



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 10:04 AM UTC

PDB ID : 8F2U / pdb_00008f2u
EMDB ID : EMD-28827
Title : Human CCC complex
Authors : Healy, M.D.; McNally, K.E.; Butkovic, R.; Chilton, M.; Kato, K.; Sacharz, J.; McConville, C.; Moody, E.R.R.; Shaw, S.; Planelles-Herrero, V.J.; Kada-palakere, S.Y.; Ross, J.; Borucu, U.; Palmer, C.S.; Chen, K.; Croll, T.I.; Hall, R.J.; Caruana, N.J.; Ghai, R.; Nguyen, T.H.D.; Heesom, K.J.; Saitoh, S.; Berger, I.; Berger-Schaffitzel, C.; Williams, T.A.; Stroud, D.A.; Derivery, E.; Collins, B.M.; Cullen, P.J.
Deposited on : 2022-11-08
Resolution : 3.53 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.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

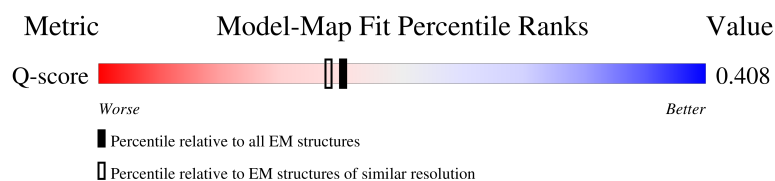
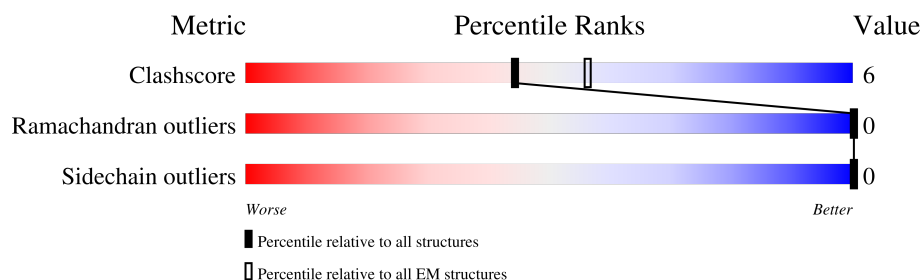
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.53 Å.

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



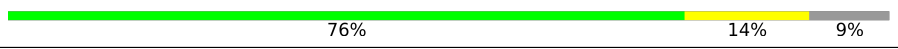
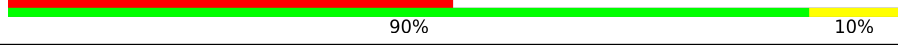
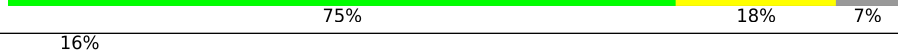
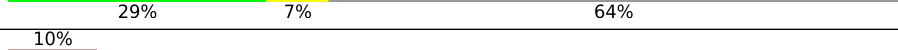
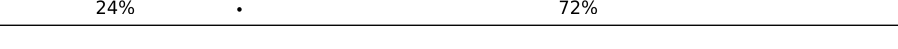
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12947 (3.03 - 4.02)

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	190	45% 84% 14% .
2	B	199	10% 86% 14%
3	C	195	. 88% 12%

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Mol	Chain	Length	Quality of chain
4	D	199	
5	E	260	
6	F	85	
7	G	200	
8	H	183	
9	I	198	
10	J	212	
11	N	631	
12	T	627	

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 17684 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 COMM domain-containing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	187	Total	C	N	O	S	0	0
			1466	928	251	282	5		

- Molecule 2 is a protein called COMM domain-containing protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	199	Total	C	N	O	S	0	0
			1601	1012	285	300	4		

- Molecule 3 is a protein called COMM domain-containing protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	195	Total	C	N	O	S	0	0
			1555	977	268	302	8		

- Molecule 4 is a protein called COMM domain-containing protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	199	Total	C	N	O	S	0	0
			1520	960	261	287	12		

- Molecule 5 is a protein called COMM domain-containing protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	205	Total	C	N	O	S	0	0
			1598	1009	287	295	7		

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	225	GLY	-	expression tag	UNP Q9GZQ3
E	226	SER	-	expression tag	UNP Q9GZQ3
E	227	LEU	-	expression tag	UNP Q9GZQ3

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Chain	Residue	Modelled	Actual	Comment	Reference
E	228	PHE	-	expression tag	UNP Q9GZQ3
E	229	GLN	-	expression tag	UNP Q9GZQ3
E	230	GLY	-	expression tag	UNP Q9GZQ3
E	231	PRO	-	expression tag	UNP Q9GZQ3
E	232	TRP	-	expression tag	UNP Q9GZQ3
E	233	SER	-	expression tag	UNP Q9GZQ3
E	234	HIS	-	expression tag	UNP Q9GZQ3
E	235	PRO	-	expression tag	UNP Q9GZQ3
E	236	GLN	-	expression tag	UNP Q9GZQ3
E	237	PHE	-	expression tag	UNP Q9GZQ3
E	238	GLU	-	expression tag	UNP Q9GZQ3
E	239	LYS	-	expression tag	UNP Q9GZQ3
E	240	GLY	-	expression tag	UNP Q9GZQ3
E	241	GLY	-	expression tag	UNP Q9GZQ3
E	242	GLY	-	expression tag	UNP Q9GZQ3
E	243	SER	-	expression tag	UNP Q9GZQ3
E	244	GLY	-	expression tag	UNP Q9GZQ3
E	245	GLY	-	expression tag	UNP Q9GZQ3
E	246	GLY	-	expression tag	UNP Q9GZQ3
E	247	SER	-	expression tag	UNP Q9GZQ3
E	248	GLY	-	expression tag	UNP Q9GZQ3
E	249	GLY	-	expression tag	UNP Q9GZQ3
E	250	SER	-	expression tag	UNP Q9GZQ3
E	251	SER	-	expression tag	UNP Q9GZQ3
E	252	ALA	-	expression tag	UNP Q9GZQ3
E	253	TRP	-	expression tag	UNP Q9GZQ3
E	254	SER	-	expression tag	UNP Q9GZQ3
E	255	HIS	-	expression tag	UNP Q9GZQ3
E	256	PRO	-	expression tag	UNP Q9GZQ3
E	257	GLN	-	expression tag	UNP Q9GZQ3
E	258	PHE	-	expression tag	UNP Q9GZQ3
E	259	GLU	-	expression tag	UNP Q9GZQ3
E	260	LYS	-	expression tag	UNP Q9GZQ3

- Molecule 6 is a protein called COMM domain-containing protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	77	Total	C	N	O	S	0	0
			617	397	101	114	5		

- Molecule 7 is a protein called COMM domain-containing protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	200	Total	C	N	O	S	0	0
			1583	1014	262	298	9		

- Molecule 8 is a protein called COMM domain-containing protein 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	179	Total	C	N	O	S	0	0
			1449	927	246	270	6		

- Molecule 9 is a protein called COMM domain-containing protein 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	198	Total	C	N	O	S	0	0
			1526	955	264	299	8		

- Molecule 10 is a protein called COMM domain-containing protein 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	198	Total	C	N	O	S	0	0
			1589	1010	274	301	4		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	203	HIS	-	expression tag	UNP Q9Y6G5
J	204	HIS	-	expression tag	UNP Q9Y6G5
J	205	HIS	-	expression tag	UNP Q9Y6G5
J	206	HIS	-	expression tag	UNP Q9Y6G5
J	207	HIS	-	expression tag	UNP Q9Y6G5
J	208	HIS	-	expression tag	UNP Q9Y6G5
J	209	HIS	-	expression tag	UNP Q9Y6G5
J	210	HIS	-	expression tag	UNP Q9Y6G5
J	211	HIS	-	expression tag	UNP Q9Y6G5
J	212	HIS	-	expression tag	UNP Q9Y6G5

- Molecule 11 is a protein called Coiled-coil domain-containing protein 93.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	N	225	Total	C	N	O	S	0	0
			1816	1155	310	343	8		

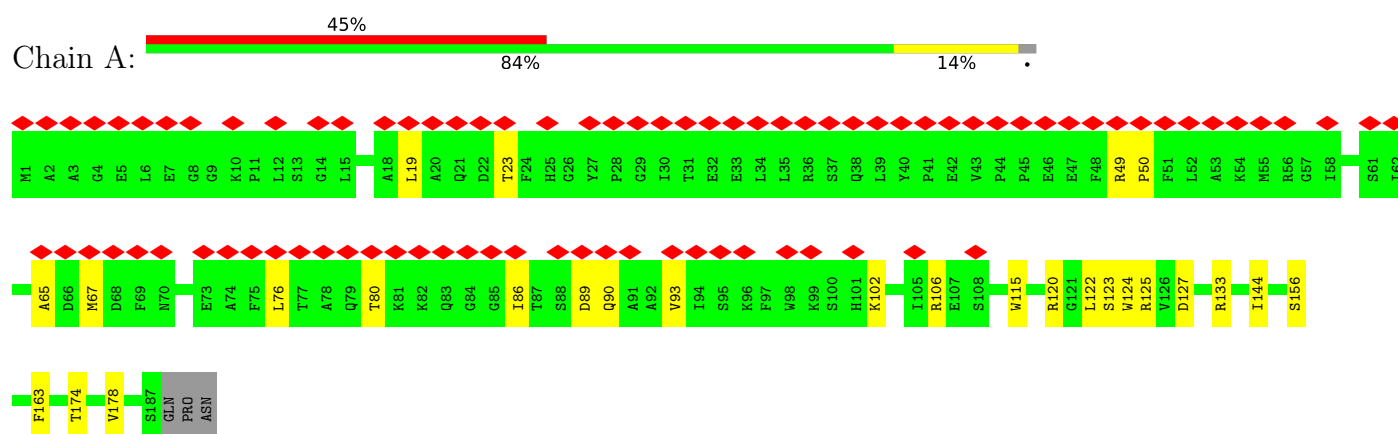
- Molecule 12 is a protein called Coiled-coil domain-containing protein 22.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	T	174	Total	C	N	O	S	0	0
			1364	854	267	242	1		

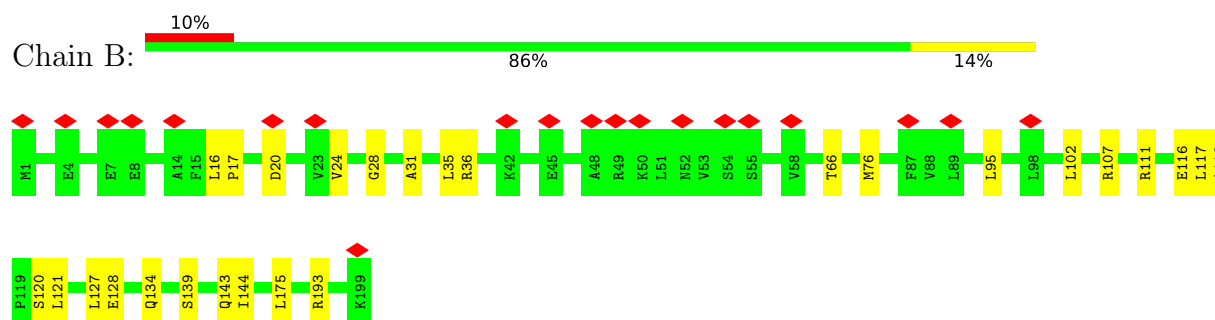
3 Residue-property plots [i](#)

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.

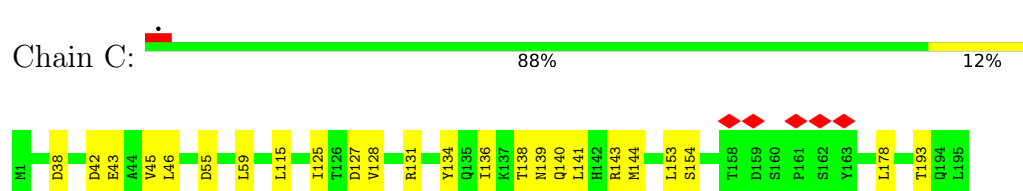
- Molecule 1: COMM domain-containing protein 1



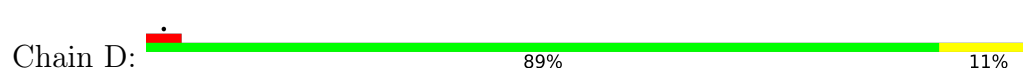
- Molecule 2: COMM domain-containing protein 2



- Molecule 3: COMM domain-containing protein 3

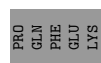
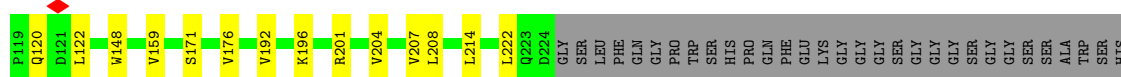


- Molecule 4: COMM domain-containing protein 4

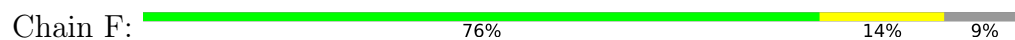




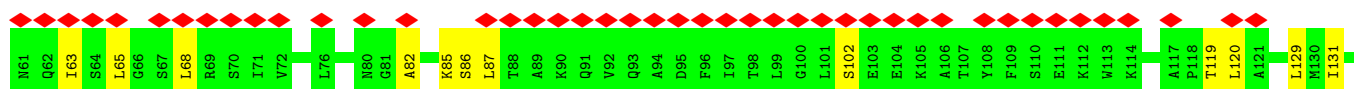
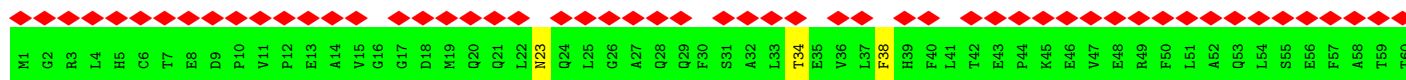
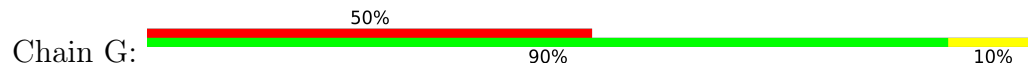
- Molecule 5: COMM domain-containing protein 5



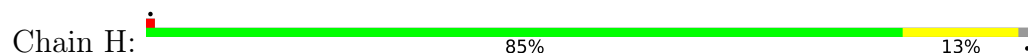
- Molecule 6: COMM domain-containing protein 6



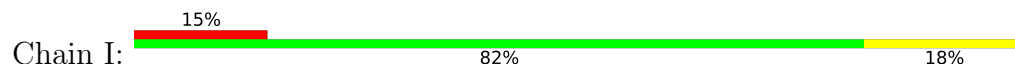
- Molecule 7: COMM domain-containing protein 7



- Molecule 8: COMM domain-containing protein 8



- Molecule 9: COMM domain-containing protein 9



GLY
ARG
VAL
ARG
GLU
ALA

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	20034	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 ($e^-/\text{\AA}^2$)	43.14	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.066	Depositor
Minimum map value	-0.035	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.01	Depositor
Map size ($\text{\AA}$)	286.176, 286.176, 286.176	wwPDB
Map dimensions	264, 264, 264	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.084, 1.084, 1.084	Depositor

5 Model quality

5.1 Standard geometry

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	0.12	0/1493	0.31	0/2011
2	B	0.10	0/1626	0.25	0/2198
3	C	0.11	0/1584	0.28	0/2142
4	D	0.11	0/1542	0.28	0/2080
5	E	0.12	0/1624	0.37	2/2198 (0.1%)
6	F	0.13	0/629	0.31	0/849
7	G	0.12	0/1612	0.32	0/2176
8	H	0.10	0/1476	0.25	0/1994
9	I	0.12	0/1543	0.31	0/2087
10	J	0.14	0/1614	0.37	1/2176 (0.0%)
11	N	0.13	0/1848	0.35	0/2489
12	T	0.13	0/1398	0.36	0/1901
All	All	0.12	0/17989	0.32	3/24301 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	113	LEU	CA-C-N	6.16	133.31	121.54
5	E	113	LEU	C-N-CA	6.16	133.31	121.54
10	J	8	ILE	CG1-CB-CG2	5.33	126.70	110.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1466	0	1474	24	0
2	B	1601	0	1638	28	0
3	C	1555	0	1540	22	0
4	D	1520	0	1573	16	0
5	E	1598	0	1638	30	0
6	F	617	0	619	11	0
7	G	1583	0	1603	18	0
8	H	1449	0	1476	14	0
9	I	1526	0	1578	29	0
10	J	1589	0	1620	30	0
11	N	1816	0	1836	37	0
12	T	1364	0	1383	14	0
All	All	17684	0	17978	228	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 6.

All (228) 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)
3:C:46:LEU:HD12	3:C:59:LEU:HD21	1.52	0.90
9:I:42:LEU:HD22	9:I:61:LEU:HD13	1.53	0.87
11:N:120:VAL:HG22	11:N:124:VAL:HG23	1.59	0.83
7:G:136:ASP:OD1	7:G:137:MET:N	2.12	0.82
7:G:23:ASN:OD1	7:G:102:SER:OG	1.98	0.81
2:B:16:LEU:HD12	2:B:24:VAL:HG22	1.61	0.80
10:J:188:TYR:OH	11:N:201:THR:OG1	1.98	0.80
7:G:63:ILE:HG22	7:G:68:LEU:HD11	1.66	0.78
10:J:8:ILE:HB	10:J:95:GLN:HE22	1.49	0.77
11:N:292:GLU:OE2	11:N:296:LYS:NZ	2.15	0.77
2:B:24:VAL:HG11	2:B:95:LEU:HD11	1.67	0.77
3:C:55:ASP:OD2	12:T:181:ARG:NH2	2.18	0.77
2:B:117:LEU:HD11	11:N:169:VAL:HG11	1.67	0.76
5:E:48:PHE:CD1	5:E:122:LEU:HD22	2.23	0.73
4:D:5:PHE:O	4:D:78:SER:OG	2.08	0.72
4:D:18:GLU:O	4:D:21:THR:OG1	2.09	0.71
3:C:139:ASN:OD1	10:J:139:TRP:NE1	2.23	0.71
8:H:48:SER:OG	8:H:49:GLU:OE1	2.09	0.69
8:H:15:LEU:HD23	8:H:16:PRO:O	1.93	0.68
9:I:17:LYS:HD2	9:I:50:LEU:HD22	1.75	0.68
2:B:76:MET:SD	2:B:107:ARG:NH1	2.67	0.67
1:A:19:LEU:O	1:A:23:THR:HG22	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:84:THR:HG21	12:T:276:LEU:HD23	1.77	0.66
10:J:58:GLN:O	10:J:62:SER:N	2.29	0.66
5:E:171:SER:O	10:J:125:ARG:NH1	2.30	0.65
11:N:85:ALA:HB1	11:N:89:LYS:NZ	2.12	0.64
12:T:148:ARG:NH1	12:T:156:GLN:O	2.31	0.64
2:B:193:ARG:NH1	5:E:222:LEU:O	2.31	0.64
2:B:118:ALA:HB2	3:C:138:THR:HG21	1.80	0.64
1:A:65:ALA:HB3	1:A:67:MET:SD	2.37	0.64
9:I:119:SER:OG	9:I:122:ARG:NH2	2.30	0.64
12:T:232:THR:HA	12:T:235:LEU:HD22	1.80	0.64
1:A:178:VAL:HG22	6:F:24:TRP:CE2	2.33	0.63
7:G:82:ALA:O	7:G:86:SER:N	2.31	0.63
11:N:30:ILE:HG23	11:N:31:LEU:HD12	1.80	0.63
7:G:63:ILE:CG2	7:G:68:LEU:HD11	2.29	0.63
5:E:111:ASP:O	5:E:114:GLN:NE2	2.31	0.63
4:D:170:GLN:NE2	4:D:171:PRO:O	2.32	0.62
1:A:76:LEU:O	1:A:80:THR:OG1	2.11	0.62
9:I:139:ILE:HG21	9:I:142:MET:CE	2.30	0.62
9:I:32:PHE:O	9:I:69:ARG:NH2	2.33	0.62
8:H:49:GLU:OE1	8:H:49:GLU:N	2.33	0.61
12:T:123:SER:O	12:T:127:LEU:HD23	1.99	0.61
2:B:117:LEU:HD13	3:C:140:GLN:HG3	1.82	0.61
6:F:21:ASP:OD2	6:F:23:GLN:NE2	2.34	0.61
9:I:139:ILE:HD13	9:I:142:MET:HE2	1.82	0.61
2:B:35:LEU:HD21	2:B:66:THR:HG23	1.82	0.60
8:H:29:ASP:OD1	8:H:97:ARG:NH2	2.32	0.60
1:A:122:LEU:HD22	6:F:71:PHE:CD1	2.37	0.60
3:C:127:ASP:OD1	3:C:154:SER:OG	2.11	0.60
2:B:175:LEU:HD11	3:C:125:ILE:HD12	1.84	0.59
1:A:120:ARG:NH2	1:A:156:SER:OG	2.35	0.59
8:H:15:LEU:HD21	8:H:19:LEU:C	2.28	0.59
9:I:22:ASP:OD2	9:I:23:VAL:N	2.36	0.58
8:H:160:MET:HE1	8:H:168:LEU:HD23	1.85	0.58
10:J:201:LEU:O	11:N:274:SER:OG	2.22	0.57
2:B:175:LEU:HD11	3:C:125:ILE:CD1	2.34	0.57
2:B:116:GLU:OE1	2:B:116:GLU:N	2.38	0.57
7:G:137:MET:CE	9:I:181:MET:HE2	2.34	0.57
4:D:126:LEU:HD23	4:D:127:ARG:N	2.20	0.57
8:H:13:GLN:OE1	8:H:83:ASN:N	2.37	0.57
6:F:81:VAL:O	6:F:84:THR:HG22	2.05	0.57
1:A:133:ARG:NH1	9:I:126:LEU:O	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:N:162:LYS:O	11:N:166:ILE:HG13	2.04	0.56
11:N:273:SER:O	11:N:277:GLN:N	2.37	0.56
1:A:125:ARG:NH1	7:G:129:LEU:O	2.38	0.56
1:A:123:SER:HB2	7:G:129:LEU:HD21	1.88	0.56
9:I:155:GLU:OE1	9:I:156:ASP:N	2.38	0.56
9:I:8:HIS:NE2	9:I:62:GLN:OE1	2.38	0.56
11:N:292:GLU:O	11:N:296:LYS:N	2.38	0.55
7:G:85:LYS:HD2	7:G:87:LEU:HD21	1.88	0.55
9:I:125:ASP:OD1	9:I:126:LEU:N	2.40	0.55
5:E:36:MET:HG3	5:E:85:LEU:HD12	1.89	0.55
10:J:23:ASN:ND2	10:J:100:HIS:O	2.38	0.55
9:I:96:ASN:OD1	9:I:97:LEU:N	2.40	0.54
5:E:204:VAL:O	5:E:208:LEU:HD23	2.06	0.54
9:I:56:GLU:O	9:I:60:LEU:HD23	2.07	0.54
11:N:97:MET:HE1	11:N:123:LEU:HD21	1.88	0.54
1:A:122:LEU:HD22	6:F:71:PHE:HD1	1.73	0.54
10:J:99:ILE:CG2	10:J:99:ILE:O	2.55	0.54
12:T:267:ILE:HG22	12:T:267:ILE:O	2.08	0.54
5:E:115:GLU:O	5:E:118:ILE:N	2.40	0.53
9:I:76:LEU:HD22	9:I:81:ALA:HB1	1.90	0.53
9:I:22:ASP:OD2	9:I:23:VAL:HG23	2.08	0.53
3:C:141:LEU:HD23	3:C:144:MET:SD	2.49	0.53
4:D:149:SER:OG	4:D:151:GLU:OE1	2.25	0.53
9:I:17:LYS:CD	9:I:50:LEU:HD22	2.37	0.53
5:E:201:ARG:NE	10:J:192:GLU:OE2	2.36	0.53
10:J:99:ILE:O	10:J:99:ILE:HG22	2.09	0.53
10:J:75:ILE:HG23	10:J:109:PHE:CZ	2.44	0.53
2:B:31:ALA:O	2:B:35:LEU:HD23	2.09	0.52
5:E:192:VAL:O	5:E:192:VAL:HG13	2.08	0.52
11:N:27:LEU:HA	11:N:30:ILE:HG22	1.92	0.52
2:B:111:ARG:NH2	3:C:143:ARG:O	2.41	0.52
5:E:159:VAL:HG12	5:E:176:VAL:HG22	1.92	0.51
7:G:131:ILE:HG23	7:G:131:ILE:O	2.11	0.51
11:N:275:VAL:O	11:N:278:ILE:HG22	2.10	0.51
10:J:49:PHE:HE2	10:J:72:LEU:HD22	1.74	0.51
11:N:50:PHE:O	11:N:54:VAL:HG12	2.11	0.51
7:G:191:ARG:O	7:G:194:THR:OG1	2.26	0.50
4:D:116:PRO:HA	4:D:119:LYS:HG2	1.93	0.50
11:N:87:SER:HA	11:N:90:ILE:HG22	1.92	0.50
3:C:45:VAL:HG23	3:C:46:LEU:HD23	1.93	0.50
11:N:31:LEU:O	11:N:35:VAL:HG23	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:16:LEU:CD1	2:B:24:VAL:HG22	2.37	0.50
1:A:80:THR:HG21	1:A:86:ILE:HG12	1.95	0.49
7:G:137:MET:HE2	9:I:181:MET:HE2	1.94	0.49
9:I:42:LEU:CD2	9:I:61:LEU:HD13	2.35	0.49
1:A:89:ASP:O	1:A:93:VAL:HG23	2.13	0.48
11:N:44:ILE:HG22	11:N:52:LYS:HE2	1.96	0.48
2:B:127:LEU:HD12	2:B:128:GLU:N	2.28	0.48
2:B:20:ASP:O	2:B:24:VAL:HG23	2.14	0.48
4:D:93:LEU:HD23	4:D:96:LEU:HD12	1.96	0.47
5:E:77:LEU:HD22	5:E:81:GLN:OE1	2.14	0.47
5:E:48:PHE:CE1	5:E:122:LEU:HD22	2.50	0.47
10:J:38:LEU:HD12	10:J:39:GLN:N	2.29	0.47
8:H:83:ASN:OD1	8:H:84:SER:N	2.47	0.47
8:H:17:ALA:HB1	8:H:85:LEU:HD22	1.97	0.47
11:N:27:LEU:O	11:N:31:LEU:HD13	2.15	0.47
4:D:64:ASP:OD1	11:N:139:ARG:NH1	2.48	0.47
5:E:36:MET:CG	5:E:85:LEU:HD12	2.45	0.47
9:I:139:ILE:HG21	9:I:142:MET:HE3	1.97	0.47
11:N:66:PHE:CE2	11:N:97:MET:HE3	2.50	0.47
11:N:120:VAL:HG22	11:N:124:VAL:CG2	2.38	0.47
5:E:39:LEU:HD12	5:E:81:GLN:CG	2.46	0.46
7:G:119:THR:HG23	7:G:120:LEU:HD12	1.96	0.46
10:J:68:LEU:HD12	10:J:69:HIS:N	2.29	0.46
9:I:30:GLU:OE2	9:I:42:LEU:HD12	2.16	0.46
4:D:22:LEU:O	4:D:22:LEU:HD23	2.16	0.46
5:E:196:LYS:HG3	10:J:134:LEU:HD22	1.96	0.46
4:D:18:GLU:HB2	4:D:71:VAL:HG21	1.98	0.46
10:J:166:ASN:ND2	10:J:173:GLU:OE1	2.42	0.46
5:E:39:LEU:HD12	5:E:81:GLN:HG3	1.96	0.46
7:G:68:LEU:HD12	7:G:68:LEU:H	1.81	0.46
2:B:120:SER:C	2:B:121:LEU:HD12	2.41	0.46
3:C:45:VAL:HG23	3:C:46:LEU:CD2	2.46	0.46
5:E:87:ALA:HB2	12:T:143:VAL:HG12	1.97	0.46
5:E:207:VAL:HG22	10:J:139:TRP:CE3	2.51	0.46
7:G:137:MET:HE3	9:I:181:MET:HE2	1.96	0.46
1:A:125:ARG:NH2	1:A:127:ASP:OD2	2.49	0.45
7:G:139:TRP:HE1	9:I:188:ILE:HD11	1.81	0.45
9:I:121:PRO:HB3	9:I:153:ILE:HG23	1.98	0.45
11:N:66:PHE:CD2	11:N:97:MET:HE3	2.51	0.45
3:C:38:ASP:O	12:T:202:ARG:NH1	2.49	0.45
3:C:134:TYR:HB2	10:J:145:MET:HE3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:TRP:CZ3	4:D:158:ARG:HB2	2.52	0.45
8:H:131:ASP:OD1	8:H:131:ASP:N	2.49	0.45
11:N:85:ALA:HB1	11:N:89:LYS:HZ3	1.81	0.45
2:B:134:GLN:OE1	2:B:143:GLN:NE2	2.49	0.45
10:J:9:LEU:HD13	10:J:99:ILE:HG13	1.99	0.45
3:C:131:ARG:HG3	10:J:147:HIS:HB3	1.99	0.45
1:A:49:ARG:N	1:A:50:PRO:CD	2.80	0.44
5:E:107:ASP:HA	5:E:110:ARG:NH2	2.32	0.44
5:E:176:VAL:HB	5:E:192:VAL:HG13	1.99	0.44
10:J:107:GLU:HA	10:J:110:VAL:HG12	2.00	0.44
2:B:143:GLN:O	2:B:144:ILE:HD13	2.17	0.44
4:D:57:ASP:OD1	4:D:57:ASP:N	2.49	0.44
11:N:61:ILE:HG23	11:N:97:MET:SD	2.57	0.44
3:C:193:THR:HG23	12:T:135:ARG:HB2	2.00	0.44
4:D:34:CYS:HA	4:D:37:VAL:HG12	2.00	0.44
6:F:38:LEU:HD21	6:F:40:TYR:HE1	1.82	0.44
5:E:208:LEU:HD22	10:J:184:LEU:HD23	1.98	0.44
1:A:86:ILE:HG22	1:A:90:GLN:OE1	2.17	0.44
5:E:54:PHE:CZ	5:E:67:ALA:HB1	2.53	0.44
10:J:19:VAL:HG11	10:J:99:ILE:HG22	2.00	0.44
4:D:93:LEU:HA	4:D:96:LEU:HD12	2.00	0.43
9:I:46:THR:HG21	9:I:57:ALA:HB2	2.00	0.43
12:T:261:GLY:HA2	12:T:265:ALA:HB3	1.99	0.43
1:A:102:LYS:C	1:A:106:ARG:HE	2.26	0.43
1:A:174:THR:O	1:A:178:VAL:HG23	2.19	0.43
6:F:85:VAL:O	6:F:85:VAL:HG13	2.19	0.43
11:N:67:ASP:O	11:N:96:ARG:NE	2.52	0.43
5:E:48:PHE:CZ	5:E:89:MET:HE1	2.53	0.43
1:A:125:ARG:N	1:A:144:ILE:O	2.48	0.43
3:C:128:VAL:HG12	3:C:153:LEU:HD23	2.00	0.43
5:E:112:GLN:C	5:E:114:GLN:H	2.26	0.43
12:T:171:VAL:HG12	12:T:192:VAL:HG11	2.01	0.43
8:H:47:GLU:O	8:H:51:TRP:N	2.44	0.43
9:I:62:GLN:NE2	9:I:66:ARG:HE	2.17	0.43
1:A:102:LYS:O	1:A:106:ARG:NE	2.50	0.42
1:A:124:TRP:CG	6:F:78:ILE:HD11	2.54	0.42
2:B:36:ARG:O	11:N:161:ARG:CG	2.67	0.42
2:B:121:LEU:HD23	5:E:148:TRP:CZ3	2.55	0.42
12:T:225:ASP:O	12:T:229:VAL:HG12	2.19	0.42
2:B:127:LEU:CD2	3:C:178:LEU:HD12	2.50	0.42
5:E:60:GLN:HB2	5:E:62:GLU:OE1	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:N:80:ILE:O	11:N:84:ILE:HG12	2.20	0.42
9:I:52:VAL:HG21	9:I:56:GLU:OE1	2.20	0.42
2:B:28:GLY:HA3	2:B:102:LEU:HD21	2.02	0.42
2:B:139:SER:OG	3:C:115:LEU:O	2.28	0.42
10:J:115:SER:OG	10:J:116:MET:N	2.53	0.42
2:B:127:LEU:HD12	2:B:128:GLU:H	1.85	0.42
9:I:189:ARG:NH1	11:N:293:TYR:OH	2.53	0.42
2:B:16:LEU:N	2:B:17:PRO:HD2	2.35	0.42
10:J:65:LYS:HA	10:J:68:LEU:HD21	2.02	0.41
7:G:34:THR:HG22	7:G:38:PHE:CZ	2.55	0.41
10:J:189:ASN:OD1	11:N:197:ARG:NH1	2.51	0.41
2:B:117:LEU:HD11	11:N:169:VAL:CG1	2.43	0.41
5:E:35:ALA:O	5:E:39:LEU:HD23	2.19	0.41
3:C:42:ASP:CG	3:C:43:GLU:H	2.28	0.41
10:J:118:GLN:HA	10:J:121:VAL:HG12	2.01	0.41
12:T:287:ALA:HB1	12:T:288:PRO:HD2	2.01	0.41
11:N:166:ILE:HA	11:N:169:VAL:HG12	2.03	0.41
7:G:65:LEU:HA	7:G:68:LEU:HD13	2.03	0.41
9:I:133:LYS:O	9:I:142:MET:HG3	2.21	0.41
11:N:117:PHE:O	11:N:121:GLN:NE2	2.49	0.41
4:D:22:LEU:HD23	4:D:22:LEU:C	2.46	0.41
4:D:161:VAL:HG22	4:D:170:GLN:O	2.21	0.41
5:E:115:GLU:CD	5:E:120:GLN:HG2	2.46	0.41
6:F:33:ASP:N	6:F:33:ASP:OD1	2.53	0.41
11:N:57:MET:O	11:N:61:ILE:HG13	2.21	0.41
11:N:70:VAL:HG11	11:N:89:LYS:HG2	2.01	0.41
8:H:80:ASN:OD1	8:H:81:GLN:N	2.53	0.40
8:H:108:GLU:O	8:H:111:ALA:HB3	2.21	0.40
10:J:38:LEU:HD13	10:J:116:MET:HB2	2.03	0.40
1:A:163:PHE:CE1	6:F:19:LEU:HD21	2.56	0.40
2:B:117:LEU:HD13	3:C:140:GLN:CG	2.48	0.40
3:C:136:ILE:HD13	5:E:214:LEU:HD21	2.02	0.40
5:E:115:GLU:HA	5:E:118:ILE:HB	2.02	0.40
10:J:17:LYS:NZ	10:J:70:LEU:HD13	2.36	0.40
10:J:92:LEU:O	10:J:96:LEU:HD12	2.22	0.40
11:N:87:SER:O	11:N:90:ILE:HG22	2.21	0.40
11:N:91:VAL:O	11:N:95:PRO:CD	2.70	0.40
1:A:67:MET:SD	1:A:67:MET:N	2.94	0.40
8:H:9:LEU:HD11	8:H:61:PHE:CD2	2.57	0.40
1:A:49:ARG:N	1:A:50:PRO:HD2	2.36	0.40
11:N:185:HIS:ND1	11:N:185:HIS:O	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:T:249:GLN:O	12:T:253:THR:HG22	2.21	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	185/190 (97%)	176 (95%)	9 (5%)	0	100	100
2	B	197/199 (99%)	194 (98%)	3 (2%)	0	100	100
3	C	193/195 (99%)	187 (97%)	6 (3%)	0	100	100
4	D	197/199 (99%)	197 (100%)	0	0	100	100
5	E	203/260 (78%)	198 (98%)	5 (2%)	0	100	100
6	F	75/85 (88%)	73 (97%)	2 (3%)	0	100	100
7	G	198/200 (99%)	195 (98%)	3 (2%)	0	100	100
8	H	177/183 (97%)	173 (98%)	4 (2%)	0	100	100
9	I	196/198 (99%)	189 (96%)	7 (4%)	0	100	100
10	J	196/212 (92%)	191 (97%)	5 (3%)	0	100	100
11	N	221/631 (35%)	216 (98%)	5 (2%)	0	100	100
12	T	172/627 (27%)	159 (92%)	13 (8%)	0	100	100
All	All	2210/3179 (70%)	2148 (97%)	62 (3%)	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	160/163 (98%)	160 (100%)	0	100	100
2	B	180/180 (100%)	180 (100%)	0	100	100
3	C	174/174 (100%)	174 (100%)	0	100	100
4	D	170/170 (100%)	170 (100%)	0	100	100
5	E	174/213 (82%)	174 (100%)	0	100	100
6	F	69/76 (91%)	69 (100%)	0	100	100
7	G	176/176 (100%)	176 (100%)	0	100	100
8	H	161/165 (98%)	161 (100%)	0	100	100
9	I	175/175 (100%)	175 (100%)	0	100	100
10	J	176/189 (93%)	176 (100%)	0	100	100
11	N	202/563 (36%)	202 (100%)	0	100	100
12	T	145/538 (27%)	145 (100%)	0	100	100
All	All	1962/2782 (70%)	1962 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	79	GLN
2	B	155	ASN
2	B	161	ASN
2	B	174	HIS
3	C	76	HIS
3	C	106	ASN
4	D	102	HIS
5	E	114	GLN
6	F	52	HIS
7	G	93	GLN
8	H	43	HIS
8	H	78	GLN
10	J	69	HIS
10	J	95	GLN

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Mol	Chain	Res	Type
10	J	150	GLN
11	N	23	GLN
11	N	101	HIS
11	N	115	HIS
12	T	153	GLN
12	T	209	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.

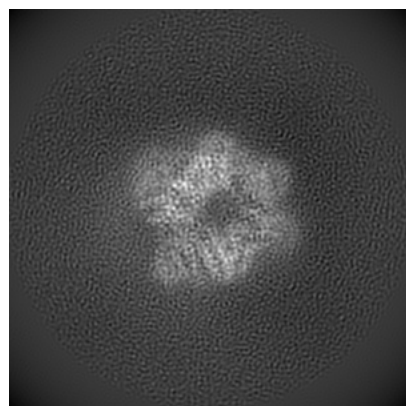
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-28827. These allow visual inspection of the internal detail of the map and identification of artifacts.

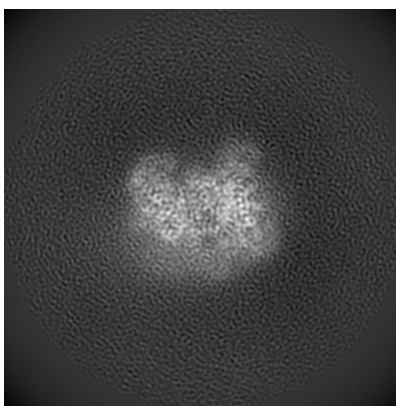
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

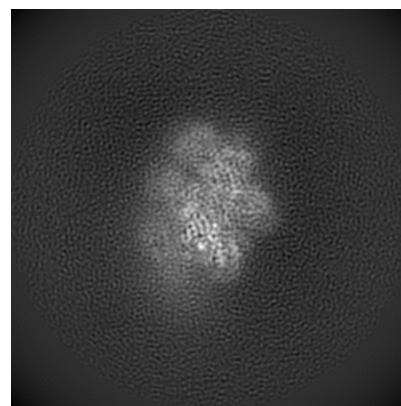
6.1.1 Primary map



X

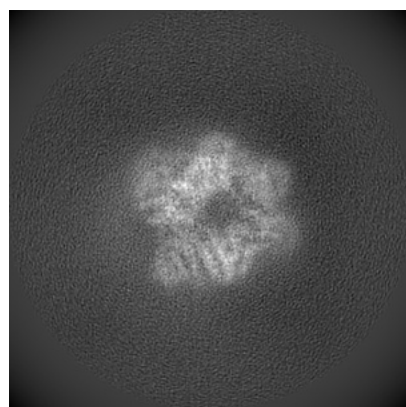


Y

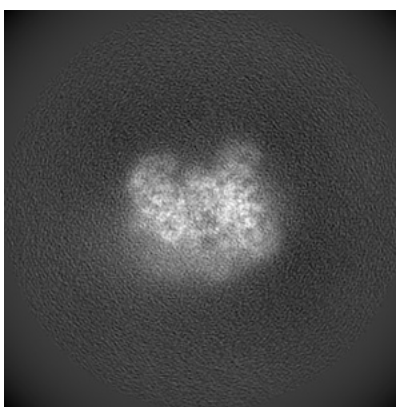


Z

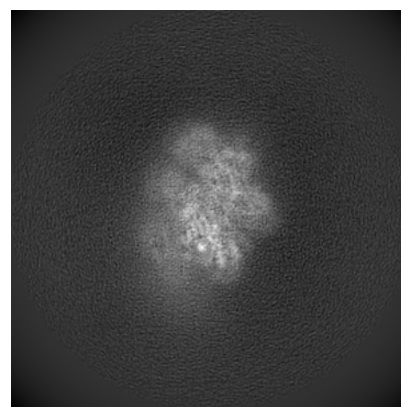
6.1.2 Raw map



X



Y

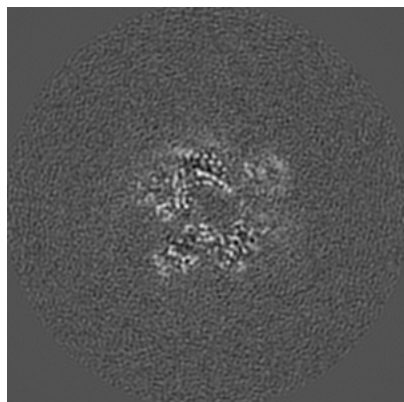


Z

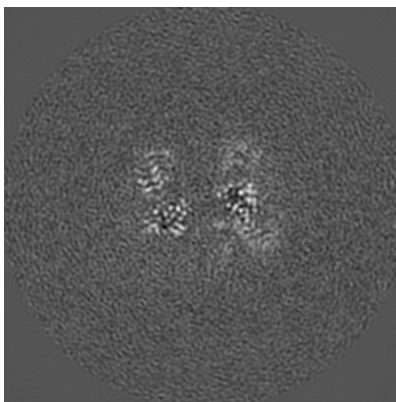
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

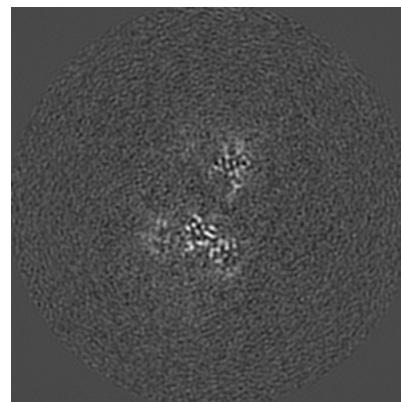
6.2.1 Primary map



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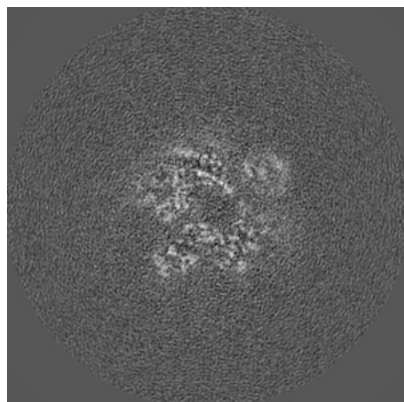


Y Index: 132

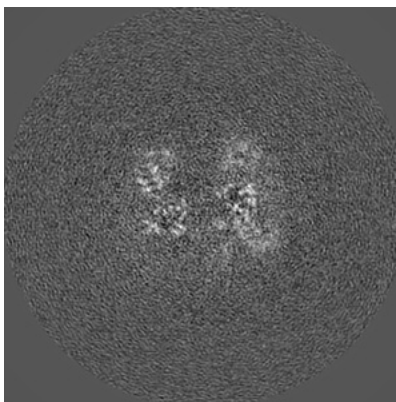


Z Index: 132

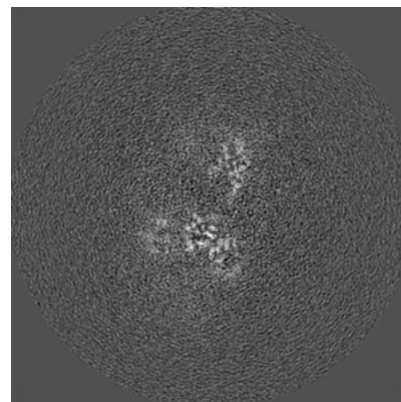
6.2.2 Raw map



X Index: 132



Y Index: 132

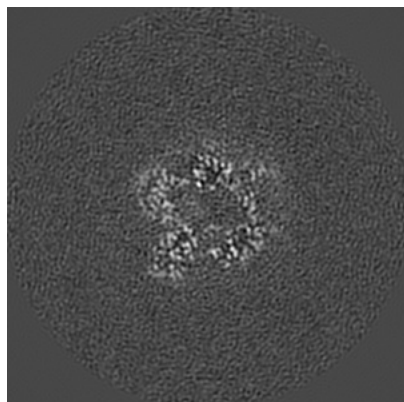


Z Index: 132

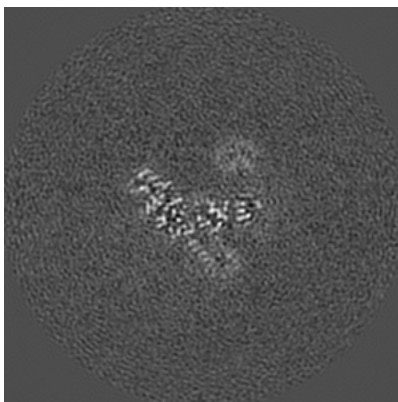
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

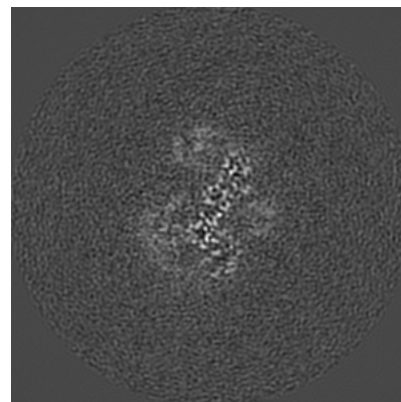
6.3.1 Primary map



X Index: 137

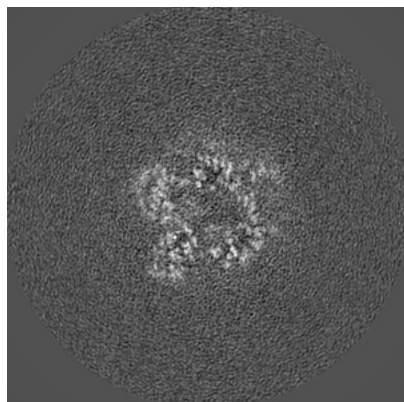


Y Index: 121

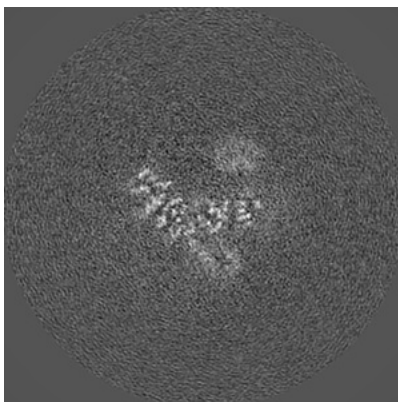


Z Index: 146

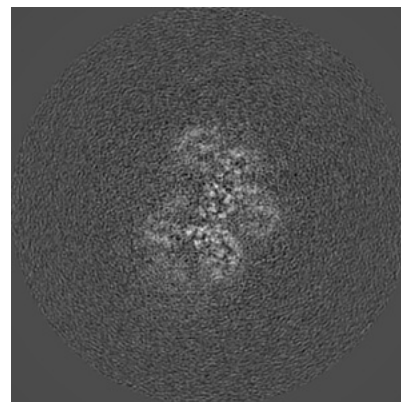
6.3.2 Raw map



X Index: 137



Y Index: 121

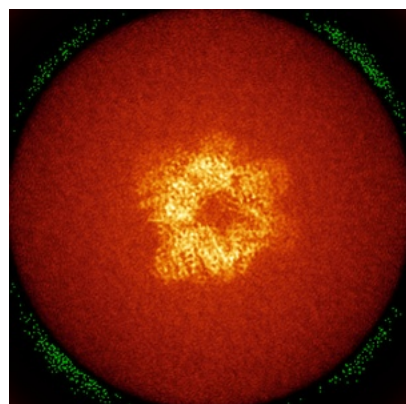


Z Index: 148

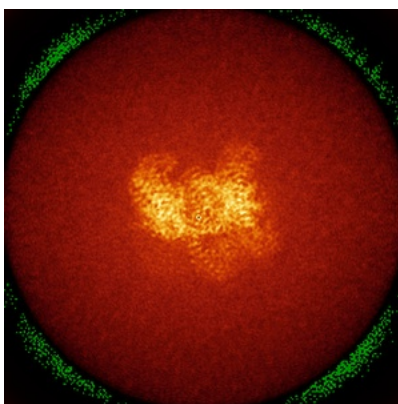
The images above show the largest variance slices of the map in three orthogonal directions.

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

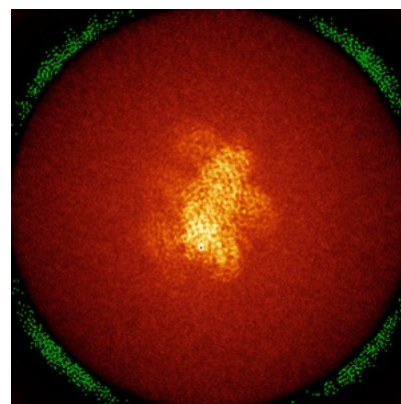
6.4.1 Primary map



X

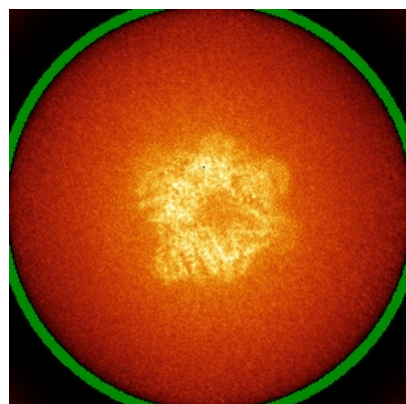


Y

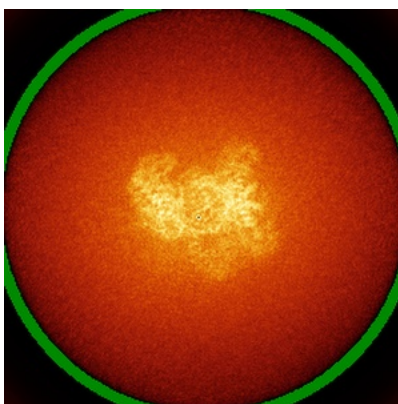


Z

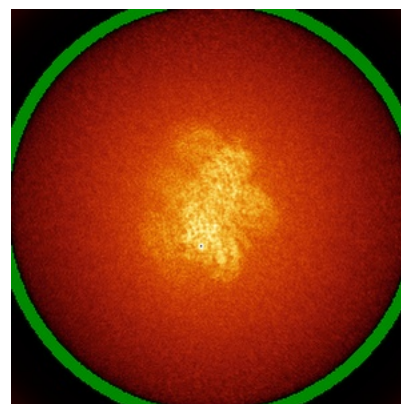
6.4.2 Raw map



X



Y

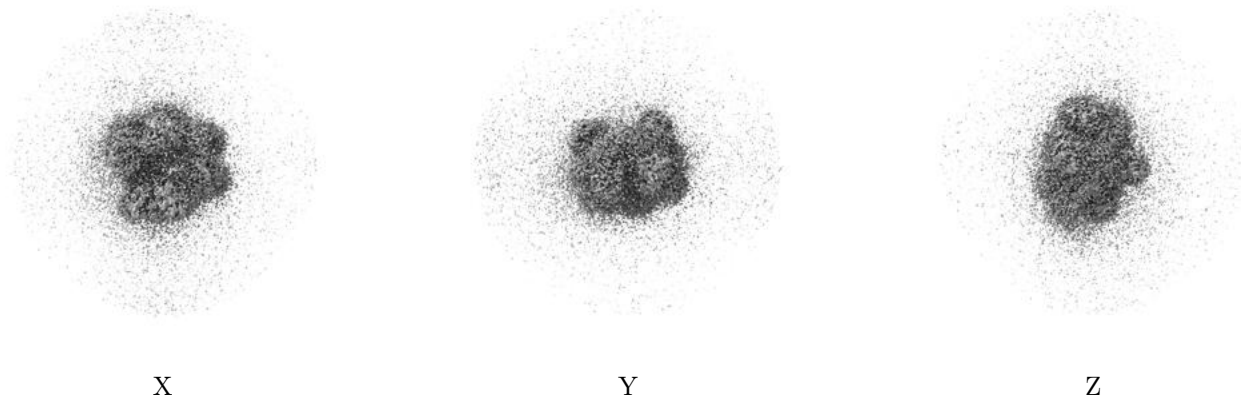


Z

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

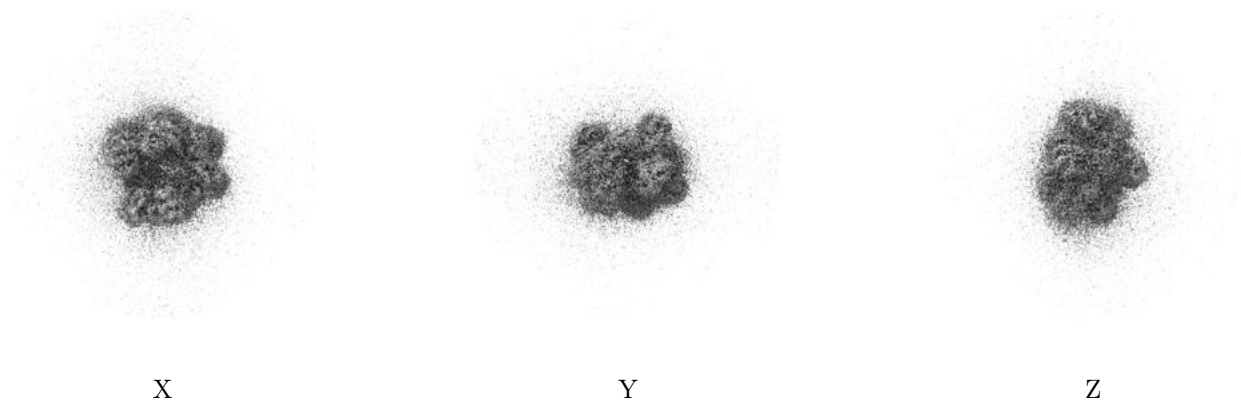
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

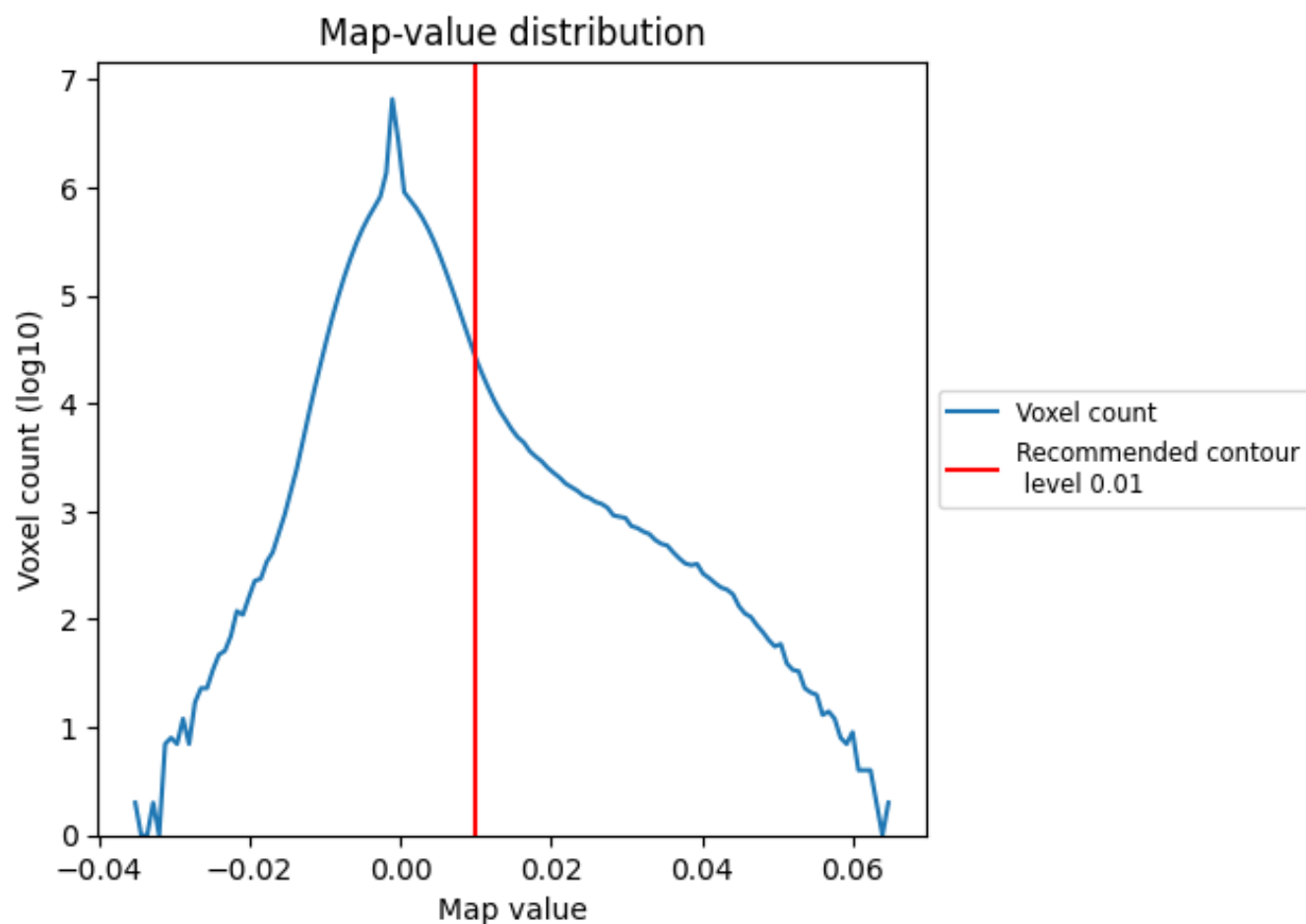
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

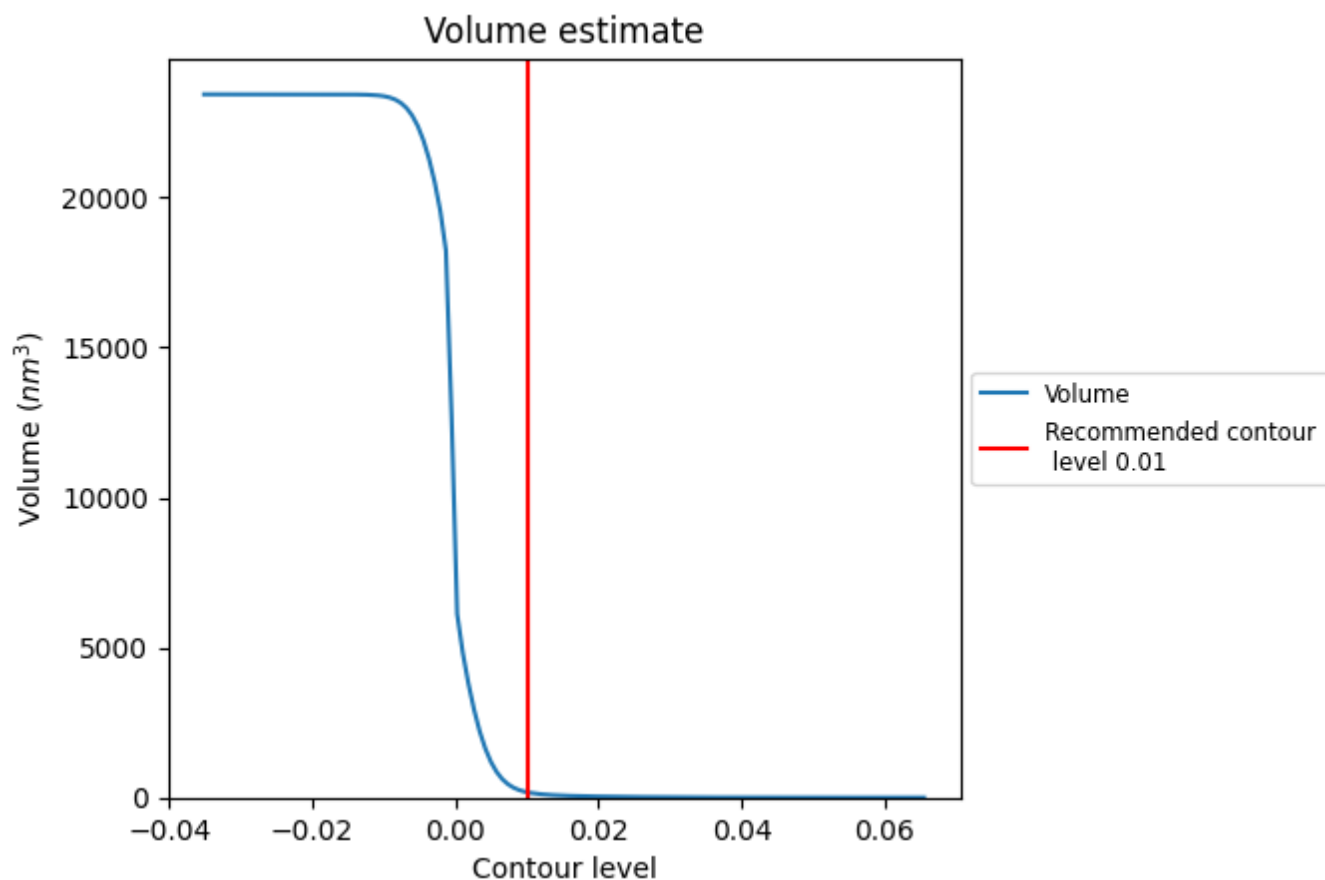
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

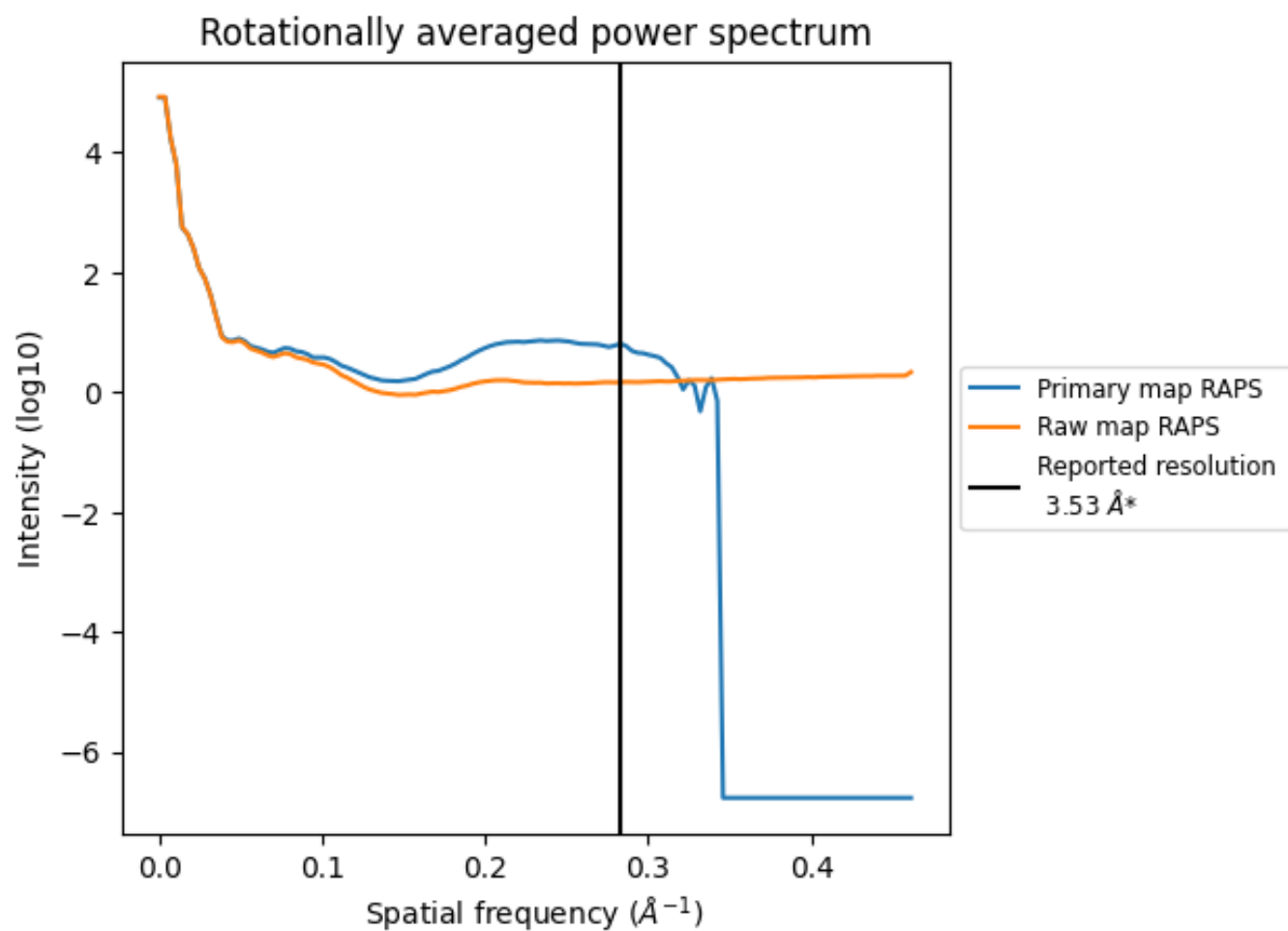
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 181 nm³; this corresponds to an approximate mass of 163 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 ⓘ

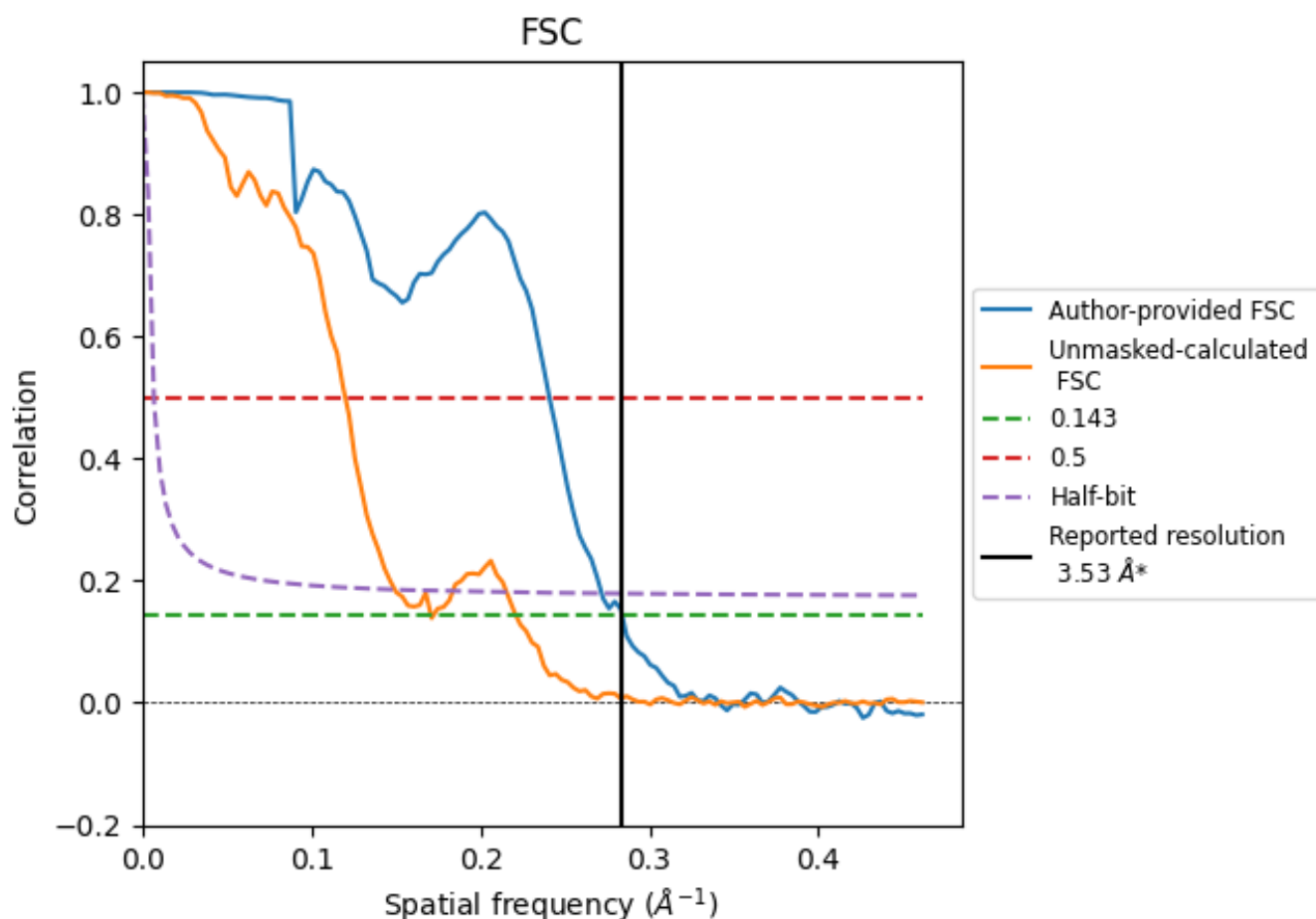


*Reported resolution corresponds to spatial frequency of 0.283 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.283 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

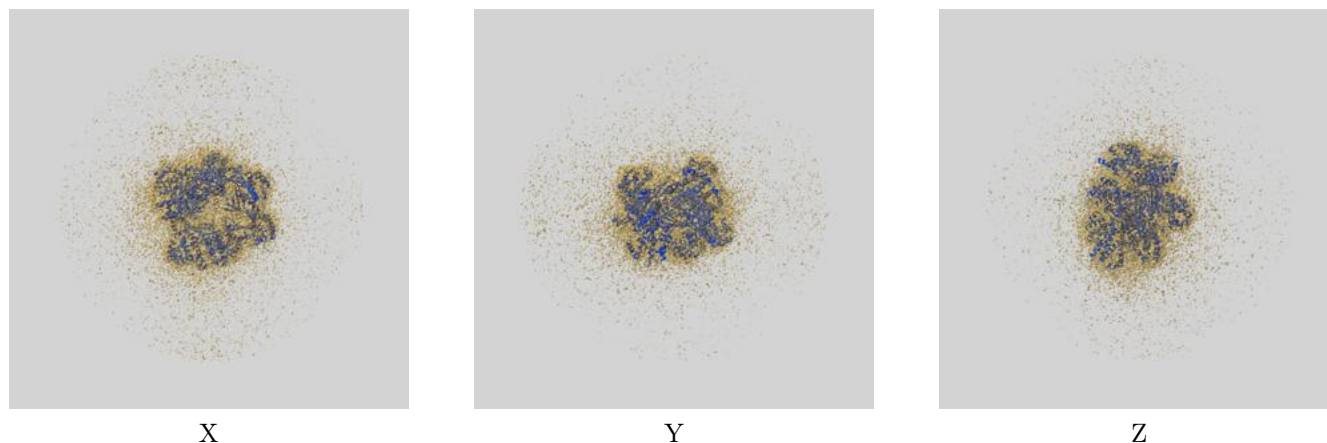
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.53	-	-
Author-provided FSC curve	3.52	4.15	3.68
Unmasked-calculated*	5.85	8.33	6.69

*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 5.85 differs from the reported value 3.53 by more than 10 %

9 Map-model fit [i](#)

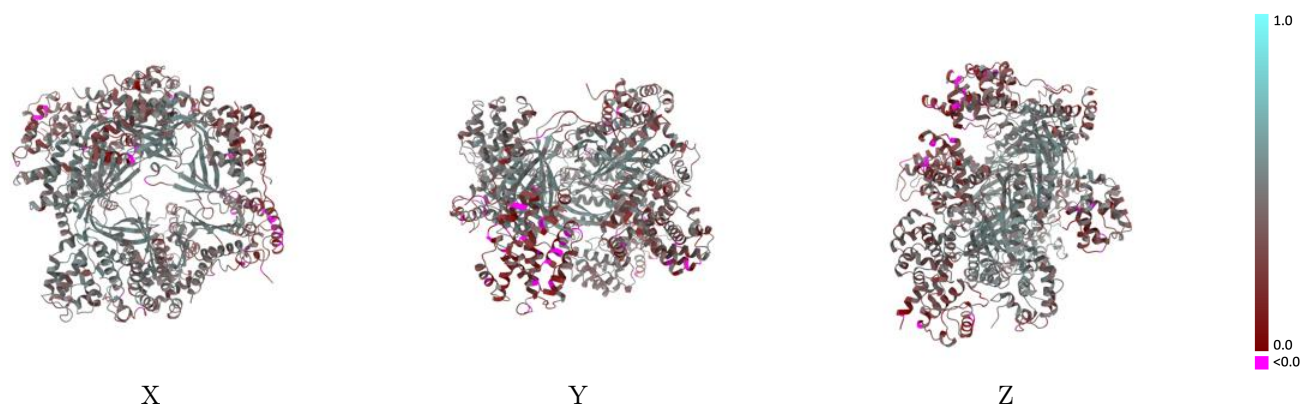
This section contains information regarding the fit between EMDB map EMD-28827 and PDB model 8F2U. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



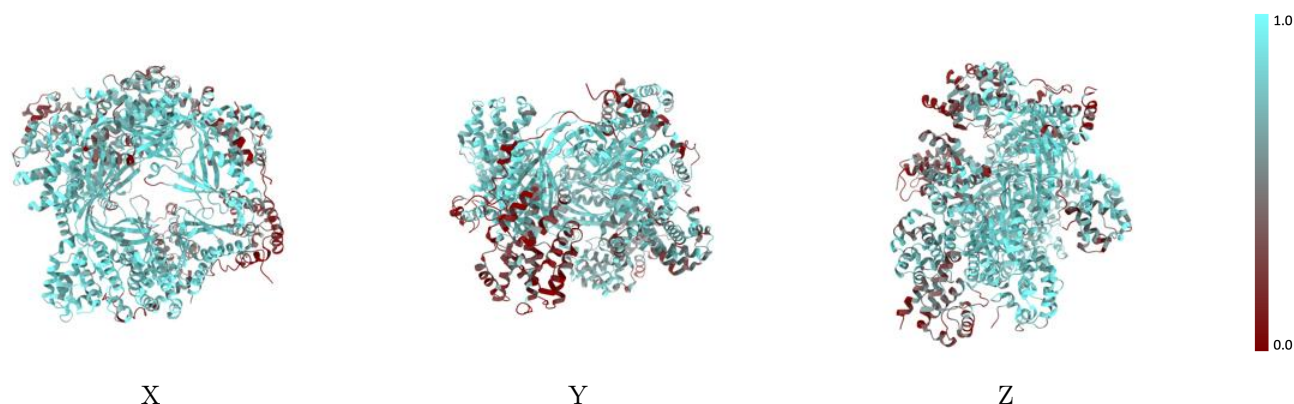
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



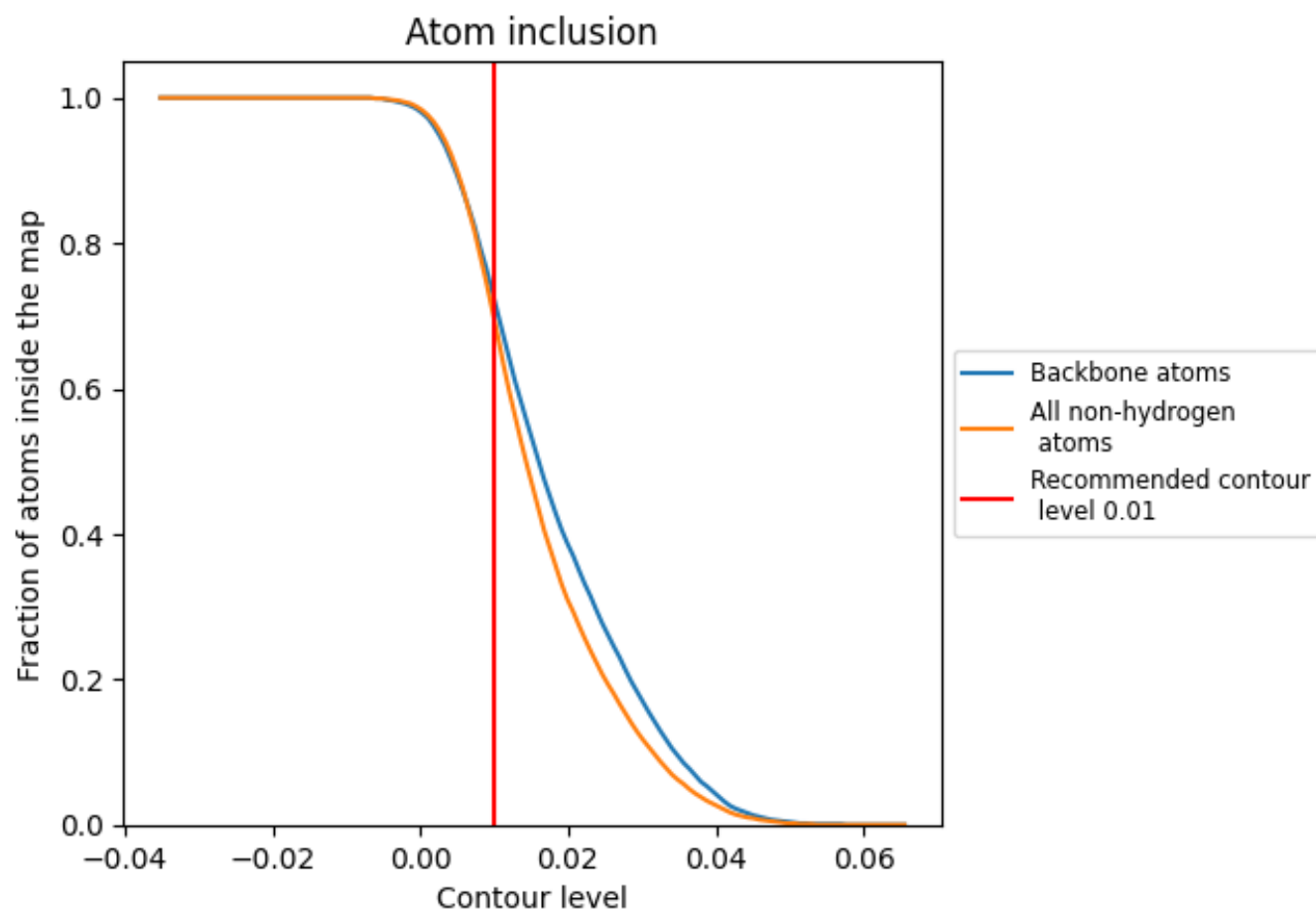
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).

9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 70% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6960	0.4080
A	0.5060	0.3460
B	0.7580	0.4270
C	0.8510	0.4840
D	0.7900	0.4500
E	0.8470	0.4710
F	0.8720	0.4880
G	0.4860	0.3050
H	0.8540	0.4830
I	0.7130	0.3880
J	0.7550	0.4040
N	0.4540	0.3270
T	0.6000	0.3800

