



Full wwPDB EM Validation Report ⓘ

Nov 13, 2022 – 09:53 AM EST

PDB ID : 6X4S
EMDB ID : EMD-22042
Title : MCU-EMRE complex of a metazoan mitochondrial calcium uniporter
Authors : Long, S.B.; Wang, C.; Baradaran, R.
Deposited on : 2020-05-22
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
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

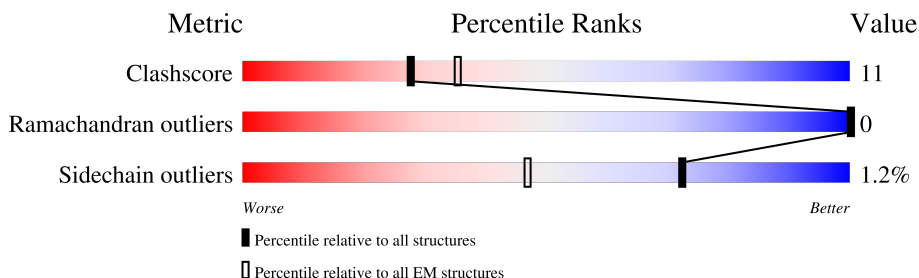
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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	243	<div> <div>5%</div> <div>50%</div> <div>13%</div> <div>37%</div> </div>
1	B	243	<div> <div>6%</div> <div>46%</div> <div>16%</div> <div>38%</div> </div>
1	C	243	<div> <div>5%</div> <div>49%</div> <div>14%</div> <div>37%</div> </div>
1	D	243	<div> <div>5%</div> <div>45%</div> <div>17%</div> <div>38%</div> </div>
1	E	243	<div> <div>8%</div> <div>90%</div> </div>
1	F	243	<div> <div>9%</div> <div>90%</div> </div>
1	G	243	<div> <div>9%</div> <div>90%</div> </div>
1	H	243	<div> <div>8%</div> <div>90%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5373 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 Calcium uniporter protein, Protein EMRE homolog, mitochondrial-like Protein fusion.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	152	Total	C	N	O	S	0	0
			1158	758	192	204	4		
1	B	151	Total	C	N	O	S	0	0
			1170	764	191	211	4		
1	C	152	Total	C	N	O	S	0	0
			1155	755	192	204	4		
1	D	151	Total	C	N	O	S	0	0
			1165	760	191	211	3		
1	E	25	Total	C	N	O		0	0
			181	121	31	29			
1	F	25	Total	C	N	O		0	0
			181	121	31	29			
1	G	25	Total	C	N	O		0	0
			181	121	31	29			
1	H	25	Total	C	N	O		0	0
			181	121	31	29			

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	159	GLY	-	expression tag	UNP D6WIX5
A	160	PRO	-	expression tag	UNP D6WIX5
A	161	THR	-	expression tag	UNP D6WIX5
A	162	ALA	-	expression tag	UNP D6WIX5
A	163	ALA	-	expression tag	UNP D6WIX5
A	164	ALA	-	expression tag	UNP D6WIX5
A	165	LEU	-	expression tag	UNP D6WIX5
A	349	SER	-	linker	UNP D6WIX5
A	350	GLY	-	linker	UNP D6WIX5
A	351	SER	-	linker	UNP D6WIX5
A	352	GLY	-	linker	UNP D6WIX5
A	353	SER	-	linker	UNP D6WIX5
A	354	GLY	-	linker	UNP D6WIX5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	355	GLU	-	linker	UNP D6WIX5
A	356	ASN	-	linker	UNP D6WIX5
A	357	LEU	-	linker	UNP D6WIX5
A	358	TYR	-	linker	UNP D6WIX5
A	359	PHE	-	linker	UNP D6WIX5
A	360	GLN	-	linker	UNP D6WIX5
A	361	GLY	-	linker	UNP D6WIX5
B	159	GLY	-	expression tag	UNP D6WIX5
B	160	PRO	-	expression tag	UNP D6WIX5
B	161	THR	-	expression tag	UNP D6WIX5
B	162	ALA	-	expression tag	UNP D6WIX5
B	163	ALA	-	expression tag	UNP D6WIX5
B	164	ALA	-	expression tag	UNP D6WIX5
B	165	LEU	-	expression tag	UNP D6WIX5
B	349	SER	-	linker	UNP D6WIX5
B	350	GLY	-	linker	UNP D6WIX5
B	351	SER	-	linker	UNP D6WIX5
B	352	GLY	-	linker	UNP D6WIX5
B	353	SER	-	linker	UNP D6WIX5
B	354	GLY	-	linker	UNP D6WIX5
B	355	GLU	-	linker	UNP D6WIX5
B	356	ASN	-	linker	UNP D6WIX5
B	357	LEU	-	linker	UNP D6WIX5
B	358	TYR	-	linker	UNP D6WIX5
B	359	PHE	-	linker	UNP D6WIX5
B	360	GLN	-	linker	UNP D6WIX5
B	361	GLY	-	linker	UNP D6WIX5
C	159	GLY	-	expression tag	UNP D6WIX5
C	160	PRO	-	expression tag	UNP D6WIX5
C	161	THR	-	expression tag	UNP D6WIX5
C	162	ALA	-	expression tag	UNP D6WIX5
C	163	ALA	-	expression tag	UNP D6WIX5
C	164	ALA	-	expression tag	UNP D6WIX5
C	165	LEU	-	expression tag	UNP D6WIX5
C	349	SER	-	linker	UNP D6WIX5
C	350	GLY	-	linker	UNP D6WIX5
C	351	SER	-	linker	UNP D6WIX5
C	352	GLY	-	linker	UNP D6WIX5
C	353	SER	-	linker	UNP D6WIX5
C	354	GLY	-	linker	UNP D6WIX5
C	355	GLU	-	linker	UNP D6WIX5
C	356	ASN	-	linker	UNP D6WIX5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	357	LEU	-	linker	UNP D6WIX5
C	358	TYR	-	linker	UNP D6WIX5
C	359	PHE	-	linker	UNP D6WIX5
C	360	GLN	-	linker	UNP D6WIX5
C	361	GLY	-	linker	UNP D6WIX5
D	159	GLY	-	expression tag	UNP D6WIX5
D	160	PRO	-	expression tag	UNP D6WIX5
D	161	THR	-	expression tag	UNP D6WIX5
D	162	ALA	-	expression tag	UNP D6WIX5
D	163	ALA	-	expression tag	UNP D6WIX5
D	164	ALA	-	expression tag	UNP D6WIX5
D	165	LEU	-	expression tag	UNP D6WIX5
D	349	SER	-	linker	UNP D6WIX5
D	350	GLY	-	linker	UNP D6WIX5
D	351	SER	-	linker	UNP D6WIX5
D	352	GLY	-	linker	UNP D6WIX5
D	353	SER	-	linker	UNP D6WIX5
D	354	GLY	-	linker	UNP D6WIX5
D	355	GLU	-	linker	UNP D6WIX5
D	356	ASN	-	linker	UNP D6WIX5
D	357	LEU	-	linker	UNP D6WIX5
D	358	TYR	-	linker	UNP D6WIX5
D	359	PHE	-	linker	UNP D6WIX5
D	360	GLN	-	linker	UNP D6WIX5
D	361	GLY	-	linker	UNP D6WIX5
E	-150	GLY	-	expression tag	UNP D6WIX5
E	-149	PRO	-	expression tag	UNP D6WIX5
E	-148	THR	-	expression tag	UNP D6WIX5
E	-147	ALA	-	expression tag	UNP D6WIX5
E	-146	ALA	-	expression tag	UNP D6WIX5
E	-145	ALA	-	expression tag	UNP D6WIX5
E	-144	LEU	-	expression tag	UNP D6WIX5
E	40	SER	-	linker	UNP D6WIX5
E	41	GLY	-	linker	UNP D6WIX5
E	42	SER	-	linker	UNP D6WIX5
E	43	GLY	-	linker	UNP D6WIX5
E	44	SER	-	linker	UNP D6WIX5
E	45	GLY	-	linker	UNP D6WIX5
E	46	GLU	-	linker	UNP D6WIX5
E	47	ASN	-	linker	UNP D6WIX5
E	48	LEU	-	linker	UNP D6WIX5
E	49	TYR	-	linker	UNP D6WIX5

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Chain	Residue	Modelled	Actual	Comment	Reference
E	50	PHE	-	linker	UNP D6WIX5
E	51	GLN	-	linker	UNP D6WIX5
E	52	GLY	-	linker	UNP D6WIX5
F	-150	GLY	-	expression tag	UNP D6WIX5
F	-149	PRO	-	expression tag	UNP D6WIX5
F	-148	THR	-	expression tag	UNP D6WIX5
F	-147	ALA	-	expression tag	UNP D6WIX5
F	-146	ALA	-	expression tag	UNP D6WIX5
F	-145	ALA	-	expression tag	UNP D6WIX5
F	-144	LEU	-	expression tag	UNP D6WIX5
F	40	SER	-	linker	UNP D6WIX5
F	41	GLY	-	linker	UNP D6WIX5
F	42	SER	-	linker	UNP D6WIX5
F	43	GLY	-	linker	UNP D6WIX5
F	44	SER	-	linker	UNP D6WIX5
F	45	GLY	-	linker	UNP D6WIX5
F	46	GLU	-	linker	UNP D6WIX5
F	47	ASN	-	linker	UNP D6WIX5
F	48	LEU	-	linker	UNP D6WIX5
F	49	TYR	-	linker	UNP D6WIX5
F	50	PHE	-	linker	UNP D6WIX5
F	51	GLN	-	linker	UNP D6WIX5
F	52	GLY	-	linker	UNP D6WIX5
G	-150	GLY	-	expression tag	UNP D6WIX5
G	-149	PRO	-	expression tag	UNP D6WIX5
G	-148	THR	-	expression tag	UNP D6WIX5
G	-147	ALA	-	expression tag	UNP D6WIX5
G	-146	ALA	-	expression tag	UNP D6WIX5
G	-145	ALA	-	expression tag	UNP D6WIX5
G	-144	LEU	-	expression tag	UNP D6WIX5
G	40	SER	-	linker	UNP D6WIX5
G	41	GLY	-	linker	UNP D6WIX5
G	42	SER	-	linker	UNP D6WIX5
G	43	GLY	-	linker	UNP D6WIX5
G	44	SER	-	linker	UNP D6WIX5
G	45	GLY	-	linker	UNP D6WIX5
G	46	GLU	-	linker	UNP D6WIX5
G	47	ASN	-	linker	UNP D6WIX5
G	48	LEU	-	linker	UNP D6WIX5
G	49	TYR	-	linker	UNP D6WIX5
G	50	PHE	-	linker	UNP D6WIX5
G	51	GLN	-	linker	UNP D6WIX5

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Chain	Residue	Modelled	Actual	Comment	Reference
G	52	GLY	-	linker	UNP D6WIX5
H	-150	GLY	-	expression tag	UNP D6WIX5
H	-149	PRO	-	expression tag	UNP D6WIX5
H	-148	THR	-	expression tag	UNP D6WIX5
H	-147	ALA	-	expression tag	UNP D6WIX5
H	-146	ALA	-	expression tag	UNP D6WIX5
H	-145	ALA	-	expression tag	UNP D6WIX5
H	-144	LEU	-	expression tag	UNP D6WIX5
H	40	SER	-	linker	UNP D6WIX5
H	41	GLY	-	linker	UNP D6WIX5
H	42	SER	-	linker	UNP D6WIX5
H	43	GLY	-	linker	UNP D6WIX5
H	44	SER	-	linker	UNP D6WIX5
H	45	GLY	-	linker	UNP D6WIX5
H	46	GLU	-	linker	UNP D6WIX5
H	47	ASN	-	linker	UNP D6WIX5
H	48	LEU	-	linker	UNP D6WIX5
H	49	TYR	-	linker	UNP D6WIX5
H	50	PHE	-	linker	UNP D6WIX5
H	51	GLN	-	linker	UNP D6WIX5
H	52	GLY	-	linker	UNP D6WIX5

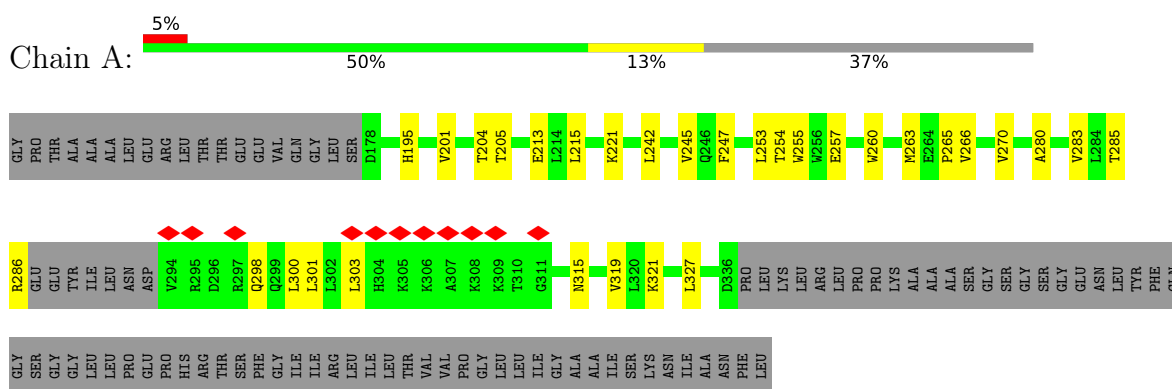
- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total	Ca	0
			1	1	

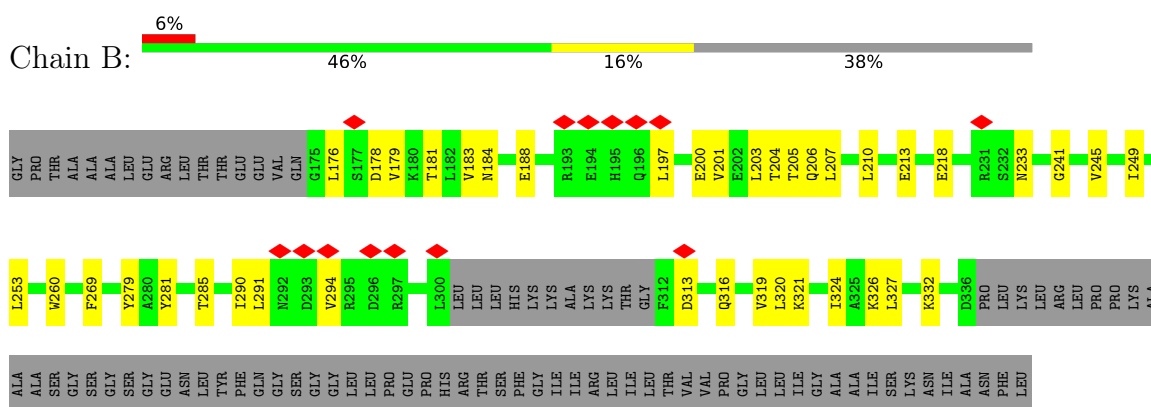
3 Residue-property plots

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

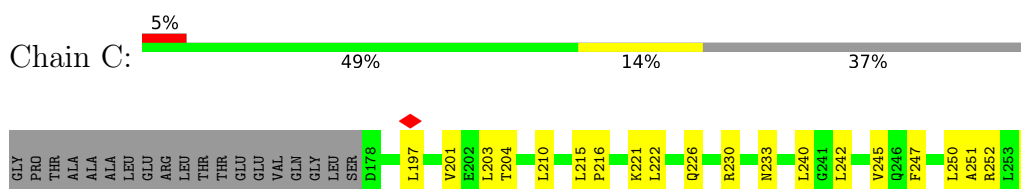
- Molecule 1: Calcium uniporter protein, Protein EMRE homolog, mitochondrial-like Protein fusion

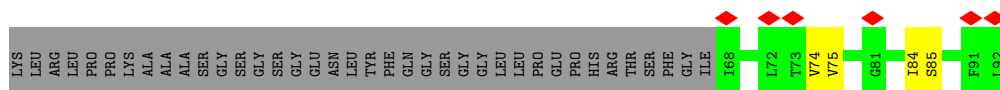


- Molecule 1: Calcium uniporter protein, Protein EMRE homolog, mitochondrial-like Protein fusion



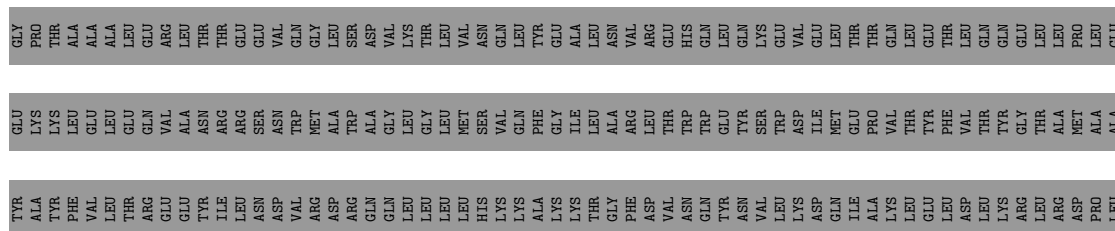
- Molecule 1: Calcium uniporter protein, Protein EMRE homolog, mitochondrial-like Protein fusion





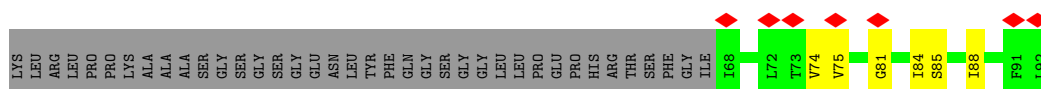
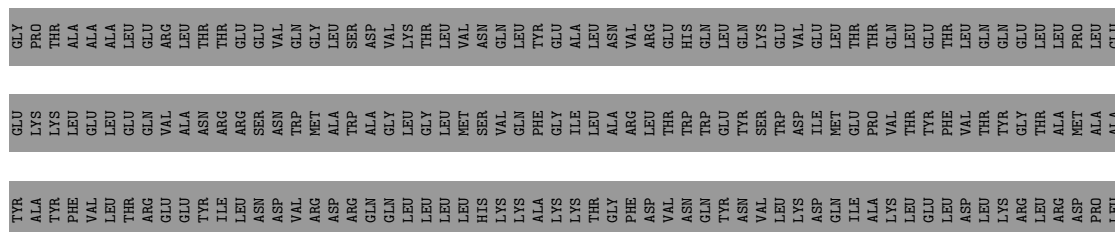
- Molecule 1: Calcium uniporter protein, Protein EMRE homolog, mitochondrial-like Protein fusion

Chain G:  90%



- Molecule 1: Calcium uniporter protein, Protein EMRE homolog, mitochondrial-like Protein fusion

Chain H:  8%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	52493	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 ($e^-/\text{\AA}^2$)	1.9	Depositor
Minimum defocus (nm)	-1000	Depositor
Maximum defocus (nm)	-3000	Depositor
Magnification	22500	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.107	Depositor
Minimum map value	-0.061	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	330.752, 330.752, 330.752	wwPDB
Map dimensions	304, 304, 304	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.088, 1.088, 1.088	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: CA

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	0.38	0/1181	0.48	0/1614
1	B	0.37	0/1192	0.45	0/1627
1	C	0.37	0/1178	0.46	0/1610
1	D	0.36	0/1187	0.49	0/1621
1	E	0.30	0/182	0.54	0/247
1	F	0.30	0/182	0.54	0/247
1	G	0.30	0/182	0.54	0/247
1	H	0.30	0/182	0.54	0/247
All	All	0.36	0/5466	0.48	0/7460

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	1158	0	1099	24	0
1	B	1170	0	1120	33	0
1	C	1155	0	1090	30	0
1	D	1165	0	1106	35	0
1	E	181	0	205	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	181	0	205	4	0
1	G	181	0	205	1	0
1	H	181	0	205	6	0
2	A	1	0	0	0	0
All	All	5373	0	5235	113	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 11.

All (113) 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:C:226:GLN:HE21	1:C:230:ARG:HH21	1.28	0.78
1:C:226:GLN:NE2	1:C:230:ARG:NH2	2.36	0.73
1:C:226:GLN:NE2	1:C:230:ARG:HH21	1.88	0.72
1:C:226:GLN:HE21	1:C:230:ARG:NH2	1.90	0.70
1:C:266:VAL:O	1:C:270:VAL:HG23	1.96	0.65
1:B:203:LEU:HD22	1:B:327:LEU:HD11	1.78	0.65
1:A:266:VAL:O	1:A:270:VAL:HG23	1.98	0.64
1:D:210:LEU:HB3	1:D:324:ILE:HG12	1.82	0.61
1:C:272:TYR:OH	1:D:246:GLN:NE2	2.34	0.60
1:B:313:ASP:HB3	1:B:316:GLN:HG2	1.84	0.59
1:A:285:THR:HG23	1:A:286:ARG:HG3	1.85	0.59
1:B:241:GLY:O	1:B:245:VAL:HG23	2.04	0.57
1:B:210:LEU:HB2	1:B:324:ILE:HD13	1.86	0.57
1:C:197:LEU:H	1:C:197:LEU:HD23	1.70	0.57
1:A:213:GLU:OE2	1:B:332:LYS:HD2	2.05	0.56
1:A:254:THR:HG22	1:A:263:MET:HB3	1.87	0.56
1:A:265:PRO:HB3	1:B:260:TRP:CE3	2.41	0.56
1:D:218:GLU:OE1	1:D:221:LYS:HE2	2.07	0.55
1:D:249:ILE:HG23	1:H:85:SER:HB3	1.88	0.55
1:D:320:LEU:O	1:D:324:ILE:HG13	2.07	0.55
1:B:213:GLU:HG3	1:B:320:LEU:HD21	1.88	0.54
1:D:200:GLU:O	1:D:204:THR:HG23	2.08	0.54
1:A:253:LEU:HB3	1:A:263:MET:SD	2.48	0.53
1:B:201:VAL:O	1:B:205:THR:HG23	2.09	0.52
1:B:269:PHE:CE2	1:C:254:THR:HG21	2.44	0.52
1:D:210:LEU:HD12	1:D:327:LEU:HD12	1.92	0.51
1:C:203:LEU:HD11	1:C:327:LEU:HD22	1.91	0.51
1:D:180:LYS:O	1:D:183:VAL:HG12	2.11	0.51
1:A:321:LYS:HD3	1:D:315:ASN:ND2	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:LEU:O	1:A:245:VAL:HG12	2.12	0.50
1:C:201:VAL:HA	1:C:204:THR:HG22	1.93	0.50
1:D:201:VAL:O	1:D:205:THR:HG23	2.11	0.50
1:A:260:TRP:CE3	1:D:265:PRO:HB3	2.47	0.50
1:C:251:ALA:HA	1:C:254:THR:HG22	1.94	0.49
1:B:179:VAL:O	1:B:183:VAL:HG23	2.12	0.49
1:B:178:ASP:O	1:B:181:THR:OG1	2.22	0.49
1:D:281:TYR:O	1:D:285:THR:HG23	2.13	0.49
1:A:298:GLN:O	1:A:301:LEU:HG	2.14	0.47
1:B:281:TYR:O	1:B:285:THR:HG23	2.15	0.47
1:B:197:LEU:O	1:B:201:VAL:HG23	2.13	0.47
1:B:249:ILE:HD11	1:F:84:ILE:HD11	1.96	0.47
1:A:221:LYS:HG3	1:A:300:LEU:HD11	1.96	0.47
1:B:320:LEU:HD13	1:C:329:LEU:HD21	1.97	0.47
1:A:201:VAL:HA	1:A:204:THR:HG22	1.97	0.47
1:G:74:VAL:HG13	1:G:75:VAL:N	2.30	0.47
1:A:201:VAL:O	1:A:205:THR:HG22	2.16	0.46
1:C:210:LEU:HD22	1:C:320:LEU:HD11	1.97	0.46
1:E:74:VAL:HG13	1:E:75:VAL:N	2.31	0.46
1:D:203:LEU:HD23	1:D:331:LEU:HD13	1.97	0.46
1:D:249:ILE:HD11	1:H:84:ILE:HD11	1.96	0.46
1:F:74:VAL:HG13	1:F:75:VAL:N	2.31	0.46
1:H:74:VAL:HG13	1:H:75:VAL:N	2.31	0.46
1:D:249:ILE:HG12	1:H:81:GLY:O	2.15	0.46
1:D:246:GLN:OE1	1:D:274:THR:OG1	2.29	0.46
1:C:242:LEU:O	1:C:245:VAL:HG12	2.16	0.46
1:C:203:LEU:CD1	1:C:327:LEU:HD22	2.46	0.45
1:C:280:ALA:O	1:C:283:VAL:HG12	2.15	0.45
1:B:253:LEU:HG	1:F:85:SER:HB2	1.98	0.45
1:C:222:LEU:HD12	1:C:222:LEU:HA	1.78	0.45
1:A:303:LEU:HD12	1:A:303:LEU:HA	1.72	0.45
1:B:279:TYR:HE2	1:C:240:LEU:HB2	1.80	0.45
1:B:201:VAL:O	1:B:204:THR:OG1	2.25	0.45
1:C:315:ASN:OD1	1:D:321:LYS:HD3	2.17	0.45
1:B:269:PHE:HD1	1:C:247:PHE:CE2	2.36	0.44
1:E:80:ILE:HD13	1:E:80:ILE:HA	1.88	0.44
1:A:257:GLU:OE1	1:E:89:ALA:HB1	2.17	0.44
1:C:221:LYS:HB2	1:C:312:PHE:CE1	2.52	0.44
1:B:326:LYS:HE3	1:B:326:LYS:HB2	1.78	0.44
1:H:88:ILE:HD12	1:H:88:ILE:HA	1.90	0.44
1:A:315:ASN:O	1:A:319:VAL:HG12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:PHE:HD2	1:D:272:TYR:CD1	2.37	0.43
1:A:280:ALA:O	1:A:283:VAL:HG12	2.18	0.43
1:C:279:TYR:HD2	1:D:240:LEU:HD13	1.83	0.43
1:A:215:LEU:HD12	1:A:215:LEU:HA	1.81	0.43
1:C:197:LEU:O	1:C:201:VAL:HG22	2.18	0.43
1:D:284:LEU:HD23	1:D:284:LEU:HA	1.80	0.43
1:D:332:LYS:HB2	1:D:332:LYS:HE3	1.74	0.43
1:B:200:GLU:O	1:B:204:THR:HG23	2.19	0.43
1:B:249:ILE:HD11	1:F:84:ILE:CD1	2.48	0.43
1:B:316:GLN:HA	1:B:319:VAL:HG12	2.01	0.42
1:D:264:GLU:N	1:D:265:PRO:HD2	2.34	0.42
1:B:176:LEU:HD12	1:B:176:LEU:HA	1.86	0.42
1:D:210:LEU:HD22	1:D:320:LEU:HD11	2.01	0.42
1:D:280:ALA:HB1	1:E:70:LEU:HD11	2.01	0.42
1:A:327:LEU:HA	1:A:327:LEU:HD12	1.77	0.42
1:C:252:ARG:NH2	1:C:257:GLU:OE2	2.52	0.42
1:D:219:GLU:OE2	1:D:219:GLU:HA	2.19	0.42
1:B:207:LEU:HD23	1:B:324:ILE:HD11	2.02	0.42
1:B:210:LEU:HD23	1:C:333:ARG:NH2	2.34	0.42
1:D:286:ARG:O	1:D:290:ILE:HG12	2.19	0.42
1:A:195:HIS:CE1	1:D:180:LYS:HD3	2.55	0.42
1:D:253:LEU:HD23	1:D:253:LEU:HA	1.79	0.41
1:C:279:TYR:HE2	1:D:240:LEU:HB2	1.85	0.41
1:A:263:MET:HG3	1:A:266:VAL:HB	2.01	0.41
1:A:253:LEU:HD23	1:A:253:LEU:HA	1.84	0.41
1:B:205:THR:OG1	1:B:206:GLN:NE2	2.53	0.41
1:D:244:SER:HB2	1:H:74:VAL:HG23	2.01	0.41
1:D:327:LEU:HD23	1:D:327:LEU:HA	1.76	0.41
1:B:249:ILE:HD13	1:B:249:ILE:HG21	1.79	0.41
1:B:290:ILE:HG13	1:B:291:LEU:N	2.35	0.41
1:A:315:ASN:ND2	1:B:321:LYS:HD3	2.36	0.41
1:B:184:ASN:O	1:B:188:GLU:HG2	2.21	0.41
1:C:251:ALA:O	1:C:254:THR:HG22	2.21	0.41
1:D:224:LEU:O	1:D:227:VAL:HG12	2.21	0.41
1:D:291:LEU:HA	1:D:294:VAL:HG12	2.02	0.41
1:C:250:LEU:HD23	1:C:250:LEU:HA	1.78	0.41
1:D:263:MET:HG3	1:D:266:VAL:HB	2.02	0.41
1:E:88:ILE:HD12	1:E:88:ILE:HA	1.90	0.41
1:C:215:LEU:HB3	1:C:216:PRO:HD3	2.03	0.40
1:C:221:LYS:HE2	1:C:221:LYS:HB3	1.98	0.40
1:B:290:ILE:O	1:B:294:VAL:HG12	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:313:ASP:HB3	1:D:316:GLN:HG2	2.02	0.40
1:B:253:LEU:HD23	1:B:253:LEU:HA	1.84	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	148/243 (61%)	143 (97%)	5 (3%)	0	100	100
1	B	147/243 (60%)	145 (99%)	2 (1%)	0	100	100
1	C	148/243 (61%)	144 (97%)	4 (3%)	0	100	100
1	D	147/243 (60%)	145 (99%)	2 (1%)	0	100	100
1	E	23/243 (10%)	23 (100%)	0	0	100	100
1	F	23/243 (10%)	23 (100%)	0	0	100	100
1	G	23/243 (10%)	23 (100%)	0	0	100	100
1	H	23/243 (10%)	23 (100%)	0	0	100	100
All	All	682/1944 (35%)	669 (98%)	13 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	108/207 (52%)	107 (99%)	1 (1%)	78	90
1	B	113/207 (55%)	111 (98%)	2 (2%)	59	81
1	C	107/207 (52%)	105 (98%)	2 (2%)	57	80
1	D	111/207 (54%)	110 (99%)	1 (1%)	78	90
1	E	19/207 (9%)	19 (100%)	0	100	100
1	F	19/207 (9%)	19 (100%)	0	100	100
1	G	19/207 (9%)	19 (100%)	0	100	100
1	H	19/207 (9%)	19 (100%)	0	100	100
All	All	515/1656 (31%)	509 (99%)	6 (1%)	72	87

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	255	TRP
1	B	218	GLU
1	B	233	ASN
1	C	233	ASN
1	C	255	TRP
1	D	237	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	195	HIS
1	A	315	ASN
1	B	206	GLN
1	C	226	GLN
1	C	246	GLN
1	D	206	GLN
1	D	246	GLN
1	D	315	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

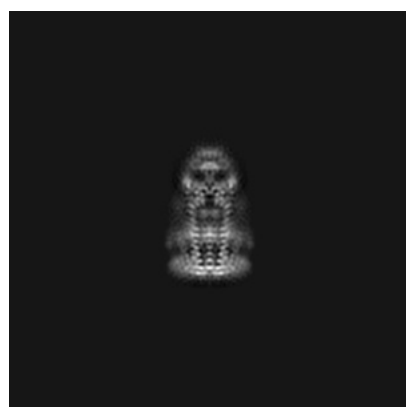
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22042. These allow visual inspection of the internal detail of the map and identification of artifacts.

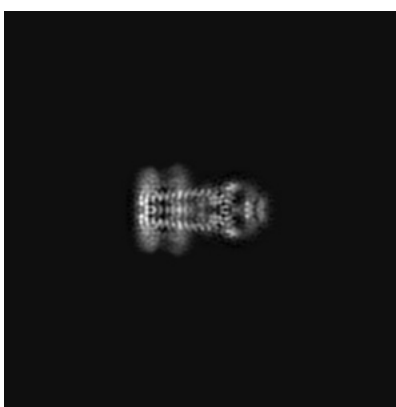
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

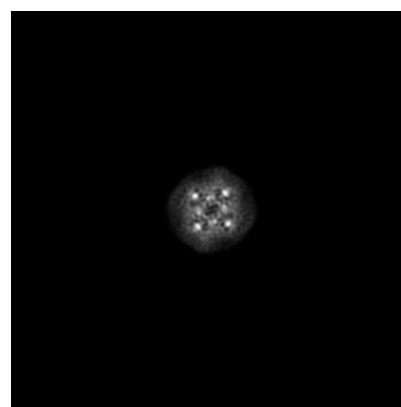
6.1.1 Primary map



X



Y



Z

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

6.2 Central slices [i](#)

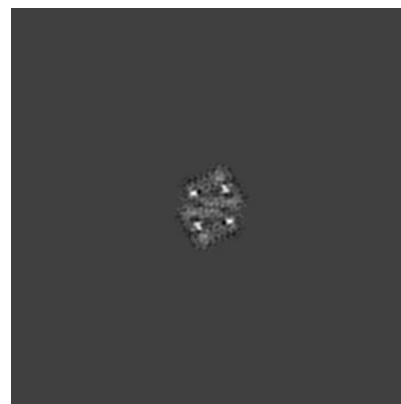
6.2.1 Primary map



X Index: 152



Y Index: 152

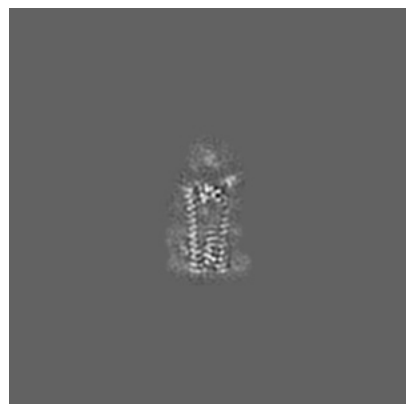


Z Index: 152

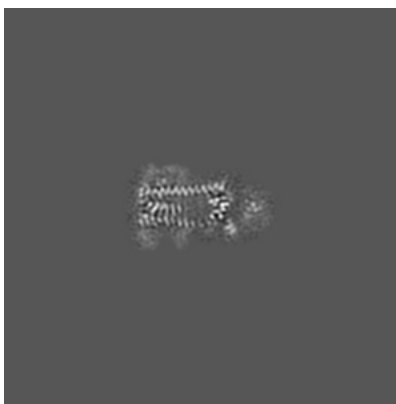
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

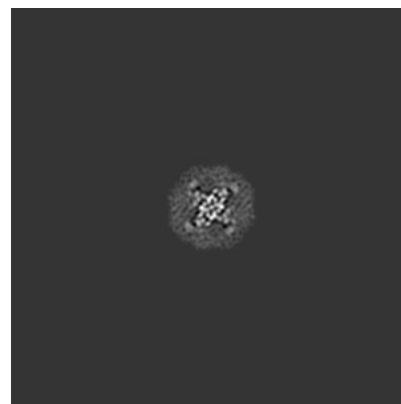
6.3.1 Primary map



X Index: 142



Y Index: 142

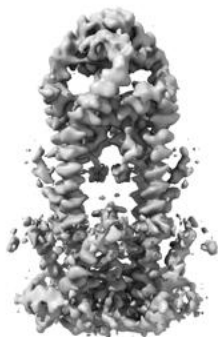


Z Index: 108

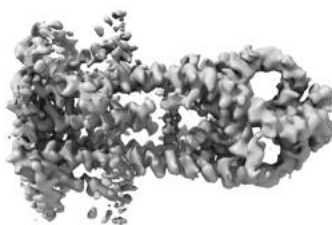
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

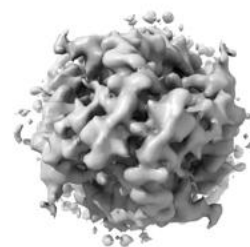
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

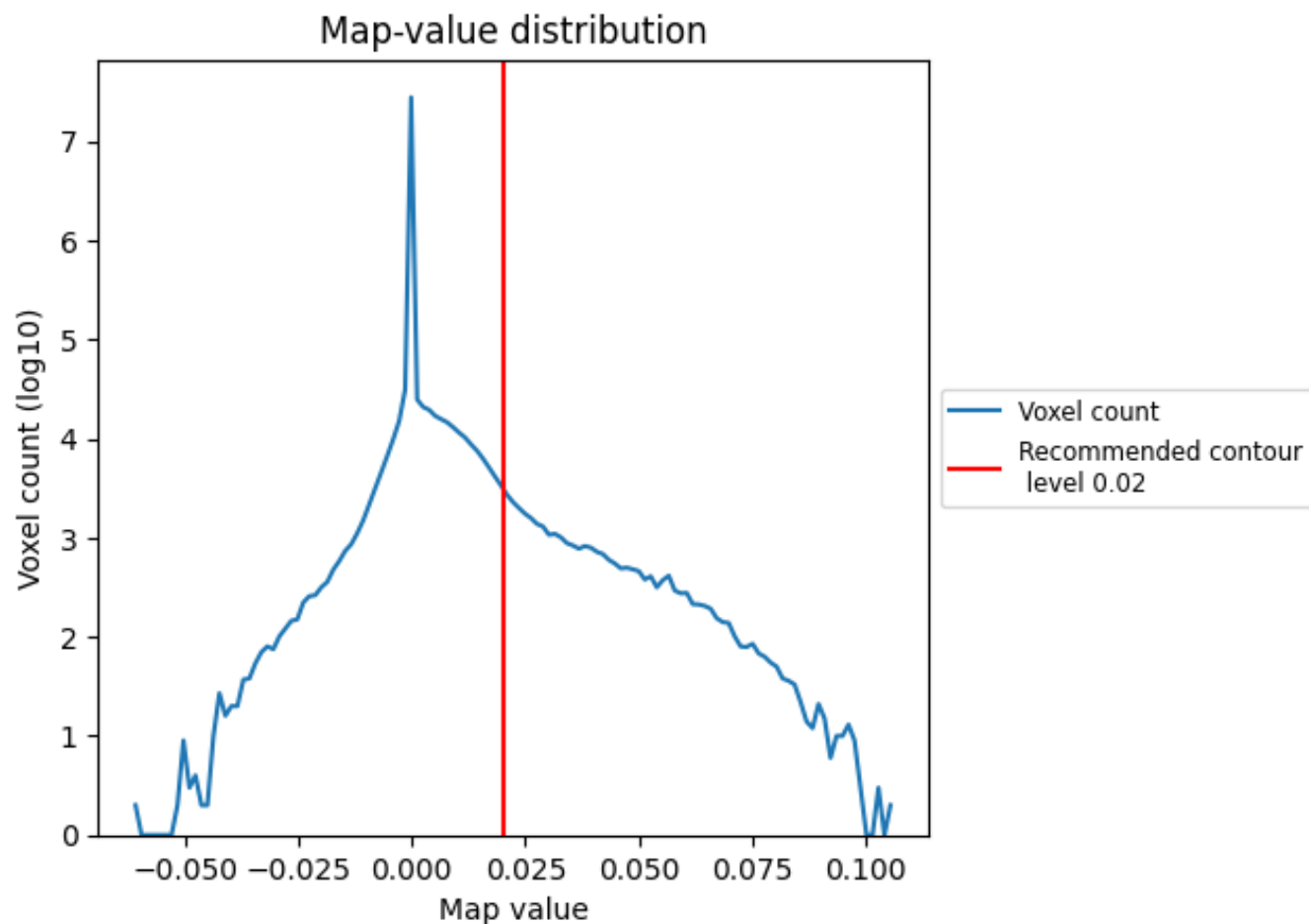
6.5 Mask visualisation

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

7 Map analysis [i](#)

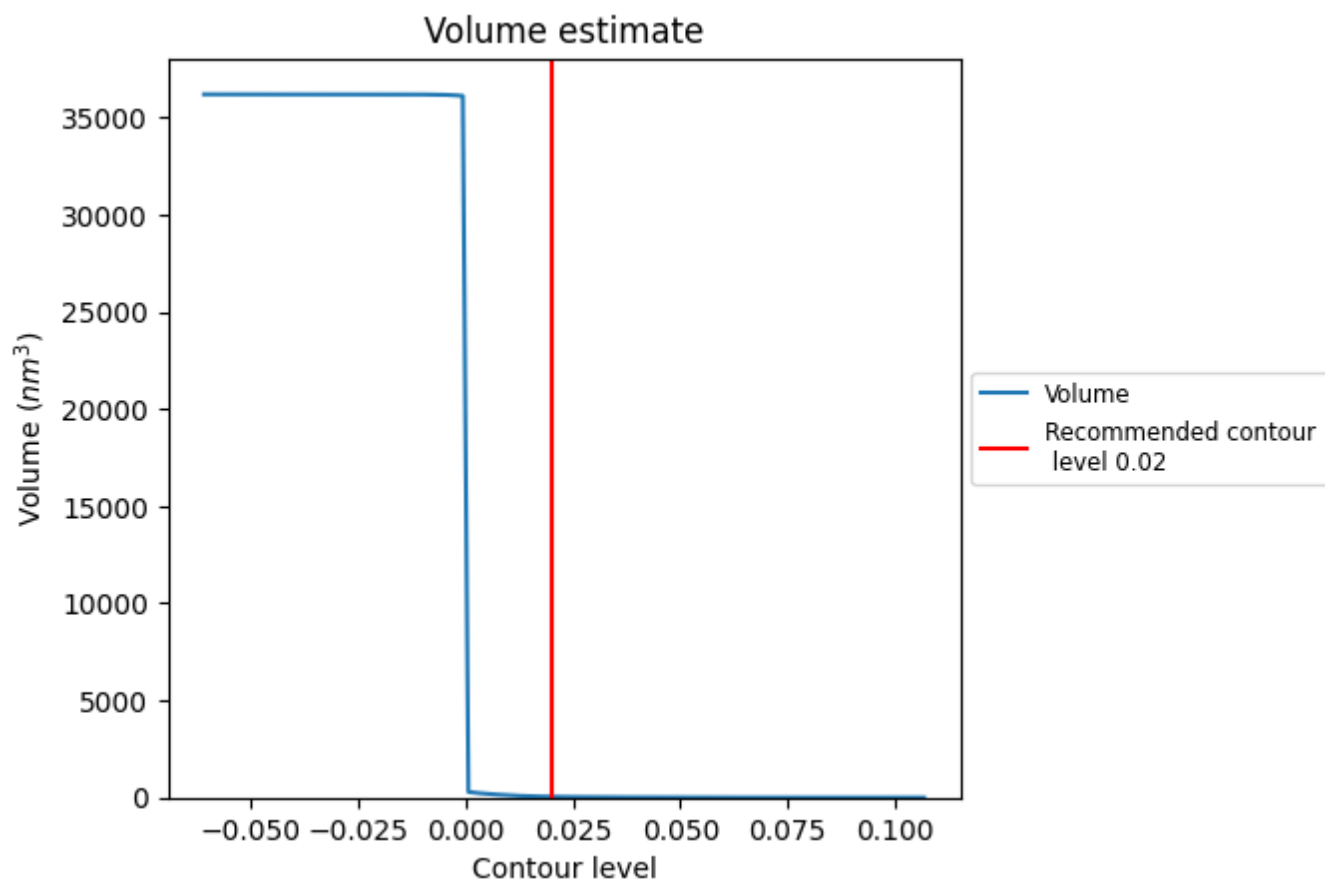
This section contains the results of statistical analysis of the map.

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.

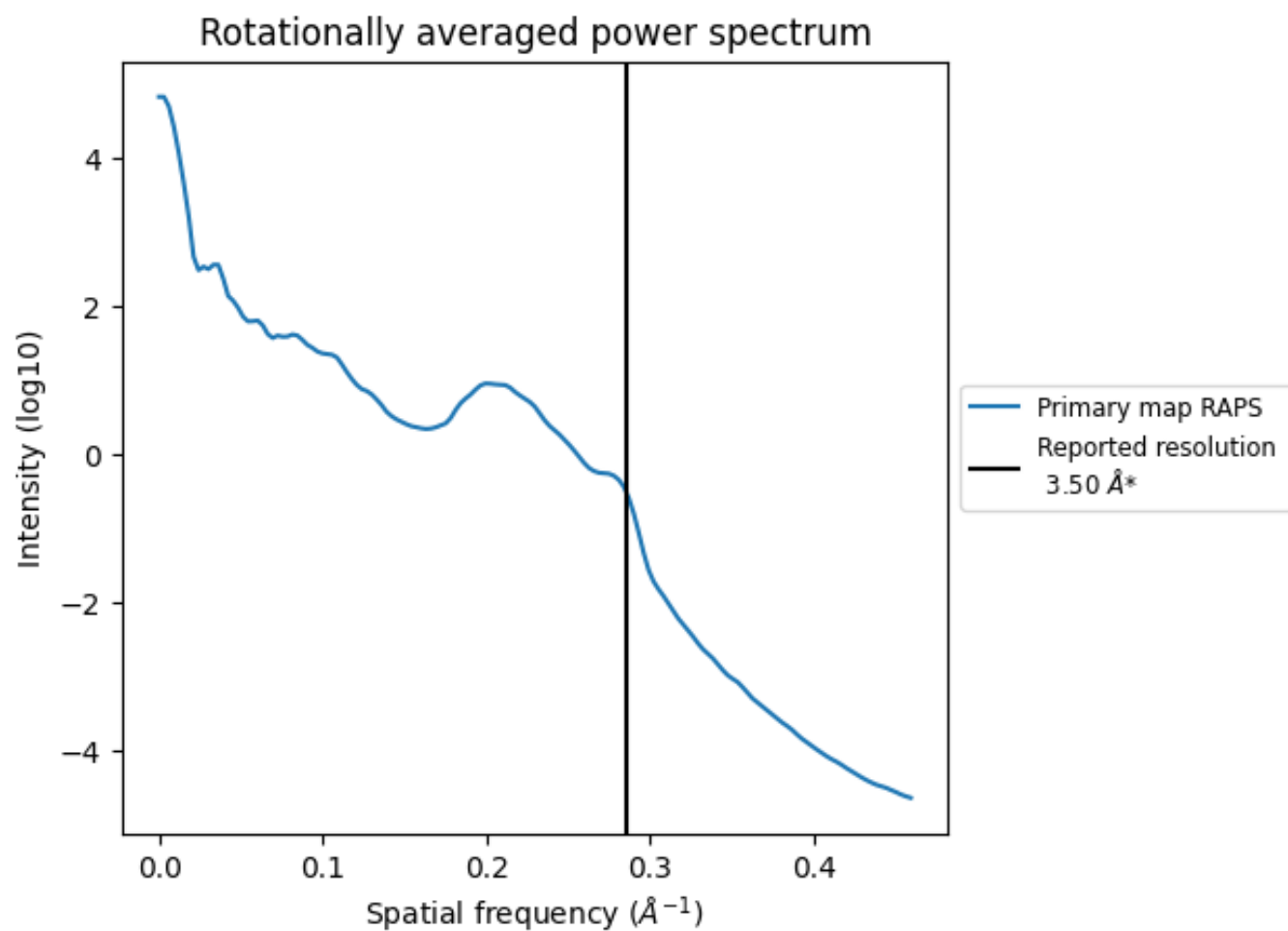
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 41 nm^3 ; this corresponds to an approximate mass of 37 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 0.286 Å⁻¹

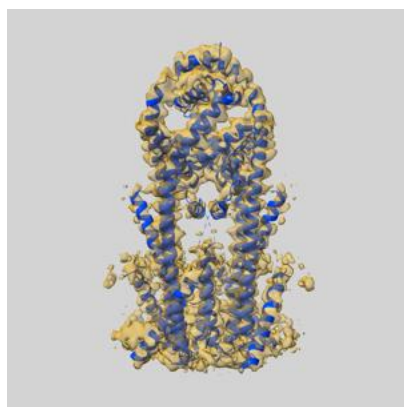
8 Fourier-Shell correlation ⓘ

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

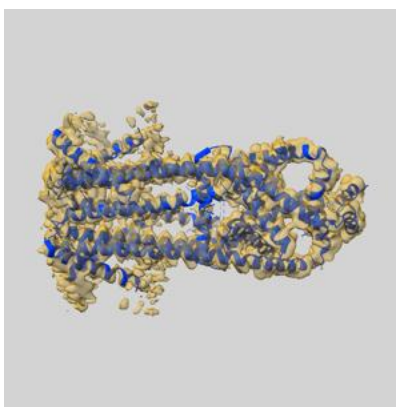
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-22042 and PDB model 6X4S. Per-residue inclusion information can be found in section [3](#) on page [8](#).

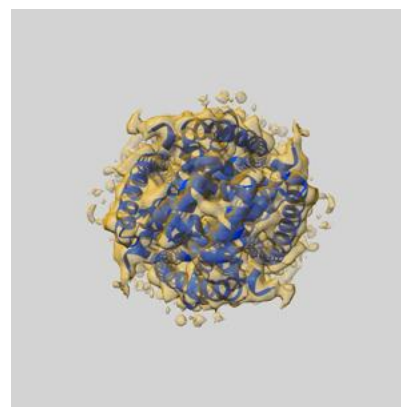
9.1 Map-model overlay [i](#)



X



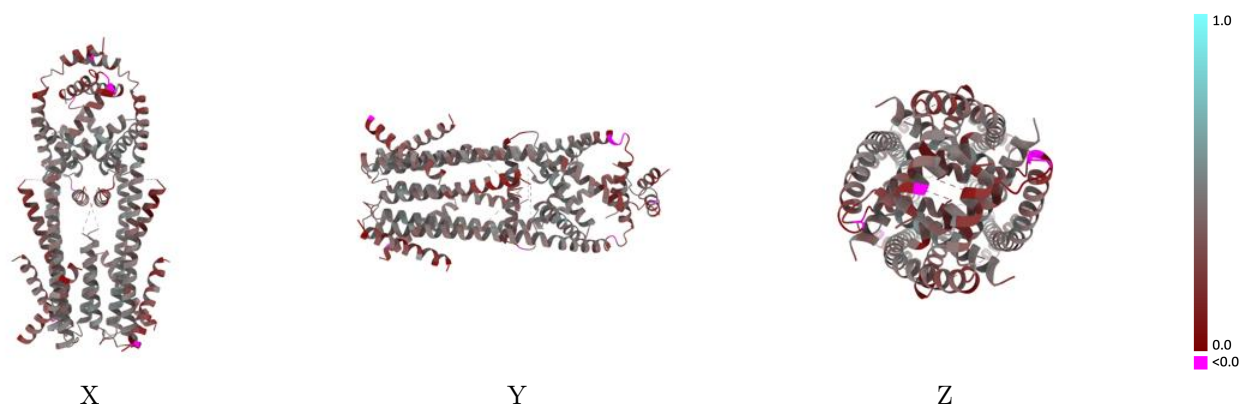
Y



Z

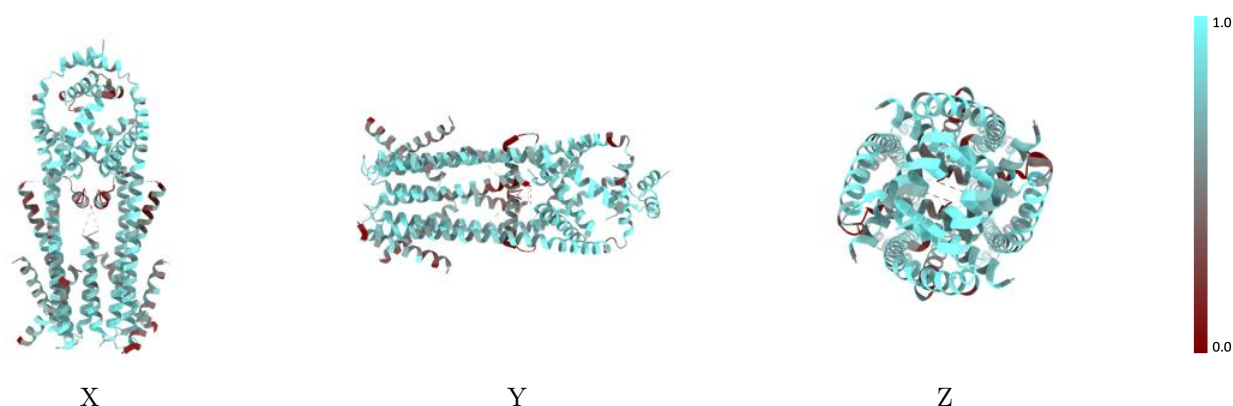
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



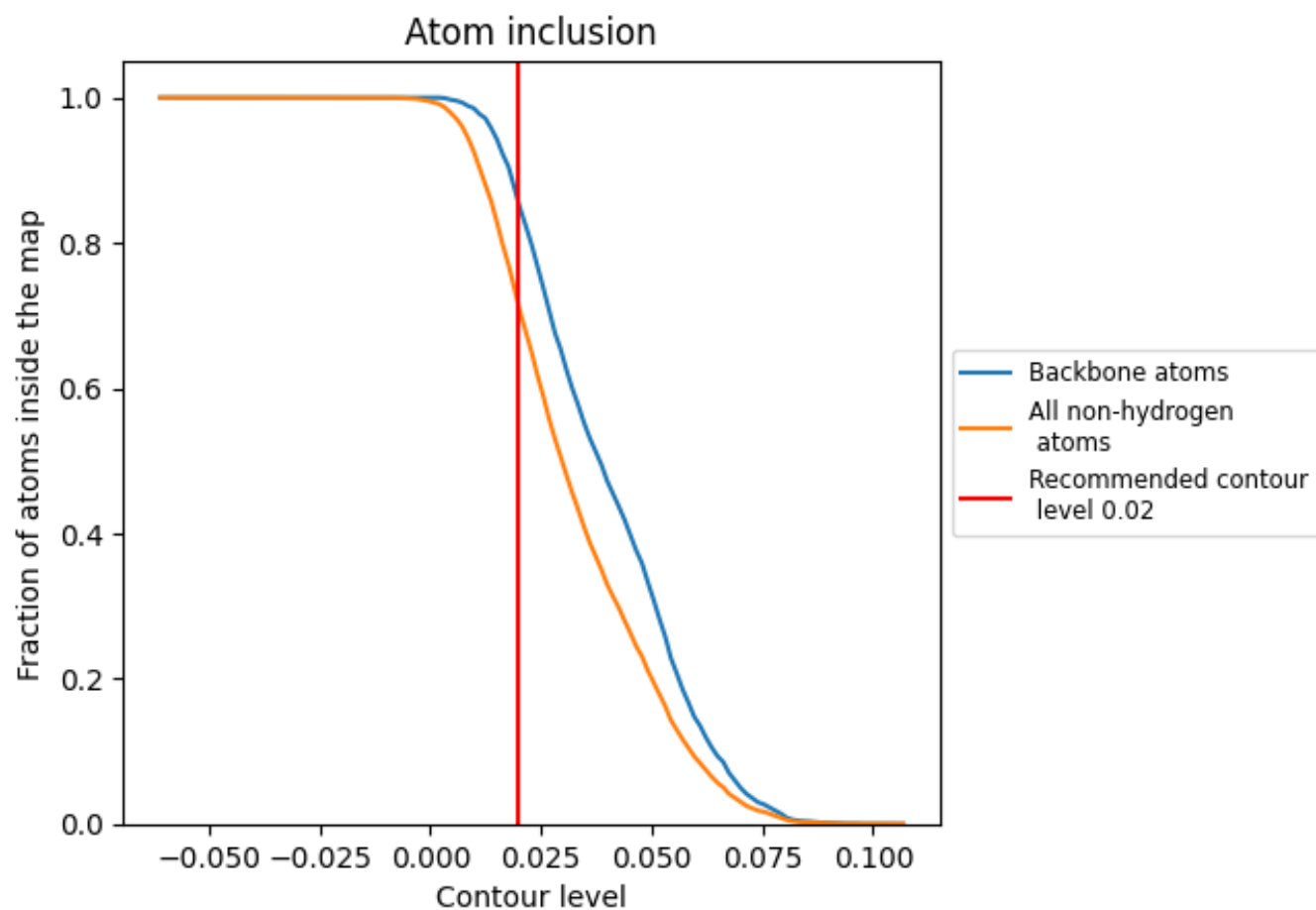
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 71% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7124	<div></div> 0.3720
A	<div></div> 0.7546	<div></div> 0.3960
B	<div></div> 0.7297	<div></div> 0.3790
C	<div></div> 0.7590	<div></div> 0.3970
D	<div></div> 0.7391	<div></div> 0.3910
E	<div></div> 0.5084	<div></div> 0.2470
F	<div></div> 0.4916	<div></div> 0.2600
G	<div></div> 0.5084	<div></div> 0.2440
H	<div></div> 0.4972	<div></div> 0.2460

1.0

0.0

<0.0