Full wwPDB EM Validation Report (i)

Mar 11, 2024 – 01:35 AM EDT

PDB ID	:	6UCU
EMDB ID	:	EMD-20728
Title	:	Cryo-EM structure of the mitochondrial TOM complex from yeast (dimer)
Authors	:	Park, E.; Tucker, K.
Deposited on	:	2019-09-17
Resolution	:	3.06 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (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:

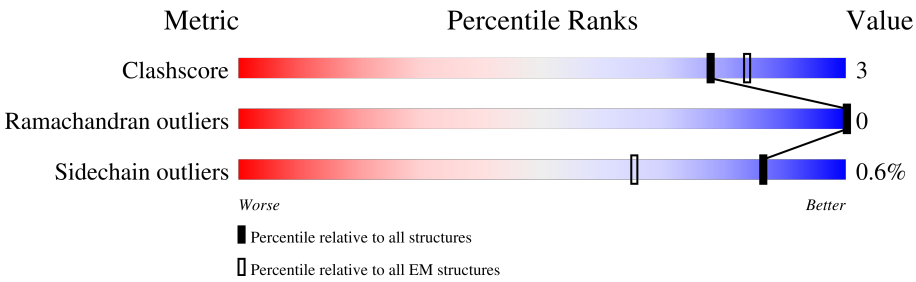
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.06 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	397	8% 70% 7% • 23%
1	I	397	8% 70% 7% • 23%
2	B	162	10% 30% • 69%
2	J	162	10% 30% • 69%
3	C	50	30% 58% 16% 26%
3	K	50	28% 58% 16% 26%
4	D	61	10% 51% 7% 43%
4	L	61	10% 52% 5% 43%

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Mol	Chain	Length	Quality of chain
5	E	60	37% 82% • 17%
5	M	60	37% 82% • 17%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 9610 atoms, of which 1412 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 Mitochondrial import receptor subunit TOM40.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	307	2369	1494	402	466	7	0	0
1	I	307	2369	1494	402	466	7	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	388	GLY	-	expression tag	UNP P23644
A	389	GLY	-	expression tag	UNP P23644
A	390	TRP	-	expression tag	UNP P23644
A	391	SER	-	expression tag	UNP P23644
A	392	HIS	-	expression tag	UNP P23644
A	393	PRO	-	expression tag	UNP P23644
A	394	GLN	-	expression tag	UNP P23644
A	395	PHE	-	expression tag	UNP P23644
A	396	GLU	-	expression tag	UNP P23644
A	397	LYS	-	expression tag	UNP P23644
I	388	GLY	-	expression tag	UNP P23644
I	389	GLY	-	expression tag	UNP P23644
I	390	TRP	-	expression tag	UNP P23644
I	391	SER	-	expression tag	UNP P23644
I	392	HIS	-	expression tag	UNP P23644
I	393	PRO	-	expression tag	UNP P23644
I	394	GLN	-	expression tag	UNP P23644
I	395	PHE	-	expression tag	UNP P23644
I	396	GLU	-	expression tag	UNP P23644
I	397	LYS	-	expression tag	UNP P23644

- Molecule 2 is a protein called Mitochondrial import receptor subunit TOM22.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	50	Total 387	C 249	N 61	O 76	S 1	0	0
2	J	50	Total 387	C 249	N 61	O 76	S 1	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	153	GLY	-	expression tag	UNP P49334
B	154	GLY	-	expression tag	UNP P49334
B	155	HIS	-	expression tag	UNP P49334
B	156	HIS	-	expression tag	UNP P49334
B	157	HIS	-	expression tag	UNP P49334
B	158	HIS	-	expression tag	UNP P49334
B	159	HIS	-	expression tag	UNP P49334
B	160	HIS	-	expression tag	UNP P49334
B	161	HIS	-	expression tag	UNP P49334
B	162	HIS	-	expression tag	UNP P49334
J	153	GLY	-	expression tag	UNP P49334
J	154	GLY	-	expression tag	UNP P49334
J	155	HIS	-	expression tag	UNP P49334
J	156	HIS	-	expression tag	UNP P49334
J	157	HIS	-	expression tag	UNP P49334
J	158	HIS	-	expression tag	UNP P49334
J	159	HIS	-	expression tag	UNP P49334
J	160	HIS	-	expression tag	UNP P49334
J	161	HIS	-	expression tag	UNP P49334
J	162	HIS	-	expression tag	UNP P49334

- Molecule 3 is a protein called Mitochondrial import receptor subunit TOM5.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	37	Total 303	C 201	N 52	O 49	S 1	0	0
3	K	37	Total 303	C 201	N 52	O 49	S 1	0	0

- Molecule 4 is a protein called Mitochondrial import receptor subunit TOM6.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	35	Total 267	C 180	N 39	O 46	S 2	0	0

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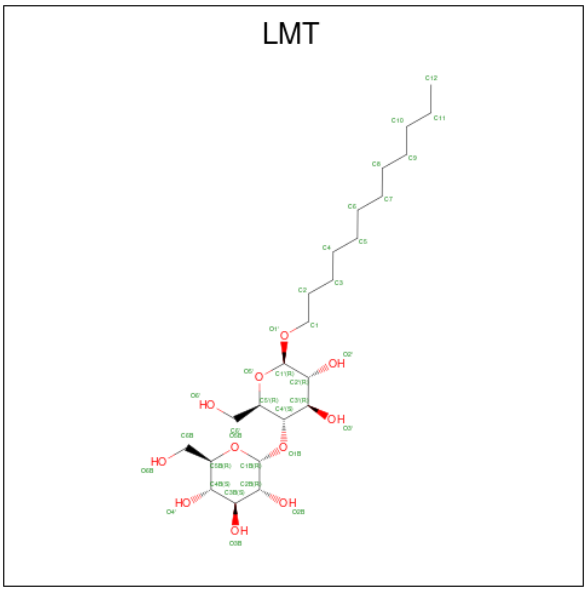
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	L	35	267	180	39	46	2	0	0

- Molecule 5 is a protein called Mitochondrial import receptor subunit TOM7.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	E	50	393	260	69	64	0	0
5	M	50	393	260	69	64	0	0

- Molecule 6 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	H	
6	A	1	35	12	23	0
6	A	1	35	12	23	0
6	A	1	35	12	23	0
6	A	1	35	12	23	0
6	A	1	35	12	23	0
6	A	1	35	12	23	0

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Mol	Chain	Residues	Atoms	AltConf
6	A	1	Total C H 35 12 23	0
6	A	1	Total C H 35 12 23	0
6	A	1	Total C H 35 12 23	0
6	A	1	Total C H 35 12 23	0
6	A	1	Total C H 35 12 23	0
6	A	1	Total C H 35 12 23	0
6	A	1	Total C H 35 12 23	0
6	A	1	Total C H O 80 24 45 11	0
6	A	1	Total C H 35 12 23	0
6	A	1	Total C H 35 12 23	0
6	A	1	Total C H 35 12 23	0
6	B	1	Total C H 26 9 17	0
6	B	1	Total C H 35 12 23	0
6	B	1	Total C H 35 12 23	0
6	B	1	Total C H 35 12 23	0
6	C	1	Total C H 35 12 23	0
6	C	1	Total C H 35 12 23	0
6	D	1	Total C H 35 12 23	0
6	D	1	Total C H 35 12 23	0
6	D	1	Total C H 35 12 23	0
6	E	1	Total C H 35 12 23	0

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Mol	Chain	Residues	Atoms	AltConf
6	E	1	Total C H 35 12 23	0
6	E	1	Total C H 35 12 23	0
6	E	1	Total C H 35 12 23	0
6	I	1	Total C H O 80 24 45 11	0
6	I	1	Total C H 35 12 23	0
6	I	1	Total C H 35 12 23	0
6	I	1	Total C H 35 12 23	0
6	I	1	Total C H 35 12 23	0
6	I	1	Total C H 35 12 23	0
6	I	1	Total C H 35 12 23	0
6	I	1	Total C H 35 12 23	0
6	I	1	Total C H 35 12 23	0
6	I	1	Total C H 35 12 23	0
6	I	1	Total C H 35 12 23	0
6	I	1	Total C H 35 12 23	0
6	I	1	Total C H 35 12 23	0
6	I	1	Total C H 35 12 23	0
6	I	1	Total C H 35 12 23	0
6	I	1	Total C H 35 12 23	0
6	J	1	Total C H 26 9 17	0

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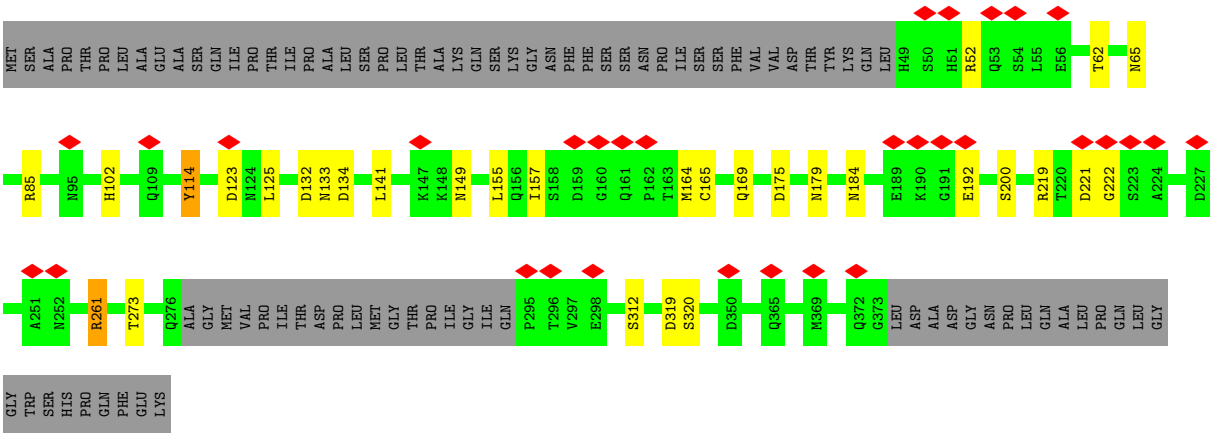
Mol	Chain	Residues	Atoms			AltConf
			Total	C	H	
6	J	1	35	12	23	0
			Total	C	H	
6	J	1	35	12	23	0
			Total	C	H	
6	J	1	35	12	23	0
			Total	C	H	
6	K	1	35	12	23	0
			Total	C	H	
6	K	1	35	12	23	0
			Total	C	H	
6	L	1	35	12	23	0
			Total	C	H	
6	L	1	35	12	23	0
			Total	C	H	
6	L	1	35	12	23	0
			Total	C	H	
6	M	1	35	12	23	0
			Total	C	H	
6	M	1	35	12	23	0
			Total	C	H	
6	M	1	35	12	23	0
			Total	C	H	
6	M	1	35	12	23	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.

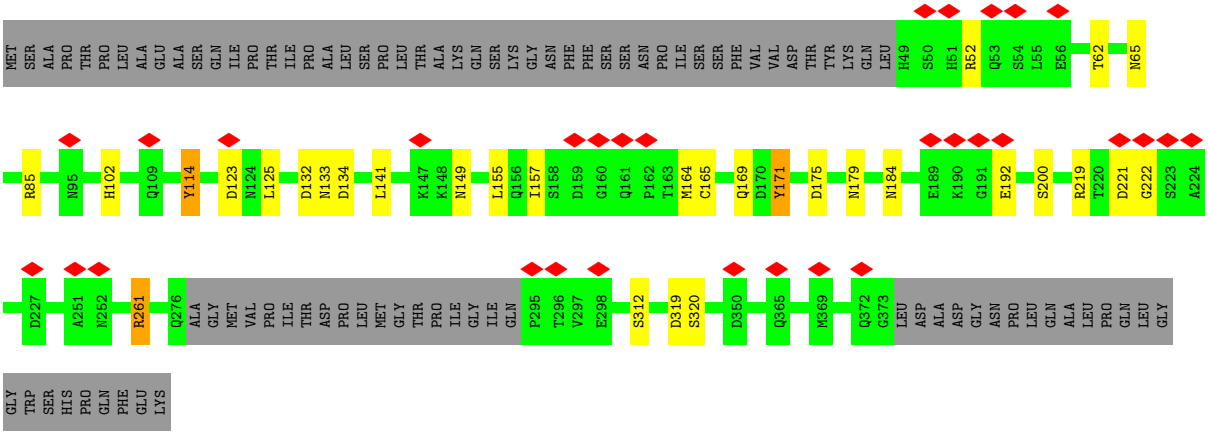
• Molecule 1: Mitochondrial import receptor subunit TOM40

Chain A:



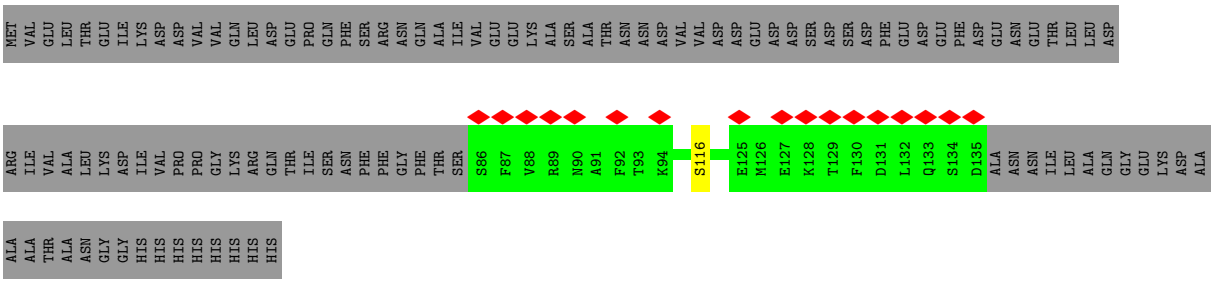
• Molecule 1: Mitochondrial import receptor subunit TOM40

Chain I:



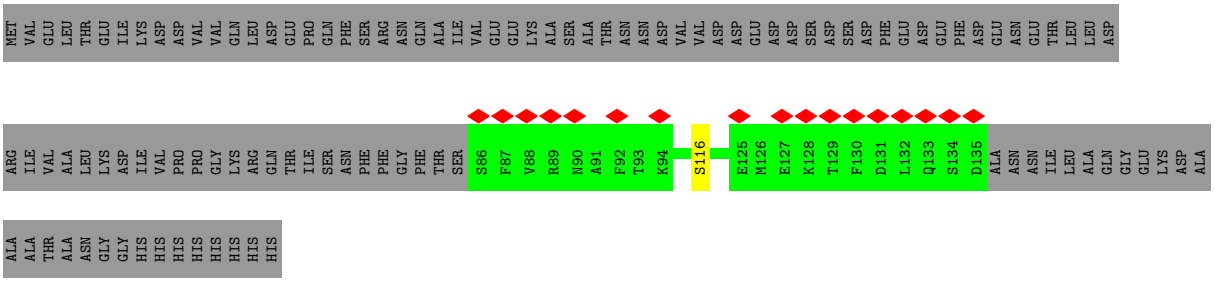
• Molecule 2: Mitochondrial import receptor subunit TOM22

Chain B:



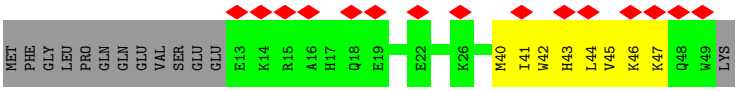
• Molecule 2: Mitochondrial import receptor subunit TOM22

Chain J:



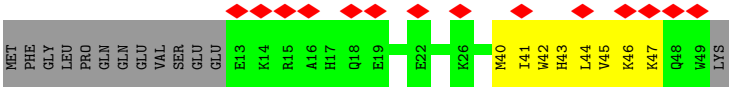
• Molecule 3: Mitochondrial import receptor subunit TOM5

Chain C:



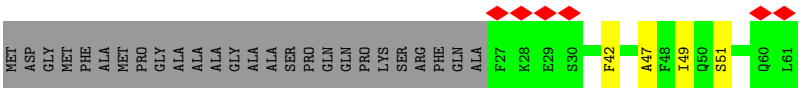
• Molecule 3: Mitochondrial import receptor subunit TOM5

Chain K:



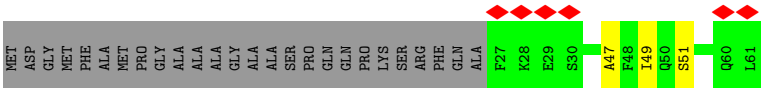
• Molecule 4: Mitochondrial import receptor subunit TOM6

Chain D:



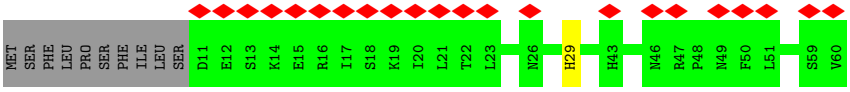
• Molecule 4: Mitochondrial import receptor subunit TOM6

Chain L:



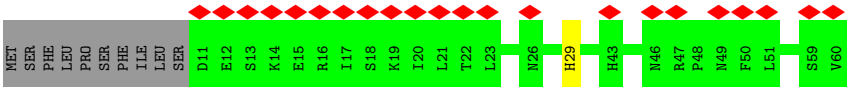
• Molecule 5: Mitochondrial import receptor subunit TOM7

Chain E:



• Molecule 5: Mitochondrial import receptor subunit TOM7

Chain M:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	160577	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	61	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	5.757	Depositor
Minimum map value	-3.888	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.109	Depositor
Recommended contour level	1.0	Depositor
Map size (Å)	294.4, 294.4, 294.4	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.15, 1.15, 1.15	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

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	0.44	0/2413	0.68	4/3265 (0.1%)
1	I	0.45	0/2413	0.70	5/3265 (0.2%)
2	B	0.30	0/392	0.50	0/532
2	J	0.30	0/392	0.50	0/532
3	C	0.29	0/313	0.42	0/426
3	K	0.30	0/313	0.42	0/426
4	D	0.37	0/274	0.52	0/372
4	L	0.37	0/274	0.52	0/372
5	E	0.34	0/407	0.55	0/560
5	M	0.34	0/407	0.55	0/560
All	All	0.41	0/7598	0.63	9/10310 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	114	TYR	CB-CG-CD2	-7.47	116.52	121.00
1	I	114	TYR	CB-CG-CD2	-7.47	116.52	121.00
1	A	134	ASP	CB-CG-OD1	6.87	124.48	118.30
1	I	134	ASP	CB-CG-OD1	6.87	124.48	118.30
1	I	171	TYR	CB-CG-CD2	-6.85	116.89	121.00
1	A	141	LEU	CB-CG-CD2	6.57	122.17	111.00
1	I	141	LEU	CB-CG-CD2	6.57	122.17	111.00
1	A	114	TYR	CB-CG-CD1	5.56	124.34	121.00
1	I	114	TYR	CB-CG-CD1	5.56	124.34	121.00

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	2369	0	2309	18	0
1	I	2369	0	2309	19	0
2	B	387	0	396	1	0
2	J	387	0	396	2	0
3	C	303	0	294	5	0
3	K	303	0	294	6	0
4	D	267	0	271	3	0
4	L	267	0	271	2	0
5	E	393	0	385	2	0
5	M	393	0	385	2	0
6	A	227	413	412	0	0
6	B	45	86	86	0	0
6	C	24	46	46	0	0
6	D	36	69	69	0	0
6	E	48	92	92	0	0
6	I	227	413	412	0	0
6	J	45	86	86	0	0
6	K	24	46	46	0	0
6	L	36	69	69	0	0
6	M	48	92	92	0	0
All	All	8198	1412	8720	49	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 3.

All (49) 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:I:179:ASN:OD1	1:I:200:SER:OG	2.02	0.76
1:A:179:ASN:OD1	1:A:200:SER:OG	2.02	0.74
1:I:261:ARG:NH1	4:L:49:ILE:O	2.23	0.72
1:A:261:ARG:NH1	4:D:49:ILE:O	2.22	0.71
1:I:192:GLU:OE1	1:I:219:ARG:NH1	2.23	0.71
1:A:192:GLU:OE1	1:A:219:ARG:NH1	2.23	0.70
1:I:149:ASN:OD1	1:I:169:GLN:NE2	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:ASN:OD1	1:A:169:GLN:NE2	2.26	0.68
1:A:157:ILE:HG21	5:E:29:HIS:CD2	2.32	0.65
1:I:157:ILE:HG21	5:M:29:HIS:CD2	2.32	0.64
1:A:312:SER:OG	2:B:116:SER:OG	2.20	0.59
1:I:157:ILE:HG21	5:M:29:HIS:HD2	1.69	0.58
1:I:312:SER:HG	2:J:116:SER:HG	1.44	0.56
1:A:157:ILE:HG21	5:E:29:HIS:HD2	1.69	0.56
3:K:40:MET:O	3:K:44:LEU:HD23	2.07	0.54
3:C:40:MET:O	3:C:44:LEU:HD23	2.07	0.54
1:I:52:ARG:NH1	1:I:175:ASP:OD2	2.42	0.52
1:A:52:ARG:NH1	1:A:175:ASP:OD2	2.43	0.51
1:A:102:HIS:ND1	1:A:114:TYR:OH	2.37	0.50
1:A:164:MET:HG2	1:A:184:ASN:HD21	1.75	0.50
1:I:164:MET:HG2	1:I:184:ASN:HD21	1.75	0.50
4:D:47:ALA:O	4:D:51:SER:HB3	2.12	0.50
4:L:47:ALA:O	4:L:51:SER:HB3	2.12	0.50
1:A:319:ASP:OD1	1:A:320:SER:N	2.45	0.49
1:I:319:ASP:OD1	1:I:320:SER:N	2.45	0.49
1:I:123:ASP:N	1:I:123:ASP:OD1	2.47	0.48
3:K:41:ILE:O	3:K:45:VAL:HG23	2.14	0.48
3:K:43:HIS:CD2	3:K:47:LYS:HD2	2.48	0.48
1:I:312:SER:OG	2:J:116:SER:OG	2.20	0.48
3:C:43:HIS:CD2	3:C:47:LYS:HD2	2.49	0.47
3:C:42:TRP:HE1	3:C:46:LYS:HD2	1.80	0.47
1:A:123:ASP:N	1:A:123:ASP:OD1	2.47	0.47
3:C:41:ILE:O	3:C:45:VAL:HG23	2.14	0.47
3:K:43:HIS:O	3:K:47:LYS:HG3	2.15	0.47
1:I:62:THR:OG1	1:I:65:ASN:OD1	2.28	0.46
3:C:43:HIS:O	3:C:47:LYS:HG3	2.15	0.46
1:A:125:LEU:C	1:A:125:LEU:HD23	2.37	0.46
1:A:62:THR:OG1	1:A:65:ASN:OD1	2.28	0.45
3:K:42:TRP:HE1	3:K:46:LYS:HD2	1.80	0.44
1:I:125:LEU:C	1:I:125:LEU:HD23	2.37	0.44
1:A:132:ASP:OD1	1:A:133:ASN:N	2.51	0.44
1:I:132:ASP:OD1	1:I:133:ASN:N	2.51	0.44
1:I:102:HIS:ND1	1:I:114:TYR:OH	2.37	0.43
1:I:155:LEU:CD2	1:I:165:CYS:HB3	2.48	0.43
1:A:155:LEU:CD2	1:A:165:CYS:HB3	2.48	0.43
1:A:221:ASP:OD1	1:A:222:GLY:N	2.53	0.41
1:A:273:THR:HG1	4:D:42:PHE:HD1	1.68	0.41
1:I:52:ARG:HD3	3:K:40:MET:CG	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:221:ASP:OD1	1:I:222:GLY:N	2.53	0.41

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	303/397 (76%)	293 (97%)	10 (3%)	0	100	100
1	I	303/397 (76%)	293 (97%)	10 (3%)	0	100	100
2	B	48/162 (30%)	48 (100%)	0	0	100	100
2	J	48/162 (30%)	48 (100%)	0	0	100	100
3	C	35/50 (70%)	35 (100%)	0	0	100	100
3	K	35/50 (70%)	35 (100%)	0	0	100	100
4	D	33/61 (54%)	33 (100%)	0	0	100	100
4	L	33/61 (54%)	33 (100%)	0	0	100	100
5	E	48/60 (80%)	45 (94%)	3 (6%)	0	100	100
5	M	48/60 (80%)	45 (94%)	3 (6%)	0	100	100
All	All	934/1460 (64%)	908 (97%)	26 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	258/335 (77%)	256 (99%)	2 (1%)	81	91
1	I	258/335 (77%)	255 (99%)	3 (1%)	71	87
2	B	44/141 (31%)	44 (100%)	0	100	100
2	J	44/141 (31%)	44 (100%)	0	100	100
3	C	29/44 (66%)	29 (100%)	0	100	100
3	K	29/44 (66%)	29 (100%)	0	100	100
4	D	28/44 (64%)	28 (100%)	0	100	100
4	L	28/44 (64%)	28 (100%)	0	100	100
5	E	42/56 (75%)	42 (100%)	0	100	100
5	M	42/56 (75%)	42 (100%)	0	100	100
All	All	802/1240 (65%)	797 (99%)	5 (1%)	86	93

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

Mol	Chain	Res	Type
1	A	85	ARG
1	A	261	ARG
1	I	85	ARG
1	I	171	TYR
1	I	261	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	ASN
3	C	43	HIS
5	E	29	HIS
1	I	95	ASN
3	K	43	HIS
5	M	29	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

60 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	$\#\|Z\| > 2$
6	LMT	L	102	-	11,11,36	0.26	0	10,10,47	0.74	0
6	LMT	I	417	-	11,11,36	0.21	0	10,10,47	0.69	0
6	LMT	K	102	-	11,11,36	0.29	0	10,10,47	0.74	0
6	LMT	A	402	-	11,11,36	0.27	0	10,10,47	0.72	0
6	LMT	C	102	-	11,11,36	0.29	0	10,10,47	0.73	0
6	LMT	B	203	-	11,11,36	0.22	0	10,10,47	0.62	0
6	LMT	E	104	-	11,11,36	0.28	0	10,10,47	0.77	0
6	LMT	A	409	-	11,11,36	0.25	0	10,10,47	0.66	0
6	LMT	I	413	-	11,11,36	0.25	0	10,10,47	0.66	0
6	LMT	I	401	-	36,36,36	1.19	4 (11%)	47,47,47	1.26	4 (8%)
6	LMT	I	411	-	11,11,36	0.28	0	10,10,47	0.71	0
6	LMT	I	414	-	11,11,36	0.24	0	10,10,47	0.64	0
6	LMT	I	404	-	11,11,36	0.27	0	10,10,47	0.72	0
6	LMT	L	103	-	11,11,36	0.29	0	10,10,47	0.75	0
6	LMT	A	406	-	11,11,36	0.26	0	10,10,47	0.71	0
6	LMT	A	412	-	11,11,36	0.21	0	10,10,47	0.67	0
6	LMT	A	404	-	11,11,36	0.25	0	10,10,47	0.72	0
6	LMT	D	102	-	11,11,36	0.26	0	10,10,47	0.74	0
6	LMT	A	401	-	11,11,36	0.27	0	10,10,47	0.70	0
6	LMT	E	102	-	11,11,36	0.25	0	10,10,47	0.73	0
6	LMT	A	416	-	11,11,36	0.33	0	10,10,47	0.77	0
6	LMT	M	101	-	11,11,36	0.25	0	10,10,47	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	LMT	A	413	-	11,11,36	0.21	0	10,10,47	0.69	0
6	LMT	M	104	-	11,11,36	0.25	0	10,10,47	0.73	0
6	LMT	B	204	-	11,11,36	0.27	0	10,10,47	0.73	0
6	LMT	A	415	-	11,11,36	0.24	0	10,10,47	0.70	0
6	LMT	I	406	-	11,11,36	0.27	0	10,10,47	0.72	0
6	LMT	D	101	-	11,11,36	0.20	0	10,10,47	0.60	0
6	LMT	I	412	-	11,11,36	0.26	0	10,10,47	0.72	0
6	LMT	I	409	-	11,11,36	0.26	0	10,10,47	0.73	0
6	LMT	I	415	-	11,11,36	0.27	0	10,10,47	0.68	0
6	LMT	I	416	-	11,11,36	0.21	0	10,10,47	0.67	0
6	LMT	A	405	-	11,11,36	0.26	0	10,10,47	0.73	0
6	LMT	E	103	-	11,11,36	0.25	0	10,10,47	0.77	0
6	LMT	B	201	-	8,8,36	0.25	0	7,7,47	0.66	0
6	LMT	J	202	-	11,11,36	0.21	0	10,10,47	0.66	0
6	LMT	I	408	-	11,11,36	0.25	0	10,10,47	0.72	0
6	LMT	M	102	-	11,11,36	0.28	0	10,10,47	0.77	0
6	LMT	I	405	-	11,11,36	0.27	0	10,10,47	0.70	0
6	LMT	E	101	-	11,11,36	0.24	0	10,10,47	0.69	0
6	LMT	A	410	-	11,11,36	0.24	0	10,10,47	0.64	0
6	LMT	I	402	-	11,11,36	0.24	0	10,10,47	0.70	0
6	LMT	A	403	-	11,11,36	0.23	0	10,10,47	0.69	0
6	LMT	C	101	-	11,11,36	0.26	0	10,10,47	0.71	0
6	LMT	L	101	-	11,11,36	0.20	0	10,10,47	0.60	0
6	LMT	J	204	-	11,11,36	0.27	0	10,10,47	0.73	0
6	LMT	A	408	-	11,11,36	0.26	0	10,10,47	0.72	0
6	LMT	I	410	-	11,11,36	0.26	0	10,10,47	0.71	0
6	LMT	B	202	-	11,11,36	0.21	0	10,10,47	0.66	0
6	LMT	M	103	-	11,11,36	0.24	0	10,10,47	0.69	0
6	LMT	A	411	-	11,11,36	0.27	0	10,10,47	0.68	0
6	LMT	A	414	-	36,36,36	1.19	4 (11%)	47,47,47	1.26	4 (8%)
6	LMT	I	407	-	11,11,36	0.23	0	10,10,47	0.69	0
6	LMT	A	417	-	11,11,36	0.27	0	10,10,47	0.72	0
6	LMT	I	403	-	11,11,36	0.33	0	10,10,47	0.77	0
6	LMT	A	407	-	11,11,36	0.27	0	10,10,47	0.71	0
6	LMT	J	201	-	8,8,36	0.25	0	7,7,47	0.66	0
6	LMT	D	103	-	11,11,36	0.29	0	10,10,47	0.75	0
6	LMT	K	101	-	11,11,36	0.26	0	10,10,47	0.71	0
6	LMT	J	203	-	11,11,36	0.22	0	10,10,47	0.62	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
6	LMT	L	102	-	-	2/9/9/61	-
6	LMT	I	417	-	-	2/9/9/61	-
6	LMT	K	102	-	-	1/9/9/61	-
6	LMT	A	402	-	-	2/9/9/61	-
6	LMT	C	102	-	-	1/9/9/61	-
6	LMT	B	203	-	-	4/9/9/61	-
6	LMT	E	104	-	-	1/9/9/61	-
6	LMT	A	409	-	-	3/9/9/61	-
6	LMT	I	413	-	-	3/9/9/61	-
6	LMT	I	401	-	-	9/21/61/61	0/2/2/2
6	LMT	I	411	-	-	3/9/9/61	-
6	LMT	I	414	-	-	3/9/9/61	-
6	LMT	I	404	-	-	3/9/9/61	-
6	LMT	L	103	-	-	2/9/9/61	-
6	LMT	A	406	-	-	3/9/9/61	-
6	LMT	A	412	-	-	3/9/9/61	-
6	LMT	A	404	-	-	4/9/9/61	-
6	LMT	D	102	-	-	2/9/9/61	-
6	LMT	A	401	-	-	3/9/9/61	-
6	LMT	E	102	-	-	1/9/9/61	-
6	LMT	A	416	-	-	1/9/9/61	-
6	LMT	M	101	-	-	1/9/9/61	-
6	LMT	A	413	-	-	2/9/9/61	-
6	LMT	M	104	-	-	1/9/9/61	-
6	LMT	B	204	-	-	1/9/9/61	-
6	LMT	A	415	-	-	1/9/9/61	-
6	LMT	I	406	-	-	2/9/9/61	-
6	LMT	D	101	-	-	3/9/9/61	-
6	LMT	I	412	-	-	2/9/9/61	-
6	LMT	I	409	-	-	3/9/9/61	-
6	LMT	I	415	-	-	3/9/9/61	-
6	LMT	I	416	-	-	3/9/9/61	-
6	LMT	A	405	-	-	3/9/9/61	-
6	LMT	E	103	-	-	1/9/9/61	-
6	LMT	B	201	-	-	1/6/6/61	-
6	LMT	J	202	-	-	4/9/9/61	-
6	LMT	I	408	-	-	4/9/9/61	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	LMT	M	102	-	-	1/9/9/61	-
6	LMT	I	405	-	-	3/9/9/61	-
6	LMT	E	101	-	-	2/9/9/61	-
6	LMT	A	410	-	-	3/9/9/61	-
6	LMT	I	402	-	-	1/9/9/61	-
6	LMT	A	403	-	-	2/9/9/61	-
6	LMT	C	101	-	-	3/9/9/61	-
6	LMT	L	101	-	-	3/9/9/61	-
6	LMT	J	204	-	-	1/9/9/61	-
6	LMT	A	408	-	-	2/9/9/61	-
6	LMT	I	410	-	-	3/9/9/61	-
6	LMT	B	202	-	-	4/9/9/61	-
6	LMT	M	103	-	-	2/9/9/61	-
6	LMT	A	411	-	-	3/9/9/61	-
6	LMT	A	414	-	-	9/21/61/61	0/2/2/2
6	LMT	I	407	-	-	2/9/9/61	-
6	LMT	A	417	-	-	3/9/9/61	-
6	LMT	I	403	-	-	1/9/9/61	-
6	LMT	A	407	-	-	3/9/9/61	-
6	LMT	J	201	-	-	1/6/6/61	-
6	LMT	D	103	-	-	2/9/9/61	-
6	LMT	K	101	-	-	3/9/9/61	-
6	LMT	J	203	-	-	4/9/9/61	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	414	LMT	O3'-C3'	-2.84	1.36	1.43
6	I	401	LMT	O3'-C3'	-2.84	1.36	1.43
6	A	414	LMT	O2B-C2B	-2.38	1.37	1.43
6	I	401	LMT	O2B-C2B	-2.38	1.37	1.43
6	A	414	LMT	O2'-C2'	-2.32	1.37	1.43
6	I	401	LMT	O2'-C2'	-2.32	1.37	1.43
6	A	414	LMT	O3B-C3B	-2.31	1.37	1.43
6	I	401	LMT	O3B-C3B	-2.31	1.37	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	414	LMT	C3'-C4'-C5'	-3.23	103.53	110.93
6	I	401	LMT	C3'-C4'-C5'	-3.23	103.53	110.93
6	A	414	LMT	O5B-C5B-C4B	3.06	115.25	109.69
6	I	401	LMT	O5B-C5B-C4B	3.06	115.25	109.69
6	A	414	LMT	C1'-C2'-C3'	2.74	115.70	110.00
6	I	401	LMT	C1'-C2'-C3'	2.74	115.70	110.00
6	A	414	LMT	C2'-C3'-C4'	2.16	114.61	109.68
6	I	401	LMT	C2'-C3'-C4'	2.16	114.61	109.68

There are no chirality outliers.

All (152) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	414	LMT	C2'-C1'-O1'-C1
6	A	414	LMT	O5'-C1'-O1'-C1
6	I	401	LMT	C2'-C1'-O1'-C1
6	I	401	LMT	O5'-C1'-O1'-C1
6	A	414	LMT	C2B-C1B-O1B-C4'
6	I	401	LMT	C2B-C1B-O1B-C4'
6	A	414	LMT	O5B-C1B-O1B-C4'
6	I	401	LMT	O5B-C1B-O1B-C4'
6	A	414	LMT	O1'-C1-C2-C3
6	I	401	LMT	O1'-C1-C2-C3
6	E	101	LMT	C3-C4-C5-C6
6	M	103	LMT	C3-C4-C5-C6
6	B	203	LMT	C11-C10-C9-C8
6	J	203	LMT	C11-C10-C9-C8
6	D	102	LMT	C5-C6-C7-C8
6	L	102	LMT	C5-C6-C7-C8
6	A	403	LMT	C7-C8-C9-C10
6	C	101	LMT	C7-C8-C9-C10
6	I	407	LMT	C7-C8-C9-C10
6	K	101	LMT	C7-C8-C9-C10
6	A	405	LMT	C6-C7-C8-C9
6	I	409	LMT	C6-C7-C8-C9
6	D	101	LMT	C5-C6-C7-C8
6	L	101	LMT	C5-C6-C7-C8
6	A	403	LMT	C3-C4-C5-C6
6	I	407	LMT	C3-C4-C5-C6
6	A	415	LMT	C7-C8-C9-C10
6	I	402	LMT	C7-C8-C9-C10
6	A	413	LMT	C6-C7-C8-C9
6	B	204	LMT	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
6	I	417	LMT	C6-C7-C8-C9
6	J	204	LMT	C7-C8-C9-C10
6	B	203	LMT	C5-C6-C7-C8
6	J	203	LMT	C5-C6-C7-C8
6	E	103	LMT	C3-C4-C5-C6
6	M	101	LMT	C3-C4-C5-C6
6	A	410	LMT	C6-C7-C8-C9
6	I	414	LMT	C6-C7-C8-C9
6	A	404	LMT	C7-C8-C9-C10
6	I	408	LMT	C7-C8-C9-C10
6	A	406	LMT	C4-C5-C6-C7
6	I	410	LMT	C4-C5-C6-C7
6	D	101	LMT	C1-C2-C3-C4
6	L	101	LMT	C1-C2-C3-C4
6	A	401	LMT	C9-C10-C11-C12
6	A	411	LMT	C6-C7-C8-C9
6	I	405	LMT	C9-C10-C11-C12
6	I	415	LMT	C6-C7-C8-C9
6	A	406	LMT	C11-C10-C9-C8
6	I	410	LMT	C11-C10-C9-C8
6	A	411	LMT	C9-C10-C11-C12
6	I	415	LMT	C9-C10-C11-C12
6	A	414	LMT	O5B-C5B-C6B-O6B
6	I	401	LMT	O5B-C5B-C6B-O6B
6	A	407	LMT	C11-C10-C9-C8
6	I	411	LMT	C11-C10-C9-C8
6	A	407	LMT	C7-C8-C9-C10
6	I	411	LMT	C7-C8-C9-C10
6	A	405	LMT	C4-C5-C6-C7
6	I	409	LMT	C4-C5-C6-C7
6	E	104	LMT	C3-C4-C5-C6
6	M	102	LMT	C3-C4-C5-C6
6	C	102	LMT	C7-C8-C9-C10
6	K	102	LMT	C7-C8-C9-C10
6	A	410	LMT	C4-C5-C6-C7
6	B	202	LMT	C7-C8-C9-C10
6	I	414	LMT	C4-C5-C6-C7
6	J	202	LMT	C7-C8-C9-C10
6	A	402	LMT	C6-C7-C8-C9
6	B	202	LMT	C6-C7-C8-C9
6	I	406	LMT	C6-C7-C8-C9
6	J	202	LMT	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
6	A	408	LMT	C6-C7-C8-C9
6	I	410	LMT	C7-C8-C9-C10
6	I	412	LMT	C6-C7-C8-C9
6	A	406	LMT	C7-C8-C9-C10
6	A	412	LMT	C11-C10-C9-C8
6	I	416	LMT	C11-C10-C9-C8
6	A	417	LMT	C3-C4-C5-C6
6	I	404	LMT	C3-C4-C5-C6
6	A	409	LMT	C6-C7-C8-C9
6	I	413	LMT	C6-C7-C8-C9
6	A	407	LMT	C4-C5-C6-C7
6	I	411	LMT	C4-C5-C6-C7
6	B	202	LMT	C3-C4-C5-C6
6	J	202	LMT	C3-C4-C5-C6
6	A	401	LMT	C1-C2-C3-C4
6	I	405	LMT	C1-C2-C3-C4
6	A	412	LMT	C6-C7-C8-C9
6	I	416	LMT	C6-C7-C8-C9
6	A	411	LMT	C4-C5-C6-C7
6	I	415	LMT	C4-C5-C6-C7
6	E	101	LMT	C7-C8-C9-C10
6	M	103	LMT	C7-C8-C9-C10
6	A	410	LMT	C9-C10-C11-C12
6	I	414	LMT	C9-C10-C11-C12
6	C	101	LMT	C3-C4-C5-C6
6	K	101	LMT	C3-C4-C5-C6
6	A	408	LMT	C5-C6-C7-C8
6	I	412	LMT	C5-C6-C7-C8
6	D	102	LMT	C3-C4-C5-C6
6	L	102	LMT	C3-C4-C5-C6
6	A	402	LMT	C4-C5-C6-C7
6	I	406	LMT	C4-C5-C6-C7
6	A	414	LMT	C3-C4-C5-C6
6	I	401	LMT	C3-C4-C5-C6
6	A	414	LMT	C1-C2-C3-C4
6	I	401	LMT	C1-C2-C3-C4
6	A	414	LMT	C6-C7-C8-C9
6	A	417	LMT	C6-C7-C8-C9
6	I	401	LMT	C6-C7-C8-C9
6	I	404	LMT	C6-C7-C8-C9
6	C	101	LMT	C9-C10-C11-C12
6	K	101	LMT	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
6	B	203	LMT	C7-C8-C9-C10
6	J	203	LMT	C7-C8-C9-C10
6	B	202	LMT	C11-C10-C9-C8
6	J	202	LMT	C11-C10-C9-C8
6	A	404	LMT	C2-C3-C4-C5
6	I	408	LMT	C2-C3-C4-C5
6	D	103	LMT	C7-C8-C9-C10
6	L	103	LMT	C7-C8-C9-C10
6	A	401	LMT	C4-C5-C6-C7
6	I	405	LMT	C4-C5-C6-C7
6	A	405	LMT	C11-C10-C9-C8
6	I	409	LMT	C11-C10-C9-C8
6	A	416	LMT	C7-C8-C9-C10
6	I	403	LMT	C7-C8-C9-C10
6	A	404	LMT	C6-C7-C8-C9
6	I	408	LMT	C6-C7-C8-C9
6	B	201	LMT	C7-C8-C9-C10
6	J	201	LMT	C7-C8-C9-C10
6	A	409	LMT	C9-C10-C11-C12
6	I	413	LMT	C9-C10-C11-C12
6	E	102	LMT	C4-C5-C6-C7
6	M	104	LMT	C4-C5-C6-C7
6	A	412	LMT	C3-C4-C5-C6
6	I	416	LMT	C3-C4-C5-C6
6	D	101	LMT	C4-C5-C6-C7
6	L	101	LMT	C4-C5-C6-C7
6	A	404	LMT	C5-C6-C7-C8
6	I	408	LMT	C5-C6-C7-C8
6	A	409	LMT	C5-C6-C7-C8
6	I	413	LMT	C5-C6-C7-C8
6	A	417	LMT	C4-C5-C6-C7
6	I	404	LMT	C4-C5-C6-C7
6	A	413	LMT	C1-C2-C3-C4
6	I	417	LMT	C1-C2-C3-C4
6	B	203	LMT	C3-C4-C5-C6
6	J	203	LMT	C3-C4-C5-C6
6	D	103	LMT	C6-C7-C8-C9
6	L	103	LMT	C6-C7-C8-C9

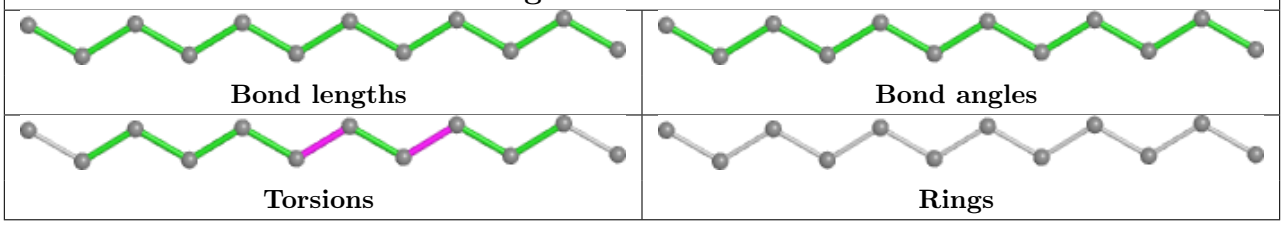
There are no ring outliers.

No monomer is involved in short contacts.

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 L 102



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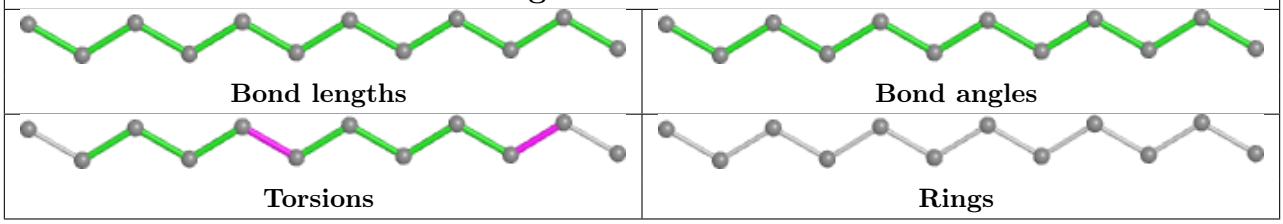
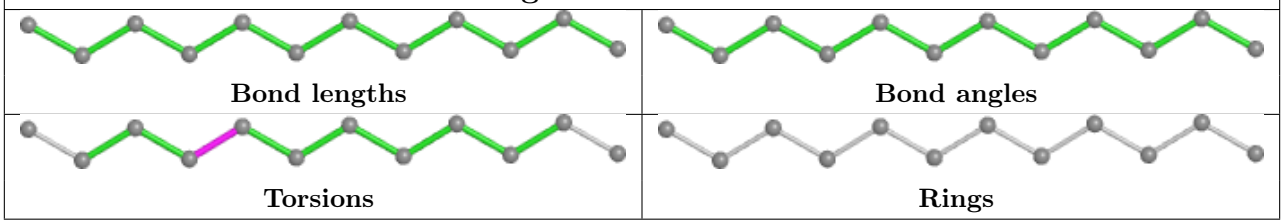


Ligand LMT K 102



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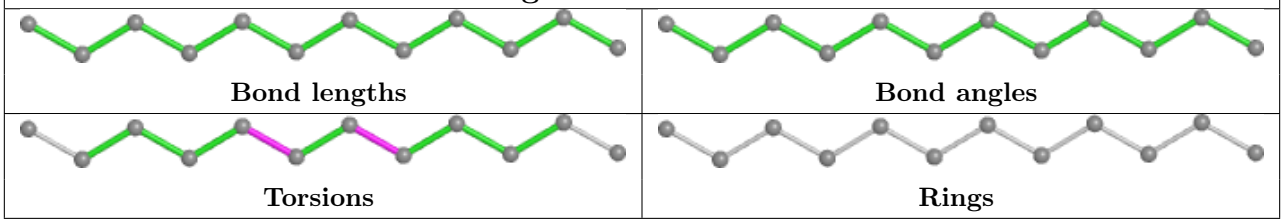

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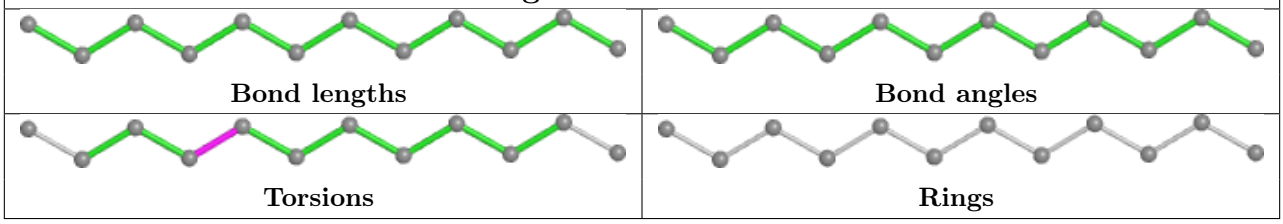

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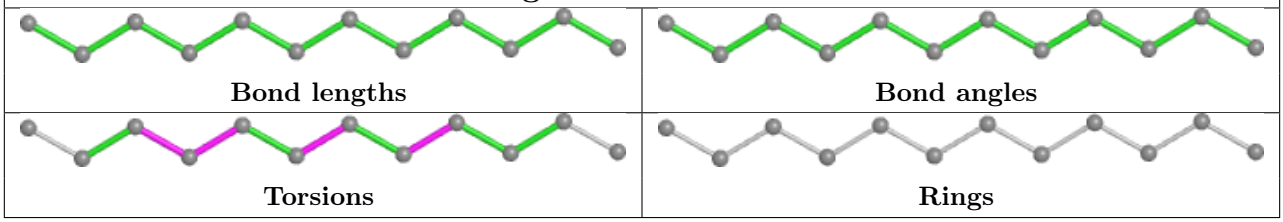

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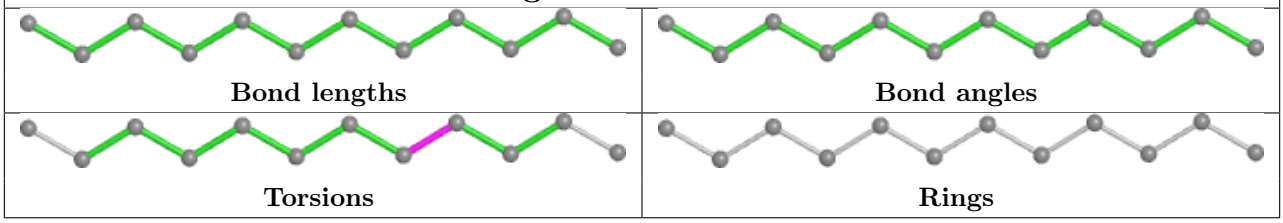

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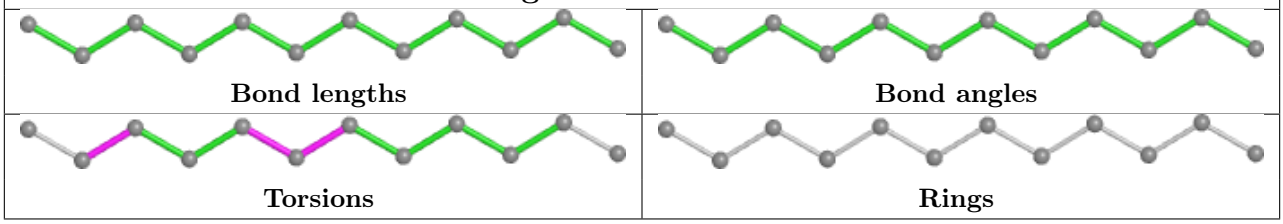

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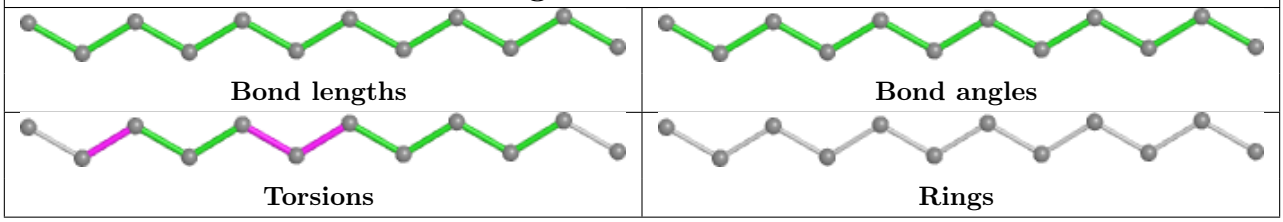

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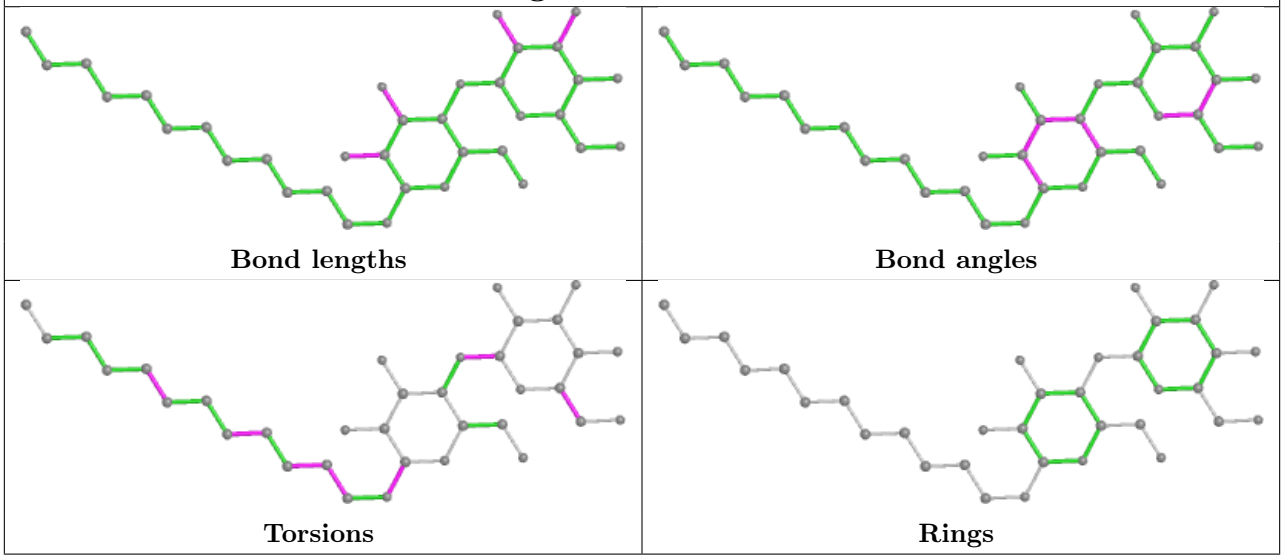

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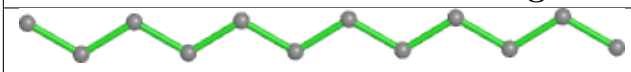
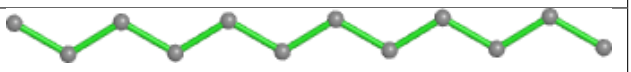
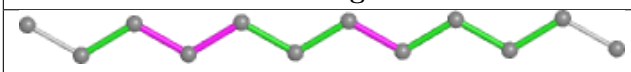
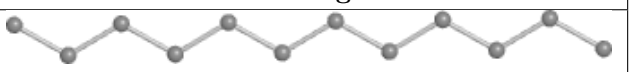
 Bond lengths	 Bond angles
 Torsions	 Rings

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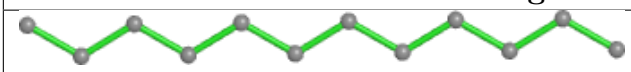
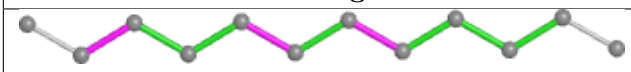
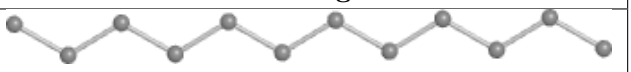
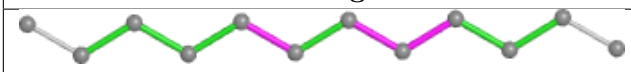
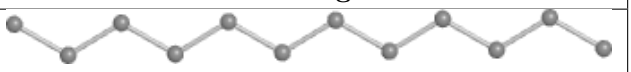
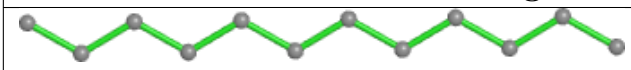
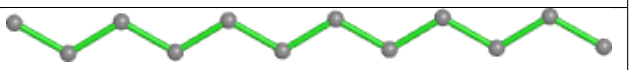
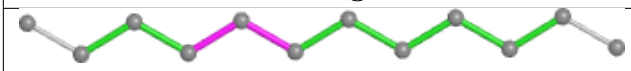
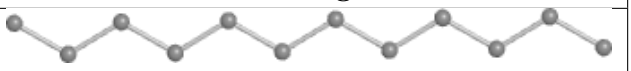
 Bond lengths	Bond angles
 Torsions	 Rings

Ligand LMT I 404	
Bond lengths	Bond angles
 Torsions	 Rings

Ligand LMT L 103	
 Bond lengths	 Bond angles
 Torsions	 Rings

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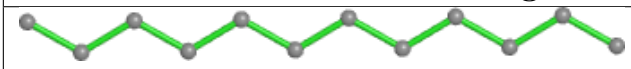
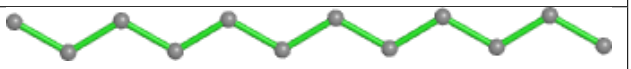
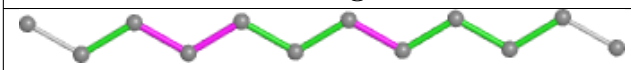
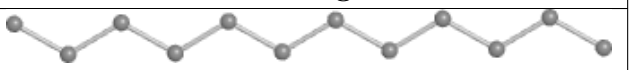
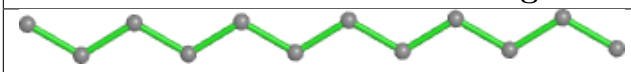
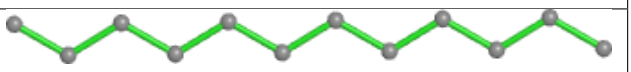
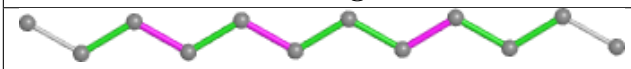
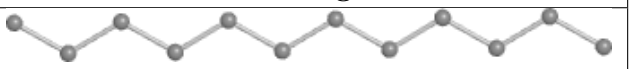
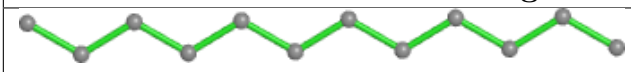
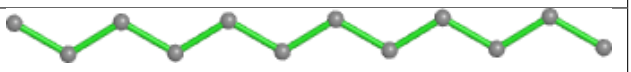
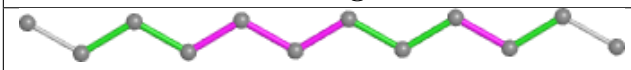
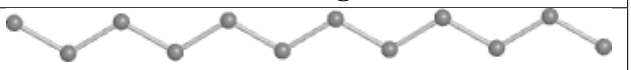
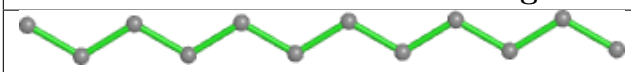
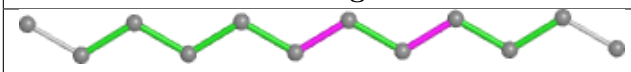
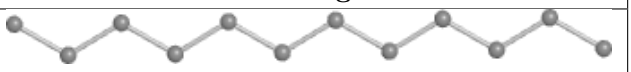
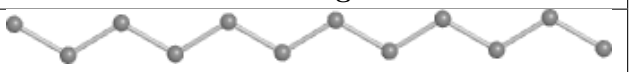
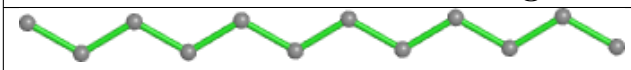
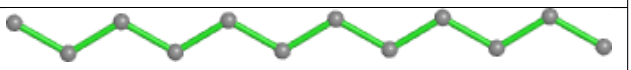
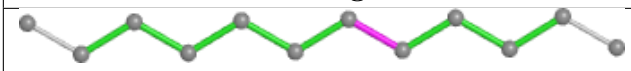
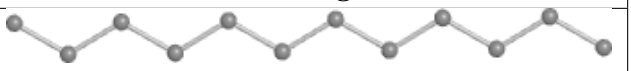
 Bond lengths	 Bond angles
 Torsions	 Rings

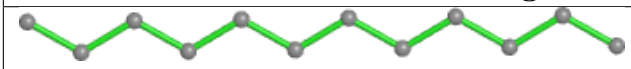
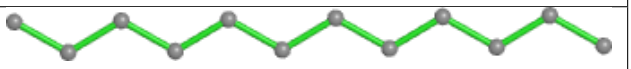
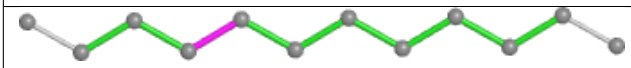
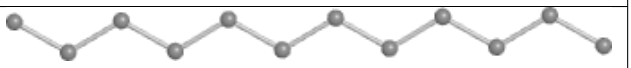
Ligand LMT A 412	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMT A 404	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMT D 102	
 Bond lengths	Bond angles
 Torsions	 Rings

Ligand LMT A 401	
Bond lengths	Bond angles
Torsions	 Rings

Ligand LMT E 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMT A 416	
 Bond lengths	 Bond angles
 Torsions	 Rings

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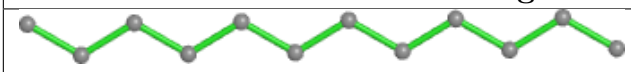
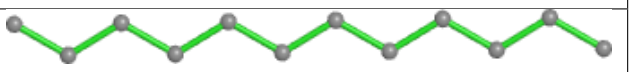
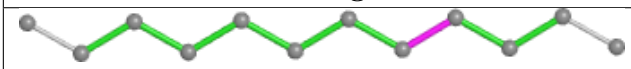
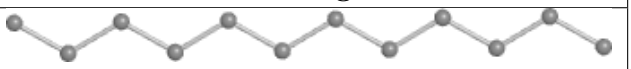
 Bond lengths	 Bond angles
 Torsions	 Rings

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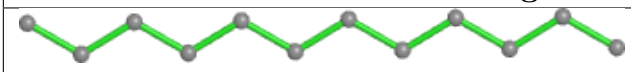
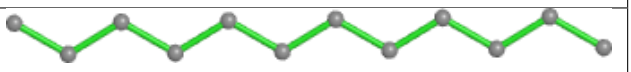
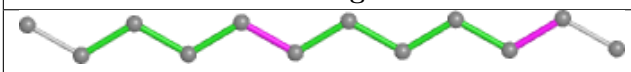
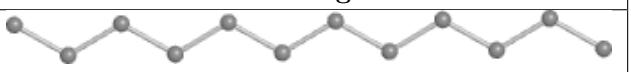
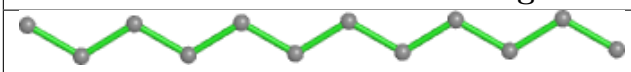
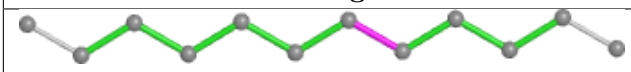
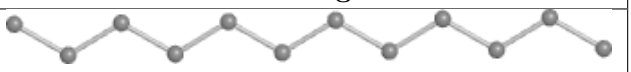
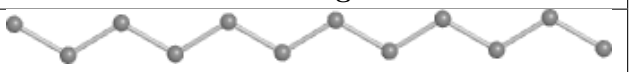
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMT M 104	
 Bond lengths	Bond angles
 Torsions	 Rings

Ligand LMT B 204	
Bond lengths	Bond angles
Torsions	 Rings

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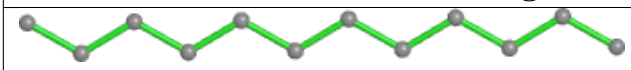
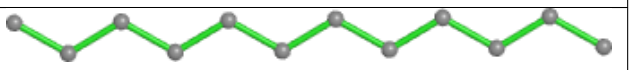
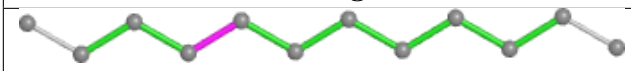
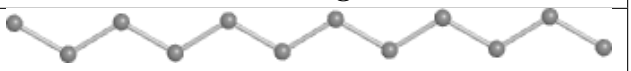
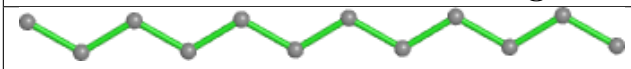
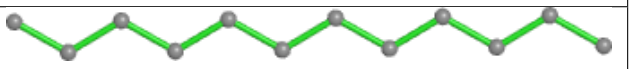
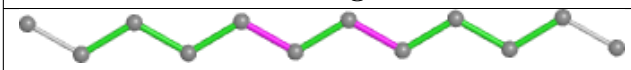
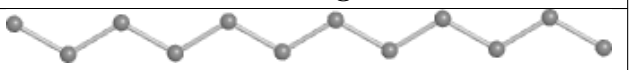
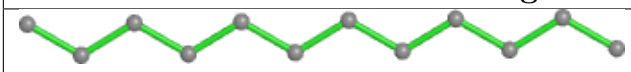
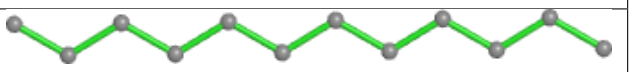
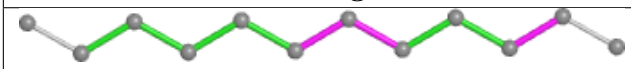
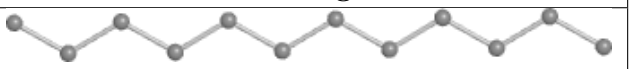
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMT I 406	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMT D 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

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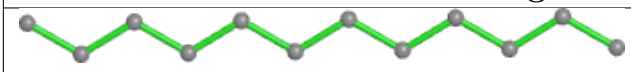
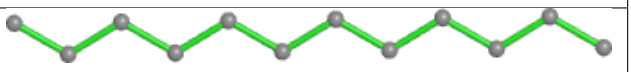
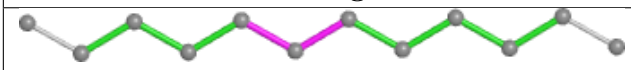
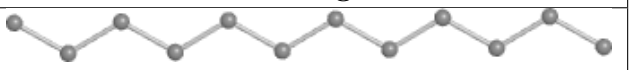
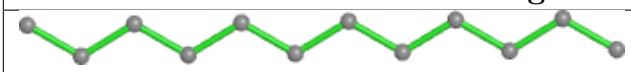
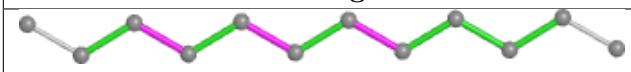
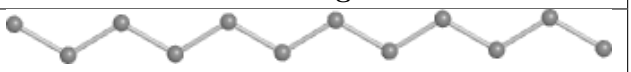
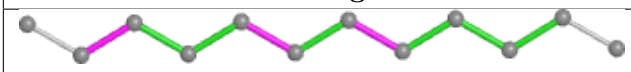
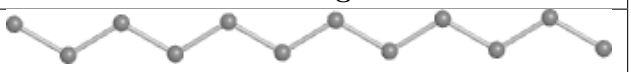
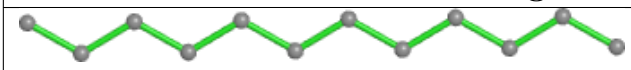
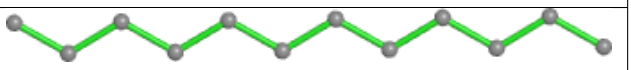
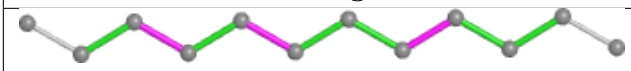
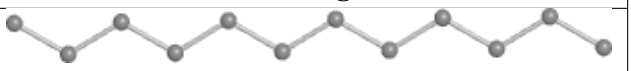
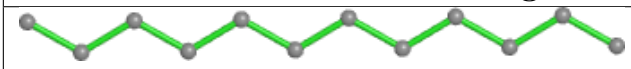
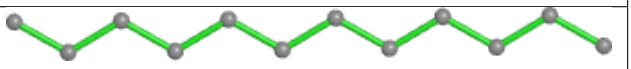
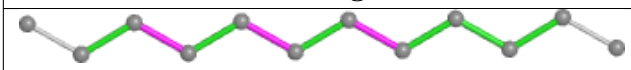
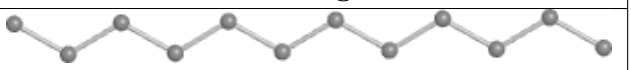
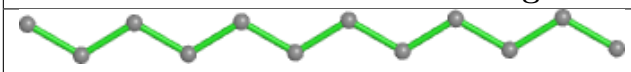
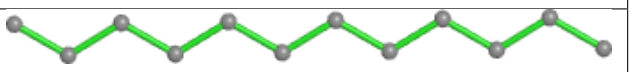
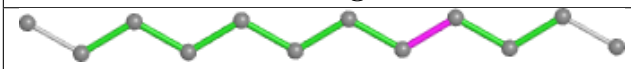
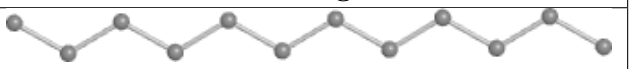
 Bond lengths	 Bond angles
 Torsions	 Rings

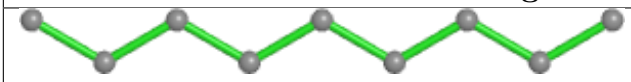
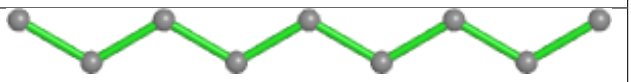
Ligand LMT I 409	
 Bond lengths	Bond angles
 Torsions	 Rings

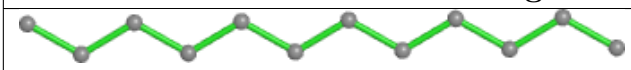
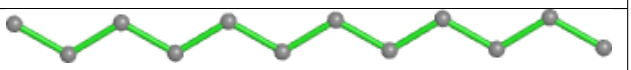
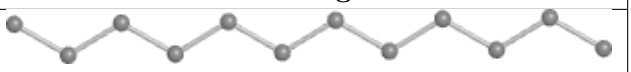
Ligand LMT I 415	
Bond lengths	Bond angles
 Torsions	 Rings

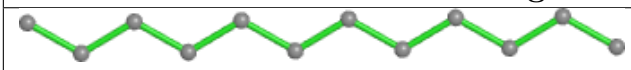
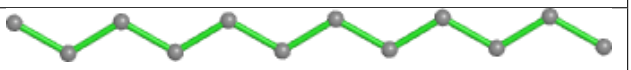
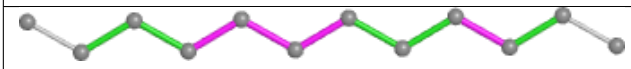
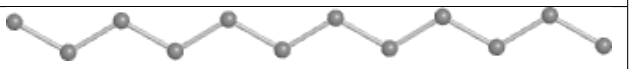
Ligand LMT I 416	
 Bond lengths	 Bond angles
 Torsions	 Rings

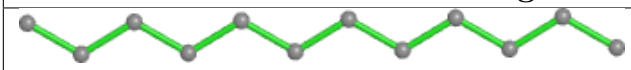
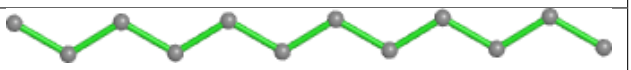
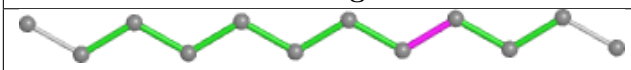
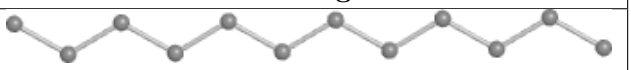
Ligand LMT A 405	
 Bond lengths	 Bond angles
 Torsions	 Rings

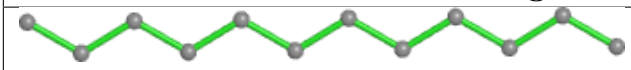
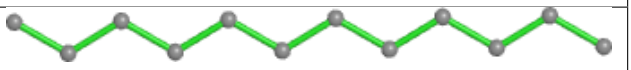
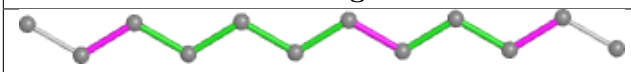
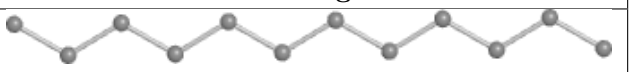
Ligand LMT E 103	
 Bond lengths	 Bond angles
 Torsions	 Rings

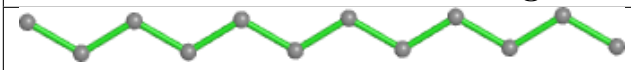
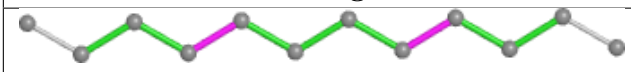
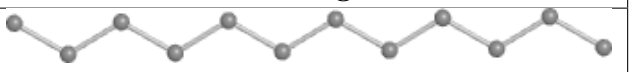
Ligand LMT B 201	
 Bond lengths	 Bond angles
Torsions	Rings

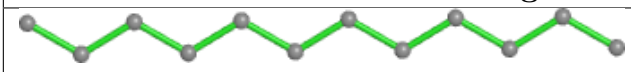
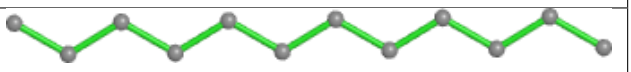
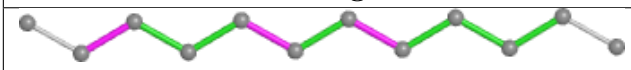
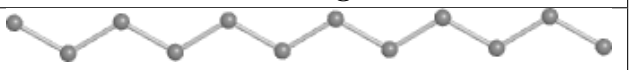
Ligand LMT J 202	
 Bond lengths	 Bond angles
Torsions	 Rings

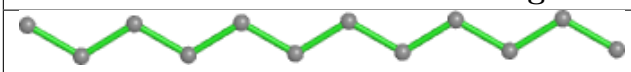
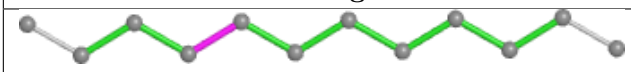
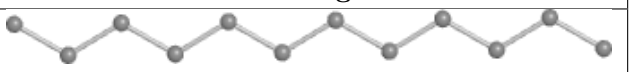
Ligand LMT I 408	
 Bond lengths	 Bond angles
 Torsions	 Rings

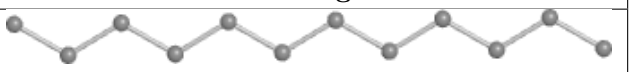
Ligand LMT M 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

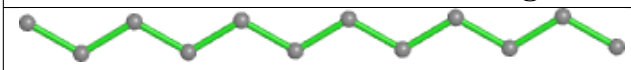
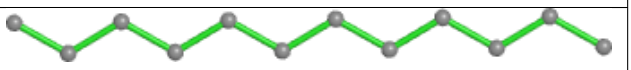
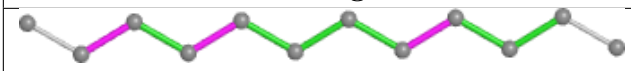
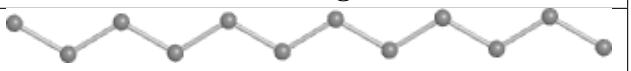
Ligand LMT I 405	
 Bond lengths	 Bond angles
 Torsions	 Rings

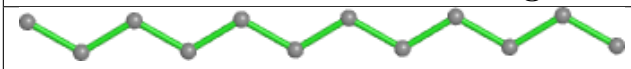
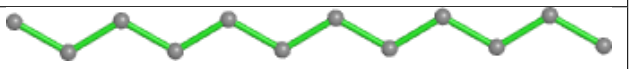
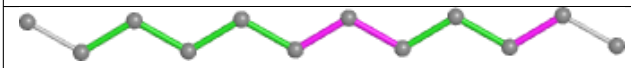
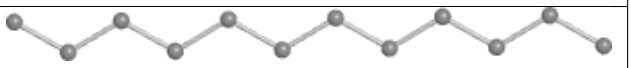
Ligand LMT E 101	
 Bond lengths	Bond angles
 Torsions	 Rings

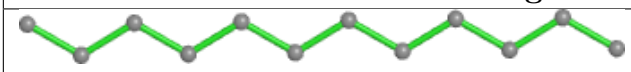
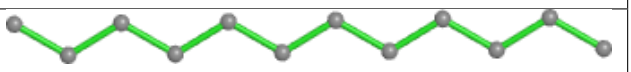
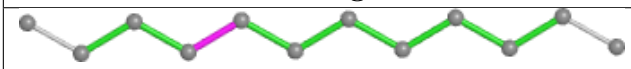
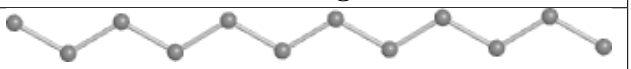
Ligand LMT A 410	
 Bond lengths	 Bond angles
 Torsions	 Rings

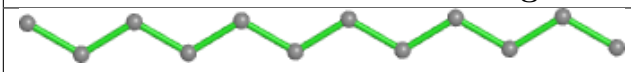
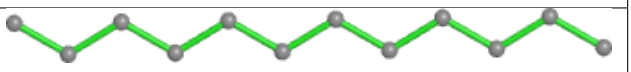
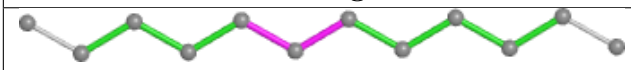
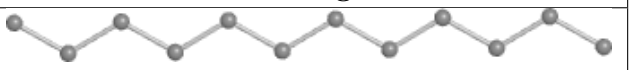
Ligand LMT I 402	
 Bond lengths	Bond angles
 Torsions	 Rings

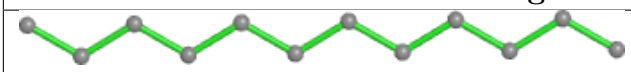
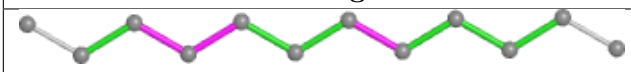
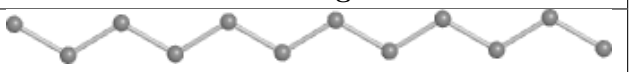
Ligand LMT A 403	
Bond lengths	Bond angles
Torsions	 Rings

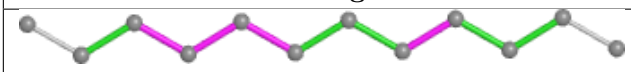
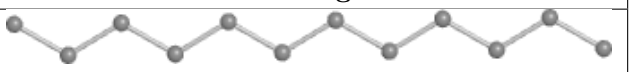
Ligand LMT C 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

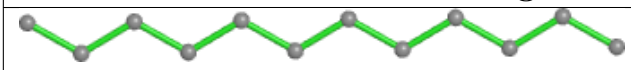
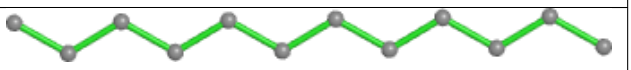
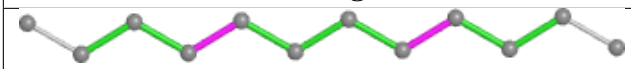
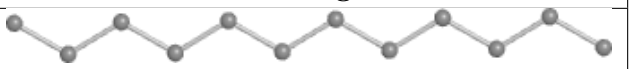
Ligand LMT L 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

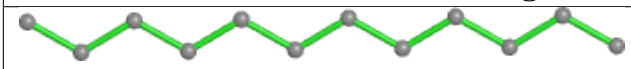
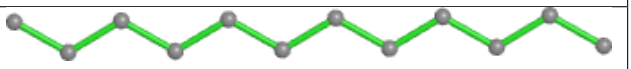
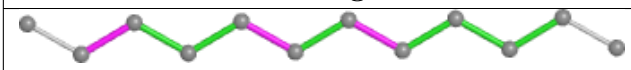
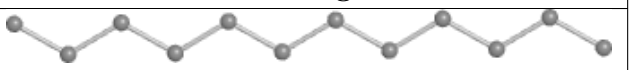
Ligand LMT J 204	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMT A 408	
 Bond lengths	 Bond angles
 Torsions	 Rings

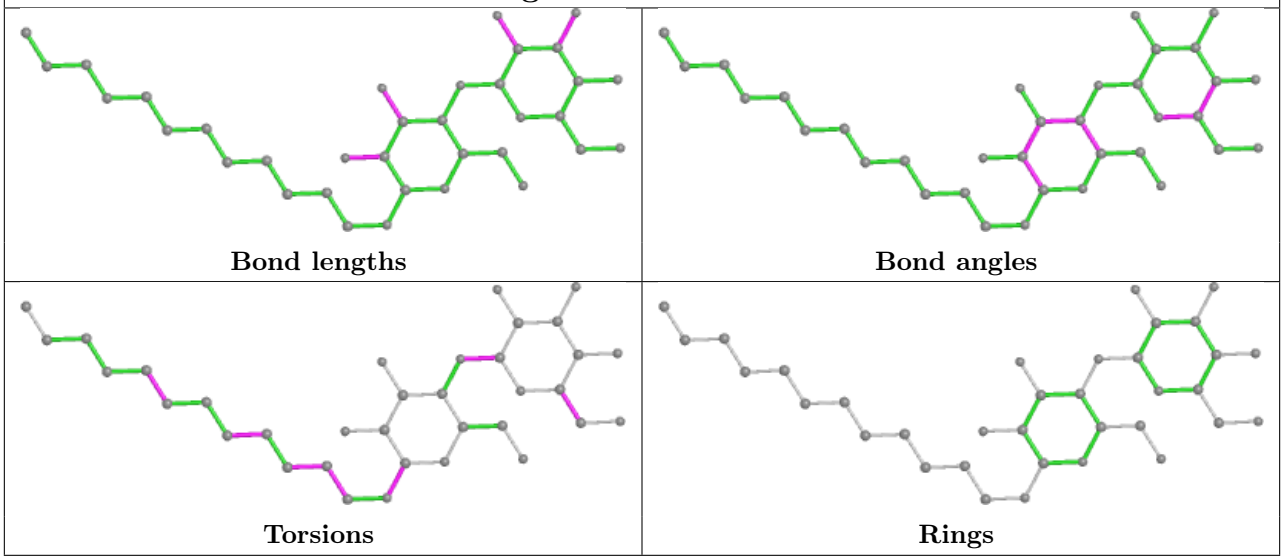
Ligand LMT I 410	
 Bond lengths	Bond angles
 Torsions	 Rings

Ligand LMT B 202	
Bond lengths	Bond angles
 Torsions	 Rings

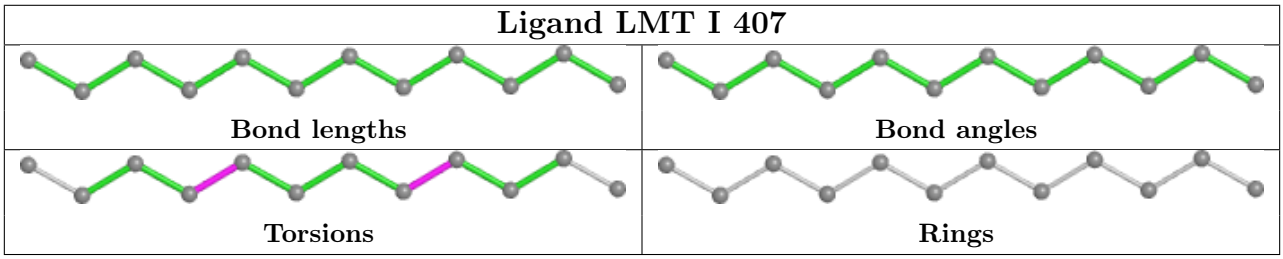
Ligand LMT M 103	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMT A 411	
 Bond lengths	 Bond angles
 Torsions	 Rings

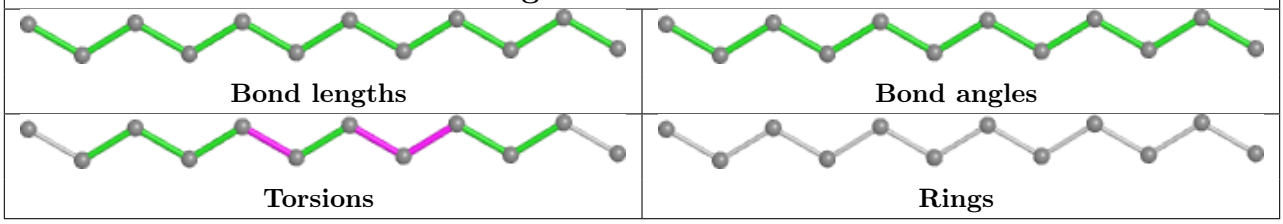
Ligand LMT A 414



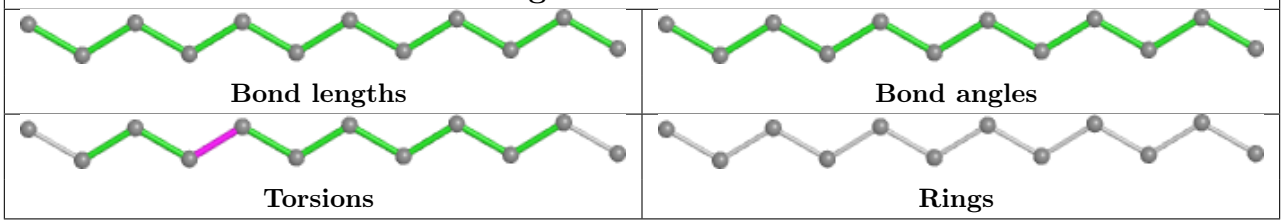
Ligand LMT I 407



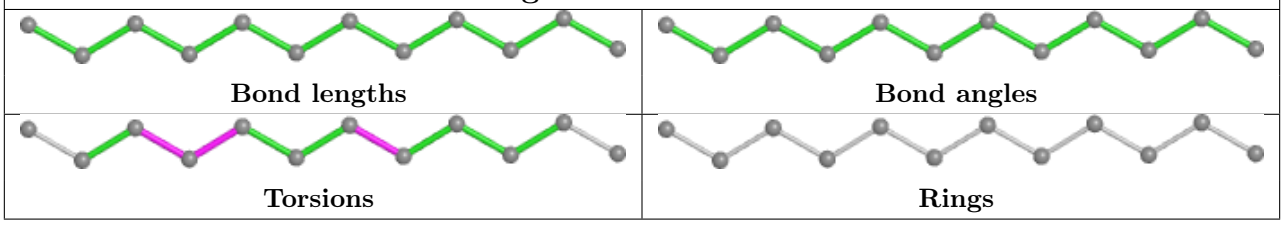
Ligand LMT A 417

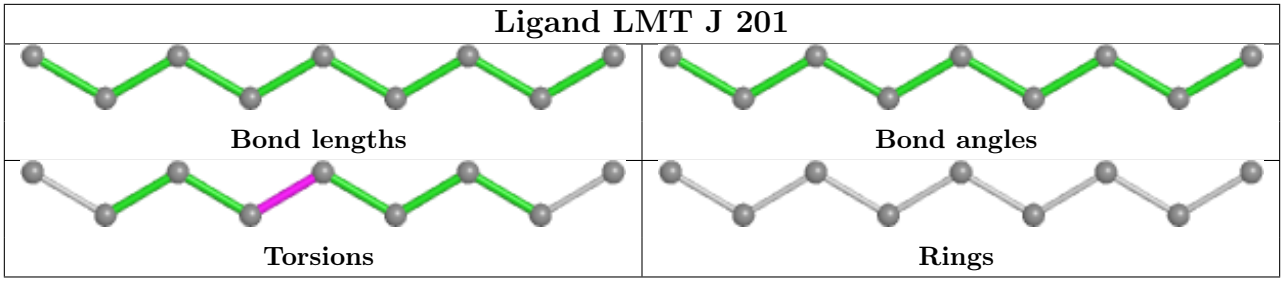


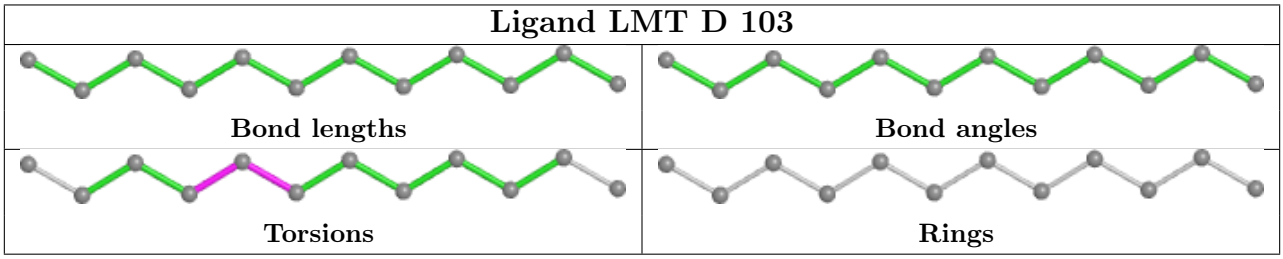
Ligand LMT I 403

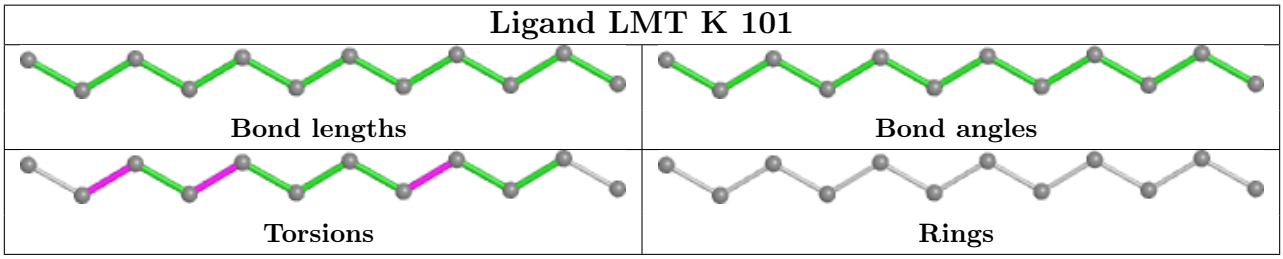


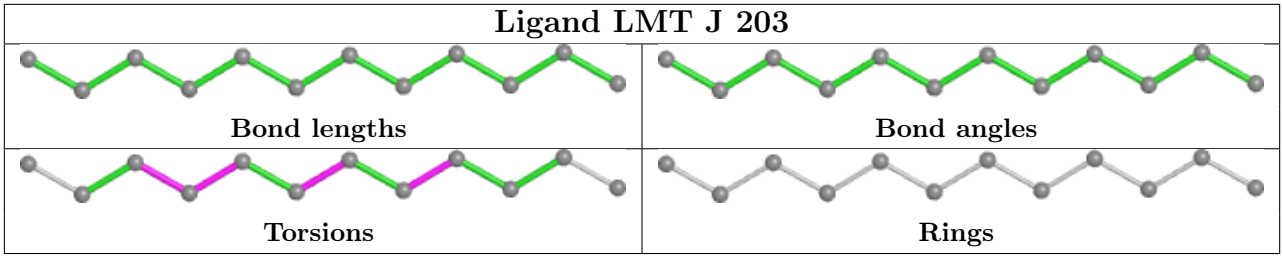
Ligand LMT A 407











5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

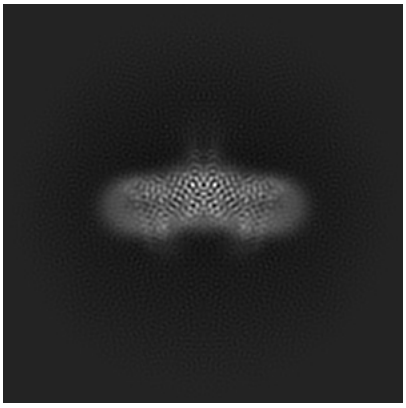
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-20728. These allow visual inspection of the internal detail of the map and identification of artifacts.

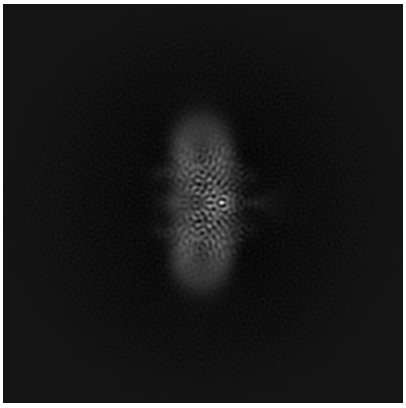
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

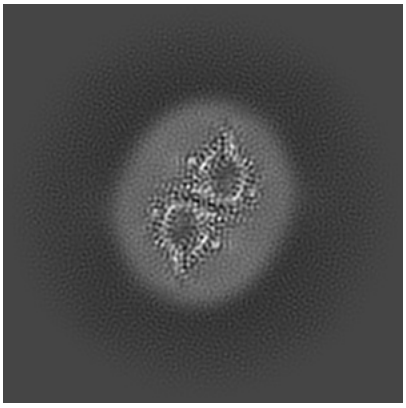
6.1.1 Primary map



X



Y

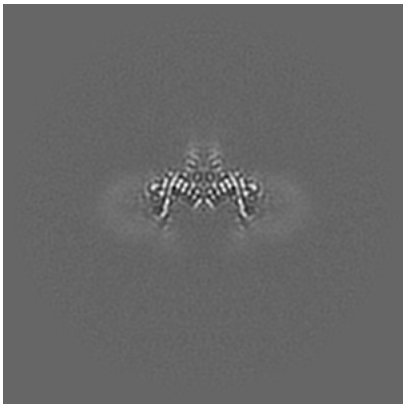


Z

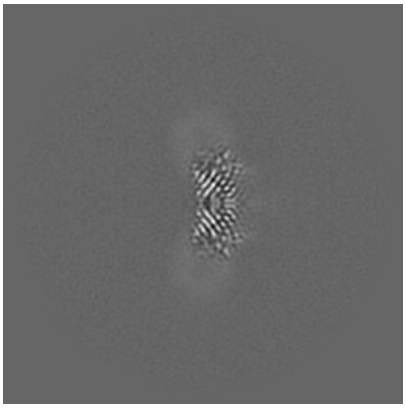
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

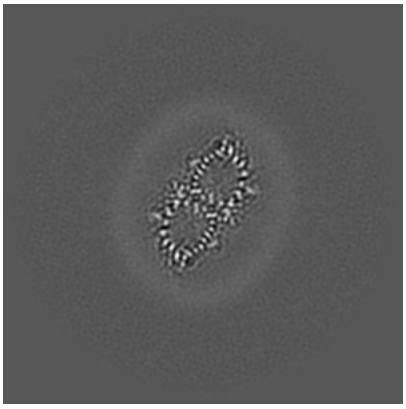
6.2.1 Primary map



X Index: 128



Y Index: 128

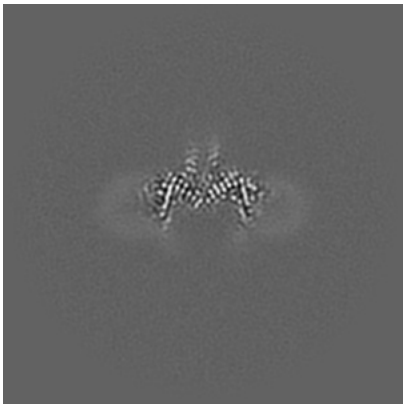


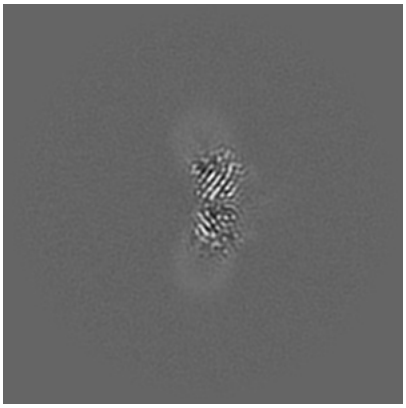
Z Index: 128

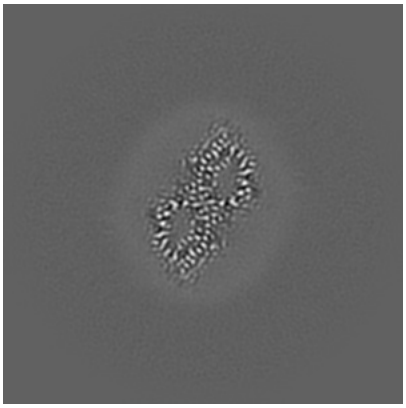
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 129

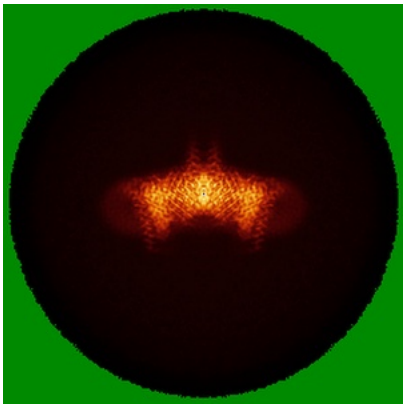

Y Index: 129

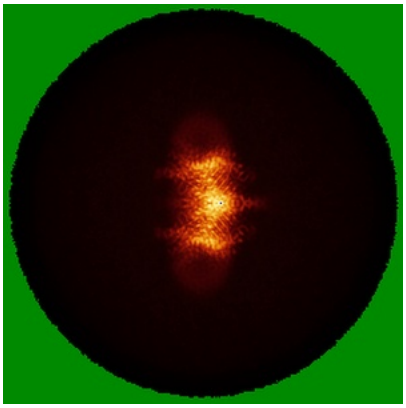

Z Index: 134

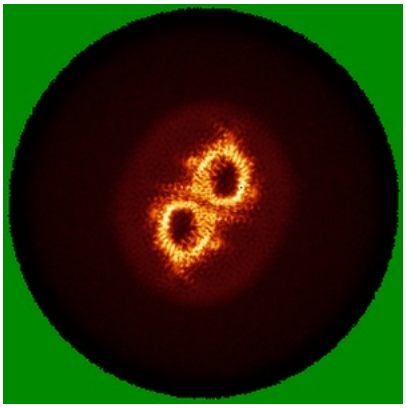
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map


X


Y


Z

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

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 1.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

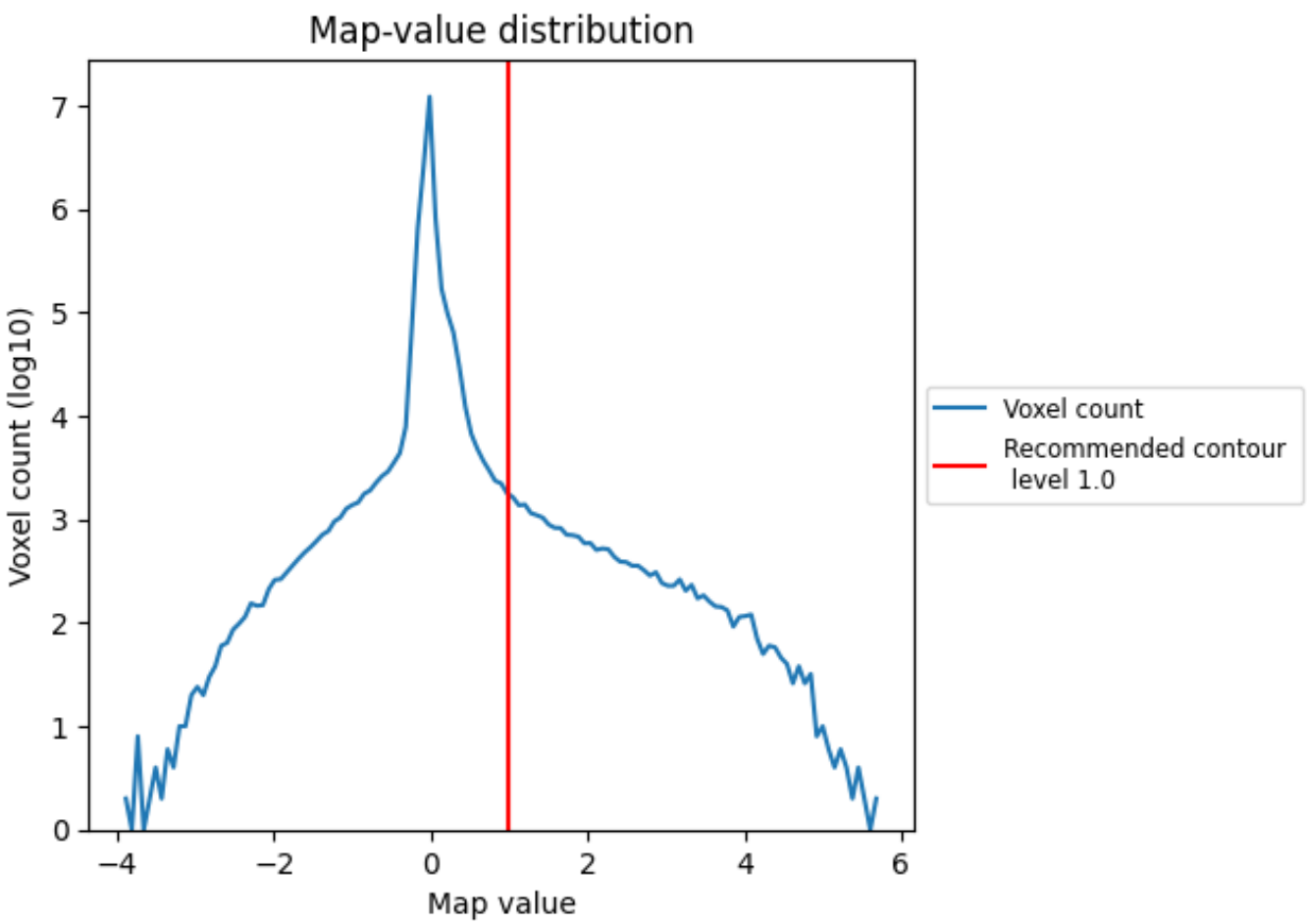
6.6 Mask visualisation (i)

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

7 Map analysis (i)

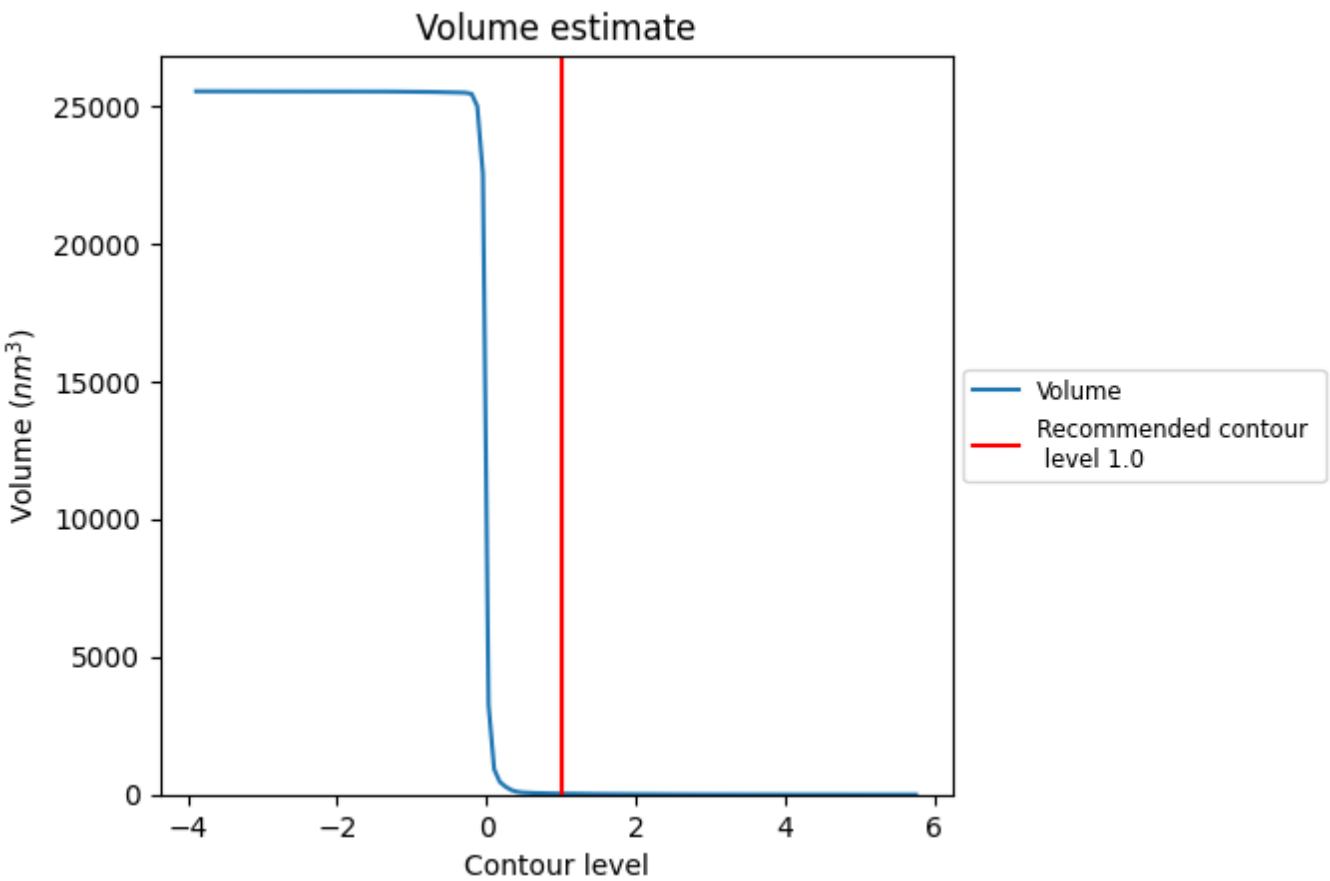
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

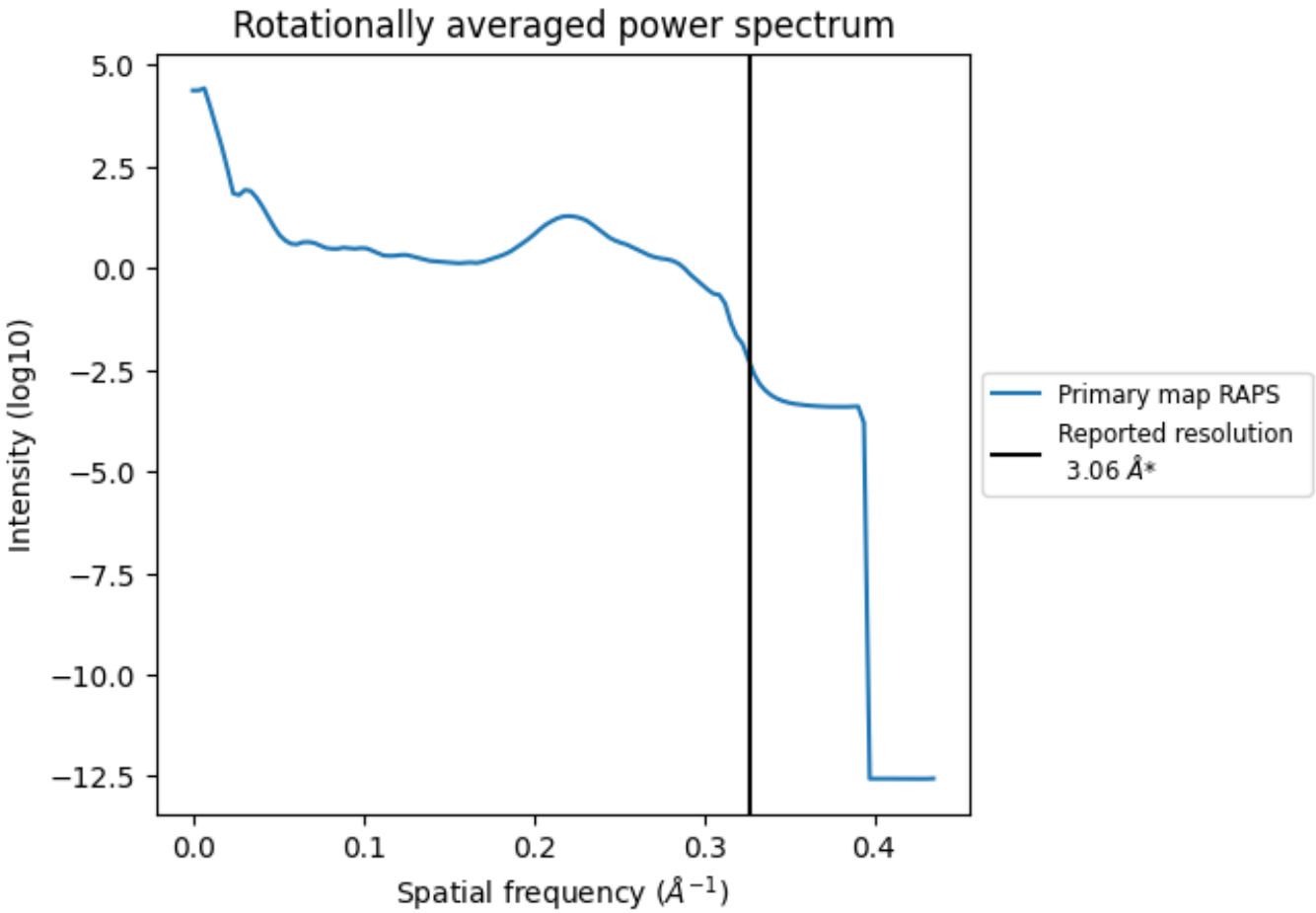
7.2 Volume estimate (i)



The volume at the recommended contour level is 34 nm^3; this corresponds to an approximate mass of 31 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)

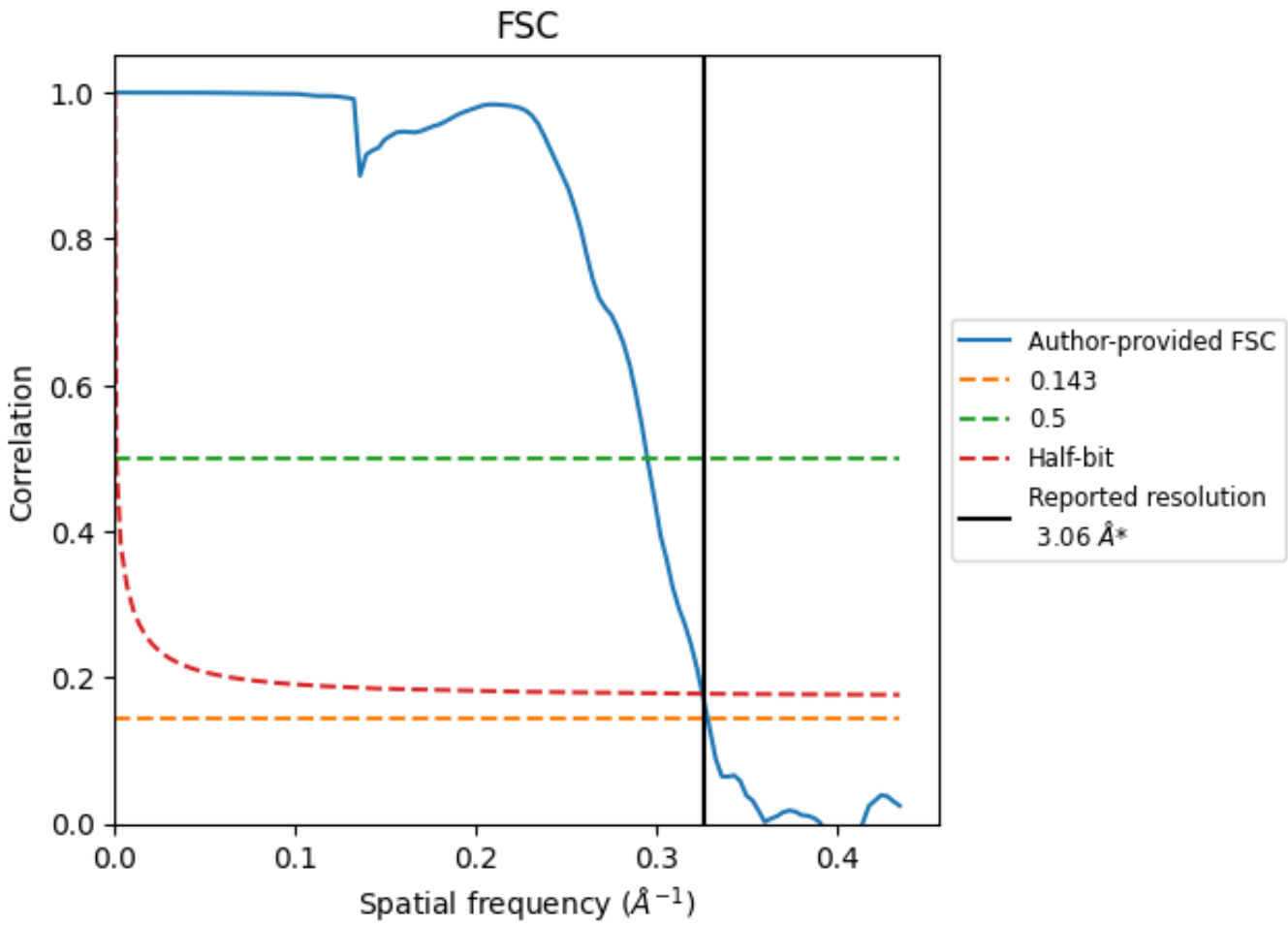


*Reported resolution corresponds to spatial frequency of 0.327 Å^{-1}

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 0.327 Å^{-1}

8.2 Resolution estimates (i)

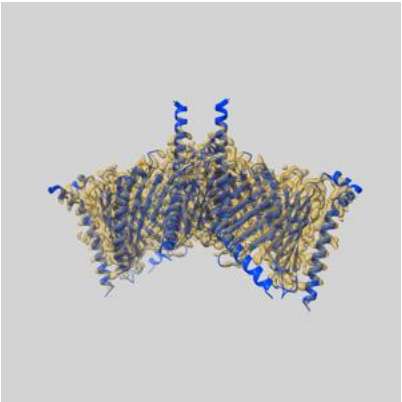
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.06	-	-
Author-provided FSC curve	3.04	3.39	3.07
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

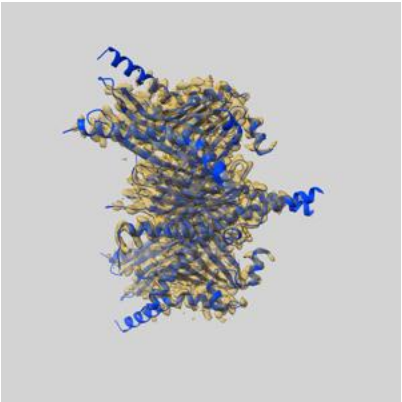
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-20728 and PDB model 6UCU. Per-residue inclusion information can be found in section 3 on page 10.

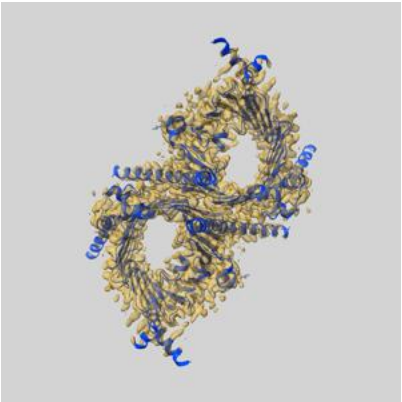
9.1 Map-model overlay (i)



X



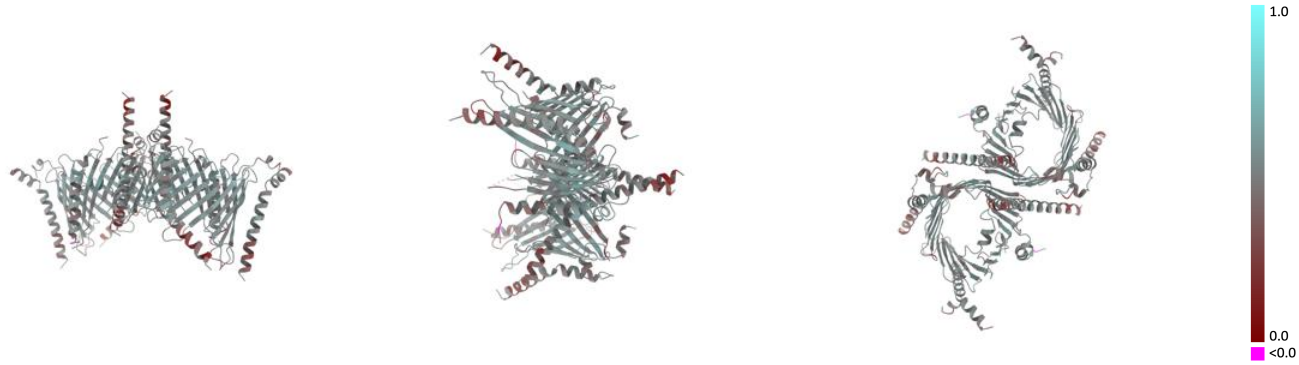
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.0 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.

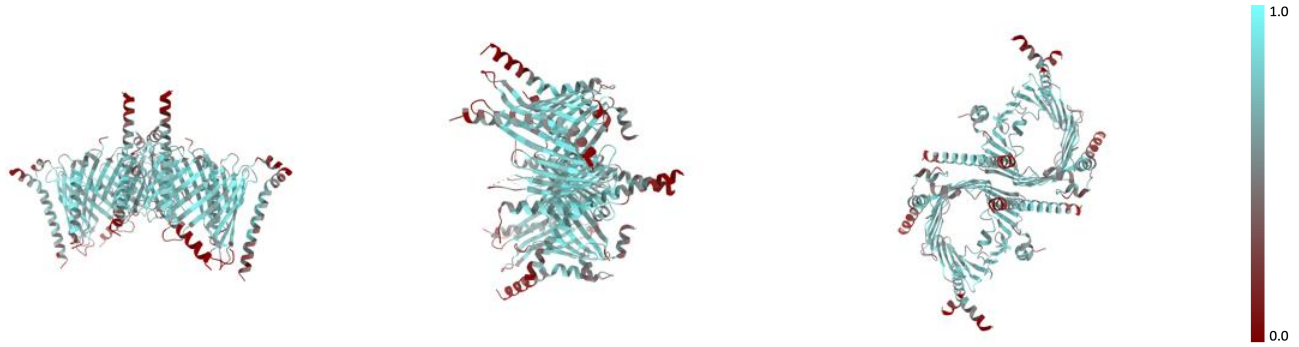
9.2 Q-score mapped to coordinate model (i)



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.

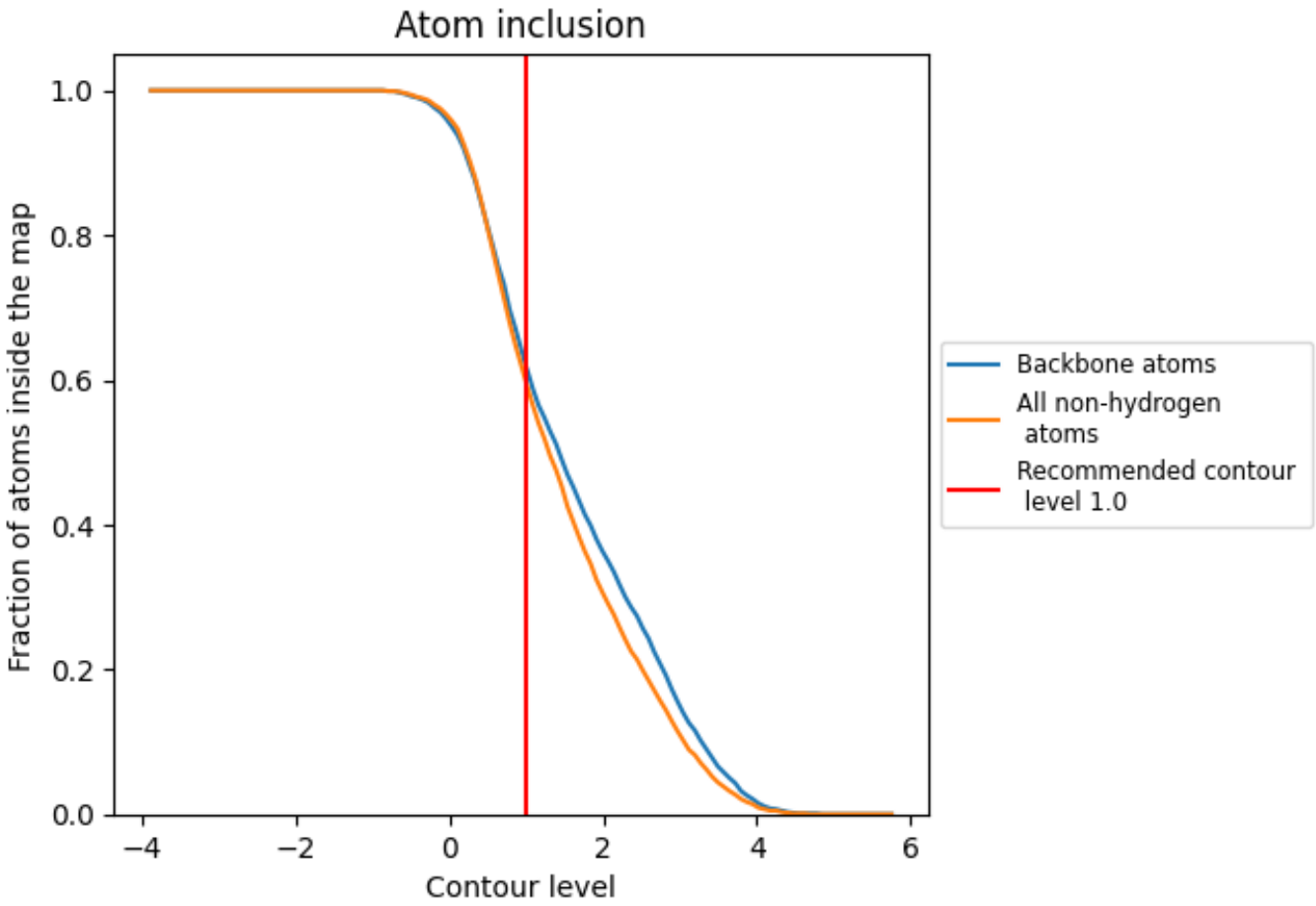
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (1.0).

9.4 Atom inclusion (i)



At the recommended contour level, 62% of all backbone atoms, 60% 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 (1.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5950	0.4920
A	0.6610	0.5150
B	0.4550	0.4390
C	0.4680	0.4560
D	0.5430	0.4830
E	0.4270	0.4480
I	0.6610	0.5140
J	0.4550	0.4320
K	0.4710	0.4580
L	0.5430	0.4800
M	0.4270	0.4510