



Full wwPDB EM Validation Report ⓘ

Dec 17, 2022 – 02:47 pm GMT

PDB ID : 6ZBB
EMDB ID : EMD-11149
Title : bovine ATP synthase Fo domain
Authors : Spikes, T.; Montgomery, M.G.; Walker, J.E.
Deposited on : 2020-06-08
Resolution : 3.61 Å(reported)
Based on initial models : 5ARA, 2XND

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 : 1.8.4, 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) : 2.31.3

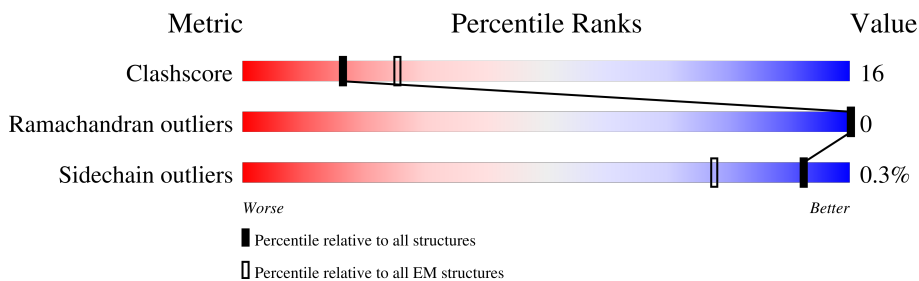
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.61 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	8	66	6% (red), 47% (green), 15% (yellow), 38% (grey)
2	K	75	33% (red), 75% (green), 24% (yellow), . (grey)
2	L	75	45% (red), 61% (green), 37% (yellow), . (grey)
2	M	75	31% (red), 64% (green), 36% (yellow)
2	N	75	20% (red), 65% (green), 35% (yellow)
2	O	75	35% (red), 69% (green), 31% (yellow)
2	P	75	37% (red), 72% (green), 27% (yellow), . (grey)
2	Q	75	25% (red), 64% (green), 36% (yellow)

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Mol	Chain	Length	Quality of chain
2	R	75	
3	a	226	
4	b	214	
5	d	160	
6	e	70	
7	f	87	
8	g	102	
9	j	60	
10	k	57	

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 21505 atoms, of which 11015 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 ATP synthase protein 8.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	8	41	696	231	352	52	58	3	0	0

- Molecule 2 is a protein called ATP synthase F(0) complex subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	K	74	1079	351	550	82	93	3	0	0
2	L	74	1078	351	549	82	93	3	0	0
2	M	75	1095	356	558	83	94	4	0	0
2	N	75	1095	356	558	83	94	4	0	0
2	O	75	1095	356	558	83	94	4	0	0
2	P	74	1079	351	550	82	93	3	0	0
2	Q	75	1095	356	558	83	94	4	0	0
2	R	75	1095	356	558	83	94	4	0	0

- Molecule 3 is a protein called ATP synthase subunit a.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	a	224	3557	1146	1832	273	295	11	0	0

- Molecule 4 is a protein called ATP synthase F(0) complex subunit B1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
4	b	112	1791	584	910	134	162	1	0	0

- Molecule 5 is a protein called ATP synthase subunit d, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
5	d	51	893	290	444	73	84	2	0	0

- Molecule 6 is a protein called ATP synthase subunit e, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
6	e	57	975	301	500	91	82	1	0	0

- Molecule 7 is a protein called ATP synthase subunit f, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
7	f	83	1411	456	718	120	114	3	0	0

- Molecule 8 is a protein called ATP synthase subunit g, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
8	g	79	1291	420	662	100	108	1	0	0

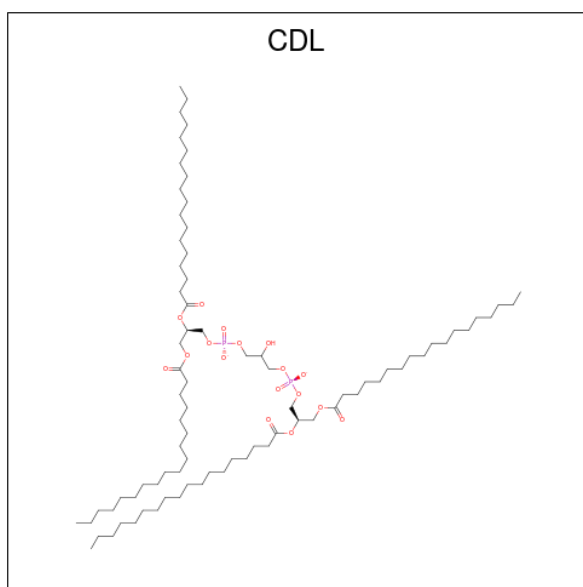
- Molecule 9 is a protein called ATP synthase subunit ATP5MPL, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
9	j	48	828	267	428	66	65	2	0	0

- Molecule 10 is a protein called ATP synthase membrane subunit DAPIT, mitochondrial.

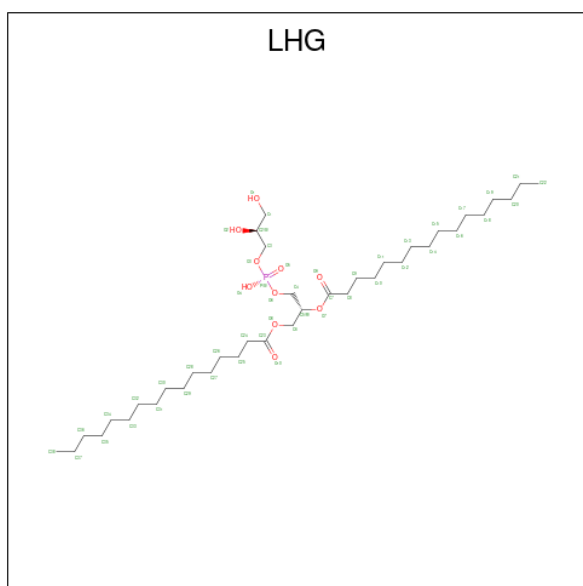
Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
10	k	36	596	192	307	47	48	2	0	0

- Molecule 11 is CARDIOLIPIN (three-letter code: CDL) (formula: C₈₁H₁₅₆O₁₇P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	O	P	
11	a	1	Total	C	H	O	P	0
			185	65	101	17	2	
11	b	1	Total	C	H	O	P	0
			361	123	200	34	4	
11	b	1	Total	C	H	O	P	0
			361	123	200	34	4	

- Molecule 12 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).

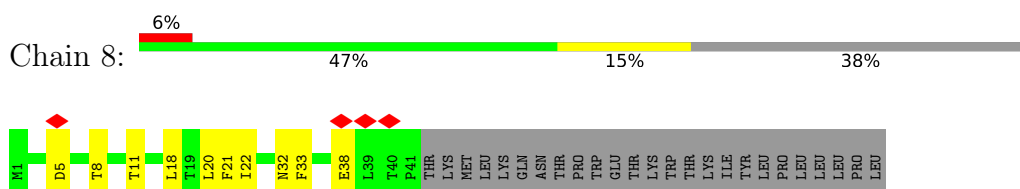


Mol	Chain	Residues	Atoms					AltConf
12	f	1	Total	C	H	O	P	0
			210	66	122	20	2	
12	f	1	Total	C	H	O	P	0
			210	66	122	20	2	

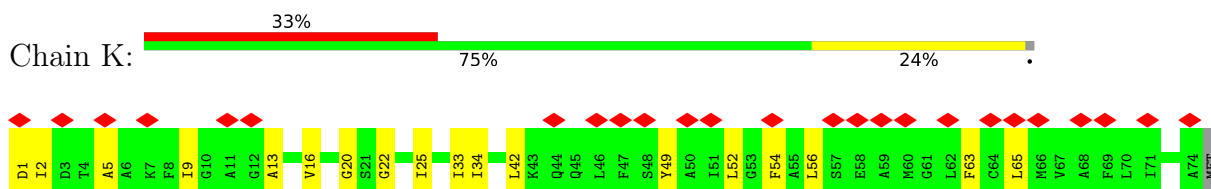
3 Residue-property plots [i](#)

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

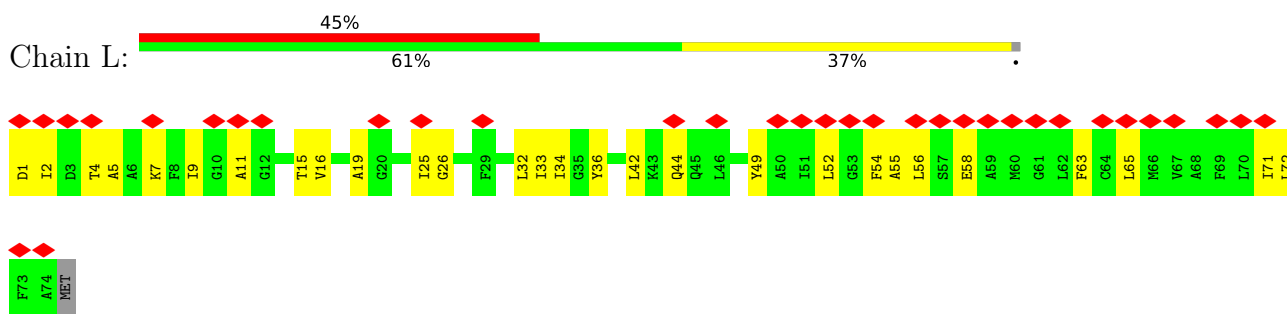
- Molecule 1: ATP synthase protein 8



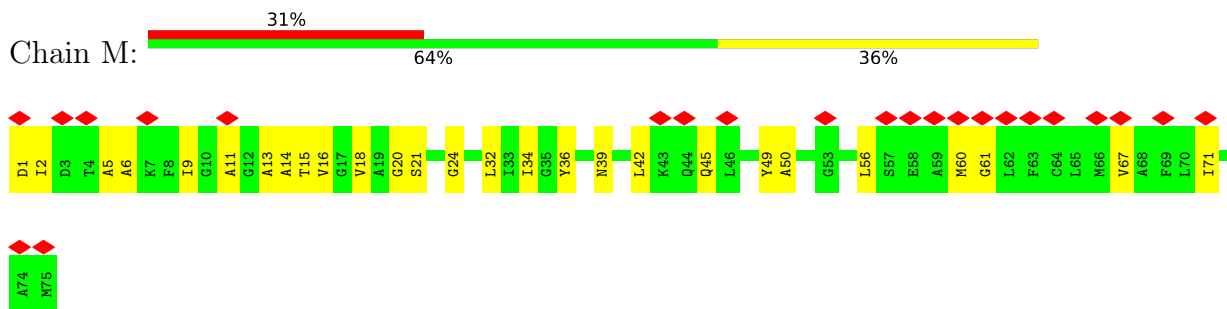
- Molecule 2: ATP synthase F(0) complex subunit C1, mitochondrial



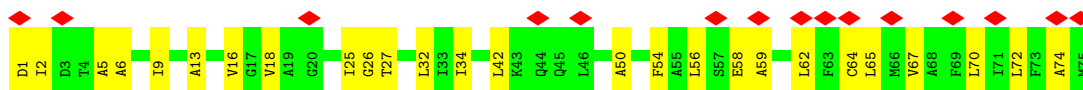
- Molecule 2: ATP synthase F(0) complex subunit C1, mitochondrial



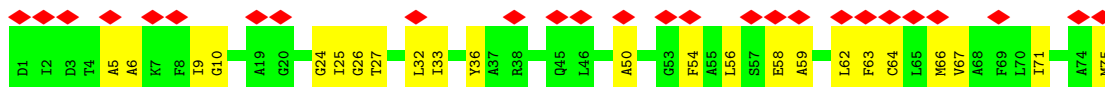
- Molecule 2: ATP synthase F(0) complex subunit C1, mitochondrial



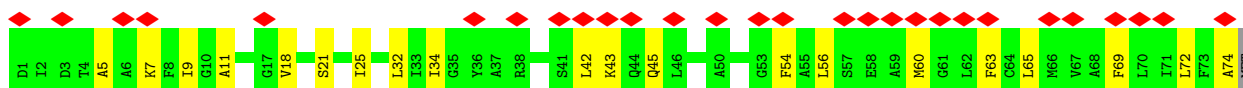
- Molecule 2: ATP synthase F(0) complex subunit C1, mitochondrial



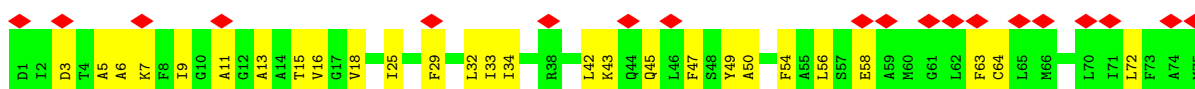
- Molecule 2: ATP synthase F(0) complex subunit C1, mitochondrial



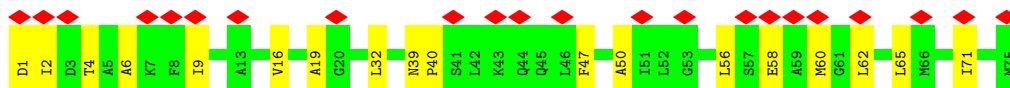
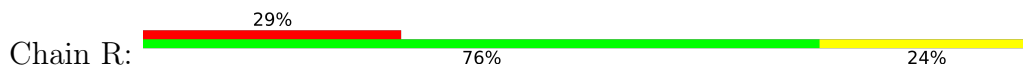
- Molecule 2: ATP synthase F(0) complex subunit C1, mitochondrial



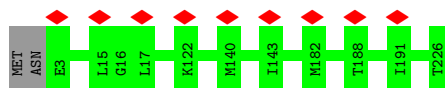
- Molecule 2: ATP synthase F(0) complex subunit C1, mitochondrial



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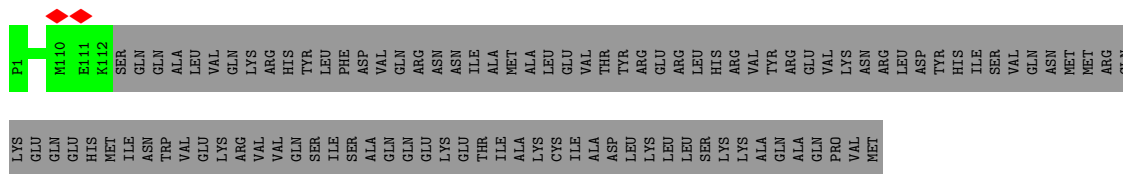


- Molecule 3: ATP synthase subunit a

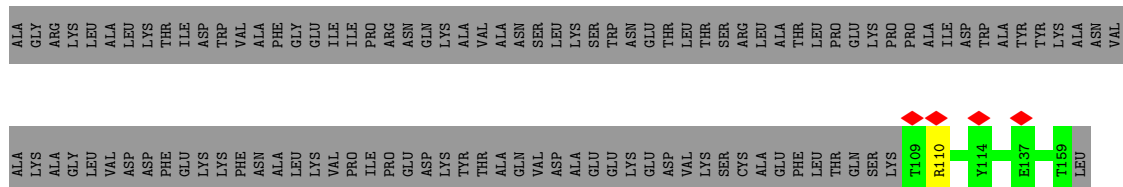


- Molecule 4: ATP synthase F(0) complex subunit B1, mitochondrial

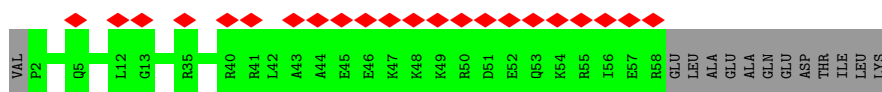
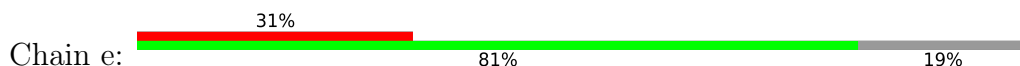




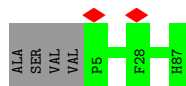
• Molecule 5: ATP synthase subunit d, mitochondrial



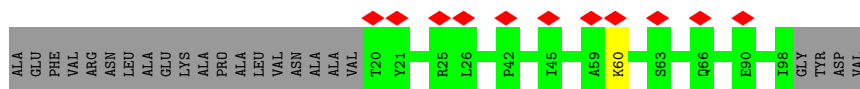
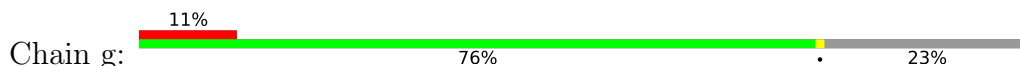
• Molecule 6: ATP synthase subunit e, mitochondrial



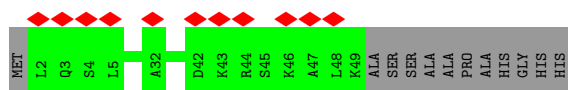
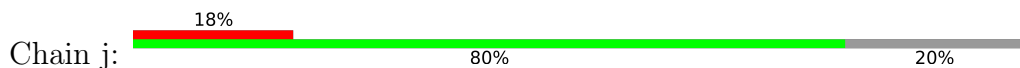
• Molecule 7: ATP synthase subunit f, mitochondrial



• Molecule 8: ATP synthase subunit g, mitochondrial

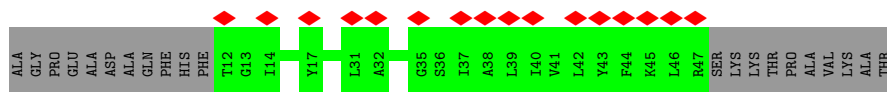


• Molecule 9: ATP synthase subunit ATP5MPL, mitochondrial



• Molecule 10: ATP synthase membrane subunit DAPIT, mitochondrial





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	253473	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 ($e^-/\text{\AA}^2$)	4.6	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.081	Depositor
Minimum map value	-0.040	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0197	Depositor
Map size (Å)	524.0, 524.0, 524.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.048, 1.048, 1.048	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: LHG, M3L, CDL

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	8	0.41	0/355	0.47	0/483
2	K	0.33	0/526	0.45	0/711
2	L	0.34	0/526	0.46	0/711
2	M	0.34	0/534	0.52	0/721
2	N	0.37	0/534	0.51	0/721
2	O	0.34	0/534	0.51	0/721
2	P	0.32	0/526	0.51	0/711
2	Q	0.34	0/534	0.47	0/721
2	R	0.33	0/534	0.47	0/721
3	a	0.35	0/1763	0.50	0/2412
4	b	0.37	0/902	0.47	0/1221
5	d	0.35	0/461	0.49	0/622
6	e	0.31	0/483	0.44	0/642
7	f	0.40	0/711	0.42	0/952
8	g	0.30	0/646	0.42	0/879
9	j	0.38	0/410	0.43	0/552
10	k	0.29	0/294	0.39	0/395
All	All	0.35	0/10273	0.47	0/13896

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	8	344	352	352	6	0
2	K	529	550	549	26	0
2	L	529	549	549	37	0
2	M	537	558	559	40	0
2	N	537	558	558	38	0
2	O	537	558	559	35	0
2	P	529	550	549	27	0
2	Q	537	558	559	34	0
2	R	537	558	559	32	0
3	a	1725	1832	1852	0	0
4	b	881	910	910	0	0
5	d	449	444	444	0	0
6	e	475	500	500	0	0
7	f	693	718	718	0	0
8	g	629	662	662	0	0
9	j	400	428	428	0	0
10	k	289	307	307	0	0
11	a	84	101	115	0	0
11	b	161	200	216	0	0
12	f	88	122	122	0	0
All	All	10490	11015	11067	181	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 16.

All (181) 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:N:9:ILE:HD13	2:O:9:ILE:HG22	1.46	0.97
1:8:32:ASN:OD1	1:8:33:PHE:N	2.10	0.84
2:Q:72:LEU:HD11	2:R:71:ILE:HD11	1.61	0.81
2:N:9:ILE:CD1	2:O:9:ILE:HG22	2.13	0.77
2:N:13:ALA:O	2:N:16:VAL:HG12	1.84	0.77
2:O:25:ILE:HD11	2:P:56:LEU:HD22	1.67	0.76
2:O:36:TYR:OH	2:P:42:LEU:HD22	1.87	0.75
2:Q:56:LEU:HD23	2:Q:56:LEU:O	1.87	0.74
2:K:42:LEU:HD11	2:R:40:PRO:HG3	1.68	0.74
2:N:72:LEU:HD22	2:O:71:ILE:HD11	1.70	0.73
2:Q:11:ALA:O	2:Q:15:THR:HG23	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:13:ALA:O	2:Q:16:VAL:HG12	1.89	0.71
2:R:32:LEU:HD12	2:R:50:ALA:HB2	1.71	0.71
2:P:9:ILE:HD12	2:Q:9:ILE:HG21	1.71	0.71
2:N:54:PHE:CE1	2:O:56:LEU:HD21	2.27	0.70
2:N:54:PHE:HE1	2:O:56:LEU:HD21	1.56	0.70
2:N:9:ILE:HD13	2:O:9:ILE:CG2	2.21	0.69
2:M:45:GLN:NE2	2:M:49:TYR:OH	2.26	0.68
2:O:25:ILE:HD11	2:P:56:LEU:CD2	2.24	0.68
2:M:16:VAL:CG2	2:N:16:VAL:HG13	2.24	0.68
2:P:9:ILE:HD12	2:Q:9:ILE:CG2	2.25	0.67
2:M:1:ASP:OD2	2:M:2:ILE:N	2.27	0.67
2:L:65:LEU:HD11	2:M:67:VAL:HG21	1.79	0.65
2:O:32:LEU:HD12	2:O:50:ALA:CB	2.26	0.64
2:K:9:ILE:HD12	2:L:9:ILE:HG21	1.80	0.64
2:N:25:ILE:HG21	2:O:56:LEU:HD22	1.79	0.63
2:N:5:ALA:HB1	2:O:6:ALA:HB2	1.81	0.62
2:P:65:LEU:HD21	2:Q:63:PHE:CE1	2.34	0.62
2:Q:54:PHE:CZ	2:R:56:LEU:HD11	2.35	0.62
2:L:1:ASP:OD1	2:L:2:ILE:N	2.32	0.62
2:R:1:ASP:OD1	2:R:2:ILE:N	2.32	0.62
2:N:62:LEU:HD11	2:O:63:PHE:HZ	1.64	0.61
2:K:13:ALA:O	2:K:16:VAL:HG22	2.01	0.61
1:8:8:THR:O	1:8:11:THR:HG22	2.01	0.60
2:K:1:ASP:OD1	2:K:2:ILE:N	2.34	0.60
2:P:5:ALA:HB1	2:Q:6:ALA:HB2	1.82	0.60
2:N:9:ILE:HD12	2:O:10:GLY:HA2	1.83	0.60
2:K:63:PHE:CE2	2:R:65:LEU:HD22	2.36	0.59
2:N:56:LEU:O	2:N:59:ALA:HB3	2.02	0.59
2:N:32:LEU:HD12	2:N:50:ALA:CB	2.33	0.58
2:M:36:TYR:CZ	2:N:42:LEU:HD21	2.39	0.58
2:P:54:PHE:CZ	2:Q:56:LEU:HD21	2.39	0.58
2:K:25:ILE:HD11	2:K:54:PHE:CE2	2.39	0.58
2:L:36:TYR:OH	2:M:42:LEU:HD22	2.04	0.57
2:M:13:ALA:O	2:M:16:VAL:HG12	2.04	0.56
2:K:65:LEU:HD11	2:L:63:PHE:CE1	2.41	0.56
2:P:18:VAL:O	2:P:21:SER:OG	2.19	0.56
2:M:11:ALA:O	2:M:15:THR:HG23	2.06	0.56
2:M:18:VAL:HG12	2:M:61:GLY:HA2	1.87	0.56
2:K:33:ILE:HG21	2:L:32:LEU:HA	1.89	0.55
2:Q:25:ILE:HD12	2:Q:54:PHE:CD1	2.41	0.55
2:R:32:LEU:HD12	2:R:50:ALA:CB	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:16:VAL:CG2	2:R:16:VAL:HG13	2.37	0.55
2:K:16:VAL:HG23	2:R:16:VAL:HG23	1.89	0.54
2:M:16:VAL:HG23	2:N:16:VAL:HG13	1.89	0.54
2:L:9:ILE:HD12	2:M:9:ILE:HG21	1.90	0.54
2:O:5:ALA:O	2:O:9:ILE:HG12	2.08	0.54
2:L:9:ILE:CD1	2:M:9:ILE:HB	2.38	0.53
2:M:18:VAL:HG12	2:M:61:GLY:O	2.09	0.53
2:O:9:ILE:HD12	2:P:9:ILE:HG23	1.91	0.53
2:Q:72:LEU:CD1	2:R:71:ILE:HD11	2.35	0.53
2:M:34:ILE:HD11	2:N:34:ILE:HB	1.91	0.52
2:R:32:LEU:C	2:R:32:LEU:HD23	2.30	0.52
2:M:18:VAL:CG2	2:N:64:CYS:SG	2.98	0.52
2:N:62:LEU:HD11	2:O:63:PHE:CZ	2.44	0.52
2:L:7:LYS:NZ	2:L:71:ILE:O	2.43	0.52
2:M:21:SER:OG	2:M:61:GLY:N	2.43	0.52
2:K:9:ILE:HD12	2:L:9:ILE:CG2	2.40	0.52
2:K:63:PHE:HE2	2:R:65:LEU:HD22	1.75	0.52
2:M:9:ILE:CD1	2:N:9:ILE:CG2	2.88	0.52
2:M:5:ALA:HB3	2:N:2:ILE:HD12	1.92	0.51
2:P:65:LEU:HD21	2:Q:63:PHE:HE1	1.75	0.51
2:L:11:ALA:HB2	2:L:72:LEU:HD21	1.92	0.51
2:L:16:VAL:HG13	2:M:16:VAL:HG13	1.93	0.51
2:L:1:ASP:O	2:L:4:THR:OG1	2.21	0.50
1:8:18:LEU:HA	1:8:22:ILE:HD12	1.94	0.50
2:Q:29:PHE:CE1	2:R:56:LEU:HD23	2.47	0.50
2:Q:33:ILE:HG21	2:R:32:LEU:HA	1.94	0.50
2:P:18:VAL:HG21	2:Q:64:CYS:SG	2.52	0.49
1:8:20:LEU:HD23	1:8:21:PHE:CD1	2.48	0.49
2:K:33:ILE:HD11	2:L:49:TYR:HB3	1.94	0.49
2:K:34:ILE:HD11	2:L:34:ILE:HB	1.95	0.49
2:K:49:TYR:HH	2:R:47:PHE:HD1	1.61	0.49
2:L:9:ILE:HD12	2:M:9:ILE:CG2	2.42	0.49
2:Q:16:VAL:HG23	2:R:16:VAL:HG13	1.95	0.49
2:K:9:ILE:HG21	2:R:9:ILE:CD1	2.43	0.48
2:L:42:LEU:O	2:L:44:GLN:N	2.46	0.48
2:Q:9:ILE:HD13	2:R:9:ILE:HG12	1.95	0.48
2:R:6:ALA:HA	2:R:9:ILE:HG22	1.96	0.48
2:O:58:GLU:OE2	2:O:58:GLU:HA	2.13	0.48
2:O:56:LEU:O	2:O:59:ALA:HB3	2.14	0.48
2:K:52:LEU:O	2:K:56:LEU:HD23	2.14	0.48
2:N:27:THR:HA	2:O:27:THR:HG21	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:32:LEU:HD12	2:M:50:ALA:HB2	1.95	0.47
2:Q:54:PHE:CE1	2:R:56:LEU:HD11	2.49	0.47
2:Q:25:ILE:HD12	2:Q:54:PHE:HD1	1.79	0.47
2:L:5:ALA:HB1	2:M:6:ALA:HB2	1.97	0.47
2:M:36:TYR:OH	2:N:42:LEU:HD21	2.15	0.47
2:R:39:ASN:OD1	2:R:39:ASN:O	2.33	0.47
2:M:15:THR:HG21	2:N:67:VAL:HG11	1.96	0.47
2:L:25:ILE:HG23	2:L:54:PHE:HD1	1.79	0.47
2:M:16:VAL:HG21	2:N:16:VAL:HG13	1.94	0.47
2:L:15:THR:HG21	2:M:14:ALA:HB1	1.97	0.46
2:K:25:ILE:HD11	2:K:54:PHE:CD2	2.49	0.46
2:L:54:PHE:CE1	2:M:56:LEU:HD23	2.50	0.46
2:R:58:GLU:O	2:R:62:LEU:HD23	2.15	0.46
2:P:60:MET:O	2:P:63:PHE:CD1	2.69	0.46
2:O:32:LEU:HD23	2:O:32:LEU:C	2.35	0.46
2:L:19:ALA:O	2:M:20:GLY:HA3	2.16	0.46
2:R:1:ASP:O	2:R:4:THR:OG1	2.18	0.46
2:P:69:PHE:HA	2:P:72:LEU:HD13	1.97	0.46
2:L:15:THR:HG21	2:M:14:ALA:CB	2.45	0.46
2:K:5:ALA:O	2:K:9:ILE:HG12	2.16	0.46
2:P:7:LYS:NZ	2:P:74:ALA:O	2.32	0.45
2:K:22:GLY:O	2:K:25:ILE:HG22	2.16	0.45
2:L:5:ALA:O	2:L:9:ILE:HG12	2.16	0.45
2:L:16:VAL:HG22	2:M:16:VAL:HG12	1.98	0.45
2:P:34:ILE:HD11	2:Q:34:ILE:HB	1.97	0.45
2:K:9:ILE:CD1	2:L:9:ILE:HB	2.46	0.45
2:O:32:LEU:HD12	2:O:50:ALA:HB3	1.96	0.45
2:O:33:ILE:HD12	2:P:32:LEU:HA	1.99	0.45
2:L:52:LEU:C	2:L:52:LEU:HD23	2.38	0.45
2:L:58:GLU:OE2	2:M:60:MET:CE	2.65	0.45
2:N:16:VAL:O	2:N:16:VAL:HG22	2.17	0.45
2:N:32:LEU:HD12	2:N:50:ALA:HB2	1.99	0.44
2:P:60:MET:HG2	2:P:63:PHE:HE1	1.83	0.44
2:P:42:LEU:O	2:P:43:M3L:C	2.66	0.44
2:N:1:ASP:OD1	2:N:2:ILE:N	2.51	0.44
2:N:5:ALA:HB1	2:O:6:ALA:CB	2.47	0.44
2:O:9:ILE:CD1	2:P:9:ILE:HG23	2.47	0.44
2:K:9:ILE:HG21	2:R:9:ILE:HD12	1.98	0.44
2:K:63:PHE:CZ	2:R:65:LEU:HD22	2.53	0.44
2:P:11:ALA:CB	2:P:72:LEU:HD12	2.48	0.44
2:M:71:ILE:O	2:M:71:ILE:HG22	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:3:ASP:O	2:Q:7:LYS:HG2	2.18	0.44
2:N:65:LEU:HD12	2:N:65:LEU:HA	1.87	0.43
2:P:54:PHE:CZ	2:Q:56:LEU:CD2	3.01	0.43
2:O:64:CYS:O	2:O:67:VAL:HG12	2.18	0.43
2:Q:45:GLN:HG3	2:Q:49:TYR:CZ	2.54	0.43
2:L:33:ILE:HG21	2:M:32:LEU:HA	2.00	0.43
2:O:54:PHE:HE1	2:P:56:LEU:HD22	1.83	0.43
2:L:55:ALA:O	2:L:58:GLU:HB2	2.18	0.43
2:O:59:ALA:O	2:O:62:LEU:HG	2.19	0.43
2:K:54:PHE:CZ	2:L:56:LEU:HD12	2.54	0.43
2:N:72:LEU:HD13	2:O:71:ILE:CD1	2.49	0.43
2:P:42:LEU:O	2:P:45:GLN:N	2.52	0.43
2:Q:58:GLU:OE2	2:R:60:MET:HE1	2.18	0.43
2:N:58:GLU:CG	2:N:62:LEU:HD23	2.49	0.43
2:M:45:GLN:HG3	2:M:49:TYR:CZ	2.54	0.42
2:O:66:MET:HE3	2:O:66:MET:HB3	1.87	0.42
2:Q:42:LEU:O	2:Q:43:M3L:C	2.68	0.42
2:O:25:ILE:HG23	2:O:26:GLY:N	2.34	0.42
2:O:62:LEU:HD12	2:O:63:PHE:N	2.34	0.42
2:M:39:ASN:ND2	2:M:42:LEU:HD12	2.35	0.42
2:Q:5:ALA:HB1	2:R:6:ALA:HB2	2.02	0.42
2:N:70:LEU:O	2:N:74:ALA:N	2.53	0.42
2:L:7:LYS:NZ	2:L:72:LEU:O	2.44	0.41
2:P:25:ILE:HD13	2:P:54:PHE:HE1	1.85	0.41
2:Q:18:VAL:CG1	2:R:60:MET:HG3	2.50	0.41
1:8:5:ASP:OD1	1:8:5:ASP:C	2.59	0.41
2:L:1:ASP:N	2:L:4:THR:OG1	2.32	0.41
2:Q:32:LEU:HD21	2:Q:47:PHE:CE1	2.55	0.41
2:Q:54:PHE:CE1	2:R:56:LEU:HD21	2.55	0.41
2:K:20:GLY:HA3	2:R:19:ALA:HA	2.02	0.41
2:L:26:GLY:HA3	2:M:24:GLY:HA2	2.03	0.41
2:N:32:LEU:C	2:N:32:LEU:HD23	2.41	0.41
2:P:60:MET:O	2:P:63:PHE:CE1	2.74	0.41
2:L:5:ALA:HB1	2:M:6:ALA:CB	2.51	0.41
2:M:60:MET:N	2:M:60:MET:SD	2.93	0.41
2:Q:58:GLU:OE2	2:Q:58:GLU:HA	2.21	0.41
1:8:38:GLU:H	1:8:38:GLU:CD	2.25	0.41
2:L:58:GLU:OE2	2:M:60:MET:HE1	2.21	0.40
2:N:18:VAL:HB	2:O:64:CYS:SG	2.61	0.40
2:N:26:GLY:HA3	2:O:24:GLY:HA2	2.03	0.40
2:Q:9:ILE:HD13	2:R:9:ILE:HG23	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:42:LEU:HD11	2:R:40:PRO:CG	2.46	0.40
2:K:65:LEU:HD21	2:L:63:PHE:HE1	1.86	0.40
2:M:5:ALA:O	2:N:6:ALA:HB1	2.20	0.40
2:N:58:GLU:HG3	2:N:62:LEU:HD23	2.03	0.40
2:O:9:ILE:HD12	2:P:9:ILE:CG2	2.51	0.40
2:Q:32:LEU:HD22	2:Q:50:ALA:CB	2.51	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	8	39/66 (59%)	35 (90%)	4 (10%)	0	100	100
2	K	71/75 (95%)	68 (96%)	3 (4%)	0	100	100
2	L	71/75 (95%)	67 (94%)	4 (6%)	0	100	100
2	M	72/75 (96%)	68 (94%)	4 (6%)	0	100	100
2	N	72/75 (96%)	69 (96%)	3 (4%)	0	100	100
2	O	72/75 (96%)	66 (92%)	6 (8%)	0	100	100
2	P	71/75 (95%)	71 (100%)	0	0	100	100
2	Q	72/75 (96%)	69 (96%)	3 (4%)	0	100	100
2	R	72/75 (96%)	67 (93%)	5 (7%)	0	100	100
3	a	222/226 (98%)	202 (91%)	20 (9%)	0	100	100
4	b	110/214 (51%)	104 (94%)	6 (6%)	0	100	100
5	d	49/160 (31%)	42 (86%)	7 (14%)	0	100	100
6	e	55/70 (79%)	54 (98%)	1 (2%)	0	100	100
7	f	81/87 (93%)	76 (94%)	5 (6%)	0	100	100
8	g	77/102 (76%)	73 (95%)	4 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	j	46/60 (77%)	43 (94%)	3 (6%)	0	100	100
10	k	34/57 (60%)	32 (94%)	2 (6%)	0	100	100
All	All	1286/1642 (78%)	1206 (94%)	80 (6%)	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	8	41/66 (62%)	41 (100%)	0	100	100
2	K	49/50 (98%)	49 (100%)	0	100	100
2	L	49/50 (98%)	49 (100%)	0	100	100
2	M	50/50 (100%)	50 (100%)	0	100	100
2	N	50/50 (100%)	50 (100%)	0	100	100
2	O	50/50 (100%)	49 (98%)	1 (2%)	55	79
2	P	49/50 (98%)	49 (100%)	0	100	100
2	Q	50/50 (100%)	50 (100%)	0	100	100
2	R	50/50 (100%)	50 (100%)	0	100	100
3	a	198/200 (99%)	198 (100%)	0	100	100
4	b	96/190 (50%)	96 (100%)	0	100	100
5	d	51/142 (36%)	50 (98%)	1 (2%)	55	79
6	e	48/59 (81%)	48 (100%)	0	100	100
7	f	72/75 (96%)	72 (100%)	0	100	100
8	g	67/83 (81%)	66 (98%)	1 (2%)	65	83
9	j	42/49 (86%)	42 (100%)	0	100	100
10	k	31/46 (67%)	31 (100%)	0	100	100
All	All	1043/1310 (80%)	1040 (100%)	3 (0%)	92	97

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	O	75	MET
5	d	110	ARG
8	g	60	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	8	25	GLN
2	M	45	GLN
3	a	56	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](#)

8 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
2	M3L	Q	43	2	10,11,12	0.46	0	9,14,16	0.52	0
2	M3L	M	43	2	10,11,12	0.59	0	9,14,16	0.44	0
2	M3L	O	43	2	10,11,12	0.55	0	9,14,16	0.55	0
2	M3L	L	43	2	10,11,12	0.49	0	9,14,16	0.34	0
2	M3L	K	43	2	10,11,12	0.53	0	9,14,16	0.62	0
2	M3L	P	43	2	10,11,12	0.44	0	9,14,16	0.52	0
2	M3L	R	43	2	10,11,12	0.48	0	9,14,16	0.42	0
2	M3L	N	43	2	10,11,12	0.48	0	9,14,16	0.49	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
2	M3L	Q	43	2	-	1/9/10/12	-
2	M3L	M	43	2	-	2/9/10/12	-
2	M3L	O	43	2	-	4/9/10/12	-
2	M3L	L	43	2	-	3/9/10/12	-
2	M3L	K	43	2	-	0/9/10/12	-
2	M3L	P	43	2	-	1/9/10/12	-
2	M3L	R	43	2	-	2/9/10/12	-
2	M3L	N	43	2	-	0/9/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	M	43	M3L	N-CA-CB-CG
2	O	43	M3L	N-CA-CB-CG
2	O	43	M3L	C-CA-CB-CG
2	R	43	M3L	O-C-CA-CB
2	L	43	M3L	CA-CB-CG-CD
2	L	43	M3L	CG-CD-CE-NZ
2	L	43	M3L	CE-CD-CG-CB
2	M	43	M3L	C-CA-CB-CG
2	R	43	M3L	CE-CD-CG-CB
2	O	43	M3L	CE-CD-CG-CB
2	Q	43	M3L	CA-CB-CG-CD
2	O	43	M3L	CG-CD-CE-NZ
2	P	43	M3L	CE-CD-CG-CB

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Q	43	M3L	1	0
2	P	43	M3L	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 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
12	LHG	f	102	-	48,48,48	0.61	1 (2%)	51,54,54	1.22	5 (9%)
11	CDL	a	301	-	83,83,99	0.98	7 (8%)	89,95,111	1.11	4 (4%)
12	LHG	f	101	-	38,38,48	0.69	1 (2%)	41,44,54	1.31	5 (12%)
11	CDL	b	301	-	77,77,99	1.00	6 (7%)	83,89,111	1.12	4 (4%)
11	CDL	b	302	-	82,82,99	0.98	6 (7%)	88,94,111	1.15	4 (4%)

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
12	LHG	f	102	-	-	16/53/53/53	-
11	CDL	a	301	-	-	28/94/94/110	-
12	LHG	f	101	-	-	15/43/43/53	-
11	CDL	b	301	-	-	38/88/88/110	-
11	CDL	b	302	-	-	35/93/93/110	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	b	301	CDL	OA6-CA4	-2.76	1.39	1.46
11	b	302	CDL	OA6-CA4	-2.76	1.39	1.46
11	a	301	CDL	OB8-CB7	2.63	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	b	301	CDL	OB8-CB7	2.61	1.41	1.33
11	b	302	CDL	OB8-CB7	2.57	1.40	1.33
11	a	301	CDL	OA6-CA4	-2.54	1.40	1.46
11	a	301	CDL	OB6-CB4	-2.53	1.40	1.46
11	b	301	CDL	OB6-CB4	-2.47	1.40	1.46
11	b	302	CDL	OB6-CB4	-2.45	1.40	1.46
11	a	301	CDL	OB6-CB5	2.43	1.41	1.34
11	b	302	CDL	OB6-CB5	2.41	1.41	1.34
11	b	302	CDL	OA8-CA7	2.37	1.40	1.33
11	b	301	CDL	OB6-CB5	2.36	1.41	1.34
11	a	301	CDL	OA8-CA7	2.33	1.40	1.33
11	a	301	CDL	OA8-CA6	-2.27	1.40	1.45
11	b	301	CDL	OA8-CA7	2.27	1.40	1.33
12	f	101	LHG	O7-C5	-2.23	1.41	1.46
11	b	301	CDL	OA8-CA6	-2.23	1.40	1.45
11	a	301	CDL	OA6-CA5	2.16	1.40	1.34
11	b	302	CDL	OA8-CA6	-2.07	1.40	1.45
12	f	102	LHG	O7-C5	-2.03	1.41	1.46

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	b	302	CDL	OB6-CB5-C51	4.44	121.07	111.50
11	b	302	CDL	OA6-CA5-C11	4.26	120.68	111.50
12	f	101	LHG	O4-P-O5	4.22	133.10	112.24
12	f	102	LHG	O4-P-O5	4.21	133.03	112.24
11	a	301	CDL	OA6-CA5-C11	4.08	120.29	111.50
11	b	301	CDL	OA6-CA5-C11	3.91	119.92	111.50
11	a	301	CDL	OB6-CB5-C51	3.89	119.88	111.50
11	b	301	CDL	OB6-CB5-C51	3.79	119.66	111.50
12	f	102	LHG	O8-C23-C24	2.77	120.59	111.91
11	b	302	CDL	OA8-CA7-C31	2.76	120.56	111.91
12	f	101	LHG	O8-C23-C24	2.75	120.52	111.91
11	b	301	CDL	OA8-CA7-C31	2.63	120.16	111.91
11	a	301	CDL	OA8-CA7-C31	2.50	119.76	111.91
11	b	302	CDL	OB8-CB7-C71	2.49	119.73	111.91
11	b	301	CDL	OB8-CB7-C71	2.45	119.59	111.91
12	f	101	LHG	C11-C10-C9	-2.44	102.05	114.42
11	a	301	CDL	OB8-CB7-C71	2.34	119.27	111.91
12	f	102	LHG	C11-C10-C9	-2.28	102.86	114.42
12	f	101	LHG	C27-C26-C25	-2.22	103.15	114.42
12	f	102	LHG	C20-C19-C18	-2.14	103.56	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	f	101	LHG	C18-C17-C16	-2.10	103.75	114.42
12	f	102	LHG	C27-C26-C25	-2.01	104.22	114.42

There are no chirality outliers.

All (132) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	b	301	CDL	CA2-OA2-PA1-OA3
11	b	301	CDL	CA2-OA2-PA1-OA4
11	b	301	CDL	CA2-OA2-PA1-OA5
11	b	301	CDL	C11-CA5-OA6-CA4
11	b	301	CDL	CB2-OB2-PB2-OB3
11	b	301	CDL	CB3-OB5-PB2-OB3
11	b	301	CDL	OB5-CB3-CB4-OB6
11	b	301	CDL	C51-CB5-OB6-CB4
11	b	302	CDL	C1-CA2-OA2-PA1
11	b	302	CDL	CA2-OA2-PA1-OA3
11	b	302	CDL	CA2-OA2-PA1-OA4
11	b	302	CDL	CB2-OB2-PB2-OB3
11	b	302	CDL	CB2-OB2-PB2-OB4
11	b	302	CDL	CB3-OB5-PB2-OB2
11	b	302	CDL	CB3-OB5-PB2-OB3
11	b	302	CDL	CB3-OB5-PB2-OB4
11	b	302	CDL	OB6-CB4-CB6-OB8
12	f	101	LHG	C3-O3-P-O5
12	f	102	LHG	C1-C2-C3-O3
11	a	301	CDL	OA9-CA7-OA8-CA6
11	b	301	CDL	OA7-CA5-OA6-CA4
11	b	301	CDL	OB7-CB5-OB6-CB4
11	a	301	CDL	C31-CA7-OA8-CA6
11	b	301	CDL	O1-C1-CA2-OA2
12	f	102	LHG	O2-C2-C3-O3
11	b	302	CDL	C71-C72-C73-C74
12	f	101	LHG	C7-C8-C9-C10
11	b	302	CDL	CA5-C11-C12-C13
11	a	301	CDL	CA7-C31-C32-C33
11	b	301	CDL	CB5-C51-C52-C53
12	f	102	LHG	C7-C8-C9-C10
11	a	301	CDL	CA5-C11-C12-C13
11	a	301	CDL	CB5-C51-C52-C53
11	a	301	CDL	C11-CA5-OA6-CA4
11	b	301	CDL	CB2-OB2-PB2-OB5

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Mol	Chain	Res	Type	Atoms
11	b	301	CDL	CB3-OB5-PB2-OB2
11	b	302	CDL	CA2-OA2-PA1-OA5
11	b	302	CDL	CB2-OB2-PB2-OB5
12	f	101	LHG	C23-C24-C25-C26
11	b	301	CDL	CB2-C1-CA2-OA2
11	a	301	CDL	OA7-CA5-OA6-CA4
12	f	102	LHG	C28-C29-C30-C31
11	a	301	CDL	C1-CB2-OB2-PB2
11	b	301	CDL	C19-C20-C21-C22
12	f	102	LHG	O1-C1-C2-C3
11	b	301	CDL	C40-C41-C42-C43
11	b	302	CDL	C60-C61-C62-C63
11	b	302	CDL	C13-C14-C15-C16
12	f	101	LHG	C4-C5-C6-O8
11	b	302	CDL	C73-C74-C75-C76
12	f	101	LHG	C13-C14-C15-C16
11	b	301	CDL	C21-C22-C23-C24
11	b	301	CDL	C37-C38-C39-C40
11	b	301	CDL	C42-C43-C44-C45
11	b	302	CDL	C11-CA5-OA6-CA4
11	a	301	CDL	C75-C76-C77-C78
11	b	302	CDL	C53-C54-C55-C56
12	f	102	LHG	C5-C4-O6-P
11	a	301	CDL	C74-C75-C76-C77
11	b	302	CDL	OA7-CA5-OA6-CA4
11	b	302	CDL	C54-C55-C56-C57
12	f	102	LHG	C15-C16-C17-C18
11	a	301	CDL	C12-C13-C14-C15
11	a	301	CDL	C71-CB7-OB8-CB6
11	a	301	CDL	C13-C14-C15-C16
12	f	101	LHG	C27-C28-C29-C30
11	a	301	CDL	OB5-CB3-CB4-CB6
11	b	301	CDL	OB5-CB3-CB4-CB6
11	b	302	CDL	C71-CB7-OB8-CB6
11	b	301	CDL	C1-CA2-OA2-PA1
12	f	101	LHG	C2-C3-O3-P
12	f	102	LHG	C11-C12-C13-C14
11	b	301	CDL	CB3-CB4-CB6-OB8
11	b	302	CDL	CB3-CB4-CB6-OB8
12	f	102	LHG	O6-C4-C5-O7
11	a	301	CDL	OB9-CB7-OB8-CB6
12	f	102	LHG	O6-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
11	a	301	CDL	C33-C34-C35-C36
11	b	302	CDL	C40-C41-C42-C43
11	b	301	CDL	CA3-CA4-CA6-OA8
11	b	302	CDL	OB9-CB7-OB8-CB6
12	f	102	LHG	C31-C32-C33-C34
12	f	101	LHG	O1-C1-C2-O2
12	f	101	LHG	O1-C1-C2-C3
11	b	302	CDL	C16-C17-C18-C19
11	a	301	CDL	CA2-OA2-PA1-OA5
11	b	302	CDL	CA3-OA5-PA1-OA2
12	f	101	LHG	C3-O3-P-O6
11	b	301	CDL	C53-C54-C55-C56
11	b	301	CDL	CB2-OB2-PB2-OB4
11	b	301	CDL	CB3-OB5-PB2-OB4
12	f	102	LHG	C29-C30-C31-C32
11	a	301	CDL	OB5-CB3-CB4-OB6
11	b	301	CDL	C13-C14-C15-C16
11	b	301	CDL	OB6-CB4-CB6-OB8
12	f	101	LHG	O7-C5-C6-O8
12	f	101	LHG	C10-C11-C12-C13
11	a	301	CDL	C14-C15-C16-C17
11	a	301	CDL	C60-C61-C62-C63
11	a	301	CDL	C53-C54-C55-C56
12	f	102	LHG	C14-C15-C16-C17
11	b	302	CDL	C11-C12-C13-C14
11	a	301	CDL	C1-CA2-OA2-PA1
11	b	302	CDL	CB4-CB3-OB5-PB2
11	a	301	CDL	CB3-OB5-PB2-OB2
11	b	301	CDL	C22-C23-C24-C25
12	f	102	LHG	C13-C14-C15-C16
11	b	301	CDL	C32-C33-C34-C35
11	b	301	CDL	OA6-CA4-CA6-OA8
12	f	101	LHG	C16-C17-C18-C19
11	b	301	CDL	C17-C18-C19-C20
12	f	102	LHG	O1-C1-C2-O2
11	b	301	CDL	C74-C75-C76-C77
11	b	302	CDL	C58-C59-C60-C61
11	a	301	CDL	C52-C53-C54-C55
11	a	301	CDL	C59-C60-C61-C62
11	b	301	CDL	C15-C16-C17-C18
11	b	302	CDL	C12-C11-CA5-OA6
11	b	301	CDL	C51-C52-C53-C54

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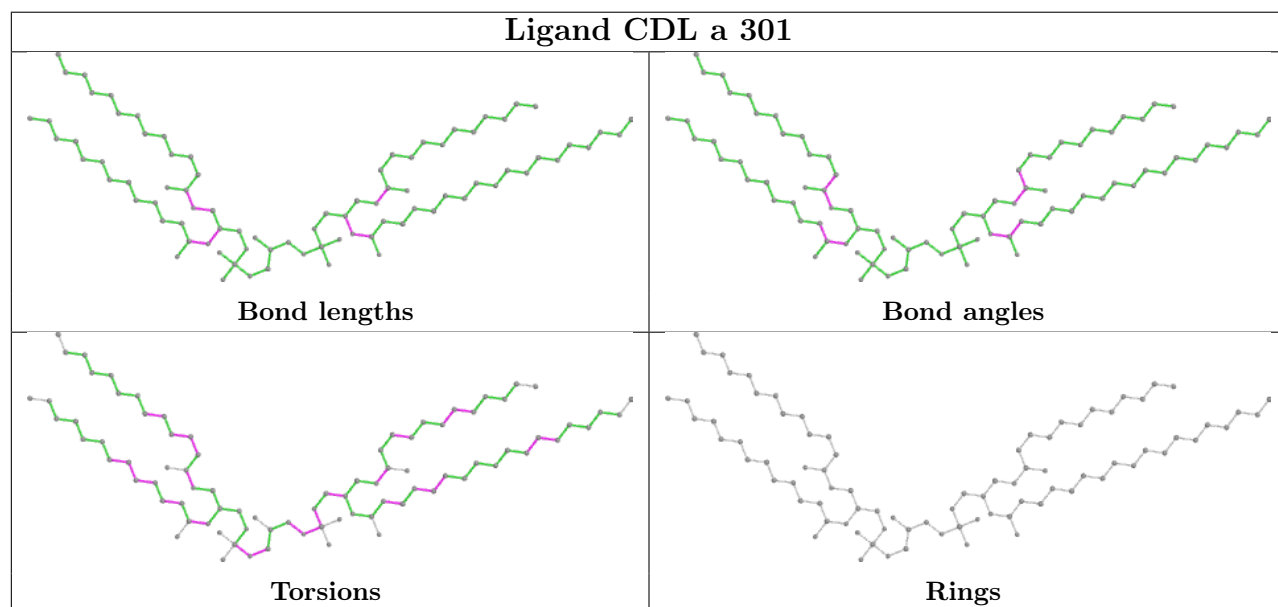
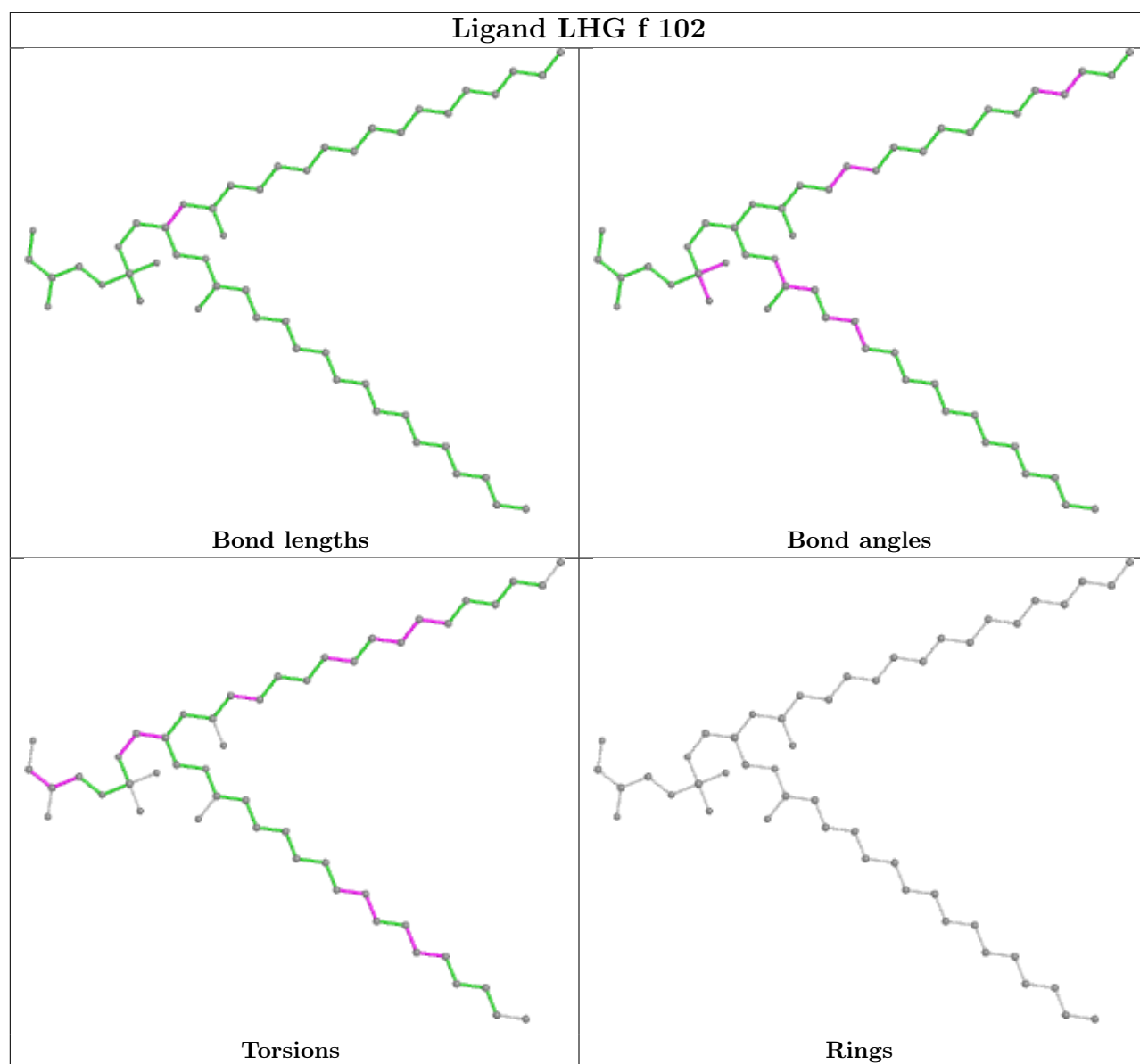
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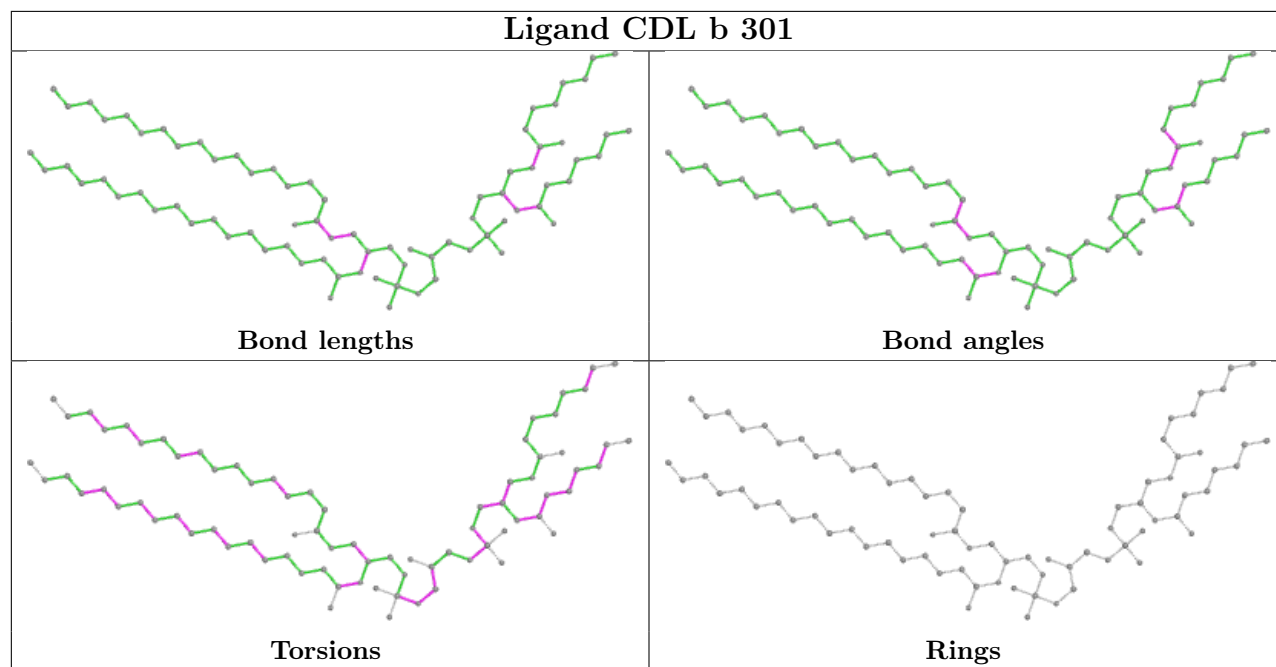
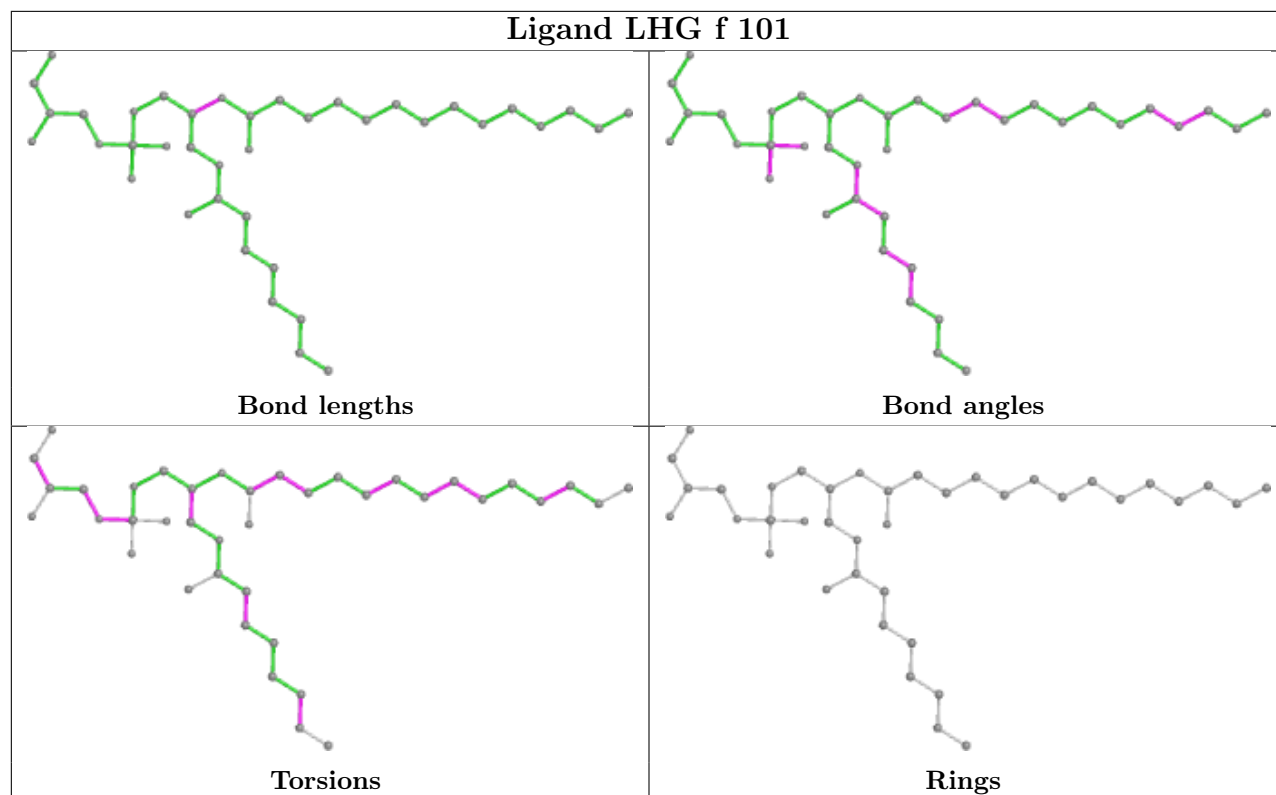
Mol	Chain	Res	Type	Atoms
11	b	302	CDL	C32-C31-CA7-OA8
11	b	302	CDL	C32-C31-CA7-OA9
11	b	302	CDL	C33-C34-C35-C36
11	a	301	CDL	CB2-OB2-PB2-OB3
11	a	301	CDL	C71-C72-C73-C74
11	b	302	CDL	C59-C60-C61-C62
12	f	102	LHG	C32-C33-C34-C35
12	f	101	LHG	C12-C13-C14-C15
12	f	101	LHG	O9-C7-C8-C9
11	b	302	CDL	CA4-CA3-OA5-PA1
11	a	301	CDL	C31-C32-C33-C34
11	b	301	CDL	C52-C51-CB5-OB6
11	b	301	CDL	C52-C51-CB5-OB7

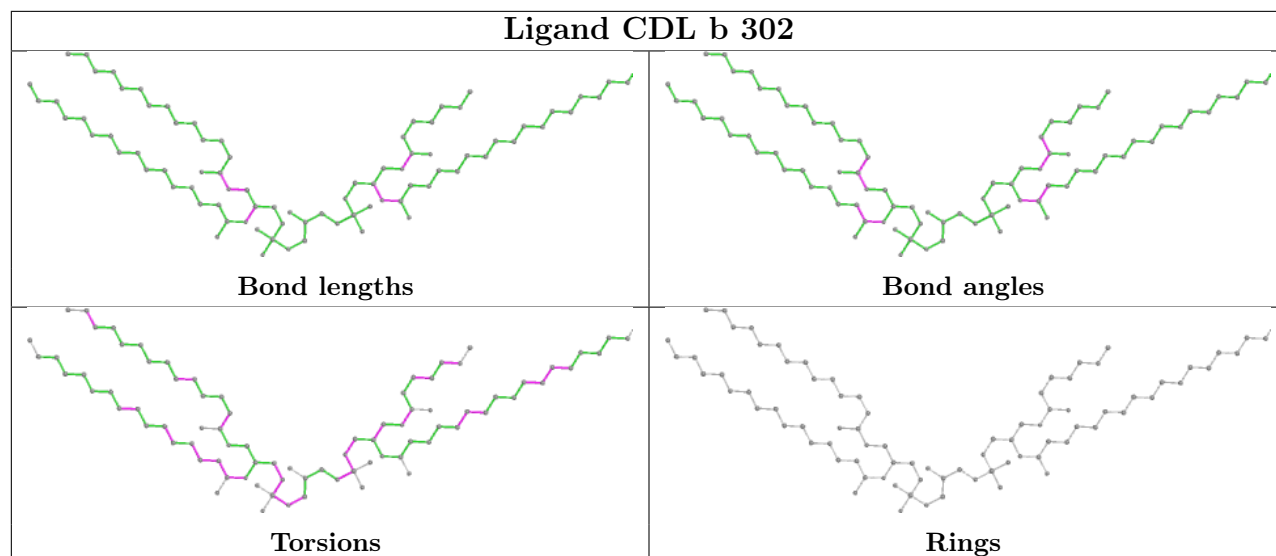
There are no ring outliers.

No monomer is involved in short contacts.

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

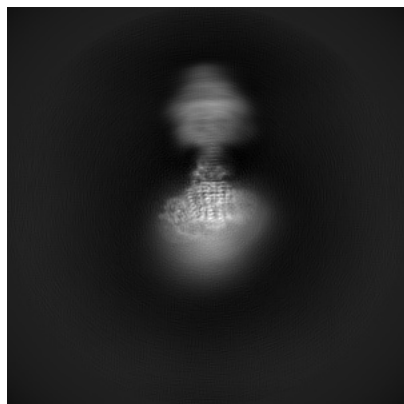
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11149. These allow visual inspection of the internal detail of the map and identification of artifacts.

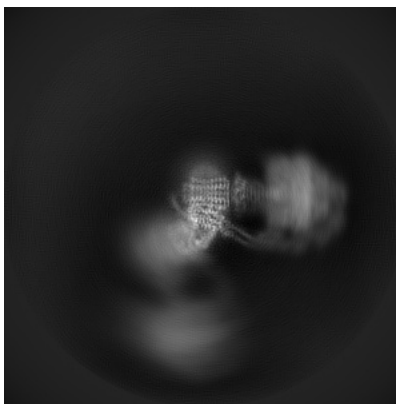
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

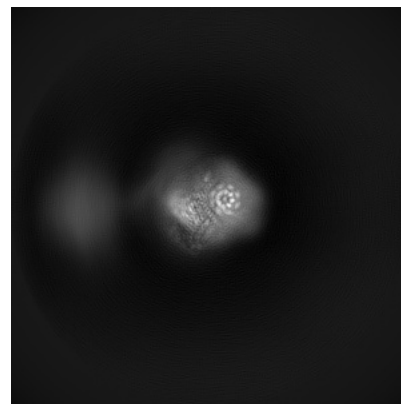
6.1.1 Primary map



X

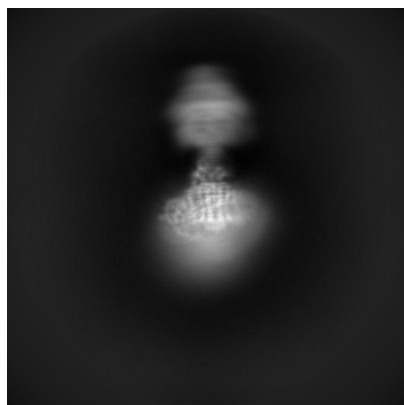


Y

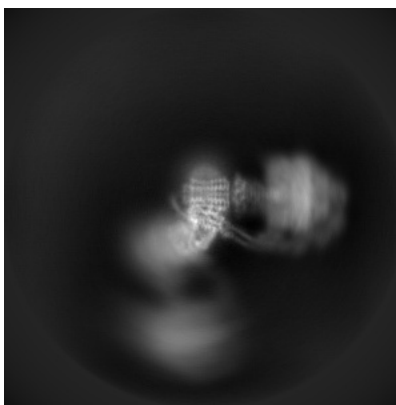


Z

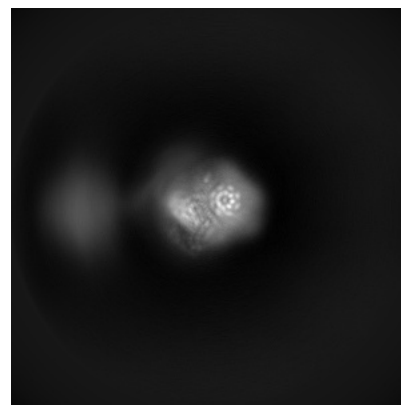
6.1.2 Raw map



X



Y

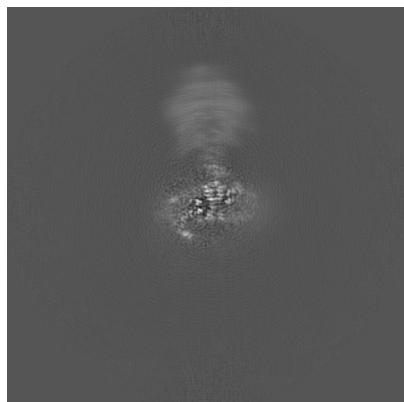


Z

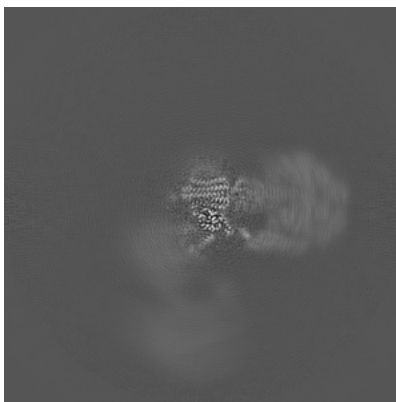
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

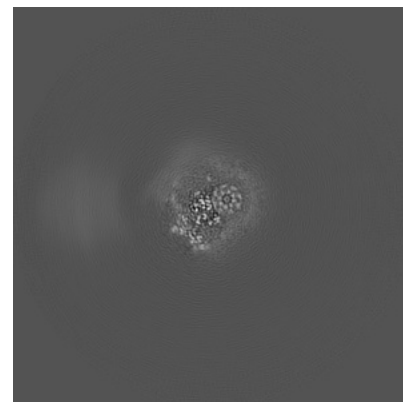
6.2.1 Primary map



X Index: 250

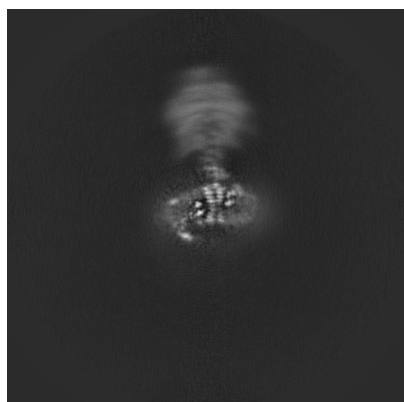


Y Index: 250

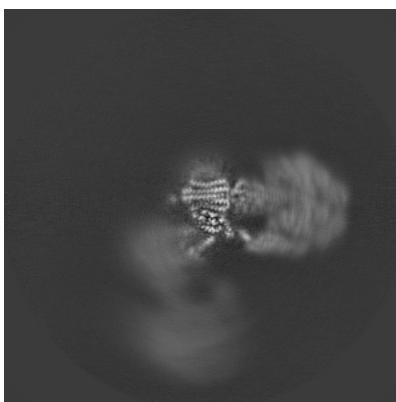


Z Index: 250

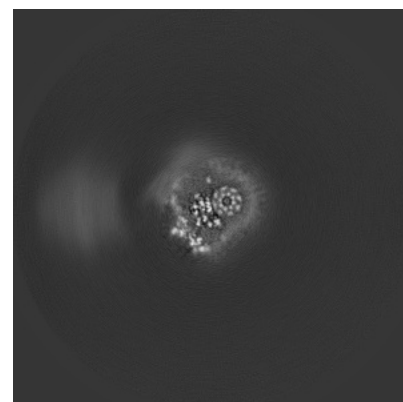
6.2.2 Raw map



X Index: 250



Y Index: 250

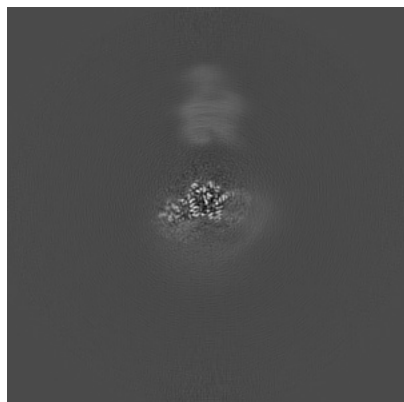


Z Index: 250

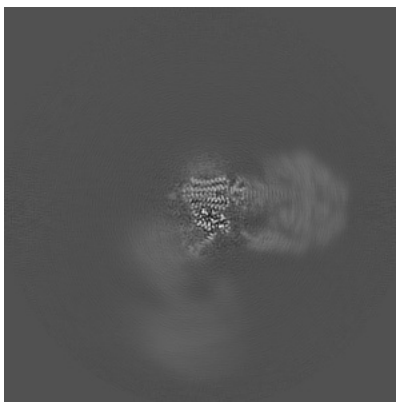
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

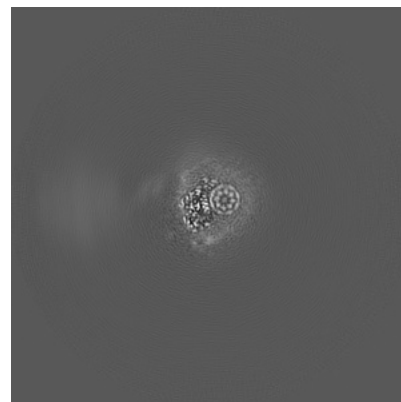
6.3.1 Primary map



X Index: 232

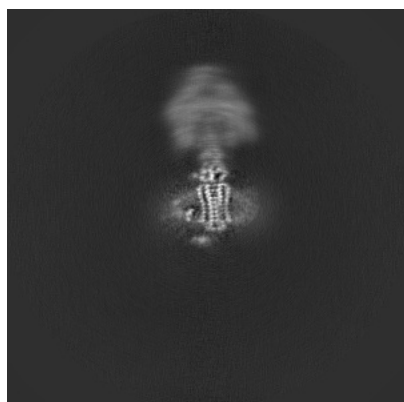


Y Index: 252

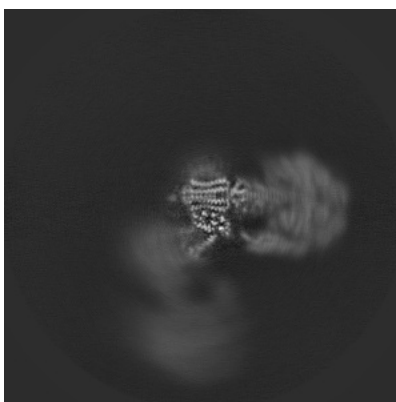


Z Index: 260

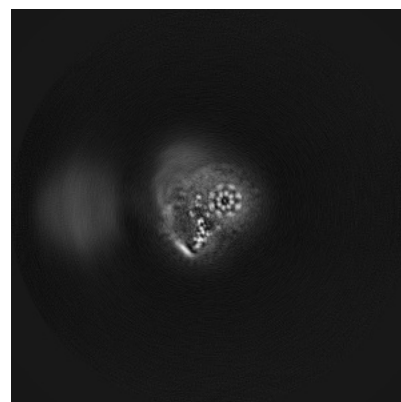
6.3.2 Raw map



X Index: 260



Y Index: 252



Z Index: 235

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



The images above show the 3D surface view of the map at the recommended contour level 0.0197. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

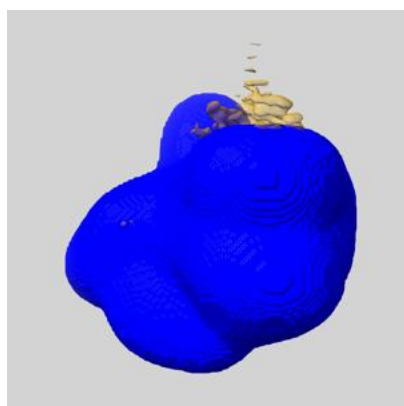
6.5 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

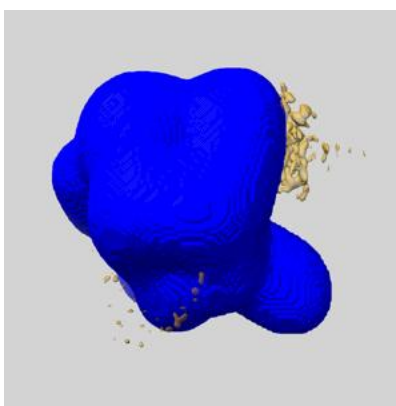
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

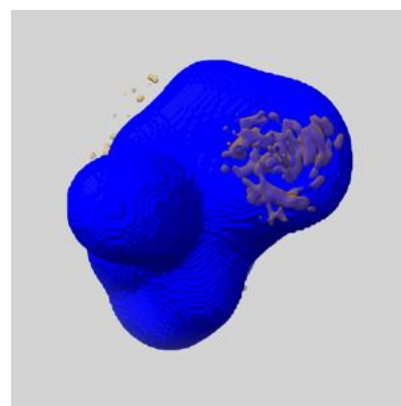
6.5.1 emd_11149_msk_1.map [i](#)



X



Y

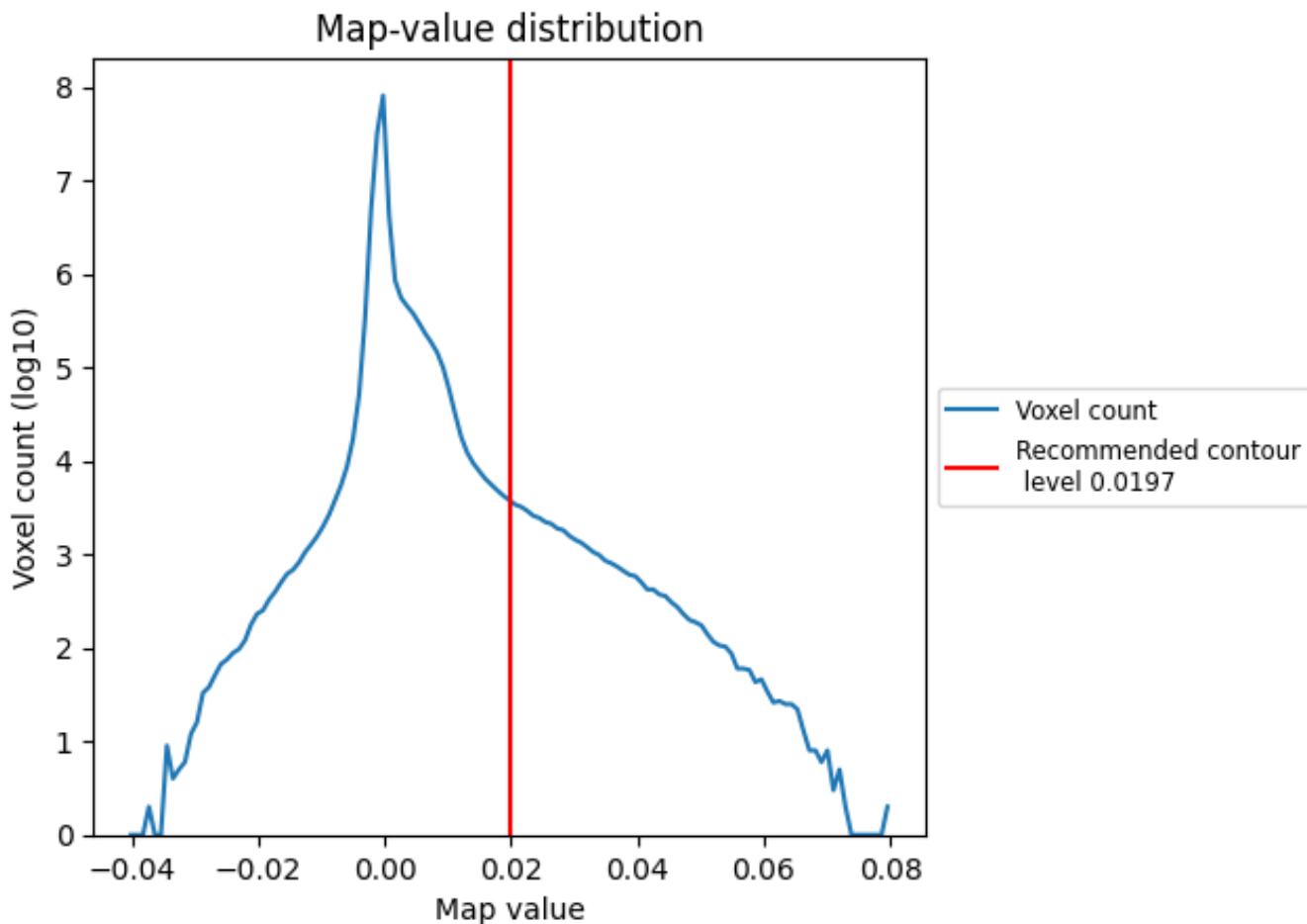


Z

7 Map analysis [i](#)

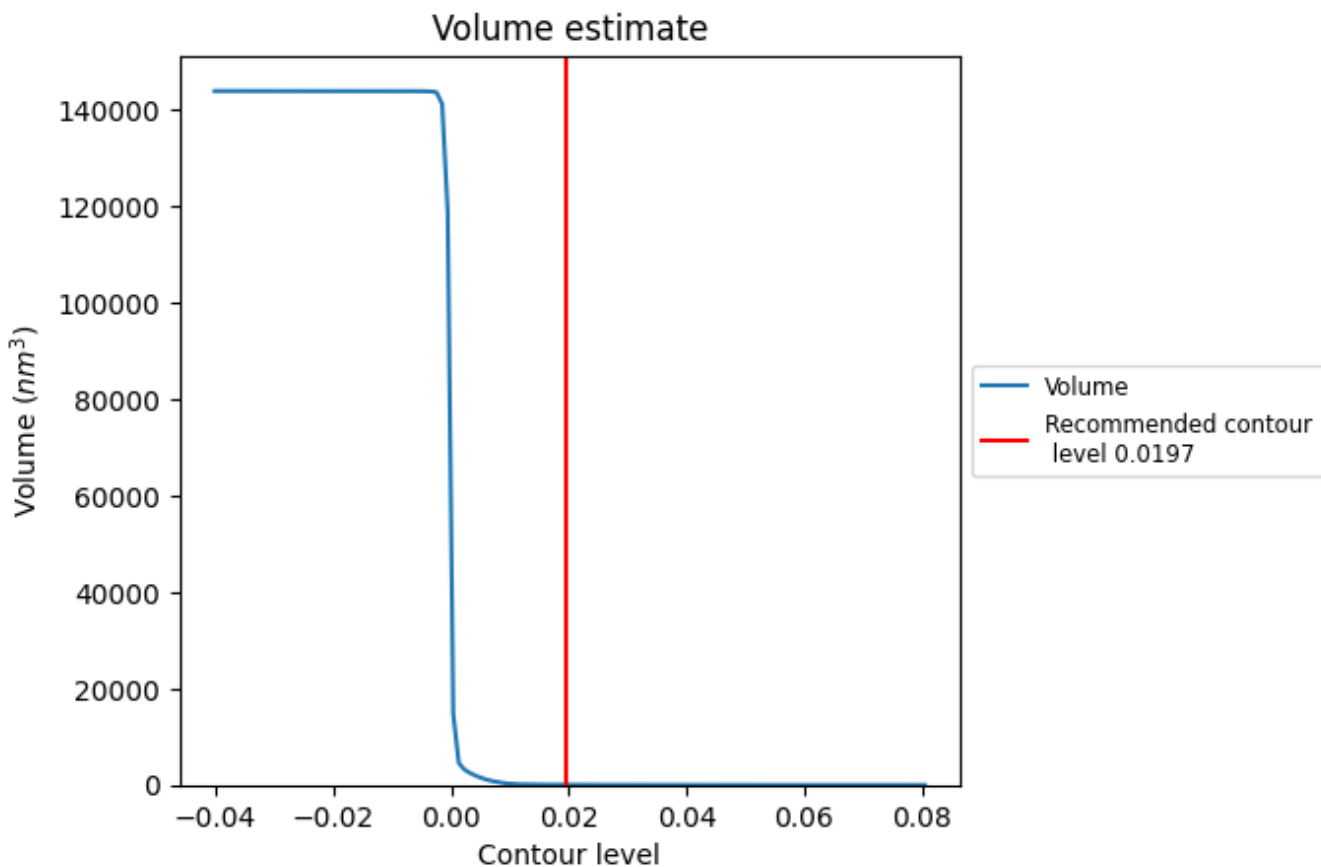
This section contains the results of statistical analysis of the map.

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.

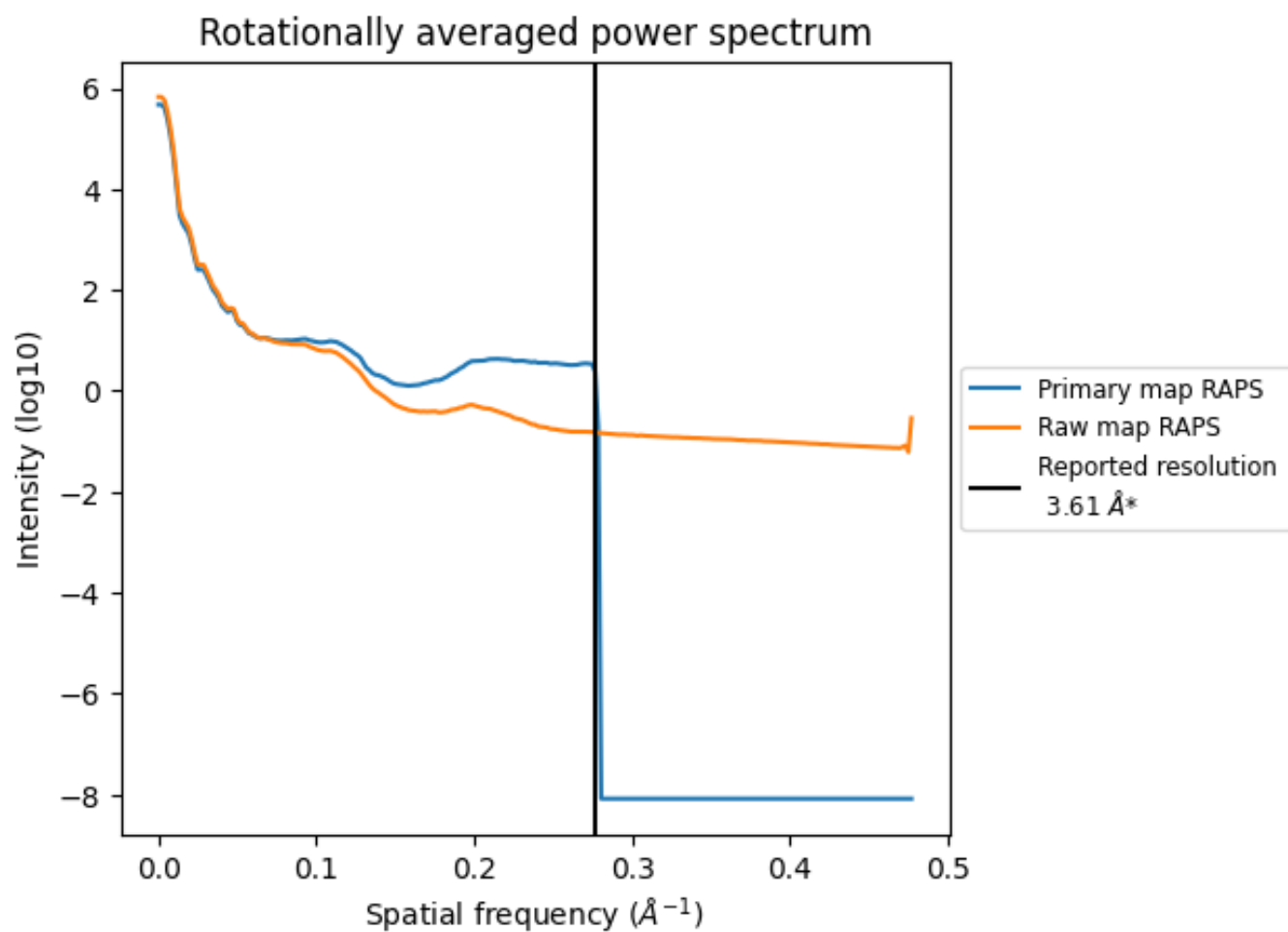
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 49 nm³; this corresponds to an approximate mass of 45 kDa.

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

7.3 Rotationally averaged power spectrum i

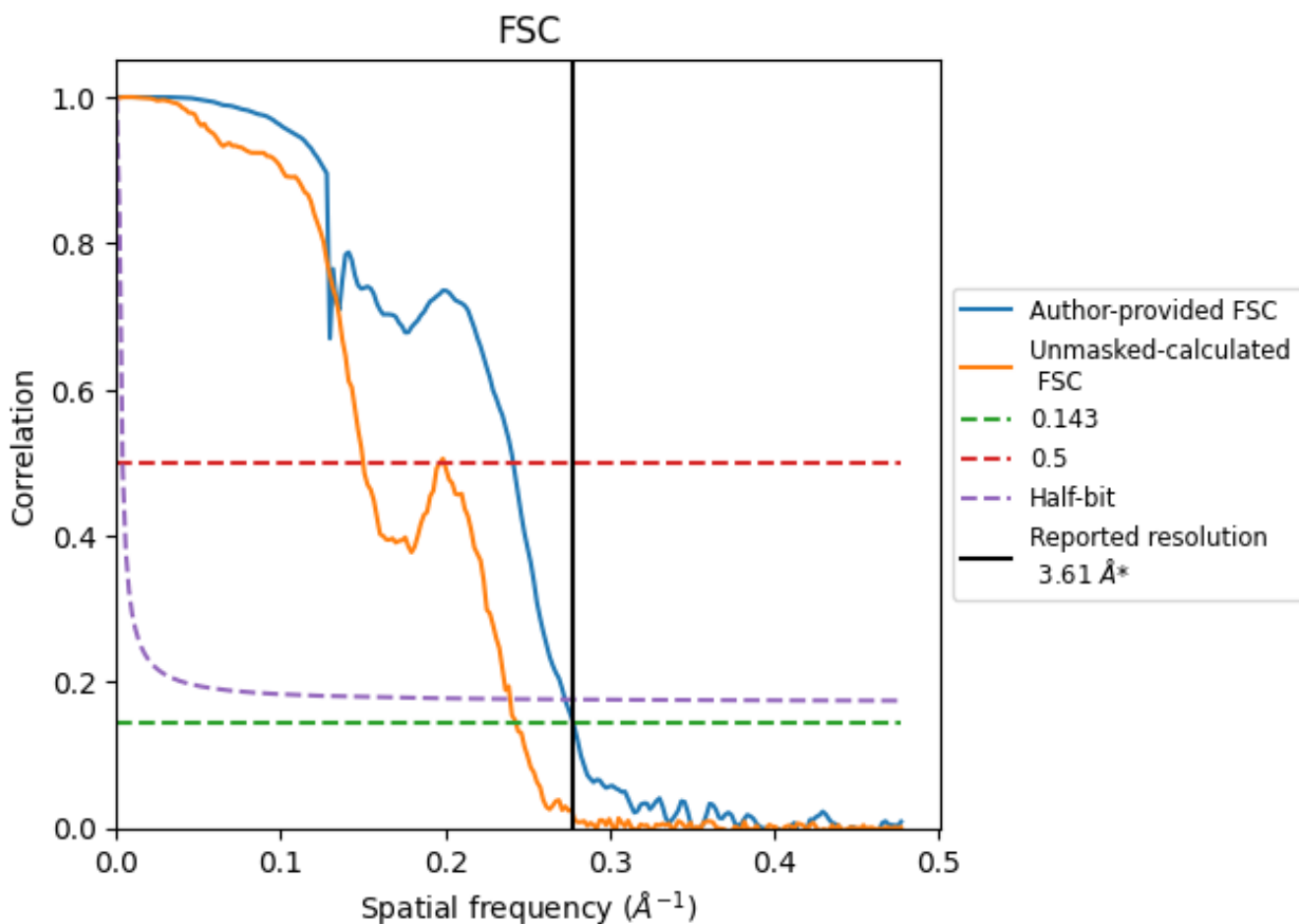


*Reported resolution corresponds to spatial frequency of 0.277 Å⁻¹

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 0.277 \AA^{-1}

8.2 Resolution estimates [i](#)

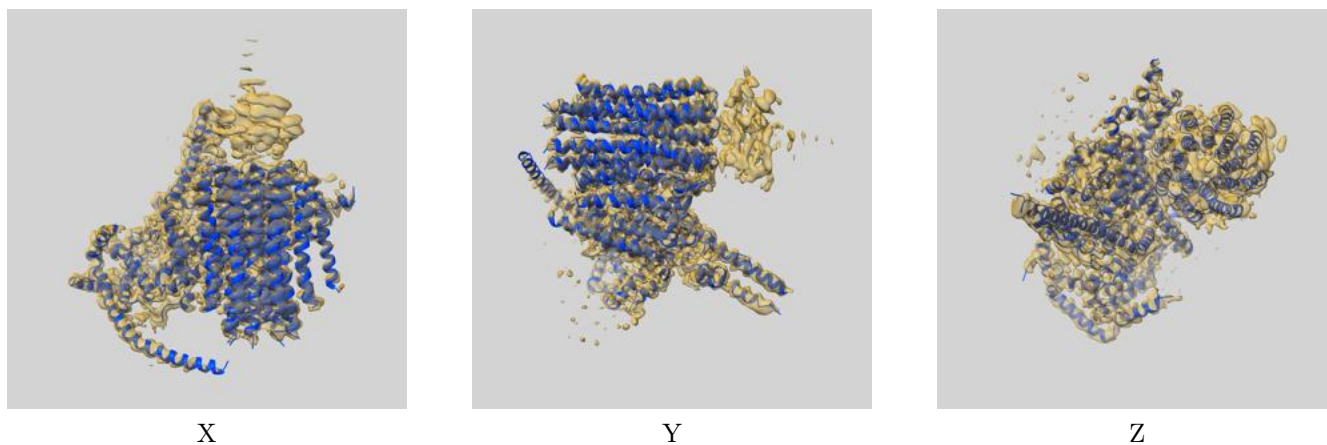
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.61	-	-
Author-provided FSC curve	3.60	4.15	3.67
Unmasked-calculated*	4.12	6.67	4.18

*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 4.12 differs from the reported value 3.61 by more than 10 %

9 Map-model fit [i](#)

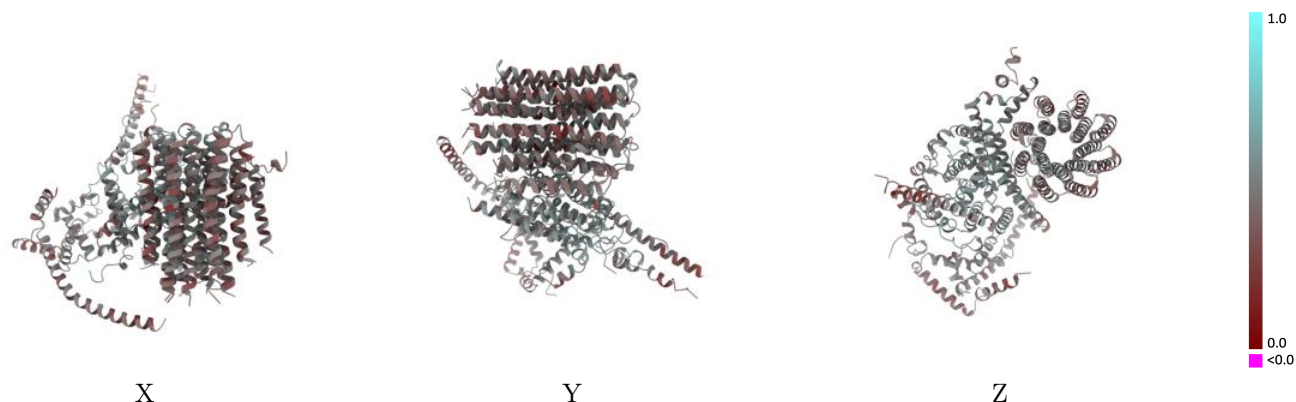
This section contains information regarding the fit between EMDB map EMD-11149 and PDB model 6ZBB. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



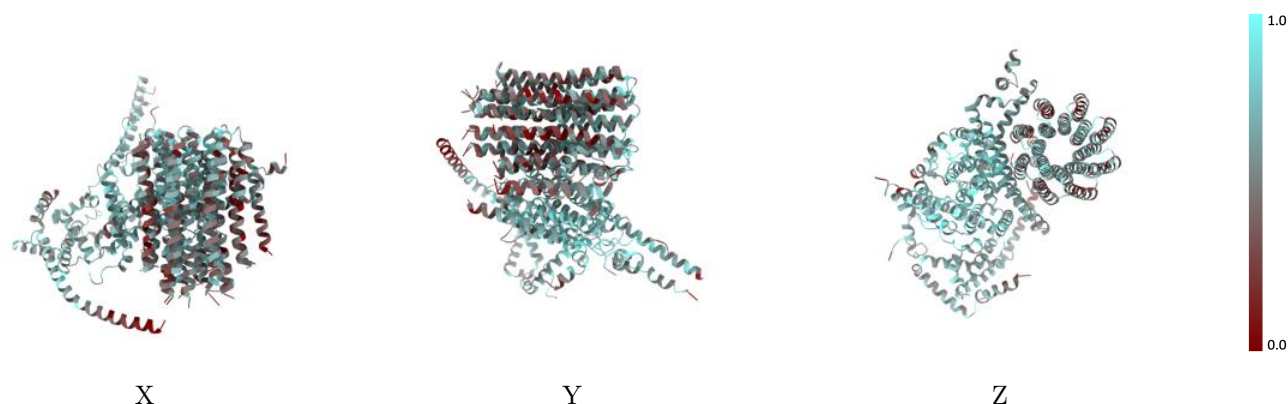
The images above show the 3D surface view of the map at the recommended contour level 0.0197 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



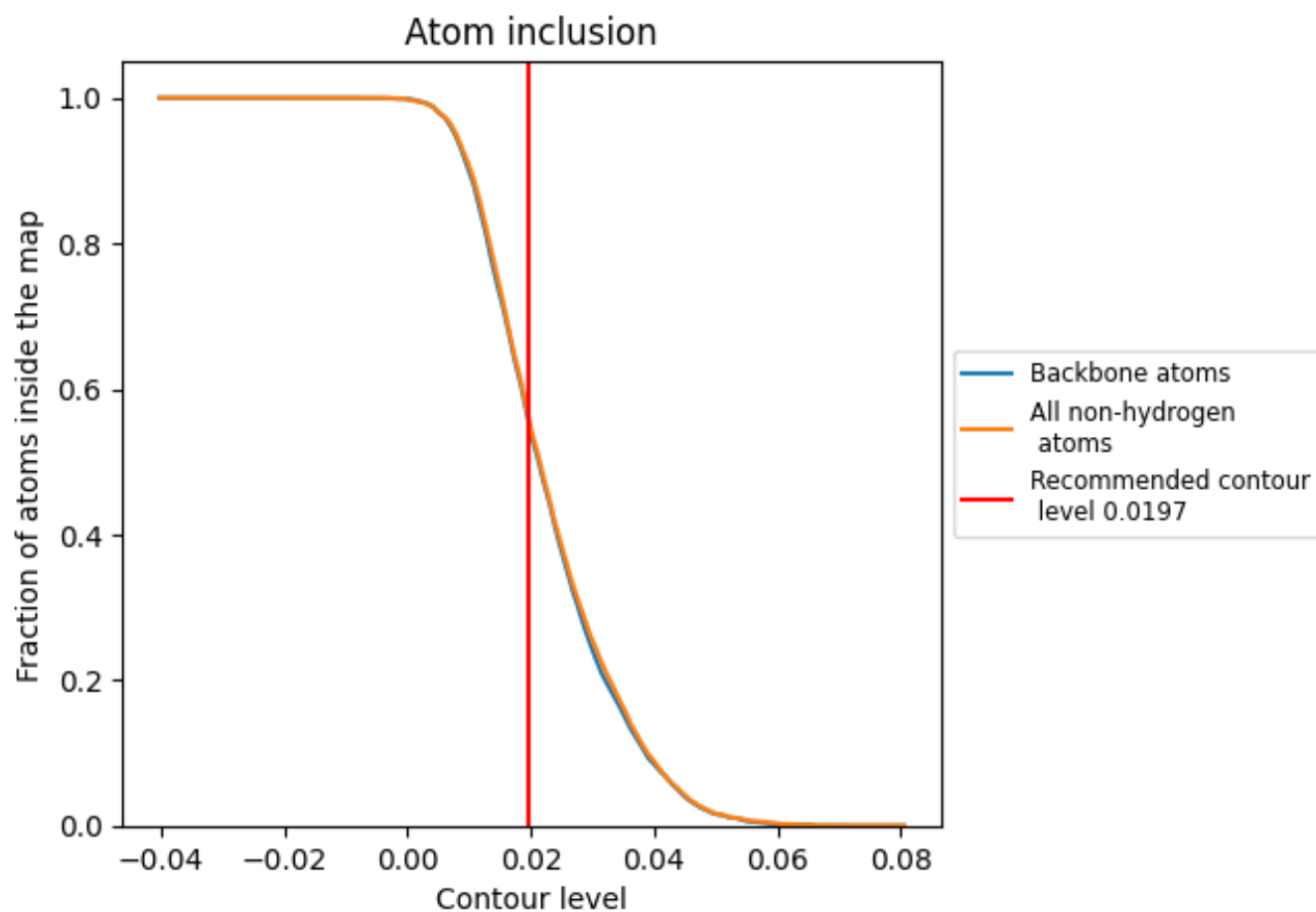
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0197).





































9.4 Atom inclusion [i](#)



At the recommended contour level, 55% of all backbone atoms, 56% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.0197) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5586	 0.4500
8	 0.7310	 0.5210
K	 0.4648	 0.4030
L	 0.4171	 0.3950
M	 0.5084	 0.4310
N	 0.5760	 0.4420
O	 0.4765	 0.4230
P	 0.4495	 0.3960
Q	 0.5291	 0.4250
R	 0.5197	 0.4110
a	 0.6871	 0.5070
b	 0.6470	 0.4820
d	 0.6765	 0.4480
e	 0.4725	 0.4070
f	 0.6350	 0.4960
g	 0.5858	 0.4030
j	 0.5990	 0.4660
k	 0.4128	 0.4150

