



Full wwPDB EM Validation Report ⓘ

Mar 12, 2026 – 05:19 PM UTC

PDB ID : 8D2S / pdb_00008d2s
EMDB ID : EMD-27148
Title : Zebrafish MFSD2A isoform B in inward open ligand bound conformation
Authors : Nguyen, C.; Lei, H.T.; Lai, L.T.F.; Gallentino, M.J.; Mu, X.; Matthies, D.; Gonen, T.
Deposited on : 2022-05-30
Resolution : 2.90 Å(reported)
Based on initial model : 7MJS

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

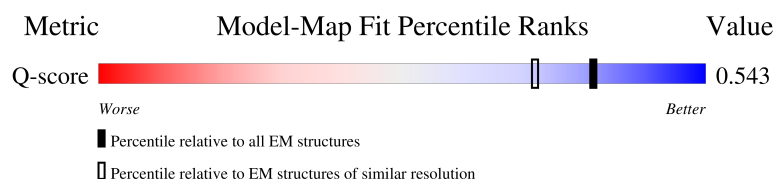
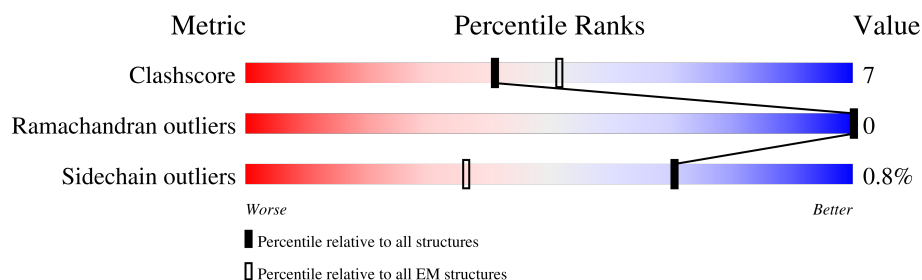
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13054 (2.40 - 3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	508	18% 79% 14% 6%
2	B	201	12% 83% 17%
3	C	203	10% 87% 13%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7071 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 Sodium-dependent lysophosphatidylcholine symporter 1-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	475	Total	C	N	O	S	5	0
			3577	2374	562	617	24		

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	MET	-	initiating methionine	UNP Q6DEJ6
A	3	HIS	-	expression tag	UNP Q6DEJ6
A	4	HIS	-	expression tag	UNP Q6DEJ6
A	5	HIS	-	expression tag	UNP Q6DEJ6
A	6	HIS	-	expression tag	UNP Q6DEJ6
A	7	HIS	-	expression tag	UNP Q6DEJ6
A	8	HIS	-	expression tag	UNP Q6DEJ6
A	9	HIS	-	expression tag	UNP Q6DEJ6
A	10	HIS	-	expression tag	UNP Q6DEJ6
A	11	HIS	-	expression tag	UNP Q6DEJ6
A	12	HIS	-	expression tag	UNP Q6DEJ6
A	13	GLU	-	expression tag	UNP Q6DEJ6
A	14	ASN	-	expression tag	UNP Q6DEJ6
A	15	LEU	-	expression tag	UNP Q6DEJ6
A	16	TYR	-	expression tag	UNP Q6DEJ6
A	17	PHE	-	expression tag	UNP Q6DEJ6
A	18	GLN	-	expression tag	UNP Q6DEJ6
A	19	GLY	-	expression tag	UNP Q6DEJ6
A	20	GLY	-	expression tag	UNP Q6DEJ6
A	21	SER	-	expression tag	UNP Q6DEJ6
A	214	GLN	ASN	engineered mutation	UNP Q6DEJ6
A	225	GLN	ASN	engineered mutation	UNP Q6DEJ6
A	509	GLN	ASN	engineered mutation	UNP Q6DEJ6

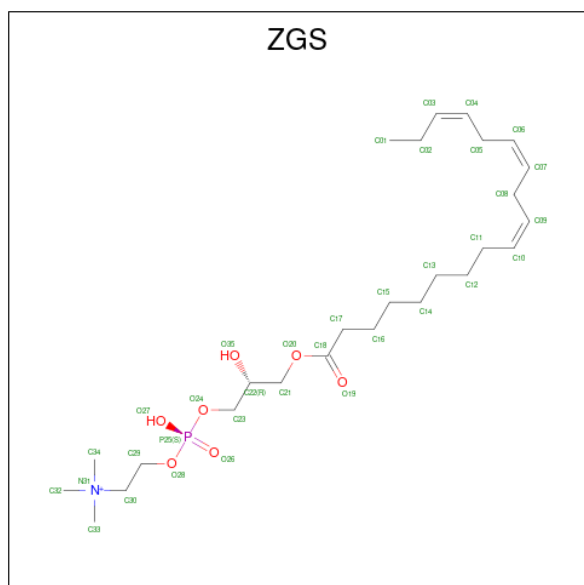
- Molecule 2 is a protein called FAB light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	201	Total	C	N	O	S	0	0
			1423	892	250	273	8		

- Molecule 3 is a protein called FAB heavy chain.

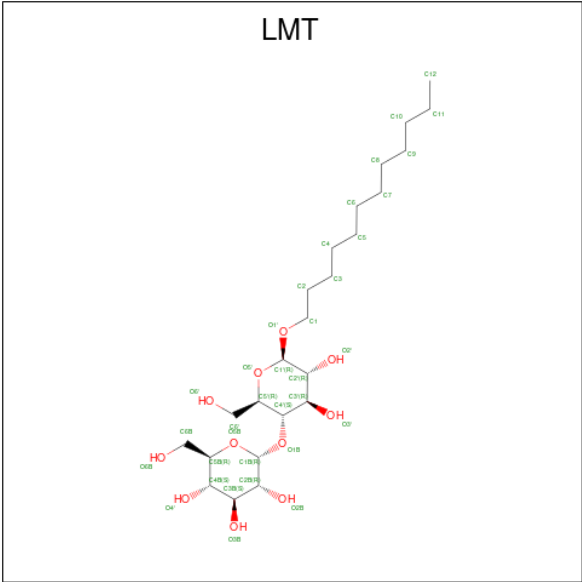
Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	203	Total	C	N	O	S	1	0
			1443	919	255	265	4		

- Molecule 4 is [(2 {R})-2-oxidanyl-3-[oxidanyl-2-(trimethyl- $\text{N}^{\{4\}}$ -azanyl)ethoxy]phosphoryl]oxy-propyl] (9 {Z},12 {Z},15 {Z})-octadeca-9,12,15-trienoate (CCD ID: ZGS) (formula: $\text{C}_{26}\text{H}_{49}\text{NO}_7\text{P}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			35	26	1	7	1	
4	A	1	Total	C	N	O	P	0
			35	26	1	7	1	
4	A	1	Total	C	N	O	P	0
			35	26	1	7	1	

- Molecule 5 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $\text{C}_{24}\text{H}_{46}\text{O}_{11}$).



Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	C	O	0
			35	24	11	
5	A	1	Total	C	O	0
			13	12	1	
5	A	1	Total	C	O	0
			24	18	6	
5	A	1	Total	C	O	0
			35	24	11	
5	A	1	Total	C	O	0
			35	24	11	
5	A	1	Total	C	O	0
			35	24	11	
5	A	1	Total	C	O	0
			35	24	11	
5	A	1	Total	C	O	0
			35	24	11	
5	A	1	Total	C	O	0
			24	18	6	
5	A	1	Total	C	O	0
			24	18	6	
5	A	1	Total	C	O	1
			70	48	22	
5	A	1	Total	C	O	0
			13	12	1	

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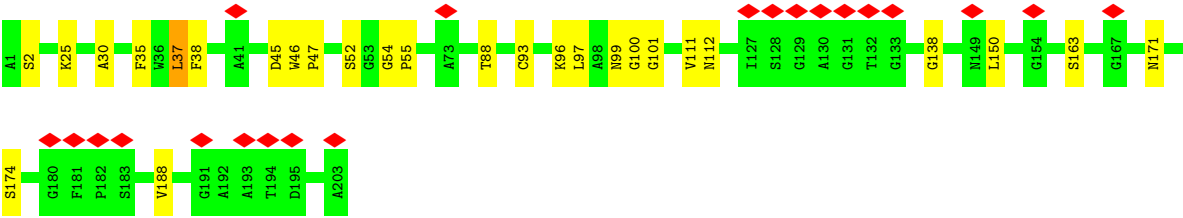
Mol	Chain	Residues	Atoms	AltConf
5	A	1	Total C O 13 12 1	0
5	A	1	Total C O 24 18 6	0
5	A	1	Total C 10 10	0

- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	AltConf
7	A	22	Total O 22 22	0
7	C	5	Total O 5 5	0



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	295580	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; Patch CTF	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	7.629	Depositor
Minimum map value	-4.508	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.075	Depositor
Recommended contour level	0.97	Depositor
Map size (Å)	324.096, 324.096, 324.096	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.84400004, 0.84400004, 0.84400004	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: LMT, ZGS, NA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.21	0/3674	0.37	0/5030
2	B	0.13	0/1460	0.37	0/1991
3	C	0.13	0/1483	0.34	0/2021
All	All	0.18	0/6617	0.36	0/9042

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3577	0	3468	56	0
2	B	1423	0	1337	21	0
3	C	1443	0	1384	18	0
4	A	105	0	0	7	0
5	A	495	0	694	13	0
6	A	1	0	0	0	0
7	A	22	0	0	0	0
7	C	5	0	0	0	0
All	All	7071	0	6883	96	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 7.

All (96) 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:295:VAL:HG23	1:A:424:PHE:HE1	1.46	0.81
1:A:291:TYR:HE1	1:A:410:PHE:HB2	1.50	0.77
1:A:296:MET:HB3	1:A:485:ILE:HD13	1.70	0.72
2:B:87:LEU:HD11	2:B:94:PHE:HB3	1.73	0.69
1:A:295:VAL:HG23	1:A:424:PHE:CE1	2.26	0.69
1:A:291:TYR:CE1	1:A:410:PHE:HB2	2.28	0.68
1:A:296:MET:HB2	1:A:485:ILE:HG21	1.74	0.68
1:A:73:PRO:HB2	1:A:448:ASP:HB2	1.75	0.68
1:A:429:VAL:HG13	1:A:433:LYS:NZ	2.12	0.64
2:B:174:ILE:HG23	2:B:178:ASP:HB3	1.78	0.64
1:A:308:LEU:O	1:A:312:PHE:HB2	1.98	0.63
3:C:38:PHE:HB3	3:C:45:ASP:HB2	1.82	0.62
3:C:138:GLY:HA2	3:C:174:SER:O	1.99	0.61
2:B:56:VAL:HG12	2:B:57:ALA:N	2.15	0.61
1:A:433:LYS:HA	4:A:601:ZGS:C32	2.31	0.61
2:B:110:GLN:HB3	2:B:133:PRO:HD2	1.83	0.60
1:A:295:VAL:CG2	1:A:424:PHE:CE1	2.85	0.60
3:C:96:LYS:HD2	3:C:101:GLY:HA2	1.83	0.60
1:A:290:PRO:HG3	1:A:490:PRO:HG2	1.83	0.59
1:A:67:ASP:HB3	1:A:455:ARG:HH11	1.67	0.58
2:B:109:PRO:HA	2:B:135:TRP:HB3	1.85	0.58
2:B:81:LEU:HD13	2:B:103:PRO:HG3	1.85	0.58
1:A:185:VAL:HG13	4:A:602:ZGS:C03	2.34	0.58
1:A:53:THR:OG1	1:A:152:GLN:NE2	2.30	0.56
1:A:103:TRP:HE3	1:A:108[B]:ARG:HG3	1.71	0.56
1:A:181:MET:HG2	4:A:602:ZGS:C17	2.36	0.56
3:C:35:PHE:HD2	3:C:46:TRP:HE1	1.54	0.55
1:A:331:LEU:HD21	5:A:604:LMT:H72	1.89	0.55
3:C:88:THR:HG23	3:C:112:ASN:HA	1.90	0.54
1:A:37:VAL:HG21	5:A:611:LMT:H6D	1.89	0.54
1:A:429:VAL:HG13	1:A:433:LYS:HZ2	1.72	0.54
3:C:37:LEU:HA	3:C:47:PRO:HD2	1.90	0.54
1:A:197:GLN:NE2	5:A:604:LMT:O6'	2.41	0.53
1:A:307:LEU:HD13	1:A:439:SER:HB3	1.90	0.53
1:A:159:TYR:OH	1:A:180:ARG:HD3	2.11	0.51
1:A:181:MET:HE2	4:A:602:ZGS:C16	2.40	0.51
1:A:77:SER:HB3	1:A:444:THR:HB	1.91	0.51
2:B:188:ALA:O	2:B:195:PRO:HA	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:ILE:HD12	5:A:610:LMT:H102	1.93	0.51
1:A:365:VAL:HG13	1:A:476:ILE:HD13	1.93	0.51
1:A:245:GLY:HA3	5:A:616[A]:LMT:H81	1.92	0.50
1:A:189:LEU:HD22	1:A:338:THR:HG21	1.93	0.50
2:B:13:ALA:N	2:B:102:ASN:O	2.35	0.50
2:B:49:TRP:H	2:B:89:PHE:HZ	1.60	0.50
1:A:344:TRP:CE2	1:A:394:ALA:HB2	2.47	0.50
2:B:85:TRP:HD1	2:B:96:PHE:HB3	1.76	0.50
1:A:210:GLU:OE2	3:C:35:PHE:HZ	1.95	0.50
2:B:56:VAL:CG1	2:B:57:ALA:N	2.74	0.49
3:C:35:PHE:O	3:C:93:CYS:HA	2.13	0.49
1:A:324:ASN:O	1:A:327:GLN:NE2	2.41	0.48
3:C:97:LEU:HD23	3:C:100:GLY:H	1.78	0.48
2:B:132:LEU:HD23	2:B:139:ILE:HD13	1.95	0.48
1:A:433:LYS:HG2	4:A:601:ZGS:C30	2.44	0.47
1:A:198:ILE:HD11	5:A:606:LMT:H52	1.95	0.47
1:A:189:LEU:HB2	4:A:602:ZGS:C01	2.45	0.47
1:A:439:SER:HA	5:A:609:LMT:H102	1.97	0.47
1:A:308:LEU:HD11	1:A:368:LEU:HD11	1.97	0.46
1:A:80:LEU:HD13	1:A:440:LEU:HG	1.98	0.46
5:A:608:LMT:H4B	3:C:97:LEU:HD13	1.97	0.46
1:A:452:TYR:O	3:C:99:ASN:ND2	2.35	0.46
1:A:334:MET:HB3	4:A:602:ZGS:C01	2.46	0.45
1:A:400:TRP:HH2	1:A:425:TYR:CE1	2.35	0.45
3:C:2:SER:HA	3:C:25:LYS:O	2.17	0.45
3:C:163:SER:HA	3:C:171:ASN:O	2.17	0.45
3:C:150:LEU:HG	3:C:188:VAL:HG12	1.98	0.44
1:A:115:LEU:HD12	5:A:613:LMT:H72	1.99	0.44
1:A:67:ASP:OD1	1:A:452:TYR:OH	2.34	0.44
2:B:116:PRO:HD3	2:B:128:VAL:HG22	1.98	0.44
1:A:469:ILE:HG23	1:A:473:ALA:HB3	1.99	0.43
2:B:47:THR:HG21	2:B:62:ALA:HB3	2.00	0.43
1:A:87:ASP:HB2	1:A:149:GLN:NE2	2.33	0.43
2:B:126:ALA:HB3	2:B:174:ILE:O	2.18	0.43
2:B:85:TRP:CD1	2:B:96:PHE:HB3	2.52	0.43
3:C:35:PHE:CE1	3:C:96:LYS:HB2	2.53	0.43
1:A:72:ASP:OD2	1:A:74:PHE:HB3	2.17	0.43
1:A:292:ALA:O	1:A:296:MET:HG2	2.18	0.43
5:A:609:LMT:H1B	5:A:609:LMT:H3'	1.79	0.43
1:A:197:GLN:HB2	5:A:605:LMT:H61	2.00	0.42
3:C:30:ALA:HA	3:C:52:SER:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:GLY:HA2	1:A:157:VAL:HG11	2.01	0.42
1:A:304:ALA:HB2	1:A:478:LEU:HB2	2.00	0.42
2:B:135:TRP:HZ2	2:B:168:MET:HB2	1.84	0.42
3:C:88:THR:HA	3:C:111:VAL:O	2.20	0.42
5:A:608:LMT:H1B	5:A:608:LMT:H3'	1.88	0.42
1:A:364:VAL:HG22	1:A:368:LEU:HG	2.02	0.42
2:B:36:ASN:HB2	2:B:46:LEU:HD11	2.00	0.42
1:A:183:VAL:O	1:A:186:LEU:N	2.52	0.41
1:A:357:VAL:HG12	1:A:398:LEU:HB3	2.02	0.41
3:C:54:GLY:HA3	3:C:55:PRO:HD3	1.79	0.41
1:A:393:ALA:O	1:A:397:LEU:HB3	2.20	0.41
2:B:46:LEU:HA	2:B:56:VAL:HG21	2.03	0.41
1:A:57:ILE:HG23	1:A:61:LEU:HD22	2.02	0.41
2:B:30:SER:HA	2:B:69:PHE:CE2	2.56	0.41
2:B:132:LEU:O	2:B:167:ALA:HA	2.20	0.41
1:A:183:VAL:O	1:A:184:GLU:C	2.63	0.40
5:A:605:LMT:H122	5:A:605:LMT:H91	1.80	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	478/508 (94%)	465 (97%)	13 (3%)	0	100	100
2	B	199/201 (99%)	183 (92%)	16 (8%)	0	100	100
3	C	202/203 (100%)	187 (93%)	15 (7%)	0	100	100
All	All	879/912 (96%)	835 (95%)	44 (5%)	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	359/436 (82%)	358 (100%)	1 (0%)	86	96
2	B	134/144 (93%)	131 (98%)	3 (2%)	45	77
3	C	133/138 (96%)	132 (99%)	1 (1%)	73	90
All	All	626/718 (87%)	621 (99%)	5 (1%)	70	90

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	406	VAL
2	B	67	THR
2	B	88	LEU
2	B	174	ILE
3	C	37	LEU

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

Mol	Chain	Res	Type
1	A	156	HIS
1	A	197	GLN
1	A	234	GLN
1	A	414	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 1 is monoatomic - leaving 21 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
5	LMT	A	604	-	36,36,36	1.28	4 (11%)	47,47,47	0.98	1 (2%)
4	ZGS	A	603	-	34,34,34	1.06	3 (8%)	39,41,41	1.53	7 (17%)
5	LMT	A	607	-	36,36,36	1.28	4 (11%)	47,47,47	0.93	1 (2%)
5	LMT	A	620	-	9,9,36	0.94	0	8,8,47	0.81	0
5	LMT	A	616[A]	-	36,36,36	1.31	4 (11%)	47,47,47	1.31	5 (10%)
5	LMT	A	610	-	36,36,36	1.27	4 (11%)	47,47,47	1.18	4 (8%)
5	LMT	A	615	-	24,24,36	1.26	2 (8%)	29,29,47	1.41	3 (10%)
5	LMT	A	612	-	36,36,36	1.29	4 (11%)	47,47,47	1.08	4 (8%)
5	LMT	A	618	-	12,12,36	0.89	0	11,11,47	0.84	0
4	ZGS	A	602	6	34,34,34	1.03	4 (11%)	39,41,41	1.94	13 (33%)
4	ZGS	A	601	-	34,34,34	1.13	4 (11%)	39,41,41	2.19	11 (28%)
5	LMT	A	605	-	12,12,36	0.88	0	11,11,47	0.85	0
5	LMT	A	619	-	24,24,36	1.24	2 (8%)	29,29,47	0.85	0
5	LMT	A	614	-	24,24,36	1.23	2 (8%)	29,29,47	0.81	0
5	LMT	A	613	-	36,36,36	1.28	4 (11%)	47,47,47	1.08	3 (6%)
5	LMT	A	609	-	36,36,36	1.29	4 (11%)	47,47,47	0.93	1 (2%)
5	LMT	A	611	-	36,36,36	1.27	4 (11%)	47,47,47	1.34	4 (8%)
5	LMT	A	617	-	12,12,36	0.89	0	11,11,47	0.83	0
5	LMT	A	608	-	36,36,36	1.29	3 (8%)	47,47,47	1.05	2 (4%)
5	LMT	A	606	-	24,24,36	1.25	2 (8%)	29,29,47	0.83	0
5	LMT	A	616[B]	-	36,36,36	1.30	4 (11%)	47,47,47	1.37	6 (12%)

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
5	LMT	A	604	-	-	11/21/61/61	0/2/2/2
4	ZGS	A	603	-	-	12/36/36/36	-
5	LMT	A	607	-	-	9/21/61/61	0/2/2/2
5	LMT	A	620	-	-	4/7/7/61	-
5	LMT	A	616[A]	-	-	7/21/61/61	0/2/2/2
5	LMT	A	610	-	-	7/21/61/61	0/2/2/2
5	LMT	A	615	-	-	8/15/35/61	0/1/1/2
5	LMT	A	612	-	-	10/21/61/61	0/2/2/2
5	LMT	A	618	-	-	5/10/10/61	-
4	ZGS	A	602	6	-	22/36/36/36	-
4	ZGS	A	601	-	-	20/36/36/36	-
5	LMT	A	605	-	-	5/10/10/61	-
5	LMT	A	619	-	-	9/15/35/61	0/1/1/2
5	LMT	A	614	-	-	9/15/35/61	0/1/1/2
5	LMT	A	613	-	-	11/21/61/61	0/2/2/2
5	LMT	A	609	-	-	15/21/61/61	0/2/2/2
5	LMT	A	611	-	-	10/21/61/61	0/2/2/2
5	LMT	A	617	-	-	6/10/10/61	-
5	LMT	A	608	-	-	7/21/61/61	0/2/2/2
5	LMT	A	606	-	-	6/15/35/61	0/1/1/2
5	LMT	A	616[B]	-	-	11/21/61/61	0/2/2/2

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	608	LMT	O5'-C1'	4.25	1.52	1.41
5	A	616[B]	LMT	O5'-C1'	4.13	1.52	1.41
5	A	609	LMT	O5'-C1'	4.11	1.52	1.41
5	A	612	LMT	O5'-C1'	4.09	1.52	1.41
5	A	606	LMT	O5'-C1'	4.08	1.52	1.41
5	A	604	LMT	O5'-C1'	4.08	1.52	1.41
5	A	619	LMT	O5'-C1'	4.07	1.52	1.41
5	A	613	LMT	O5'-C1'	4.06	1.52	1.41
5	A	615	LMT	O5'-C1'	4.00	1.52	1.41
5	A	611	LMT	O5B-C1B	3.95	1.52	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	614	LMT	O5'-C1'	3.95	1.52	1.41
5	A	607	LMT	O5'-C1'	3.92	1.51	1.41
5	A	616[A]	LMT	O5'-C1'	3.90	1.51	1.41
5	A	616[B]	LMT	O5B-C1B	3.87	1.51	1.41
5	A	609	LMT	O5B-C1B	3.86	1.51	1.41
5	A	610	LMT	O5'-C1'	3.83	1.51	1.41
5	A	612	LMT	O5B-C1B	3.83	1.51	1.41
5	A	611	LMT	O5'-C1'	3.83	1.51	1.41
5	A	616[A]	LMT	O5B-C1B	3.82	1.51	1.41
5	A	607	LMT	O5B-C1B	3.80	1.51	1.41
5	A	610	LMT	O5B-C1B	3.77	1.51	1.41
5	A	604	LMT	O5B-C1B	3.76	1.51	1.41
5	A	608	LMT	O5B-C1B	3.76	1.51	1.41
5	A	613	LMT	O5B-C1B	3.63	1.51	1.41
4	A	601	ZGS	O20-C18	3.12	1.42	1.33
4	A	603	ZGS	O20-C18	2.78	1.41	1.33
5	A	616[A]	LMT	O5B-C5B	2.71	1.51	1.44
5	A	616[B]	LMT	O5B-C5B	2.54	1.50	1.44
4	A	602	ZGS	O20-C21	-2.39	1.39	1.45
5	A	613	LMT	O5B-C5B	2.37	1.50	1.44
5	A	607	LMT	O5B-C5B	2.33	1.50	1.44
5	A	608	LMT	O5B-C5B	2.32	1.50	1.44
5	A	604	LMT	O5B-C5B	2.32	1.50	1.44
4	A	603	ZGS	P25-O28	2.31	1.68	1.59
5	A	609	LMT	O5B-C5B	2.31	1.50	1.44
5	A	611	LMT	O5B-C5B	2.31	1.50	1.44
5	A	612	LMT	O5B-C5B	2.29	1.50	1.44
4	A	602	ZGS	P25-O24	2.25	1.68	1.59
5	A	610	LMT	O5B-C5B	2.23	1.49	1.44
5	A	616[A]	LMT	O1'-C1'	-2.21	1.36	1.40
4	A	602	ZGS	C23-C22	2.21	1.58	1.51
5	A	613	LMT	O1'-C1'	-2.15	1.36	1.40
5	A	614	LMT	O1'-C1'	-2.15	1.36	1.40
5	A	612	LMT	O1'-C1'	-2.14	1.36	1.40
5	A	619	LMT	O1'-C1'	-2.14	1.36	1.40
5	A	607	LMT	O1'-C1'	-2.14	1.36	1.40
4	A	601	ZGS	P25-O24	2.13	1.67	1.59
5	A	615	LMT	O1'-C1'	-2.12	1.36	1.40
5	A	616[B]	LMT	O1'-C1'	-2.11	1.36	1.40
5	A	610	LMT	O1'-C1'	-2.11	1.36	1.40
4	A	602	ZGS	O20-C18	2.10	1.39	1.33
5	A	606	LMT	O1'-C1'	-2.09	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	611	LMT	O1'-C1'	-2.09	1.36	1.40
4	A	603	ZGS	C30-C29	2.07	1.57	1.51
5	A	604	LMT	O1'-C1'	-2.06	1.36	1.40
4	A	601	ZGS	C30-C29	2.03	1.57	1.51
5	A	609	LMT	O1'-C1'	-2.02	1.36	1.40
4	A	601	ZGS	P25-O26	-2.01	1.43	1.50

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	601	ZGS	O28-P25-O26	-6.74	82.22	108.94
4	A	601	ZGS	C06-C05-C04	5.16	137.41	112.02
5	A	616[A]	LMT	O5B-C5B-C4B	4.87	118.48	109.70
4	A	602	ZGS	C06-C05-C04	4.24	132.91	112.02
5	A	611	LMT	C2'-C3'-C4'	4.19	119.19	109.68
4	A	601	ZGS	C08-C07-C06	4.08	157.97	123.57
4	A	603	ZGS	C06-C05-C04	4.06	132.03	112.02
5	A	611	LMT	C1'-C2'-C3'	4.00	118.44	110.01
4	A	601	ZGS	C11-C10-C09	3.92	154.21	124.83
5	A	615	LMT	O5'-C5'-C4'	3.91	116.75	109.70
5	A	615	LMT	C3'-C4'-C5'	3.80	117.13	110.23
4	A	603	ZGS	C11-C10-C09	3.64	152.08	124.83
4	A	603	ZGS	C08-C07-C06	3.48	152.93	123.57
5	A	616[B]	LMT	C1B-O1B-C4'	-3.47	109.75	117.98
5	A	616[B]	LMT	O5B-C5B-C4B	3.43	115.89	109.70
4	A	603	ZGS	C05-C04-C03	3.43	152.52	123.57
4	A	601	ZGS	C34-N31-C32	3.35	117.78	108.98
5	A	616[B]	LMT	C4B-C3B-C2B	3.34	116.69	110.83
4	A	602	ZGS	C08-C07-C06	3.30	151.43	123.57
5	A	613	LMT	C1B-O1B-C4'	-3.27	110.23	117.98
5	A	616[A]	LMT	C3B-C4B-C5B	3.21	116.06	110.23
4	A	602	ZGS	C15-C16-C17	-3.20	101.36	113.13
5	A	610	LMT	C1B-O1B-C4'	-3.19	110.43	117.98
5	A	604	LMT	C1B-O1B-C4'	-3.15	110.51	117.98
4	A	602	ZGS	C11-C10-C09	3.15	148.41	124.83
5	A	612	LMT	C1B-O1B-C4'	-3.11	110.60	117.98
4	A	602	ZGS	O35-C22-C23	3.08	120.34	109.70
4	A	602	ZGS	C16-C17-C18	-3.06	102.47	113.69
5	A	615	LMT	C4'-C3'-C2'	3.06	116.20	110.83
5	A	610	LMT	O5'-C5'-C4'	3.02	115.97	109.72
4	A	601	ZGS	C05-C04-C03	3.02	149.02	123.57
4	A	601	ZGS	C33-N31-C32	-3.01	101.06	108.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	613	LMT	C3B-C4B-C5B	2.91	115.51	110.23
5	A	616[B]	LMT	C3B-C4B-C5B	2.90	115.49	110.23
5	A	609	LMT	C1B-O1B-C4'	-2.78	111.38	117.98
5	A	607	LMT	C1B-O1B-C4'	-2.78	111.39	117.98
5	A	616[A]	LMT	C1B-O1B-C4'	-2.78	111.39	117.98
4	A	602	ZGS	C05-C04-C03	2.75	146.80	123.57
4	A	601	ZGS	O20-C18-C17	2.75	120.22	111.83
5	A	612	LMT	C2'-C3'-C4'	2.74	115.91	109.68
4	A	602	ZGS	C23-C22-C21	-2.74	104.77	112.65
5	A	610	LMT	C3'-C4'-C5'	2.73	116.97	110.93
5	A	610	LMT	C2'-C3'-C4'	2.72	115.86	109.68
5	A	608	LMT	C2'-C3'-C4'	2.69	115.78	109.68
5	A	616[A]	LMT	C1B-O5B-C5B	2.67	118.92	113.72
5	A	616[B]	LMT	C1B-C2B-C3B	2.53	115.33	110.01
4	A	602	ZGS	C02-C03-C04	-2.48	111.48	126.42
4	A	601	ZGS	C29-C30-N31	-2.41	108.09	115.82
4	A	603	ZGS	C29-C30-N31	-2.38	108.17	115.82
5	A	611	LMT	O1B-C4'-C3'	2.35	113.21	107.23
4	A	602	ZGS	C05-C06-C07	-2.34	103.79	123.57
4	A	603	ZGS	C02-C03-C04	-2.34	112.36	126.42
5	A	613	LMT	O5B-C5B-C4B	2.34	113.91	109.70
4	A	603	ZGS	O20-C18-C17	2.32	118.90	111.83
5	A	608	LMT	C1'-C2'-C3'	2.29	114.83	110.01
5	A	611	LMT	C1'-O5'-C5'	-2.24	109.34	113.72
5	A	616[A]	LMT	C6B-C5B-C4B	-2.21	107.58	113.02
4	A	601	ZGS	C05-C06-C07	-2.20	104.97	123.57
4	A	602	ZGS	P25-O24-C23	-2.19	108.77	121.35
4	A	602	ZGS	C09-C08-C07	-2.17	101.35	112.02
5	A	616[B]	LMT	C2'-C3'-C4'	2.15	114.56	109.68
4	A	602	ZGS	C34-N31-C33	2.12	114.55	108.98
5	A	612	LMT	O5'-C1'-C2'	2.10	114.69	110.37
4	A	601	ZGS	O27-P25-O28	2.03	116.75	107.57
5	A	612	LMT	C1'-C2'-C3'	2.01	114.23	110.01

There are no chirality outliers.

All (204) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	602	ZGS	C22-C23-O24-P25
4	A	602	ZGS	O28-C29-C30-N31
4	A	602	ZGS	C23-O24-P25-O26
4	A	602	ZGS	C23-O24-P25-O27

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Mol	Chain	Res	Type	Atoms
4	A	602	ZGS	C23-O24-P25-O28
4	A	602	ZGS	C29-O28-P25-O24
4	A	602	ZGS	C29-O28-P25-O26
4	A	602	ZGS	C29-O28-P25-O27
4	A	603	ZGS	C17-C18-O20-C21
4	A	603	ZGS	O19-C18-O20-C21
4	A	603	ZGS	C30-C29-O28-P25
4	A	603	ZGS	C23-O24-P25-O26
4	A	603	ZGS	C23-O24-P25-O27
4	A	603	ZGS	C23-O24-P25-O28
5	A	604	LMT	C2'-C1'-O1'-C1
5	A	604	LMT	O5'-C1'-O1'-C1
5	A	608	LMT	O5'-C1'-O1'-C1
5	A	609	LMT	O5'-C1'-O1'-C1
5	A	613	LMT	C2'-C1'-O1'-C1
5	A	613	LMT	O5'-C1'-O1'-C1
5	A	612	LMT	O5B-C1B-O1B-C4'
5	A	615	LMT	O5'-C5'-C6'-O6'
5	A	611	LMT	C3'-C4'-O1B-C1B
5	A	612	LMT	O5'-C5'-C6'-O6'
5	A	616[A]	LMT	O5'-C5'-C6'-O6'
5	A	608	LMT	C3'-C4'-O1B-C1B
5	A	613	LMT	O5'-C5'-C6'-O6'
4	A	601	ZGS	O35-C22-C23-O24
4	A	601	ZGS	C17-C18-O20-C21
4	A	601	ZGS	O19-C18-O20-C21
5	A	615	LMT	C4'-C5'-C6'-O6'
5	A	607	LMT	O5B-C5B-C6B-O6B
5	A	619	LMT	O5'-C5'-C6'-O6'
5	A	612	LMT	O5B-C5B-C6B-O6B
5	A	613	LMT	C4'-C5'-C6'-O6'
5	A	616[A]	LMT	C4'-C5'-C6'-O6'
5	A	616[A]	LMT	O5B-C5B-C6B-O6B
5	A	612	LMT	C4'-C5'-C6'-O6'
5	A	610	LMT	O5'-C1'-O1'-C1
5	A	615	LMT	O5'-C1'-O1'-C1
5	A	619	LMT	O5'-C1'-O1'-C1
4	A	601	ZGS	C21-C22-C23-O24
5	A	606	LMT	O5'-C5'-C6'-O6'
4	A	601	ZGS	C29-C30-N31-C32
5	A	614	LMT	C4'-C5'-C6'-O6'
5	A	610	LMT	C2'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
5	A	615	LMT	C2'-C1'-O1'-C1
5	A	619	LMT	C2'-C1'-O1'-C1
4	A	602	ZGS	O35-C22-C23-O24
5	A	609	LMT	C4B-C5B-C6B-O6B
4	A	602	ZGS	C17-C18-O20-C21
5	A	616[B]	LMT	O5'-C5'-C6'-O6'
5	A	604	LMT	O5'-C5'-C6'-O6'
5	A	616[B]	LMT	O5B-C5B-C6B-O6B
4	A	601	ZGS	C15-C16-C17-C18
5	A	610	LMT	O5'-C5'-C6'-O6'
5	A	604	LMT	C4'-C5'-C6'-O6'
5	A	614	LMT	O5'-C5'-C6'-O6'
5	A	616[B]	LMT	O1'-C1-C2-C3
5	A	607	LMT	C4'-C5'-C6'-O6'
5	A	612	LMT	C4B-C5B-C6B-O6B
4	A	602	ZGS	O19-C18-O20-C21
5	A	607	LMT	C4B-C5B-C6B-O6B
5	A	619	LMT	C4'-C5'-C6'-O6'
4	A	602	ZGS	C21-C22-C23-O24
5	A	608	LMT	O1'-C1-C2-C3
5	A	609	LMT	O5B-C5B-C6B-O6B
5	A	614	LMT	O5'-C1'-O1'-C1
5	A	608	LMT	C2-C1-O1'-C1'
5	A	616[A]	LMT	C2-C3-C4-C5
5	A	605	LMT	C3-C4-C5-C6
5	A	611	LMT	C3-C4-C5-C6
5	A	619	LMT	O1'-C1-C2-C3
5	A	615	LMT	C11-C10-C9-C8
4	A	601	ZGS	C11-C12-C13-C14
5	A	615	LMT	C2-C3-C4-C5
5	A	607	LMT	C2-C3-C4-C5
5	A	609	LMT	C3'-C4'-O1B-C1B
5	A	617	LMT	C1-C2-C3-C4
5	A	617	LMT	C2-C3-C4-C5
5	A	609	LMT	C5'-C4'-O1B-C1B
5	A	607	LMT	O5'-C5'-C6'-O6'
5	A	614	LMT	O1'-C1-C2-C3
5	A	609	LMT	C11-C10-C9-C8
5	A	619	LMT	C3-C4-C5-C6
5	A	609	LMT	C3-C4-C5-C6
5	A	612	LMT	C3-C4-C5-C6
5	A	611	LMT	C5'-C4'-O1B-C1B

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Mol	Chain	Res	Type	Atoms
5	A	604	LMT	O5B-C5B-C6B-O6B
5	A	611	LMT	O5B-C1B-O1B-C4'
5	A	608	LMT	C6-C7-C8-C9
5	A	609	LMT	C4-C5-C6-C7
4	A	602	ZGS	C10-C11-C12-C13
5	A	610	LMT	C4B-C5B-C6B-O6B
5	A	607	LMT	C5-C6-C7-C8
5	A	609	LMT	C2-C3-C4-C5
5	A	609	LMT	C6-C7-C8-C9
4	A	602	ZGS	C13-C14-C15-C16
5	A	604	LMT	C5-C6-C7-C8
5	A	607	LMT	O1'-C1-C2-C3
5	A	616[B]	LMT	O5B-C1B-O1B-C4'
5	A	618	LMT	C3-C4-C5-C6
5	A	614	LMT	C3-C4-C5-C6
4	A	602	ZGS	C15-C16-C17-C18
5	A	615	LMT	C3-C4-C5-C6
4	A	601	ZGS	C14-C15-C16-C17
5	A	608	LMT	C7-C8-C9-C10
5	A	616[A]	LMT	C1-C2-C3-C4
5	A	612	LMT	C1-C2-C3-C4
4	A	603	ZGS	C10-C11-C12-C13
5	A	607	LMT	C3-C4-C5-C6
5	A	610	LMT	O1'-C1-C2-C3
5	A	619	LMT	C5-C6-C7-C8
5	A	619	LMT	C6-C7-C8-C9
5	A	611	LMT	C6-C7-C8-C9
5	A	610	LMT	O5B-C5B-C6B-O6B
5	A	609	LMT	C5-C6-C7-C8
5	A	604	LMT	C2-C3-C4-C5
5	A	606	LMT	C4'-C5'-C6'-O6'
5	A	613	LMT	C3-C4-C5-C6
4	A	603	ZGS	C15-C16-C17-C18
5	A	620	LMT	C3-C4-C5-C6
4	A	601	ZGS	C12-C13-C14-C15
5	A	609	LMT	O1'-C1-C2-C3
5	A	617	LMT	C5-C6-C7-C8
5	A	616[B]	LMT	C4'-C5'-C6'-O6'
5	A	618	LMT	C11-C10-C9-C8
5	A	614	LMT	C6-C7-C8-C9
5	A	620	LMT	C5-C6-C7-C8
4	A	601	ZGS	C16-C17-C18-O20

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Mol	Chain	Res	Type	Atoms
4	A	601	ZGS	C03-C04-C05-C06
4	A	601	ZGS	C07-C08-C09-C10
4	A	602	ZGS	C03-C04-C05-C06
4	A	602	ZGS	C07-C08-C09-C10
4	A	603	ZGS	C06-C07-C08-C09
5	A	613	LMT	C5-C6-C7-C8
5	A	613	LMT	C11-C10-C9-C8
5	A	614	LMT	C1-C2-C3-C4
5	A	613	LMT	C9-C10-C11-C12
4	A	601	ZGS	C01-C02-C03-C04
5	A	606	LMT	C5-C6-C7-C8
5	A	612	LMT	C9-C10-C11-C12
5	A	614	LMT	C5-C6-C7-C8
5	A	616[B]	LMT	C6-C7-C8-C9
5	A	608	LMT	C5'-C4'-O1B-C1B
4	A	602	ZGS	C30-C29-O28-P25
5	A	618	LMT	C5-C6-C7-C8
5	A	611	LMT	C11-C10-C9-C8
5	A	620	LMT	C6-C7-C8-C9
4	A	601	ZGS	O28-C29-C30-N31
4	A	603	ZGS	O28-C29-C30-N31
5	A	616[A]	LMT	C5-C6-C7-C8
5	A	605	LMT	C2-C3-C4-C5
5	A	611	LMT	C2B-C1B-O1B-C4'
5	A	604	LMT	C3'-C4'-O1B-C1B
5	A	604	LMT	C9-C10-C11-C12
5	A	615	LMT	C6-C7-C8-C9
4	A	602	ZGS	O20-C21-C22-O35
5	A	611	LMT	O1'-C1-C2-C3
4	A	601	ZGS	C10-C11-C12-C13
4	A	602	ZGS	C29-C30-N31-C32
5	A	611	LMT	C9-C10-C11-C12
5	A	616[A]	LMT	C4B-C5B-C6B-O6B
4	A	601	ZGS	C22-C23-O24-P25
5	A	604	LMT	C5'-C4'-O1B-C1B
5	A	616[B]	LMT	C2B-C1B-O1B-C4'
4	A	602	ZGS	C29-C30-N31-C33
5	A	606	LMT	C3-C4-C5-C6
5	A	610	LMT	C3-C4-C5-C6
5	A	606	LMT	O5'-C1'-O1'-C1
5	A	618	LMT	O1'-C1-C2-C3
4	A	603	ZGS	C01-C02-C03-C04

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Mol	Chain	Res	Type	Atoms
5	A	613	LMT	C2-C1-O1'-C1'
5	A	609	LMT	O5B-C1B-O1B-C4'
4	A	601	ZGS	C09-C10-C11-C12
4	A	601	ZGS	C29-C30-N31-C33
5	A	616[B]	LMT	C1-C2-C3-C4
5	A	616[B]	LMT	C5-C6-C7-C8
5	A	619	LMT	C11-C10-C9-C8
5	A	613	LMT	C2-C3-C4-C5
5	A	617	LMT	O1'-C1-C2-C3
4	A	603	ZGS	C07-C08-C09-C10
5	A	613	LMT	O5B-C5B-C6B-O6B
5	A	605	LMT	C5-C6-C7-C8
4	A	601	ZGS	C16-C17-C18-O19
5	A	612	LMT	C5-C6-C7-C8
5	A	618	LMT	C6-C7-C8-C9
5	A	612	LMT	O1'-C1-C2-C3
5	A	617	LMT	C3-C4-C5-C6
5	A	611	LMT	C4'-C5'-C6'-O6'
5	A	616[B]	LMT	C11-C10-C9-C8
5	A	606	LMT	O1'-C1-C2-C3
5	A	604	LMT	C6-C7-C8-C9
4	A	602	ZGS	C29-C30-N31-C34
5	A	617	LMT	C6-C7-C8-C9
5	A	607	LMT	C9-C10-C11-C12
5	A	620	LMT	C9-C10-C11-C12
5	A	616[B]	LMT	C2-C3-C4-C5
5	A	614	LMT	C2-C3-C4-C5
5	A	605	LMT	C11-C10-C9-C8
4	A	601	ZGS	C29-C30-N31-C34
5	A	609	LMT	C7-C8-C9-C10
5	A	609	LMT	C2B-C1B-O1B-C4'
5	A	605	LMT	C9-C10-C11-C12

There are no ring outliers.

11 monomers are involved in 20 short contacts:

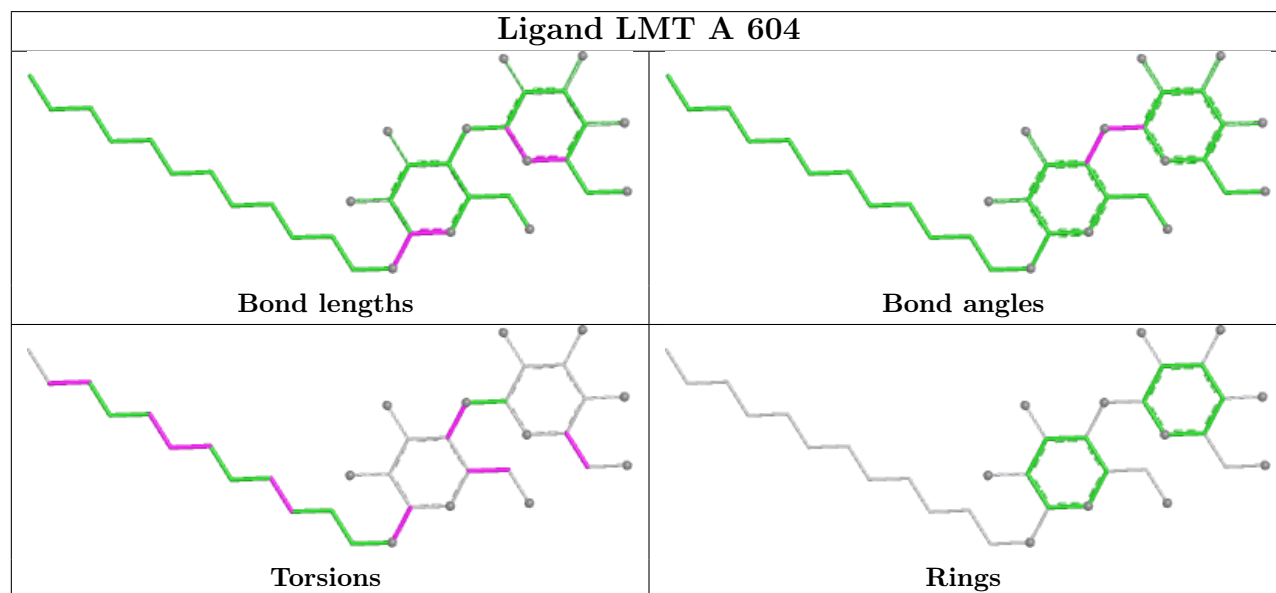
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	604	LMT	2	0
5	A	616[A]	LMT	1	0
5	A	610	LMT	1	0
4	A	602	ZGS	5	0
4	A	601	ZGS	2	0

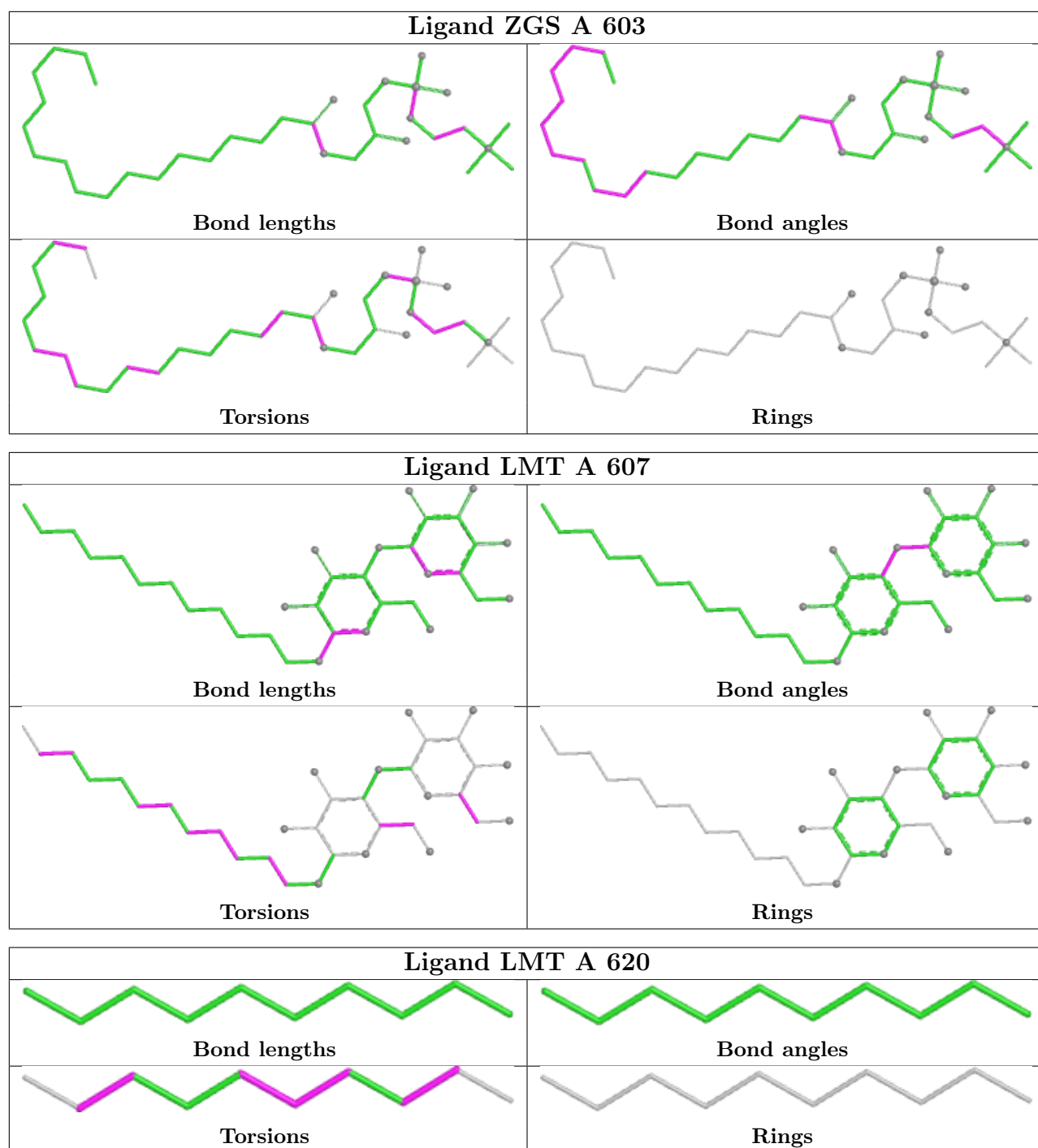
Continued on next page...

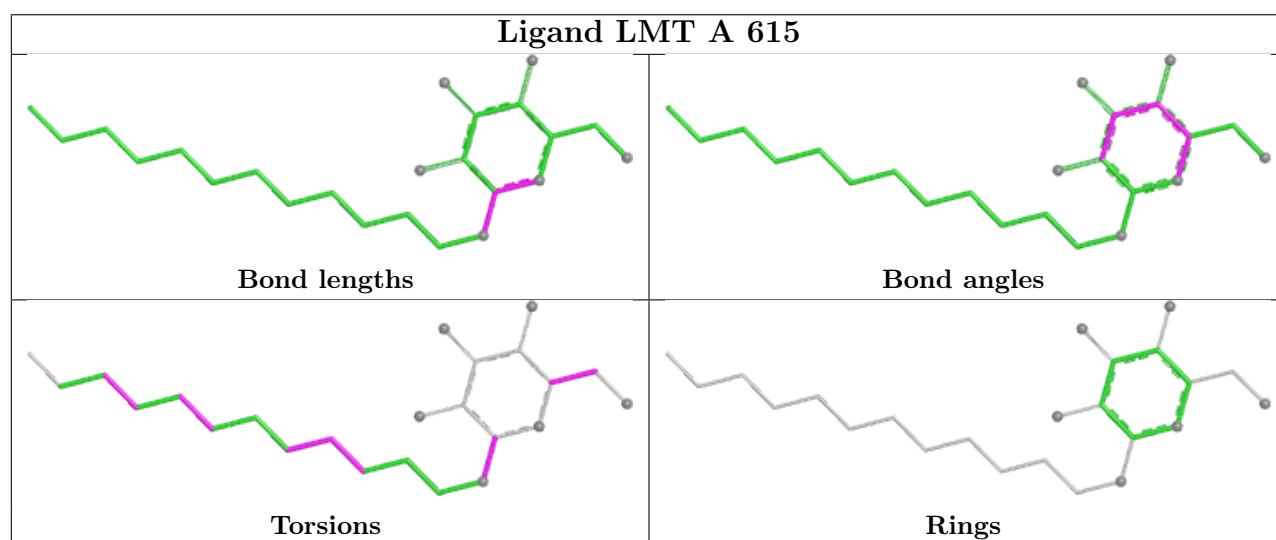
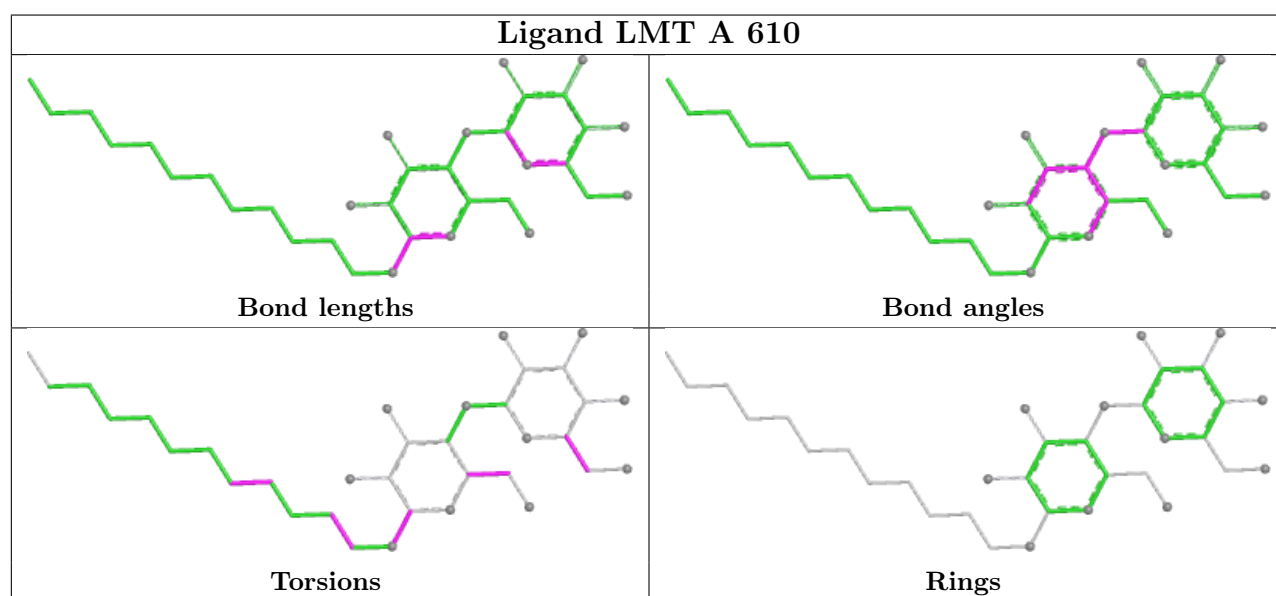
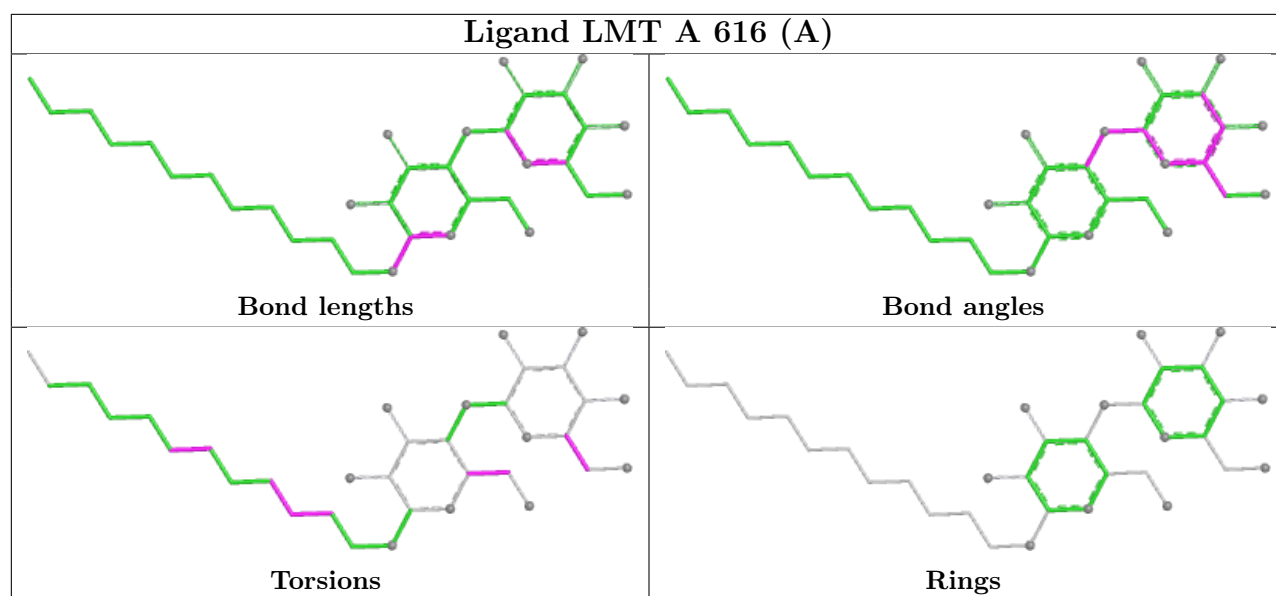
Continued from previous page...

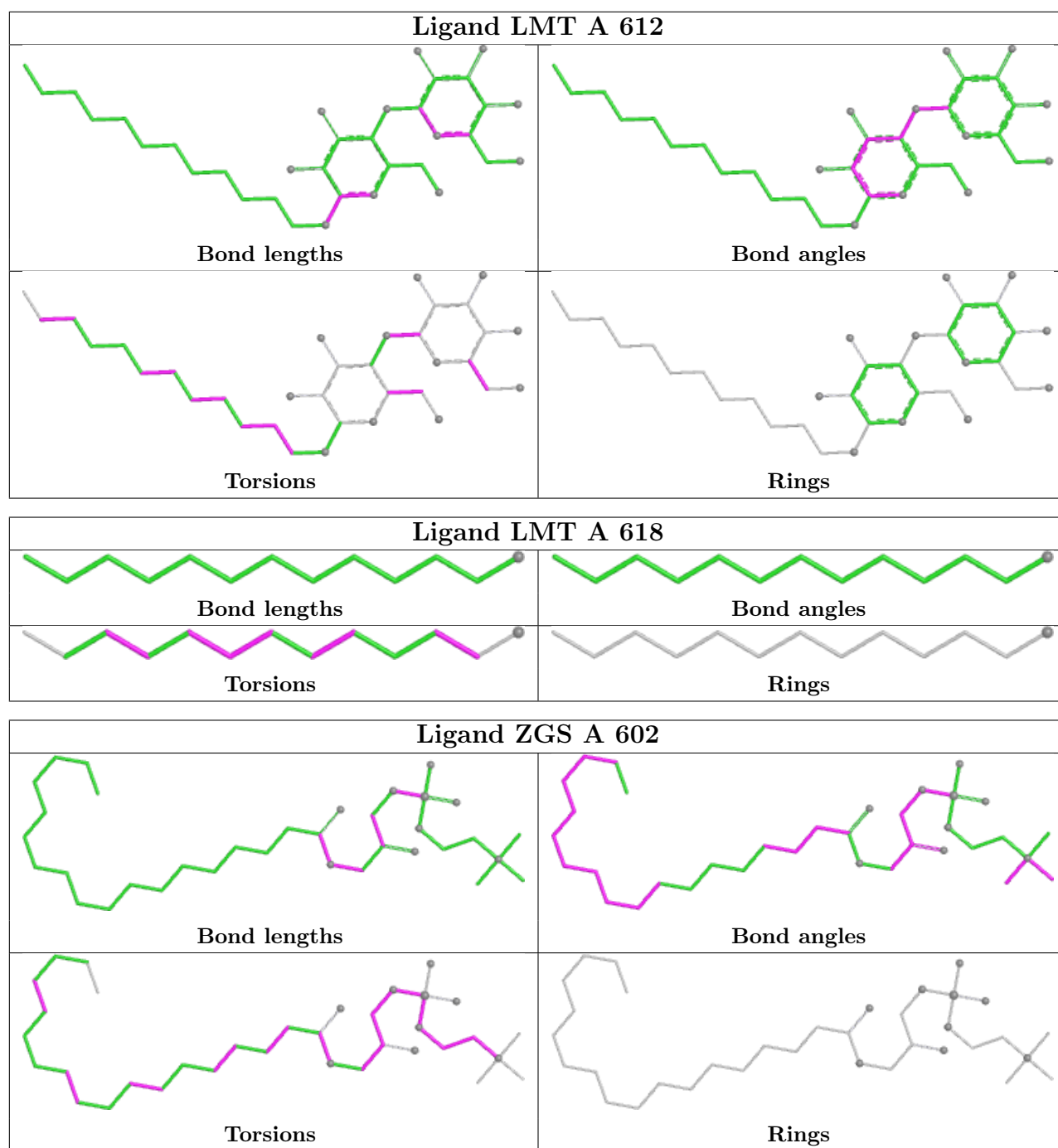
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	605	LMT	2	0
5	A	613	LMT	1	0
5	A	609	LMT	2	0
5	A	611	LMT	1	0
5	A	608	LMT	2	0
5	A	606	LMT	1	0

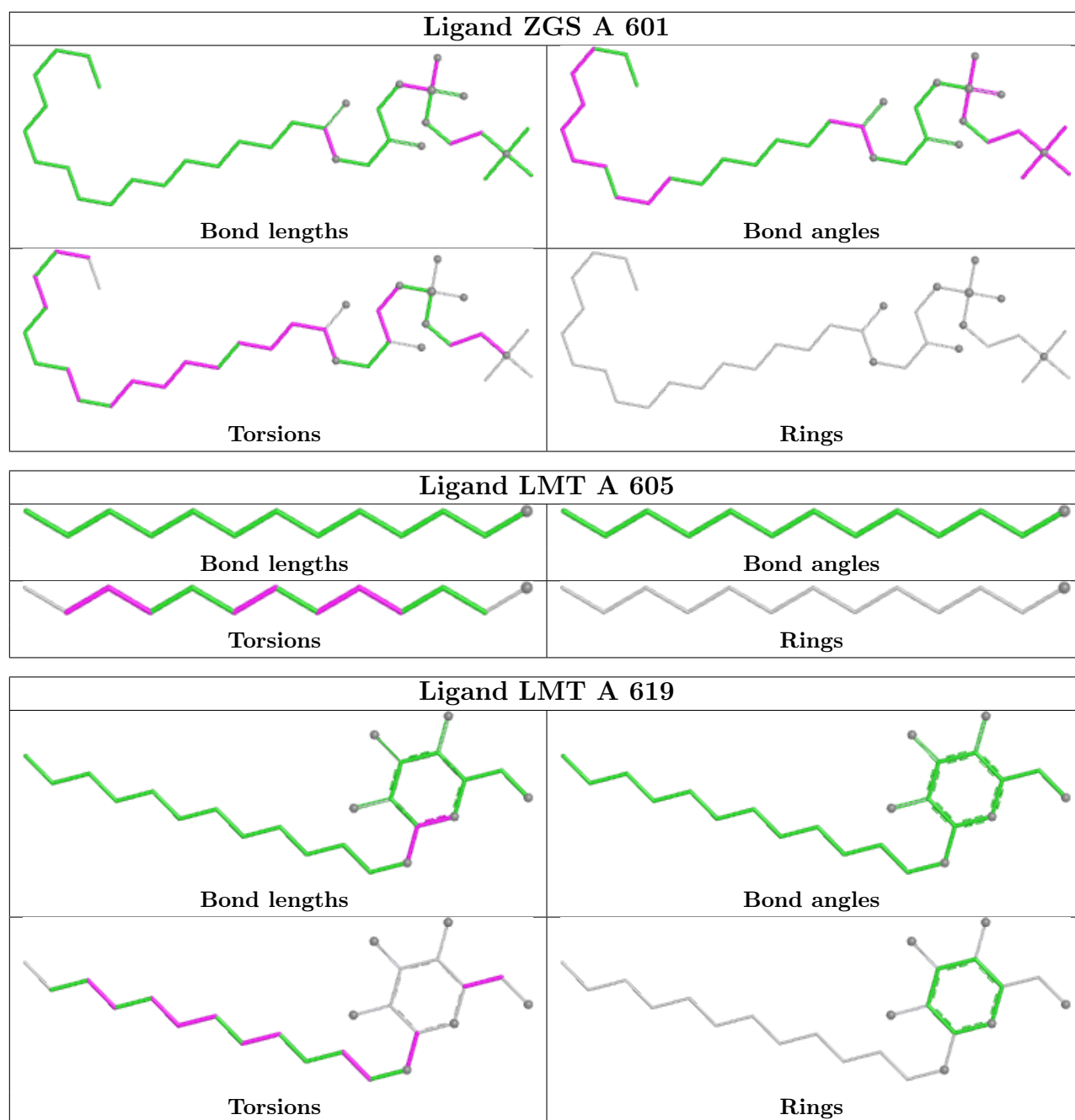
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

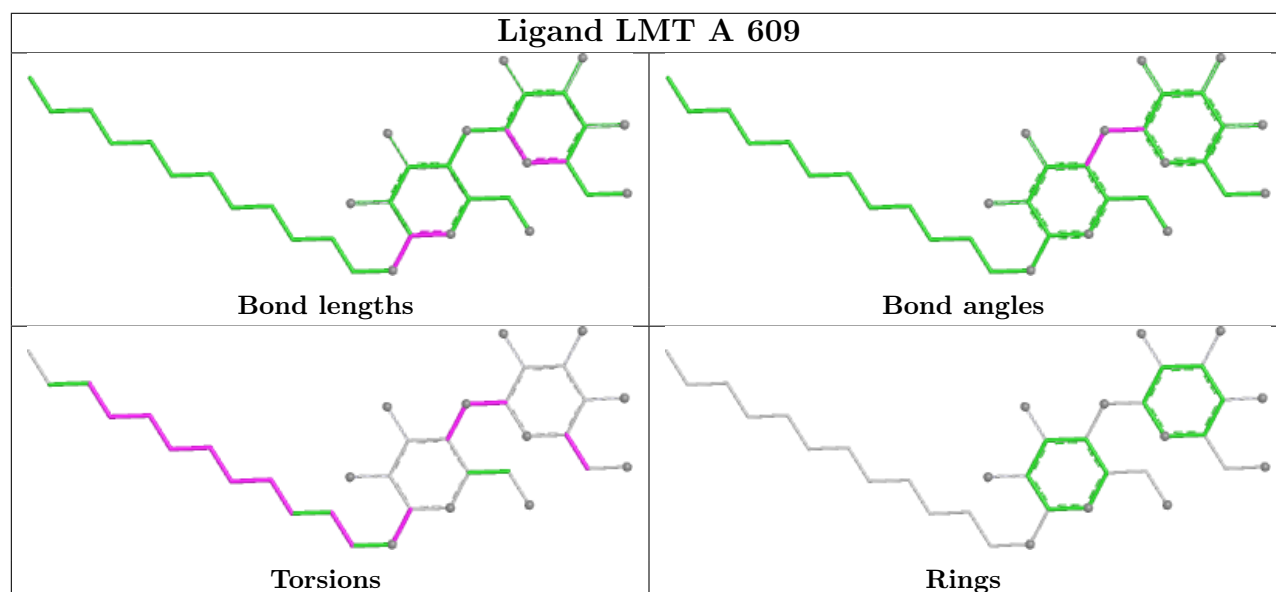
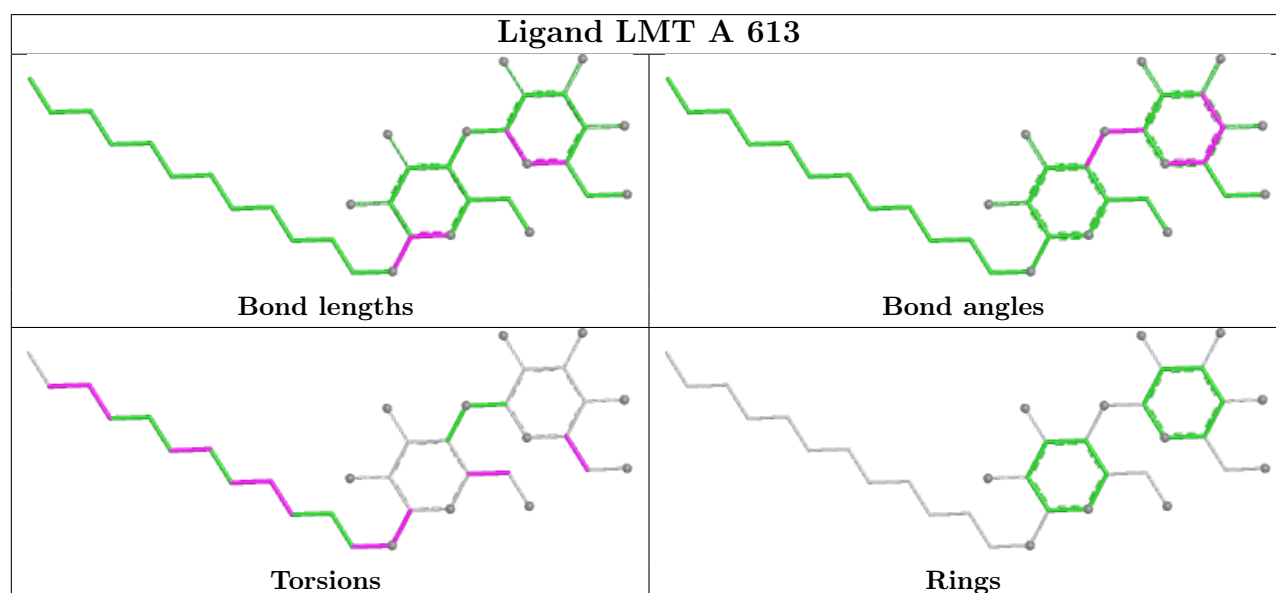
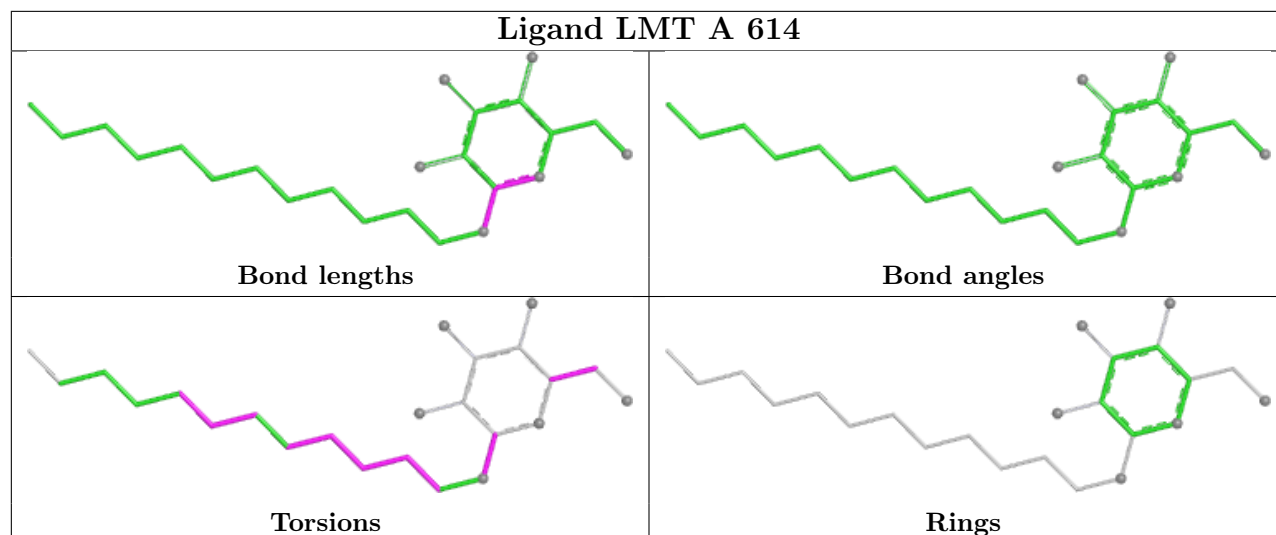


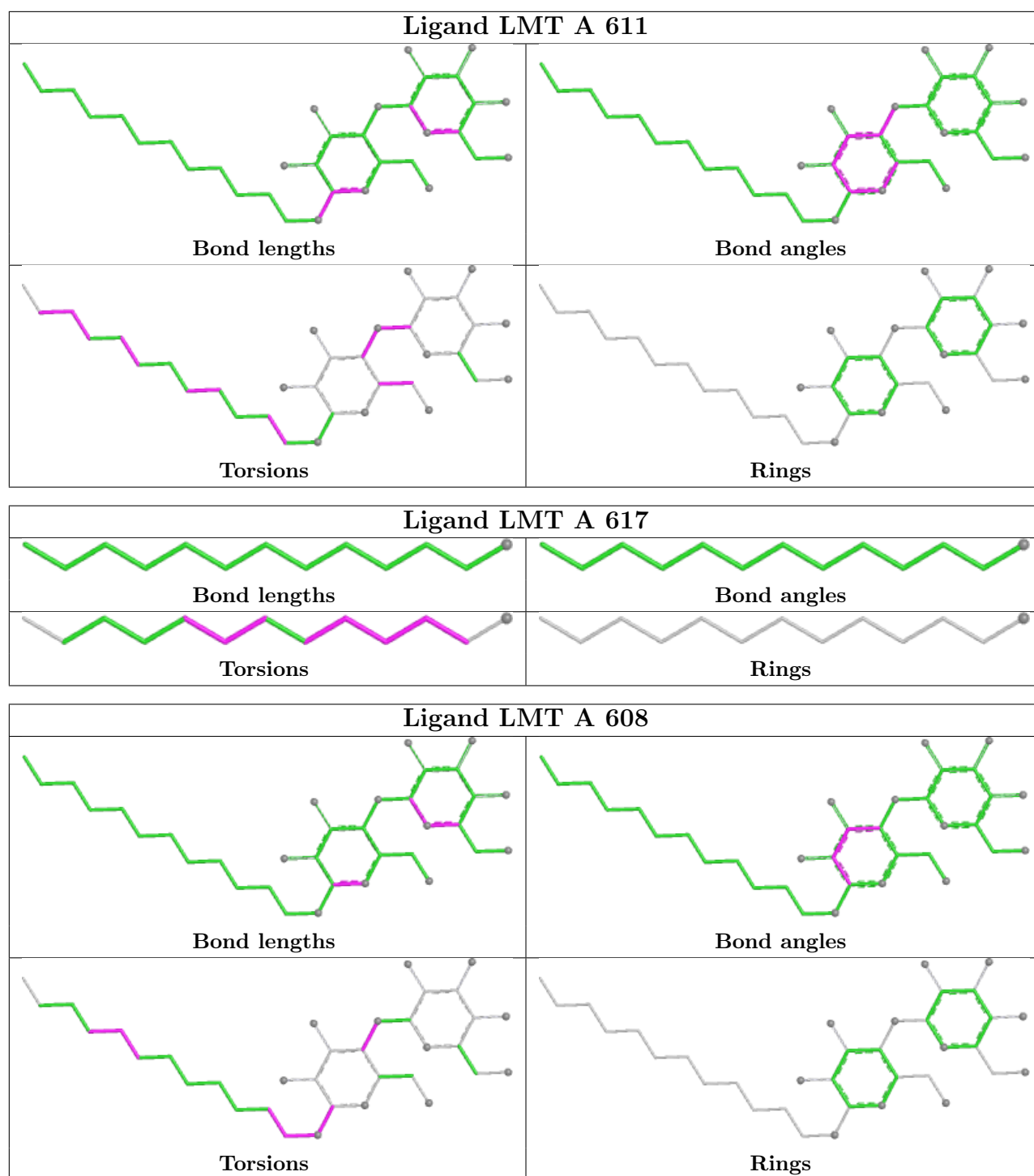


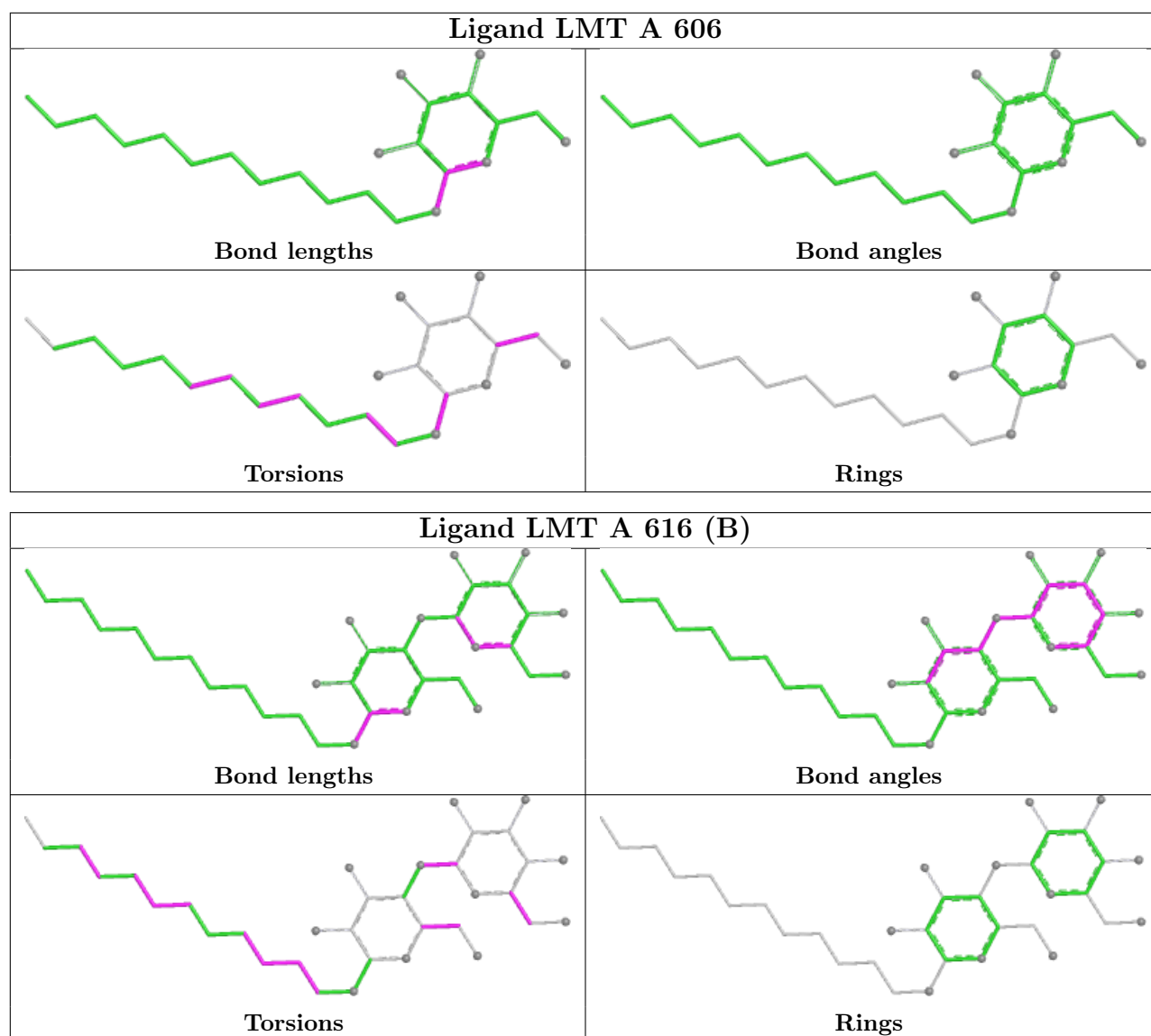












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27148. These allow visual inspection of the internal detail of the map and identification of artifacts.

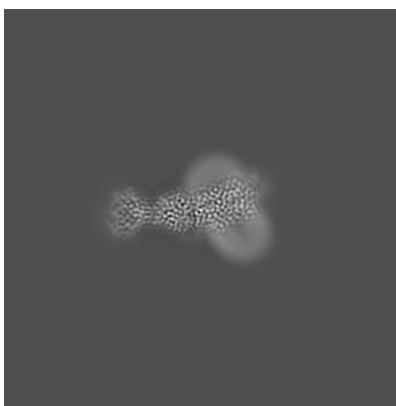
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

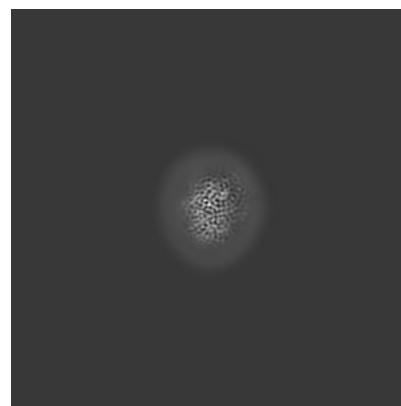
6.1.1 Primary map



X

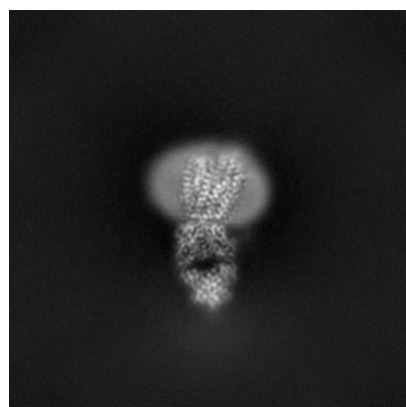


Y

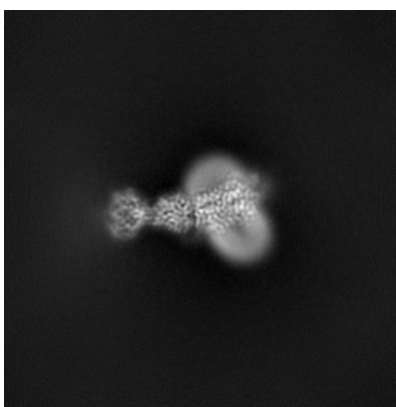


Z

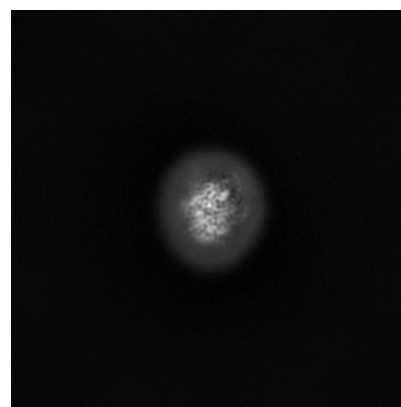
6.1.2 Raw map



X



Y



Z

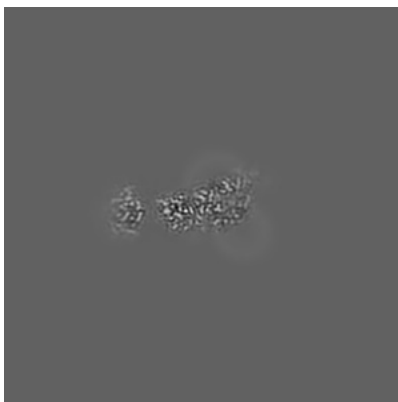
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

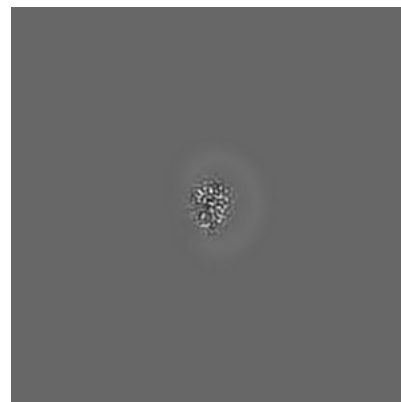
6.2.1 Primary map



X Index: 192

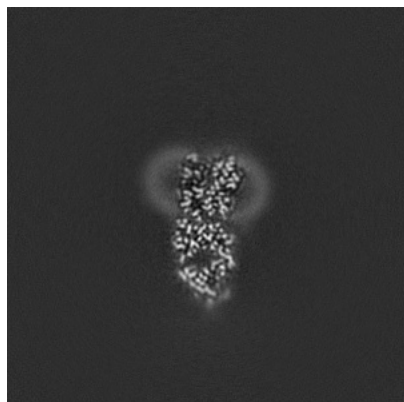


Y Index: 192

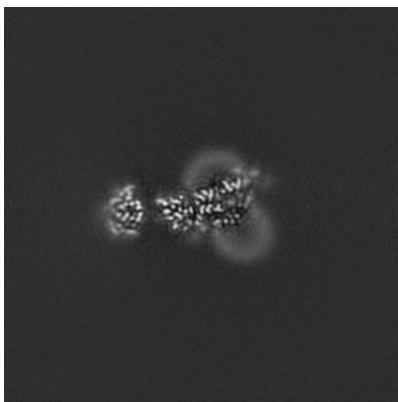


Z Index: 192

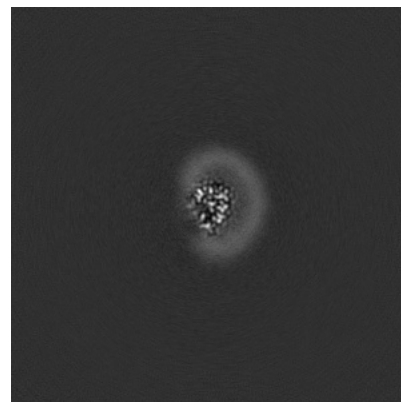
6.2.2 Raw map



X Index: 192



Y Index: 192



Z Index: 192

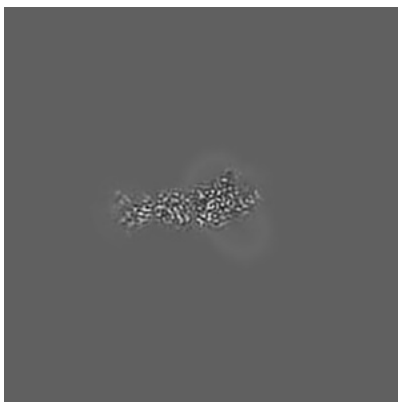
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

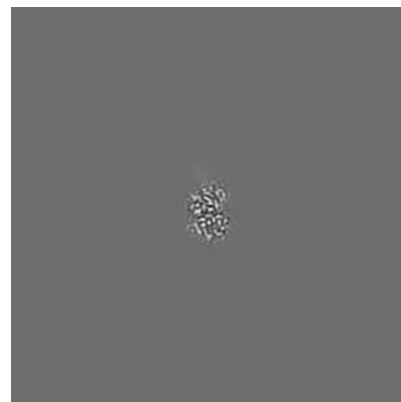
6.3.1 Primary map



X Index: 192

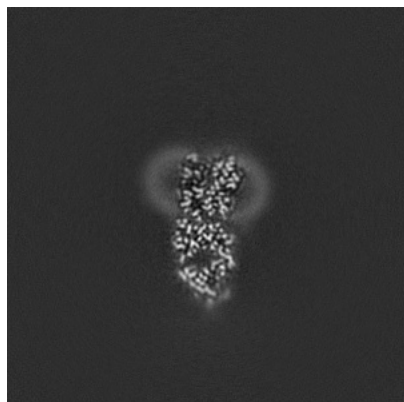


Y Index: 204

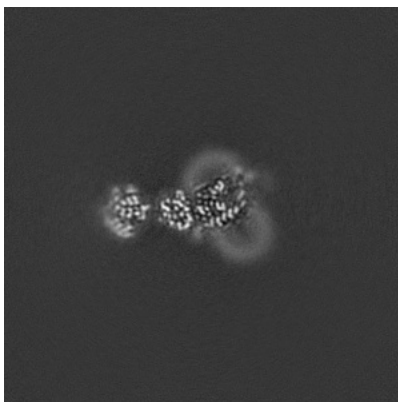


Z Index: 165

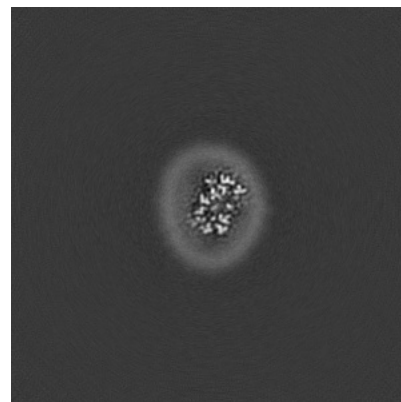
6.3.2 Raw map



X Index: 192



Y Index: 197

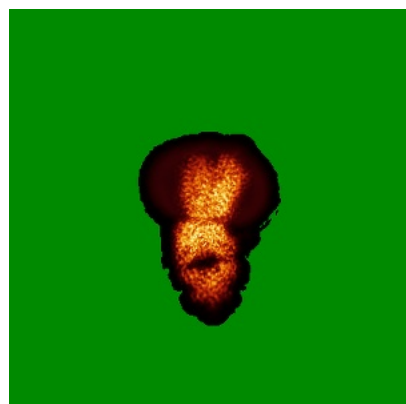


Z Index: 216

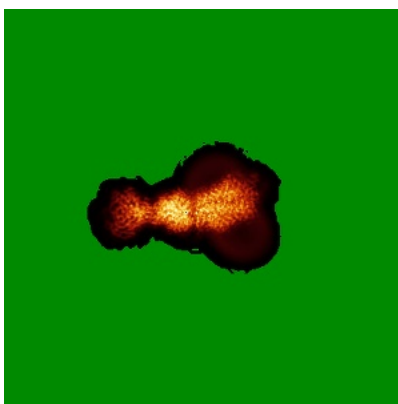
The images above show the largest variance slices of the map in three orthogonal directions.

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

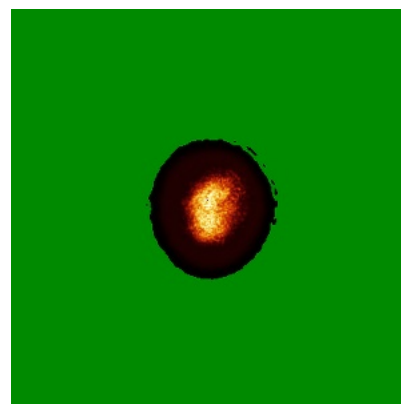
6.4.1 Primary map



X

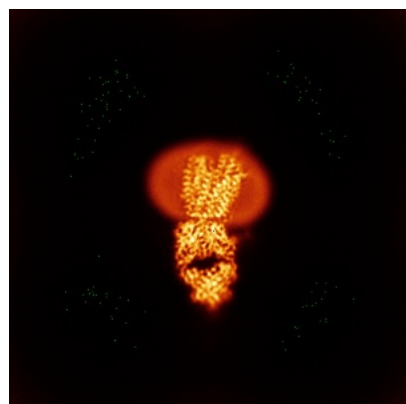


Y

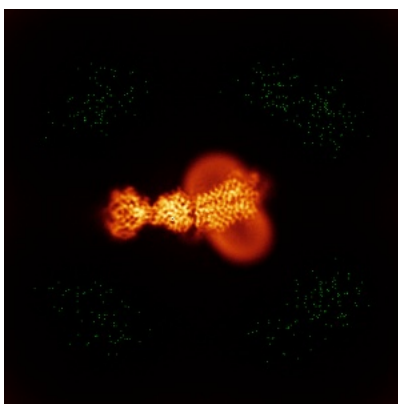


Z

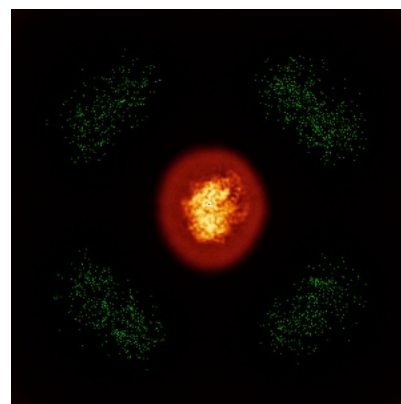
6.4.2 Raw map



X



Y

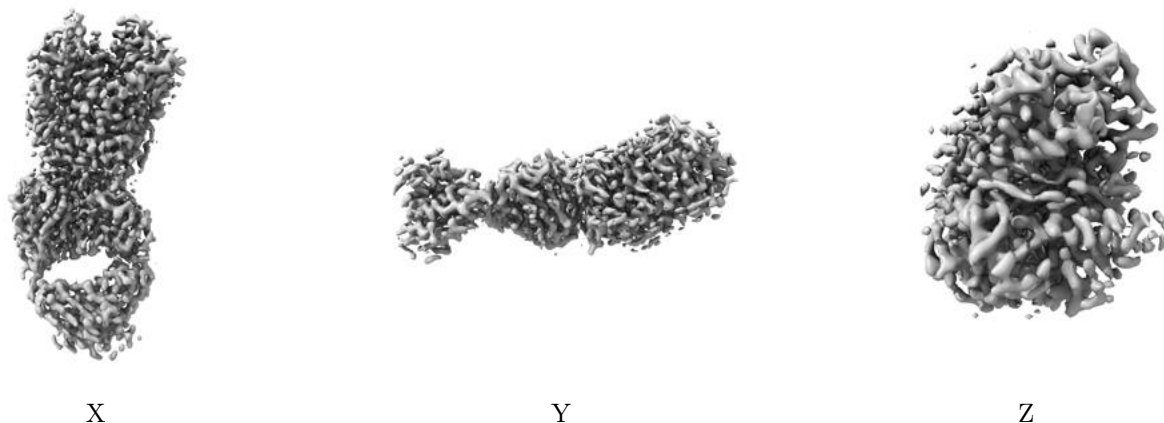


Z

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.

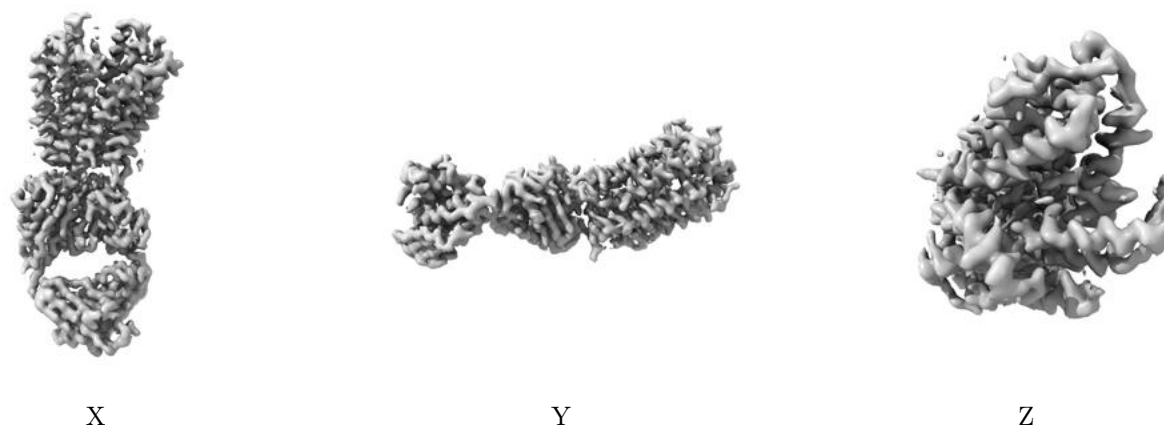
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.97. 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.

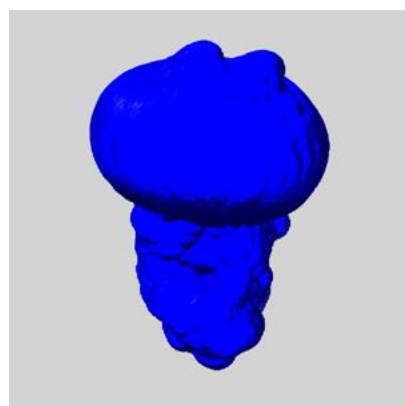
6.6 Mask visualisation [i](#)

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

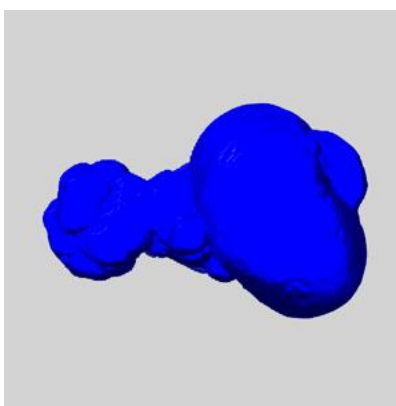
A mask typically either:

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

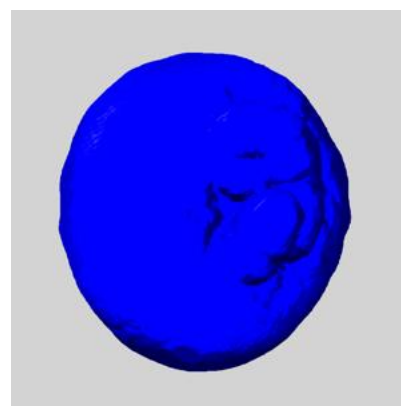
6.6.1 emd_27148_msk_1.map [i](#)



X



Y

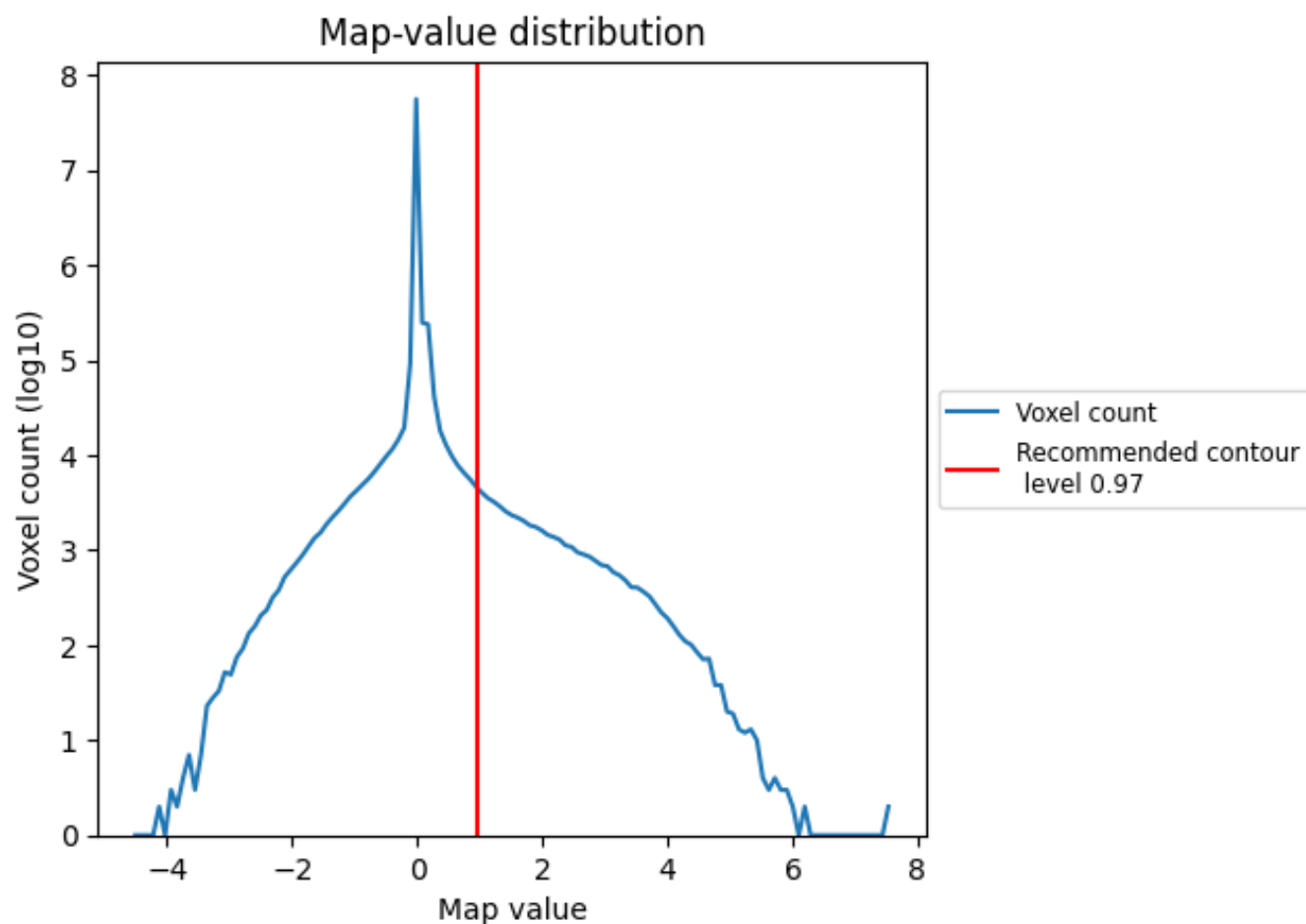


Z

7 Map analysis [i](#)

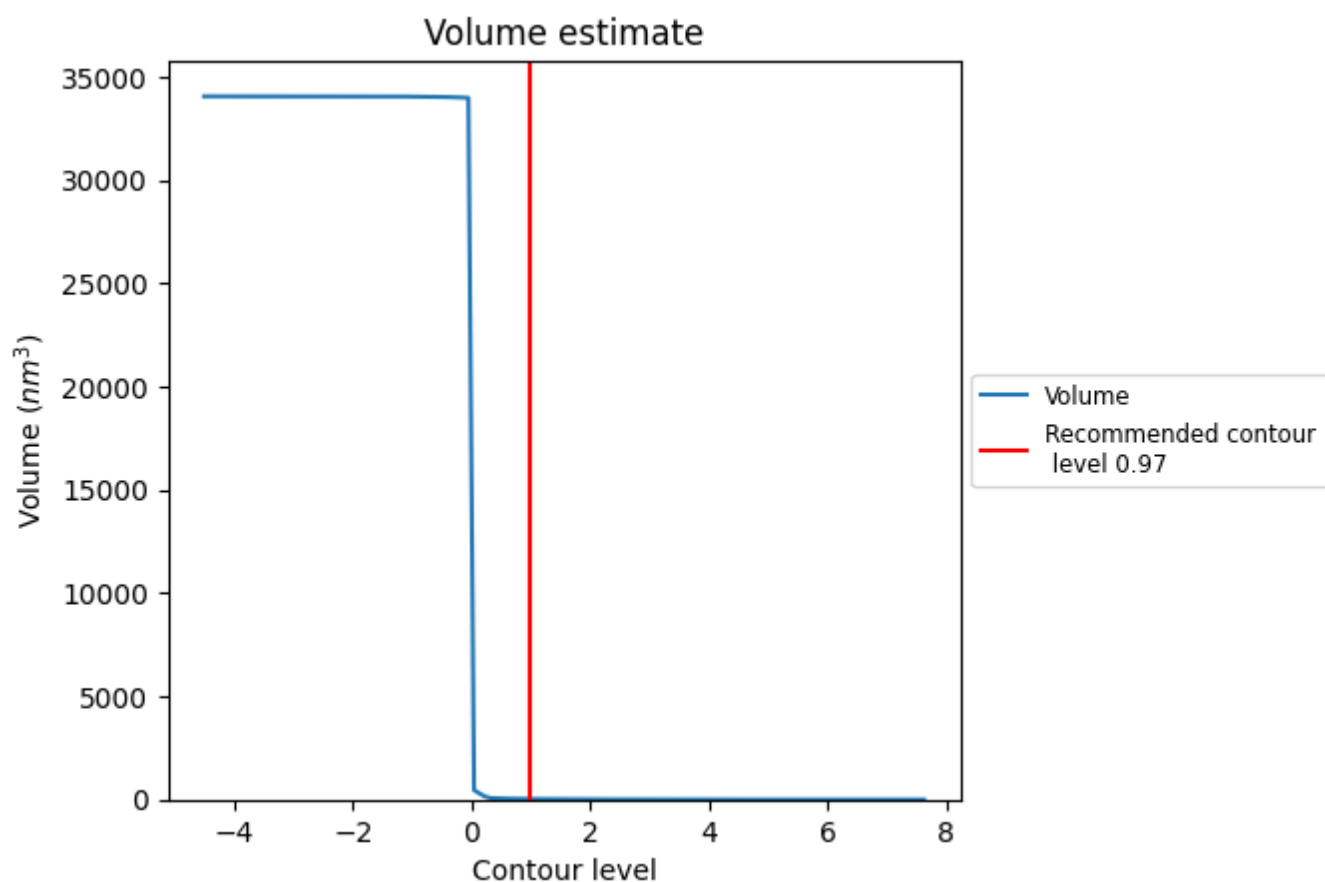
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

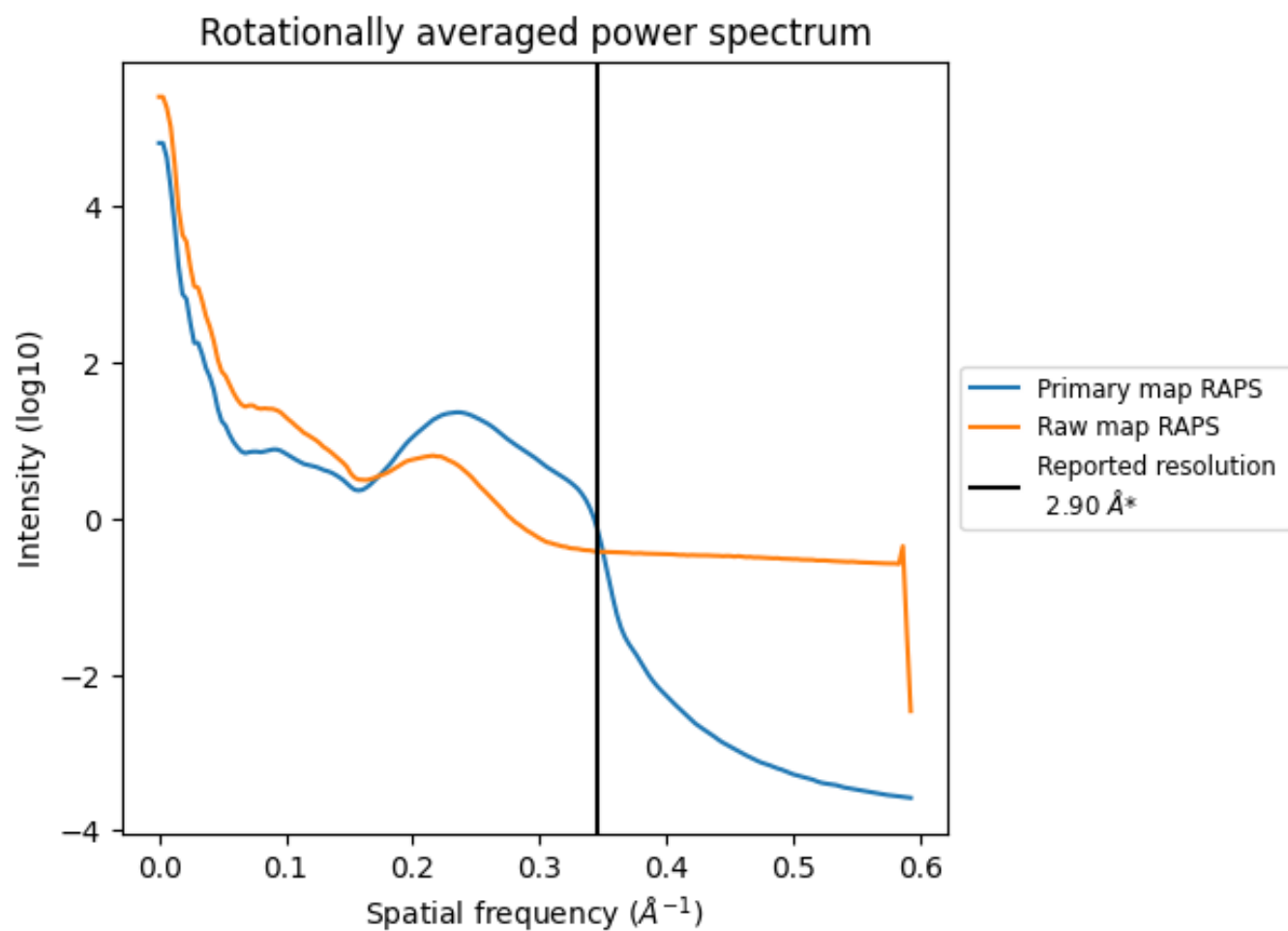
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 28 nm^3 ; this corresponds to an approximate mass of 26 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

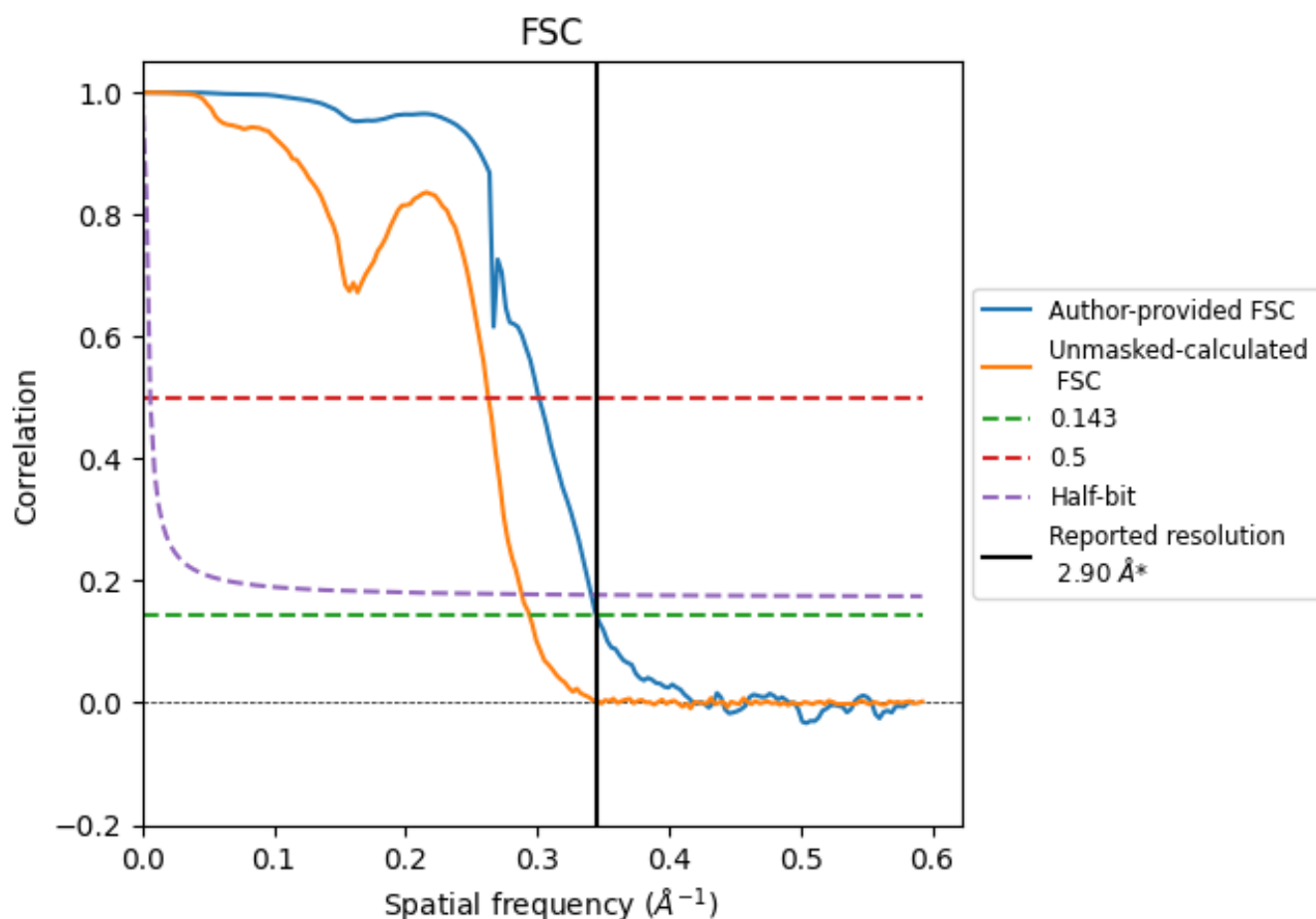


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

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 0.345 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

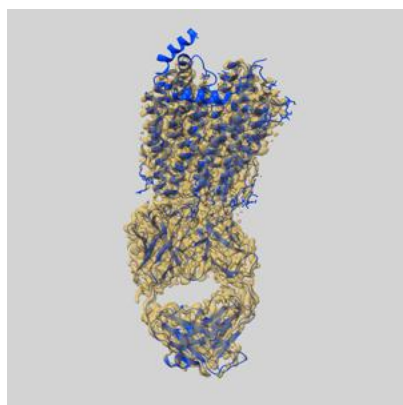
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.90	3.32	2.93
Unmasked-calculated*	3.40	3.80	3.47

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

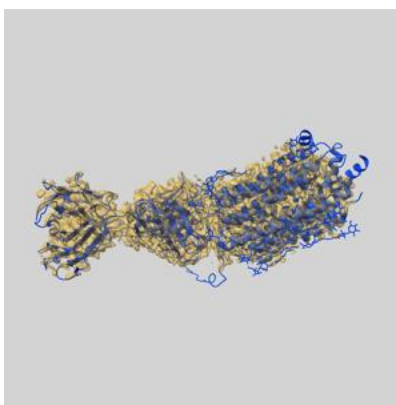
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-27148 and PDB model 8D2S. Per-residue inclusion information can be found in section [3](#) on page [7](#).

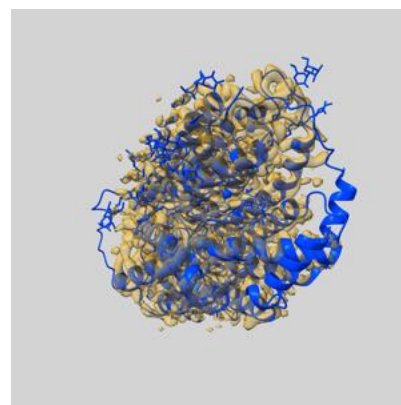
9.1 Map-model overlay [i](#)



X



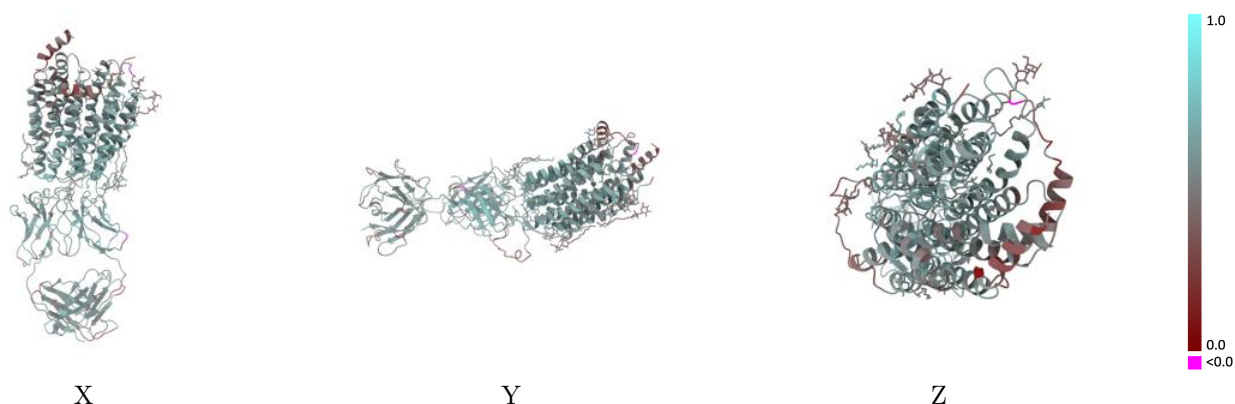
Y



Z

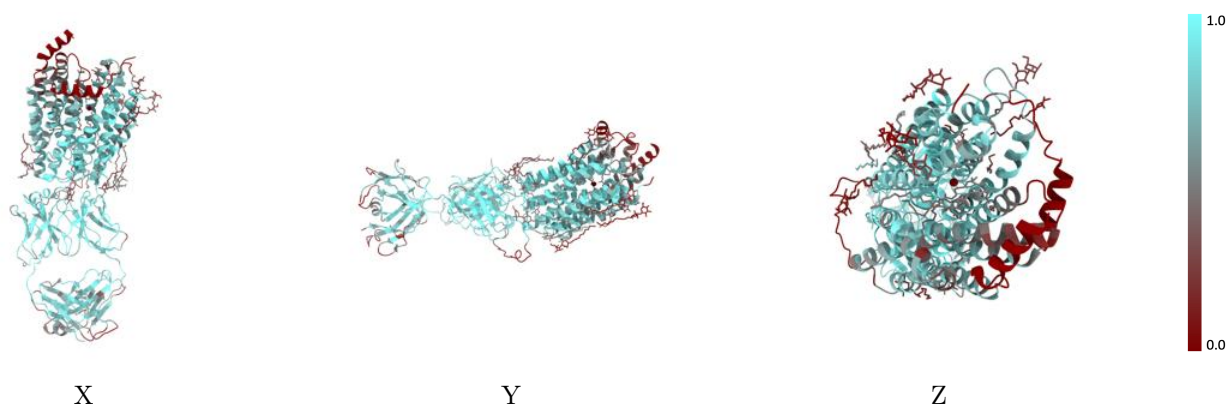
The images above show the 3D surface view of the map at the recommended contour level 0.97 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



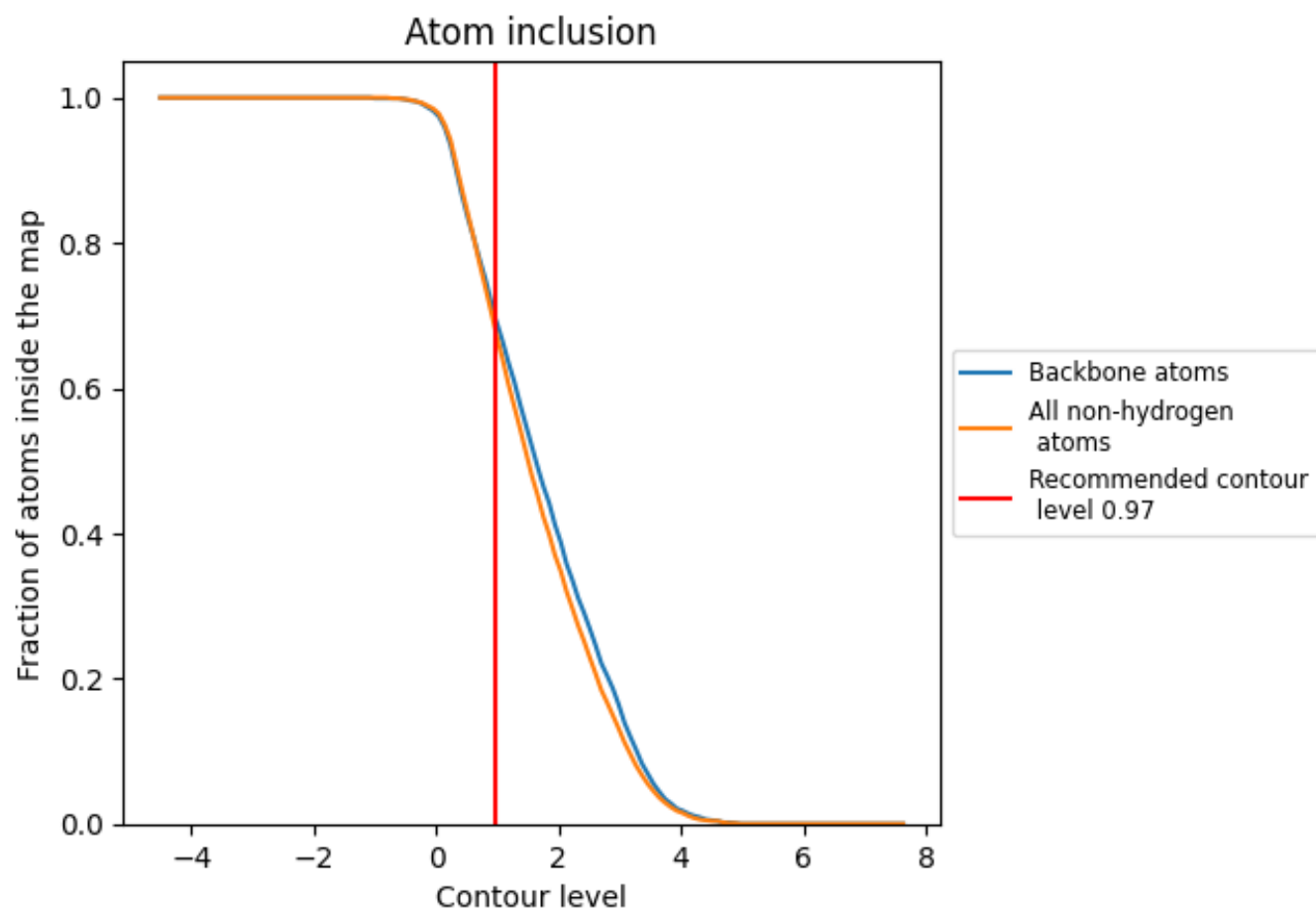
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.97).

9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 68% 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 (0.97) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6780	0.5430
A	0.6320	0.5410
B	0.7550	0.5500
C	0.7430	0.5420

