



Full wwPDB EM Validation Report ⓘ

Aug 16, 2026 – 04:31 pm BST

PDB ID : 9SAS / pdb_00009sas
EMDB ID : EMD-54696
Title : Chlorophyll synthase in complex with the LHC-like protein HliD, apo state
Authors : Shvarev, D.; Hitchcock, A.; Sobotka, R.
Deposited on : 2025-08-07
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.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

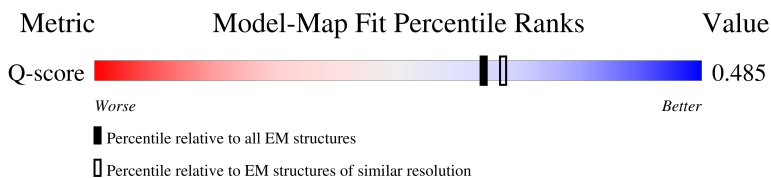
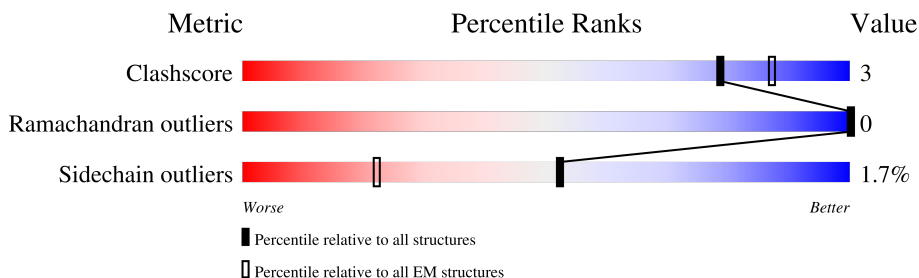
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14717 (2.90 - 3.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	40	
1	B	40	
2	C	295	
2	D	295	

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
5	A1JR2	C	401	X	-	-	-
5	A1JR2	D	401	X	-	-	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 5874 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.

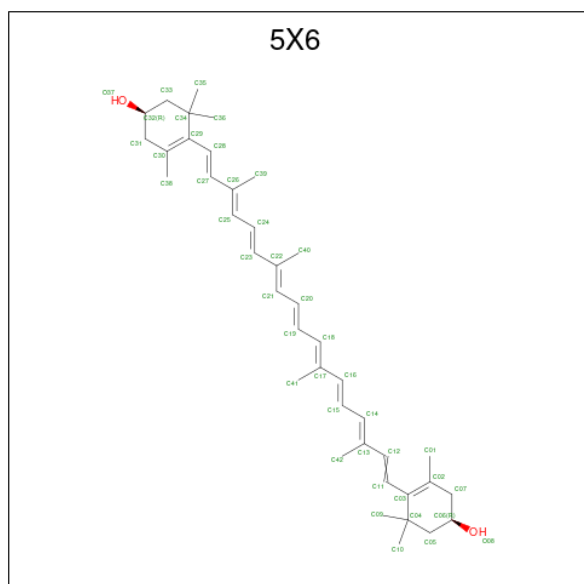
- Molecule 1 is a protein called High light-inducible protein HliD.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	40	Total	C	N	O	S	0	0
			317	213	51	52	1		
1	B	40	Total	C	N	O	S	0	0
			317	213	51	52	1		

- Molecule 2 is a protein called Chlorophyll a synthase.

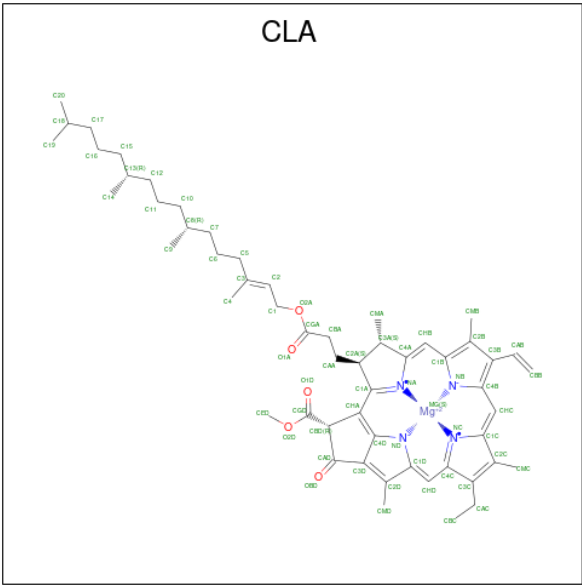
Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	295	Total	C	N	O	S	0	0
			2278	1517	357	391	13		
2	D	295	Total	C	N	O	S	0	0
			2278	1517	357	391	13		

- Molecule 3 is Zeaxanthin (CCD ID: 5X6) (formula: $C_{40}H_{56}O_2$) (labeled as "Ligand of Interest" by depositor).



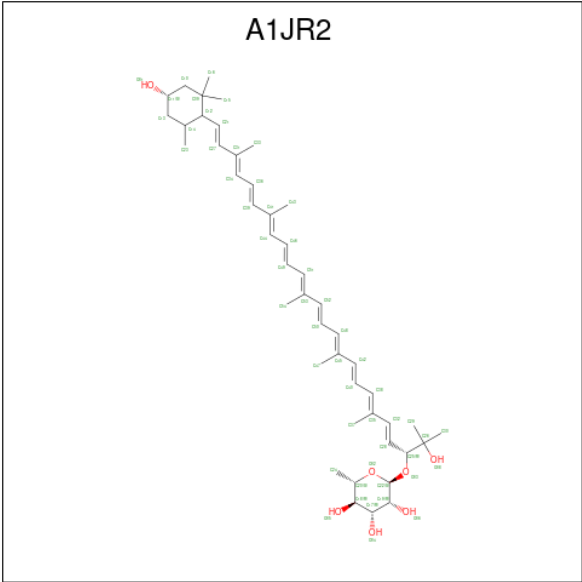
Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total	C	O	0
			42	40	2	
3	B	1	Total	C	O	0
			42	40	2	

- Molecule 4 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



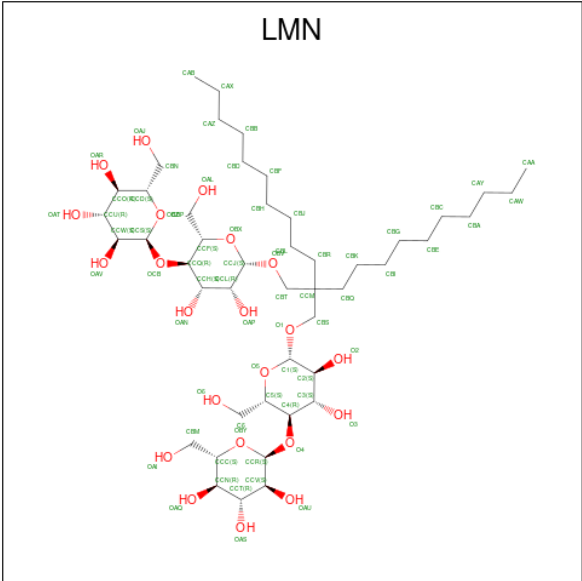
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
4	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
4	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
4	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 5 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: $C_{46}H_{68}O_7$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 6 is Lauryl Maltose Neopentyl Glycol (CCD ID: LMN) (formula: $C_{47}H_{88}O_{22}$) (labeled as "Ligand of Interest" by depositor).



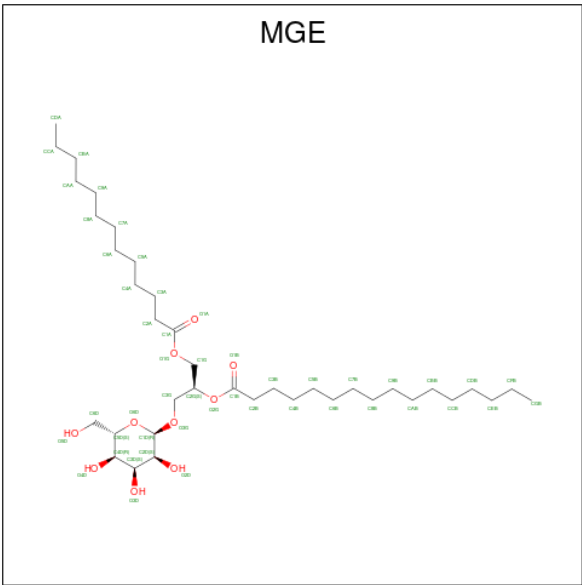
Mol	Chain	Residues	Atoms			AltConf
6	C	1	Total	C	O	0
			69	47	22	

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

- Molecule 7 is (1S)-2-(ALPHA-L-ALLOPYRANOSYLOXY)-1-[(TRIDECANOYLOXY)METHYL]ETHYL PALMITATE (CCD ID: MGE) (formula: C₃₈H₇₂O₁₀) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
7	C	1	Total	C	O	0
			48	38	10	
7	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:  90% 10%

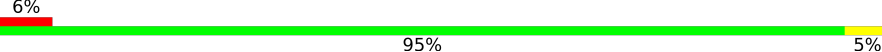


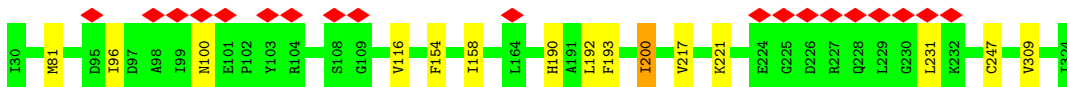
- Molecule 1: High light-inducible protein HliD

Chain B:  75% 25%



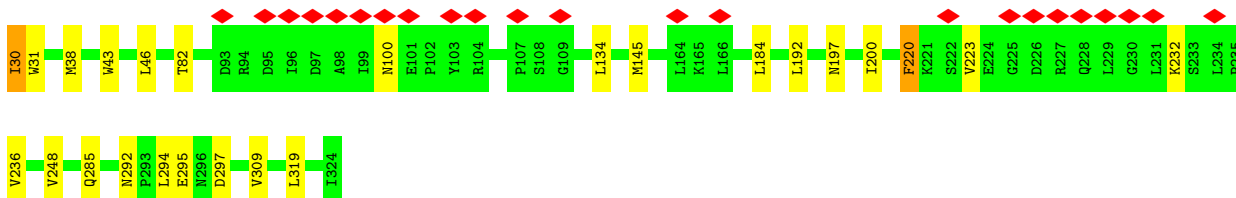
- Molecule 2: Chlorophyll a synthase

Chain C:  6% 95% 5%



- Molecule 2: Chlorophyll a synthase

Chain D:  8% 92% 8%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	354715	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	0.216	Depositor
Minimum map value	-0.089	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: LMN, A1JR2, MGE, 5X6, CLA

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	0.09	0/325	0.19	0/438
1	B	0.09	0/325	0.23	0/438
2	C	0.09	0/2342	0.25	0/3203
2	D	0.09	0/2342	0.26	0/3203
All	All	0.09	0/5334	0.25	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	317	0	320	3	0
1	B	317	0	320	7	0
2	C	2278	0	2331	11	0
2	D	2278	0	2331	12	0
3	A	42	0	0	0	0
3	B	42	0	0	0	0
4	A	130	0	143	2	0
4	B	130	0	144	1	0
5	C	53	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	53	0	0	0	0
6	C	69	0	88	2	0
6	D	69	0	88	0	0
7	C	48	0	72	0	0
7	D	48	0	72	0	0
All	All	5874	0	5909	33	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 (33) 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:C:154:PHE:O	2:C:158:ILE:HG23	1.95	0.65
2:D:232:LYS:HE3	2:D:232:LYS:HA	1.80	0.64
2:D:46:LEU:HD22	2:D:82:THR:OG1	1.98	0.64
2:C:221:LYS:HA	2:C:221:LYS:HE2	1.85	0.56
2:C:309:VAL:HG11	6:C:402:LMN:CBJ	2.39	0.52
2:C:81:MET:HA	2:C:81:MET:HE2	1.92	0.50
2:C:96:ILE:O	2:C:96:ILE:HG22	2.10	0.50
2:C:217:VAL:HG23	2:C:247:CYS:SG	2.52	0.50
1:B:29:GLY:O	1:B:33:MET:HG3	2.13	0.49
2:D:200:ILE:HD13	2:D:319:LEU:HD23	1.95	0.48
2:C:96:ILE:HG22	2:C:100:ASN:OD1	2.14	0.47
2:C:309:VAL:HG11	6:C:402:LMN:HBJA	1.96	0.47
1:A:21:ASN:C	4:A:102:CLA:HMA1	2.40	0.47
1:B:21:ASN:C	4:B:102:CLA:HMA1	2.40	0.47
2:D:100:ASN:OD1	2:D:100:ASN:C	2.57	0.47
2:D:220:PHE:O	2:D:223:VAL:HG23	2.16	0.46
1:B:39:ILE:O	1:B:43:GLU:OE1	2.34	0.46
2:D:134:LEU:HD21	2:D:192:LEU:HD22	1.97	0.46
2:C:190:HIS:CD2	2:C:200:ILE:HG21	2.52	0.44
2:D:248:VAL:HG13	2:D:285:GLN:OE1	2.17	0.44
1:B:50:VAL:HG13	1:B:51:LEU:N	2.33	0.43
2:D:30:ILE:HD12	2:D:31:TRP:N	2.33	0.43
1:B:54:LEU:O	1:B:54:LEU:HD12	2.18	0.43
1:A:35:GLY:O	1:A:39:ILE:HG13	2.18	0.43
1:B:26:LYS:O	1:B:30:ARG:HG3	2.19	0.42
2:D:197:ASN:O	2:D:200:ILE:HG22	2.19	0.42
2:D:145:MET:HE3	2:D:145:MET:HA	2.02	0.42
1:A:28:ASN:C	1:B:33:MET:HE2	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:103:CLA:H112	4:A:103:CLA:H91	1.87	0.41
2:C:231:LEU:O	2:C:231:LEU:HD12	2.21	0.41
2:C:192:LEU:O	2:C:193:PHE:HB2	2.20	0.41
2:D:292:ASN:O	2:D:295:GLU:O	2.38	0.41
2:D:38:MET:HE2	2:D:43:TRP:CZ2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	38/40 (95%)	38 (100%)	0	0	100	100
1	B	38/40 (95%)	36 (95%)	2 (5%)	0	100	100
2	C	293/295 (99%)	280 (96%)	13 (4%)	0	100	100
2	D	293/295 (99%)	282 (96%)	11 (4%)	0	100	100
All	All	662/670 (99%)	636 (96%)	26 (4%)	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	31/31 (100%)	31 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	31/31 (100%)	31 (100%)	0	100	100
2	C	238/238 (100%)	236 (99%)	2 (1%)	73	77
2	D	238/238 (100%)	231 (97%)	7 (3%)	37	60
All	All	538/538 (100%)	529 (98%)	9 (2%)	52	67

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	116	VAL
2	C	200	ILE
2	D	30	ILE
2	D	184	LEU
2	D	220	PHE
2	D	236	VAL
2	D	294	LEU
2	D	297	ASP
2	D	309	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	168	GLN
2	C	228	GLN
2	C	255	GLN
2	C	281	GLN
2	D	321	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

12 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	A1JR2	D	401	-	53,54,54	1.32	3 (5%)	64,75,75	1.45	3 (4%)
6	LMN	C	402	-	72,72,72	0.52	0	96,98,98	0.96	5 (5%)
4	CLA	B	103	1	69,73,73	1.26	7 (10%)	83,113,113	1.33	9 (10%)
5	A1JR2	C	401	-	53,54,54	1.34	3 (5%)	64,75,75	1.50	3 (4%)
3	5X6	B	101	-	43,43,43	0.12	0	58,60,60	0.46	0
4	CLA	A	103	1	69,73,73	1.26	7 (10%)	83,113,113	1.30	8 (9%)
7	MGE	C	403	-	48,48,48	0.48	0	56,56,56	0.60	0
6	LMN	D	402	-	72,72,72	0.52	0	96,98,98	0.85	2 (2%)
3	5X6	A	101	-	43,43,43	0.14	0	58,60,60	0.39	0
7	MGE	D	403	-	48,48,48	0.46	0	56,56,56	0.64	1 (1%)
4	CLA	A	102	1	69,73,73	1.25	9 (13%)	83,113,113	1.29	7 (8%)
4	CLA	B	102	1	69,73,73	1.25	8 (11%)	83,113,113	1.27	8 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	A1JR2	D	401	-	2/2/16/33	6/45/84/84	0/2/2/2
6	LMN	C	402	-	-	24/50/130/130	0/4/4/4
5	A1JR2	C	401	-	2/2/16/33	8/45/84/84	0/2/2/2
4	CLA	B	103	1	-	16/39/115/115	-
3	5X6	B	101	-	-	0/29/67/67	0/2/2/2
4	CLA	A	103	1	-	14/39/115/115	-
4	CLA	B	102	1	-	10/39/115/115	-
7	MGE	C	403	-	-	8/43/63/63	0/1/1/1
6	LMN	D	402	-	-	19/50/130/130	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	5X6	A	101	-	-	0/29/67/67	0/2/2/2
7	MGE	D	403	-	-	12/43/63/63	0/1/1/1
4	CLA	A	102	1	-	15/39/115/115	-

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	401	A1JR2	C12-C14	-8.79	1.34	1.54
5	C	401	A1JR2	C12-C14	-8.75	1.34	1.54
4	B	103	CLA	C1D-ND	3.77	1.42	1.37
4	B	102	CLA	C1D-ND	3.75	1.42	1.37
4	A	103	CLA	C1D-ND	3.71	1.42	1.37
4	A	102	CLA	C1D-ND	3.68	1.42	1.37
4	B	103	CLA	C4B-NB	3.51	1.42	1.37
4	A	103	CLA	C4B-NB	3.47	1.42	1.37
4	B	102	CLA	C4B-NB	3.26	1.41	1.37
4	A	102	CLA	C4B-NB	3.15	1.41	1.37
4	B	103	CLA	C3B-C4B	3.13	1.50	1.42
4	A	103	CLA	C3B-C4B	3.11	1.50	1.42
5	C	401	A1JR2	C12-C21	-3.07	1.46	1.50
4	A	102	CLA	C4D-ND	-2.93	1.33	1.37
4	B	102	CLA	C3B-C4B	2.93	1.49	1.42
4	A	103	CLA	C4D-ND	-2.86	1.33	1.37
4	B	102	CLA	C4D-ND	-2.86	1.33	1.37
4	A	102	CLA	C3B-C4B	2.80	1.49	1.42
4	B	103	CLA	C4D-ND	-2.80	1.33	1.37
4	A	102	CLA	C1B-C2B	2.78	1.49	1.43
4	B	102	CLA	C1B-C2B	2.62	1.49	1.43
5	D	401	A1JR2	C12-C21	-2.52	1.46	1.50
4	A	103	CLA	C1B-C2B	2.52	1.49	1.43
4	B	103	CLA	C1B-C2B	2.49	1.49	1.43
5	C	401	A1JR2	C09-C12	-2.47	1.53	1.55
5	D	401	A1JR2	C09-C12	-2.39	1.53	1.55
4	B	102	CLA	CHC-C1C	2.38	1.43	1.38
4	A	102	CLA	CHC-C1C	2.26	1.43	1.38
4	B	103	CLA	CHC-C1C	2.24	1.43	1.38
4	A	103	CLA	CHC-C1C	2.23	1.43	1.38
4	B	103	CLA	CMD-C2D	-2.07	1.46	1.50
4	A	102	CLA	MG-NB	-2.06	2.01	2.05
4	B	102	CLA	MG-NB	-2.05	2.01	2.05
4	A	103	CLA	CMD-C2D	-2.05	1.46	1.50
4	A	102	CLA	CMD-C2D	-2.04	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	102	CLA	CMD-C2D	-2.01	1.46	1.50
4	A	102	CLA	CMC-C2C	-2.01	1.46	1.50

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	401	A1JR2	C13-C14-C12	9.54	120.68	109.72
5	D	401	A1JR2	C13-C14-C12	9.22	120.33	109.72
4	A	102	CLA	C4A-NA-C1A	6.52	109.64	106.71
4	B	103	CLA	C4A-NA-C1A	6.31	109.55	106.71
4	B	102	CLA	C4A-NA-C1A	6.13	109.46	106.71
5	D	401	A1JR2	C23-C14-C12	6.06	124.55	112.60
4	A	103	CLA	C4A-NA-C1A	6.03	109.42	106.71
5	C	401	A1JR2	C23-C14-C12	6.03	124.50	112.60
6	D	402	LMN	CCR-O4-C4	3.91	127.65	117.96
6	C	402	LMN	CBS-O1-C1	3.37	122.12	113.36
4	B	102	CLA	C3B-C4B-NB	-3.06	107.68	110.52
4	A	103	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
4	A	103	CLA	C9-C8-C10	2.87	121.68	111.29
4	B	103	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
6	C	402	LMN	CCS-OCB-CCQ	2.85	125.02	117.96
4	B	102	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
4	A	102	CLA	C3B-C4B-NB	-2.80	107.91	110.52
4	A	102	CLA	O2D-CGD-O1D	-2.78	118.39	123.84
4	B	103	CLA	C3B-C4B-NB	-2.64	108.07	110.52
4	A	103	CLA	C3B-C4B-NB	-2.61	108.09	110.52
4	B	102	CLA	CHB-C4A-NA	2.58	128.08	124.51
4	B	103	CLA	C9-C8-C10	2.52	120.42	111.29
6	C	402	LMN	CCR-OBV-CCC	2.44	118.47	113.69
4	A	102	CLA	CHB-C4A-NA	2.44	127.88	124.51
4	B	103	CLA	CHB-C4A-NA	2.38	127.81	124.51
4	B	103	CLA	O2A-CGA-O1A	-2.38	117.59	123.59
4	B	103	CLA	CAA-C2A-C1A	-2.38	104.19	111.97
4	A	103	CLA	O2A-CGA-O1A	-2.37	117.61	123.59
4	A	103	CLA	CAA-C2A-C1A	-2.24	104.63	111.97
4	A	103	CLA	CHB-C4A-NA	2.22	127.58	124.51
5	D	401	A1JR2	C23-C14-C13	2.18	115.10	111.18
4	B	102	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
4	A	102	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
4	A	102	CLA	C9-C8-C10	2.11	118.95	111.29
6	D	402	LMN	CBT-OBV-CCJ	2.11	118.83	113.36
6	C	402	LMN	O1-C1-C2	2.10	111.59	108.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	103	CLA	C2A-C1A-CHA	2.09	127.52	123.86
4	B	102	CLA	C9-C8-C10	2.09	118.86	111.29
4	B	102	CLA	C9-C8-C7	2.08	118.83	111.29
4	A	102	CLA	C9-C8-C7	2.07	118.79	111.29
4	A	103	CLA	C9-C8-C7	2.06	118.76	111.29
4	B	102	CLA	CHD-C1D-ND	-2.04	122.58	124.45
7	D	403	MGE	C2G-O2G-C1B	2.04	122.81	117.79
4	B	103	CLA	C9-C8-C7	2.03	118.63	111.29
5	C	401	A1JR2	C23-C14-C13	2.02	114.82	111.18
6	C	402	LMN	CBT-OBV-CCJ	2.02	118.61	113.36

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	C	401	A1JR2	C14
5	C	401	A1JR2	C12
5	D	401	A1JR2	C14
5	D	401	A1JR2	C12

All (132) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	102	CLA	C2B-C3B-CAB-CBB
4	A	102	CLA	C4B-C3B-CAB-CBB
4	A	103	CLA	C1A-C2A-CAA-CBA
4	A	103	CLA	C11-C10-C8-C9
4	B	102	CLA	C2B-C3B-CAB-CBB
4	B	102	CLA	C4B-C3B-CAB-CBB
4	B	103	CLA	C1A-C2A-CAA-CBA
5	C	401	A1JR2	C14-C12-C21-C27
5	C	401	A1JR2	C28-C25-C26-O08
5	C	401	A1JR2	C28-C32-C35-C37
5	C	401	A1JR2	C28-C32-C35-C38
5	D	401	A1JR2	C09-C12-C21-C27
5	D	401	A1JR2	C28-C32-C35-C37
5	D	401	A1JR2	C28-C32-C35-C38
6	C	402	LMN	C2-C1-O1-CBS
6	C	402	LMN	O5-C1-O1-CBS
6	C	402	LMN	CBK-CBQ-CCM-CBR
6	C	402	LMN	CBK-CBQ-CCM-CBS
6	C	402	LMN	CCM-CBT-OBV-CCJ
6	C	402	LMN	OBV-CBT-CCM-CBQ

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Mol	Chain	Res	Type	Atoms
6	C	402	LMN	OBV-CBT-CCM-CBR
6	D	402	LMN	C2-C1-O1-CBS
6	D	402	LMN	O5-C1-O1-CBS
6	D	402	LMN	CBK-CBQ-CCM-CBR
6	D	402	LMN	CBK-CBQ-CCM-CBS
6	D	402	LMN	CBK-CBQ-CCM-CBT
6	D	402	LMN	OBX-CCJ-OBV-CBT
7	D	403	MGE	C2B-C1B-O2G-C2G
6	C	402	LMN	CCH-CCQ-OCB-CCS
6	C	402	LMN	OBY-CCR-O4-C4
6	D	402	LMN	C3-C4-O4-CCR
6	D	402	LMN	C4-C5-C6-O6
4	A	102	CLA	CBD-CGD-O2D-CED
7	C	403	MGE	O1A-C1A-O1G-C1G
7	D	403	MGE	O1A-C1A-O1G-C1G
6	C	402	LMN	C4-C5-C6-O6
7	C	403	MGE	C2A-C1A-O1G-C1G
7	D	403	MGE	C2A-C1A-O1G-C1G
6	D	402	LMN	CCH-CCQ-OCB-CCS
6	D	402	LMN	O5-C5-C6-O6
6	C	402	LMN	O5-C5-C6-O6
7	D	403	MGE	O1B-C1B-O2G-C2G
4	A	102	CLA	CBA-CGA-O2A-C1
4	A	103	CLA	CBA-CGA-O2A-C1
4	B	102	CLA	CBA-CGA-O2A-C1
4	B	103	CLA	CBA-CGA-O2A-C1
6	D	402	LMN	CCL-CCJ-OBV-CBT
4	A	103	CLA	O1A-CGA-O2A-C1
4	B	103	CLA	O1A-CGA-O2A-C1
4	B	102	CLA	C11-C10-C8-C9
4	B	103	CLA	C11-C10-C8-C9
4	A	102	CLA	O1A-CGA-O2A-C1
4	B	102	CLA	O1A-CGA-O2A-C1
4	A	102	CLA	C15-C16-C17-C18
4	A	102	CLA	O1D-CGD-O2D-CED
6	C	402	LMN	OBV-CBT-CCM-CBS
6	C	402	LMN	CBJ-CBL-CBR-CCM
4	B	102	CLA	C13-C15-C16-C17
6	D	402	LMN	CBA-CBC-CBE-CBG
7	D	403	MGE	C1G-C2G-O2G-C1B
6	C	402	LMN	CBH-CBJ-CBL-CBR
6	C	402	LMN	CBI-CBK-CBQ-CCM

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Mol	Chain	Res	Type	Atoms
4	A	102	CLA	C11-C10-C8-C9
4	B	103	CLA	C8-C10-C11-C12
6	C	402	LMN	CAY-CBA-CBC-CBE
6	D	402	LMN	CBC-CBE-CBG-CBI
7	C	403	MGE	C5A-C6A-C7A-C8A
4	A	103	CLA	C3A-C2A-CAA-CBA
4	B	102	CLA	C15-C16-C17-C18
6	C	402	LMN	C5-C4-O4-CCR
7	D	403	MGE	C4A-C5A-C6A-C7A
4	A	103	CLA	C15-C16-C17-C18
5	C	401	A1JR2	O03-C25-C26-C30
6	C	402	LMN	OAJ-CBN-CCD-OBZ
6	C	402	LMN	OAI-CBM-CCC-OBY
7	C	403	MGE	O6D-C5D-C6D-O5D
6	D	402	LMN	OAI-CBM-CCC-OBY
7	C	403	MGE	C1B-C2B-C3B-C4B
6	C	402	LMN	CBK-CBQ-CCM-CBT
7	D	403	MGE	C1G-C2G-C3G-O3G
6	C	402	LMN	C3-C4-O4-CCR
7	D	403	MGE	C2A-C3A-C4A-C5A
4	A	102	CLA	C13-C15-C16-C17
6	C	402	LMN	OAL-CBP-CCF-OBX
4	B	103	CLA	C12-C13-C15-C16
4	A	103	CLA	C8-C10-C11-C12
4	A	103	CLA	C4-C3-C5-C6
4	A	103	CLA	C2-C3-C5-C6
4	B	103	CLA	C3A-C2A-CAA-CBA
4	B	103	CLA	C5-C6-C7-C8
7	D	403	MGE	C3B-C4B-C5B-C6B
6	D	402	LMN	CBG-CBI-CBK-CBQ
5	D	401	A1JR2	C14-C12-C21-C27
6	D	402	LMN	CCF-CCQ-OCB-CCS
4	A	102	CLA	C6-C7-C8-C10
4	B	102	CLA	C6-C7-C8-C10
7	C	403	MGE	C3B-C4B-C5B-C6B
4	A	102	CLA	C5-C6-C7-C8
4	A	102	CLA	CAD-CBD-CGD-O2D
7	C	403	MGE	O6D-C1D-O3G-C3G
7	D	403	MGE	O2G-C2G-C3G-O3G
5	C	401	A1JR2	O03-C25-C28-C32
5	C	401	A1JR2	C26-C25-C28-C32
4	B	103	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
4	B	103	CLA	C14-C13-C15-C16
6	D	402	LMN	CBB-CBD-CBF-CBH
4	A	103	CLA	CAA-CBA-CGA-O2A
4	B	103	CLA	CAA-CBA-CGA-O2A
7	D	403	MGE	C2D-C1D-O3G-C3G
4	B	103	CLA	C4-C3-C5-C6
4	B	102	CLA	C3-C5-C6-C7
4	B	102	CLA	C5-C6-C7-C8
7	D	403	MGE	O6D-C1D-O3G-C3G
4	A	102	CLA	C2-C1-O2A-CGA
4	B	103	CLA	C2-C1-O2A-CGA
4	A	103	CLA	C5-C6-C7-C8
6	C	402	LMN	CBE-CBG-CBI-CBK
6	C	402	LMN	CBF-CBH-CBJ-CBL
4	B	103	CLA	C2-C3-C5-C6
6	D	402	LMN	CBD-CBF-CBH-CBJ
4	A	103	CLA	C2-C1-O2A-CGA
6	D	402	LMN	CBL-CBR-CCM-CBT
4	B	103	CLA	CAD-CBD-CGD-O2D
5	D	401	A1JR2	C28-C25-C26-O08
7	C	403	MGE	C9B-CAB-CBB-CCB
4	B	103	CLA	C10-C11-C12-C13
4	A	103	CLA	C6-C7-C8-C10
5	D	401	A1JR2	O03-C25-C26-C30
4	A	102	CLA	C11-C12-C13-C15
4	A	103	CLA	C12-C13-C15-C16
4	A	102	CLA	C3-C5-C6-C7
5	C	401	A1JR2	C21-C27-C31-C34

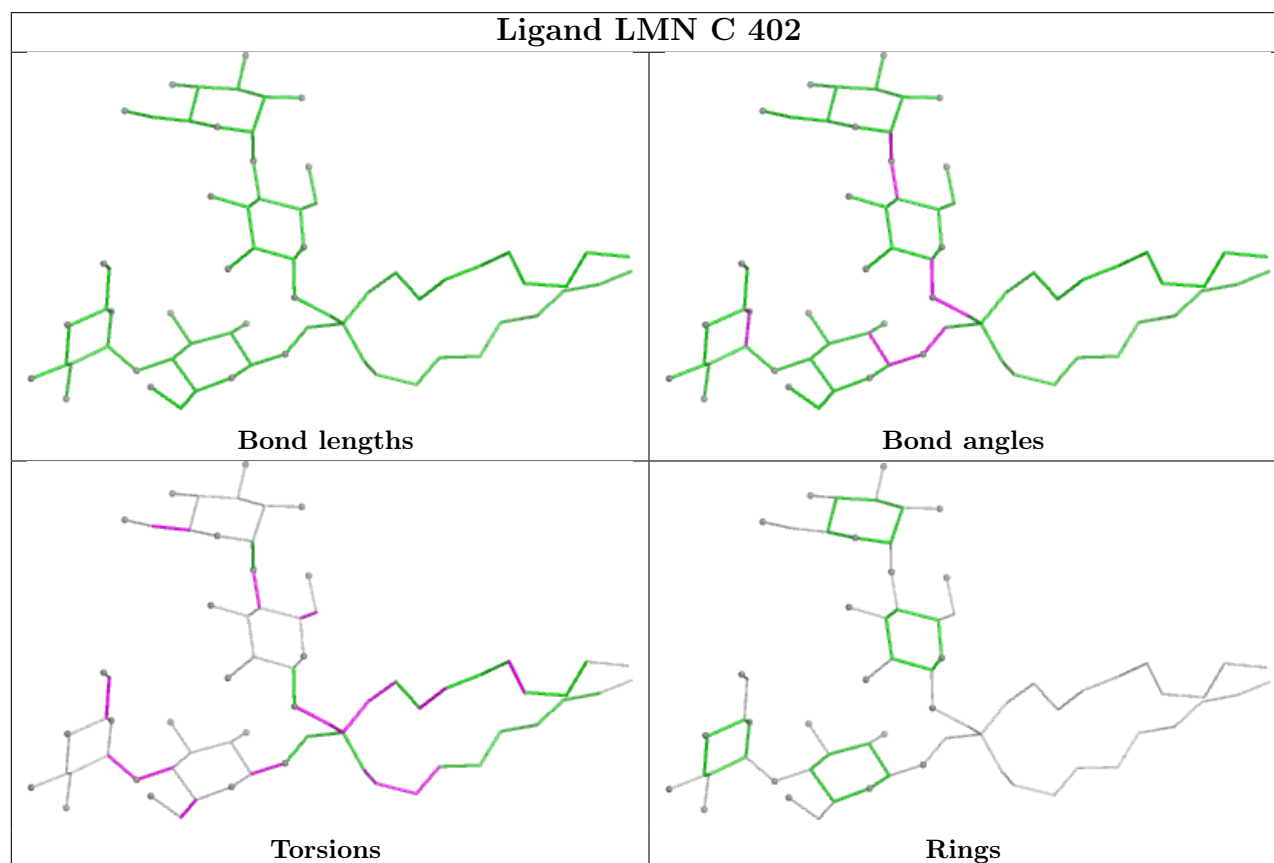
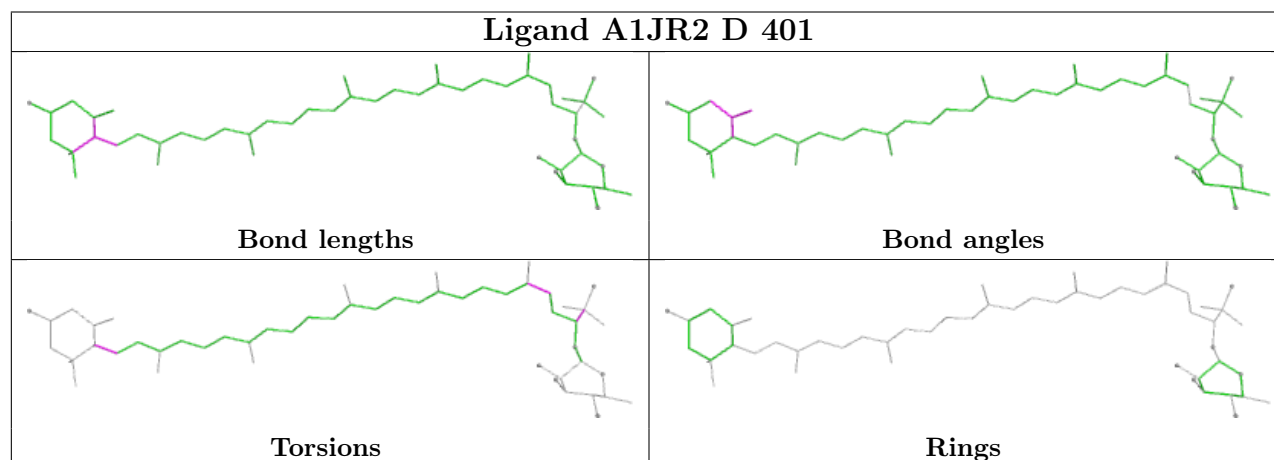
There are no ring outliers.

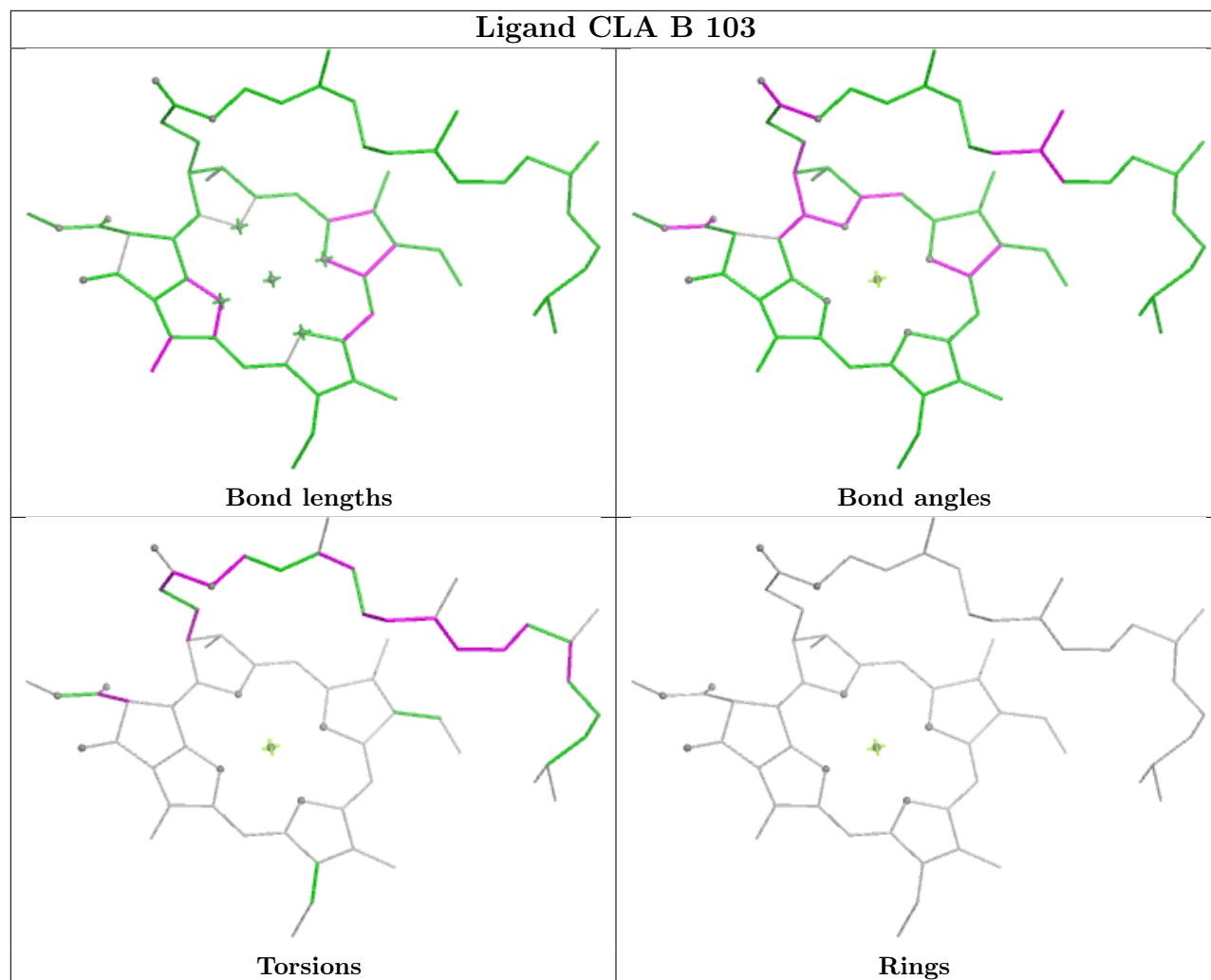
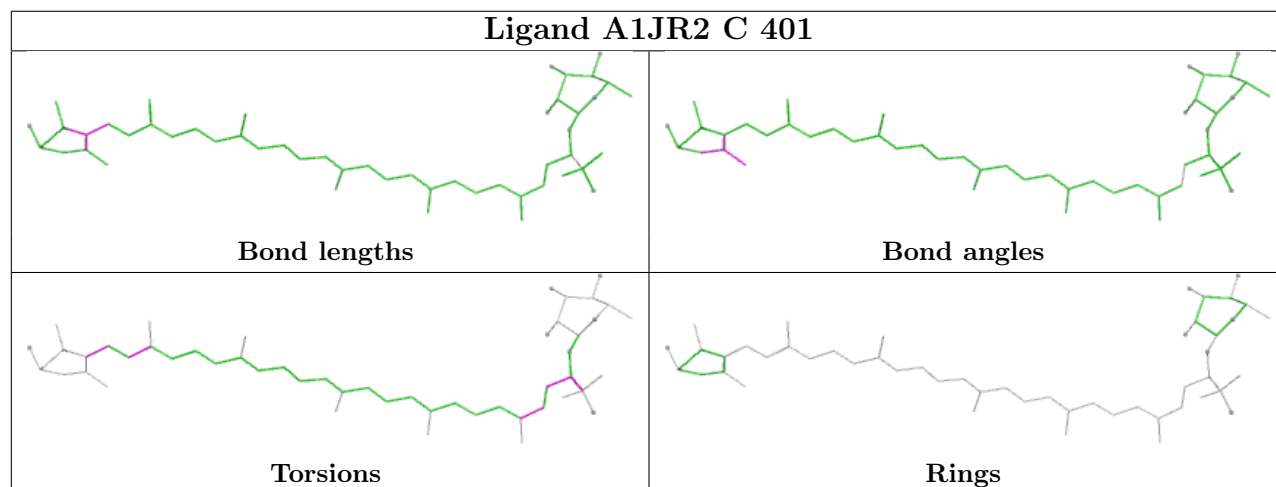
4 monomers are involved in 5 short contacts:

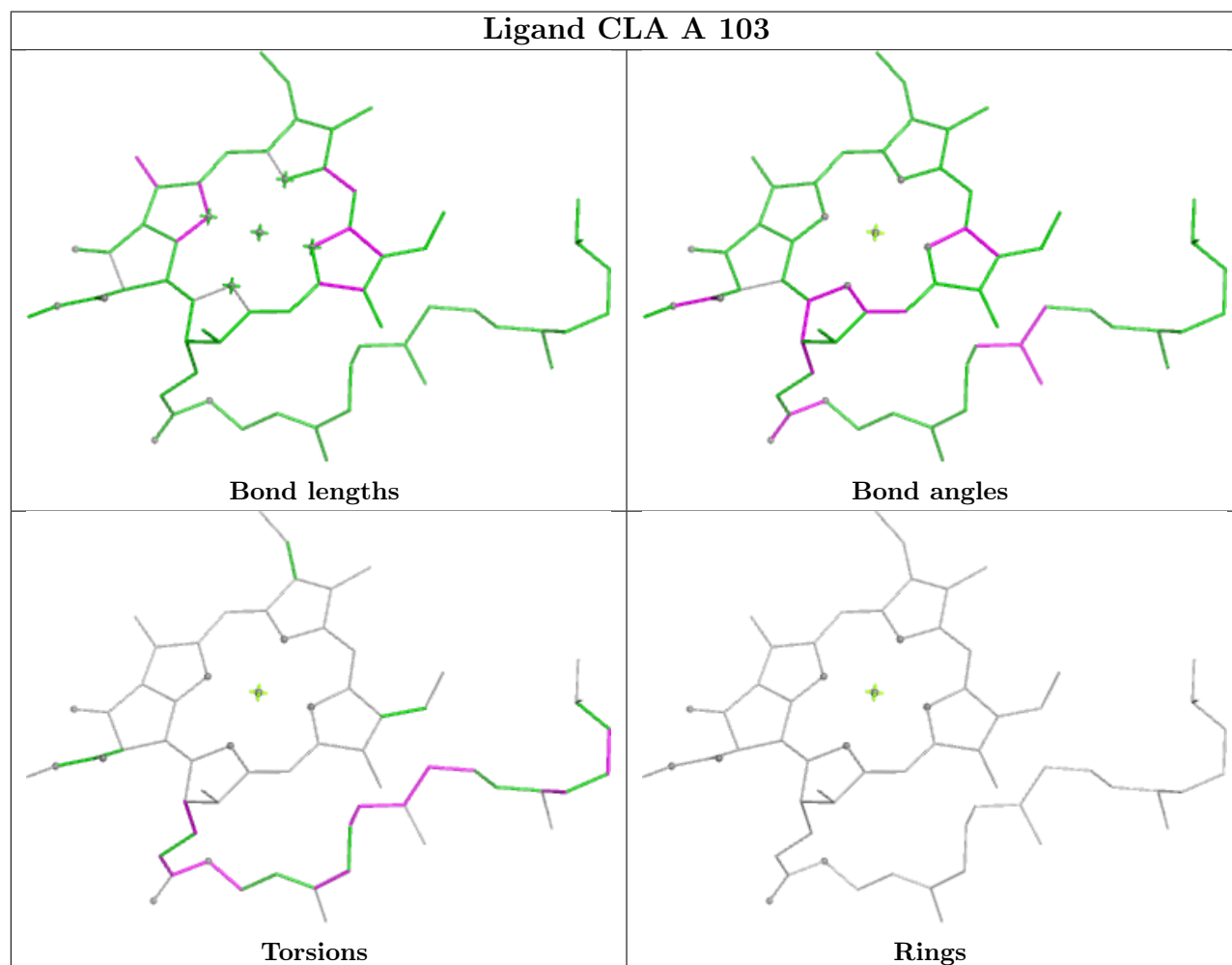
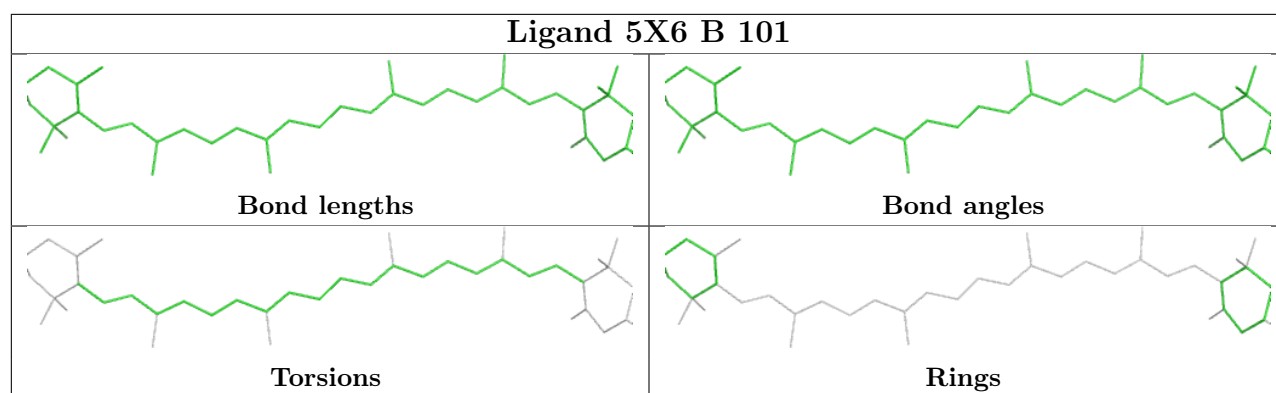
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	402	LMN	2	0
4	A	103	CLA	1	0
4	A	102	CLA	1	0
4	B	102	CLA	1	0

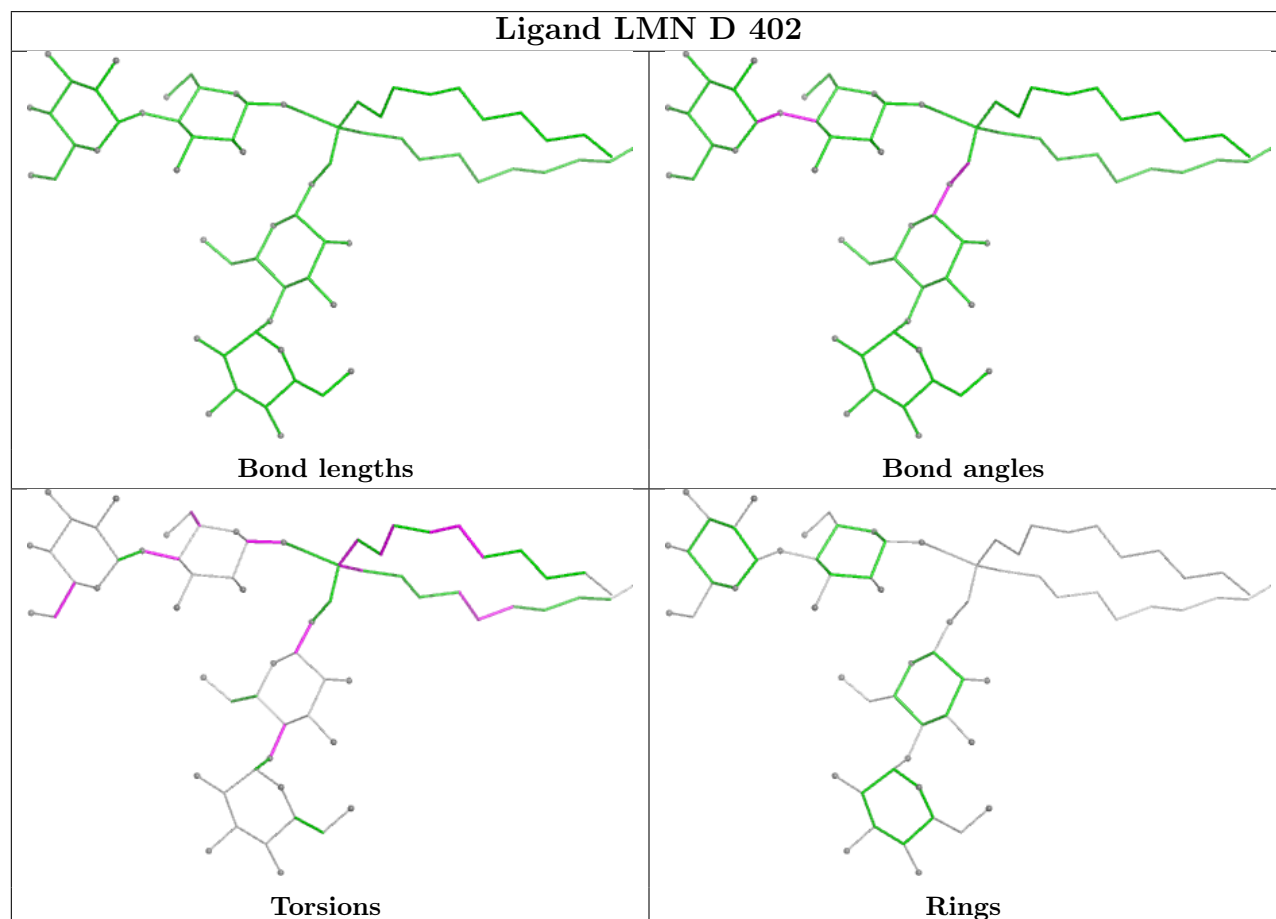
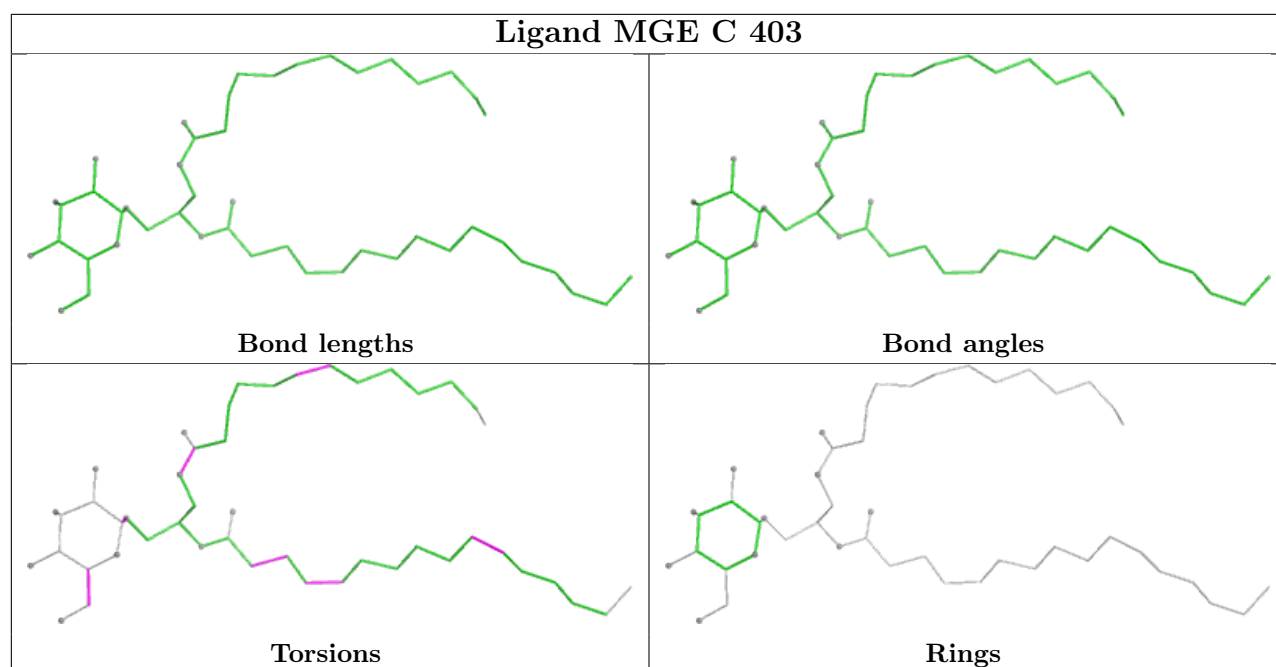
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

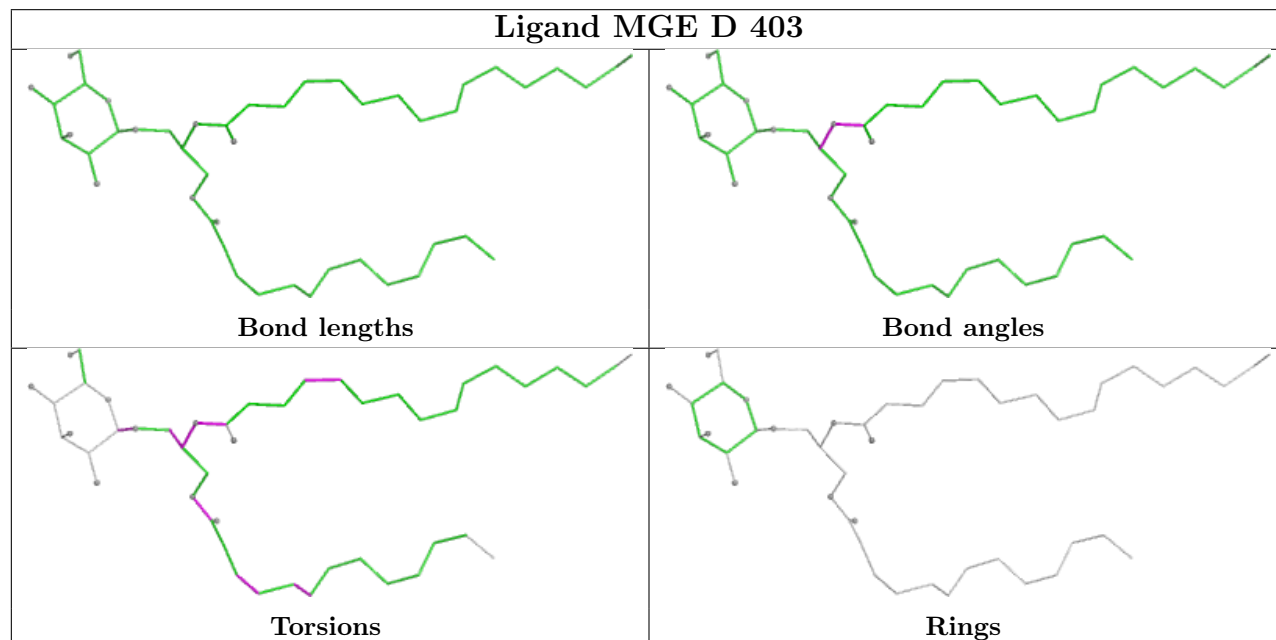
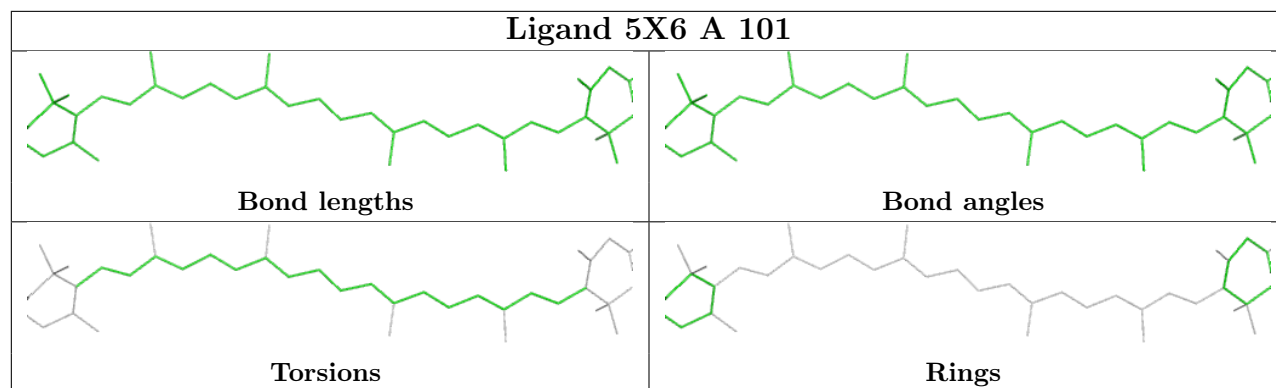
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

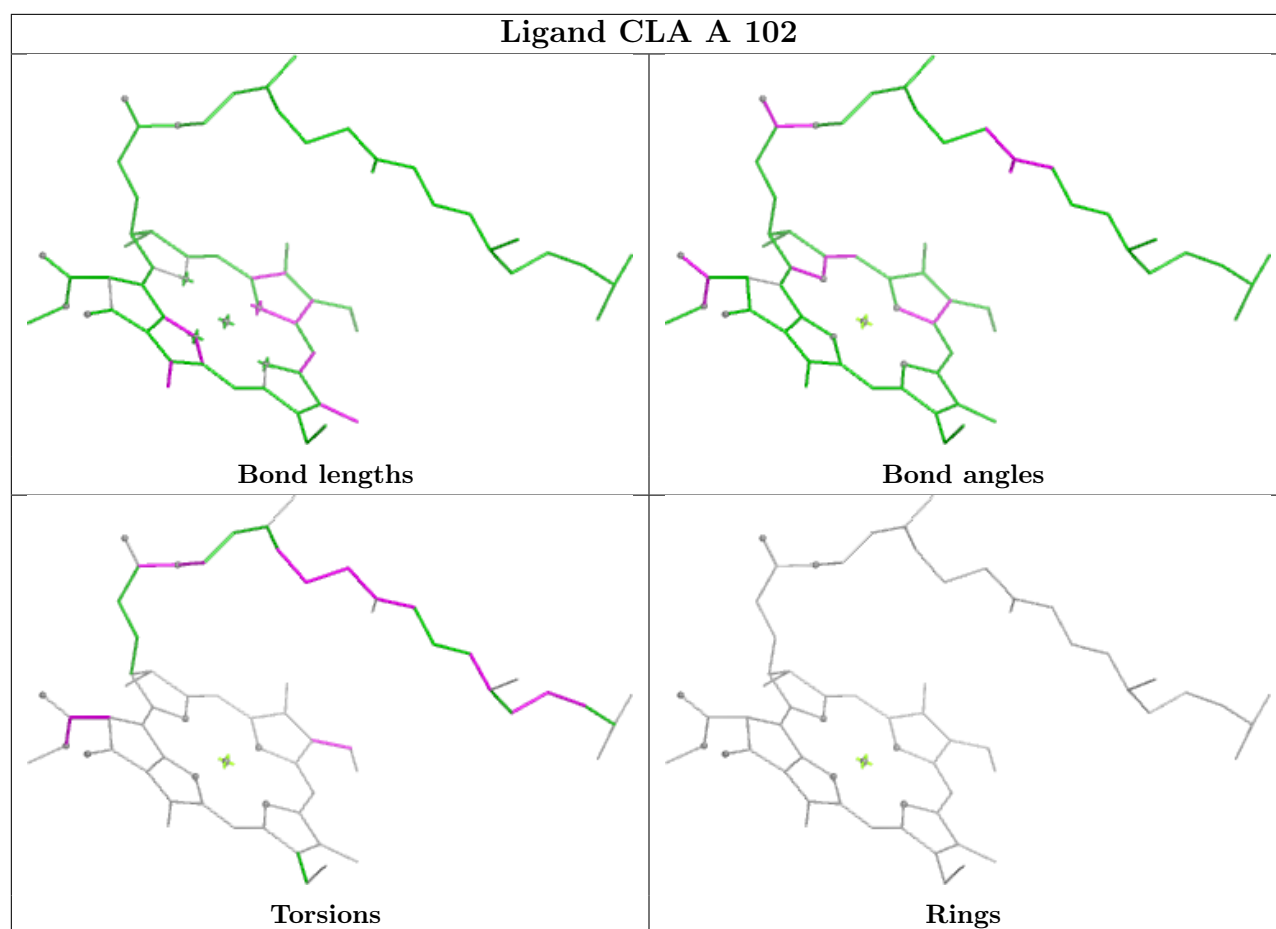


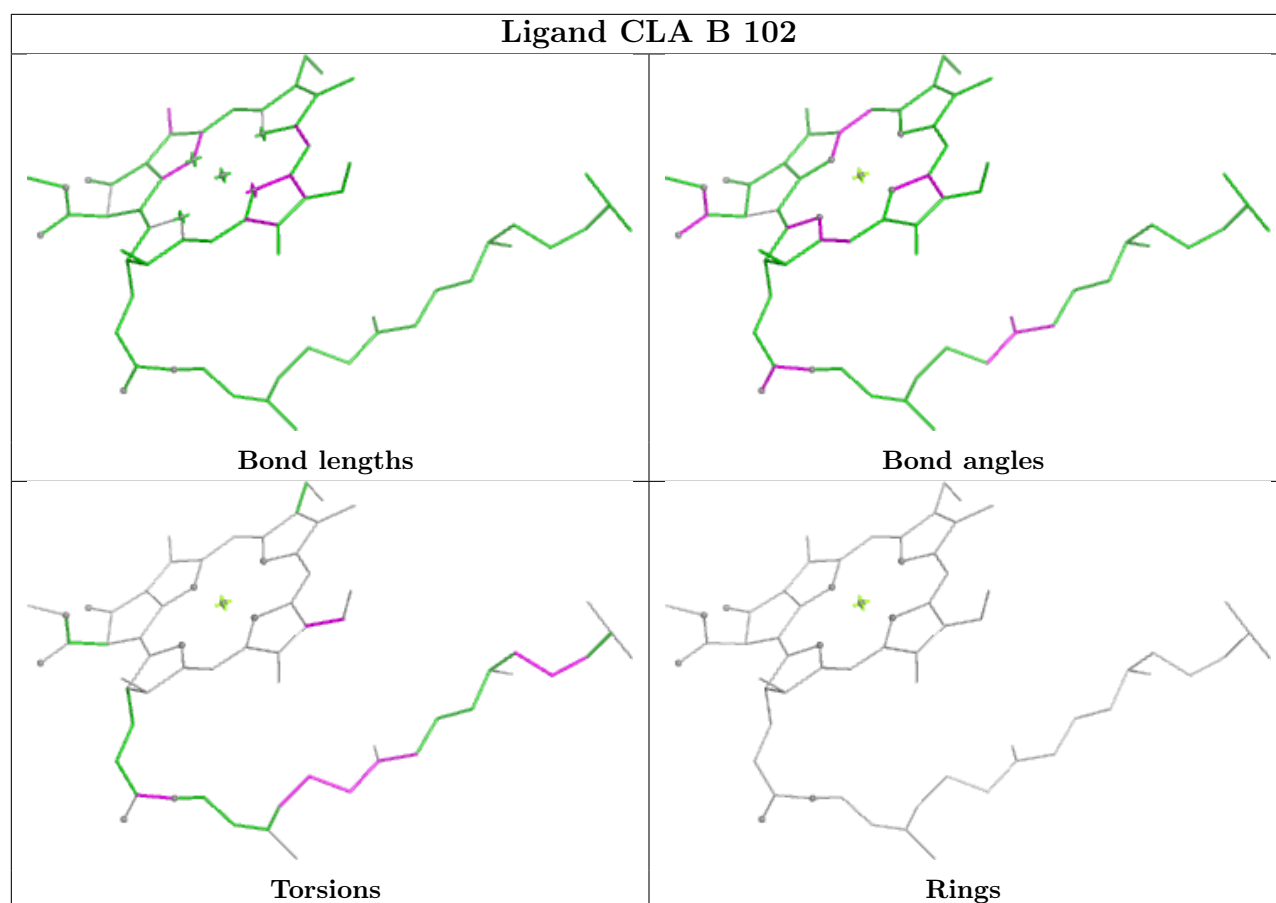
Ligand CLA B 103**Ligand A1JR2 C 401**











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-54696. These allow visual inspection of the internal detail of the map and identification of artifacts.

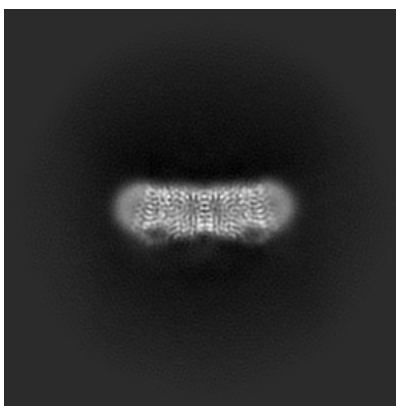
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

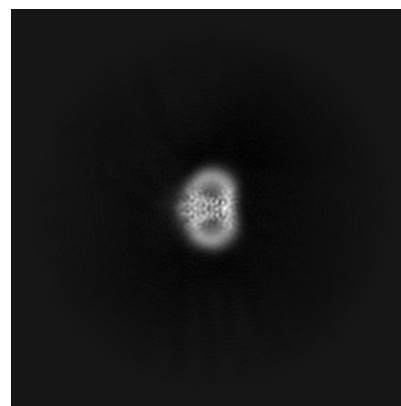
6.1.1 Primary map



X

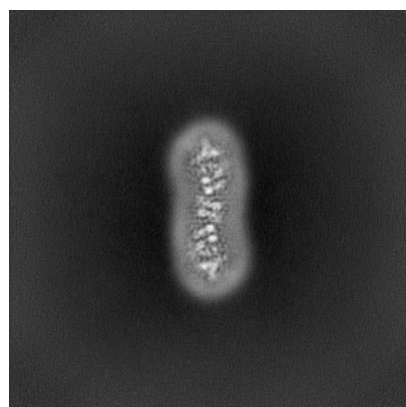


Y

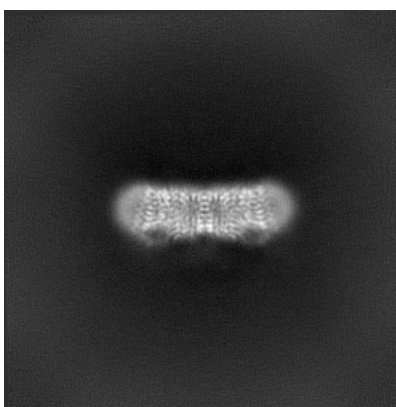


Z

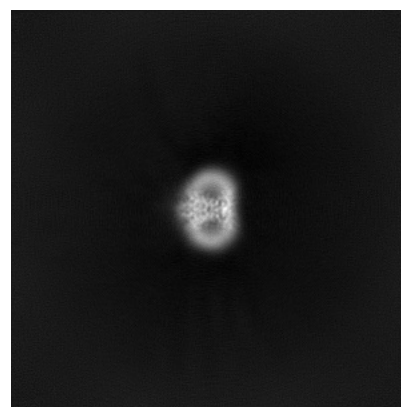
6.1.2 Raw map



X



Y

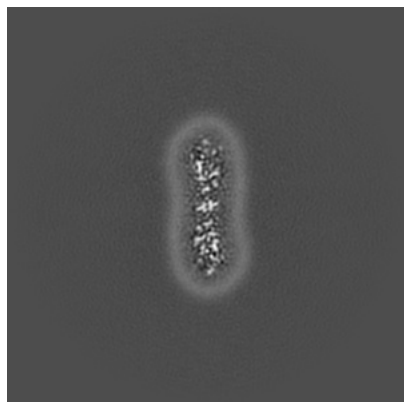


Z

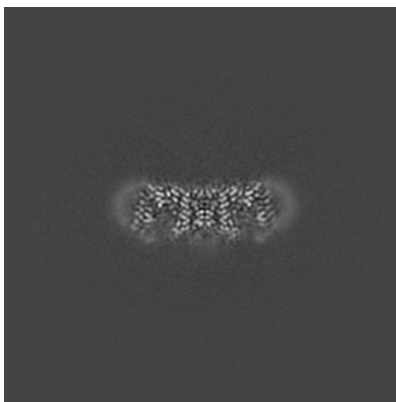
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

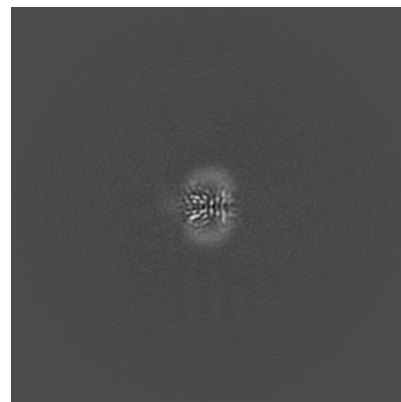
6.2.1 Primary map



X Index: 256

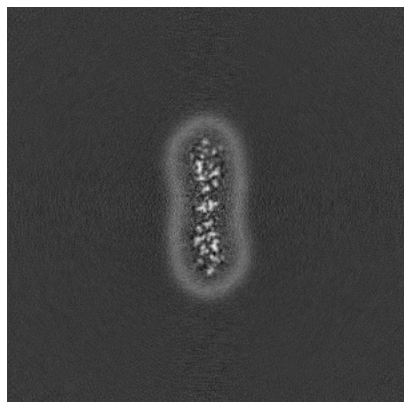


Y Index: 256

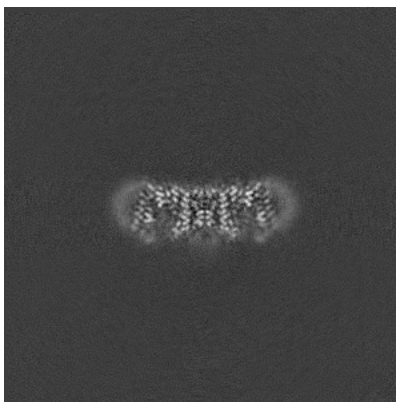


Z Index: 256

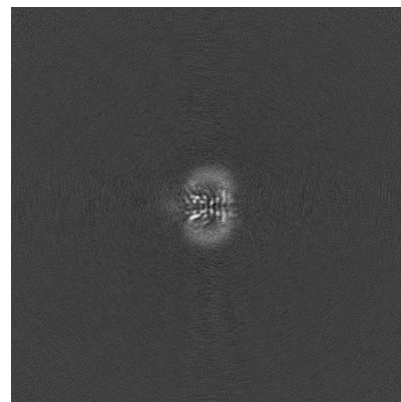
6.2.2 Raw map



X Index: 256



Y Index: 256

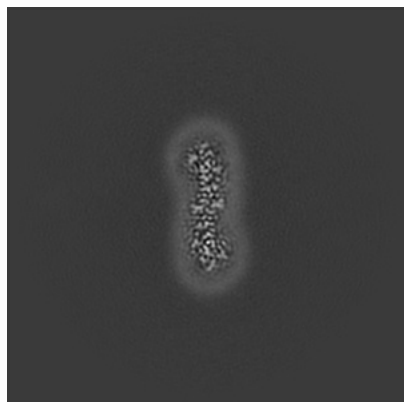


Z Index: 256

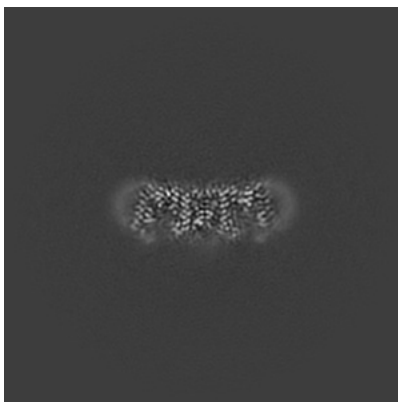
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

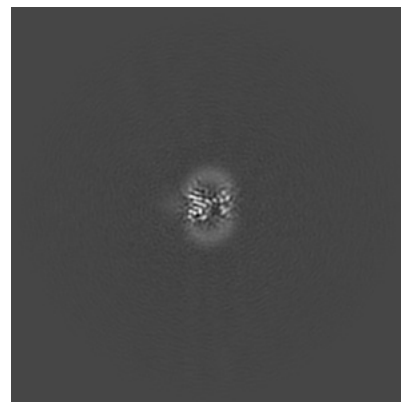
6.3.1 Primary map



X Index: 272

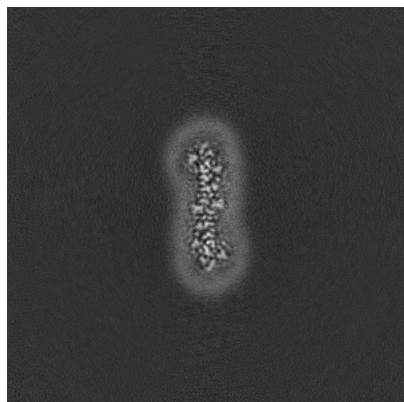


Y Index: 257

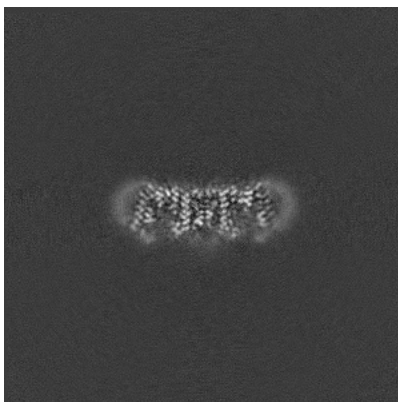


Z Index: 264

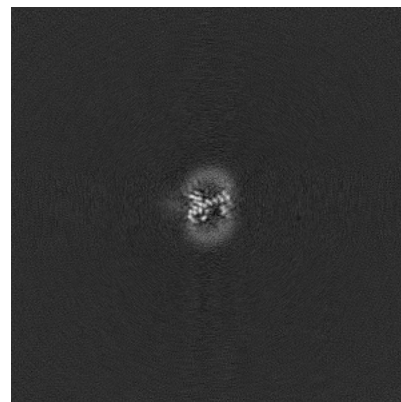
6.3.2 Raw map



X Index: 272



Y Index: 257

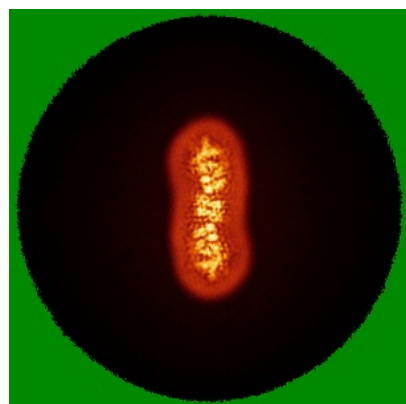


Z Index: 263

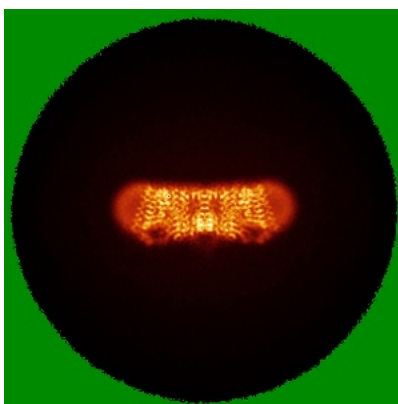
The images above show the largest variance slices of the map in three orthogonal directions.

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

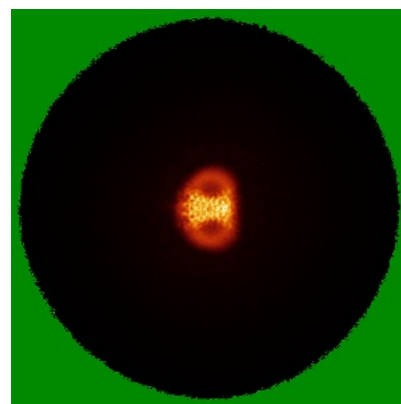
6.4.1 Primary map



X

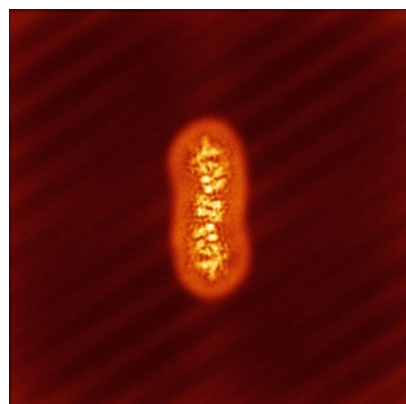


Y

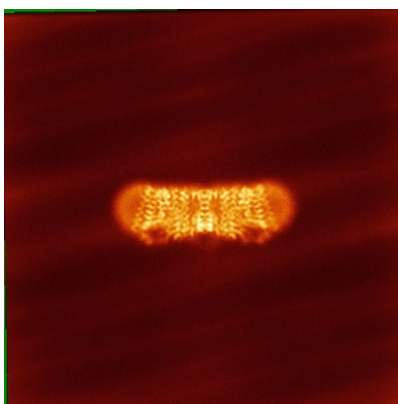


Z

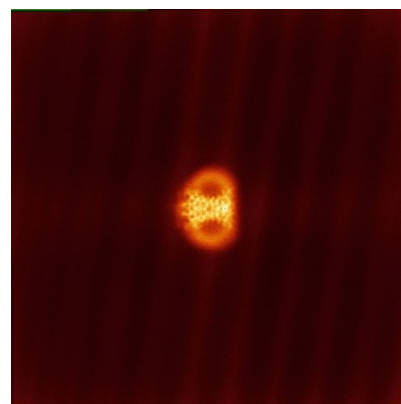
6.4.2 Raw map



X



Y

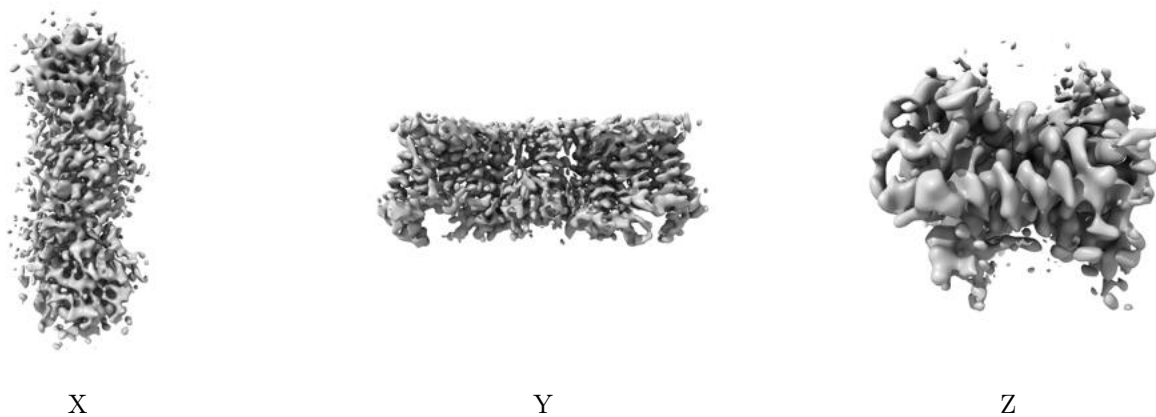


Z

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.

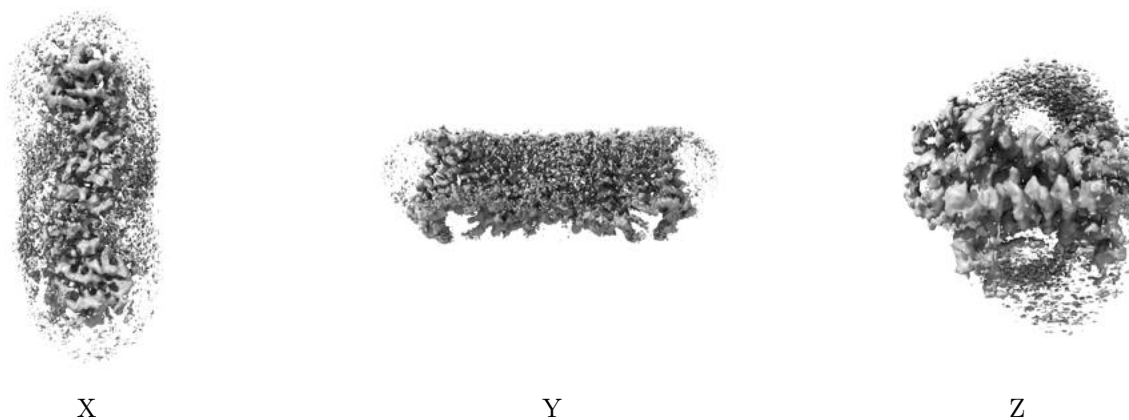
6.5 Orthogonal surface views [i](#)

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.

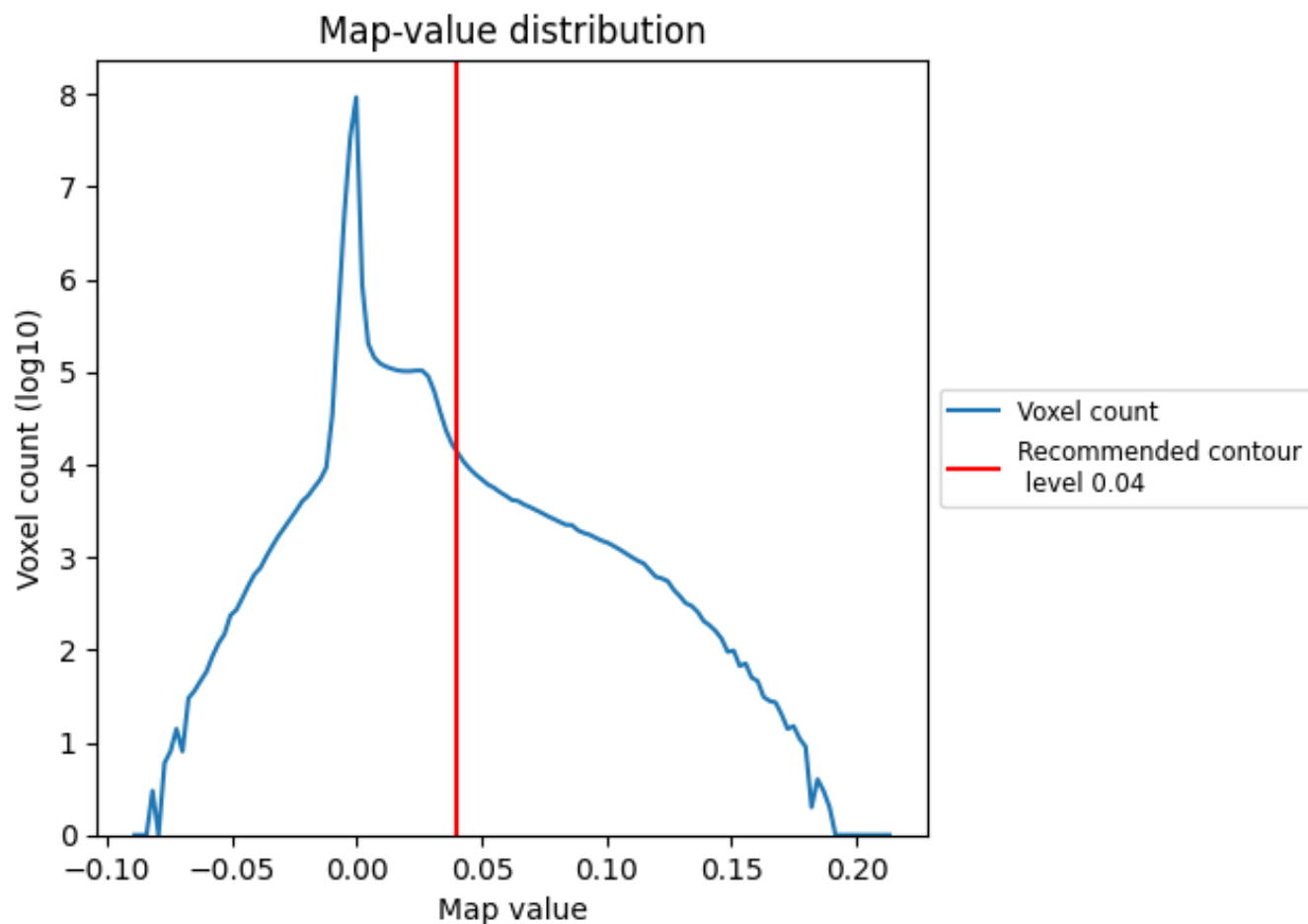
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

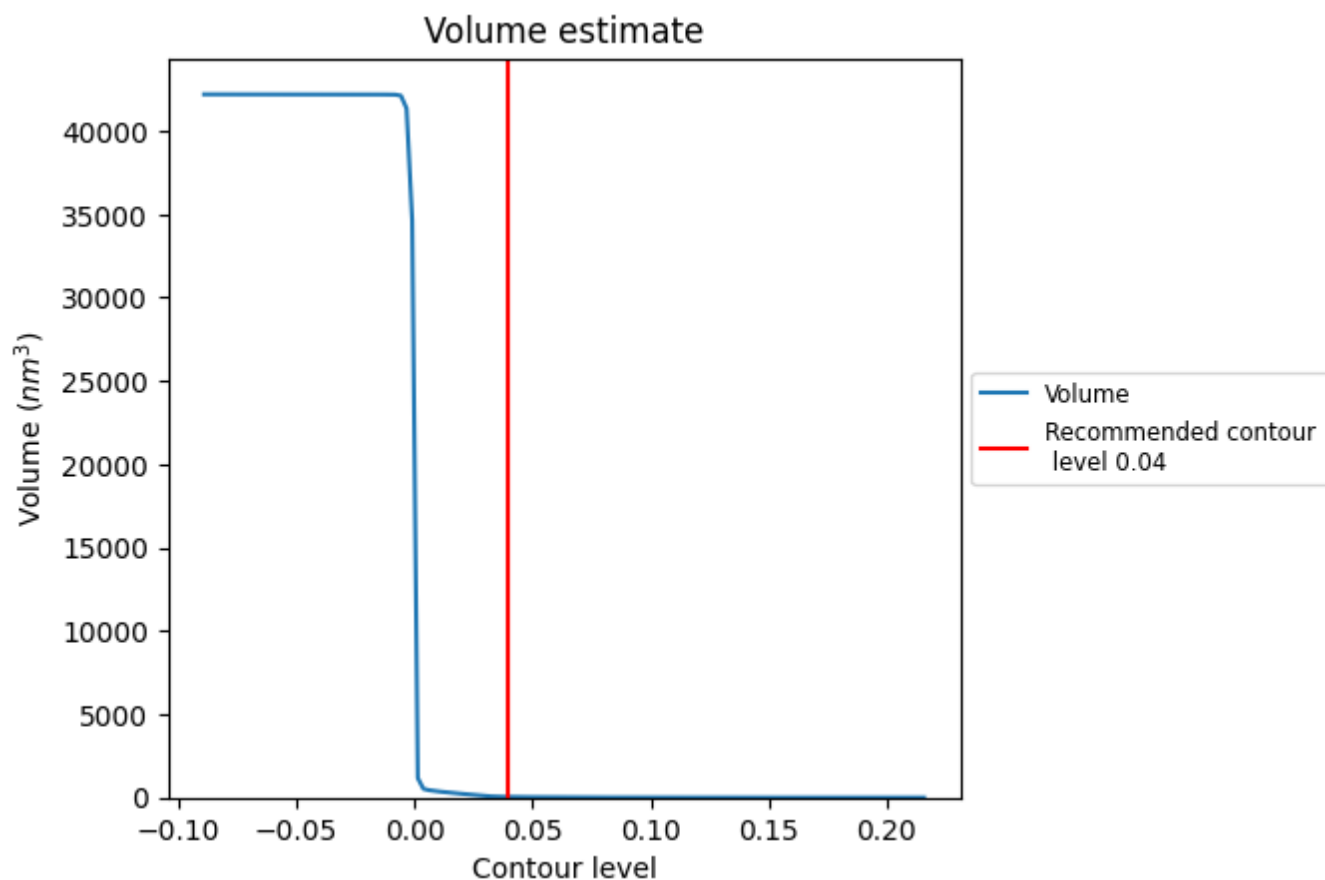
This section contains the results of statistical analysis of the map.

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.

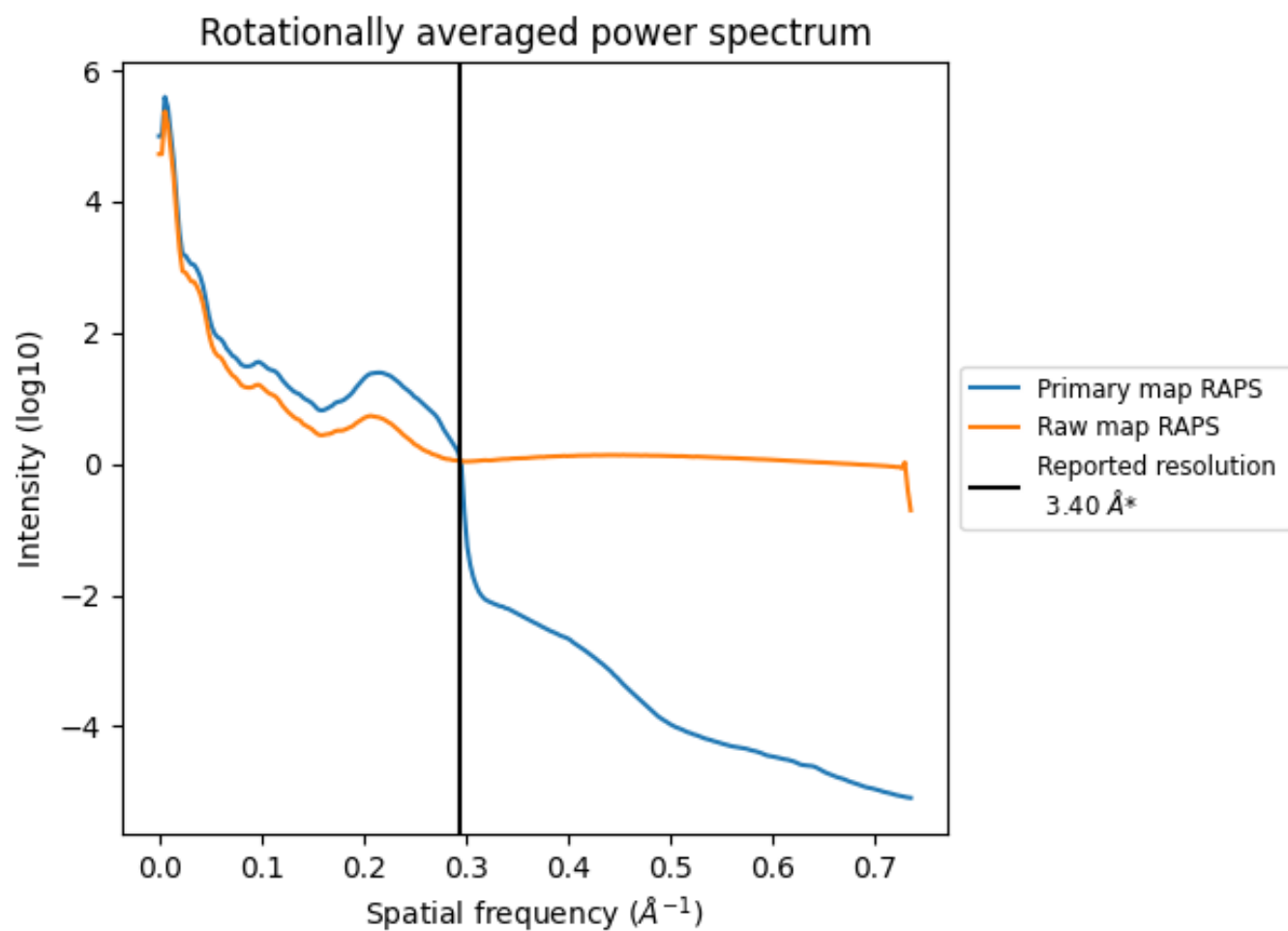
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 40 nm^3 ; this corresponds to an approximate mass of 36 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 ⓘ

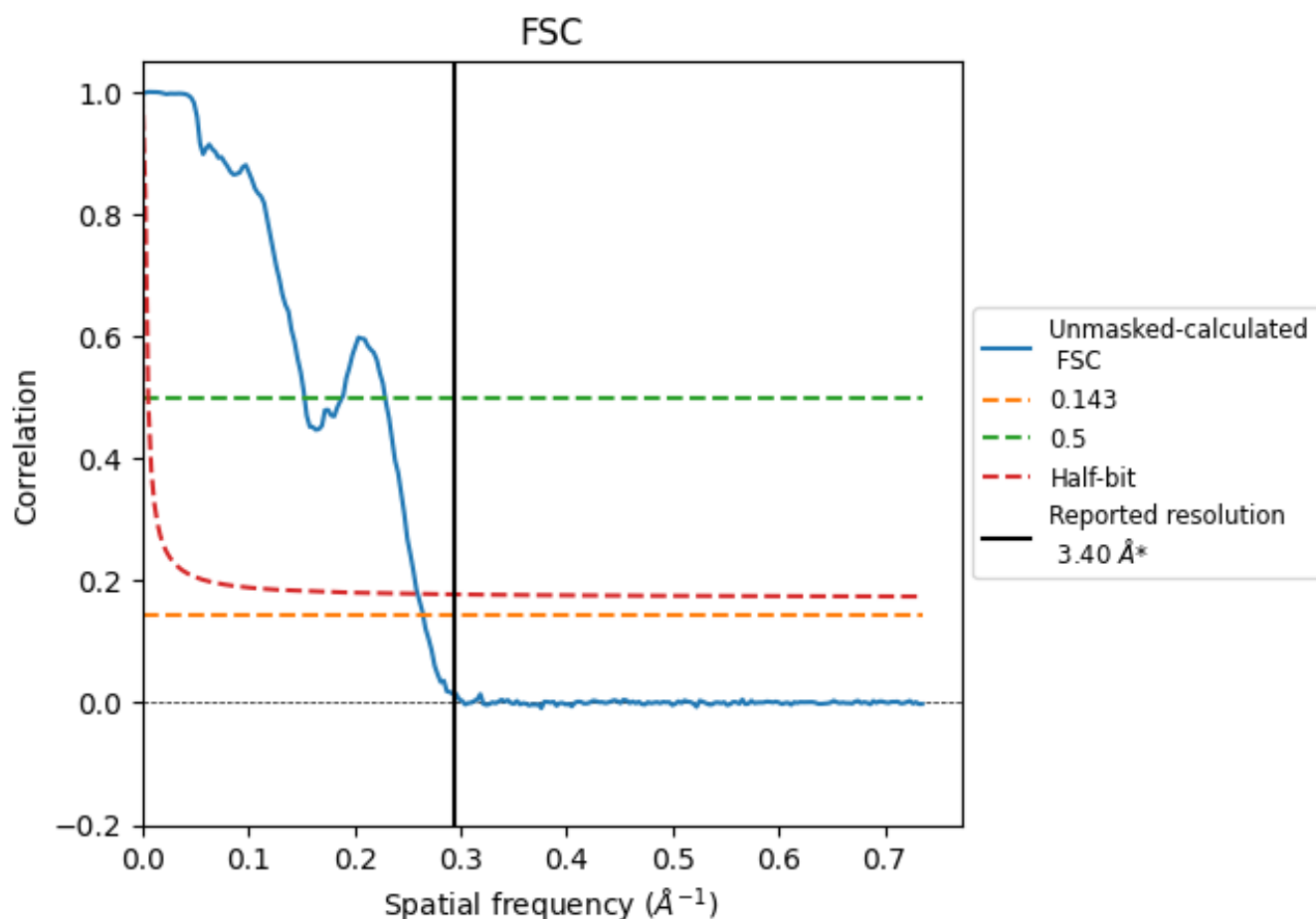


*Reported resolution corresponds to spatial frequency of 0.294 $\text{\AA}^{-1}$

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 $0.294 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

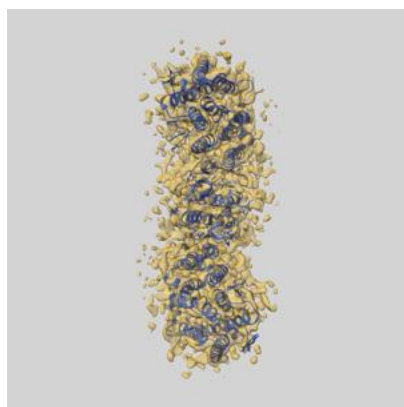
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.78	6.54	3.85

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.78 differs from the reported value 3.4 by more than 10 %

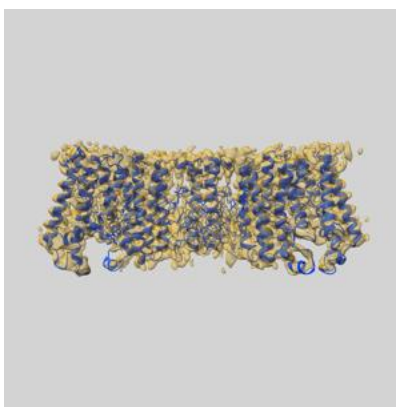
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-54696 and PDB model 9SAS. Per-residue inclusion information can be found in section [3](#) on page [8](#).

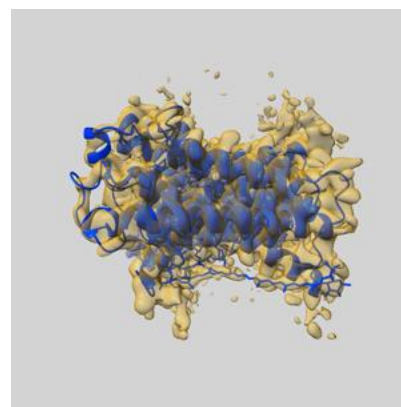
9.1 Map-model overlay [i](#)



X



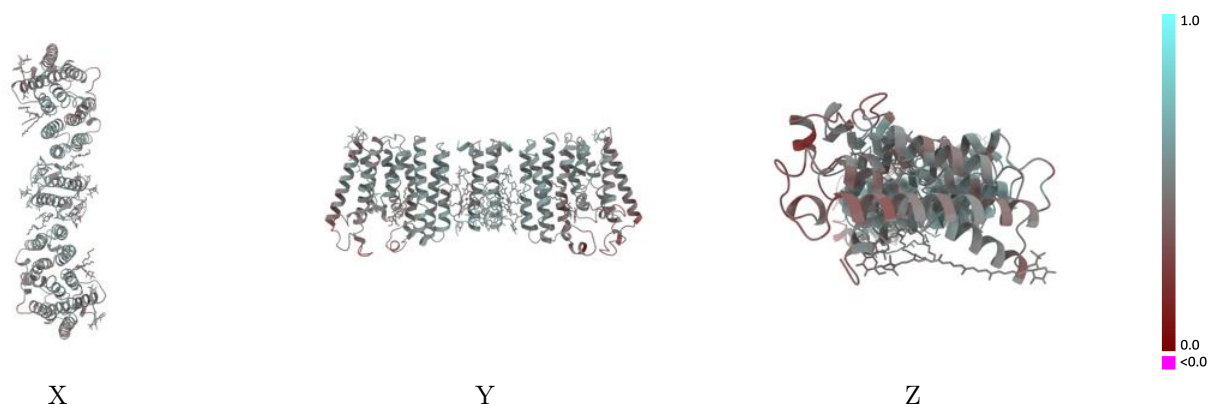
Y



Z

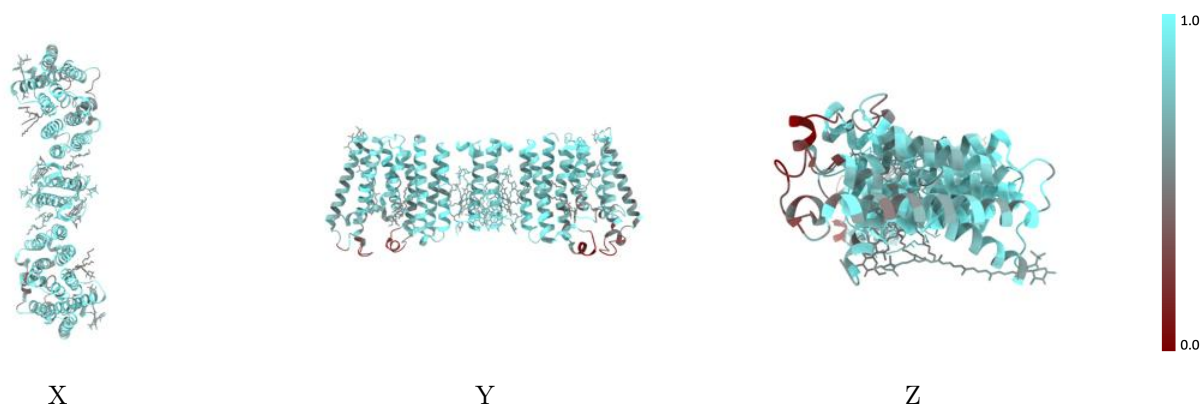
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



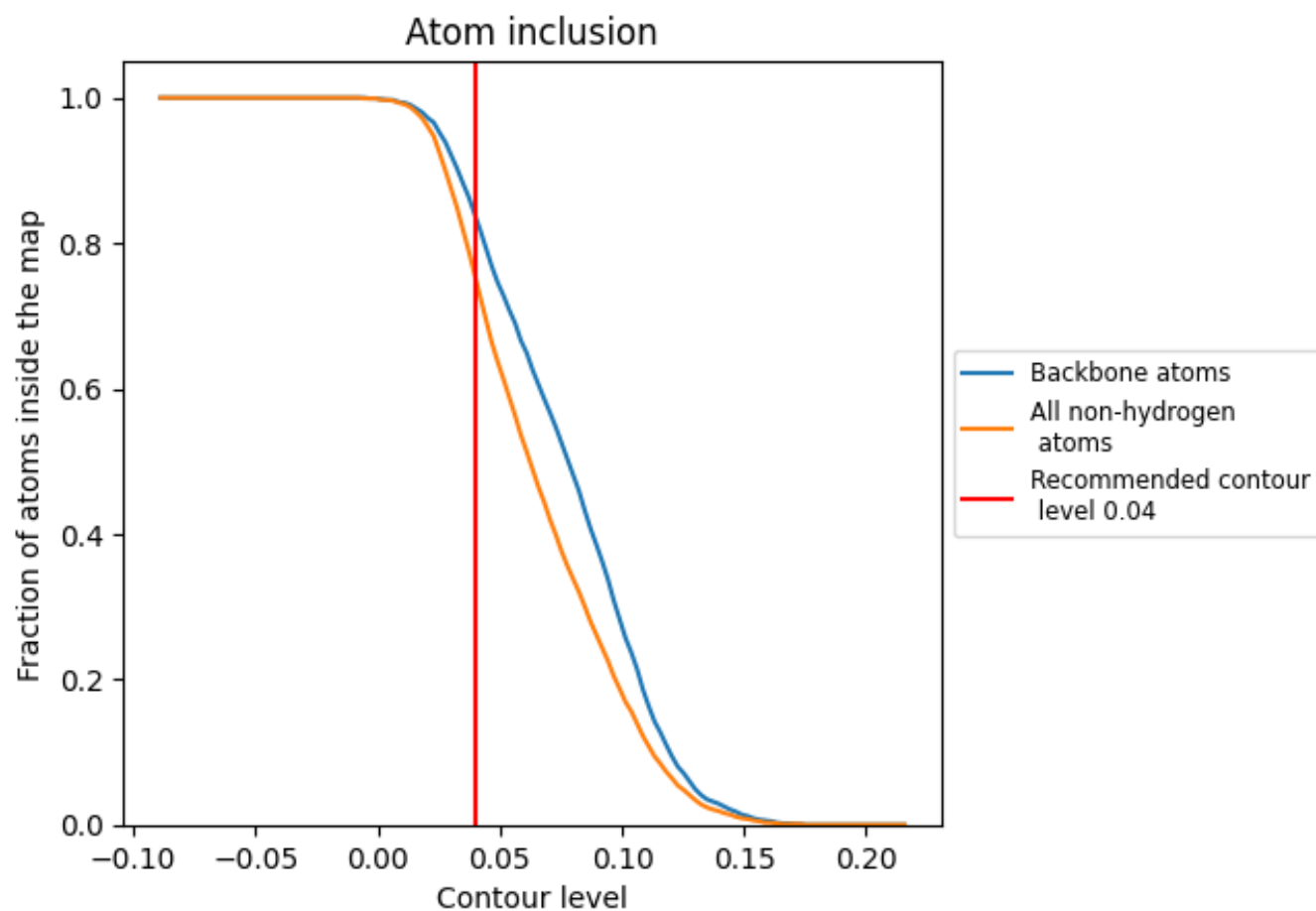
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 84% of all backbone atoms, 75% 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	0.7520	0.4850
A	0.8210	0.5260
B	0.8150	0.5310
C	0.7480	0.4800
D	0.7290	0.4730

