



Full wwPDB EM Validation Report ⓘ

Mar 26, 2025 – 03:02 PM JST

PDB ID : 9INH
EMDB ID : EMD-60707
Title : Cryo-EM structure of human XPR1 in complex with InsP6 in outward-facing state (SPX visible)-in the presence of KIDINS220-1-432 and 10 mM KH₂PO₄
Authors : Zuo, P.; Liang, L.; Yin, Y.
Deposited on : 2024-07-06
Resolution : 3.68 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.dev117
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41.2

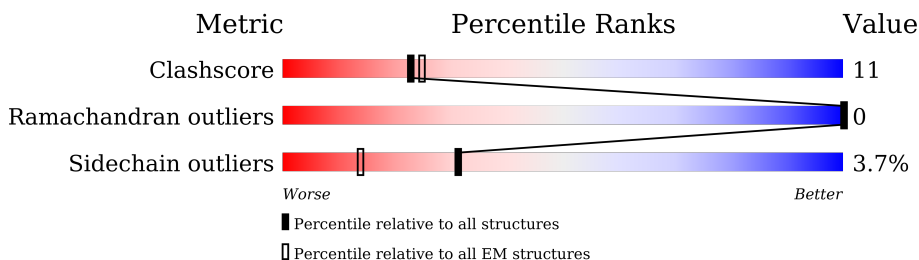
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.68 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	704	<div> <div>17%</div> <div>61%</div> <div>24%</div> <div>•</div> <div>14%</div> </div>
1	D	704	<div> <div>17%</div> <div>63%</div> <div>23%</div> <div>•</div> <div>13%</div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10933 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.

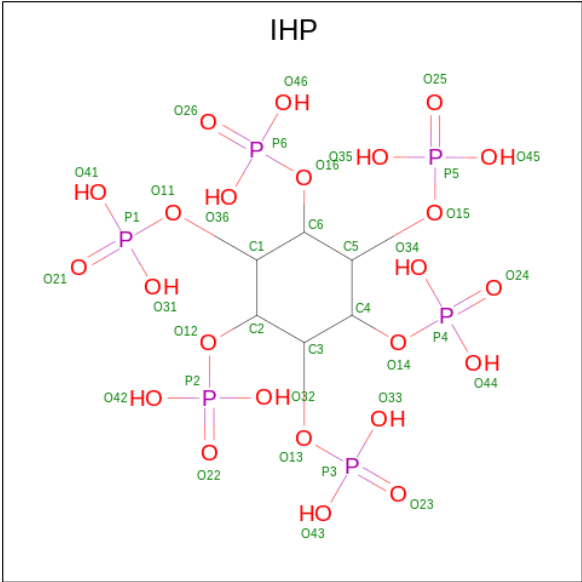
- Molecule 1 is a protein called Solute carrier family 53 member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	606	Total	C	N	O	S	0	0
			5030	3312	829	868	21		
1	D	609	Total	C	N	O	S	0	0
			5059	3332	835	871	21		

There are 16 discrepancies between the modelled and reference sequences:

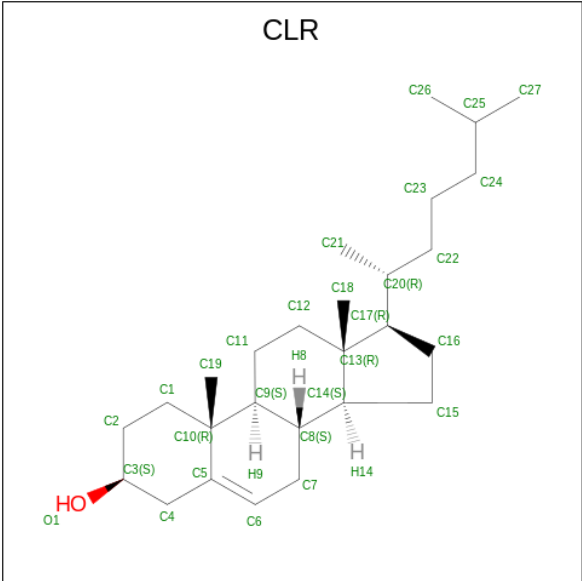
Chain	Residue	Modelled	Actual	Comment	Reference
A	697	SER	-	expression tag	UNP Q9UBH6
A	698	ARG	-	expression tag	UNP Q9UBH6
A	699	GLU	-	expression tag	UNP Q9UBH6
A	700	ASN	-	expression tag	UNP Q9UBH6
A	701	LEU	-	expression tag	UNP Q9UBH6
A	702	TYR	-	expression tag	UNP Q9UBH6
A	703	PHE	-	expression tag	UNP Q9UBH6
A	704	GLN	-	expression tag	UNP Q9UBH6
D	697	SER	-	expression tag	UNP Q9UBH6
D	698	ARG	-	expression tag	UNP Q9UBH6
D	699	GLU	-	expression tag	UNP Q9UBH6
D	700	ASN	-	expression tag	UNP Q9UBH6
D	701	LEU	-	expression tag	UNP Q9UBH6
D	702	TYR	-	expression tag	UNP Q9UBH6
D	703	PHE	-	expression tag	UNP Q9UBH6
D	704	GLN	-	expression tag	UNP Q9UBH6

- Molecule 2 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: C₆H₁₈O₂₄P₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	O	P	0
			36	6	24	6	
2	D	1	Total	C	O	P	0
			36	6	24	6	

- Molecule 3 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$) (labeled as "Ligand of Interest" by depositor).



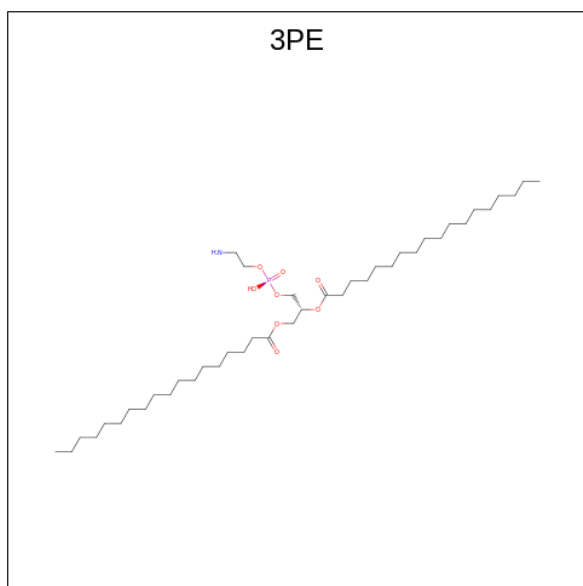
Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	O		0
			28	27	1		

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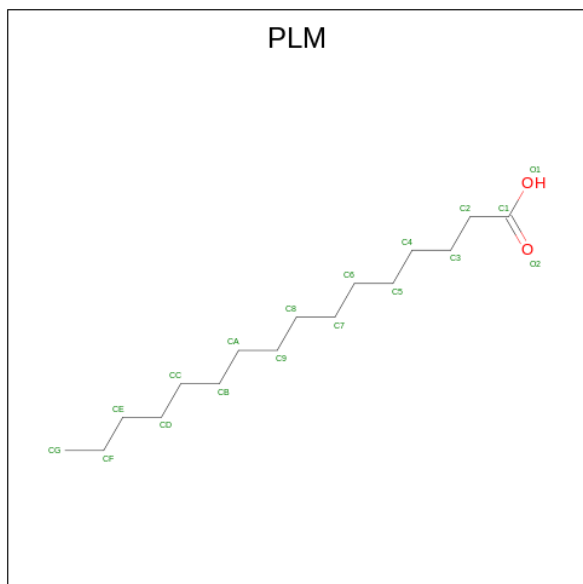
Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total	C	O	0
			28	27	1	
3	A	1	Total	C	O	0
			28	27	1	
3	A	1	Total	C	O	0
			28	27	1	
3	A	1	Total	C	O	0
			28	27	1	
3	A	1	Total	C	O	0
			28	27	1	
3	D	1	Total	C	O	0
			28	27	1	
3	D	1	Total	C	O	0
			28	27	1	
3	D	1	Total	C	O	0
			28	27	1	
3	D	1	Total	C	O	0
			28	27	1	
3	D	1	Total	C	O	0
			28	27	1	

- Molecule 4 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$) (labeled as "Ligand of Interest" by depositor).



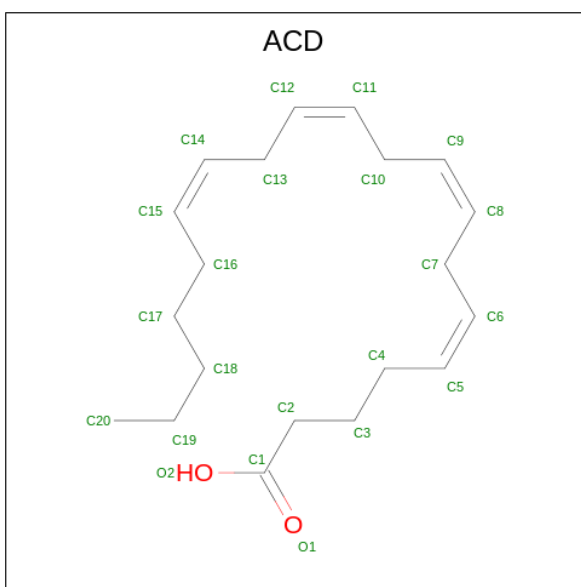
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
4	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
4	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
4	D	1	Total	C	N	O	P	0
			51	41	1	8	1	
4	D	1	Total	C	N	O	P	0
			51	41	1	8	1	
4	D	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 5 is PALMITIC ACID (three-letter code: PLM) (formula: $C_{16}H_{32}O_2$) (labeled as "Ligand of Interest" by depositor).



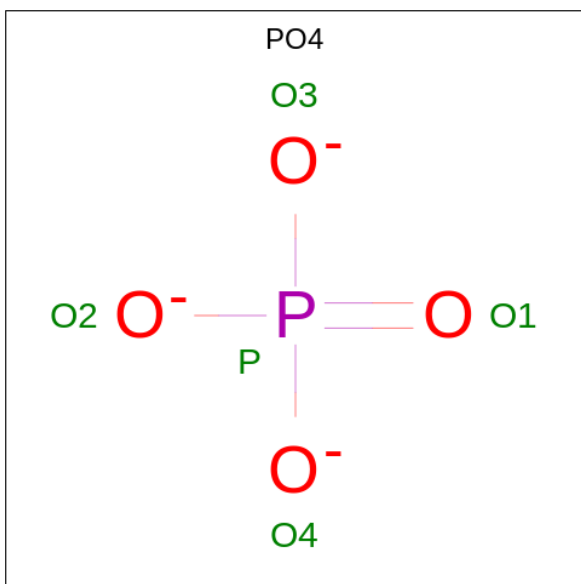
Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	C	O	0
			18	16	2	
5	D	1	Total	C	O	0
			18	16	2	

- Molecule 6 is ARACHIDONIC ACID (three-letter code: ACD) (formula: $C_{20}H_{32}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total	C	O	0
			22	20	2	
6	D	1	Total	C	O	0
			22	20	2	

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P) (labeled as "Ligand of Interest" by depositor).



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

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Mol	Chain	Residues	Atoms			AltConf
7	A	1	Total	O	P	0
			5	4	1	
7	A	1	Total	O	P	0
			5	4	1	
7	A	1	Total	O	P	0
			5	4	1	
7	A	1	Total	O	P	0
			5	4	1	
7	D	1	Total	O	P	0
			5	4	1	
7	D	1	Total	O	P	0
			5	4	1	
7	D	1	Total	O	P	0
			5	4	1	
7	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	79995	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.019	Depositor
Minimum map value	-1.416	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	387.84003, 387.84003, 387.84003	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.808, 0.808, 0.808	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, 3PE, IHP, ACD, PLM, CLR

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	0.29	0/5175	0.48	0/7014
1	D	0.29	0/5204	0.49	0/7053
All	All	0.29	0/10379	0.49	0/14067

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

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	5030	0	4994	115	0
1	D	5059	0	5036	120	0
2	A	36	0	6	1	0
2	D	36	0	6	5	0
3	A	168	0	276	7	0
3	D	168	0	276	2	0
4	A	153	0	246	4	0
4	D	153	0	246	11	0
5	A	18	0	31	1	0
5	D	18	0	31	1	0
6	A	22	0	31	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	22	0	31	0	0
7	A	25	0	0	0	0
7	D	25	0	0	0	0
All	All	10933	0	11210	244	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 11.

All (244) 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:A:146:GLN:HE22	1:A:191:ILE:HG23	1.45	0.80
1:A:122:ARG:O	1:A:125:HIS:ND1	2.28	0.67
1:A:157:ARG:HH22	1:A:181:GLU:HG3	1.60	0.66
1:D:404:SER:HA	1:D:407:LEU:HD12	1.78	0.66
1:D:277:LEU:HD11	1:D:597:ALA:HB1	1.77	0.65
1:D:534:TRP:HB3	1:D:536:LEU:HD13	1.78	0.65
1:A:398:ASP:OD1	1:A:604:ARG:NH1	2.30	0.65
1:D:545:THR:HG1	1:D:560:TYR:HH	1.43	0.64
1:D:146:GLN:NE2	1:D:191:ILE:HG13	2.13	0.64
1:A:192:ASN:HA	1:A:195:ILE:HD12	1.79	0.64
1:A:63:GLU:HG3	1:A:175:TRP:HZ2	1.64	0.62
1:D:57:LYS:HA	1:D:60:GLN:HE21	1.63	0.62
1:D:2:LYS:NZ	2:D:801:IHP:O21	2.33	0.62
1:A:44:GLU:HG2	1:A:48:LYS:HE3	1.81	0.62
1:A:404:SER:HA	1:A:407:LEU:HD12	1.82	0.61
1:A:161:LYS:HB3	1:A:176:ARG:HH12	1.66	0.61
1:D:259:LEU:HD21	1:D:265:ILE:HG21	1.81	0.61
1:A:207:GLU:HB3	1:A:210:ASP:HB3	1.83	0.60
1:A:482:LYS:HG3	1:A:525:THR:HG22	1.84	0.60
1:D:51:PHE:O	1:D:55:GLU:HG2	2.01	0.59
1:D:251:LEU:HD11	1:D:331:LEU:HD23	1.85	0.59
1:D:16:ARG:HD2	1:D:17:LYS:HD3	1.85	0.59
4:A:817:3PE:H372	3:D:812:CLR:H151	1.84	0.59
1:A:202:VAL:HG22	1:A:206:LEU:HD12	1.84	0.58
1:A:2:LYS:NZ	2:A:801:IHP:O21	2.35	0.58
1:D:125:HIS:HA	1:D:128:ILE:HD12	1.85	0.58
1:A:190:LYS:O	1:A:193:GLN:HG3	2.03	0.58
3:A:806:CLR:H151	4:D:802:3PE:H372	1.87	0.57
1:D:142:LEU:O	1:D:146:GLN:HG2	2.05	0.57
1:D:202:VAL:HG21	1:D:218:LEU:HD21	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:279:ILE:HD13	1:D:324:GLY:HA2	1.86	0.57
1:A:447:VAL:O	1:A:451:VAL:HG22	2.05	0.57
1:D:308:ARG:NH2	2:D:801:IHP:O35	2.38	0.57
1:A:23:GLU:HA	1:A:26:LYS:HE2	1.86	0.57
4:D:814:3PE:H2F2	4:D:814:3PE:H3B2	1.86	0.57
1:A:41:VAL:HG12	1:A:42:THR:HG23	1.87	0.57
1:A:157:ARG:CZ	1:A:176:ARG:HB2	2.35	0.57
1:D:73:TYR:CD1	1:D:185:PHE:HA	2.40	0.57
1:D:99:LYS:O	1:D:103:GLY:N	2.35	0.56
1:D:250:THR:HG22	4:D:802:3PE:H282	1.86	0.56
1:A:385:PRO:O	1:A:465:ARG:NH1	2.39	0.56
1:A:173:ALA:O	1:A:176:ARG:HG2	2.05	0.56
1:A:347:TYR:HB2	1:A:348:PRO:HD3	1.86	0.56
1:D:525:THR:HG23	1:D:570:ARG:HH11	1.71	0.55
1:A:600:GLU:OE2	1:A:603:ARG:NH2	2.40	0.55
1:D:190:LYS:HA	1:D:193:GLN:HG3	1.88	0.55
1:D:303:PHE:HE2	1:D:612:LEU:HD11	1.72	0.55
1:D:374:LEU:HD13	4:D:809:3PE:H232	1.89	0.55
1:A:259:LEU:HD21	1:A:265:ILE:HG21	1.88	0.55
1:A:100:GLU:HA	1:A:104:VAL:HG13	1.89	0.54
1:A:569:LEU:HD11	1:A:599:LEU:HB3	1.90	0.54
1:D:162:LYS:NZ	2:D:801:IHP:O42	2.37	0.54
1:A:135:PHE:CD1	1:A:206:LEU:HD11	2.43	0.54
1:A:515:ILE:HD11	1:A:577:ILE:HD13	1.88	0.54
1:D:61:THR:O	1:D:65:GLU:HG2	2.08	0.54
1:D:19:TYR:HD2	1:D:148:TYR:HD1	1.54	0.54
1:A:235:PHE:HE2	5:A:809:PLM:HA2	1.74	0.53
1:A:361:ASN:HB3	1:A:371:ARG:NH1	2.23	0.53
1:D:263:ARG:HH21	1:D:432:ASN:HA	1.74	0.53
1:D:481:GLY:O	1:D:485:THR:HG23	2.08	0.53
1:D:389:VAL:CG2	1:D:466:ARG:HG2	2.39	0.53
1:D:569:LEU:HD11	1:D:599:LEU:HB3	1.89	0.53
1:D:368:TYR:CE2	1:D:369:LYS:HG2	2.44	0.53
1:D:305:LEU:HD22	4:D:809:3PE:H12	1.91	0.53
1:D:73:TYR:HD1	1:D:185:PHE:HA	1.73	0.52
1:A:146:GLN:O	1:A:150:ASN:ND2	2.37	0.52
4:A:808:3PE:H2F2	4:A:808:3PE:H3B2	1.92	0.52
1:D:202:VAL:HG22	1:D:206:LEU:HD12	1.90	0.52
1:A:232:TRP:HD1	1:A:236:ARG:HH21	1.58	0.52
1:D:583:THR:HG23	1:D:585:LEU:H	1.73	0.52
1:A:191:ILE:HD12	1:A:194:LEU:HD12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:158:LYS:HZ1	2:D:801:IHP:H4	1.74	0.52
1:D:292:TRP:CZ2	1:D:612:LEU:HD12	2.45	0.52
1:A:285:LEU:CD2	4:A:803:3PE:H362	2.40	0.51
1:A:191:ILE:O	1:A:194:LEU:HB2	2.11	0.51
1:D:173:ALA:HA	1:D:176:ARG:HE	1.75	0.51
1:D:20:ILE:HG13	1:D:25:PHE:CE1	2.45	0.51
1:D:146:GLN:HE22	1:D:191:ILE:HG13	1.73	0.51
1:D:402:SER:OG	1:D:604:ARG:NE	2.39	0.51
1:D:517:PHE:HA	1:D:520:ILE:HG22	1.92	0.51
1:A:20:ILE:HG13	1:A:25:PHE:HE2	1.75	0.51
1:A:250:THR:HG22	4:A:817:3PE:H282	1.92	0.51
1:D:146:GLN:HE21	1:D:195:ILE:CD1	2.22	0.51
1:A:360:ILE:HG13	1:A:361:ASN:H	1.76	0.51
1:D:44:GLU:HG2	1:D:48:LYS:HE3	1.91	0.51
1:D:135:PHE:HA	1:D:138:PHE:HB3	1.91	0.51
1:D:536:LEU:HD23	1:D:563:ILE:HD11	1.93	0.51
1:D:173:ALA:HA	1:D:176:ARG:NE	2.26	0.51
1:A:73:TYR:HD2	1:A:185:PHE:HA	1.75	0.50
1:D:389:VAL:HG21	1:D:466:ARG:HG2	1.93	0.50
1:A:214:ALA:O	1:A:218:LEU:HG	2.11	0.50
1:A:132:LYS:HG2	1:A:206:LEU:HD13	1.93	0.50
1:A:525:THR:HB	1:A:570:ARG:HH21	1.76	0.50
1:A:251:LEU:HD11	1:A:331:LEU:HD23	1.93	0.50
1:D:91:LEU:HG	1:D:205:GLU:OE2	2.11	0.50
1:D:291:GLY:HA3	1:D:609:PHE:HE1	1.77	0.50
1:D:518:TYR:CE1	1:D:573:TRP:HB2	2.47	0.50
1:A:466:ARG:HB3	1:A:476:HIS:CE1	2.47	0.49
1:D:57:LYS:HZ3	1:D:58:PHE:HE1	1.58	0.49
1:A:433:ASN:ND2	1:A:435:GLU:O	2.44	0.49
1:D:235:PHE:HE2	5:D:815:PLM:HA2	1.76	0.49
1:A:310:ASN:N	1:A:310:ASN:OD1	2.46	0.49
1:D:7:LEU:HA	1:D:10:HIS:CE1	2.48	0.49
1:D:59:PHE:CZ	1:D:171:ARG:HG3	2.48	0.49
1:D:32:ALA:HA	1:D:35:GLN:HB2	1.94	0.49
1:A:499:HIS:HB3	1:A:507:THR:OG1	2.13	0.49
1:A:135:PHE:HA	1:A:138:PHE:HB3	1.94	0.48
1:A:303:PHE:HE2	1:A:612:LEU:HD11	1.78	0.48
1:D:122:ARG:HA	1:D:125:HIS:CD2	2.48	0.48
1:A:395:TRP:NE1	1:A:608:ASN:OD1	2.37	0.48
1:D:585:LEU:HD23	1:D:587:HIS:H	1.77	0.48
1:D:306:ASN:HD21	1:D:308:ARG:NE	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:LEU:HA	1:A:10:HIS:CE1	2.49	0.48
1:D:515:ILE:HD11	1:D:577:ILE:HG12	1.95	0.48
1:D:171:ARG:NH1	1:D:174:ASP:OD1	2.48	0.47
1:D:266:TRP:CE3	1:D:266:TRP:HA	2.49	0.47
1:D:499:HIS:HB3	1:D:507:THR:HB	1.95	0.47
1:A:484:SER:HA	1:A:487:PHE:HD1	1.80	0.47
1:D:395:TRP:NE1	1:D:608:ASN:OD1	2.35	0.47
1:D:300:VAL:HG11	1:D:307:PRO:HA	1.96	0.47
1:A:13:PRO:O	1:A:17:LYS:NZ	2.34	0.47
1:A:22:TYR:O	1:A:26:LYS:HG3	2.14	0.47
1:A:272:TYR:HB3	1:A:327:TRP:HE1	1.80	0.47
1:A:395:TRP:O	1:A:399:GLN:HG2	2.15	0.47
1:D:202:VAL:HA	1:D:206:LEU:HB2	1.95	0.47
1:A:66:LEU:HD11	1:A:179:HIS:HB3	1.96	0.47
1:A:555:GLN:HG3	1:A:557:ALA:H	1.78	0.47
1:A:368:TYR:CE2	1:A:369:LYS:HG2	2.50	0.47
1:D:177:VAL:O	1:D:181:GLU:HB2	2.15	0.47
1:D:299:HIS:O	1:D:303:PHE:HB2	2.15	0.47
1:D:310:ASN:OD1	1:D:310:ASN:N	2.47	0.46
1:D:398:ASP:OD1	1:D:604:ARG:NH1	2.47	0.46
3:A:806:CLR:H71	4:D:802:3PE:H351	1.98	0.46
1:D:418:SER:HA	3:D:816:CLR:H6	1.97	0.46
1:A:183:ALA:HB3	1:A:185:PHE:CE1	2.50	0.46
1:A:552:VAL:HG23	1:A:617:LEU:HD11	1.96	0.46
1:D:78:ALA:O	1:D:81:GLN:HG2	2.15	0.46
1:A:240:PHE:HA	1:A:325:ILE:HD11	1.98	0.46
1:D:122:ARG:O	1:D:126:ARG:HG3	2.16	0.45
4:D:809:3PE:H221	4:D:809:3PE:H341	1.98	0.45
1:A:292:TRP:CZ2	1:A:612:LEU:HD12	2.51	0.45
1:D:173:ALA:O	1:D:176:ARG:HG2	2.15	0.45
1:D:537:PHE:HE1	1:D:546:PHE:HB3	1.81	0.45
3:A:806:CLR:H162	3:A:806:CLR:H221	1.76	0.45
1:D:142:LEU:HD22	1:D:191:ILE:HD11	1.97	0.45
1:A:11:ILE:HG23	1:A:19:TYR:HE1	1.81	0.45
1:D:260:GLU:HG3	1:D:262:ASP:H	1.82	0.45
1:A:172:GLY:C	1:A:176:ARG:HE	2.19	0.45
1:A:279:ILE:HD13	1:A:324:GLY:HA2	1.98	0.45
1:A:282:LEU:HD23	1:A:282:LEU:HA	1.81	0.44
1:A:356:VAL:O	1:A:360:ILE:HG12	2.17	0.44
1:A:548:ARG:NH1	1:A:613:GLU:OE2	2.50	0.44
1:A:16:ARG:HA	1:A:19:TYR:CD1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:ASP:O	1:A:46:THR:OG1	2.32	0.44
1:D:203:THR:HG21	1:D:211:ARG:HD2	1.98	0.44
1:A:127:ASN:O	1:A:131:LEU:HD13	2.17	0.44
1:A:303:PHE:CE2	1:A:612:LEU:HD11	2.53	0.44
1:D:282:LEU:HD23	1:D:282:LEU:HA	1.83	0.44
1:D:603:ARG:HG3	1:D:603:ARG:HH11	1.83	0.44
1:A:31:SER:OG	1:D:122:ARG:NH1	2.51	0.44
1:D:291:GLY:HA3	1:D:609:PHE:CE1	2.52	0.44
1:D:395:TRP:O	1:D:399:GLN:HG2	2.18	0.44
1:A:134:ALA:O	1:A:137:GLU:HG2	2.18	0.44
1:D:153:PHE:O	1:D:157:ARG:HG2	2.18	0.44
1:D:569:LEU:HB3	1:D:603:ARG:HG3	1.99	0.44
1:A:25:PHE:CD1	1:A:25:PHE:N	2.85	0.44
1:D:19:TYR:HD2	1:D:148:TYR:CD1	2.32	0.44
1:D:158:LYS:NZ	2:D:801:IHP:H4	2.33	0.44
1:A:266:TRP:HA	1:A:266:TRP:CE3	2.53	0.43
1:A:360:ILE:O	1:A:371:ARG:NH1	2.51	0.43
1:A:513:LEU:HA	1:A:516:VAL:HB	1.99	0.43
1:A:537:PHE:HE1	1:A:546:PHE:HB3	1.82	0.43
3:A:802:CLR:H263	3:A:802:CLR:H232	1.83	0.43
1:A:8:SER:HA	1:A:11:ILE:HD12	2.00	0.43
1:D:99:LYS:HA	1:D:102:THR:HB	2.00	0.43
1:A:153:PHE:O	1:A:157:ARG:HG2	2.18	0.43
1:A:369:LYS:HB3	1:A:369:LYS:HE3	1.83	0.43
1:D:73:TYR:O	1:D:73:TYR:CD2	2.71	0.43
1:D:272:TYR:CD1	1:D:331:LEU:HD13	2.53	0.43
1:A:232:TRP:HZ3	4:D:814:3PE:H2	1.84	0.43
1:D:136:SER:OG	1:D:137:GLU:OE1	2.36	0.43
4:D:814:3PE:H322	4:D:814:3PE:H241	2.00	0.43
1:D:429:LEU:HD12	1:D:429:LEU:HA	1.87	0.43
1:A:52:ALA:O	1:A:55:GLU:HG3	2.19	0.43
1:A:561:CYS:HB3	3:A:802:CLR:H232	2.00	0.43
1:A:473:ALA:O	1:A:477:LEU:HB2	2.18	0.43
1:A:543:GLU:OE2	1:A:543:GLU:N	2.26	0.43
1:D:78:ALA:O	1:D:82:ARG:HG3	2.19	0.43
1:A:422:LYS:HD3	1:A:422:LYS:HA	1.80	0.43
1:D:518:TYR:OH	1:D:574:THR:N	2.52	0.42
1:A:345:TYR:CD2	1:A:421:LEU:HD11	2.53	0.42
1:A:399:GLN:OE1	1:A:608:ASN:ND2	2.52	0.42
1:D:59:PHE:CE2	1:D:171:ARG:HG3	2.54	0.42
1:A:135:PHE:HD1	1:A:206:LEU:HD11	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:359:LEU:HD13	4:D:809:3PE:H292	2.00	0.42
1:D:547:LEU:HD23	1:D:551:ILE:HG21	2.02	0.42
1:A:62:CYS:O	1:A:66:LEU:HB2	2.19	0.42
1:A:339:ILE:HG22	1:A:341:VAL:HG12	2.01	0.42
1:A:418:SER:HA	3:A:810:CLR:H6	2.01	0.42
1:A:484:SER:HA	1:A:487:PHE:CD1	2.54	0.42
1:D:126:ARG:O	1:D:129:LYS:HG2	2.20	0.42
1:A:11:ILE:HG23	1:A:19:TYR:CE1	2.55	0.42
1:D:157:ARG:HH22	1:D:181:GLU:HG3	1.85	0.42
1:D:521:SER:O	1:D:525:THR:HG22	2.20	0.42
1:A:348:PRO:HG2	1:A:429:LEU:HD21	2.01	0.42
1:A:408:MET:HG3	1:A:448:ARG:NH1	2.34	0.42
1:A:172:GLY:HA3	1:A:176:ARG:HH21	1.85	0.42
1:D:22:TYR:OH	1:D:158:LYS:HB3	2.19	0.42
1:D:326:LEU:HD23	1:D:326:LEU:HA	1.81	0.42
1:A:277:LEU:HD11	1:A:597:ALA:HB1	2.00	0.41
1:A:87:LEU:HD13	1:A:135:PHE:CD2	2.55	0.41
1:D:585:LEU:HB3	1:D:588:SER:HB3	2.02	0.41
1:D:264:SER:HB3	1:D:434:SER:HA	2.02	0.41
1:D:464:LEU:HD23	1:D:464:LEU:HA	1.83	0.41
1:A:518:TYR:OH	1:A:574:THR:HG23	2.21	0.41
1:A:575:ILE:O	1:A:579:ILE:HG13	2.21	0.41
1:A:98:GLN:O	1:A:102:THR:N	2.54	0.41
1:A:354:PHE:HA	1:A:357:PHE:HB3	2.01	0.41
1:D:303:PHE:HB3	1:D:305:LEU:HG	2.01	0.41
1:D:466:ARG:HB3	1:D:476:HIS:CE1	2.55	0.41
3:A:810:CLR:H162	3:A:810:CLR:H221	1.49	0.41
1:A:76:LYS:HA	1:A:76:LYS:HD3	1.83	0.41
1:D:248:ASN:HD22	4:D:814:3PE:H3D1	1.85	0.41
1:A:4:ALA:HB1	1:A:26:LYS:NZ	2.36	0.41
1:A:122:ARG:O	1:A:126:ARG:HG3	2.20	0.41
1:D:544:ASN:ND2	1:D:549:GLU:O	2.53	0.41
1:A:87:LEU:O	1:A:90:GLU:HG2	2.21	0.41
1:A:597:ALA:HB3	1:A:598:PRO:HD3	2.03	0.41
1:D:540:ASN:OD1	1:D:549:GLU:HB2	2.21	0.41
1:A:429:LEU:HD12	1:A:429:LEU:HA	1.95	0.41
1:D:157:ARG:HA	1:D:157:ARG:HD3	1.91	0.41
1:D:190:LYS:O	1:D:194:LEU:HG	2.21	0.41
1:D:19:TYR:CD2	1:D:148:TYR:HD1	2.37	0.40
1:A:60:GLN:O	1:A:64:LYS:HG2	2.21	0.40
1:D:190:LYS:HB3	1:D:193:GLN:HE21	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:273:ARG:HB3	1:D:409:ASP:OD1	2.21	0.40
1:D:576:GLN:O	1:D:580:THR:HG22	2.21	0.40
1:A:211:ARG:O	1:A:215:MET:HG2	2.20	0.40
1:A:375:LEU:HD23	1:A:375:LEU:HA	1.86	0.40
1:A:457:TRP:HA	1:A:487:PHE:HZ	1.86	0.40
1:D:100:GLU:HA	1:D:104:VAL:HB	2.03	0.40
1:D:83:ARG:NH1	1:D:83:ARG:HA	2.37	0.40
1:D:347:TYR:HB2	1:D:348:PRO:HD3	2.03	0.40
1:D:548:ARG:NH2	1:D:613:GLU:OE1	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	600/704 (85%)	580 (97%)	20 (3%)	0	100	100
1	D	603/704 (86%)	586 (97%)	17 (3%)	0	100	100
All	All	1203/1408 (85%)	1166 (97%)	37 (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	537/629 (85%)	516 (96%)	21 (4%)	27	53
1	D	541/629 (86%)	522 (96%)	19 (4%)	31	56
All	All	1078/1258 (86%)	1038 (96%)	40 (4%)	31	54

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	TYR
1	A	54	PHE
1	A	65	GLU
1	A	72	PHE
1	A	84	PHE
1	A	127	ASN
1	A	135	PHE
1	A	163	HIS
1	A	185	PHE
1	A	232	TRP
1	A	241	CYS
1	A	326	LEU
1	A	354	PHE
1	A	394	PHE
1	A	441	HIS
1	A	502	ARG
1	A	524	TYR
1	A	573	TRP
1	A	605	PHE
1	A	613	GLU
1	A	624	ARG
1	D	1	MET
1	D	22	TYR
1	D	50	TYR
1	D	54	PHE
1	D	73	TYR
1	D	104	VAL
1	D	135	PHE
1	D	232	TRP
1	D	263	ARG
1	D	326	LEU
1	D	335	PHE
1	D	394	PHE
1	D	441	HIS
1	D	466	ARG

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Mol	Chain	Res	Type
1	D	510	PHE
1	D	524	TYR
1	D	603	ARG
1	D	605	PHE
1	D	609	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	GLN
1	A	149	GLN
1	D	60	GLN
1	D	248	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

34 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
7	PO4	A	815	-	4,4,4	0.95	0	6,6,6	0.45	0
3	CLR	A	805	-	31,31,31	0.38	0	48,48,48	0.79	1 (2%)
7	PO4	A	816	-	4,4,4	0.95	0	6,6,6	0.47	0
3	CLR	A	810	-	31,31,31	0.37	0	48,48,48	0.45	0
4	3PE	A	817	-	50,50,50	0.52	0	53,55,55	0.53	1 (1%)
7	PO4	A	812	-	4,4,4	0.99	0	6,6,6	0.45	0
3	CLR	D	812	-	31,31,31	0.39	0	48,48,48	0.62	0
7	PO4	D	805	-	4,4,4	0.98	0	6,6,6	0.46	0
2	IHP	D	801	-	36,36,36	1.48	6 (16%)	54,60,60	0.83	3 (5%)
3	CLR	D	816	-	31,31,31	0.36	0	48,48,48	0.48	0
3	CLR	A	806	-	31,31,31	0.38	0	48,48,48	0.61	0
4	3PE	A	803	-	50,50,50	0.28	0	53,55,55	0.30	0
7	PO4	D	803	-	4,4,4	0.97	0	6,6,6	0.50	0
4	3PE	D	814	-	50,50,50	0.51	0	53,55,55	0.55	1 (1%)
6	ACD	A	811	-	21,21,21	0.56	0	21,21,21	0.59	0
7	PO4	D	807	-	4,4,4	0.97	0	6,6,6	0.38	0
7	PO4	D	806	-	4,4,4	0.94	0	6,6,6	0.43	0
3	CLR	D	808	-	31,31,31	0.39	0	48,48,48	0.54	0
3	CLR	A	802	-	31,31,31	0.40	0	48,48,48	0.57	0
6	ACD	D	817	-	21,21,21	0.55	0	21,21,21	0.58	0
3	CLR	A	804	-	31,31,31	0.38	0	48,48,48	0.49	0
3	CLR	D	810	-	31,31,31	0.38	0	48,48,48	0.51	0
4	3PE	D	802	-	50,50,50	0.51	0	53,55,55	0.54	1 (1%)
3	CLR	A	807	-	31,31,31	0.39	0	48,48,48	0.52	0
4	3PE	D	809	-	50,50,50	0.51	0	53,55,55	0.58	1 (1%)
5	PLM	D	815	-	17,17,17	0.83	1 (5%)	17,17,17	0.75	2 (11%)
4	3PE	A	808	-	50,50,50	0.51	0	53,55,55	0.54	1 (1%)
2	IHP	A	801	-	36,36,36	1.49	6 (16%)	54,60,60	0.83	2 (3%)
7	PO4	A	813	-	4,4,4	0.96	0	6,6,6	0.45	0
7	PO4	A	814	-	4,4,4	0.98	0	6,6,6	0.42	0
3	CLR	D	813	-	31,31,31	0.40	0	48,48,48	0.53	0
3	CLR	D	811	-	31,31,31	0.38	0	48,48,48	0.75	0
7	PO4	D	804	-	4,4,4	0.95	0	6,6,6	0.42	0
5	PLM	A	809	-	17,17,17	0.85	1 (5%)	17,17,17	0.75	2 (11%)

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	CLR	A	805	-	-	6/10/68/68	0/4/4/4
3	CLR	A	810	-	-	7/10/68/68	0/4/4/4
4	3PE	A	817	-	-	13/54/54/54	-
3	CLR	D	812	-	-	5/10/68/68	0/4/4/4
2	IHP	D	801	-	-	9/30/54/54	0/1/1/1
3	CLR	D	816	-	-	7/10/68/68	0/4/4/4
3	CLR	A	806	-	-	3/10/68/68	0/4/4/4
4	3PE	A	803	-	-	24/54/54/54	-
4	3PE	D	814	-	-	25/54/54/54	-
6	ACD	A	811	-	-	3/19/19/19	-
3	CLR	D	808	-	-	8/10/68/68	0/4/4/4
3	CLR	A	802	-	-	6/10/68/68	0/4/4/4
6	ACD	D	817	-	-	3/19/19/19	-
3	CLR	A	804	-	-	2/10/68/68	0/4/4/4
3	CLR	D	810	-	-	2/10/68/68	0/4/4/4
4	3PE	D	802	-	-	12/54/54/54	-
3	CLR	A	807	-	-	5/10/68/68	0/4/4/4
4	3PE	D	809	-	-	26/54/54/54	-
5	PLM	D	815	-	-	6/15/15/15	-
4	3PE	A	808	-	-	26/54/54/54	-
2	IHP	A	801	-	-	11/30/54/54	0/1/1/1
3	CLR	D	813	-	-	5/10/68/68	0/4/4/4
3	CLR	D	811	-	-	6/10/68/68	0/4/4/4
5	PLM	A	809	-	-	4/15/15/15	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	IHP	P4-O14	3.49	1.65	1.59
2	D	801	IHP	P4-O14	3.42	1.65	1.59
2	A	801	IHP	P2-O12	3.16	1.65	1.59
2	A	801	IHP	P1-O11	3.14	1.65	1.59
2	D	801	IHP	P3-O13	3.14	1.65	1.59
2	D	801	IHP	P6-O16	3.13	1.65	1.59
2	A	801	IHP	P6-O16	3.13	1.65	1.59
2	D	801	IHP	P2-O12	3.12	1.65	1.59
2	A	801	IHP	P3-O13	3.09	1.65	1.59
2	D	801	IHP	P1-O11	3.08	1.65	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	801	IHP	P5-O15	3.04	1.65	1.59
2	A	801	IHP	P5-O15	3.01	1.65	1.59
5	A	809	PLM	C2-C1	2.64	1.56	1.50
5	D	815	PLM	C2-C1	2.58	1.56	1.50

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	IHP	C6-C5-C4	2.50	115.89	110.41
2	A	801	IHP	C6-C5-C4	2.49	115.85	110.41
4	D	814	3PE	O12-P-O14	2.38	124.00	112.24
4	A	808	3PE	O12-P-O14	2.38	124.00	112.24
4	D	802	3PE	O12-P-O14	2.34	123.79	112.24
4	A	817	3PE	O12-P-O14	2.32	123.72	112.24
4	D	809	3PE	O12-P-O14	2.29	123.57	112.24
5	D	815	PLM	O1-C1-O2	2.26	128.93	123.30
5	A	809	PLM	O1-C1-O2	2.23	128.87	123.30
3	A	805	CLR	C13-C17-C20	2.17	122.88	119.49
2	D	801	IHP	C5-C6-C1	2.12	115.05	110.41
2	D	801	IHP	C6-C1-C2	2.06	114.93	110.41
5	A	809	PLM	O2-C1-C2	-2.05	116.50	123.08
5	D	815	PLM	O2-C1-C2	-2.01	116.63	123.08
2	A	801	IHP	C6-C1-C2	2.00	114.80	110.41

There are no chirality outliers.

All (224) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	IHP	C3-C2-O12-P2
2	A	801	IHP	C2-C3-O13-P3
2	A	801	IHP	C5-C4-O14-P4
2	A	801	IHP	C6-O16-P6-O46
2	D	801	IHP	C5-C4-O14-P4
3	A	807	CLR	C13-C17-C20-C21
3	A	807	CLR	C16-C17-C20-C22
4	A	803	3PE	C1-O11-P-O13
4	A	803	3PE	C22-C21-O21-C2
4	A	808	3PE	C1-O11-P-O12
4	A	808	3PE	C11-O13-P-O14
4	A	808	3PE	O13-C11-C12-N
4	A	808	3PE	C22-C21-O21-C2
4	A	817	3PE	O13-C11-C12-N

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Mol	Chain	Res	Type	Atoms
4	A	817	3PE	C22-C21-O21-C2
4	D	802	3PE	C11-O13-P-O14
4	D	802	3PE	O13-C11-C12-N
4	D	809	3PE	C1-O11-P-O13
4	D	809	3PE	C11-O13-P-O14
4	D	809	3PE	C22-C21-O21-C2
4	D	814	3PE	O13-C11-C12-N
4	D	814	3PE	C22-C21-O21-C2
6	A	811	ACD	C11-C12-C13-C14
6	D	817	ACD	C11-C12-C13-C14
4	A	803	3PE	O32-C31-O31-C3
4	D	809	3PE	O32-C31-O31-C3
3	A	807	CLR	C16-C17-C20-C21
3	A	810	CLR	C16-C17-C20-C21
3	A	810	CLR	C13-C17-C20-C21
3	D	816	CLR	C13-C17-C20-C21
3	A	807	CLR	C13-C17-C20-C22
4	A	803	3PE	O22-C21-O21-C2
4	A	808	3PE	O22-C21-O21-C2
4	A	817	3PE	O22-C21-O21-C2
4	D	809	3PE	O22-C21-O21-C2
4	D	814	3PE	O22-C21-O21-C2
4	A	803	3PE	C32-C31-O31-C3
3	A	804	CLR	C21-C20-C22-C23
3	D	808	CLR	C21-C20-C22-C23
3	D	810	CLR	C21-C20-C22-C23
3	D	816	CLR	C16-C17-C20-C21
3	A	810	CLR	C13-C17-C20-C22
3	D	816	CLR	C13-C17-C20-C22
4	D	809	3PE	C32-C31-O31-C3
4	A	808	3PE	O32-C31-O31-C3
3	A	810	CLR	C16-C17-C20-C22
3	D	816	CLR	C16-C17-C20-C22
3	D	813	CLR	C13-C17-C20-C22
3	D	808	CLR	C17-C20-C22-C23
3	D	810	CLR	C17-C20-C22-C23
4	A	808	3PE	C32-C31-O31-C3
3	A	802	CLR	C21-C20-C22-C23
3	A	804	CLR	C17-C20-C22-C23
3	A	810	CLR	C17-C20-C22-C23
3	D	811	CLR	C17-C20-C22-C23
3	D	816	CLR	C17-C20-C22-C23

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Mol	Chain	Res	Type	Atoms
3	A	807	CLR	C21-C20-C22-C23
3	A	810	CLR	C21-C20-C22-C23
3	A	805	CLR	C17-C20-C22-C23
3	A	806	CLR	C17-C20-C22-C23
3	D	812	CLR	C17-C20-C22-C23
3	A	806	CLR	C22-C23-C24-C25
3	A	810	CLR	C22-C23-C24-C25
3	D	808	CLR	C22-C23-C24-C25
3	D	816	CLR	C22-C23-C24-C25
3	D	811	CLR	C21-C20-C22-C23
3	D	813	CLR	C21-C20-C22-C23
3	D	816	CLR	C21-C20-C22-C23
3	D	812	CLR	C22-C23-C24-C25
3	A	802	CLR	C20-C22-C23-C24
3	A	802	CLR	C17-C20-C22-C23
3	A	805	CLR	C21-C20-C22-C23
4	A	803	3PE	C31-C32-C33-C34
3	D	813	CLR	C16-C17-C20-C21
3	A	802	CLR	C22-C23-C24-C25
3	D	813	CLR	C13-C17-C20-C21
4	A	808	3PE	C1-O11-P-O13
4	A	808	3PE	C11-O13-P-O11
3	D	813	CLR	C16-C17-C20-C22
4	D	809	3PE	C3E-C3F-C3G-C3H
4	D	814	3PE	C34-C35-C36-C37
5	D	815	PLM	C3-C4-C5-C6
4	D	814	3PE	C25-C26-C27-C28
5	A	809	PLM	CB-CC-CD-CE
4	D	814	3PE	C32-C31-O31-C3
4	D	802	3PE	C21-C22-C23-C24
4	A	808	3PE	C35-C36-C37-C38
4	D	814	3PE	C35-C36-C37-C38
2	A	801	IHP	C1-C2-O12-P2
2	A	801	IHP	C4-C3-O13-P3
2	D	801	IHP	C2-C3-O13-P3
2	D	801	IHP	C4-C3-O13-P3
4	A	817	3PE	C22-C23-C24-C25
4	A	817	3PE	C3C-C3D-C3E-C3F
3	A	805	CLR	C22-C23-C24-C25
4	D	814	3PE	O32-C31-O31-C3
5	A	809	PLM	C3-C4-C5-C6
4	D	814	3PE	C3D-C3E-C3F-C3G

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Mol	Chain	Res	Type	Atoms
4	D	814	3PE	C26-C27-C28-C29
4	D	809	3PE	C11-O13-P-O11
4	D	809	3PE	C22-C23-C24-C25
4	D	814	3PE	C3A-C3B-C3C-C3D
4	D	809	3PE	C27-C28-C29-C2A
4	D	809	3PE	C2A-C2B-C2C-C2D
4	A	808	3PE	C2F-C2G-C2H-C2I
4	D	809	3PE	C35-C36-C37-C38
4	D	814	3PE	C33-C34-C35-C36
4	A	803	3PE	C2D-C2E-C2F-C2G
4	A	803	3PE	C3E-C3F-C3G-C3H
3	D	811	CLR	C20-C22-C23-C24
3	D	811	CLR	C22-C23-C24-C25
3	A	805	CLR	C20-C22-C23-C24
4	A	803	3PE	C3F-C3G-C3H-C3I
4	D	814	3PE	C2F-C2G-C2H-C2I
4	A	803	3PE	C33-C34-C35-C36
4	D	809	3PE	C3C-C3D-C3E-C3F
4	A	808	3PE	C1-C2-C3-O31
4	D	814	3PE	C1-O11-P-O13
6	A	811	ACD	C11-C10-C9-C8
6	A	811	ACD	C12-C13-C14-C15
6	D	817	ACD	C11-C10-C9-C8
6	D	817	ACD	C12-C13-C14-C15
3	D	812	CLR	C21-C20-C22-C23
3	D	811	CLR	C23-C24-C25-C26
3	D	811	CLR	C23-C24-C25-C27
2	A	801	IHP	C3-O13-P3-O23
2	D	801	IHP	C3-O13-P3-O23
4	D	809	3PE	C28-C29-C2A-C2B
4	A	817	3PE	C21-C22-C23-C24
4	A	808	3PE	C37-C38-C39-C3A
4	D	802	3PE	C32-C31-O31-C3
3	D	808	CLR	C13-C17-C20-C22
4	A	803	3PE	C22-C23-C24-C25
4	D	814	3PE	C1-C2-C3-O31
3	A	806	CLR	C21-C20-C22-C23
5	D	815	PLM	CB-CC-CD-CE
4	A	808	3PE	O21-C2-C3-O31
4	D	802	3PE	O21-C2-C3-O31
4	D	814	3PE	O21-C2-C3-O31
4	D	814	3PE	C2E-C2F-C2G-C2H

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Mol	Chain	Res	Type	Atoms
2	A	801	IHP	C4-O14-P4-O44
2	D	801	IHP	C3-C2-O12-P2
2	D	801	IHP	C4-O14-P4-O44
3	D	808	CLR	C16-C17-C20-C22
4	D	809	3PE	C29-C2A-C2B-C2C
4	A	803	3PE	C24-C25-C26-C27
4	A	803	3PE	C11-O13-P-O11
4	A	817	3PE	C1-O11-P-O13
4	A	808	3PE	C2-C1-O11-P
4	A	803	3PE	C1-O11-P-O12
4	A	808	3PE	C11-O13-P-O12
4	D	809	3PE	C1-O11-P-O12
3	A	805	CLR	C23-C24-C25-C27
4	A	803	3PE	C32-C33-C34-C35
4	D	802	3PE	C1-C2-C3-O31
4	D	802	3PE	O32-C31-O31-C3
4	D	809	3PE	C37-C38-C39-C3A
4	D	809	3PE	C34-C35-C36-C37
3	D	808	CLR	C13-C17-C20-C21
4	A	808	3PE	C25-C26-C27-C28
4	D	809	3PE	C36-C37-C38-C39
4	A	803	3PE	C1-C2-O21-C21
4	A	803	3PE	C3-C2-O21-C21
4	D	809	3PE	C3-C2-O21-C21
4	D	809	3PE	C3B-C3C-C3D-C3E
4	D	814	3PE	C27-C28-C29-C2A
4	D	809	3PE	C23-C24-C25-C26
4	A	817	3PE	C11-O13-P-O11
4	D	802	3PE	C11-O13-P-O11
4	D	802	3PE	C2F-C2G-C2H-C2I
4	A	803	3PE	C36-C37-C38-C39
3	A	805	CLR	C23-C24-C25-C26
5	D	815	PLM	O2-C1-C2-C3
4	D	809	3PE	C3F-C3G-C3H-C3I
3	D	808	CLR	C16-C17-C20-C21
5	D	815	PLM	C6-C7-C8-C9
4	A	808	3PE	C3C-C3D-C3E-C3F
4	A	808	3PE	C2B-C2C-C2D-C2E
5	D	815	PLM	O1-C1-C2-C3
4	A	808	3PE	C3F-C3G-C3H-C3I
4	A	803	3PE	C3C-C3D-C3E-C3F
4	A	808	3PE	C38-C39-C3A-C3B

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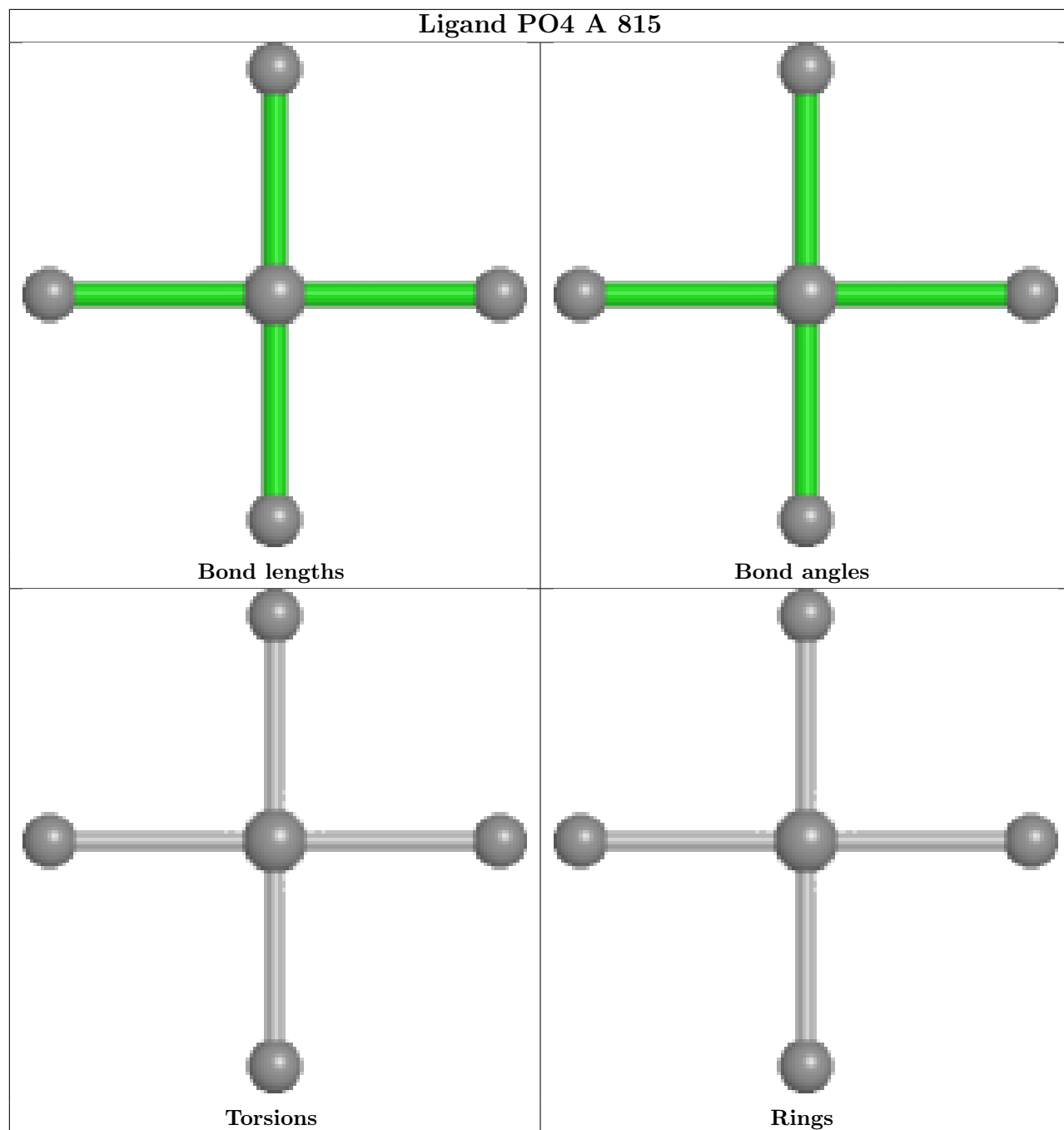
Mol	Chain	Res	Type	Atoms
4	D	814	3PE	C3E-C3F-C3G-C3H
4	D	802	3PE	C3D-C3E-C3F-C3G
4	A	817	3PE	C3D-C3E-C3F-C3G
4	D	814	3PE	C2B-C2C-C2D-C2E
4	D	814	3PE	C23-C24-C25-C26
2	A	801	IHP	C2-O12-P2-O22
4	A	808	3PE	C3D-C3E-C3F-C3G
4	D	814	3PE	O21-C21-C22-C23
4	D	809	3PE	C2D-C2E-C2F-C2G
4	D	802	3PE	O31-C31-C32-C33
4	A	803	3PE	C3B-C3C-C3D-C3E
4	A	817	3PE	O31-C31-C32-C33
5	D	815	PLM	C8-C9-CA-CB
4	A	808	3PE	C2E-C2F-C2G-C2H
4	A	803	3PE	O11-C1-C2-O21
4	A	808	3PE	O21-C21-C22-C23
4	A	817	3PE	O21-C2-C3-O31
2	A	801	IHP	C2-O12-P2-O32
2	A	801	IHP	C2-O12-P2-O42
2	D	801	IHP	C1-C2-O12-P2
2	D	801	IHP	C2-O12-P2-O32
2	D	801	IHP	C3-O13-P3-O33
3	A	802	CLR	C16-C17-C20-C22
3	D	812	CLR	C16-C17-C20-C22
4	A	808	3PE	O22-C21-C22-C23
4	A	808	3PE	C2D-C2E-C2F-C2G
3	D	812	CLR	C13-C17-C20-C21
4	A	817	3PE	O32-C31-C32-C33
3	A	802	CLR	C13-C17-C20-C21
3	D	808	CLR	C23-C24-C25-C26
4	D	814	3PE	C21-C22-C23-C24
4	A	803	3PE	C2A-C2B-C2C-C2D
4	D	809	3PE	C11-O13-P-O12
4	D	814	3PE	C1-O11-P-O12
4	A	803	3PE	C23-C24-C25-C26
4	D	802	3PE	O32-C31-C32-C33
4	D	809	3PE	C1-C2-O21-C21
4	D	814	3PE	O22-C21-C22-C23
4	A	817	3PE	C25-C26-C27-C28
5	A	809	PLM	C1-C2-C3-C4
4	A	803	3PE	O31-C31-C32-C33
5	A	809	PLM	C4-C5-C6-C7

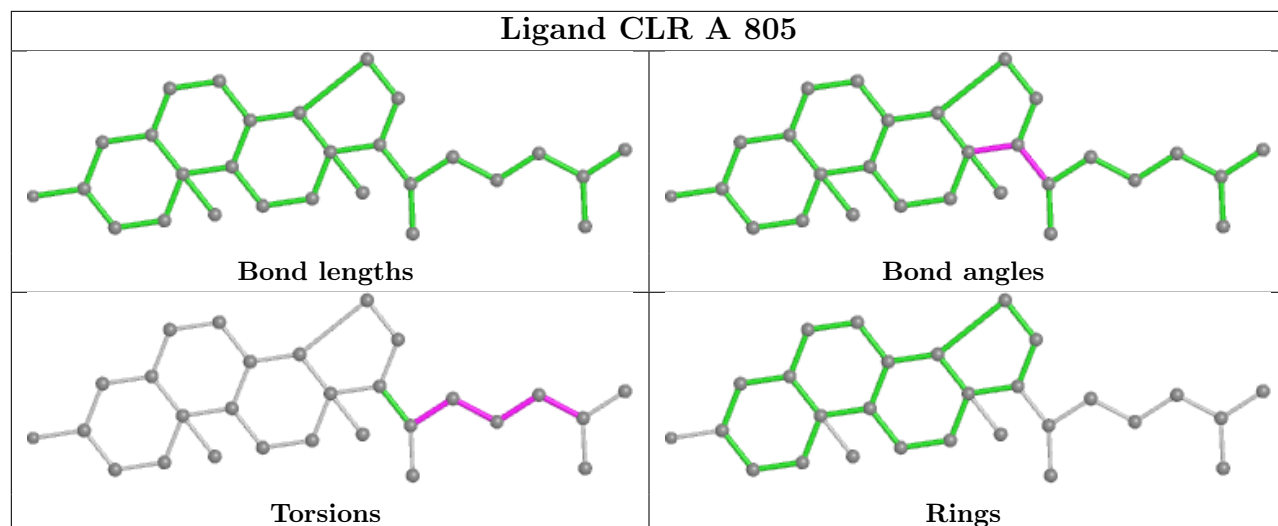
There are no ring outliers.

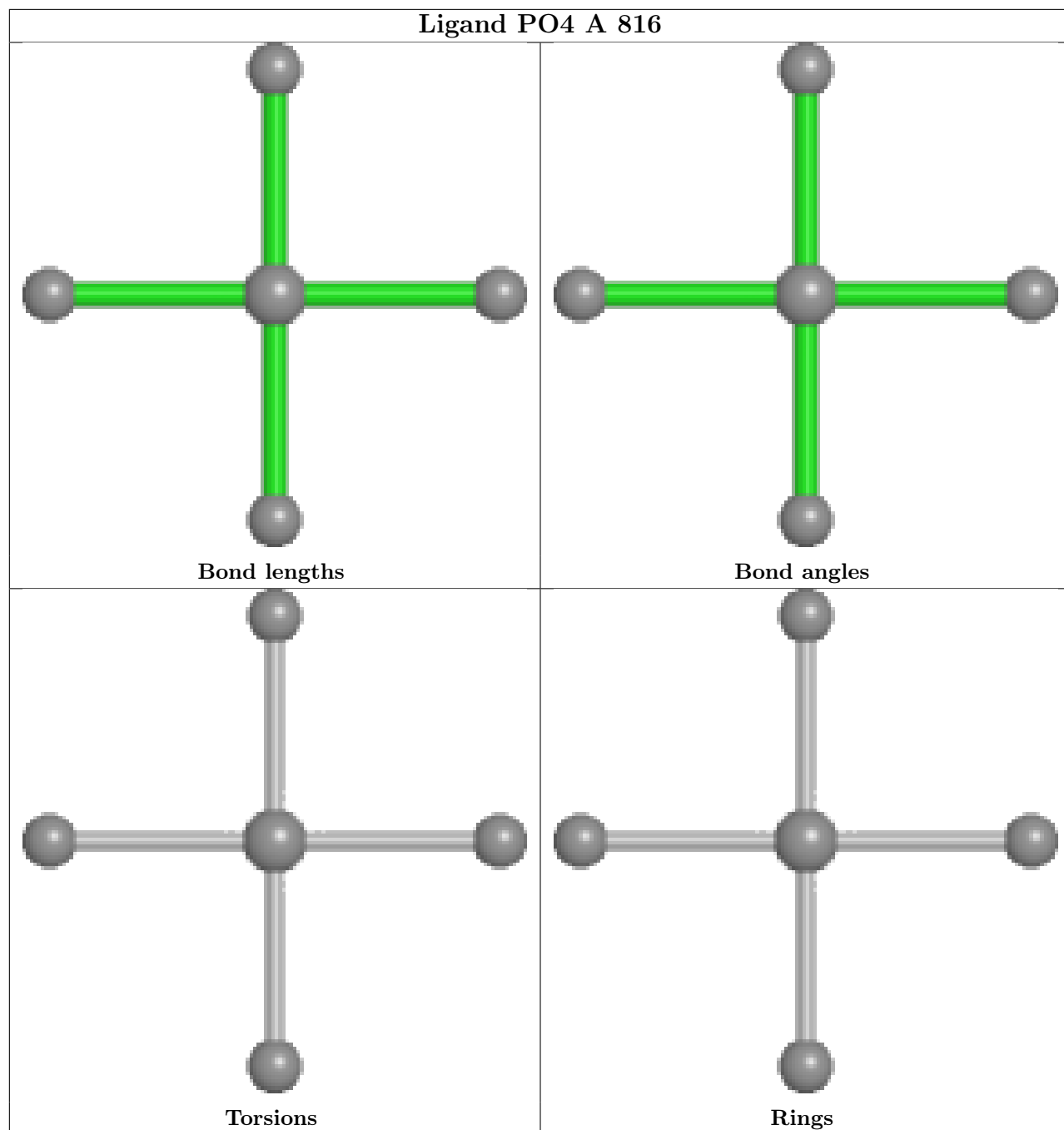
15 monomers are involved in 29 short contacts:

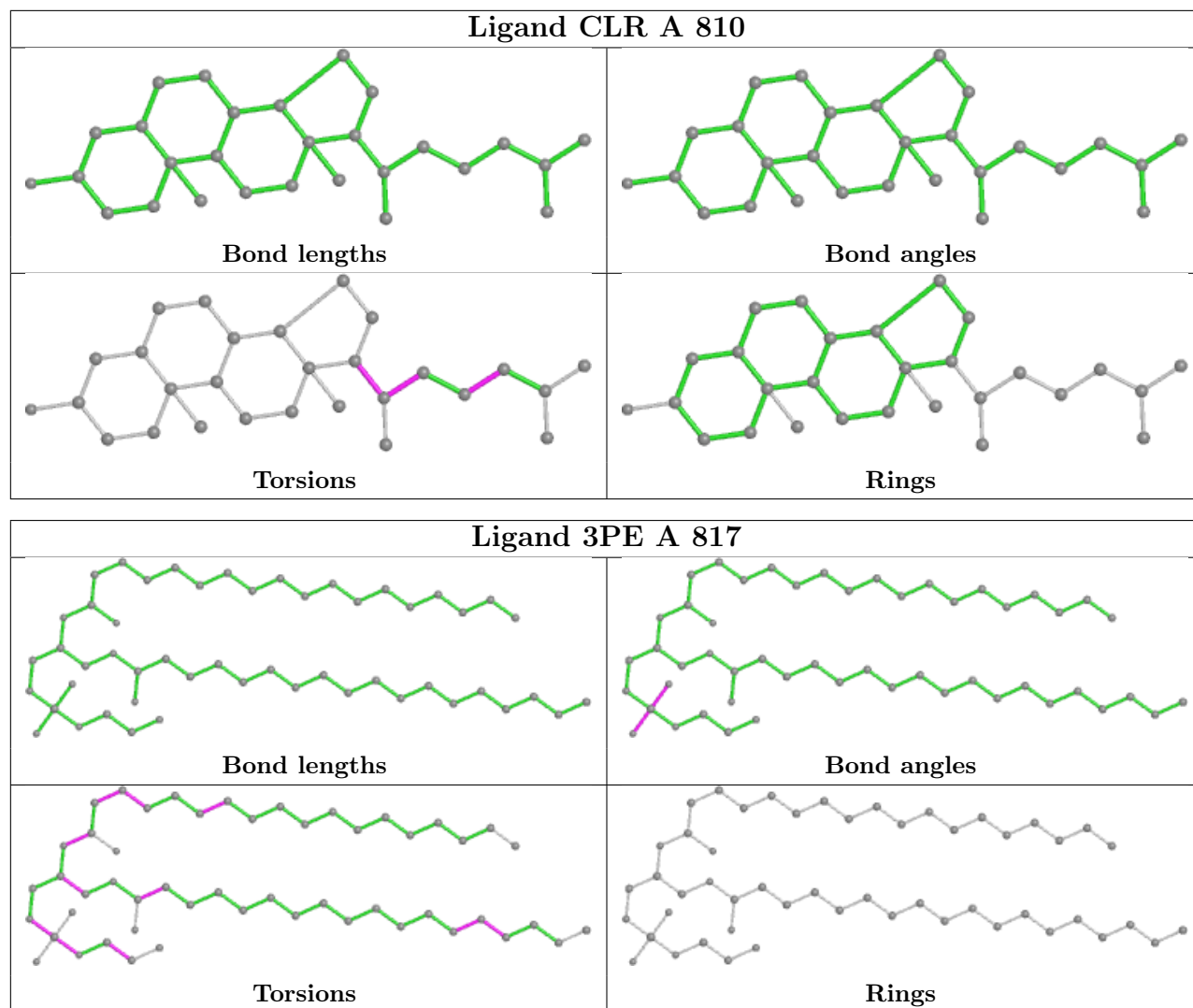
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	810	CLR	2	0
4	A	817	3PE	2	0
3	D	812	CLR	1	0
2	D	801	IHP	5	0
3	D	816	CLR	1	0
3	A	806	CLR	3	0
4	A	803	3PE	1	0
4	D	814	3PE	4	0
3	A	802	CLR	2	0
4	D	802	3PE	3	0
4	D	809	3PE	4	0
5	D	815	PLM	1	0
4	A	808	3PE	1	0
2	A	801	IHP	1	0
5	A	809	PLM	1	0

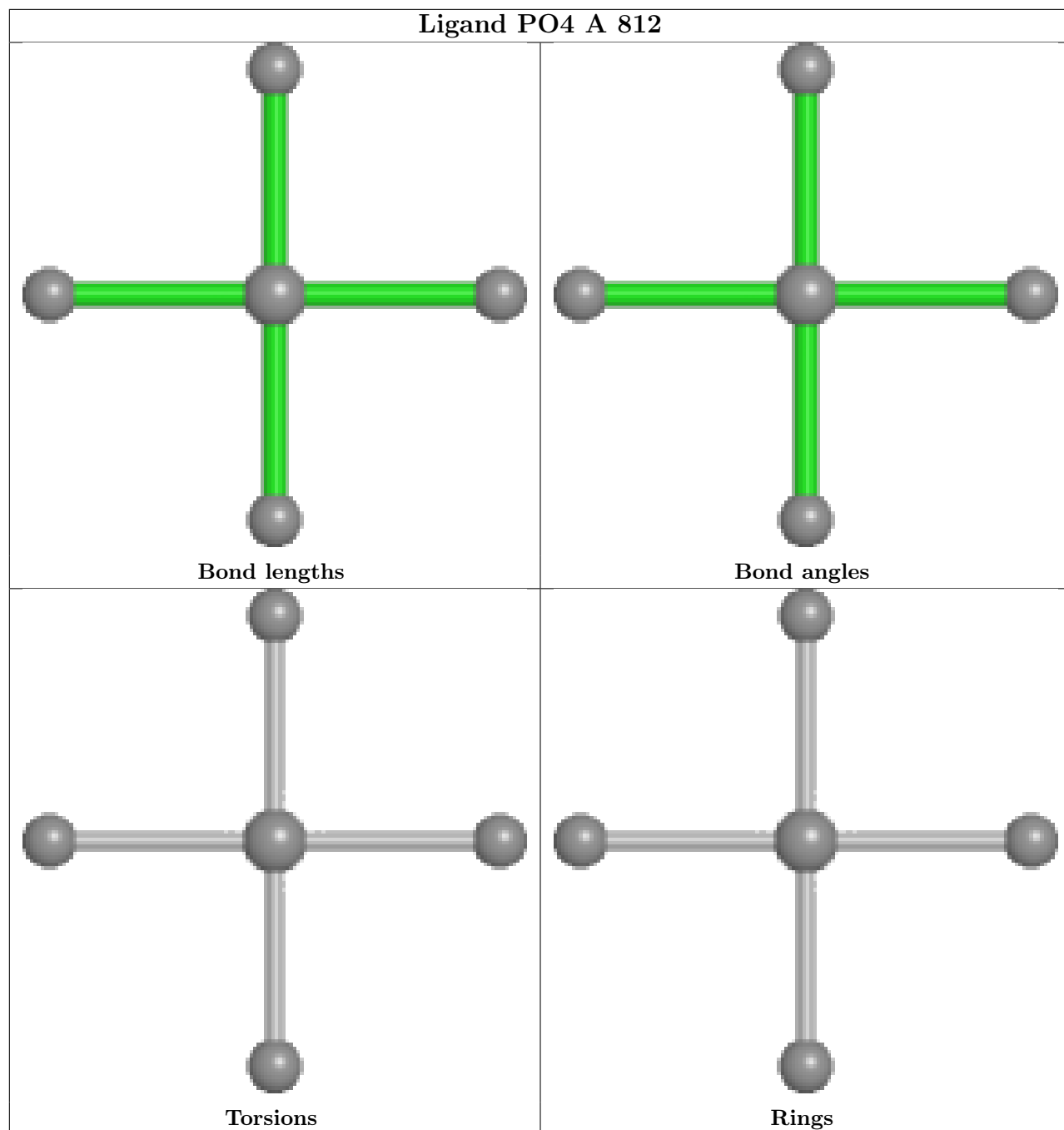
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

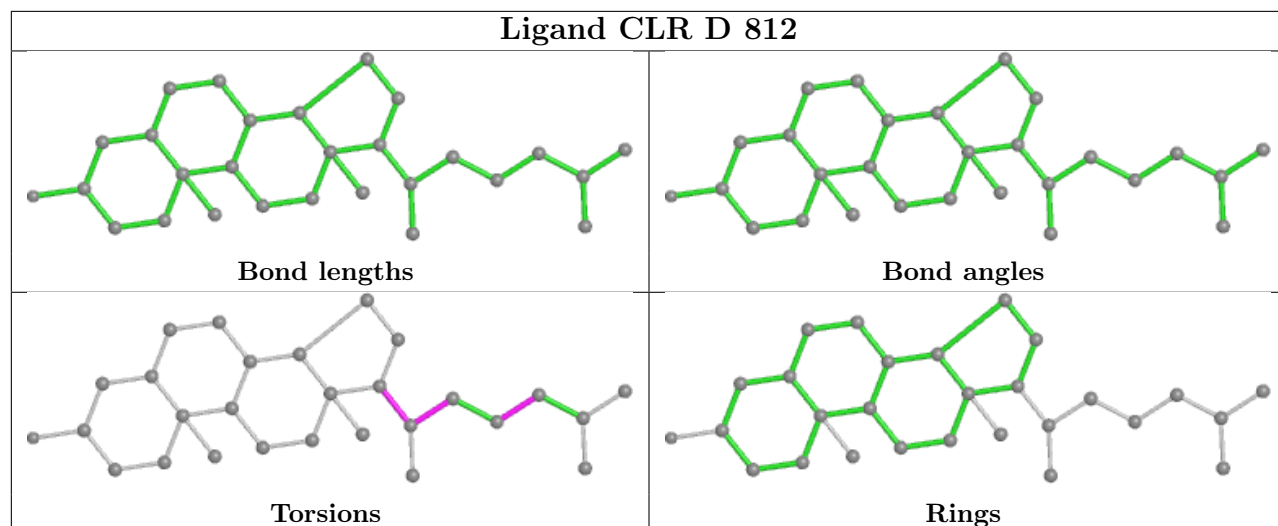


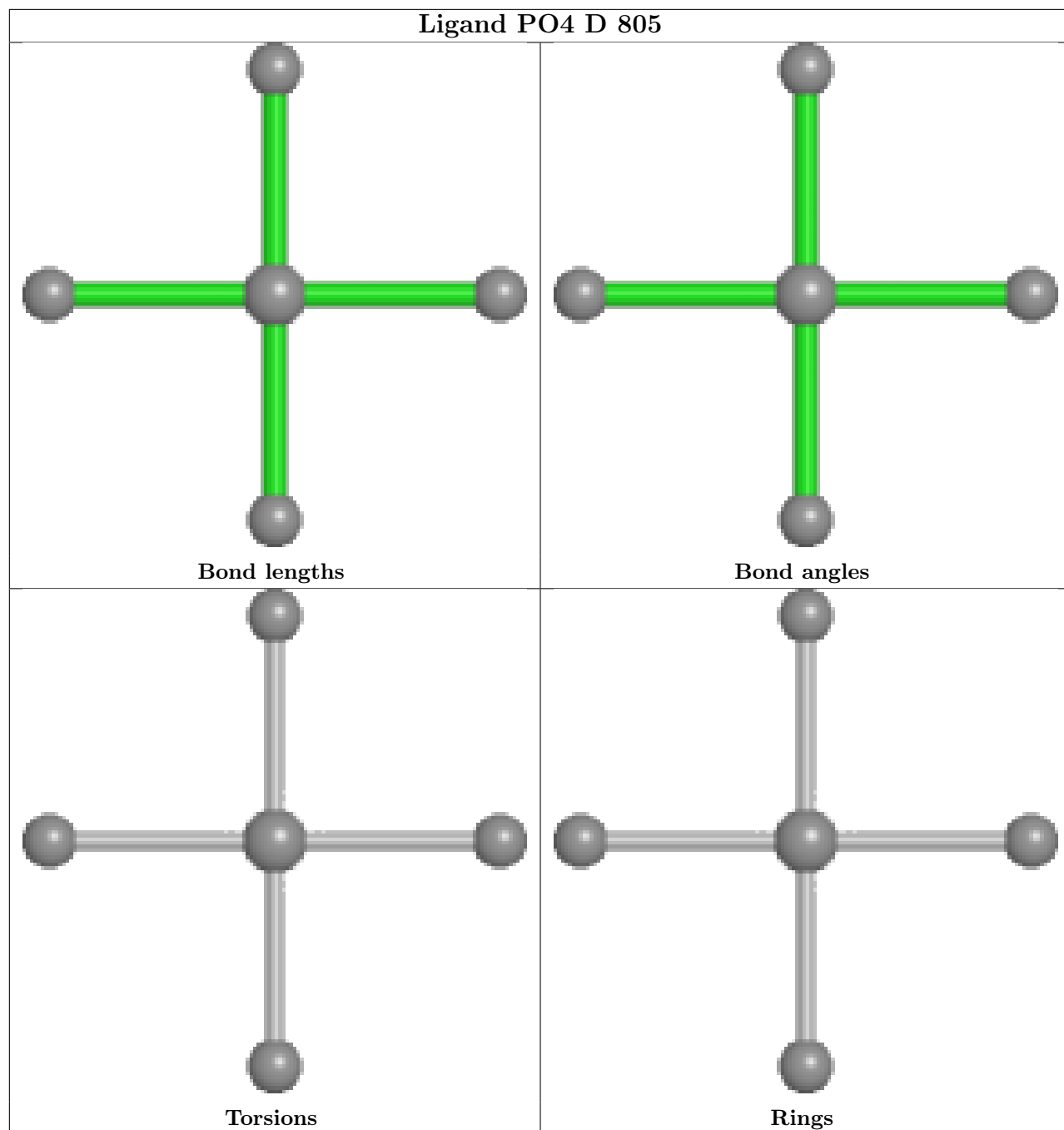




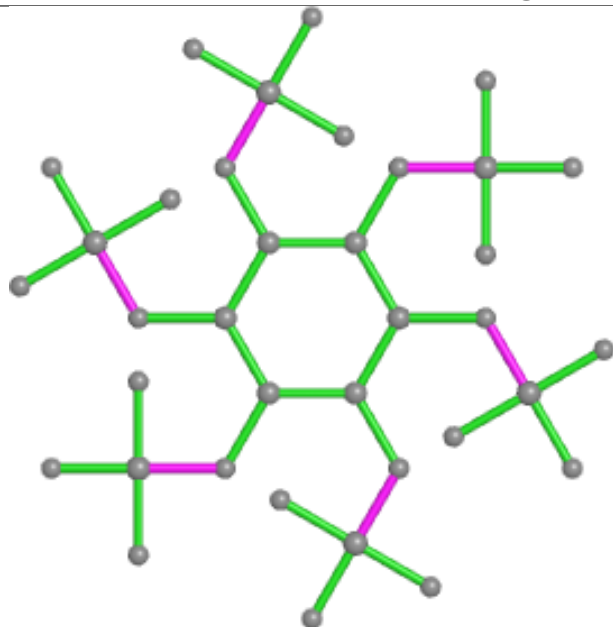




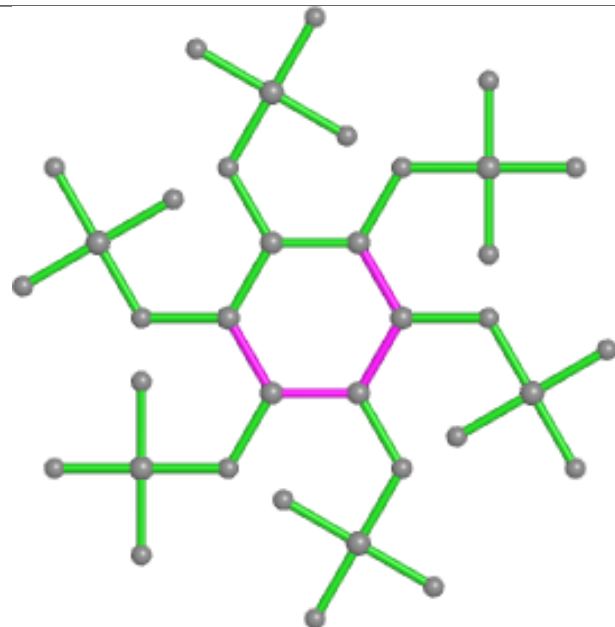




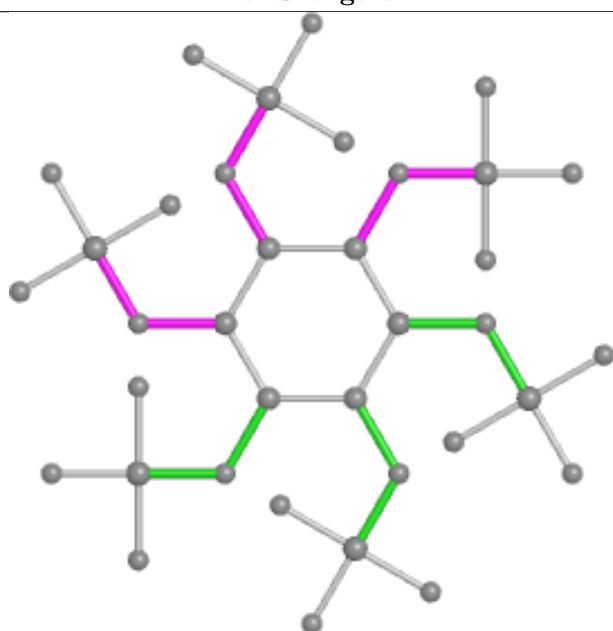
Ligand IHP D 801



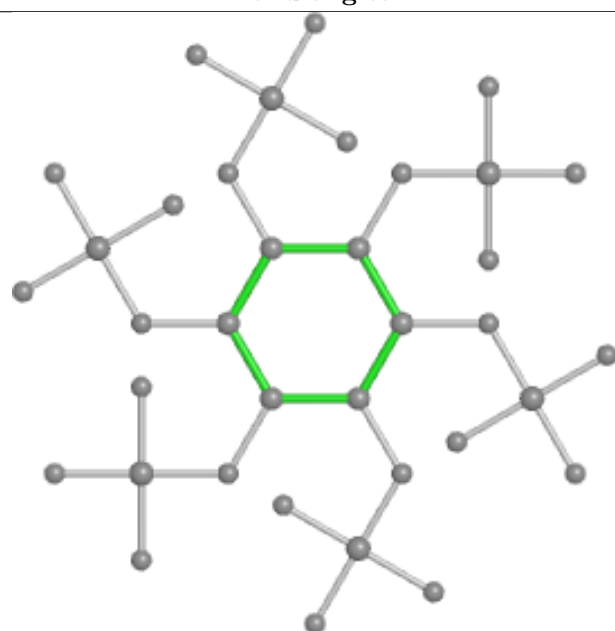
Bond lengths



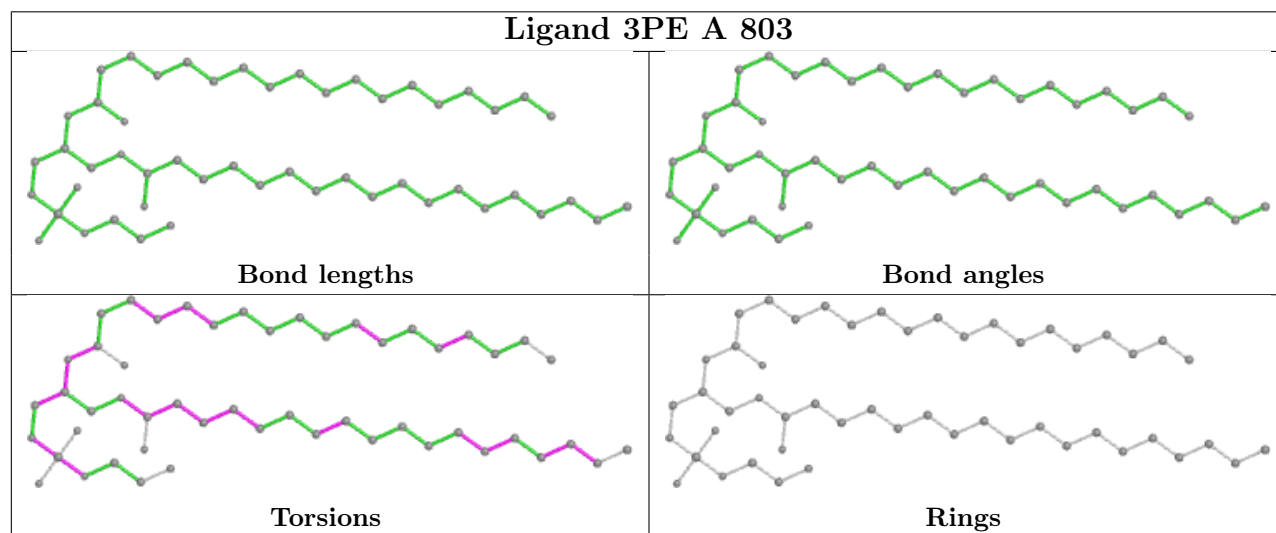
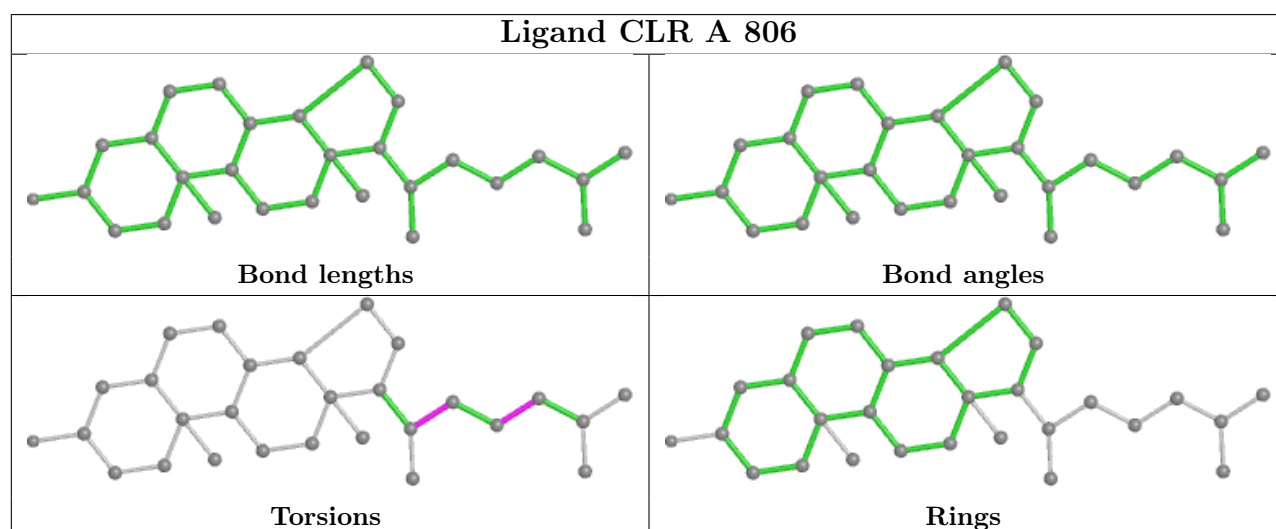
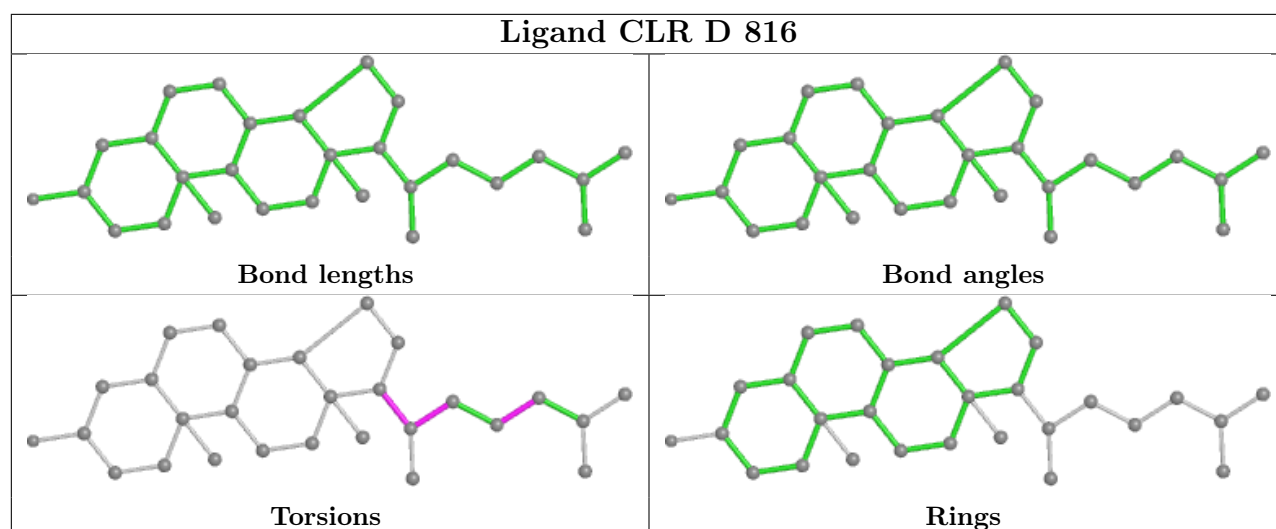
Bond angles

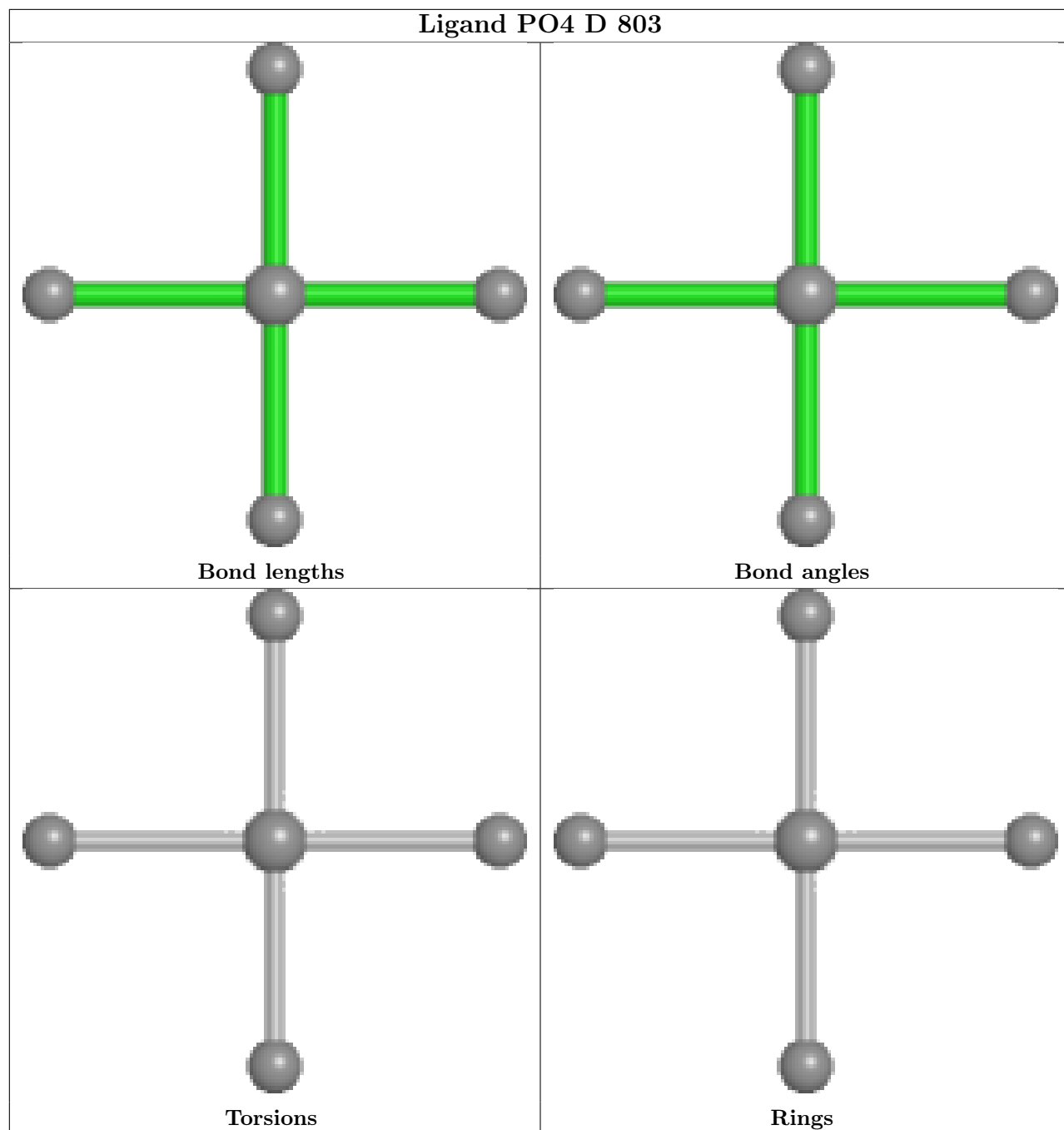


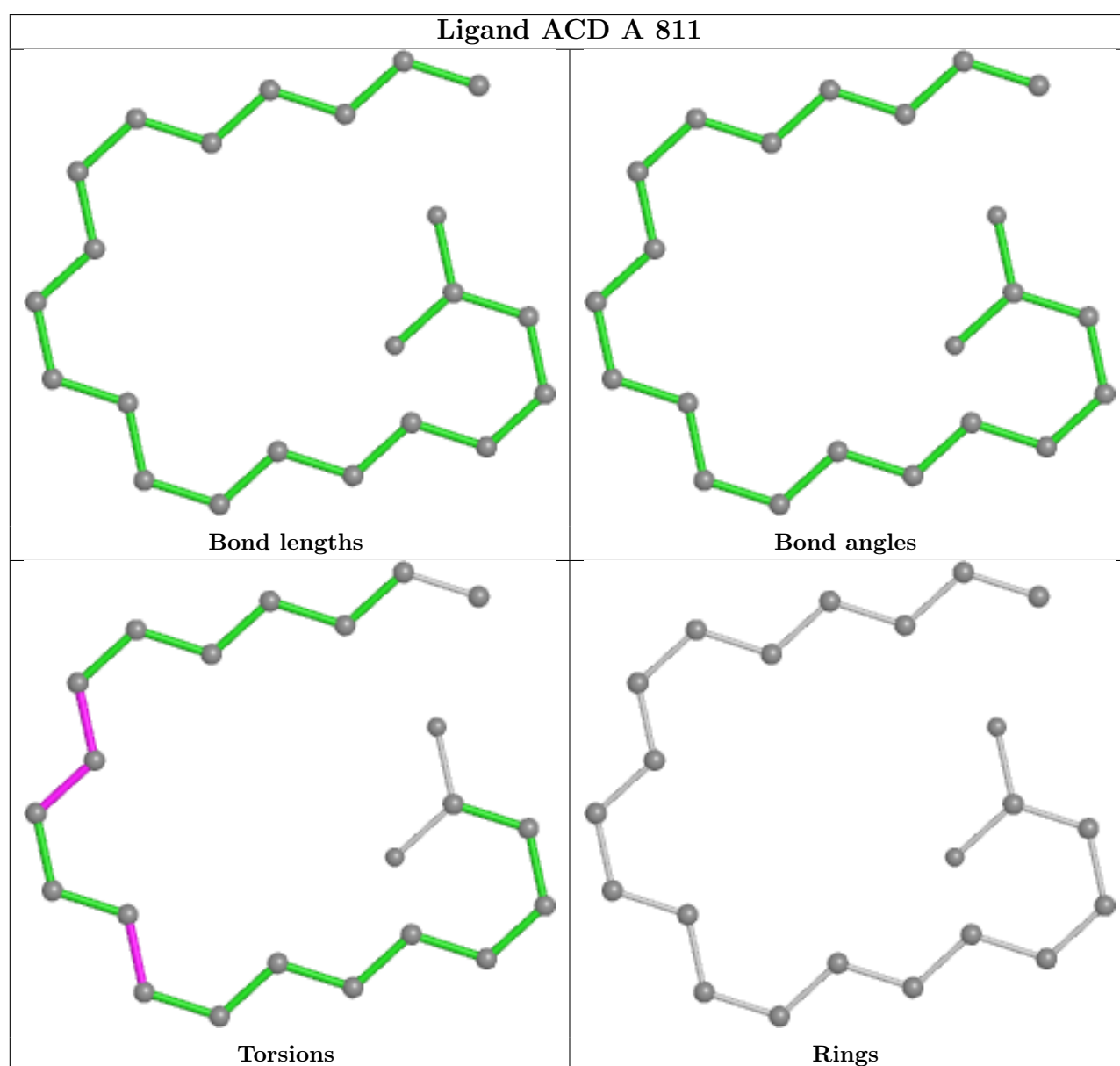
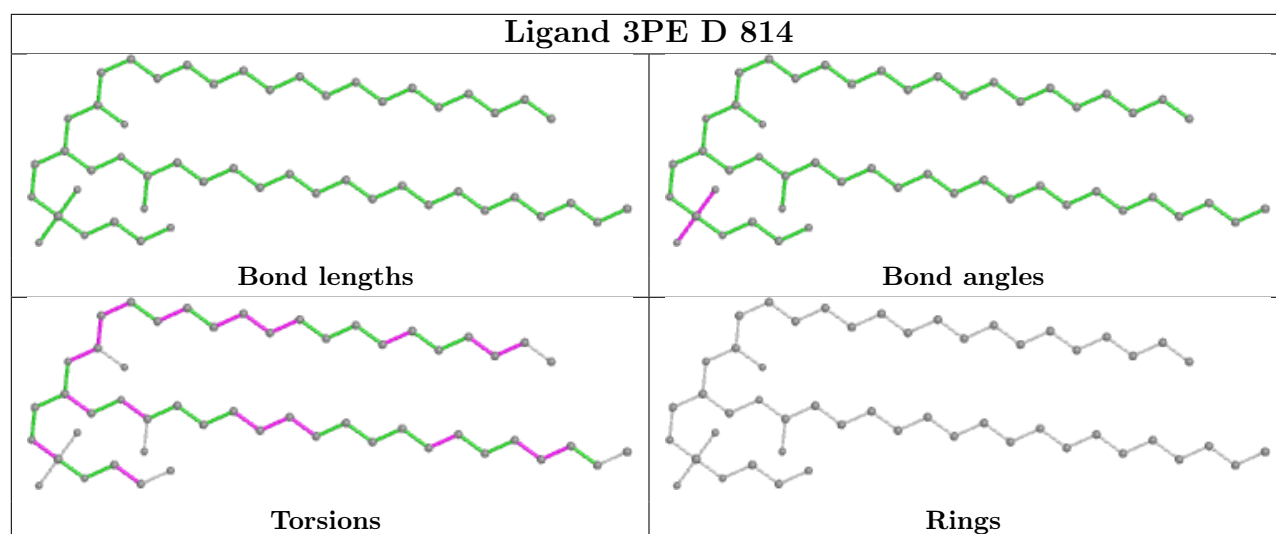
Torsions

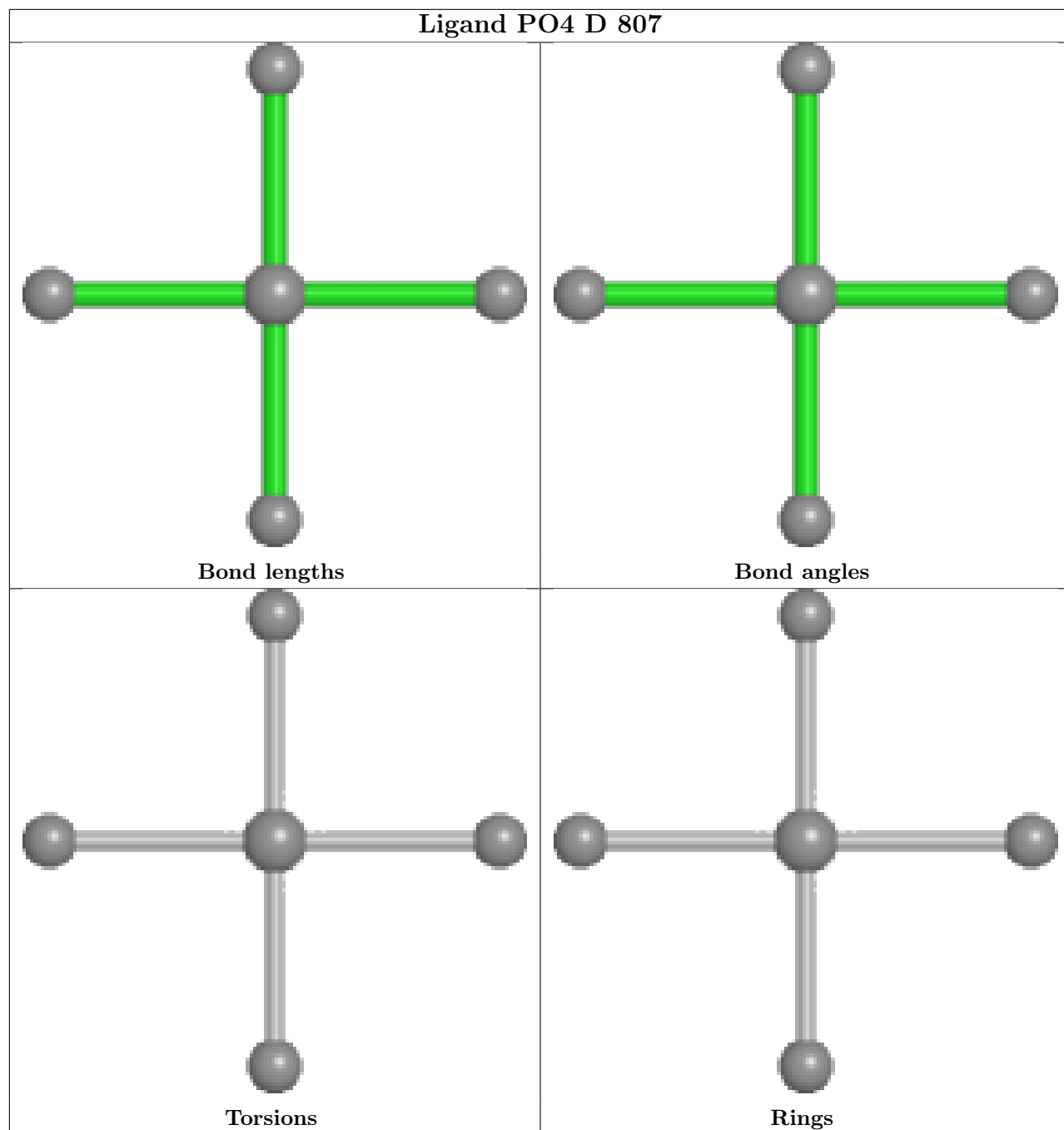


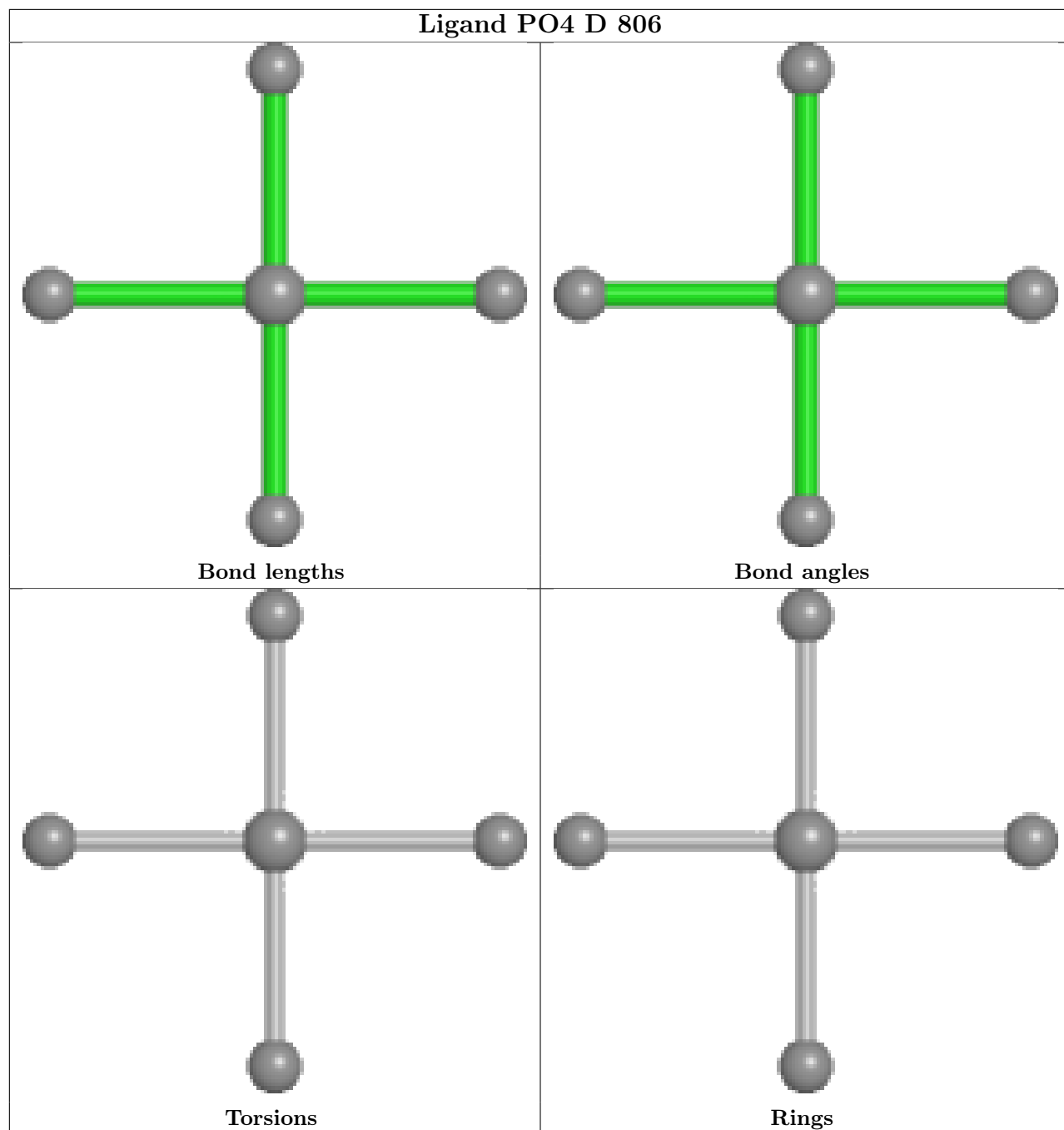
Rings

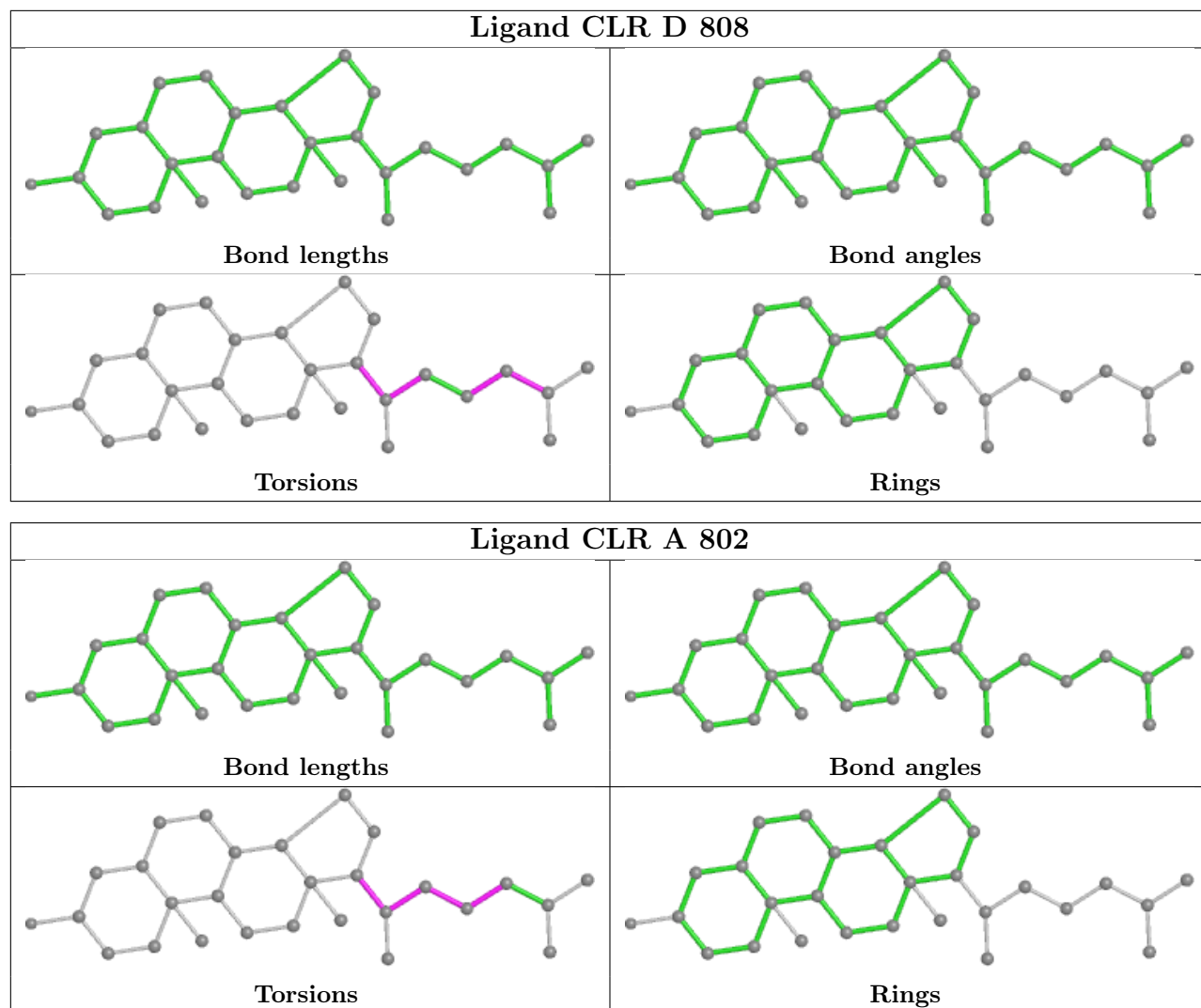


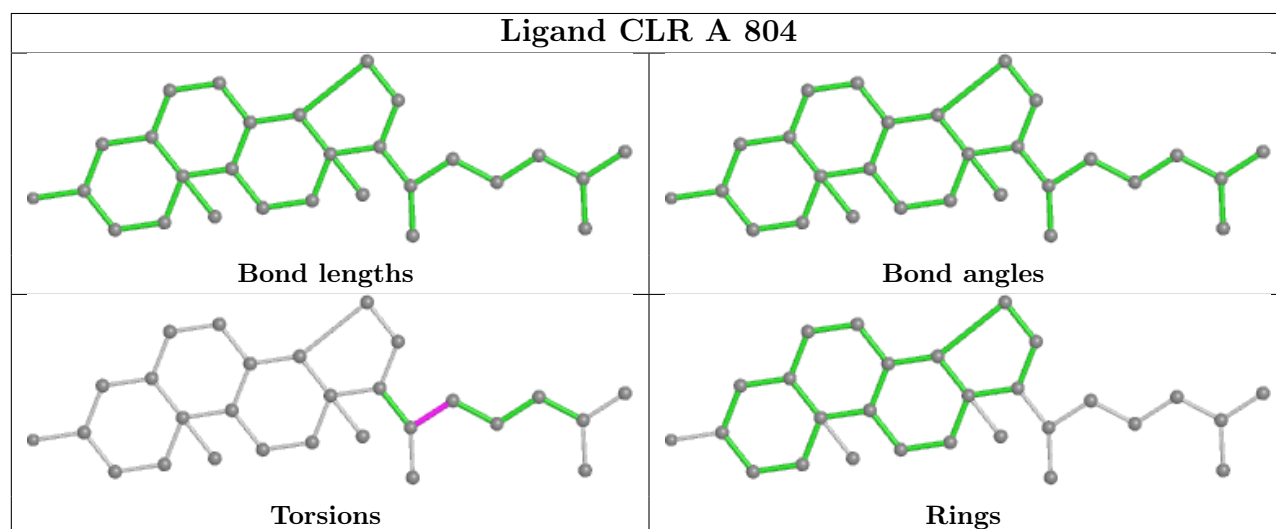
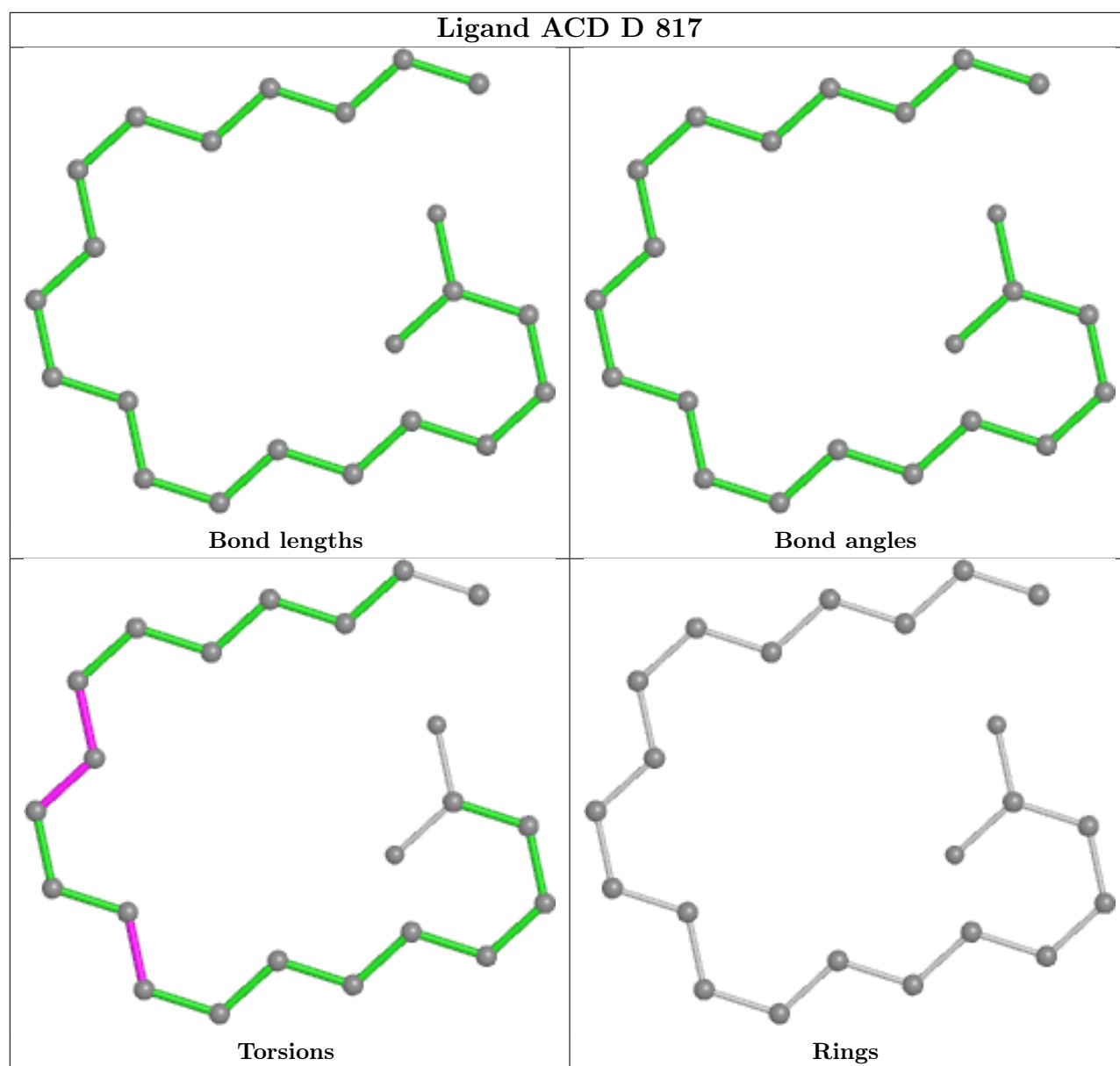


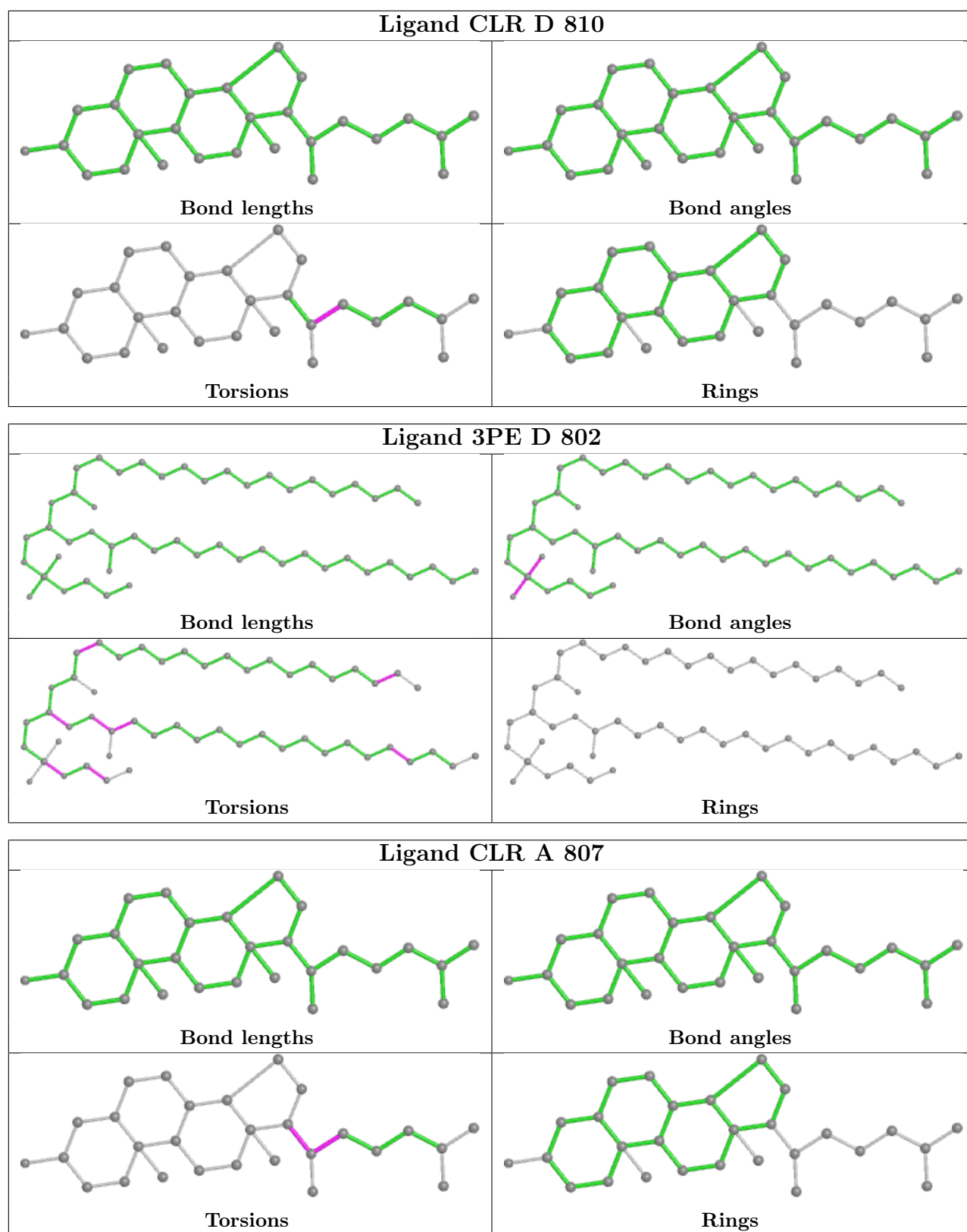


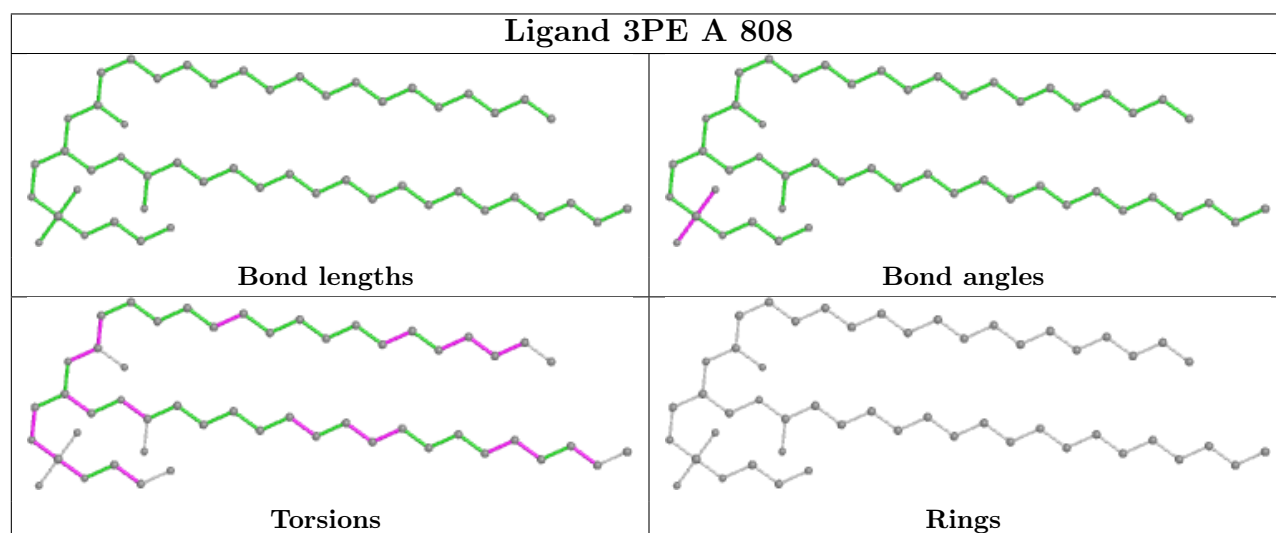
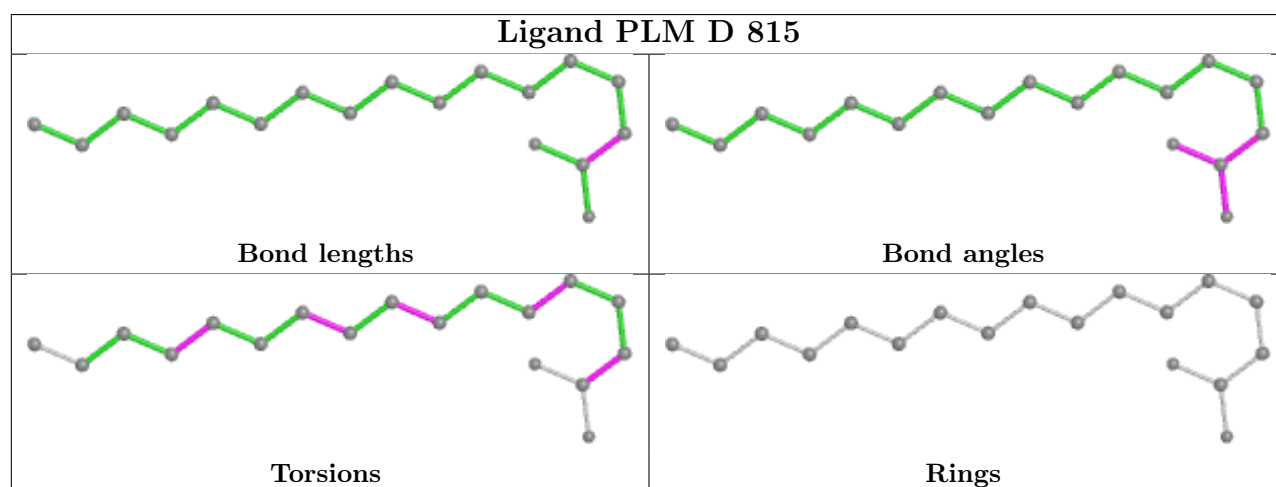
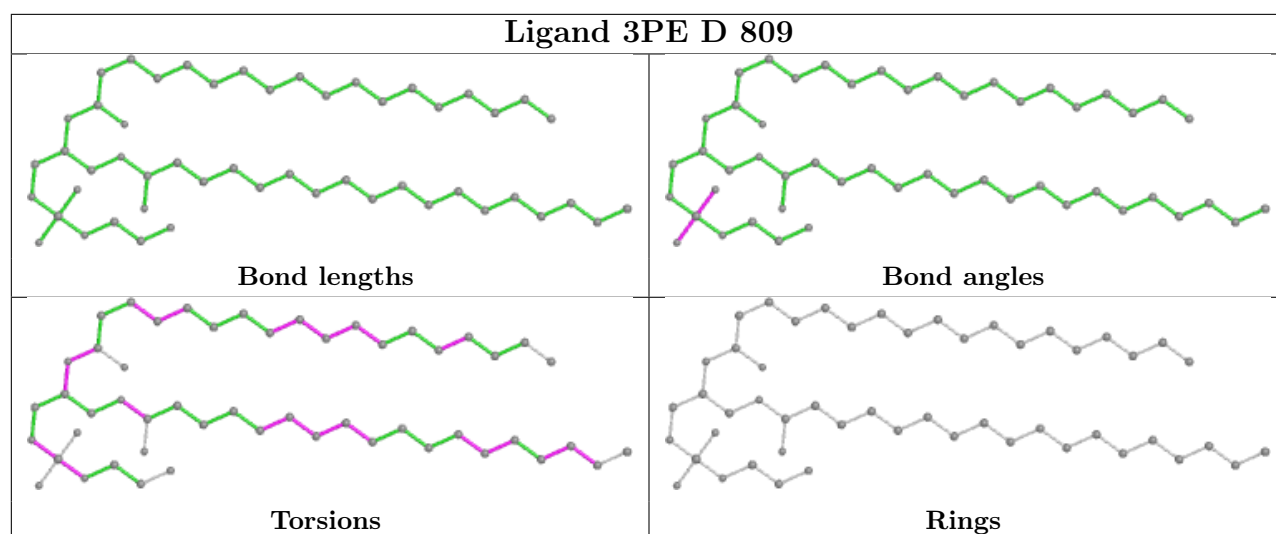




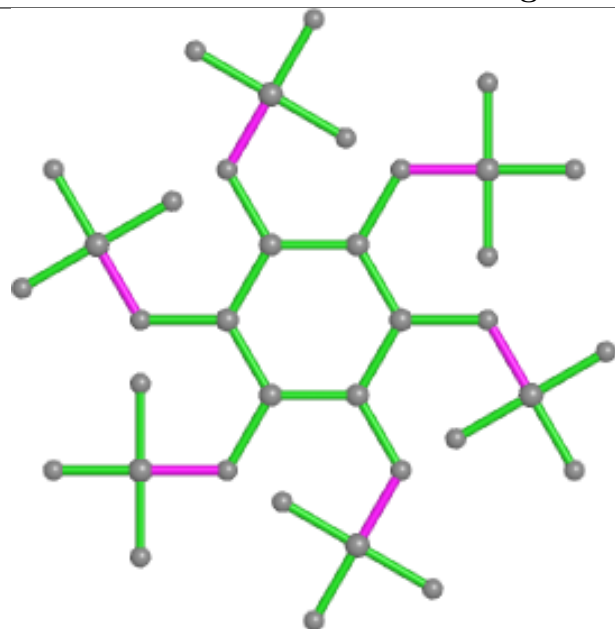




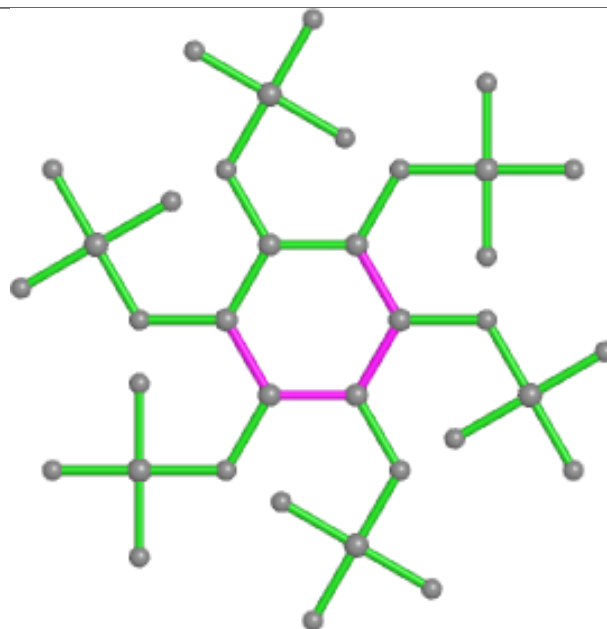




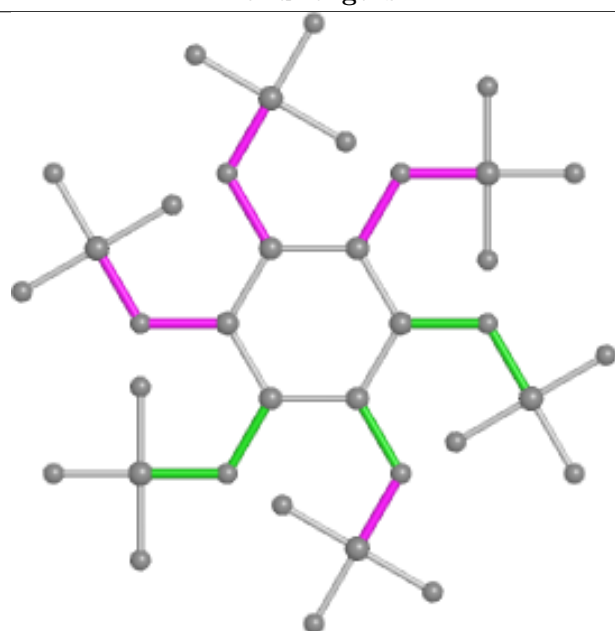
Ligand IHP A 801



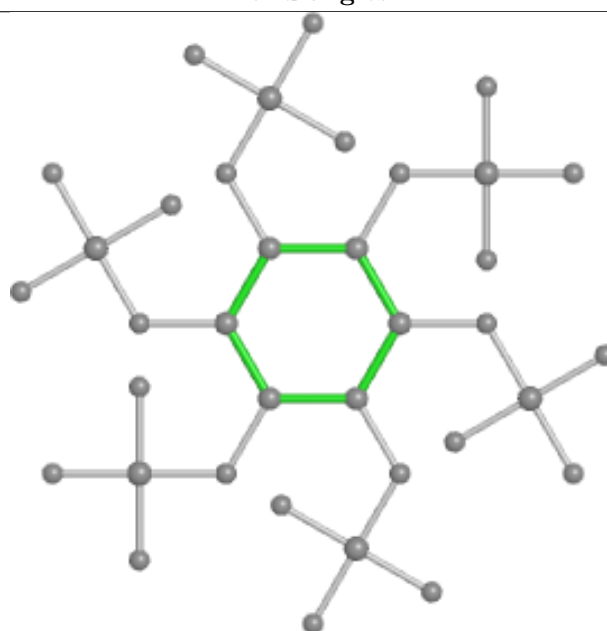
Bond lengths



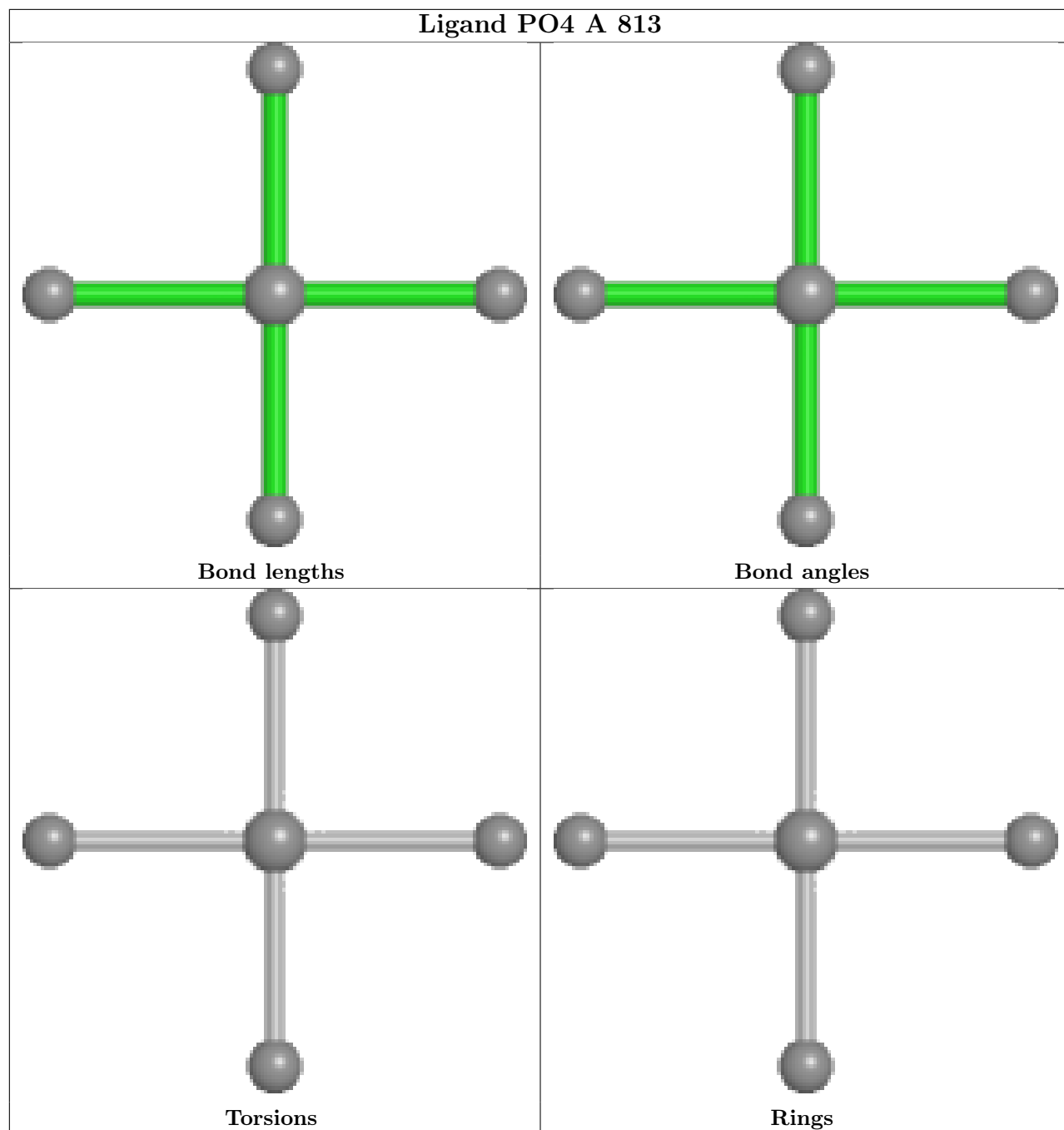
Bond angles

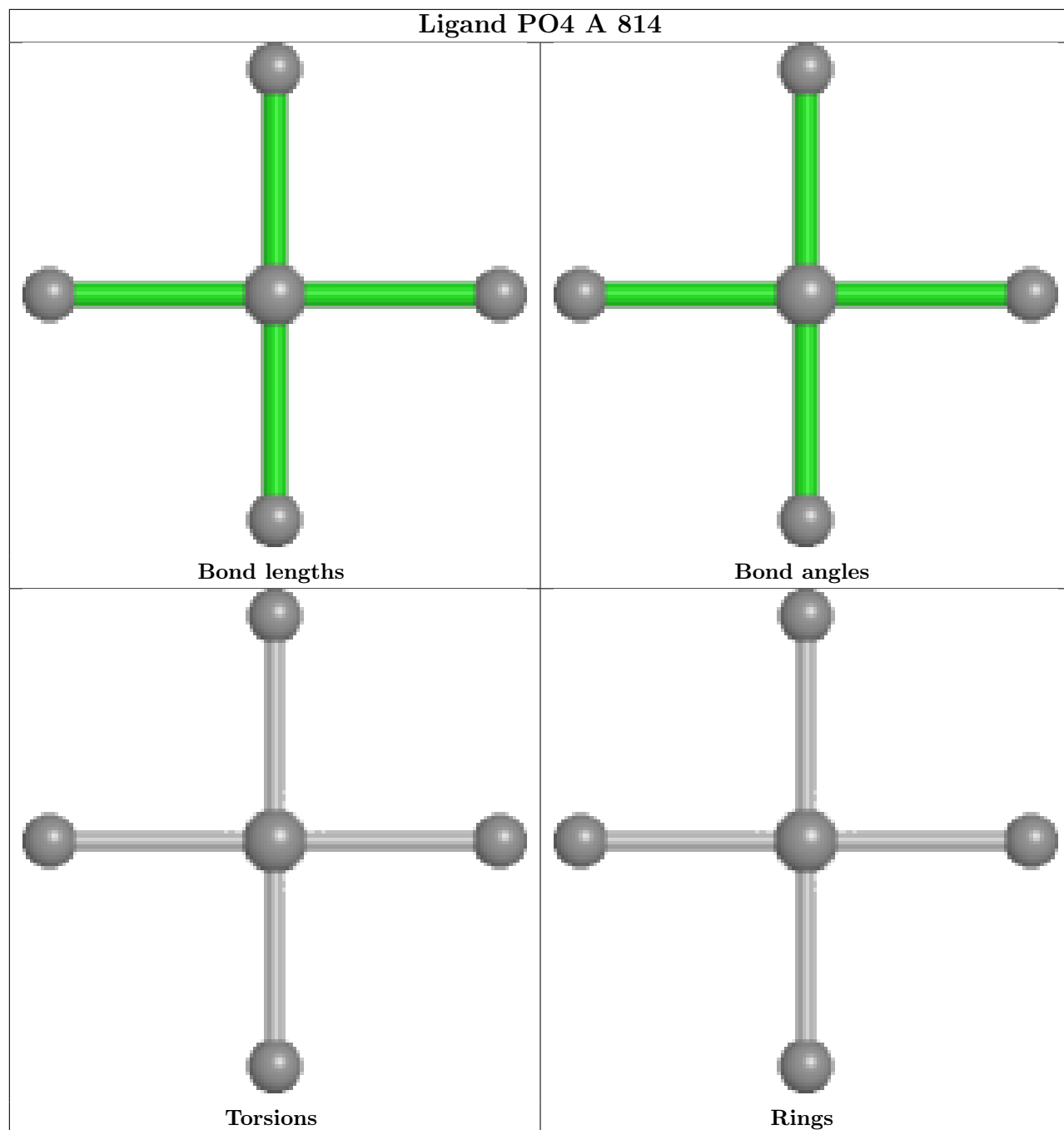


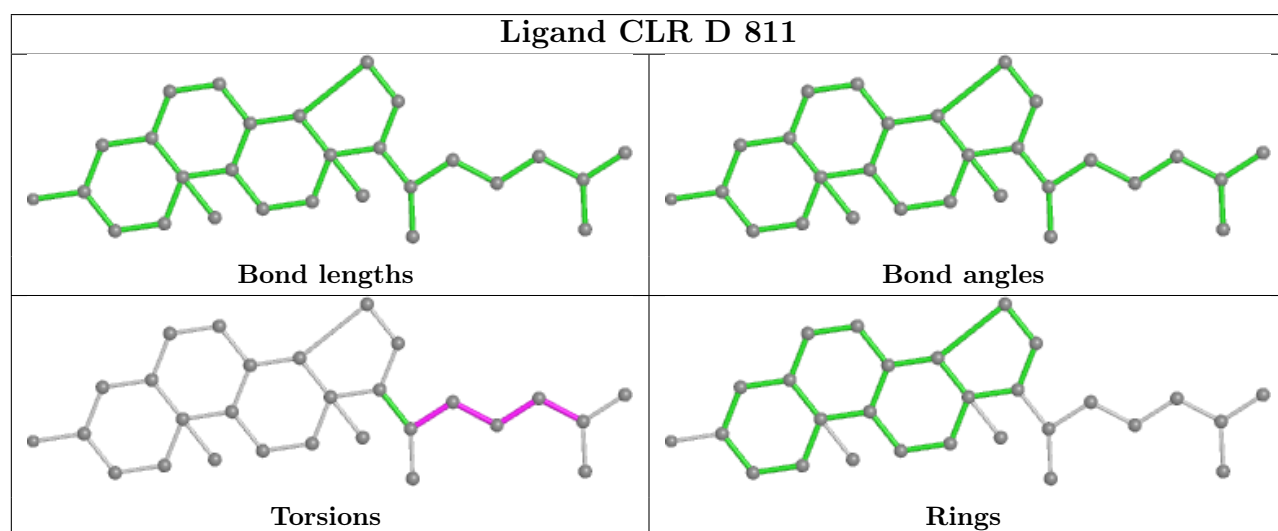
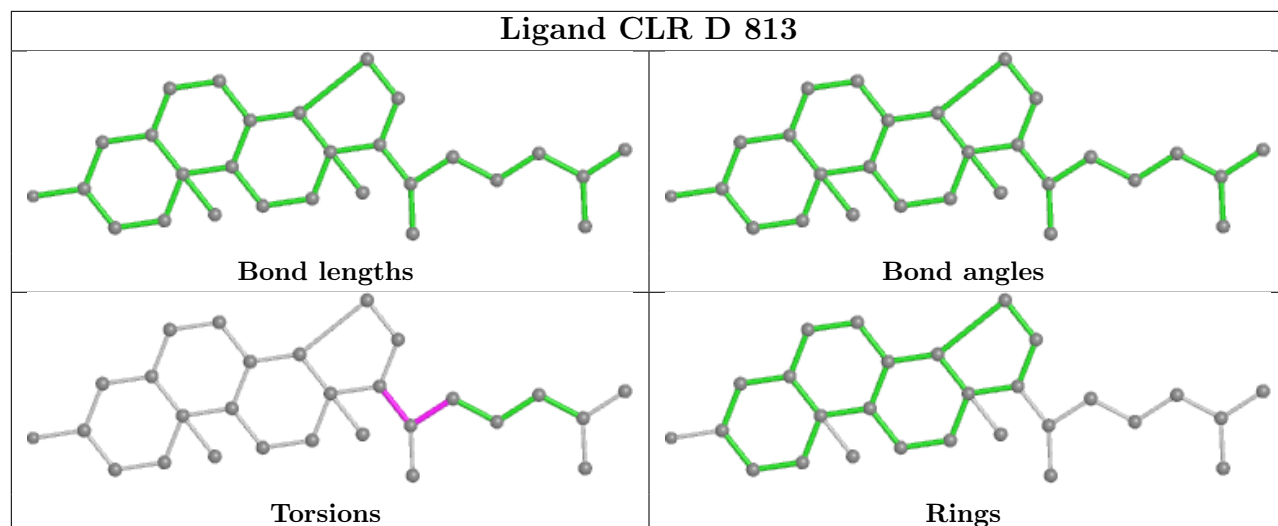
Torsions

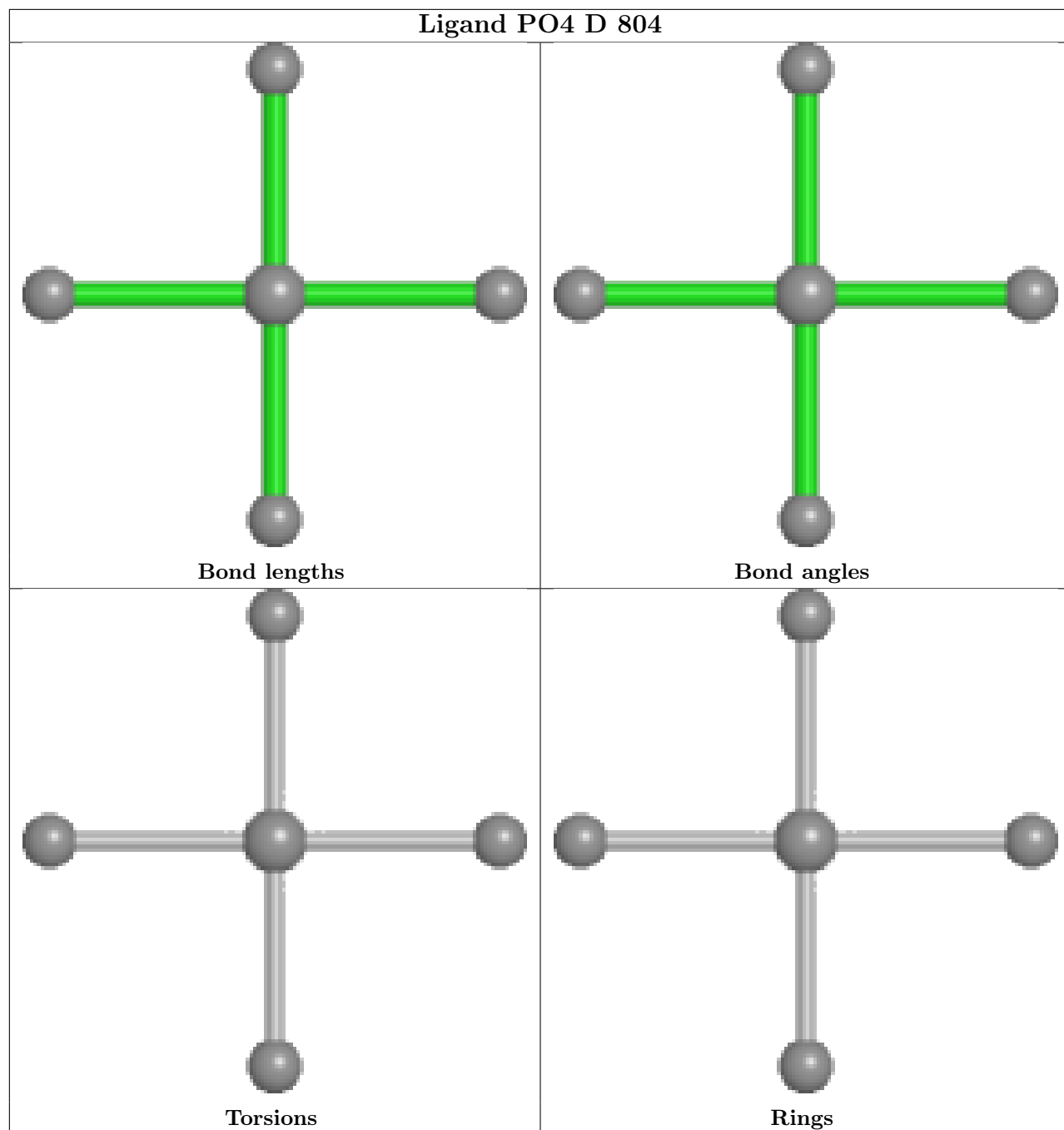


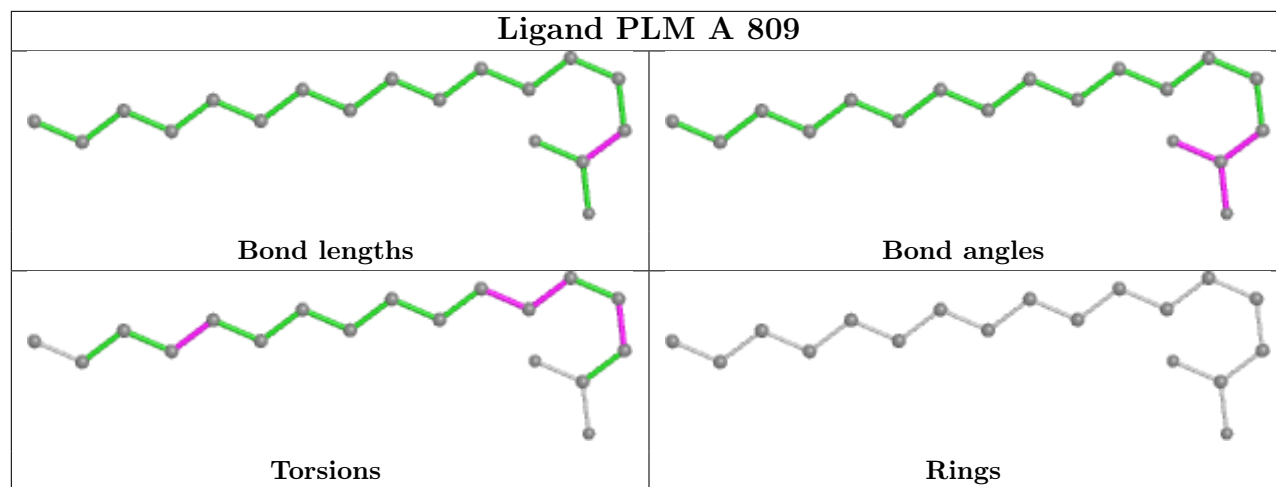
Rings











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.

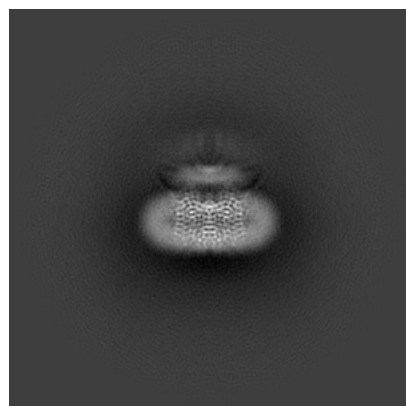
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60707. These allow visual inspection of the internal detail of the map and identification of artifacts.

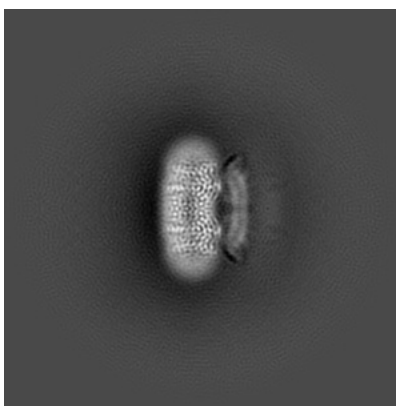
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

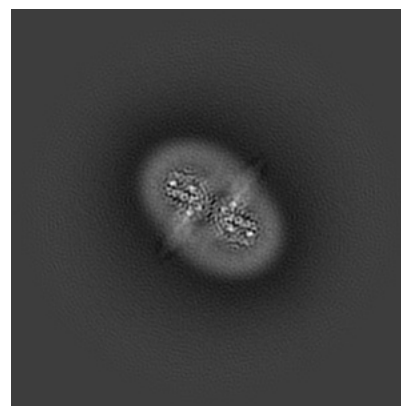
6.1.1 Primary map



X

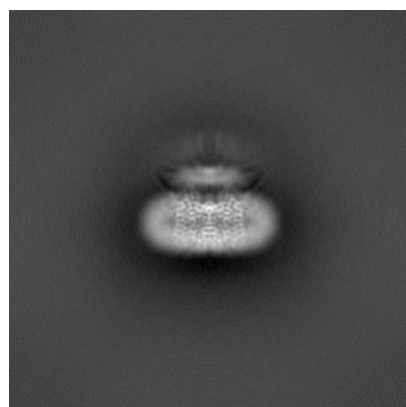


Y

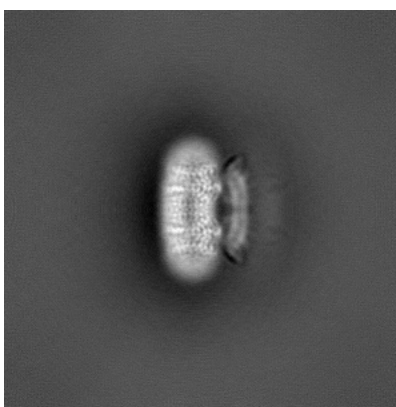


Z

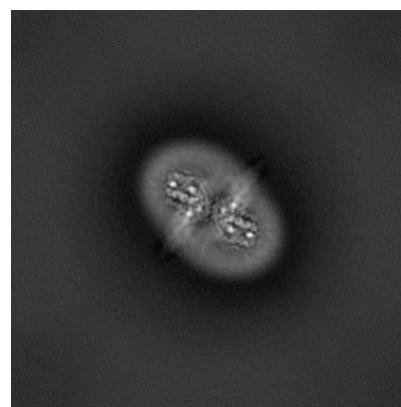
6.1.2 Raw map



X



Y

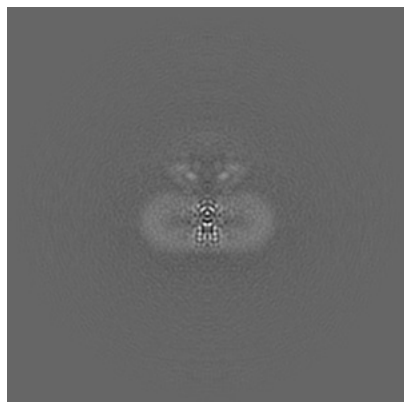


Z

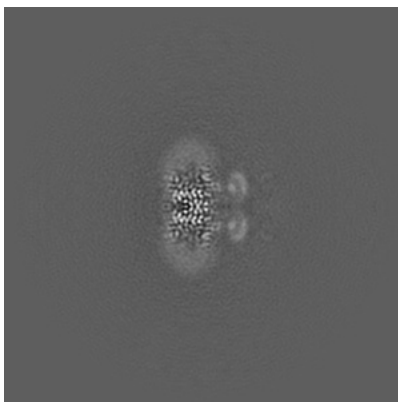
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

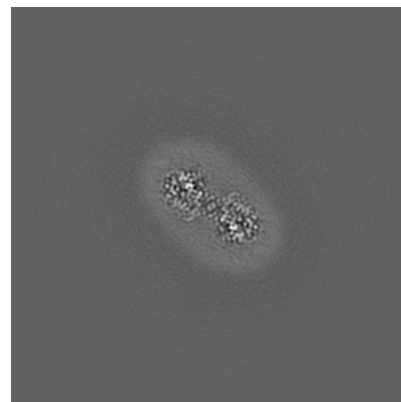
6.2.1 Primary map



X Index: 240

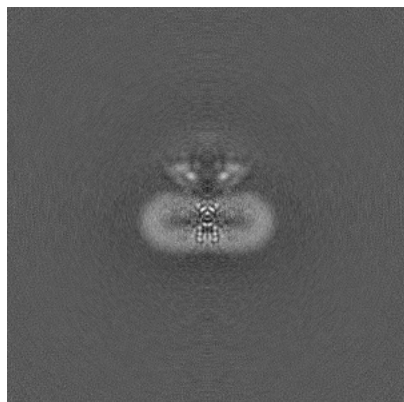


Y Index: 240

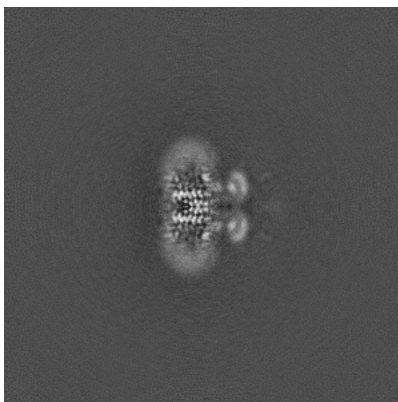


Z Index: 240

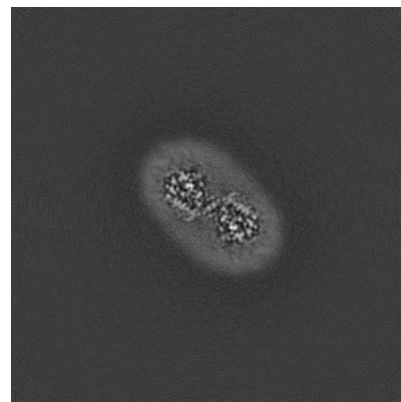
6.2.2 Raw map



X Index: 240



Y Index: 240

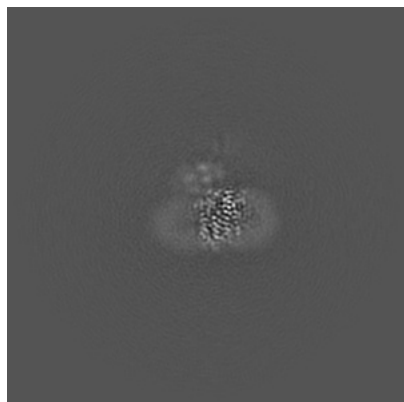


Z Index: 240

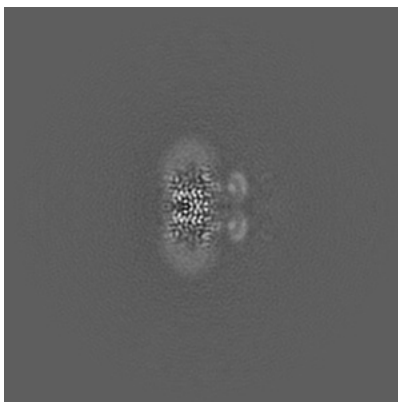
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

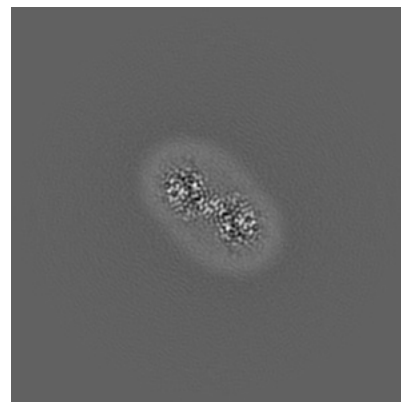
6.3.1 Primary map



X Index: 215

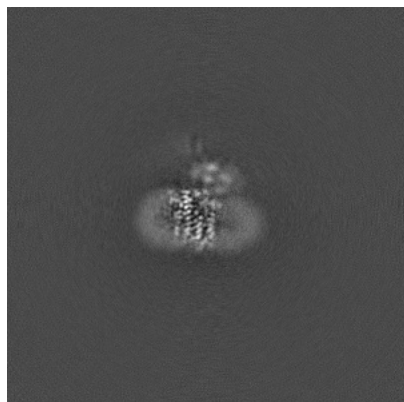


Y Index: 240

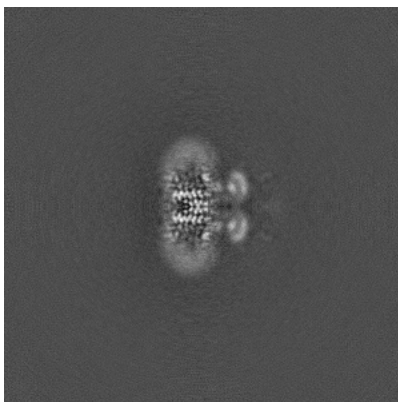


Z Index: 237

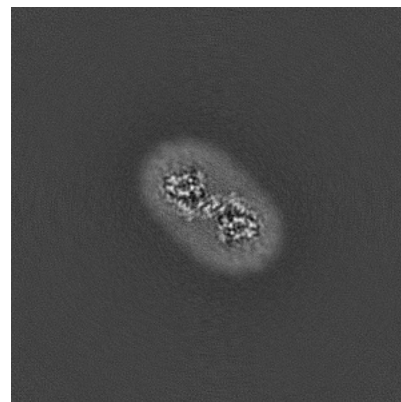
6.3.2 Raw map



X Index: 265



Y Index: 240

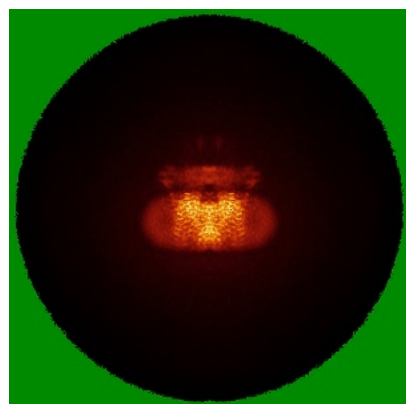


Z Index: 242

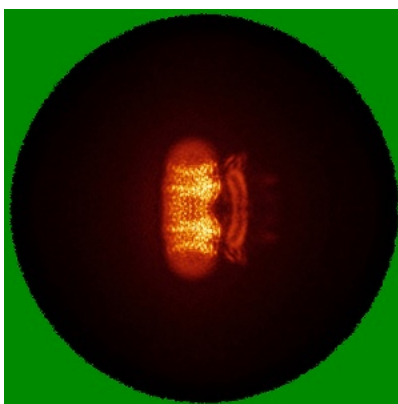
The images above show the largest variance slices of the map in three orthogonal directions.

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

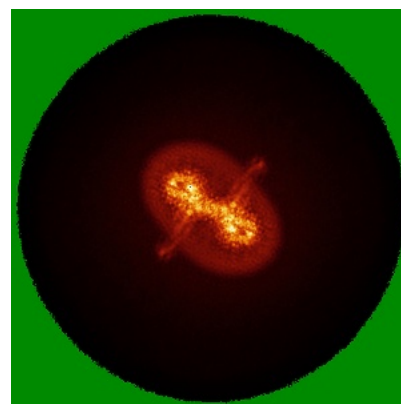
6.4.1 Primary map



X

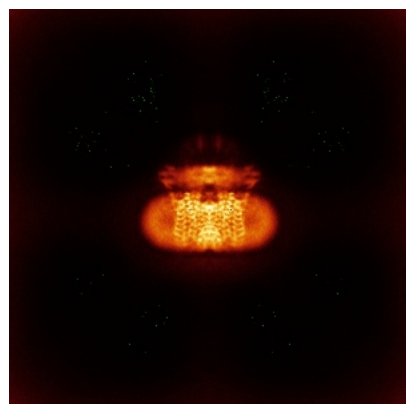


Y

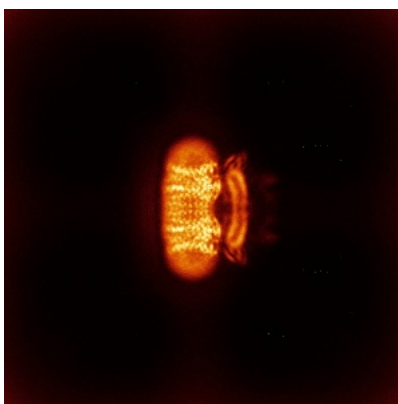


Z

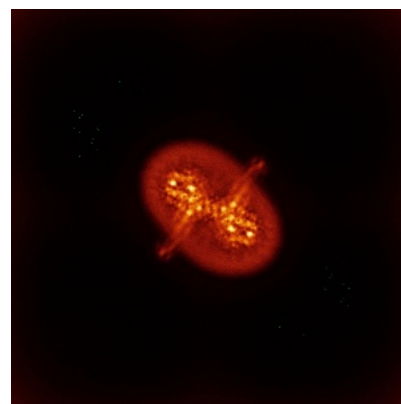
6.4.2 Raw map



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 0.2. 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.

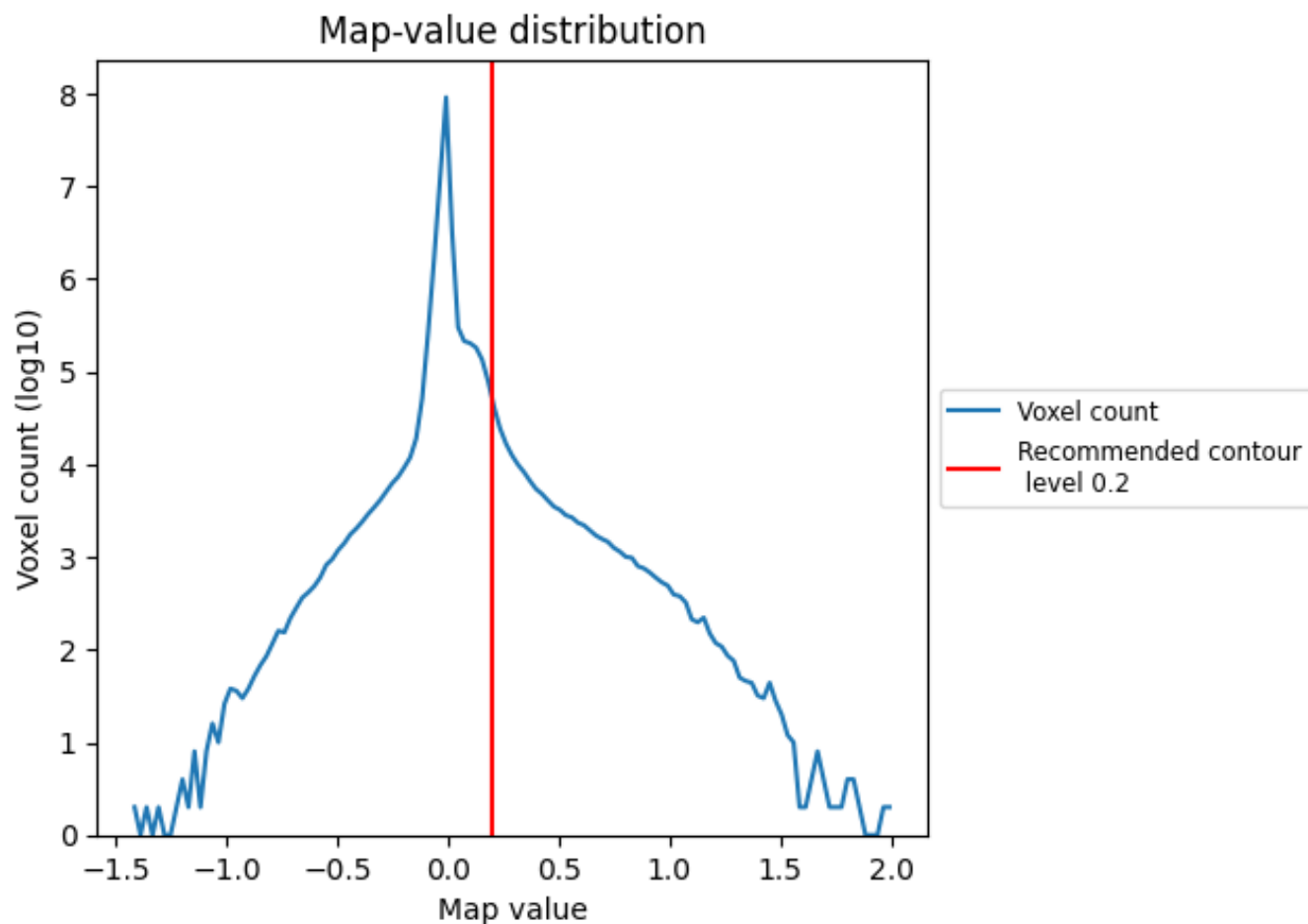
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

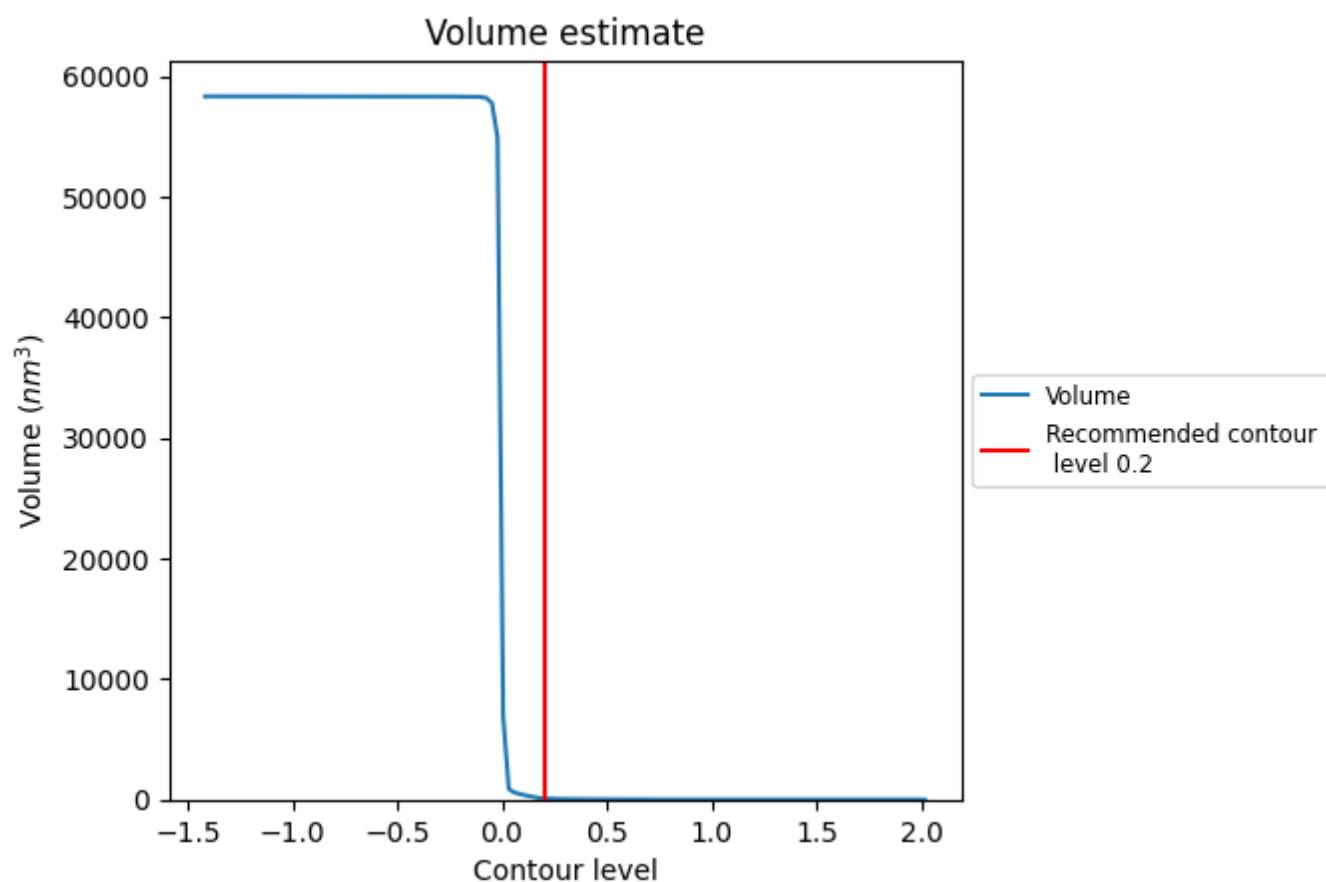
This section contains the results of statistical analysis of the map.

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.

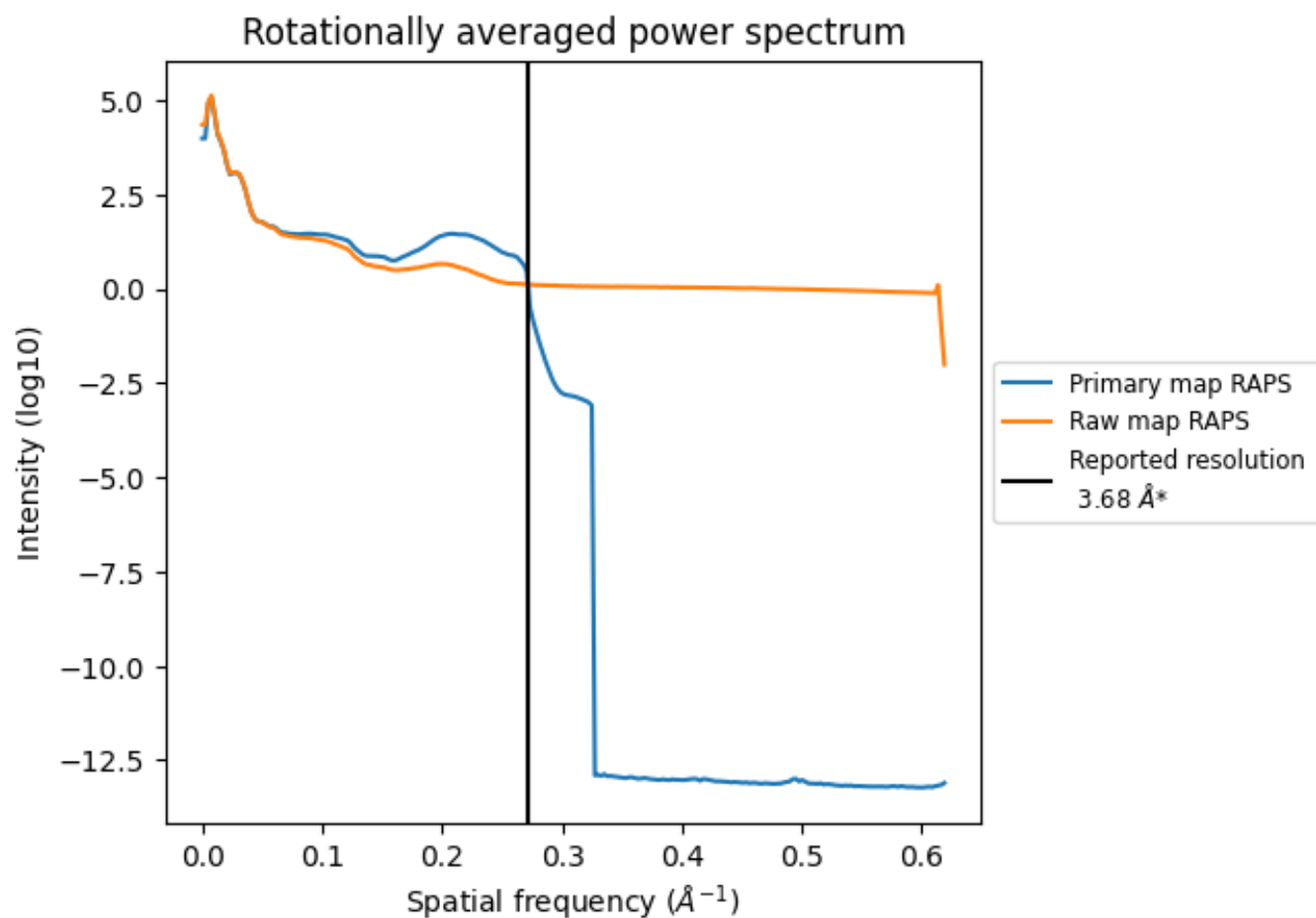
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 99 nm³; this corresponds to an approximate mass of 89 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 ⓘ

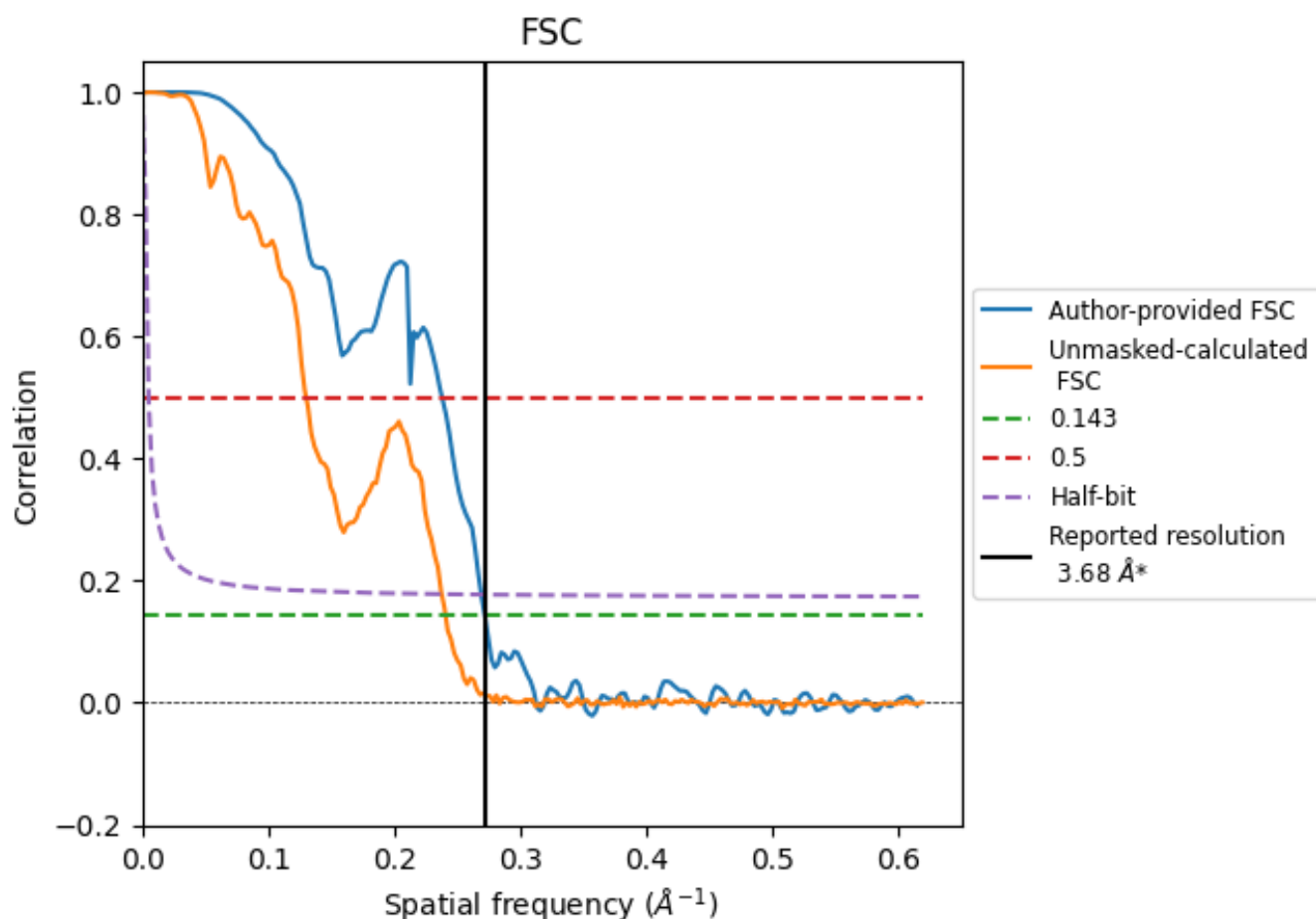


*Reported resolution corresponds to spatial frequency of 0.272 Å⁻¹

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 0.272 \AA^{-1}

8.2 Resolution estimates [i](#)

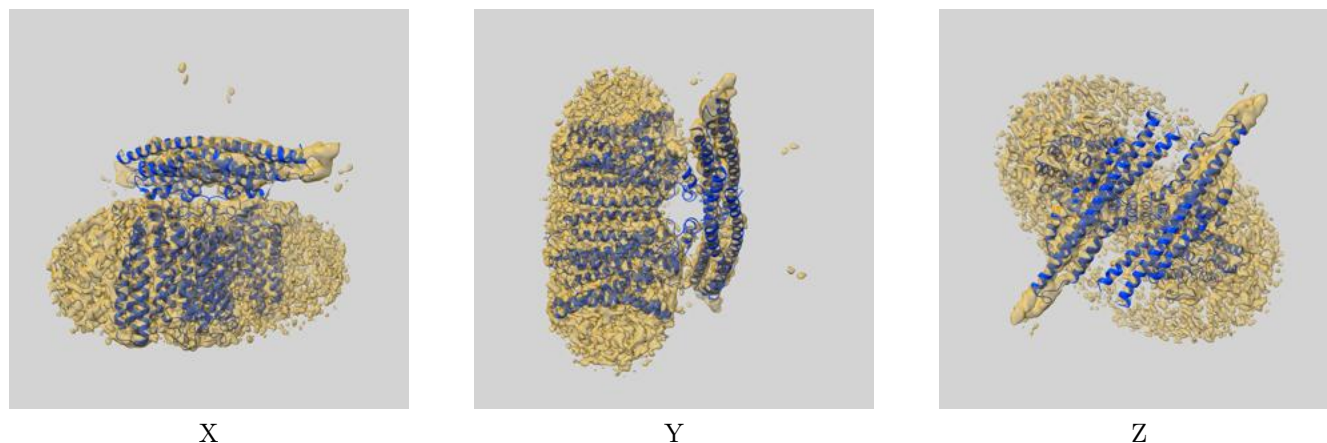
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.68	-	-
Author-provided FSC curve	3.68	4.20	3.72
Unmasked-calculated*	4.15	7.69	4.21

*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 4.15 differs from the reported value 3.68 by more than 10 %

9 Map-model fit [i](#)

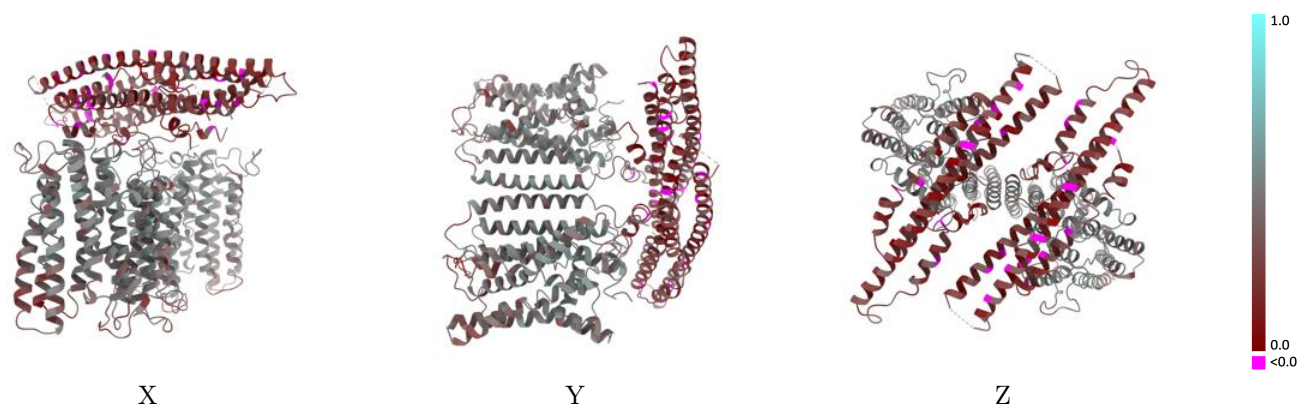
This section contains information regarding the fit between EMDB map EMD-60707 and PDB model 9INH. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



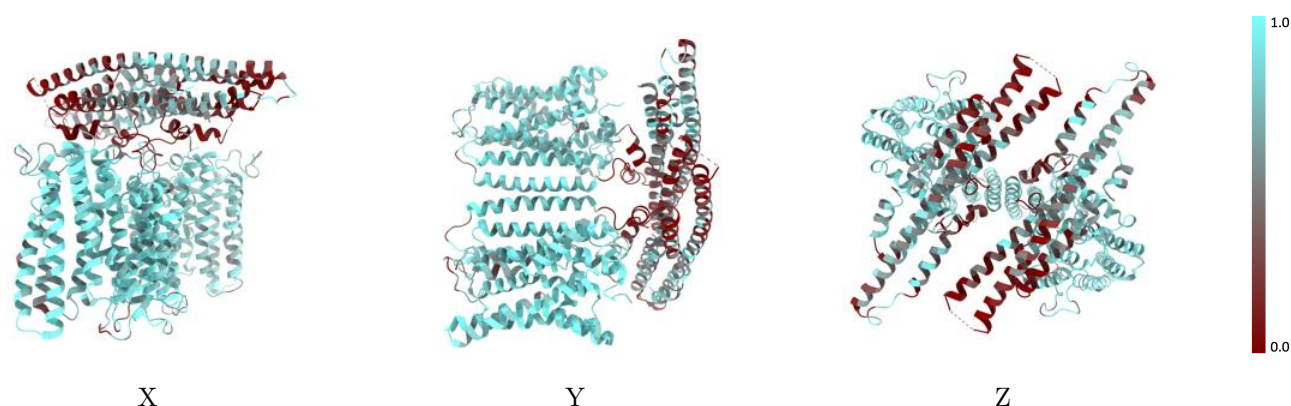
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



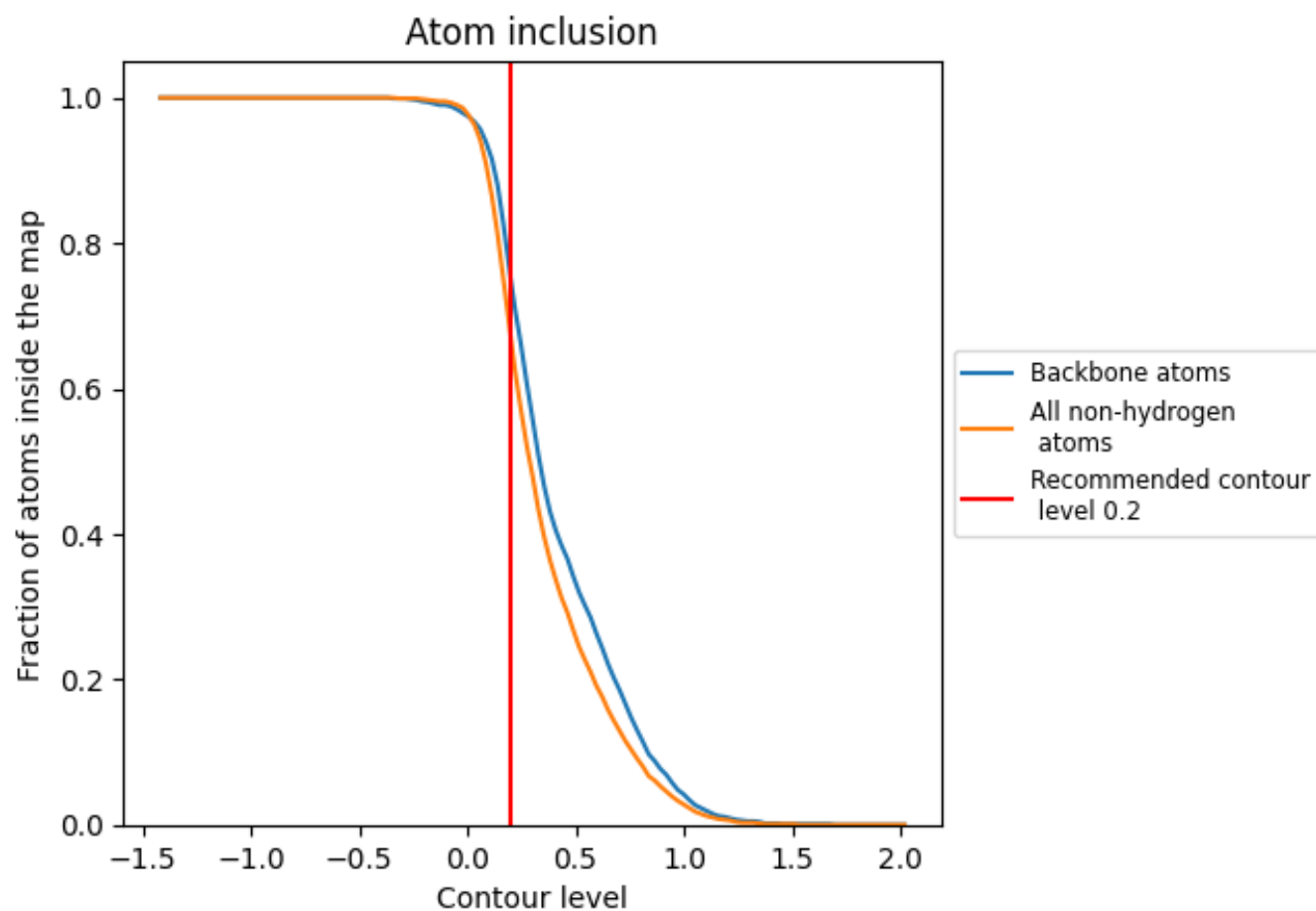
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 67% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6720	<div></div> 0.3700
A	<div></div> 0.6690	<div></div> 0.3700
D	<div></div> 0.6750	<div></div> 0.3710

