



Full wwPDB EM Validation Report ⓘ

Apr 5, 2026 – 10:33 PM UTC

PDB ID : 9W0X / pdb_00009w0x
EMDB ID : EMD-65520
Title : Cryo-EM structure of a Fungal XPR1
Authors : Shen, H.Z.; Yang, H.; Wang, Y.C.
Deposited on : 2025-07-24
Resolution : 2.90 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

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

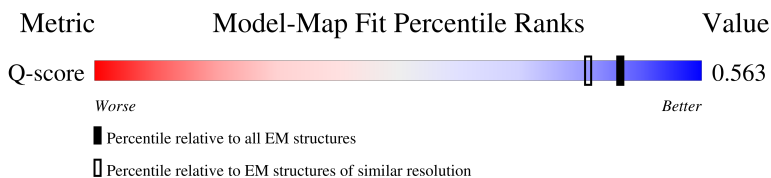
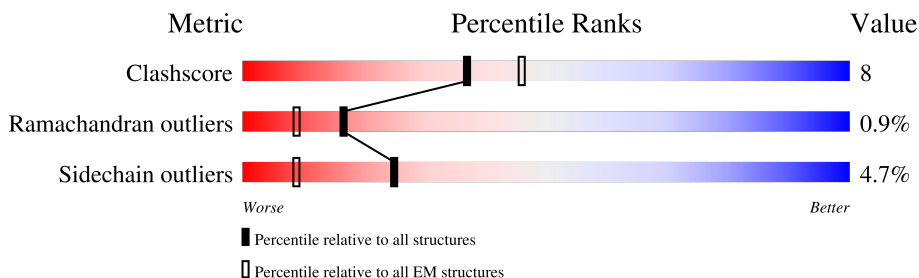
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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	13054 (2.40 - 3.40)

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	707	
1	D	707	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PO4	A	713	-	-	X	-
4	PO4	D	713	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10436 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 Protein SYG1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	595	Total	C	N	O	S	0	0
			5028	3328	846	832	22		
1	D	595	Total	C	N	O	S	0	0
			5028	3328	846	832	22		

There are 52 discrepancies between the modelled and reference sequences:

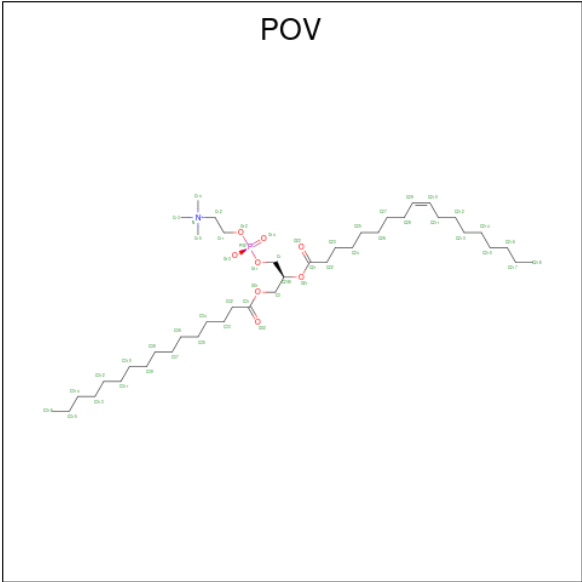
Chain	Residue	Modelled	Actual	Comment	Reference
A	-24	MET	-	initiating methionine	UNP Q9UU86
A	-23	ASP	-	expression tag	UNP Q9UU86
A	-22	TYR	-	expression tag	UNP Q9UU86
A	-21	LYS	-	expression tag	UNP Q9UU86
A	-20	ASP	-	expression tag	UNP Q9UU86
A	-19	ASP	-	expression tag	UNP Q9UU86
A	-18	ASP	-	expression tag	UNP Q9UU86
A	-17	ASP	-	expression tag	UNP Q9UU86
A	-16	LYS	-	expression tag	UNP Q9UU86
A	-15	GLY	-	expression tag	UNP Q9UU86
A	-14	GLY	-	expression tag	UNP Q9UU86
A	-13	SER	-	expression tag	UNP Q9UU86
A	-12	GLY	-	expression tag	UNP Q9UU86
A	-11	SER	-	expression tag	UNP Q9UU86
A	-10	GLY	-	expression tag	UNP Q9UU86
A	-9	GLY	-	expression tag	UNP Q9UU86
A	-8	SER	-	expression tag	UNP Q9UU86
A	-7	GLY	-	expression tag	UNP Q9UU86
A	-6	SER	-	expression tag	UNP Q9UU86
A	-5	GLY	-	expression tag	UNP Q9UU86
A	-4	SER	-	expression tag	UNP Q9UU86
A	-3	SER	-	expression tag	UNP Q9UU86
A	-2	GLY	-	expression tag	UNP Q9UU86
A	-1	SER	-	expression tag	UNP Q9UU86
A	0	THR	-	expression tag	UNP Q9UU86
A	1	GLY	-	expression tag	UNP Q9UU86

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-24	MET	-	initiating methionine	UNP Q9UU86
D	-23	ASP	-	expression tag	UNP Q9UU86
D	-22	TYR	-	expression tag	UNP Q9UU86
D	-21	LYS	-	expression tag	UNP Q9UU86
D	-20	ASP	-	expression tag	UNP Q9UU86
D	-19	ASP	-	expression tag	UNP Q9UU86
D	-18	ASP	-	expression tag	UNP Q9UU86
D	-17	ASP	-	expression tag	UNP Q9UU86
D	-16	LYS	-	expression tag	UNP Q9UU86
D	-15	GLY	-	expression tag	UNP Q9UU86
D	-14	GLY	-	expression tag	UNP Q9UU86
D	-13	SER	-	expression tag	UNP Q9UU86
D	-12	GLY	-	expression tag	UNP Q9UU86
D	-11	SER	-	expression tag	UNP Q9UU86
D	-10	GLY	-	expression tag	UNP Q9UU86
D	-9	GLY	-	expression tag	UNP Q9UU86
D	-8	SER	-	expression tag	UNP Q9UU86
D	-7	GLY	-	expression tag	UNP Q9UU86
D	-6	SER	-	expression tag	UNP Q9UU86
D	-5	GLY	-	expression tag	UNP Q9UU86
D	-4	SER	-	expression tag	UNP Q9UU86
D	-3	SER	-	expression tag	UNP Q9UU86
D	-2	GLY	-	expression tag	UNP Q9UU86
D	-1	SER	-	expression tag	UNP Q9UU86
D	0	THR	-	expression tag	UNP Q9UU86
D	1	GLY	-	expression tag	UNP Q9UU86

- Molecule 2 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (CCD ID: POV) (formula: C₄₂H₈₂NO₈P).



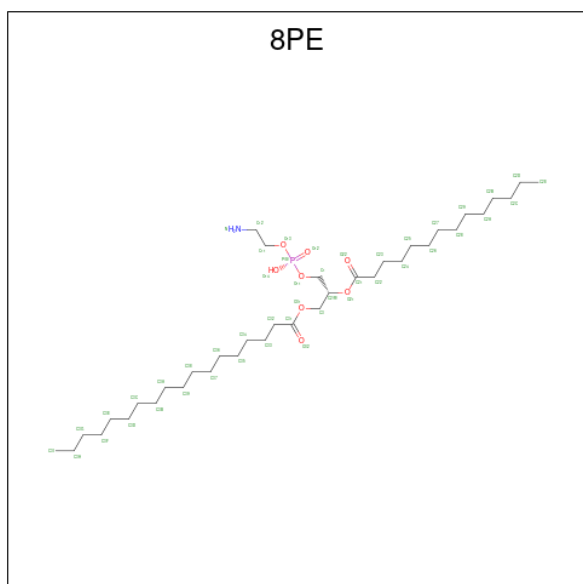
Mol	Chain	Residues	Atoms			AltConf
2	A	1	Total	C	O	0
			16	14	2	
2	A	1	Total	C	O	0
			20	18	2	
2	A	1	Total	C	O	0
			15	13	2	
2	A	1	Total	C	O	0
			14	12	2	
2	A	1	Total	C	O	0
			16	14	2	
2	A	1	Total	C	O	0
			12	10	2	
2	A	1	Total	C	O	0
			13	11	2	
2	A	1	Total	C	O	0
			15	13	2	
2	A	1	Total	C	O	0
			11	9	2	
2	D	1	Total	C	O	0
			16	14	2	
2	D	1	Total	C	O	0
			20	18	2	
2	D	1	Total	C	O	0
			15	13	2	
2	D	1	Total	C	O	0
			14	12	2	
2	D	1	Total	C	O	0
			16	14	2	

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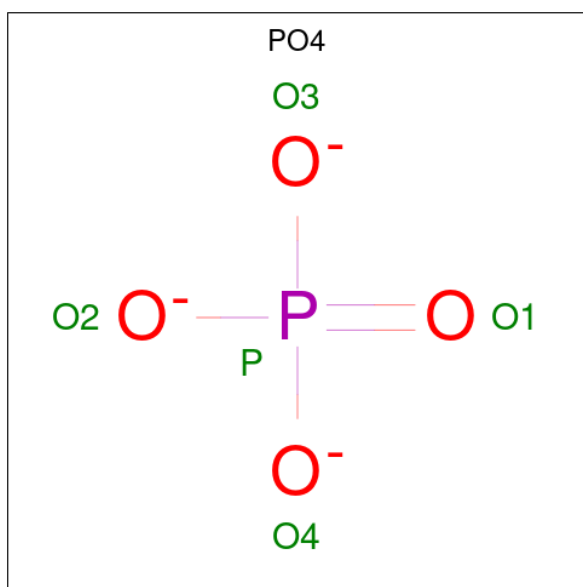
Mol	Chain	Residues	Atoms			AltConf
2	D	1	Total	C	O	0
			12	10	2	
2	D	1	Total	C	O	0
			13	11	2	
2	D	1	Total	C	O	0
			15	13	2	
2	D	1	Total	C	O	0
			11	9	2	

- Molecule 3 is (2R)-3-{[(S)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-2-(tetradecanoyloxy) propyl octadecanoate (CCD ID: 8PE) (formula: C₃₇H₇₄NO₈P).

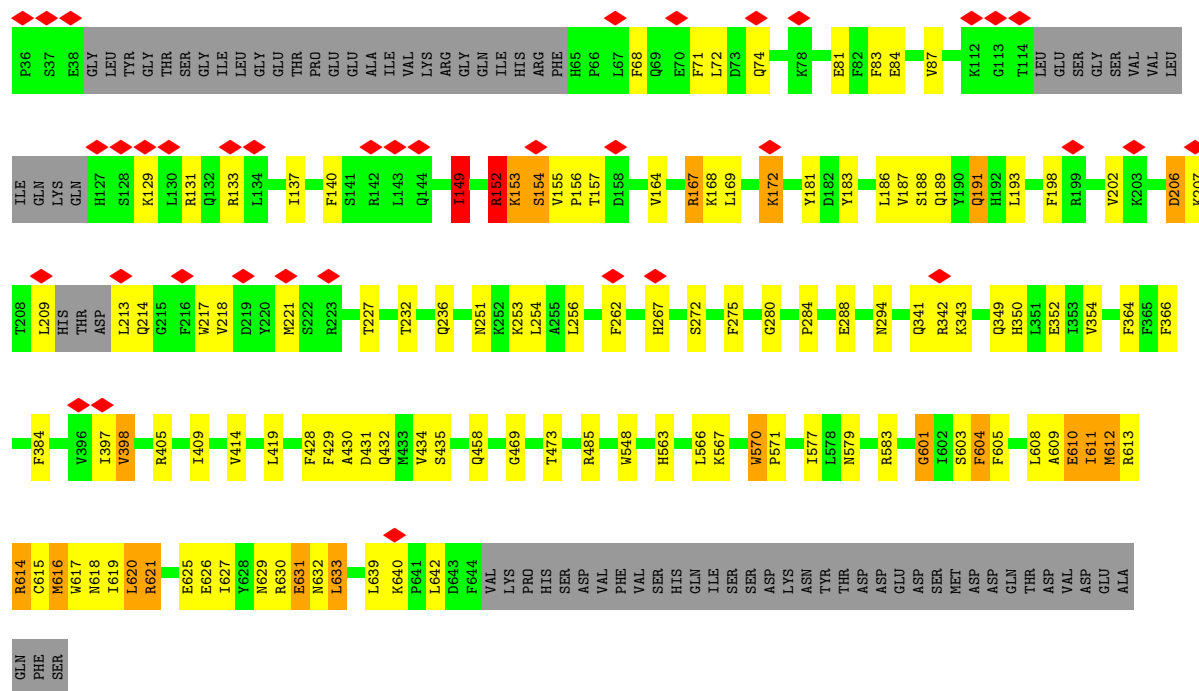


Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			43	33	1	8	1	
3	D	1	Total	C	N	O	P	0
			43	33	1	8	1	

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total	O	P	0
			5	4	1	
4	A	1	Total	O	P	0
			5	4	1	
4	A	1	Total	O	P	0
			5	4	1	
4	D	1	Total	O	P	0
			5	4	1	
4	D	1	Total	O	P	0
			5	4	1	
4	D	1	Total	O	P	0
			5	4	1	



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	210108	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)	1500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	5.451	Depositor
Minimum map value	-3.333	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.077	Depositor
Recommended contour level	0.739	Depositor
Map size (\AA)	391.32, 391.32, 391.32	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.087, 1.087, 1.087	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: POV, PO4, 8PE

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	0.69	22/5179 (0.4%)	0.65	14/6999 (0.2%)
1	D	0.69	22/5179 (0.4%)	0.65	14/6999 (0.2%)
All	All	0.69	44/10358 (0.4%)	0.65	28/13998 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	1
All	All	0	2

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	612	MET	C-O	9.75	1.35	1.24
1	A	612	MET	C-O	9.73	1.35	1.24
1	A	632	ASN	CA-C	-9.53	1.40	1.52
1	D	632	ASN	CA-C	-9.53	1.40	1.52
1	D	630	ARG	CA-C	-8.44	1.42	1.52
1	A	149	ILE	CA-C	-8.43	1.44	1.52
1	A	630	ARG	CA-C	-8.43	1.42	1.52
1	D	149	ILE	CA-C	-8.39	1.44	1.52
1	A	604	PHE	N-CA	-8.02	1.36	1.46
1	D	604	PHE	N-CA	-7.99	1.36	1.46
1	D	614	ARG	C-O	-7.81	1.15	1.24
1	A	614	ARG	C-O	-7.78	1.15	1.24
1	A	617	TRP	CA-C	-6.92	1.44	1.52
1	D	617	TRP	CA-C	-6.92	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	618	ASN	CA-C	-6.90	1.44	1.52
1	D	618	ASN	CA-C	-6.89	1.44	1.52
1	A	609	ALA	CA-CB	-6.80	1.42	1.53
1	D	609	ALA	CA-CB	-6.78	1.42	1.53
1	A	630	ARG	C-O	-6.47	1.16	1.24
1	D	630	ARG	C-O	-6.39	1.16	1.24
1	D	157	THR	N-CA	-6.20	1.38	1.46
1	A	612	MET	CA-CB	-6.18	1.43	1.53
1	D	612	MET	CA-CB	-6.18	1.43	1.53
1	A	630	ARG	CA-CB	-6.17	1.43	1.53
1	D	630	ARG	CA-CB	-6.17	1.43	1.53
1	A	614	ARG	CA-C	-6.14	1.44	1.52
1	D	614	ARG	CA-C	-6.14	1.44	1.52
1	A	157	THR	N-CA	-6.14	1.38	1.46
1	A	157	THR	CA-C	-6.10	1.45	1.52
1	D	157	THR	CA-C	-6.09	1.45	1.52
1	A	604	PHE	CA-C	-5.61	1.45	1.52
1	D	604	PHE	CA-C	-5.58	1.45	1.52
1	D	631	GLU	CA-CB	-5.58	1.43	1.53
1	A	631	GLU	CA-CB	-5.56	1.43	1.53
1	D	610	GLU	CA-CB	-5.43	1.44	1.53
1	A	610	GLU	CA-CB	-5.42	1.44	1.53
1	A	614	ARG	C-N	-5.26	1.27	1.33
1	A	601	GLY	CA-C	-5.26	1.44	1.51
1	D	614	ARG	C-N	-5.25	1.27	1.33
1	D	601	GLY	CA-C	-5.25	1.44	1.51
1	A	617	TRP	C-O	-5.21	1.18	1.24
1	A	154	SER	CA-C	-5.14	1.45	1.52
1	D	154	SER	CA-C	-5.14	1.45	1.52
1	D	617	TRP	C-O	-5.11	1.18	1.24

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	632	ASN	N-CA-C	-9.67	101.61	113.50
1	A	632	ASN	N-CA-C	-9.66	101.62	113.50
1	A	631	GLU	N-CA-C	8.00	122.61	113.01
1	D	631	GLU	N-CA-C	7.98	122.58	113.01
1	D	610	GLU	N-CA-C	7.03	118.94	111.28
1	A	610	GLU	N-CA-C	7.02	118.93	111.28
1	A	153	LYS	N-CA-C	-6.58	96.78	110.80
1	D	153	LYS	N-CA-C	-6.56	96.83	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	620	LEU	N-CA-C	6.29	119.12	111.82
1	D	620	LEU	N-CA-C	6.27	119.09	111.82
1	D	612	MET	N-CA-C	6.25	118.10	111.28
1	A	612	MET	N-CA-C	6.25	118.09	111.28
1	A	626	GLU	N-CA-C	6.22	118.58	111.11
1	D	626	GLU	N-CA-C	6.20	118.54	111.11
1	A	619	ILE	N-CA-C	6.15	116.81	110.36
1	D	619	ILE	N-CA-C	6.13	116.80	110.36
1	A	17	SER	N-CA-C	-5.99	106.95	114.56
1	D	17	SER	N-CA-C	-5.99	106.95	114.56
1	D	626	GLU	CB-CA-C	-5.52	101.98	110.81
1	A	626	GLU	CB-CA-C	-5.51	102.00	110.81
1	A	612	MET	N-CA-CB	-5.50	102.03	110.12
1	D	612	MET	N-CA-CB	-5.49	102.05	110.12
1	A	149	ILE	CA-C-N	-5.02	113.57	119.84
1	A	149	ILE	C-N-CA	-5.02	113.57	119.84
1	A	616	MET	N-CA-C	5.02	116.75	111.28
1	D	616	MET	N-CA-C	5.02	116.75	111.28
1	D	149	ILE	CA-C-N	-5.01	113.58	119.84
1	D	149	ILE	C-N-CA	-5.01	113.58	119.84

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	294	ASN	Peptide
1	D	294	ASN	Peptide

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	5028	0	5020	79	0
1	D	5028	0	5020	82	0
2	A	132	0	182	1	0
2	D	132	0	182	0	0
3	A	43	0	59	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	43	0	59	0	0
4	A	15	0	0	2	0
4	D	15	0	0	2	0
All	All	10436	0	10522	160	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 8.

All (160) 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:D:218:VAL:HA	1:D:221:MET:HE2	1.65	0.78
1:A:218:VAL:HA	1:A:221:MET:HE2	1.65	0.77
1:A:188:SER:HB2	1:A:232:THR:HG21	1.76	0.66
1:D:188:SER:HB2	1:D:232:THR:HG21	1.76	0.65
1:A:168:LYS:HE3	1:A:341:GLN:H	1.64	0.63
1:D:189:GLN:O	1:D:193:LEU:HG	1.99	0.61
1:A:189:GLN:O	1:A:193:LEU:HG	1.99	0.61
1:D:168:LYS:HE3	1:D:341:GLN:H	1.64	0.61
1:D:155:VAL:HB	1:D:156:PRO:HD2	1.83	0.60
1:D:397:ILE:HG23	1:D:398:VAL:HG23	1.84	0.60
1:A:397:ILE:HG23	1:A:398:VAL:HG23	1.84	0.60
1:A:155:VAL:HB	1:A:156:PRO:HD2	1.83	0.59
1:A:428:PHE:O	1:A:432:GLN:HG2	2.03	0.59
1:D:428:PHE:O	1:D:432:GLN:HG2	2.03	0.59
1:A:342:ARG:HH11	1:A:343:LYS:HD3	1.69	0.58
1:D:608:LEU:O	1:D:612:MET:HG3	2.05	0.57
1:D:149:ILE:HG21	1:D:633:LEU:CD1	2.35	0.57
1:A:608:LEU:O	1:A:612:MET:HG3	2.05	0.57
1:A:149:ILE:HG21	1:A:633:LEU:CD1	2.35	0.56
1:D:342:ARG:HH11	1:D:343:LYS:HD3	1.69	0.56
1:A:364:PHE:HD2	1:A:384:PHE:HB2	1.70	0.56
1:D:364:PHE:HD2	1:D:384:PHE:HB2	1.70	0.56
1:A:272:SER:HA	1:A:275:PHE:CE2	2.42	0.55
1:D:349:GLN:O	1:D:352:GLU:HG2	2.08	0.54
1:D:272:SER:HA	1:D:275:PHE:CE2	2.42	0.54
1:A:12:VAL:HB	1:A:15:TRP:HB2	1.90	0.54
1:D:12:VAL:HB	1:D:15:TRP:HB2	1.90	0.54
1:A:349:GLN:O	1:A:352:GLU:HG2	2.08	0.54
1:D:202:VAL:HG21	1:D:217:TRP:CD2	2.44	0.53
1:A:72:LEU:HD21	1:A:217:TRP:HD1	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:563:HIS:HD2	1:A:631:GLU:OE2	1.92	0.53
1:D:18:ALA:O	1:D:19:TYR:HB2	2.09	0.53
1:A:18:ALA:O	1:A:19:TYR:HB2	2.09	0.53
1:D:570:TRP:CG	1:D:571:PRO:HD3	2.44	0.53
1:A:72:LEU:HD21	1:A:217:TRP:CD1	2.43	0.53
1:D:72:LEU:HD21	1:D:217:TRP:CD1	2.43	0.53
1:A:81:GLU:O	1:A:84:GLU:HG3	2.09	0.53
1:D:72:LEU:HD21	1:D:217:TRP:HD1	1.73	0.53
1:D:81:GLU:O	1:D:84:GLU:HG3	2.09	0.53
1:A:202:VAL:HG21	1:A:217:TRP:CD2	2.44	0.52
1:D:563:HIS:HD2	1:D:631:GLU:OE2	1.92	0.52
1:D:430:ALA:O	1:D:434:VAL:HG23	2.10	0.52
1:A:570:TRP:CG	1:A:571:PRO:HD3	2.44	0.52
1:A:430:ALA:O	1:A:434:VAL:HG23	2.10	0.52
1:D:570:TRP:H	1:D:571:PRO:CD	2.24	0.51
1:A:469:GLY:O	1:A:473:THR:HG23	2.11	0.51
1:A:149:ILE:HG21	1:A:633:LEU:HD11	1.93	0.51
1:D:469:GLY:O	1:D:473:THR:HG23	2.11	0.51
1:D:149:ILE:HG21	1:D:633:LEU:HD11	1.93	0.51
1:A:570:TRP:H	1:A:571:PRO:CD	2.24	0.51
1:D:435:SER:OG	1:D:614:ARG:NH1	2.44	0.50
1:A:435:SER:OG	1:A:614:ARG:NH1	2.44	0.50
1:D:405:ARG:O	1:D:409:ILE:HG13	2.13	0.49
1:A:154:SER:OG	1:A:155:VAL:N	2.42	0.49
1:A:133:ARG:HD2	1:A:137:ILE:CD1	2.43	0.49
1:D:251:ASN:HD22	1:D:254:LEU:HB2	1.78	0.49
1:D:26:LYS:HA	1:D:29:ILE:HB	1.95	0.49
1:A:405:ARG:O	1:A:409:ILE:HG13	2.12	0.48
1:D:621:ARG:NH1	1:D:625:GLU:OE2	2.46	0.48
1:D:288:GLU:HG2	1:D:366:PHE:HE1	1.78	0.48
1:A:621:ARG:NH1	1:A:625:GLU:OE2	2.46	0.48
1:D:133:ARG:HD2	1:D:137:ILE:CD1	2.43	0.48
1:D:639:LEU:HD23	1:D:640:LYS:H	1.79	0.48
1:A:26:LYS:HA	1:A:29:ILE:HB	1.95	0.48
1:A:288:GLU:HG2	1:A:366:PHE:HE1	1.78	0.48
1:A:639:LEU:HD23	1:A:640:LYS:N	2.29	0.48
1:A:570:TRP:CD2	1:A:571:PRO:HD3	2.49	0.47
1:A:639:LEU:HD23	1:A:640:LYS:H	1.79	0.47
1:A:251:ASN:HD22	1:A:254:LEU:HB2	1.78	0.47
1:D:570:TRP:CD2	1:D:571:PRO:HD3	2.48	0.47
1:D:639:LEU:HD23	1:D:640:LYS:N	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:154:SER:OG	1:D:155:VAL:N	2.42	0.47
1:A:167:ARG:H	1:A:167:ARG:HG2	1.48	0.47
1:A:253:LYS:HD2	1:A:253:LYS:N	2.30	0.47
1:D:253:LYS:HD2	1:D:253:LYS:N	2.30	0.47
1:D:627:ILE:O	1:D:631:GLU:HG3	2.15	0.47
1:A:625:GLU:O	1:A:629:ASN:ND2	2.48	0.46
1:A:187:VAL:O	1:A:191:GLN:HG2	2.16	0.46
1:D:24:LYS:HB3	1:D:71:PHE:HZ	1.81	0.46
1:D:611:ILE:HD13	1:D:611:ILE:HA	1.83	0.46
1:D:625:GLU:O	1:D:629:ASN:ND2	2.48	0.46
1:A:627:ILE:O	1:A:631:GLU:HG3	2.15	0.46
1:D:187:VAL:O	1:D:191:GLN:HG2	2.16	0.46
1:D:20:PHE:CG	1:D:21:ASP:N	2.84	0.45
1:D:614:ARG:HH22	4:D:713:PO4:P	2.39	0.45
1:A:24:LYS:HB3	1:A:71:PHE:HZ	1.81	0.45
1:D:342:ARG:HD2	1:D:343:LYS:HD3	1.99	0.45
1:A:198:PHE:HB3	1:A:217:TRP:CZ2	2.52	0.45
1:A:566:LEU:HD23	1:A:566:LEU:HA	1.83	0.45
1:D:24:LYS:HD2	1:D:71:PHE:CE1	2.52	0.45
1:A:24:LYS:HD2	1:A:71:PHE:CE1	2.52	0.45
1:A:342:ARG:HD2	1:A:343:LYS:HD3	1.99	0.45
1:A:614:ARG:HH22	4:A:713:PO4:P	2.39	0.45
1:A:350:HIS:O	1:A:354:VAL:HG23	2.18	0.44
1:A:20:PHE:CG	1:A:21:ASP:N	2.84	0.44
1:D:181:TYR:CE1	1:D:236:GLN:HG2	2.52	0.44
1:D:198:PHE:HB3	1:D:217:TRP:CZ2	2.52	0.44
1:A:83:PHE:O	1:A:87:VAL:HG23	2.17	0.44
1:A:181:TYR:CE1	1:A:236:GLN:HG2	2.52	0.44
1:D:251:ASN:ND2	1:D:254:LEU:HB2	2.32	0.44
1:D:169:LEU:HD12	1:D:169:LEU:HA	1.85	0.44
1:D:172:LYS:HA	1:D:172:LYS:HD2	1.85	0.44
1:D:350:HIS:O	1:D:354:VAL:HG23	2.18	0.44
1:D:83:PHE:O	1:D:87:VAL:HG23	2.17	0.44
1:A:251:ASN:ND2	1:A:254:LEU:HB2	2.32	0.44
1:A:570:TRP:H	1:A:571:PRO:HD2	1.82	0.44
1:D:152:ARG:HE	1:D:152:ARG:HB2	1.51	0.44
1:D:570:TRP:H	1:D:571:PRO:HD2	1.82	0.43
1:D:603:SER:O	1:D:604:PHE:C	2.59	0.43
1:A:23:LYS:HA	1:A:23:LYS:HD3	1.70	0.43
1:A:24:LYS:HD2	1:A:71:PHE:HE1	1.84	0.43
1:A:603:SER:O	1:A:604:PHE:C	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:167:ARG:H	1:D:167:ARG:HG2	1.48	0.43
1:D:601:GLY:O	1:D:605:PHE:HD2	2.01	0.43
1:A:129:LYS:HE3	1:A:129:LYS:HB3	1.79	0.43
1:D:24:LYS:HD2	1:D:71:PHE:HE1	1.84	0.43
1:A:414:VAL:HG21	1:A:429:PHE:HB3	2.01	0.43
1:A:479:ARG:HA	1:A:479:ARG:HD2	1.87	0.43
1:D:27:LYS:HD2	1:D:27:LYS:C	2.44	0.43
1:A:27:LYS:HD2	1:A:27:LYS:C	2.44	0.42
1:A:213:LEU:HD23	1:A:213:LEU:HA	1.83	0.42
1:D:579:ASN:O	1:D:583:ARG:HG3	2.19	0.42
1:A:601:GLY:O	1:A:605:PHE:HD2	2.01	0.42
1:D:23:LYS:HA	1:D:23:LYS:HD3	1.70	0.42
1:D:567:LYS:HD2	1:D:567:LYS:HA	1.84	0.42
1:D:405:ARG:HG3	1:D:405:ARG:HH11	1.84	0.42
1:D:164:VAL:HG21	1:D:169:LEU:HD13	2.01	0.42
1:D:275:PHE:C	1:D:275:PHE:CD1	2.97	0.42
1:D:405:ARG:HG3	1:D:405:ARG:NH1	2.35	0.42
1:D:566:LEU:HD23	1:D:566:LEU:HA	1.83	0.42
1:A:164:VAL:HG21	1:A:169:LEU:HD13	2.01	0.42
1:A:611:ILE:HD13	1:A:611:ILE:HA	1.83	0.42
1:D:414:VAL:HG21	1:D:429:PHE:HB3	2.01	0.42
1:D:614:ARG:NH2	4:D:713:PO4:O4	2.53	0.42
1:A:614:ARG:NH2	4:A:713:PO4:O4	2.53	0.42
1:A:186:LEU:HD21	1:D:262:PHE:HZ	1.83	0.42
1:A:262:PHE:HZ	1:D:186:LEU:HD21	1.84	0.42
1:A:405:ARG:HG3	1:A:405:ARG:NH1	2.35	0.42
1:A:405:ARG:HG3	1:A:405:ARG:HH11	1.84	0.42
1:D:206:ASP:HB3	1:D:207:LYS:H	1.63	0.42
1:A:275:PHE:CD1	1:A:275:PHE:C	2.97	0.41
1:D:131:ARG:HH21	1:D:485:ARG:NE	2.18	0.41
1:A:579:ASN:O	1:A:583:ARG:HG3	2.19	0.41
1:D:149:ILE:O	1:D:149:ILE:HG13	2.21	0.41
1:D:254:LEU:HD12	1:D:254:LEU:HA	1.85	0.41
1:D:24:LYS:HB3	1:D:71:PHE:CZ	2.56	0.41
1:D:183:TYR:O	1:D:187:VAL:HG23	2.21	0.41
1:A:183:TYR:O	1:A:187:VAL:HG23	2.21	0.41
1:D:129:LYS:HE3	1:D:129:LYS:HB3	1.79	0.41
1:D:419:LEU:HD23	1:D:419:LEU:HA	1.92	0.41
1:A:131:ARG:HH21	1:A:485:ARG:NE	2.18	0.41
1:A:149:ILE:O	1:A:149:ILE:HG13	2.21	0.41
1:A:318:LEU:HD23	1:A:318:LEU:HA	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:GLY:O	1:A:284:PRO:HD2	2.22	0.40
1:D:213:LEU:HB3	1:D:214:GLN:H	1.67	0.40
1:A:14:GLU:HG2	1:A:15:TRP:HD1	1.87	0.40
1:A:548:TRP:CD1	1:A:548:TRP:N	2.90	0.40
1:D:280:GLY:O	1:D:284:PRO:HD2	2.21	0.40
1:A:597:GLN:H	1:A:597:GLN:HG2	1.74	0.40
2:A:705:POV:H22A	2:A:705:POV:H25	1.98	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	587/707 (83%)	553 (94%)	29 (5%)	5 (1%)	14	41
1	D	587/707 (83%)	553 (94%)	29 (5%)	5 (1%)	14	41
All	All	1174/1414 (83%)	1106 (94%)	58 (5%)	10 (1%)	16	41

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	206	ASP
1	A	570	TRP
1	D	206	ASP
1	D	570	TRP
1	A	152	ARG
1	D	152	ARG
1	A	140	PHE
1	D	140	PHE
1	A	398	VAL
1	D	398	VAL

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	540/634 (85%)	515 (95%)	25 (5%)	24	57
1	D	540/634 (85%)	514 (95%)	26 (5%)	23	55
All	All	1080/1268 (85%)	1029 (95%)	51 (5%)	25	56

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ILE
1	A	68	PHE
1	A	74	GLN
1	A	149	ILE
1	A	152	ARG
1	A	153	LYS
1	A	167	ARG
1	A	172	LYS
1	A	191	GLN
1	A	209	LEU
1	A	227	THR
1	A	256	LEU
1	A	431	ASP
1	A	458	GLN
1	A	548	TRP
1	A	577	ILE
1	A	610	GLU
1	A	611	ILE
1	A	613	ARG
1	A	615	CYS
1	A	616	MET
1	A	620	LEU
1	A	621	ARG
1	A	633	LEU
1	A	642	LEU
1	D	28	ILE
1	D	68	PHE

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Mol	Chain	Res	Type
1	D	74	GLN
1	D	149	ILE
1	D	152	ARG
1	D	153	LYS
1	D	167	ARG
1	D	172	LYS
1	D	191	GLN
1	D	209	LEU
1	D	227	THR
1	D	256	LEU
1	D	267	HIS
1	D	431	ASP
1	D	458	GLN
1	D	548	TRP
1	D	577	ILE
1	D	610	GLU
1	D	611	ILE
1	D	613	ARG
1	D	615	CYS
1	D	616	MET
1	D	620	LEU
1	D	621	ARG
1	D	633	LEU
1	D	642	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	194	ASN
1	A	214	GLN
1	A	251	ASN
1	A	298	GLN
1	A	410	GLN
1	A	549	ASN
1	A	563	HIS
1	A	597	GLN
1	A	629	ASN
1	D	194	ASN
1	D	214	GLN
1	D	251	ASN
1	D	267	HIS
1	D	298	GLN

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Mol	Chain	Res	Type
1	D	304	GLN
1	D	410	GLN
1	D	549	ASN
1	D	563	HIS
1	D	597	GLN
1	D	629	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

26 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	POV	D	708	-	12,12,51	1.35	1 (8%)	12,12,59	1.12	1 (8%)
4	PO4	A	713	-	4,4,4	0.99	0	6,6,6	0.48	0
2	POV	A	709	-	14,14,51	1.23	1 (7%)	14,14,59	1.00	0
3	8PE	D	707	-	42,42,46	1.00	2 (4%)	45,47,51	1.01	2 (4%)
2	POV	A	701	-	15,15,51	1.19	1 (6%)	15,15,59	0.98	0
4	PO4	D	713	-	4,4,4	0.98	0	6,6,6	0.47	0
2	POV	A	705	-	15,15,51	1.19	1 (6%)	15,15,59	0.96	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	POV	A	704	-	13,13,51	1.28	1 (7%)	13,13,59	1.07	1 (7%)
3	8PE	A	707	-	42,42,46	1.00	2 (4%)	45,47,51	1.01	1 (2%)
2	POV	D	709	-	14,14,51	1.23	1 (7%)	14,14,59	1.00	0
2	POV	D	704	-	13,13,51	1.29	1 (7%)	13,13,59	1.08	1 (7%)
4	PO4	D	711	-	4,4,4	1.01	0	6,6,6	0.49	0
2	POV	A	708	-	12,12,51	1.34	1 (8%)	12,12,59	1.12	1 (8%)
2	POV	D	701	-	15,15,51	1.19	1 (6%)	15,15,59	0.98	0
2	POV	D	705	-	15,15,51	1.20	1 (6%)	15,15,59	0.97	0
4	PO4	A	712	-	4,4,4	1.05	0	6,6,6	0.47	0
2	POV	A	710	-	10,10,51	1.45	1 (10%)	10,10,59	1.15	1 (10%)
2	POV	D	710	-	10,10,51	1.45	1 (10%)	10,10,59	1.15	1 (10%)
2	POV	D	703	-	14,14,51	1.23	1 (7%)	14,14,59	1.00	0
2	POV	A	702	-	19,19,51	1.06	1 (5%)	19,19,59	0.92	0
4	PO4	D	712	-	4,4,4	1.05	0	6,6,6	0.47	0
2	POV	A	706	-	11,11,51	1.40	1 (9%)	11,11,59	1.15	1 (9%)
4	PO4	A	711	-	4,4,4	1.01	0	6,6,6	0.49	0
2	POV	D	702	-	19,19,51	1.07	1 (5%)	19,19,59	0.92	0
2	POV	A	703	-	14,14,51	1.23	1 (7%)	14,14,59	1.00	0
2	POV	D	706	-	11,11,51	1.40	1 (9%)	11,11,59	1.15	1 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	POV	D	708	-	-	4/10/10/55	-
2	POV	A	709	-	-	6/12/12/55	-
3	8PE	D	707	-	-	14/46/46/50	-
2	POV	A	701	-	-	2/13/13/55	-
2	POV	A	705	-	-	4/13/13/55	-
2	POV	A	704	-	-	2/11/11/55	-
3	8PE	A	707	-	-	14/46/46/50	-
2	POV	D	709	-	-	6/12/12/55	-
2	POV	D	704	-	-	2/11/11/55	-
2	POV	A	708	-	-	3/10/10/55	-
2	POV	D	701	-	-	2/13/13/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	POV	D	705	-	-	4/13/13/55	-
2	POV	A	710	-	-	2/8/8/55	-
2	POV	D	710	-	-	2/8/8/55	-
2	POV	D	703	-	-	1/12/12/55	-
2	POV	A	702	-	-	4/17/17/55	-
2	POV	A	706	-	-	3/9/9/55	-
2	POV	D	702	-	-	4/17/17/55	-
2	POV	A	703	-	-	1/12/12/55	-
2	POV	D	706	-	-	3/9/9/55	-

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	708	POV	O21-C21	4.57	1.45	1.30
2	D	702	POV	O21-C21	4.56	1.45	1.30
2	D	704	POV	O21-C21	4.56	1.45	1.30
2	A	708	POV	O21-C21	4.55	1.45	1.30
2	D	701	POV	O21-C21	4.55	1.45	1.30
2	D	705	POV	O21-C21	4.55	1.45	1.30
2	A	701	POV	O21-C21	4.54	1.45	1.30
2	A	702	POV	O21-C21	4.54	1.45	1.30
2	A	710	POV	O31-C31	4.53	1.45	1.30
2	A	705	POV	O21-C21	4.53	1.45	1.30
2	A	704	POV	O21-C21	4.53	1.45	1.30
2	A	706	POV	O21-C21	4.53	1.45	1.30
2	D	710	POV	O31-C31	4.53	1.45	1.30
2	A	703	POV	O21-C21	4.53	1.45	1.30
2	D	706	POV	O21-C21	4.52	1.45	1.30
2	D	703	POV	O21-C21	4.52	1.45	1.30
2	A	709	POV	O31-C31	4.52	1.45	1.30
2	D	709	POV	O31-C31	4.52	1.45	1.30
3	A	707	8PE	O31-C31	4.16	1.45	1.33
3	D	707	8PE	O31-C31	4.16	1.45	1.33
3	A	707	8PE	O21-C21	4.14	1.46	1.34
3	D	707	8PE	O21-C21	4.14	1.46	1.34

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	707	8PE	O21-C21-C22	3.72	119.53	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	707	8PE	O21-C21-C22	3.70	119.49	111.48
2	D	706	POV	C23-C22-C21	-2.06	109.13	114.51
2	D	710	POV	C33-C32-C31	-2.06	109.13	114.51
2	A	706	POV	C23-C22-C21	-2.06	109.14	114.51
2	A	710	POV	C33-C32-C31	-2.06	109.14	114.51
2	A	708	POV	O21-C21-C22	2.03	120.42	114.00
2	D	708	POV	O21-C21-C22	2.03	120.40	114.00
2	D	704	POV	O21-C21-C22	2.02	120.39	114.00
2	A	704	POV	O21-C21-C22	2.02	120.37	114.00
3	D	707	8PE	C2-O21-C21	-2.01	112.99	117.80

There are no chirality outliers.

All (83) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	707	8PE	C1-O11-P-O13
3	A	707	8PE	C11-O13-P-O11
3	A	707	8PE	O13-C11-C12-N
3	D	707	8PE	C1-O11-P-O13
3	D	707	8PE	C11-O13-P-O11
3	D	707	8PE	O13-C11-C12-N
3	A	707	8PE	C36-C37-C38-C39
3	D	707	8PE	C36-C37-C38-C39
2	A	708	POV	C23-C24-C25-C26
2	D	708	POV	C23-C24-C25-C26
2	A	709	POV	C311-C310-C39-C38
2	D	709	POV	C311-C310-C39-C38
3	A	707	8PE	C1-C2-C3-O31
3	D	707	8PE	C1-C2-C3-O31
2	A	709	POV	C33-C34-C35-C36
2	D	709	POV	C33-C34-C35-C36
2	A	702	POV	C26-C27-C28-C29
2	D	702	POV	C26-C27-C28-C29
3	A	707	8PE	C39-C3A-C3B-C3C
3	D	707	8PE	C39-C3A-C3B-C3C
3	A	707	8PE	C22-C23-C24-C25
3	D	707	8PE	C22-C23-C24-C25
3	A	707	8PE	O21-C2-C3-O31
3	D	707	8PE	O21-C2-C3-O31
2	A	708	POV	C21-C22-C23-C24
2	D	708	POV	C21-C22-C23-C24
3	A	707	8PE	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
3	D	707	8PE	C23-C24-C25-C26
3	A	707	8PE	O11-C1-C2-C3
3	D	707	8PE	O11-C1-C2-C3
2	A	705	POV	C23-C24-C25-C26
2	A	709	POV	C39-C310-C311-C312
2	D	705	POV	C23-C24-C25-C26
2	D	709	POV	C39-C310-C311-C312
2	A	706	POV	C21-C22-C23-C24
2	D	706	POV	C21-C22-C23-C24
3	A	707	8PE	O11-C1-C2-O21
3	D	707	8PE	O11-C1-C2-O21
3	A	707	8PE	C1-O11-P-O12
3	A	707	8PE	C11-O13-P-O12
3	D	707	8PE	C1-O11-P-O12
3	D	707	8PE	C11-O13-P-O12
3	D	707	8PE	C35-C36-C37-C38
3	A	707	8PE	C35-C36-C37-C38
2	A	705	POV	O22-C21-C22-C23
2	D	705	POV	O22-C21-C22-C23
2	A	702	POV	O22-C21-C22-C23
2	A	704	POV	O22-C21-C22-C23
2	A	709	POV	O32-C31-C32-C33
2	A	710	POV	O31-C31-C32-C33
2	D	702	POV	O22-C21-C22-C23
2	D	704	POV	O22-C21-C22-C23
2	D	709	POV	O32-C31-C32-C33
2	D	710	POV	O31-C31-C32-C33
2	D	709	POV	C34-C35-C36-C37
2	A	709	POV	C34-C35-C36-C37
2	A	710	POV	O32-C31-C32-C33
2	D	710	POV	O32-C31-C32-C33
2	A	704	POV	O21-C21-C22-C23
2	D	705	POV	C22-C23-C24-C25
2	D	705	POV	O21-C21-C22-C23
2	A	705	POV	C22-C23-C24-C25
2	A	702	POV	O21-C21-C22-C23
2	A	705	POV	O21-C21-C22-C23
2	D	702	POV	O21-C21-C22-C23
2	D	704	POV	O21-C21-C22-C23
2	A	709	POV	O31-C31-C32-C33
2	D	709	POV	O31-C31-C32-C33
2	A	702	POV	C214-C215-C216-C217

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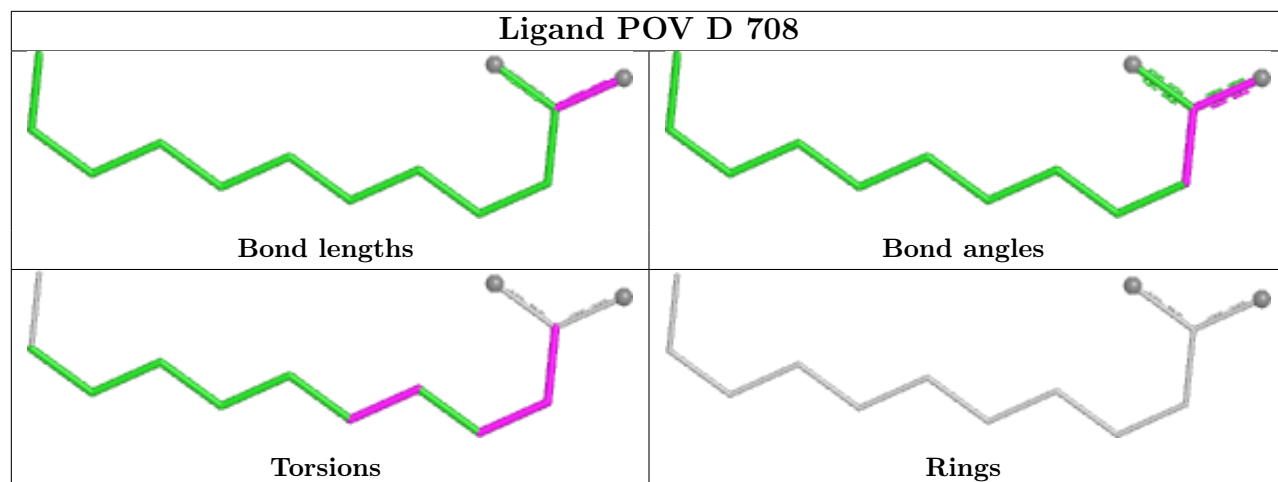
Mol	Chain	Res	Type	Atoms
2	D	702	POV	C214-C215-C216-C217
2	A	701	POV	C27-C28-C29-C210
2	D	701	POV	C27-C28-C29-C210
2	A	701	POV	C29-C210-C211-C212
2	D	701	POV	C29-C210-C211-C212
2	A	706	POV	O22-C21-C22-C23
2	D	706	POV	O22-C21-C22-C23
2	A	706	POV	O21-C21-C22-C23
2	D	706	POV	O21-C21-C22-C23
2	D	703	POV	C24-C25-C26-C27
2	A	703	POV	C24-C25-C26-C27
2	A	708	POV	O21-C21-C22-C23
2	D	708	POV	O21-C21-C22-C23
2	D	708	POV	O22-C21-C22-C23

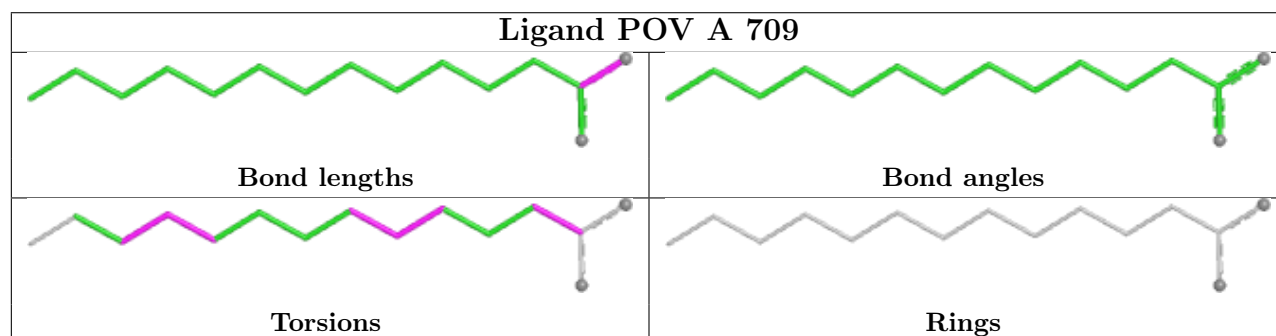
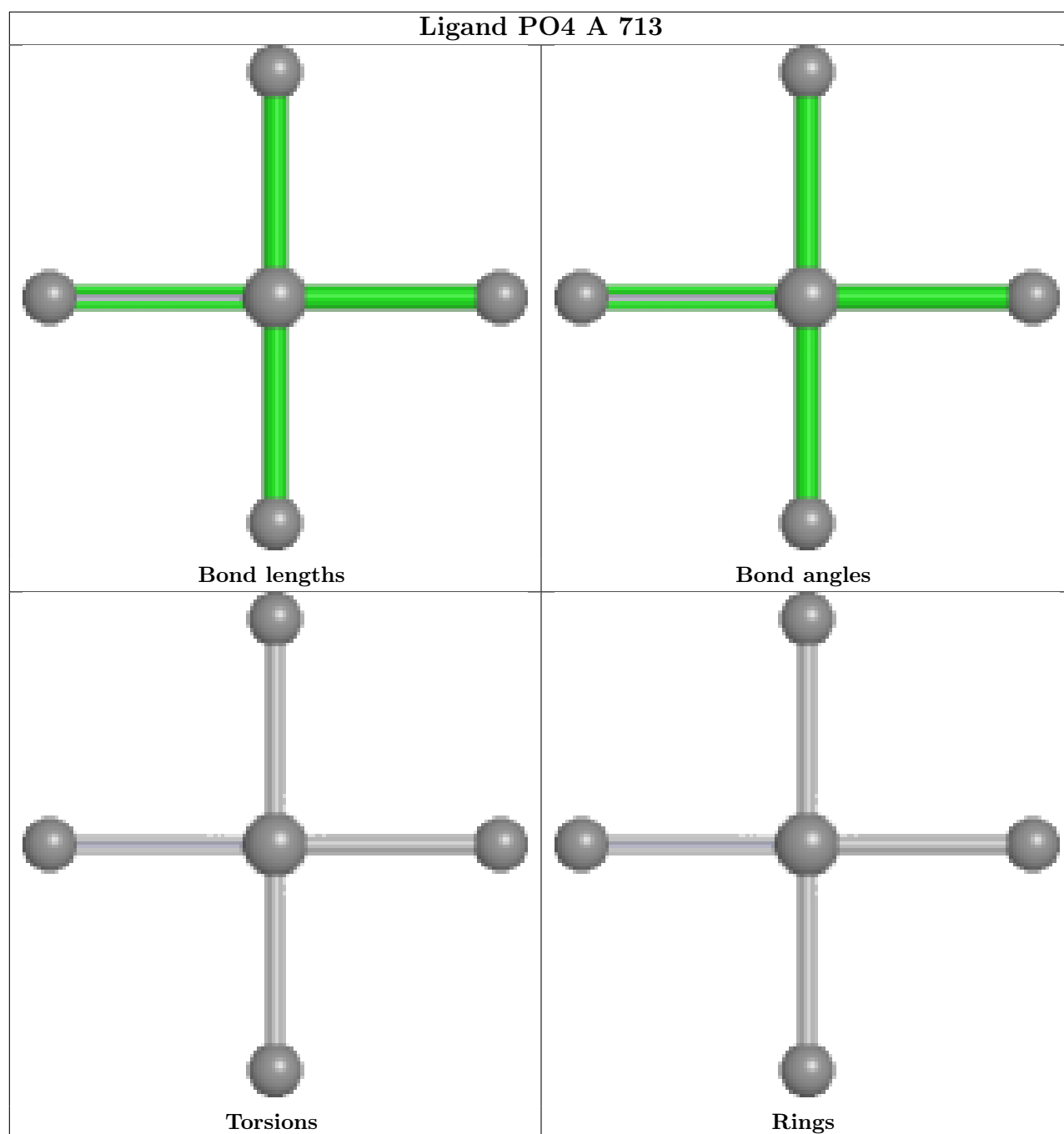
There are no ring outliers.

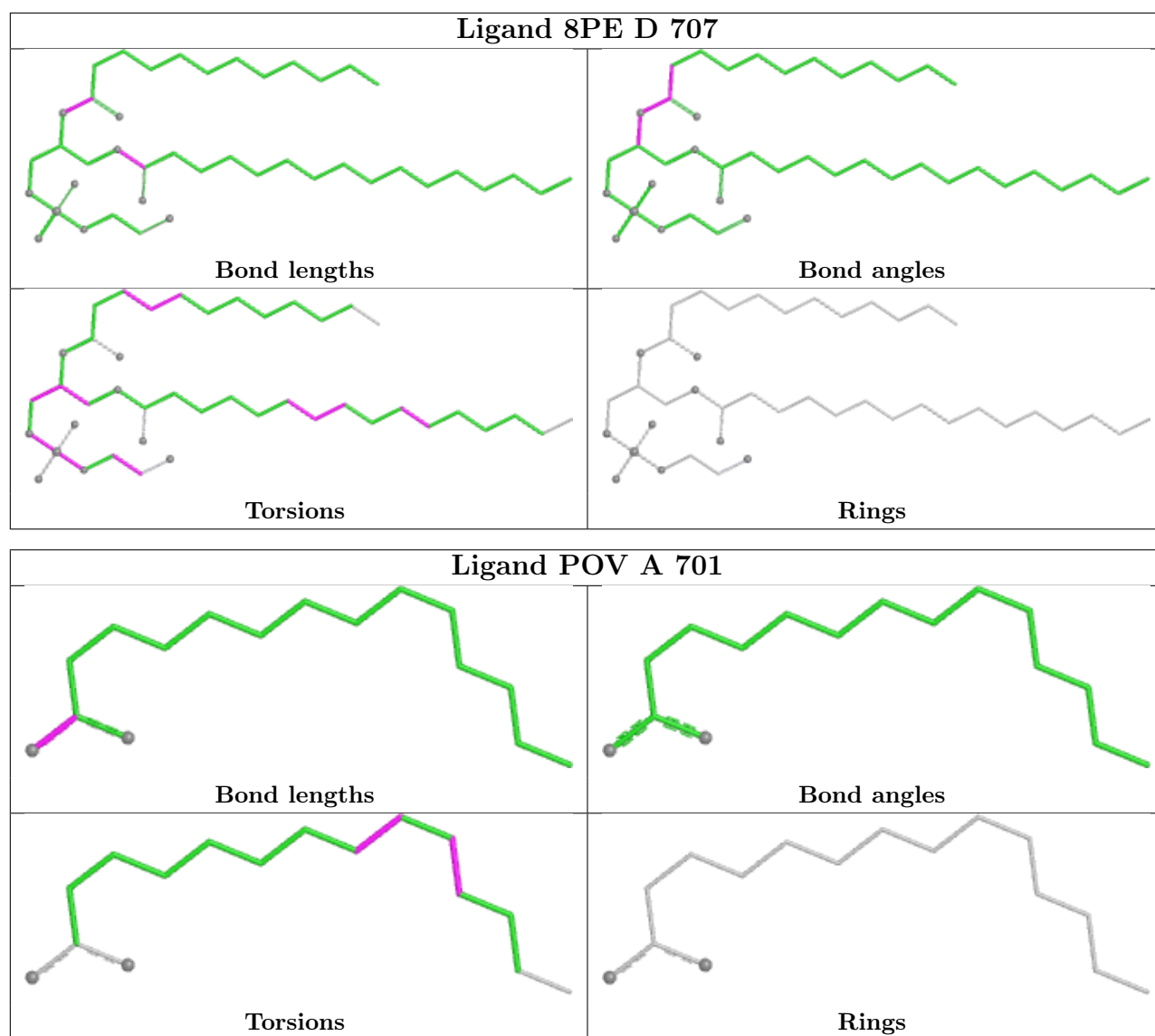
3 monomers are involved in 5 short contacts:

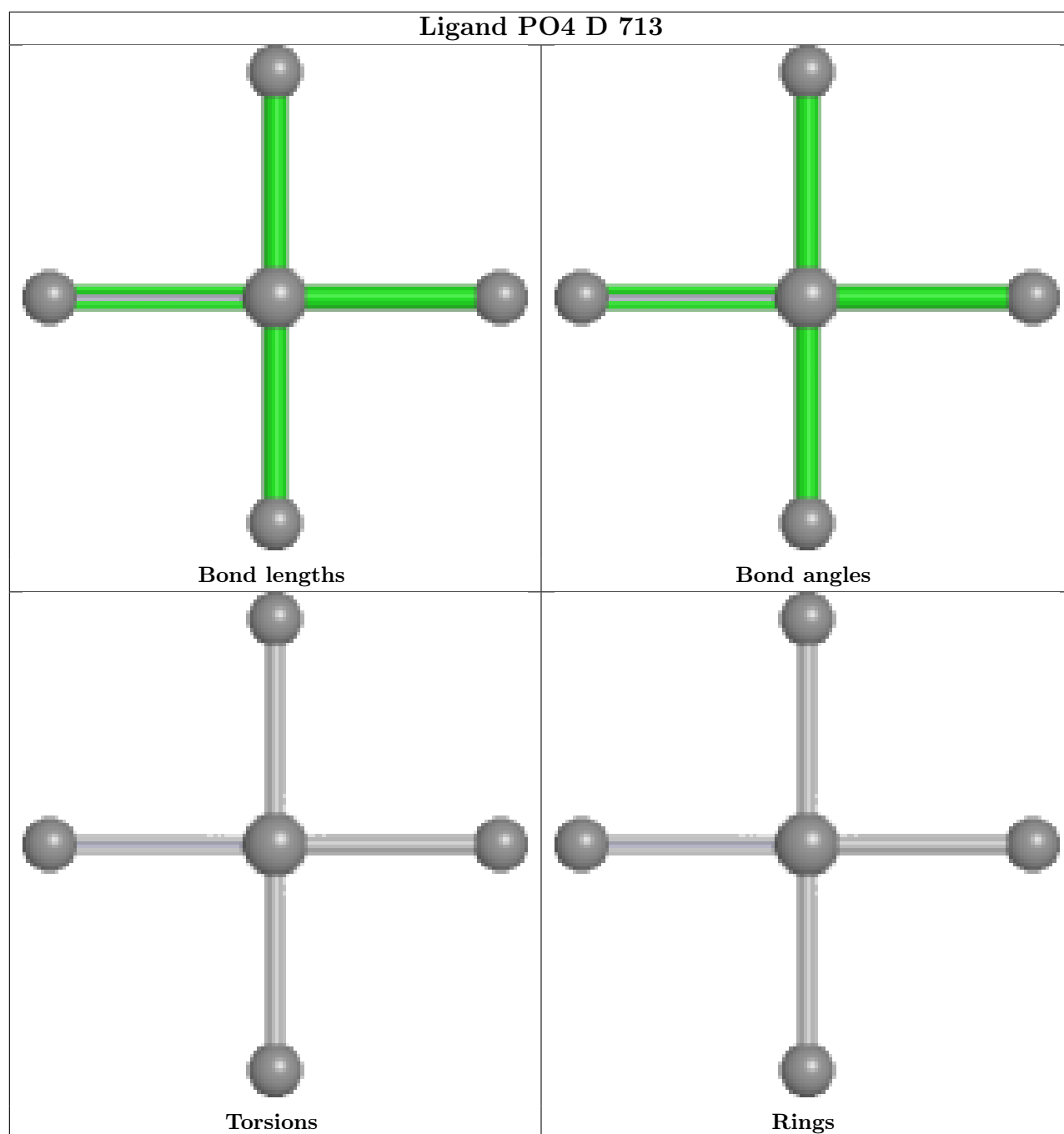
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	713	PO4	2	0
4	D	713	PO4	2	0
2	A	705	POV	1	0

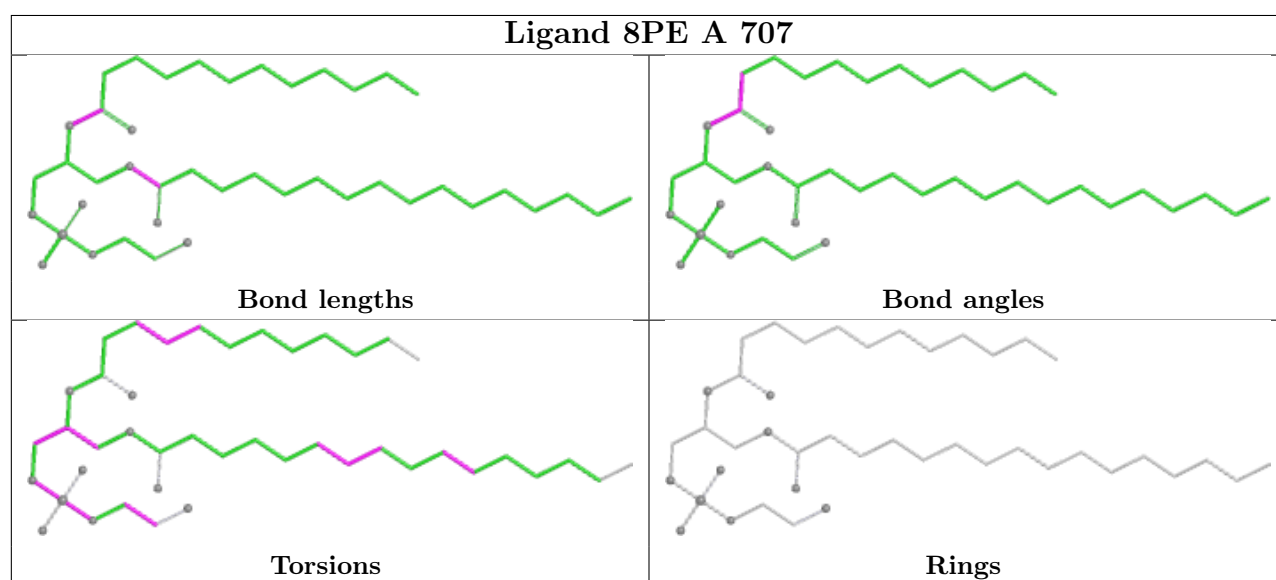
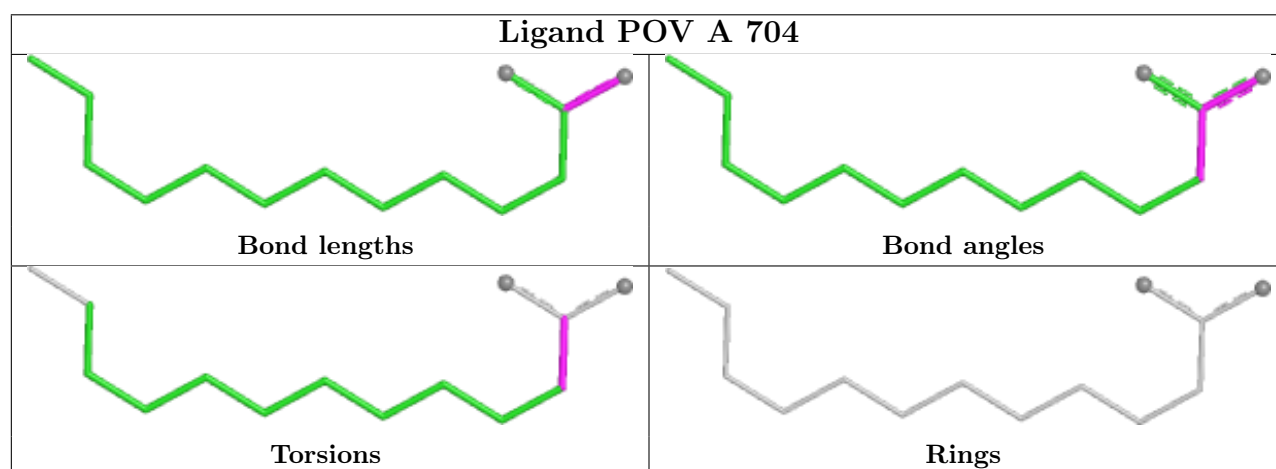
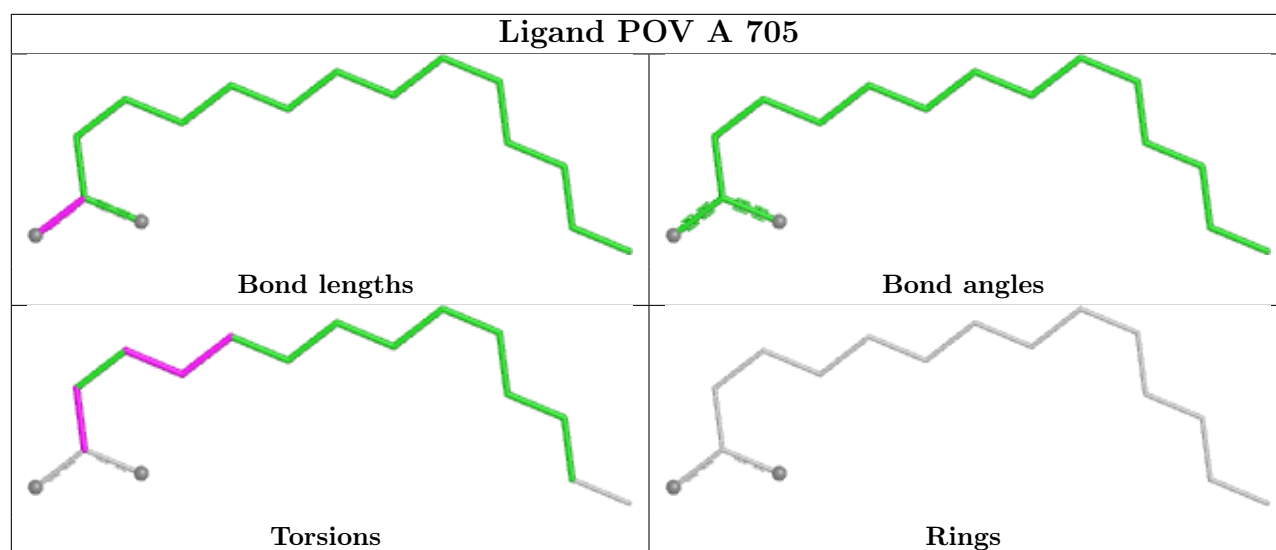
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

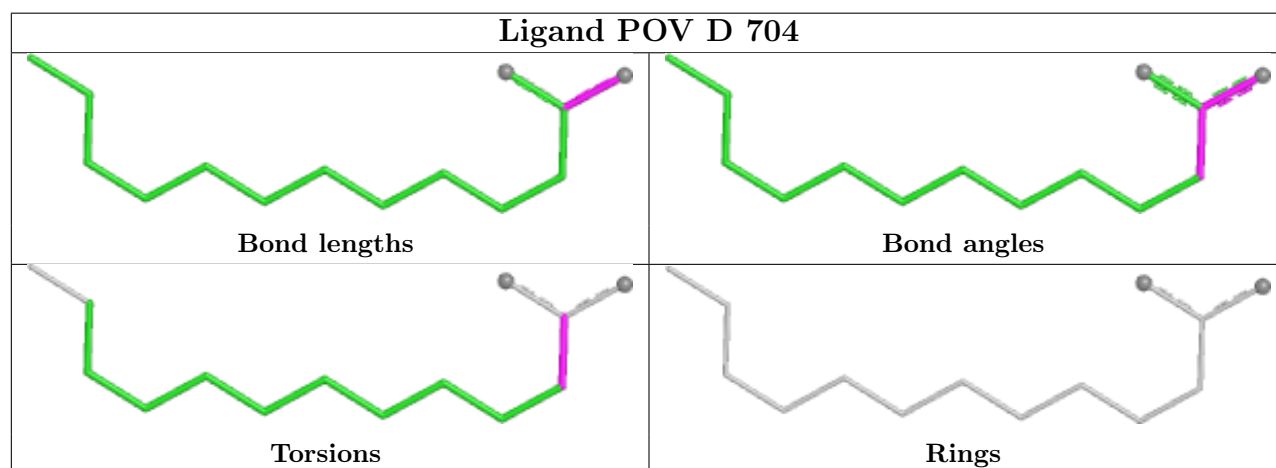
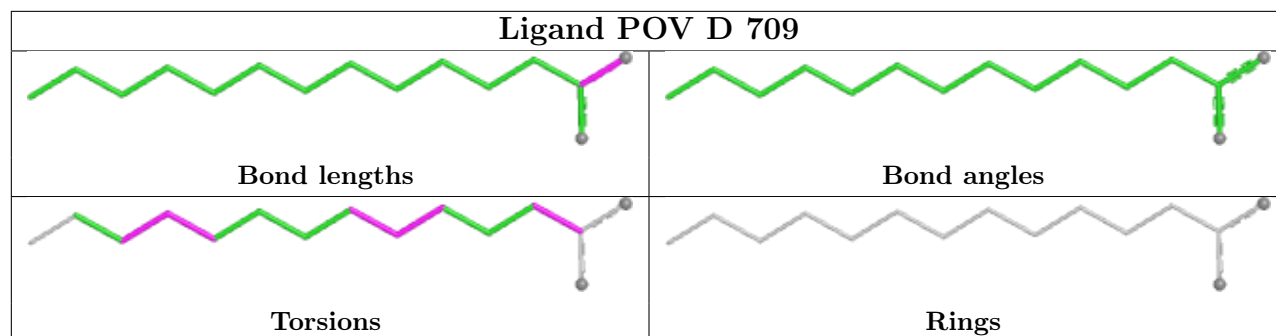


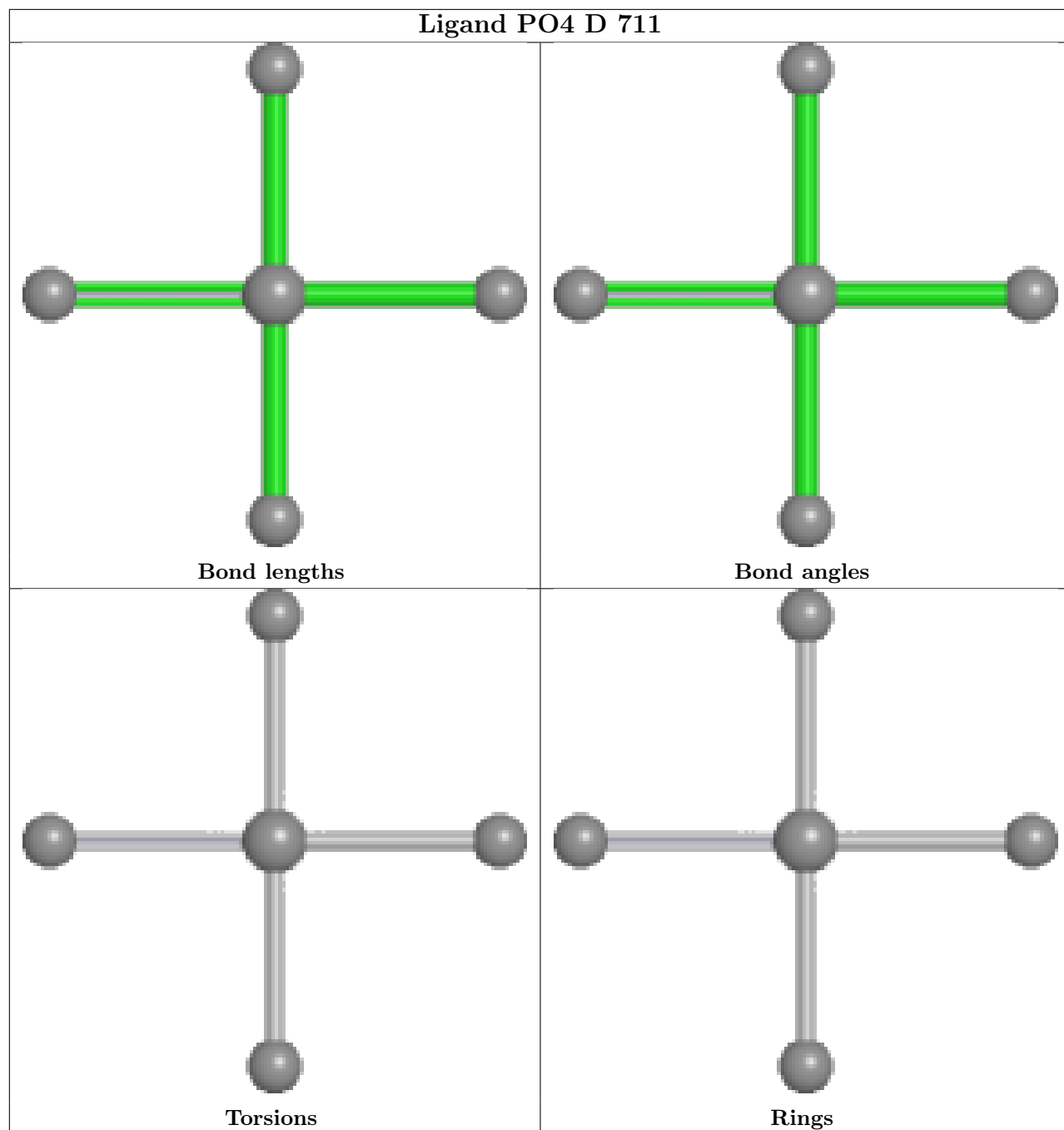


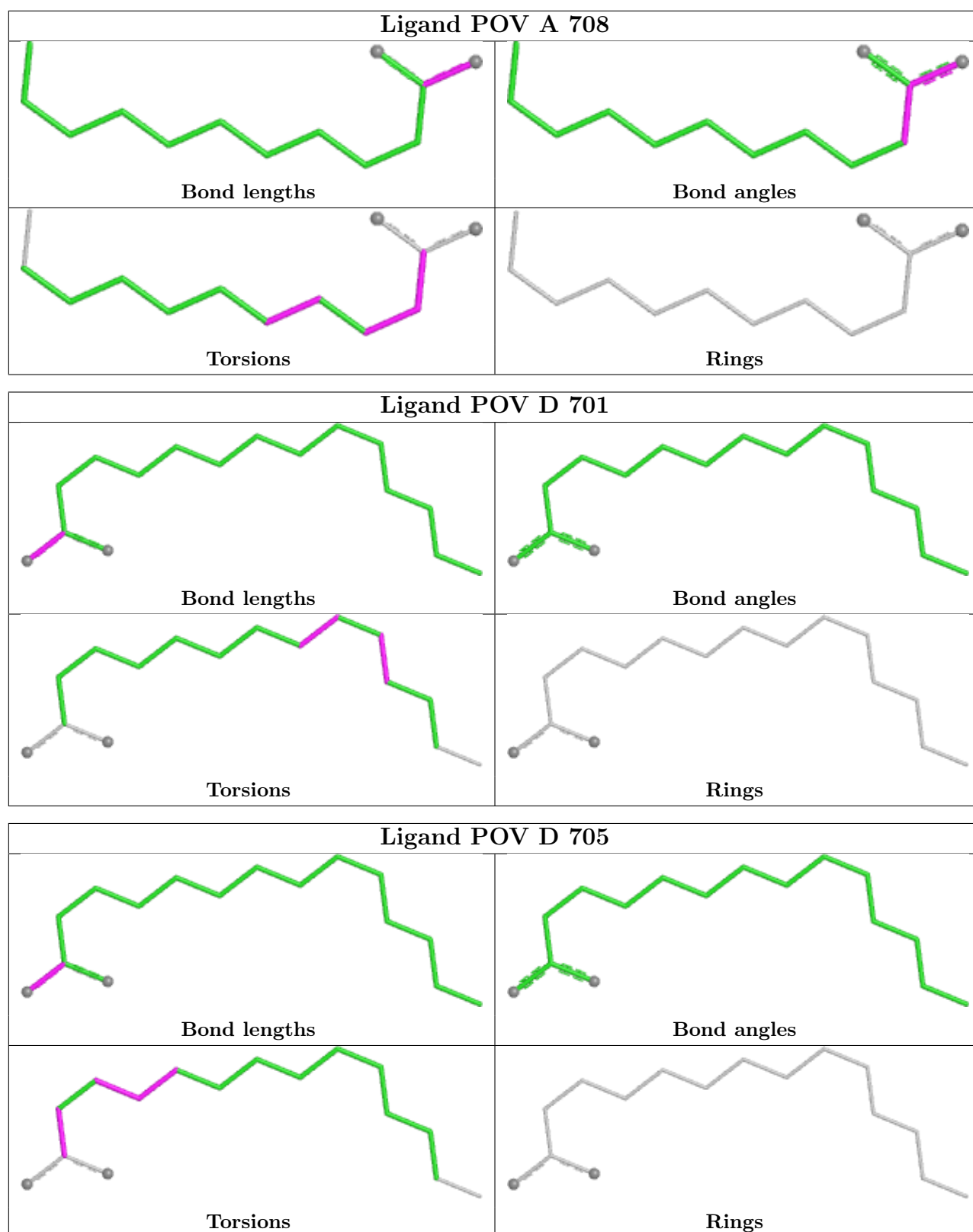


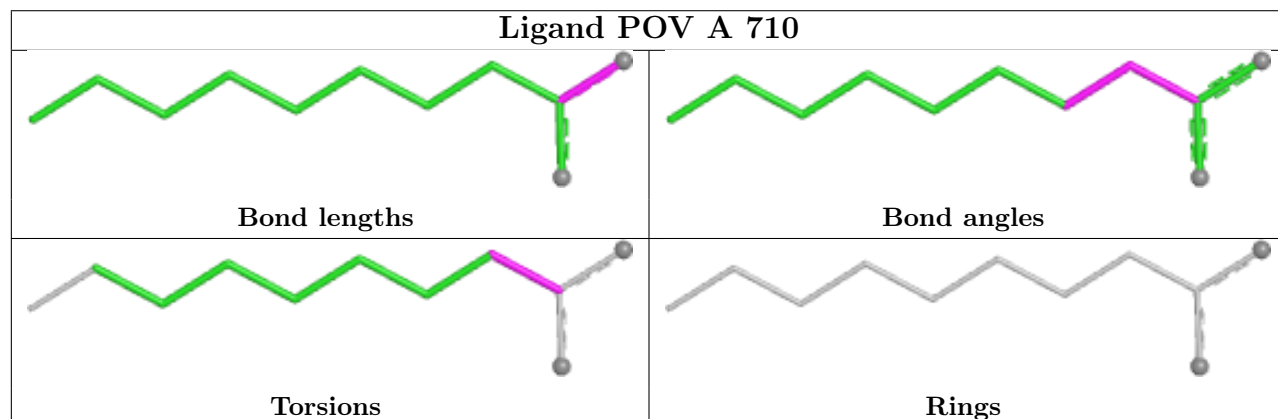
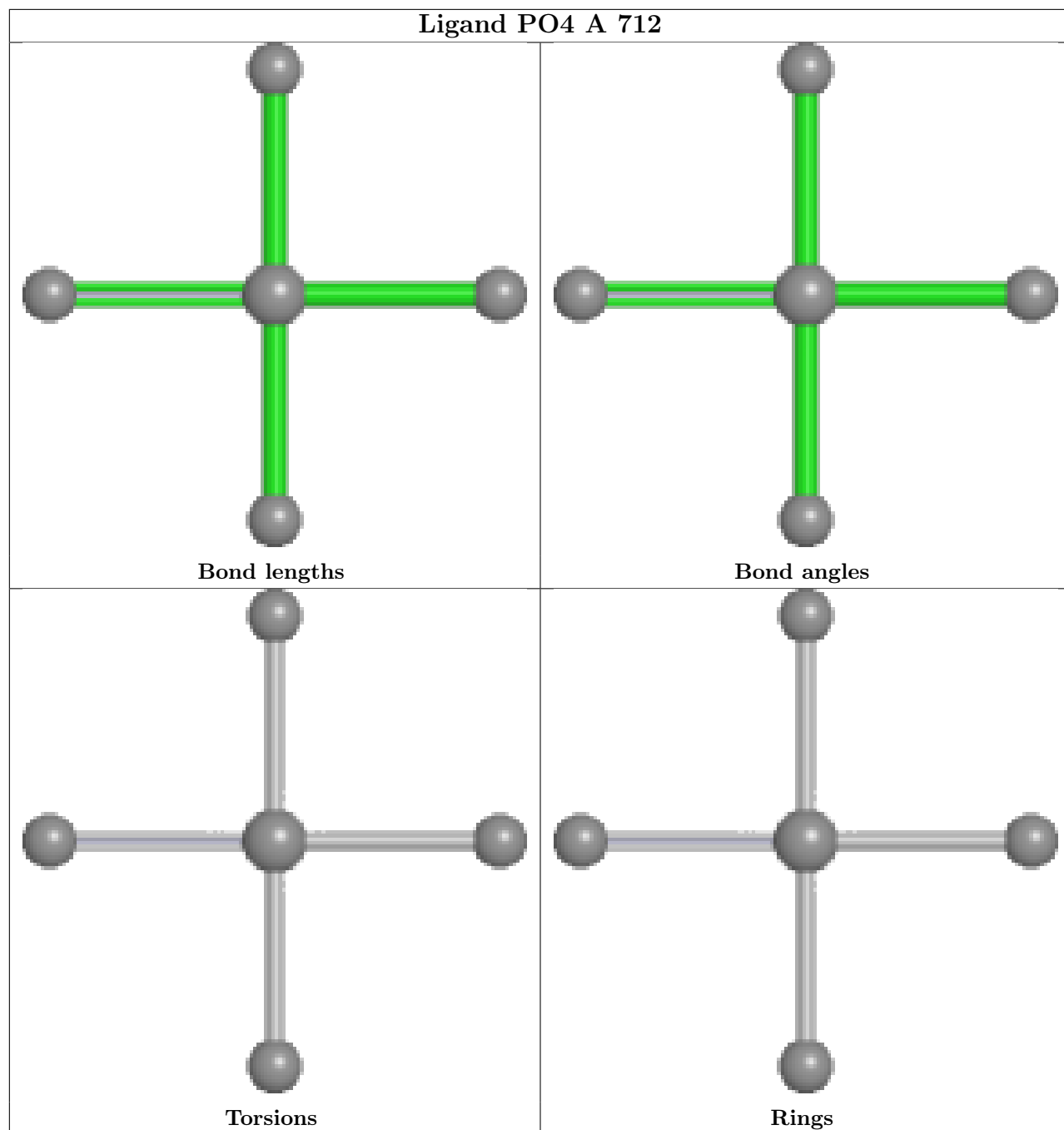


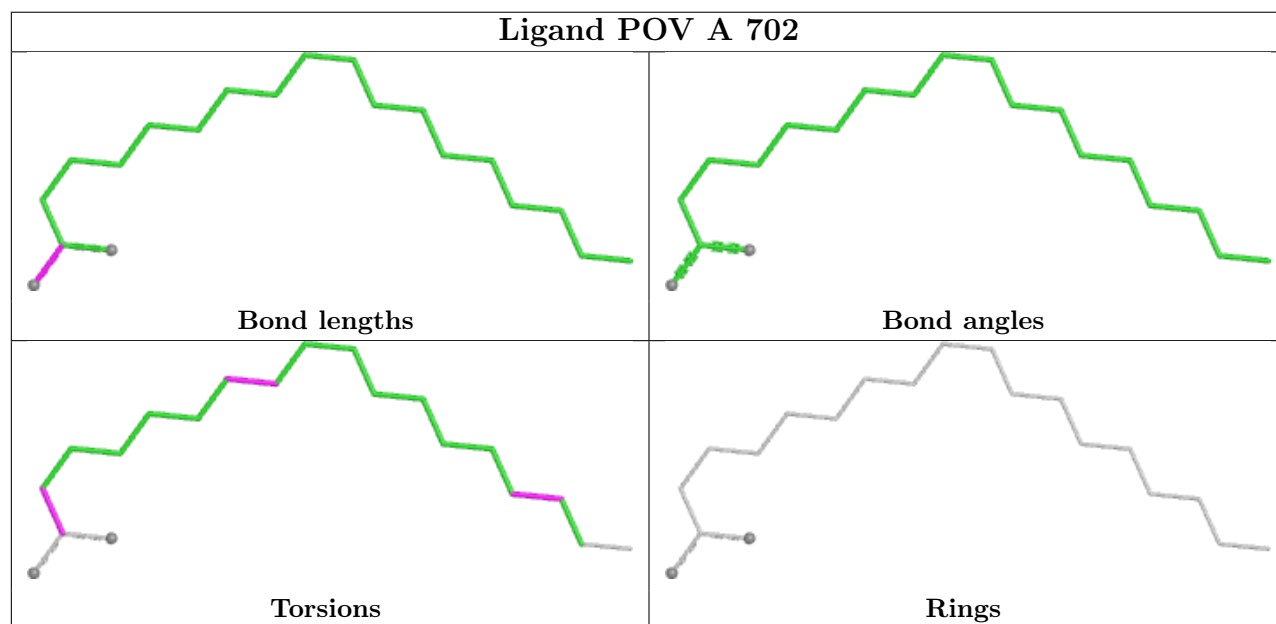
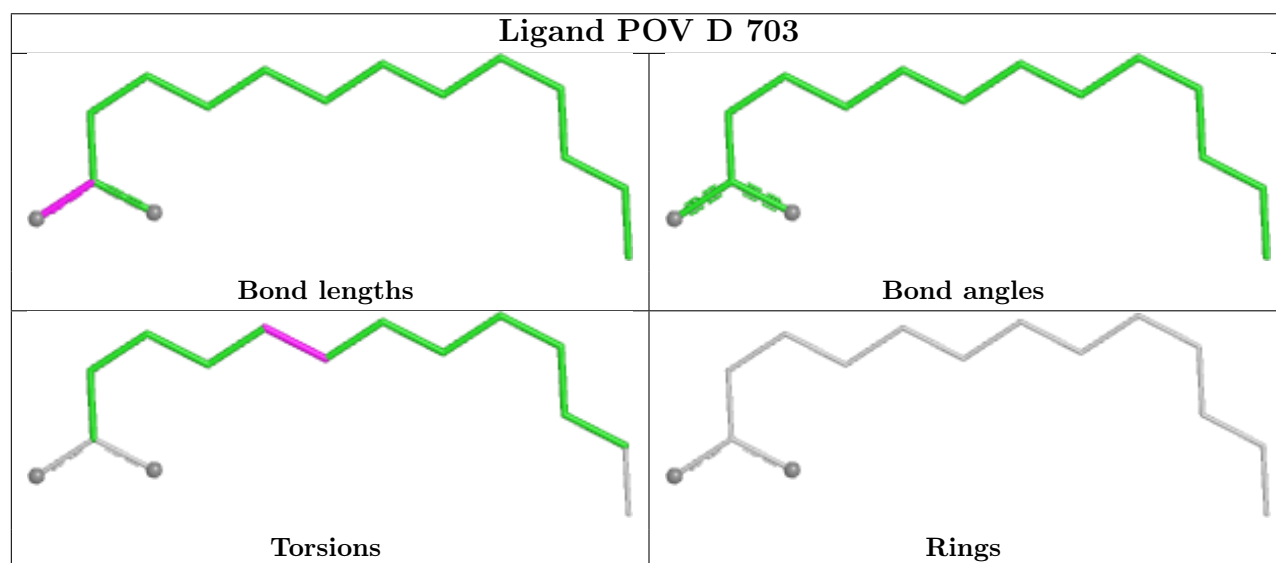
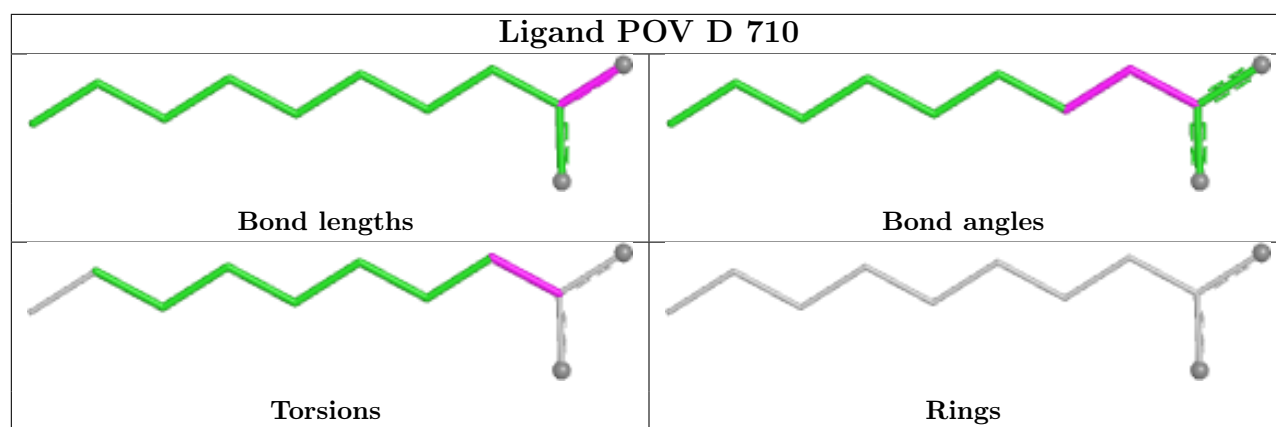


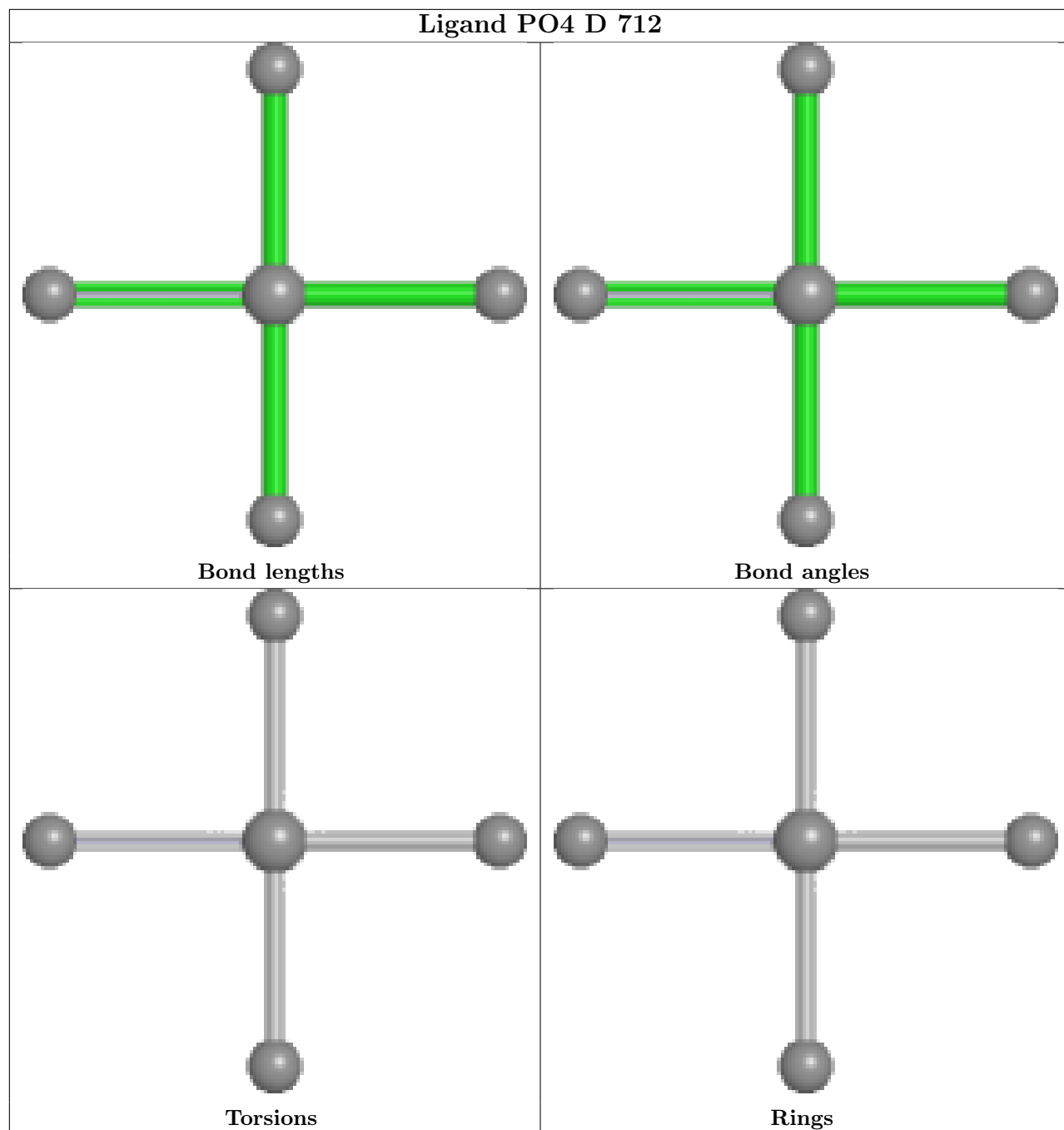


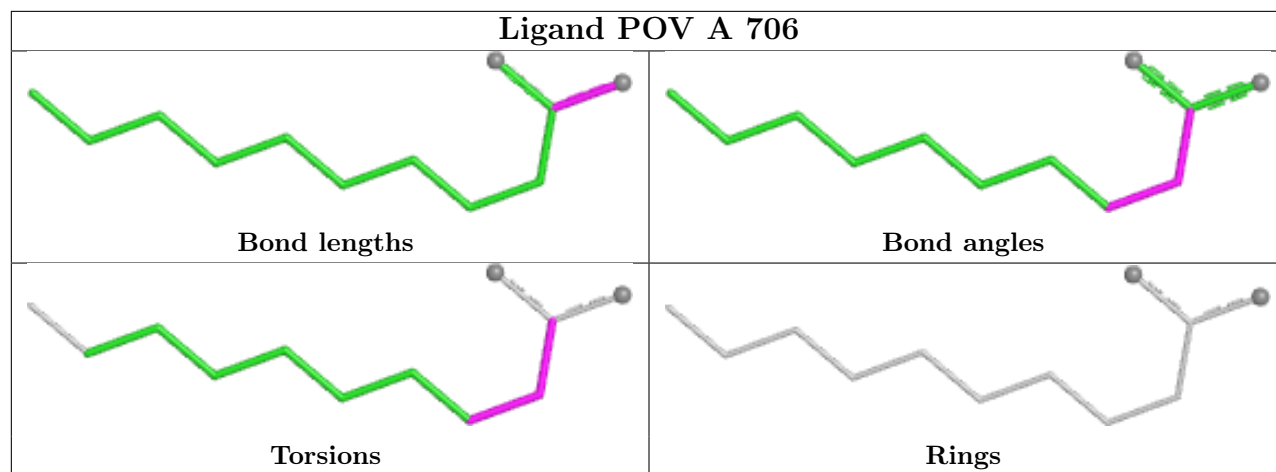


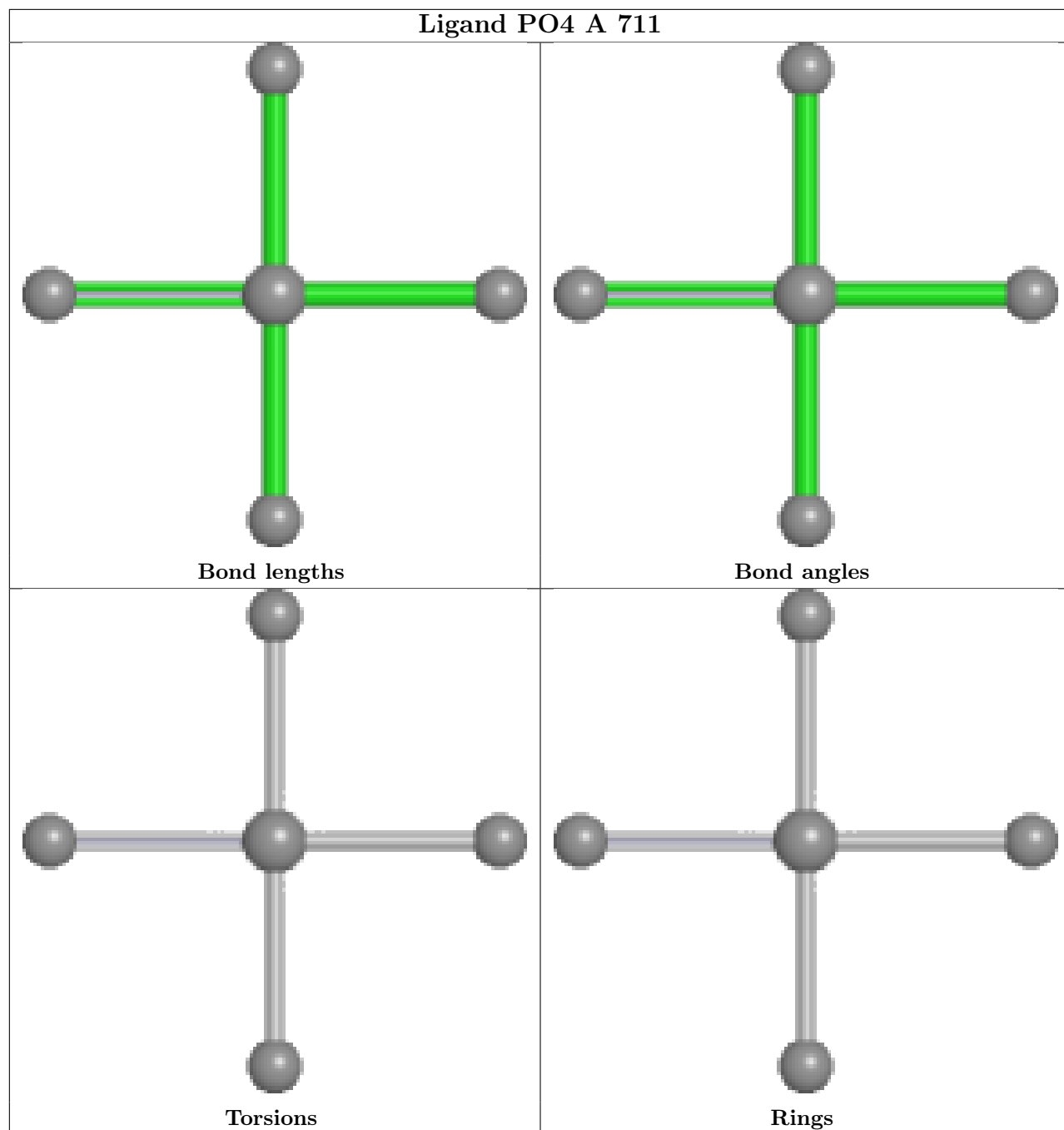


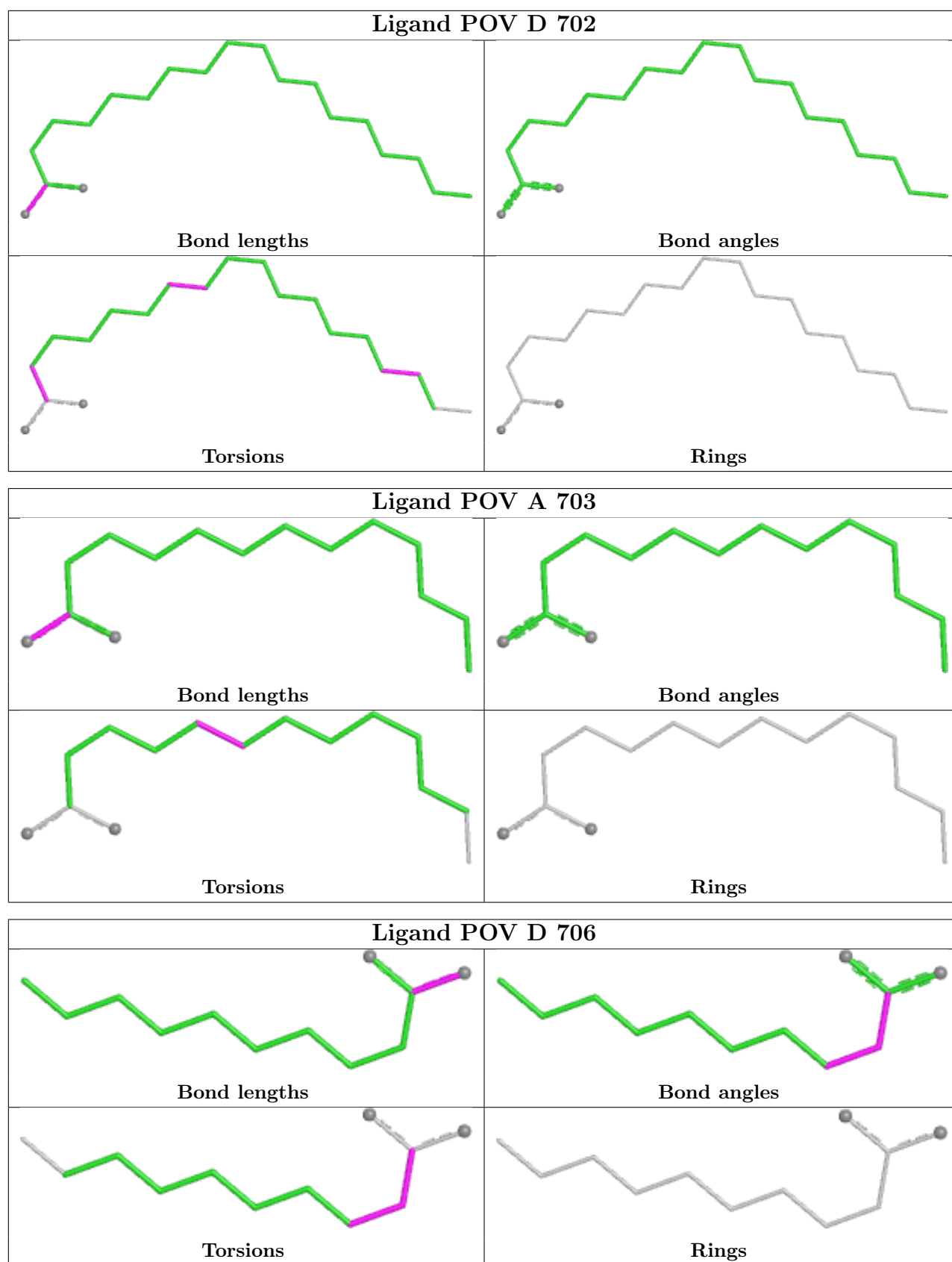












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

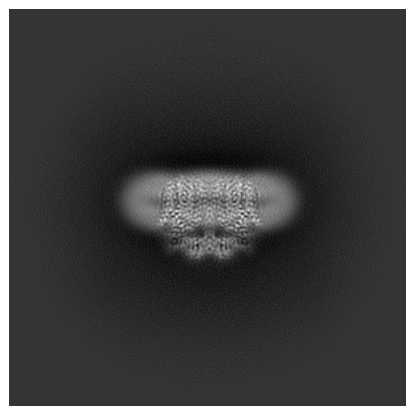
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-65520. These allow visual inspection of the internal detail of the map and identification of artifacts.

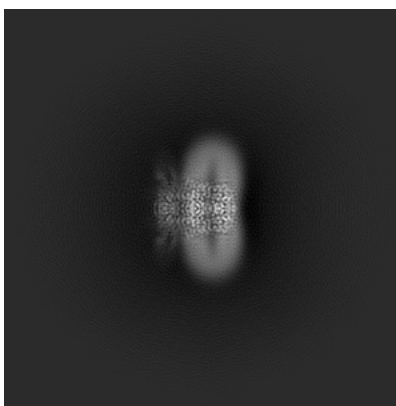
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

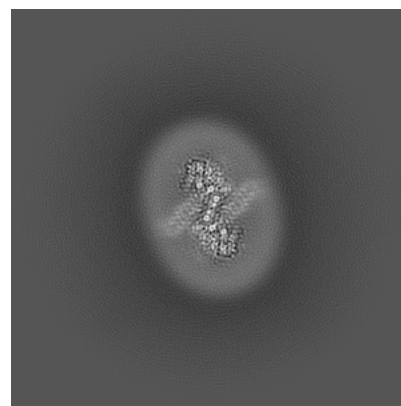
6.1.1 Primary map



X

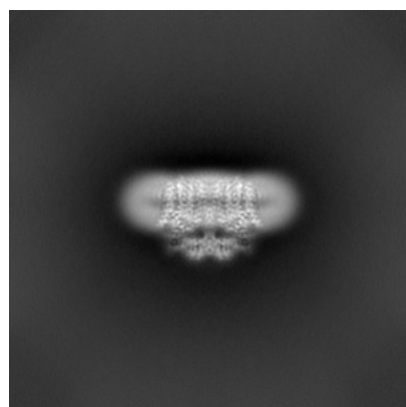


Y

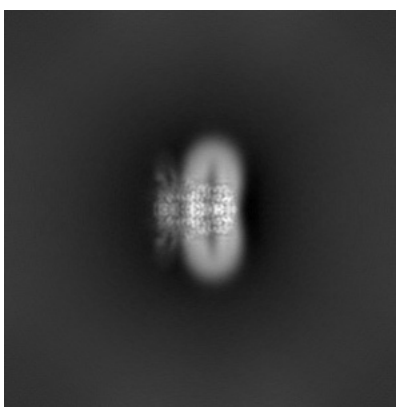


Z

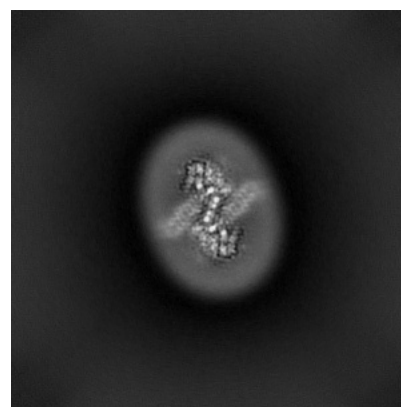
6.1.2 Raw map



X



Y

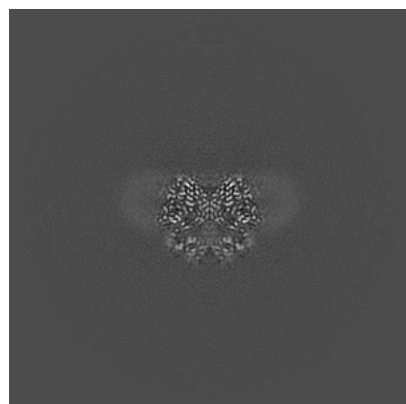


Z

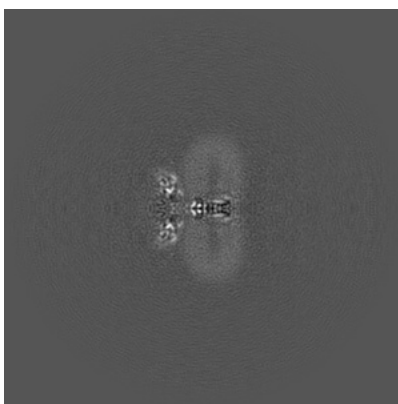
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

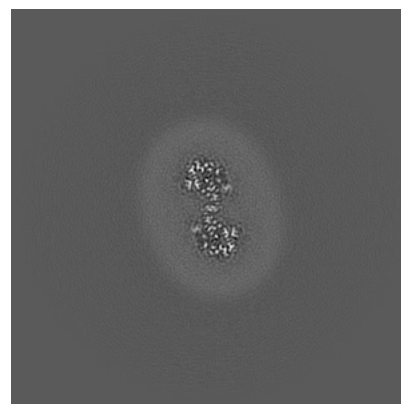
6.2.1 Primary map



X Index: 180

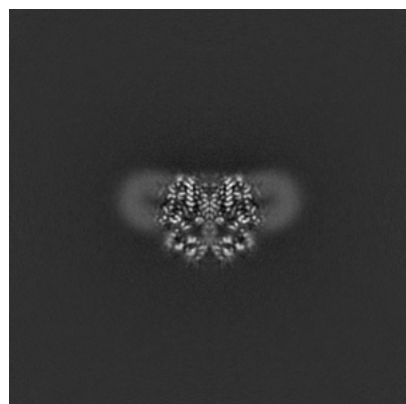


Y Index: 180

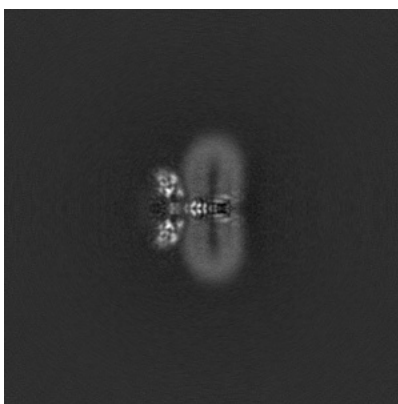


Z Index: 180

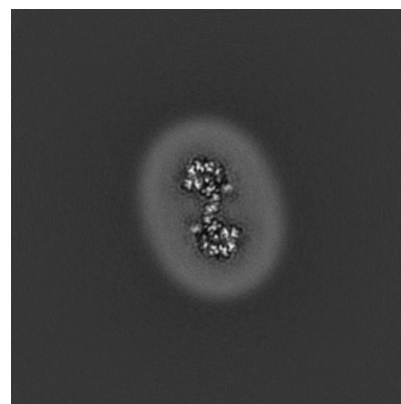
6.2.2 Raw map



X Index: 180



Y Index: 180

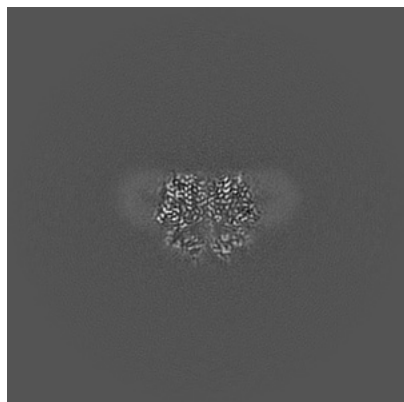


Z Index: 180

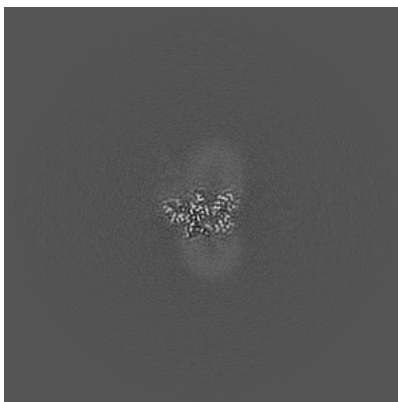
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

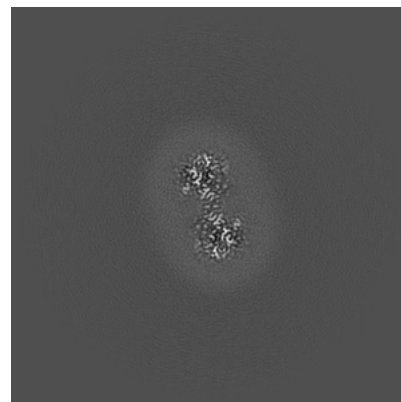
6.3.1 Primary map



X Index: 181

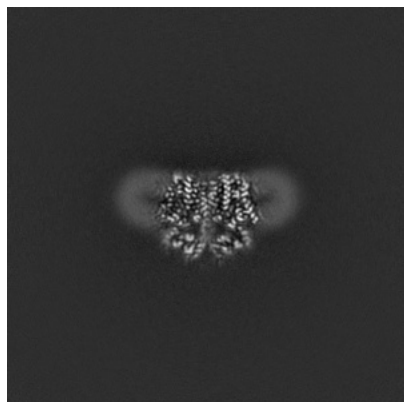


Y Index: 207

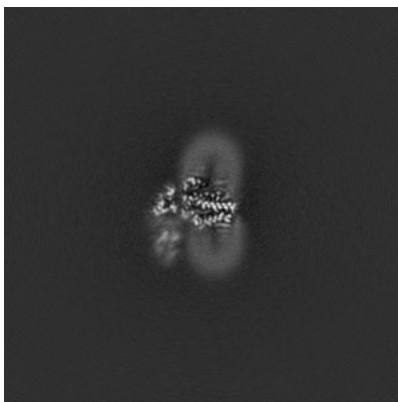


Z Index: 170

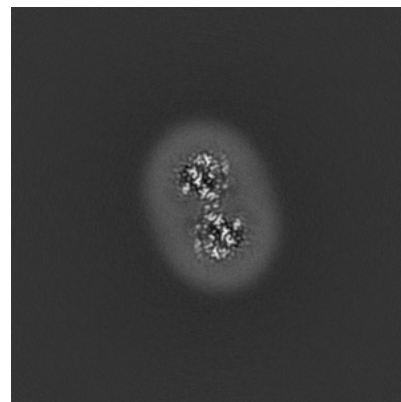
6.3.2 Raw map



X Index: 179



Y Index: 163

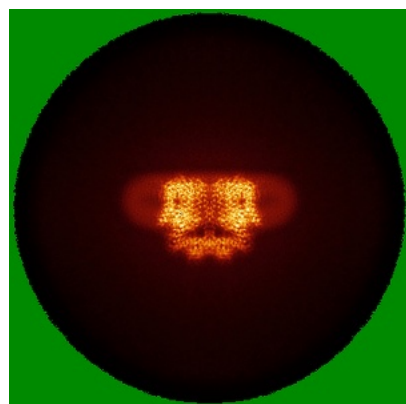


Z Index: 170

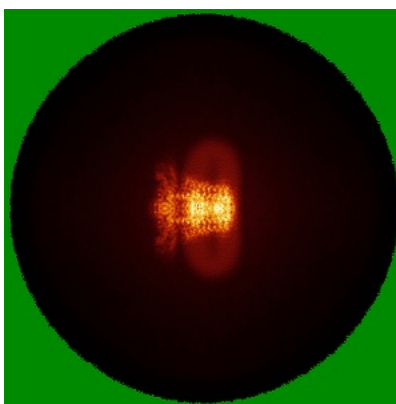
The images above show the largest variance slices of the map in three orthogonal directions.

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

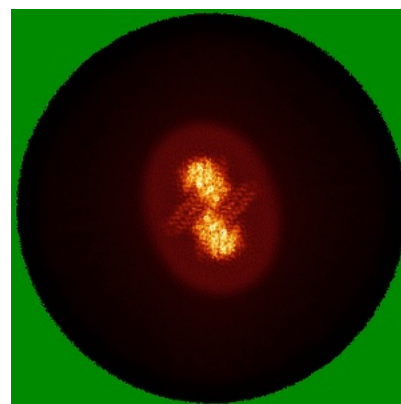
6.4.1 Primary map



X

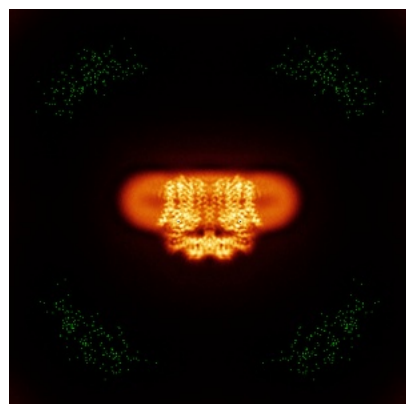


Y

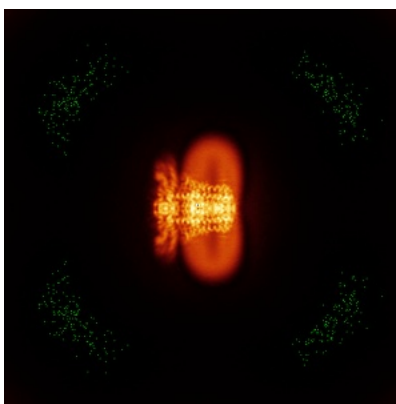


Z

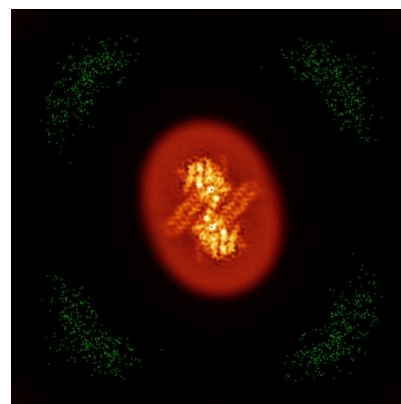
6.4.2 Raw map



X



Y

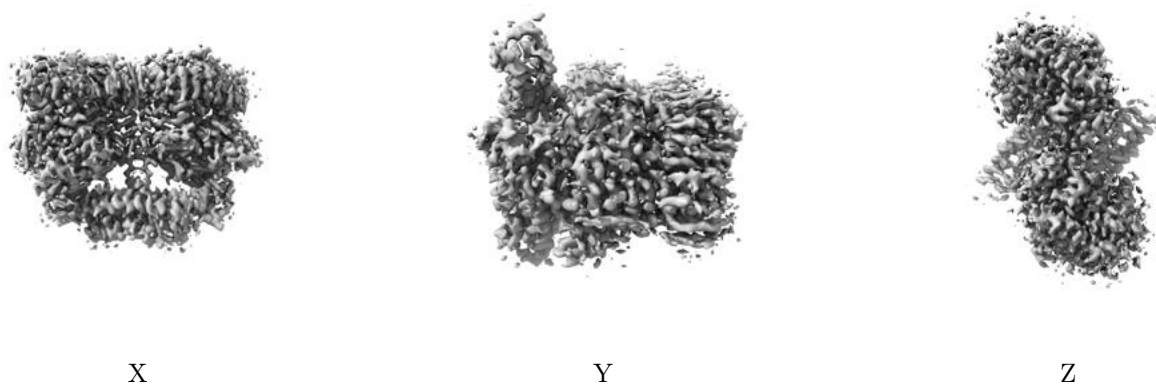


Z

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.

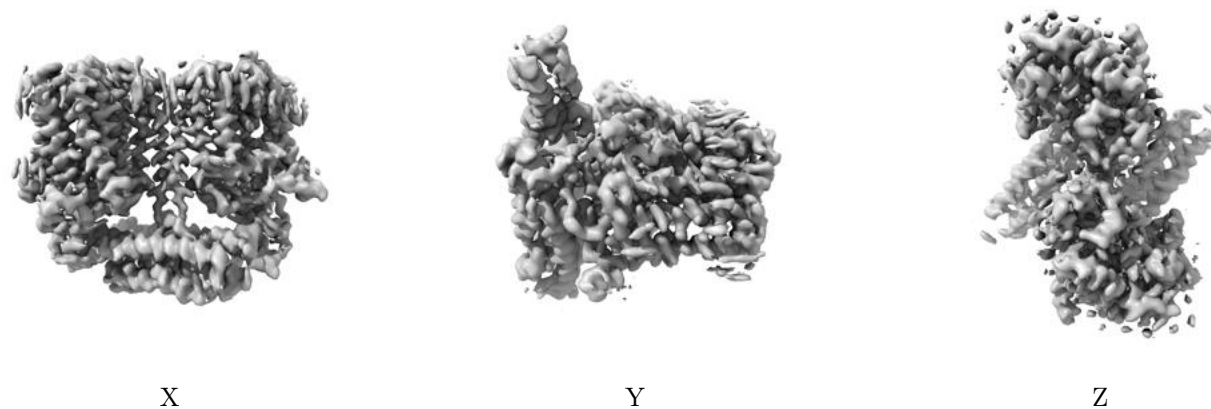
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.739. 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.

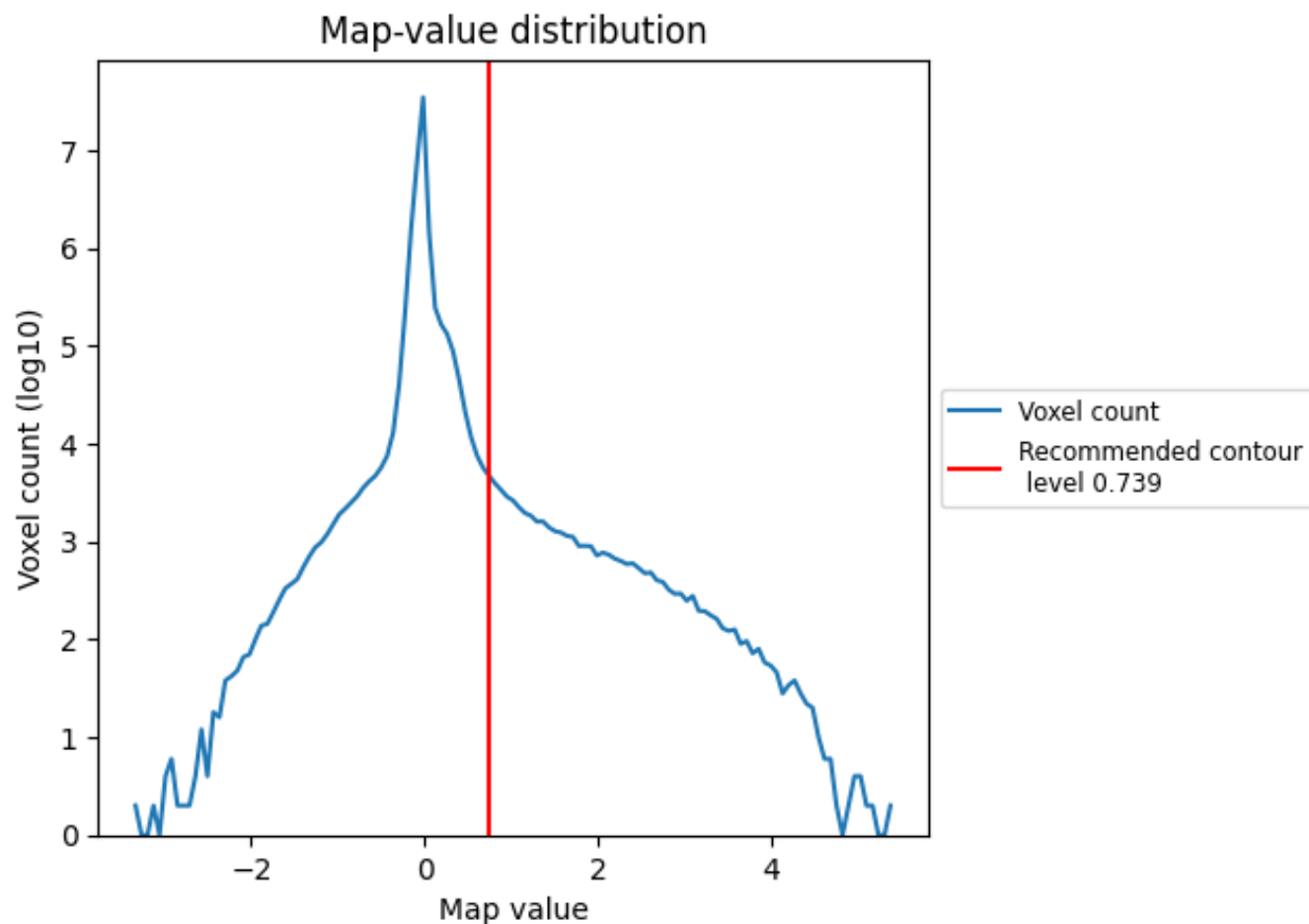
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

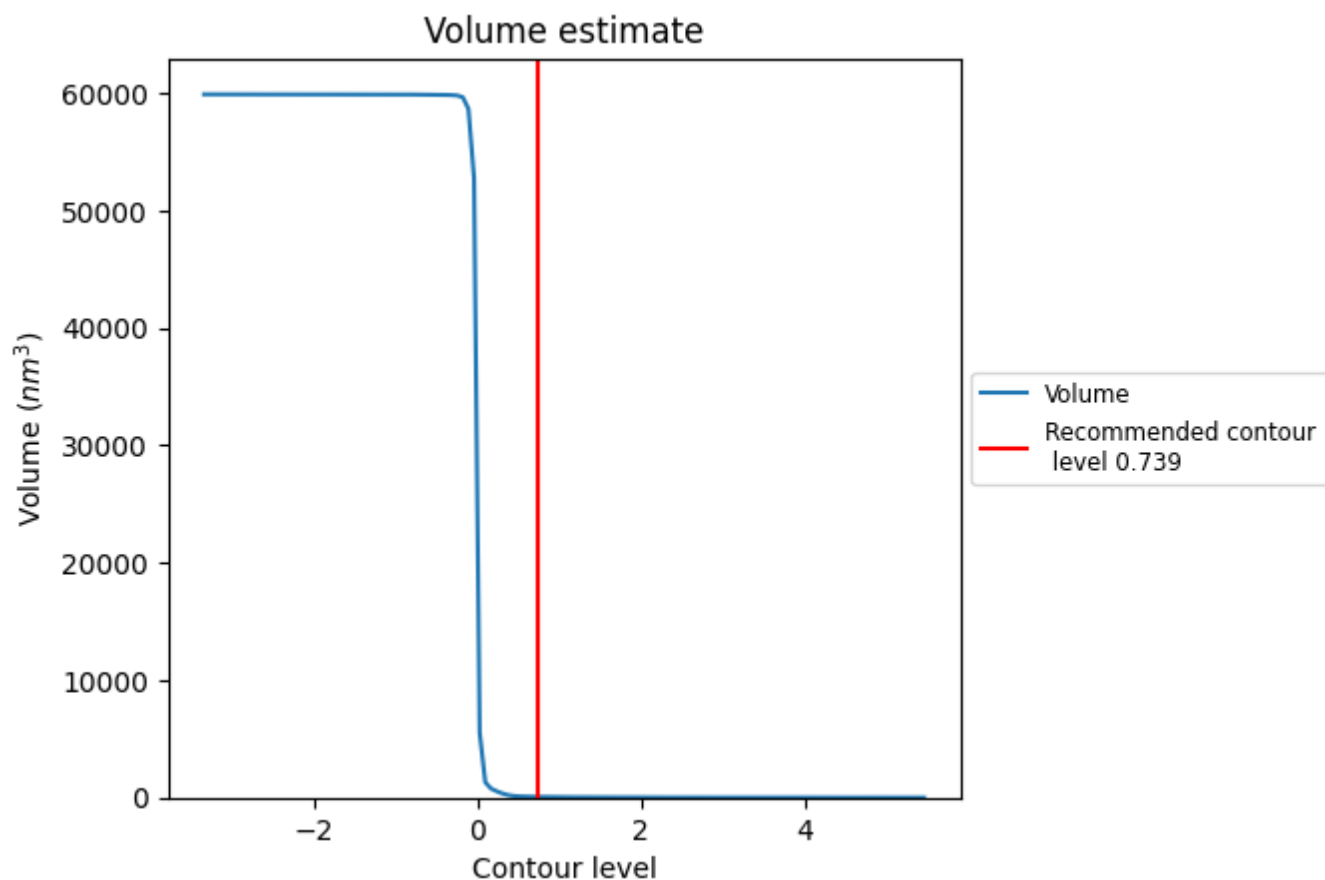
This section contains the results of statistical analysis of the map.

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.

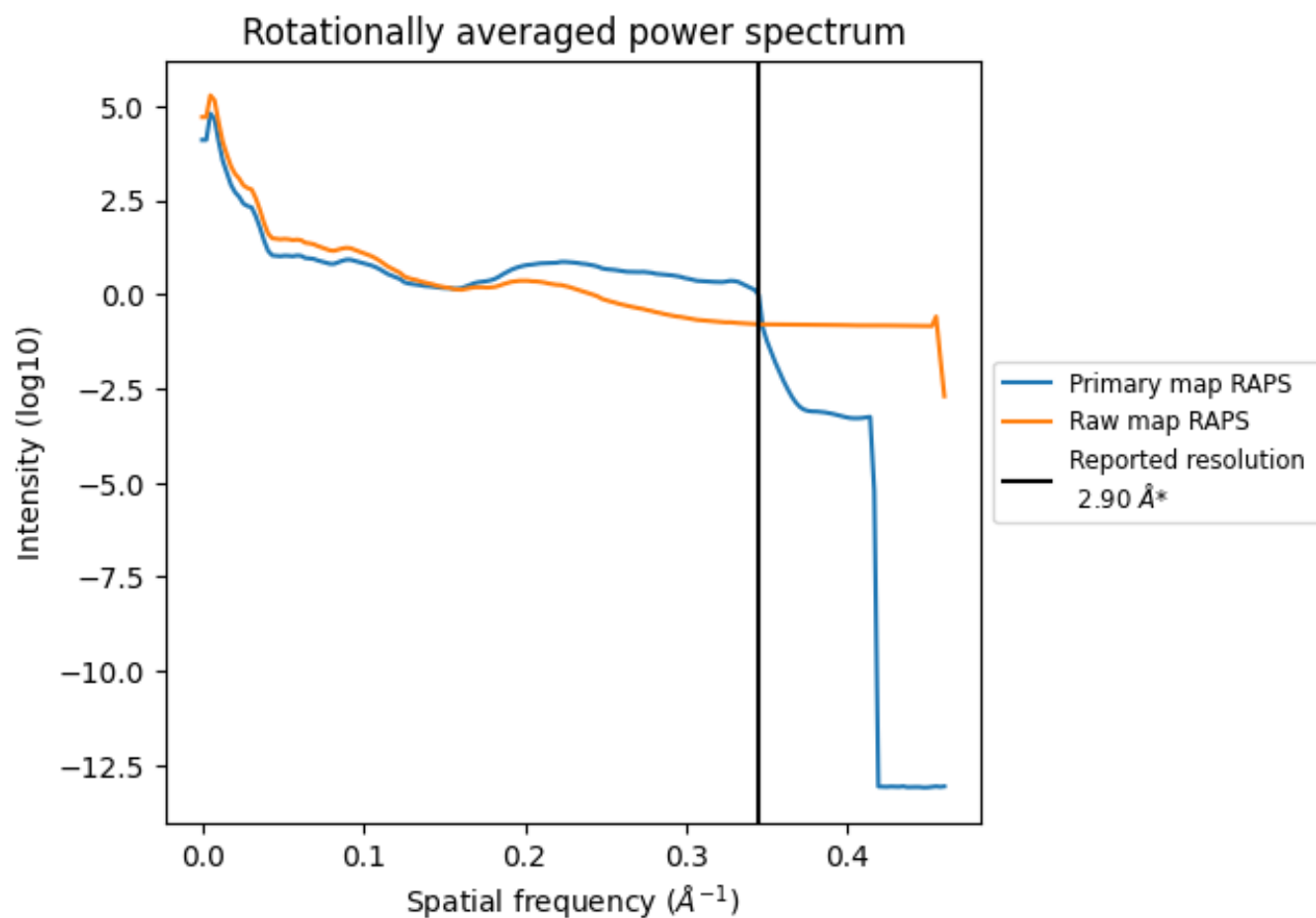
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 60 nm³; this corresponds to an approximate mass of 54 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 ⓘ

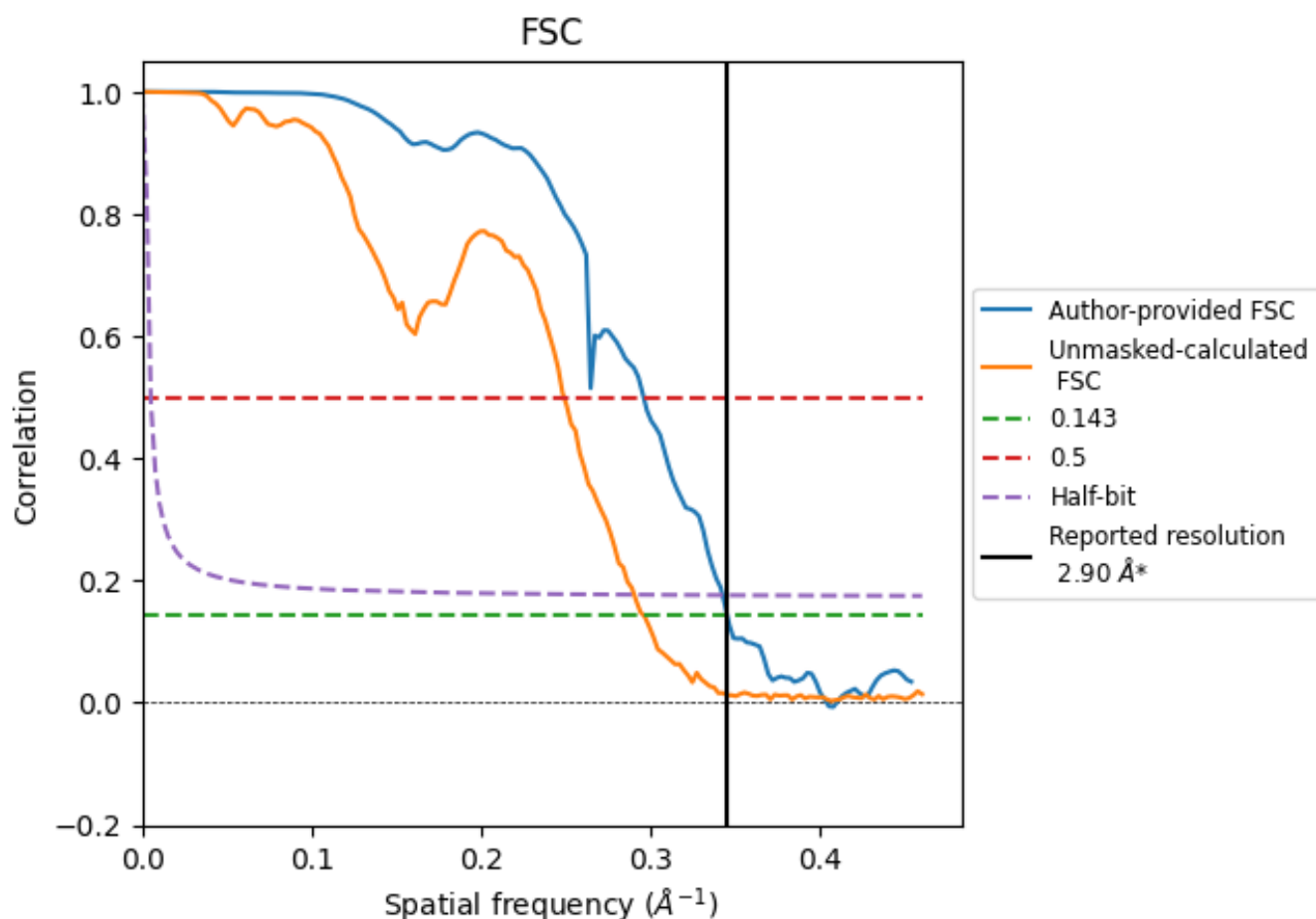


*Reported resolution corresponds to spatial frequency of 0.345 \AA^{-1}

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 0.345 \AA^{-1}

8.2 Resolution estimates [i](#)

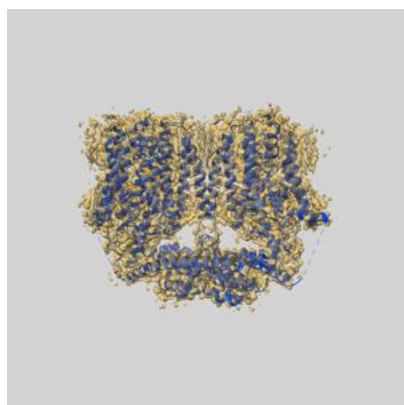
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.90	3.38	2.92
Unmasked-calculated*	3.38	4.02	3.45

*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 3.38 differs from the reported value 2.9 by more than 10 %

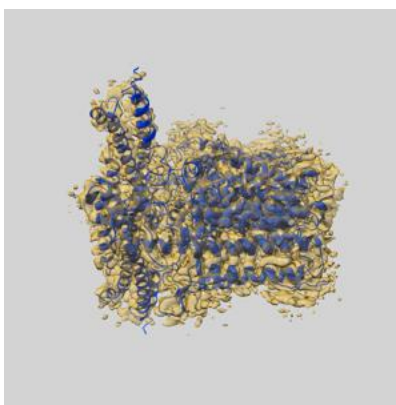
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-65520 and PDB model 9W0X. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

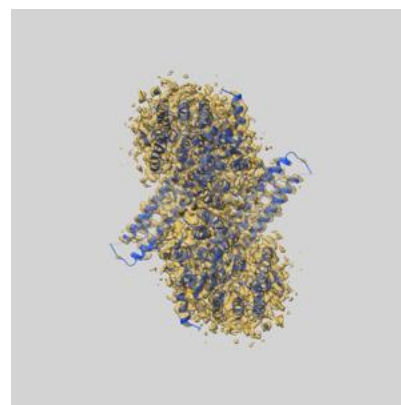
9.1 Map-model overlay [i](#)



X



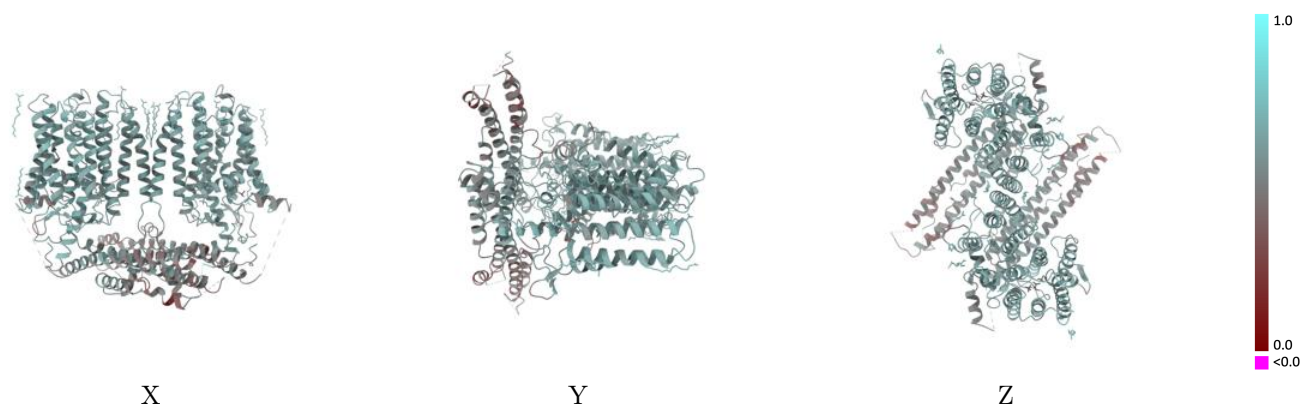
Y



Z

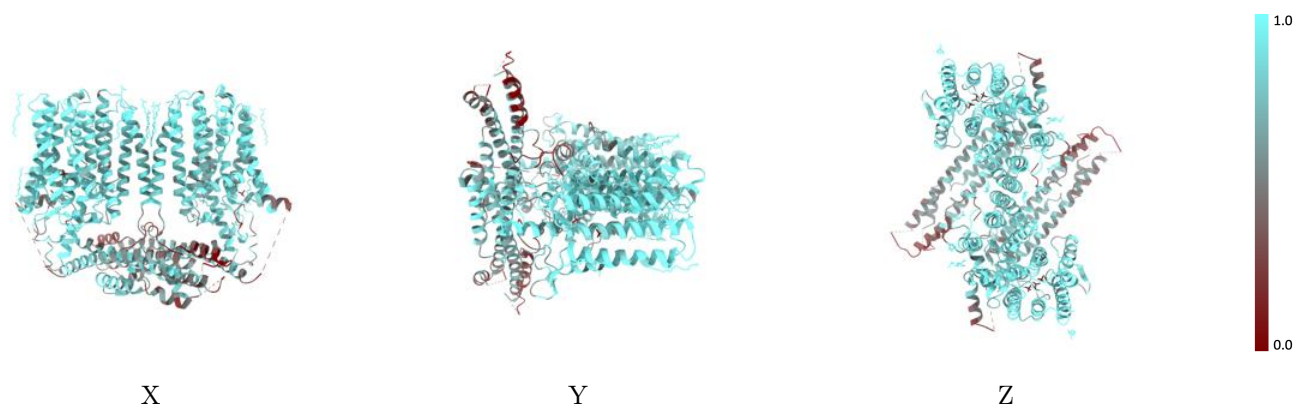
The images above show the 3D surface view of the map at the recommended contour level 0.739 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



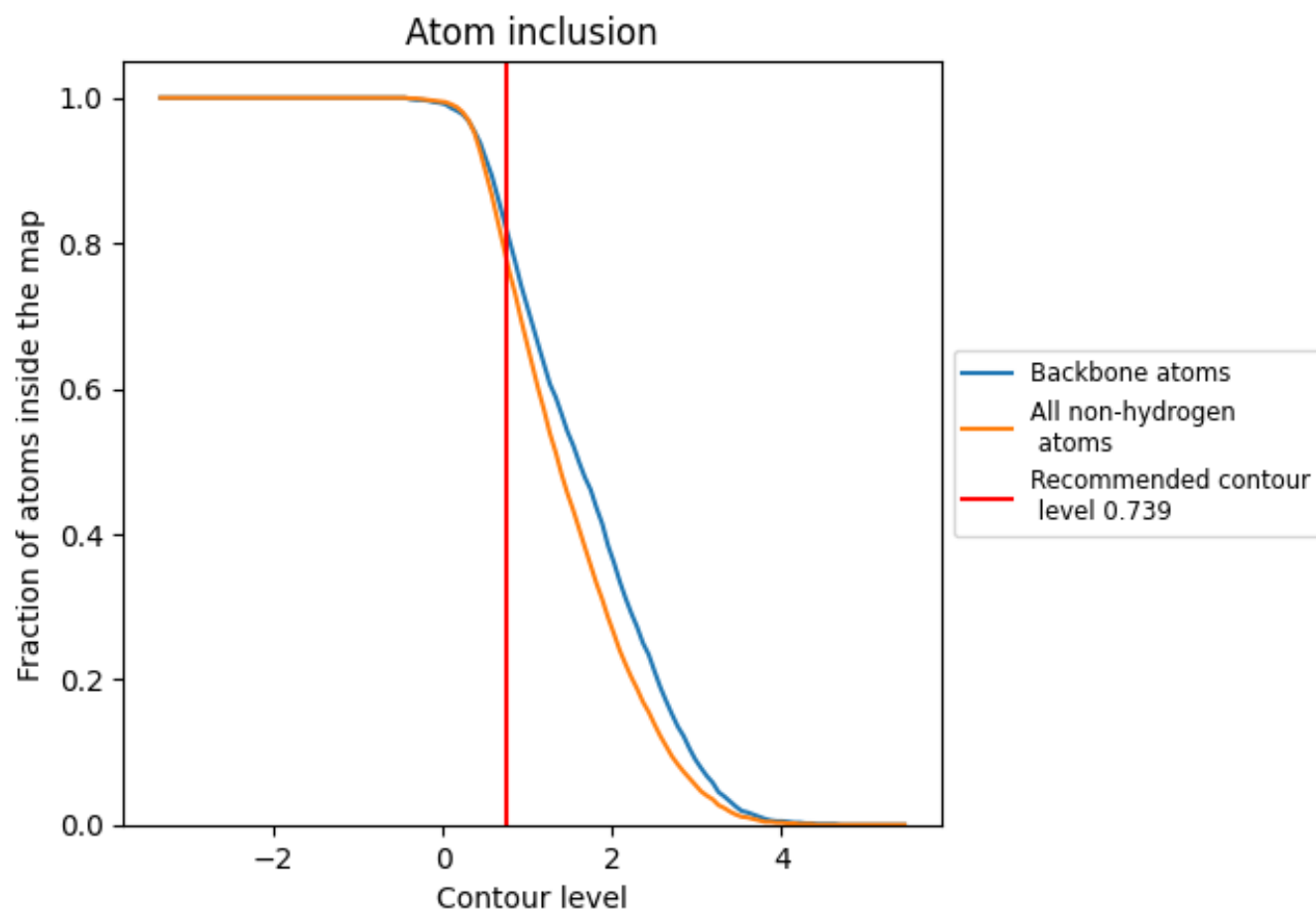
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.739).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 78% 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 (0.739) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7830	<div></div> 0.5630
A	<div></div> 0.7830	<div></div> 0.5620
D	<div></div> 0.7830	<div></div> 0.5630

