



Full wwPDB EM Validation Report ⓘ

Aug 10, 2026 – 06:22 pm BST

PDB ID : 9SAU / pdb_00009sau
EMDB ID : EMD-54697
Title : Chlorophyll synthase in complex with the LHC-like protein HliD, GGPP-bound state
Authors : Shvarev, D.; Hitchcock, A.; Sobotka, R.
Deposited on : 2025-08-07
Resolution : 3.60 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.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

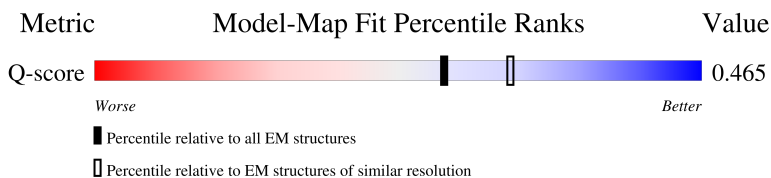
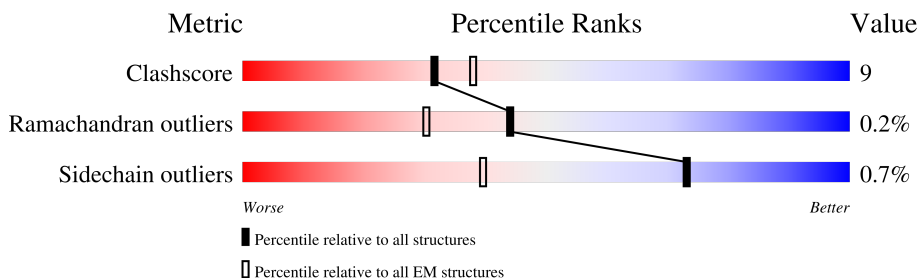
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12797 (3.10 - 4.10)

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	41	 76% 24%
1	B	41	 71% 29%
2	C	294	 83% 17%
2	D	294	 83% 17%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	A1JR2	C	402	X	-	-	-
6	A1JR2	D	402	X	-	-	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 5930 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.

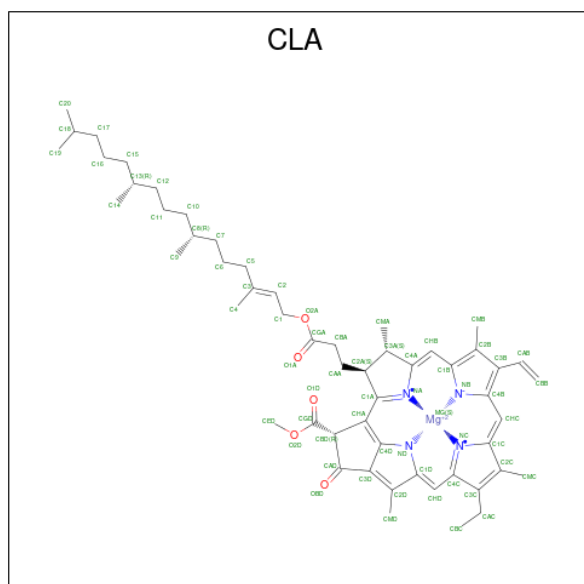
- Molecule 1 is a protein called High light-inducible protein HliD.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	41	Total	C	N	O	S	0	0
			325	219	52	53	1		
1	B	41	Total	C	N	O	S	0	0
			325	219	52	53	1		

- Molecule 2 is a protein called Chlorophyll a synthase.

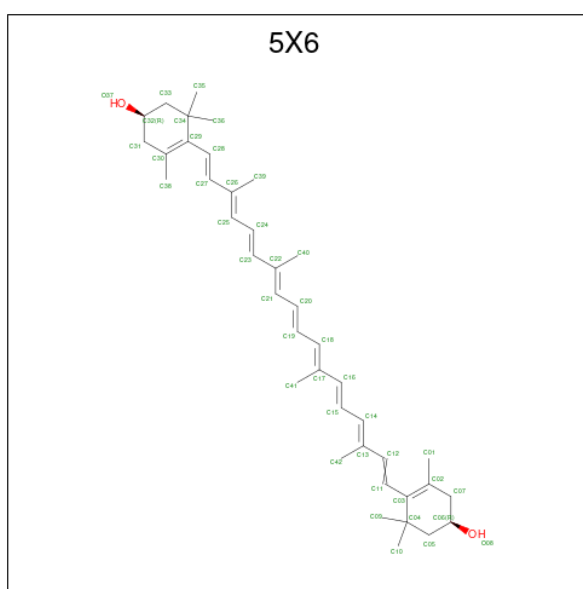
Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	294	Total	C	N	O	S	0	0
			2269	1511	356	389	13		
2	D	294	Total	C	N	O	S	0	0
			2269	1511	356	389	13		

- Molecule 3 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



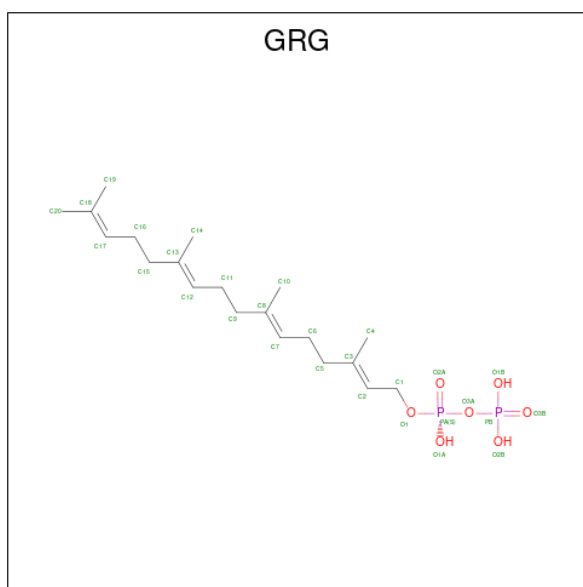
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 4 is Zeaxanthin (CCD ID: 5X6) (formula: $C_{40}H_{56}O_2$) (labeled as "Ligand of Interest" by depositor).



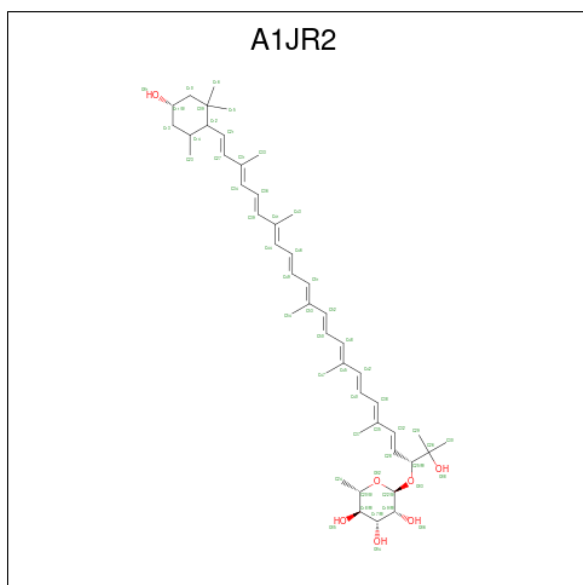
Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	O		0
			42	40	2		
4	B	1	Total	C	O		0
			42	40	2		

- Molecule 5 is GERANYLGERANYL DIPHOSPHATE (CCD ID: GRG) (formula: $C_{20}H_{36}O_7P_2$) (labeled as "Ligand of Interest" by depositor).



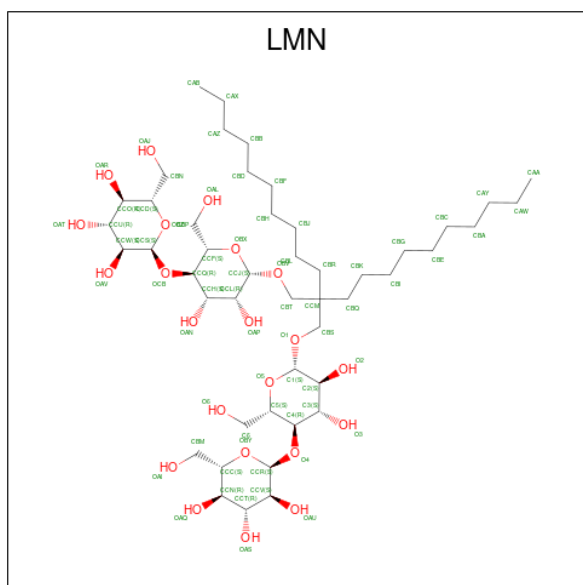
Mol	Chain	Residues	Atoms				AltConf
5	C	1	Total	C	O	P	0
			29	20	7	2	
5	D	1	Total	C	O	P	0
			29	20	7	2	

- Molecule 6 is (2 {S},3 {R},4 {R},5 {R},6 {S})-2-[(3 {R},4 {E},6 {E},8 {E},10 {E},12 {E},14 {E},16 {E},18 {E},20 {E},22 {E},24 {E})-2,6,10,14,19,23-hexamethyl-2-oxidanyl-25-[(4 {S})-2,2,6-trimethyl-4-oxidanyl-cyclohexyl]pentacos-4,6,8,10,12,14,16,18,20,22,24-undec-2-en-3-yl]oxy-6-methyl-oxane-3,4,5-triol (CCD ID: A1JR2) (formula: C₄₆H₆₈O₇) (labeled as "Ligand of Interest" by depositor).



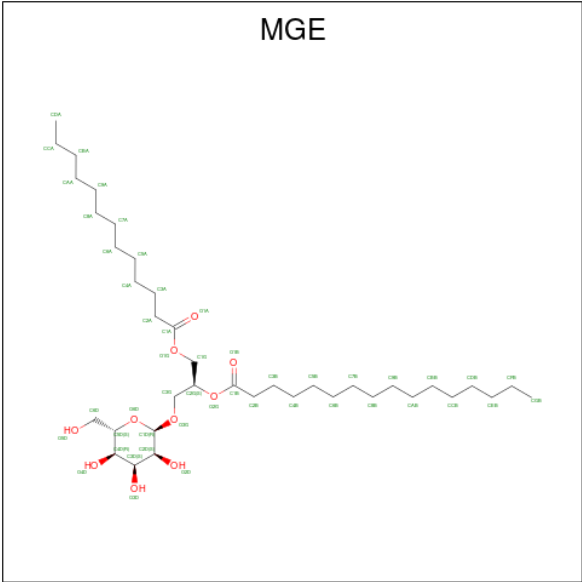
Mol	Chain	Residues	Atoms			AltConf
6	C	1	Total	C	O	0
			53	46	7	
6	D	1	Total	C	O	0
			53	46	7	

- Molecule 7 is Lauryl Maltose Neopentyl Glycol (CCD ID: LMN) (formula: $C_{47}H_{88}O_{22}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
7	C	1	Total	C	O	0
			69	47	22	
7	D	1	Total	C	O	0
			69	47	22	

- Molecule 8 is (1S)-2-(ALPHA-L-ALLOPYRANOSYLOXY)-1-[(TRIDECANOYLOXY)METHYL]ETHYL PALMITATE (CCD ID: MGE) (formula: $C_{38}H_{72}O_{10}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
8	C	1	Total	C	O	0
			48	38	10	
8	D	1	Total	C	O	0
			48	38	10	

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: High light-inducible protein HliD

Chain A:  76% 24%



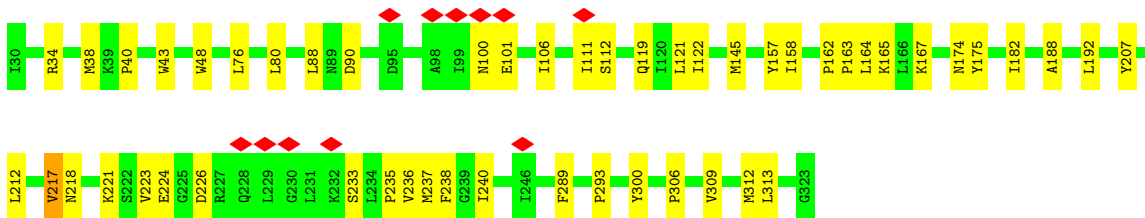
- Molecule 1: High light-inducible protein HliD

Chain B:  71% 29%



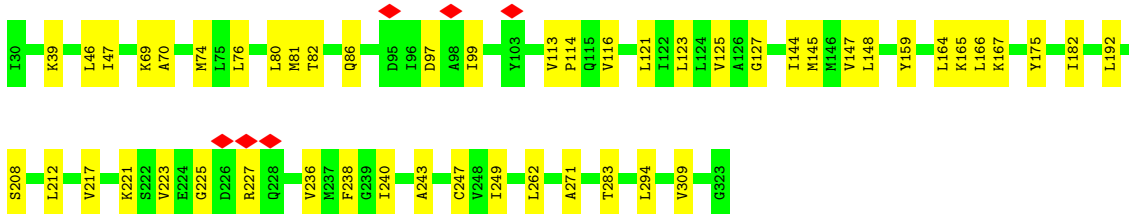
- Molecule 2: Chlorophyll a synthase

Chain C:  83% 17%



- Molecule 2: Chlorophyll a synthase

Chain D:  83% 17%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	254925	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.166	Depositor
Minimum map value	-0.073	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	348.16, 348.16, 348.16	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.68, 0.68, 0.68	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: A1JR2, LMN, MGE, 5X6, CLA, GRG

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	0.16	0/333	0.32	0/449
1	B	0.18	0/333	0.31	0/449
2	C	0.17	0/2333	0.37	0/3192
2	D	0.16	0/2333	0.35	0/3192
All	All	0.17	0/5332	0.35	0/7282

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	325	0	331	14	0
1	B	325	0	331	13	0
2	C	2269	0	2320	34	0
2	D	2269	0	2320	36	0
3	A	130	0	144	7	0
3	B	130	0	144	8	0
4	A	42	0	0	1	0
4	B	42	0	0	1	0
5	C	29	0	33	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	29	0	33	3	0
6	C	53	0	0	0	0
6	D	53	0	0	0	0
7	C	69	0	88	4	0
7	D	69	0	88	2	0
8	C	48	0	72	0	0
8	D	48	0	72	2	0
All	All	5930	0	5976	103	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 9.

All (103) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:39:LYS:HG3	2:D:86:GLN:HE21	1.46	0.80
2:D:47:ILE:HG12	2:D:74:MET:HB3	1.72	0.71
2:C:306:PRO:HG3	7:C:403:LMN:HBJ	1.75	0.69
2:C:218:ASN:HD21	7:C:403:LMN:HCT	1.57	0.68
2:C:309:VAL:HA	2:C:312:MET:HE3	1.80	0.62
2:D:159:TYR:HD1	2:D:166:LEU:HB2	1.64	0.62
2:D:69:LYS:HG2	2:D:192:LEU:HD11	1.80	0.62
2:D:159:TYR:HA	2:D:166:LEU:HG	1.83	0.60
2:D:238:PHE:HB2	2:D:243:ALA:HB2	1.85	0.58
2:D:159:TYR:HE2	5:D:401:GRG:HC42	1.68	0.57
2:D:121:LEU:O	2:D:125:VAL:HG22	2.05	0.56
2:C:158:ILE:HD11	2:C:164:LEU:HD11	1.87	0.56
2:D:165:LYS:HZ2	2:D:167:LYS:HG3	1.70	0.56
2:C:48:TRP:HZ2	2:C:313:LEU:HB2	1.72	0.55
2:D:227:ARG:HE	2:D:236:VAL:HG22	1.73	0.54
2:C:165:LYS:HE3	2:C:167:LYS:HD3	1.88	0.54
1:B:28:ASN:HD21	3:B:102:CLA:C1A	2.21	0.53
1:A:33:MET:HE1	3:B:101:CLA:HHC	1.91	0.53
1:B:43:GLU:HG3	1:B:49:GLY:HA2	1.91	0.53
2:D:159:TYR:CD1	2:D:166:LEU:HB2	2.43	0.52
1:B:38:LEU:O	1:B:42:ILE:HG13	2.09	0.52
2:C:38:MET:HG2	2:C:43:TRP:HZ2	1.75	0.52
2:C:226:ASP:HB2	2:C:236:VAL:HG11	1.92	0.52
2:C:309:VAL:HG11	7:C:403:LMN:HBIA	1.92	0.52
2:C:119:GLN:HA	2:C:122:ILE:HG22	1.93	0.51
1:A:29:GLY:HA2	1:B:33:MET:HE2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:306:PRO:HA	2:C:309:VAL:HG12	1.94	0.49
2:C:182:ILE:HD11	2:C:207:TYR:C	2.37	0.49
2:C:48:TRP:CZ2	2:C:313:LEU:HB2	2.49	0.48
1:B:21:ASN:C	3:B:101:CLA:HMA1	2.39	0.48
1:B:25:GLU:OE1	3:B:101:CLA:NA	2.47	0.47
1:A:30:ARG:HD3	8:D:404:MGE:H3A2	1.97	0.47
2:C:289:PHE:CE1	2:C:293:PRO:HB3	2.49	0.47
1:A:33:MET:CE	3:B:101:CLA:HHC	2.45	0.47
2:C:90:ASP:HB3	2:C:106:ILE:HD12	1.97	0.47
2:C:237:MET:HE1	2:C:238:PHE:CD2	2.49	0.47
2:C:174:ASN:HB3	2:C:212:LEU:HG	1.97	0.47
2:D:164:LEU:O	2:D:166:LEU:HD23	2.15	0.46
1:A:21:ASN:C	3:A:101:CLA:HMA1	2.40	0.46
2:C:217:VAL:HG21	2:C:300:TYR:HE2	1.80	0.46
2:D:46:LEU:HD22	2:D:82:THR:OG1	2.15	0.46
1:A:33:MET:HG2	4:B:103:5X6:C19	2.46	0.46
1:A:29:GLY:CA	1:B:33:MET:HE2	2.46	0.45
2:C:224:GLU:HA	2:C:224:GLU:OE1	2.15	0.45
1:A:25:GLU:CD	3:A:101:CLA:NB	2.74	0.45
2:D:69:LYS:HD2	2:D:192:LEU:HD21	1.97	0.45
2:D:113:VAL:O	2:D:116:VAL:HG12	2.15	0.45
2:D:221:LYS:HA	2:D:221:LYS:HE2	1.99	0.45
2:C:40:PRO:HA	2:C:43:TRP:CE2	2.52	0.45
2:C:111:ILE:H	2:C:111:ILE:HD12	1.81	0.45
2:D:97:ASP:C	2:D:99:ILE:H	2.24	0.45
4:A:103:5X6:C19	1:B:33:MET:HG2	2.47	0.45
2:D:294:LEU:HD23	2:D:294:LEU:HA	1.77	0.44
1:A:28:ASN:OD1	3:A:102:CLA:NA	2.51	0.44
2:C:223:VAL:HG23	2:C:235:PRO:HB2	1.99	0.44
2:D:175:TYR:HA	2:D:212:LEU:HB2	1.98	0.44
5:D:401:GRG:H201	5:D:401:GRG:H162	1.77	0.44
1:A:27:LEU:HD12	1:A:27:LEU:HA	1.83	0.44
3:A:102:CLA:H93	3:A:102:CLA:H62	1.74	0.44
7:D:403:LMN:HBTA	7:D:403:LMN:HBKA	1.55	0.44
2:C:233:SER:O	2:C:236:VAL:HG22	2.17	0.44
2:D:240:ILE:HG12	2:D:294:LEU:HG	2.00	0.44
1:B:25:GLU:OE1	3:B:101:CLA:NB	2.51	0.43
2:D:70:ALA:O	2:D:74:MET:HE2	2.18	0.43
2:D:76:LEU:O	2:D:81:MET:HB2	2.18	0.43
2:C:34:ARG:HD2	2:C:119:GLN:OE1	2.18	0.43
2:D:123:LEU:HD23	2:D:123:LEU:HA	1.78	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:182:ILE:HD13	2:D:208:SER:HA	1.99	0.43
2:C:162:PRO:N	2:C:163:PRO:HD2	2.33	0.43
2:C:76:LEU:HA	2:C:80:LEU:HB2	2.01	0.43
2:C:237:MET:HE2	2:C:237:MET:C	2.44	0.43
2:C:100:ASN:HB3	2:C:101:GLU:OE2	2.19	0.43
2:D:144:ILE:HA	2:D:147:VAL:HG22	2.01	0.43
3:A:102:CLA:HBB1	3:A:102:CLA:HHC	2.00	0.42
1:A:25:GLU:HB2	3:A:101:CLA:C1B	2.49	0.42
1:A:38:LEU:HD11	8:D:404:MGE:H133	2.00	0.42
1:B:36:PHE:O	1:B:39:ILE:HG22	2.19	0.42
1:A:33:MET:HG3	1:B:32:ALA:CB	2.50	0.42
2:C:121:LEU:HD12	2:C:121:LEU:HA	1.83	0.42
5:C:401:GRG:H162	5:C:401:GRG:H201	1.77	0.42
2:D:80:LEU:HD23	2:D:127:GLY:HA2	2.01	0.42
5:C:401:GRG:H141	5:C:401:GRG:HC7	2.00	0.42
2:D:69:LYS:CG	2:D:192:LEU:HD11	2.45	0.42
2:D:217:VAL:HG23	2:D:247:CYS:SG	2.59	0.42
1:A:50:VAL:O	1:A:54:LEU:HG	2.20	0.41
2:C:175:TYR:HB2	2:C:212:LEU:HD12	2.02	0.41
7:C:403:LMN:HBQA	7:C:403:LMN:HBL	1.80	0.41
2:D:223:VAL:C	2:D:225:GLY:H	2.27	0.41
2:C:88:LEU:HD21	2:C:157:TYR:HA	2.01	0.41
2:C:217:VAL:HG21	2:C:300:TYR:CE2	2.55	0.41
2:D:249:ILE:HD13	2:D:249:ILE:HA	1.89	0.41
1:B:30:ARG:HA	1:B:33:MET:HE3	2.02	0.41
2:D:145:MET:HE3	2:D:145:MET:HA	2.01	0.41
2:C:145:MET:HE1	2:C:188:ALA:O	2.21	0.41
2:C:182:ILE:HD11	2:C:207:TYR:O	2.20	0.41
2:D:148:LEU:HD23	2:D:148:LEU:HA	1.94	0.41
2:D:262:LEU:HB3	2:D:271:ALA:HB2	2.03	0.41
5:D:401:GRG:HC11	5:D:401:GRG:HC41	1.92	0.41
3:A:102:CLA:HAA1	2:D:283:THR:HG21	2.02	0.40
2:D:113:VAL:N	2:D:114:PRO:HD2	2.36	0.40
1:B:28:ASN:HD21	3:B:102:CLA:CHA	2.34	0.40
3:B:101:CLA:H91	3:B:101:CLA:H112	1.88	0.40
2:D:309:VAL:HG11	7:D:403:LMN:HBJA	2.02	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	39/41 (95%)	37 (95%)	2 (5%)	0	100	100
1	B	39/41 (95%)	37 (95%)	2 (5%)	0	100	100
2	C	292/294 (99%)	275 (94%)	16 (6%)	1 (0%)	36	65
2	D	292/294 (99%)	273 (94%)	19 (6%)	0	100	100
All	All	662/670 (99%)	622 (94%)	39 (6%)	1 (0%)	44	72

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	112	SER

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	32/32 (100%)	32 (100%)	0	100	100
1	B	32/32 (100%)	32 (100%)	0	100	100
2	C	237/237 (100%)	233 (98%)	4 (2%)	53	69
2	D	237/237 (100%)	237 (100%)	0	100	100
All	All	538/538 (100%)	534 (99%)	4 (1%)	73	78

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	192	LEU
2	C	217	VAL
2	C	221	LYS
2	C	240	ILE

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

Mol	Chain	Res	Type
2	C	89	ASN
2	C	139	GLN
2	D	86	GLN
2	D	255	GLN
2	D	281	GLN
2	D	301	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

14 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GRG	C	401	-	26,28,28	1.56	5 (19%)	33,37,37	4.32	15 (45%)
6	A1JR2	C	402	-	53,54,54	1.35	3 (5%)	64,75,75	1.45	3 (4%)
4	5X6	B	103	-	43,43,43	0.20	0	58,60,60	0.52	1 (1%)
4	5X6	A	103	-	43,43,43	0.17	0	58,60,60	0.49	1 (1%)
7	LMN	C	403	-	72,72,72	0.55	0	96,98,98	0.69	1 (1%)
7	LMN	D	403	-	72,72,72	0.50	0	96,98,98	1.04	8 (8%)
6	A1JR2	D	402	-	53,54,54	1.33	3 (5%)	64,75,75	1.45	3 (4%)
3	CLA	B	102	1	69,73,73	1.26	10 (14%)	83,113,113	1.25	5 (6%)
3	CLA	A	102	1	69,73,73	1.26	9 (13%)	83,113,113	1.25	5 (6%)
8	MGE	D	404	-	48,48,48	0.49	0	56,56,56	0.61	0
5	GRG	D	401	-	26,28,28	1.55	5 (19%)	33,37,37	4.30	15 (45%)
3	CLA	B	101	1	69,73,73	1.24	10 (14%)	83,113,113	1.24	6 (7%)
3	CLA	A	101	1	69,73,73	1.28	10 (14%)	83,113,113	1.26	4 (4%)
8	MGE	C	404	-	48,48,48	0.47	0	56,56,56	0.66	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	A1JR2	C	402	-	2/2/16/33	4/45/84/84	0/2/2/2
5	GRG	C	401	-	-	7/31/31/31	-
4	5X6	B	103	-	-	0/29/67/67	0/2/2/2
4	5X6	A	103	-	-	0/29/67/67	0/2/2/2
7	LMN	C	403	-	-	11/50/130/130	0/4/4/4
7	LMN	D	403	-	-	26/50/130/130	0/4/4/4
6	A1JR2	D	402	-	2/2/16/33	6/45/84/84	0/2/2/2
3	CLA	B	102	1	-	9/39/115/115	-
3	CLA	A	102	1	-	13/39/115/115	-
8	MGE	D	404	-	-	14/43/63/63	0/1/1/1
5	GRG	D	401	-	-	6/31/31/31	-
3	CLA	B	101	1	-	13/39/115/115	-
3	CLA	A	101	1	-	11/39/115/115	-
8	MGE	C	404	-	-	8/43/63/63	0/1/1/1

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	402	A1JR2	C12-C14	-8.77	1.34	1.54
6	C	402	A1JR2	C12-C14	-8.75	1.34	1.54
3	A	102	CLA	C1D-ND	3.65	1.42	1.37
3	A	101	CLA	C1D-ND	3.63	1.42	1.37
3	B	102	CLA	C1D-ND	3.62	1.42	1.37
6	C	402	A1JR2	C12-C21	-3.47	1.45	1.50
3	A	101	CLA	C4B-NB	3.46	1.42	1.37
3	B	102	CLA	C4B-NB	3.45	1.42	1.37
3	A	102	CLA	C4B-NB	3.43	1.42	1.37
3	B	101	CLA	C1D-ND	3.39	1.42	1.37
3	B	101	CLA	C4D-ND	-3.17	1.33	1.37
3	B	102	CLA	C3B-C4B	3.10	1.50	1.42
3	A	102	CLA	C3B-C4B	3.09	1.50	1.42
3	A	102	CLA	C4D-ND	-3.07	1.33	1.37
3	B	102	CLA	C4D-ND	-3.04	1.33	1.37
3	A	101	CLA	C4D-ND	-2.98	1.33	1.37
3	A	101	CLA	C3B-C4B	2.92	1.49	1.42
3	B	101	CLA	C4B-NB	2.91	1.41	1.37
3	B	101	CLA	C3B-C4B	2.90	1.49	1.42
6	D	402	A1JR2	C12-C21	-2.82	1.46	1.50
5	D	401	GRG	C9-C8	2.69	1.56	1.51
5	C	401	GRG	C9-C8	2.69	1.56	1.51
3	A	101	CLA	C1B-C2B	2.67	1.49	1.43
5	C	401	GRG	C15-C13	2.65	1.56	1.51
5	D	401	GRG	C15-C13	2.64	1.56	1.51
6	D	402	A1JR2	C09-C12	-2.54	1.53	1.55
3	B	101	CLA	C1B-C2B	2.52	1.49	1.43
3	A	102	CLA	C1B-C2B	2.49	1.49	1.43
6	C	402	A1JR2	C09-C12	-2.47	1.53	1.55
3	B	102	CLA	C1B-C2B	2.42	1.48	1.43
3	B	101	CLA	MG-NB	-2.41	2.01	2.05
3	A	101	CLA	MG-NB	-2.22	2.01	2.05
5	C	401	GRG	C5-C3	2.21	1.55	1.51
3	B	101	CLA	CMD-C2D	-2.21	1.46	1.50
3	A	101	CLA	CHC-C1C	2.19	1.43	1.38
3	B	101	CLA	CHC-C1C	2.17	1.42	1.38
3	B	102	CLA	CMD-C2D	-2.17	1.46	1.50
3	A	101	CLA	CMC-C2C	-2.15	1.46	1.50
3	A	101	CLA	CMD-C2D	-2.13	1.46	1.50
5	C	401	GRG	C1-C2	2.13	1.55	1.49
5	D	401	GRG	C1-C2	2.12	1.55	1.49
5	D	401	GRG	C5-C3	2.11	1.55	1.51
3	A	101	CLA	CMB-C2B	-2.10	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	102	CLA	CMD-C2D	-2.10	1.46	1.50
3	B	102	CLA	MG-NB	-2.09	2.01	2.05
3	B	102	CLA	CHC-C1C	2.09	1.42	1.38
5	D	401	GRG	C10-C8	2.09	1.56	1.50
3	B	102	CLA	CMC-C2C	-2.08	1.46	1.50
3	A	102	CLA	CMB-C2B	-2.08	1.46	1.50
3	A	102	CLA	CHC-C1C	2.08	1.42	1.38
3	B	102	CLA	CMB-C2B	-2.07	1.46	1.50
3	B	101	CLA	CMC-C2C	-2.05	1.46	1.50
3	B	101	CLA	CMB-C2B	-2.05	1.46	1.50
3	A	102	CLA	MG-NB	-2.03	2.01	2.05
5	C	401	GRG	C10-C8	2.02	1.55	1.50

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	401	GRG	C14-C13-C15	-12.40	94.41	115.27
5	D	401	GRG	C14-C13-C15	-12.25	94.66	115.27
5	C	401	GRG	C10-C8-C9	-11.80	95.42	115.27
5	D	401	GRG	C10-C8-C9	-11.70	95.60	115.27
6	C	402	A1JR2	C13-C14-C12	9.36	120.48	109.72
6	D	402	A1JR2	C13-C14-C12	9.18	120.27	109.72
5	D	401	GRG	C19-C18-C20	-8.65	95.51	114.60
5	C	401	GRG	C19-C18-C20	-8.64	95.53	114.60
3	A	101	CLA	C4A-NA-C1A	6.60	109.67	106.71
3	A	102	CLA	C4A-NA-C1A	6.55	109.65	106.71
5	C	401	GRG	C11-C12-C13	-6.41	112.23	127.66
3	B	102	CLA	C4A-NA-C1A	6.40	109.58	106.71
5	D	401	GRG	C6-C7-C8	-6.37	112.33	127.66
5	D	401	GRG	C11-C12-C13	-6.35	112.36	127.66
6	D	402	A1JR2	C23-C14-C12	6.10	124.63	112.60
6	C	402	A1JR2	C23-C14-C12	6.03	124.49	112.60
3	B	101	CLA	C4A-NA-C1A	5.99	109.40	106.71
5	C	401	GRG	C6-C7-C8	-5.95	113.32	127.66
5	C	401	GRG	C15-C13-C12	5.71	132.68	121.12
5	D	401	GRG	C15-C13-C12	5.64	132.53	121.12
5	D	401	GRG	C9-C8-C7	5.39	132.03	121.12
5	C	401	GRG	C9-C8-C7	5.32	131.89	121.12
5	C	401	GRG	C16-C17-C18	-4.75	111.50	127.75
5	D	401	GRG	C16-C17-C18	-4.74	111.54	127.75
5	C	401	GRG	C14-C13-C12	3.60	132.91	123.68
5	D	401	GRG	C14-C13-C12	3.56	132.80	123.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	403	LMN	O1-C1-C2	3.52	113.79	108.30
5	C	401	GRG	C10-C8-C7	3.51	132.69	123.68
5	D	401	GRG	C10-C8-C7	3.39	132.37	123.68
5	C	401	GRG	C19-C18-C17	3.37	132.37	122.65
5	D	401	GRG	C19-C18-C17	3.34	132.31	122.65
5	D	401	GRG	C1-C2-C3	-3.33	120.28	126.04
5	D	401	GRG	C20-C18-C17	3.30	132.19	122.65
5	C	401	GRG	C20-C18-C17	3.27	132.10	122.65
5	C	401	GRG	PA-O3A-PB	-3.12	122.11	132.83
3	A	101	CLA	C3B-C4B-NB	-3.09	107.64	110.52
7	D	403	LMN	CBS-O1-C1	3.05	121.30	113.36
7	D	403	LMN	CCR-OBY-CCC	3.01	119.59	113.69
5	C	401	GRG	C1-C2-C3	-2.89	121.04	126.04
3	A	102	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
3	B	102	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
5	C	401	GRG	C4-C3-C5	2.81	120.00	115.27
3	B	101	CLA	C3B-C4B-NB	-2.72	107.99	110.52
3	B	101	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
3	A	101	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
5	D	401	GRG	C4-C3-C5	2.64	119.71	115.27
3	B	102	CLA	C3B-C4B-NB	-2.62	108.08	110.52
4	B	103	5X6	C05-C06-C07	2.53	113.77	110.30
4	A	103	5X6	C05-C06-C07	2.48	113.69	110.30
3	A	102	CLA	C3B-C4B-NB	-2.45	108.24	110.52
3	B	101	CLA	CHB-C4A-NA	2.44	127.89	124.51
3	A	101	CLA	CHB-C4A-NA	2.44	127.88	124.51
7	D	403	LMN	O2-C2-C3	-2.38	104.84	110.35
7	D	403	LMN	CCR-O4-C4	2.38	123.84	117.96
3	B	102	CLA	CHB-C4A-NA	2.36	127.77	124.51
5	D	401	GRG	PA-O3A-PB	-2.32	124.85	132.83
3	A	102	CLA	CHB-C4A-NA	2.27	127.65	124.51
7	D	403	LMN	C3-C4-C5	-2.25	105.77	110.93
3	A	102	CLA	C1-C2-C3	-2.24	122.17	126.04
7	D	403	LMN	CBT-OBV-CCJ	2.18	119.03	113.36
3	B	102	CLA	C1-C2-C3	-2.18	122.28	126.04
3	B	101	CLA	CMB-C2B-C1B	-2.17	122.06	125.37
6	D	402	A1JR2	C23-C14-C13	2.15	115.05	111.18
3	B	101	CLA	O2A-CGA-O1A	-2.13	118.20	123.59
6	C	402	A1JR2	C23-C14-C13	2.13	115.01	111.18
7	D	403	LMN	OBV-CCJ-CCL	-2.11	105.00	108.30
7	C	403	LMN	O2-C2-C3	-2.08	105.54	110.35

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	C	402	A1JR2	C14
6	C	402	A1JR2	C12
6	D	402	A1JR2	C14
6	D	402	A1JR2	C12

All (128) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	102	CLA	C1A-C2A-CAA-CBA
3	A	102	CLA	CBD-CGD-O2D-CED
3	B	102	CLA	C1A-C2A-CAA-CBA
3	B	102	CLA	C3A-C2A-CAA-CBA
5	C	401	GRG	C1-O1-PA-O1A
5	C	401	GRG	C1-O1-PA-O2A
5	D	401	GRG	C1-O1-PA-O3A
6	C	402	A1JR2	O03-C25-C28-C32
6	C	402	A1JR2	C26-C25-C28-C32
6	C	402	A1JR2	C28-C32-C35-C37
6	C	402	A1JR2	C28-C32-C35-C38
6	D	402	A1JR2	C09-C12-C21-C27
6	D	402	A1JR2	C28-C32-C35-C37
6	D	402	A1JR2	C28-C32-C35-C38
7	D	403	LMN	C2-C1-O1-CBS
7	D	403	LMN	CBK-CBQ-CCM-CBR
7	D	403	LMN	CBK-CBQ-CCM-CBS
7	D	403	LMN	CBK-CBQ-CCM-CBT
7	D	403	LMN	O1-CBS-CCM-CBQ
7	D	403	LMN	OBV-CBT-CCM-CBQ
7	D	403	LMN	OBV-CBT-CCM-CBR
3	A	101	CLA	O1A-CGA-O2A-C1
7	D	403	LMN	OBY-CCR-O4-C4
3	A	102	CLA	O1D-CGD-O2D-CED
3	B	101	CLA	CBD-CGD-O2D-CED
3	B	101	CLA	O1A-CGA-O2A-C1
8	D	404	MGE	O1A-C1A-O1G-C1G
3	B	101	CLA	C3-C5-C6-C7
3	B	102	CLA	C3-C5-C6-C7
3	A	101	CLA	CBA-CGA-O2A-C1
8	D	404	MGE	C2A-C1A-O1G-C1G
7	D	403	LMN	C4-C5-C6-O6
7	D	403	LMN	CCH-CCQ-OCB-CCS
3	B	101	CLA	CBA-CGA-O2A-C1
7	C	403	LMN	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	D	403	LMN	O5-C5-C6-O6
3	A	101	CLA	CBD-CGD-O2D-CED
3	A	101	CLA	C3-C5-C6-C7
7	D	403	LMN	CAW-CAY-CBA-CBC
7	D	403	LMN	OBV-CBT-CCM-CBS
3	B	101	CLA	O1D-CGD-O2D-CED
7	C	403	LMN	O5-C5-C6-O6
7	C	403	LMN	CCH-CCQ-OCB-CCS
8	D	404	MGE	C1B-C2B-C3B-C4B
7	C	403	LMN	CBI-CBK-CBQ-CCM
7	D	403	LMN	CBJ-CBL-CBR-CCM
8	D	404	MGE	C2B-C1B-O2G-C2G
3	B	102	CLA	CBA-CGA-O2A-C1
3	B	101	CLA	C5-C6-C7-C8
7	C	403	LMN	CBJ-CBL-CBR-CCM
5	C	401	GRG	C12-C11-C9-C8
5	D	401	GRG	C12-C11-C9-C8
3	A	102	CLA	C5-C6-C7-C8
3	A	102	CLA	CBA-CGA-O2A-C1
8	D	404	MGE	O1B-C1B-O2G-C2G
7	C	403	LMN	CBG-CBI-CBK-CBQ
3	A	102	CLA	C16-C17-C18-C20
3	A	102	CLA	O1A-CGA-O2A-C1
3	B	102	CLA	O1A-CGA-O2A-C1
3	A	102	CLA	C16-C17-C18-C19
7	D	403	LMN	O5-C1-O1-CBS
8	D	404	MGE	C5A-C6A-C7A-C8A
3	A	102	CLA	C3A-C2A-CAA-CBA
7	D	403	LMN	CBD-CBF-CBH-CBJ
7	D	403	LMN	CBI-CBK-CBQ-CCM
5	C	401	GRG	C12-C13-C15-C16
7	C	403	LMN	CCF-CCQ-OCB-CCS
5	C	401	GRG	C14-C13-C15-C16
5	D	401	GRG	C12-C13-C15-C16
3	A	101	CLA	O1D-CGD-O2D-CED
7	D	403	LMN	CBF-CBH-CBJ-CBL
7	C	403	LMN	OAI-CBM-CCC-OBY
7	D	403	LMN	O1-CBS-CCM-CBT
5	D	401	GRG	C14-C13-C15-C16
8	D	404	MGE	O6D-C5D-C6D-O5D
7	D	403	LMN	CBB-CBD-CBF-CBH
3	B	101	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
3	A	101	CLA	C12-C13-C15-C16
3	B	101	CLA	C6-C7-C8-C10
3	A	102	CLA	C14-C13-C15-C16
3	B	101	CLA	C6-C7-C8-C9
3	B	101	CLA	C15-C16-C17-C18
3	B	101	CLA	C16-C17-C18-C20
3	B	102	CLA	C13-C15-C16-C17
6	D	402	A1JR2	O02-C22-O03-C25
7	D	403	LMN	CCF-CCQ-OCB-CCS
3	A	101	CLA	C6-C7-C8-C10
3	A	102	CLA	C12-C13-C15-C16
7	D	403	LMN	O1-CBS-CCM-CBR
3	B	101	CLA	C13-C15-C16-C17
8	C	404	MGE	C8A-C9A-CAA-CBA
6	D	402	A1JR2	C19-C22-O03-C25
5	D	401	GRG	C1-O1-PA-O1A
5	D	401	GRG	C1-O1-PA-O2A
8	C	404	MGE	C1B-C2B-C3B-C4B
8	C	404	MGE	C7A-C8A-C9A-CAA
8	C	404	MGE	C9A-CAA-CBA-CCA
3	B	102	CLA	C12-C13-C15-C16
3	A	101	CLA	C6-C7-C8-C9
8	C	404	MGE	C3A-C4A-C5A-C6A
3	A	101	CLA	C5-C6-C7-C8
7	D	403	LMN	C5-C4-O4-CCR
3	A	101	CLA	C14-C13-C15-C16
8	D	404	MGE	C4B-C5B-C6B-C7B
8	D	404	MGE	C4A-C5A-C6A-C7A
8	C	404	MGE	O1B-C1B-O2G-C2G
7	D	403	LMN	CBC-CBE-CBG-CBI
7	C	403	LMN	OBX-CCJ-OBV-CBT
3	B	102	CLA	CAA-CBA-CGA-O2A
8	C	404	MGE	C2G-C3G-O3G-C1D
6	D	402	A1JR2	C14-C12-C21-C27
3	B	102	CLA	C14-C13-C15-C16
3	A	101	CLA	CAD-CBD-CGD-O2D
3	B	101	CLA	CAD-CBD-CGD-O2D
8	D	404	MGE	O1G-C1A-C2A-C3A
5	C	401	GRG	C1-O1-PA-O3A
7	C	403	LMN	O1-CBS-CCM-CBQ
7	C	403	LMN	OBV-CBT-CCM-CBR
5	C	401	GRG	C10-C8-C9-C11

Continued on next page...

Continued from previous page...

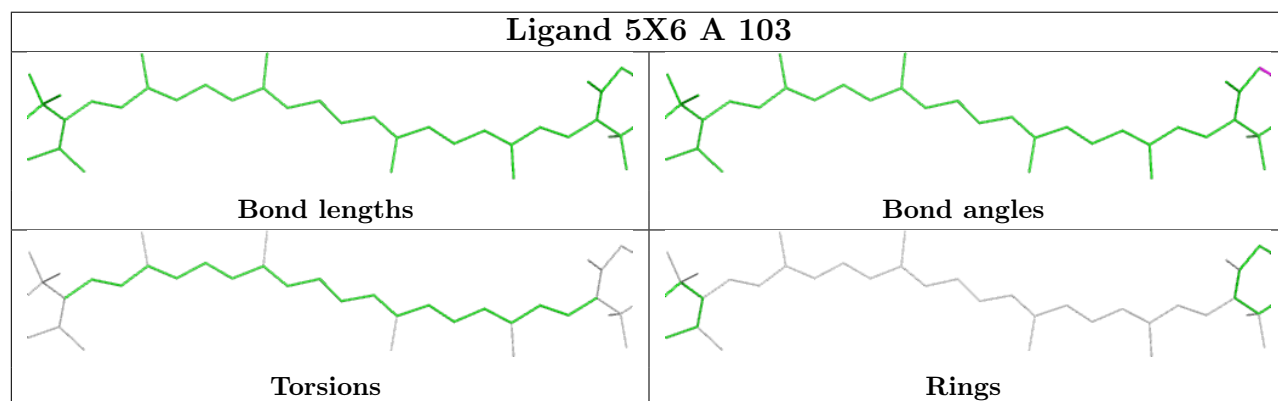
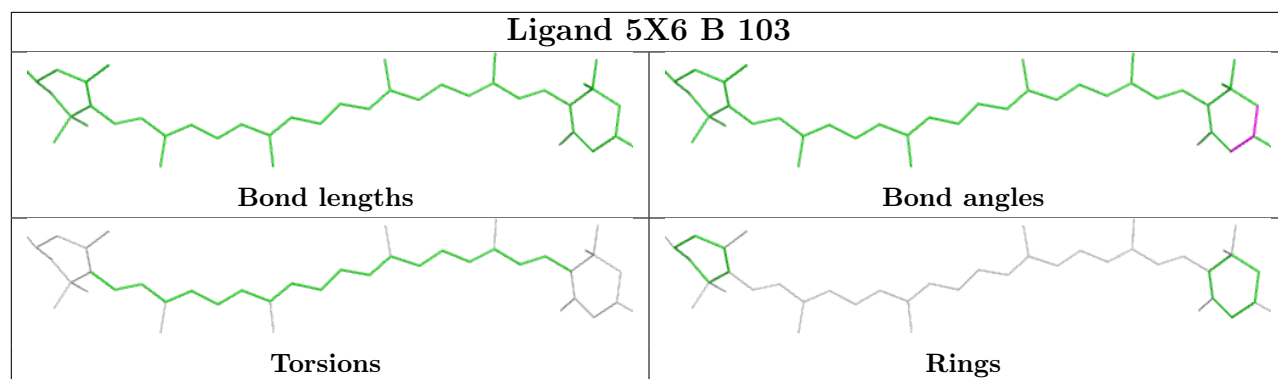
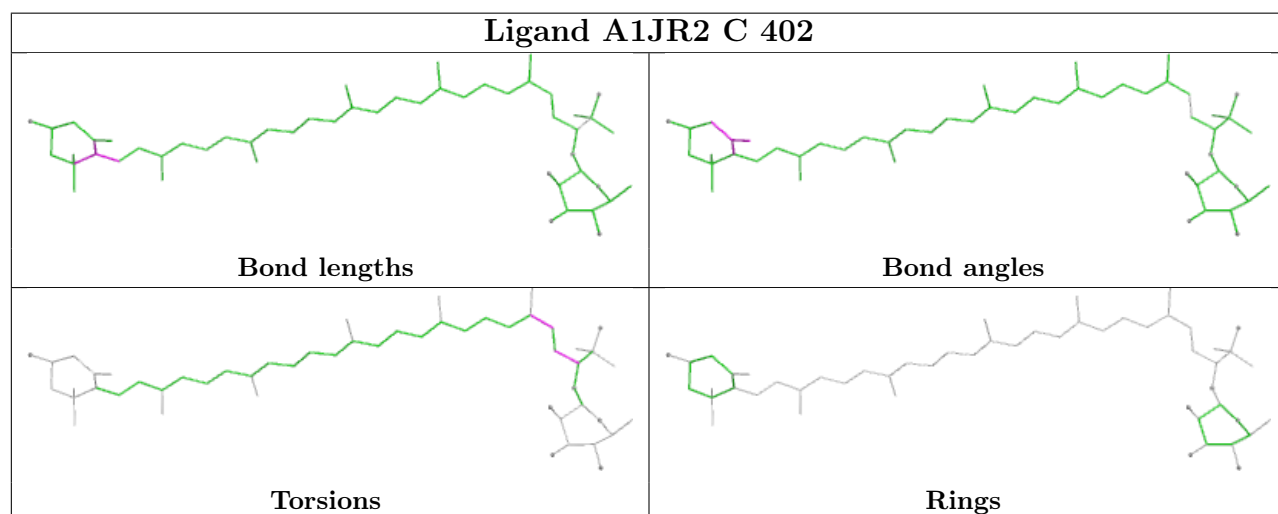
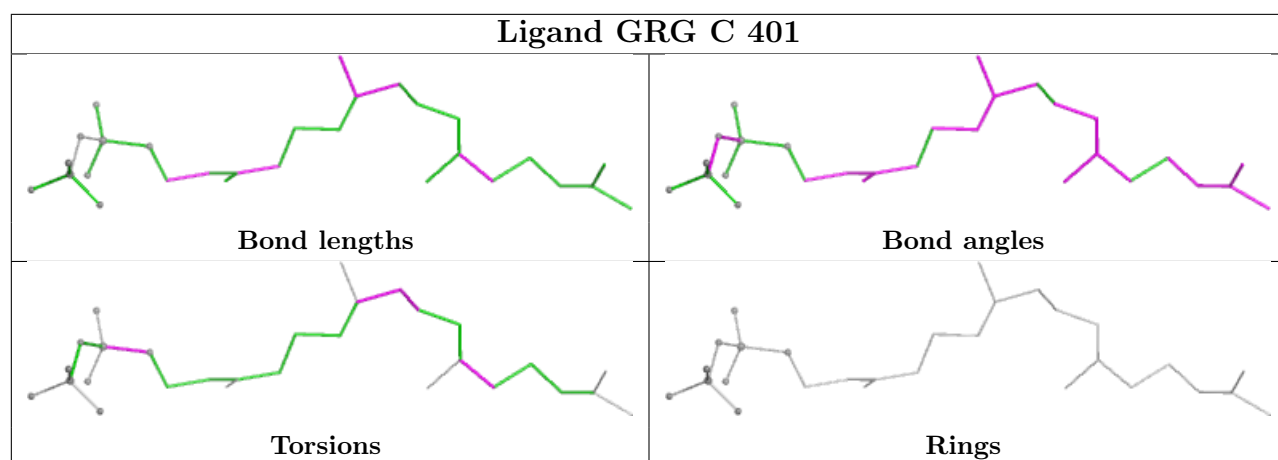
Mol	Chain	Res	Type	Atoms
8	C	404	MGE	C2B-C1B-O2G-C2G
7	D	403	LMN	C3-C4-O4-CCR
8	D	404	MGE	C9B-CAB-CBB-CCB
3	A	102	CLA	CAA-CBA-CGA-O2A
3	A	102	CLA	C15-C16-C17-C18
8	D	404	MGE	O1A-C1A-C2A-C3A
8	D	404	MGE	O2G-C1B-C2B-C3B
8	D	404	MGE	O1B-C1B-C2B-C3B
7	D	403	LMN	CAX-CAZ-CBB-CBD

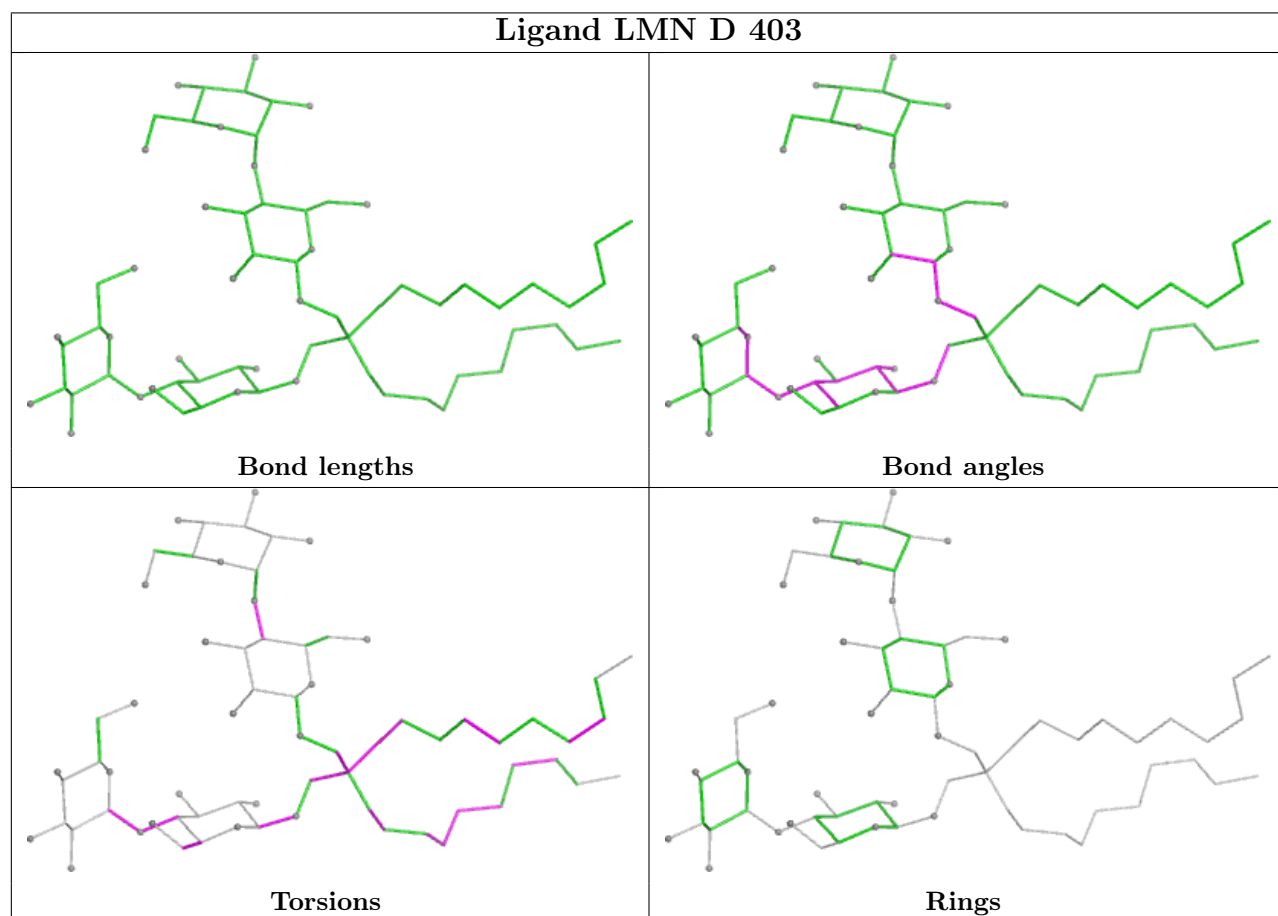
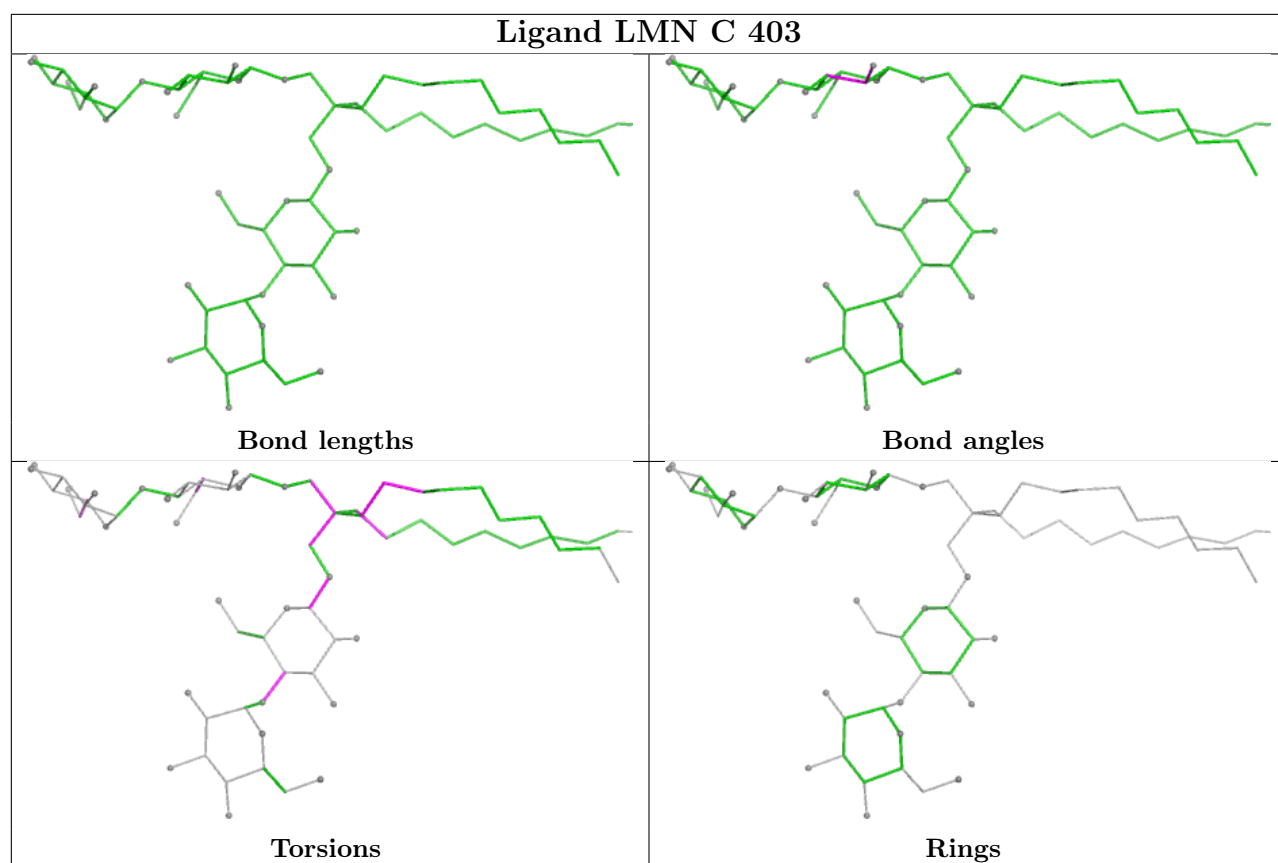
There are no ring outliers.

11 monomers are involved in 30 short contacts:

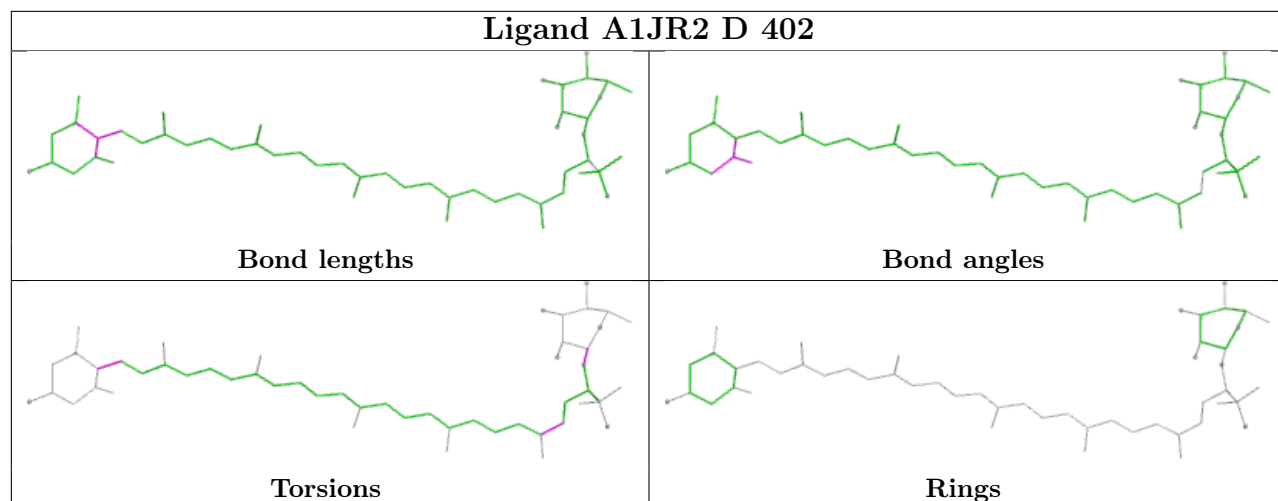
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	401	GRG	2	0
4	B	103	5X6	1	0
4	A	103	5X6	1	0
7	C	403	LMN	4	0
7	D	403	LMN	2	0
3	B	102	CLA	2	0
3	A	102	CLA	4	0
8	D	404	MGE	2	0
5	D	401	GRG	3	0
3	B	101	CLA	6	0
3	A	101	CLA	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

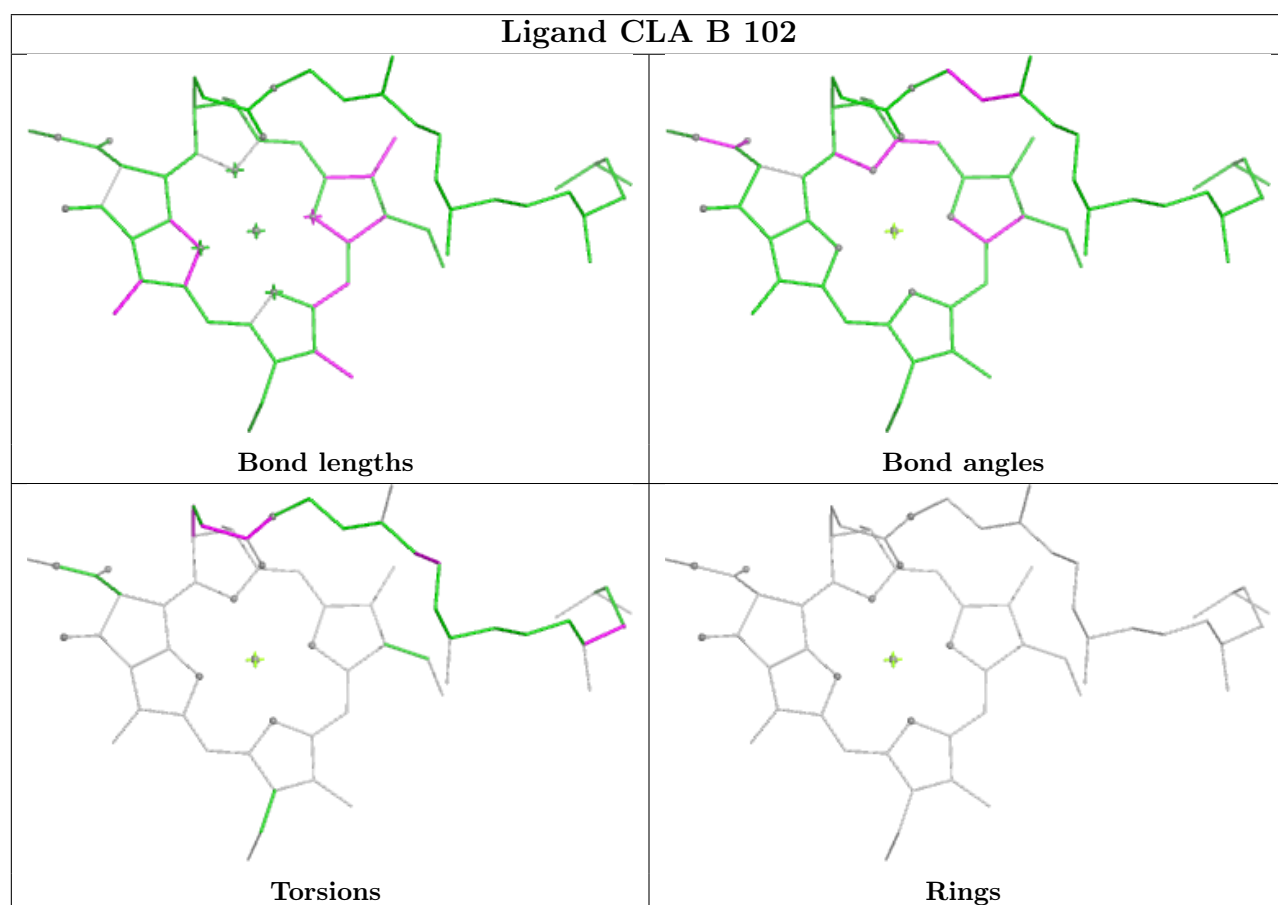


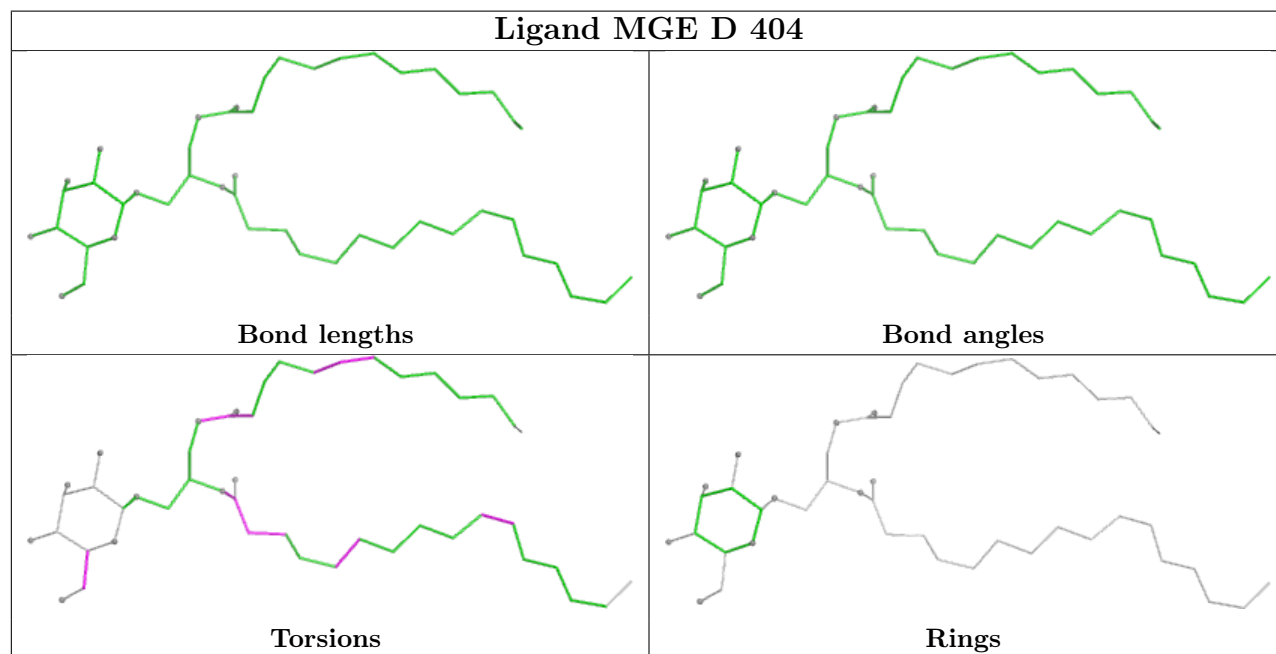
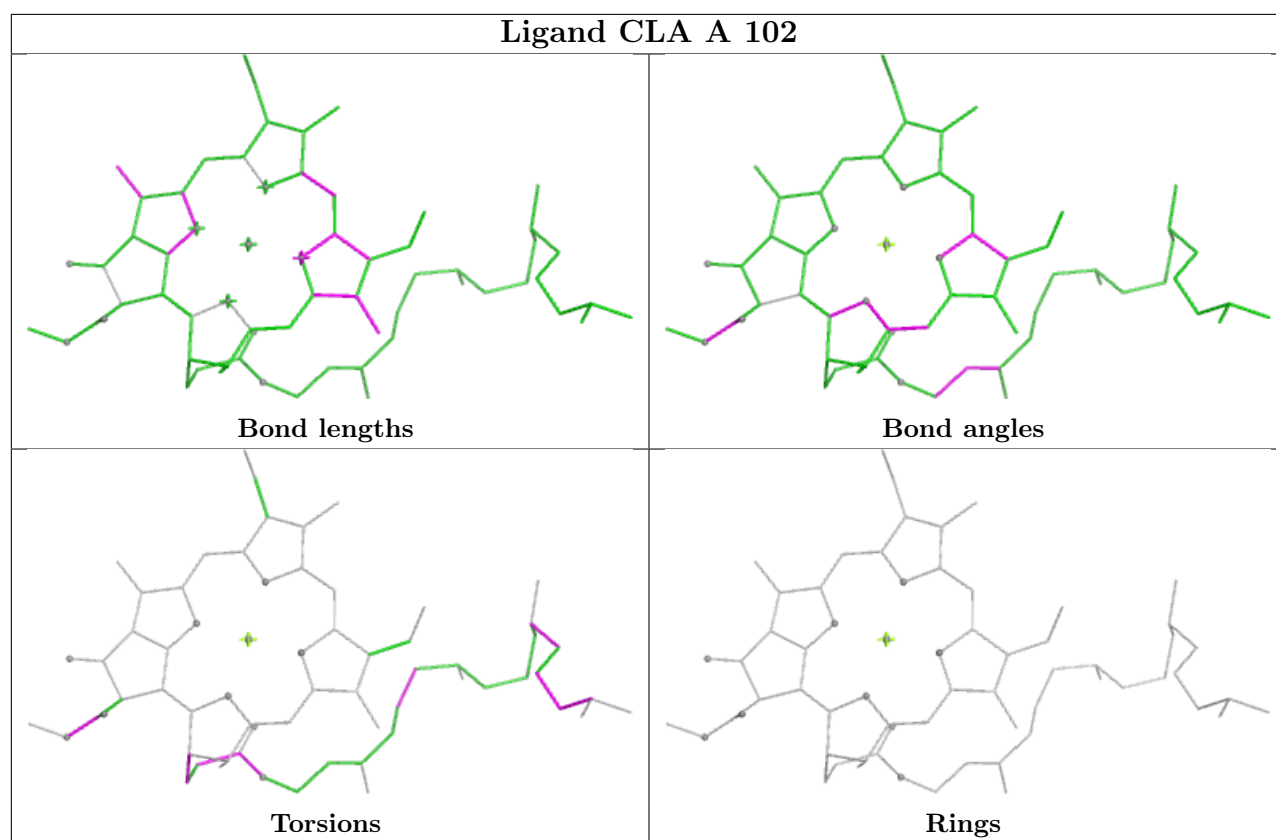


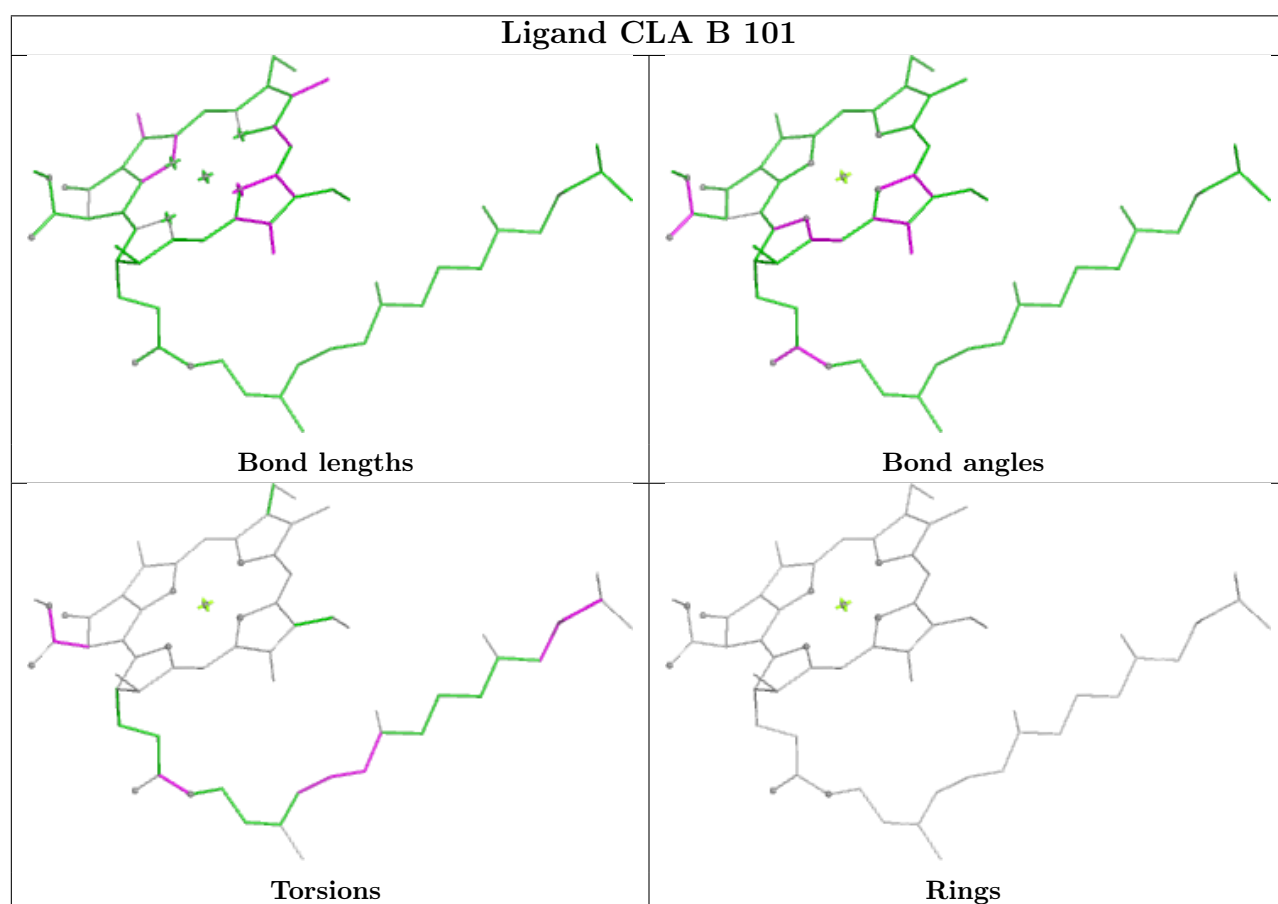
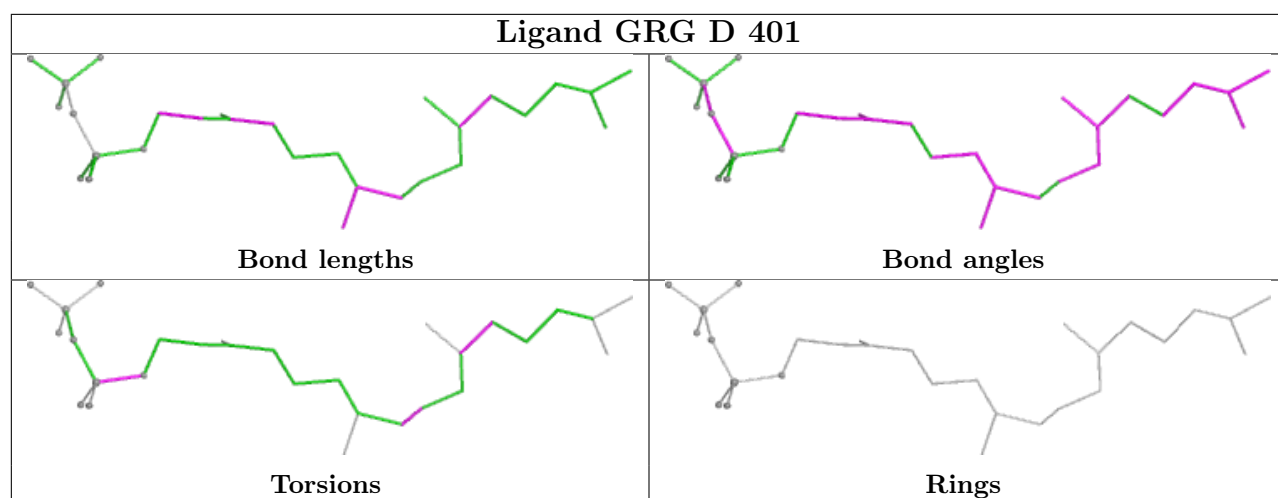
Ligand A1JR2 D 402

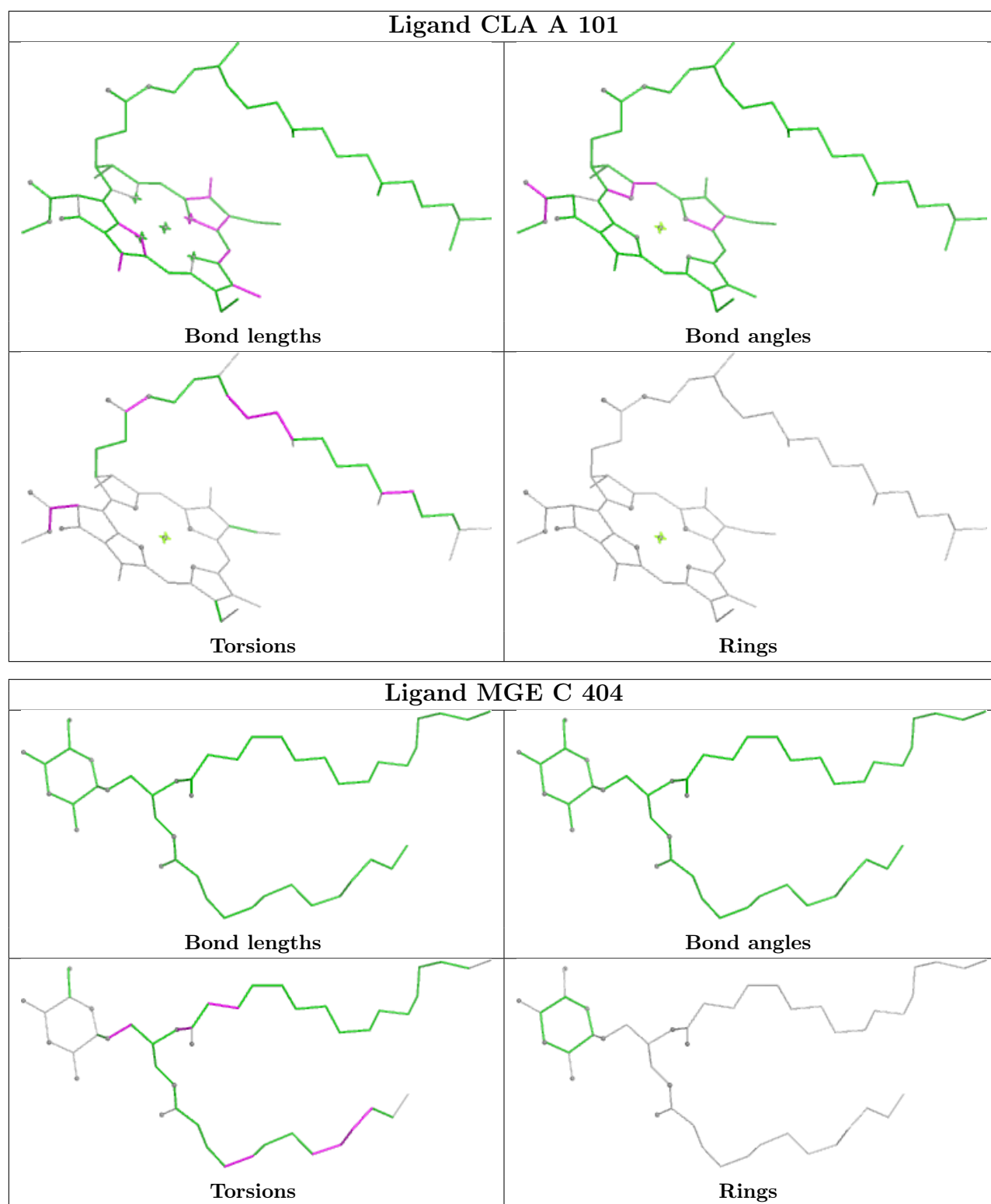


Ligand CLA B 102









5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

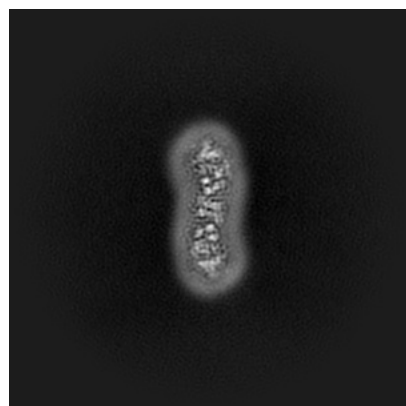
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54697. These allow visual inspection of the internal detail of the map and identification of artifacts.

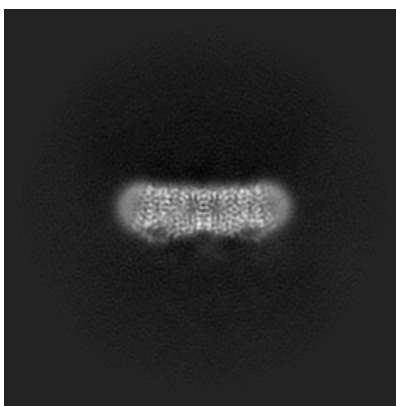
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

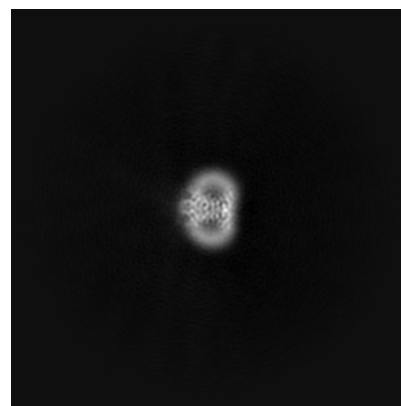
6.1.1 Primary map



X

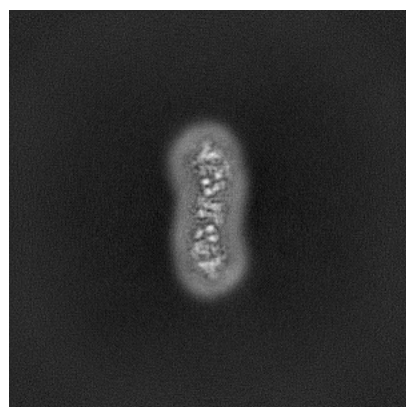


Y

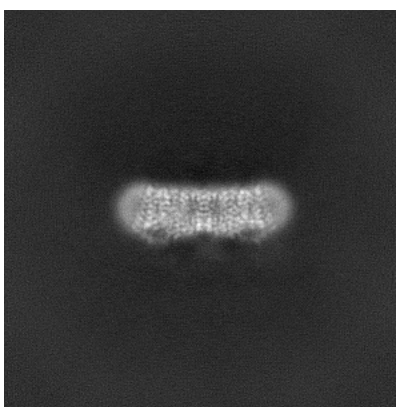


Z

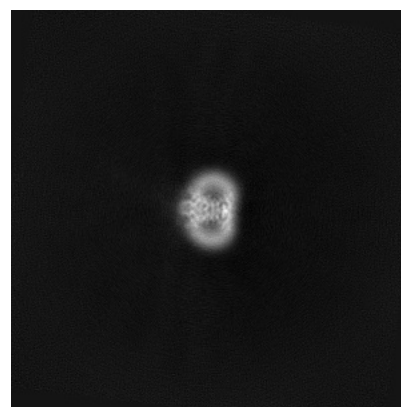
6.1.2 Raw map



X



Y

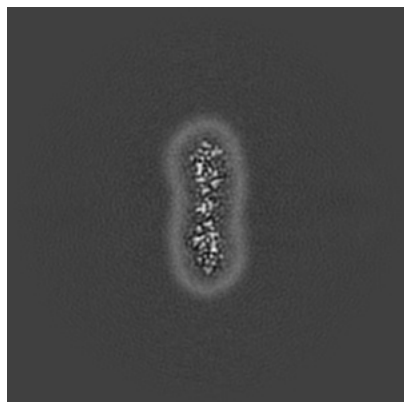


Z

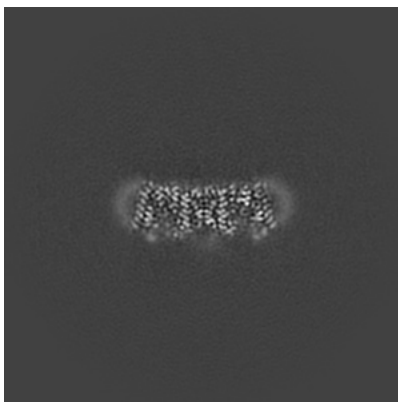
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

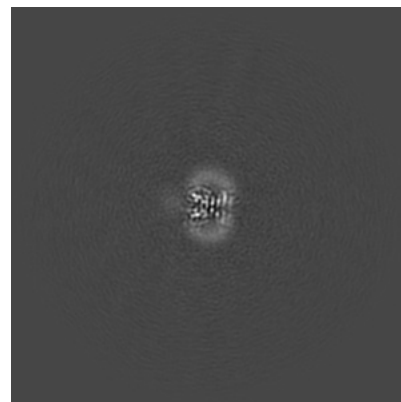
6.2.1 Primary map



X Index: 256

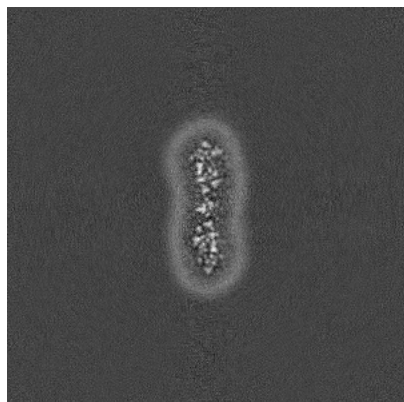


Y Index: 256

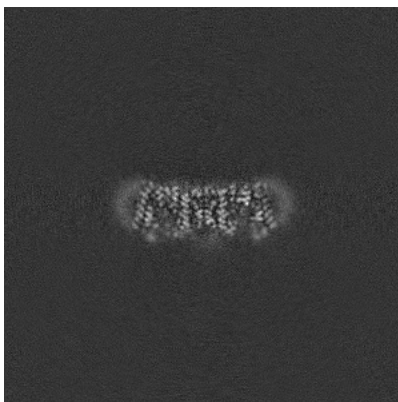


Z Index: 256

6.2.2 Raw map



X Index: 256



Y Index: 256

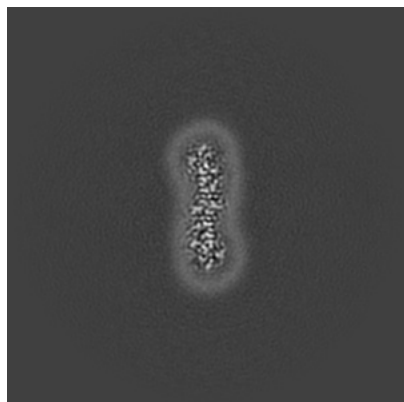


Z Index: 256

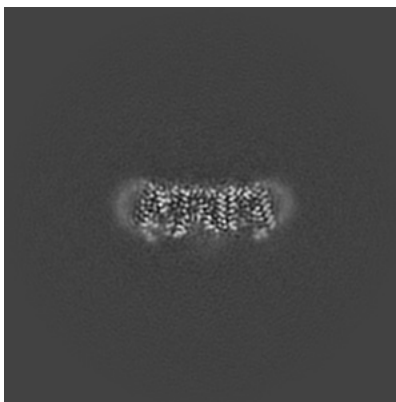
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

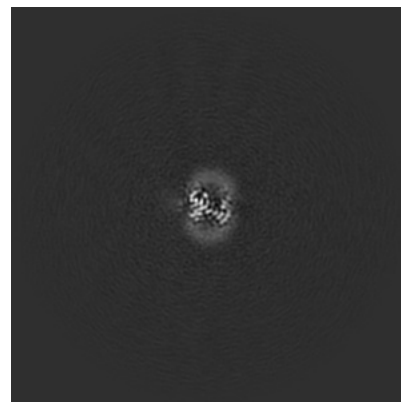
6.3.1 Primary map



X Index: 272

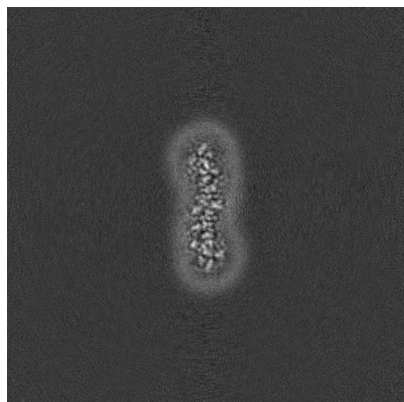


Y Index: 253

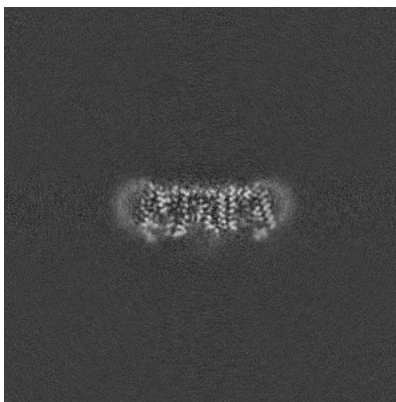


Z Index: 249

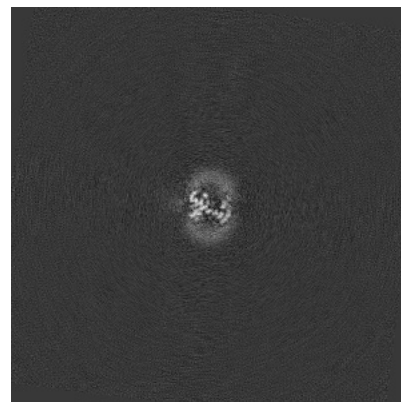
6.3.2 Raw map



X Index: 273



Y Index: 253



Z Index: 249

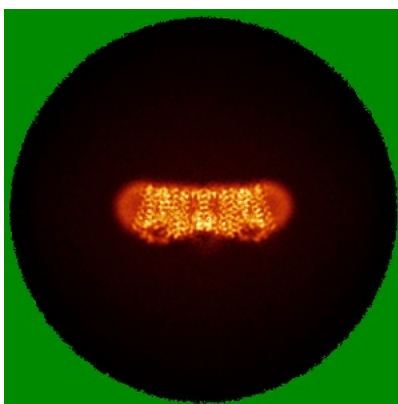
The images above show the largest variance slices of the map in three orthogonal directions.

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

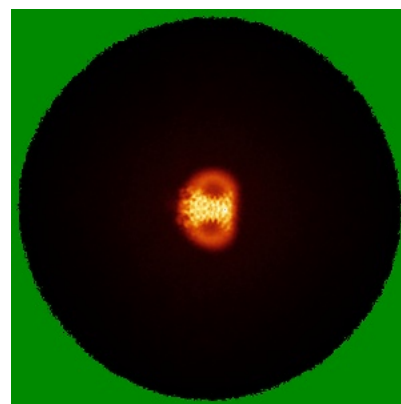
6.4.1 Primary map



X

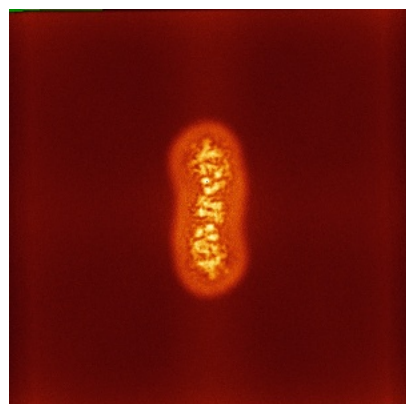


Y

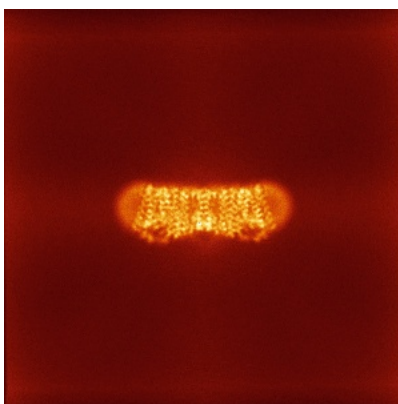


Z

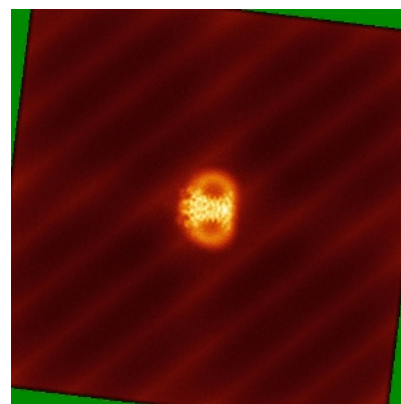
6.4.2 Raw map



X



Y

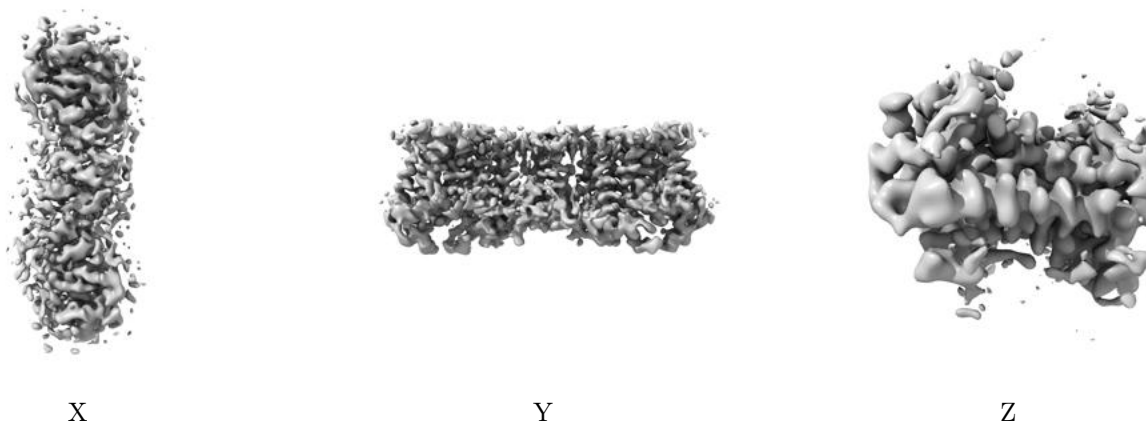


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

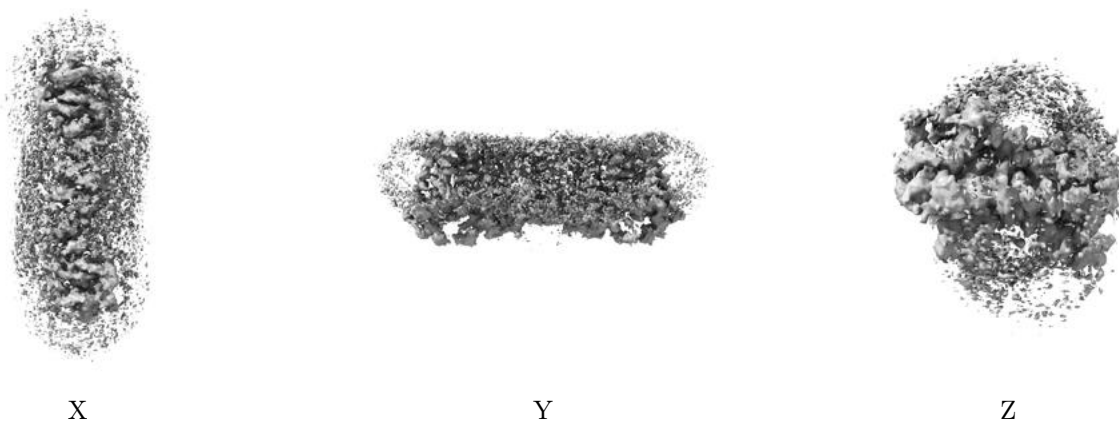
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

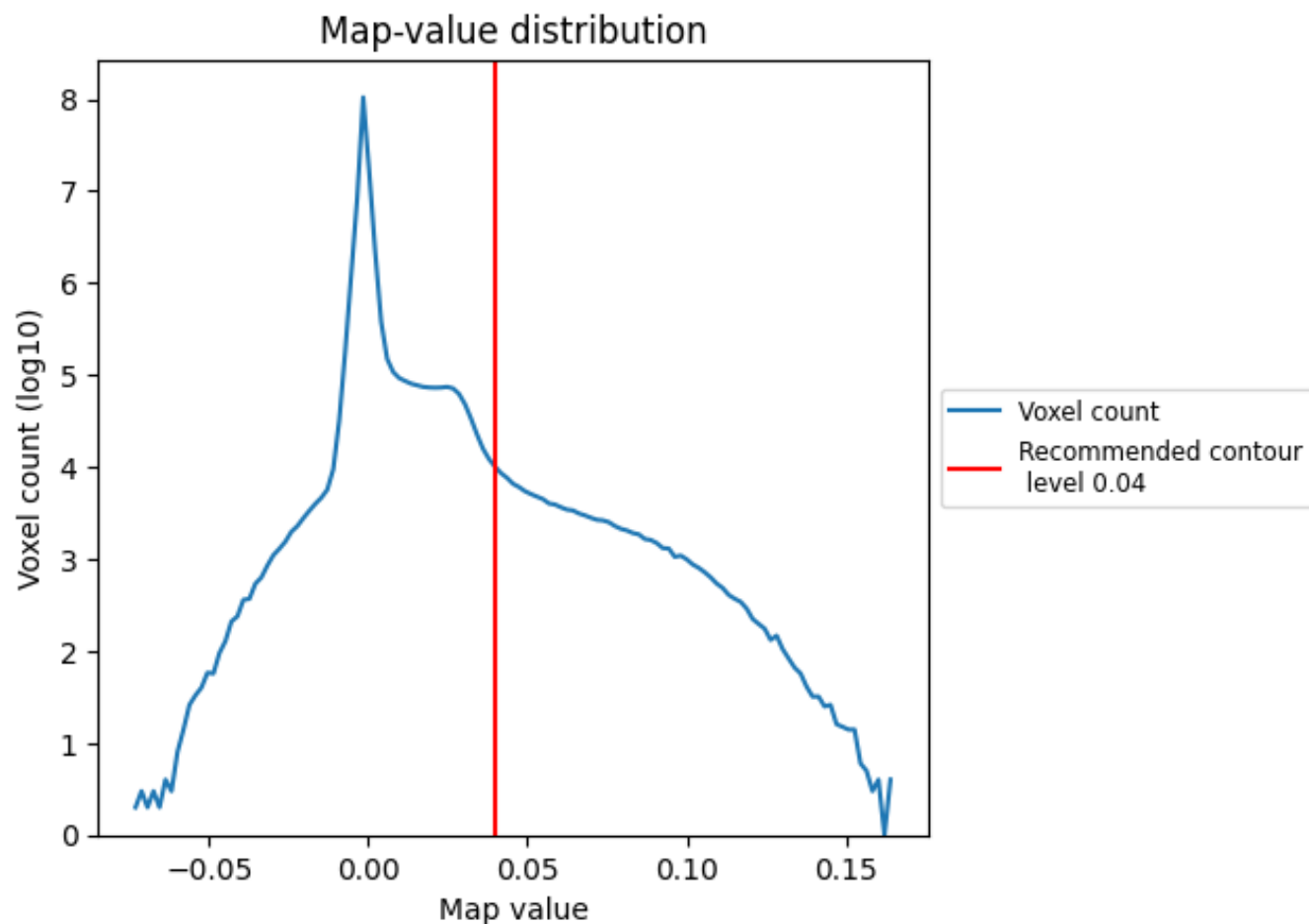
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

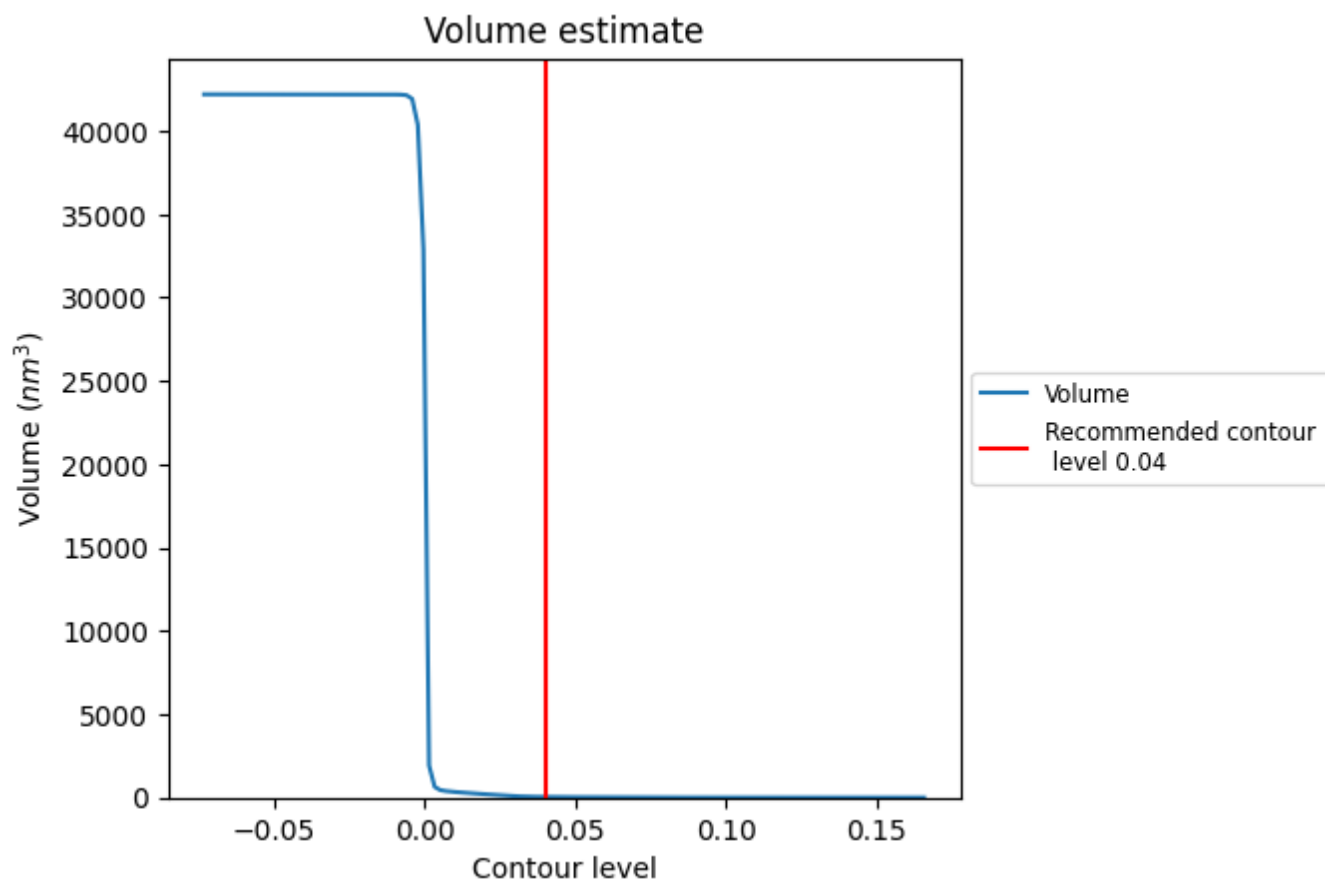
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

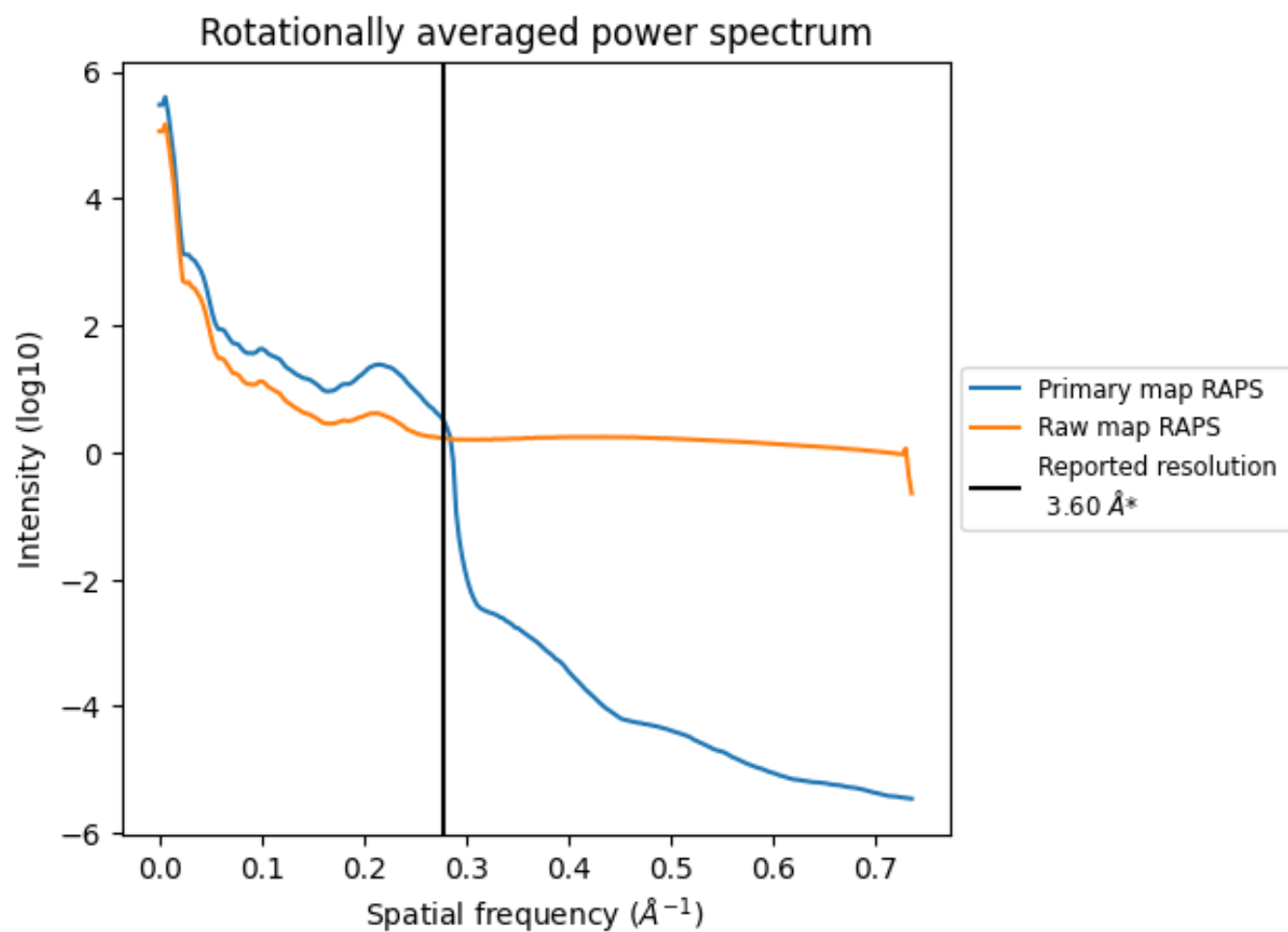
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 38 nm^3 ; this corresponds to an approximate mass of 34 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 ⓘ

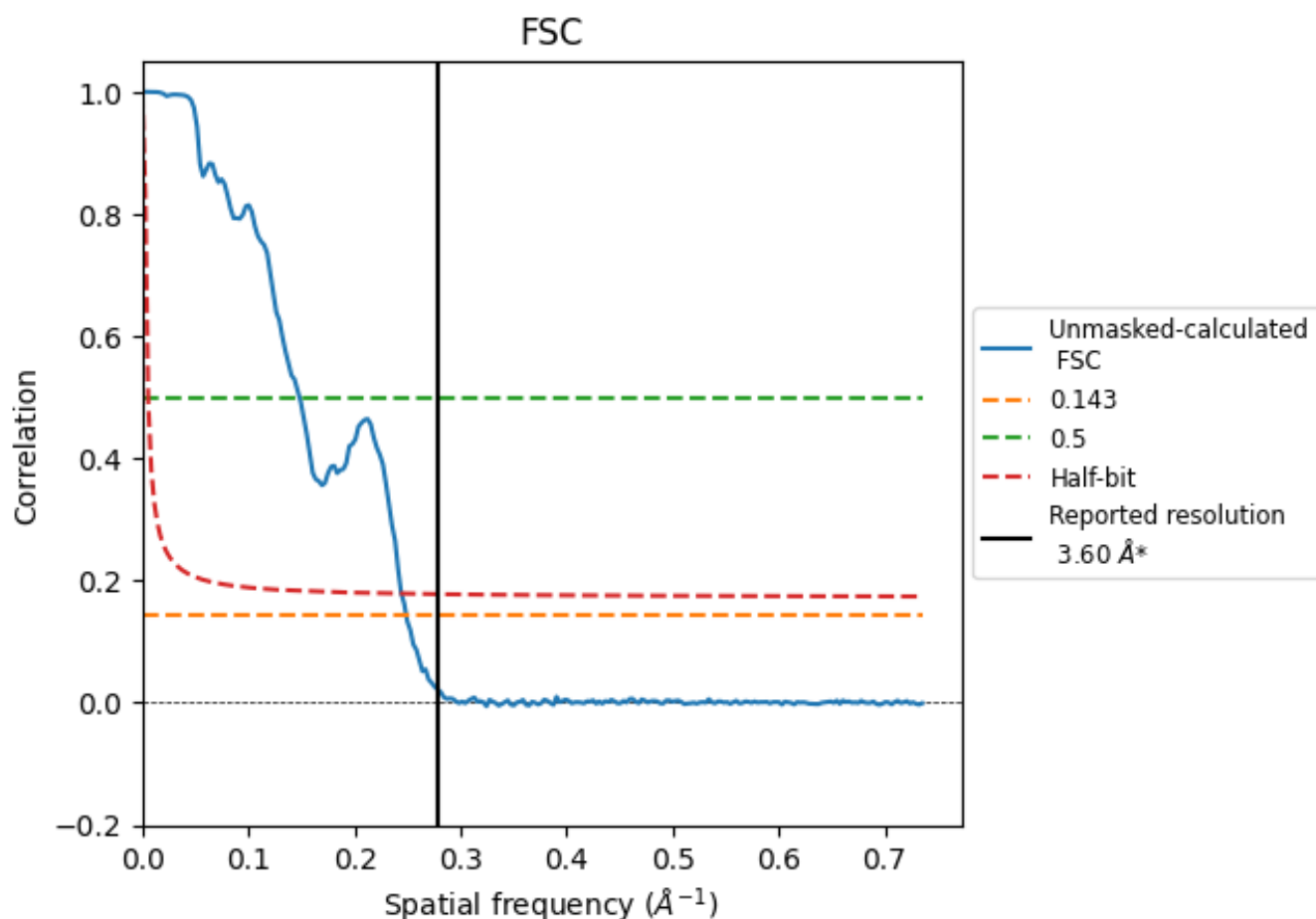


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

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 0.278 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

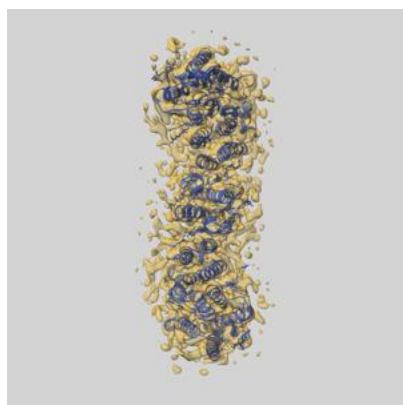
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.02	6.75	4.09

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.02 differs from the reported value 3.6 by more than 10 %

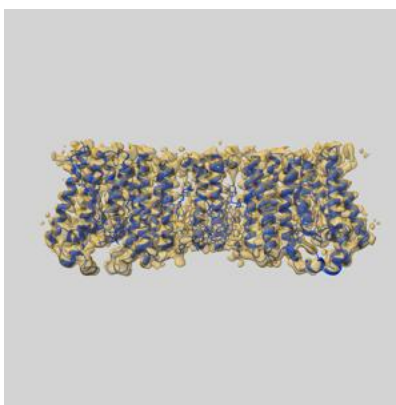
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-54697 and PDB model 9SAU. Per-residue inclusion information can be found in section [3](#) on page [9](#).

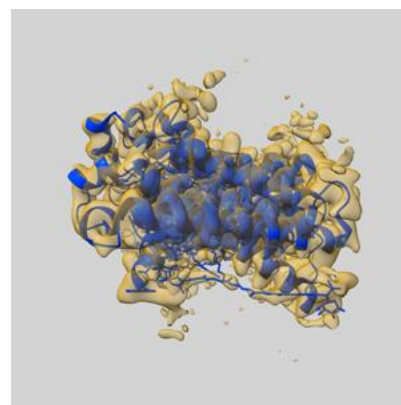
9.1 Map-model overlay [i](#)



X



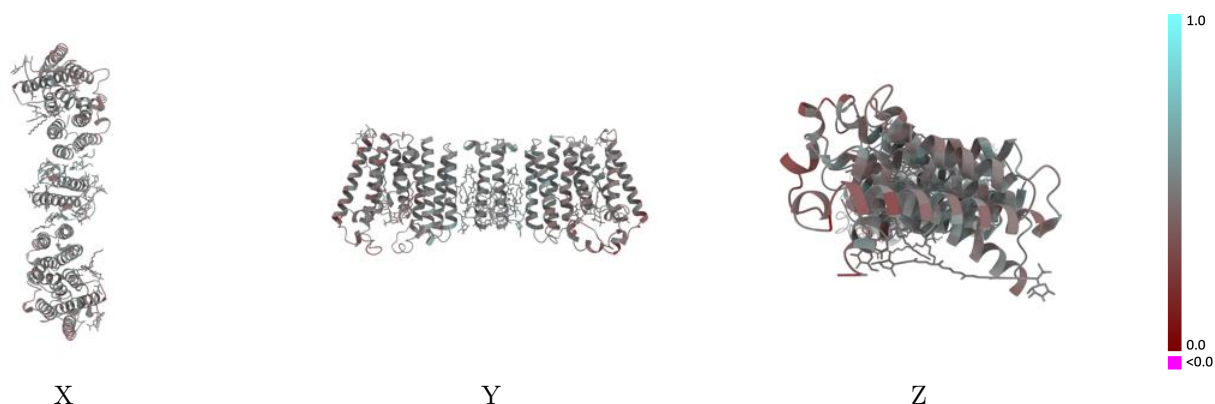
Y



Z

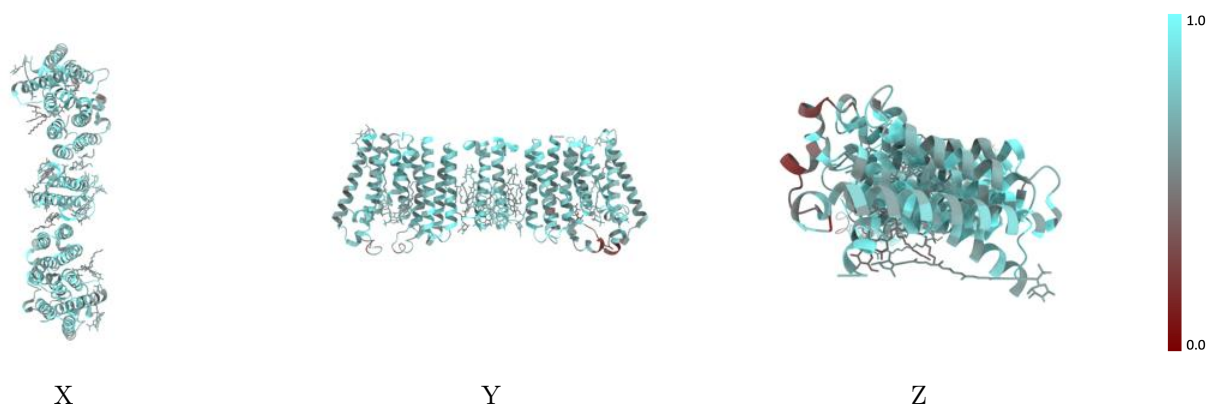
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



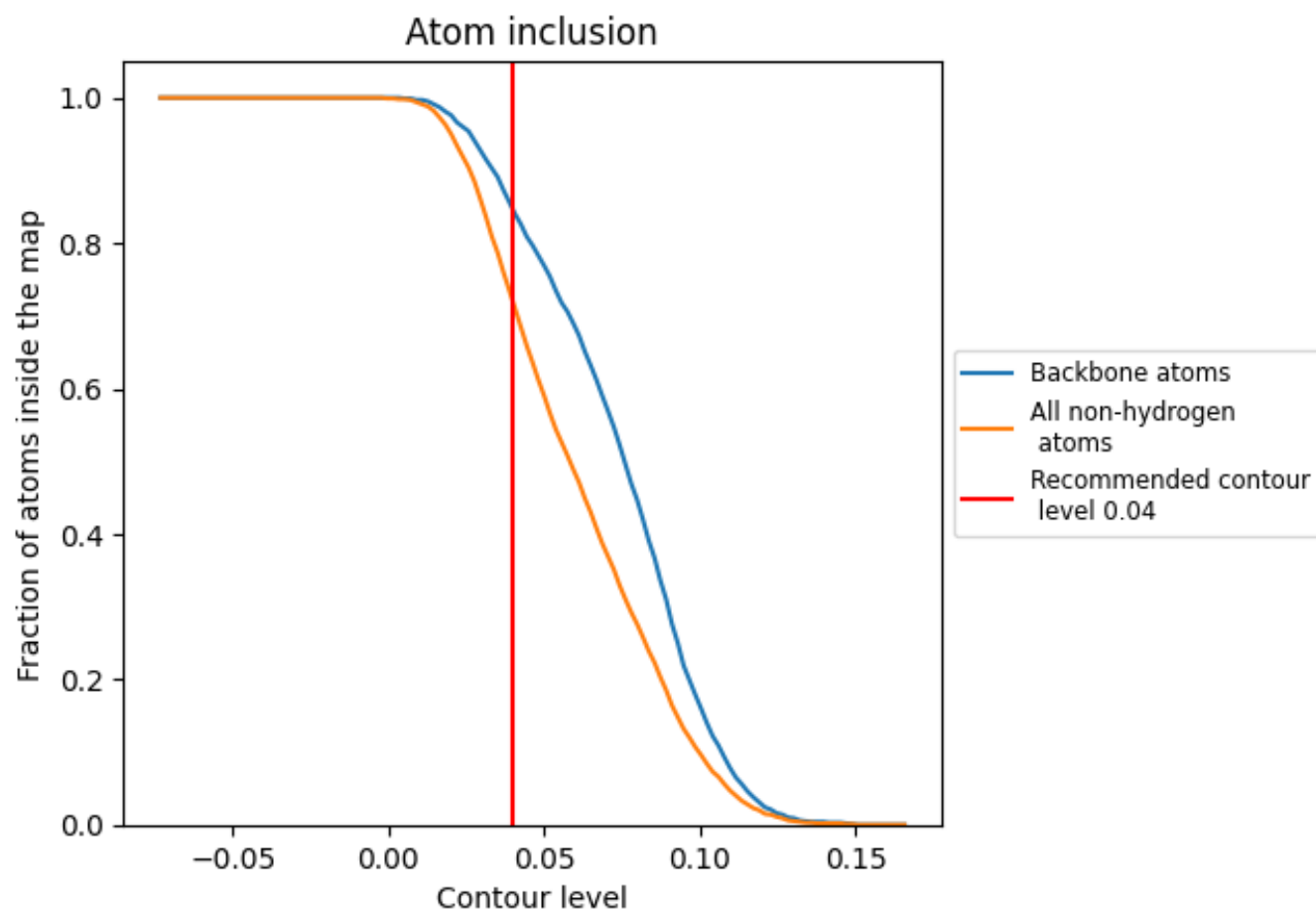
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 85% of all backbone atoms, 72% 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	0.7210	0.4650
A	0.7730	0.4940
B	0.7460	0.4970
C	0.7090	0.4580
D	0.7180	0.4590

