



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 08:16 PM UTC

PDB ID : 9IUC / pdb_00009iuc
EMDB ID : EMD-60897
Title : Cryo-EM structure of human XPR1 in complex with InsP6 in closed state - in the presence of KIDINS220-1-432 without substrate KH2PO4
Authors : Zuo, P.; Liang, L.; Yin, Y.
Deposited on : 2024-07-20
Resolution : 3.80 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

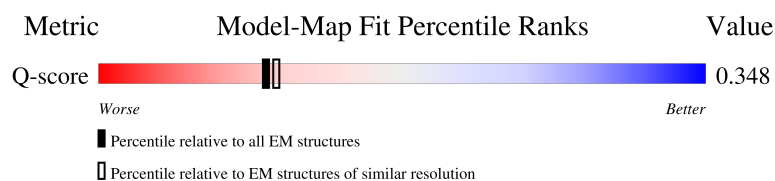
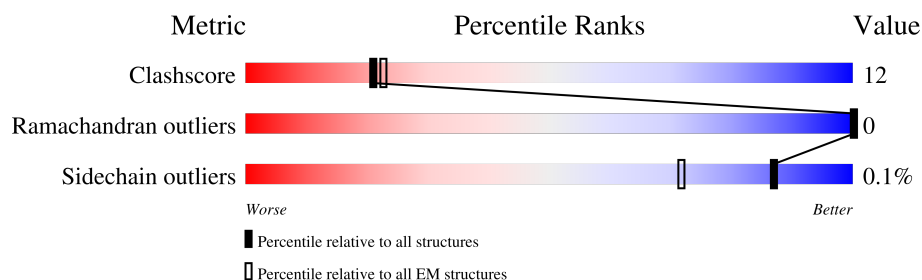
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

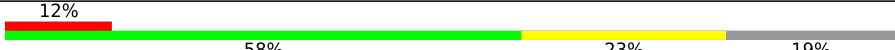
The reported resolution of this entry is 3.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10198 (3.30 - 4.30)

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	
1	B	704	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10360 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	570	Total	C	N	O	S	0	0
			4765	3155	780	810	20		
1	B	570	Total	C	N	O	S	0	0
			4765	3155	780	810	20		

There are 16 discrepancies between the modelled and reference sequences:

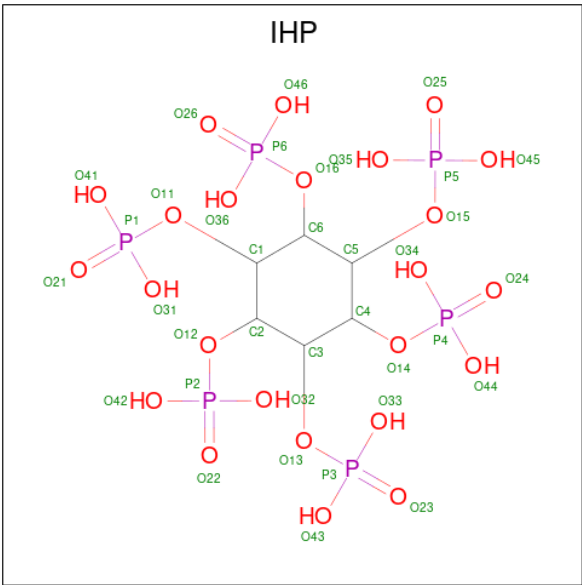
Chain	Residue	Modelled	Actual	Comment	Reference
A	697	SER	-	expression tag	UNP Q9UBH6
A	698	ARG	-	expression tag	UNP Q9UBH6
A	699	GLU	-	expression tag	UNP Q9UBH6
A	700	ASN	-	expression tag	UNP Q9UBH6
A	701	LEU	-	expression tag	UNP Q9UBH6
A	702	TYR	-	expression tag	UNP Q9UBH6
A	703	PHE	-	expression tag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

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



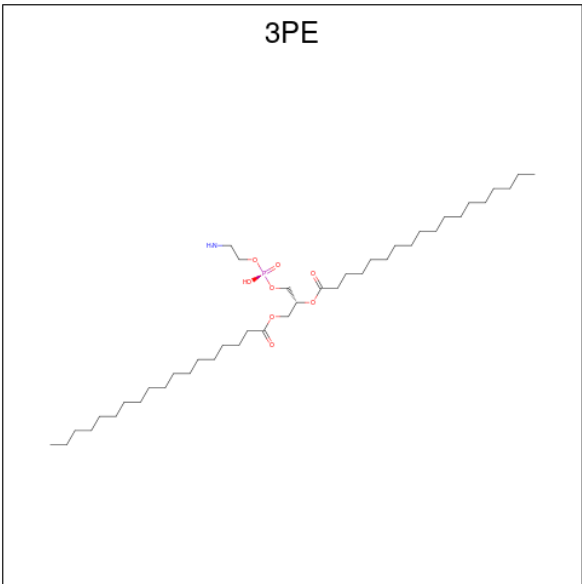
Mol	Chain	Residues	Atoms			AltConf
2	A	1	Total	C	O	0
			28	27	1	
2	A	1	Total	C	O	0
			28	27	1	
2	A	1	Total	C	O	0
			28	27	1	
2	A	1	Total	C	O	0
			28	27	1	
2	A	1	Total	C	O	0
			28	27	1	
2	A	1	Total	C	O	0
			28	27	1	
2	B	1	Total	C	O	0
			28	27	1	
2	B	1	Total	C	O	0
			28	27	1	
2	B	1	Total	C	O	0
			28	27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

- Molecule 3 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: $C_6H_{18}O_{24}P_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	O	P	0
			36	6	24	6	
3	B	1	Total	C	O	P	0
			36	6	24	6	

- Molecule 4 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: C₄₁H₈₂NO₈P) (labeled as "Ligand of Interest" by depositor).



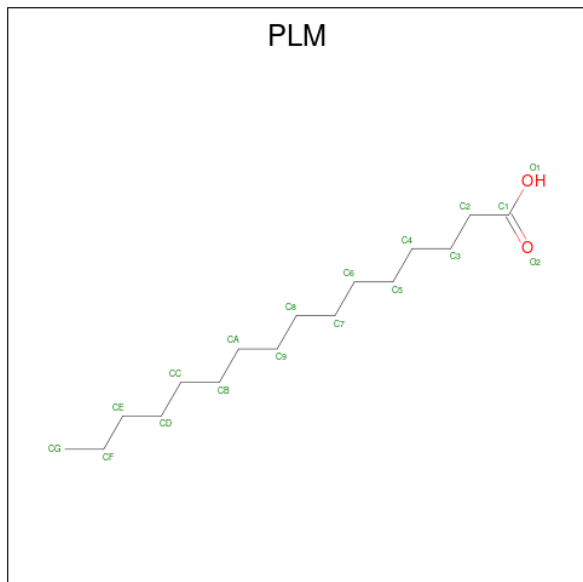
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			51	41	1	8	1	

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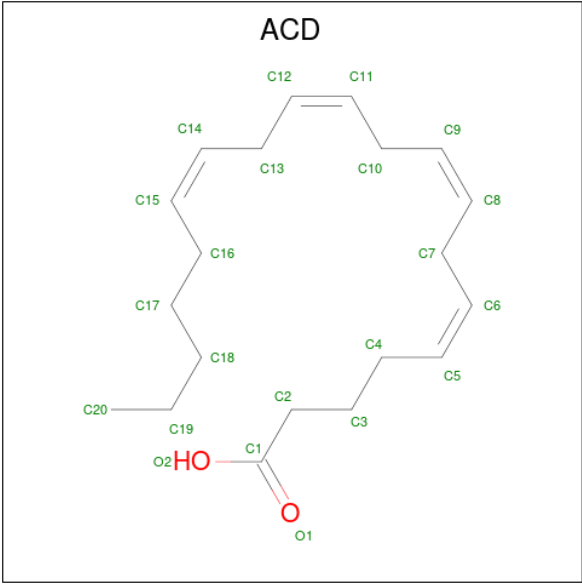
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
4	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
4	B	1	Total	C	N	O	P	0
			51	41	1	8	1	
4	B	1	Total	C	N	O	P	0
			51	41	1	8	1	
4	B	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 5 is PALMITIC ACID (CCD ID: 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	A	1	Total	C	O	0
			18	16	2	
5	B	1	Total	C	O	0
			18	16	2	
5	B	1	Total	C	O	0
			18	16	2	

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

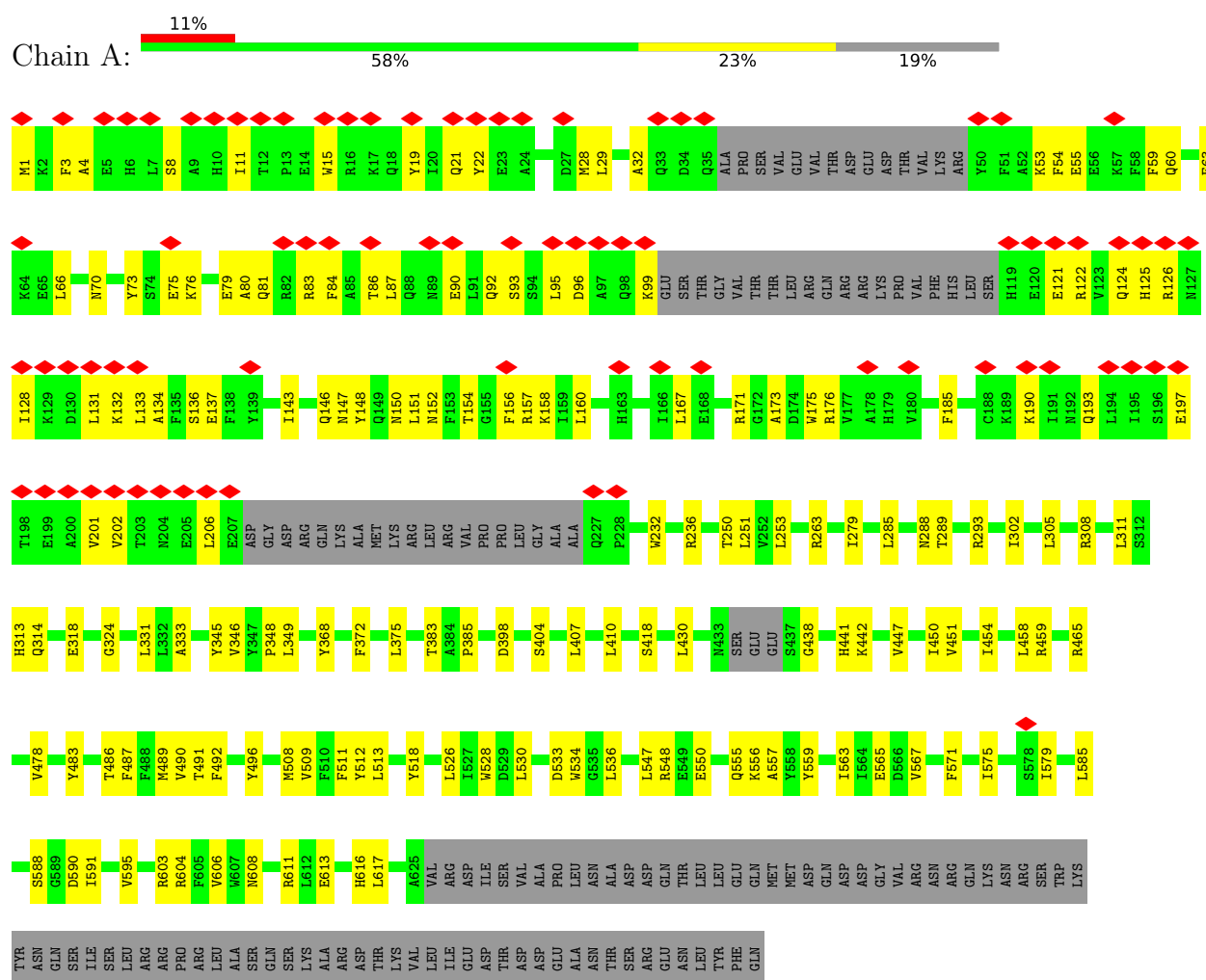


Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total	C	O	0
			22	20	2	
6	B	1	Total	C	O	0
			22	20	2	

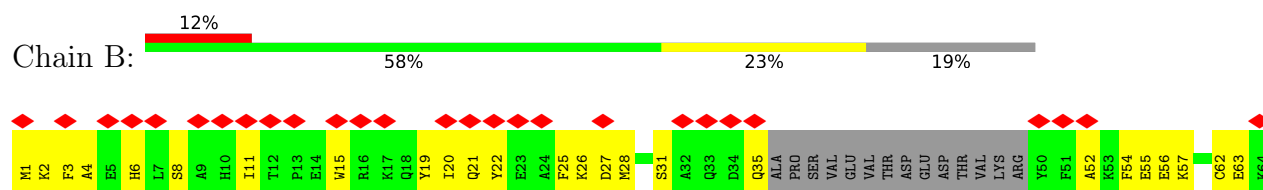
3 Residue-property plots

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



LYS	VAL	LEU	ILE	GLU	ASP	THR	ASP	ASP	GLU	GLU	ALA	ASN	ASN	THR	SER	ARG	GLN	ASN	LEU	LEU	TYR	PHE	GLN																																		
AG25	VAL	ARG	ILE	ASP	ILE	SER	VAL	ALA	PRO	ASP	LEU	ALA	ASN	ALA	ASP	ASP	GLN	THR	ASN	LEU	LEU	TYR	PHE	GLN																																	
Y524	T525	L526	D533	W534	G535	F537	L536	D538	K539	W540	A541	T545	F546	L547	R548	E549	E550	Q555	K556	A557	E565	D566	V567	I568	L569	R570	F571	T574	S578	L585	P586	H587	S588	G589	D590	I591	L599	R603	V606	W607	N608	R611	L612	E613	H616	L617											
L359	L374	P385	W395	D398	M408	D409	L410	E411	Y412	Y417	L429	L430	P431	N432	N433	SER	GLU	GLU	S437	G438	I439	C440	H441	K442	R448	R459	R465	R472	Y483	F488	T491	Y496	D506	F511	W514	F517	Y518	I519	I520	S521																	
A200	V201	V202	T203	N204	E205	L206	E207	ASP	GLY	ASP	ARG	GLN	LYS	ALA	MET	LYS	ARG	LEU	ARG	VAL	PRO	PRO	LEU	GLY	ALA	ALA	Q227	P228	L251	A255	R263	W266	P267	I279	W292	I302	L305	R308	G324	L331	L332	A333	C334	F335	F336	L349											
K132	L133	E137	F138	Y139	L140	S141	L142	I143	L144	L145	Q146	N147	Y148	Q149	N150	L151	N152	F153	T154	G155	F156	R157	K158	I159	L160	K161	K162	H163	D164	K165	I166	L167	R171	D174	W175	R176	V177	A178	H179	V180	E181	V182	F185	C188	K189	K190	I191	L194	I195	S196	E197	T198	E199				
W70	Y73	S74	E75	K76	A80	Q81	R82	R83	F84	A85	T86	L87	N88	N89	E90	L91	Q92	S93	S94	L95	D96	A97	Q98	K99	GLU	SER	THR	GLY	VAL	THR	THR	LEU	ARG	GLN	ARG	ARG	LYS	PRO	PRO	VAL	PHE	HIS	LEU	SER	H119	E120	E121	R122	V123	Q124	H125	R126	N127	I128	K129	D130	L131

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	88082	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)	200	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	0.663	Depositor
Minimum map value	-0.472	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.055	Depositor
Map size ($\text{\AA}$)	296.0, 296.0, 296.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.74, 0.74, 0.74	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.18	0/4905	0.44	3/6646 (0.0%)
1	B	0.14	0/4905	0.35	1/6646 (0.0%)
All	All	0.16	0/9810	0.40	4/13292 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	59	PHE	N-CA-C	-8.12	103.37	113.28
1	A	60	GLN	N-CA-C	-5.55	106.68	113.50
1	B	88	GLN	N-CA-C	-5.18	105.53	111.07
1	A	590	ASP	N-CA-C	5.01	116.55	111.14

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4765	0	4733	116	0
1	B	4765	0	4733	124	0
2	A	196	0	322	11	0
2	B	140	0	230	3	0
3	A	36	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	36	0	6	3	0
4	A	153	0	246	8	0
4	B	153	0	246	7	0
5	A	36	0	62	0	0
5	B	36	0	62	0	0
6	A	22	0	31	0	0
6	B	22	0	31	1	0
All	All	10360	0	10708	250	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 12.

All (250) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:PHE:HA	1:B:28:MET:HE1	1.62	0.81
1:B:143:ILE:HA	1:B:146:GLN:HE22	1.48	0.77
1:A:489:MET:HE1	1:A:518:TYR:HA	1.71	0.72
1:A:548:ARG:NH1	1:A:613:GLU:OE2	2.25	0.69
1:B:491:THR:HG22	2:B:905:CLR:H71	1.73	0.68
1:A:368:TYR:HD2	1:A:372:PHE:HE2	1.42	0.68
1:A:132:LYS:HG2	1:A:206:LEU:HD22	1.74	0.68
1:A:533:ASP:OD1	1:A:611:ARG:NH1	2.27	0.68
1:B:534:TRP:O	1:B:548:ARG:NH1	2.27	0.66
1:B:533:ASP:OD1	1:B:611:ARG:NH1	2.29	0.66
1:B:526:LEU:HD21	1:B:567:VAL:HG22	1.77	0.66
1:A:143:ILE:O	1:A:147:ASN:ND2	2.28	0.66
1:B:202:VAL:HG22	1:B:206:LEU:HD12	1.76	0.66
1:A:171:ARG:O	1:A:175:TRP:N	2.30	0.65
1:B:161:LYS:C	1:B:165:LYS:HZ3	2.04	0.64
1:B:161:LYS:HA	1:B:164:ASP:HB2	1.78	0.64
1:A:19:TYR:O	1:A:21:GLN:NE2	2.30	0.64
1:A:202:VAL:HG22	1:A:206:LEU:HD12	1.80	0.64
1:A:438:GLY:O	1:A:441:HIS:ND1	2.29	0.63
1:A:550:GLU:N	1:A:550:GLU:OE2	2.32	0.62
1:A:143:ILE:HA	1:A:146:GLN:HE21	1.65	0.62
1:A:575:ILE:O	1:A:579:ILE:HG12	2.00	0.62
1:A:3:PHE:HD1	1:A:308:ARG:HE	1.48	0.62
1:A:492:PHE:HE2	1:A:513:LEU:HD12	1.64	0.62
1:B:92:GLN:O	1:B:96:ASP:N	2.28	0.61
1:B:154:THR:HA	1:B:157:ARG:HE	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:GLU:HA	1:A:66:LEU:HB3	1.82	0.61
1:B:1:MET:N	3:B:903:IHP:O41	2.34	0.61
1:A:534:TRP:HB3	1:A:536:LEU:HD23	1.82	0.61
1:A:263:ARG:NH2	1:A:430:LEU:O	2.35	0.60
1:A:385:PRO:O	1:A:465:ARG:NH1	2.35	0.60
1:B:263:ARG:NH2	1:B:430:LEU:O	2.36	0.59
1:B:514:TRP:NE1	1:B:578:SER:OG	2.28	0.59
1:A:550:GLU:HB2	1:A:617:LEU:HD21	1.84	0.59
1:A:491:THR:HG22	2:A:804:CLR:H71	1.84	0.58
1:A:447:VAL:O	1:A:451:VAL:HG12	2.03	0.58
4:B:901:3PE:H371	4:B:901:3PE:H2A2	1.85	0.57
1:B:132:LYS:HG2	1:B:206:LEU:HD22	1.85	0.57
1:B:156:PHE:O	1:B:160:LEU:HG	2.04	0.56
1:B:125:HIS:HA	1:B:128:ILE:HB	1.87	0.56
1:A:63:GLU:HG3	1:A:175:TRP:HZ2	1.71	0.56
1:B:548:ARG:NH2	1:B:613:GLU:OE2	2.39	0.56
1:A:92:GLN:H	1:A:92:GLN:CD	2.13	0.55
1:A:125:HIS:HA	1:A:128:ILE:HB	1.88	0.55
1:B:171:ARG:O	1:B:175:TRP:N	2.40	0.55
1:A:154:THR:O	1:A:158:LYS:HG2	2.07	0.54
2:A:806:CLR:H151	4:B:901:3PE:H372	1.89	0.54
1:B:138:PHE:HA	1:B:141:SER:HB3	1.89	0.54
1:A:404:SER:HA	1:A:407:LEU:HD12	1.89	0.54
1:A:509:VAL:HA	1:A:512:TYR:CD2	2.42	0.54
1:A:8:SER:HA	1:A:11:ILE:HD12	1.89	0.54
2:A:806:CLR:H6	4:B:901:3PE:H331	1.90	0.54
1:A:55:GLU:HG3	1:A:167:LEU:HD12	1.89	0.53
1:B:157:ARG:O	1:B:161:LYS:HG2	2.07	0.53
1:B:550:GLU:HB2	1:B:617:LEU:HD21	1.91	0.53
1:B:28:MET:HA	1:B:31:SER:HB3	1.90	0.53
1:B:81:GLN:HA	1:B:84:PHE:HB2	1.90	0.53
4:A:813:3PE:H331	2:A:814:CLR:H6	1.90	0.53
1:A:148:TYR:O	1:A:152:ASN:ND2	2.42	0.52
1:B:121:GLU:HA	1:B:124:GLN:HB3	1.92	0.52
1:B:2:LYS:NZ	3:B:903:IHP:O21	2.42	0.52
1:A:126:ARG:NH1	1:B:27:ASP:OD2	2.42	0.52
1:B:8:SER:HA	1:B:11:ILE:HD12	1.90	0.52
1:B:19:TYR:O	1:B:21:GLN:NE2	2.42	0.52
1:B:202:VAL:HA	1:B:206:LEU:HB2	1.92	0.52
1:B:63:GLU:HG3	1:B:175:TRP:HZ2	1.74	0.52
1:A:128:ILE:O	1:A:132:LYS:HG3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:PHE:O	1:B:142:LEU:N	2.33	0.52
1:A:81:GLN:HA	1:A:84:PHE:HB2	1.92	0.51
1:A:450:ILE:HD13	2:A:804:CLR:H181	1.91	0.51
1:A:73:TYR:CD2	1:A:185:PHE:HA	2.45	0.51
1:B:308:ARG:O	1:B:308:ARG:NE	2.36	0.51
1:A:588:SER:HA	1:A:591:ILE:HG22	1.92	0.51
1:B:73:TYR:CD2	1:B:185:PHE:HA	2.45	0.51
1:A:346:VAL:HA	1:A:349:LEU:HD13	1.92	0.51
1:A:232:TRP:HZ3	4:B:908:3PE:H2	1.75	0.51
1:A:279:ILE:HD13	1:A:324:GLY:HA2	1.93	0.51
1:B:148:TYR:O	1:B:152:ASN:ND2	2.44	0.51
1:A:526:LEU:HD21	1:A:567:VAL:HG22	1.92	0.51
4:A:813:3PE:H3B1	1:B:333:ALA:HB2	1.93	0.50
1:B:302:ILE:HD11	1:B:616:HIS:HB2	1.93	0.50
1:B:534:TRP:HB3	1:B:536:LEU:HD23	1.94	0.50
1:B:536:LEU:HD12	1:B:547:LEU:HA	1.93	0.50
1:A:146:GLN:O	1:A:150:ASN:ND2	2.43	0.50
1:A:250:THR:HG21	4:B:901:3PE:H281	1.94	0.50
1:A:486:THR:O	1:A:490:VAL:HG23	2.11	0.50
1:B:308:ARG:HE	1:B:308:ARG:C	2.18	0.50
1:A:398:ASP:OD2	1:A:483:TYR:OH	2.28	0.50
1:A:1:MET:CE	1:A:3:PHE:H	2.25	0.50
1:A:534:TRP:O	1:A:548:ARG:NH2	2.41	0.50
1:B:569:LEU:HD11	1:B:599:LEU:HD22	1.94	0.50
1:A:32:ALA:HB2	1:A:54:PHE:CE2	2.47	0.50
1:B:96:ASP:HA	1:B:99:LYS:HD2	1.92	0.49
1:A:313:HIS:CD2	1:A:314:GLN:HG3	2.48	0.49
1:B:349:LEU:HD11	1:B:417:TYR:HE2	1.78	0.49
1:B:410:LEU:HD11	2:B:910:CLR:H273	1.94	0.49
1:B:438:GLY:H	1:B:441:HIS:CE1	2.31	0.49
1:B:146:GLN:O	1:B:150:ASN:N	2.31	0.49
1:A:288:ASN:HD21	1:A:608:ASN:HB3	1.78	0.49
1:B:506:ASP:OD1	1:B:506:ASP:N	2.36	0.49
1:A:122:ARG:HA	1:A:125:HIS:NE2	2.27	0.49
1:B:570:ARG:HE	1:B:603:ARG:NH1	2.10	0.49
1:A:80:ALA:O	1:A:84:PHE:N	2.44	0.48
1:A:92:GLN:O	1:A:96:ASP:N	2.35	0.48
1:A:372:PHE:HA	1:A:375:LEU:HD12	1.94	0.48
1:A:90:GLU:O	1:A:93:SER:OG	2.29	0.48
1:B:52:ALA:HA	1:B:55:GLU:HG3	1.95	0.48
1:A:345:TYR:O	1:A:348:PRO:HD2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:813:3PE:H391	4:A:813:3PE:H2A2	1.95	0.47
1:A:492:PHE:CE2	1:A:513:LEU:HD12	2.46	0.47
1:A:15:TRP:HZ2	1:A:76:LYS:HE3	1.79	0.47
1:B:128:ILE:O	1:B:132:LYS:HG3	2.13	0.47
1:B:174:ASP:O	1:B:178:ALA:N	2.38	0.47
1:B:349:LEU:HD12	1:B:349:LEU:H	1.80	0.47
1:B:525:THR:HG23	1:B:570:ARG:HH11	1.80	0.47
1:A:19:TYR:CE1	1:A:148:TYR:HA	2.50	0.47
1:B:6:HIS:CD2	1:B:308:ARG:HD3	2.49	0.47
1:A:556:LYS:HA	1:A:559:TYR:HD2	1.79	0.47
1:A:96:ASP:HA	1:A:99:LYS:HD2	1.96	0.47
1:A:496:TYR:CZ	1:A:511:PHE:HD2	2.32	0.47
1:A:508:MET:HG3	1:A:512:TYR:CZ	2.50	0.47
1:B:176:ARG:O	1:B:181:GLU:N	2.45	0.47
1:B:412:TYR:CZ	1:B:441:HIS:HB3	2.50	0.46
1:A:92:GLN:HA	1:A:95:LEU:HB2	1.97	0.46
1:A:555:GLN:HG3	1:A:557:ALA:H	1.80	0.46
4:A:813:3PE:H272	4:A:813:3PE:H371	1.98	0.46
1:B:251:LEU:HD11	1:B:331:LEU:HG	1.97	0.46
1:B:55:GLU:OE1	1:B:56:GLU:HG3	2.15	0.46
1:A:333:ALA:HB2	4:B:901:3PE:H3B1	1.98	0.46
1:B:408:MET:SD	1:B:448:ARG:NE	2.79	0.46
1:B:488:PHE:HB3	1:B:517:PHE:HD2	1.81	0.46
1:B:520:ILE:O	1:B:524:TYR:HB2	2.15	0.46
1:B:585:LEU:HB3	1:B:588:SER:HB3	1.96	0.46
1:B:1:MET:SD	1:B:2:LYS:N	2.89	0.46
1:B:398:ASP:OD2	1:B:483:TYR:OH	2.33	0.46
1:B:550:GLU:N	1:B:550:GLU:OE1	2.49	0.46
2:A:810:CLR:H162	2:A:810:CLR:H221	1.78	0.46
1:A:173:ALA:HA	1:A:176:ARG:HE	1.81	0.45
1:A:251:LEU:HD11	1:A:331:LEU:HG	1.98	0.45
1:B:266:TRP:HB2	1:B:267:PRO:HD3	1.97	0.45
1:B:588:SER:HA	1:B:591:ILE:HG22	1.98	0.45
2:B:910:CLR:H162	2:B:910:CLR:H221	1.74	0.45
1:A:134:ALA:HA	1:A:137:GLU:OE1	2.16	0.45
1:A:121:GLU:HA	1:A:124:GLN:HB3	1.98	0.45
1:A:190:LYS:O	1:A:193:GLN:HG2	2.15	0.45
4:A:813:3PE:H361	1:B:336:PHE:HD2	1.80	0.45
1:A:3:PHE:CG	1:A:3:PHE:O	2.70	0.45
1:B:4:ALA:HA	1:B:22:TYR:CD2	2.51	0.45
1:B:612:LEU:HD23	1:B:612:LEU:HA	1.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:LEU:HA	1:A:288:ASN:HB2	1.98	0.45
1:A:410:LEU:HD11	2:A:810:CLR:H273	1.99	0.45
1:A:236:ARG:NH1	1:A:318:GLU:OE1	2.49	0.45
1:A:530:LEU:HD11	1:A:563:ILE:HG12	1.99	0.45
1:A:536:LEU:HD12	1:A:547:LEU:HA	1.98	0.45
1:A:92:GLN:OE1	1:A:92:GLN:N	2.31	0.45
1:A:197:GLU:O	1:A:201:VAL:HG12	2.17	0.45
4:A:813:3PE:H2C1	4:A:813:3PE:H292	1.73	0.45
1:A:90:GLU:HB3	1:A:131:LEU:HD21	1.97	0.45
1:A:383:THR:O	1:A:383:THR:OG1	2.34	0.45
1:B:1:MET:CE	1:B:3:PHE:H	2.30	0.45
1:B:538:ASP:OD1	1:B:539:LYS:N	2.50	0.45
1:A:173:ALA:HA	1:A:176:ARG:NE	2.31	0.44
1:B:54:PHE:HA	1:B:57:LYS:HG2	1.99	0.44
1:B:292:TRP:CZ2	1:B:612:LEU:HD12	2.52	0.44
1:A:603:ARG:O	1:A:606:VAL:HG12	2.17	0.44
1:B:31:SER:O	1:B:35:GLN:N	2.48	0.44
1:B:156:PHE:O	1:B:159:ILE:HG22	2.16	0.44
1:A:143:ILE:HG23	1:A:146:GLN:NE2	2.32	0.44
1:A:591:ILE:O	1:A:595:VAL:HG23	2.18	0.44
1:B:549:GLU:HB3	1:B:550:GLU:OE1	2.16	0.44
1:A:285:LEU:O	1:A:289:THR:HG23	2.18	0.44
1:A:585:LEU:HB3	1:A:588:SER:HB3	1.99	0.44
1:B:20:ILE:HG13	1:B:25:PHE:HE2	1.81	0.44
1:B:555:GLN:HG3	1:B:557:ALA:H	1.82	0.44
1:B:521:SER:O	1:B:525:THR:HG22	2.18	0.44
1:A:83:ARG:HA	1:A:86:THR:HB	2.00	0.43
2:A:801:CLR:H211	2:A:801:CLR:H232	1.80	0.43
1:B:541:ALA:HB1	1:B:545:THR:HA	2.00	0.43
1:A:53:LYS:HD3	1:A:53:LYS:N	2.32	0.43
1:A:487:PHE:HD2	2:A:804:CLR:H221	1.84	0.43
1:A:28:MET:SD	1:A:29:LEU:HD23	2.59	0.43
1:B:54:PHE:HD1	1:B:167:LEU:HD11	1.83	0.43
1:B:122:ARG:HA	1:B:125:HIS:CD2	2.53	0.43
1:B:162:LYS:HG3	1:B:166:ILE:HD12	2.00	0.43
1:A:147:ASN:HB2	1:A:151:LEU:HG	2.00	0.43
1:B:526:LEU:HD11	1:B:567:VAL:HG13	1.99	0.43
1:A:311:LEU:HD23	1:A:311:LEU:HA	1.83	0.43
1:A:565:GLU:HB2	2:A:801:CLR:H242	2.01	0.43
1:B:359:LEU:HD11	1:B:374:LEU:HD23	2.00	0.43
1:B:472:ARG:HE	1:B:472:ARG:HB3	1.68	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:565:GLU:OE1	1:B:606:VAL:HG11	2.19	0.43
1:A:518:TYR:OH	1:A:571:PHE:O	2.37	0.43
1:B:126:ARG:O	1:B:129:LYS:HG2	2.19	0.43
1:B:143:ILE:HA	1:B:146:GLN:NE2	2.27	0.43
1:A:253:LEU:HD23	1:A:253:LEU:HA	1.79	0.42
1:A:454:ILE:O	1:A:458:LEU:HG	2.19	0.42
1:B:570:ARG:O	1:B:574:THR:HG23	2.18	0.42
1:A:305:LEU:HD23	1:A:305:LEU:HA	1.87	0.42
1:A:311:LEU:HB2	4:A:803:3PE:H32	2.01	0.42
1:A:478:VAL:HB	1:A:528:TRP:HZ3	1.84	0.42
1:B:305:LEU:HD23	1:B:305:LEU:HA	1.85	0.42
1:B:151:LEU:O	1:B:155:GLY:N	2.51	0.42
1:B:617:LEU:HD12	1:B:617:LEU:HA	1.91	0.42
1:A:441:HIS:HE1	1:A:442:LYS:HE3	1.85	0.42
1:B:385:PRO:O	1:B:465:ARG:NH1	2.48	0.42
1:B:62:CYS:HB3	1:B:175:TRP:CH2	2.55	0.42
1:B:137:GLU:O	1:B:141:SER:N	2.40	0.42
1:B:146:GLN:H	1:B:146:GLN:CD	2.26	0.42
1:B:150:ASN:OD1	1:B:151:LEU:N	2.53	0.42
1:A:87:LEU:HA	1:A:90:GLU:HB2	2.01	0.42
1:B:279:ILE:HD13	1:B:324:GLY:HA2	2.00	0.42
1:B:459:ARG:HB3	1:B:483:TYR:CE2	2.55	0.42
1:A:157:ARG:HG3	1:A:158:LYS:HD2	2.02	0.42
1:B:4:ALA:HB1	1:B:26:LYS:HD2	2.02	0.42
1:A:66:LEU:HD12	1:A:185:PHE:CE2	2.55	0.41
1:B:80:ALA:O	1:B:84:PHE:N	2.50	0.41
1:B:96:ASP:OD1	1:B:99:LYS:NZ	2.44	0.41
1:B:266:TRP:CH2	6:B:911:ACD:H42	2.54	0.41
1:A:418:SER:HA	2:A:810:CLR:H6	2.03	0.41
1:B:2:LYS:HZ3	3:B:903:IHP:P1	2.43	0.41
1:B:15:TRP:HZ2	1:B:76:LYS:HE3	1.84	0.41
1:B:19:TYR:CE2	1:B:148:TYR:HA	2.55	0.41
1:A:302:ILE:HD11	1:A:616:HIS:HB2	2.01	0.41
1:B:70:ASN:OD1	1:B:185:PHE:N	2.53	0.41
1:B:131:LEU:HD23	1:B:131:LEU:HA	1.89	0.41
1:B:161:LYS:O	1:B:164:ASP:N	2.51	0.41
1:A:293:ARG:HH21	1:A:313:HIS:CE1	2.39	0.41
1:B:255:ALA:HB2	1:B:335:PHE:HE2	1.84	0.41
1:A:4:ALA:HA	1:A:22:TYR:CD2	2.55	0.41
1:A:75:GLU:O	1:A:79:GLU:HG2	2.21	0.41
1:B:555:GLN:OE1	1:B:556:LYS:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:TRP:CE2	1:B:612:LEU:HD12	2.56	0.41
1:A:66:LEU:HA	1:A:185:PHE:HE2	1.86	0.41
1:A:156:PHE:O	1:A:160:LEU:HG	2.21	0.41
1:A:447:VAL:HA	1:A:450:ILE:HG22	2.02	0.41
4:A:803:3PE:H3D2	4:A:803:3PE:H3G1	1.88	0.41
1:B:518:TYR:OH	1:B:571:PHE:O	2.30	0.41
1:A:70:ASN:OD1	1:A:185:PHE:N	2.54	0.41
1:A:133:LEU:HD12	1:A:136:SER:OG	2.20	0.41
1:B:429:LEU:HD12	1:B:429:LEU:HA	1.95	0.41
1:B:439:ILE:HA	1:B:442:LYS:HD2	2.03	0.40
1:B:496:TYR:CZ	1:B:511:PHE:HD2	2.38	0.40
1:A:398:ASP:OD1	1:A:604:ARG:NH1	2.54	0.40
1:A:459:ARG:HB3	1:A:483:TYR:CD2	2.57	0.40
1:B:84:PHE:HE2	1:B:142:LEU:HD21	1.86	0.40
1:B:228:PRO:HA	4:B:908:3PE:H121	2.03	0.40
1:B:83:ARG:HD3	1:B:86:THR:HB	2.03	0.40
1:B:408:MET:HE2	1:B:408:MET:HB2	1.94	0.40
1:B:585:LEU:O	1:B:589:GLY:N	2.54	0.40
1:B:395:TRP:HZ2	1:B:608:ASN:HD21	1.67	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	560/704 (80%)	544 (97%)	16 (3%)	0	100	100
1	B	560/704 (80%)	539 (96%)	21 (4%)	0	100	100
All	All	1120/1408 (80%)	1083 (97%)	37 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	508/629 (81%)	508 (100%)	0	100	100
1	B	508/629 (81%)	507 (100%)	1 (0%)	87	87
All	All	1016/1258 (81%)	1015 (100%)	1 (0%)	87	89

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	87	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	GLN
1	A	313	HIS
1	A	479	ASN
1	A	499	HIS
1	B	119	HIS
1	B	146	GLN
1	B	147	ASN
1	B	163	HIS
1	B	387	HIS
1	B	576	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
4	3PE	A	803	-	50,50,50	0.51	0	53,55,55	0.54	1 (1%)
5	PLM	B	909	-	17,17,17	0.89	1 (5%)	17,17,17	0.73	2 (11%)
6	ACD	B	911	-	21,21,21	0.58	0	21,21,21	0.55	0
3	IHP	B	903	-	36,36,36	1.57	6 (16%)	60,60,60	1.00	4 (6%)
2	CLR	A	806	-	31,31,31	0.38	0	48,48,48	0.59	0
4	3PE	B	901	-	50,50,50	0.51	0	53,55,55	0.57	2 (3%)
4	3PE	B	908	-	50,50,50	0.52	0	53,55,55	0.58	1 (1%)
3	IHP	A	802	-	36,36,36	1.56	6 (16%)	60,60,60	0.98	2 (3%)
5	PLM	A	812	-	17,17,17	0.93	1 (5%)	17,17,17	0.73	2 (11%)
2	CLR	A	805	-	31,31,31	0.38	0	48,48,48	0.66	0
2	CLR	A	814	-	31,31,31	0.37	0	48,48,48	0.54	0
2	CLR	B	902	-	31,31,31	0.37	0	48,48,48	0.67	0
2	CLR	A	801	-	31,31,31	0.36	0	48,48,48	0.70	0
2	CLR	A	804	-	31,31,31	0.40	0	48,48,48	0.51	0
2	CLR	B	910	-	31,31,31	0.35	0	48,48,48	0.46	0
4	3PE	A	808	-	50,50,50	0.51	0	53,55,55	0.56	1 (1%)
2	CLR	A	810	-	31,31,31	0.35	0	48,48,48	0.48	0
2	CLR	B	906	-	31,31,31	0.38	0	48,48,48	0.66	0
6	ACD	A	811	-	21,21,21	0.58	0	21,21,21	0.58	0
4	3PE	A	813	-	50,50,50	0.51	0	53,55,55	0.54	1 (1%)
2	CLR	B	907	-	31,31,31	0.38	0	48,48,48	0.53	0
5	PLM	A	809	-	17,17,17	0.90	1 (5%)	17,17,17	0.74	2 (11%)
5	PLM	B	912	-	17,17,17	0.92	1 (5%)	17,17,17	0.73	2 (11%)
4	3PE	B	904	-	50,50,50	0.52	0	53,55,55	0.54	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CLR	B	905	-	31,31,31	0.40	0	48,48,48	0.49	0
2	CLR	A	807	-	31,31,31	0.38	0	48,48,48	0.51	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
4	3PE	A	803	-	-	26/54/54/54	-
5	PLM	B	909	-	-	4/15/15/15	-
6	ACD	B	911	-	-	5/19/19/19	-
3	IHP	B	903	-	-	8/30/54/54	0/1/1/1
2	CLR	A	806	-	-	4/10/68/68	0/4/4/4
4	3PE	B	901	-	-	21/54/54/54	-
4	3PE	B	908	-	-	20/54/54/54	-
3	IHP	A	802	-	-	8/30/54/54	0/1/1/1
5	PLM	A	812	-	-	2/15/15/15	-
2	CLR	A	805	-	-	6/10/68/68	0/4/4/4
2	CLR	A	814	-	-	5/10/68/68	0/4/4/4
2	CLR	B	902	-	-	5/10/68/68	0/4/4/4
2	CLR	A	801	-	-	6/10/68/68	0/4/4/4
2	CLR	A	804	-	-	2/10/68/68	0/4/4/4
2	CLR	B	910	-	-	7/10/68/68	0/4/4/4
4	3PE	A	808	-	-	19/54/54/54	-
2	CLR	A	810	-	-	7/10/68/68	0/4/4/4
2	CLR	B	906	-	-	6/10/68/68	0/4/4/4
6	ACD	A	811	-	-	4/19/19/19	-
4	3PE	A	813	-	-	18/54/54/54	-
2	CLR	B	907	-	-	8/10/68/68	0/4/4/4
5	PLM	A	809	-	-	5/15/15/15	-
5	PLM	B	912	-	-	2/15/15/15	-
4	3PE	B	904	-	-	26/54/54/54	-
2	CLR	B	905	-	-	1/10/68/68	0/4/4/4
2	CLR	A	807	-	-	7/10/68/68	0/4/4/4

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	802	IHP	P4-O14	3.59	1.65	1.59
3	B	903	IHP	P4-O14	3.56	1.65	1.59
3	B	903	IHP	P2-O12	3.39	1.65	1.59
3	A	802	IHP	P5-O15	3.37	1.65	1.59
3	A	802	IHP	P1-O11	3.36	1.65	1.59
3	B	903	IHP	P6-O16	3.35	1.65	1.59
3	B	903	IHP	P1-O11	3.34	1.65	1.59
3	A	802	IHP	P2-O12	3.31	1.65	1.59
3	A	802	IHP	P6-O16	3.28	1.65	1.59
3	B	903	IHP	P5-O15	3.28	1.65	1.59
3	B	903	IHP	P3-O13	3.23	1.65	1.59
3	A	802	IHP	P3-O13	3.20	1.65	1.59
5	A	812	PLM	C2-C1	2.95	1.57	1.50
5	B	912	PLM	C2-C1	2.93	1.57	1.50
5	A	809	PLM	C2-C1	2.81	1.57	1.50
5	B	909	PLM	C2-C1	2.76	1.57	1.50

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802	IHP	C6-C5-C4	2.62	116.17	110.43
3	B	903	IHP	C6-C5-C4	2.49	115.89	110.43
4	B	904	3PE	O12-P-O14	2.44	123.80	112.44
3	A	802	IHP	C5-C6-C1	2.43	115.76	110.43
4	A	803	3PE	O12-P-O14	2.43	123.74	112.44
4	A	813	3PE	O12-P-O14	2.43	123.73	112.44
4	A	808	3PE	O12-P-O14	2.43	123.73	112.44
4	B	901	3PE	O12-P-O14	2.41	123.66	112.44
4	B	908	3PE	O12-P-O14	2.39	123.56	112.44
3	B	903	IHP	C5-C6-C1	2.37	115.62	110.43
5	A	809	PLM	O1-C1-O2	2.16	128.88	123.33
5	B	909	PLM	O1-C1-O2	2.15	128.86	123.33
5	A	812	PLM	O1-C1-O2	2.13	128.81	123.33
5	B	912	PLM	O1-C1-O2	2.12	128.79	123.33
3	B	903	IHP	C6-C1-C2	2.11	115.05	110.43
4	B	901	3PE	C2-O21-C21	2.07	122.76	117.80
5	A	809	PLM	O2-C1-C2	-2.06	116.57	123.09
5	B	909	PLM	O2-C1-C2	-2.04	116.61	123.09
3	B	903	IHP	P5-O15-C5	-2.04	117.99	123.43
5	A	812	PLM	O2-C1-C2	-2.03	116.65	123.09
5	B	912	PLM	O2-C1-C2	-2.03	116.65	123.09

There are no chirality outliers.

All (232) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	802	IHP	C5-C4-O14-P4
3	B	903	IHP	C2-C3-O13-P3
3	B	903	IHP	C4-C3-O13-P3
3	B	903	IHP	C5-C4-O14-P4
4	A	803	3PE	C1-O11-P-O13
4	A	803	3PE	C1-O11-P-O14
4	A	803	3PE	C11-O13-P-O14
4	A	803	3PE	O11-C1-C2-O21
4	A	803	3PE	C22-C21-O21-C2
4	A	808	3PE	C1-O11-P-O14
4	A	808	3PE	O13-C11-C12-N
4	A	808	3PE	O22-C21-O21-C2
4	A	808	3PE	C22-C21-O21-C2
4	A	813	3PE	C1-O11-P-O13
4	A	813	3PE	C1-O11-P-O14
4	A	813	3PE	O13-C11-C12-N
4	A	813	3PE	C22-C21-O21-C2
4	B	901	3PE	C1-O11-P-O14
4	B	901	3PE	O13-C11-C12-N
4	B	901	3PE	C22-C21-O21-C2
4	B	904	3PE	C1-O11-P-O13
4	B	904	3PE	C1-O11-P-O14
4	B	904	3PE	C11-O13-P-O11
4	B	904	3PE	C11-O13-P-O14
4	B	904	3PE	O11-C1-C2-O21
4	B	904	3PE	C22-C21-O21-C2
4	B	908	3PE	C1-O11-P-O14
4	B	908	3PE	O13-C11-C12-N
4	B	908	3PE	C22-C21-O21-C2
4	A	803	3PE	O32-C31-O31-C3
4	B	904	3PE	O32-C31-O31-C3
4	A	803	3PE	O22-C21-O21-C2
4	A	813	3PE	O22-C21-O21-C2
4	B	901	3PE	O22-C21-O21-C2
4	B	904	3PE	O22-C21-O21-C2
4	B	908	3PE	O22-C21-O21-C2
2	B	910	CLR	C13-C17-C20-C22
4	A	803	3PE	C32-C31-O31-C3
4	B	904	3PE	C32-C31-O31-C3
2	A	805	CLR	C17-C20-C22-C23
2	A	810	CLR	C17-C20-C22-C23
2	B	906	CLR	C17-C20-C22-C23

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Mol	Chain	Res	Type	Atoms
2	A	814	CLR	C21-C20-C22-C23
2	B	910	CLR	C21-C20-C22-C23
2	A	814	CLR	C17-C20-C22-C23
2	B	910	CLR	C17-C20-C22-C23
4	B	908	3PE	C32-C31-O31-C3
2	A	805	CLR	C21-C20-C22-C23
2	B	906	CLR	C21-C20-C22-C23
4	B	908	3PE	O32-C31-O31-C3
2	A	806	CLR	C17-C20-C22-C23
2	B	910	CLR	C13-C17-C20-C21
4	A	803	3PE	C29-C2A-C2B-C2C
4	B	908	3PE	C27-C28-C29-C2A
2	A	810	CLR	C22-C23-C24-C25
2	A	806	CLR	C22-C23-C24-C25
2	B	902	CLR	C22-C23-C24-C25
2	A	814	CLR	C22-C23-C24-C25
3	A	802	IHP	C3-C2-O12-P2
4	A	808	3PE	C27-C28-C29-C2A
2	A	810	CLR	C21-C20-C22-C23
2	A	810	CLR	C13-C17-C20-C22
4	B	904	3PE	C29-C2A-C2B-C2C
2	A	807	CLR	C13-C17-C20-C22
2	B	905	CLR	C17-C20-C22-C23
4	A	813	3PE	C22-C23-C24-C25
2	B	910	CLR	C16-C17-C20-C21
2	B	910	CLR	C22-C23-C24-C25
4	B	904	3PE	C33-C34-C35-C36
4	B	908	3PE	C25-C26-C27-C28
2	B	910	CLR	C16-C17-C20-C22
4	B	908	3PE	C34-C35-C36-C37
4	B	901	3PE	C21-C22-C23-C24
4	B	904	3PE	C31-C32-C33-C34
4	A	813	3PE	C27-C28-C29-C2A
4	A	803	3PE	C31-C32-C33-C34
4	A	808	3PE	C32-C31-O31-C3
4	A	803	3PE	C27-C28-C29-C2A
5	B	909	PLM	C3-C4-C5-C6
4	A	803	3PE	C33-C34-C35-C36
4	A	803	3PE	C24-C25-C26-C27
4	B	901	3PE	C2B-C2C-C2D-C2E
2	B	907	CLR	C21-C20-C22-C23
4	A	803	3PE	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
4	B	901	3PE	C22-C23-C24-C25
2	A	805	CLR	C23-C24-C25-C26
3	A	802	IHP	C1-C2-O12-P2
2	A	804	CLR	C17-C20-C22-C23
2	A	810	CLR	C13-C17-C20-C21
4	B	908	3PE	C35-C36-C37-C38
2	A	807	CLR	C16-C17-C20-C21
4	A	803	3PE	C35-C36-C37-C38
4	A	808	3PE	O32-C31-O31-C3
4	A	808	3PE	C34-C35-C36-C37
2	A	807	CLR	C13-C17-C20-C21
2	B	907	CLR	C13-C17-C20-C22
4	A	803	3PE	O11-C1-C2-C3
4	B	904	3PE	O11-C1-C2-C3
4	B	904	3PE	C27-C28-C29-C2A
2	B	906	CLR	C23-C24-C25-C26
2	A	810	CLR	C16-C17-C20-C21
4	A	808	3PE	C1-C2-C3-O31
4	B	904	3PE	C3C-C3D-C3E-C3F
4	A	803	3PE	C3C-C3D-C3E-C3F
2	B	907	CLR	C16-C17-C20-C21
2	A	801	CLR	C13-C17-C20-C21
4	A	813	3PE	C2E-C2F-C2G-C2H
4	A	808	3PE	C25-C26-C27-C28
2	B	907	CLR	C13-C17-C20-C21
2	A	807	CLR	C21-C20-C22-C23
2	A	807	CLR	C16-C17-C20-C22
2	A	810	CLR	C16-C17-C20-C22
4	A	808	3PE	C2F-C2G-C2H-C2I
4	A	808	3PE	C26-C27-C28-C29
4	B	904	3PE	C32-C33-C34-C35
4	B	901	3PE	C3F-C3G-C3H-C3I
4	B	908	3PE	C2F-C2G-C2H-C2I
4	B	904	3PE	C21-C22-C23-C24
4	A	803	3PE	C22-C23-C24-C25
4	B	908	3PE	C26-C27-C28-C29
2	A	801	CLR	C16-C17-C20-C21
2	A	801	CLR	C13-C17-C20-C22
4	A	813	3PE	C3C-C3D-C3E-C3F
4	B	901	3PE	C35-C36-C37-C38
4	B	904	3PE	C36-C37-C38-C39
2	B	902	CLR	C13-C17-C20-C21

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Mol	Chain	Res	Type	Atoms
5	A	809	PLM	C1-C2-C3-C4
4	A	808	3PE	C2B-C2C-C2D-C2E
4	B	901	3PE	C2D-C2E-C2F-C2G
2	B	907	CLR	C16-C17-C20-C22
2	B	902	CLR	C13-C17-C20-C22
4	A	808	3PE	C35-C36-C37-C38
4	A	803	3PE	C21-C22-C23-C24
4	B	904	3PE	C24-C25-C26-C27
4	B	901	3PE	C2C-C2D-C2E-C2F
4	A	813	3PE	C23-C24-C25-C26
2	B	906	CLR	C20-C22-C23-C24
2	B	907	CLR	C20-C22-C23-C24
4	B	904	3PE	C22-C23-C24-C25
2	A	805	CLR	C20-C22-C23-C24
2	A	805	CLR	C23-C24-C25-C27
2	A	801	CLR	C22-C23-C24-C25
2	B	906	CLR	C23-C24-C25-C27
4	B	908	3PE	C2B-C2C-C2D-C2E
2	A	801	CLR	C16-C17-C20-C22
4	A	808	3PE	O21-C2-C3-O31
4	B	908	3PE	O21-C2-C3-O31
2	B	902	CLR	C16-C17-C20-C21
4	A	813	3PE	C28-C29-C2A-C2B
3	B	903	IHP	C3-O13-P3-O23
3	A	802	IHP	C2-C3-O13-P3
2	B	902	CLR	C16-C17-C20-C22
2	B	906	CLR	C22-C23-C24-C25
4	A	803	3PE	C1-O11-P-O12
4	A	803	3PE	C11-O13-P-O11
4	A	803	3PE	C11-O13-P-O12
4	B	901	3PE	C11-O13-P-O14
4	B	904	3PE	C1-O11-P-O12
4	B	904	3PE	C11-O13-P-O12
4	B	901	3PE	C27-C28-C29-C2A
4	A	813	3PE	C37-C38-C39-C3A
2	A	805	CLR	C22-C23-C24-C25
4	A	803	3PE	C2A-C2B-C2C-C2D
4	A	813	3PE	C29-C2A-C2B-C2C
4	B	908	3PE	C1-C2-C3-O31
2	A	807	CLR	C23-C24-C25-C26
3	B	903	IHP	C3-C2-O12-P2
3	B	903	IHP	C4-O14-P4-O44

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Mol	Chain	Res	Type	Atoms
2	B	907	CLR	C23-C24-C25-C26
2	A	806	CLR	C21-C20-C22-C23
2	A	807	CLR	C23-C24-C25-C27
4	A	813	3PE	C33-C34-C35-C36
4	B	901	3PE	C2F-C2G-C2H-C2I
6	A	811	ACD	O1-C1-C2-C3
6	A	811	ACD	O2-C1-C2-C3
4	B	901	3PE	C3-C2-O21-C21
4	A	803	3PE	C3E-C3F-C3G-C3H
5	B	909	PLM	O2-C1-C2-C3
5	B	912	PLM	O1-C1-C2-C3
5	A	812	PLM	O1-C1-C2-C3
3	A	802	IHP	C2-C1-O11-P1
3	A	802	IHP	C4-C3-O13-P3
3	B	903	IHP	C2-C1-O11-P1
4	B	904	3PE	C3E-C3F-C3G-C3H
2	B	907	CLR	C23-C24-C25-C27
6	B	911	ACD	C5-C6-C7-C8
6	B	911	ACD	C6-C7-C8-C9
6	B	911	ACD	C12-C13-C14-C15
4	B	908	3PE	C3B-C3C-C3D-C3E
3	A	802	IHP	C2-O12-P2-O22
5	B	909	PLM	C4-C5-C6-C7
5	A	812	PLM	O2-C1-C2-C3
5	B	912	PLM	O2-C1-C2-C3
5	A	809	PLM	C3-C4-C5-C6
4	B	901	3PE	O11-C1-C2-O21
5	B	909	PLM	O1-C1-C2-C3
6	B	911	ACD	O2-C1-C2-C3
2	A	806	CLR	C20-C22-C23-C24
4	B	904	3PE	C2A-C2B-C2C-C2D
4	B	901	3PE	C25-C26-C27-C28
6	A	811	ACD	C2-C3-C4-C5
4	A	813	3PE	C35-C36-C37-C38
6	B	911	ACD	O1-C1-C2-C3
4	A	808	3PE	C21-C22-C23-C24
2	A	801	CLR	C21-C20-C22-C23
2	A	804	CLR	C23-C24-C25-C26
4	A	803	3PE	C36-C37-C38-C39
4	A	803	3PE	C28-C29-C2A-C2B
4	B	901	3PE	C2A-C2B-C2C-C2D
5	A	809	PLM	CC-CD-CE-CF

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Mol	Chain	Res	Type	Atoms
4	B	908	3PE	O21-C21-C22-C23
4	A	813	3PE	O31-C31-C32-C33
4	B	901	3PE	O31-C31-C32-C33
4	B	904	3PE	C28-C29-C2A-C2B
5	A	809	PLM	O1-C1-C2-C3
3	A	802	IHP	C4-O14-P4-O44
3	B	903	IHP	C6-O16-P6-O46
4	A	808	3PE	O21-C21-C22-C23
5	A	809	PLM	O2-C1-C2-C3
4	A	813	3PE	C3F-C3G-C3H-C3I
4	B	908	3PE	C3-C2-O21-C21
6	A	811	ACD	C3-C4-C5-C6
4	B	908	3PE	O22-C21-C22-C23
4	B	908	3PE	C29-C2A-C2B-C2C
4	A	813	3PE	O32-C31-C32-C33
4	A	808	3PE	O22-C21-C22-C23
4	B	901	3PE	C2E-C2F-C2G-C2H
4	B	901	3PE	O32-C31-C32-C33
4	B	904	3PE	O31-C31-C32-C33
4	A	808	3PE	C29-C2A-C2B-C2C
2	A	814	CLR	C16-C17-C20-C22
2	A	814	CLR	C13-C17-C20-C21

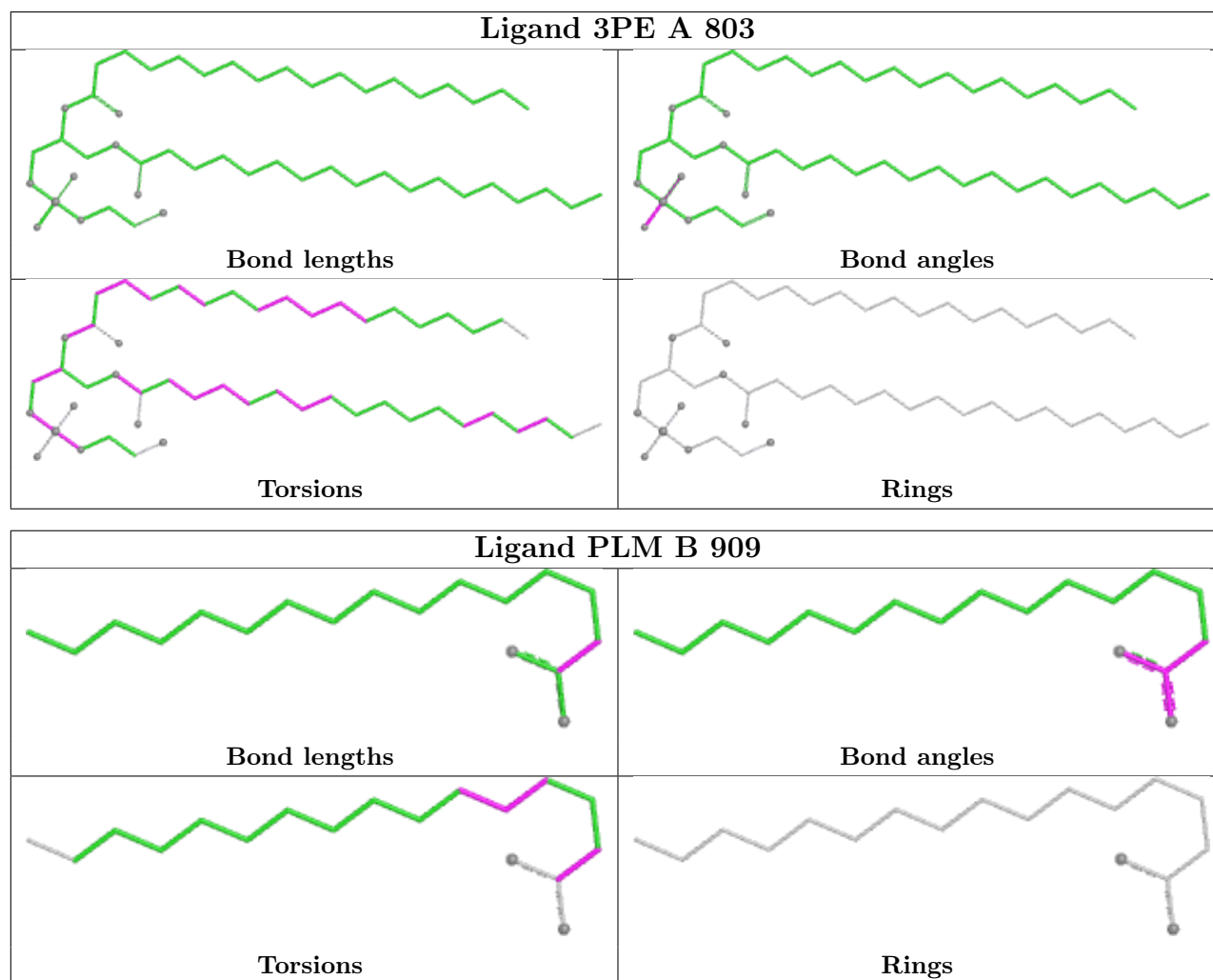
There are no ring outliers.

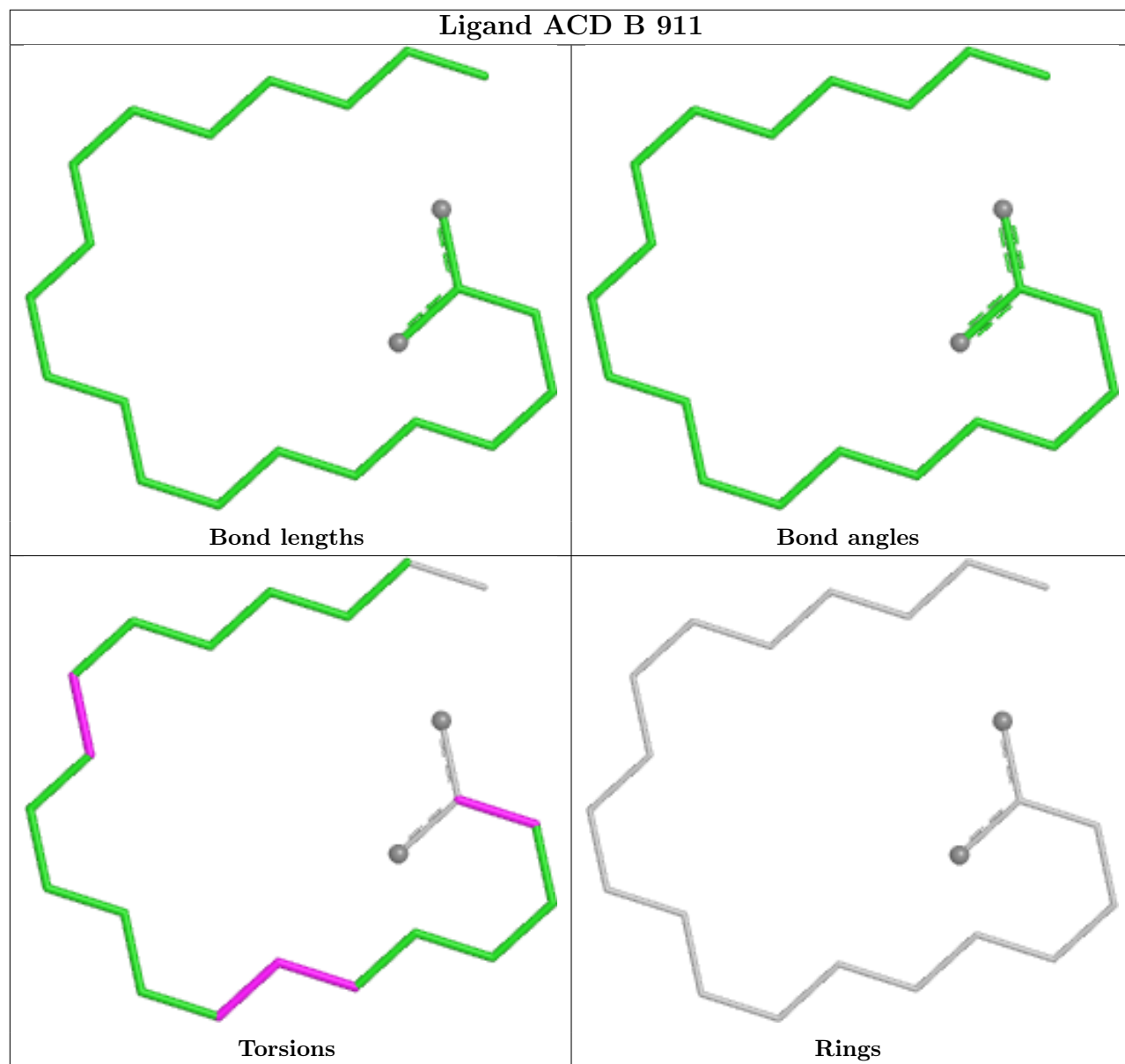
13 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	803	3PE	2	0
6	B	911	ACD	1	0
3	B	903	IHP	3	0
2	A	806	CLR	2	0
4	B	901	3PE	5	0
4	B	908	3PE	2	0
2	A	814	CLR	1	0
2	A	801	CLR	2	0
2	A	804	CLR	3	0
2	B	910	CLR	2	0
2	A	810	CLR	3	0
4	A	813	3PE	6	0
2	B	905	CLR	1	0

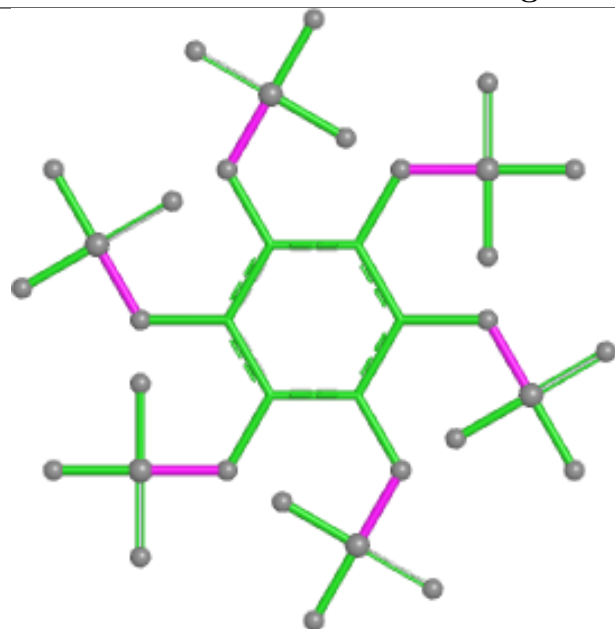
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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.

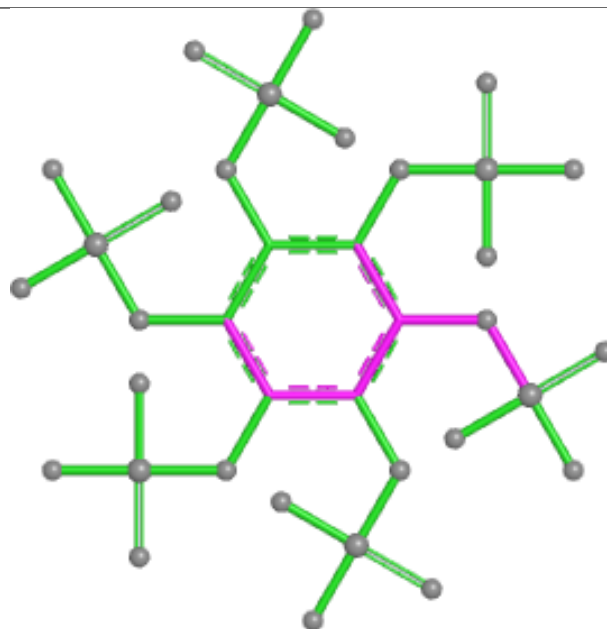




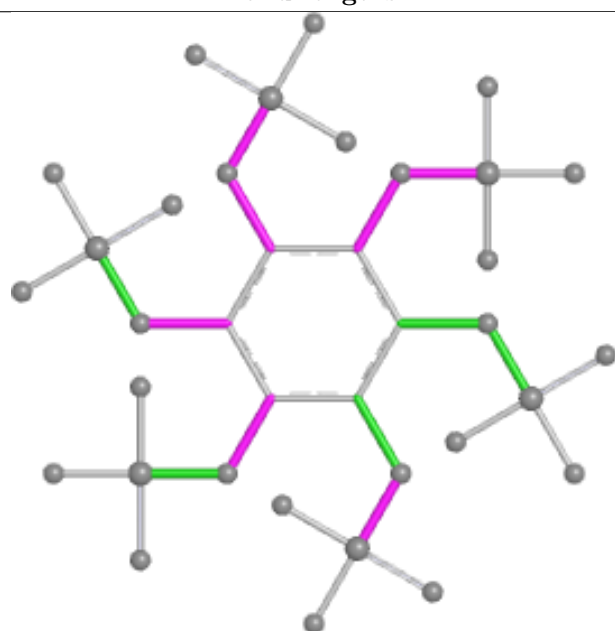
Ligand IHP B 903



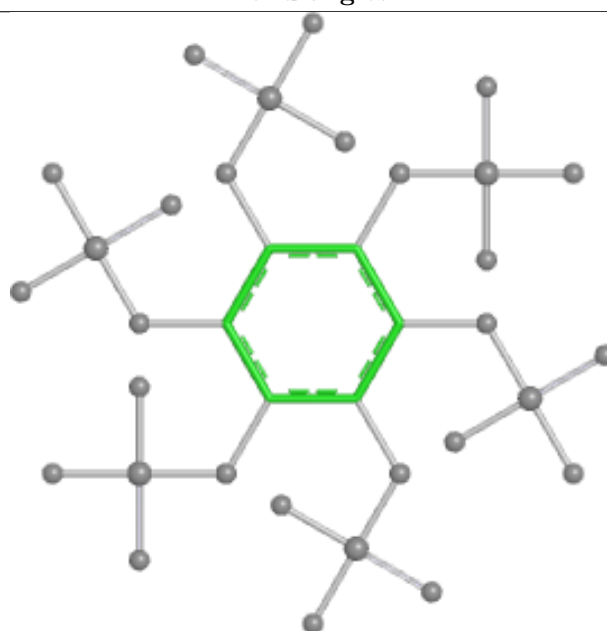
Bond lengths



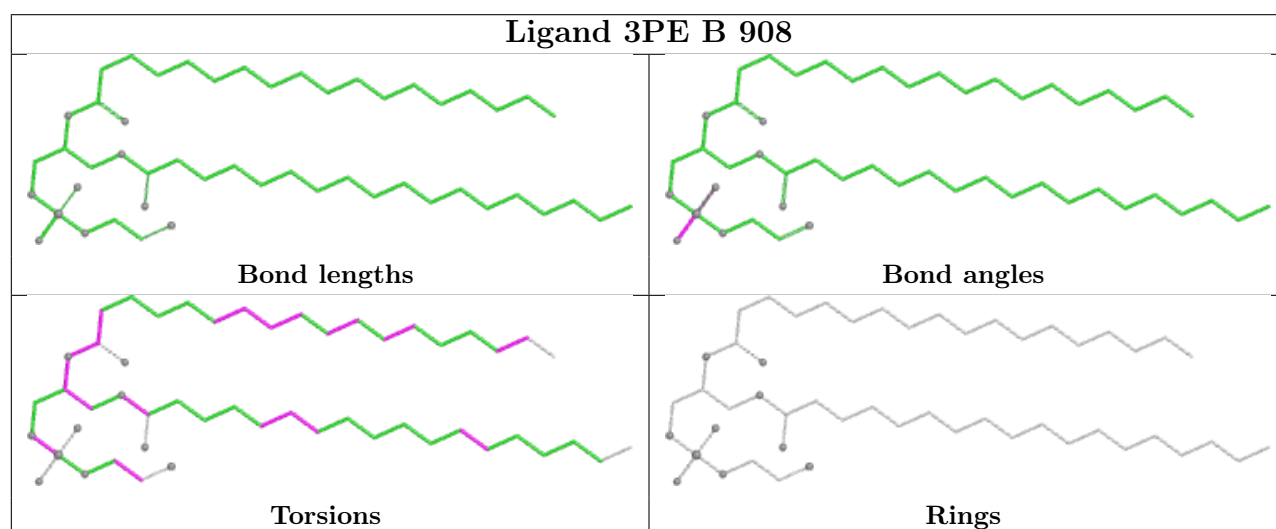
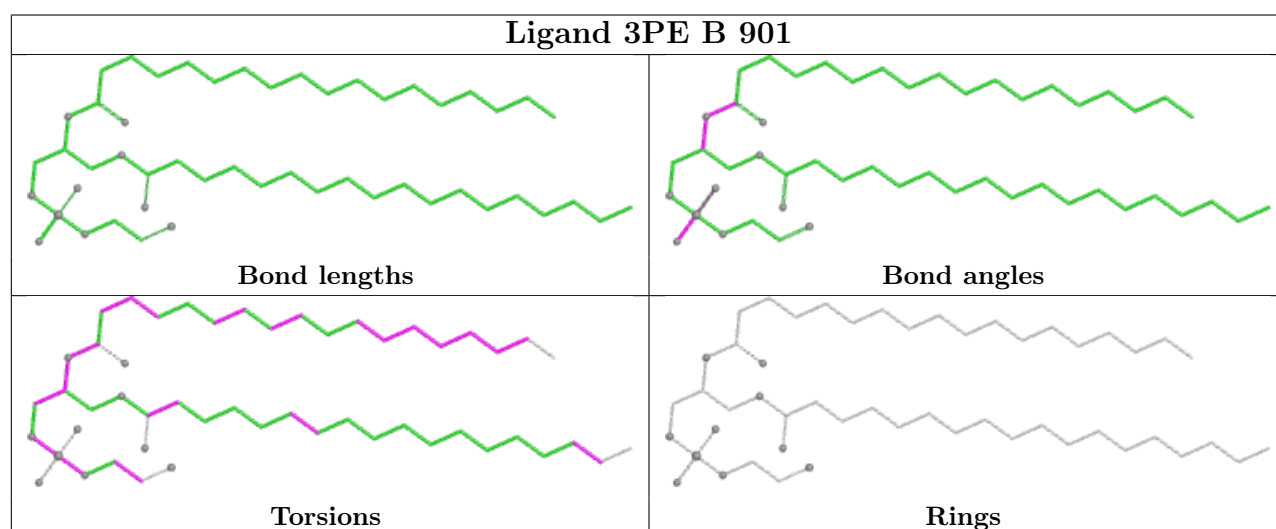
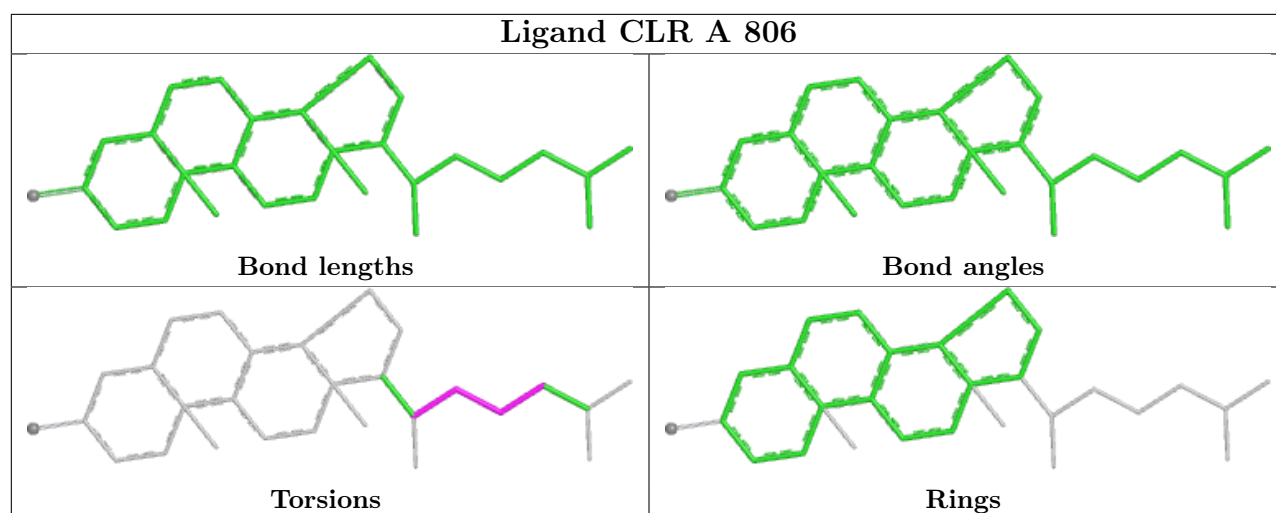
Bond angles



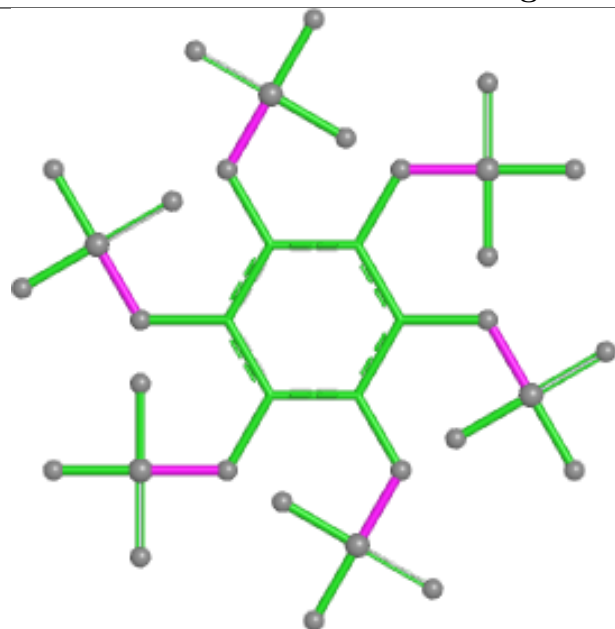
Torsions



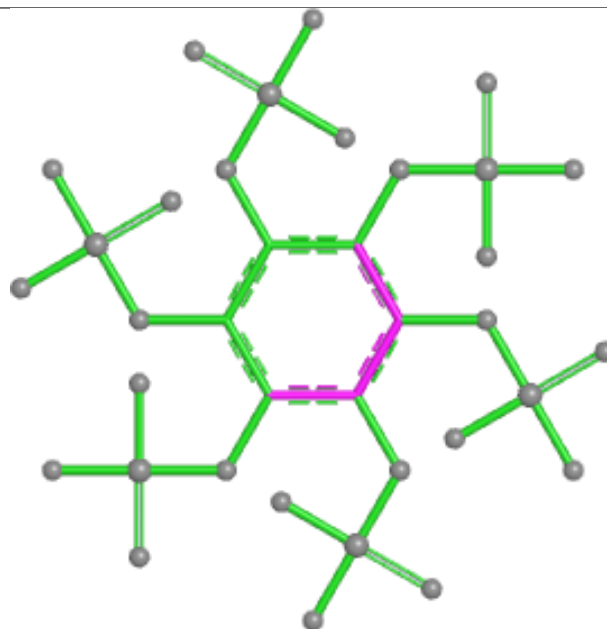
Rings



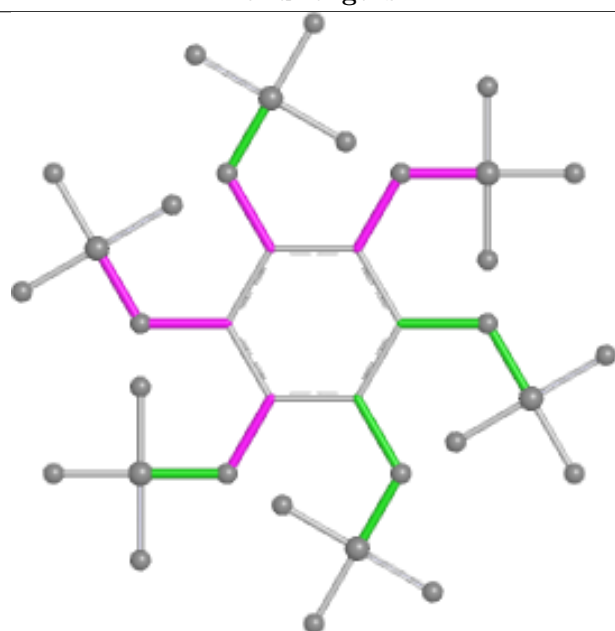
Ligand IHP A 802



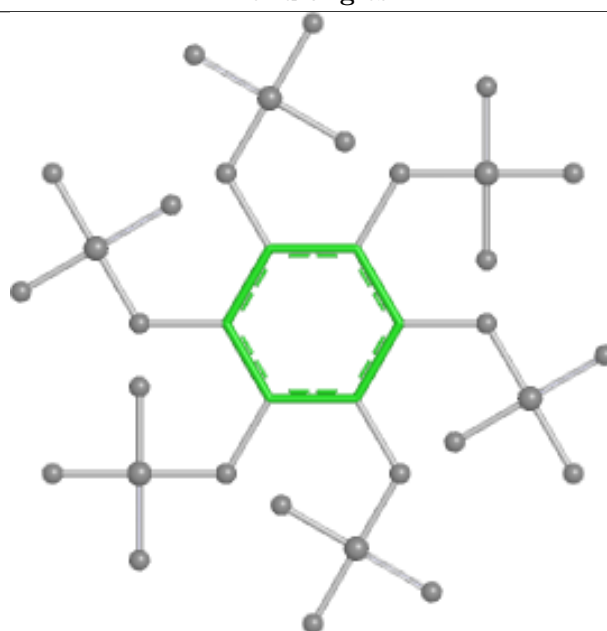
Bond lengths



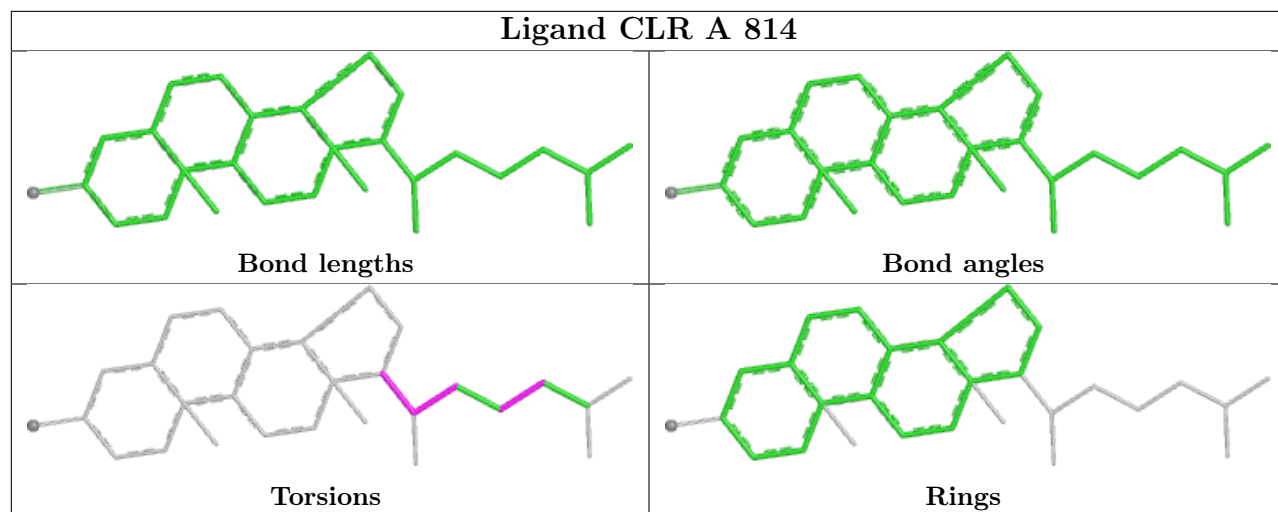
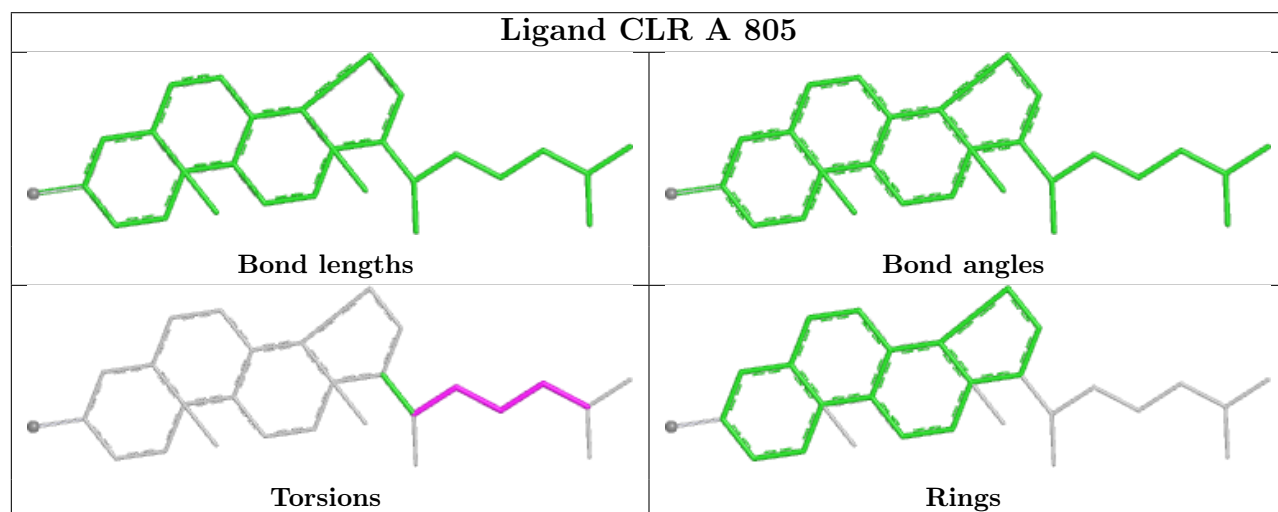
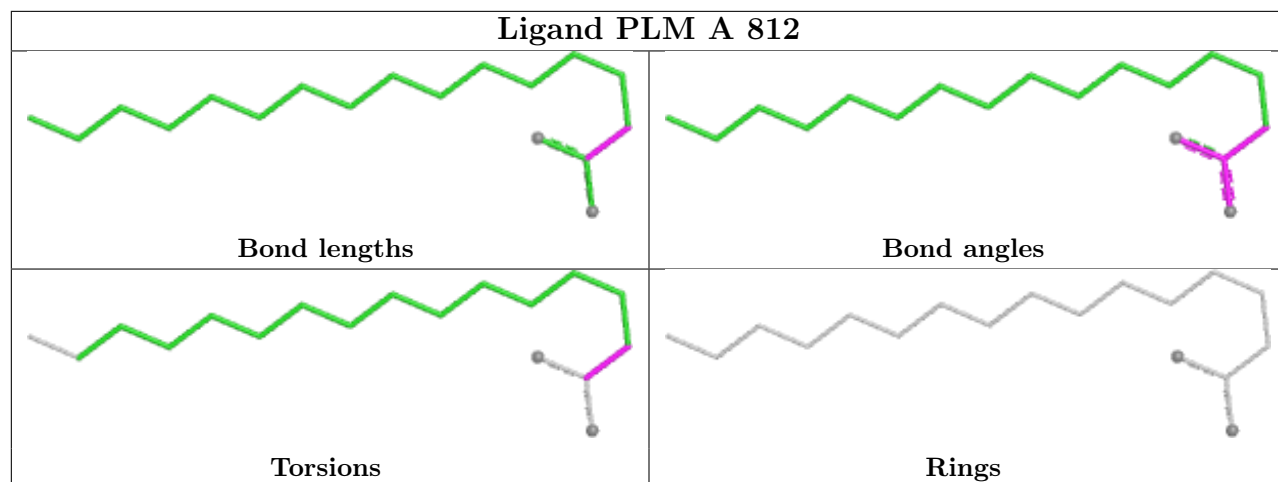
Bond angles

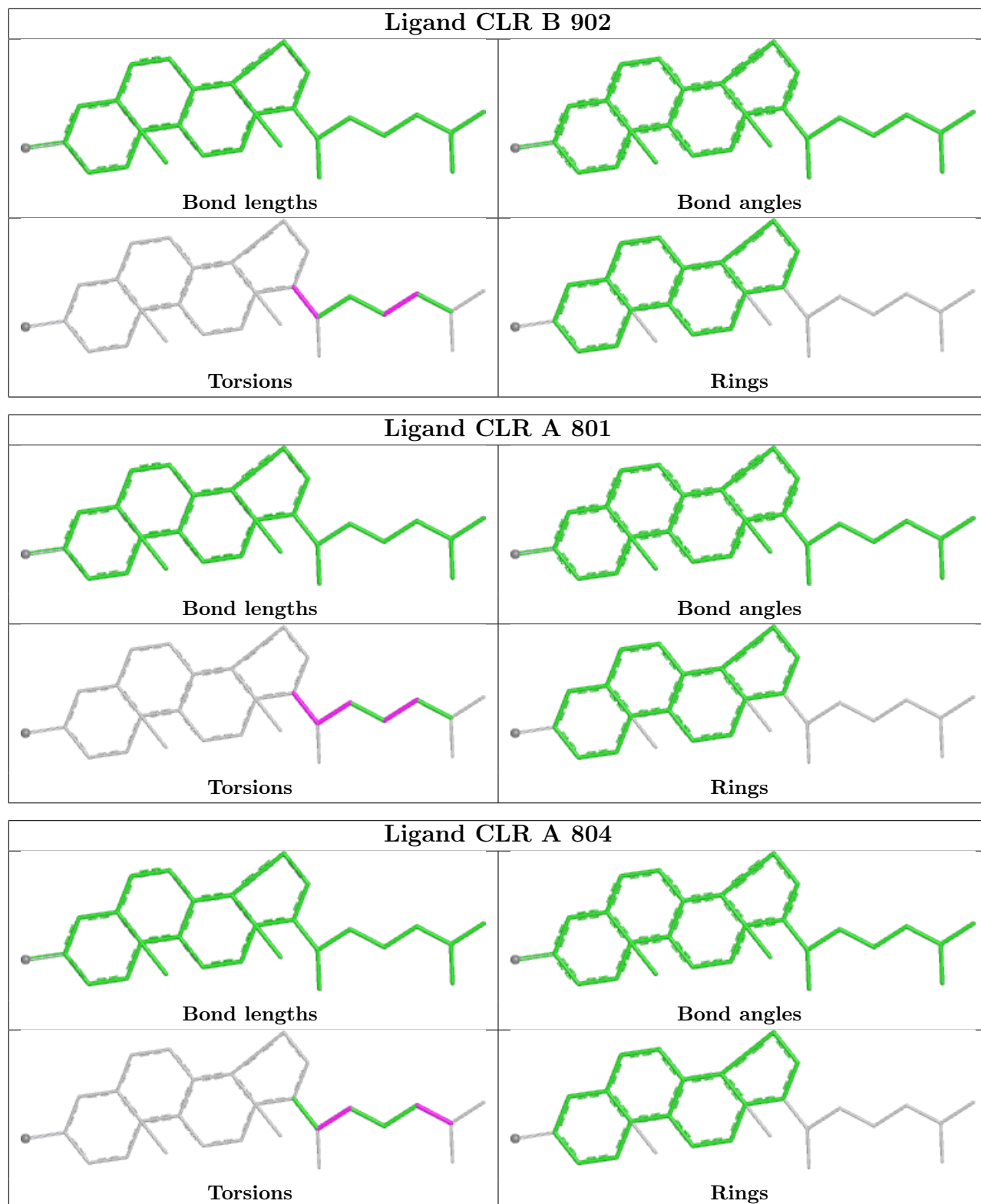


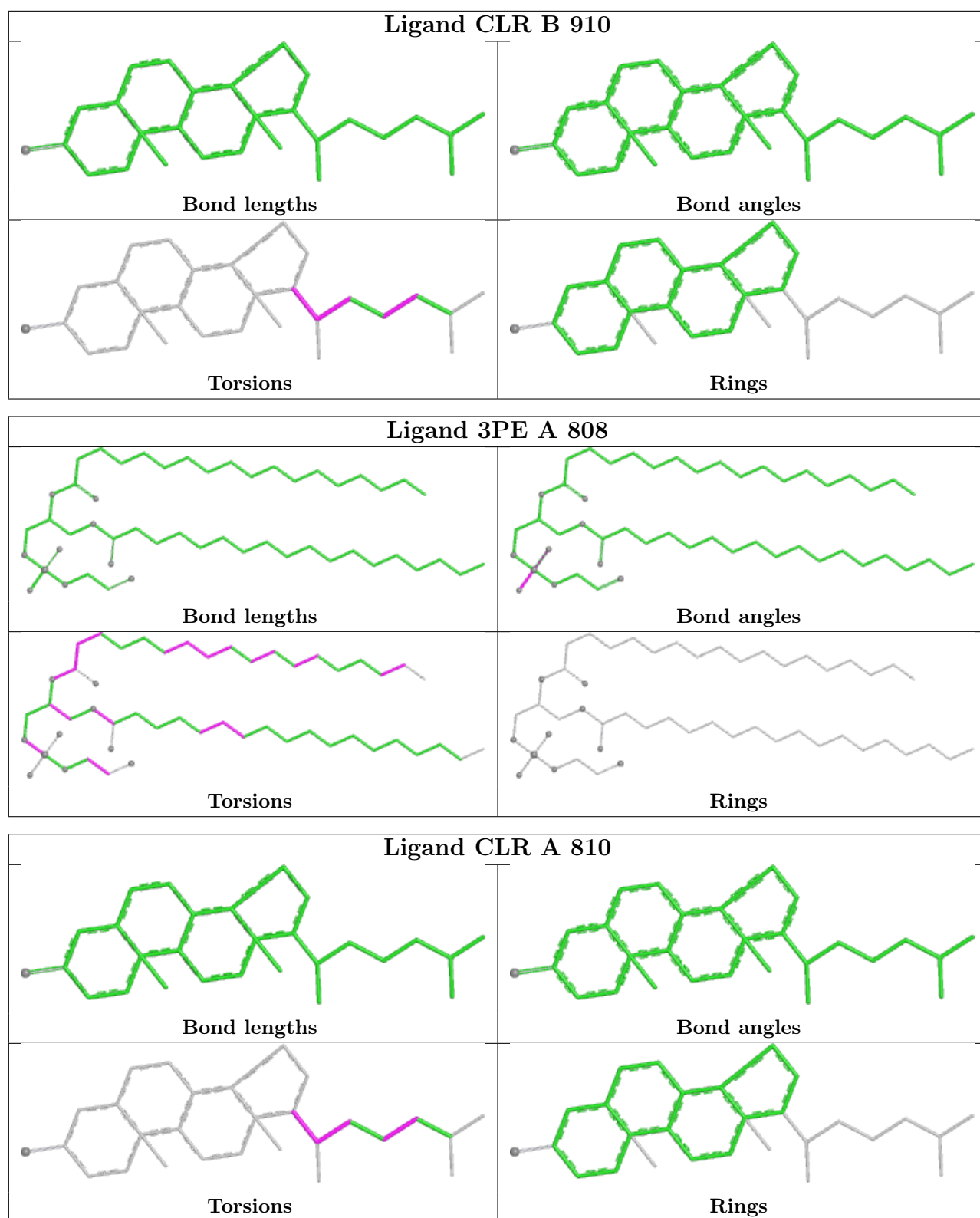
Torsions

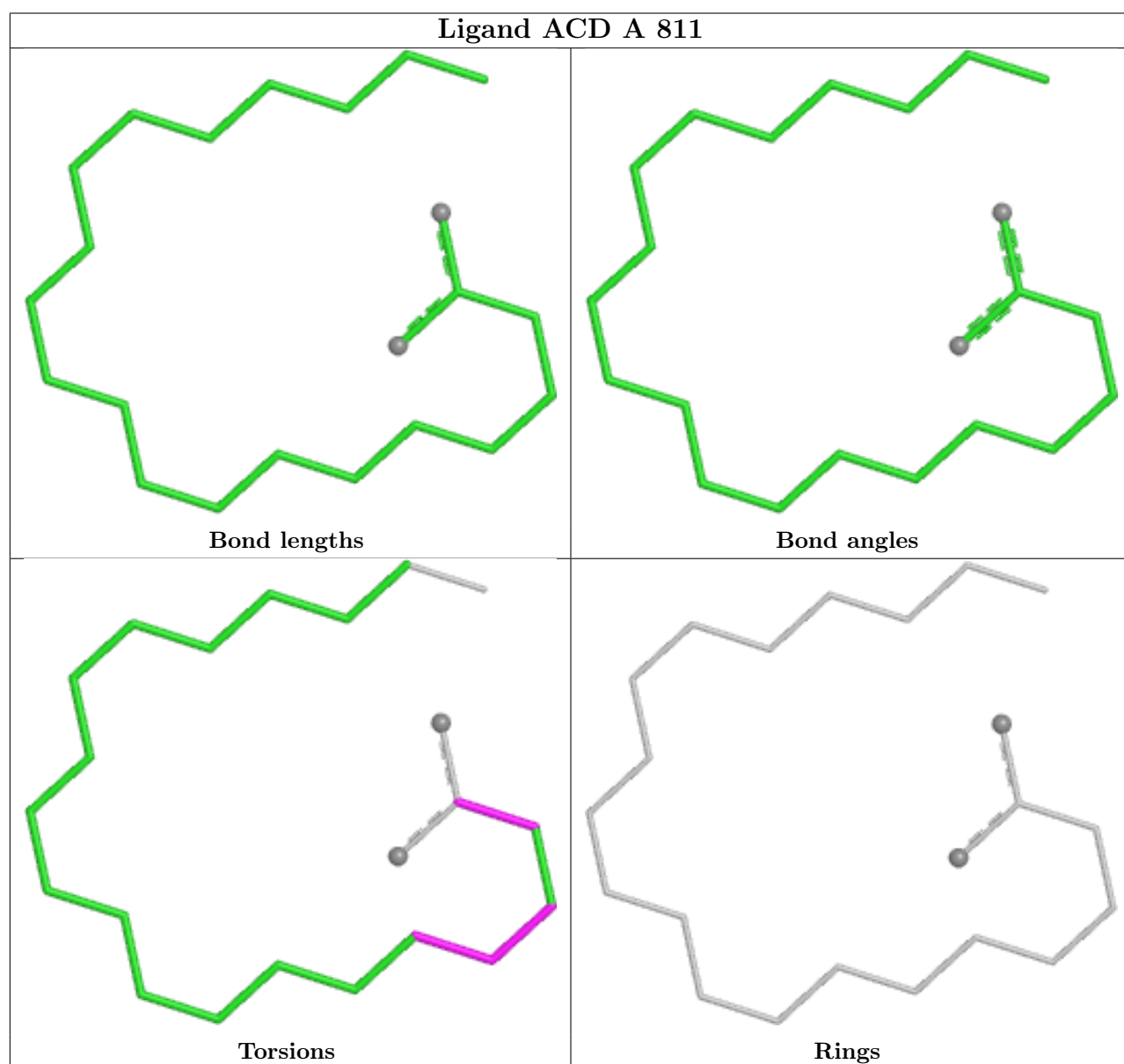
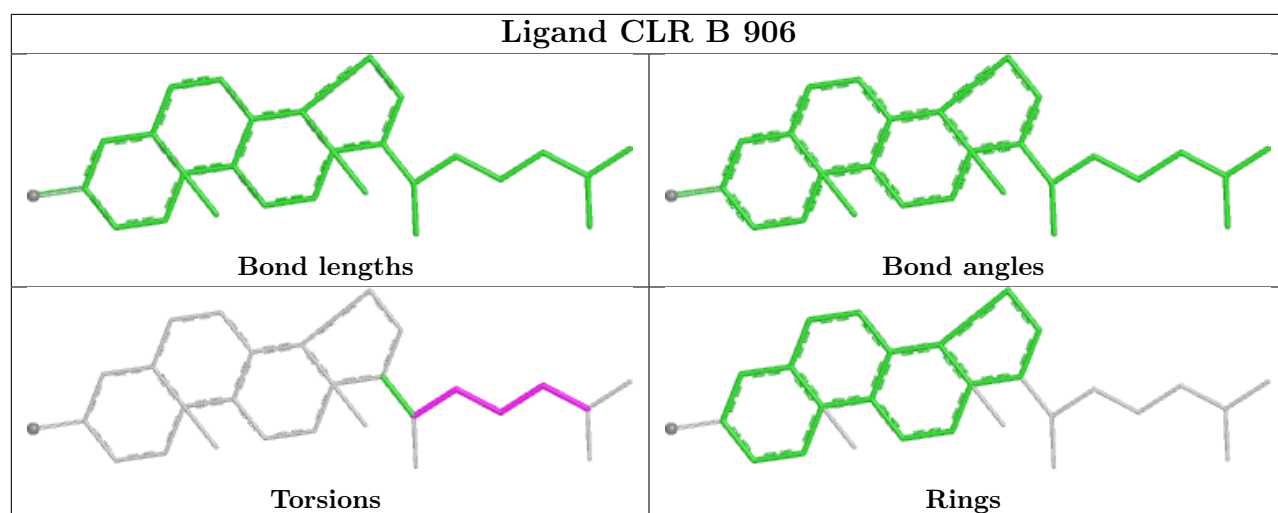


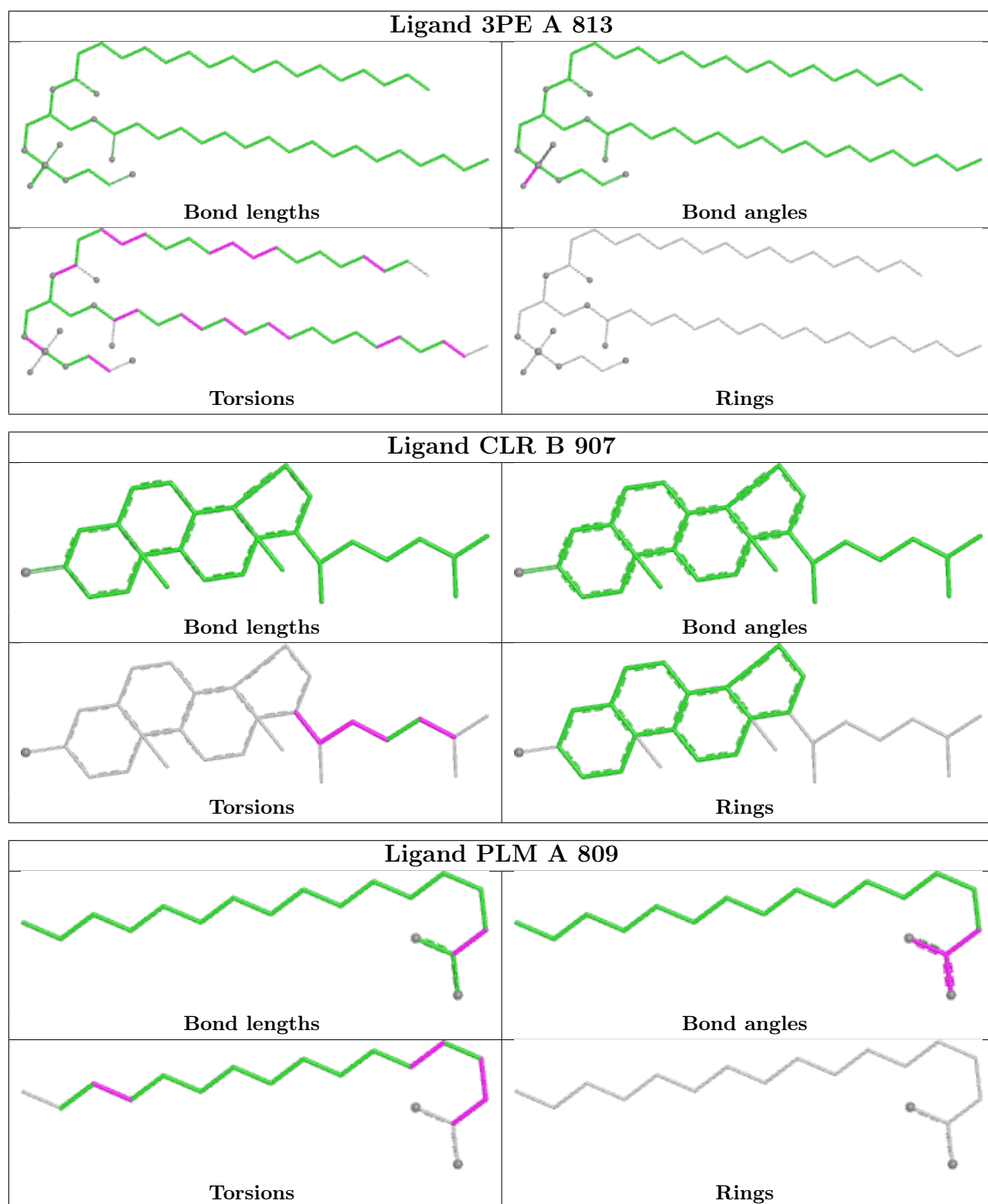
Rings

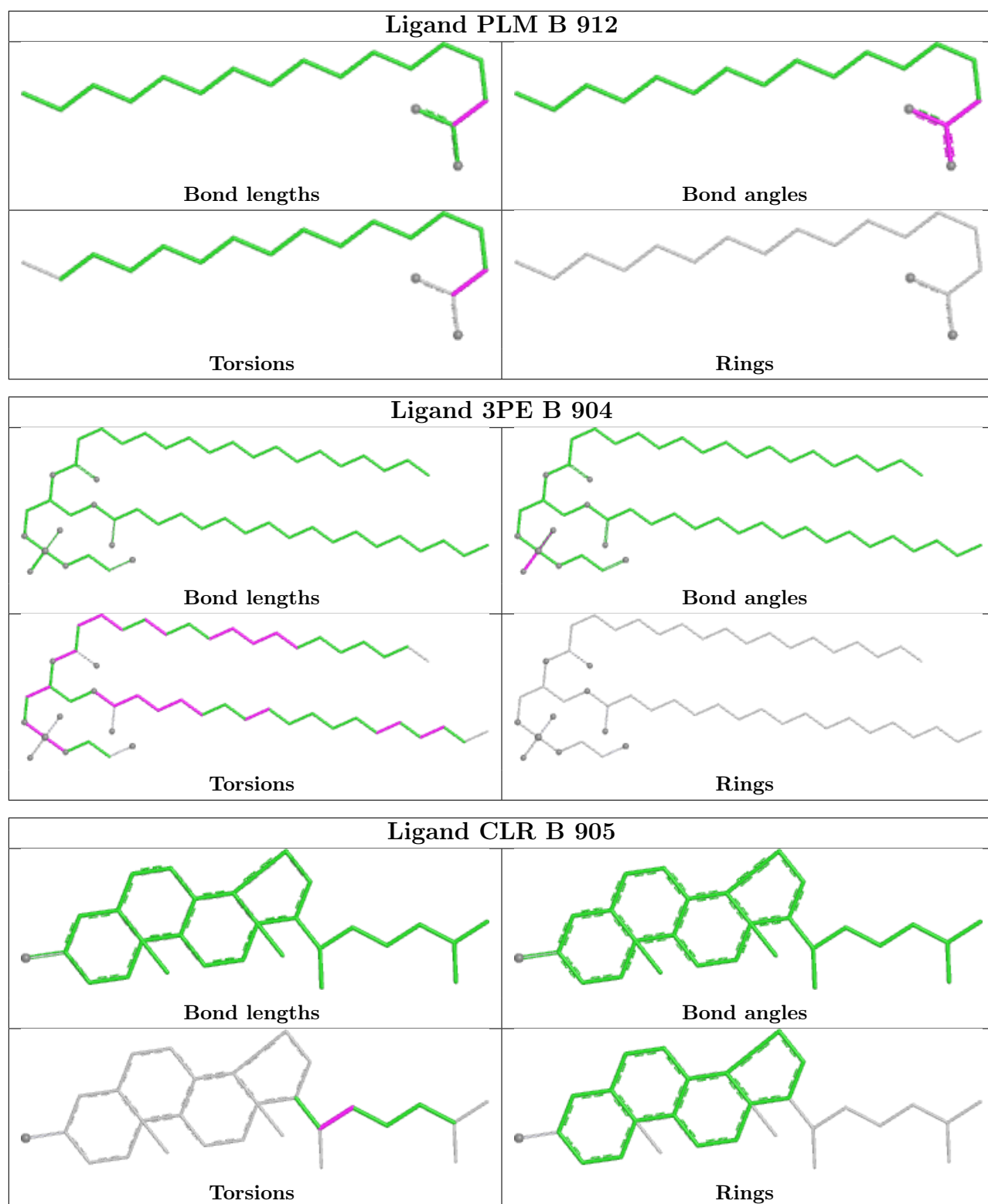


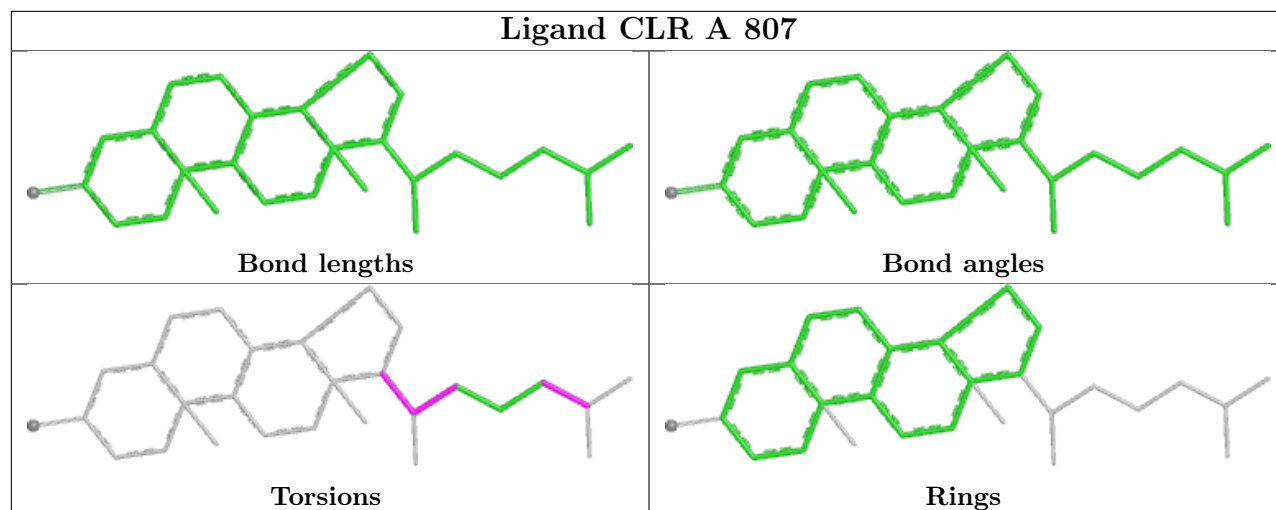












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

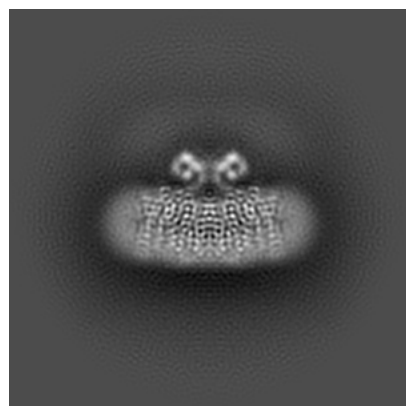
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60897. These allow visual inspection of the internal detail of the map and identification of artifacts.

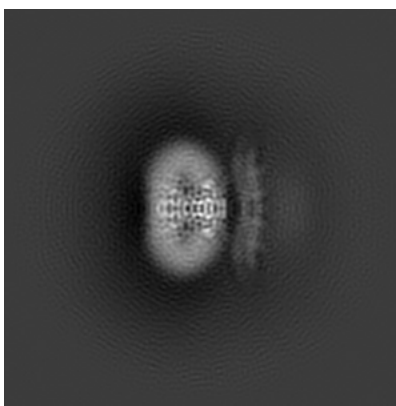
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

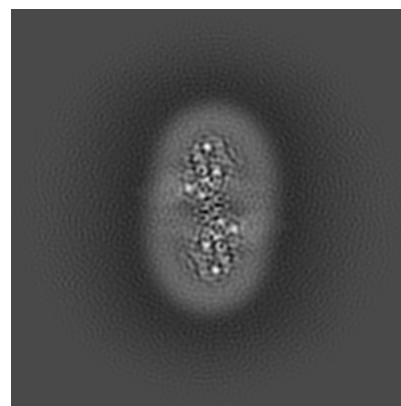
6.1.1 Primary map



X

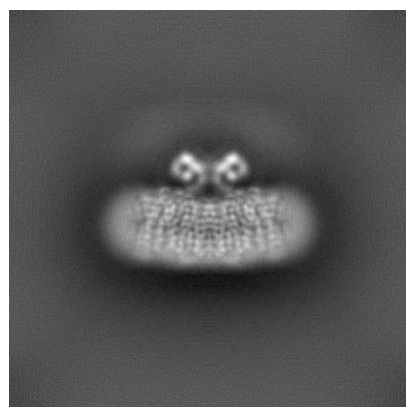


Y

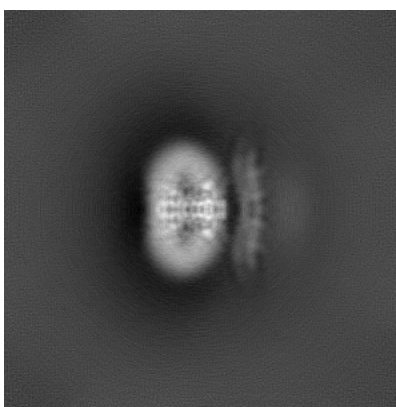


Z

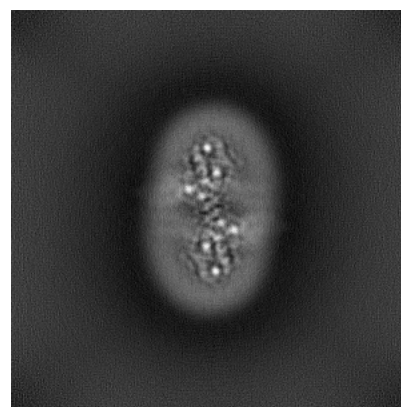
6.1.2 Raw map



X



Y

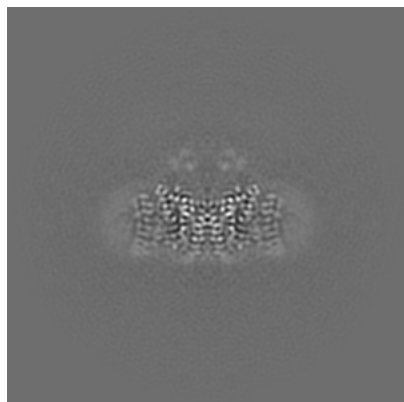


Z

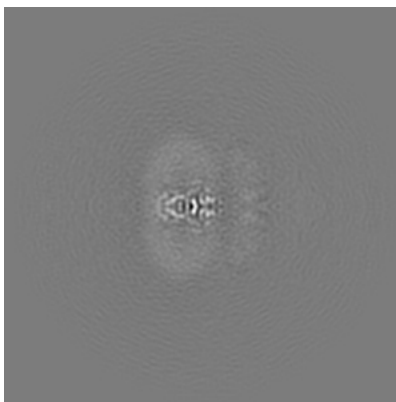
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

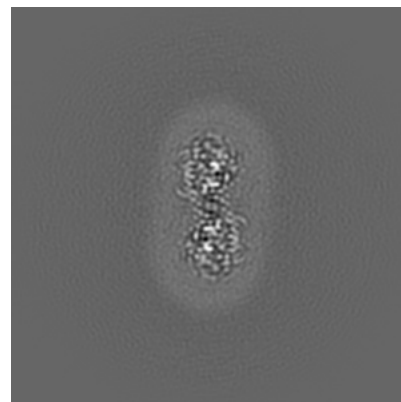
6.2.1 Primary map



X Index: 200

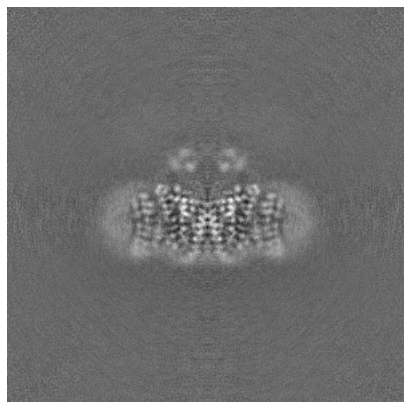


Y Index: 200

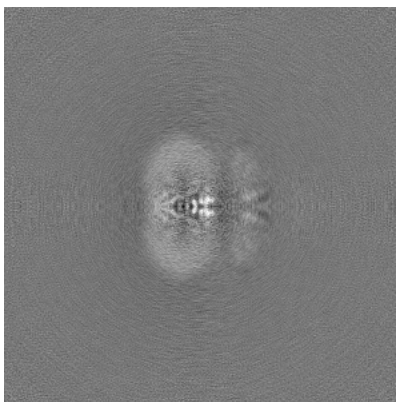


Z Index: 200

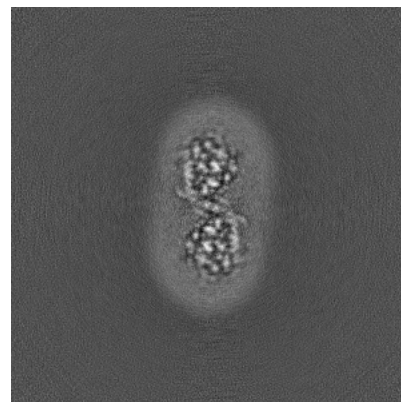
6.2.2 Raw map



X Index: 200



Y Index: 200

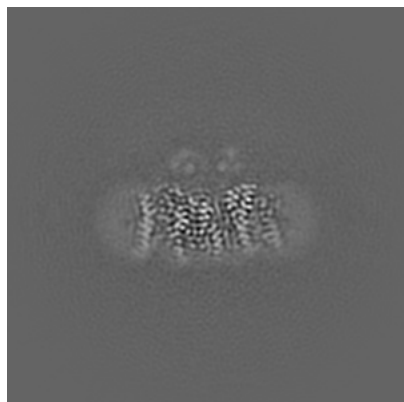


Z Index: 200

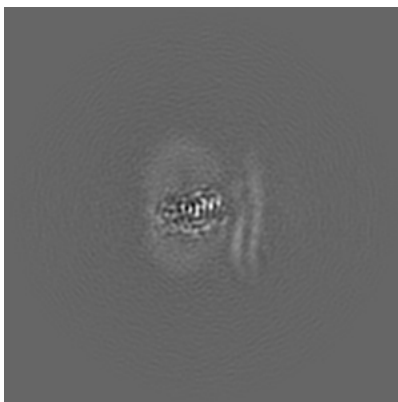
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

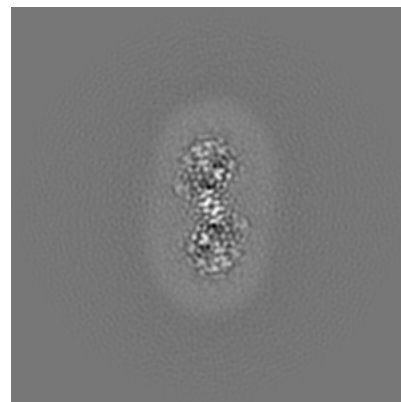
6.3.1 Primary map



X Index: 204

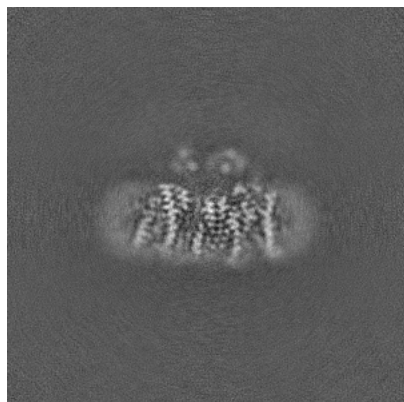


Y Index: 223

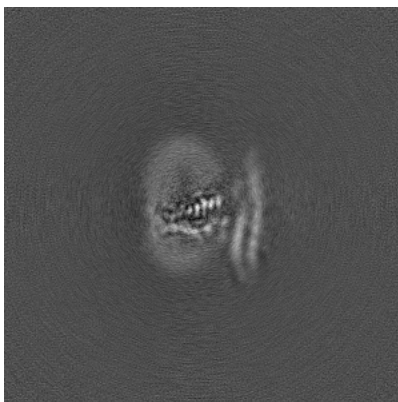


Z Index: 196

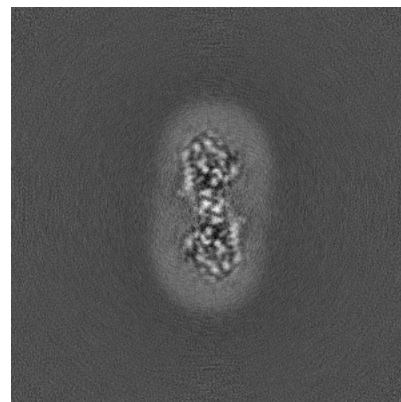
6.3.2 Raw map



X Index: 195



Y Index: 222

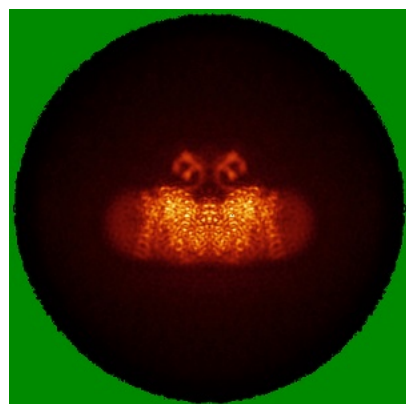


Z Index: 203

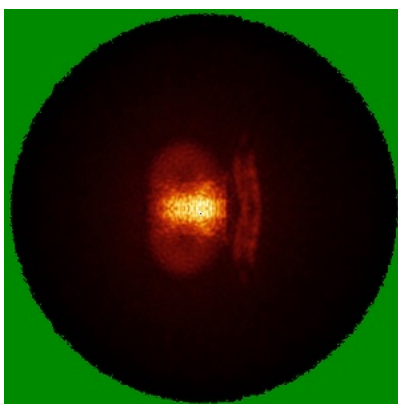
The images above show the largest variance slices of the map in three orthogonal directions.

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

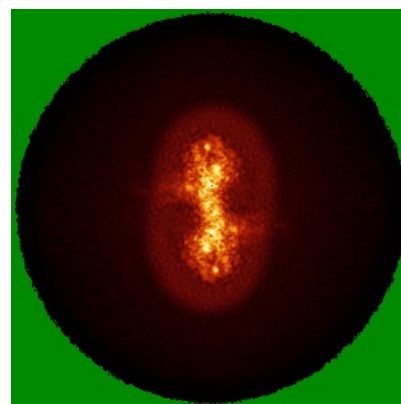
6.4.1 Primary map



X

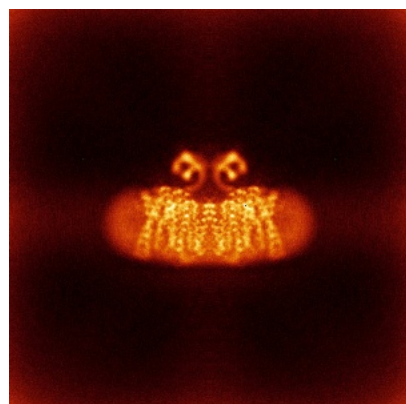


Y

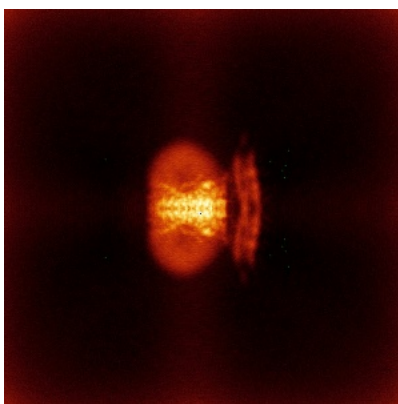


Z

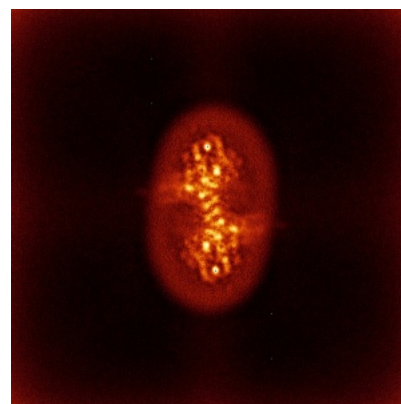
6.4.2 Raw map



X



Y

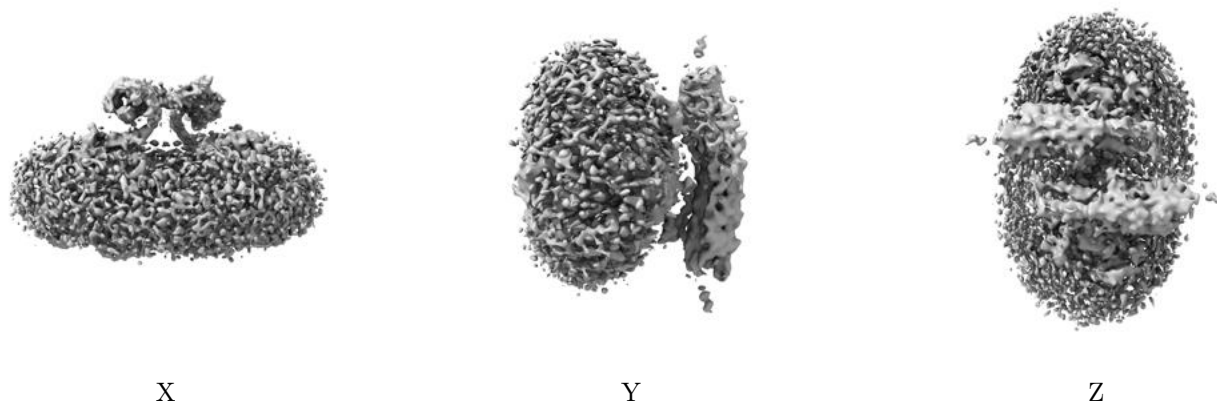


Z

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.

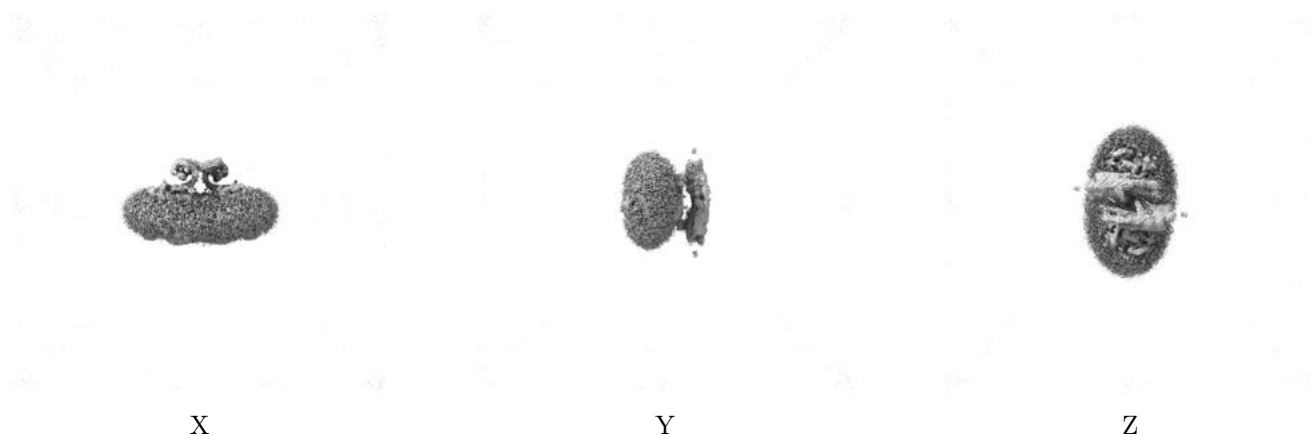
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.055. 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.

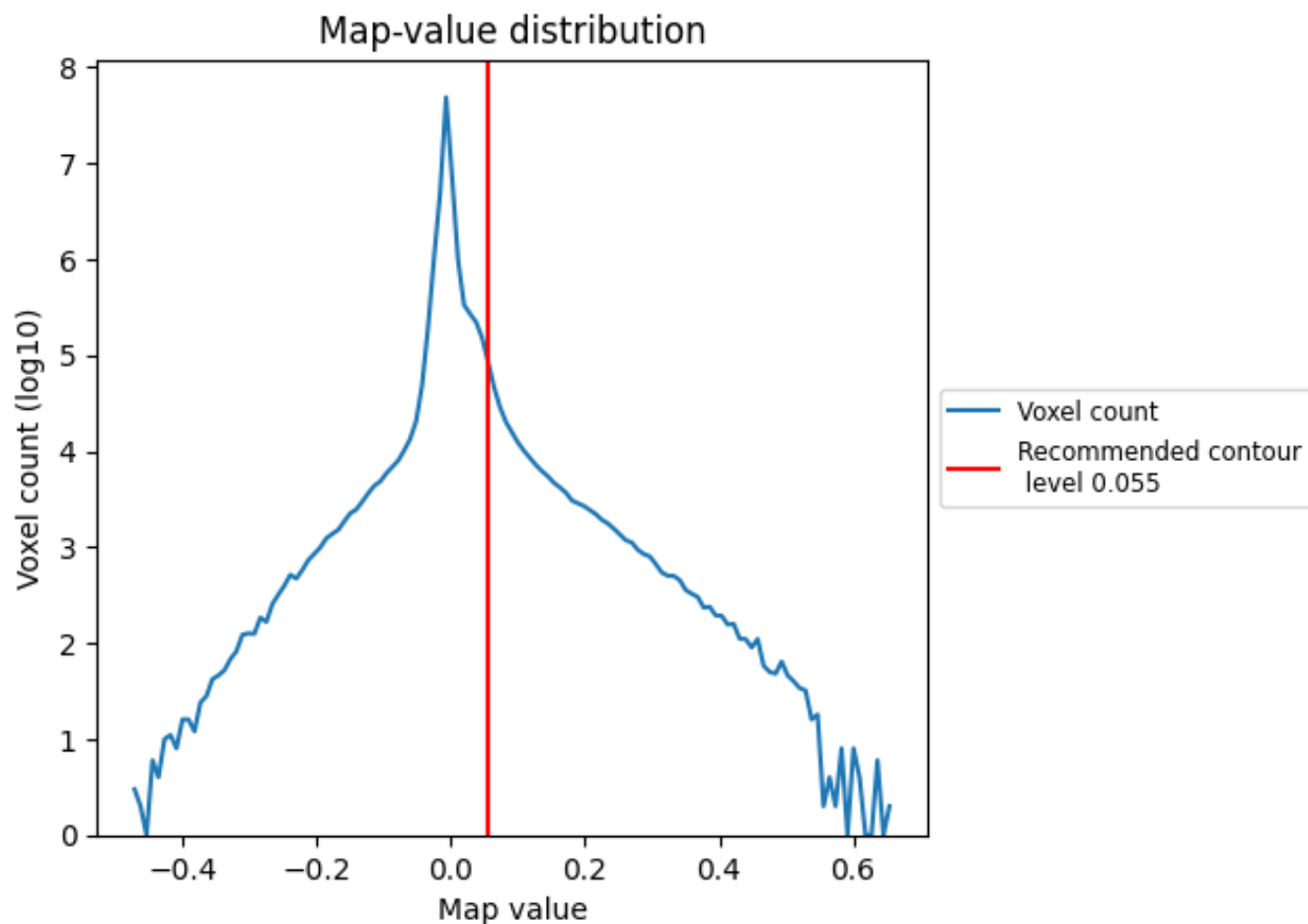
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

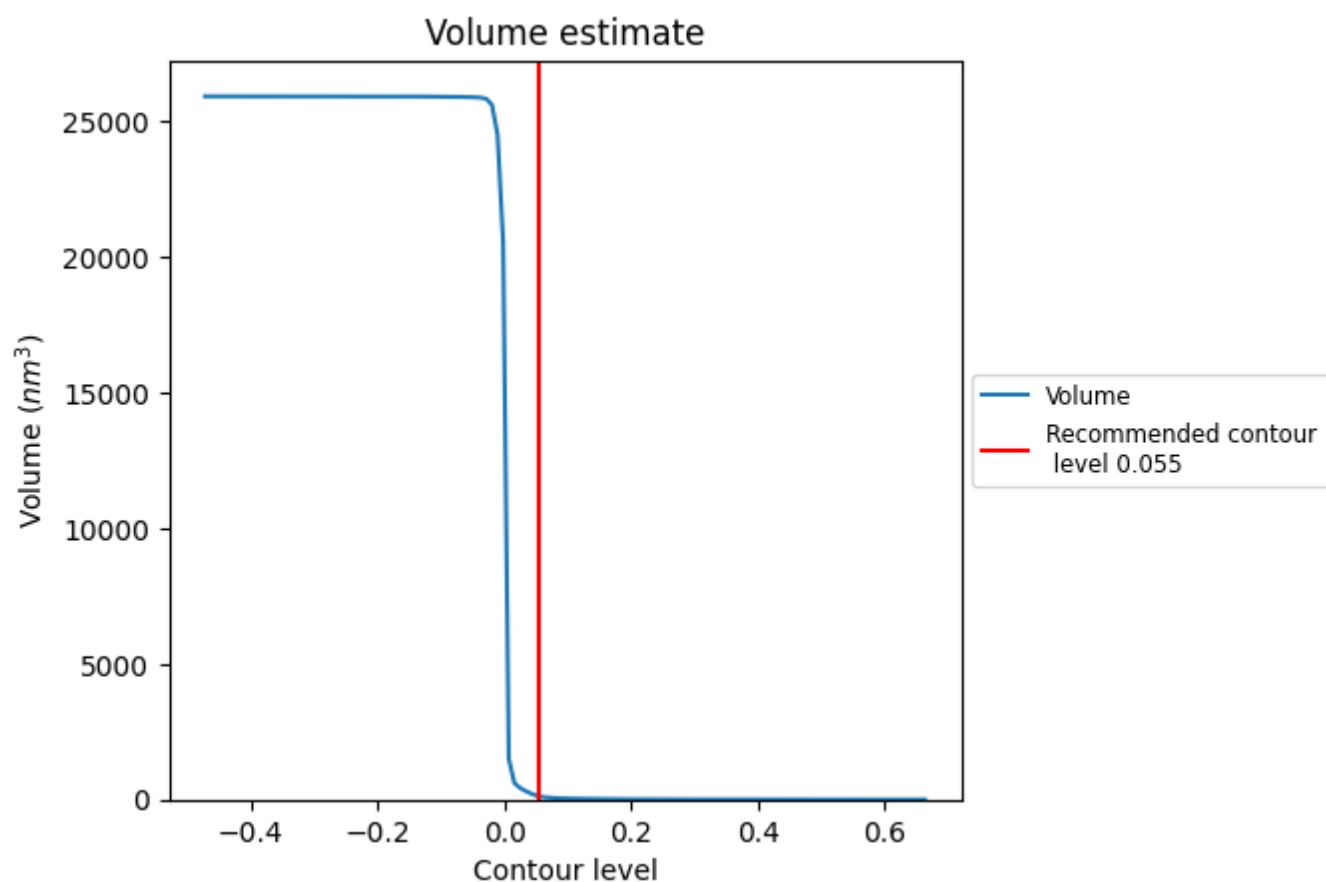
This section contains the results of statistical analysis of the map.

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.

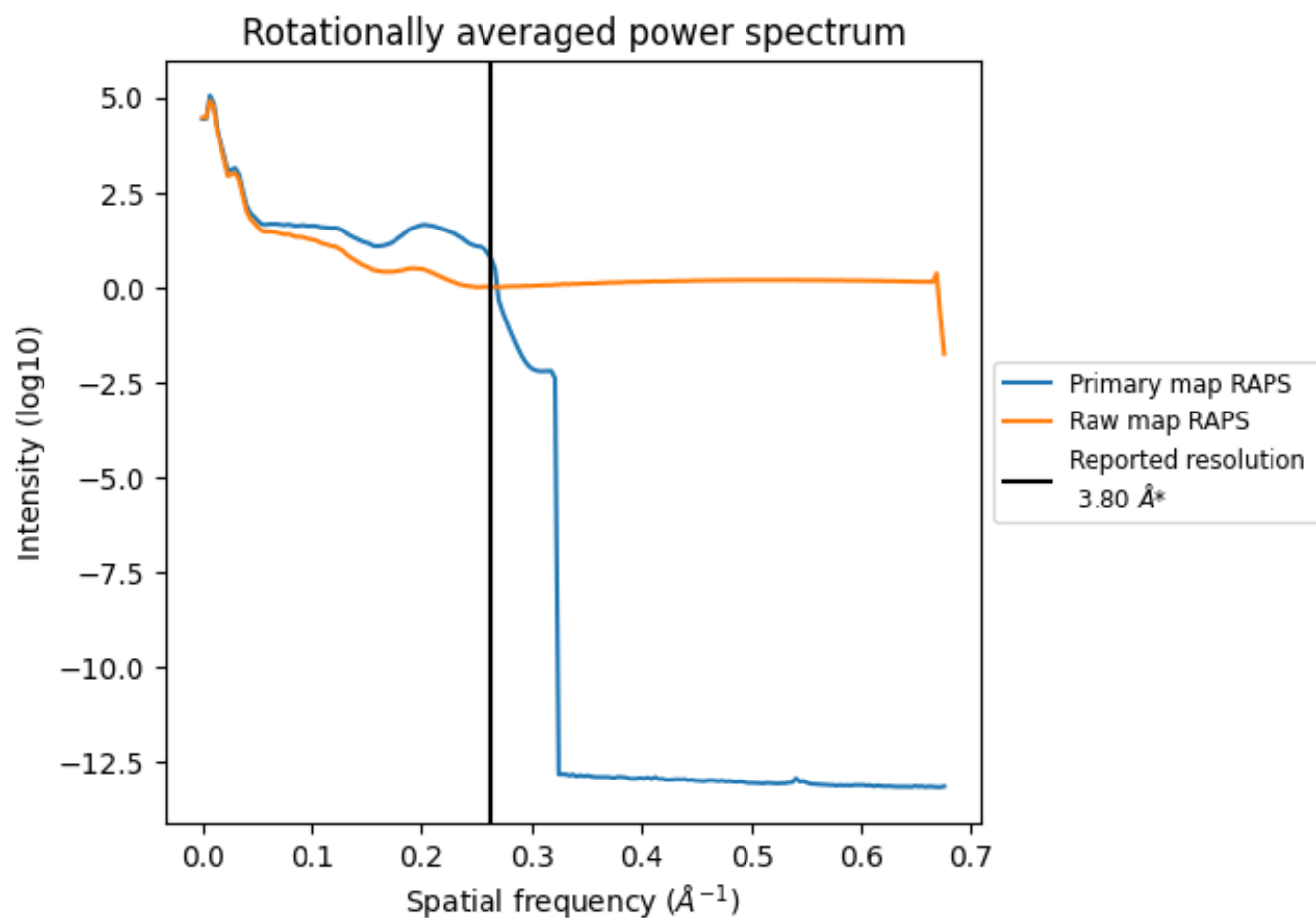
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 121 nm³; this corresponds to an approximate mass of 109 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 ⓘ

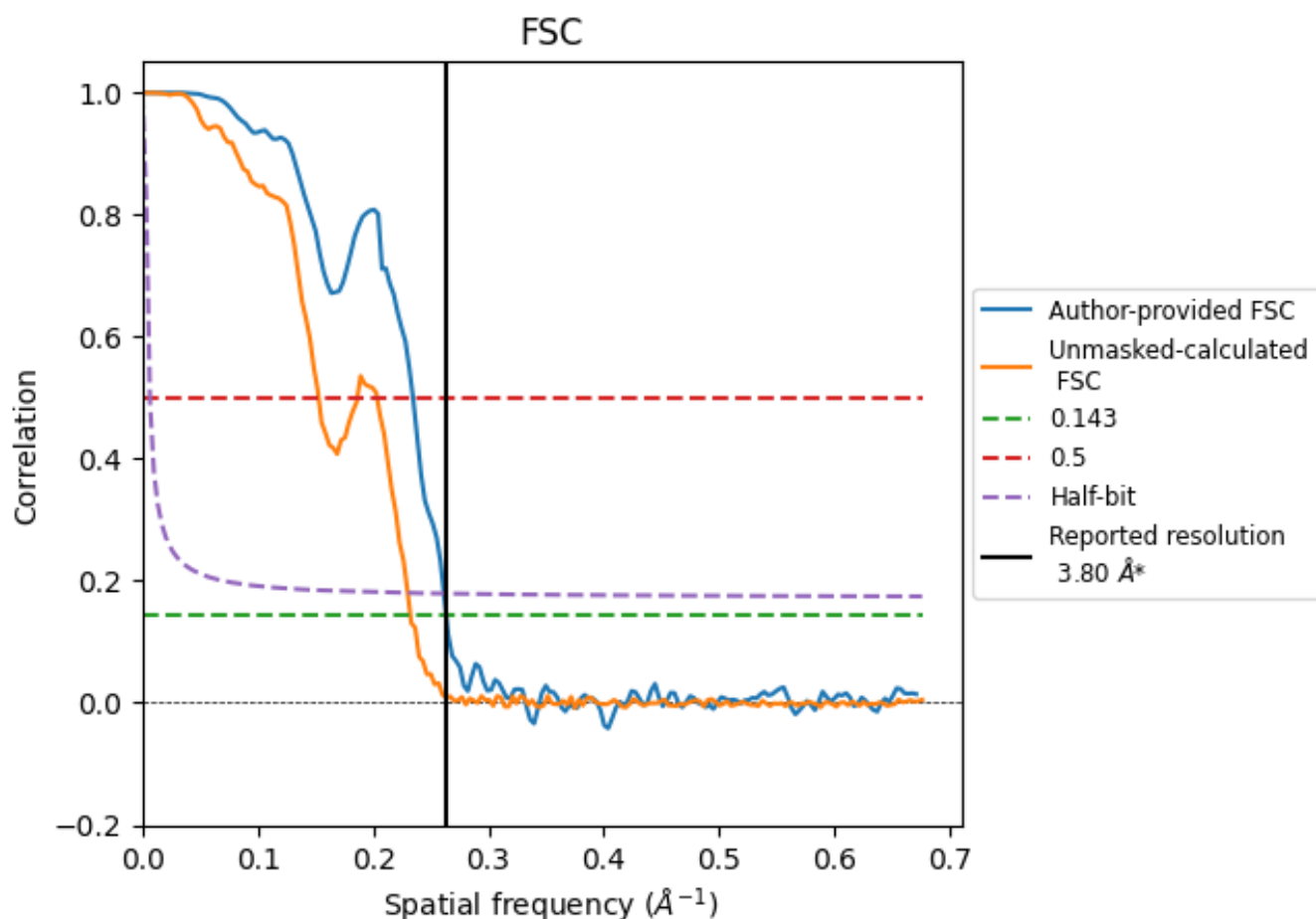


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

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 0.263 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

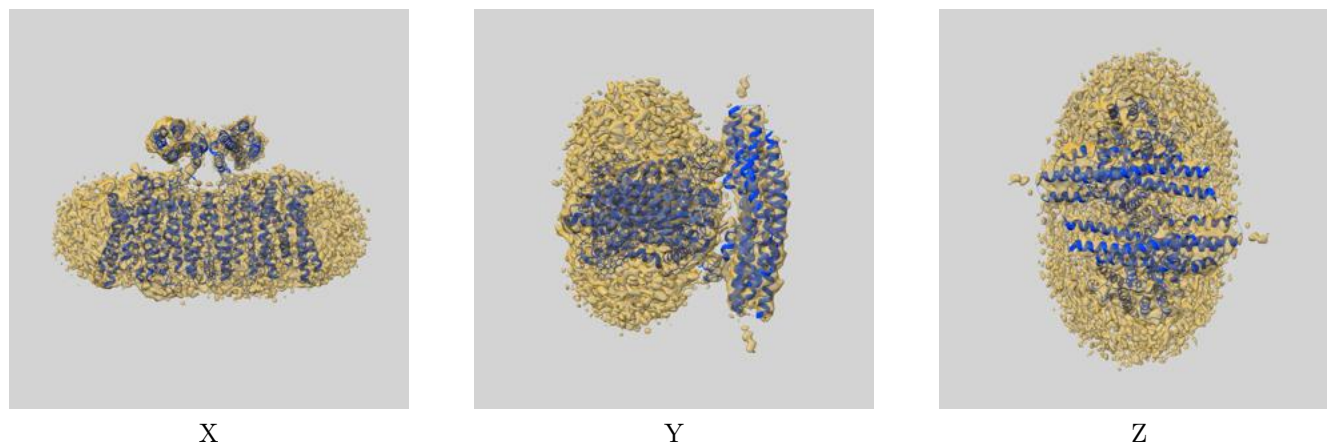
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.80	4.26	3.83
Unmasked-calculated*	4.30	6.54	4.35

*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 4.30 differs from the reported value 3.8 by more than 10 %

9 Map-model fit [i](#)

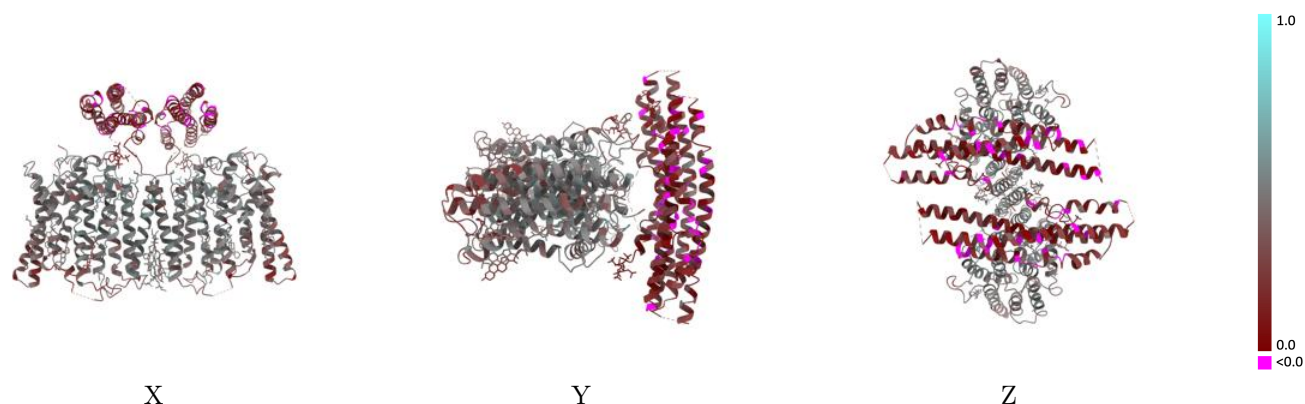
This section contains information regarding the fit between EMDB map EMD-60897 and PDB model 9IUC. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



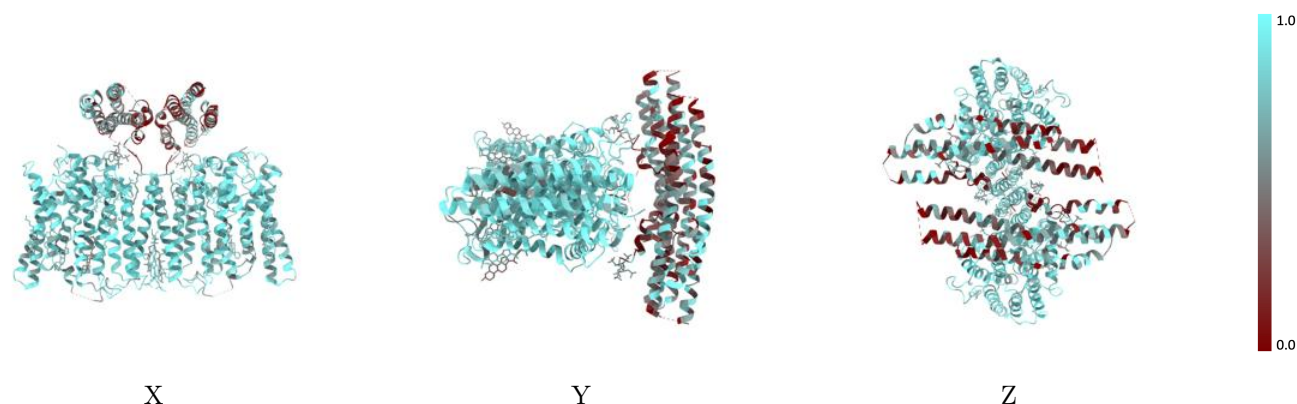
The images above show the 3D surface view of the map at the recommended contour level 0.055 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



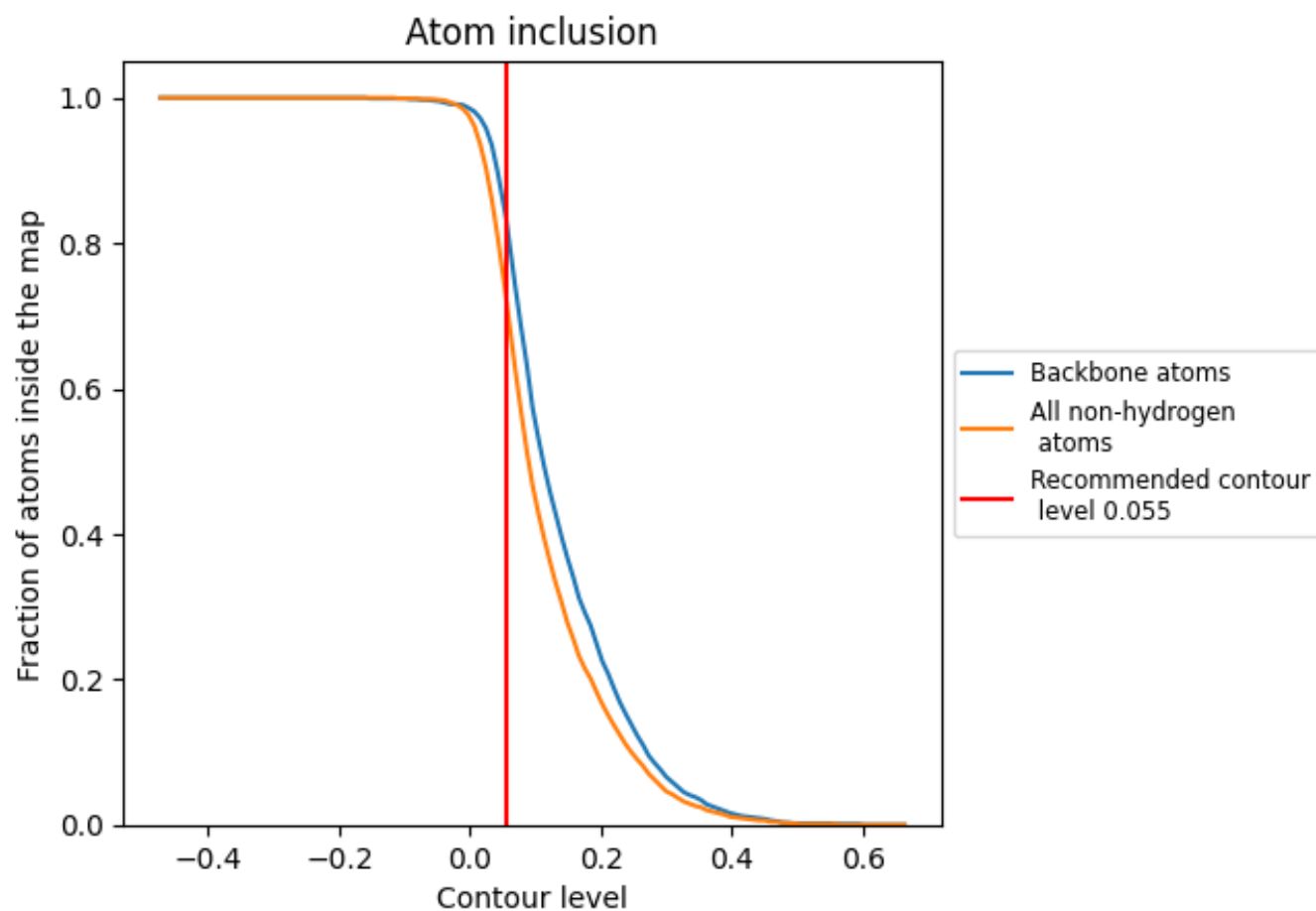
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.055).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 73% 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 (0.055) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7260	0.3480
A	0.7220	0.3440
B	0.7300	0.3510

