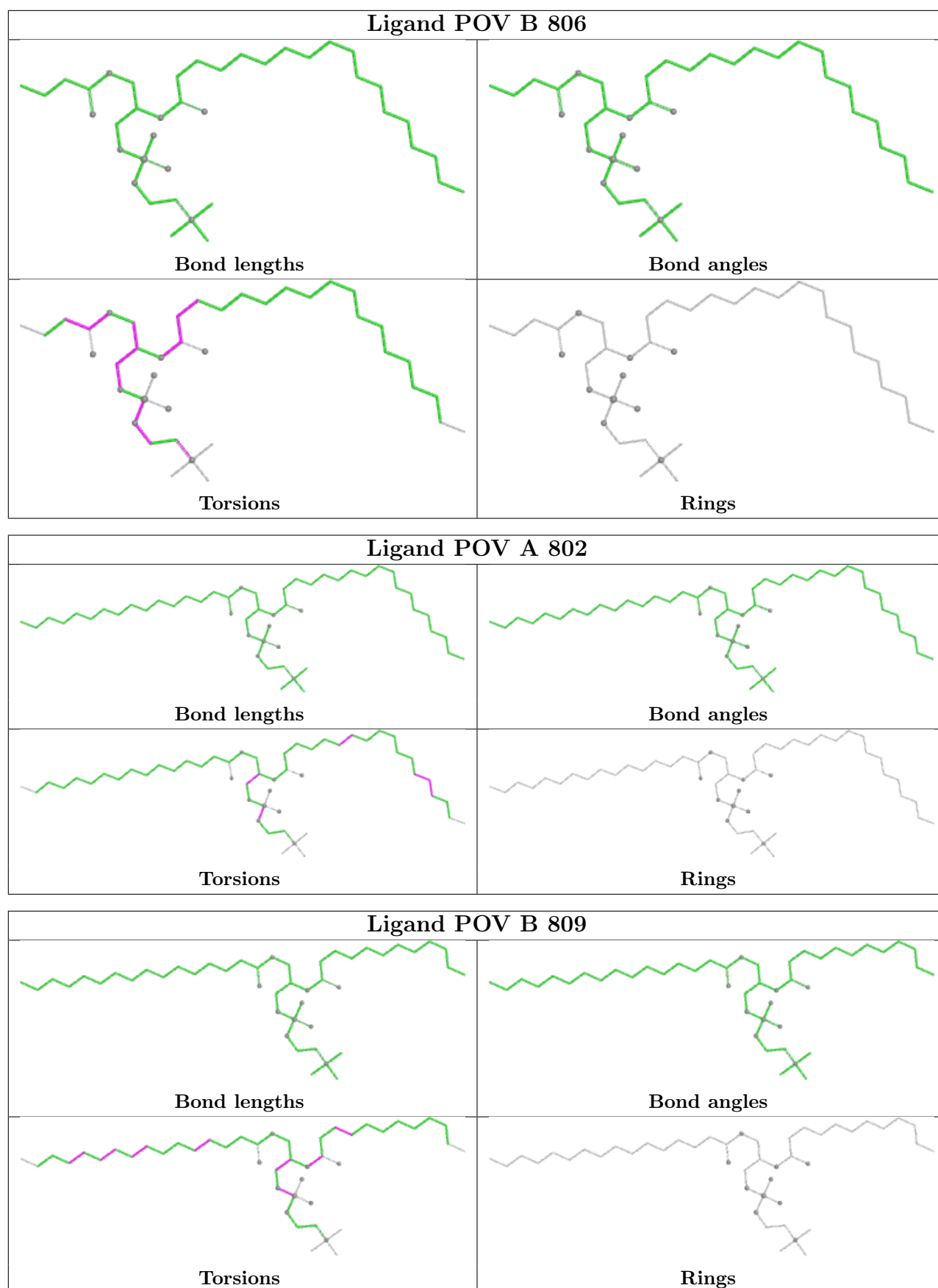


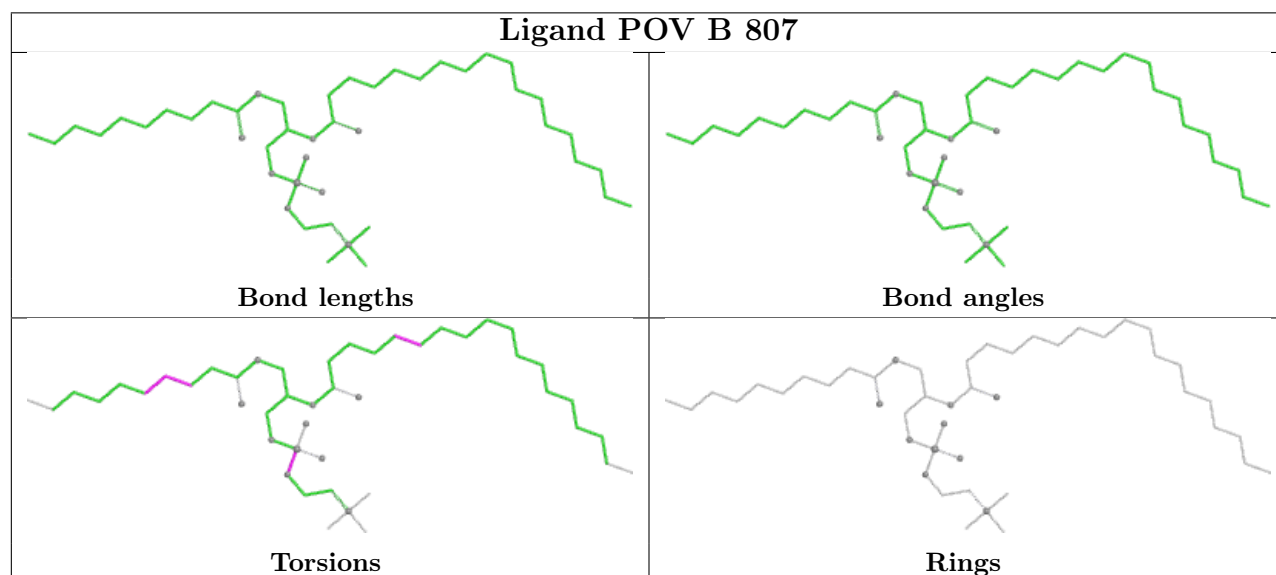
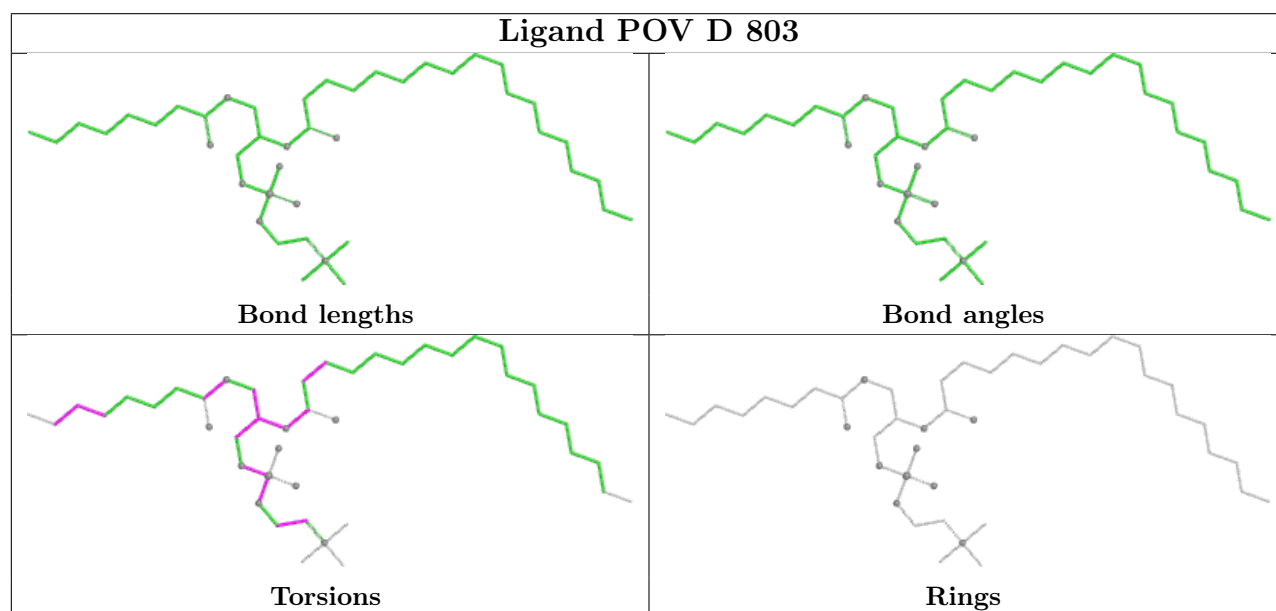
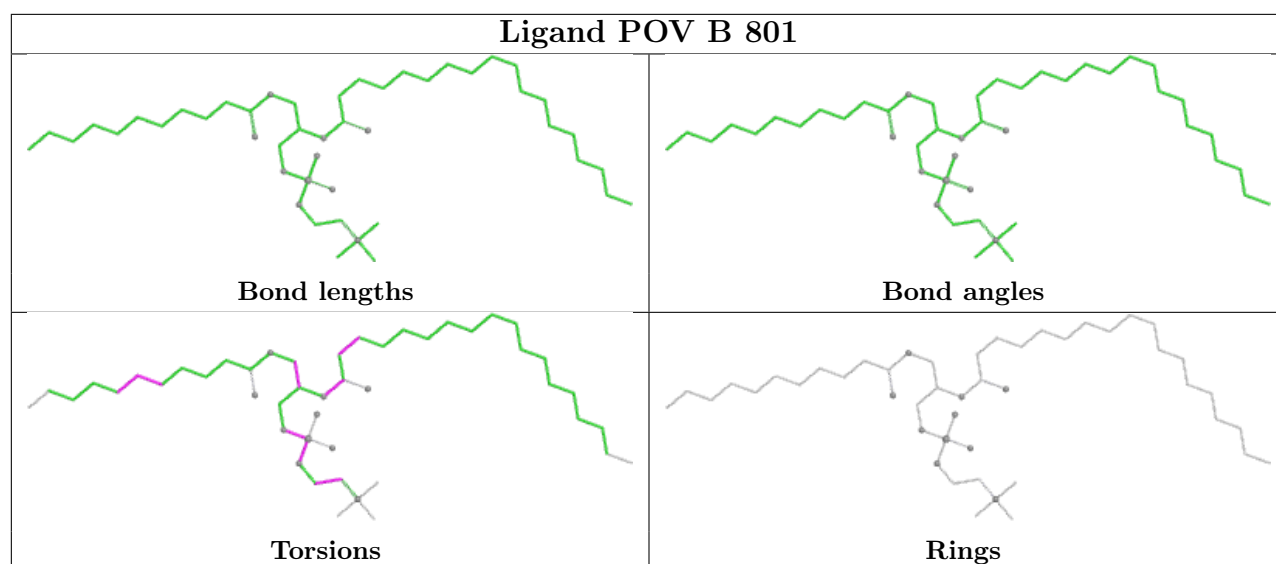


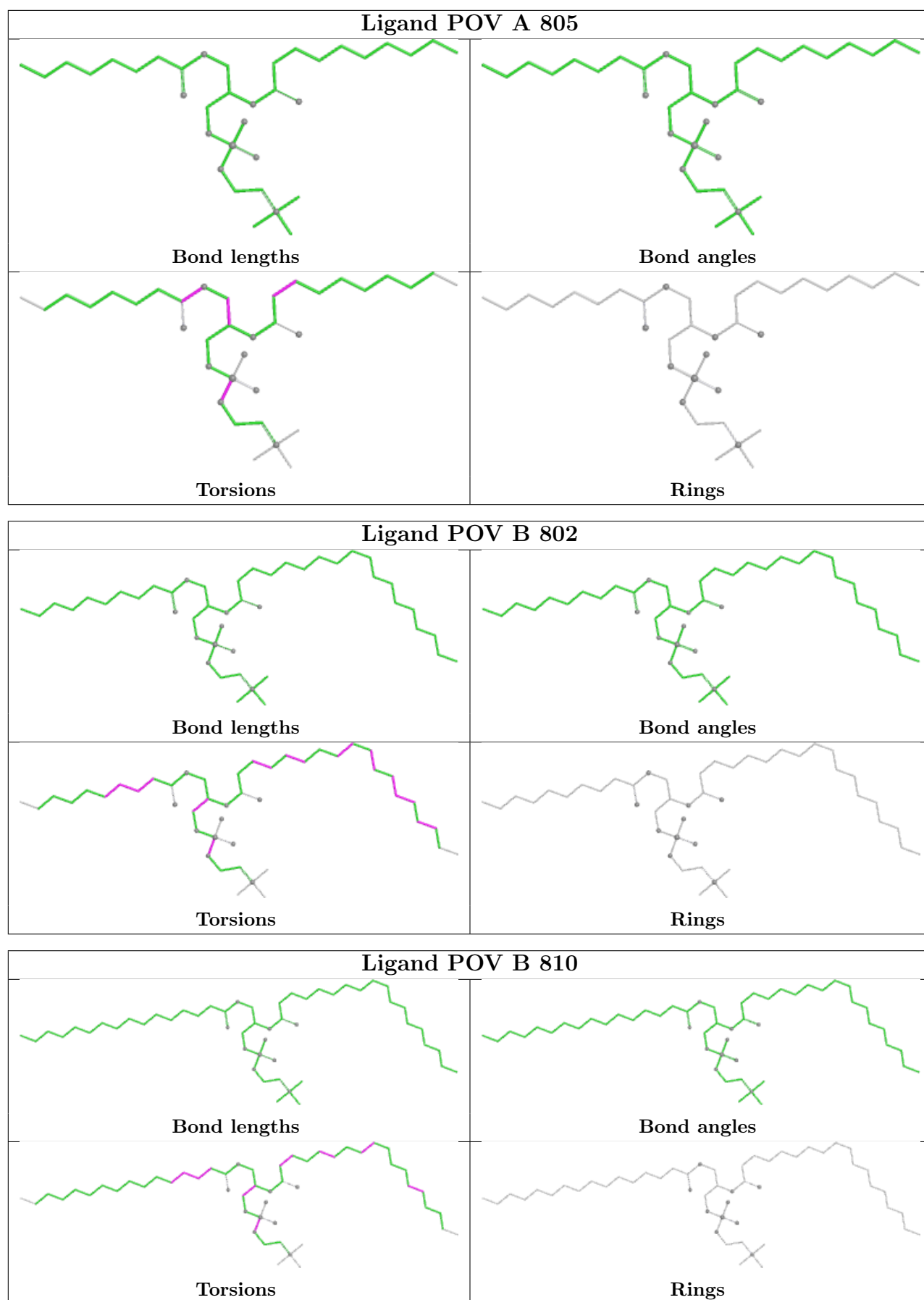


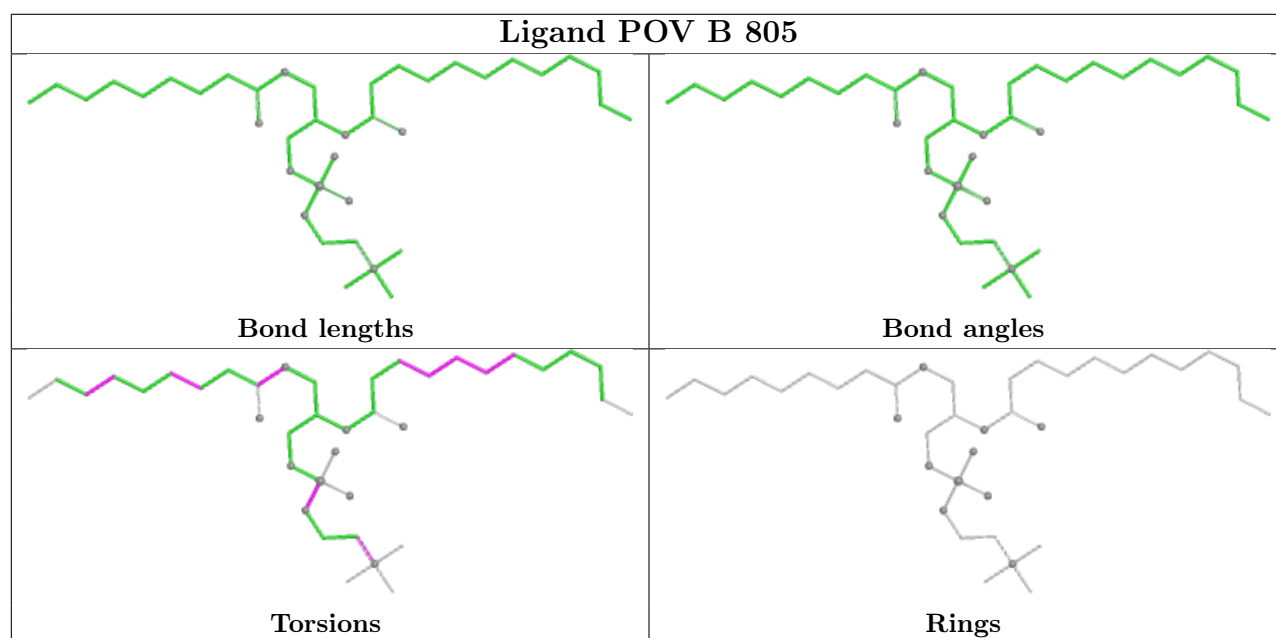
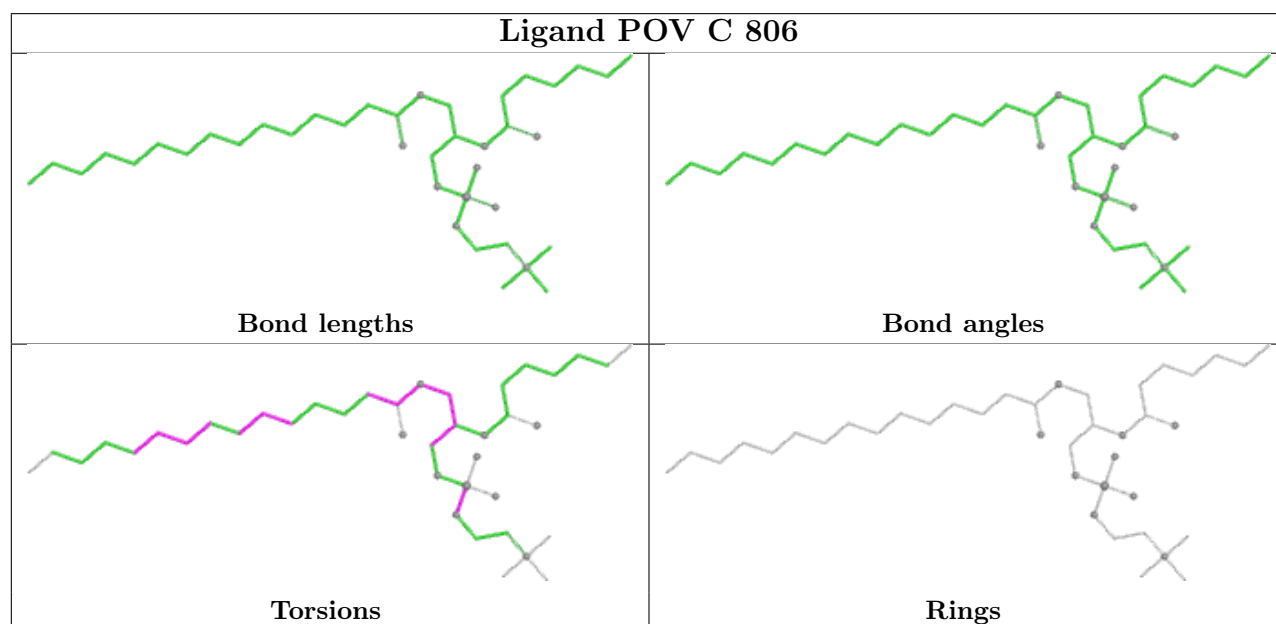
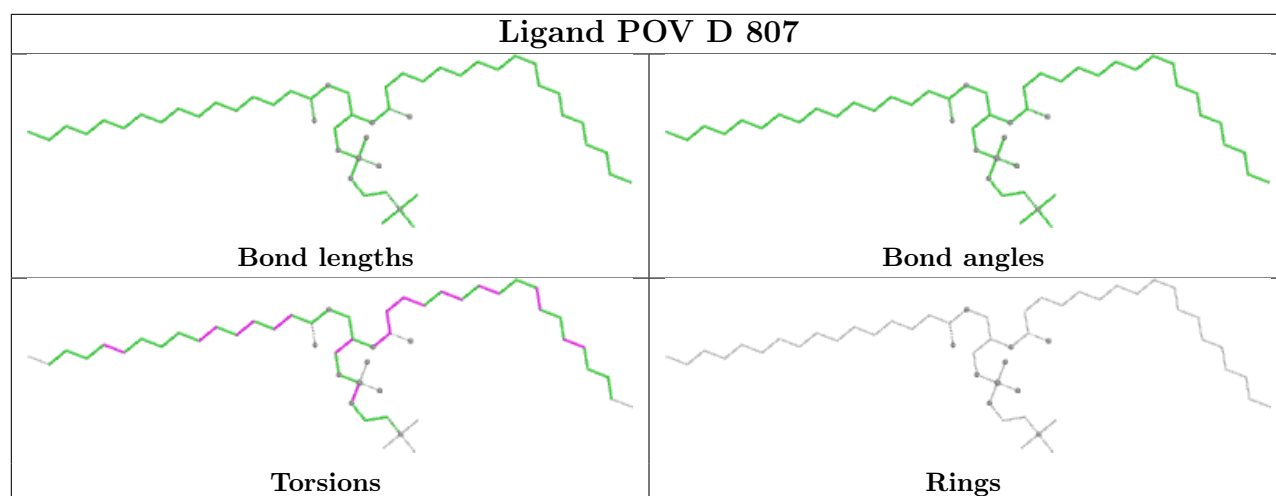


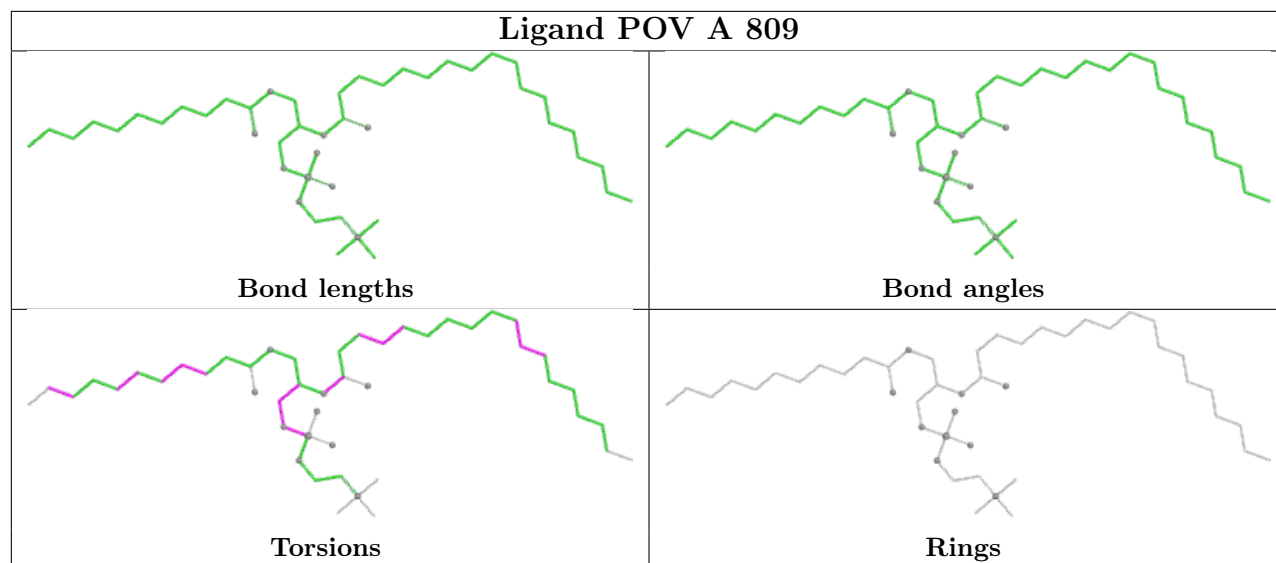












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

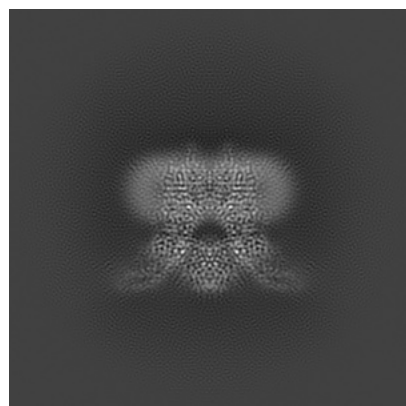
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40181. These allow visual inspection of the internal detail of the map and identification of artifacts.

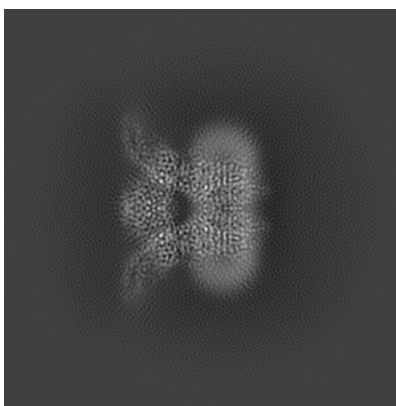
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

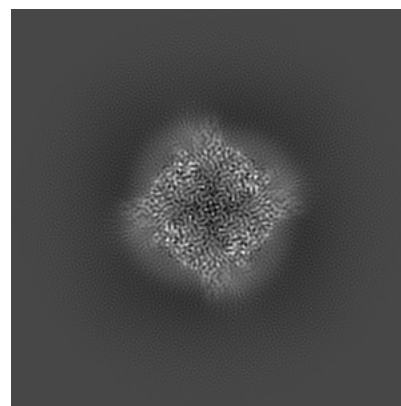
6.1.1 Primary map



X

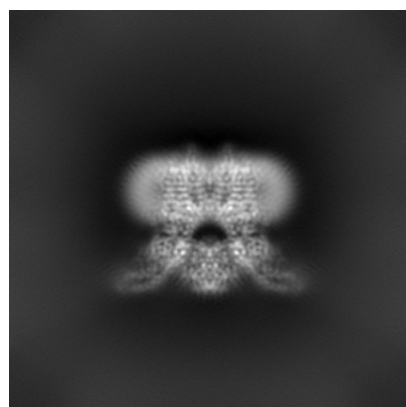


Y

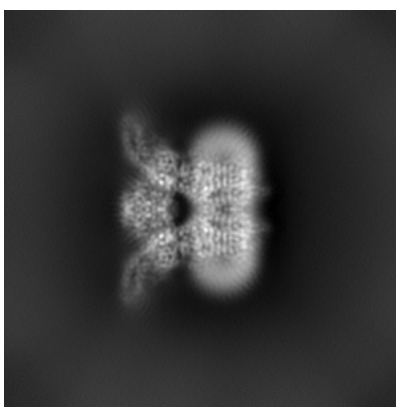


Z

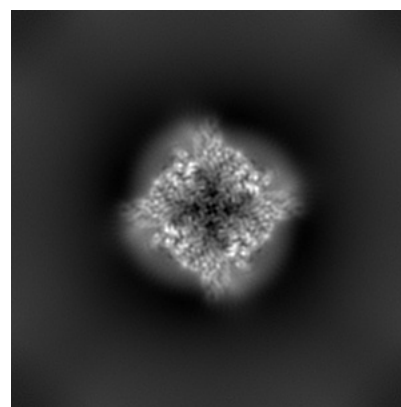
6.1.2 Raw map



X



Y

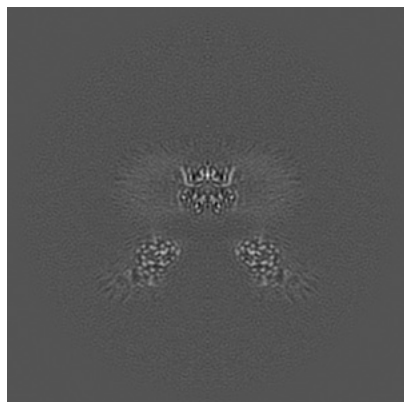


Z

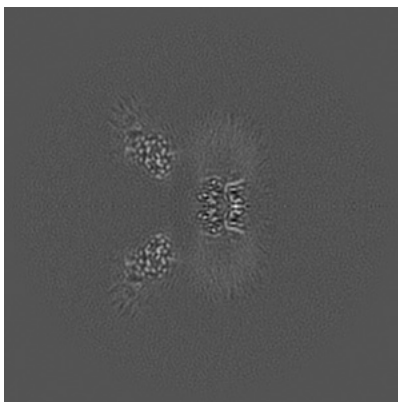
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

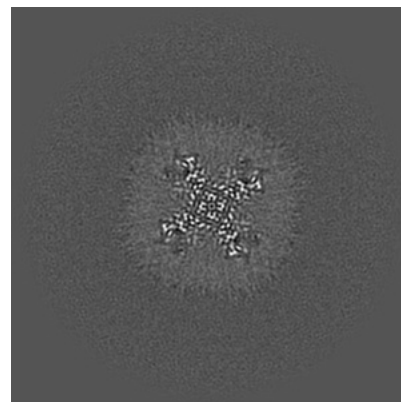
6.2.1 Primary map



X Index: 140

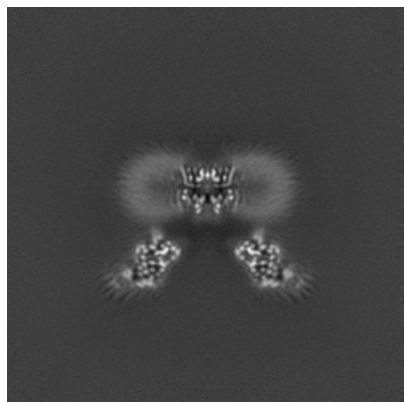


Y Index: 140

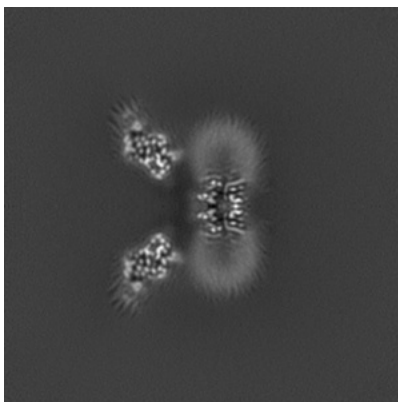


Z Index: 140

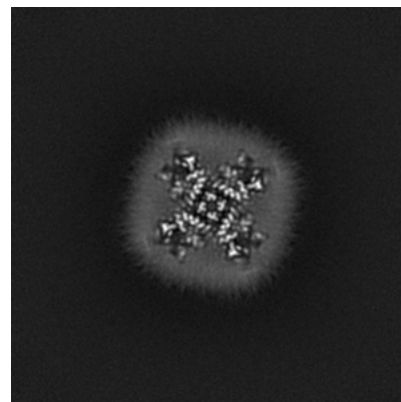
6.2.2 Raw map



X Index: 140



Y Index: 140

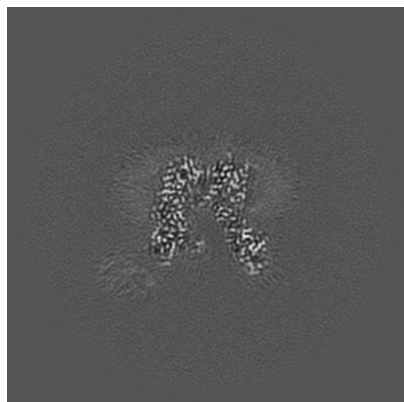


Z Index: 140

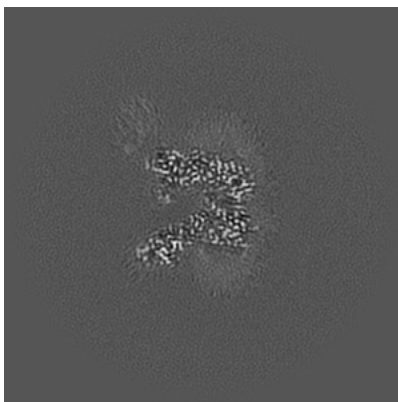
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

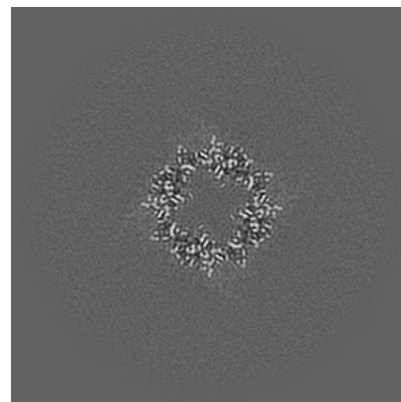
6.3.1 Primary map



X Index: 157

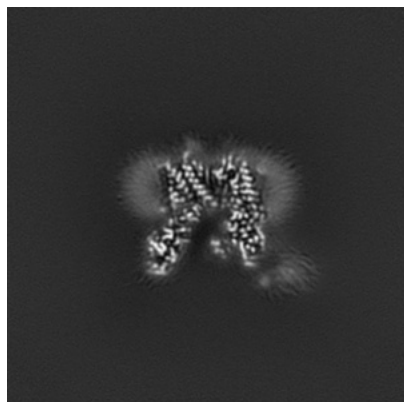


Y Index: 157

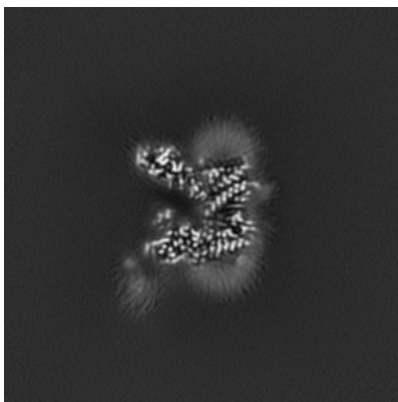


Z Index: 112

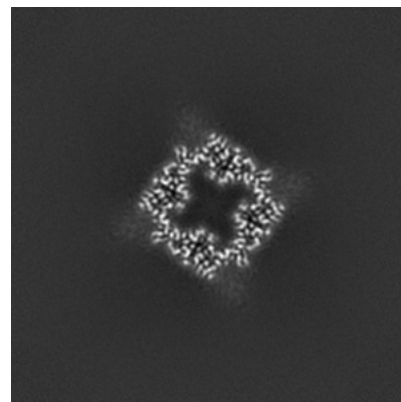
6.3.2 Raw map



X Index: 123



Y Index: 123

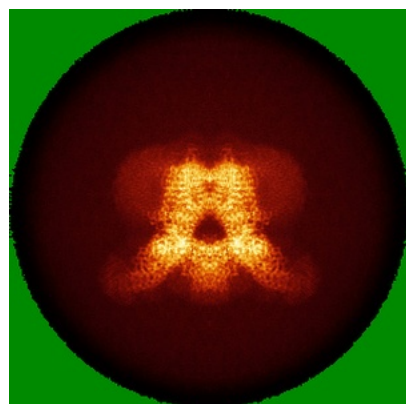


Z Index: 109

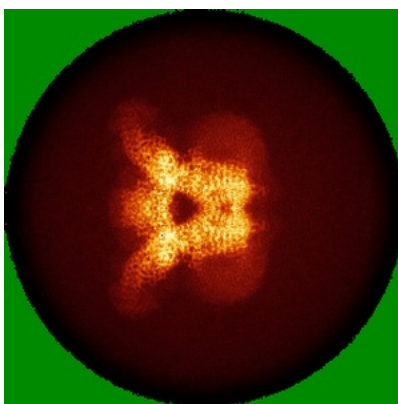
The images above show the largest variance slices of the map in three orthogonal directions.

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

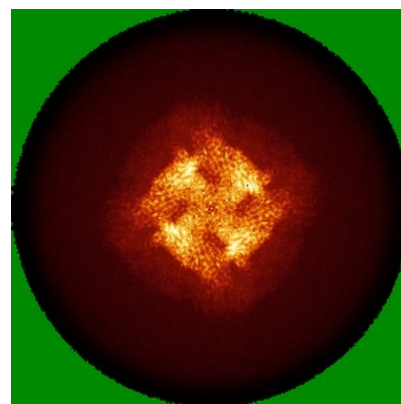
6.4.1 Primary map



X

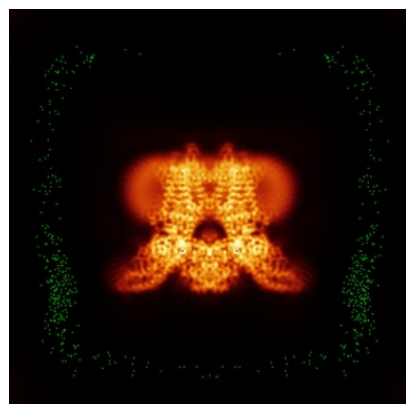


Y

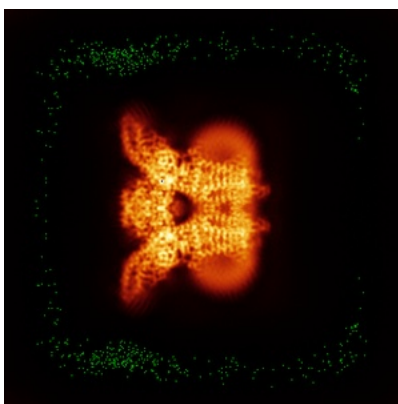


Z

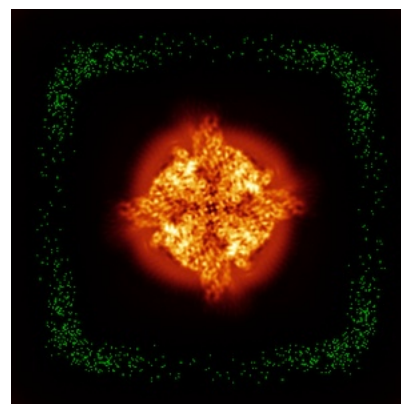
6.4.2 Raw map



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](#)

This section was not generated.

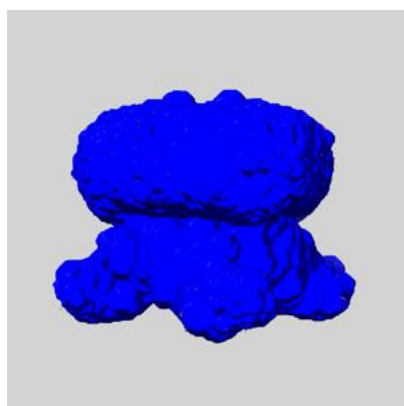
6.6 Mask visualisation [i](#)

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

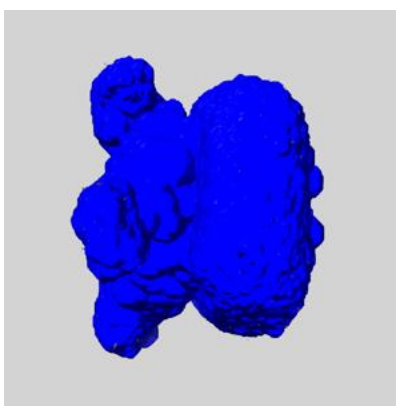
A mask typically either:

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

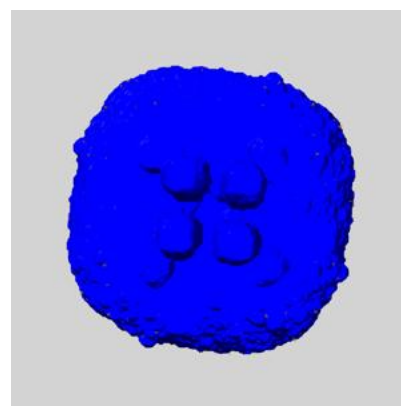
6.6.1 emd_40181_msk_1.map [i](#)



X



Y

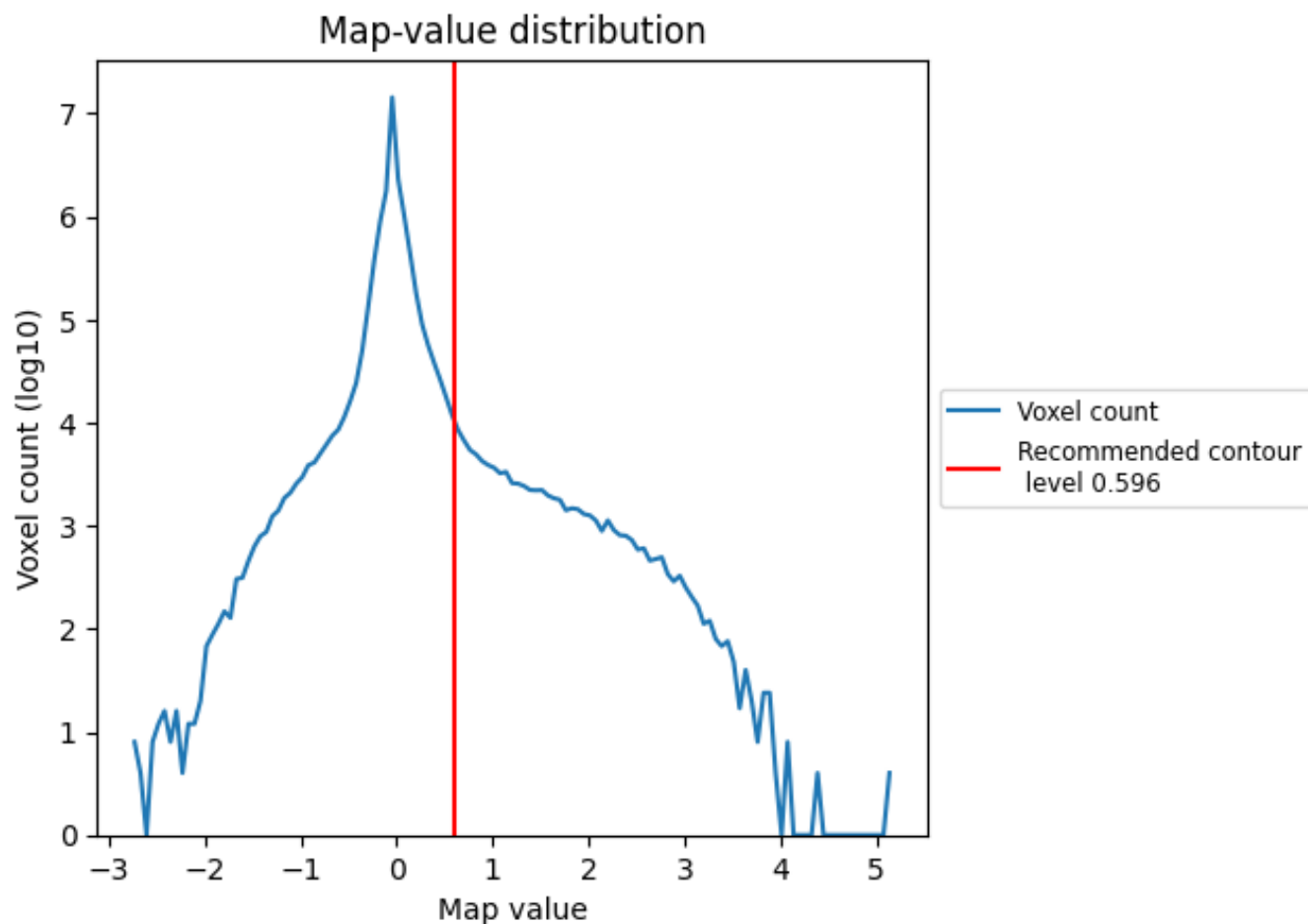


Z

7 Map analysis [i](#)

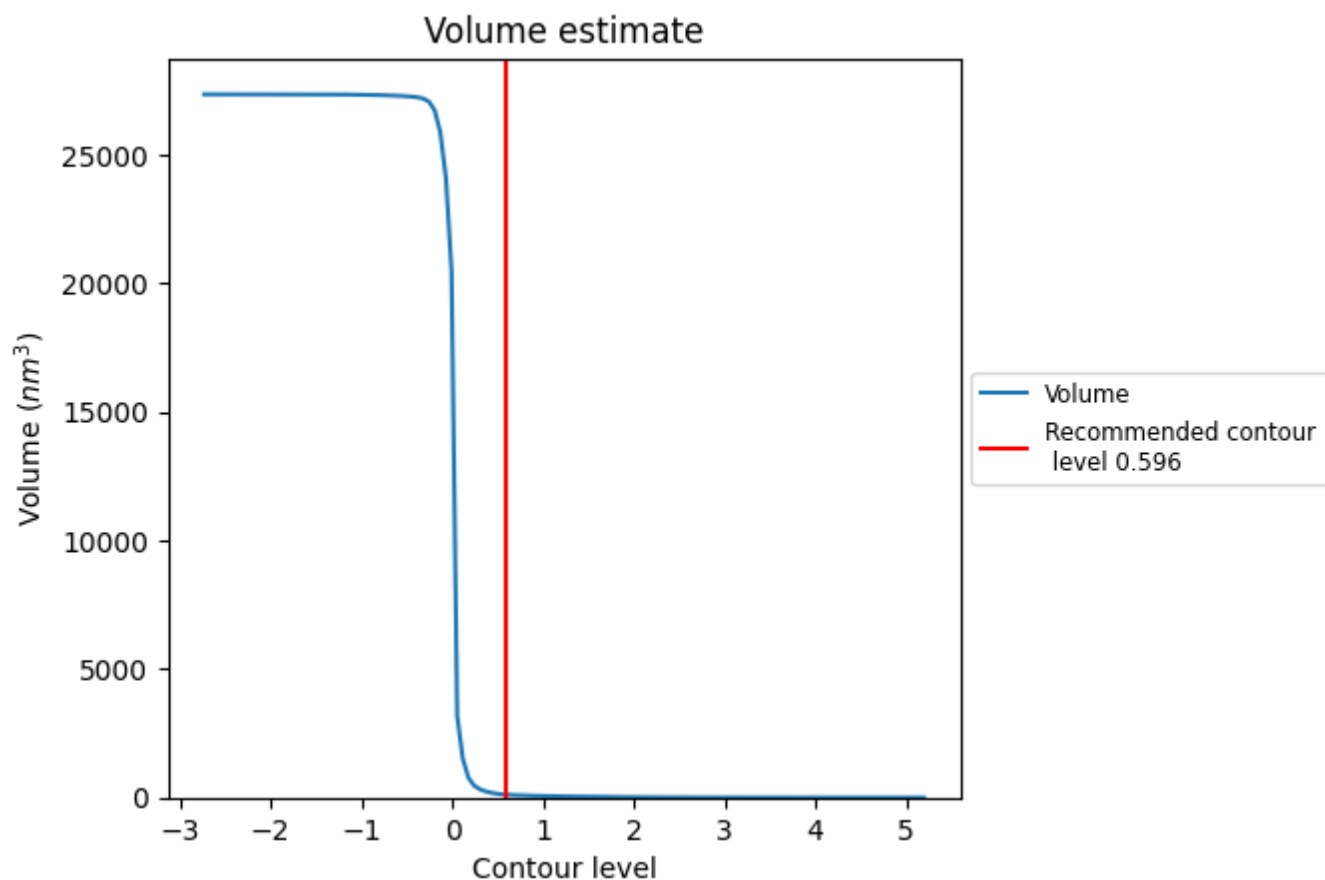
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

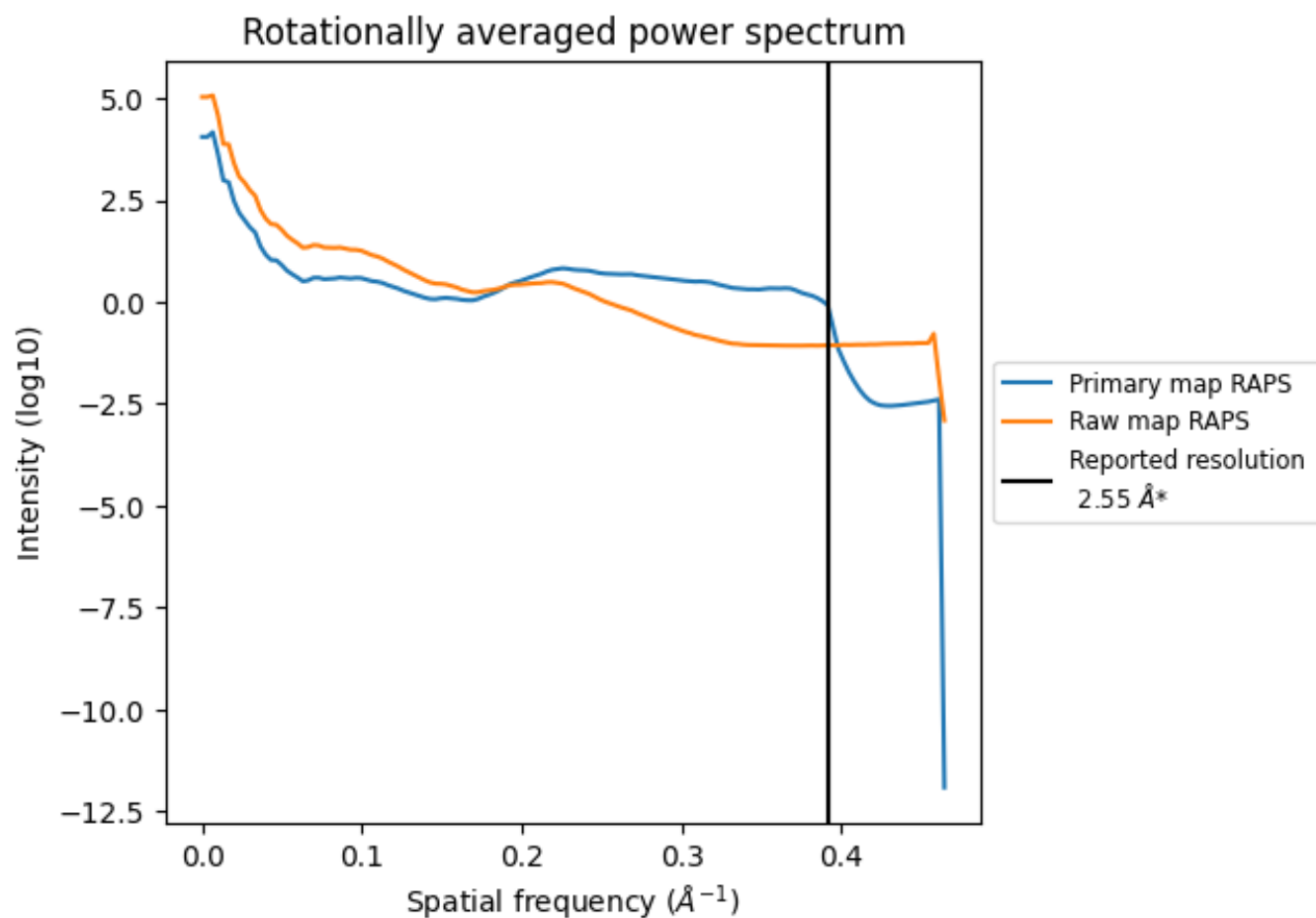
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 113 nm³; this corresponds to an approximate mass of 102 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 ⓘ

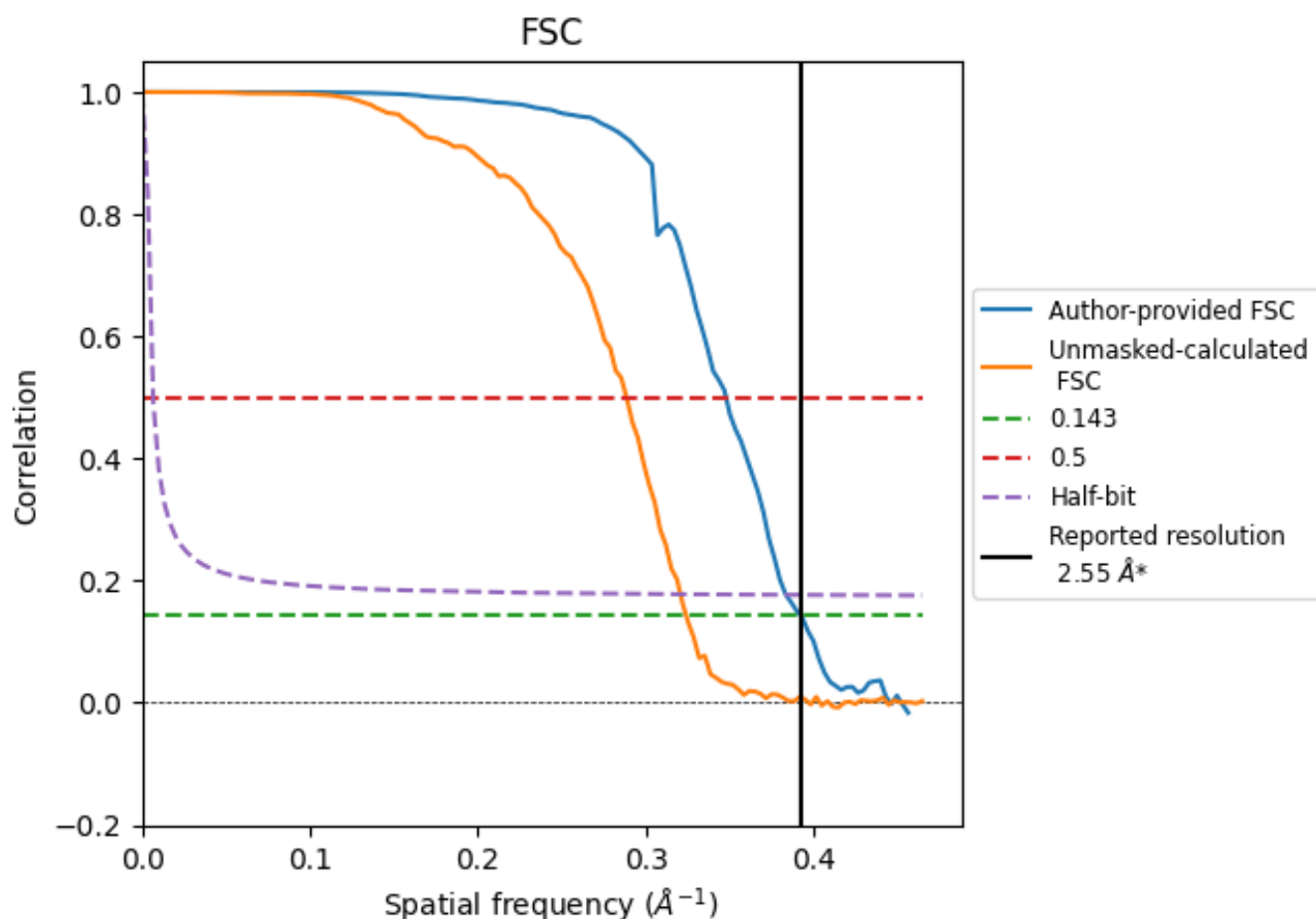


*Reported resolution corresponds to spatial frequency of 0.392 Å⁻¹

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 0.392 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

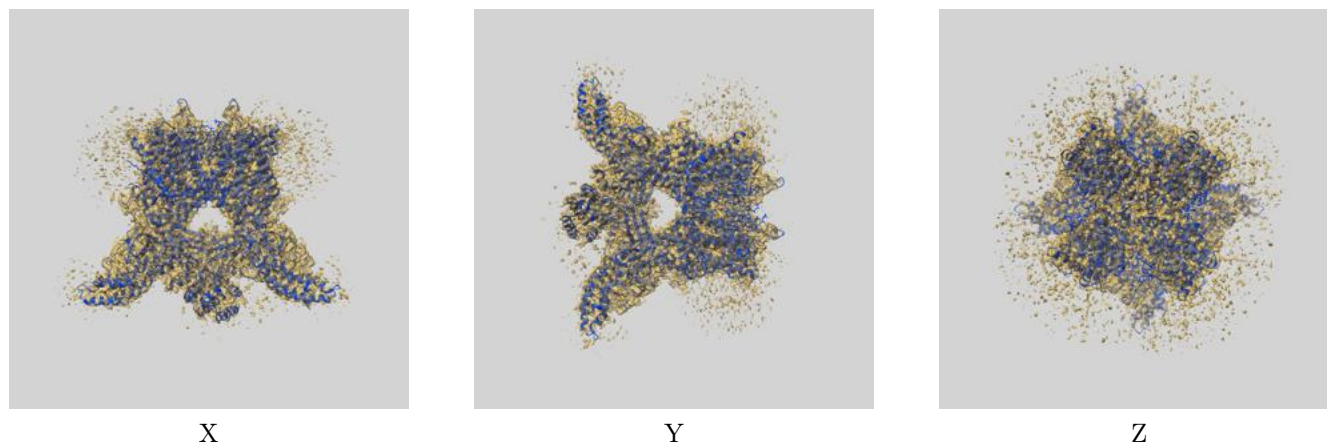
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.55	-	-
Author-provided FSC curve	2.55	2.88	2.61
Unmasked-calculated*	3.09	3.47	3.12

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.09 differs from the reported value 2.55 by more than 10 %

9 Map-model fit [i](#)

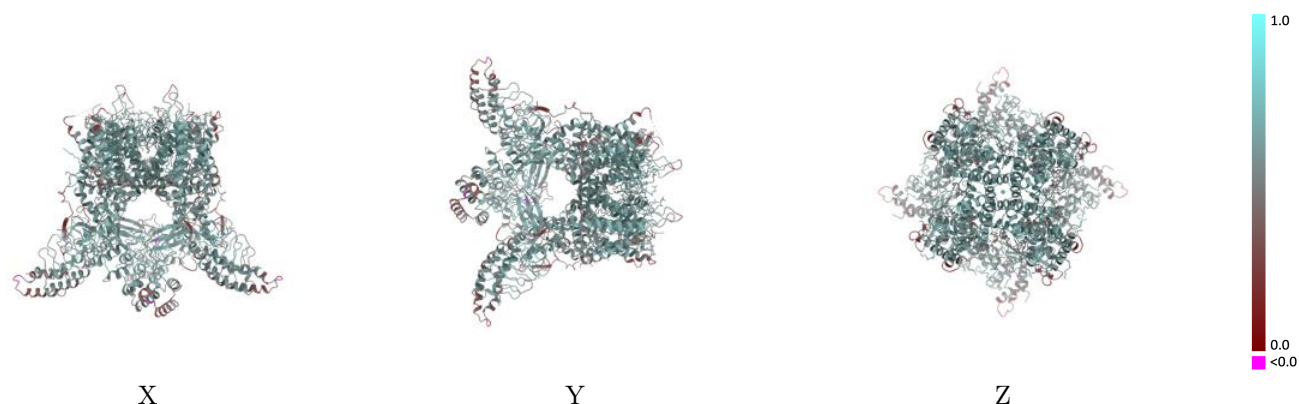
This section contains information regarding the fit between EMDB map EMD-40181 and PDB model 8GKA. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



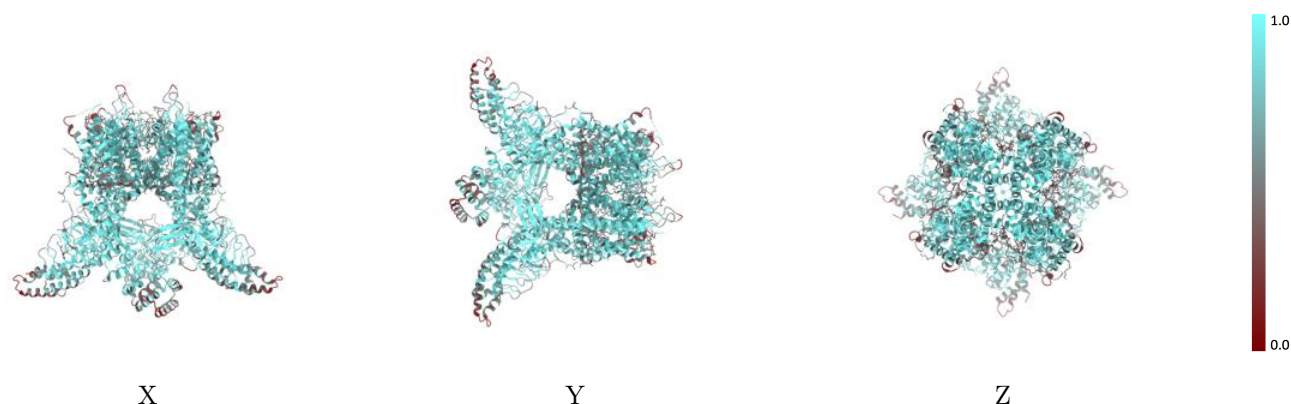
The images above show the 3D surface view of the map at the recommended contour level 0.596 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



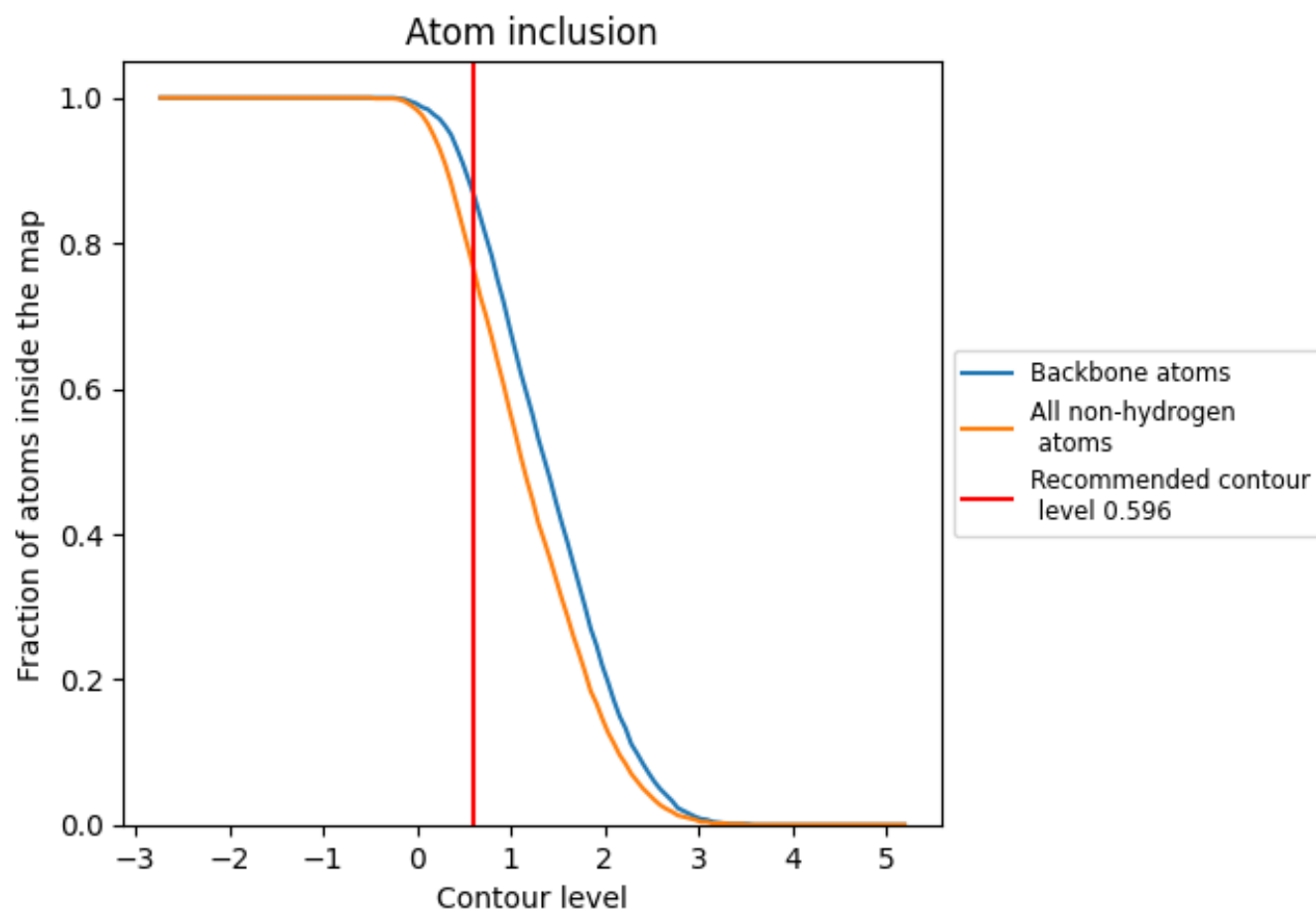
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.596).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 77% 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 (0.596) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7690	0.5530
A	0.7700	0.5520
B	0.7660	0.5530
C	0.7750	0.5540
D	0.7660	0.5520

