



Full wwPDB EM Validation Report ⓘ

Nov 6, 2022 – 06:15 PM EST

PDB ID : 6CNM
EMDB ID : EMD-7537
Title : Cryo-EM structure of the human SK4/calmodulin channel complex
Authors : Lee, C.H.; MacKinnon, R.
Deposited on : 2018-03-08
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43
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 : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

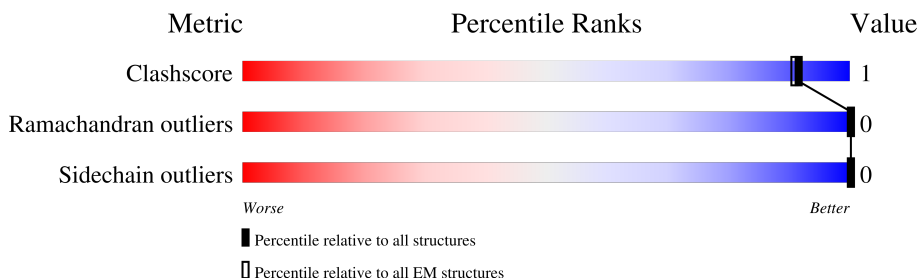
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY





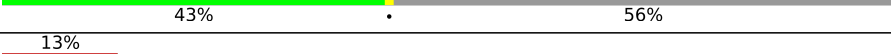
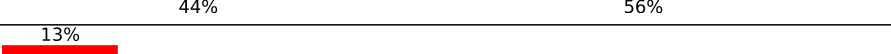
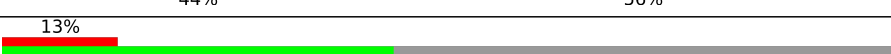

The reported resolution of this entry is 3.40 Å.

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)
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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	427	
1	B	427	
1	C	427	
1	D	427	
2	E	149	
2	F	149	
2	G	149	
2	H	149	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12541 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 Intermediate conductance calcium-activated potassium channel protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	359	Total	C	N	O	S	0	0
			2694	1746	487	442	19		
1	B	359	Total	C	N	O	S	0	0
			2694	1746	487	442	19		
1	C	359	Total	C	N	O	S	0	0
			2694	1746	487	442	19		
1	D	359	Total	C	N	O	S	0	0
			2694	1746	487	442	19		

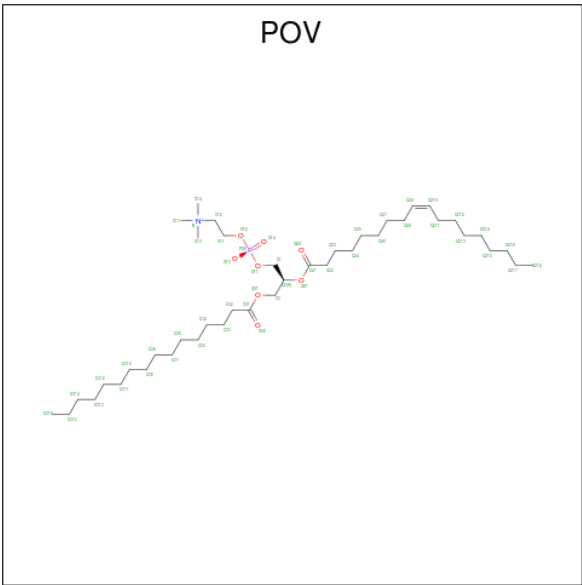
- Molecule 2 is a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	66	Total	C	N	O	S	0	0
			363	227	66	69	1		
2	F	66	Total	C	N	O	S	0	0
			363	227	66	69	1		
2	G	66	Total	C	N	O	S	0	0
			363	227	66	69	1		
2	H	66	Total	C	N	O	S	0	0
			363	227	66	69	1		

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

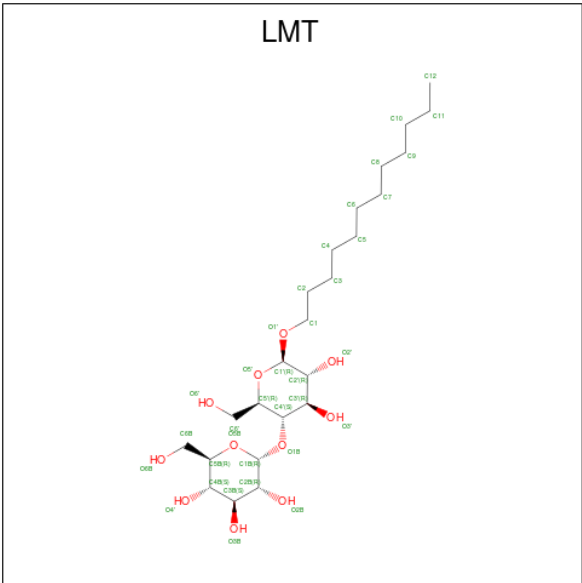
Mol	Chain	Residues	Atoms		AltConf
3	A	5	Total	K	0
			5	5	

- Molecule 4 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylamm onio)ethyl phosphate (three-letter code: POV) (formula: C₄₂H₈₂NO₈P).



Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	O	P	0
			21	12	8	1	
4	B	1	Total	C	O	P	0
			21	12	8	1	
4	C	1	Total	C	O	P	0
			21	12	8	1	
4	D	1	Total	C	O	P	0
			21	12	8	1	

- Molecule 5 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).

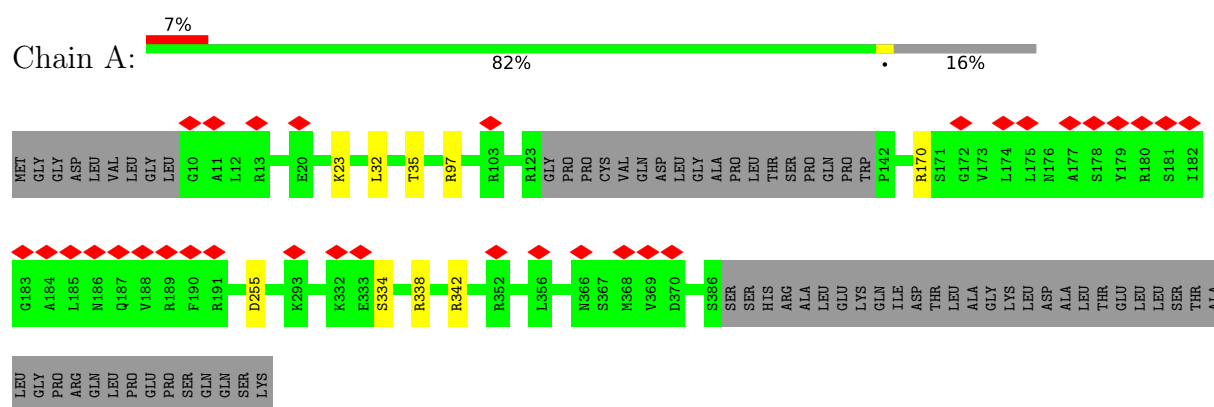


Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	C	O	0
			56	39	17	
5	A	1	Total	C	O	0
			56	39	17	
5	B	1	Total	C	O	0
			56	39	17	
5	B	1	Total	C	O	0
			56	39	17	
5	C	1	Total	C	O	0
			56	39	17	
5	C	1	Total	C	O	0
			56	39	17	
5	D	1	Total	C	O	0
			56	39	17	
5	D	1	Total	C	O	0
			56	39	17	

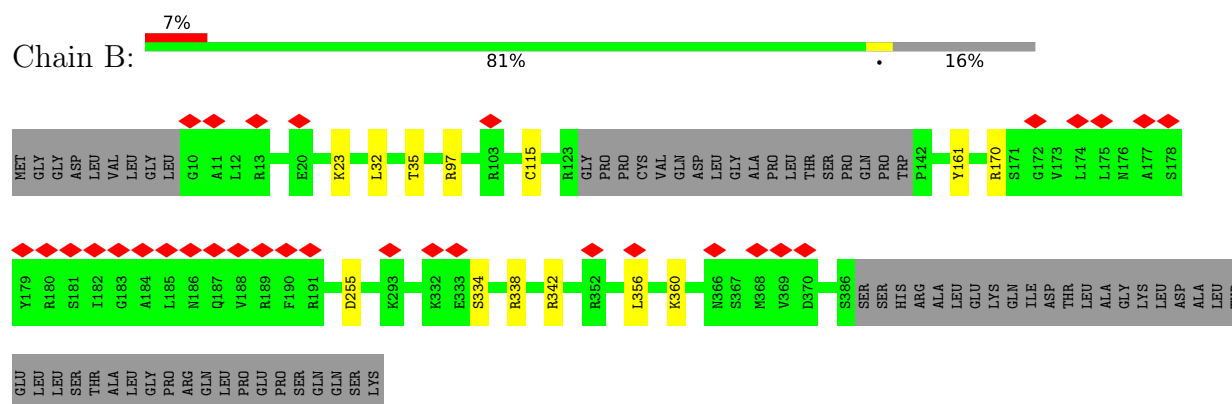
3 Residue-property plots

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

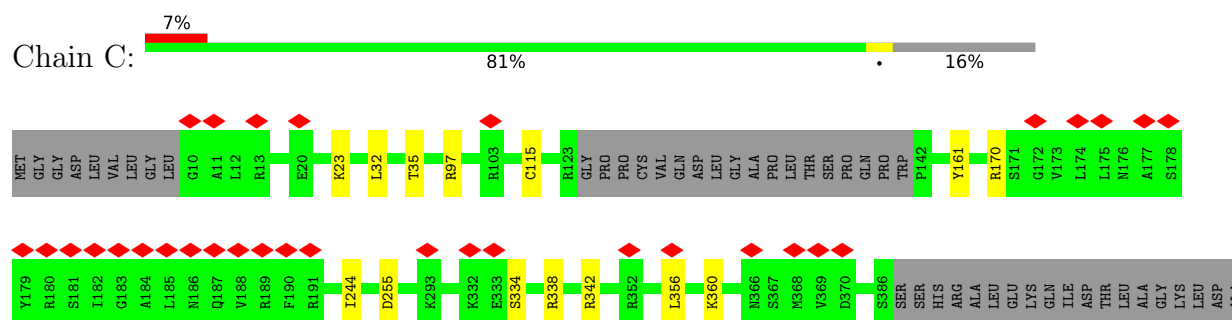
- Molecule 1: Intermediate conductance calcium-activated potassium channel protein 4



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LEU THR GLU LEU LEU SER THR ALA GLY PRO ARG GLN LEU PRO GLU PRO GLN SER LYS

- Molecule 1: Intermediate conductance calcium-activated potassium channel protein 4

Chain D: 

MET GLY GLY ASP LEU VAL LEU GLY LEU G10 A11 L12 R13 E20 K23 L32 T35 R97 R103 C115 R123 GLY PRO PRO CYS VAL GLN ASP LEU GLY ALA PRO LEU THR SER PRO GLN TRP P142 Y161 R170 S171 G172 V173 L174 L175 N176 A177 S178
 Y179 R180 S181 I182 G183 A184 L185 N186 Q187 V188 R189 F190 R191 D255 K293 K332 E333 S334 R338 R342 R352 L356 K360 N366 S367 M368 V369 D370 S386 SER SER HIS ARG ALA LEU LYS GLN ILE ASP THR LEU ALA GLY LYS LEU ASP ALA THR
 GLU LEU LEU SER THR ALA LEU PRO GLN LEU PRO GLU PRO SER GLN SER LYS

- Molecule 2: Calmodulin-1

Chain E: 

MET ALA ASP GLN THR LEU THR ALA GLU GLN ALA ILE LEU ALA GLU PHE MET PHE LYS GLU ALA PHE SER LYS PHE ASP ASP LYS ASP GLY ASP ASP GLY THR ILE THR LYS GLU LEU ARG SER LEU GLY GLN THR VAL MET ARG SER LEU GLY GLN THR ASN PRO THR GLU ALA LEU GLN ASP MET ILE ASN VAL ASP ALA GLY
 ASN GLY THR ILE ASP PHE PRO GLU PHE THR ALA ARG LYS MET LYS MET ASP THR ASP S81 D93 K94 D95 G96 N97 G98 E119 E120 V121 D122 I125 R126 A127 A128 D129 I130 D131 G132 D133 G134 Q135 E140 Q143 T146 ALA LYS

- Molecule 2: Calmodulin-1

Chain F: 

MET ALA ASP GLN THR LEU THR ALA GLU GLN ALA ILE LEU ALA GLU PHE MET PHE LYS GLU ALA PHE SER LYS PHE ASP ASP LYS ASP GLY ASP ASP GLY THR ILE THR LYS GLU LEU ARG SER LEU GLY GLN THR VAL MET ARG SER LEU GLY GLN THR ASN PRO THR GLU ALA LEU GLN ASP MET ILE ASN VAL ASP ALA GLY
 ASN GLY THR ILE ASP PHE PRO GLU PHE THR ALA ARG LYS MET LYS MET ASP THR ASP S81 D93 K94 D95 G96 N97 G98 E119 E120 V121 D122 E127 A128 D129 I130 D131 G132 D133 G134 Q135 E140 Q143 T146 ALA LYS

- Molecule 2: Calmodulin-1

Chain G: 

MET ALA ASP GLN THR LEU THR ALA GLU GLN ALA ILE LEU ALA GLU PHE MET PHE LYS GLU ALA PHE SER LYS PHE ASP ASP LYS ASP GLY ASP ASP GLY THR ILE THR LYS GLU LEU ARG SER LEU GLY GLN THR VAL MET ARG SER LEU GLY GLN THR ASN PRO THR GLU ALA LEU GLN ASP MET ILE ASN VAL ASP ALA GLY
 ASN GLY THR ILE ASP PHE PRO GLU PHE THR ALA ARG LYS MET LYS MET ASP THR ASP S81 D93 K94 D95 G96 N97 G98 E119 E120 V121 D122 E127 A128 D129 I130 D131 G132 D133 G134 Q135 E140 Q143 T146 ALA LYS

- Molecule 2: Calmodulin-1

Chain H: 

ASN	GLY	THR	ILE	ASP	PHE	PRO	GLU	GLU	PHE	LEU	THR	MET	MET	ALA	ARG	LYS	MET	LYS	ASP	THR	ASP	SS1	D93	K94	D95	G96	N97	E119	E120	E127	A128	D129	I130	D131	G132	D133	G134	Q135	E140	Q143	M144	M145	T146	ALA	LYS														
MET	ALA	ASP	GLN	LEU	THR	GLU	GLU	GLN	ILE	ALA	GLU	PHE	LYS	GLU	ALA	PHE	LYS	SER	LEU	PHE	ASP	LYS	ASP	GLY	ASP	GLY	THR	ILE	THR	THR	LYS	GLU	LEU	GLY	THR	VAL	ARG	SER	LEU	GLY	GLN	ASN	PRO	THR	GLU	ALA	GLU	LEU	GLN	ASP	MET	ILE	ASN	GLU	VAL	ASP	ALA	ASP	GLY

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	42422	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	75	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.234	Depositor
Minimum map value	-0.128	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	309.0, 309.0, 309.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.03, 1.03, 1.03	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: POV, K, 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	0.41	0/2749	0.56	0/3730
1	B	0.41	0/2749	0.56	0/3730
1	C	0.41	0/2749	0.56	0/3730
1	D	0.41	0/2749	0.56	0/3730
2	E	0.28	0/366	0.43	0/504
2	F	0.28	0/366	0.43	0/504
2	G	0.28	0/366	0.43	0/504
2	H	0.28	0/366	0.43	0/504
All	All	0.39	0/12460	0.55	0/16936

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2694	0	2691	6	0
1	B	2694	0	2691	8	0
1	C	2694	0	2691	9	0
1	D	2694	0	2691	8	0
2	E	363	0	214	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	363	0	214	0	0
2	G	363	0	214	0	0
2	H	363	0	214	0	0
3	A	5	0	0	0	0
4	A	21	0	15	2	0
4	B	21	0	15	2	0
4	C	21	0	15	2	0
4	D	21	0	15	2	0
5	A	56	0	66	0	0
5	B	56	0	66	0	0
5	C	56	0	66	0	0
5	D	56	0	66	0	0
All	All	12541	0	11944	36	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 1.

All (36) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:CYS:SG	1:B:161:TYR:OH	2.61	0.58
4:D:1101:POV:H22	4:D:1101:POV:H32A	1.88	0.55
4:A:1101:POV:H32A	4:A:1101:POV:H22	1.89	0.55
1:D:115:CYS:SG	1:D:161:TYR:OH	2.61	0.55
4:C:1101:POV:H22	4:C:1101:POV:H32A	1.89	0.53
4:B:1101:POV:H32A	4:B:1101:POV:H22	1.89	0.53
4:A:1101:POV:H22	4:A:1101:POV:C32	2.43	0.49
4:D:1101:POV:H22	4:D:1101:POV:C32	2.42	0.49
4:B:1101:POV:H22	4:B:1101:POV:C32	2.43	0.49
4:C:1101:POV:H22	4:C:1101:POV:C32	2.43	0.47
1:D:255:ASP:N	1:D:255:ASP:OD1	2.48	0.47
1:A:255:ASP:N	1:A:255:ASP:OD1	2.48	0.46
1:A:342:ARG:NH2	1:C:97:ARG:O	2.50	0.45
1:B:334:SER:O	1:B:338:ARG:NH2	2.50	0.45
1:B:97:ARG:O	1:D:342:ARG:NH2	2.50	0.45
1:C:334:SER:O	1:C:338:ARG:NH2	2.50	0.45
1:D:334:SER:O	1:D:338:ARG:NH2	2.50	0.45
1:B:255:ASP:N	1:B:255:ASP:OD1	2.48	0.44
1:C:255:ASP:OD1	1:C:255:ASP:N	2.48	0.44
1:B:342:ARG:NH2	1:D:97:ARG:O	2.50	0.44
1:C:32:LEU:HA	1:C:35:THR:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:LEU:HA	1:B:35:THR:HG22	2.00	0.44
1:D:32:LEU:HA	1:D:35:THR:HG22	2.00	0.44
1:A:32:LEU:HA	1:A:35:THR:HG22	2.00	0.44
1:C:23:LYS:HE3	1:C:170:ARG:HG2	1.99	0.44
1:A:97:ARG:O	1:C:342:ARG:NH2	2.50	0.43
1:D:23:LYS:HE3	1:D:170:ARG:HG2	2.00	0.43
1:A:334:SER:O	1:A:338:ARG:NH2	2.51	0.43
1:A:23:LYS:HE3	1:A:170:ARG:HG2	1.99	0.43
1:B:356:LEU:O	1:B:360:LYS:NZ	2.43	0.43
1:B:23:LYS:HE3	1:B:170:ARG:HG2	1.99	0.42
1:C:244:ILE:HD13	1:C:244:ILE:HA	1.91	0.42
1:C:356:LEU:O	1:C:360:LYS:NZ	2.45	0.42
1:C:115:CYS:SG	1:C:161:TYR:OH	2.61	0.41
1:D:356:LEU:O	1:D:360:LYS:NZ	2.46	0.41
2:E:125:ILE:O	2:E:129:ASP:CB	2.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	355/427 (83%)	338 (95%)	17 (5%)	0	100	100
1	B	355/427 (83%)	338 (95%)	17 (5%)	0	100	100
1	C	355/427 (83%)	338 (95%)	17 (5%)	0	100	100
1	D	355/427 (83%)	338 (95%)	17 (5%)	0	100	100
2	E	64/149 (43%)	63 (98%)	1 (2%)	0	100	100
2	F	64/149 (43%)	63 (98%)	1 (2%)	0	100	100
2	G	64/149 (43%)	63 (98%)	1 (2%)	0	100	100
2	H	64/149 (43%)	63 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1676/2304 (73%)	1604 (96%)	72 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	256/356 (72%)	256 (100%)	0	100	100
1	B	256/356 (72%)	256 (100%)	0	100	100
1	C	256/356 (72%)	256 (100%)	0	100	100
1	D	256/356 (72%)	256 (100%)	0	100	100
2	E	10/127 (8%)	10 (100%)	0	100	100
2	F	10/127 (8%)	10 (100%)	0	100	100
2	G	10/127 (8%)	10 (100%)	0	100	100
2	H	10/127 (8%)	10 (100%)	0	100	100
All	All	1064/1932 (55%)	1064 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 5 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	POV	A	1101	-	20,20,51	1.48	2 (10%)	24,25,59	1.47	4 (16%)
5	LMT	B	1103	-	21,21,36	1.23	3 (14%)	26,26,47	1.27	3 (11%)
5	LMT	D	1104	-	36,36,36	1.39	7 (19%)	47,47,47	1.20	3 (6%)
5	LMT	A	1104	-	36,36,36	1.38	7 (19%)	47,47,47	1.20	2 (4%)
5	LMT	B	1104	-	36,36,36	1.38	7 (19%)	47,47,47	1.20	2 (4%)
4	POV	B	1101	-	20,20,51	1.48	2 (10%)	24,25,59	1.47	4 (16%)
5	LMT	C	1104	-	36,36,36	1.38	7 (19%)	47,47,47	1.20	2 (4%)
5	LMT	C	1103	-	21,21,36	1.23	2 (9%)	26,26,47	1.28	3 (11%)
4	POV	D	1101	-	20,20,51	1.48	2 (10%)	24,25,59	1.47	4 (16%)
4	POV	C	1101	-	20,20,51	1.47	2 (10%)	24,25,59	1.47	4 (16%)
5	LMT	D	1103	-	21,21,36	1.23	2 (9%)	26,26,47	1.28	3 (11%)
5	LMT	A	1103	-	21,21,36	1.23	2 (9%)	26,26,47	1.28	3 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	POV	A	1101	-	-	9/22/22/55	-
5	LMT	B	1103	-	-	6/12/32/61	0/1/1/2
5	LMT	D	1104	-	-	7/21/61/61	0/2/2/2
5	LMT	A	1104	-	-	7/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	LMT	B	1104	-	-	7/21/61/61	0/2/2/2
4	POV	B	1101	-	-	9/22/22/55	-
5	LMT	C	1104	-	-	7/21/61/61	0/2/2/2
5	LMT	C	1103	-	-	6/12/32/61	0/1/1/2
4	POV	D	1101	-	-	9/22/22/55	-
4	POV	C	1101	-	-	9/22/22/55	-
5	LMT	D	1103	-	-	6/12/32/61	0/1/1/2
5	LMT	A	1103	-	-	6/12/32/61	0/1/1/2

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1101	POV	O31-C31	4.30	1.45	1.33
4	D	1101	POV	O31-C31	4.29	1.45	1.33
4	A	1101	POV	O31-C31	4.29	1.45	1.33
4	C	1101	POV	O31-C31	4.27	1.45	1.33
4	A	1101	POV	O21-C21	4.11	1.45	1.34
4	D	1101	POV	O21-C21	4.10	1.45	1.34
4	C	1101	POV	O21-C21	4.09	1.45	1.34
4	B	1101	POV	O21-C21	4.09	1.45	1.34
5	A	1103	LMT	O3'-C3'	-2.94	1.36	1.43
5	B	1103	LMT	O3'-C3'	-2.91	1.36	1.43
5	D	1104	LMT	O3'-C3'	-2.90	1.36	1.43
5	C	1104	LMT	O3'-C3'	-2.90	1.36	1.43
5	B	1104	LMT	O2'-C2'	-2.90	1.36	1.43
5	C	1103	LMT	O3'-C3'	-2.90	1.36	1.43
5	D	1104	LMT	O2'-C2'	-2.90	1.36	1.43
5	A	1104	LMT	O2'-C2'	-2.90	1.36	1.43
5	D	1103	LMT	O3'-C3'	-2.89	1.36	1.43
5	A	1104	LMT	O3'-C3'	-2.89	1.36	1.43
5	C	1104	LMT	O2'-C2'	-2.89	1.36	1.43
5	B	1104	LMT	O3'-C3'	-2.86	1.36	1.43
5	D	1104	LMT	O1'-C1'	-2.76	1.35	1.40
5	B	1104	LMT	O1'-C1'	-2.75	1.35	1.40
5	C	1104	LMT	O1'-C1'	-2.70	1.35	1.40
5	A	1104	LMT	O1'-C1'	-2.70	1.35	1.40
5	B	1104	LMT	O2B-C2B	-2.58	1.36	1.43
5	D	1104	LMT	O2B-C2B	-2.58	1.36	1.43
5	A	1104	LMT	O2B-C2B	-2.58	1.36	1.43
5	C	1104	LMT	O2B-C2B	-2.57	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1104	LMT	O3B-C3B	-2.46	1.37	1.43
5	D	1104	LMT	O4'-C4B	-2.45	1.37	1.43
5	D	1104	LMT	O3B-C3B	-2.45	1.37	1.43
5	A	1104	LMT	O4'-C4B	-2.43	1.37	1.43
5	A	1104	LMT	O3B-C3B	-2.42	1.37	1.43
5	C	1104	LMT	O4'-C4B	-2.42	1.37	1.43
5	C	1103	LMT	O1'-C1'	-2.42	1.36	1.40
5	B	1104	LMT	O3B-C3B	-2.41	1.37	1.43
5	B	1104	LMT	O4'-C4B	-2.40	1.37	1.43
5	A	1103	LMT	O1'-C1'	-2.39	1.36	1.40
5	D	1103	LMT	O1'-C1'	-2.36	1.36	1.40
5	B	1103	LMT	O1'-C1'	-2.35	1.36	1.40
5	A	1104	LMT	O5'-C5'	-2.13	1.39	1.44
5	C	1104	LMT	O5'-C5'	-2.13	1.39	1.44
5	B	1104	LMT	O5'-C5'	-2.12	1.39	1.44
5	D	1104	LMT	O5'-C5'	-2.11	1.39	1.44
5	B	1103	LMT	C3'-C2'	2.02	1.57	1.52

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1101	POV	O21-C21-C22	4.02	120.17	111.50
4	C	1101	POV	O21-C21-C22	4.02	120.17	111.50
4	B	1101	POV	O21-C21-C22	4.02	120.17	111.50
4	A	1101	POV	O21-C21-C22	4.02	120.16	111.50
5	C	1104	LMT	C1'-O5'-C5'	-3.58	106.66	113.69
5	D	1104	LMT	C1'-O5'-C5'	-3.58	106.67	113.69
5	A	1104	LMT	C1'-O5'-C5'	-3.57	106.69	113.69
5	B	1104	LMT	C1'-O5'-C5'	-3.56	106.71	113.69
5	B	1104	LMT	C2'-C3'-C4'	3.47	117.60	109.68
5	D	1104	LMT	C2'-C3'-C4'	3.46	117.58	109.68
5	A	1104	LMT	C2'-C3'-C4'	3.46	117.58	109.68
5	C	1104	LMT	C2'-C3'-C4'	3.45	117.56	109.68
5	D	1103	LMT	C4'-C3'-C2'	3.16	116.35	110.82
5	A	1103	LMT	C4'-C3'-C2'	3.14	116.31	110.82
5	B	1103	LMT	C4'-C3'-C2'	3.13	116.28	110.82
5	C	1103	LMT	C4'-C3'-C2'	3.12	116.27	110.82
5	D	1103	LMT	O5'-C5'-C4'	2.86	114.88	109.69
5	C	1103	LMT	O5'-C5'-C4'	2.85	114.87	109.69
5	A	1103	LMT	O5'-C5'-C4'	2.84	114.85	109.69
5	B	1103	LMT	O5'-C5'-C4'	2.80	114.78	109.69
5	A	1103	LMT	O5'-C1'-C2'	-2.70	104.62	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1103	LMT	O5'-C1'-C2'	-2.69	104.65	110.35
5	D	1103	LMT	O5'-C1'-C2'	-2.69	104.65	110.35
5	B	1103	LMT	O5'-C1'-C2'	-2.67	104.69	110.35
4	B	1101	POV	O31-C31-C32	2.64	120.19	111.91
4	C	1101	POV	O31-C31-C32	2.63	120.17	111.91
4	D	1101	POV	O31-C31-C32	2.63	120.15	111.91
4	A	1101	POV	O31-C31-C32	2.62	120.14	111.91
4	A	1101	POV	C2-O21-C21	-2.45	111.75	117.79
4	D	1101	POV	C2-O21-C21	-2.43	111.81	117.79
4	C	1101	POV	C2-O21-C21	-2.42	111.83	117.79
4	B	1101	POV	C2-O21-C21	-2.42	111.83	117.79
4	B	1101	POV	O13-P-O14	2.37	119.97	110.68
4	A	1101	POV	O13-P-O14	2.37	119.96	110.68
4	D	1101	POV	O13-P-O14	2.37	119.94	110.68
4	C	1101	POV	O13-P-O14	2.36	119.93	110.68
5	D	1104	LMT	O5B-C5B-C6B	2.00	111.41	106.44

There are no chirality outliers.

All (88) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1101	POV	C1-O11-P-O12
4	A	1101	POV	C1-O11-P-O13
4	A	1101	POV	C22-C21-O21-C2
4	B	1101	POV	C1-O11-P-O12
4	B	1101	POV	C1-O11-P-O13
4	B	1101	POV	C22-C21-O21-C2
4	C	1101	POV	C1-O11-P-O12
4	C	1101	POV	C1-O11-P-O13
4	C	1101	POV	C22-C21-O21-C2
4	D	1101	POV	C1-O11-P-O12
4	D	1101	POV	C1-O11-P-O13
4	D	1101	POV	C22-C21-O21-C2
4	A	1101	POV	O22-C21-O21-C2
4	B	1101	POV	O22-C21-O21-C2
4	C	1101	POV	O22-C21-O21-C2
4	D	1101	POV	O22-C21-O21-C2
5	B	1104	LMT	O5B-C5B-C6B-O6B
5	C	1104	LMT	O5B-C5B-C6B-O6B
5	A	1104	LMT	O5B-C5B-C6B-O6B
5	D	1104	LMT	O5B-C5B-C6B-O6B
5	A	1103	LMT	O5'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
5	B	1103	LMT	O5'-C1'-O1'-C1
5	C	1103	LMT	O5'-C1'-O1'-C1
5	D	1103	LMT	O5'-C1'-O1'-C1
4	A	1101	POV	C32-C31-O31-C3
4	B	1101	POV	C32-C31-O31-C3
4	C	1101	POV	C32-C31-O31-C3
4	D	1101	POV	C32-C31-O31-C3
4	A	1101	POV	O32-C31-O31-C3
4	B	1101	POV	O32-C31-O31-C3
4	C	1101	POV	O32-C31-O31-C3
4	D	1101	POV	O32-C31-O31-C3
5	A	1103	LMT	C2'-C1'-O1'-C1
5	B	1103	LMT	C2'-C1'-O1'-C1
5	C	1103	LMT	C2'-C1'-O1'-C1
5	D	1103	LMT	C2'-C1'-O1'-C1
5	B	1104	LMT	C4B-C5B-C6B-O6B
5	C	1104	LMT	C4B-C5B-C6B-O6B
5	A	1104	LMT	C4B-C5B-C6B-O6B
5	A	1103	LMT	C2-C1-O1'-C1'
5	B	1103	LMT	C2-C1-O1'-C1'
5	C	1103	LMT	C2-C1-O1'-C1'
5	D	1104	LMT	C4B-C5B-C6B-O6B
5	A	1103	LMT	O1'-C1-C2-C3
5	B	1103	LMT	O1'-C1-C2-C3
5	C	1103	LMT	O1'-C1-C2-C3
5	D	1103	LMT	O1'-C1-C2-C3
5	C	1104	LMT	O5'-C5'-C6'-O6'
5	D	1103	LMT	C3-C4-C5-C6
5	B	1103	LMT	C3-C4-C5-C6
5	C	1103	LMT	C3-C4-C5-C6
5	C	1104	LMT	C6-C7-C8-C9
5	A	1103	LMT	C3-C4-C5-C6
5	B	1104	LMT	C6-C7-C8-C9
5	A	1104	LMT	C6-C7-C8-C9
5	A	1104	LMT	O5'-C5'-C6'-O6'
5	B	1104	LMT	O5'-C5'-C6'-O6'
5	D	1104	LMT	C6-C7-C8-C9
4	A	1101	POV	O11-C1-C2-C3
4	B	1101	POV	O11-C1-C2-C3
4	C	1101	POV	O11-C1-C2-C3
4	D	1101	POV	O11-C1-C2-C3
5	D	1104	LMT	O5'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
5	D	1103	LMT	C2-C1-O1'-C1'
4	A	1101	POV	O11-C1-C2-O21
4	B	1101	POV	O11-C1-C2-O21
4	C	1101	POV	O11-C1-C2-O21
4	D	1101	POV	O11-C1-C2-O21
5	A	1104	LMT	O1'-C1-C2-C3
5	B	1104	LMT	O1'-C1-C2-C3
5	C	1104	LMT	O1'-C1-C2-C3
5	D	1104	LMT	O1'-C1-C2-C3
4	A	1101	POV	C3-C2-O21-C21
4	B	1101	POV	C3-C2-O21-C21
4	C	1101	POV	C3-C2-O21-C21
4	D	1101	POV	C3-C2-O21-C21
5	A	1104	LMT	C2-C3-C4-C5
5	C	1104	LMT	C2-C3-C4-C5
5	B	1104	LMT	C2-C3-C4-C5
5	D	1104	LMT	C2-C3-C4-C5
5	C	1104	LMT	C11-C10-C9-C8
5	B	1104	LMT	C11-C10-C9-C8
5	A	1104	LMT	C11-C10-C9-C8
5	D	1104	LMT	C11-C10-C9-C8
5	D	1103	LMT	C2-C3-C4-C5
5	C	1103	LMT	C2-C3-C4-C5
5	B	1103	LMT	C2-C3-C4-C5
5	A	1103	LMT	C2-C3-C4-C5

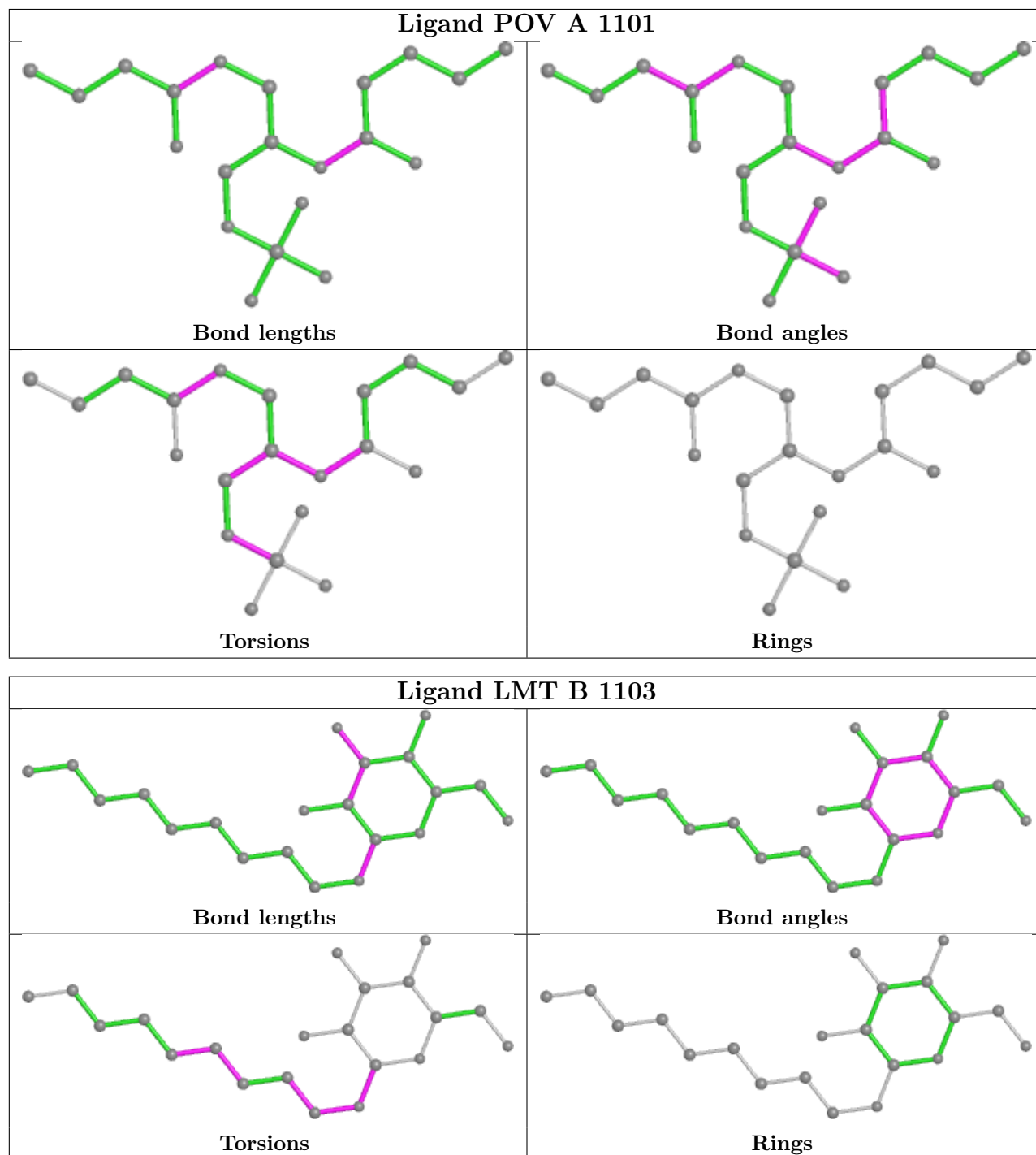
There are no ring outliers.

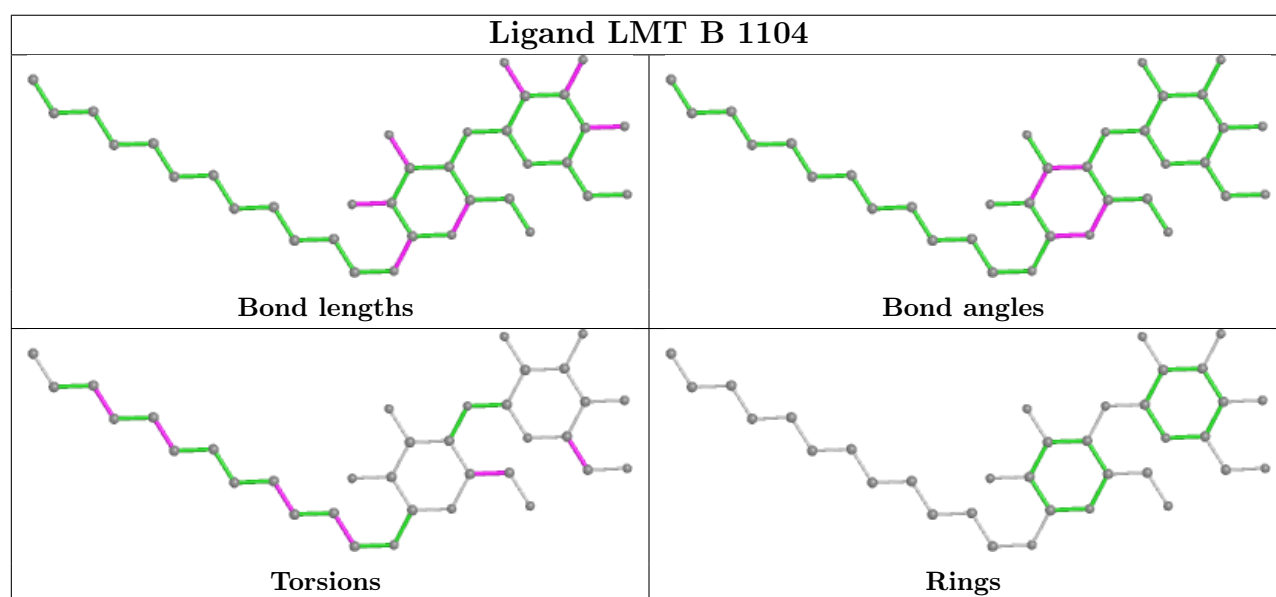
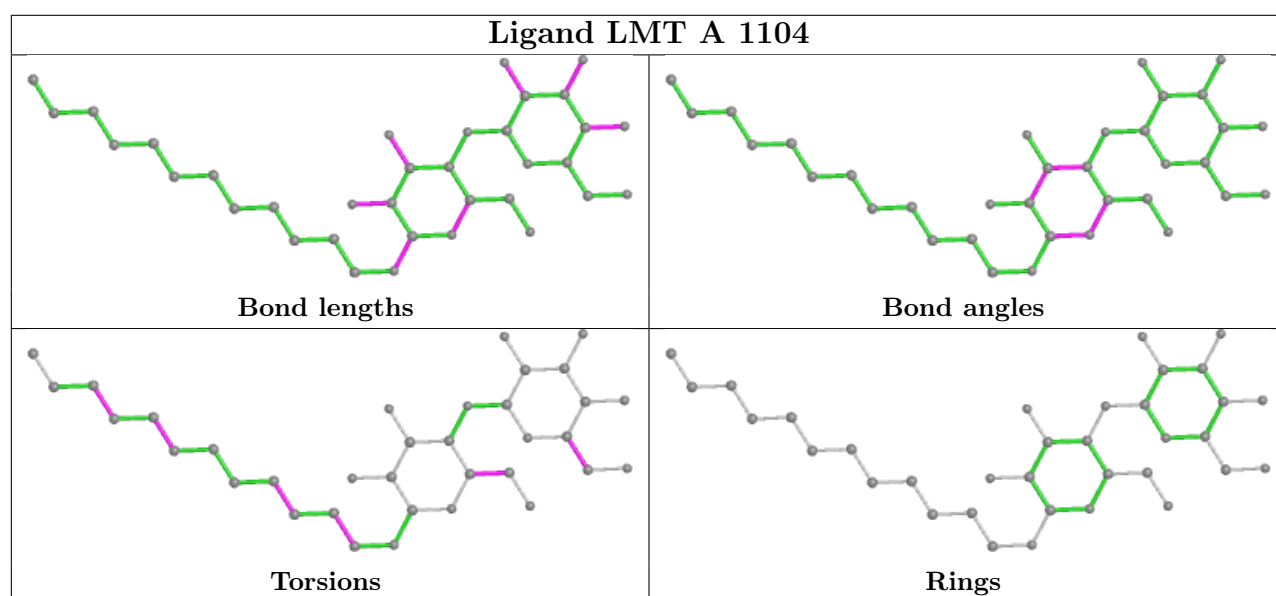
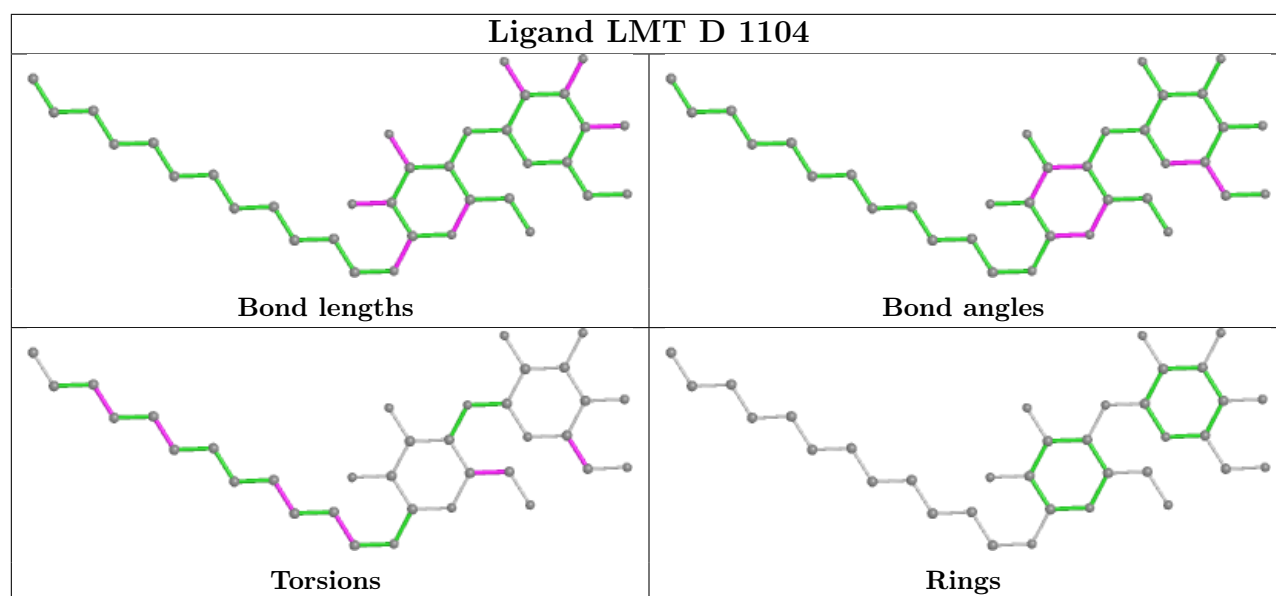
4 monomers are involved in 8 short contacts:

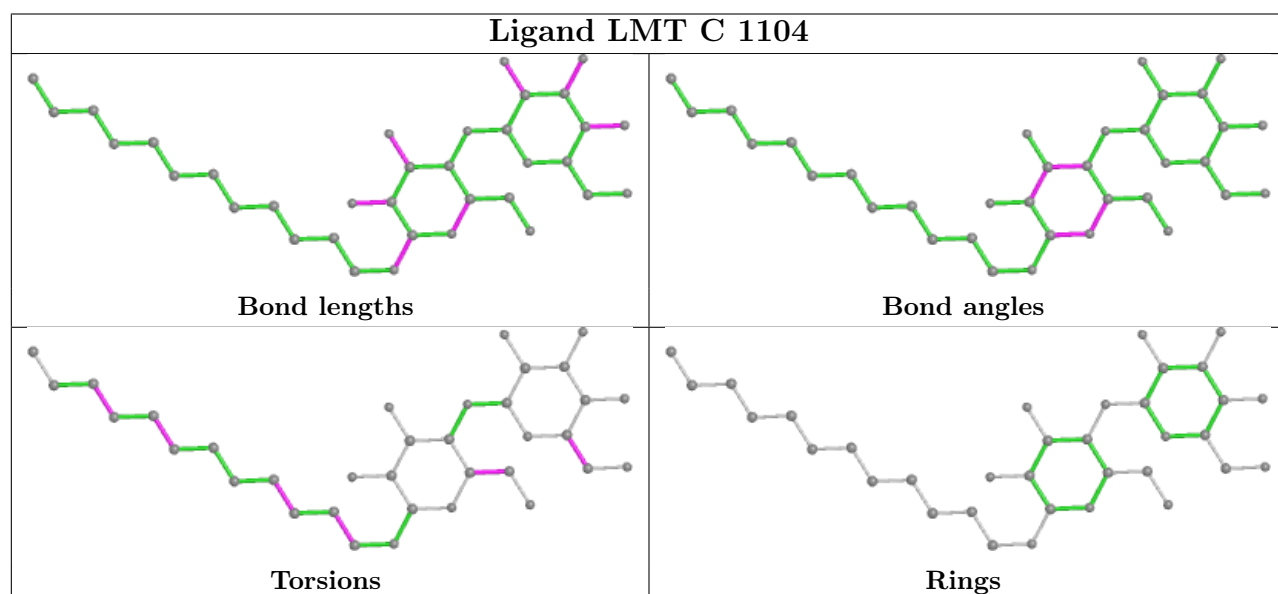
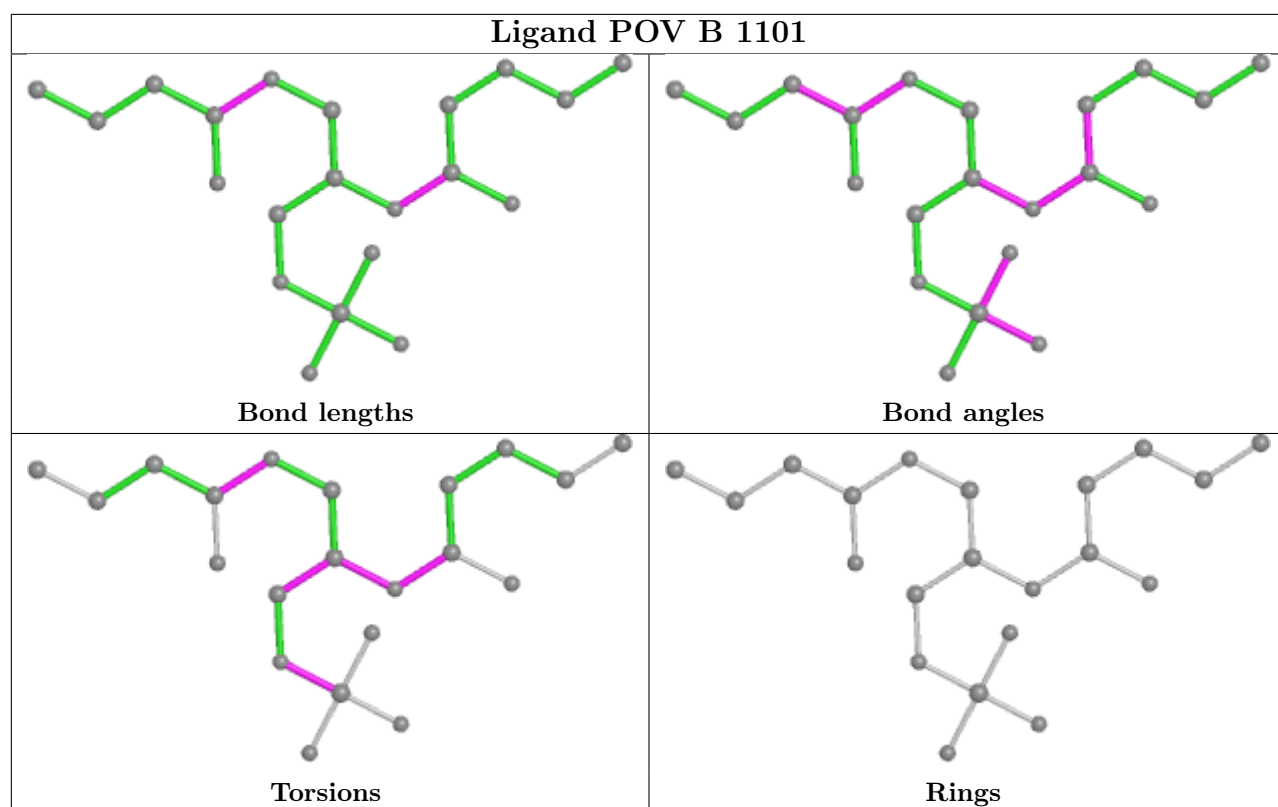
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1101	POV	2	0
4	B	1101	POV	2	0
4	D	1101	POV	2	0
4	C	1101	POV	2	0

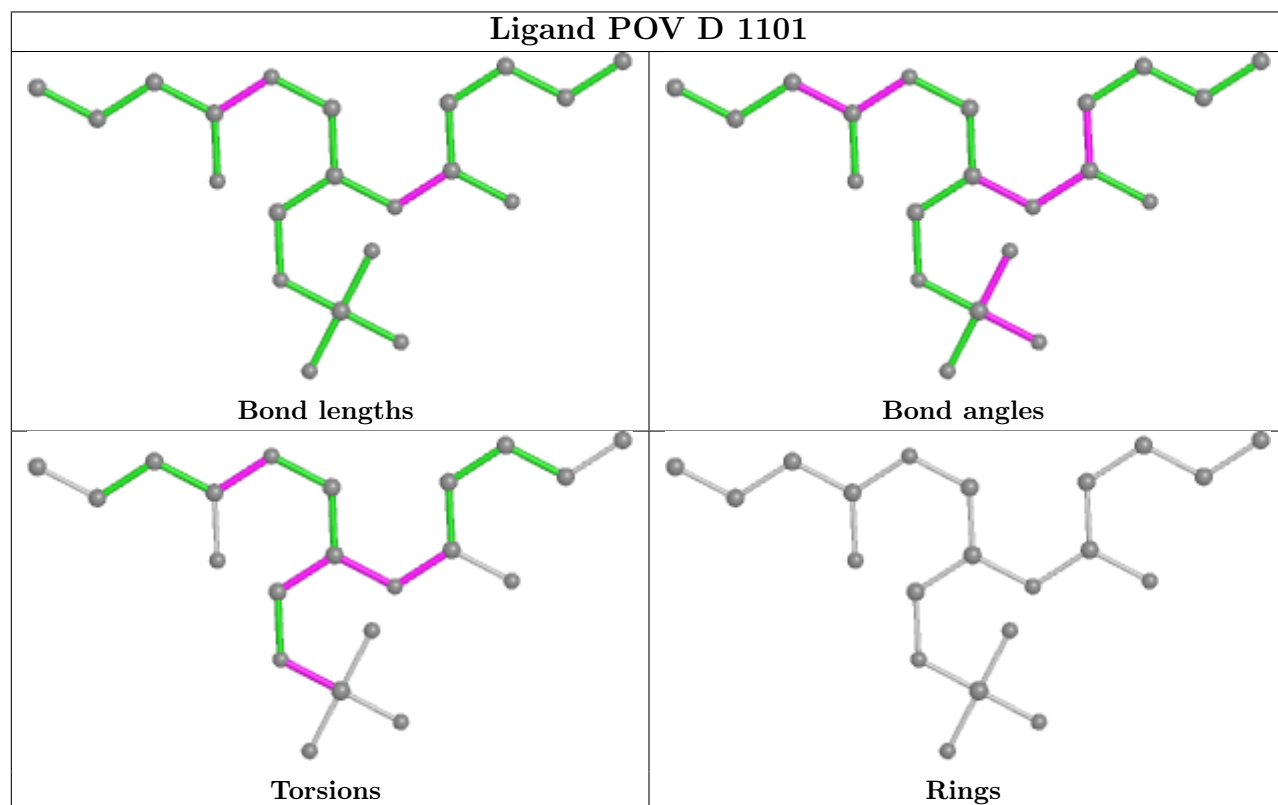
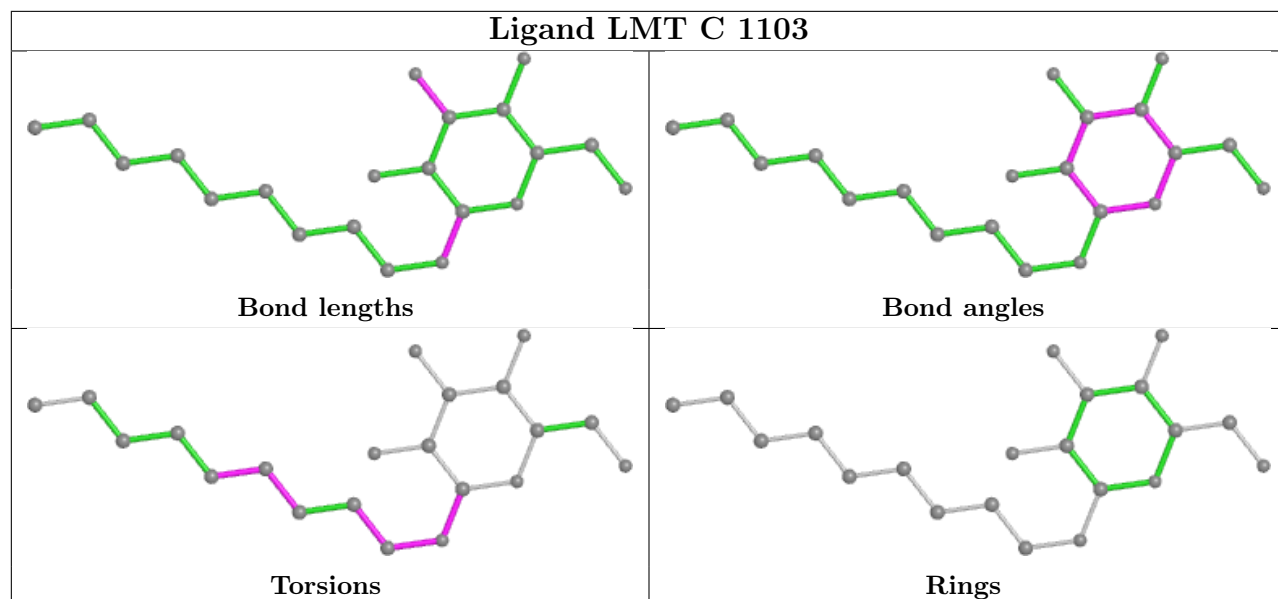
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

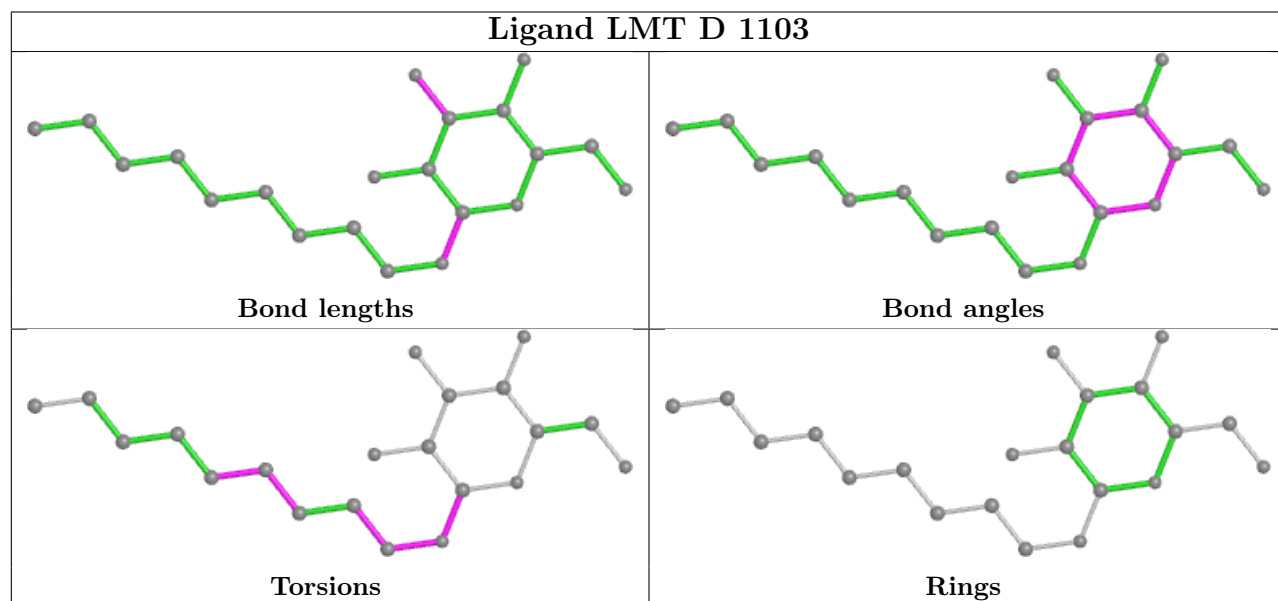
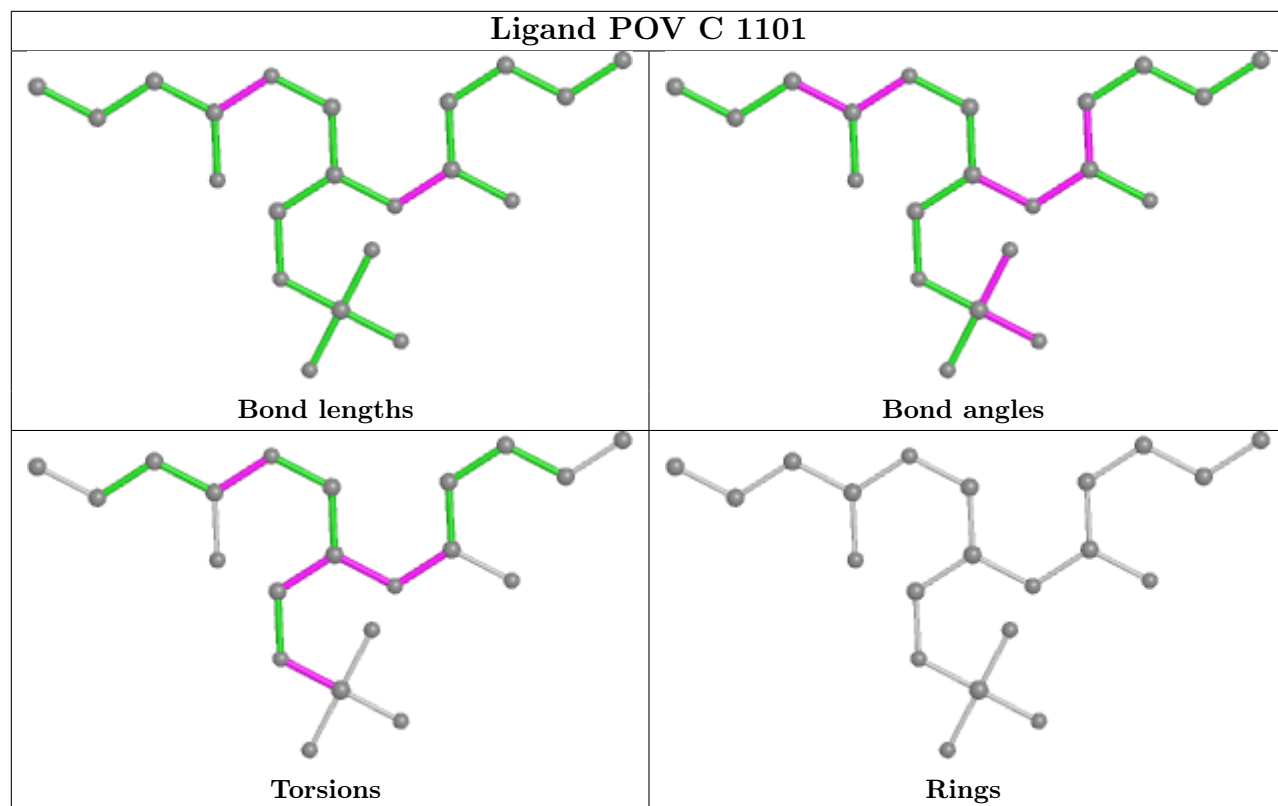
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

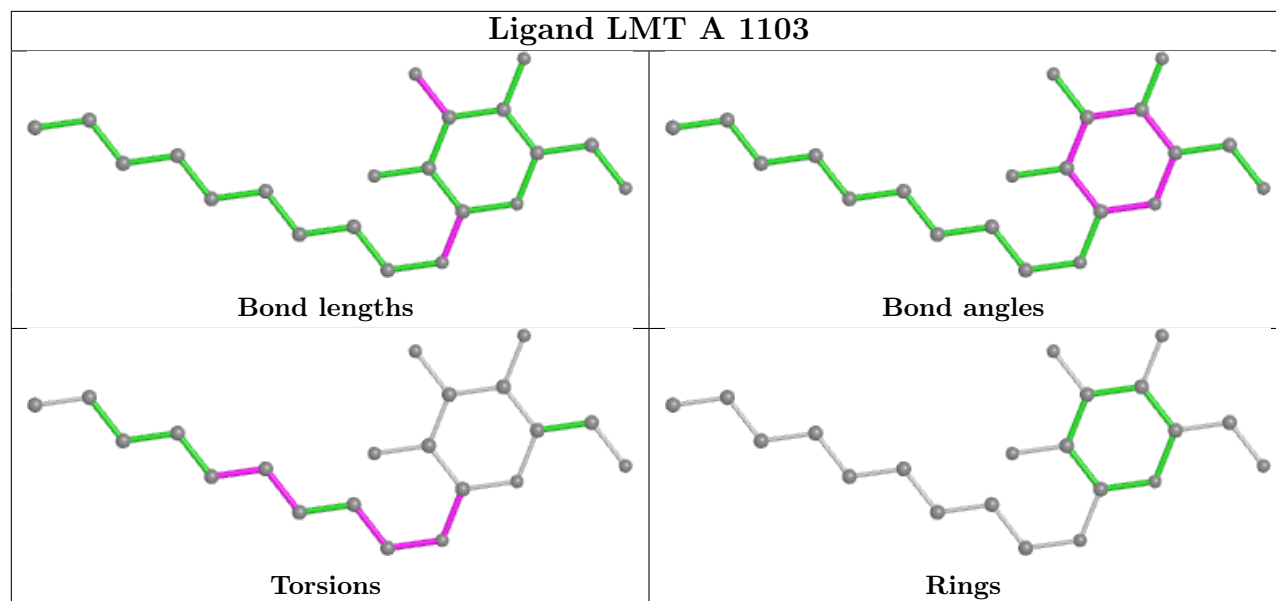












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

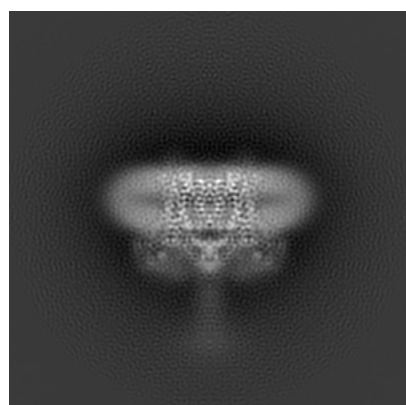
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7537. These allow visual inspection of the internal detail of the map and identification of artifacts.

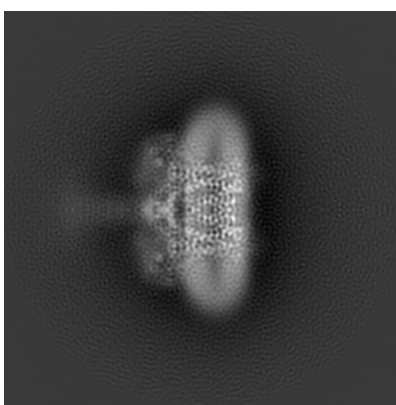
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

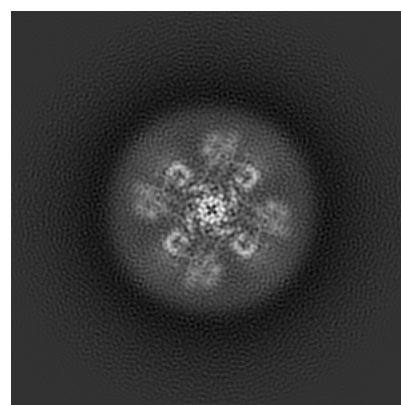
6.1.1 Primary map



X



Y

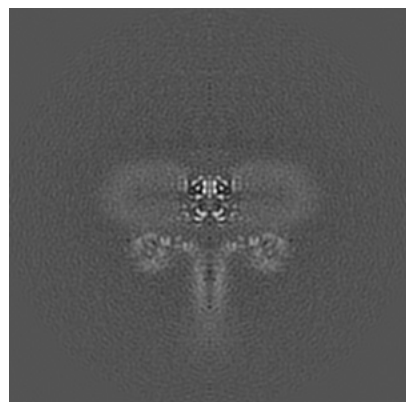


Z

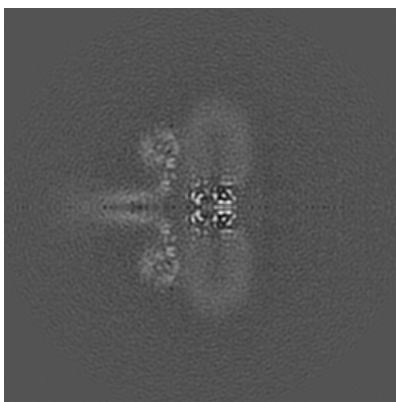
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

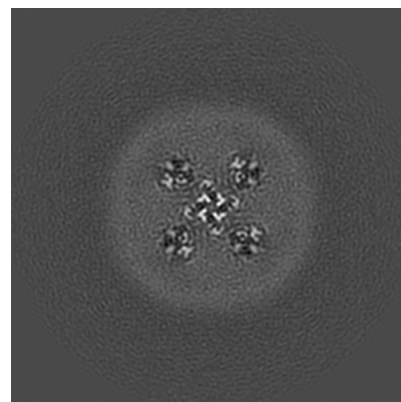
6.2.1 Primary map



X Index: 150



Y Index: 150

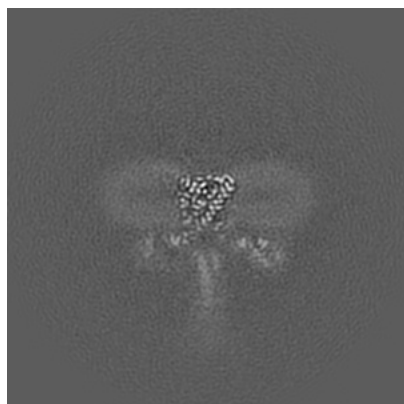


Z Index: 150

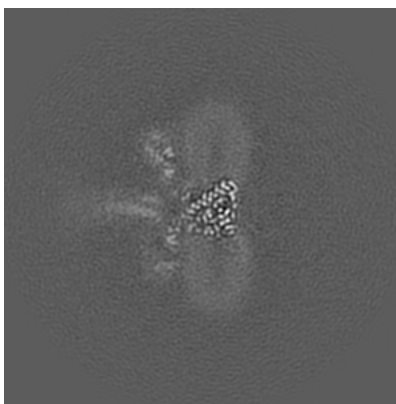
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

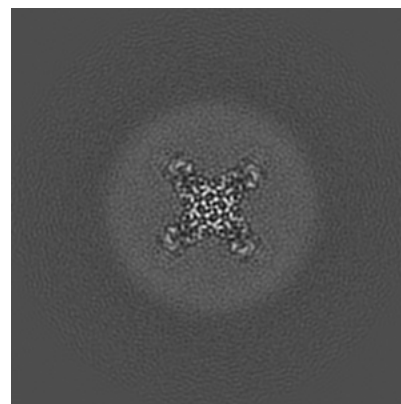
6.3.1 Primary map



X Index: 156



Y Index: 144



Z Index: 167

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

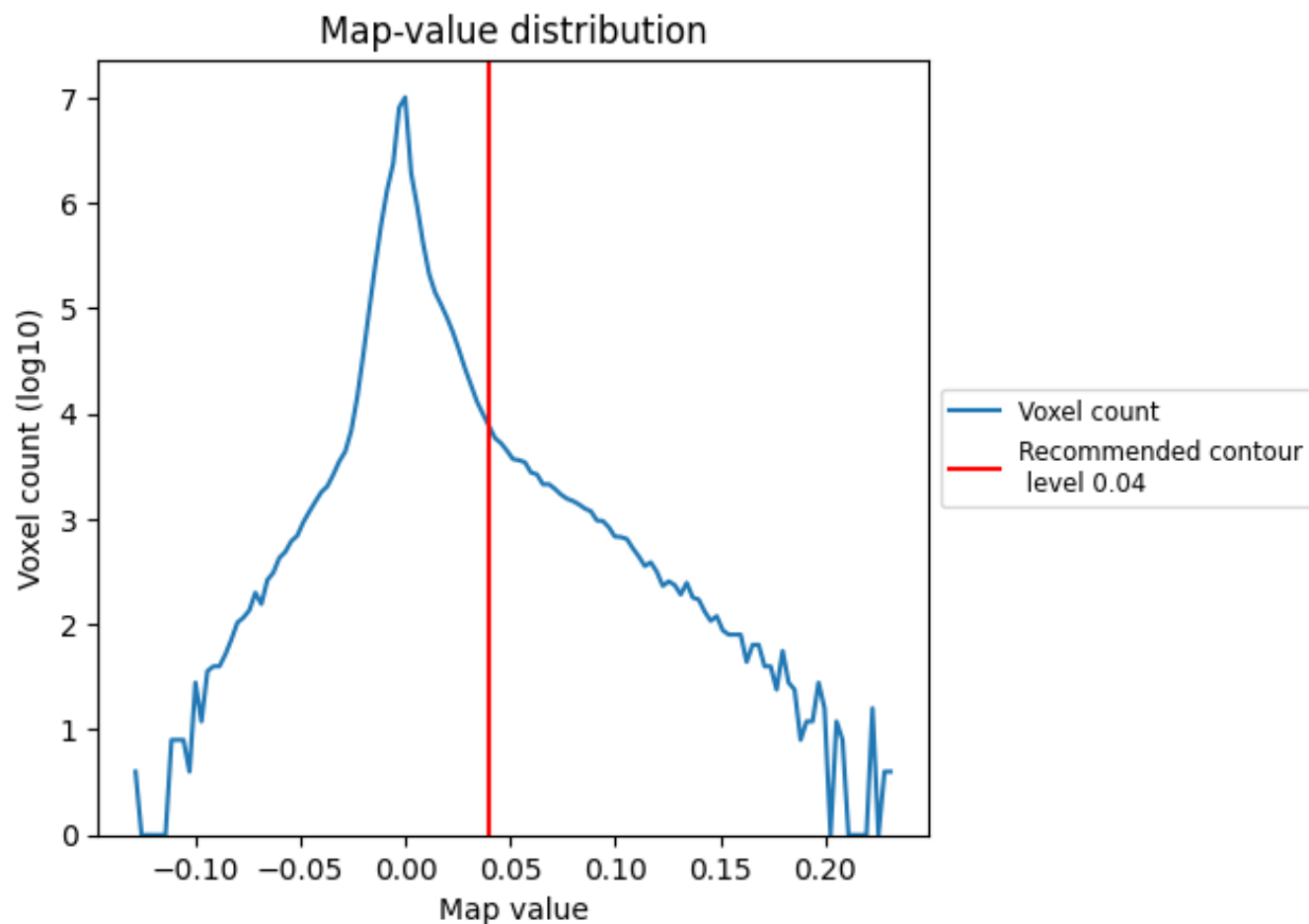
6.5 Mask visualisation

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

7 Map analysis [i](#)

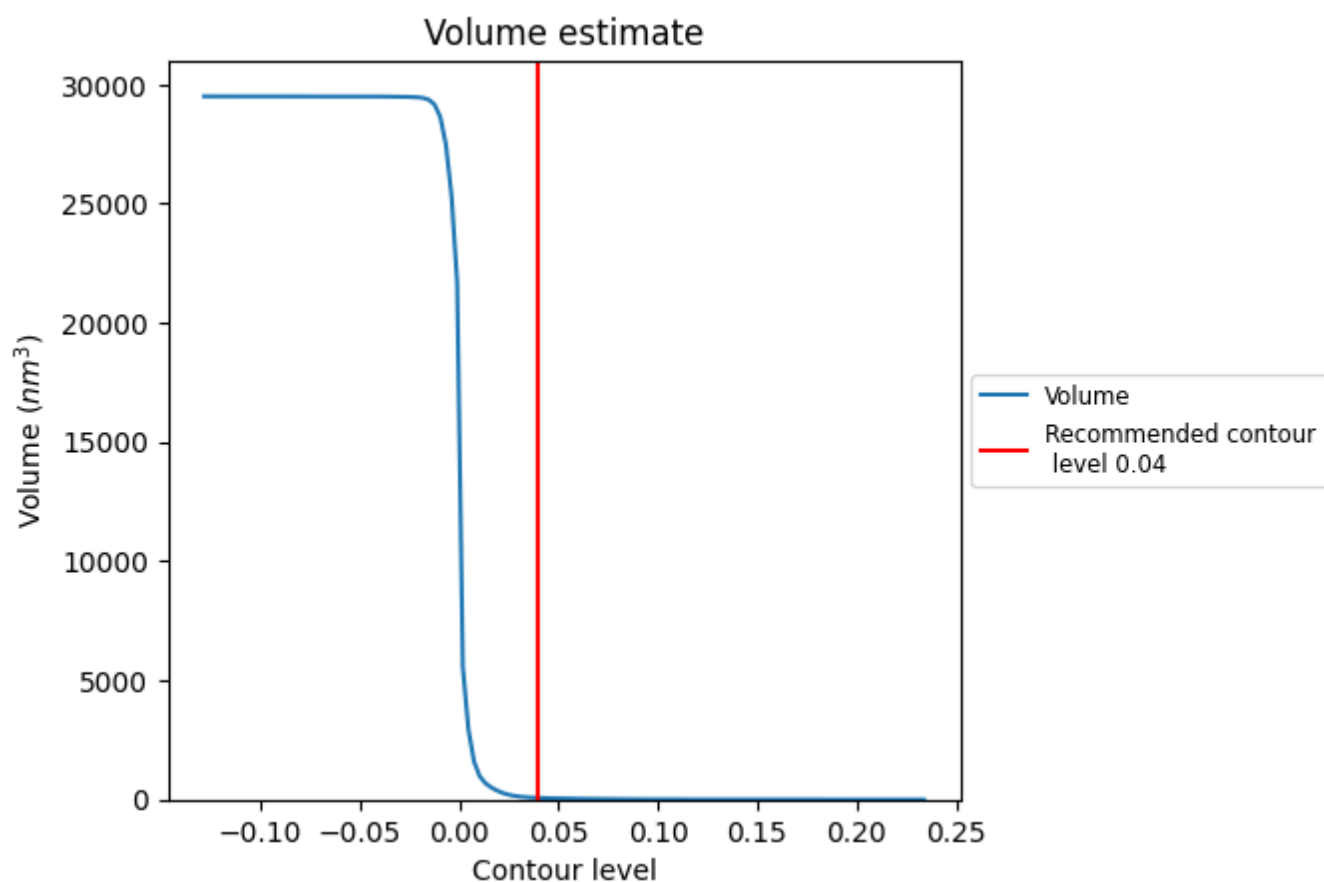
This section contains the results of statistical analysis of the map.

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.

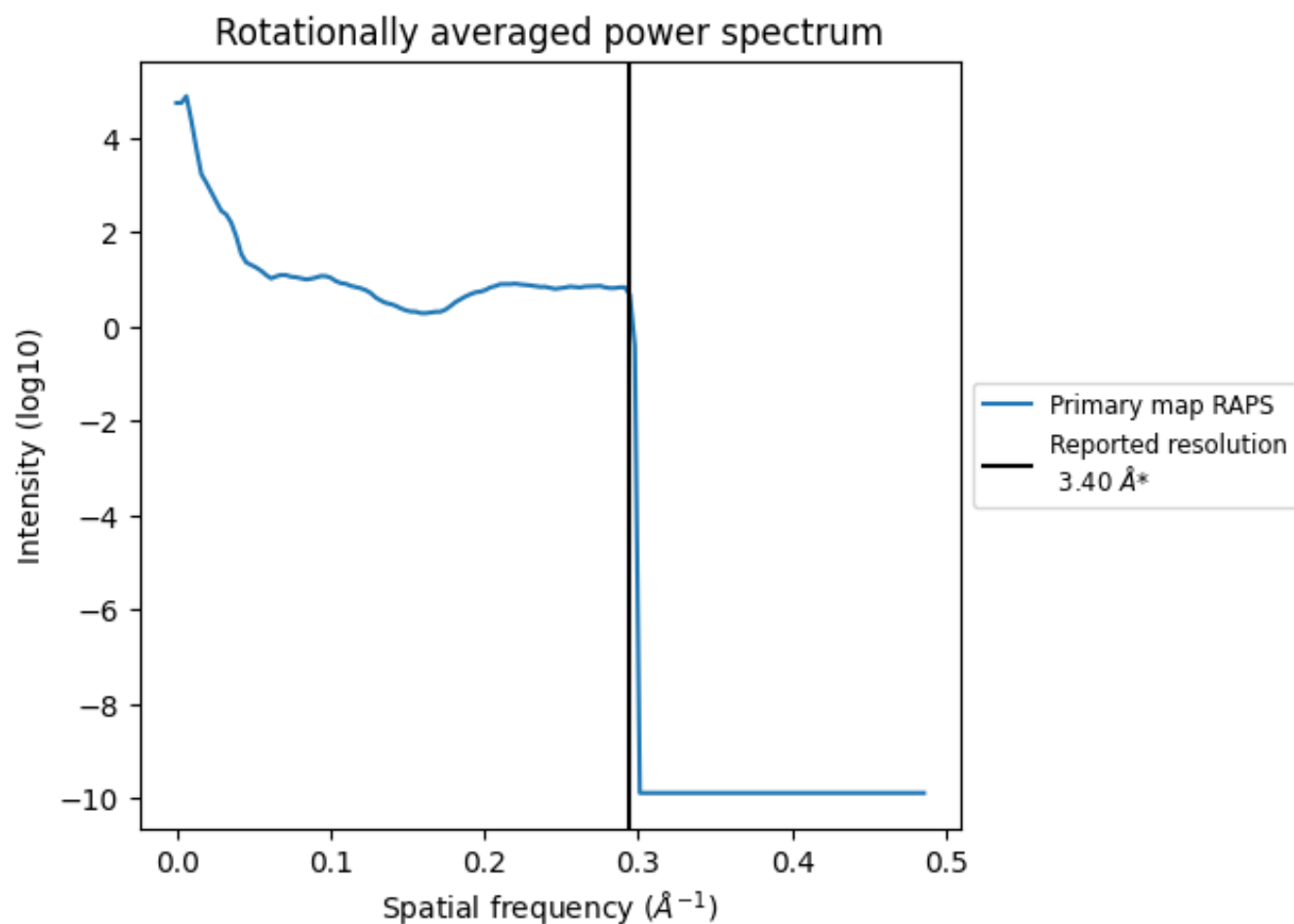
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 70 nm^3 ; this corresponds to an approximate mass of 63 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

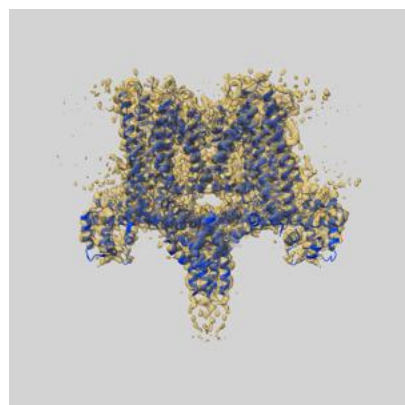
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

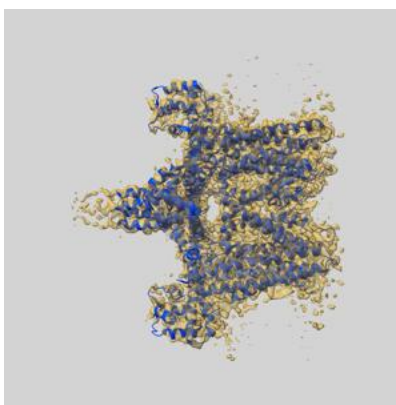
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-7537 and PDB model 6CNM. Per-residue inclusion information can be found in section [3](#) on page [6](#).

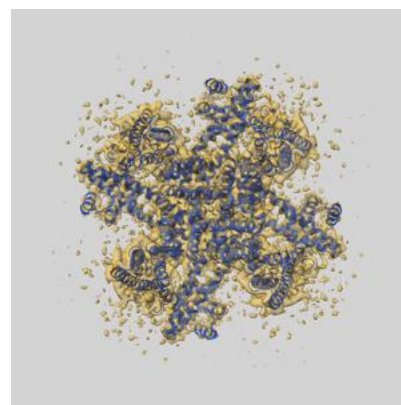
9.1 Map-model overlay [i](#)



X



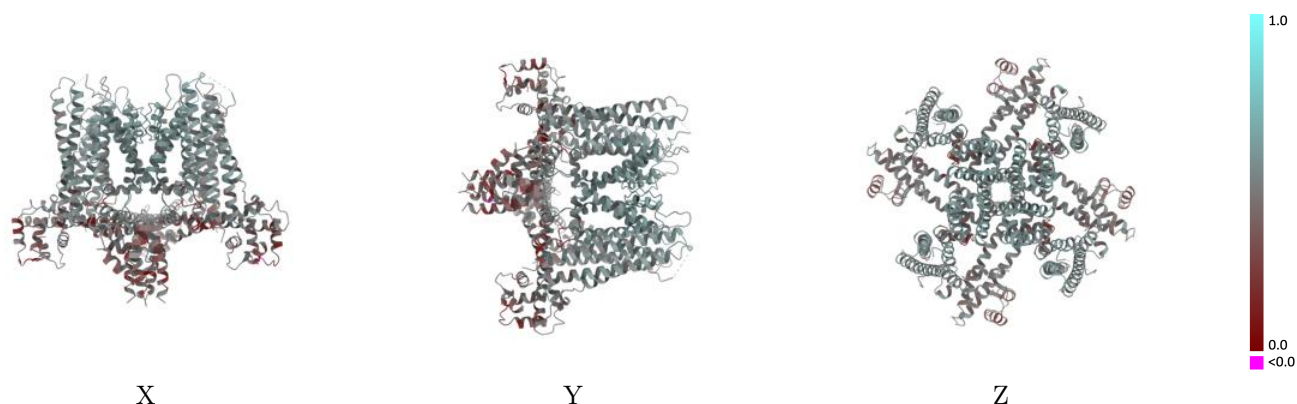
Y



Z

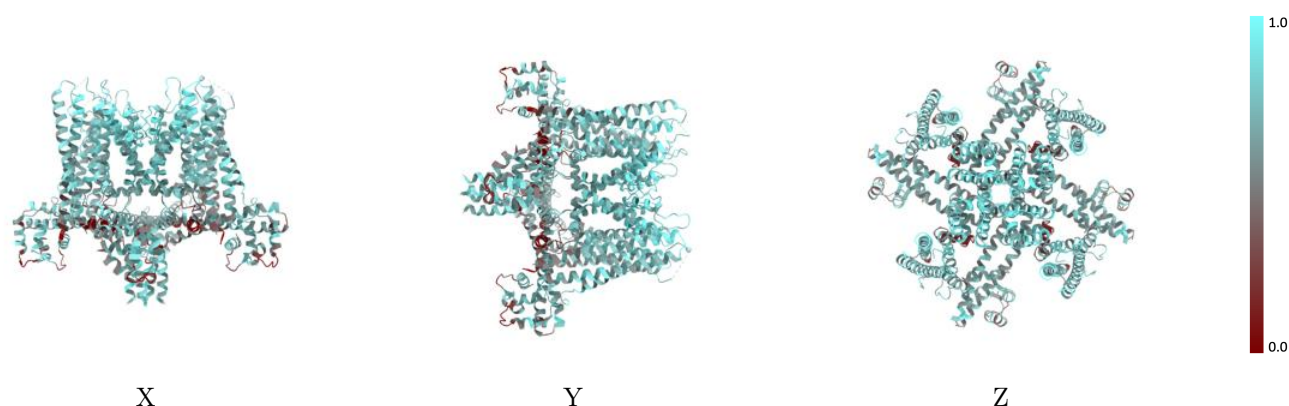
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



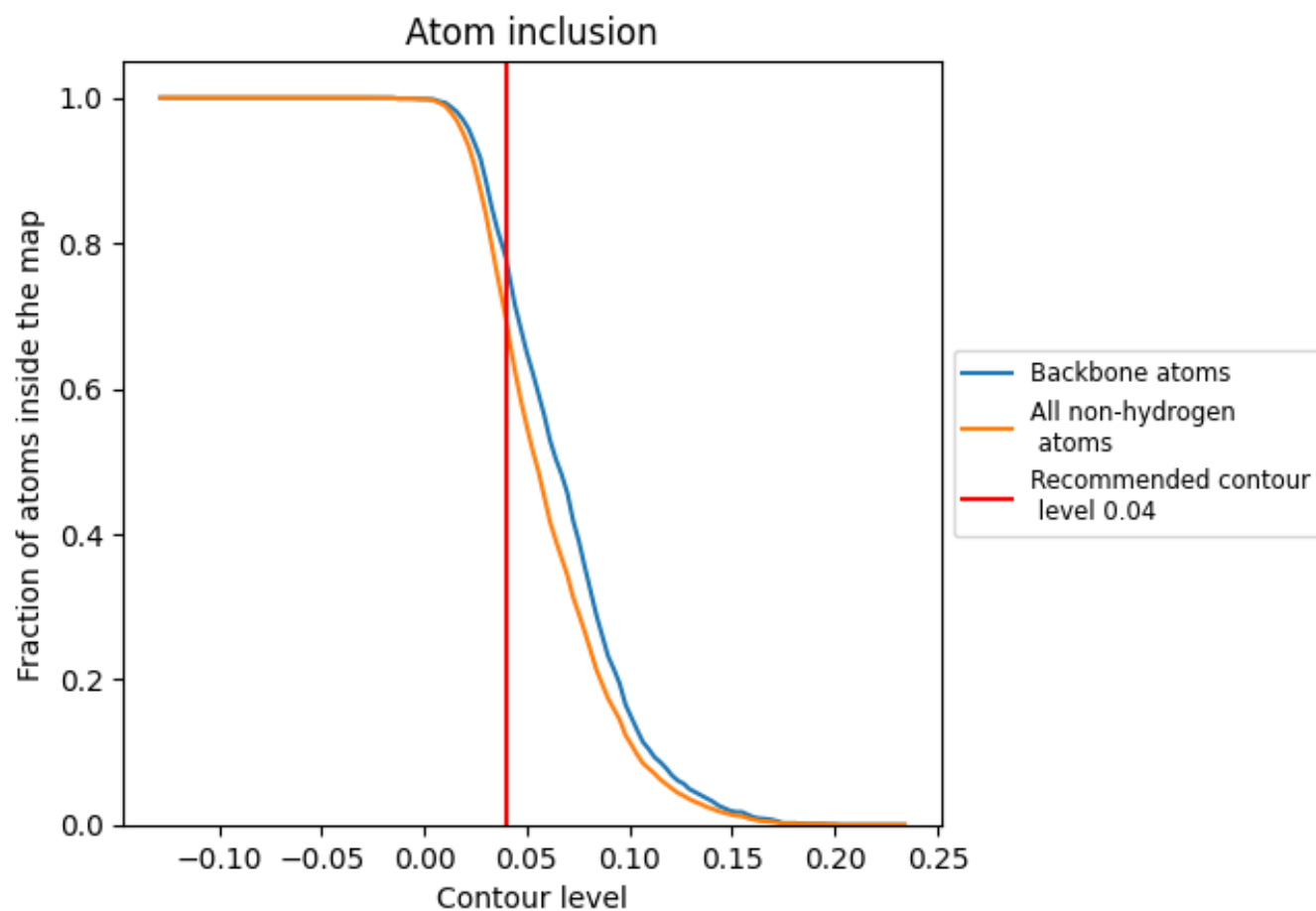
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 69% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6946	<div></div> 0.4930
A	<div></div> 0.7090	<div></div> 0.5060
B	<div></div> 0.7107	<div></div> 0.5040
C	<div></div> 0.7103	<div></div> 0.5050
D	<div></div> 0.7092	<div></div> 0.5050
E	<div></div> 0.5801	<div></div> 0.3990
F	<div></div> 0.5801	<div></div> 0.4000
G	<div></div> 0.5829	<div></div> 0.3980
H	<div></div> 0.5801	<div></div> 0.3950

1.0

0.0

<0.0