Full wwPDB EM Validation Report

Mar 8, 2026 – 12:41 AM UTC

PDB ID	:	8D2W / pdb_00008d2w
EMDB ID	:	EMD-27152
Title	:	Zebrafish MFSD2A isoform B in inward open ligand 2B 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	:	3.40 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 (i) 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 (1)) were used in the production of this report:

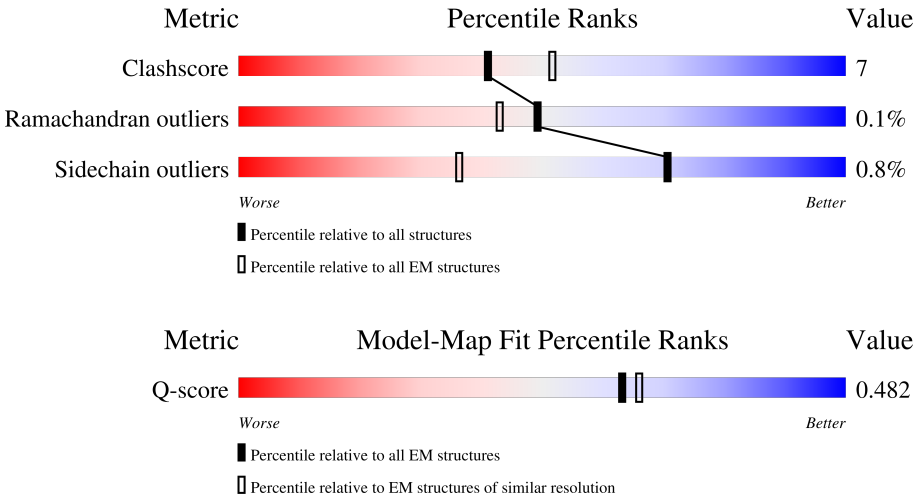
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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 3.40 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	14717 (2.90 - 3.90)

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 <=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	17% 77% 13% 9%
2	B	201	9% 88% 12%
3	C	203	8% 87% 13%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 6858 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
			Total	C	N	O	S		
1	A	460	3442	2295	529	594	24	2	0

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

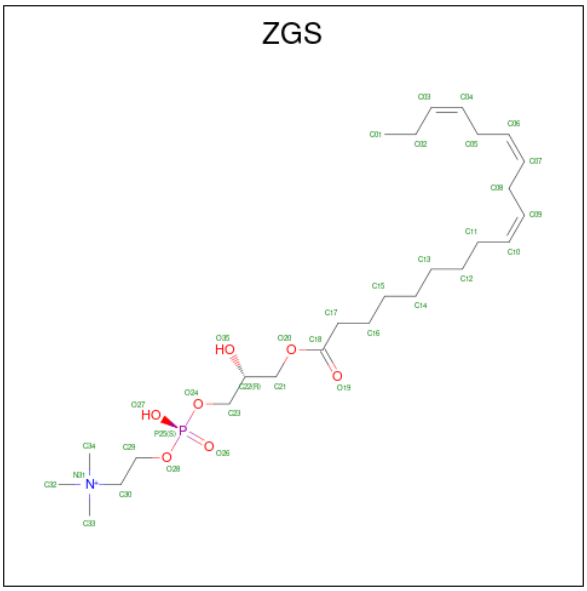
- Molecule 2 is a protein called FAB light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	201	Total	C	N	O	S	1	0
			1404	884	247	267	6		

- Molecule 3 is a protein called FAB heavy chain.

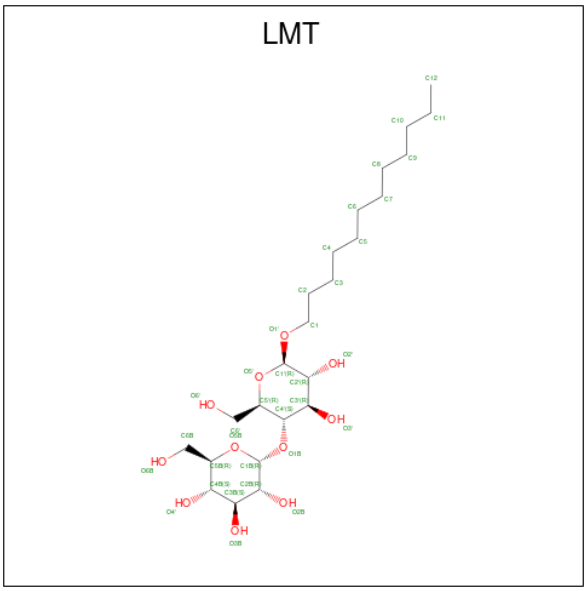
Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	203	Total	C	N	O	S	1	0
			1419	906	249	260	4		

- Molecule 4 is [(2 {R})-2-oxidanyl-3-[oxidanyl-[2-(trimethyl-$l^{4}-azanyl)ethoxy]phosphoryl]oxy-propyl] (9 {Z},12 {Z},15 {Z})-octadeca-9,12,15-trienoate (CCD ID: ZGS) (formula: $C_{26}H_{49}NO_7P$) (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	

- Molecule 5 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	C	O	1
			70	48	22	
5	A	1	Total	C	O	1
			70	48	22	
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	1
			70	48	22	
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
			13	12	1	
5	A	1	Total	C	O	0
			13	12	1	
5	A	1	Total	C	O	0
			13	12	1	

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Mol	Chain	Residues	Atoms			AltConf
5	C	1	Total 35	C 24	O 11	0

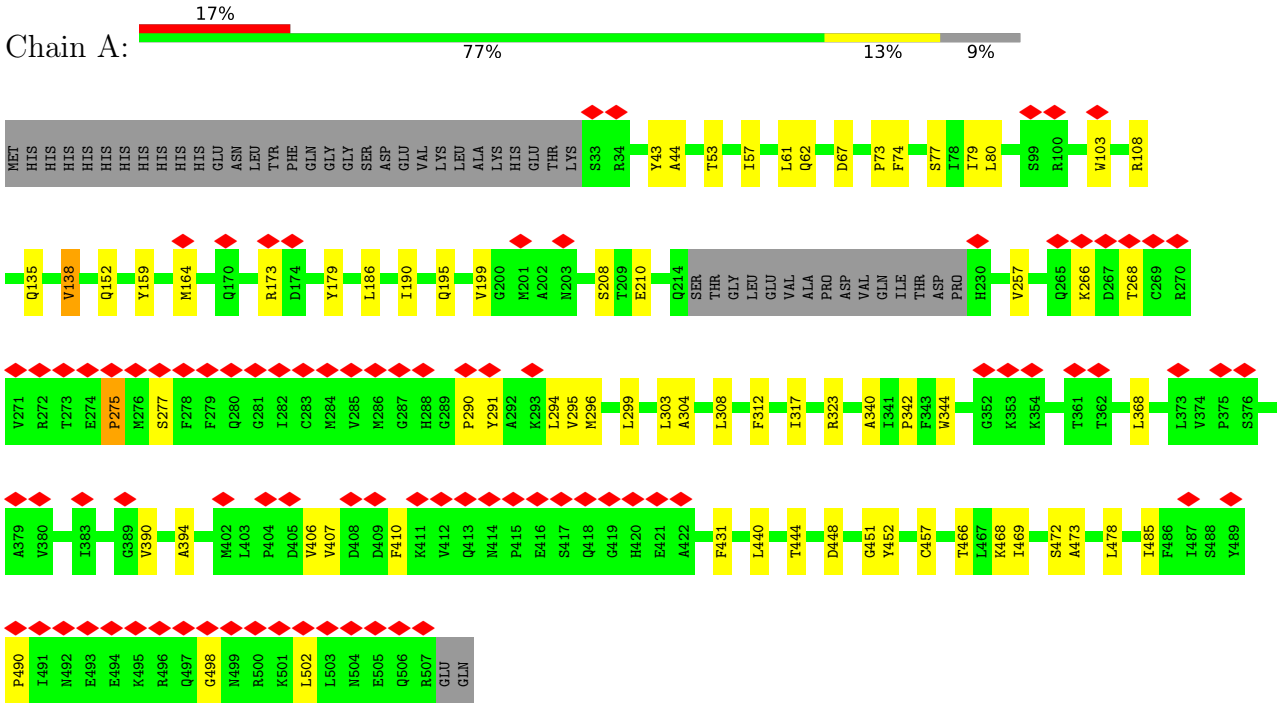
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		AltConf
6	A	5	Total 5	O 5	0

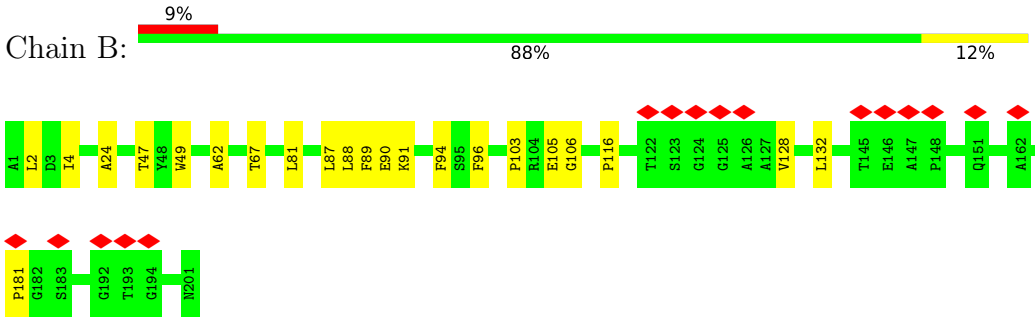
3 Residue-property plots (i)

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.

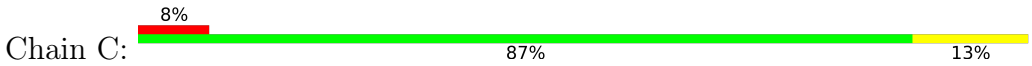
• Molecule 1: Sodium-dependent lysophosphatidylcholine symporter 1-B

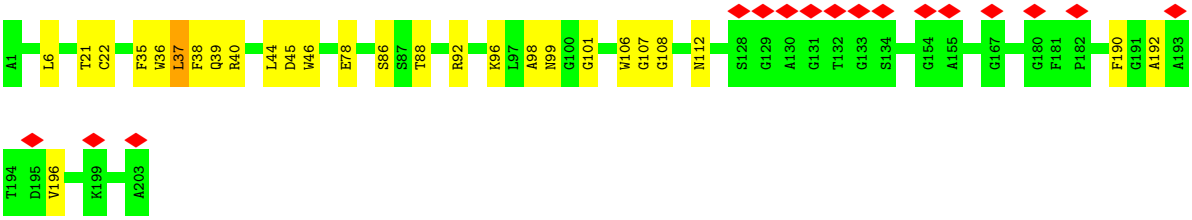


• Molecule 2: FAB light chain



• Molecule 3: FAB heavy chain




A1
L6
T21
C22
F35
W36
L37
F38
Q39
R40
L44
D45
W46
E78
S86
S87
T88
R92
K96
L97
A98
N99
G100
G101
W106
G107
G108
N112
S128
G129
A130
G131
T132
G133
S134
G154
A155
G167
G180
F181
P182
F190
G191
A192
A193
T194
D195
V196
K199
A203

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	76700	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	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	5.283	Depositor
Minimum map value	-2.250	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.045	Depositor
Recommended contour level	0.6	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LMT, ZGS

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	0.19	0/3534	0.38	0/4843
2	B	0.18	0/1442	0.47	0/1973
3	C	0.17	0/1459	0.41	0/1993
All	All	0.19	0/6435	0.41	0/8809

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3442	0	3346	51	0
2	B	1404	0	1284	18	0
3	C	1419	0	1331	17	0
4	A	35	0	0	1	0
5	A	518	0	708	14	0
5	C	35	0	46	2	0
6	A	5	0	0	0	0
All	All	6858	0	6715	93	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 (93) 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)
2:B:4:ILE:HG12	2:B:88:LEU:HD23	1.56	0.88
2:B:87:LEU:HD11	2:B:94:PHE:HB3	1.62	0.80
2:B:88:LEU:O	2:B:88:LEU:HD12	1.86	0.74
1:A:291:TYR:CE2	1:A:410:PHE:HB2	2.24	0.72
1:A:308:LEU:O	1:A:312:PHE:HB2	1.90	0.71
2:B:4:ILE:CG1	2:B:88:LEU:HD23	2.23	0.67
1:A:299:LEU:HD11	1:A:431:PHE:HB3	1.77	0.67
1:A:291:TYR:CD2	1:A:406:VAL:HG12	2.30	0.66
2:B:87:LEU:HD13	2:B:96:PHE:CZ	2.35	0.62
1:A:73:PRO:HB2	1:A:448:ASP:HB2	1.80	0.62
1:A:290:PRO:HG3	1:A:490:PRO:HG2	1.82	0.62
3:C:35:PHE:HD2	3:C:46:TRP:HE1	1.49	0.61
1:A:468:LYS:O	1:A:472:SER:HB3	2.03	0.59
3:C:38:PHE:HB3	3:C:45:ASP:HB2	1.83	0.59
5:A:607:LMT:H82	5:A:609:LMT:H112	1.86	0.57
1:A:53:THR:OG1	1:A:152:GLN:NE2	2.36	0.57
1:A:295:VAL:O	1:A:299:LEU:HB2	2.05	0.57
3:C:39:GLN:OE1	3:C:92:ARG:NH1	2.38	0.57
3:C:39:GLN:HB2	3:C:44:LEU:HD23	1.88	0.55
1:A:135:GLN:HG3	5:A:602[A]:LMT:H5'	1.88	0.55
2:B:88:LEU:HD12	2:B:88:LEU:C	2.32	0.55
3:C:6:LEU:HD22	3:C:108:GLY:H	1.71	0.54
1:A:466:THR:HG22	5:A:606:LMT:H31	1.88	0.54
1:A:208:SER:HB2	2:B:91:LYS:HA	1.89	0.54
1:A:291:TYR:HE2	1:A:410:PHE:HB2	1.71	0.54
1:A:452:TYR:O	3:C:99:ASN:ND2	2.32	0.53
3:C:37:LEU:HB2	3:C:92:ARG:HB2	1.90	0.52
1:A:190:ILE:HD11	5:A:609:LMT:H123	1.92	0.52
3:C:40:ARG:NH1	3:C:86:SER:O	2.43	0.52
3:C:37:LEU:HD23	3:C:44:LEU:HB3	1.92	0.51
1:A:164:MET:SD	1:A:173:ARG:NH1	2.83	0.51
1:A:195:GLN:O	1:A:199:VAL:HB	2.10	0.50
1:A:266:LYS:C	1:A:268:THR:H	2.19	0.50
3:C:88:THR:HG23	3:C:112:ASN:HA	1.92	0.50
1:A:43:TYR:O	1:A:159:TYR:OH	2.28	0.50
1:A:62:GLN:NE2	1:A:444:THR:OG1	2.41	0.50
1:A:344:TRP:CE2	1:A:394:ALA:HB2	2.47	0.49
1:A:308:LEU:HD11	1:A:368:LEU:HD11	1.95	0.48
2:B:49:TRP:H	2:B:89:PHE:HZ	1.61	0.48
1:A:296:MET:HB3	1:A:485:ILE:HD13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:87:LEU:HD13	2:B:96:PHE:CE1	2.49	0.48
1:A:323:ARG:HE	1:A:457:CYS:HA	1.79	0.47
1:A:57:ILE:HG23	1:A:61:LEU:HD22	1.96	0.47
3:C:96:LYS:HD2	3:C:101:GLY:HA2	1.95	0.47
1:A:103:TRP:HE3	1:A:108:ARG:HG3	1.79	0.47
5:A:603[A]:LMT:H71	5:A:604:LMT:H82	1.96	0.47
1:A:323:ARG:HH21	1:A:457:CYS:H	1.61	0.47
1:A:67:ASP:OD1	1:A:452:TYR:OH	2.29	0.47
3:C:6:LEU:HD13	3:C:107:GLY:HA3	1.97	0.47
1:A:79:ILE:HD11	1:A:138:VAL:HA	1.96	0.46
1:A:291:TYR:HE2	1:A:406:VAL:O	1.98	0.46
1:A:257:VAL:HG22	5:A:611:LMT:H41	1.97	0.46
2:B:180:GLY:N	2:B:181:PRO:HD3	2.30	0.46
1:A:317:ILE:HG23	1:A:323:ARG:HG2	1.98	0.46
2:B:116:PRO:HD3	2:B:128:VAL:HG22	1.96	0.46
1:A:304:ALA:HB2	1:A:478:LEU:HB2	1.98	0.45
2:B:105:GLU:CD	2:B:106:GLY:H	2.24	0.45
2:B:132:LEU:O	2:B:167:ALA:HA	2.17	0.45
1:A:294:LEU:HD22	1:A:406:VAL:HG21	1.98	0.45
5:C:301:LMT:H12	5:C:301:LMT:H41	1.63	0.45
5:A:602[A]:LMT:H11	5:A:602[A]:LMT:H41	1.72	0.45
1:A:498:GLY:O	1:A:502:LEU:N	2.44	0.45
4:A:601:ZGS:O35	4:A:601:ZGS:O19	2.34	0.45
5:A:610[B]:LMT:H71	5:A:610[B]:LMT:H102	1.79	0.45
2:B:2:LEU:HB2	2:B:88:LEU:CD2	2.46	0.45
1:A:299:LEU:HD11	1:A:431:PHE:CB	2.44	0.45
1:A:44:ALA:HB2	1:A:179:TYR:HB3	1.98	0.45
1:A:451:GLY:HA2	3:C:98:ALA:HB1	1.98	0.44
1:A:208:SER:N	2:B:90:GLU:O	2.51	0.44
5:A:607:LMT:H62	5:A:609:LMT:H92	2.00	0.44
5:A:605:LMT:H71	5:A:605:LMT:H102	1.83	0.43
3:C:21:THR:HG22	3:C:78:GLU:HG2	2.00	0.43
5:A:615:LMT:H71	5:A:615:LMT:H101	1.78	0.43
2:B:24:ALA:O	2:B:67:THR:OG1	2.35	0.42
3:C:36:TRP:HA	3:C:92:ARG:O	2.19	0.42
1:A:80:LEU:HD13	1:A:440:LEU:HG	2.01	0.42
1:A:186:LEU:HD21	5:A:610[A]:LMT:H81	2.00	0.42
1:A:469:ILE:HG23	1:A:473:ALA:HB3	2.01	0.42
1:A:291:TYR:OH	1:A:407:VAL:HA	2.20	0.41
2:B:81:LEU:HD13	2:B:103:PRO:HG3	2.01	0.41
1:A:266:LYS:C	1:A:268:THR:N	2.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:190:PHE:CE2	3:C:192:ALA:HB3	2.56	0.41
5:A:610[A]:LMT:H62	5:A:610[A]:LMT:H31	1.71	0.41
1:A:340:ALA:HB2	1:A:390:VAL:HG22	2.03	0.41
3:C:92:ARG:HG2	3:C:106:TRP:HE3	1.86	0.41
1:A:77:SER:HB3	1:A:444:THR:HB	2.03	0.40
2:B:47:THR:HG21	2:B:62:ALA:HB3	2.03	0.40
5:C:301:LMT:H122	5:C:301:LMT:H92	1.77	0.40
1:A:303:LEU:HD23	1:A:303:LEU:HA	1.91	0.40
1:A:440:LEU:HD12	1:A:440:LEU:HA	1.93	0.40
1:A:342:PRO:HG3	5:A:610[B]:LMT:H32	2.03	0.40
1:A:74:PHE:O	1:A:77:SER:OG	2.38	0.40
1:A:275:PRO:C	1:A:277:SER:H	2.28	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	458/508 (90%)	443 (97%)	14 (3%)	1 (0%)	43 71
2	B	200/201 (100%)	180 (90%)	20 (10%)	0	100 100
3	C	202/203 (100%)	180 (89%)	22 (11%)	0	100 100
All	All	860/912 (94%)	803 (93%)	56 (6%)	1 (0%)	49 78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	275	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	346/436 (79%)	344 (99%)	2 (1%)	78 80
2	B	125/144 (87%)	125 (100%)	0	100 100
3	C	125/138 (91%)	122 (98%)	3 (2%)	43 62
All	All	596/718 (83%)	591 (99%)	5 (1%)	70 77

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

Mol	Chain	Res	Type
1	A	138	VAL
1	A	210	GLU
3	C	22	CYS
3	C	37	LEU
3	C	196	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	GLN
1	A	152	GLN
1	A	156	HIS
1	A	170	GLN
1	A	197	GLN
1	A	319	ASN
1	A	328	ASN
1	A	413	GLN
1	A	414	ASN
2	B	5	ASN
2	B	36	ASN
2	B	102	ASN
3	C	65	ASN
3	C	74	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

There are no oligosaccharides in this entry.

5.6 Ligand geometry

19 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	$\#\|Z\| > 2$
5	LMT	A	611	-	36,36,36	1.32	4 (11%)	47,47,47	1.51	8 (17%)
5	LMT	A	602[B]	-	36,36,36	1.29	3 (8%)	47,47,47	1.04	1 (2%)
5	LMT	A	614	-	12,12,36	0.89	0	11,11,47	0.82	0
5	LMT	A	606	-	36,36,36	1.29	4 (11%)	47,47,47	0.94	1 (2%)
4	ZGS	A	601	-	34,34,34	1.09	4 (11%)	39,41,41	1.43	6 (15%)
5	LMT	A	610[A]	-	36,36,36	1.30	4 (11%)	47,47,47	1.18	4 (8%)
5	LMT	A	603[B]	-	36,36,36	1.25	4 (11%)	47,47,47	1.12	4 (8%)
5	LMT	A	613	-	12,12,36	0.89	0	11,11,47	0.84	0
5	LMT	A	608	-	36,36,36	1.27	4 (11%)	47,47,47	0.92	1 (2%)
5	LMT	A	605	-	36,36,36	1.30	4 (11%)	47,47,47	0.93	1 (2%)
5	LMT	A	604	-	36,36,36	1.30	4 (11%)	47,47,47	1.10	3 (6%)
5	LMT	A	609	-	24,24,36	1.23	2 (8%)	29,29,47	0.85	0
5	LMT	A	607	-	36,36,36	1.28	4 (11%)	47,47,47	0.92	1 (2%)
5	LMT	A	612	-	36,36,36	1.28	4 (11%)	47,47,47	1.09	4 (8%)
5	LMT	A	610[B]	-	36,36,36	1.33	4 (11%)	47,47,47	1.14	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	LMT	A	602[A]	-	36,36,36	1.27	4 (11%)	47,47,47	1.06	4 (8%)
5	LMT	C	301	-	36,36,36	1.30	4 (11%)	47,47,47	1.12	3 (6%)
5	LMT	A	603[A]	-	36,36,36	1.31	4 (11%)	47,47,47	1.03	2 (4%)
5	LMT	A	615	-	12,12,36	0.89	0	11,11,47	0.82	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
5	LMT	A	611	-	-	6/21/61/61	0/2/2/2
5	LMT	A	602[B]	-	-	10/21/61/61	0/2/2/2
5	LMT	A	614	-	-	4/10/10/61	-
5	LMT	A	606	-	-	14/21/61/61	0/2/2/2
4	ZGS	A	601	-	-	12/36/36/36	-
5	LMT	A	610[A]	-	-	7/21/61/61	0/2/2/2
5	LMT	A	603[B]	-	-	12/21/61/61	0/2/2/2
5	LMT	A	613	-	-	5/10/10/61	-
5	LMT	A	608	-	-	6/21/61/61	0/2/2/2
5	LMT	A	605	-	-	5/21/61/61	0/2/2/2
5	LMT	A	604	-	-	10/21/61/61	0/2/2/2
5	LMT	A	609	-	-	7/15/35/61	0/1/1/2
5	LMT	A	607	-	-	10/21/61/61	0/2/2/2
5	LMT	A	612	-	-	12/21/61/61	0/2/2/2
5	LMT	A	610[B]	-	-	5/21/61/61	0/2/2/2
5	LMT	A	602[A]	-	-	8/21/61/61	0/2/2/2
5	LMT	C	301	-	-	15/21/61/61	0/2/2/2
5	LMT	A	603[A]	-	-	11/21/61/61	0/2/2/2
5	LMT	A	615	-	-	5/10/10/61	-

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	611	LMT	O5'-C1'	4.33	1.53	1.41
5	A	610[A]	LMT	O5'-C1'	4.31	1.52	1.41
5	C	301	LMT	O5'-C1'	4.28	1.52	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	610[B]	LMT	O5'-C1'	4.24	1.52	1.41
5	A	602[B]	LMT	O5'-C1'	4.12	1.52	1.41
5	A	606	LMT	O5'-C1'	4.12	1.52	1.41
5	A	612	LMT	O5'-C1'	4.11	1.52	1.41
5	A	603[A]	LMT	O5B-C1B	4.09	1.52	1.41
5	A	607	LMT	O5'-C1'	4.05	1.52	1.41
5	A	604	LMT	O5B-C1B	4.00	1.52	1.41
5	A	609	LMT	O5'-C1'	3.98	1.52	1.41
5	A	608	LMT	O5'-C1'	3.97	1.52	1.41
5	A	605	LMT	O5'-C1'	3.97	1.52	1.41
5	A	604	LMT	O5'-C1'	3.91	1.51	1.41
5	A	602[B]	LMT	O5B-C1B	3.90	1.51	1.41
5	A	611	LMT	O5B-C1B	3.86	1.51	1.41
5	A	603[B]	LMT	O5'-C1'	3.86	1.51	1.41
5	A	603[A]	LMT	O5'-C1'	3.86	1.51	1.41
5	A	605	LMT	O5B-C1B	3.86	1.51	1.41
5	A	602[A]	LMT	O5'-C1'	3.84	1.51	1.41
5	C	301	LMT	O5B-C1B	3.79	1.51	1.41
5	A	610[B]	LMT	O5B-C1B	3.76	1.51	1.41
5	A	606	LMT	O5B-C1B	3.75	1.51	1.41
5	A	610[A]	LMT	O5B-C1B	3.73	1.51	1.41
5	A	607	LMT	O5B-C1B	3.72	1.51	1.41
5	A	608	LMT	O5B-C1B	3.72	1.51	1.41
5	A	602[A]	LMT	O5B-C1B	3.66	1.51	1.41
5	A	603[B]	LMT	O5B-C1B	3.65	1.51	1.41
5	A	612	LMT	O5B-C1B	3.64	1.51	1.41
5	A	611	LMT	O5B-C5B	2.61	1.50	1.44
4	A	601	ZGS	C30-C29	2.57	1.59	1.51
4	A	601	ZGS	O20-C21	-2.55	1.39	1.45
5	A	604	LMT	O5B-C5B	2.51	1.50	1.44
4	A	601	ZGS	P25-O28	2.48	1.69	1.59
5	A	603[A]	LMT	O5B-C5B	2.42	1.50	1.44
5	A	607	LMT	O5B-C5B	2.40	1.50	1.44
5	C	301	LMT	O5B-C5B	2.37	1.50	1.44
5	A	605	LMT	O5B-C5B	2.37	1.50	1.44
5	A	610[A]	LMT	O5B-C5B	2.36	1.50	1.44
5	A	602[A]	LMT	O5B-C5B	2.35	1.50	1.44
5	A	602[B]	LMT	O5B-C5B	2.35	1.50	1.44
5	A	612	LMT	O5B-C5B	2.35	1.50	1.44
5	A	610[B]	LMT	O5B-C5B	2.32	1.50	1.44
5	A	608	LMT	O5B-C5B	2.28	1.50	1.44
5	A	602[A]	LMT	O1'-C1'	-2.23	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	605	LMT	O1'-C1'	-2.23	1.36	1.40
5	A	606	LMT	O5B-C5B	2.22	1.49	1.44
5	A	604	LMT	O1'-C1'	-2.21	1.36	1.40
5	A	612	LMT	O1'-C1'	-2.19	1.36	1.40
4	A	601	ZGS	O20-C18	2.18	1.39	1.33
5	A	606	LMT	O1'-C1'	-2.15	1.36	1.40
5	A	609	LMT	O1'-C1'	-2.15	1.36	1.40
5	A	610[A]	LMT	O1'-C1'	-2.14	1.36	1.40
5	A	603[B]	LMT	O5B-C5B	2.13	1.49	1.44
5	A	603[B]	LMT	O1'-C1'	-2.12	1.36	1.40
5	A	608	LMT	O1'-C1'	-2.12	1.36	1.40
5	A	607	LMT	O1'-C1'	-2.11	1.36	1.40
5	C	301	LMT	O1'-C1'	-2.09	1.36	1.40
5	A	611	LMT	O1'-C1'	-2.09	1.36	1.40
5	A	603[A]	LMT	O1'-C1'	-2.05	1.36	1.40
5	A	610[B]	LMT	O1'-C1'	-2.04	1.36	1.40

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	611	LMT	O5B-C5B-C4B	3.70	116.37	109.70
5	A	602[B]	LMT	C1B-O1B-C4'	-3.63	109.37	117.98
5	A	611	LMT	C4B-C3B-C2B	3.62	117.19	110.83
4	A	601	ZGS	C06-C05-C04	3.58	129.66	112.02
5	A	610[B]	LMT	C1B-O1B-C4'	-3.50	109.67	117.98
4	A	601	ZGS	C11-C10-C09	3.50	151.03	124.83
5	A	611	LMT	C1B-O1B-C4'	-3.39	109.95	117.98
5	A	610[B]	LMT	O5'-C5'-C4'	3.38	116.72	109.72
4	A	601	ZGS	C05-C04-C03	3.38	152.08	123.57
4	A	601	ZGS	C08-C07-C06	3.29	151.32	123.57
5	A	612	LMT	C1B-O1B-C4'	-3.20	110.39	117.98
5	A	606	LMT	C1B-O1B-C4'	-3.13	110.55	117.98
5	A	611	LMT	C3B-C4B-C5B	3.11	115.88	110.23
5	A	603[B]	LMT	C4B-C3B-C2B	3.04	116.17	110.83
5	A	610[A]	LMT	C2'-C3'-C4'	3.04	116.57	109.68
5	A	611	LMT	C2'-C3'-C4'	3.03	116.56	109.68
5	A	610[A]	LMT	C1B-O1B-C4'	-3.02	110.83	117.98
5	A	605	LMT	C1B-O1B-C4'	-2.98	110.90	117.98
5	A	612	LMT	C3B-C4B-C5B	2.95	115.57	110.23
5	C	301	LMT	C2'-C3'-C4'	2.94	116.36	109.68
5	A	602[A]	LMT	C1B-O1B-C4'	-2.71	111.56	117.98
5	A	611	LMT	O5'-C1'-C2'	2.71	115.93	110.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	604	LMT	C4B-C3B-C2B	2.69	115.55	110.83
5	A	608	LMT	C1B-O1B-C4'	-2.67	111.64	117.98
5	A	602[A]	LMT	O5'-C5'-C4'	2.62	115.15	109.72
5	A	603[A]	LMT	O5'-C5'-C4'	2.56	115.02	109.72
5	C	301	LMT	O5'-C1'-C2'	2.53	115.57	110.37
5	A	604	LMT	C1B-O1B-C4'	-2.52	112.01	117.98
4	A	601	ZGS	C02-C03-C04	-2.49	111.44	126.42
5	A	603[B]	LMT	C1B-O1B-C4'	-2.47	112.13	117.98
4	A	601	ZGS	O20-C18-C17	2.46	119.34	111.83
5	A	603[A]	LMT	C2'-C3'-C4'	2.44	115.22	109.68
5	A	611	LMT	C1B-C2B-C3B	2.41	115.08	110.01
5	A	610[A]	LMT	O5'-C1'-C2'	2.40	115.31	110.37
5	A	610[B]	LMT	C1'-O5'-C5'	2.37	118.34	113.72
5	A	612	LMT	O5B-C5B-C4B	2.34	113.92	109.70
5	A	611	LMT	C1'-C2'-C3'	2.33	114.91	110.01
5	A	603[B]	LMT	C2'-C3'-C4'	2.30	114.90	109.68
5	A	610[A]	LMT	C1'-C2'-C3'	2.28	114.80	110.01
5	A	607	LMT	C1B-O1B-C4'	-2.21	112.75	117.98
5	A	604	LMT	C1B-C2B-C3B	2.19	114.61	110.01
5	C	301	LMT	C1'-C2'-C3'	2.17	114.58	110.01
5	A	602[A]	LMT	C2'-C3'-C4'	2.15	114.56	109.68
5	A	603[B]	LMT	O5'-C5'-C4'	2.08	114.03	109.72
5	A	612	LMT	C4B-C3B-C2B	2.04	114.42	110.83
5	A	602[A]	LMT	C3'-C4'-C5'	2.01	115.39	110.93

There are no chirality outliers.

All (164) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	601	ZGS	C10-C11-C12-C13
4	A	601	ZGS	C29-O28-P25-O24
5	A	602[A]	LMT	C2'-C1'-O1'-C1
5	A	602[A]	LMT	C2-C1-O1'-C1'
5	A	602[B]	LMT	O5'-C1'-O1'-C1
5	A	606	LMT	C2'-C1'-O1'-C1
5	A	608	LMT	C2-C1-O1'-C1'
5	A	611	LMT	O5'-C1'-O1'-C1
5	A	612	LMT	C2-C1-O1'-C1'
5	C	301	LMT	O5B-C1B-O1B-C4'
5	A	604	LMT	O5'-C5'-C6'-O6'
5	A	603[A]	LMT	C2B-C1B-O1B-C4'
4	A	601	ZGS	C17-C18-O20-C21

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Mol	Chain	Res	Type	Atoms
5	A	607	LMT	O5'-C5'-C6'-O6'
5	A	609	LMT	O5'-C5'-C6'-O6'
5	A	610[B]	LMT	O5B-C5B-C6B-O6B
5	A	604	LMT	C4'-C5'-C6'-O6'
5	A	603[A]	LMT	O5B-C1B-O1B-C4'
4	A	601	ZGS	O19-C18-O20-C21
5	C	301	LMT	O5B-C5B-C6B-O6B
5	A	603[B]	LMT	C4B-C5B-C6B-O6B
5	A	602[A]	LMT	O5'-C1'-O1'-C1
5	A	606	LMT	O5'-C1'-O1'-C1
5	A	608	LMT	O5'-C1'-O1'-C1
5	A	610[A]	LMT	O5'-C1'-O1'-C1
5	A	612	LMT	O5'-C1'-O1'-C1
5	C	301	LMT	O5'-C1'-O1'-C1
5	A	606	LMT	C4B-C5B-C6B-O6B
5	A	607	LMT	C4'-C5'-C6'-O6'
5	A	602[B]	LMT	C2'-C1'-O1'-C1
5	A	610[A]	LMT	C2'-C1'-O1'-C1
5	A	612	LMT	C2'-C1'-O1'-C1
5	C	301	LMT	C2'-C1'-O1'-C1
5	A	602[B]	LMT	O5B-C5B-C6B-O6B
5	A	603[B]	LMT	O5B-C5B-C6B-O6B
5	A	610[B]	LMT	C4B-C5B-C6B-O6B
5	A	603[A]	LMT	O1'-C1-C2-C3
5	A	612	LMT	C4'-C5'-C6'-O6'
5	A	606	LMT	O5B-C5B-C6B-O6B
5	A	610[A]	LMT	O5B-C5B-C6B-O6B
5	A	609	LMT	C4'-C5'-C6'-O6'
5	A	607	LMT	C3'-C4'-O1B-C1B
5	A	604	LMT	C2'-C1'-O1'-C1
5	A	611	LMT	C2'-C1'-O1'-C1
5	A	604	LMT	O5'-C1'-O1'-C1
5	A	608	LMT	C4-C5-C6-C7
5	A	606	LMT	C2-C1-O1'-C1'
5	A	607	LMT	C2-C3-C4-C5
5	A	607	LMT	C5'-C4'-O1B-C1B
5	A	602[A]	LMT	C3-C4-C5-C6
5	A	604	LMT	C6-C7-C8-C9
5	A	602[A]	LMT	O1'-C1-C2-C3
4	A	601	ZGS	C14-C15-C16-C17
5	A	603[B]	LMT	C11-C10-C9-C8
5	A	608	LMT	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
5	A	603[A]	LMT	C1-C2-C3-C4
5	A	606	LMT	O1'-C1-C2-C3
5	A	614	LMT	C3-C4-C5-C6
5	A	612	LMT	O5'-C5'-C6'-O6'
5	A	604	LMT	C1-C2-C3-C4
4	A	601	ZGS	C01-C02-C03-C04
5	A	615	LMT	C6-C7-C8-C9
5	A	604	LMT	O5B-C5B-C6B-O6B
5	C	301	LMT	C4B-C5B-C6B-O6B
5	A	606	LMT	C11-C10-C9-C8
5	A	612	LMT	C3-C4-C5-C6
5	A	605	LMT	O5B-C5B-C6B-O6B
5	A	603[B]	LMT	O1'-C1-C2-C3
5	A	609	LMT	C3-C4-C5-C6
5	C	301	LMT	C11-C10-C9-C8
5	A	603[B]	LMT	C3-C4-C5-C6
5	A	607	LMT	O5B-C5B-C6B-O6B
5	C	301	LMT	O5'-C5'-C6'-O6'
5	A	609	LMT	C5-C6-C7-C8
5	A	602[B]	LMT	C5-C6-C7-C8
5	A	615	LMT	C3-C4-C5-C6
5	A	612	LMT	C6-C7-C8-C9
5	A	610[A]	LMT	C2-C3-C4-C5
5	A	602[B]	LMT	C4B-C5B-C6B-O6B
5	A	603[A]	LMT	O5B-C5B-C6B-O6B
5	A	606	LMT	C3-C4-C5-C6
5	A	611	LMT	O5B-C5B-C6B-O6B
5	A	613	LMT	C3-C4-C5-C6
5	A	606	LMT	C2-C3-C4-C5
5	A	604	LMT	C5-C6-C7-C8
5	A	614	LMT	C2-C3-C4-C5
5	A	613	LMT	C6-C7-C8-C9
5	A	602[B]	LMT	C7-C8-C9-C10
5	A	603[A]	LMT	C5-C6-C7-C8
5	A	603[A]	LMT	C3-C4-C5-C6
5	A	605	LMT	C2-C3-C4-C5
5	A	606	LMT	C9-C10-C11-C12
5	A	603[A]	LMT	O5'-C5'-C6'-O6'
5	A	608	LMT	C5-C6-C7-C8
5	C	301	LMT	C5-C6-C7-C8
5	A	603[A]	LMT	C2-C1-O1'-C1'
5	A	611	LMT	C2-C1-O1'-C1'

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Mol	Chain	Res	Type	Atoms
5	C	301	LMT	C2-C1-O1'-C1'
5	A	613	LMT	O1'-C1-C2-C3
5	A	604	LMT	C2-C3-C4-C5
5	A	603[B]	LMT	C7-C8-C9-C10
5	A	612	LMT	C5-C6-C7-C8
5	A	603[B]	LMT	O5'-C5'-C6'-O6'
5	A	611	LMT	C5-C6-C7-C8
5	A	606	LMT	C5-C6-C7-C8
5	A	612	LMT	C4-C5-C6-C7
5	A	614	LMT	O1'-C1-C2-C3
4	A	601	ZGS	C06-C07-C08-C09
4	A	601	ZGS	C07-C08-C09-C10
4	A	601	ZGS	C11-C12-C13-C14
5	A	603[B]	LMT	C6-C7-C8-C9
5	A	609	LMT	C6-C7-C8-C9
5	A	603[A]	LMT	C4'-C5'-C6'-O6'
5	A	612	LMT	C1-C2-C3-C4
5	C	301	LMT	C3-C4-C5-C6
5	A	610[A]	LMT	O1'-C1-C2-C3
5	A	612	LMT	C2-C3-C4-C5
5	A	611	LMT	C9-C10-C11-C12
5	A	603[B]	LMT	C4'-C5'-C6'-O6'
5	A	609	LMT	O1'-C1-C2-C3
5	A	613	LMT	C5-C6-C7-C8
5	A	613	LMT	C2-C3-C4-C5
4	A	601	ZGS	O28-C29-C30-N31
5	A	610[B]	LMT	C2-C1-O1'-C1'
5	C	301	LMT	O1'-C1-C2-C3
5	A	612	LMT	O5B-C5B-C6B-O6B
5	C	301	LMT	C3'-C4'-O1B-C1B
5	A	603[A]	LMT	C4-C5-C6-C7
4	A	601	ZGS	C29-O28-P25-O26
5	C	301	LMT	C1-C2-C3-C4
5	A	602[B]	LMT	O5B-C1B-O1B-C4'
5	A	610[A]	LMT	C3-C4-C5-C6
5	A	607	LMT	O1'-C1-C2-C3
5	A	610[A]	LMT	C4B-C5B-C6B-O6B
5	A	615	LMT	C7-C8-C9-C10
5	C	301	LMT	C5'-C4'-O1B-C1B
5	A	609	LMT	C2-C1-O1'-C1'
5	A	606	LMT	C1-C2-C3-C4
5	A	602[B]	LMT	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
5	A	602[B]	LMT	C11-C10-C9-C8
5	A	607	LMT	C4-C5-C6-C7
5	A	607	LMT	C9-C10-C11-C12
5	A	602[A]	LMT	C5-C6-C7-C8
5	A	608	LMT	C1-C2-C3-C4
4	A	601	ZGS	C22-C23-O24-P25
5	A	610[B]	LMT	C9-C10-C11-C12
5	A	603[B]	LMT	C4-C5-C6-C7
5	A	615	LMT	C1-C2-C3-C4
5	A	604	LMT	C11-C10-C9-C8
5	A	605	LMT	C11-C10-C9-C8
5	A	605	LMT	O5'-C1'-O1'-C1
5	A	606	LMT	C6-C7-C8-C9
5	A	614	LMT	C5-C6-C7-C8
5	A	603[B]	LMT	C2-C1-O1'-C1'
5	A	603[B]	LMT	O5'-C1'-O1'-C1
5	A	602[B]	LMT	C2B-C1B-O1B-C4'
5	C	301	LMT	C9-C10-C11-C12
5	A	615	LMT	O1'-C1-C2-C3
5	A	602[A]	LMT	C1-C2-C3-C4
5	A	606	LMT	C2B-C1B-O1B-C4'
5	A	605	LMT	O1'-C1-C2-C3
5	A	610[B]	LMT	C6-C7-C8-C9
5	A	607	LMT	C5-C6-C7-C8
5	A	602[A]	LMT	O5'-C5'-C6'-O6'

There are no ring outliers.

13 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	611	LMT	1	0
5	A	606	LMT	1	0
4	A	601	ZGS	1	0
5	A	610[A]	LMT	2	0
5	A	605	LMT	1	0
5	A	604	LMT	1	0
5	A	609	LMT	3	0
5	A	607	LMT	2	0
5	A	610[B]	LMT	2	0
5	A	602[A]	LMT	2	0
5	C	301	LMT	2	0
5	A	603[A]	LMT	1	0

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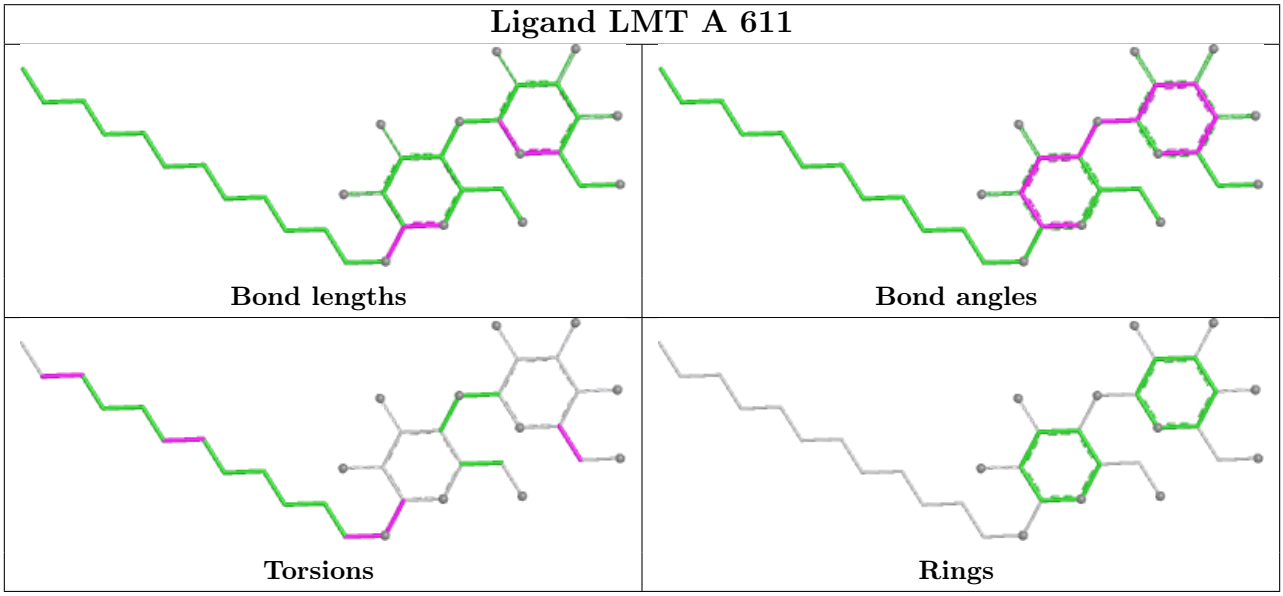
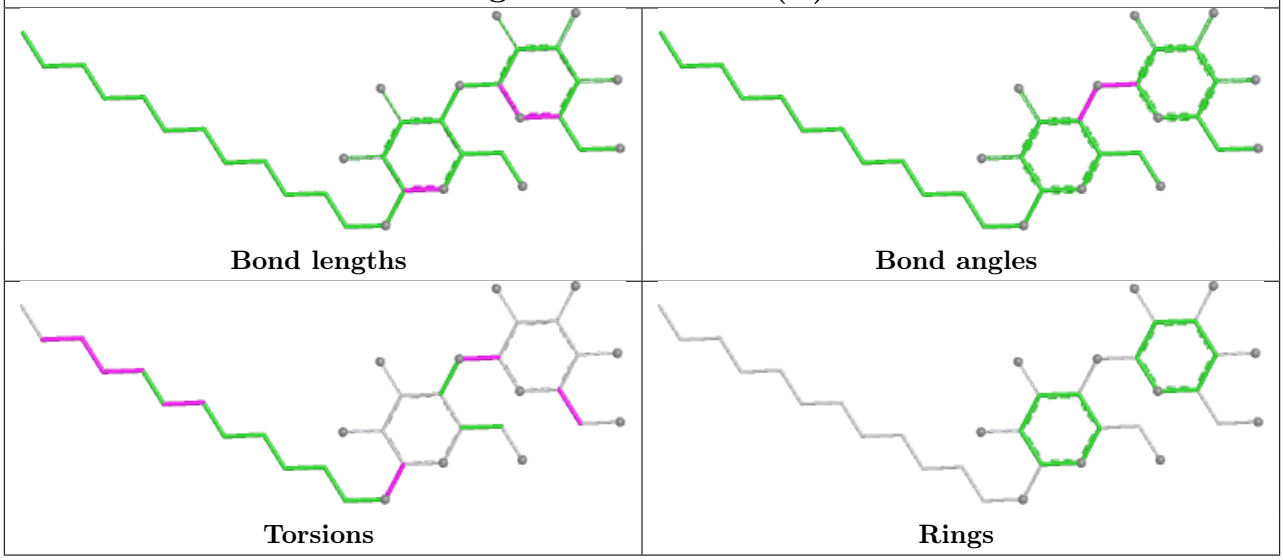
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	615	LMT	1	0

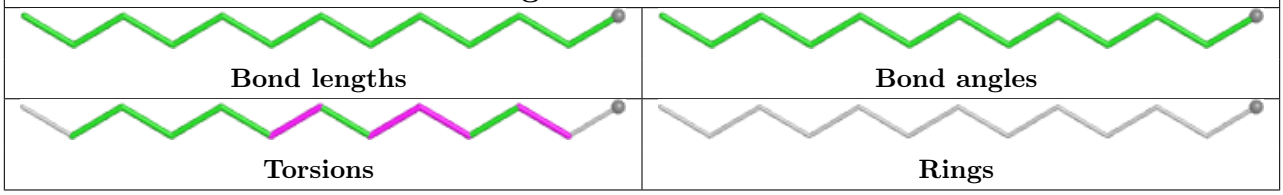
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



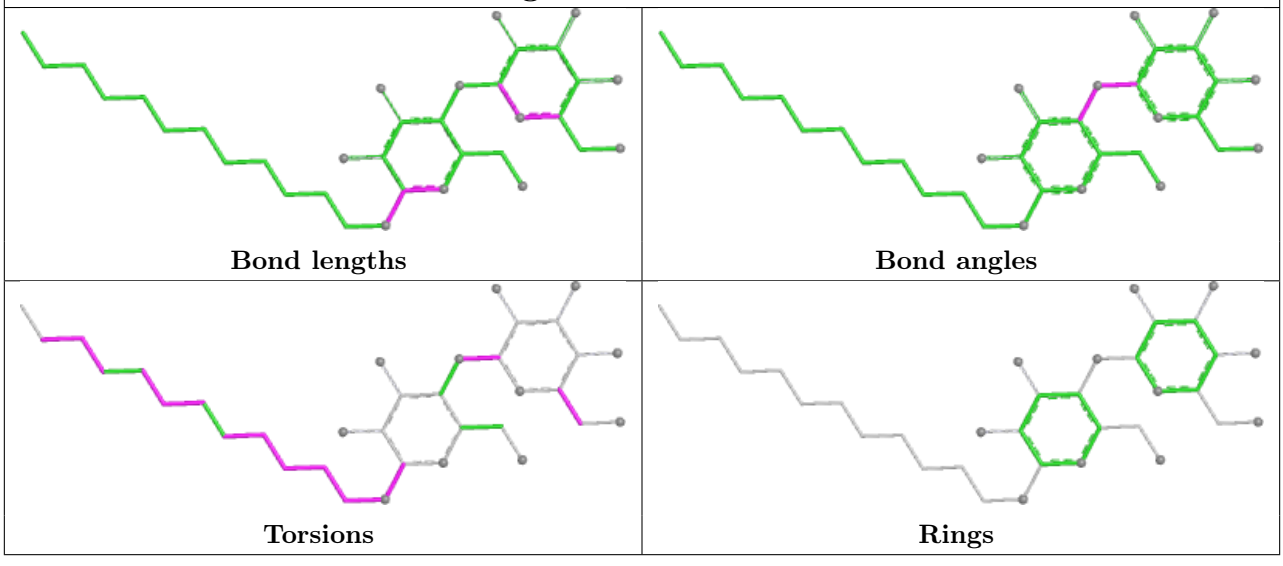
Ligand LMT A 602 (B)



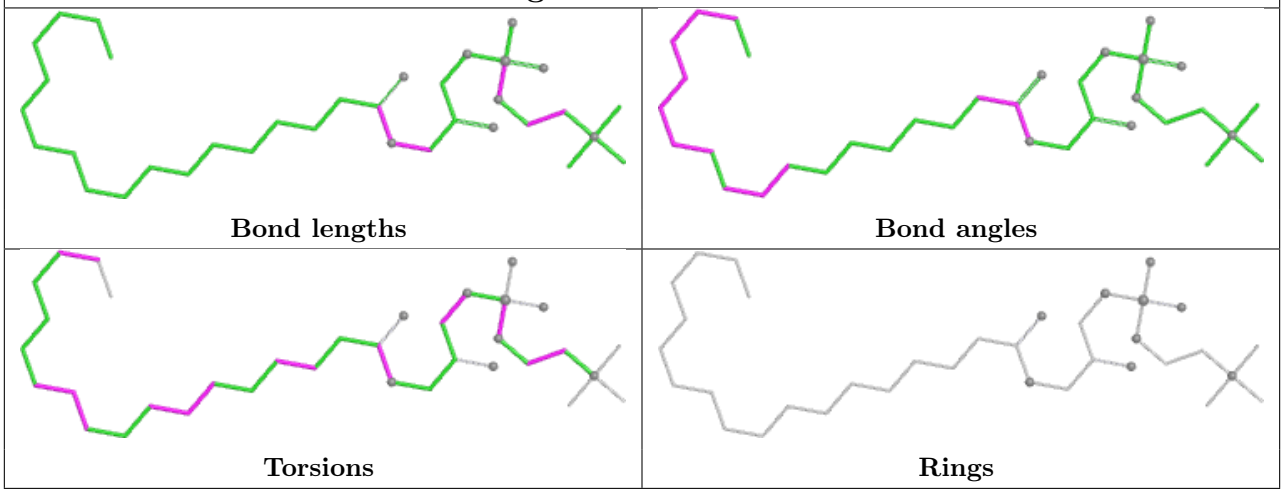
Ligand LMT A 614



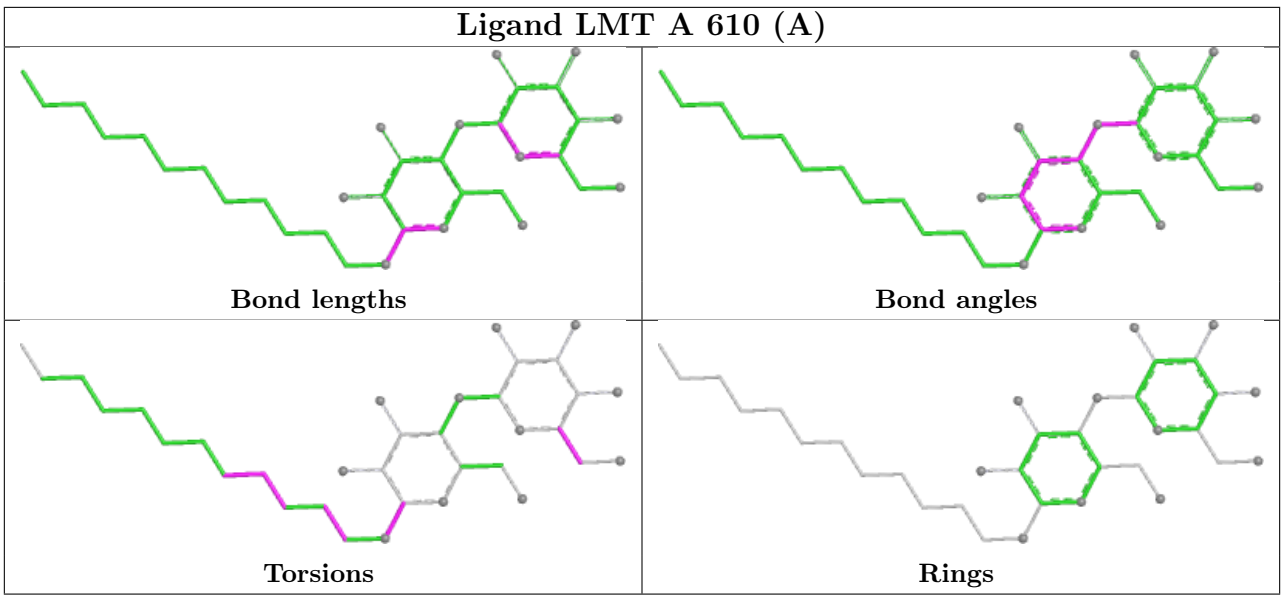
Ligand LMT A 606



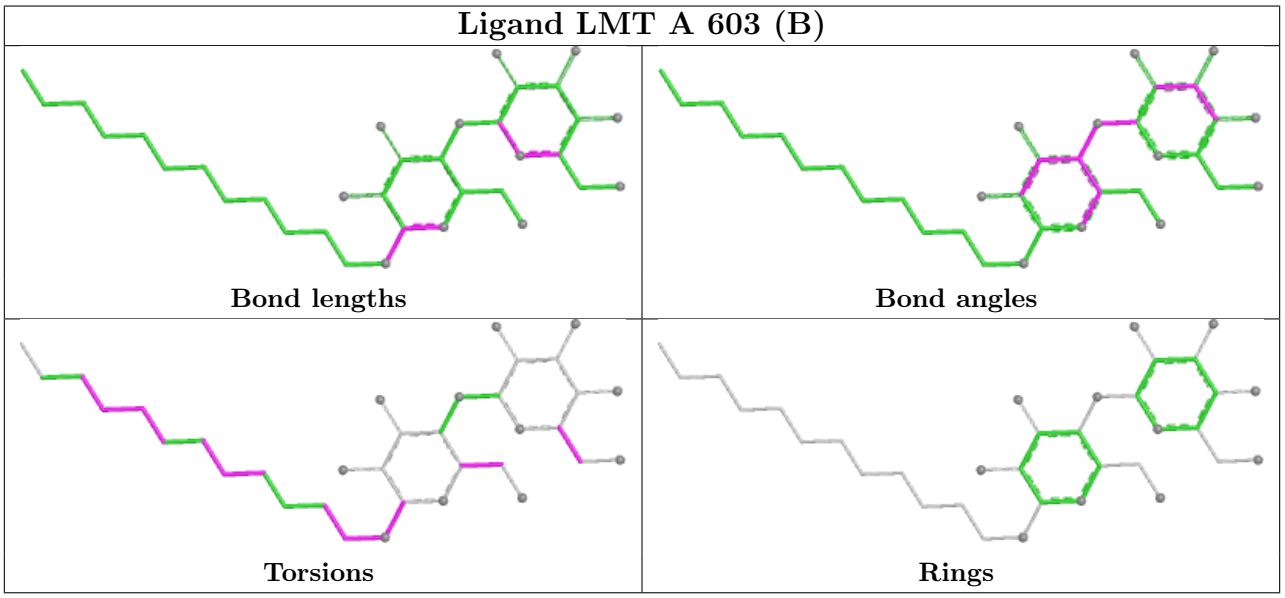
Ligand ZGS A 601



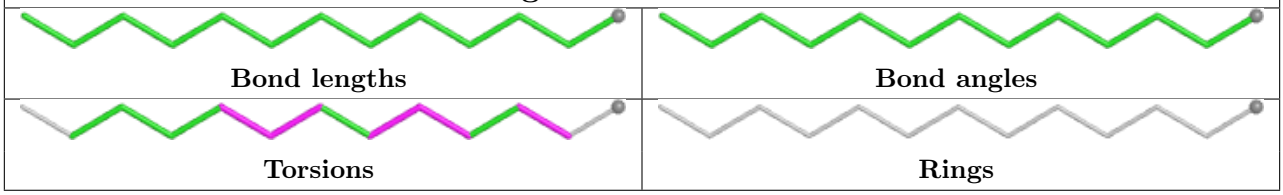
Ligand LMT A 610 (A)



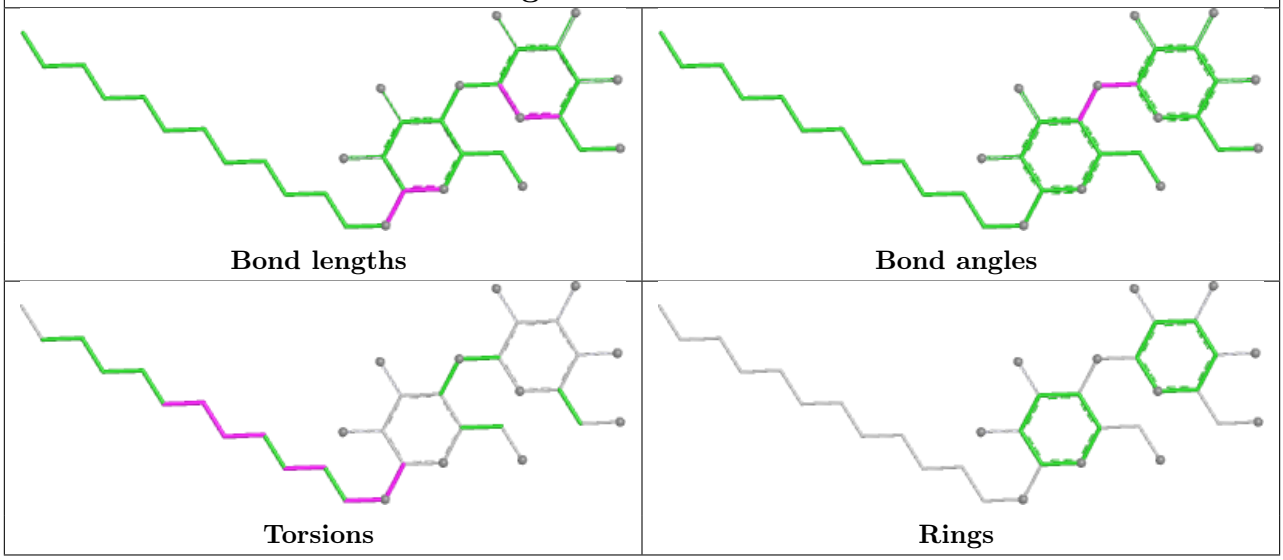
Ligand LMT A 603 (B)



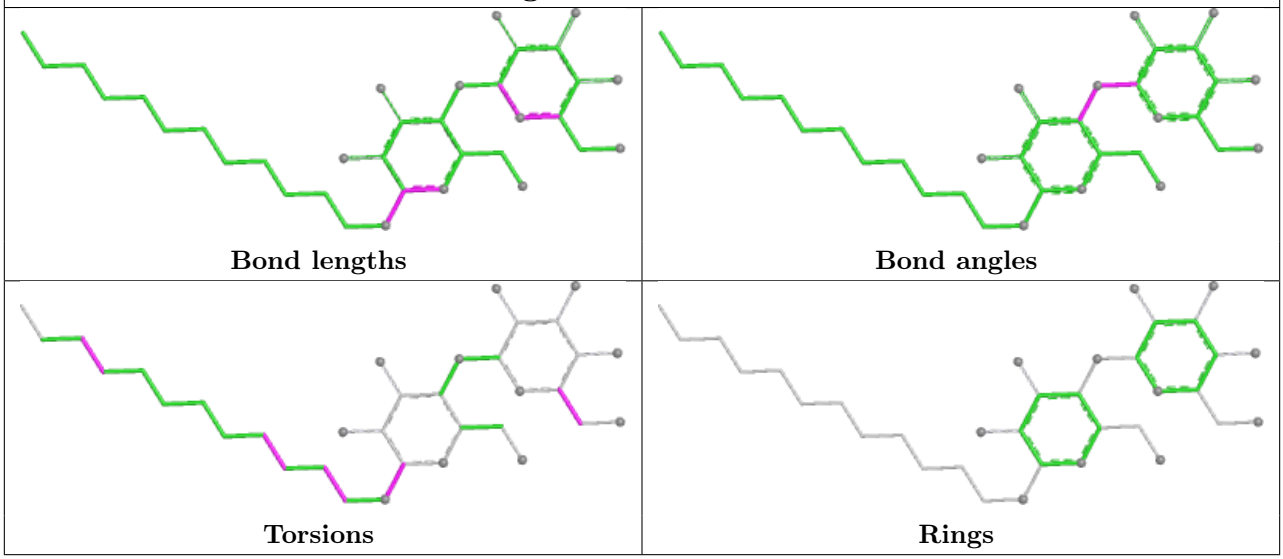
Ligand LMT A 613



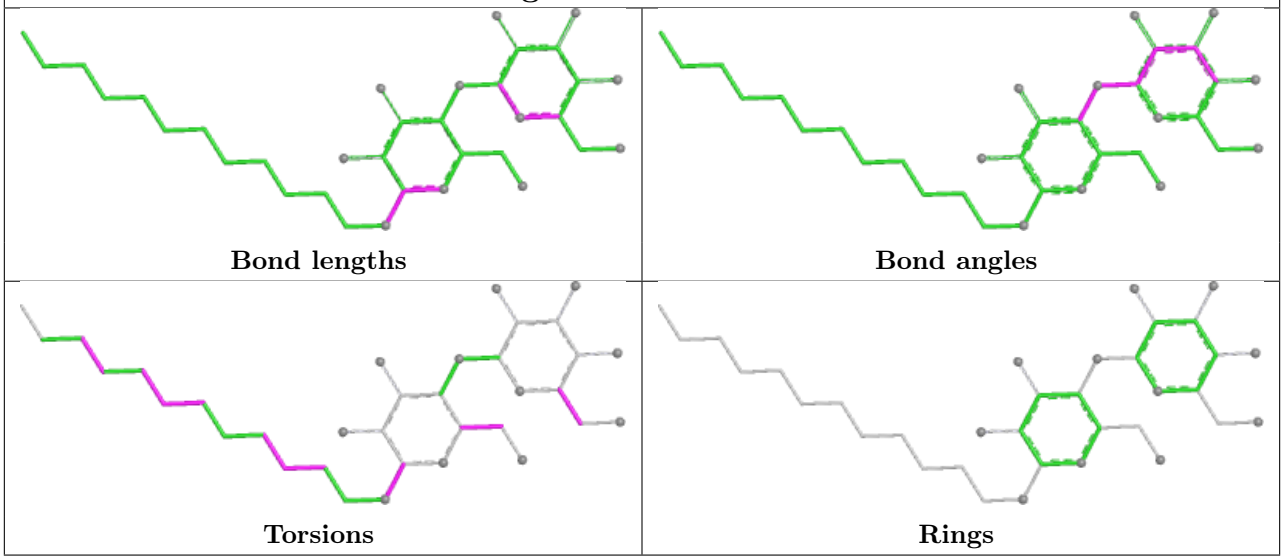
Ligand LMT A 608



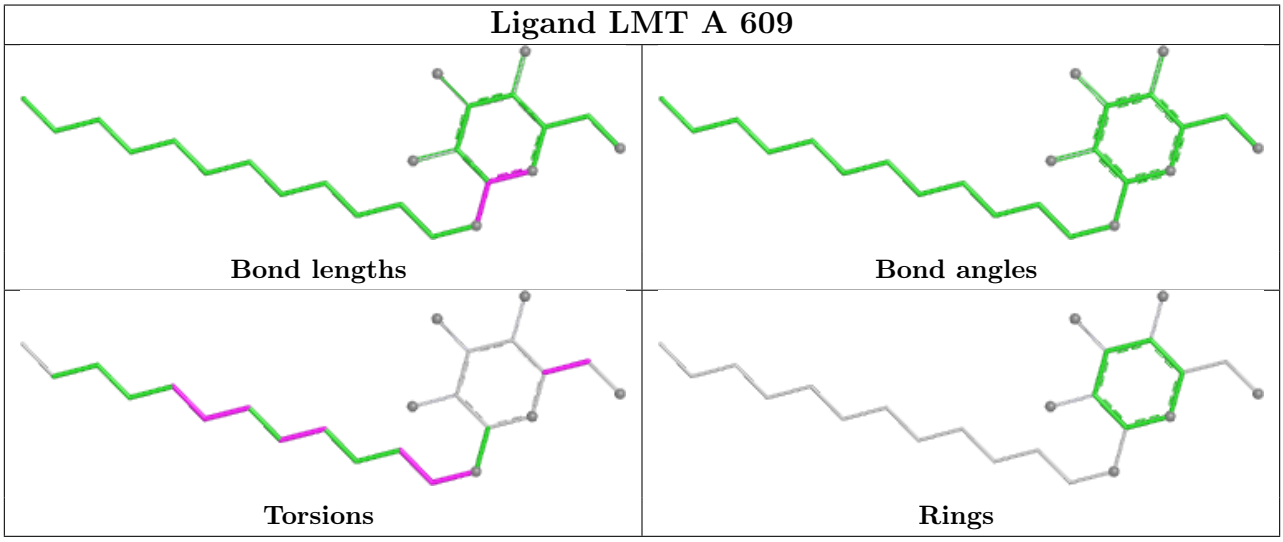
Ligand LMT A 605



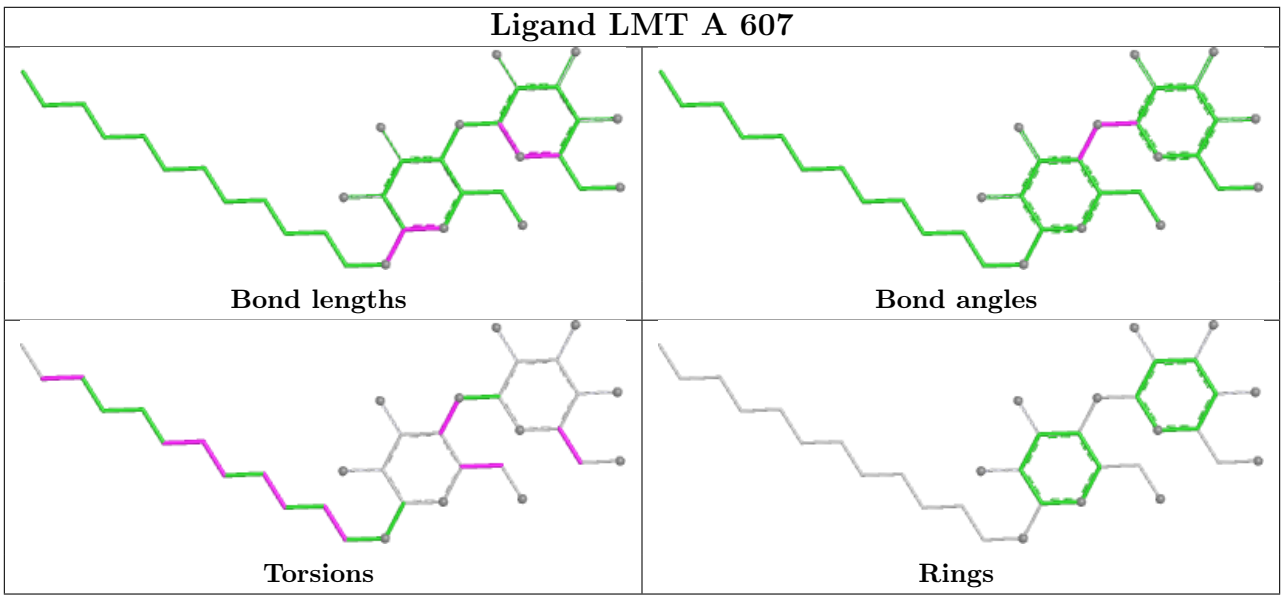
Ligand LMT A 604



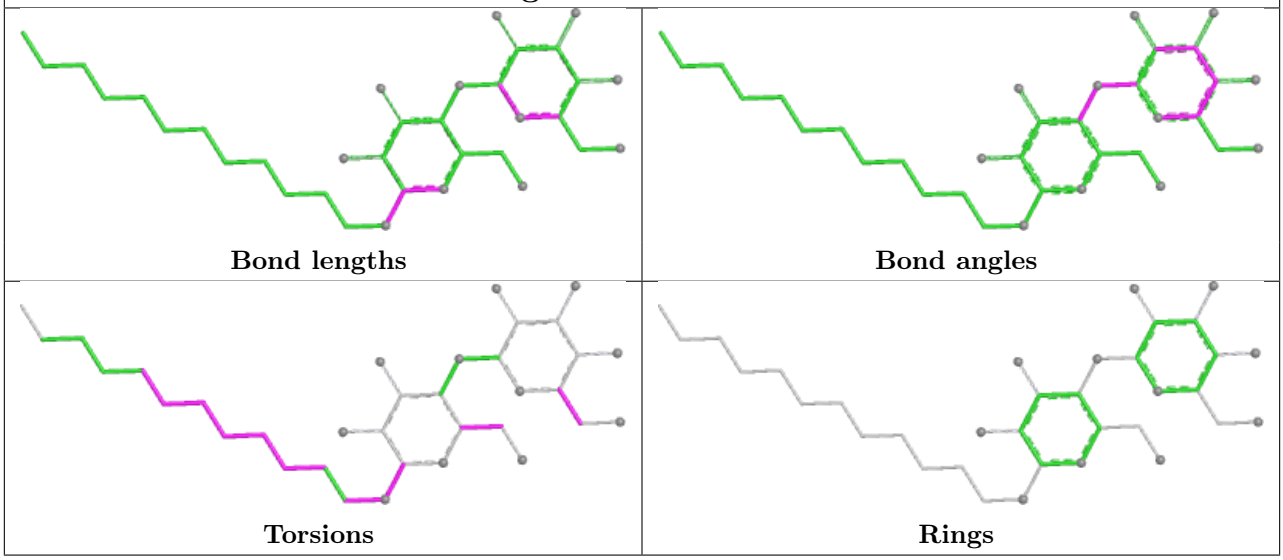
Ligand LMT A 609



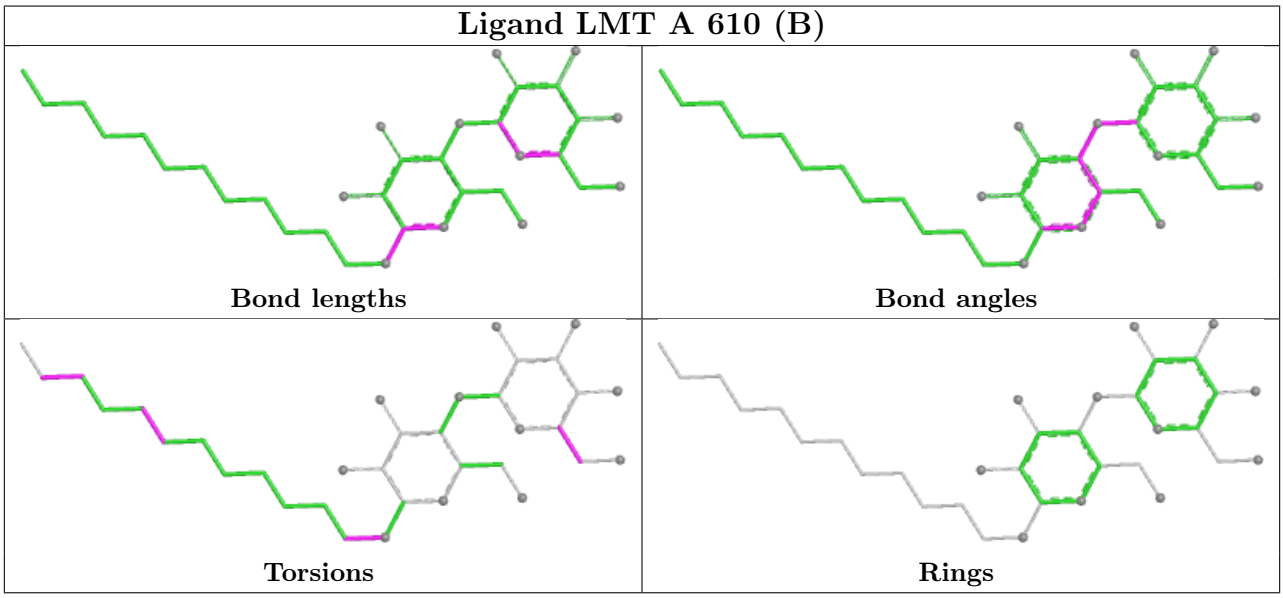
Ligand LMT A 607



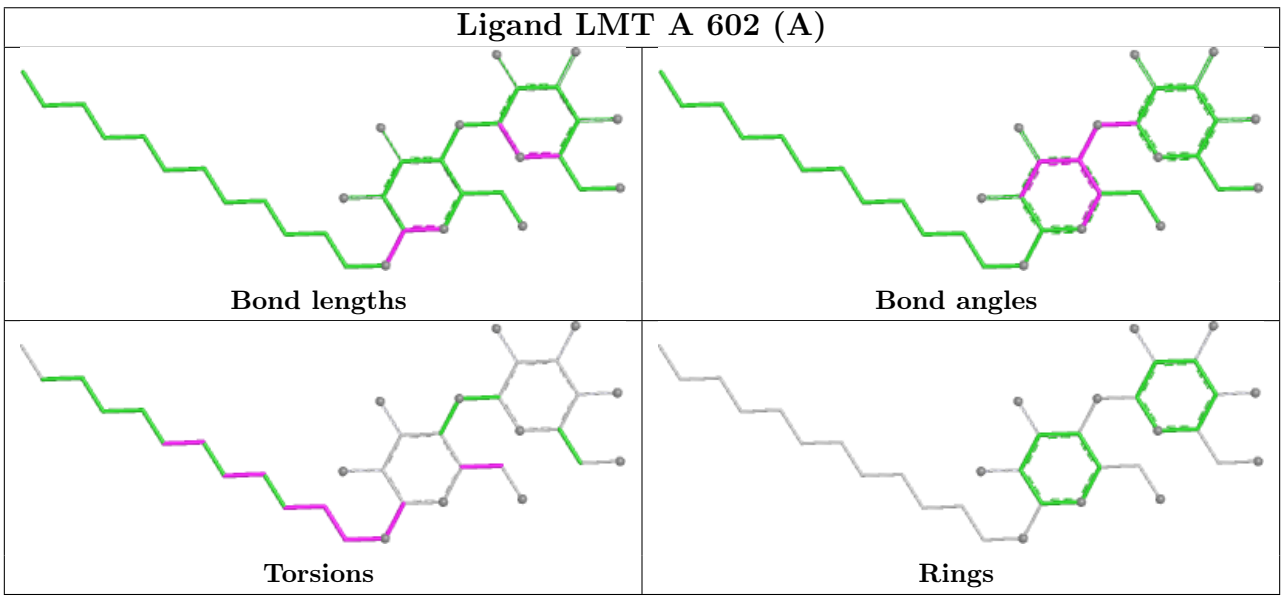
Ligand LMT A 612

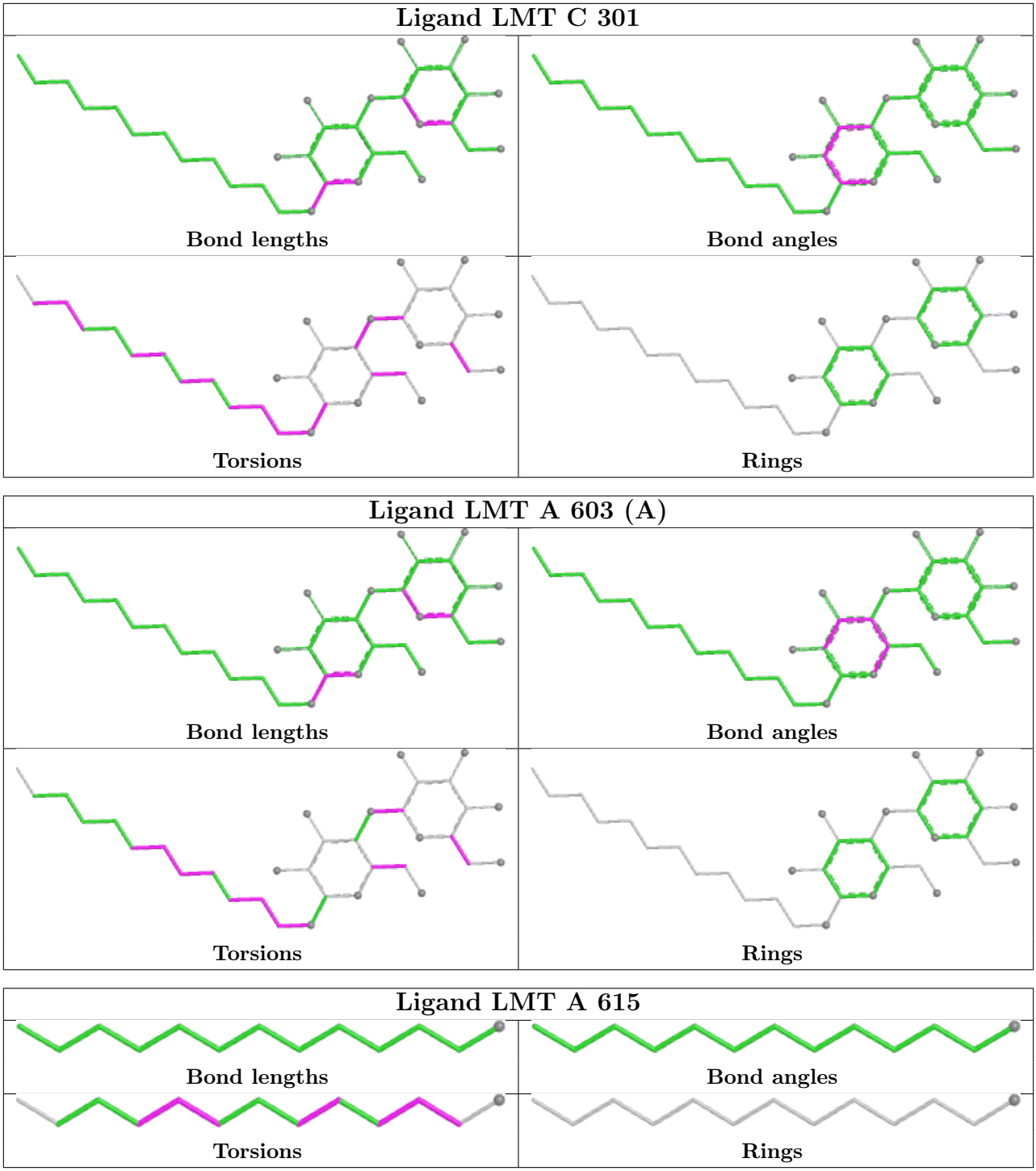


Ligand LMT A 610 (B)



Ligand LMT A 602 (A)





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

This section contains visualisations of the EMDB entry EMD-27152. These allow visual inspection of the internal detail of the map and identification of artifacts.

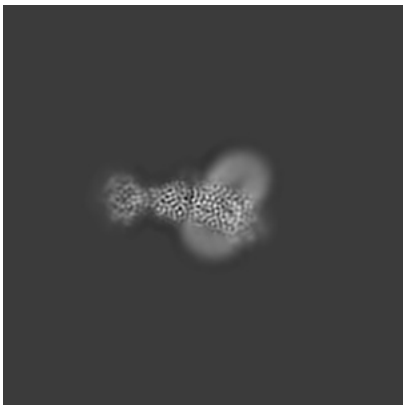
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

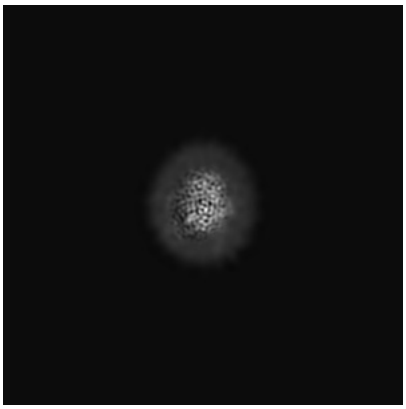
6.1.1 Primary map



X

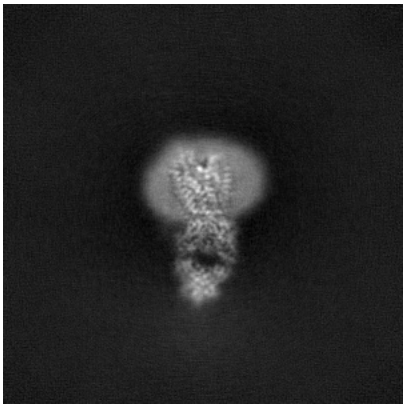


Y

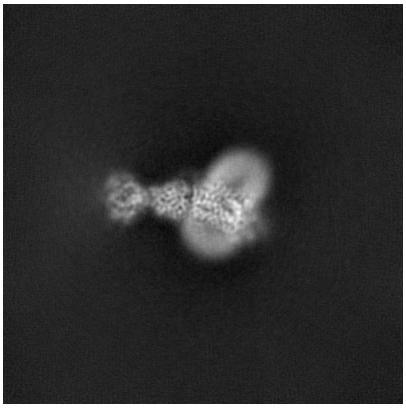


Z

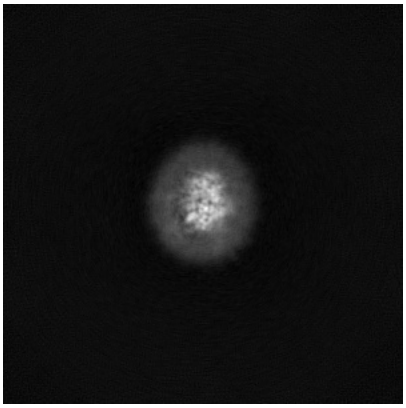
6.1.2 Raw map



X



Y

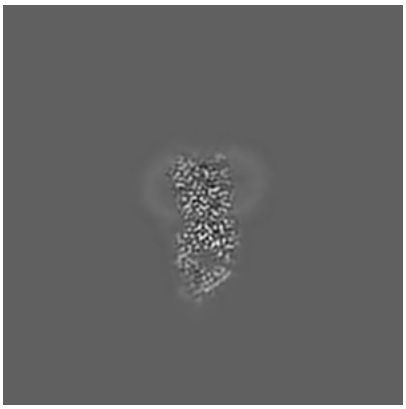


Z

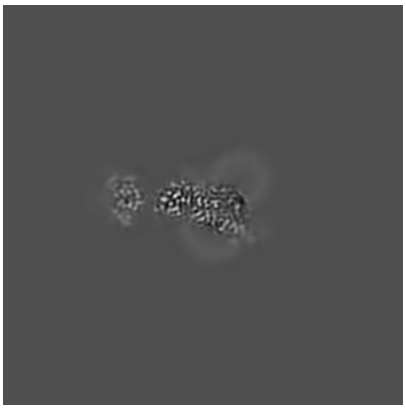
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

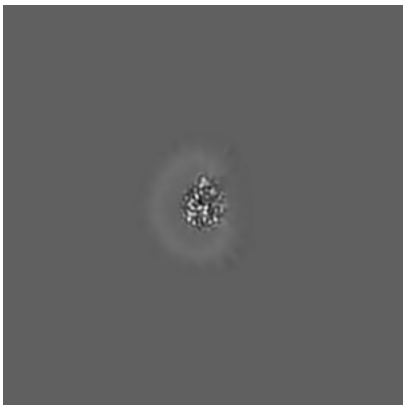
6.2.1 Primary map



X Index: 192

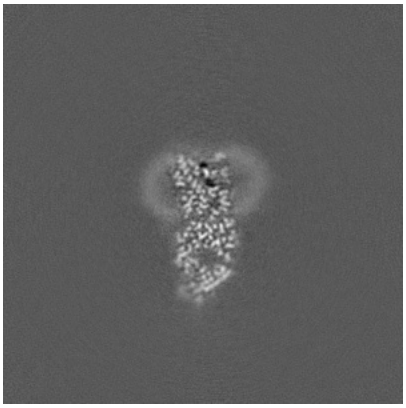


Y Index: 192

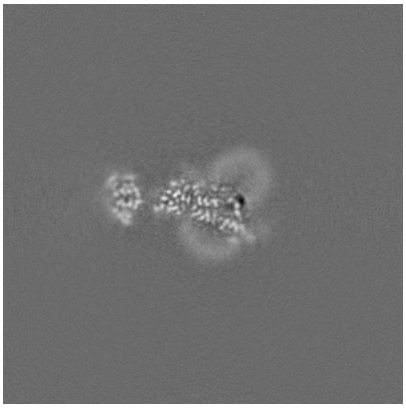


Z Index: 192

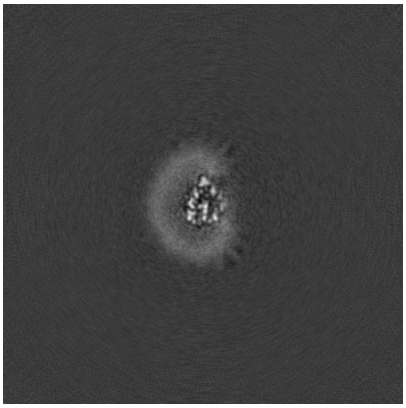
6.2.2 Raw map



X Index: 192



Y Index: 192

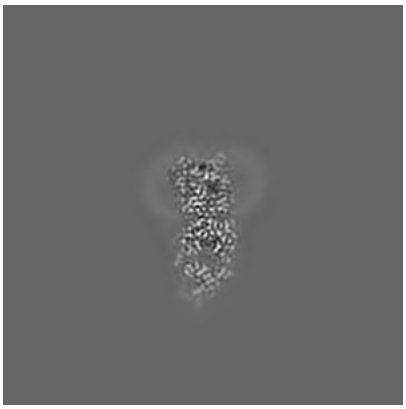


Z Index: 192

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: 194

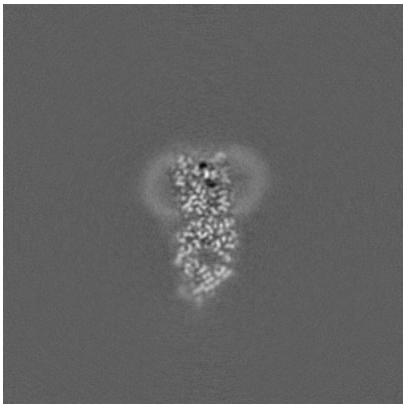


Y Index: 189

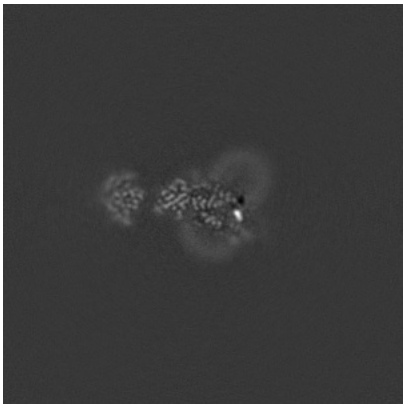


Z Index: 164

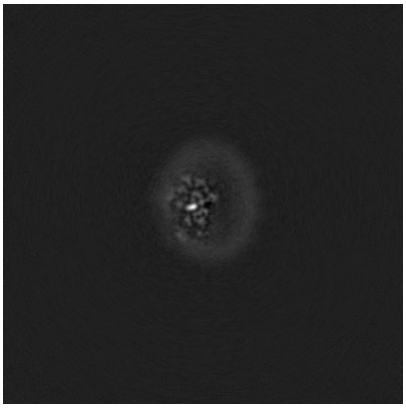
6.3.2 Raw map



X Index: 193



Y Index: 189

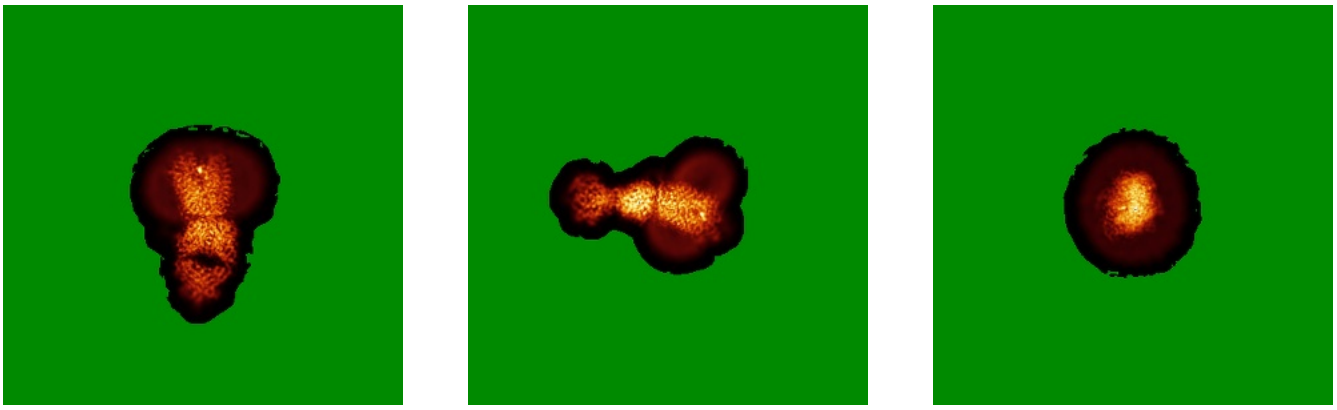


Z Index: 225

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

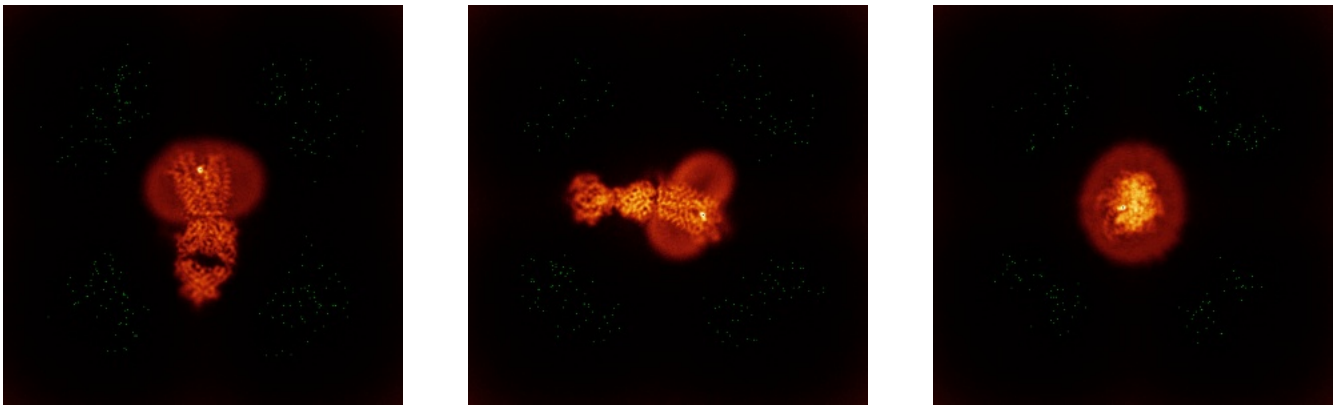
6.4 Orthogonal standard-deviation projections (False-color) (i)

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)

This section was not generated.

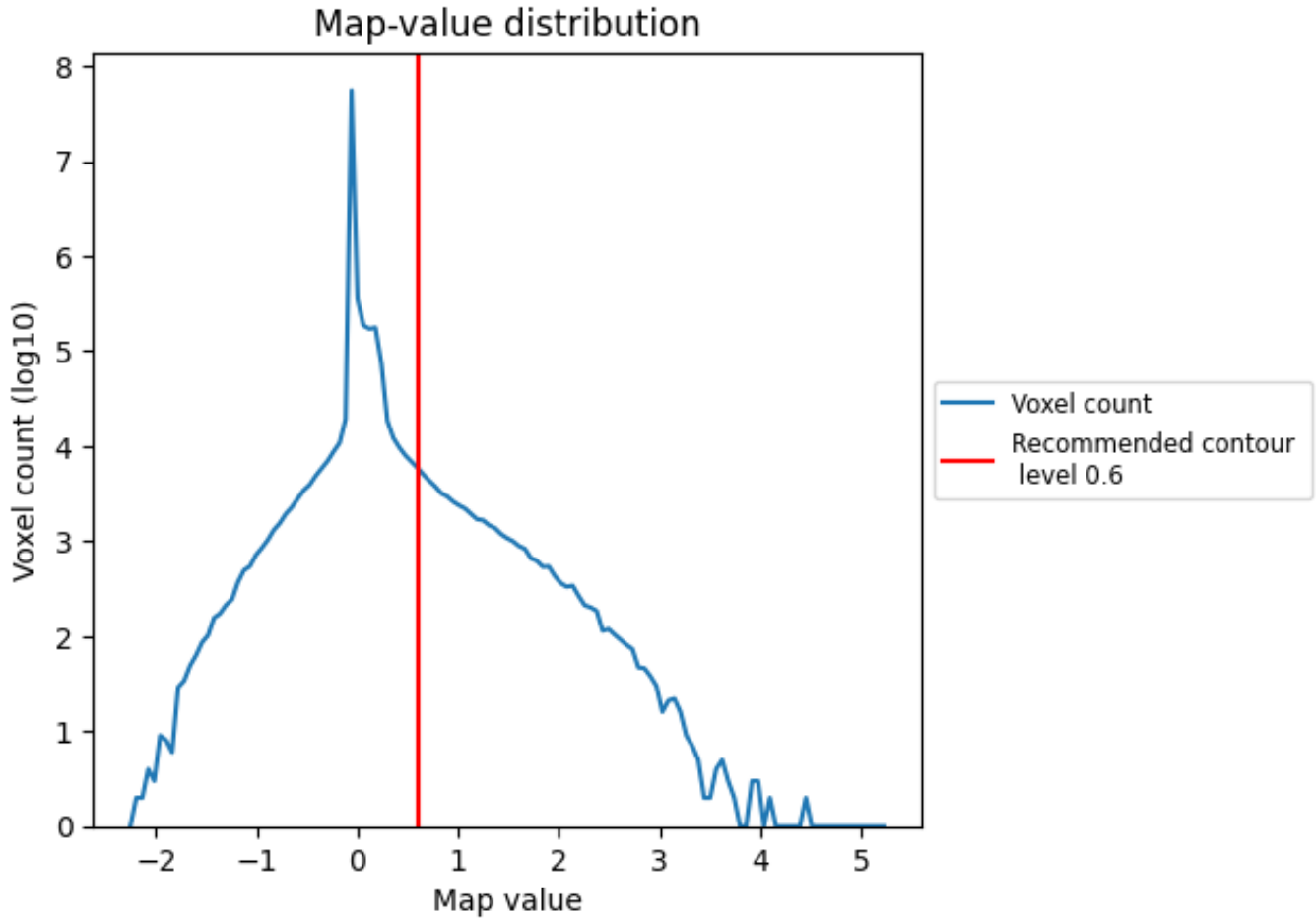
6.6 Mask visualisation (i)

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

7 Map analysis

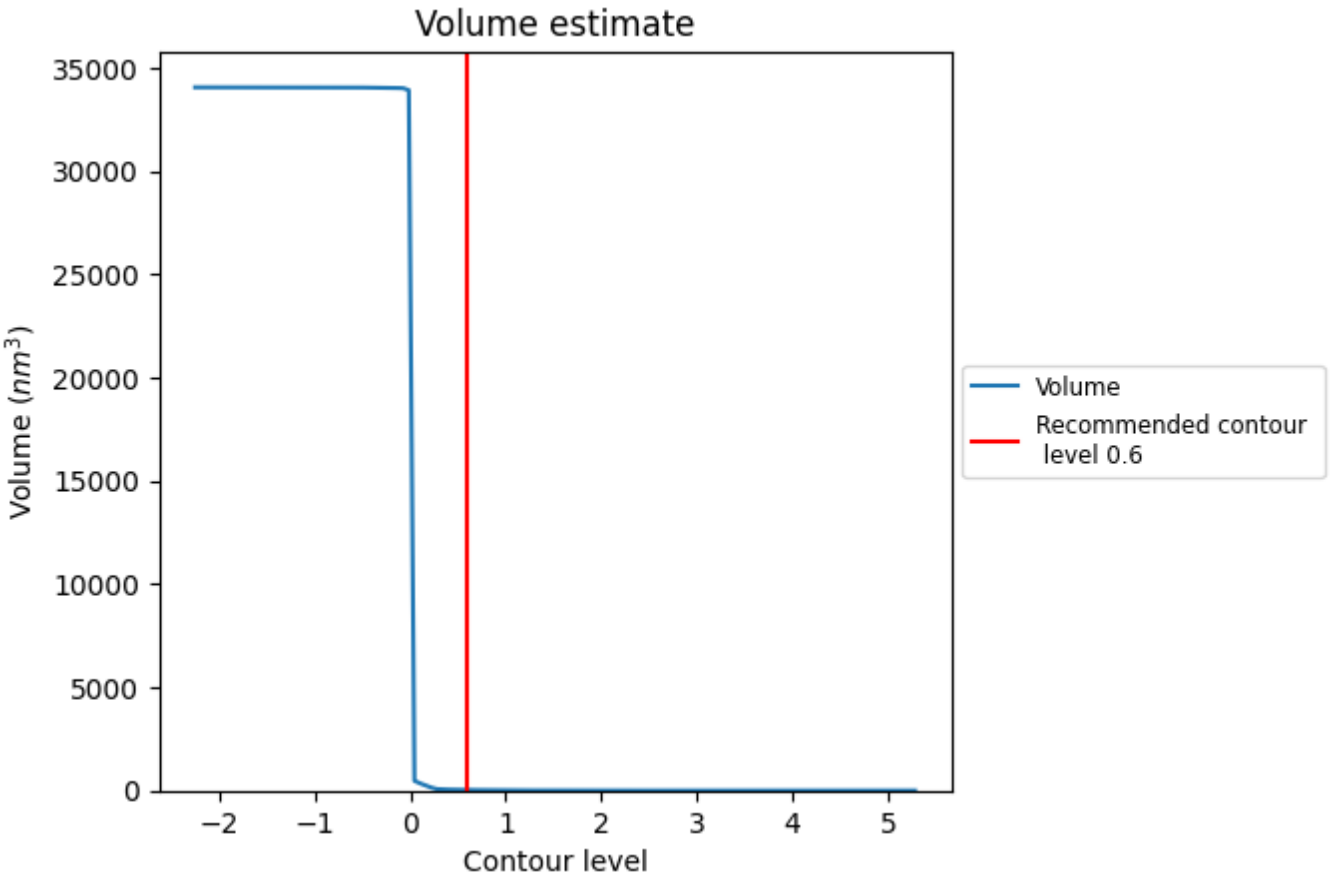
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

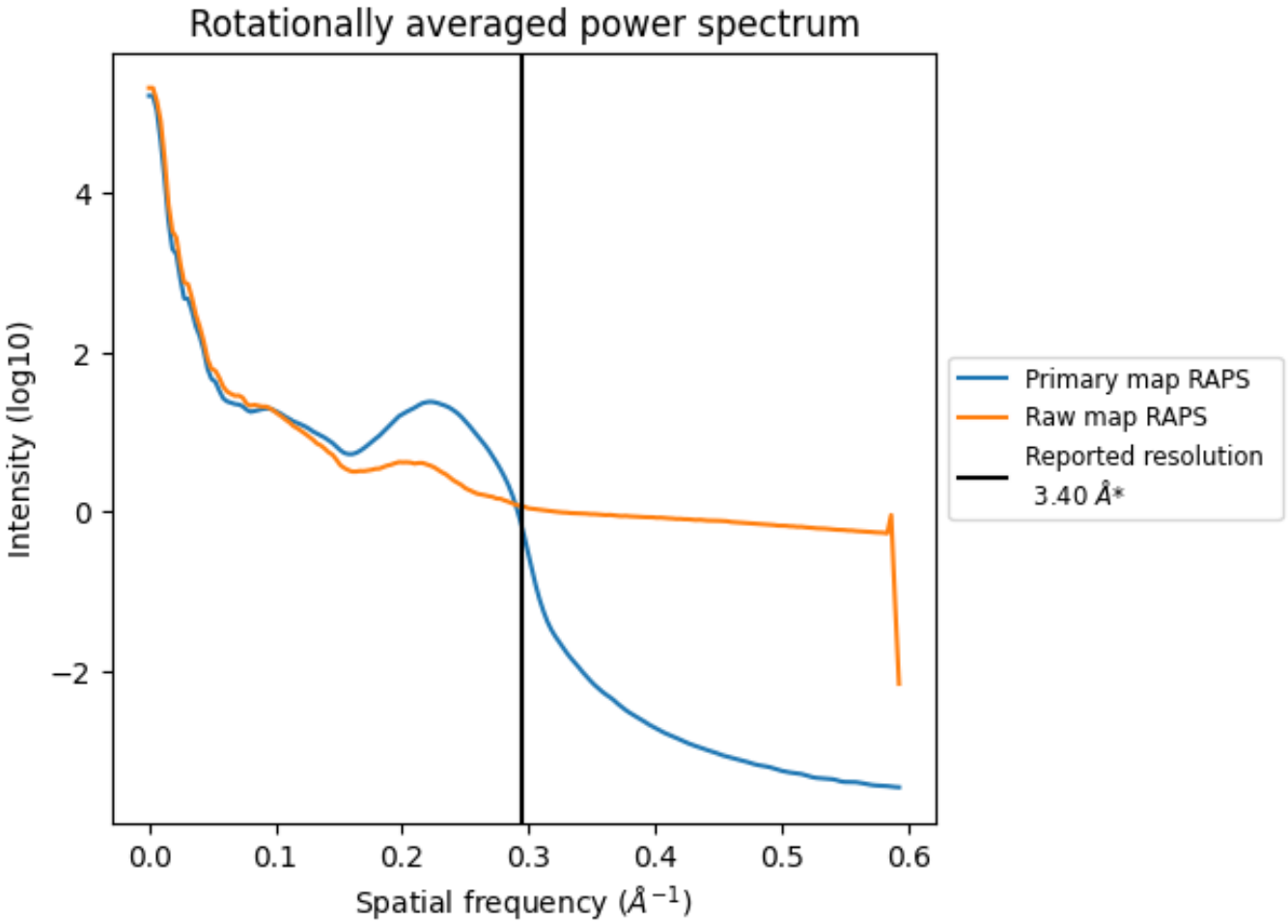
7.2 Volume estimate



The volume at the recommended contour level is 31 nm^3; this corresponds to an approximate mass of 28 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 (i)

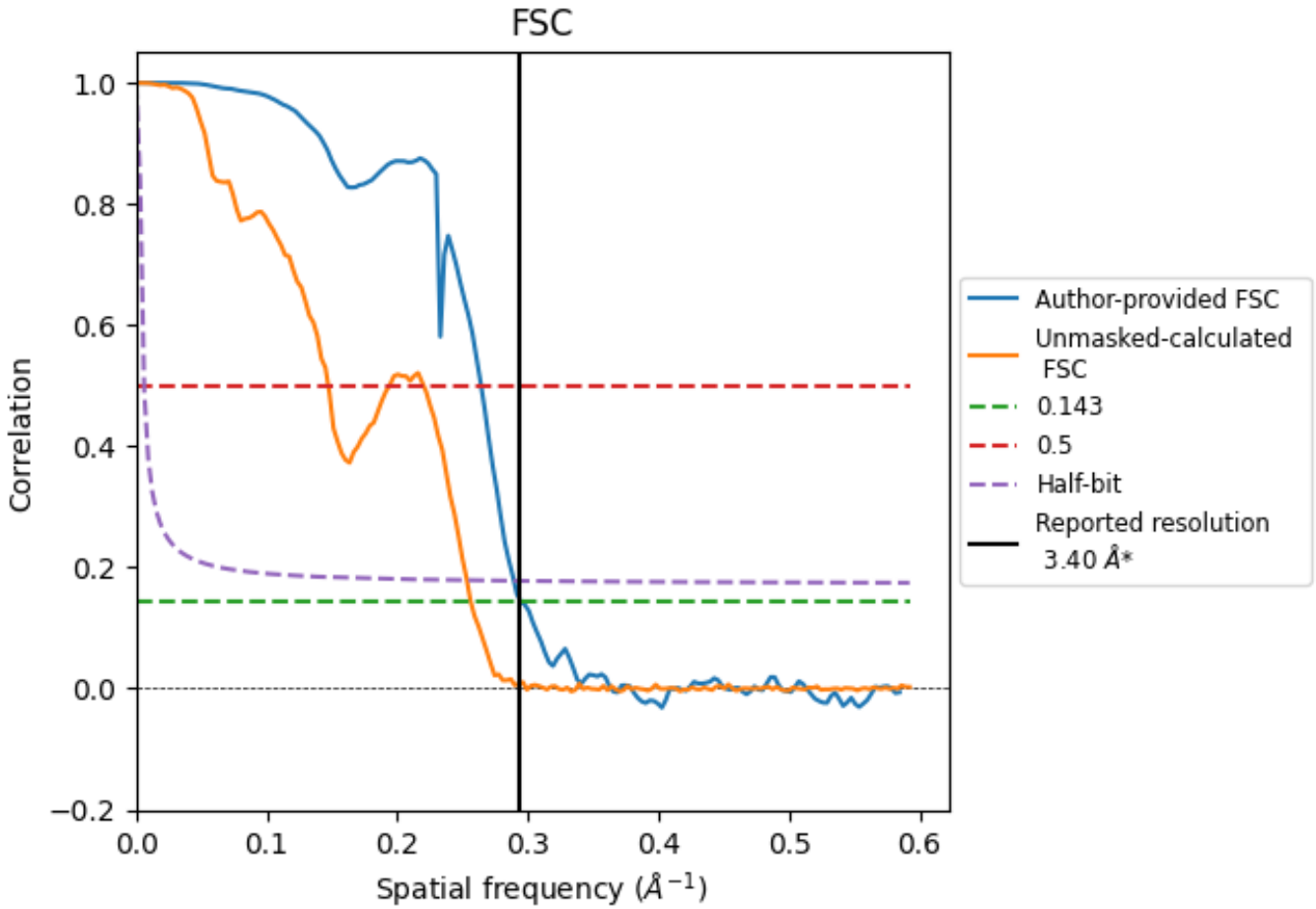


*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.39	3.79	3.46
Unmasked-calculated*	3.90	6.79	3.95

*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 3.90 differs from the reported value 3.4 by more than 10 %

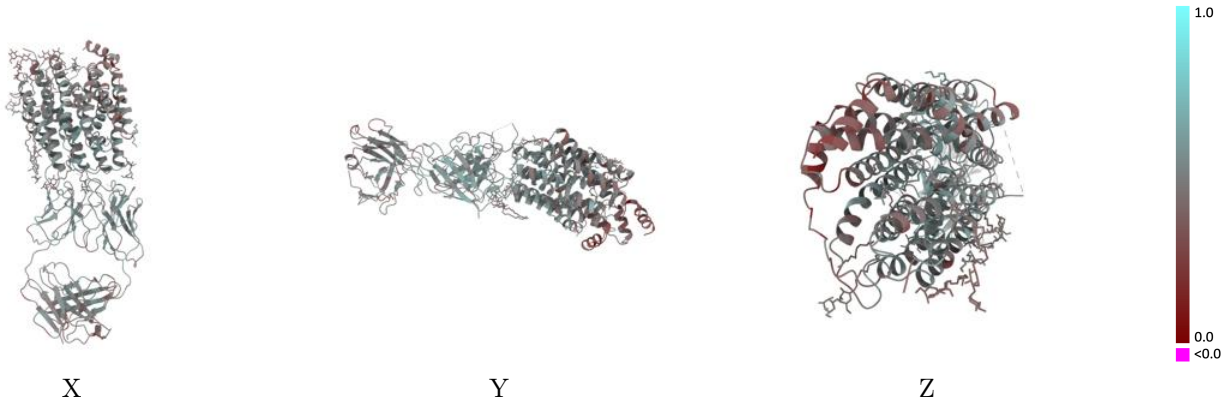
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-27152 and PDB model 8D2W. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay

This section was not generated.

9.2 Q-score mapped to coordinate model



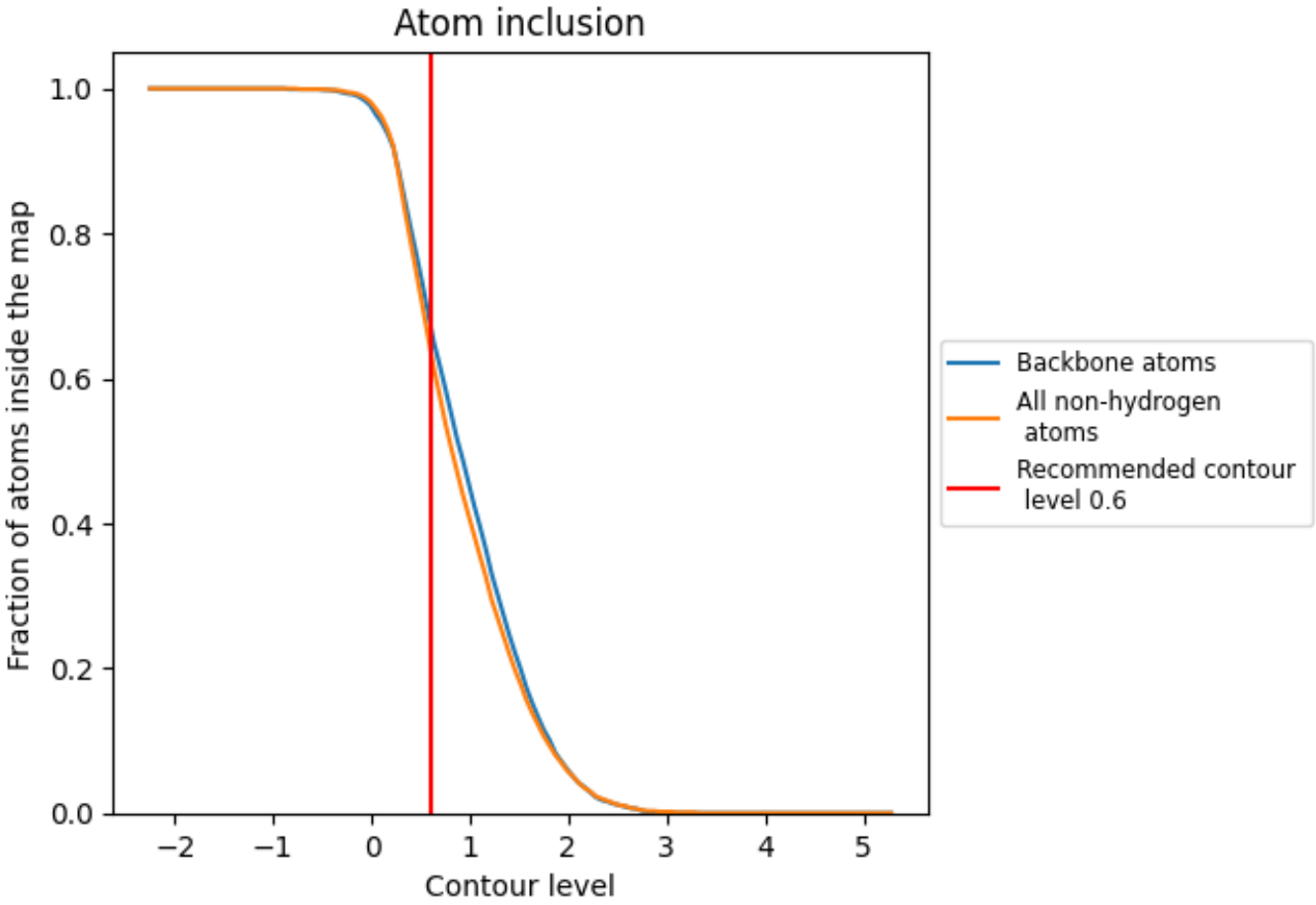
X Y Z

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

9.3 Atom inclusion mapped to coordinate model

This section was not generated.

9.4 Atom inclusion (i)



At the recommended contour level, 67% of all backbone atoms, 64% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.6) and Q-score for the entire model and for each chain.



Chain	Atom inclusion	Q-score
All	0.6390	0.4820
A	0.5870	0.4720
B	0.7230	0.4920
C	0.7070	0.4990