



Full wwPDB EM Validation Report ⓘ

Nov 13, 2022 – 08:22 PM EST

PDB ID : 6XBD
EMDB ID : EMD-22116
Title : Cryo-EM structure of MlaFEDB in nanodiscs with phospholipid substrates
Authors : Coudray, N.; Isom, G.L.; MacRae, M.R.; Saiduddin, M.; Ekiert, D.C.; Bhabha, G.
Deposited on : 2020-06-05
Resolution : 3.05 Å (reported)
Based on initial models : 5UW2, 6CM1

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

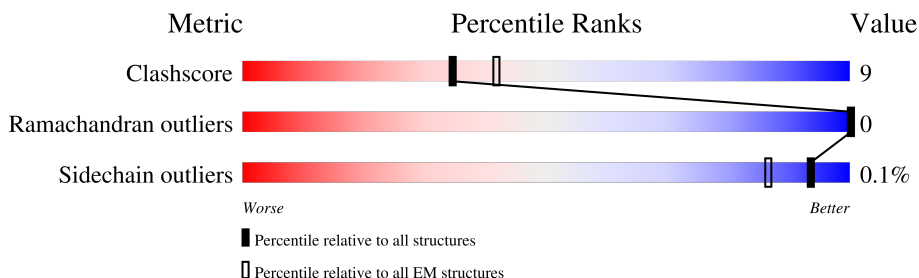
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.05 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	201	
1	B	201	
1	C	201	
1	D	201	
1	E	201	
1	F	201	
2	G	260	
2	H	260	

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Mol	Chain	Length	Quality of chain
3	I	269	<div><div></div><div>79%</div><div>19%</div><div></div></div>
3	J	269	<div><div></div><div>79%</div><div>19%</div><div></div></div>
4	K	97	<div><div></div><div>68%</div><div>30%</div><div></div></div>
4	L	97	<div><div></div><div>68%</div><div>30%</div><div></div></div>
5	M	164	<div><div></div><div>34%</div><div>75%</div><div>25%</div><div></div></div>
5	N	164	<div><div></div><div>29%</div><div>66%</div><div>29%</div><div>5%</div><div></div></div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17433 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 Phospholipid ABC transporter-binding protein MlaD.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	144	Total	C	N	O	S	0	0
			1108	715	178	213	2		
1	B	138	Total	C	N	O	S	0	0
			1063	687	170	204	2		
1	C	144	Total	C	N	O	S	0	0
			1033	652	172	208	1		
1	D	143	Total	C	N	O	S	0	0
			1096	707	177	210	2		
1	E	145	Total	C	N	O	S	0	0
			1112	718	179	213	2		
1	F	143	Total	C	N	O	S	0	0
			1028	649	171	207	1		

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	MET	-	expression tag	UNP H4UPP8
A	-16	HIS	-	expression tag	UNP H4UPP8
A	-15	HIS	-	expression tag	UNP H4UPP8
A	-14	HIS	-	expression tag	UNP H4UPP8
A	-13	HIS	-	expression tag	UNP H4UPP8
A	-12	HIS	-	expression tag	UNP H4UPP8
A	-11	HIS	-	expression tag	UNP H4UPP8
A	-10	GLN	-	expression tag	UNP H4UPP8
A	-9	HIS	-	expression tag	UNP H4UPP8
A	-8	GLN	-	expression tag	UNP H4UPP8
A	-7	HIS	-	expression tag	UNP H4UPP8
A	-6	GLU	-	expression tag	UNP H4UPP8
A	-5	ASN	-	expression tag	UNP H4UPP8
A	-4	LEU	-	expression tag	UNP H4UPP8
A	-3	TYR	-	expression tag	UNP H4UPP8
A	-2	PHE	-	expression tag	UNP H4UPP8
A	-1	GLN	-	expression tag	UNP H4UPP8
A	0	GLY	-	expression tag	UNP H4UPP8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	MET	-	expression tag	UNP H4UPP8
B	-16	HIS	-	expression tag	UNP H4UPP8
B	-15	HIS	-	expression tag	UNP H4UPP8
B	-14	HIS	-	expression tag	UNP H4UPP8
B	-13	HIS	-	expression tag	UNP H4UPP8
B	-12	HIS	-	expression tag	UNP H4UPP8
B	-11	HIS	-	expression tag	UNP H4UPP8
B	-10	GLN	-	expression tag	UNP H4UPP8
B	-9	HIS	-	expression tag	UNP H4UPP8
B	-8	GLN	-	expression tag	UNP H4UPP8
B	-7	HIS	-	expression tag	UNP H4UPP8
B	-6	GLU	-	expression tag	UNP H4UPP8
B	-5	ASN	-	expression tag	UNP H4UPP8
B	-4	LEU	-	expression tag	UNP H4UPP8
B	-3	TYR	-	expression tag	UNP H4UPP8
B	-2	PHE	-	expression tag	UNP H4UPP8
B	-1	GLN	-	expression tag	UNP H4UPP8
B	0	GLY	-	expression tag	UNP H4UPP8
C	-17	MET	-	expression tag	UNP H4UPP8
C	-16	HIS	-	expression tag	UNP H4UPP8
C	-15	HIS	-	expression tag	UNP H4UPP8
C	-14	HIS	-	expression tag	UNP H4UPP8
C	-13	HIS	-	expression tag	UNP H4UPP8
C	-12	HIS	-	expression tag	UNP H4UPP8
C	-11	HIS	-	expression tag	UNP H4UPP8
C	-10	GLN	-	expression tag	UNP H4UPP8
C	-9	HIS	-	expression tag	UNP H4UPP8
C	-8	GLN	-	expression tag	UNP H4UPP8
C	-7	HIS	-	expression tag	UNP H4UPP8
C	-6	GLU	-	expression tag	UNP H4UPP8
C	-5	ASN	-	expression tag	UNP H4UPP8
C	-4	LEU	-	expression tag	UNP H4UPP8
C	-3	TYR	-	expression tag	UNP H4UPP8
C	-2	PHE	-	expression tag	UNP H4UPP8
C	-1	GLN	-	expression tag	UNP H4UPP8
C	0	GLY	-	expression tag	UNP H4UPP8
D	-17	MET	-	expression tag	UNP H4UPP8
D	-16	HIS	-	expression tag	UNP H4UPP8
D	-15	HIS	-	expression tag	UNP H4UPP8
D	-14	HIS	-	expression tag	UNP H4UPP8
D	-13	HIS	-	expression tag	UNP H4UPP8
D	-12	HIS	-	expression tag	UNP H4UPP8

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-11	HIS	-	expression tag	UNP H4UPP8
D	-10	GLN	-	expression tag	UNP H4UPP8
D	-9	HIS	-	expression tag	UNP H4UPP8
D	-8	GLN	-	expression tag	UNP H4UPP8
D	-7	HIS	-	expression tag	UNP H4UPP8
D	-6	GLU	-	expression tag	UNP H4UPP8
D	-5	ASN	-	expression tag	UNP H4UPP8
D	-4	LEU	-	expression tag	UNP H4UPP8
D	-3	TYR	-	expression tag	UNP H4UPP8
D	-2	PHE	-	expression tag	UNP H4UPP8
D	-1	GLN	-	expression tag	UNP H4UPP8
D	0	GLY	-	expression tag	UNP H4UPP8
E	-17	MET	-	expression tag	UNP H4UPP8
E	-16	HIS	-	expression tag	UNP H4UPP8
E	-15	HIS	-	expression tag	UNP H4UPP8
E	-14	HIS	-	expression tag	UNP H4UPP8
E	-13	HIS	-	expression tag	UNP H4UPP8
E	-12	HIS	-	expression tag	UNP H4UPP8
E	-11	HIS	-	expression tag	UNP H4UPP8
E	-10	GLN	-	expression tag	UNP H4UPP8
E	-9	HIS	-	expression tag	UNP H4UPP8
E	-8	GLN	-	expression tag	UNP H4UPP8
E	-7	HIS	-	expression tag	UNP H4UPP8
E	-6	GLU	-	expression tag	UNP H4UPP8
E	-5	ASN	-	expression tag	UNP H4UPP8
E	-4	LEU	-	expression tag	UNP H4UPP8
E	-3	TYR	-	expression tag	UNP H4UPP8
E	-2	PHE	-	expression tag	UNP H4UPP8
E	-1	GLN	-	expression tag	UNP H4UPP8
E	0	GLY	-	expression tag	UNP H4UPP8
F	-17	MET	-	expression tag	UNP H4UPP8
F	-16	HIS	-	expression tag	UNP H4UPP8
F	-15	HIS	-	expression tag	UNP H4UPP8
F	-14	HIS	-	expression tag	UNP H4UPP8
F	-13	HIS	-	expression tag	UNP H4UPP8
F	-12	HIS	-	expression tag	UNP H4UPP8
F	-11	HIS	-	expression tag	UNP H4UPP8
F	-10	GLN	-	expression tag	UNP H4UPP8
F	-9	HIS	-	expression tag	UNP H4UPP8
F	-8	GLN	-	expression tag	UNP H4UPP8
F	-7	HIS	-	expression tag	UNP H4UPP8
F	-6	GLU	-	expression tag	UNP H4UPP8

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-5	ASN	-	expression tag	UNP H4UPP8
F	-4	LEU	-	expression tag	UNP H4UPP8
F	-3	TYR	-	expression tag	UNP H4UPP8
F	-2	PHE	-	expression tag	UNP H4UPP8
F	-1	GLN	-	expression tag	UNP H4UPP8
F	0	GLY	-	expression tag	UNP H4UPP8

- Molecule 2 is a protein called Phospholipid ABC transporter permease protein MlaE.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	256	Total	C	N	O	S	0	0
			1926	1261	323	330	12		
2	H	255	Total	C	N	O	S	0	0
			1918	1257	321	328	12		

- Molecule 3 is a protein called Phospholipid transport system ATP-binding protein MlaF.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	263	Total	C	N	O	S	0	0
			1996	1268	352	362	14		
3	J	263	Total	C	N	O	S	0	0
			1996	1268	352	362	14		

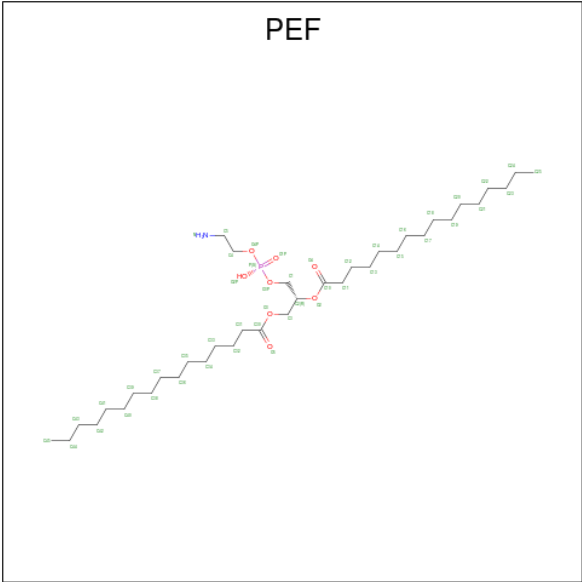
- Molecule 4 is a protein called Phospholipid ABC transporter-binding protein MlaB.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	95	Total	C	N	O	S	0	0
			734	464	124	143	3		
4	L	95	Total	C	N	O	S	0	0
			734	464	124	143	3		

- Molecule 5 is a protein called MSP1D1.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	M	164	Total	C	N	O	0	0
			821	492	164	165		
5	N	156	Total	C	N	O	0	0
			780	468	156	156		

- Molecule 6 is DI-PALMITOYL-3-SN-PHOSPHATIDYLETHANOLAMINE (three-letter code: PEF) (formula: C₃₇H₇₄NO₈P) (labeled as "Ligand of Interest" by depositor).

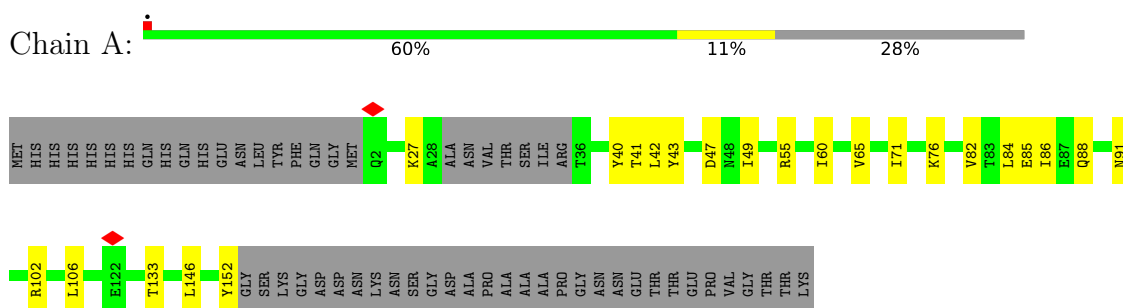


Mol	Chain	Residues	Atoms				AltConf
6	G	1	Total	C	O	P	0
			88	70	16	2	
6	G	1	Total	C	O	P	0
			88	70	16	2	

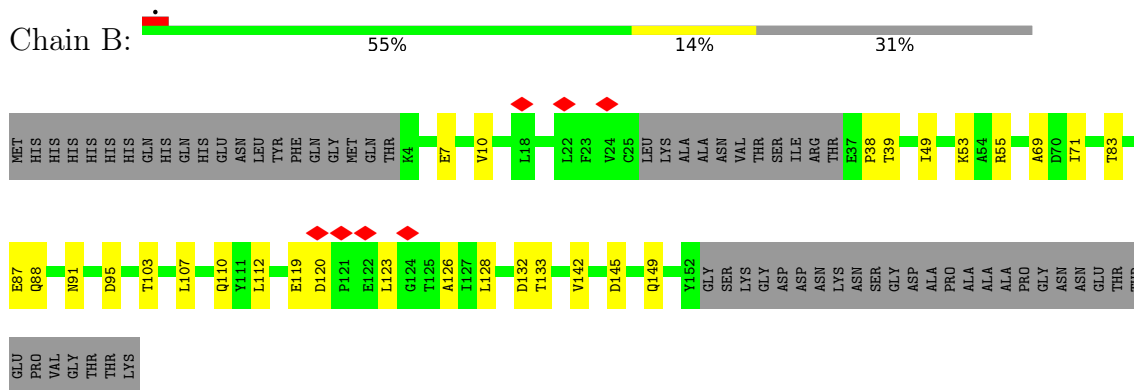
3 Residue-property plots [i](#)

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.

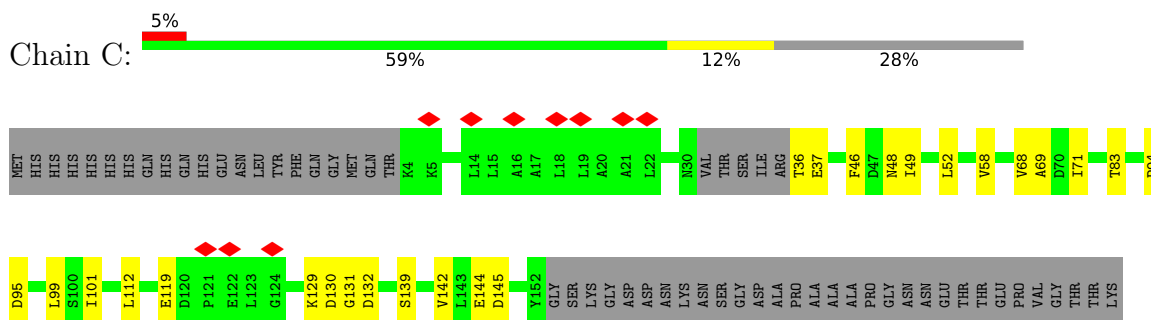
- Molecule 1: Phospholipid ABC transporter-binding protein MlaD



- Molecule 1: Phospholipid ABC transporter-binding protein MlaD

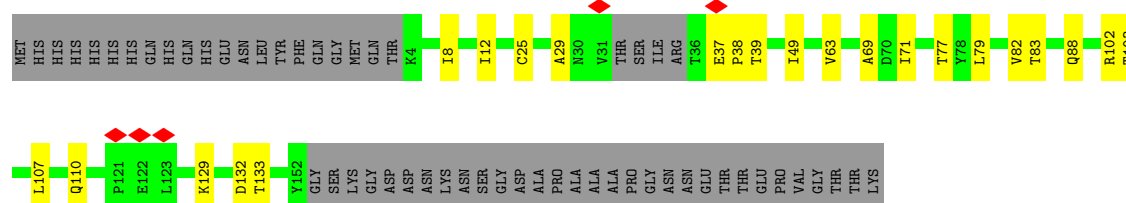


- Molecule 1: Phospholipid ABC transporter-binding protein MlaD

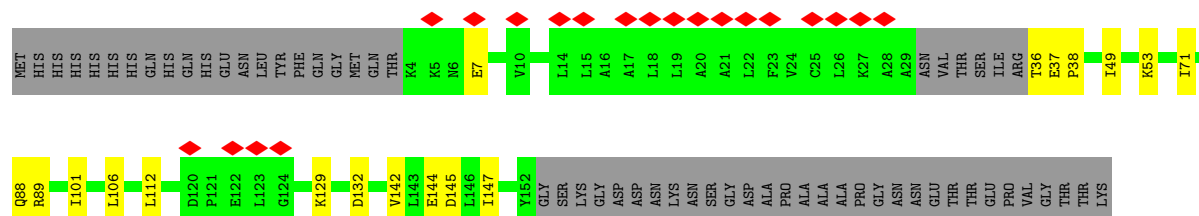


- Molecule 1: Phospholipid ABC transporter-binding protein MlaD

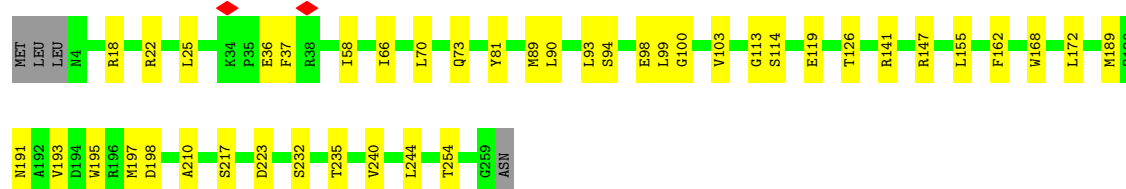
- Molecule 1: Phospholipid ABC transporter-binding protein MlaD



- Molecule 1: Phospholipid ABC transporter-binding protein MlaD

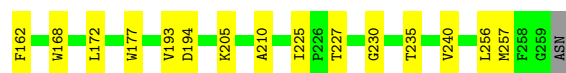


- Molecule 2: Phospholipid ABC transporter permease protein MlaE



- Molecule 2: Phospholipid ABC transporter permease protein MlaE





- Molecule 3: Phospholipid transport system ATP-binding protein MlaF

Chain I: 79% 19%



- Molecule 3: Phospholipid transport system ATP-binding protein MlaF

Chain J: 79% 19%



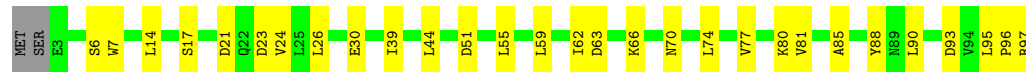
- Molecule 4: Phospholipid ABC transporter-binding protein MlaB

Chain K: 68% 30%



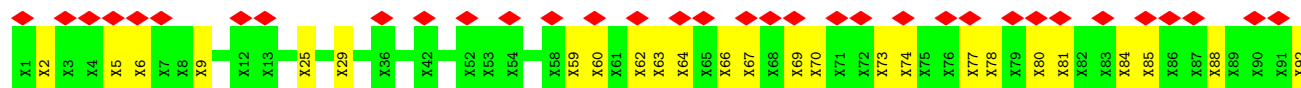
- Molecule 4: Phospholipid ABC transporter-binding protein MlaB

Chain L: 68% 30%

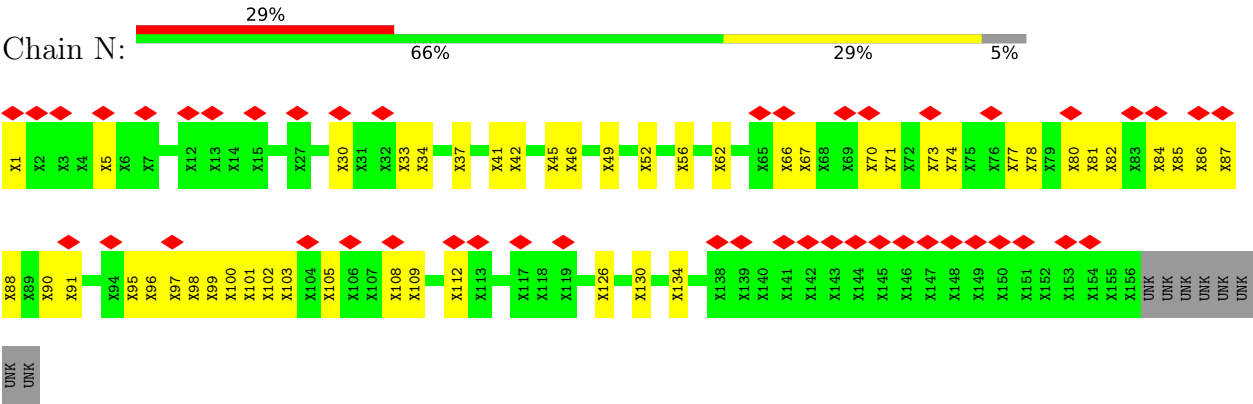


- Molecule 5: MSP1D1

Chain M: 34% 75% 25%



● Molecule 5: MSP1D1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	731205	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 ($e^-/\text{\AA}^2$)	71	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	29000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.904	Depositor
Minimum map value	-0.909	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.071	Depositor
Recommended contour level	0.27	Depositor
Map size (Å)	249.6, 249.6, 249.6	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.832, 0.832, 0.832	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: PEF

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	0.25	0/1126	0.47	0/1531
1	B	0.25	0/1081	0.43	0/1470
1	C	0.25	0/1047	0.47	0/1429
1	D	0.25	0/1113	0.43	0/1512
1	E	0.25	0/1130	0.45	0/1537
1	F	0.25	0/1042	0.47	0/1422
2	G	0.26	0/1964	0.45	0/2669
2	H	0.26	0/1956	0.44	0/2658
3	I	0.25	0/2036	0.43	0/2764
3	J	0.25	0/2036	0.43	0/2764
4	K	0.26	0/743	0.44	0/1008
4	L	0.26	0/743	0.44	0/1008
All	All	0.25	0/16017	0.44	0/21772

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	1108	0	1133	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1063	0	1082	21	0
1	C	1033	0	973	14	0
1	D	1096	0	1120	11	0
1	E	1112	0	1138	16	0
1	F	1028	0	971	21	0
2	G	1926	0	2029	46	0
2	H	1918	0	2023	37	0
3	I	1996	0	2039	30	0
3	J	1996	0	2039	32	0
4	K	734	0	755	20	0
4	L	734	0	755	21	0
5	M	821	0	166	22	0
5	N	780	0	158	29	0
6	G	88	0	134	9	0
All	All	17433	0	16515	298	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (298) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:53:LYS:CD	2:G:191:ASN:HD22	1.61	1.13
1:F:53:LYS:HD3	2:G:191:ASN:ND2	1.68	1.07
1:F:53:LYS:CD	2:G:191:ASN:ND2	2.30	0.91
1:F:53:LYS:CG	2:G:191:ASN:HD22	1.84	0.89
2:G:89:MET:HG3	2:G:193:VAL:HG21	1.53	0.87
2:H:93:LEU:HD21	2:H:193:VAL:HB	1.55	0.85
1:F:53:LYS:CG	2:G:191:ASN:ND2	2.44	0.80
1:A:55:ARG:HD3	2:G:195:TRP:HZ3	1.49	0.76
2:H:93:LEU:HD11	2:H:193:VAL:CG1	2.16	0.76
1:A:55:ARG:HE	2:G:195:TRP:HE3	1.31	0.76
1:A:43:TYR:HB2	1:A:133:THR:HG22	1.68	0.75
2:H:93:LEU:HD11	2:H:193:VAL:HG11	1.73	0.71
1:D:142:VAL:HG21	1:E:102:ARG:HD3	1.72	0.71
4:K:44:LEU:HD12	4:K:77:VAL:HG22	1.74	0.70
1:E:69:ALA:HB3	1:E:83:THR:HG23	1.75	0.69
5:N:77:UNK:O	5:N:81:UNK:N	2.24	0.69
1:A:55:ARG:HD3	2:G:195:TRP:CZ3	2.27	0.69
2:G:126:THR:O	2:G:126:THR:HG22	1.93	0.69
4:L:44:LEU:HD12	4:L:77:VAL:HG22	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:69:ALA:HB3	1:C:83:THR:HG23	1.76	0.68
5:M:66:UNK:O	5:M:70:UNK:N	2.27	0.68
4:L:6:SER:HG	4:L:17:SER:HG	1.43	0.66
2:G:58:ILE:HD12	2:H:240:VAL:HG13	1.77	0.66
4:K:6:SER:HG	4:K:17:SER:HG	1.41	0.66
1:F:53:LYS:HG2	2:G:191:ASN:HD22	1.58	0.65
2:G:240:VAL:HG13	2:H:58:ILE:HD12	1.78	0.65
2:H:114:SER:HB2	2:H:235:THR:HG23	1.77	0.65
2:G:70:LEU:HD11	2:G:99:LEU:HD12	1.79	0.64
1:F:53:LYS:HG2	2:G:191:ASN:ND2	2.13	0.64
5:N:73:UNK:O	5:N:77:UNK:N	2.30	0.64
1:B:88:GLN:NE2	1:B:91:ASN:OD1	2.31	0.64
2:G:22:ARG:NH1	2:G:223:ASP:OD2	2.31	0.64
2:G:114:SER:HB2	2:G:235:THR:HG23	1.79	0.63
2:H:70:LEU:HD11	2:H:99:LEU:HD12	1.78	0.63
3:J:22:CYS:HB3	3:J:221:LYS:HE3	1.80	0.63
5:N:130:UNK:O	5:N:134:UNK:N	2.32	0.63
5:M:74:UNK:O	5:M:78:UNK:N	2.33	0.62
5:M:99:UNK:O	5:M:103:UNK:N	2.33	0.62
1:F:37:GLU:OE2	1:F:89:ARG:NH1	2.33	0.62
3:I:22:CYS:HB3	3:I:221:LYS:HE3	1.80	0.62
1:F:129:LYS:N	1:F:132:ASP:OD2	2.31	0.62
5:N:62:UNK:O	5:N:66:UNK:N	2.33	0.62
5:N:84:UNK:O	5:N:88:UNK:N	2.33	0.61
4:K:85:ALA:HB1	4:K:90:LEU:HD12	1.82	0.61
5:N:30:UNK:O	5:N:34:UNK:N	2.33	0.61
2:G:232:SER:HB3	2:H:118:ALA:HB1	1.81	0.61
4:L:85:ALA:HB1	4:L:90:LEU:HD12	1.82	0.61
5:M:59:UNK:O	5:M:63:UNK:N	2.34	0.61
1:B:49:ILE:HD13	1:B:71:ILE:HG21	1.83	0.60
1:B:103:THR:HG22	1:B:110:GLN:HG2	1.82	0.60
5:N:81:UNK:O	5:N:85:UNK:N	2.34	0.60
2:H:227:THR:HG23	2:H:230:GLY:H	1.66	0.59
5:M:63:UNK:O	5:M:67:UNK:N	2.34	0.59
2:G:36:GLU:HA	2:G:141:ARG:HH12	1.67	0.59
5:M:77:UNK:O	5:M:81:UNK:N	2.34	0.59
1:A:71:ILE:HG12	1:A:82:VAL:HG12	1.85	0.58
4:L:7:TRP:HB2	4:L:14:LEU:HD11	1.85	0.58
5:M:69:UNK:O	5:M:73:UNK:N	2.36	0.58
1:B:53:LYS:NZ	2:H:75:TYR:OH	2.37	0.58
2:G:73:GLN:NE2	2:H:98:GLU:OE1	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:39:ILE:O	4:K:70:ASN:ND2	2.37	0.58
5:N:45:UNK:O	5:N:49:UNK:N	2.36	0.58
4:K:7:TRP:HB2	4:K:14:LEU:HD11	1.85	0.58
4:L:39:ILE:O	4:L:70:ASN:ND2	2.37	0.58
5:M:134:UNK:O	5:M:138:UNK:N	2.36	0.58
5:N:87:UNK:O	5:N:91:UNK:N	2.37	0.58
4:K:62:ILE:HD11	4:K:74:LEU:HD21	1.87	0.57
1:E:8:ILE:O	1:E:12:ILE:HG13	2.04	0.57
1:A:41:THR:HG22	1:A:85:GLU:HG2	1.86	0.57
1:E:49:ILE:HD13	1:E:71:ILE:HG21	1.87	0.57
5:N:86:UNK:O	5:N:90:UNK:N	2.38	0.57
4:L:62:ILE:HD11	4:L:74:LEU:HD21	1.87	0.57
5:N:70:UNK:O	5:N:74:UNK:N	2.38	0.56
1:D:69:ALA:HB3	1:D:83:THR:HG23	1.86	0.56
1:E:71:ILE:HG12	1:E:82:VAL:HG23	1.87	0.56
1:B:69:ALA:HB3	1:B:83:THR:HG23	1.87	0.56
2:G:89:MET:HG3	2:G:193:VAL:CG2	2.31	0.55
5:M:25:UNK:O	5:M:29:UNK:N	2.39	0.55
2:G:94:SER:HA	6:G:302:PEF:H351	1.87	0.55
5:M:62:UNK:O	5:M:66:UNK:N	2.39	0.55
1:B:10:VAL:HG11	2:G:25:LEU:HG	1.88	0.55
1:C:36:THR:OG1	1:C:37:GLU:N	2.40	0.55
5:N:105:UNK:O	5:N:109:UNK:N	2.40	0.55
2:H:93:LEU:CD1	2:H:193:VAL:HG11	2.36	0.55
1:B:55:ARG:NH2	2:H:177:TRP:O	2.40	0.55
3:I:232:LEU:O	3:I:241:ARG:NH2	2.38	0.55
1:D:49:ILE:HD13	1:D:71:ILE:HG21	1.89	0.55
2:G:155:LEU:HB3	2:G:210:ALA:HB2	1.89	0.55
2:H:155:LEU:HB3	2:H:210:ALA:HB2	1.89	0.55
3:J:95:ALA:O	3:J:157:ARG:NH1	2.40	0.54
3:J:51:LEU:HD22	3:J:167:MET:HB3	1.90	0.54
3:I:87:MET:HG2	3:I:165:LEU:HD23	1.89	0.54
3:I:95:ALA:O	3:I:157:ARG:NH1	2.41	0.54
4:L:66:LYS:NZ	4:L:93:ASP:O	2.41	0.54
1:A:55:ARG:NE	2:G:195:TRP:HE3	2.03	0.54
2:H:36:GLU:O	2:H:40:HIS:ND1	2.41	0.54
3:J:232:LEU:O	3:J:241:ARG:NH2	2.38	0.54
5:M:80:UNK:O	5:M:84:UNK:N	2.41	0.54
1:F:36:THR:OG1	1:F:37:GLU:N	2.41	0.54
1:E:103:THR:HG22	1:E:110:GLN:HG2	1.90	0.53
1:B:95:ASP:OD2	1:B:126:ALA:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:ILE:HD13	1:A:71:ILE:HG21	1.90	0.53
4:K:66:LYS:NZ	4:K:93:ASP:O	2.41	0.53
1:A:84:LEU:HD13	1:A:86:ILE:HG13	1.90	0.53
3:I:51:LEU:HD22	3:I:167:MET:HB3	1.90	0.53
5:N:97:UNK:O	5:N:101:UNK:N	2.42	0.53
3:I:151:ARG:NH2	3:I:171:PRO:O	2.41	0.53
3:J:87:MET:HG2	3:J:165:LEU:HD23	1.89	0.53
5:M:81:UNK:O	5:M:85:UNK:N	2.42	0.53
5:N:41:UNK:O	5:N:45:UNK:N	2.41	0.52
5:N:108:UNK:O	5:N:112:UNK:N	2.42	0.52
4:L:6:SER:OG	4:L:17:SER:OG	2.22	0.52
3:I:170:GLU:HG3	3:I:202:SER:HA	1.92	0.52
3:J:151:ARG:NH2	3:J:171:PRO:O	2.41	0.52
1:D:28:ALA:HA	2:H:194:ASP:CB	2.40	0.52
3:J:131:ALA:HB2	4:L:88:TYR:CD1	2.45	0.52
2:H:36:GLU:OE2	2:H:149:TRP:NE1	2.38	0.51
1:C:95:ASP:OD1	1:C:95:ASP:N	2.42	0.51
1:F:53:LYS:HB3	2:G:191:ASN:HD21	1.75	0.51
1:B:120:ASP:HB2	1:B:123:LEU:HB2	1.92	0.51
5:N:101:UNK:O	5:N:105:UNK:N	2.43	0.51
4:K:26:LEU:O	4:K:30:GLU:HG3	2.11	0.51
3:J:170:GLU:HG3	3:J:202:SER:HA	1.92	0.51
5:N:99:UNK:O	5:N:103:UNK:N	2.44	0.51
1:A:27:LYS:O	2:G:189:MET:HE3	2.11	0.51
1:E:29:ALA:HB2	2:H:256:LEU:HD23	1.92	0.51
5:M:5:UNK:O	5:M:9:UNK:N	2.44	0.51
1:C:52:LEU:HD21	1:C:68:VAL:HG21	1.93	0.51
1:E:38:PRO:HB2	1:E:88:GLN:H	1.76	0.50
1:F:53:LYS:CE	2:G:191:ASN:HD22	2.21	0.50
4:L:26:LEU:O	4:L:30:GLU:HG3	2.11	0.50
3:I:53:LEU:HD23	3:I:58:ILE:HG13	1.94	0.50
5:N:98:UNK:O	5:N:102:UNK:N	2.45	0.50
5:N:126:UNK:O	5:N:130:UNK:N	2.45	0.50
6:G:302:PEF:H221	2:H:90:LEU:HD11	1.93	0.50
3:I:131:ALA:HB2	4:K:88:TYR:CD1	2.46	0.50
1:F:101:ILE:HG12	1:F:112:LEU:HD23	1.93	0.49
4:K:23:ASP:OD1	4:K:24:VAL:HG13	2.12	0.49
1:B:132:ASP:OD1	1:B:133:THR:N	2.45	0.49
4:L:95:LEU:O	4:L:97:ARG:NH1	2.46	0.49
1:A:42:LEU:HB2	1:A:84:LEU:HD11	1.92	0.49
1:A:102:ARG:HG2	1:F:144:GLU:HG3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:53:LEU:HD23	3:J:58:ILE:HG13	1.94	0.49
4:L:23:ASP:OD1	4:L:24:VAL:HG13	2.12	0.49
1:C:94:PRO:HG3	1:C:119:GLU:HG3	1.95	0.49
2:H:119:GLU:OE2	2:H:147:ARG:NH2	2.35	0.49
4:K:95:LEU:O	4:K:97:ARG:NH1	2.46	0.49
3:I:106:VAL:HG21	3:I:129:LEU:HD21	1.95	0.49
1:E:77:THR:HG23	1:E:79:LEU:H	1.78	0.48
1:F:49:ILE:HD13	1:F:71:ILE:HG21	1.93	0.48
3:I:40:MET:HE1	3:I:209:LEU:HD21	1.95	0.48
5:N:52:UNK:O	5:N:56:UNK:N	2.45	0.48
1:D:132:ASP:OD1	1:D:133:THR:N	2.45	0.48
5:N:95:UNK:O	5:N:99:UNK:N	2.46	0.48
1:A:60:ILE:HG13	1:A:65:VAL:HG21	1.95	0.48
1:E:37:GLU:HA	1:E:39:THR:HG23	1.95	0.48
3:I:128:LYS:HE3	3:I:160:ALA:HA	1.95	0.48
3:J:128:LYS:HE3	3:J:160:ALA:HA	1.95	0.48
1:B:49:ILE:HD12	1:B:71:ILE:HD13	1.96	0.48
1:D:73:LEU:HG	1:E:63:VAL:HG11	1.95	0.48
2:G:126:THR:O	2:G:126:THR:CG2	2.61	0.48
1:A:146:LEU:HD11	1:F:147:ILE:HD13	1.96	0.48
1:D:5:LYS:NZ	2:H:49:TYR:OH	2.47	0.47
1:B:38:PRO:O	1:B:88:GLN:HB2	2.14	0.47
5:N:42:UNK:O	5:N:46:UNK:N	2.47	0.47
3:J:106:VAL:HG21	3:J:129:LEU:HD21	1.95	0.47
3:I:130:GLU:OE2	3:J:255:ARG:NH2	2.48	0.47
3:J:146:SER:OG	3:J:147:GLY:N	2.48	0.47
4:K:62:ILE:HD13	4:K:96:PRO:HD2	1.97	0.47
4:L:55:LEU:O	4:L:59:LEU:HG	2.15	0.47
1:E:132:ASP:OD1	1:E:133:THR:N	2.44	0.47
2:G:100:GLY:HA2	2:G:162:PHE:CE2	2.50	0.47
5:M:60:UNK:O	5:M:64:UNK:N	2.48	0.47
6:G:302:PEF:H332	6:G:302:PEF:H362	1.73	0.46
1:C:144:GLU:HG3	1:D:102:ARG:HG2	1.98	0.46
2:H:100:GLY:HA2	2:H:162:PHE:CE2	2.51	0.46
3:I:242:GLN:HE22	3:I:252:VAL:HB	1.81	0.46
5:M:102:UNK:O	5:M:106:UNK:N	2.48	0.46
1:F:7:GLU:O	2:H:10:GLY:HA3	2.16	0.46
5:N:67:UNK:O	5:N:71:UNK:N	2.49	0.46
1:C:49:ILE:HD13	1:C:71:ILE:HG21	1.98	0.46
1:C:58:VAL:HG22	1:C:112:LEU:HB2	1.97	0.46
1:F:142:VAL:HG23	1:F:145:ASP:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:62:ILE:HD13	4:L:96:PRO:HD2	1.97	0.46
1:C:46:PHE:HZ	1:C:99:LEU:HD23	1.81	0.46
2:G:93:LEU:HD22	2:G:198:ASP:OD2	2.15	0.46
1:E:49:ILE:HD12	1:E:71:ILE:HD13	1.97	0.46
6:G:301:PEF:H201	6:G:301:PEF:H172	1.72	0.46
2:G:66:ILE:CD1	2:G:103:VAL:HG11	2.46	0.46
3:J:40:MET:HE1	3:J:209:LEU:HD21	1.98	0.46
1:C:130:ASP:OD1	1:C:131:GLY:N	2.48	0.46
2:G:90:LEU:HD12	6:G:302:PEF:H312	1.98	0.46
2:G:36:GLU:HG2	2:G:37:PHE:HD1	1.80	0.46
3:I:146:SER:OG	3:I:147:GLY:N	2.48	0.46
4:K:21:ASP:OD1	4:K:21:ASP:N	2.49	0.46
1:B:7:GLU:HA	1:B:10:VAL:HG12	1.96	0.45
2:G:119:GLU:OE2	2:G:147:ARG:NH2	2.34	0.45
4:K:55:LEU:O	4:K:59:LEU:HG	2.15	0.45
4:L:21:ASP:OD1	4:L:21:ASP:N	2.49	0.45
1:A:27:LYS:HB3	2:G:189:MET:CE	2.47	0.45
1:A:152:TYR:HE1	1:B:149:GLN:HE22	1.62	0.45
1:D:2:GLN:N	1:D:2:GLN:OE1	2.49	0.45
1:B:7:GLU:OE2	2:G:18:ARG:HA	2.17	0.45
1:E:107:LEU:HD11	6:G:301:PEF:H212	1.99	0.45
3:I:255:ARG:NH2	3:J:130:GLU:OE2	2.49	0.45
2:H:55:SER:O	2:H:55:SER:OG	2.33	0.45
5:N:91:UNK:O	5:N:95:UNK:N	2.49	0.45
3:J:242:GLN:HE22	3:J:252:VAL:HB	1.81	0.45
1:E:25:CYS:HB3	2:H:256:LEU:HD21	1.98	0.45
3:J:39:ILE:HB	3:J:201:VAL:HG22	1.99	0.45
1:A:47:ASP:OD1	1:A:47:ASP:N	2.49	0.45
1:B:119:GLU:OE1	1:B:119:GLU:N	2.46	0.45
1:C:129:LYS:N	1:C:132:ASP:OD2	2.50	0.45
1:B:39:THR:HG22	1:B:87:GLU:HA	1.99	0.44
5:M:128:UNK:O	5:M:132:UNK:N	2.50	0.44
3:I:39:ILE:HB	3:I:201:VAL:HG22	1.99	0.44
4:K:6:SER:OG	4:K:17:SER:OG	2.22	0.44
1:D:36:THR:OG1	1:D:37:GLU:N	2.51	0.44
3:I:135:ARG:NH1	3:J:260:ASP:O	2.49	0.44
3:I:202:SER:OG	3:I:203:HIS:N	2.51	0.44
4:L:80:LYS:HB2	4:L:80:LYS:HE3	1.79	0.44
5:M:133:UNK:O	5:M:137:UNK:N	2.51	0.44
3:J:202:SER:OG	3:J:203:HIS:N	2.51	0.43
2:H:108:PHE:O	2:H:113:GLY:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:225:ILE:HG22	2:H:227:THR:HG22	2.00	0.43
3:I:101:ASN:O	3:I:105:ASN:ND2	2.45	0.43
3:I:260:ASP:O	3:J:135:ARG:NH1	2.49	0.43
5:N:96:UNK:O	5:N:100:UNK:N	2.52	0.43
2:G:36:GLU:HA	2:G:141:ARG:NH1	2.33	0.43
2:G:168:TRP:CH2	2:G:172:LEU:HD11	2.54	0.43
6:G:302:PEF:H402	2:H:99:LEU:HD11	2.00	0.43
2:H:145:SER:OG	2:H:146:PRO:HD3	2.19	0.43
1:C:101:ILE:HG12	1:C:112:LEU:HD23	2.00	0.43
2:H:168:TRP:CH2	2:H:172:LEU:HD11	2.54	0.43
5:M:88:UNK:O	5:M:92:UNK:N	2.51	0.43
2:H:135:MET:HE1	3:J:157:ARG:HH21	1.83	0.43
3:I:181:GLY:HA2	3:I:184:VAL:HG12	2.01	0.43
5:M:2:UNK:O	5:M:6:UNK:N	2.52	0.43
4:K:21:ASP:HA	4:K:51:ASP:OD1	2.19	0.43
4:L:23:ASP:OD1	4:L:24:VAL:N	2.52	0.43
5:N:80:UNK:O	5:N:84:UNK:N	2.52	0.43
3:J:181:GLY:HA2	3:J:184:VAL:HG12	2.01	0.42
2:G:113:GLY:O	2:G:217:SER:HB2	2.19	0.42
5:M:142:UNK:O	5:M:146:UNK:N	2.52	0.42
1:A:88:GLN:HE21	1:A:91:ASN:ND2	2.17	0.42
1:D:27:LYS:HA	1:D:27:LYS:HD3	1.87	0.42
4:K:82:TYR:OH	4:K:97:ARG:O	2.29	0.42
4:L:21:ASP:HA	4:L:51:ASP:OD1	2.19	0.42
1:E:129:LYS:HE2	1:E:129:LYS:HB3	1.84	0.42
3:J:92:GLN:O	3:J:151:ARG:NE	2.48	0.42
4:L:55:LEU:HD21	4:L:81:VAL:HG13	2.02	0.42
4:K:23:ASP:OD1	4:K:24:VAL:N	2.52	0.42
1:F:38:PRO:O	1:F:88:GLN:HB2	2.18	0.42
2:H:36:GLU:HB2	2:H:141:ARG:HH12	1.84	0.42
2:G:36:GLU:HG2	2:G:37:PHE:CD1	2.54	0.42
5:M:127:UNK:O	5:M:131:UNK:N	2.53	0.42
5:N:33:UNK:O	5:N:37:UNK:N	2.53	0.42
6:G:302:PEF:H361	6:G:302:PEF:H392	1.58	0.42
3:I:39:ILE:HG21	3:I:50:LEU:HD23	2.02	0.42
5:N:78:UNK:O	5:N:82:UNK:N	2.53	0.42
3:J:13:ASP:H	3:J:28:SER:HB3	1.85	0.41
1:A:76:LYS:HA	1:A:76:LYS:HD2	1.86	0.41
1:B:142:VAL:HG23	1:B:145:ASP:HB2	2.03	0.41
3:J:131:ALA:HB2	4:L:88:TYR:HD1	1.85	0.41
1:A:88:GLN:HE21	1:A:91:ASN:HD21	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:ASN:N	1:C:139:SER:OG	2.48	0.41
3:J:39:ILE:HG21	3:J:50:LEU:HD23	2.02	0.41
4:K:80:LYS:HB2	4:K:80:LYS:HE3	1.79	0.41
3:I:45:ILE:HD13	3:I:218:LEU:HD23	2.02	0.41
3:I:49:THR:HG23	3:I:58:ILE:HD11	2.03	0.41
3:I:67:PHE:HB2	3:I:72:ILE:HD11	2.02	0.41
2:H:139:PRO:O	2:H:143:VAL:HG12	2.20	0.41
3:I:100:MET:HB2	3:I:104:ASP:HB2	2.02	0.41
3:J:45:ILE:HD13	3:J:218:LEU:HD23	2.02	0.41
5:N:1:UNK:O	5:N:5:UNK:N	2.53	0.41
1:A:40:TYR:CE2	1:A:42:LEU:HD11	2.55	0.41
3:I:13:ASP:H	3:I:28:SER:HB3	1.85	0.41
3:J:137:ALA:HA	3:J:140:LEU:HD13	2.02	0.41
1:F:53:LYS:CB	2:G:191:ASN:ND2	2.84	0.41
2:H:38:ARG:HD3	2:H:38:ARG:HA	1.82	0.41
3:J:49:THR:HG23	3:J:58:ILE:HD11	2.03	0.41
4:K:55:LEU:HD21	4:K:81:VAL:HG13	2.02	0.41
2:G:81:TYR:OH	6:G:301:PEF:H121	2.21	0.41
2:G:98:GLU:OE2	2:G:254:THR:OG1	2.38	0.41
3:J:67:PHE:HB2	3:J:72:ILE:HD11	2.02	0.41
1:A:106:LEU:HD23	1:F:106:LEU:HD22	2.03	0.40
1:B:95:ASP:HA	1:B:128:LEU:HD21	2.03	0.40
1:B:107:LEU:O	2:H:82:SER:HB3	2.21	0.40
1:B:112:LEU:HD23	1:B:112:LEU:HA	1.91	0.40
5:M:156:UNK:O	5:M:160:UNK:N	2.54	0.40
1:C:142:VAL:HG23	1:C:145:ASP:OD1	2.22	0.40
2:G:99:LEU:HD23	2:G:99:LEU:HA	1.87	0.40
2:H:205:LYS:HE3	2:H:257:MET:HE1	2.02	0.40
3:J:100:MET:HB2	3:J:104:ASP:HB2	2.02	0.40
2:G:244:LEU:HD21	2:H:58:ILE:HG13	2.03	0.40
3:I:137:ALA:HA	3:I:140:LEU:HD13	2.02	0.40
3:I:266:LEU:HD13	4:L:63:ASP:HB2	2.04	0.40
3:J:85:LYS:HE2	3:J:113:HIS:ND1	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	140/201 (70%)	136 (97%)	4 (3%)	0	100	100
1	B	134/201 (67%)	129 (96%)	5 (4%)	0	100	100
1	C	140/201 (70%)	137 (98%)	3 (2%)	0	100	100
1	D	137/201 (68%)	134 (98%)	3 (2%)	0	100	100
1	E	141/201 (70%)	131 (93%)	10 (7%)	0	100	100
1	F	139/201 (69%)	132 (95%)	7 (5%)	0	100	100
2	G	254/260 (98%)	248 (98%)	6 (2%)	0	100	100
2	H	253/260 (97%)	242 (96%)	11 (4%)	0	100	100
3	I	261/269 (97%)	253 (97%)	8 (3%)	0	100	100
3	J	261/269 (97%)	253 (97%)	8 (3%)	0	100	100
4	K	93/97 (96%)	90 (97%)	3 (3%)	0	100	100
4	L	93/97 (96%)	90 (97%)	3 (3%)	0	100	100
All	All	2046/2458 (83%)	1975 (96%)	71 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	121/167 (72%)	121 (100%)	0	100	100
1	B	116/167 (70%)	116 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	100/167 (60%)	100 (100%)	0	100	100
1	D	119/167 (71%)	119 (100%)	0	100	100
1	E	121/167 (72%)	121 (100%)	0	100	100
1	F	100/167 (60%)	100 (100%)	0	100	100
2	G	205/209 (98%)	204 (100%)	1 (0%)	88	94
2	H	204/209 (98%)	204 (100%)	0	100	100
3	I	215/220 (98%)	215 (100%)	0	100	100
3	J	215/220 (98%)	215 (100%)	0	100	100
4	K	82/84 (98%)	82 (100%)	0	100	100
4	L	82/84 (98%)	82 (100%)	0	100	100
All	All	1680/2028 (83%)	1679 (100%)	1 (0%)	93	97

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	G	197	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	88	GLN
1	B	88	GLN
1	B	91	ASN
1	B	149	GLN
1	C	135	GLN
1	D	2	GLN
2	G	191	ASN
3	I	191	ASN
3	I	226	HIS
3	J	191	ASN
3	J	226	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	PEF	G	301	-	43,43,46	1.06	2 (4%)	47,48,51	0.91	2 (4%)
6	PEF	G	302	-	43,43,46	1.06	2 (4%)	47,48,51	0.93	2 (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
6	PEF	G	301	-	-	24/45/45/50	-
6	PEF	G	302	-	-	27/45/45/50	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	302	PEF	O2-C10	3.68	1.44	1.34
6	G	301	PEF	O2-C10	3.62	1.44	1.34
6	G	302	PEF	O3-C30	2.67	1.41	1.33
6	G	301	PEF	O3-C30	2.67	1.41	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	302	PEF	O2-C10-C11	3.88	119.87	111.50
6	G	301	PEF	O2-C10-C11	3.84	119.77	111.50
6	G	301	PEF	O3-C30-C31	2.67	120.29	111.91
6	G	302	PEF	O3-C30-C31	2.64	120.20	111.91

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	G	301	PEF	C31-C30-O3-C3
6	G	301	PEF	O5-C30-O3-C3
6	G	302	PEF	C31-C30-O3-C3
6	G	302	PEF	O5-C30-O3-C3
6	G	301	PEF	C34-C35-C36-C37
6	G	302	PEF	C36-C37-C38-C39
6	G	301	PEF	C17-C18-C19-C20
6	G	301	PEF	C10-C11-C12-C13
6	G	302	PEF	C11-C12-C13-C14
6	G	301	PEF	C39-C40-C41-C42
6	G	302	PEF	C21-C22-C23-C24
6	G	302	PEF	C39-C40-C41-C42
6	G	302	PEF	C12-C13-C14-C15
6	G	301	PEF	C38-C39-C40-C41
6	G	302	PEF	C31-C32-C33-C34
6	G	301	PEF	C12-C13-C14-C15
6	G	301	PEF	C21-C22-C23-C24
6	G	302	PEF	C34-C35-C36-C37
6	G	301	PEF	C42-C43-C44-C45
6	G	301	PEF	C11-C10-O2-C2
6	G	302	PEF	C42-C43-C44-C45
6	G	301	PEF	C31-C32-C33-C34
6	G	302	PEF	C35-C36-C37-C38
6	G	302	PEF	O3P-C1-C2-O2
6	G	302	PEF	C22-C23-C24-C25
6	G	301	PEF	O2-C2-C3-O3
6	G	301	PEF	C22-C23-C24-C25
6	G	302	PEF	C10-C11-C12-C13
6	G	301	PEF	C35-C36-C37-C38
6	G	302	PEF	C38-C39-C40-C41
6	G	301	PEF	O4-C10-O2-C2
6	G	301	PEF	C36-C37-C38-C39
6	G	301	PEF	C1-C2-C3-O3
6	G	302	PEF	O3P-C1-C2-C3

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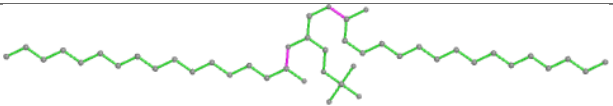
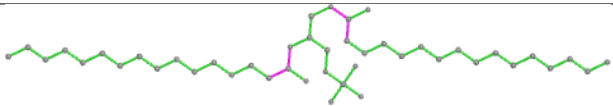
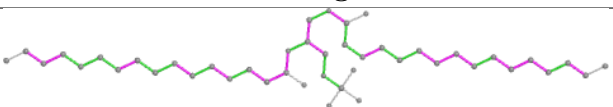
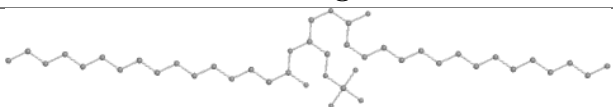
Mol	Chain	Res	Type	Atoms
6	G	302	PEF	C16-C17-C18-C19
6	G	301	PEF	C14-C15-C16-C17
6	G	302	PEF	C15-C16-C17-C18
6	G	302	PEF	O2-C2-C3-O3
6	G	302	PEF	C14-C15-C16-C17
6	G	302	PEF	C13-C14-C15-C16
6	G	301	PEF	C40-C41-C42-C43
6	G	301	PEF	O3P-C1-C2-O2
6	G	302	PEF	C30-C31-C32-C33
6	G	302	PEF	C32-C33-C34-C35
6	G	302	PEF	C1-C2-C3-O3
6	G	302	PEF	C33-C34-C35-C36
6	G	301	PEF	O3P-C1-C2-C3
6	G	301	PEF	O2-C10-C11-C12
6	G	302	PEF	O2-C10-C11-C12
6	G	301	PEF	O4-C10-C11-C12
6	G	302	PEF	O4-C10-C11-C12

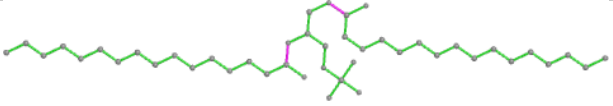
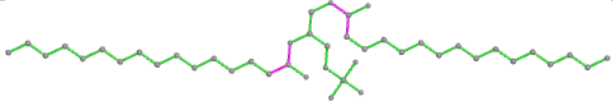
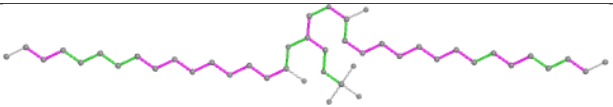
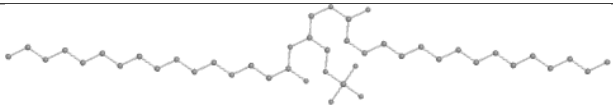
There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	G	301	PEF	3	0
6	G	302	PEF	6	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 PEF G 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PEF G 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

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.

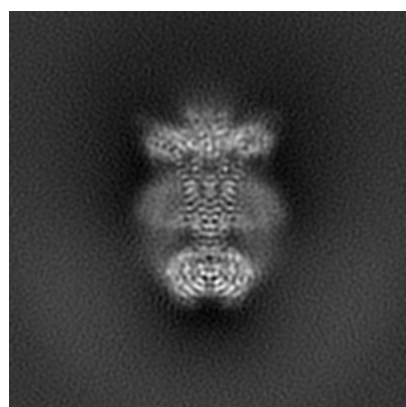
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22116. These allow visual inspection of the internal detail of the map and identification of artifacts.

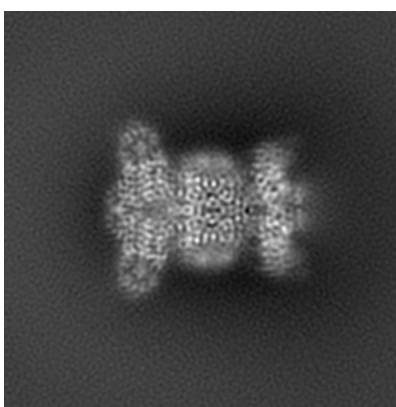
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

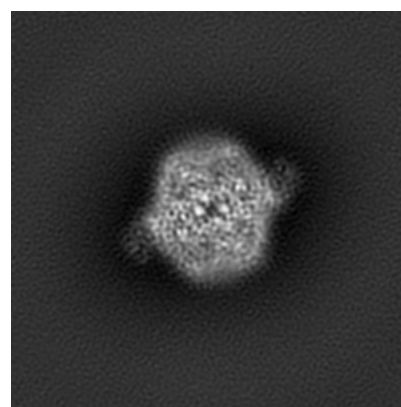
6.1.1 Primary map



X



Y

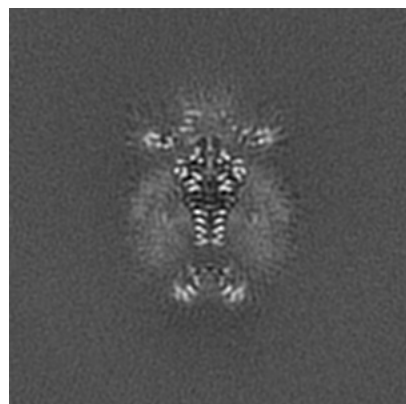


Z

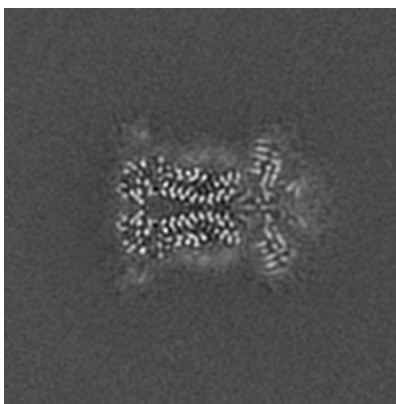
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

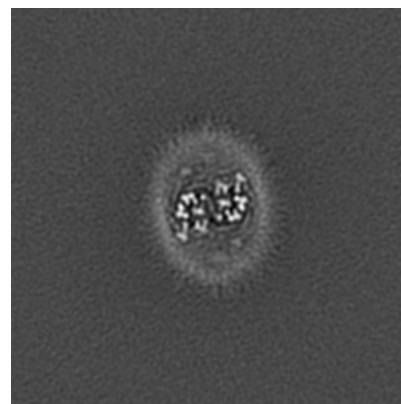
6.2.1 Primary map



X Index: 150



Y Index: 150

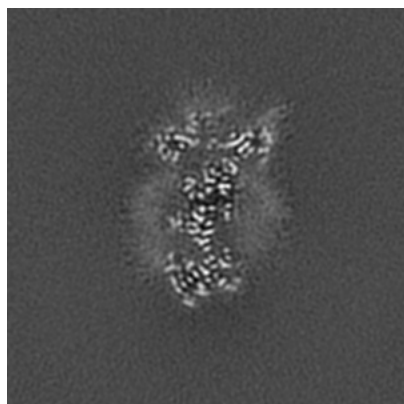


Z Index: 150

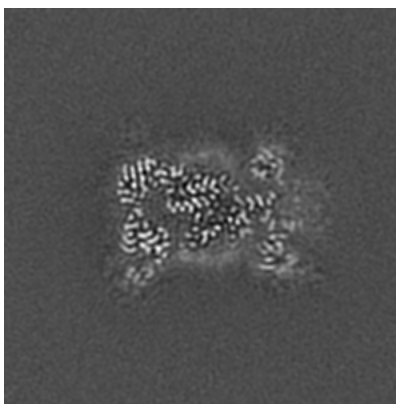
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

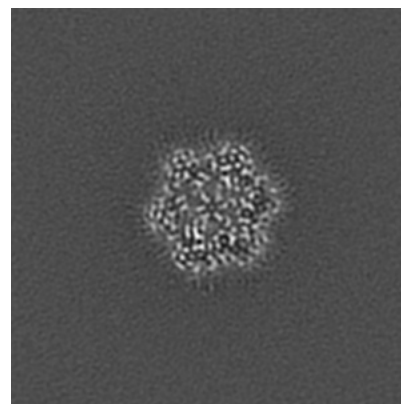
6.3.1 Primary map



X Index: 162



Y Index: 144

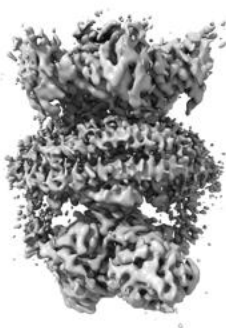


Z Index: 198

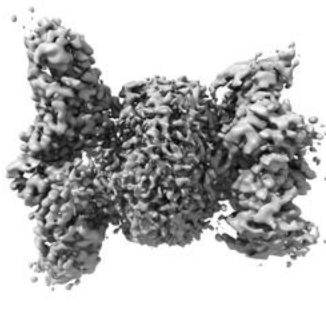
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

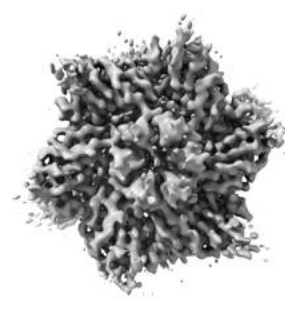
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.27. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

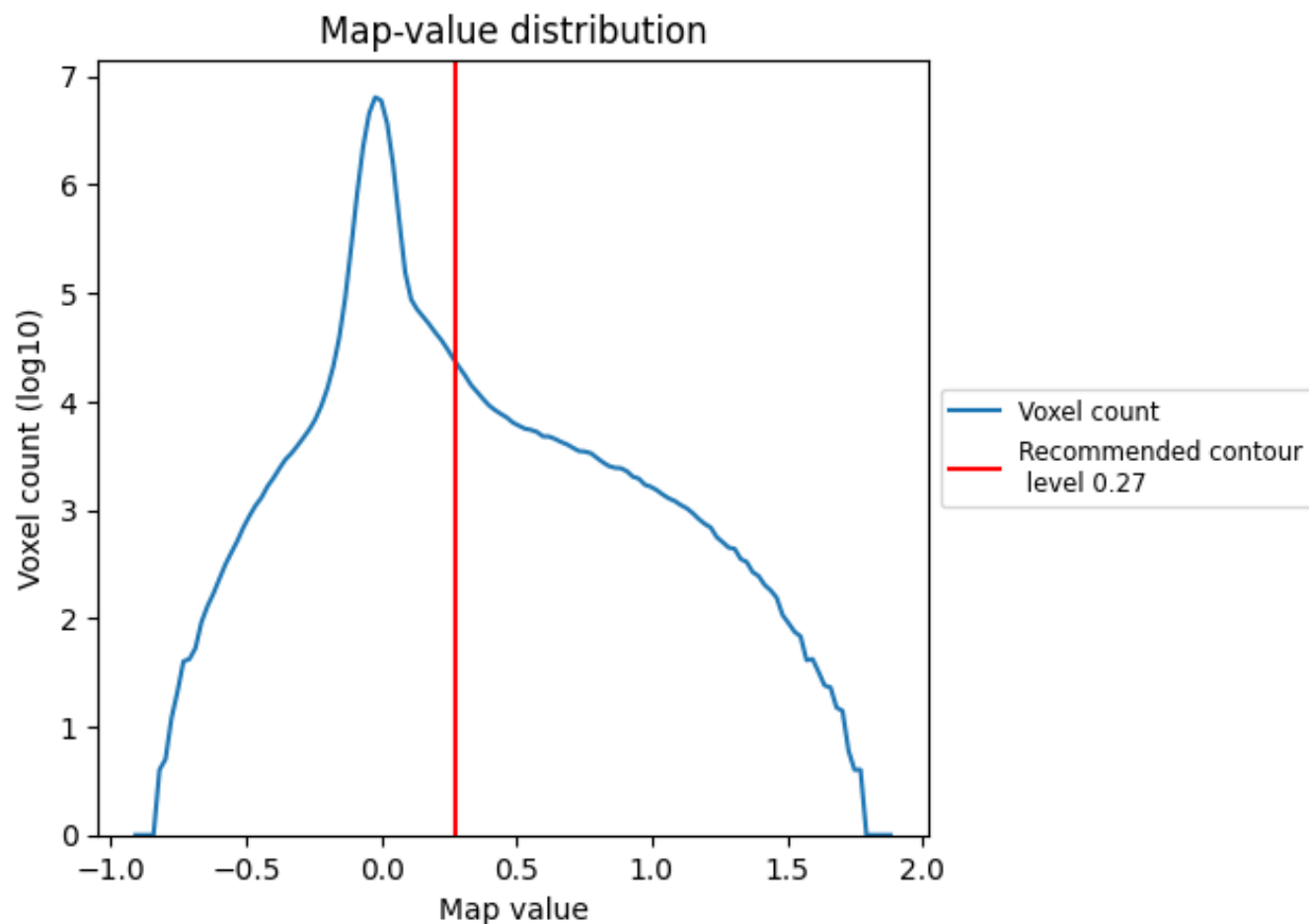
6.5 Mask visualisation

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

7 Map analysis [i](#)

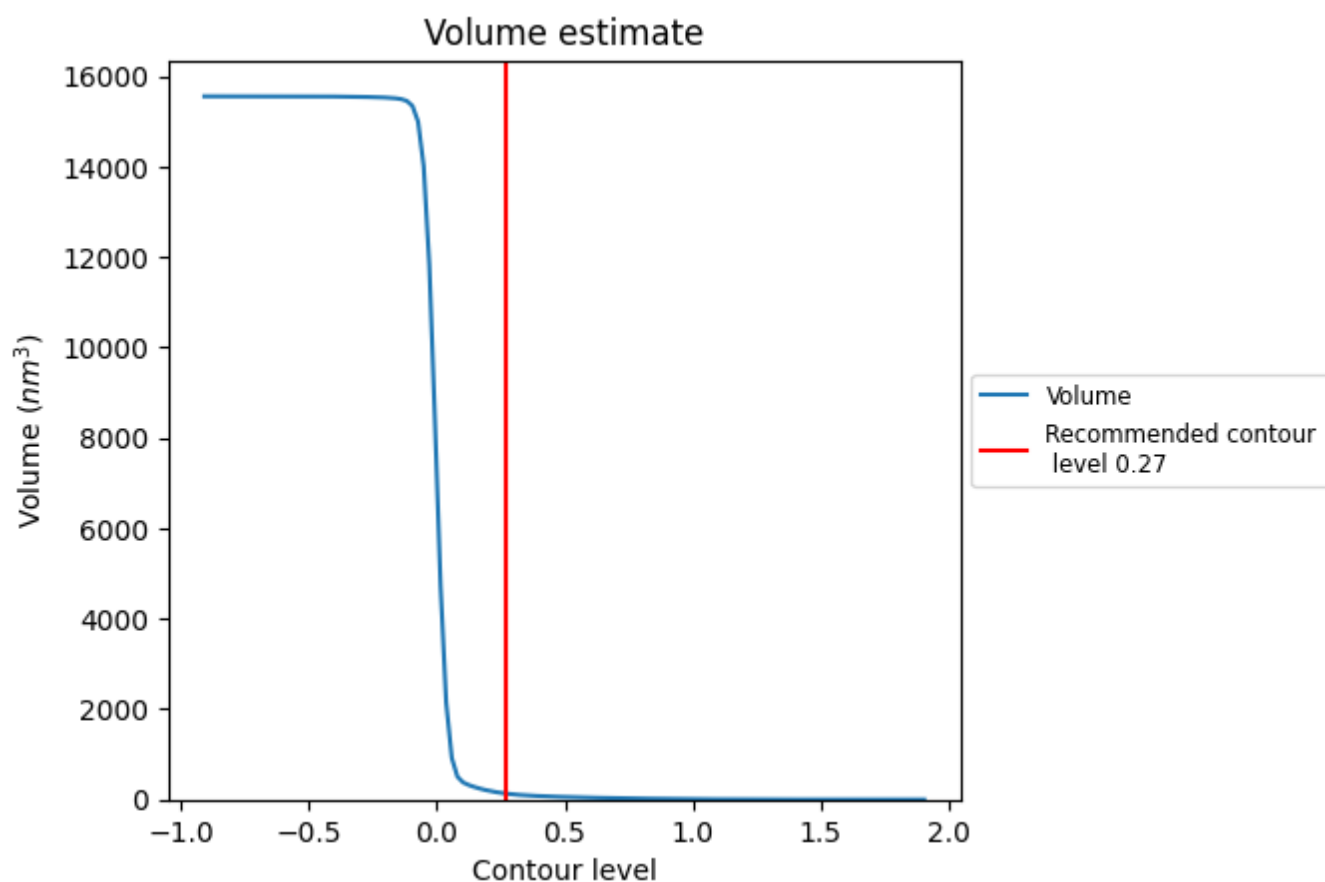
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

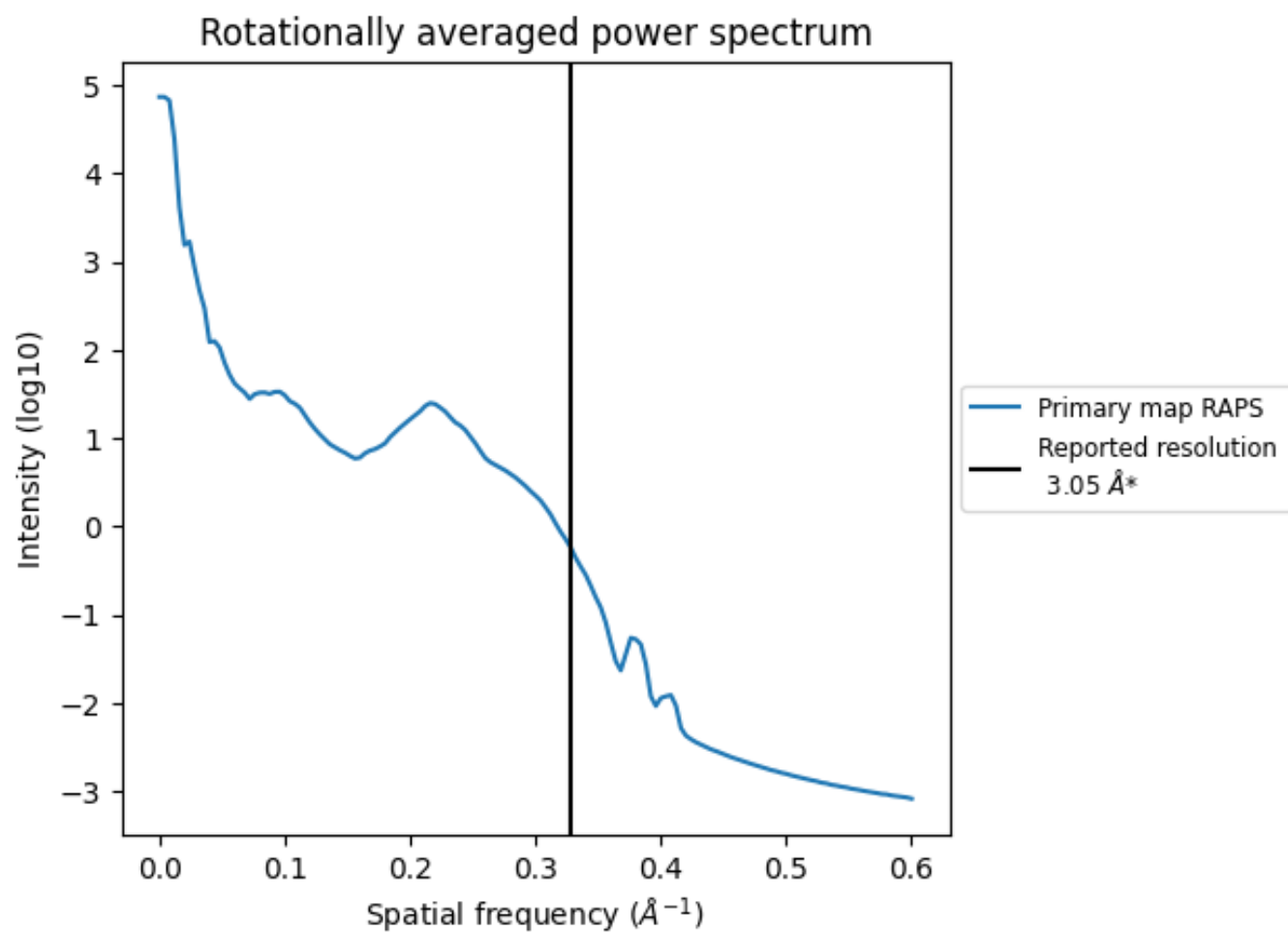
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 132 nm³; this corresponds to an approximate mass of 120 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 0.328 Å⁻¹

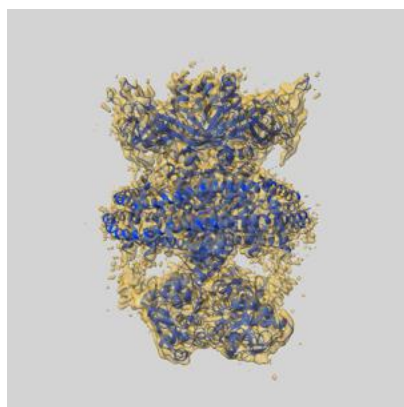
8 Fourier-Shell correlation

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

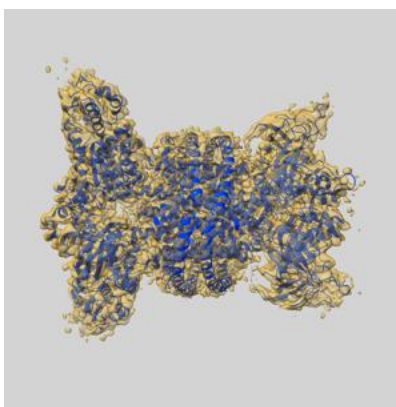
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-22116 and PDB model 6XBD. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

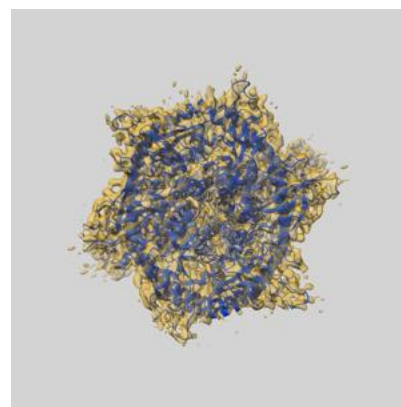
9.1 Map-model overlay [i](#)



X



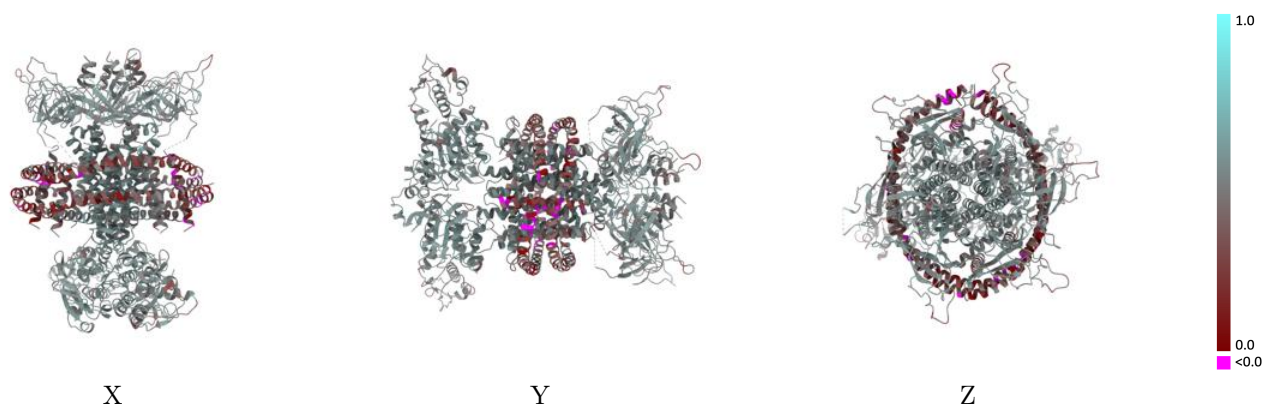
Y



Z

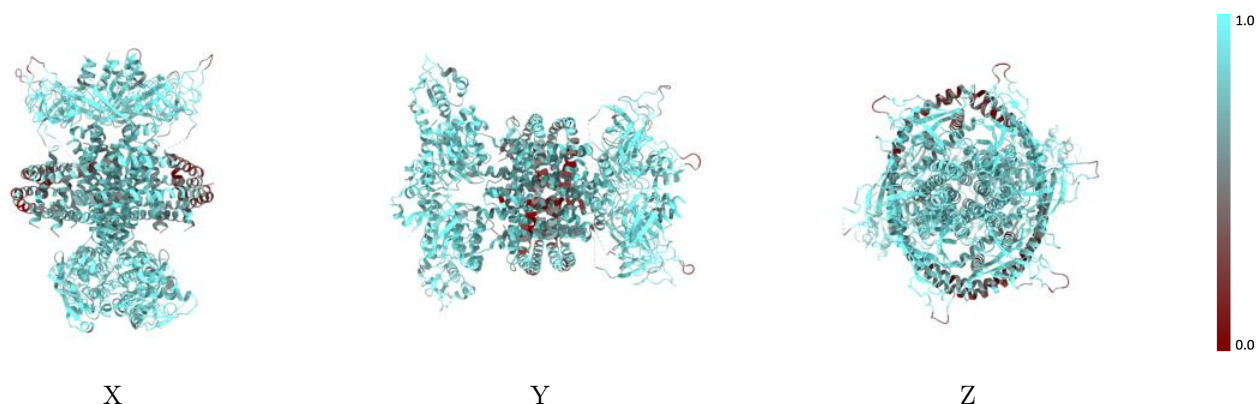
The images above show the 3D surface view of the map at the recommended contour level 0.27 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



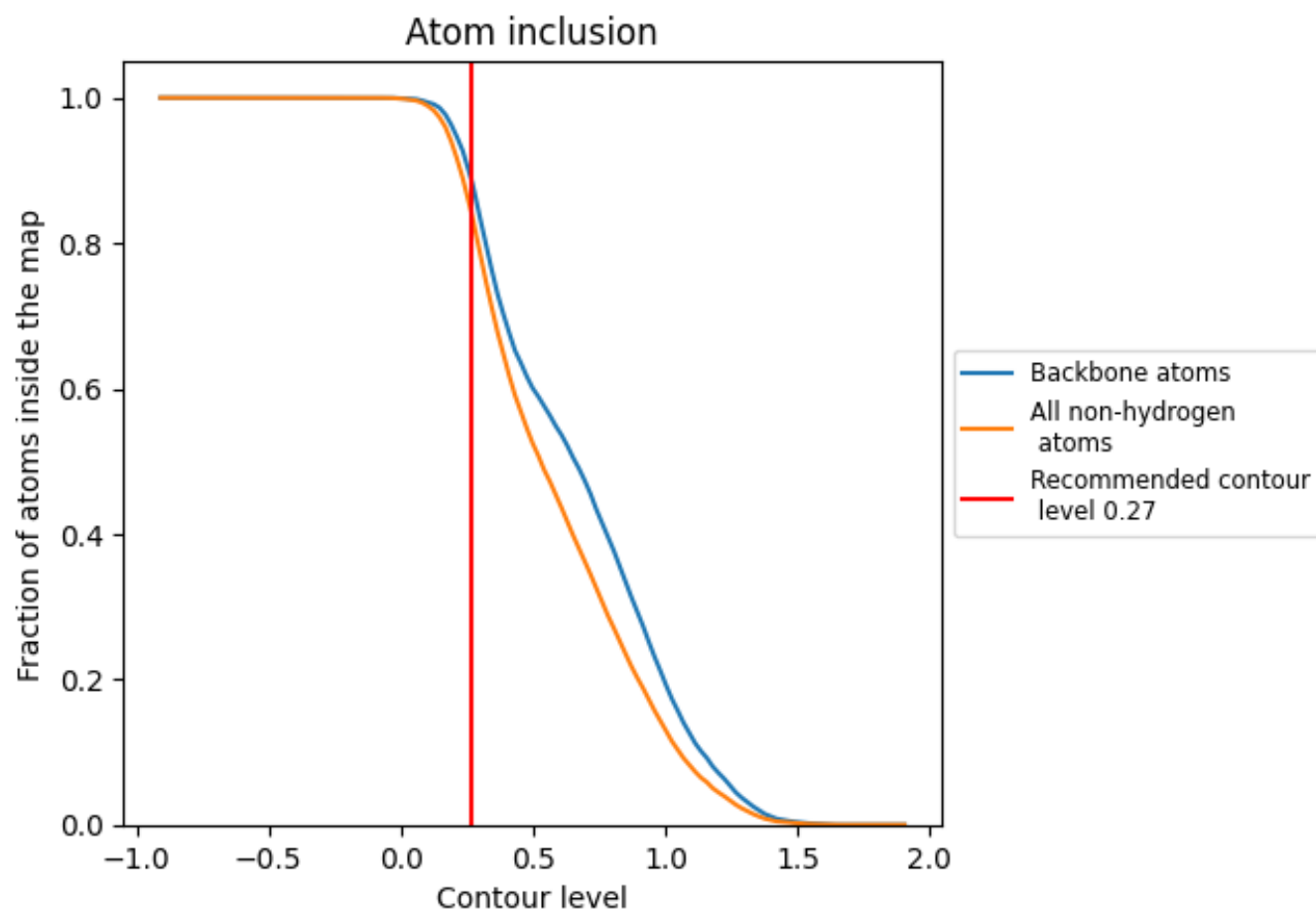
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.27).































9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 84% 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 (0.27) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8372	 0.4890
A	 0.8478	 0.5030
B	 0.8270	 0.4930
C	 0.8505	 0.4940
D	 0.8647	 0.5060
E	 0.8311	 0.4940
F	 0.8043	 0.4680
G	 0.8655	 0.5350
H	 0.8698	 0.5330
I	 0.9009	 0.5360
J	 0.8937	 0.5360
K	 0.8296	 0.4880
L	 0.8380	 0.4710
M	 0.6054	 0.2450
N	 0.6308	 0.2680

