



Full wwPDB EM Validation Report ⓘ

Mar 26, 2025 – 02:26 PM JST

PDB ID : 9INE
EMDB ID : EMD-60704
Title : Cryo-EM structure of human XPR1 in closed state in the presence of KIDINS220-1-432
Authors : Zuo, P.; Liang, L.; Yin, Y.
Deposited on : 2024-07-06
Resolution : 3.32 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

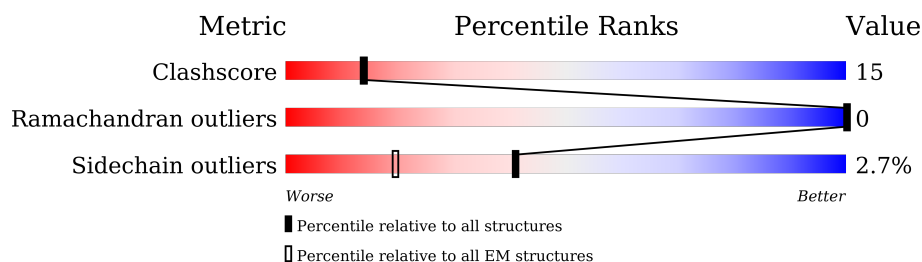
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.32 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	 6% 37% 20% 43%
1	B	704	 7% 38% 18% 43%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7520 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	B	401	Total	C	N	O	S	0	0
			3333	2233	535	549	16		
1	A	401	Total	C	N	O	S	0	0
			3333	2233	535	549	16		

There are 16 discrepancies between the modelled and reference sequences:

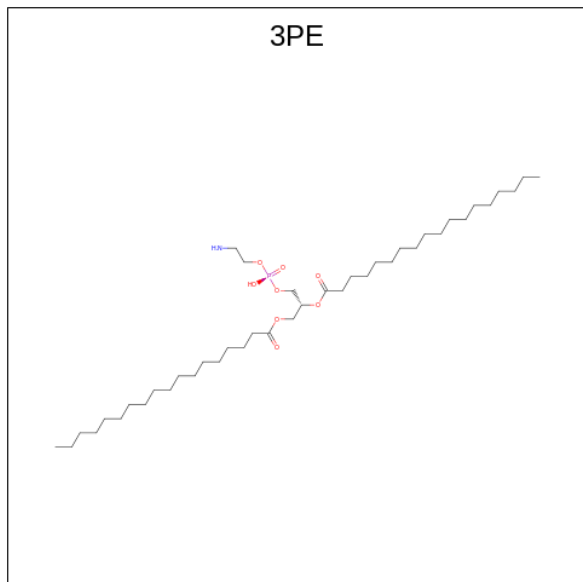
Chain	Residue	Modelled	Actual	Comment	Reference
B	697	SER	-	expression tag	UNP Q9UBH6
B	698	ARG	-	expression tag	UNP Q9UBH6
B	699	GLU	-	expression tag	UNP Q9UBH6
B	700	ASN	-	expression tag	UNP Q9UBH6
B	701	LEU	-	expression tag	UNP Q9UBH6
B	702	TYR	-	expression tag	UNP Q9UBH6
B	703	PHE	-	expression tag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

- Molecule 2 is CHOLESTEROL (three-letter code: CLR) (formula: C₂₇H₄₆O) (labeled as "Ligand of Interest" by depositor).



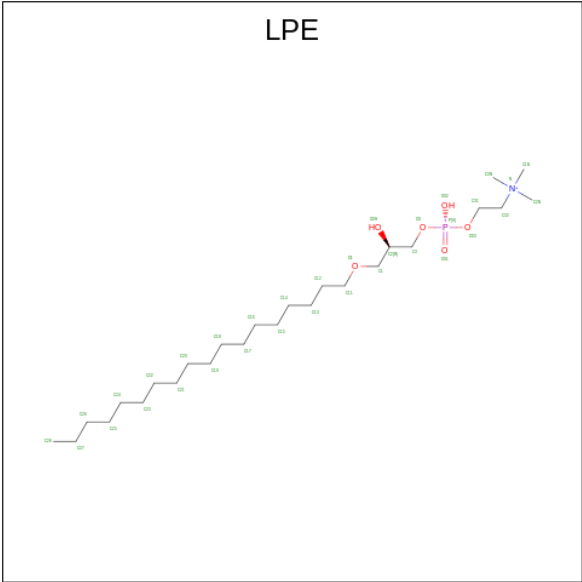
Mol	Chain	Residues	Atoms			AltConf
2	B	1	Total	C	O	0
			28	27	1	
2	B	1	Total	C	O	0
			28	27	1	
2	B	1	Total	C	O	0
			28	27	1	
2	B	1	Total	C	O	0
			28	27	1	
2	B	1	Total	C	O	0
			28	27	1	
2	B	1	Total	C	O	0
			28	27	1	
2	A	1	Total	C	O	0
			28	27	1	
2	A	1	Total	C	O	0
			28	27	1	
2	A	1	Total	C	O	0
			28	27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

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



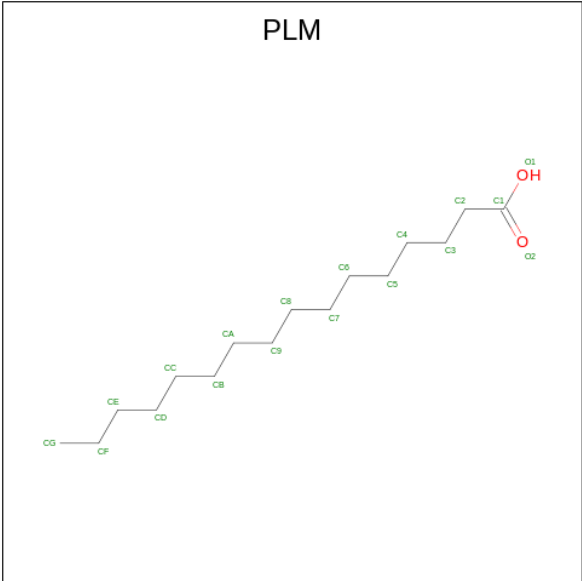
Mol	Chain	Residues	Atoms					AltConf
3	B	1	Total	C	N	O	P	0
			51	41	1	8	1	
3	B	1	Total	C	N	O	P	0
			51	41	1	8	1	
3	B	1	Total	C	N	O	P	0
			51	41	1	8	1	
3	B	1	Total	C	N	O	P	0
			51	41	1	8	1	
3	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
3	A	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 4 is 1-O-OCTADECYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: LPE) (formula: $C_{26}H_{57}NO_6P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
4	B	1	Total	C	N	O	P	0
			34	26	1	6	1	
4	A	1	Total	C	N	O	P	0
			34	26	1	6	1	

- Molecule 5 is PALMITIC ACID (three-letter code: PLM) (formula: C₁₆H₃₂O₂) (labeled as "Ligand of Interest" by depositor).



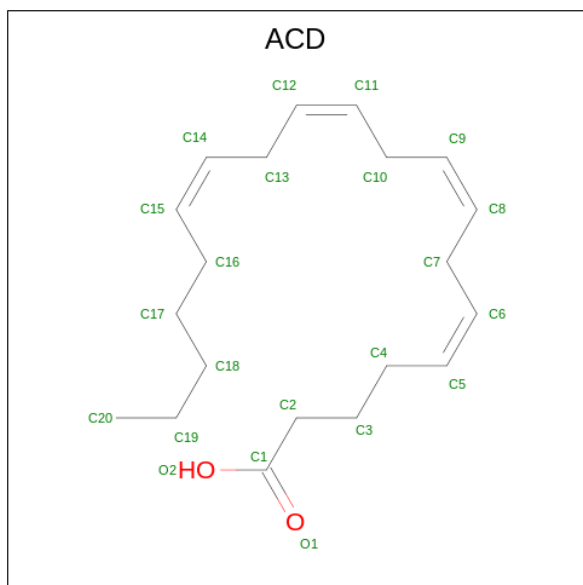
Mol	Chain	Residues	Atoms			AltConf
5	B	1	Total	C	O	0
			18	16	2	

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

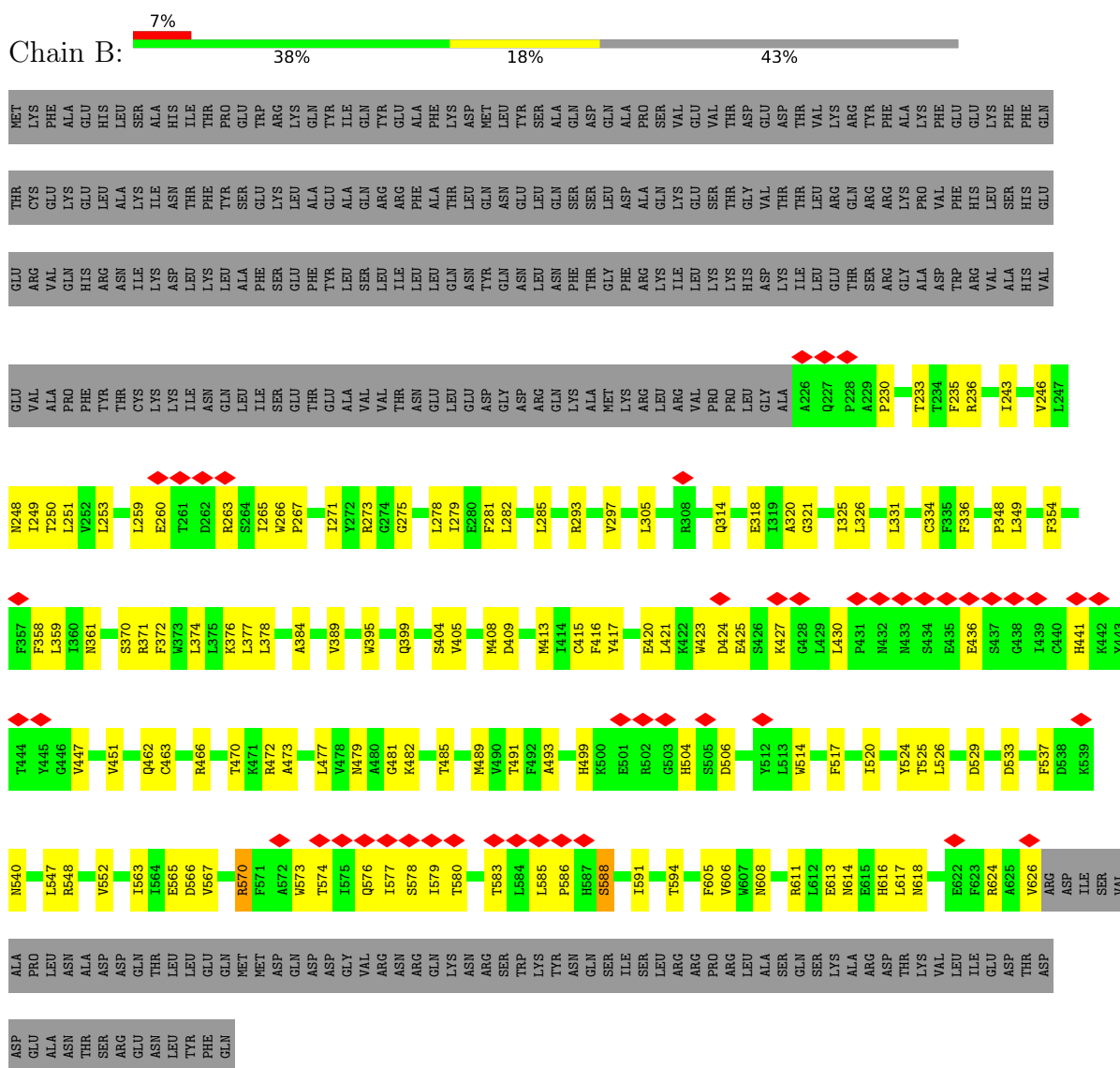
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		AltConf
7	B	4	Total	O	0
			4	4	
7	A	4	Total	O	0
			4	4	

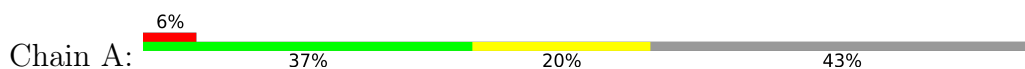
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Solute carrier family 53 member 1



- Molecule 1: Solute carrier family 53 member 1





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	187463	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)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.337	Depositor
Minimum map value	-0.831	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.165	Depositor
Map size (\AA)	377.66, 377.66, 377.66	wwPDB
Map dimensions	460, 460, 460	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.821, 0.821, 0.821	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.28	0/3444	0.47	0/4688
1	B	0.28	0/3444	0.48	0/4688
All	All	0.28	0/6888	0.47	0/9376

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	3333	0	3317	114	0
1	B	3333	0	3317	101	0
2	A	196	0	322	18	0
2	B	196	0	322	19	0
3	A	102	0	164	10	0
3	B	204	0	328	23	0
4	A	34	0	56	2	0
4	B	34	0	56	2	0
5	A	18	0	31	3	0
5	B	18	0	31	3	0
6	A	22	0	31	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	22	0	31	0	0
7	A	4	0	0	3	0
7	B	4	0	0	3	0
All	All	7520	0	8006	240	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 15.

All (240) 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:566:ASP:O	1:A:570:ARG:HB2	1.82	0.80
1:A:405:VAL:HG22	1:A:577:ILE:HG12	1.63	0.79
1:B:566:ASP:O	1:B:570:ARG:HB2	1.87	0.75
1:B:405:VAL:HG22	1:B:577:ILE:HG12	1.68	0.74
1:B:466:ARG:CD	7:B:901:HOH:O	2.34	0.74
1:A:514:TRP:HZ2	1:A:579:ILE:HG13	1.52	0.72
1:A:489:MET:HG3	1:A:579:ILE:HD11	1.72	0.71
1:B:533:ASP:OD1	1:B:611:ARG:NH2	2.25	0.69
1:A:314:GLN:HE22	3:A:806:3PE:H31	1.57	0.69
1:A:466:ARG:CD	7:A:901:HOH:O	2.41	0.69
1:A:533:ASP:OD1	1:A:611:ARG:NH2	2.25	0.68
1:B:314:GLN:HE22	3:B:807:3PE:H31	1.58	0.68
1:B:370:SER:HB3	3:B:802:3PE:H222	1.74	0.68
1:A:297:VAL:HG23	1:A:616:HIS:HB2	1.76	0.68
1:A:370:SER:HB3	3:A:802:3PE:H222	1.75	0.68
1:A:466:ARG:HD2	7:A:901:HOH:O	1.92	0.68
1:B:297:VAL:HG23	1:B:616:HIS:HB2	1.76	0.66
1:B:466:ARG:HD3	7:B:901:HOH:O	1.96	0.66
1:B:489:MET:HG3	1:B:579:ILE:HD11	1.80	0.64
1:A:358:PHE:O	1:A:371:ARG:HD3	1.98	0.64
1:B:417:TYR:HA	1:B:421:LEU:HB2	1.80	0.63
1:B:358:PHE:O	1:B:371:ARG:HD3	1.99	0.63
1:A:482:LYS:HE2	1:A:525:THR:HG22	1.80	0.63
1:B:466:ARG:HD2	7:B:901:HOH:O	1.97	0.63
1:B:482:LYS:HE2	1:B:525:THR:HG22	1.80	0.63
1:A:395:TRP:O	1:A:399:GLN:HG2	1.99	0.62
1:B:395:TRP:O	1:B:399:GLN:HG2	1.99	0.62
1:A:339:ILE:HB	1:A:342:ILE:HG22	1.81	0.62
1:A:481:GLY:HA3	2:A:808:CLR:H181	1.82	0.62
1:B:473:ALA:HA	1:B:477:LEU:HD23	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:TYR:HA	1:A:421:LEU:HB2	1.81	0.62
1:B:235:PHE:HE2	5:B:811:PLM:HA2	1.65	0.61
1:A:451:VAL:HA	1:A:454:ILE:HD12	1.82	0.61
1:B:481:GLY:HA3	2:B:809:CLR:H181	1.81	0.61
1:A:473:ALA:HA	1:A:477:LEU:HD23	1.84	0.60
1:A:235:PHE:HE2	5:A:810:PLM:HA2	1.65	0.60
1:B:361:ASN:O	1:B:371:ARG:NH1	2.35	0.59
1:B:585:LEU:HB3	1:B:586:PRO:HD3	1.85	0.59
1:A:585:LEU:HB3	1:A:586:PRO:HD3	1.84	0.58
1:B:552:VAL:HG12	1:B:613:GLU:HG3	1.86	0.58
1:A:361:ASN:O	1:A:371:ARG:NH1	2.37	0.58
1:A:236:ARG:NH2	5:A:810:PLM:O2	2.37	0.57
1:A:271:ILE:HD12	1:A:413:MET:HG3	1.86	0.57
1:B:514:TRP:CZ2	1:B:579:ILE:HG21	2.40	0.57
1:B:236:ARG:NH2	5:B:811:PLM:O2	2.37	0.57
1:A:275:GLY:O	1:A:279:ILE:HG12	2.05	0.57
1:A:411:GLU:HG3	1:A:451:VAL:HG11	1.87	0.57
1:A:552:VAL:HG12	1:A:613:GLU:HG3	1.87	0.56
3:A:802:3PE:H232	3:A:802:3PE:H361	1.87	0.56
1:B:263:ARG:NH1	1:B:430:LEU:O	2.38	0.56
1:B:359:LEU:HD11	1:B:374:LEU:HD12	1.87	0.56
1:A:359:LEU:HD11	1:A:374:LEU:HD12	1.86	0.56
4:B:810:LPE:H162	5:B:811:PLM:HG3	1.88	0.56
4:A:809:LPE:H162	5:A:810:PLM:HG3	1.88	0.56
1:B:275:GLY:O	1:B:279:ILE:HG12	2.05	0.56
3:B:802:3PE:H361	3:B:802:3PE:H232	1.89	0.55
1:B:271:ILE:HD12	1:B:413:MET:HG3	1.89	0.54
1:B:493:ALA:HB2	1:B:579:ILE:HD12	1.89	0.54
1:A:285:LEU:HD21	3:A:802:3PE:H332	1.89	0.54
1:B:285:LEU:HD21	3:B:802:3PE:H332	1.90	0.54
1:A:579:ILE:HG22	1:A:580:THR:H	1.73	0.54
1:B:248:ASN:HD22	3:B:807:3PE:H3D1	1.72	0.53
1:A:514:TRP:HE1	1:A:579:ILE:HD12	1.74	0.53
1:B:404:SER:O	1:B:408:MET:HG3	2.08	0.53
1:A:372:PHE:O	1:A:376:LYS:HG2	2.09	0.53
1:B:395:TRP:NE1	1:B:608:ASN:OD1	2.37	0.53
1:A:529:ASP:HA	1:A:533:ASP:HB2	1.91	0.53
1:A:359:LEU:HD22	3:A:802:3PE:H2C2	1.91	0.52
1:A:514:TRP:CZ2	1:A:579:ILE:HG21	2.45	0.52
1:B:359:LEU:HD22	3:B:802:3PE:H2C2	1.92	0.52
1:B:529:ASP:HA	1:B:533:ASP:HB2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:ILE:HD11	1:A:346:VAL:HG11	1.92	0.51
1:B:565:GLU:HB2	2:B:801:CLR:H25	1.93	0.51
1:B:517:PHE:HD2	2:B:809:CLR:H272	1.76	0.51
1:A:252:VAL:O	1:A:256:VAL:HG12	2.11	0.51
1:A:481:GLY:O	1:A:485:THR:HG23	2.11	0.50
1:A:267:PRO:O	1:A:271:ILE:HG12	2.12	0.50
1:A:463:CYS:SG	1:A:479:ASN:ND2	2.83	0.50
1:B:372:PHE:O	1:B:376:LYS:HG2	2.10	0.50
1:B:267:PRO:O	1:B:271:ILE:HG12	2.12	0.49
1:A:447:VAL:O	1:A:451:VAL:HG13	2.13	0.49
3:B:803:3PE:H3D1	2:B:805:CLR:H241	1.95	0.49
1:A:436:GLU:O	1:A:441:HIS:NE2	2.43	0.49
1:A:466:ARG:HD3	7:A:901:HOH:O	2.11	0.49
1:A:520:ILE:HG23	2:A:807:CLR:H242	1.95	0.49
1:B:421:LEU:HD23	1:B:423:TRP:CE2	2.48	0.48
1:A:293:ARG:HG3	1:A:293:ARG:HH11	1.78	0.48
1:A:466:ARG:NH2	1:A:621:GLY:O	2.35	0.48
1:B:250:THR:HG21	3:B:803:3PE:H381	1.94	0.48
1:A:514:TRP:CZ2	1:A:579:ILE:HG13	2.41	0.48
1:B:293:ARG:HG3	1:B:293:ARG:HH11	1.79	0.48
1:B:520:ILE:HG23	2:B:808:CLR:H242	1.95	0.48
3:B:814:3PE:H381	1:A:250:THR:HG21	1.96	0.48
1:B:389:VAL:HG11	1:B:466:ARG:HG2	1.96	0.47
1:B:305:LEU:HD13	3:B:802:3PE:H12	1.96	0.47
1:B:481:GLY:O	1:B:485:THR:HG23	2.14	0.47
1:A:281:PHE:HE2	3:A:802:3PE:H3A2	1.79	0.47
1:A:305:LEU:HD13	3:A:802:3PE:H12	1.96	0.47
1:B:576:GLN:NE2	1:B:577:ILE:HB	2.29	0.47
3:B:803:3PE:H3E2	1:A:249:ILE:HD12	1.97	0.47
1:B:293:ARG:HG3	1:B:293:ARG:NH1	2.30	0.47
1:A:421:LEU:HD23	1:A:423:TRP:CE2	2.49	0.47
1:B:579:ILE:HG22	1:B:580:THR:H	1.80	0.47
1:A:357:PHE:HA	1:A:360:ILE:HG22	1.97	0.47
1:A:451:VAL:HA	1:A:454:ILE:CD1	2.45	0.47
1:A:520:ILE:HG23	2:A:807:CLR:H262	1.96	0.47
1:B:281:PHE:HE2	3:B:802:3PE:H3A2	1.80	0.47
1:B:282:LEU:HB3	1:B:320:ALA:HB2	1.97	0.47
3:B:814:3PE:H3D1	2:A:804:CLR:H241	1.97	0.47
1:A:271:ILE:HG21	1:A:348:PRO:HB3	1.96	0.47
1:A:259:LEU:HD12	1:A:259:LEU:HA	1.83	0.47
1:A:282:LEU:HB3	1:A:320:ALA:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:574:THR:HA	1:A:578:SER:HB2	1.97	0.47
1:A:449:ALA:O	1:A:453:CYS:HB2	2.14	0.47
1:B:499:HIS:CD2	1:B:504:HIS:HB2	2.49	0.46
1:A:293:ARG:HG3	1:A:293:ARG:NH1	2.30	0.46
2:A:807:CLR:H162	2:A:807:CLR:H221	1.47	0.46
1:B:579:ILE:HG22	1:B:583:THR:HG22	1.98	0.46
2:B:809:CLR:H213	2:B:809:CLR:H231	1.85	0.46
1:B:251:LEU:HD11	1:B:331:LEU:HD23	1.97	0.46
1:B:520:ILE:HG23	2:B:808:CLR:H262	1.97	0.46
1:A:404:SER:O	1:A:408:MET:HG3	2.15	0.46
1:A:573:TRP:HE3	1:A:600:GLU:OE1	1.98	0.46
1:A:578:SER:O	1:A:579:ILE:HD13	2.15	0.46
1:B:236:ARG:NH1	1:B:318:GLU:OE1	2.49	0.46
1:B:260:GLU:N	1:B:260:GLU:OE2	2.49	0.46
1:B:463:CYS:SG	1:B:479:ASN:ND2	2.88	0.46
1:A:251:LEU:HD11	1:A:331:LEU:HD23	1.97	0.46
1:A:529:ASP:OD2	1:A:570:ARG:NH2	2.49	0.46
2:A:807:CLR:H25	2:A:807:CLR:H222	1.85	0.46
1:A:236:ARG:NH1	1:A:318:GLU:OE1	2.48	0.46
1:B:384:ALA:HB1	1:B:462:GLN:HG3	1.98	0.45
1:B:447:VAL:O	1:B:451:VAL:HG13	2.16	0.45
1:B:259:LEU:HD21	1:B:265:ILE:HD12	1.98	0.45
1:B:230:PRO:O	1:B:233:THR:HG22	2.17	0.45
1:B:266:TRP:CZ2	1:B:591:ILE:HG13	2.52	0.45
1:B:314:GLN:NE2	3:B:807:3PE:H31	2.30	0.45
1:B:462:GLN:O	1:B:466:ARG:HG3	2.17	0.45
1:B:259:LEU:HD12	1:B:259:LEU:HA	1.85	0.45
1:B:326:LEU:HD22	3:B:803:3PE:H212	1.98	0.45
1:A:230:PRO:O	1:A:233:THR:HG22	2.17	0.45
1:A:624:ARG:HG2	1:A:626:VAL:HG22	1.98	0.45
1:A:314:GLN:NE2	3:A:806:3PE:H31	2.30	0.45
1:A:424:ASP:OD1	1:A:424:ASP:N	2.50	0.45
1:A:395:TRP:NE1	1:A:608:ASN:OD1	2.50	0.44
1:B:436:GLU:O	1:B:441:HIS:NE2	2.43	0.44
1:B:624:ARG:HG2	1:B:626:VAL:HG22	1.99	0.44
1:A:266:TRP:CZ2	1:A:591:ILE:HG13	2.53	0.44
1:A:273:ARG:HD3	1:A:594:THR:HG23	1.99	0.44
2:B:805:CLR:H213	2:B:805:CLR:H231	1.84	0.44
2:A:804:CLR:H213	2:A:804:CLR:H231	1.84	0.44
2:A:804:CLR:H231	2:A:804:CLR:H272	1.85	0.44
1:A:416:PHE:CD1	1:A:420:GLU:HB3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:808:CLR:H162	2:B:808:CLR:H221	1.47	0.43
1:A:573:TRP:HB2	1:A:600:GLU:HG3	2.00	0.43
1:B:349:LEU:HD13	1:B:417:TYR:CE2	2.53	0.43
1:B:485:THR:HG22	2:B:809:CLR:H273	2.01	0.43
2:A:811:CLR:H162	2:A:811:CLR:H221	1.58	0.43
1:A:408:MET:HE3	1:A:448:ARG:HD2	2.00	0.43
1:B:273:ARG:HB3	1:B:409:ASP:OD2	2.17	0.43
1:B:273:ARG:HD3	1:B:594:THR:HG23	1.98	0.43
1:B:377:LEU:HD12	1:B:377:LEU:HA	1.85	0.43
1:A:248:ASN:HD22	3:A:806:3PE:H3D1	1.84	0.43
1:B:470:THR:HG23	1:B:472:ARG:H	1.84	0.43
3:B:803:3PE:H3I3	3:B:803:3PE:H3F1	1.90	0.43
1:A:573:TRP:O	1:A:576:GLN:HG3	2.19	0.43
1:B:537:PHE:HE2	1:B:563:ILE:HD13	1.84	0.43
1:A:425:GLU:HG2	1:A:427:LYS:H	1.84	0.43
1:B:249:ILE:HD12	3:B:814:3PE:H3E2	2.00	0.43
1:B:499:HIS:NE2	1:B:506:ASP:HB2	2.34	0.43
1:B:548:ARG:HH21	1:B:617:LEU:HD12	1.84	0.43
2:B:805:CLR:H231	2:B:805:CLR:H272	1.85	0.43
4:B:810:LPE:H11	4:B:810:LPE:H311	2.01	0.43
1:A:321:GLY:O	1:A:325:ILE:HG12	2.19	0.43
1:B:416:PHE:CD1	1:B:420:GLU:HB3	2.54	0.42
1:B:578:SER:O	1:B:579:ILE:HD13	2.19	0.42
2:B:812:CLR:H162	2:B:812:CLR:H221	1.58	0.42
1:A:400:LEU:HD22	1:A:407:LEU:HD11	2.01	0.42
1:A:459:ARG:HA	1:A:459:ARG:HD2	1.60	0.42
3:B:803:3PE:H242	1:A:253:LEU:HD23	2.01	0.42
1:B:278:LEU:HD11	3:B:802:3PE:H2C1	2.01	0.42
1:B:424:ASP:N	1:B:424:ASP:OD1	2.50	0.42
1:B:537:PHE:N	1:B:537:PHE:CD2	2.87	0.42
1:A:588:SER:HA	1:A:591:ILE:HD12	2.01	0.42
1:B:321:GLY:O	1:B:325:ILE:HG12	2.19	0.42
3:B:814:3PE:H2I2	1:A:326:LEU:HD22	2.02	0.42
1:A:565:GLU:HB2	2:A:801:CLR:H25	2.01	0.42
2:A:805:CLR:H162	2:A:805:CLR:H221	1.43	0.42
1:A:470:THR:HG23	1:A:472:ARG:H	1.84	0.42
1:A:548:ARG:HH22	1:A:613:GLU:CD	2.23	0.42
1:B:253:LEU:HD23	3:B:814:3PE:H242	2.02	0.42
1:A:263:ARG:NH1	1:A:430:LEU:O	2.53	0.42
1:A:493:ALA:HB2	1:A:579:ILE:HD12	2.01	0.42
1:B:588:SER:HA	1:B:591:ILE:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:606:VAL:HG23	2:B:801:CLR:H152	2.02	0.42
2:B:804:CLR:H213	2:B:804:CLR:H231	1.86	0.42
1:A:332:LEU:HD23	1:A:332:LEU:HA	1.90	0.42
1:A:491:THR:HG22	1:A:495:LEU:HD11	2.02	0.42
1:B:243:ILE:HG22	1:B:325:ILE:HD12	2.02	0.41
1:B:491:THR:HA	2:B:804:CLR:H151	2.01	0.41
2:B:805:CLR:H162	2:B:805:CLR:H221	1.82	0.41
1:A:491:THR:HA	2:A:803:CLR:H151	2.01	0.41
1:A:278:LEU:HD11	3:A:802:3PE:H2C1	2.02	0.41
1:A:395:TRP:CE2	1:A:399:GLN:NE2	2.86	0.41
1:B:526:LEU:HD21	1:B:567:VAL:HG22	2.01	0.41
1:B:573:TRP:NE1	1:B:574:THR:HG23	2.35	0.41
2:B:801:CLR:H213	2:B:801:CLR:H231	1.92	0.41
1:A:273:ARG:HB3	1:A:409:ASP:OD1	2.20	0.41
1:B:334:CYS:SG	1:B:348:PRO:HD3	2.61	0.41
1:B:517:PHE:CD2	2:B:809:CLR:H272	2.55	0.41
1:A:485:THR:HG22	2:A:808:CLR:H273	2.03	0.41
4:A:809:LPE:H11	4:A:809:LPE:H311	2.01	0.41
1:B:246:VAL:HG21	1:A:243:ILE:HA	2.03	0.41
1:A:499:HIS:NE2	1:A:506:ASP:HB2	2.35	0.41
1:B:493:ALA:HB1	1:B:579:ILE:HG23	2.02	0.41
1:A:415:CYS:SG	1:A:416:PHE:N	2.94	0.41
1:B:354:PHE:CD1	1:B:354:PHE:C	2.94	0.41
1:B:243:ILE:HA	1:A:246:VAL:HG21	2.02	0.41
1:B:415:CYS:SG	1:B:416:PHE:N	2.93	0.41
1:A:311:LEU:HD23	1:A:311:LEU:HA	1.92	0.41
1:A:416:PHE:HD1	1:A:420:GLU:HB3	1.85	0.41
2:A:804:CLR:H162	2:A:804:CLR:H221	1.82	0.41
1:A:349:LEU:HD11	2:A:811:CLR:H162	2.03	0.41
1:A:400:LEU:HD23	1:A:400:LEU:HA	1.88	0.41
1:A:496:TYR:CD1	1:A:511:PHE:HB2	2.56	0.41
1:A:496:TYR:CE1	1:A:511:PHE:HB2	2.56	0.41
1:B:416:PHE:HD1	1:B:420:GLU:HB3	1.86	0.40
1:B:425:GLU:HG2	1:B:427:LYS:H	1.85	0.40
1:A:243:ILE:HG22	1:A:325:ILE:HD12	2.02	0.40
1:A:519:ILE:HG23	2:A:805:CLR:H263	2.02	0.40
1:A:606:VAL:HG23	2:A:801:CLR:H152	2.03	0.40
1:B:378:LEU:HD23	1:B:378:LEU:HA	1.90	0.40
3:B:803:3PE:H31	3:B:803:3PE:H322	1.82	0.40
1:B:547:LEU:HD23	1:B:547:LEU:HA	1.90	0.40
1:A:242:GLY:O	1:A:246:VAL:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:588:SER:O	1:A:592:ILE:HG12	2.22	0.40
2:B:806:CLR:H221	2:B:806:CLR:H162	1.44	0.40
1:A:450:ILE:CD1	2:A:803:CLR:H183	2.51	0.40
3:B:814:3PE:H3I3	3:B:814:3PE:H3F1	1.90	0.40
1:A:408:MET:HE3	1:A:408:MET:HB3	1.68	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	399/704 (57%)	382 (96%)	17 (4%)	0	100	100
1	B	399/704 (57%)	381 (96%)	18 (4%)	0	100	100
All	All	798/1408 (57%)	763 (96%)	35 (4%)	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	355/629 (56%)	344 (97%)	11 (3%)	35	62
1	B	355/629 (56%)	347 (98%)	8 (2%)	45	69
All	All	710/1258 (56%)	691 (97%)	19 (3%)	41	66

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	336	PHE
1	B	524	TYR
1	B	540	ASN
1	B	570	ARG
1	B	588	SER
1	B	605	PHE
1	B	614	ASN
1	B	618	ASN
1	A	336	PHE
1	A	432	ASN
1	A	443	TYR
1	A	524	TYR
1	A	538	ASP
1	A	540	ASN
1	A	570	ARG
1	A	588	SER
1	A	596	PHE
1	A	605	PHE
1	A	614	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	399	GLN
1	A	452	GLN

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

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	CLR	B	804	-	31,31,31	0.41	0	48,48,48	0.61	0
3	3PE	A	806	-	50,50,50	0.51	0	53,55,55	0.55	1 (1%)
3	3PE	B	807	-	50,50,50	0.51	0	53,55,55	0.55	1 (1%)
4	LPE	B	810	-	33,33,33	0.90	0	37,39,39	0.91	2 (5%)
2	CLR	B	801	-	31,31,31	0.37	0	48,48,48	0.58	0
3	3PE	B	814	-	50,50,50	0.51	0	53,55,55	0.54	1 (1%)
2	CLR	B	806	-	31,31,31	0.39	0	48,48,48	0.70	0
2	CLR	A	805	-	31,31,31	0.40	0	48,48,48	0.70	1 (2%)
2	CLR	A	811	-	31,31,31	0.38	0	48,48,48	0.49	0
4	LPE	A	809	-	33,33,33	0.90	0	37,39,39	0.91	2 (5%)
2	CLR	B	808	-	31,31,31	0.36	0	48,48,48	0.60	0
5	PLM	A	810	-	17,17,17	0.90	1 (5%)	17,17,17	0.75	2 (11%)
2	CLR	A	808	-	31,31,31	0.39	0	48,48,48	0.62	0
2	CLR	A	803	-	31,31,31	0.42	0	48,48,48	0.61	0
2	CLR	A	807	-	31,31,31	0.36	0	48,48,48	0.60	0
2	CLR	B	809	-	31,31,31	0.38	0	48,48,48	0.62	0
2	CLR	B	805	-	31,31,31	0.36	0	48,48,48	0.49	0
2	CLR	A	801	-	31,31,31	0.38	0	48,48,48	0.58	0
2	CLR	A	804	-	31,31,31	0.35	0	48,48,48	0.50	0
6	ACD	A	812	-	21,21,21	0.57	0	21,21,21	0.56	0
3	3PE	B	803	-	50,50,50	0.51	0	53,55,55	0.54	1 (1%)
5	PLM	B	811	-	17,17,17	0.91	1 (5%)	17,17,17	0.75	2 (11%)
3	3PE	B	802	-	50,50,50	0.51	0	53,55,55	0.59	2 (3%)
3	3PE	A	802	-	50,50,50	0.50	0	53,55,55	0.60	2 (3%)
2	CLR	B	812	-	31,31,31	0.38	0	48,48,48	0.49	0
6	ACD	B	813	-	21,21,21	0.57	0	21,21,21	0.57	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CLR	B	804	-	-	2/10/68/68	0/4/4/4
3	3PE	A	806	-	-	24/54/54/54	-
3	3PE	B	807	-	-	25/54/54/54	-
4	LPE	B	810	-	-	16/34/34/34	-
2	CLR	B	801	-	-	4/10/68/68	0/4/4/4
3	3PE	B	814	-	-	25/54/54/54	-
2	CLR	B	806	-	-	7/10/68/68	0/4/4/4
2	CLR	A	805	-	-	7/10/68/68	0/4/4/4
2	CLR	A	811	-	-	8/10/68/68	0/4/4/4
4	LPE	A	809	-	-	16/34/34/34	-
2	CLR	B	808	-	-	8/10/68/68	0/4/4/4
5	PLM	A	810	-	-	8/15/15/15	-
2	CLR	A	808	-	-	8/10/68/68	0/4/4/4
2	CLR	A	803	-	-	2/10/68/68	0/4/4/4
2	CLR	A	807	-	-	8/10/68/68	0/4/4/4
2	CLR	B	809	-	-	8/10/68/68	0/4/4/4
2	CLR	B	805	-	-	9/10/68/68	0/4/4/4
2	CLR	A	801	-	-	4/10/68/68	0/4/4/4
2	CLR	A	804	-	-	9/10/68/68	0/4/4/4
6	ACD	A	812	-	-	3/19/19/19	-
3	3PE	B	803	-	-	24/54/54/54	-
5	PLM	B	811	-	-	8/15/15/15	-
3	3PE	B	802	-	-	24/54/54/54	-
3	3PE	A	802	-	-	24/54/54/54	-
2	CLR	B	812	-	-	8/10/68/68	0/4/4/4
6	ACD	B	813	-	-	5/19/19/19	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	811	PLM	C2-C1	2.91	1.57	1.50
5	A	810	PLM	C2-C1	2.86	1.57	1.50

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	809	LPE	C2N-N-C1N	3.89	118.98	108.97
4	B	810	LPE	C2N-N-C1N	3.88	118.95	108.97
3	B	814	3PE	O12-P-O14	2.35	123.87	112.24
3	A	806	3PE	O12-P-O14	2.35	123.86	112.24
3	B	803	3PE	O12-P-O14	2.35	123.85	112.24
3	B	807	3PE	O12-P-O14	2.35	123.84	112.24
3	A	802	3PE	O12-P-O14	2.31	123.66	112.24
3	B	802	3PE	O12-P-O14	2.31	123.66	112.24
3	A	802	3PE	C2-O21-C21	2.27	123.37	117.79
4	A	809	LPE	O32-P-O31	-2.24	101.18	112.24
4	B	810	LPE	O32-P-O31	-2.23	101.23	112.24
5	B	811	PLM	O1-C1-O2	2.22	128.84	123.30
3	B	802	3PE	C2-O21-C21	2.22	123.25	117.79
5	A	810	PLM	O1-C1-O2	2.21	128.81	123.30
5	B	811	PLM	O2-C1-C2	-2.04	116.53	123.08
5	A	810	PLM	O2-C1-C2	-2.03	116.55	123.08
2	A	805	CLR	C17-C13-C14	2.00	102.44	100.07

There are no chirality outliers.

All (294) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	802	3PE	C1-O11-P-O14
3	B	802	3PE	C11-O13-P-O12
3	B	802	3PE	C12-C11-O13-P
3	B	802	3PE	O13-C11-C12-N
3	B	802	3PE	O22-C21-O21-C2
3	B	802	3PE	C22-C21-O21-C2
3	B	803	3PE	C1-O11-P-O14
3	B	803	3PE	C11-O13-P-O14
3	B	803	3PE	O13-C11-C12-N
3	B	803	3PE	C22-C21-O21-C2
3	B	807	3PE	C1-O11-P-O14
3	B	807	3PE	C11-O13-P-O11
3	B	807	3PE	C11-O13-P-O12
3	B	807	3PE	C11-O13-P-O14
3	B	807	3PE	O13-C11-C12-N
3	B	807	3PE	O11-C1-C2-O21
3	B	807	3PE	O22-C21-O21-C2
3	B	807	3PE	C22-C21-O21-C2
3	B	814	3PE	C1-O11-P-O14
3	B	814	3PE	C11-O13-P-O14
3	B	814	3PE	O13-C11-C12-N

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Mol	Chain	Res	Type	Atoms
3	B	814	3PE	C22-C21-O21-C2
3	A	802	3PE	C1-O11-P-O14
3	A	802	3PE	C11-O13-P-O12
3	A	802	3PE	C12-C11-O13-P
3	A	802	3PE	O13-C11-C12-N
3	A	802	3PE	C22-C21-O21-C2
3	A	806	3PE	C1-O11-P-O14
3	A	806	3PE	C11-O13-P-O11
3	A	806	3PE	C11-O13-P-O12
3	A	806	3PE	C11-O13-P-O14
3	A	806	3PE	O13-C11-C12-N
3	A	806	3PE	O11-C1-C2-O21
3	A	806	3PE	O22-C21-O21-C2
3	A	806	3PE	C22-C21-O21-C2
4	B	810	LPE	O33-C31-C32-N
4	A	809	LPE	O33-C31-C32-N
2	B	812	CLR	C21-C20-C22-C23
2	A	811	CLR	C21-C20-C22-C23
3	B	803	3PE	O32-C31-O31-C3
3	B	814	3PE	O32-C31-O31-C3
2	B	808	CLR	C16-C17-C20-C21
2	A	807	CLR	C16-C17-C20-C21
2	B	808	CLR	C13-C17-C20-C21
3	A	802	3PE	O22-C21-O21-C2
2	B	801	CLR	C21-C20-C22-C23
2	B	808	CLR	C21-C20-C22-C23
2	A	801	CLR	C21-C20-C22-C23
2	A	807	CLR	C21-C20-C22-C23
2	A	807	CLR	C13-C17-C20-C21
2	B	808	CLR	C13-C17-C20-C22
2	A	807	CLR	C13-C17-C20-C22
3	B	803	3PE	C32-C31-O31-C3
3	B	814	3PE	C32-C31-O31-C3
3	B	803	3PE	O22-C21-O21-C2
3	B	814	3PE	O22-C21-O21-C2
2	B	808	CLR	C16-C17-C20-C22
2	A	807	CLR	C16-C17-C20-C22
2	B	812	CLR	C13-C17-C20-C22
2	A	811	CLR	C13-C17-C20-C22
2	B	806	CLR	C21-C20-C22-C23
2	B	809	CLR	C21-C20-C22-C23
2	A	805	CLR	C21-C20-C22-C23

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Mol	Chain	Res	Type	Atoms
2	A	808	CLR	C21-C20-C22-C23
2	B	801	CLR	C17-C20-C22-C23
2	A	801	CLR	C17-C20-C22-C23
2	A	808	CLR	C17-C20-C22-C23
2	B	805	CLR	C17-C20-C22-C23
2	B	806	CLR	C17-C20-C22-C23
2	B	808	CLR	C17-C20-C22-C23
2	B	809	CLR	C17-C20-C22-C23
2	A	804	CLR	C17-C20-C22-C23
2	A	805	CLR	C17-C20-C22-C23
4	B	810	LPE	C17-C18-C19-C20
4	A	809	LPE	C17-C18-C19-C20
4	B	810	LPE	O1-C1-C2-O2H
4	A	809	LPE	O1-C1-C2-O2H
2	B	812	CLR	C17-C20-C22-C23
2	A	807	CLR	C17-C20-C22-C23
2	A	811	CLR	C17-C20-C22-C23
2	B	809	CLR	C20-C22-C23-C24
2	A	808	CLR	C20-C22-C23-C24
2	B	812	CLR	C22-C23-C24-C25
2	A	811	CLR	C22-C23-C24-C25
4	B	810	LPE	O1-C11-C12-C13
4	A	809	LPE	O1-C11-C12-C13
2	A	811	CLR	C16-C17-C20-C22
3	A	806	3PE	C3B-C3C-C3D-C3E
2	B	805	CLR	C22-C23-C24-C25
2	B	801	CLR	C20-C22-C23-C24
2	A	801	CLR	C20-C22-C23-C24
2	A	804	CLR	C22-C23-C24-C25
3	B	802	3PE	C1-O11-P-O13
3	B	802	3PE	C11-O13-P-O11
3	B	803	3PE	C1-O11-P-O13
3	B	803	3PE	C11-O13-P-O11
3	B	814	3PE	C1-O11-P-O13
3	B	814	3PE	C11-O13-P-O11
3	A	802	3PE	C1-O11-P-O13
3	A	802	3PE	C11-O13-P-O11
2	A	811	CLR	C13-C17-C20-C21
2	B	812	CLR	C16-C17-C20-C22
2	A	805	CLR	C13-C17-C20-C22
2	B	812	CLR	C13-C17-C20-C21
3	B	803	3PE	C29-C2A-C2B-C2C

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Mol	Chain	Res	Type	Atoms
2	B	806	CLR	C13-C17-C20-C22
3	B	814	3PE	C29-C2A-C2B-C2C
4	B	810	LPE	C14-C15-C16-C17
4	A	809	LPE	C14-C15-C16-C17
4	B	810	LPE	O1-C1-C2-C3
3	B	807	3PE	C34-C35-C36-C37
3	B	807	3PE	C3B-C3C-C3D-C3E
3	A	806	3PE	C34-C35-C36-C37
3	B	803	3PE	C2B-C2C-C2D-C2E
2	B	808	CLR	C20-C22-C23-C24
3	B	814	3PE	C2B-C2C-C2D-C2E
2	A	807	CLR	C20-C22-C23-C24
3	A	806	3PE	C33-C34-C35-C36
3	B	807	3PE	C33-C34-C35-C36
3	B	807	3PE	C2D-C2E-C2F-C2G
3	A	806	3PE	C2D-C2E-C2F-C2G
2	A	811	CLR	C16-C17-C20-C21
3	B	807	3PE	C25-C26-C27-C28
4	B	810	LPE	C20-C21-C22-C23
4	A	809	LPE	C20-C21-C22-C23
2	B	809	CLR	C13-C17-C20-C22
3	B	807	3PE	C26-C27-C28-C29
3	A	806	3PE	C25-C26-C27-C28
3	A	806	3PE	C26-C27-C28-C29
2	B	801	CLR	C22-C23-C24-C25
2	B	812	CLR	C16-C17-C20-C21
5	B	811	PLM	C8-C9-CA-CB
2	A	801	CLR	C22-C23-C24-C25
3	A	802	3PE	C38-C39-C3A-C3B
5	A	810	PLM	C8-C9-CA-CB
3	B	802	3PE	C38-C39-C3A-C3B
5	A	810	PLM	C5-C6-C7-C8
2	A	808	CLR	C13-C17-C20-C22
3	B	802	3PE	C26-C27-C28-C29
3	A	802	3PE	C26-C27-C28-C29
5	B	811	PLM	C5-C6-C7-C8
3	A	802	3PE	C31-C32-C33-C34
4	A	809	LPE	O1-C1-C2-C3
2	B	806	CLR	C16-C17-C20-C22
2	A	805	CLR	C16-C17-C20-C22
3	B	802	3PE	C31-C32-C33-C34
3	B	803	3PE	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
2	A	805	CLR	C16-C17-C20-C21
3	B	814	3PE	C22-C23-C24-C25
6	B	813	ACD	C2-C3-C4-C5
6	A	812	ACD	C2-C3-C4-C5
2	B	805	CLR	C13-C17-C20-C22
2	A	804	CLR	C13-C17-C20-C22
3	A	802	3PE	C36-C37-C38-C39
3	B	807	3PE	O11-C1-C2-C3
3	A	806	3PE	O11-C1-C2-C3
3	B	802	3PE	C36-C37-C38-C39
2	B	806	CLR	C16-C17-C20-C21
3	B	802	3PE	C1-C2-C3-O31
3	A	802	3PE	C1-C2-C3-O31
4	A	809	LPE	C23-C24-C25-C26
4	B	810	LPE	C23-C24-C25-C26
3	B	814	3PE	C32-C33-C34-C35
5	A	810	PLM	C1-C2-C3-C4
3	B	803	3PE	C32-C33-C34-C35
5	B	811	PLM	C1-C2-C3-C4
2	B	805	CLR	C16-C17-C20-C21
2	B	809	CLR	C16-C17-C20-C21
2	A	804	CLR	C16-C17-C20-C21
2	A	808	CLR	C16-C17-C20-C21
2	B	805	CLR	C13-C17-C20-C21
2	B	806	CLR	C13-C17-C20-C21
2	B	809	CLR	C13-C17-C20-C21
2	A	804	CLR	C13-C17-C20-C21
2	A	805	CLR	C13-C17-C20-C21
2	A	808	CLR	C13-C17-C20-C21
2	B	809	CLR	C16-C17-C20-C22
3	A	806	3PE	C37-C38-C39-C3A
3	B	807	3PE	C29-C2A-C2B-C2C
3	A	806	3PE	C29-C2A-C2B-C2C
2	A	804	CLR	C21-C20-C22-C23
4	B	810	LPE	C22-C23-C24-C25
4	A	809	LPE	C22-C23-C24-C25
3	A	802	3PE	C22-C23-C24-C25
2	B	805	CLR	C16-C17-C20-C22
2	A	804	CLR	C16-C17-C20-C22
2	A	808	CLR	C16-C17-C20-C22
4	B	810	LPE	C25-C26-C27-C28
3	A	802	3PE	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
2	A	803	CLR	C17-C20-C22-C23
3	A	802	3PE	C21-C22-C23-C24
2	B	805	CLR	C21-C20-C22-C23
3	B	807	3PE	C37-C38-C39-C3A
3	A	802	3PE	C3D-C3E-C3F-C3G
4	A	809	LPE	C25-C26-C27-C28
3	B	802	3PE	C22-C23-C24-C25
3	B	802	3PE	C3D-C3E-C3F-C3G
4	A	809	LPE	C18-C19-C20-C21
2	B	812	CLR	C20-C22-C23-C24
2	A	811	CLR	C20-C22-C23-C24
3	B	803	3PE	C23-C24-C25-C26
3	B	814	3PE	C23-C24-C25-C26
4	B	810	LPE	C18-C19-C20-C21
6	B	813	ACD	C11-C12-C13-C14
6	B	813	ACD	C12-C13-C14-C15
6	A	812	ACD	C11-C12-C13-C14
3	B	802	3PE	C21-C22-C23-C24
3	B	802	3PE	C35-C36-C37-C38
2	A	803	CLR	C20-C22-C23-C24
2	A	804	CLR	C20-C22-C23-C24
2	B	805	CLR	C20-C22-C23-C24
3	B	802	3PE	C24-C25-C26-C27
2	A	808	CLR	C22-C23-C24-C25
3	B	803	3PE	O11-C1-C2-C3
3	B	807	3PE	C2B-C2C-C2D-C2E
3	A	806	3PE	C2B-C2C-C2D-C2E
3	A	802	3PE	C24-C25-C26-C27
2	B	809	CLR	C22-C23-C24-C25
3	B	803	3PE	O11-C1-C2-O21
3	B	814	3PE	O11-C1-C2-O21
3	A	806	3PE	C3A-C3B-C3C-C3D
3	B	802	3PE	O21-C2-C3-O31
3	A	802	3PE	O21-C2-C3-O31
2	B	804	CLR	C17-C20-C22-C23
4	B	810	LPE	C31-C32-N-C1N
3	B	802	3PE	C2E-C2F-C2G-C2H
4	B	810	LPE	C2-C1-O1-C11
4	A	809	LPE	C2-C1-O1-C11
3	A	802	3PE	C2E-C2F-C2G-C2H
3	B	802	3PE	C1-O11-P-O12
3	B	803	3PE	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
3	B	803	3PE	C11-O13-P-O12
3	B	814	3PE	C1-O11-P-O12
3	B	814	3PE	C11-O13-P-O12
3	A	802	3PE	C1-O11-P-O12
3	B	814	3PE	O11-C1-C2-C3
3	B	807	3PE	C3A-C3B-C3C-C3D
3	B	814	3PE	C31-C32-C33-C34
3	B	803	3PE	C37-C38-C39-C3A
4	A	809	LPE	C31-C32-N-C1N
3	B	803	3PE	C2C-C2D-C2E-C2F
2	B	808	CLR	C22-C23-C24-C25
3	B	803	3PE	C31-C32-C33-C34
3	B	814	3PE	C2C-C2D-C2E-C2F
3	B	802	3PE	C2B-C2C-C2D-C2E
2	B	806	CLR	C20-C22-C23-C24
2	A	805	CLR	C20-C22-C23-C24
3	B	802	3PE	C28-C29-C2A-C2B
4	B	810	LPE	C31-C32-N-C3N
4	A	809	LPE	C31-C32-N-C3N
3	A	802	3PE	C2B-C2C-C2D-C2E
3	A	802	3PE	C28-C29-C2A-C2B
6	A	812	ACD	C1-C2-C3-C4
2	A	807	CLR	C22-C23-C24-C25
3	B	807	3PE	C1-O11-P-O13
3	A	806	3PE	C1-O11-P-O13
3	B	814	3PE	C37-C38-C39-C3A
6	B	813	ACD	C1-C2-C3-C4
3	B	802	3PE	C37-C38-C39-C3A
5	B	811	PLM	CB-CC-CD-CE
5	A	810	PLM	CB-CC-CD-CE
3	B	807	3PE	C1-C2-C3-O31
3	A	806	3PE	C1-C2-C3-O31
5	B	811	PLM	C4-C5-C6-C7
3	A	802	3PE	C37-C38-C39-C3A
3	B	803	3PE	C3E-C3F-C3G-C3H
2	B	804	CLR	C20-C22-C23-C24
3	B	814	3PE	C36-C37-C38-C39
3	B	814	3PE	C3F-C3G-C3H-C3I
5	A	810	PLM	C4-C5-C6-C7
3	B	803	3PE	C3F-C3G-C3H-C3I
3	A	806	3PE	C22-C23-C24-C25
3	B	807	3PE	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
3	B	803	3PE	C36-C37-C38-C39
4	B	810	LPE	C31-C32-N-C2N
5	A	810	PLM	O1-C1-C2-C3
4	A	809	LPE	C31-C32-N-C2N
5	B	811	PLM	O1-C1-C2-C3
3	A	806	3PE	C24-C25-C26-C27
3	B	814	3PE	C3E-C3F-C3G-C3H
4	B	810	LPE	C12-C13-C14-C15
4	A	809	LPE	C12-C13-C14-C15
5	B	811	PLM	O2-C1-C2-C3
5	A	810	PLM	O2-C1-C2-C3
3	B	807	3PE	C24-C25-C26-C27
2	B	805	CLR	C23-C24-C25-C27
5	A	810	PLM	C7-C8-C9-CA
2	A	804	CLR	C23-C24-C25-C27
3	B	807	3PE	O21-C21-C22-C23
5	B	811	PLM	C7-C8-C9-CA
3	A	806	3PE	O21-C21-C22-C23
3	B	807	3PE	O22-C21-C22-C23
6	B	813	ACD	O2-C1-C2-C3
3	B	814	3PE	O21-C21-C22-C23

There are no ring outliers.

24 monomers are involved in 76 short contacts:

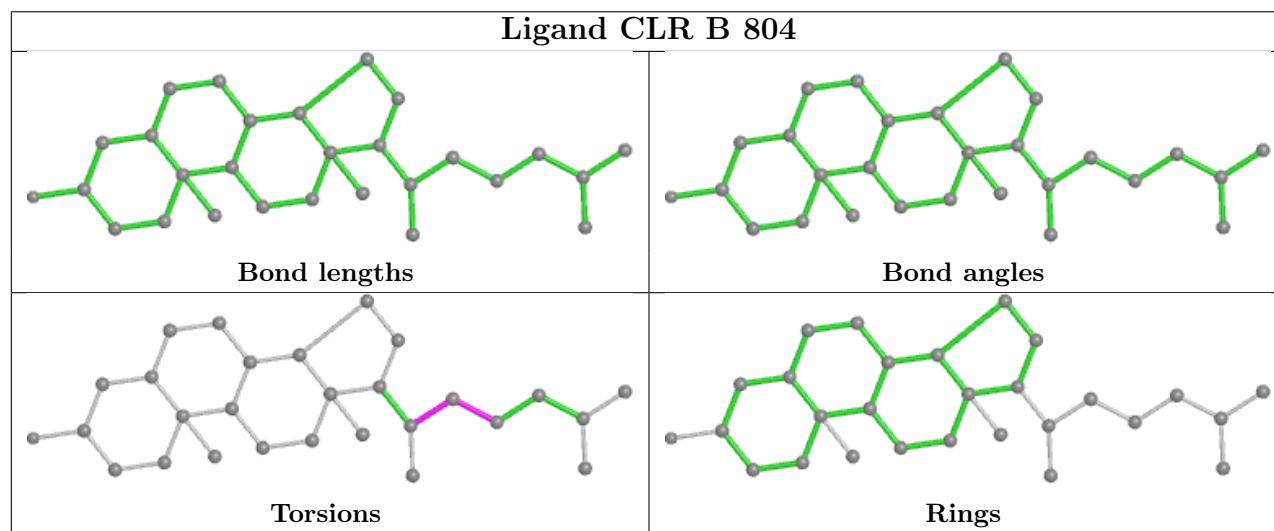
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	804	CLR	2	0
3	A	806	3PE	3	0
3	B	807	3PE	3	0
4	B	810	LPE	2	0
2	B	801	CLR	3	0
3	B	814	3PE	6	0
2	B	806	CLR	1	0
2	A	805	CLR	2	0
2	A	811	CLR	2	0
4	A	809	LPE	2	0
2	B	808	CLR	3	0
5	A	810	PLM	3	0
2	A	808	CLR	2	0
2	A	803	CLR	2	0
2	A	807	CLR	4	0
2	B	809	CLR	5	0

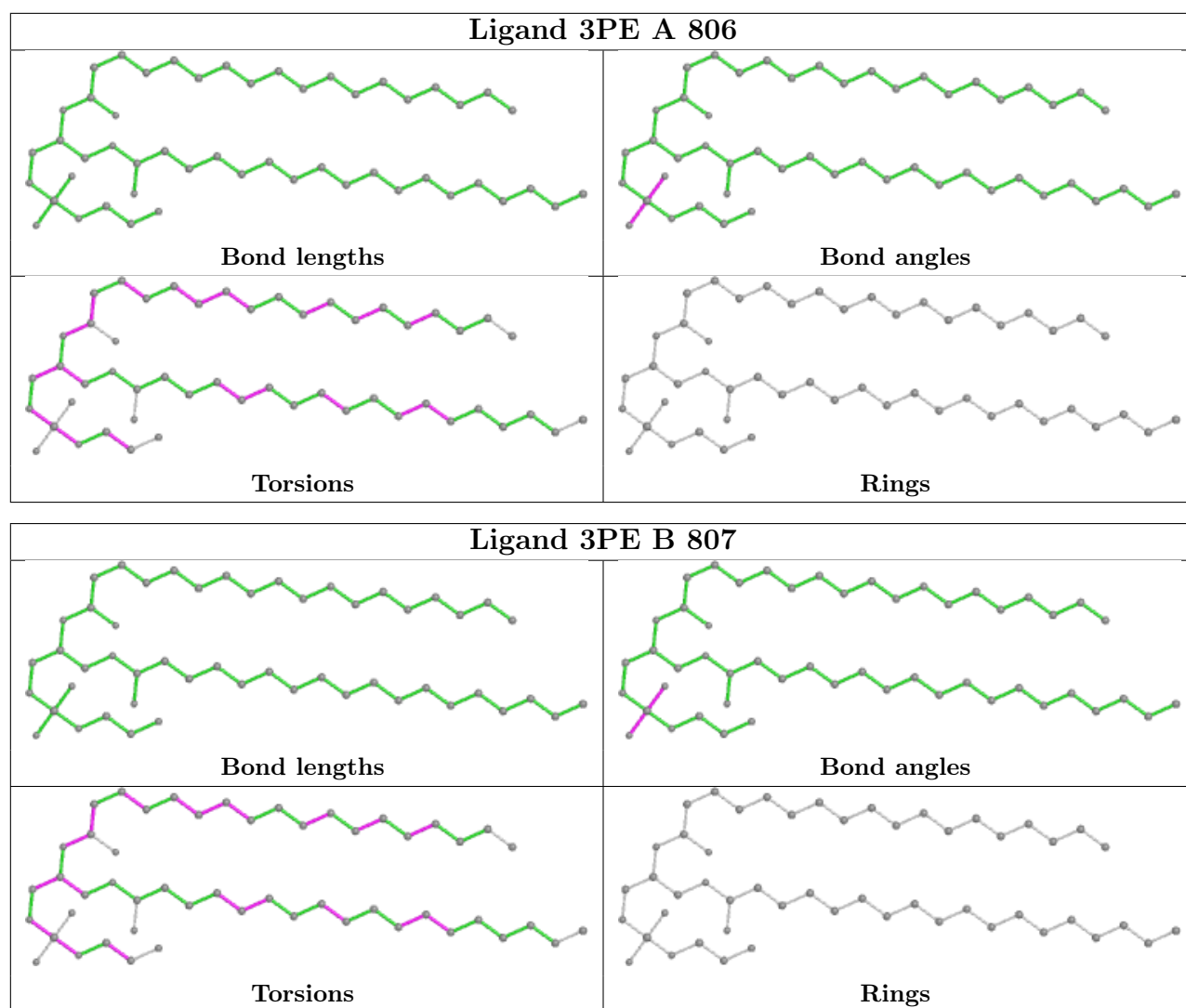
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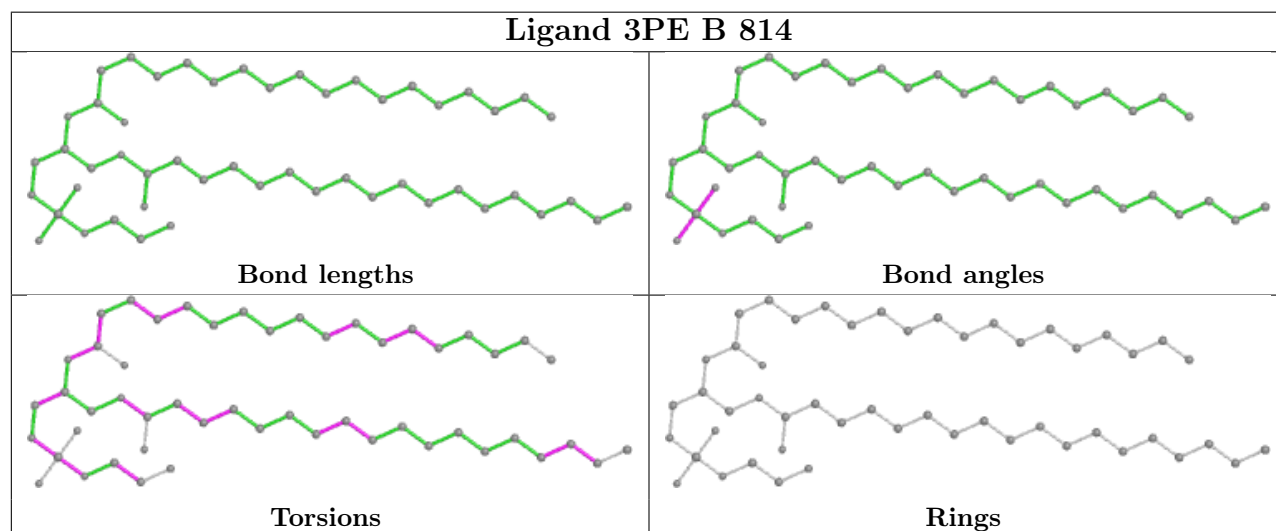
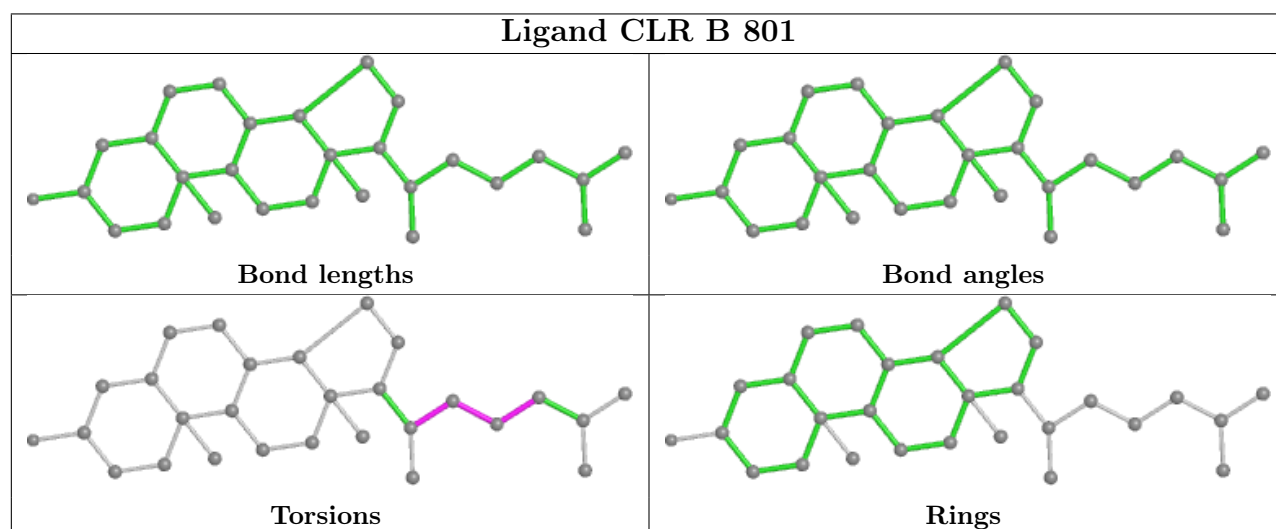
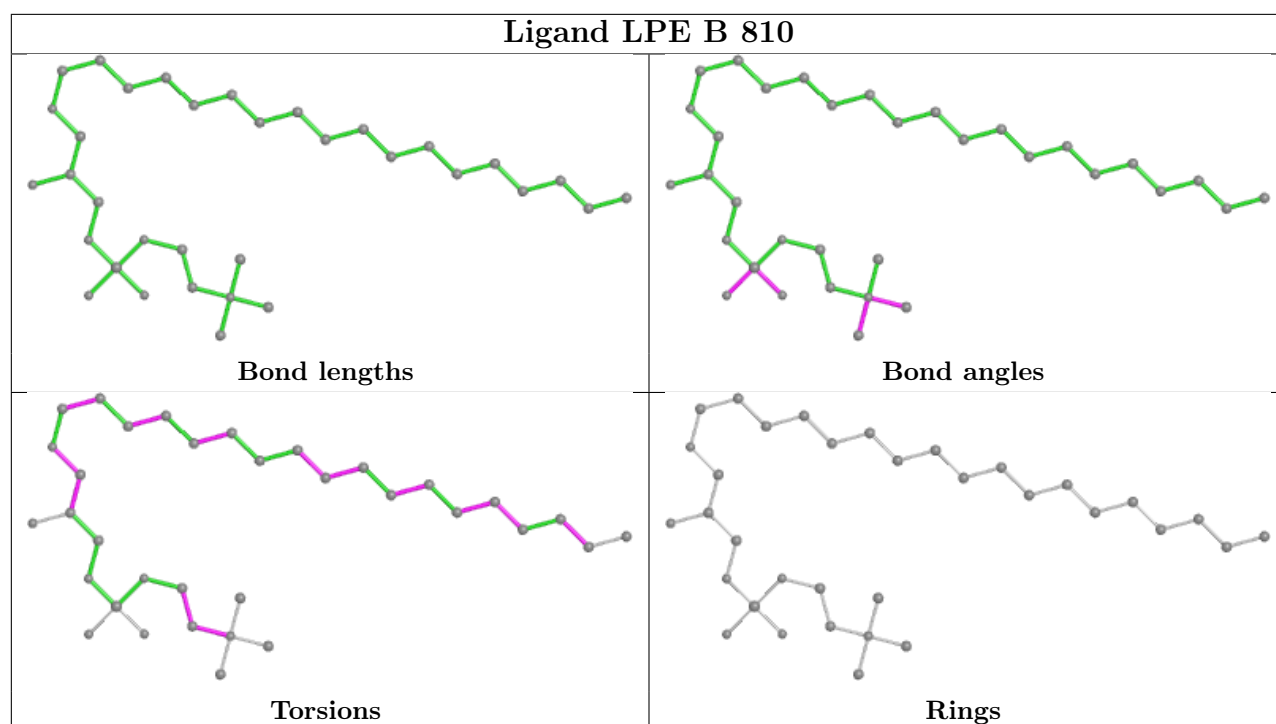
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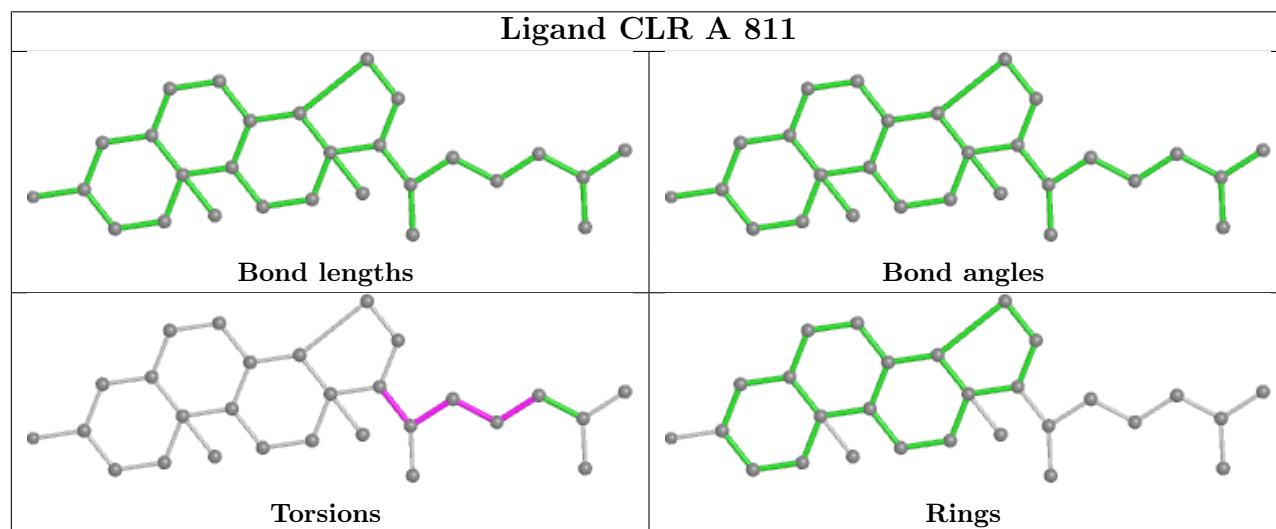
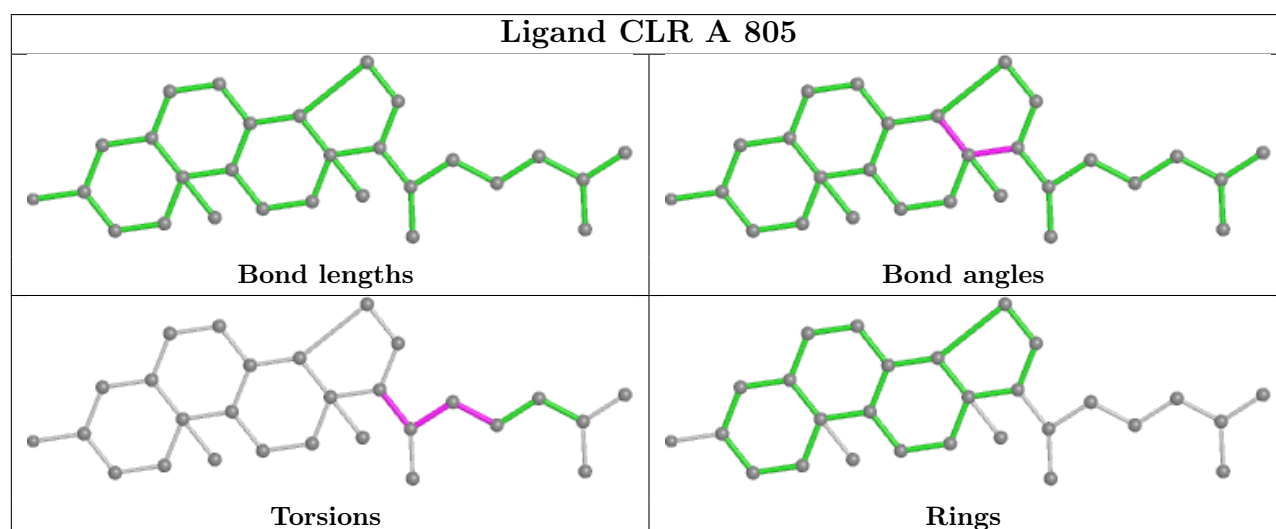
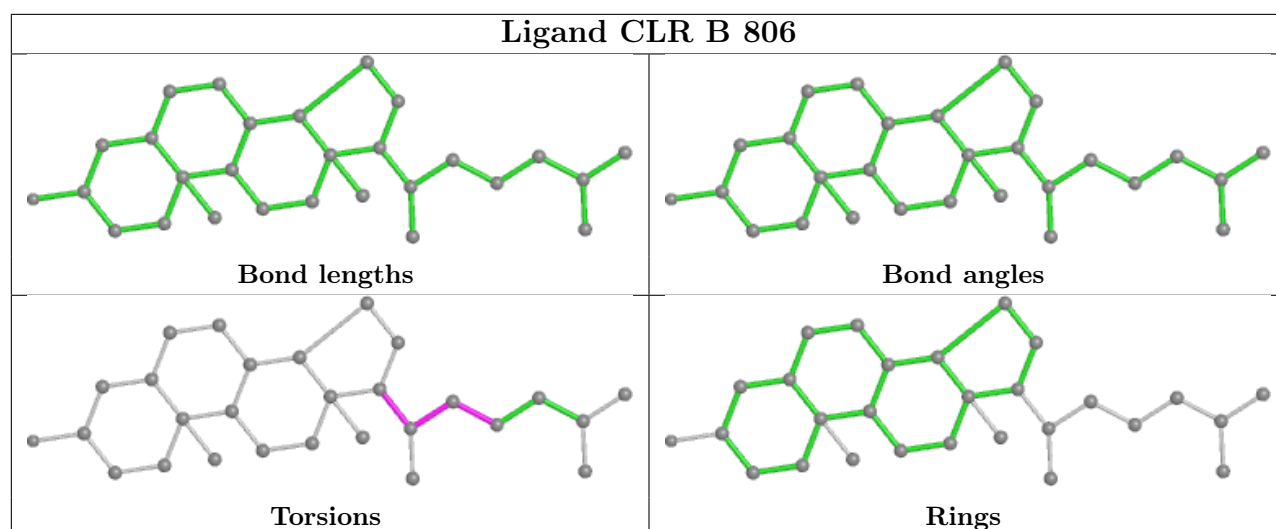
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	805	CLR	4	0
2	A	801	CLR	2	0
2	A	804	CLR	4	0
3	B	803	3PE	7	0
5	B	811	PLM	3	0
3	B	802	3PE	7	0
3	A	802	3PE	7	0
2	B	812	CLR	1	0

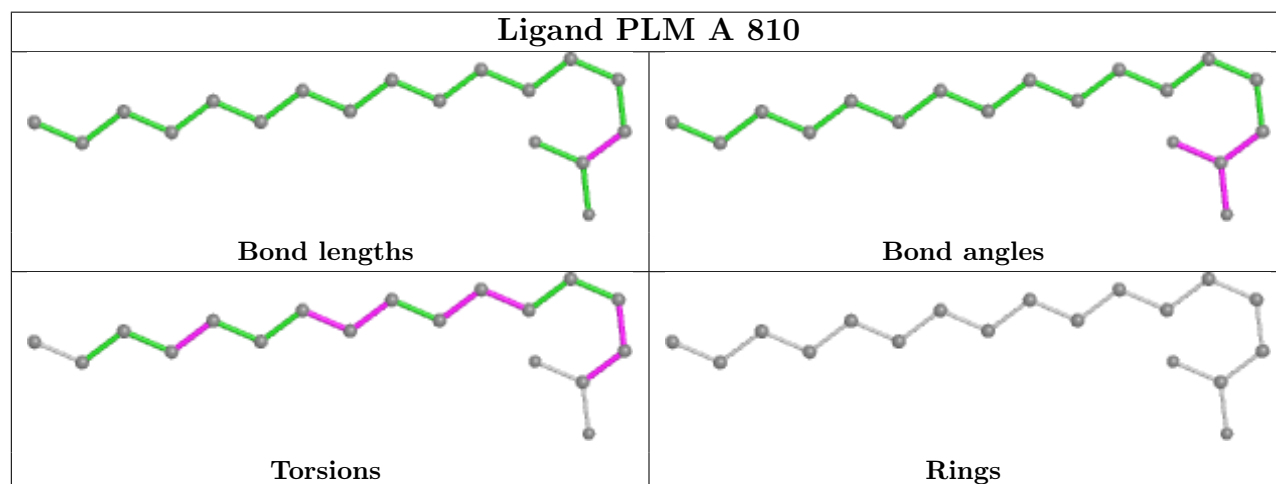
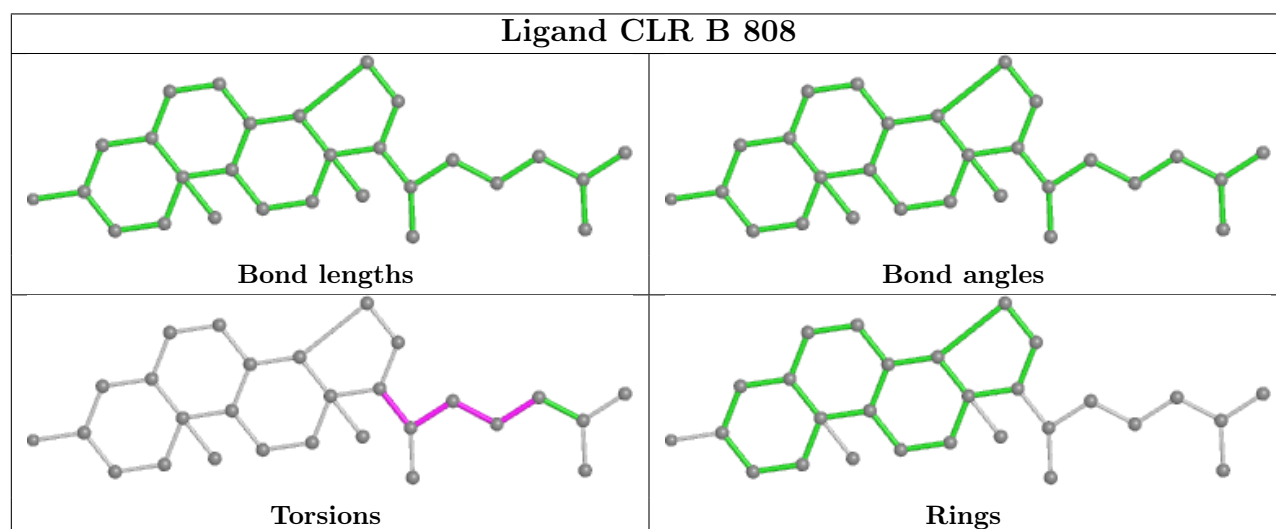
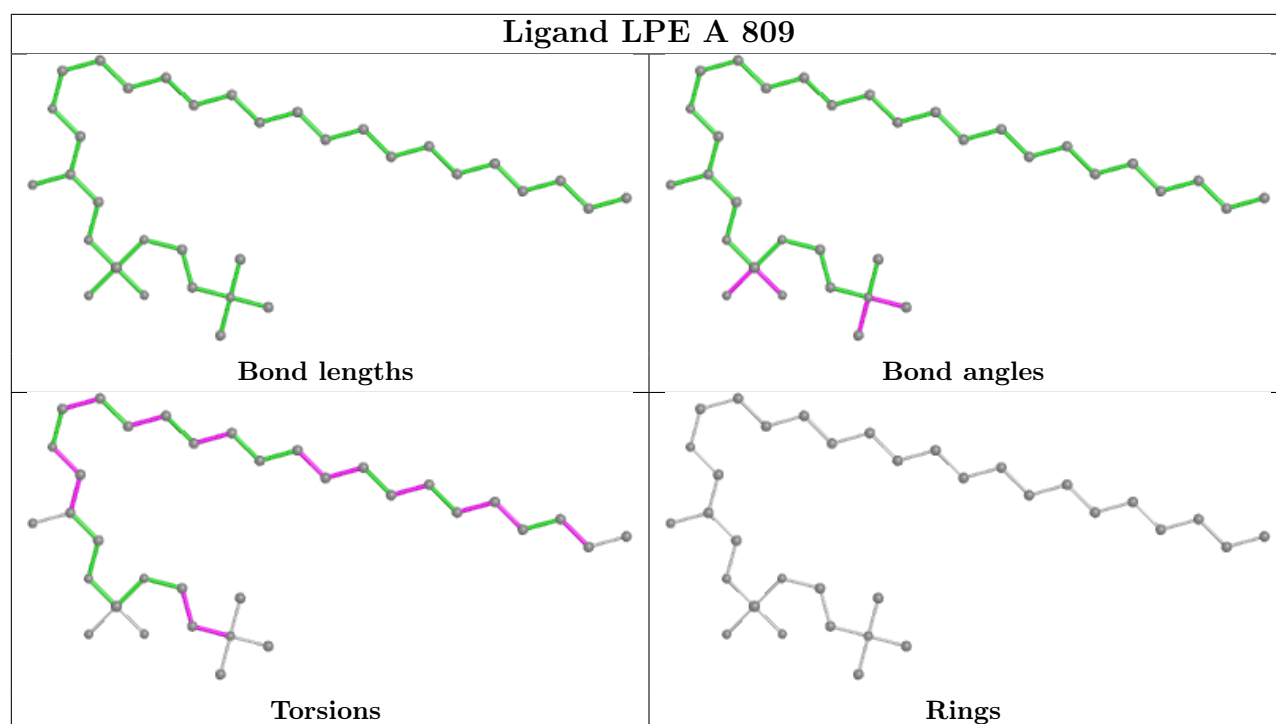
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

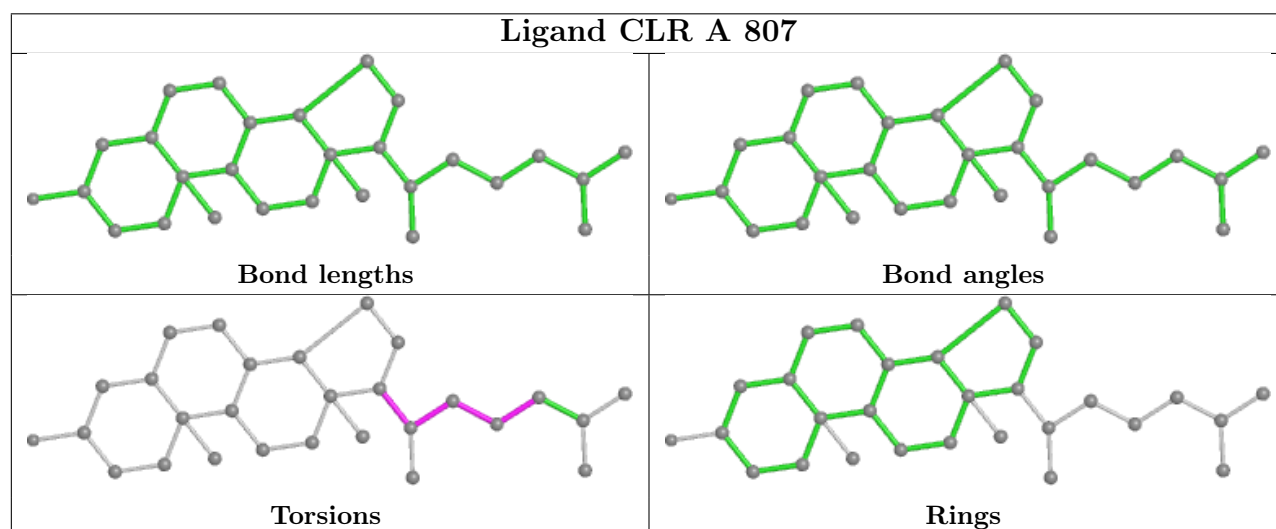
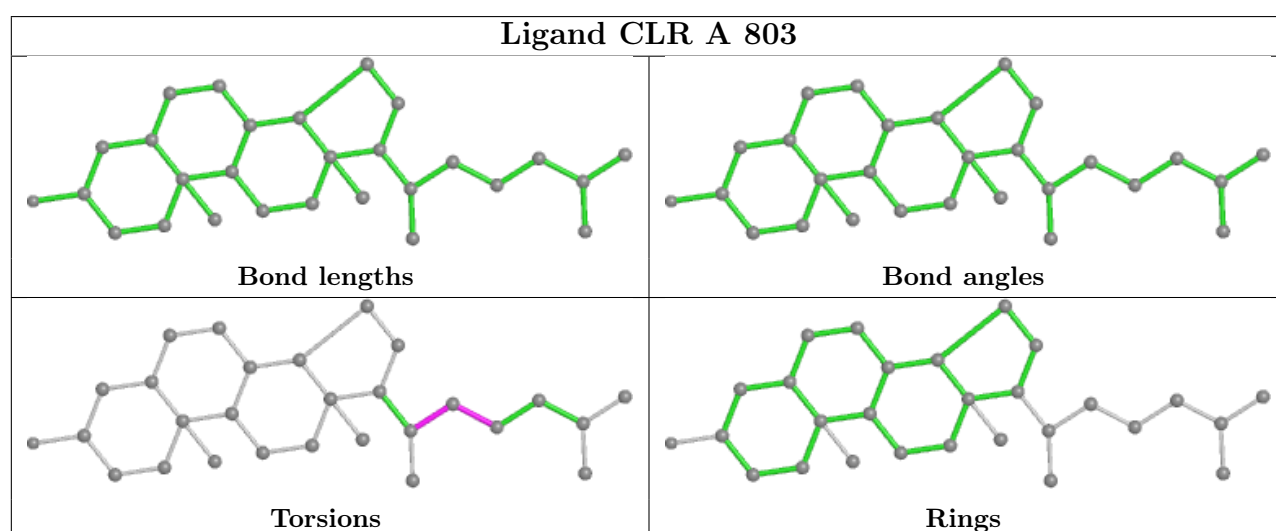
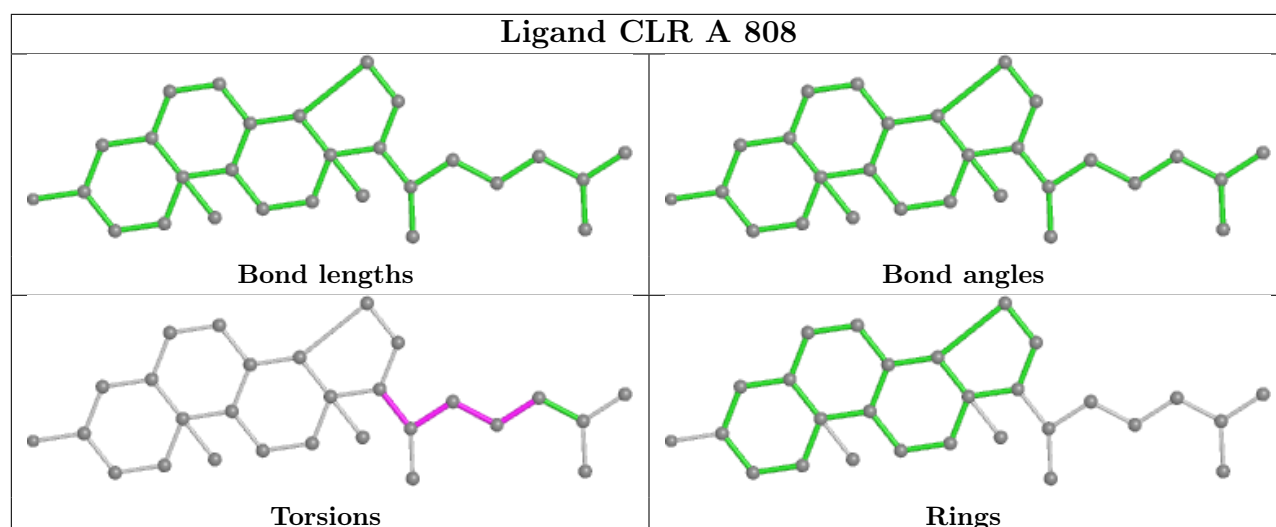


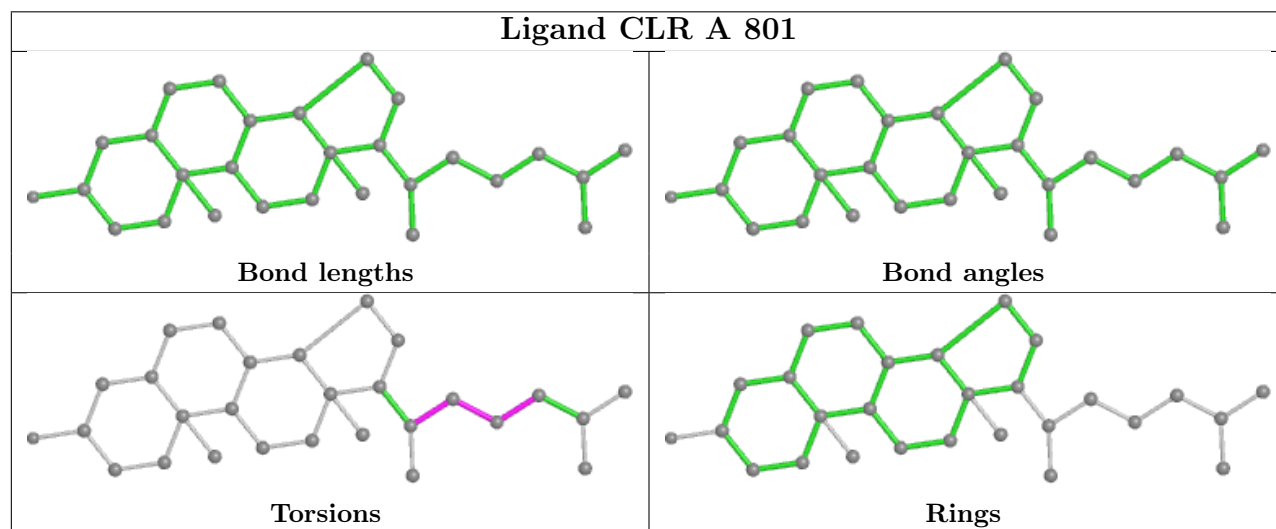
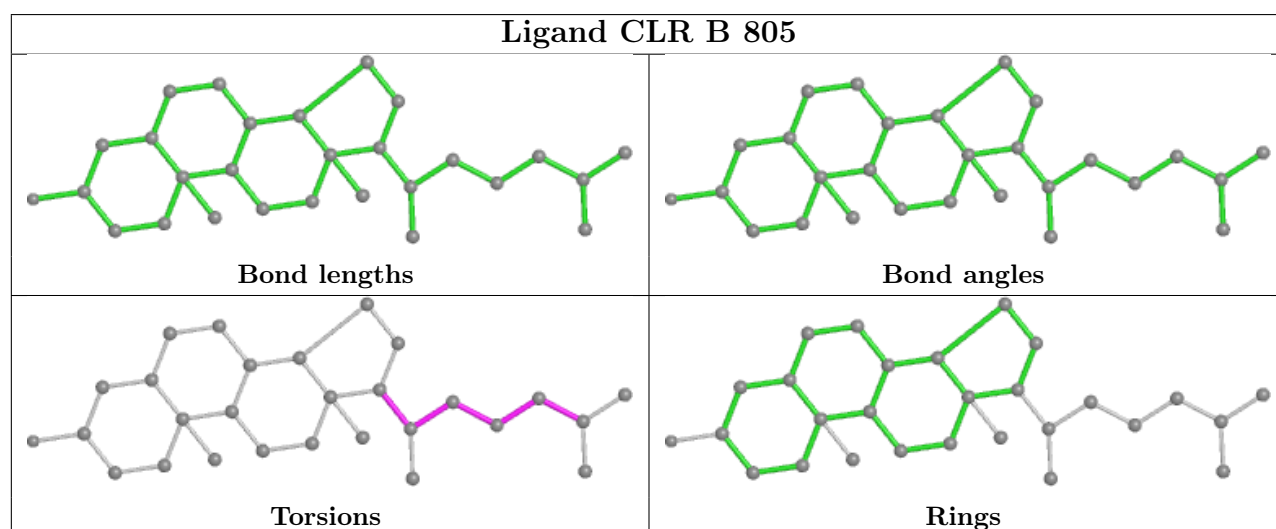
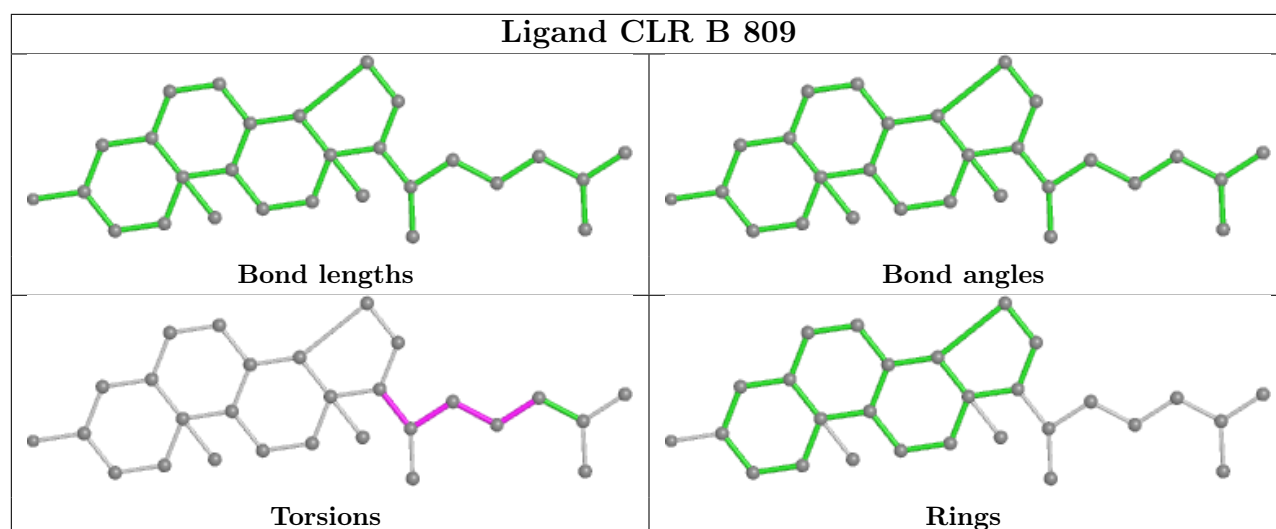


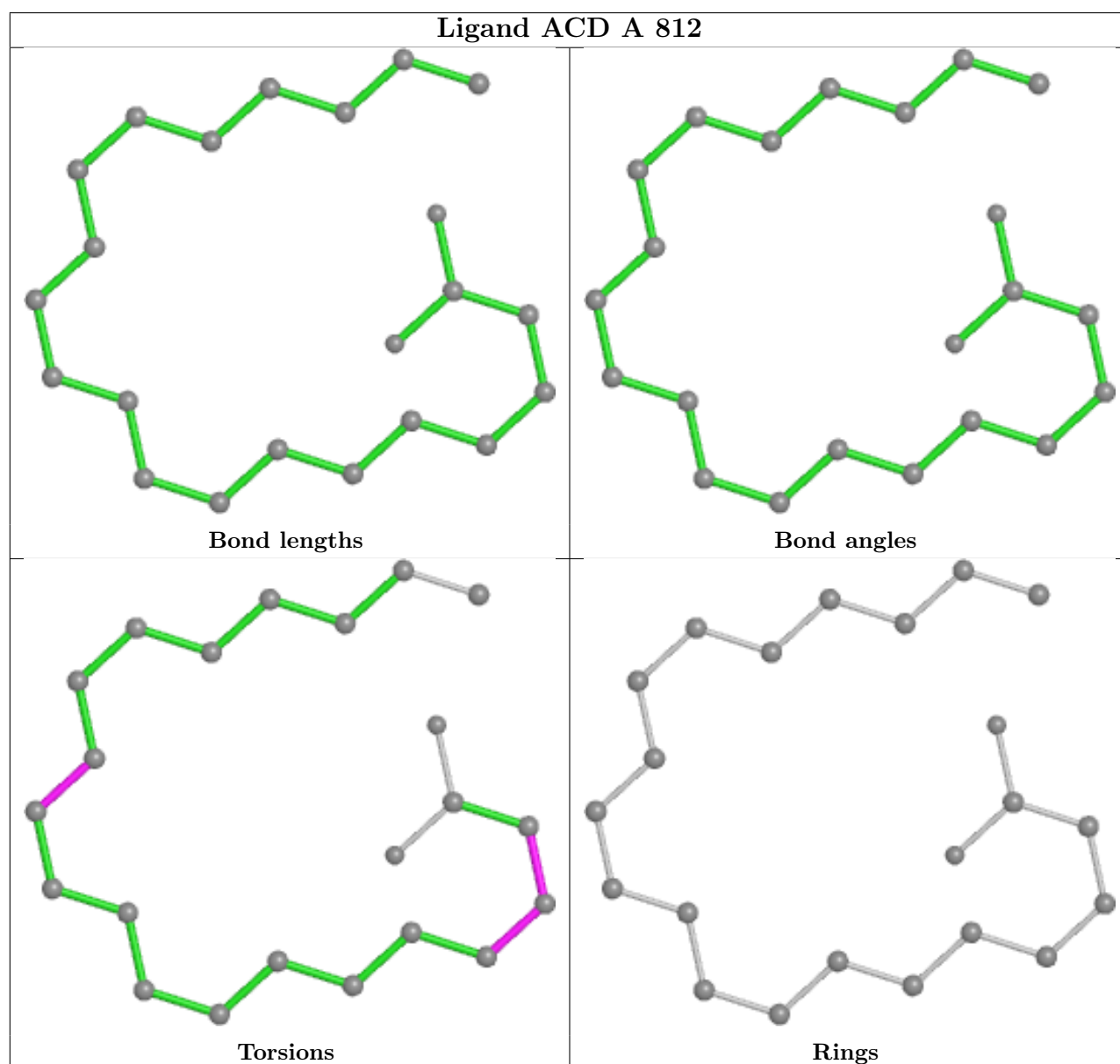
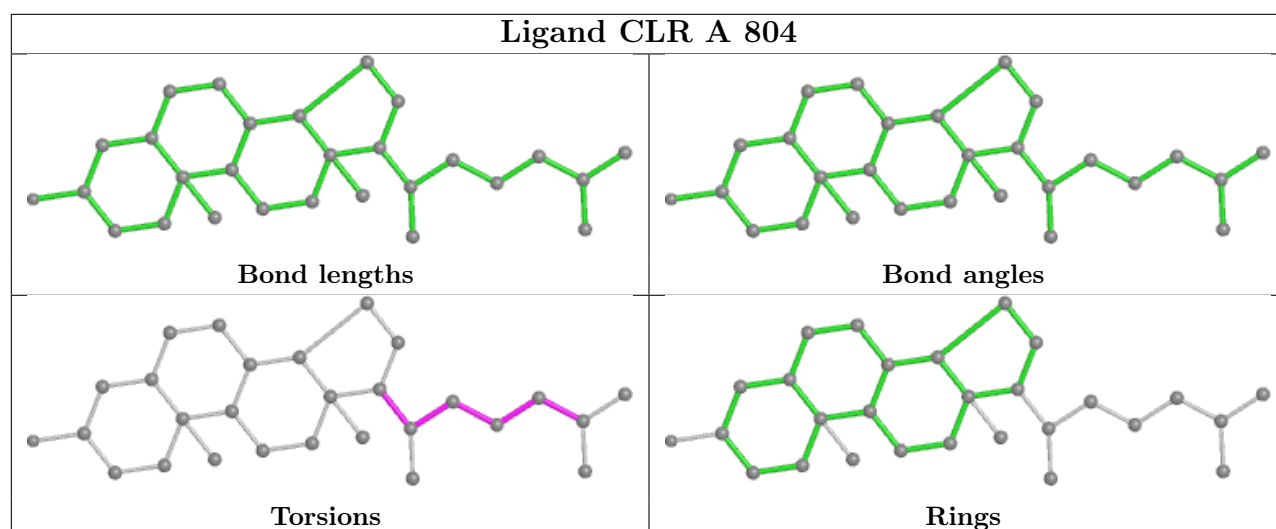


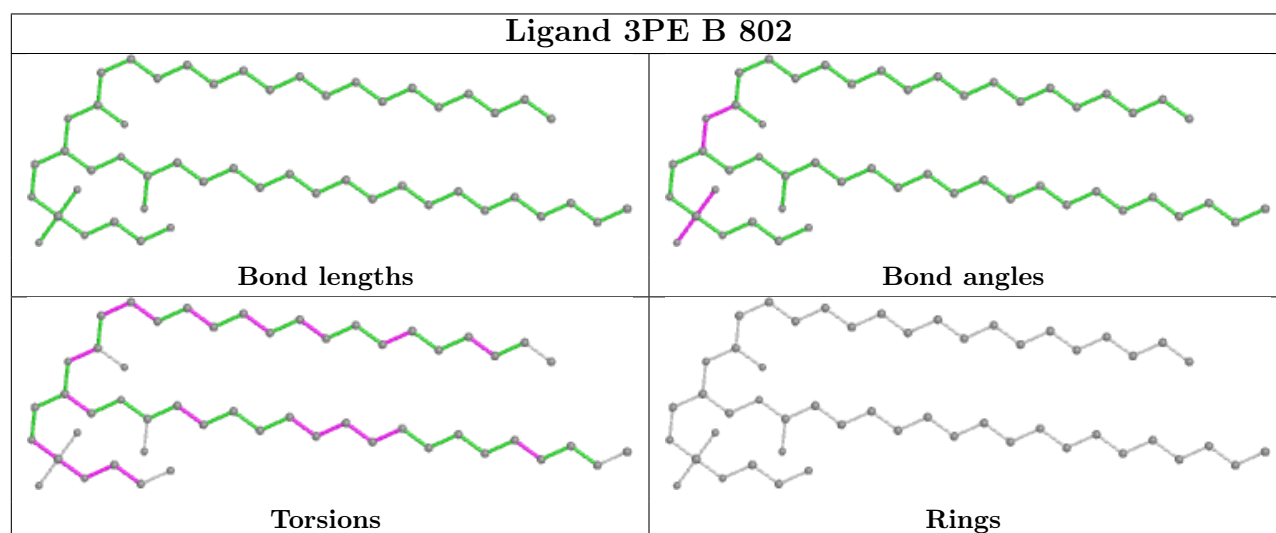
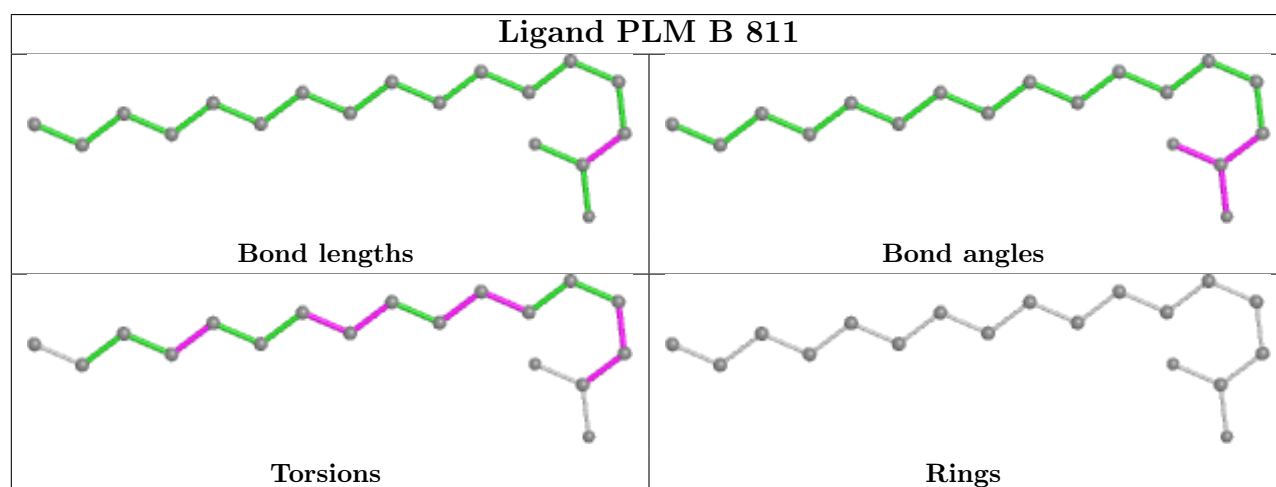
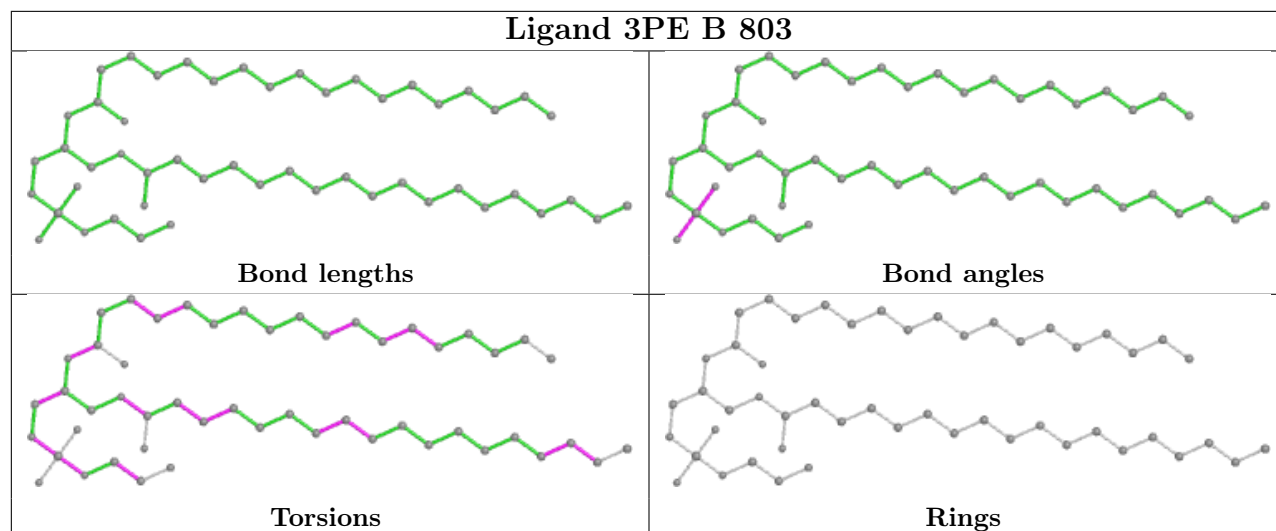


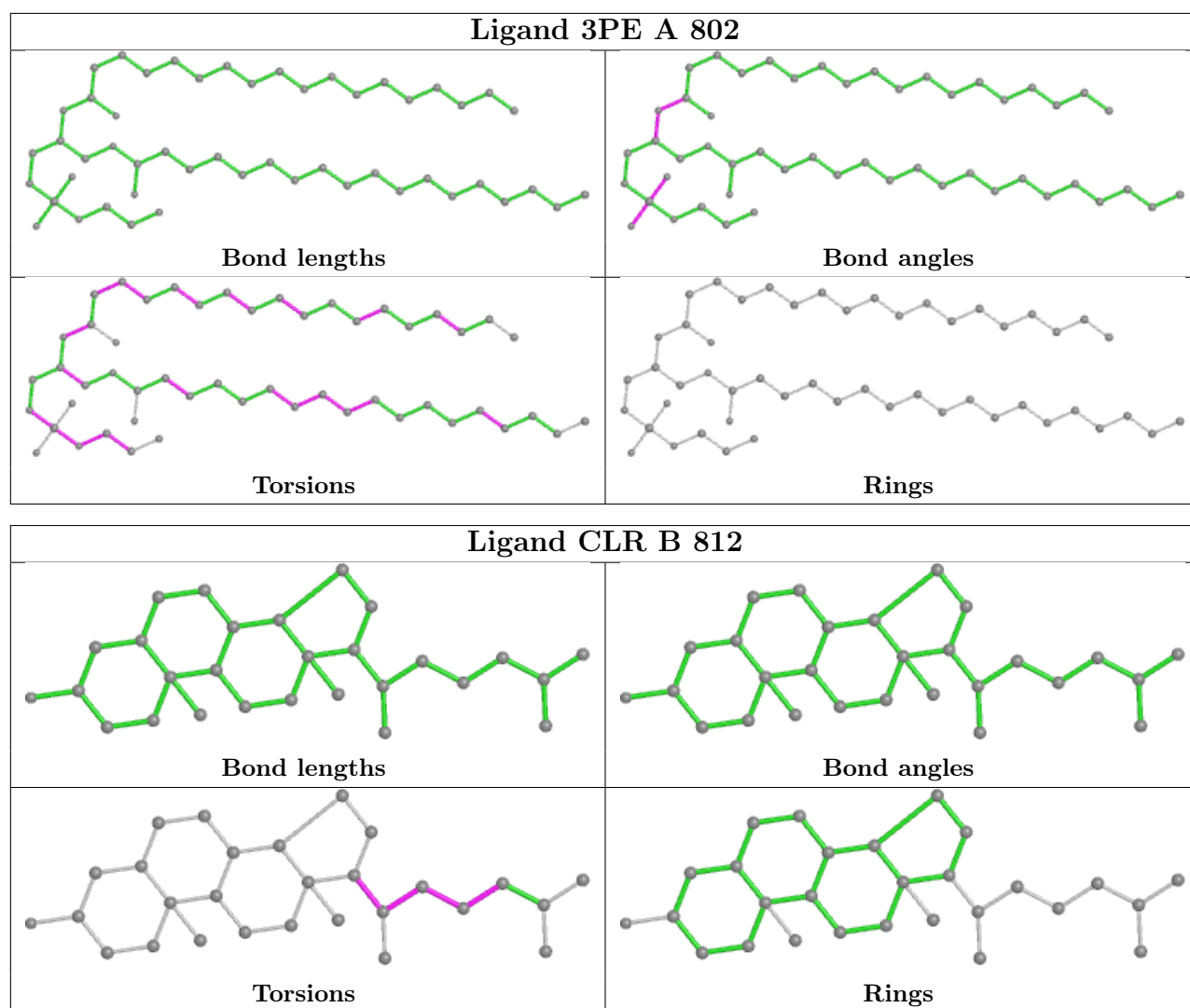


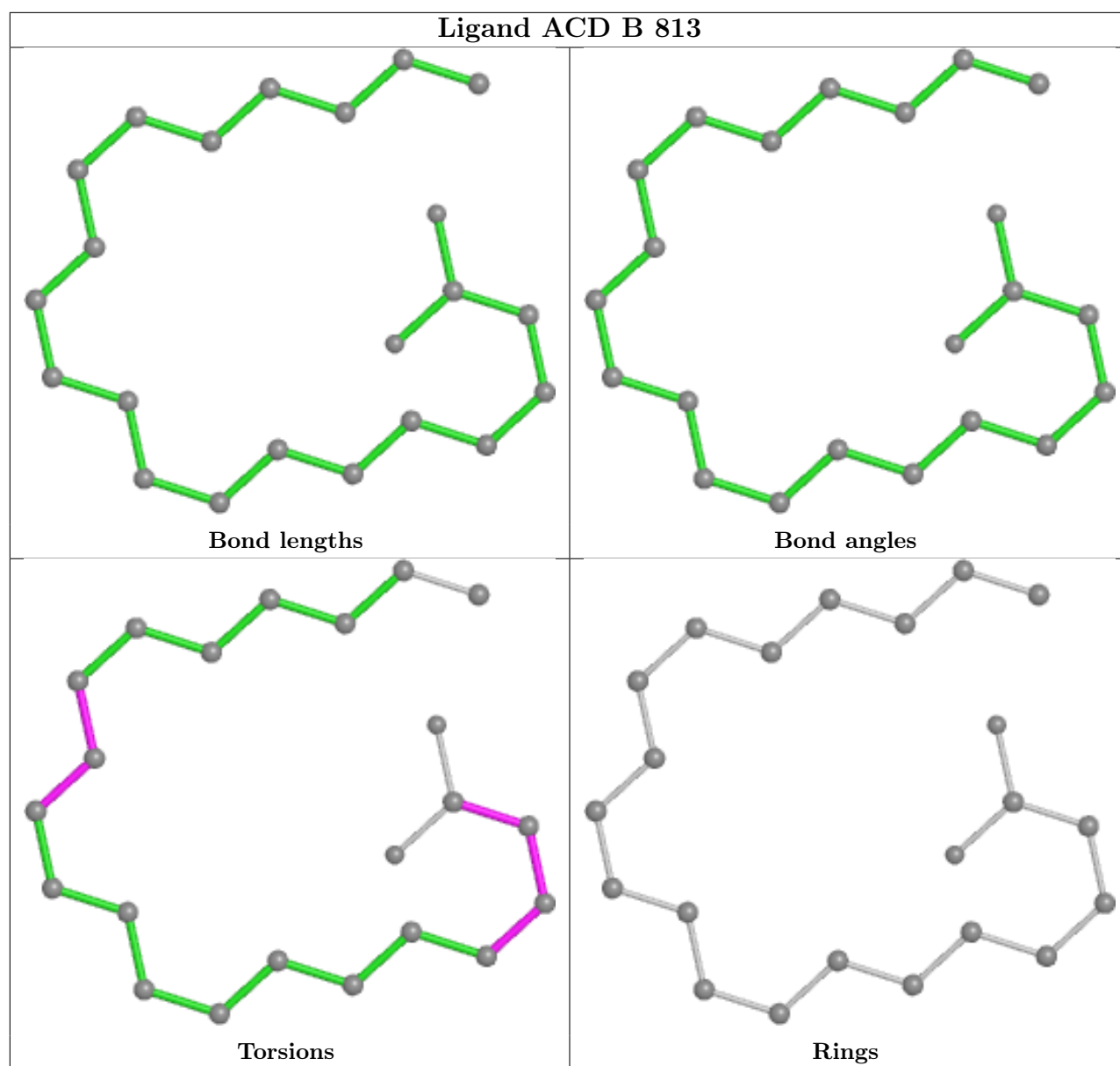












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

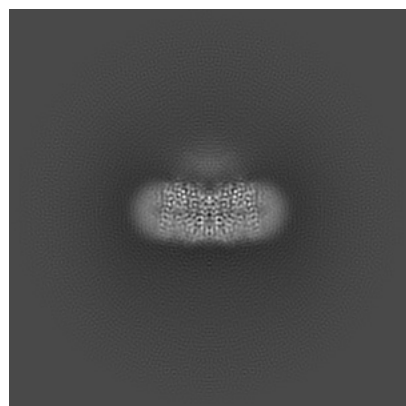
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60704. These allow visual inspection of the internal detail of the map and identification of artifacts.

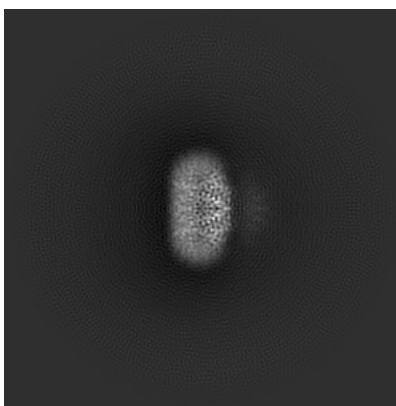
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

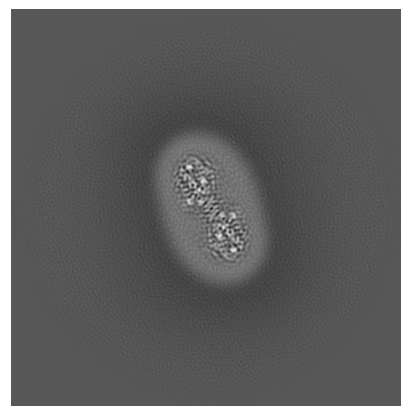
6.1.1 Primary map



X

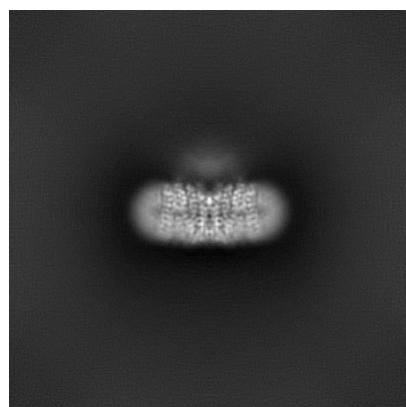


Y

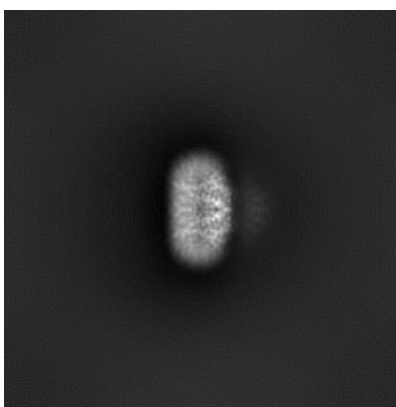


Z

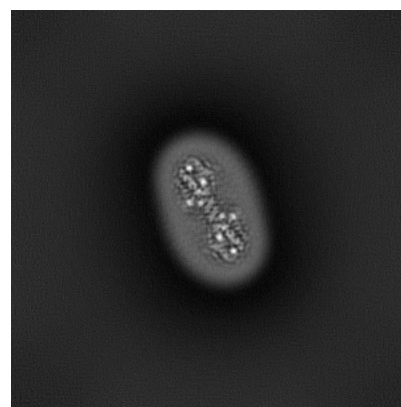
6.1.2 Raw map



X



Y

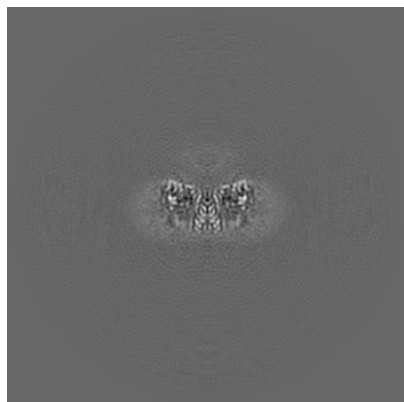


Z

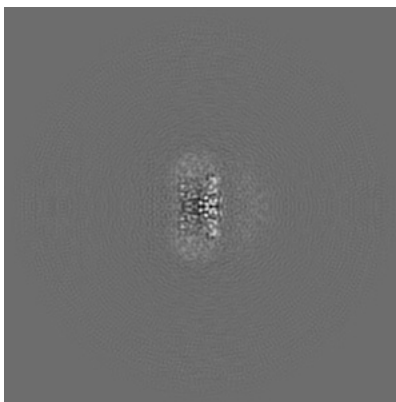
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

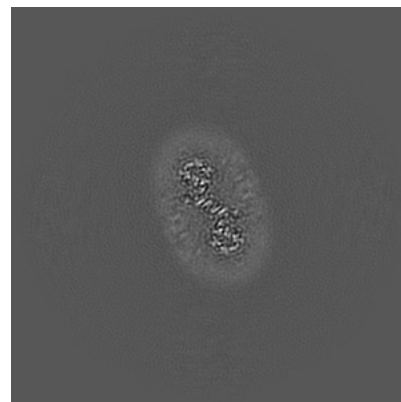
6.2.1 Primary map



X Index: 230

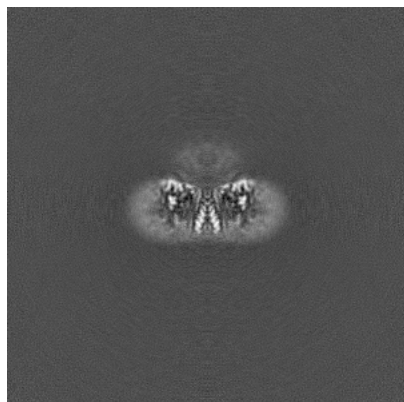


Y Index: 230

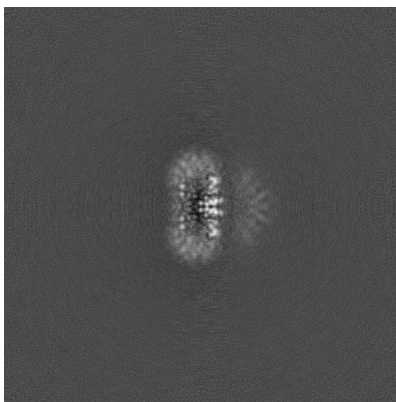


Z Index: 230

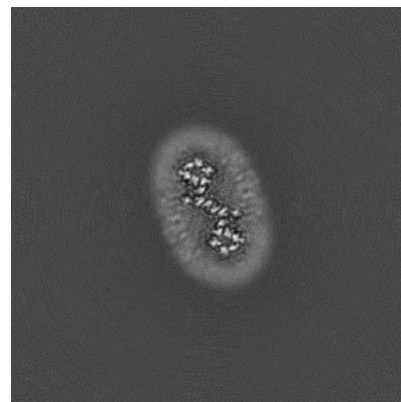
6.2.2 Raw map



X Index: 230



Y Index: 230

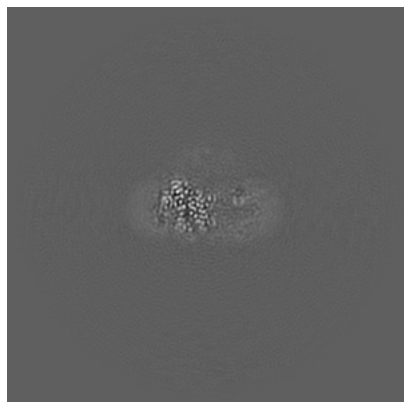


Z Index: 230

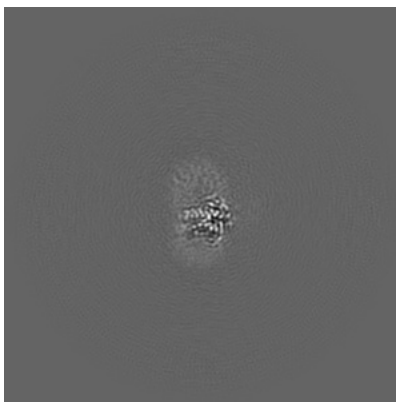
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

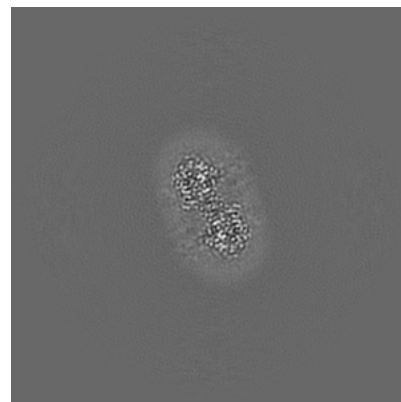
6.3.1 Primary map



X Index: 241

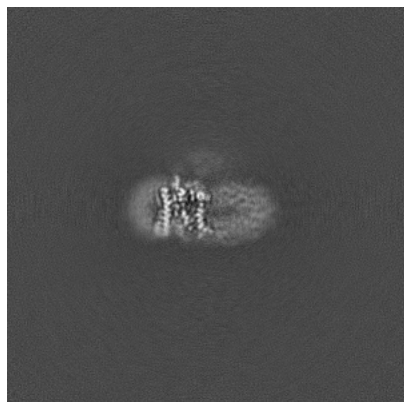


Y Index: 261

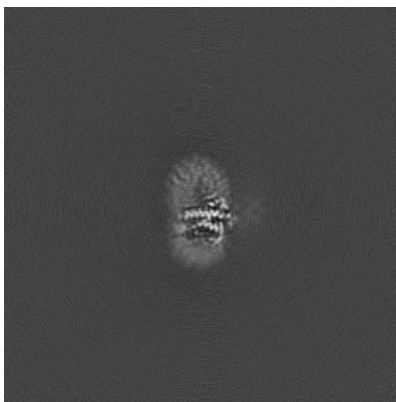


Z Index: 241

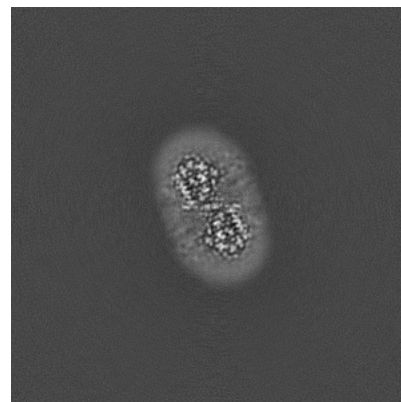
6.3.2 Raw map



X Index: 255



Y Index: 261

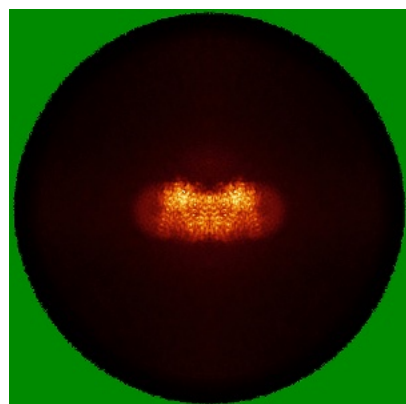


Z Index: 241

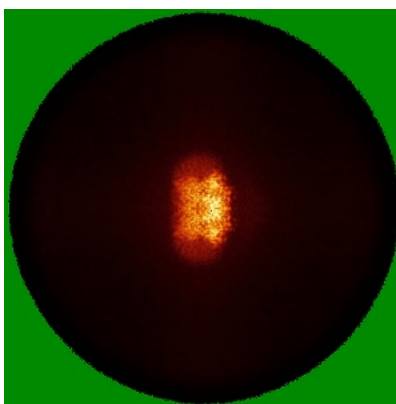
The images above show the largest variance slices of the map in three orthogonal directions.

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

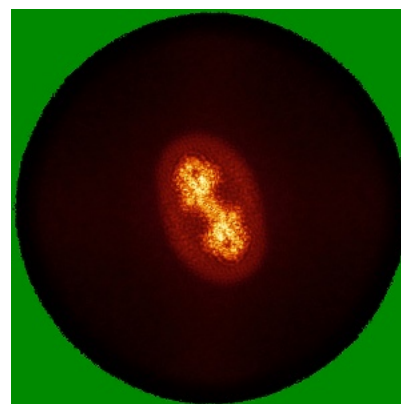
6.4.1 Primary map



X

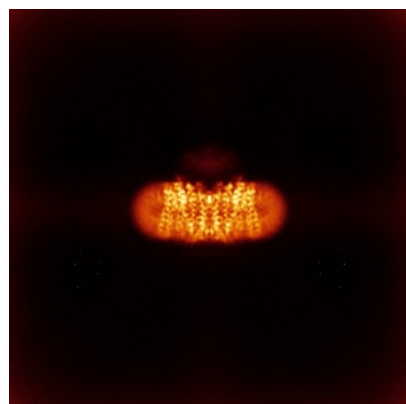


Y

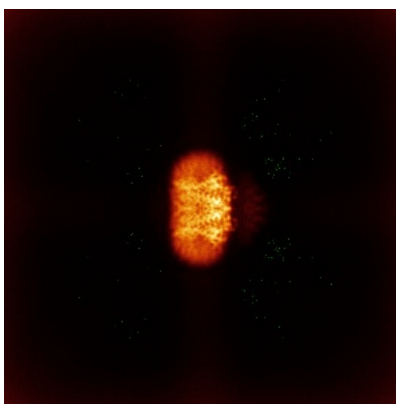


Z

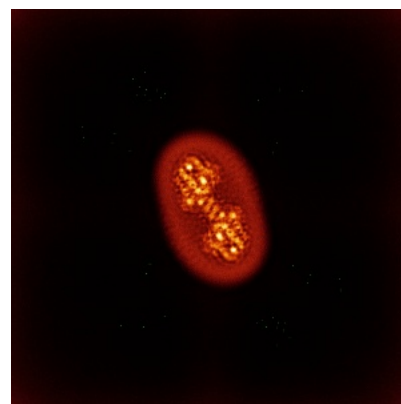
6.4.2 Raw map



X



Y

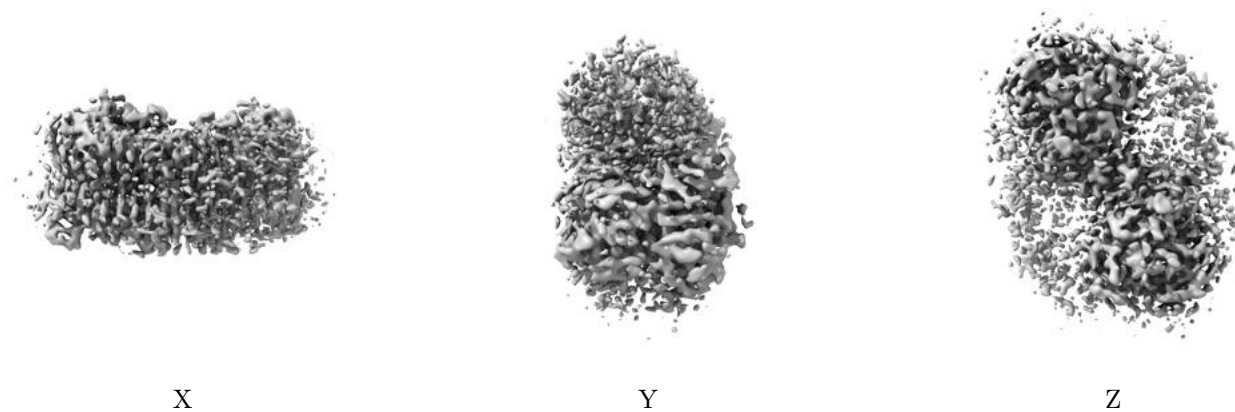


Z

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.

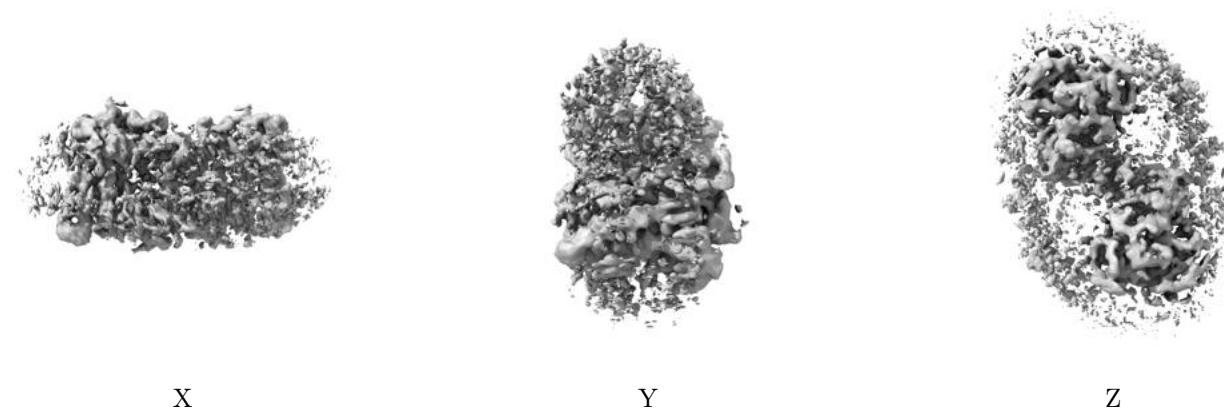
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.165. 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.

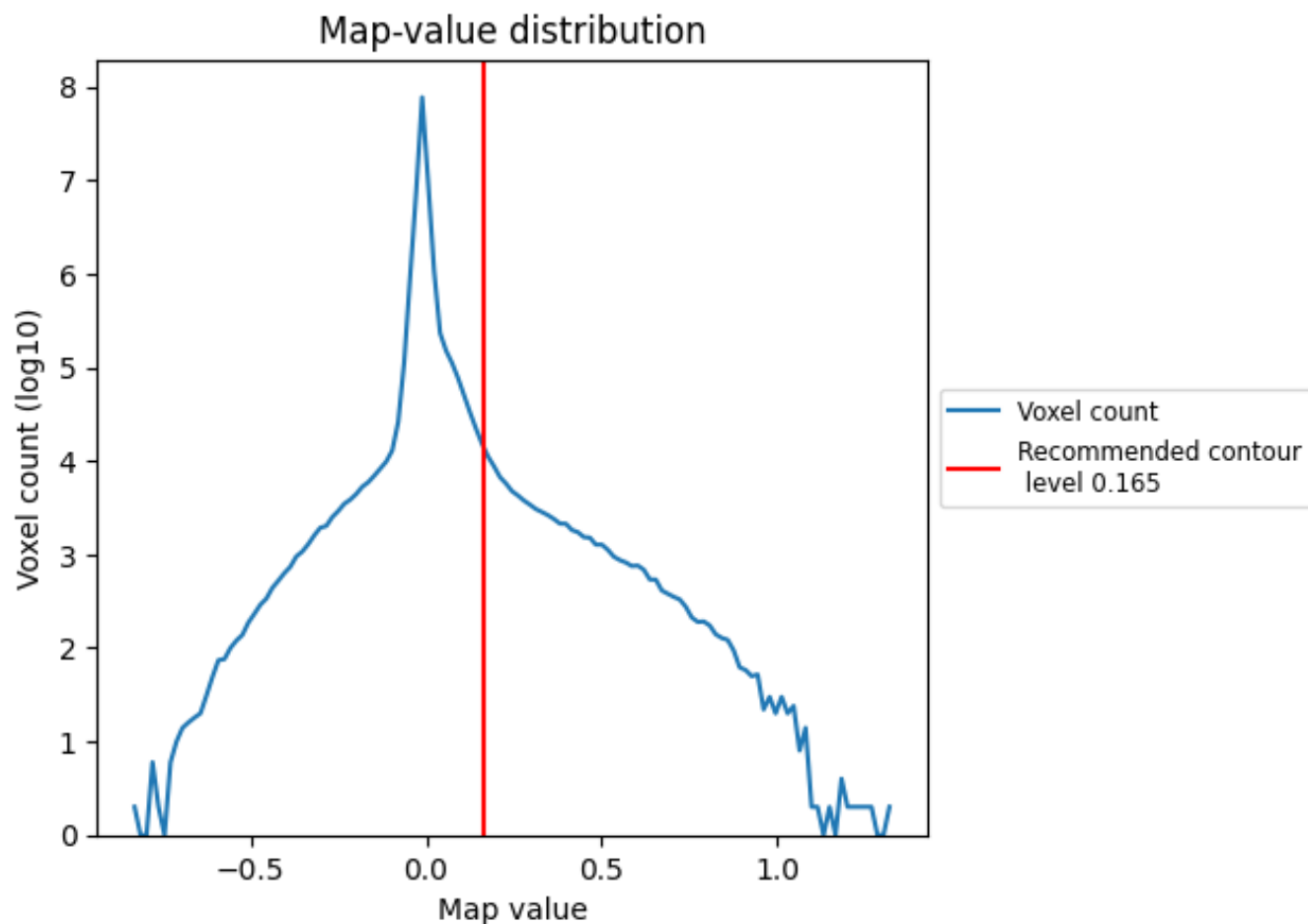
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

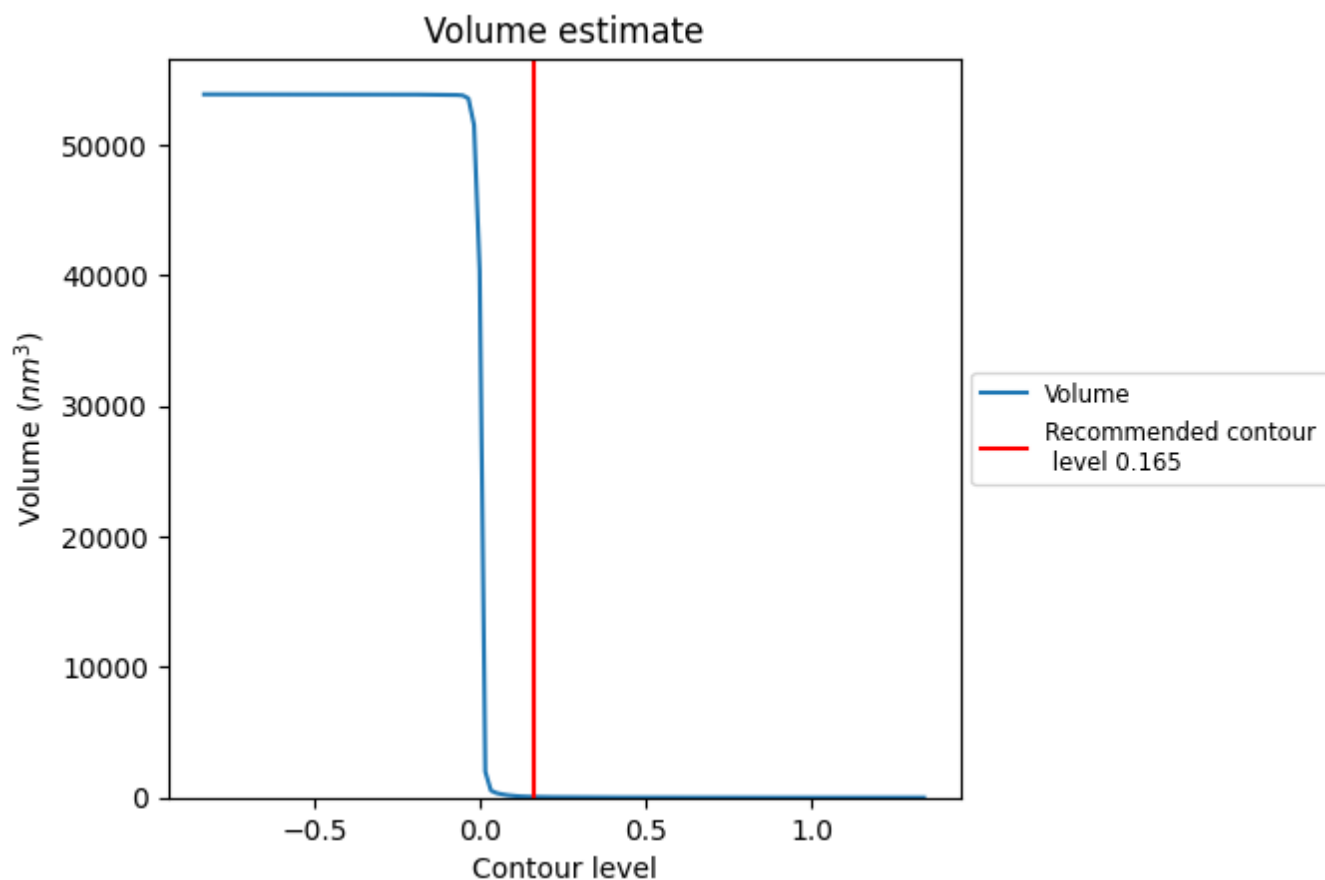
This section contains the results of statistical analysis of the map.

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.

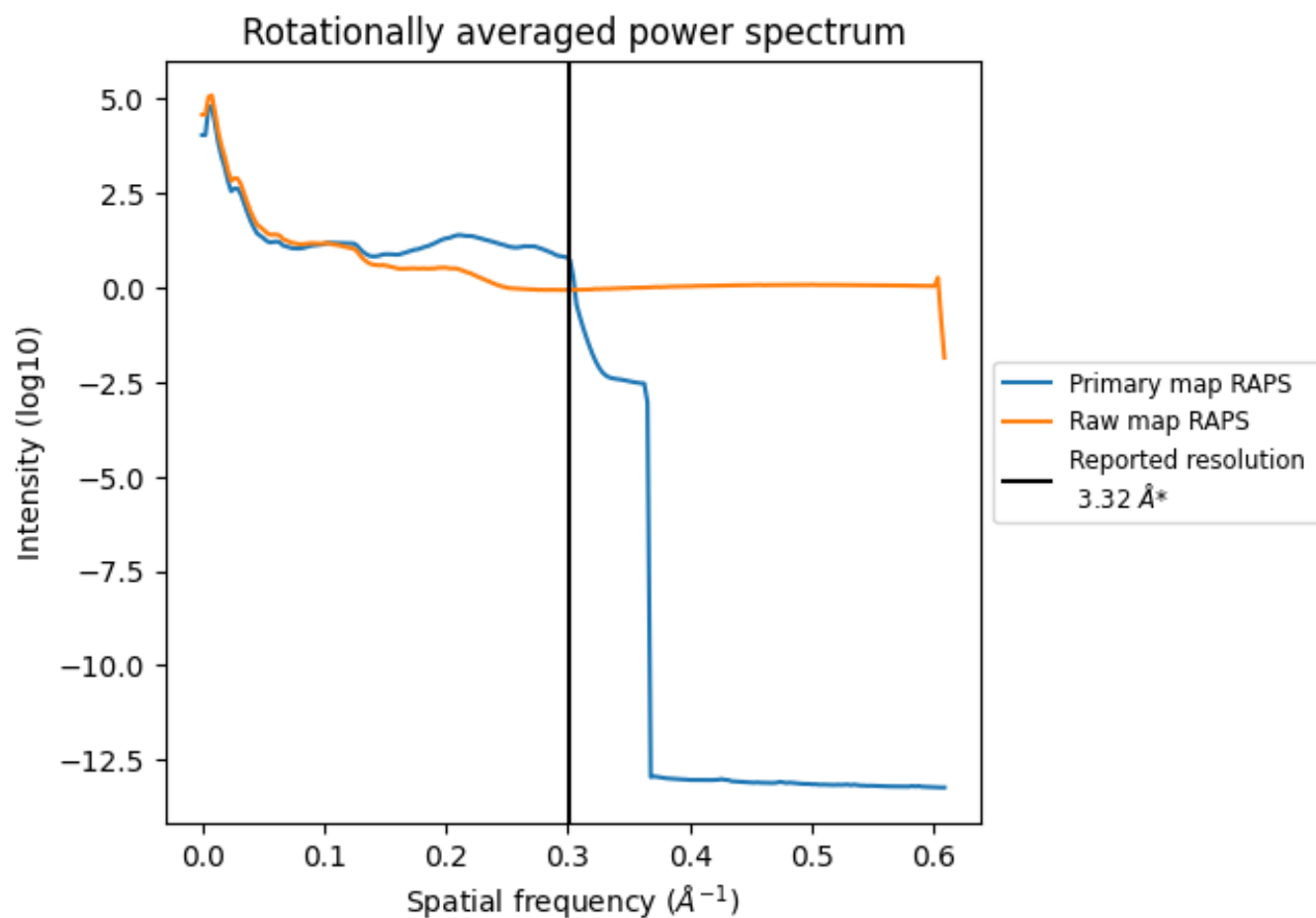
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 52 nm^3 ; this corresponds to an approximate mass of 47 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 ⓘ

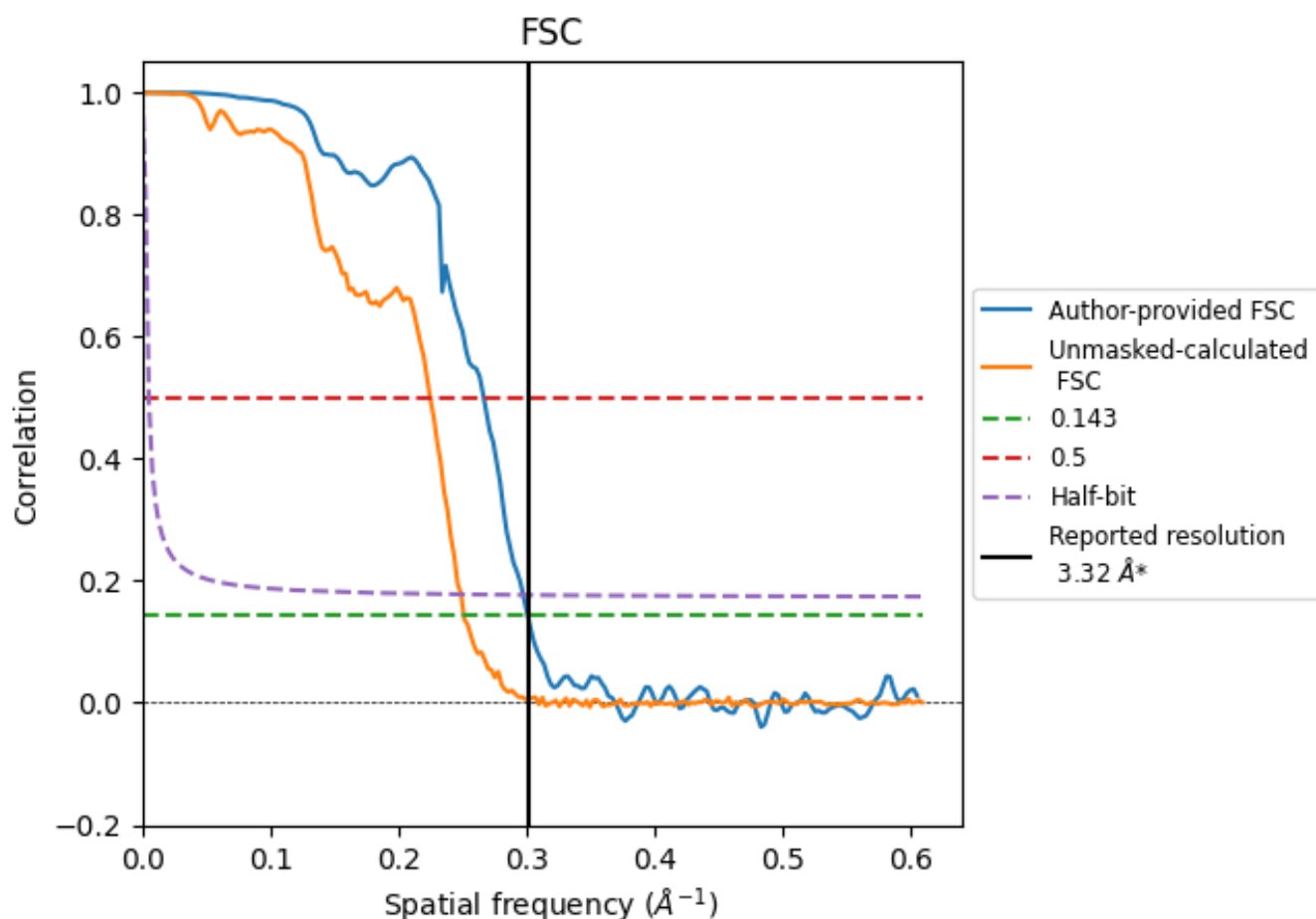


*Reported resolution corresponds to spatial frequency of 0.301 Å⁻¹

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 0.301 \AA^{-1}

8.2 Resolution estimates [i](#)

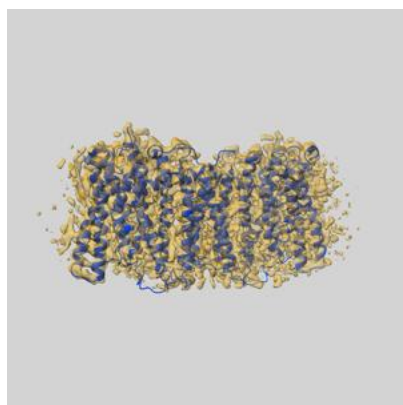
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.32	-	-
Author-provided FSC curve	3.32	3.75	3.36
Unmasked-calculated*	3.98	4.45	4.02

*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 3.98 differs from the reported value 3.32 by more than 10 %

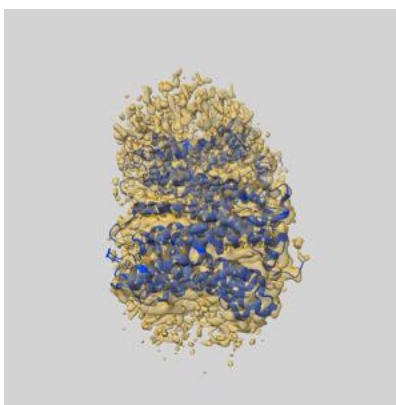
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-60704 and PDB model 9INE. Per-residue inclusion information can be found in section [3](#) on page [8](#).

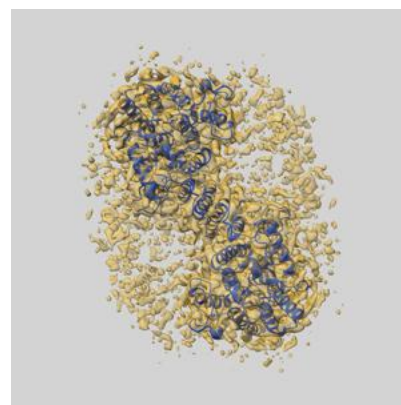
9.1 Map-model overlay [i](#)



X



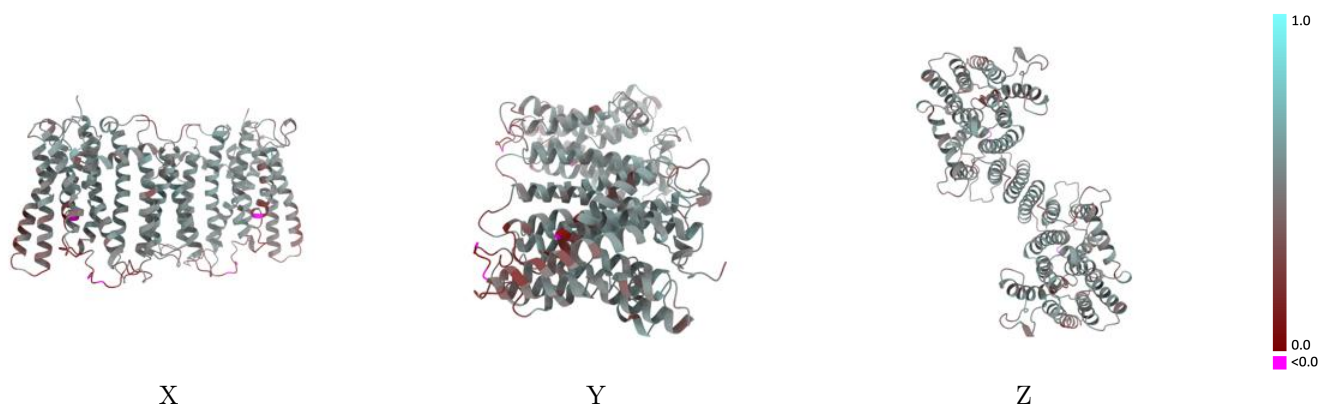
Y



Z

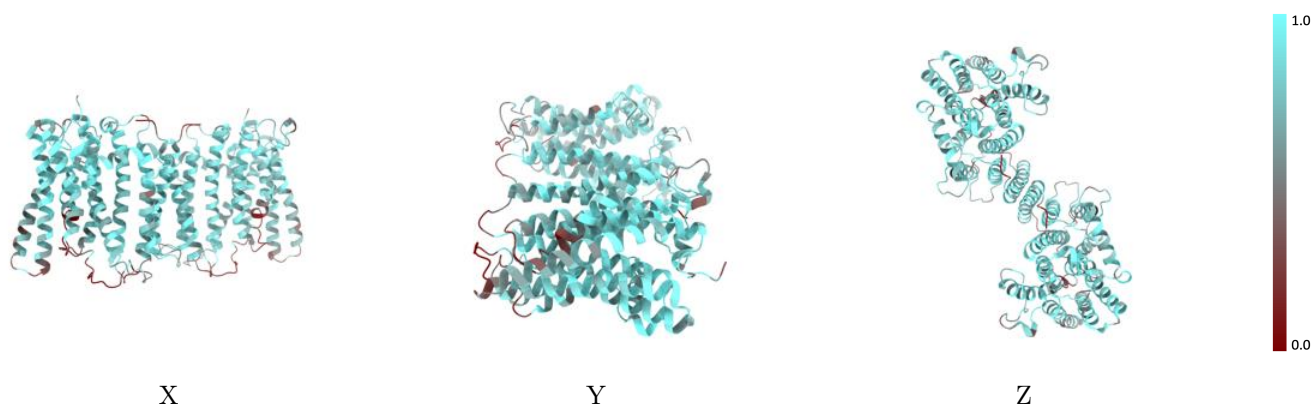
The images above show the 3D surface view of the map at the recommended contour level 0.165 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



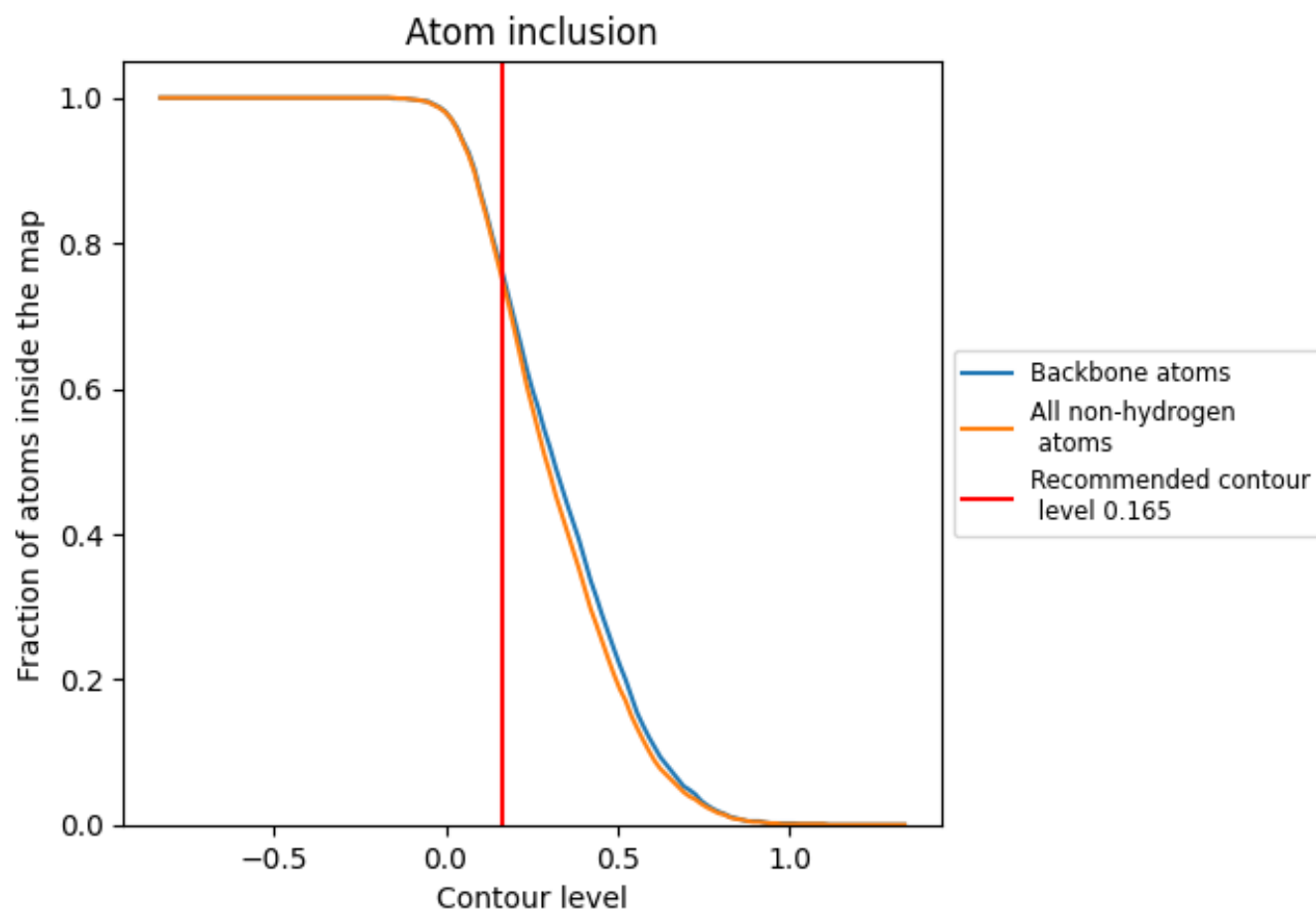
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.165).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 75% 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 (0.165) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7500	<div></div> 0.4800
A	<div></div> 0.7510	<div></div> 0.4800
B	<div></div> 0.7490	<div></div> 0.4790

