



Full wwPDB EM Validation Report ⓘ

Apr 5, 2026 – 11:52 PM UTC

PDB ID : 9RLA / pdb_00009rla
EMDB ID : EMD-54032
Title : 13S+Beta1 proteasome precursor complex
Authors : Mark, E.; Ramos, P.C.; Nunes, M.M.; Dohmen, R.J.; Wendler, P.
Deposited on : 2025-06-16
Resolution : 3.16 Å(reported)
Based on initial model : 8RVL

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:

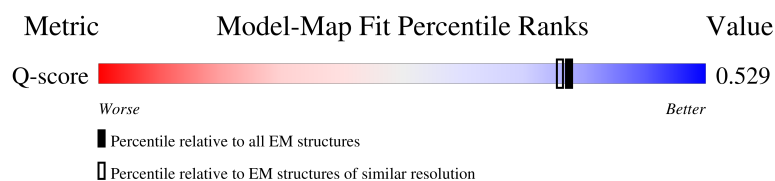
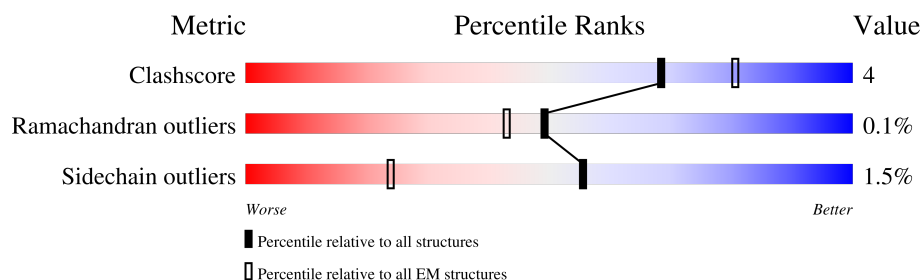
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.16 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	14474 (2.66 - 3.66)

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	252	
2	D	254	
3	E	260	
4	F	234	

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Mol	Chain	Length	Quality of chain
5	H	215	
6	3	162	
7	4	276	
8	5	267	
9	B	250	
10	C	258	
11	G	288	
12	I	261	
13	J	205	
14	K	198	

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 24539 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 Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	250	Total	C	N	O	S	0	0
			1955	1241	329	377	8		

- Molecule 2 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	250	Total	C	N	O	S	0	0
			1950	1215	342	388	5		

- Molecule 3 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	251	Total	C	N	O	S	0	0
			1934	1210	326	390	8		

- Molecule 4 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	234	Total	C	N	O	S	0	0
			1802	1134	313	350	5		

- Molecule 5 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	172	Total	C	N	O	S	0	0
			1318	837	217	257	7		

- Molecule 6 is a protein called Proteasome maturation factor UMP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	3	116	Total	C	N	O	S	0	0
			929	569	171	183	6		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	-14	ASP	-	expression tag	UNP P38293
3	-13	TYR	-	expression tag	UNP P38293
3	-12	LYS	-	expression tag	UNP P38293
3	-11	ASP	-	expression tag	UNP P38293
3	-10	ASP	-	expression tag	UNP P38293
3	-9	ASP	-	expression tag	UNP P38293
3	-8	ASP	-	expression tag	UNP P38293
3	-7	LYS	-	expression tag	UNP P38293
3	-6	HIS	-	expression tag	UNP P38293
3	-5	HIS	-	expression tag	UNP P38293
3	-4	HIS	-	expression tag	UNP P38293
3	-3	HIS	-	expression tag	UNP P38293
3	-1	HIS	-	expression tag	UNP P38293
3	0	HIS	-	expression tag	UNP P38293
3	43	PRO	-	insertion	UNP P38293
3	?	-	LEU	deletion	UNP P38293
3	126	THR	-	insertion	UNP P38293
3	?	-	THR	deletion	UNP P38293

- Molecule 7 is a protein called Proteasome chaperone 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	4	276	Total	C	N	O	S	0	0
			2130	1375	335	407	13		

- Molecule 8 is a protein called Proteasome assembly chaperone 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	5	266	Total	C	N	O	S	0	0
			2161	1396	347	410	8		

- Molecule 9 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B	248	Total	C	N	O	S	0	0
			1898	1208	313	374	3		

- Molecule 10 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	C	238	Total	C	N	O	S	0	0
			1868	1182	314	369	3		

- Molecule 11 is a protein called Probable proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	247	Total	C	N	O	S	0	0
			1917	1218	333	362	4		

- Molecule 12 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	I	225	Total	C	N	O	S	0	0
			1706	1070	295	335	6		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	20	SER	-	insertion	UNP P25043
I	?	-	CYS	deletion	UNP P25043
I	192	THR	-	insertion	UNP P25043
I	?	-	GLU	deletion	UNP P25043
I	232	THR	ALA	conflict	UNP P25043

- Molecule 13 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	J	191	Total	C	N	O	S	0	0
			1475	951	238	278	8		


- Molecule 14 is a protein called Proteasome subunit beta type-4.

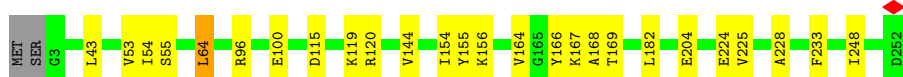
Mol	Chain	Residues	Atoms					AltConf	Trace
14	K	187	Total	C	N	O	S	0	0
			1496	952	253	285	6		

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.

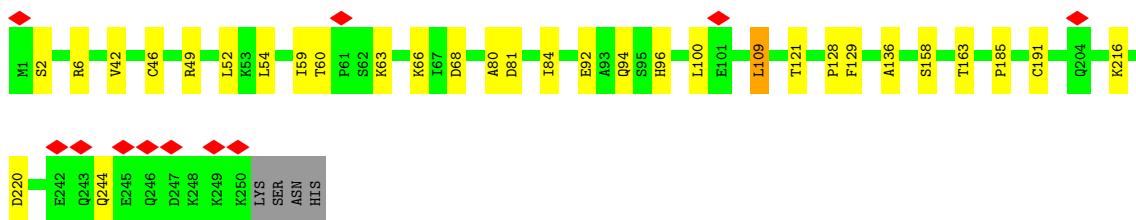
• Molecule 1: Proteasome subunit alpha type-1

Chain A: 




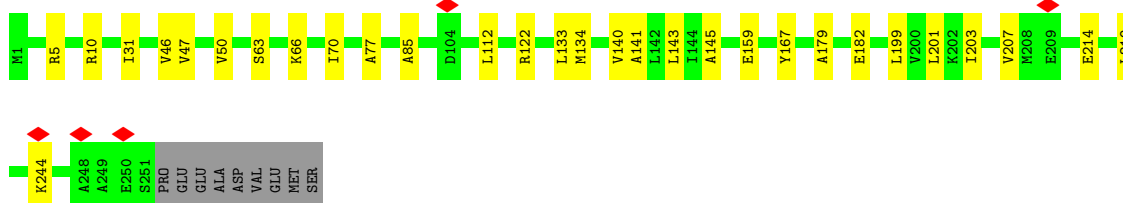
• Molecule 2: Proteasome subunit alpha type-4

Chain D: 




• Molecule 3: Proteasome subunit alpha type-5

Chain E: 

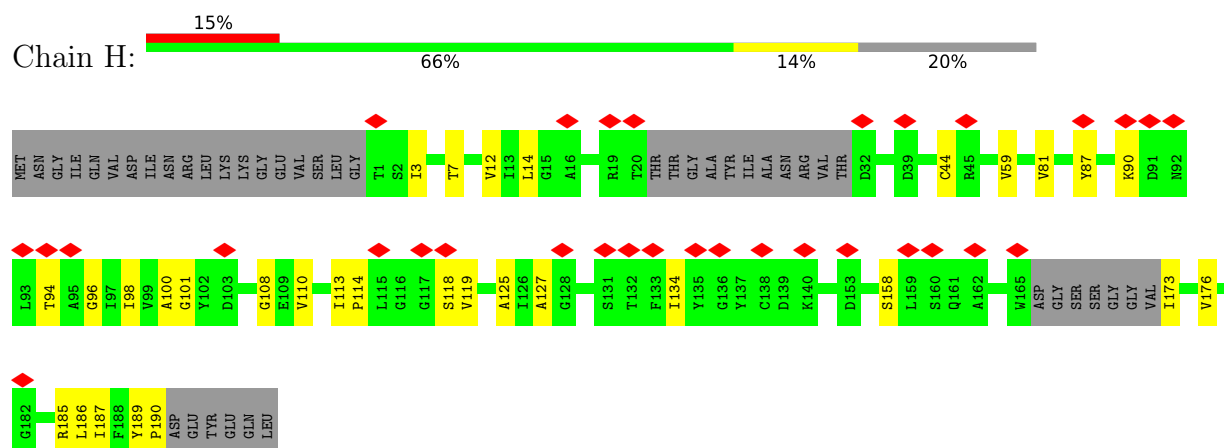


• Molecule 4: Proteasome subunit alpha type-6

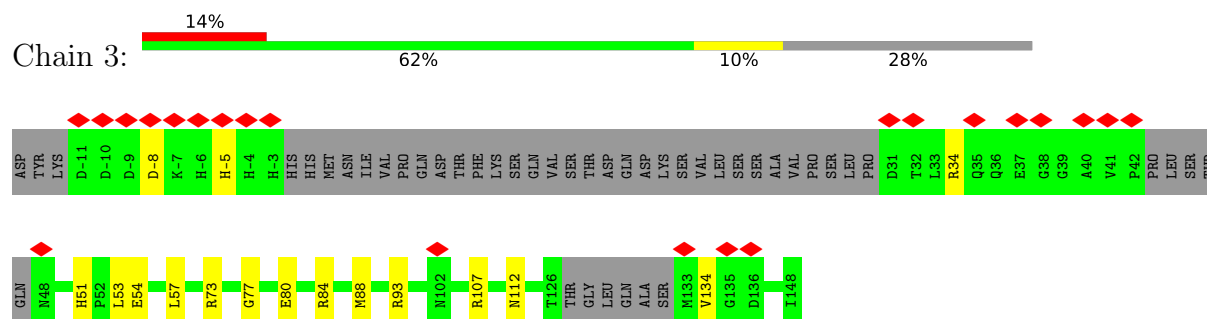
Chain F: 



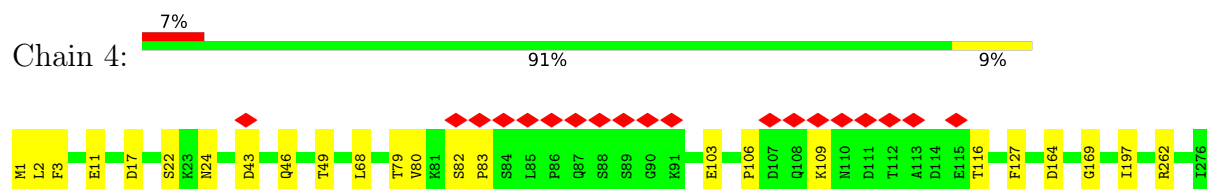
- Molecule 5: Proteasome subunit beta type-1



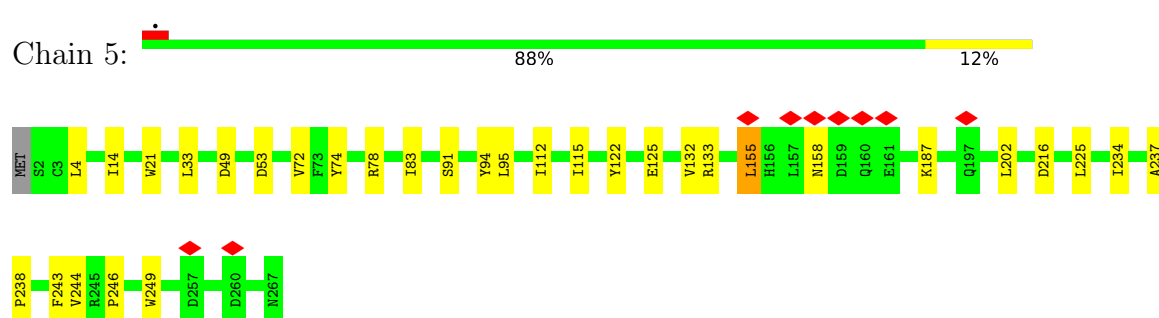
- Molecule 6: Proteasome maturation factor UMP1



- Molecule 7: Proteasome chaperone 1



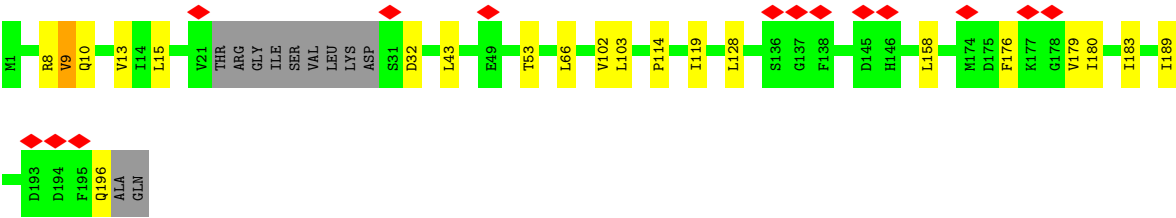
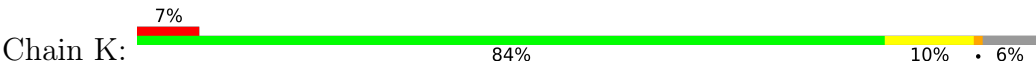
- Molecule 8: Proteasome assembly chaperone 2



- Molecule 9: Proteasome subunit alpha type-2







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	53118	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	64	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.923	Depositor
Minimum map value	-0.566	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.119	Depositor
Map size (Å)	498.0, 498.0, 498.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.996, 0.996, 0.996	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0/1993	0.26	0/2700
2	D	0.11	0/1979	0.24	0/2679
3	E	0.09	0/1961	0.24	0/2642
4	F	0.10	0/1830	0.25	0/2473
5	H	0.09	0/1343	0.23	0/1818
6	3	0.10	0/943	0.23	0/1269
7	4	0.10	0/2183	0.25	0/2969
8	5	0.10	0/2214	0.23	0/3010
9	B	0.12	0/1935	0.24	0/2621
10	C	0.12	0/1897	0.23	0/2566
11	G	0.11	0/1957	0.24	0/2643
12	I	0.10	0/1735	0.23	0/2353
13	J	0.11	0/1504	0.25	0/2031
14	K	0.10	0/1523	0.26	0/2052
All	All	0.11	0/24997	0.24	0/33826

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	1955	0	1943	17	0
2	D	1950	0	1945	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	1934	0	1906	16	0
4	F	1802	0	1809	16	0
5	H	1318	0	1276	17	0
6	3	929	0	874	11	0
7	4	2130	0	2091	15	0
8	5	2161	0	2115	17	0
9	B	1898	0	1906	16	0
10	C	1868	0	1872	15	0
11	G	1917	0	1909	9	0
12	I	1706	0	1676	13	0
13	J	1475	0	1462	12	0
14	K	1496	0	1488	9	0
All	All	24539	0	24272	179	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 4.

All (179) 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:A:119:LYS:HE3	9:B:83:ARG:HD2	1.70	0.73
5:H:96:GLY:HA2	5:H:113:ILE:O	1.89	0.73
3:E:85:ALA:HB2	3:E:140:VAL:HG21	1.69	0.72
7:4:49:THR:HG22	7:4:164:ASP:HB2	1.74	0.69
9:B:226:GLY:HA3	12:I:186:TYR:HB3	1.75	0.68
4:F:74:LEU:HD22	4:F:81:ALA:HB1	1.74	0.68
5:H:101:GLY:O	5:H:108:GLY:HA2	1.95	0.67
13:J:146:LEU:HD13	13:J:174:ALA:HB2	1.76	0.67
2:D:216:LYS:HB2	2:D:220:ASP:HB3	1.77	0.66
13:J:10:GLY:HA3	13:J:42:LYS:HE3	1.77	0.66
8:5:132:VAL:HG23	8:5:133:ARG:HG2	1.79	0.65
10:C:64:GLU:HG3	10:C:65:LYS:HG2	1.81	0.62
13:J:21:VAL:HG23	13:J:190:ILE:HB	1.80	0.62
5:H:134:ILE:HD11	5:H:158:SER:HB3	1.82	0.62
1:A:55:SER:HB3	1:A:224:GLU:HG3	1.82	0.61
14:K:15:LEU:HD12	14:K:43:LEU:HD23	1.82	0.60
13:J:63:LEU:HD11	13:J:105:VAL:HG21	1.84	0.60
1:A:228:ALA:HB2	1:A:233:PHE:HD1	1.67	0.60
7:4:24:ASN:HB3	7:4:83:PRO:HB3	1.84	0.60
4:F:63:ILE:HG21	4:F:214:ALA:HB2	1.85	0.59
14:K:32:ASP:HB2	14:K:180:ILE:HD12	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:4:169:GLY:HA3	7:4:197:ILE:HG13	1.87	0.57
2:D:158:SER:HB3	3:E:63:SER:HB3	1.86	0.56
8:5:234:ILE:HB	8:5:237:ALA:HB2	1.87	0.56
5:H:114:PRO:HD2	5:H:118:SER:H	1.70	0.56
8:5:78:ARG:HE	8:5:238:PRO:HG3	1.70	0.56
9:B:122:THR:HG22	9:B:129:PRO:HB3	1.87	0.55
14:K:8:ARG:HD3	14:K:114:PRO:HG2	1.88	0.55
3:E:201:LEU:HD21	3:E:219:LEU:HD11	1.89	0.55
11:G:24:VAL:HG11	11:G:154:SER:HB3	1.89	0.55
6:3:51:HIS:HB3	6:3:54:GLU:HG3	1.88	0.55
6:3:93:ARG:HD2	7:4:2:LEU:HD12	1.89	0.55
3:E:5:ARG:HH11	3:E:10:ARG:HH12	1.55	0.54
5:H:3:ILE:HB	5:H:127:ALA:O	2.07	0.54
4:F:54:ASP:HA	7:4:262:ARG:HH12	1.73	0.54
2:D:46:CYS:HB3	2:D:63:LYS:HD3	1.89	0.54
3:E:77:ALA:HB3	3:E:143:LEU:HB2	1.89	0.54
8:5:115:ILE:HG22	8:5:202:LEU:HD11	1.90	0.53
3:E:46:VAL:HG11	3:E:145:ALA:HB1	1.90	0.53
2:D:121:THR:HG22	2:D:128:PRO:HB3	1.91	0.53
12:I:112:SER:HB3	12:I:125:LEU:HD13	1.91	0.53
8:5:4:LEU:HD11	8:5:83:ILE:HG13	1.91	0.53
10:C:53:THR:HG23	10:C:210:ARG:HD3	1.91	0.53
8:5:122:TYR:HD2	8:5:125:GLU:HG3	1.74	0.52
5:H:87:TYR:HA	5:H:90:LYS:HB2	1.91	0.52
12:I:12:VAL:HG13	12:I:178:MET:HE2	1.91	0.52
1:A:168:ALA:HB1	1:A:182:LEU:HD13	1.93	0.52
3:E:50:VAL:HG21	3:E:66:LYS:HB2	1.93	0.51
14:K:179:VAL:HB	14:K:196:GLN:HG2	1.92	0.51
6:3:34:ARG:HA	6:3:134:VAL:HG21	1.93	0.51
2:D:42:VAL:HG11	2:D:136:ALA:HB1	1.92	0.51
8:5:155:LEU:HA	8:5:158:ASN:HB2	1.93	0.50
2:D:81:ASP:HB3	2:D:129:PHE:HD1	1.75	0.50
5:H:173:ILE:HG13	5:H:190:PRO:HD3	1.93	0.50
10:C:216:ILE:HG13	10:C:227:GLN:HG2	1.94	0.50
8:5:33:LEU:HD22	8:5:74:TYR:HB2	1.93	0.49
6:3:-8:ASP:HA	6:3:-5:HIS:HB2	1.93	0.49
13:J:27:LEU:HD11	13:J:41:GLU:HG2	1.94	0.49
14:K:9:VAL:HG23	14:K:10:GLN:H	1.77	0.49
5:H:12:VAL:HG11	5:H:100:ALA:HB1	1.95	0.49
7:4:80:VAL:HG12	7:4:82:SER:H	1.76	0.49
7:4:80:VAL:HB	7:4:116:THR:HG23	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:G:120:VAL:HG21	11:G:151:LEU:HD21	1.95	0.49
12:I:17:ASP:HB2	12:I:170:GLY:HA2	1.95	0.49
13:J:92:SER:HB2	13:J:130:ILE:HD11	1.95	0.49
5:H:87:TYR:HA	5:H:90:LYS:HE3	1.94	0.48
9:B:140:ASP:HB3	9:B:143:ASN:HB2	1.94	0.48
8:5:72:VAL:HG22	8:5:83:ILE:HG12	1.95	0.48
1:A:115:ASP:HB3	1:A:155:TYR:CZ	2.48	0.48
2:D:49:ARG:HH21	7:4:103:GLU:H	1.61	0.48
2:D:94:GLN:HG3	14:K:66:LEU:HB2	1.94	0.48
7:4:68:LEU:HD23	7:4:127:PHE:HB3	1.95	0.48
2:D:6:ARG:HH21	3:E:10:ARG:HB3	1.79	0.48
2:D:92:GLU:HB2	6:3:34:ARG:HH21	1.78	0.48
2:D:2:SER:HB2	7:4:17:ASP:HB3	1.96	0.47
2:D:54:LEU:HD13	10:C:162:ALA:HB3	1.97	0.47
6:3:80:GLU:O	6:3:84:ARG:HG2	2.14	0.47
8:5:53:ASP:HB3	8:5:244:VAL:HG11	1.96	0.47
8:5:246:PRO:HG2	8:5:249:TRP:CD1	2.49	0.47
9:B:74:VAL:HG12	9:B:135:LEU:HB2	1.96	0.47
6:3:53:LEU:HG	6:3:57:LEU:HG	1.97	0.47
7:4:106:PRO:HA	7:4:109:LYS:HE3	1.95	0.47
14:K:102:VAL:HG22	14:K:119:ILE:HB	1.96	0.47
8:5:91:SER:HB3	8:5:94:TYR:HD2	1.79	0.47
13:J:190:ILE:HG23	13:J:195:VAL:HG22	1.97	0.46
3:E:70:ILE:HG21	3:E:112:LEU:HD21	1.97	0.46
12:I:133:ALA:HB3	12:I:162:GLY:HA2	1.97	0.46
10:C:158:THR:HB	10:C:160:TRP:HE1	1.79	0.46
5:H:3:ILE:HD12	5:H:44:CYS:HB3	1.97	0.46
6:3:88:MET:HE1	6:3:107:ARG:HG3	1.97	0.46
4:F:26:LEU:HD23	4:F:149:PRO:HG2	1.97	0.46
4:F:227:GLY:O	4:F:230:VAL:HG22	2.16	0.46
1:A:156:LYS:HD2	1:A:169:THR:HG21	1.97	0.46
13:J:7:ILE:O	13:J:57:ALA:HB2	2.15	0.46
4:F:124:GLY:HA3	7:4:1:MET:HG2	1.97	0.45
8:5:4:LEU:HB2	8:5:112:ILE:HD13	1.98	0.45
12:I:230:ILE:HD11	13:J:195:VAL:HG21	1.97	0.45
10:C:107:PRO:HD2	10:C:110:ILE:HD12	1.98	0.45
11:G:193:VAL:HG13	11:G:216:ILE:HG21	1.97	0.45
10:C:213:PHE:HB3	10:C:230:PHE:CD2	2.51	0.45
11:G:50:VAL:HG12	11:G:215:GLU:HB2	1.98	0.45
11:G:151:LEU:HD12	11:G:157:TYR:HB3	1.98	0.45
12:I:124:TYR:HB2	12:I:138:LEU:HD13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:LEU:HD21	11:G:158:TRP:HB3	1.99	0.45
1:A:144:VAL:HG12	1:A:154:ILE:HG12	1.99	0.45
1:A:204:GLU:HA	1:A:248:ILE:HD11	1.99	0.45
2:D:96:HIS:NE2	2:D:100:LEU:HD12	2.32	0.45
4:F:71:GLY:HA3	4:F:222:PHE:CZ	2.51	0.45
9:B:75:TYR:HB3	9:B:82:TYR:CD1	2.52	0.44
5:H:176:VAL:HG22	5:H:185:ARG:HD3	1.99	0.44
12:I:8:PHE:HB3	12:I:151:ALA:HB2	1.98	0.44
7:4:22:SER:HB3	7:4:80:VAL:HG11	1.99	0.44
5:H:187:ILE:HG22	5:H:189:TYR:HD1	1.82	0.44
8:5:95:LEU:HD23	8:5:187:LYS:HD3	1.98	0.44
9:B:71:ILE:HG21	9:B:110:LEU:HD23	2.00	0.44
9:B:149:GLN:O	9:B:156:TYR:HA	2.17	0.44
1:A:54:ILE:HG12	1:A:225:VAL:HG22	2.00	0.44
8:5:216:ASP:HB3	11:G:4:ILE:HG21	1.98	0.44
1:A:156:LYS:HB3	1:A:166:TYR:HE1	1.82	0.44
5:H:59:VAL:HG22	5:H:81:VAL:HG12	2.00	0.44
4:F:104:ALA:HA	4:F:138:ASP:OD2	2.18	0.44
5:H:14:LEU:HD21	5:H:100:ALA:HB2	2.00	0.43
3:E:244:LYS:HE3	3:E:244:LYS:HB3	1.84	0.43
3:E:31:ILE:HD13	3:E:141:ALA:HB2	2.00	0.43
9:B:222:LEU:HD13	9:B:232:GLY:HA2	1.99	0.43
10:C:213:PHE:HB3	10:C:230:PHE:HD2	1.82	0.43
9:B:44:VAL:HG22	9:B:213:ILE:HG22	2.01	0.43
4:F:50:LYS:HD2	4:F:60:GLN:O	2.18	0.43
1:A:168:ALA:HB3	9:B:55:LEU:HD13	1.99	0.43
1:A:167:LYS:HG2	9:B:55:LEU:O	2.19	0.43
6:3:73:ARG:HA	6:3:77:GLY:O	2.18	0.43
1:A:164:VAL:HG13	1:A:166:TYR:CE1	2.54	0.42
8:5:225:LEU:HD23	8:5:243:PHE:HE2	1.84	0.42
9:B:160:LYS:HD3	9:B:179:TRP:CH2	2.54	0.42
12:I:13:VAL:HG22	12:I:177:VAL:HG22	2.01	0.42
4:F:186:PRO:HB3	4:F:215:ILE:HD11	2.01	0.42
10:C:136:ILE:HD11	10:C:165:VAL:HG22	2.01	0.42
13:J:171:LEU:HD23	13:J:171:LEU:HA	1.89	0.42
4:F:62:LYS:HE3	4:F:62:LYS:HB3	1.91	0.42
10:C:14:SER:HB3	10:C:18:ARG:H	1.84	0.42
9:B:42:GLY:HA3	9:B:185:LEU:HD13	2.00	0.42
5:H:98:ILE:HD12	5:H:125:ALA:HB1	2.01	0.42
9:B:237:LYS:HE2	9:B:237:LYS:HB3	1.82	0.42
3:E:199:LEU:O	3:E:203:ILE:HG12	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:G:88:LEU:HD23	11:G:88:LEU:HA	1.86	0.42
9:B:94:HIS:HA	9:B:98:LYS:HB3	2.02	0.42
12:I:19:ARG:HG2	12:I:169:SER:HA	2.02	0.42
13:J:16:THR:HG22	13:J:21:VAL:HG12	2.02	0.42
14:K:158:LEU:HD21	14:K:183:ILE:HD11	2.02	0.42
2:D:185:PRO:HB2	2:D:191:CYS:SG	2.60	0.41
5:H:96:GLY:CA	5:H:113:ILE:O	2.61	0.41
10:C:108:VAL:HG21	10:C:139:GLY:HA3	2.02	0.41
4:F:135:ILE:HD11	4:F:222:PHE:HE1	1.85	0.41
8:5:21:TRP:CZ3	8:5:243:PHE:HB3	2.55	0.41
12:I:70:THR:O	12:I:72:ARG:HG3	2.20	0.41
5:H:7:THR:HG23	5:H:110:VAL:HG23	2.03	0.41
1:A:96:ARG:O	1:A:100:GLU:HG2	2.21	0.41
2:D:80:ALA:O	2:D:84:ILE:HG12	2.21	0.41
3:E:179:ALA:HB2	3:E:207:VAL:HG21	2.02	0.41
4:F:72:LEU:HD23	4:F:88:LEU:HD23	2.03	0.41
2:D:109:LEU:HD12	2:D:109:LEU:HA	1.84	0.41
3:E:167:TYR:CE2	4:F:57:SER:HB3	2.55	0.41
4:F:140:SER:HB2	4:F:143:HIS:NE2	2.35	0.41
2:D:52:LEU:HD12	10:C:160:TRP:CH2	2.55	0.41
7:4:3:PHE:HA	11:G:128:SER:HB3	2.02	0.41
10:C:194:LEU:HD12	10:C:242:THR:HG21	2.02	0.41
6:3:57:LEU:HD12	12:I:-24:PHE:HZ	1.84	0.41
14:K:43:LEU:HD13	14:K:189:ILE:HD13	2.01	0.41
1:A:43:LEU:HD11	1:A:182:LEU:HD11	2.03	0.41
1:A:120:ARG:HH12	6:3:112:ASN:CG	2.28	0.41
4:F:206:LEU:HD22	4:F:211:LEU:HD13	2.02	0.41
2:D:66:LYS:HG2	2:D:68:ASP:O	2.21	0.41
10:C:44:ILE:HD11	10:C:146:TYR:HB3	2.02	0.41
10:C:66:LEU:HD23	10:C:214:ALA:HB2	2.02	0.40
7:4:43:ASP:O	7:4:46:GLN:HG2	2.21	0.40
3:E:214:GLU:H	3:E:214:GLU:CD	2.29	0.40
13:J:11:ILE:HD12	13:J:146:LEU:HD22	2.02	0.40
3:E:122:ARG:HB3	3:E:133:LEU:HB3	2.03	0.40
12:I:-2:THR:HB	12:I:33:LYS:HE2	2.03	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	248/252 (98%)	236 (95%)	12 (5%)	0	100	100
2	D	248/254 (98%)	240 (97%)	8 (3%)	0	100	100
3	E	249/260 (96%)	243 (98%)	6 (2%)	0	100	100
4	F	232/234 (99%)	223 (96%)	9 (4%)	0	100	100
5	H	166/215 (77%)	162 (98%)	4 (2%)	0	100	100
6	3	108/162 (67%)	104 (96%)	4 (4%)	0	100	100
7	4	274/276 (99%)	261 (95%)	13 (5%)	0	100	100
8	5	264/267 (99%)	253 (96%)	11 (4%)	0	100	100
9	B	246/250 (98%)	240 (98%)	6 (2%)	0	100	100
10	C	234/258 (91%)	231 (99%)	3 (1%)	0	100	100
11	G	245/288 (85%)	236 (96%)	8 (3%)	1 (0%)	30	59
12	I	219/261 (84%)	211 (96%)	8 (4%)	0	100	100
13	J	187/205 (91%)	177 (95%)	10 (5%)	0	100	100
14	K	183/198 (92%)	167 (91%)	15 (8%)	1 (0%)	24	55
All	All	3103/3380 (92%)	2984 (96%)	117 (4%)	2 (0%)	49	76

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	K	176	PHE
11	G	247	ILE

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	208/210 (99%)	206 (99%)	2 (1%)	68	76
2	D	218/226 (96%)	213 (98%)	5 (2%)	44	66
3	E	205/215 (95%)	201 (98%)	4 (2%)	48	68
4	F	193/193 (100%)	190 (98%)	3 (2%)	55	71
5	H	139/178 (78%)	136 (98%)	3 (2%)	45	67
6	3	101/150 (67%)	101 (100%)	0	100	100
7	4	240/251 (96%)	238 (99%)	2 (1%)	73	78
8	5	243/244 (100%)	240 (99%)	3 (1%)	63	74
9	B	207/209 (99%)	203 (98%)	4 (2%)	50	69
10	C	200/216 (93%)	198 (99%)	2 (1%)	68	76
11	G	204/239 (85%)	201 (98%)	3 (2%)	57	72
12	I	183/215 (85%)	181 (99%)	2 (1%)	65	75
13	J	157/173 (91%)	154 (98%)	3 (2%)	50	69
14	K	163/175 (93%)	158 (97%)	5 (3%)	35	61
All	All	2661/2894 (92%)	2620 (98%)	41 (2%)	55	72

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	VAL
1	A	64	LEU
2	D	59	ILE
2	D	60	THR
2	D	109	LEU
2	D	163	THR
2	D	244	GLN
3	E	47	VAL
3	E	134	MET
3	E	159	GLU
3	E	182	GLU
4	F	34	VAL
4	F	74	LEU
4	F	156	LEU
5	H	94	THR
5	H	119	VAL

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Mol	Chain	Res	Type
5	H	186	LEU
7	4	11	GLU
7	4	79	THR
8	5	14	ILE
8	5	49	ASP
8	5	155	LEU
9	B	30	GLN
9	B	50	LYS
9	B	211	LEU
9	B	245	ASP
10	C	53	THR
10	C	213	PHE
11	G	69	VAL
11	G	179	LEU
11	G	214	LEU
12	I	38	SER
12	I	149	GLU
13	J	7	ILE
13	J	21	VAL
13	J	58	THR
14	K	9	VAL
14	K	13	VAL
14	K	53	THR
14	K	103	LEU
14	K	128	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	176	GLN
2	D	16	HIS
2	D	94	GLN
3	E	147	HIS
3	E	180	GLN
6	3	139	HIS
7	4	225	ASN
8	5	13	ASN
8	5	154	ASN
9	B	20	GLN
10	C	233	GLN
11	G	64	ASN
11	G	248	ASN

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Mol	Chain	Res	Type
12	I	93	HIS
12	I	116	HIS
14	K	101	ASN
14	K	118	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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.

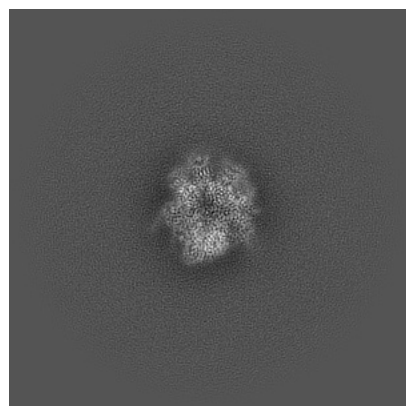
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54032. These allow visual inspection of the internal detail of the map and identification of artifacts.

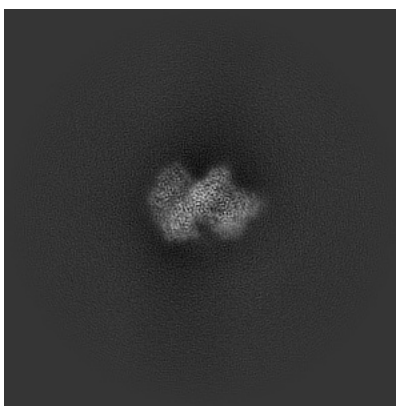
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

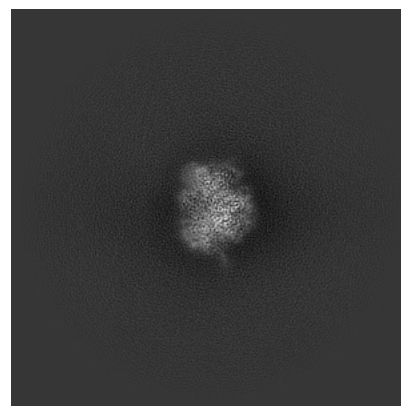
6.1.1 Primary map



X

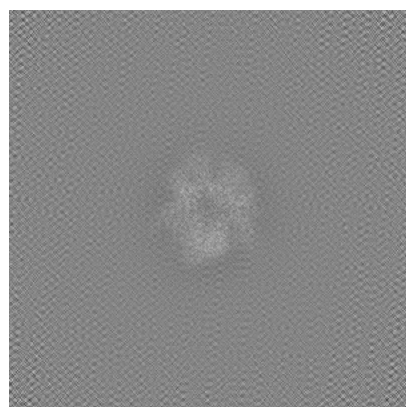


Y

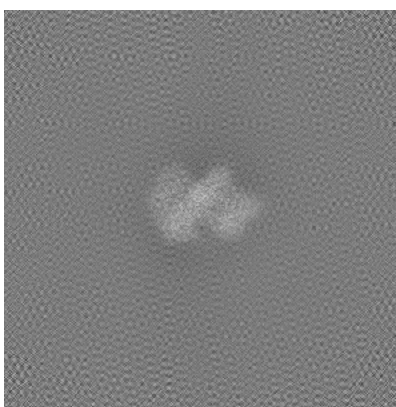


Z

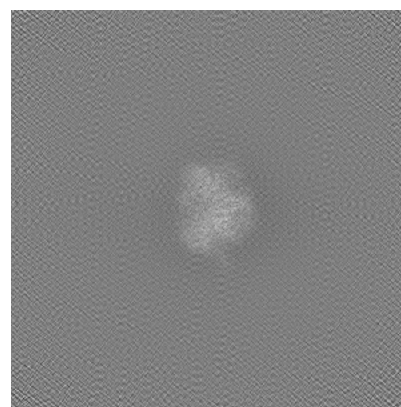
6.1.2 Raw map



X



Y

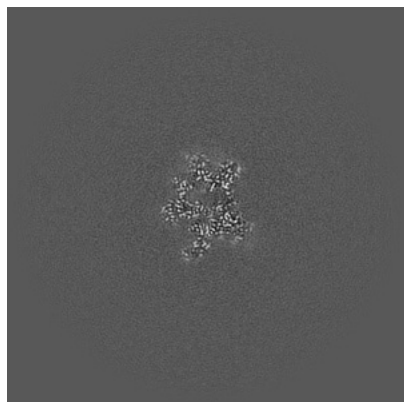


Z

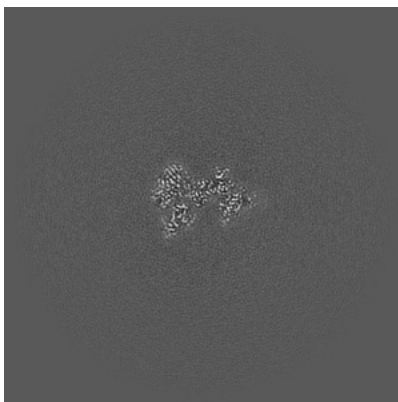
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

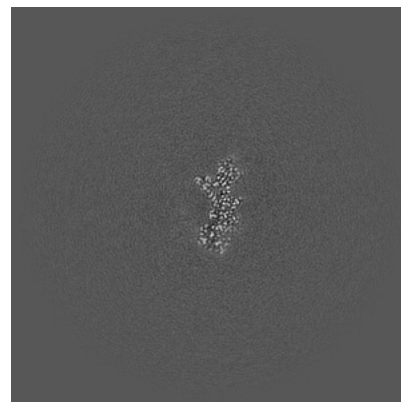
6.2.1 Primary map



X Index: 250

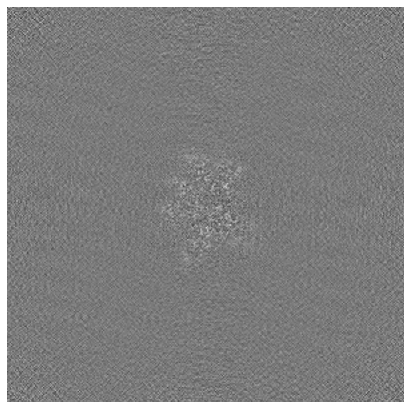


Y Index: 250

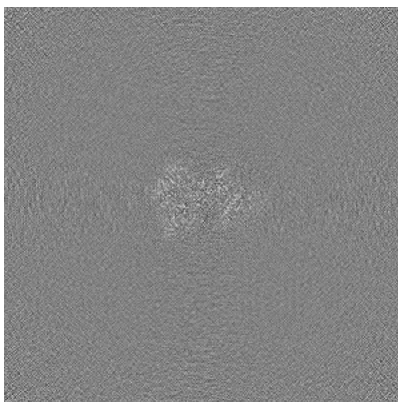


Z Index: 250

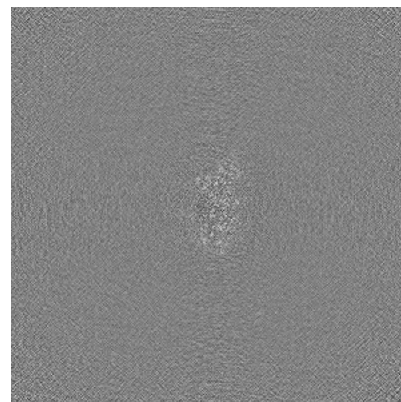
6.2.2 Raw map



X Index: 250



Y Index: 250

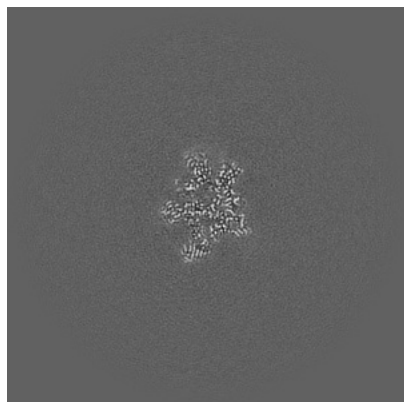


Z Index: 250

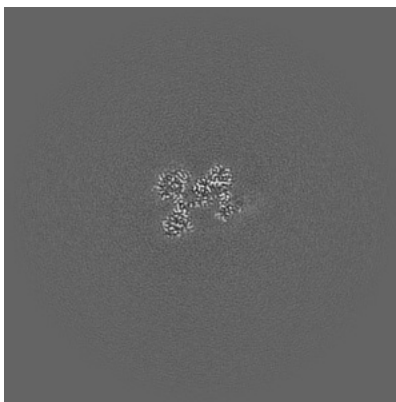
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

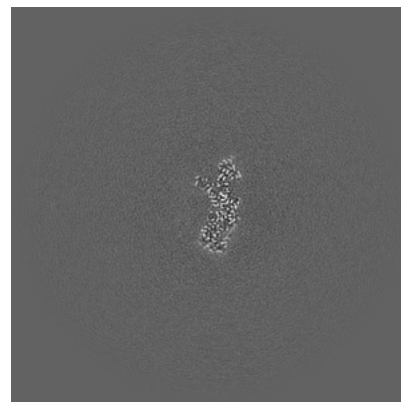
6.3.1 Primary map



X Index: 256

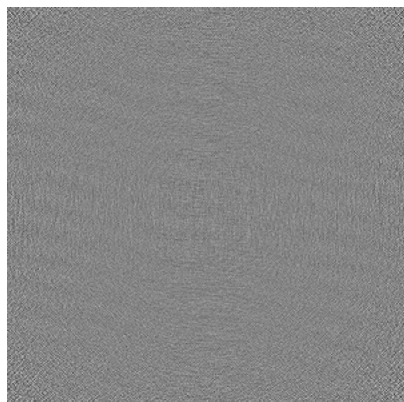


Y Index: 256

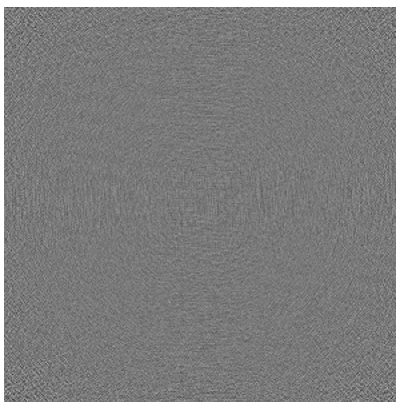


Z Index: 248

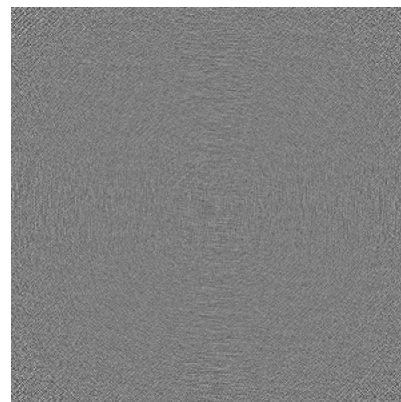
6.3.2 Raw map



X Index: 0



Y Index: 0

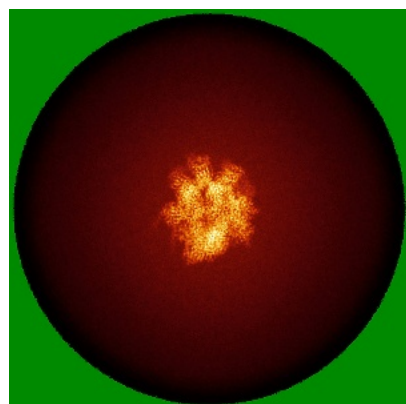


Z Index: 499

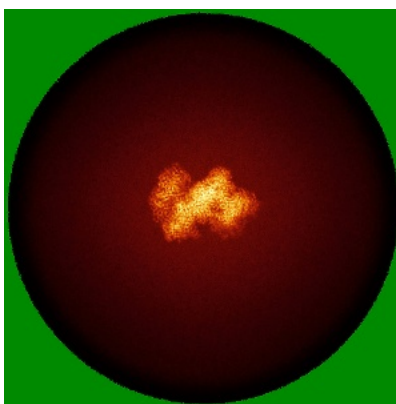
The images above show the largest variance slices of the map in three orthogonal directions.

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

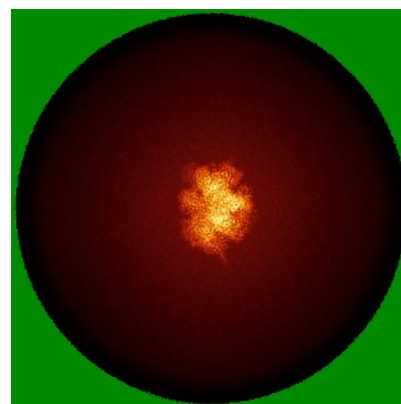
6.4.1 Primary map



X

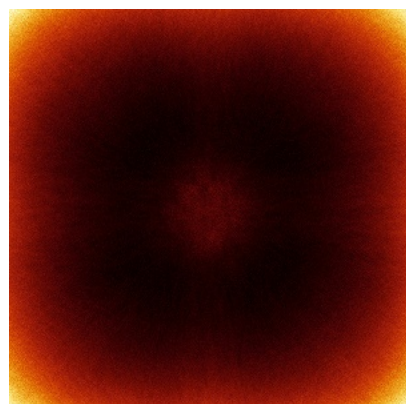


Y

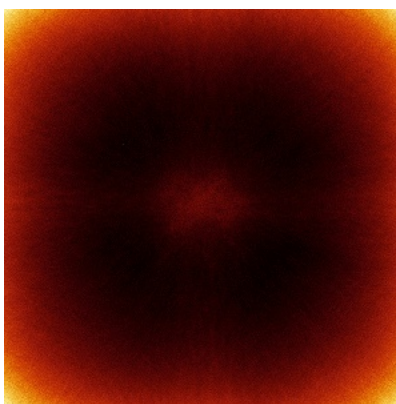


Z

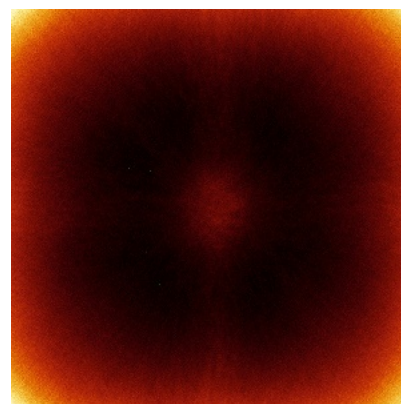
6.4.2 Raw map



X



Y



Z

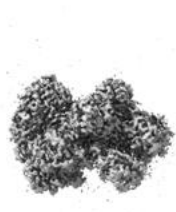
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



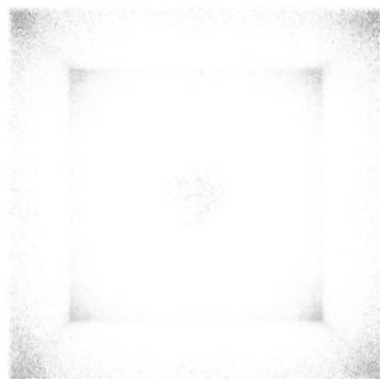
Y



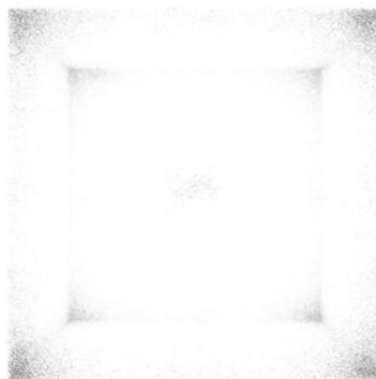
Z

The images above show the 3D surface view of the map at the recommended contour level 0.119. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

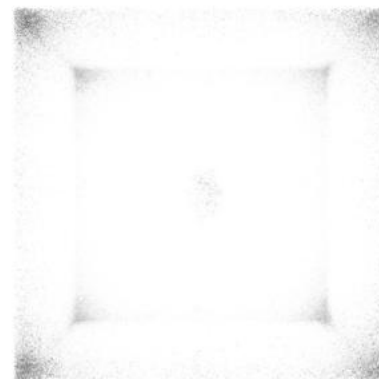
6.5.2 Raw map



X



Y



Z

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.

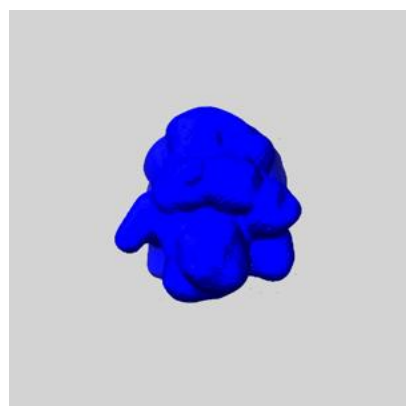
6.6 Mask visualisation [i](#)

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

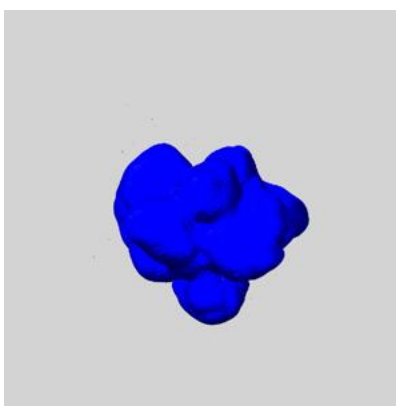
A mask typically either:

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

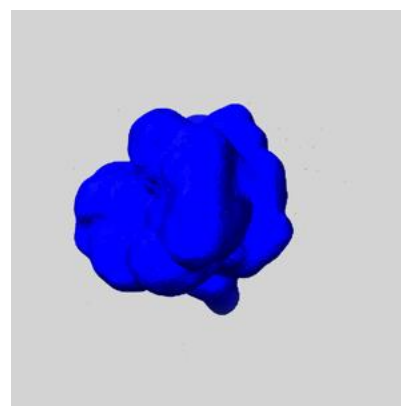
6.6.1 emd_54032_msk_1.map [i](#)



X



Y

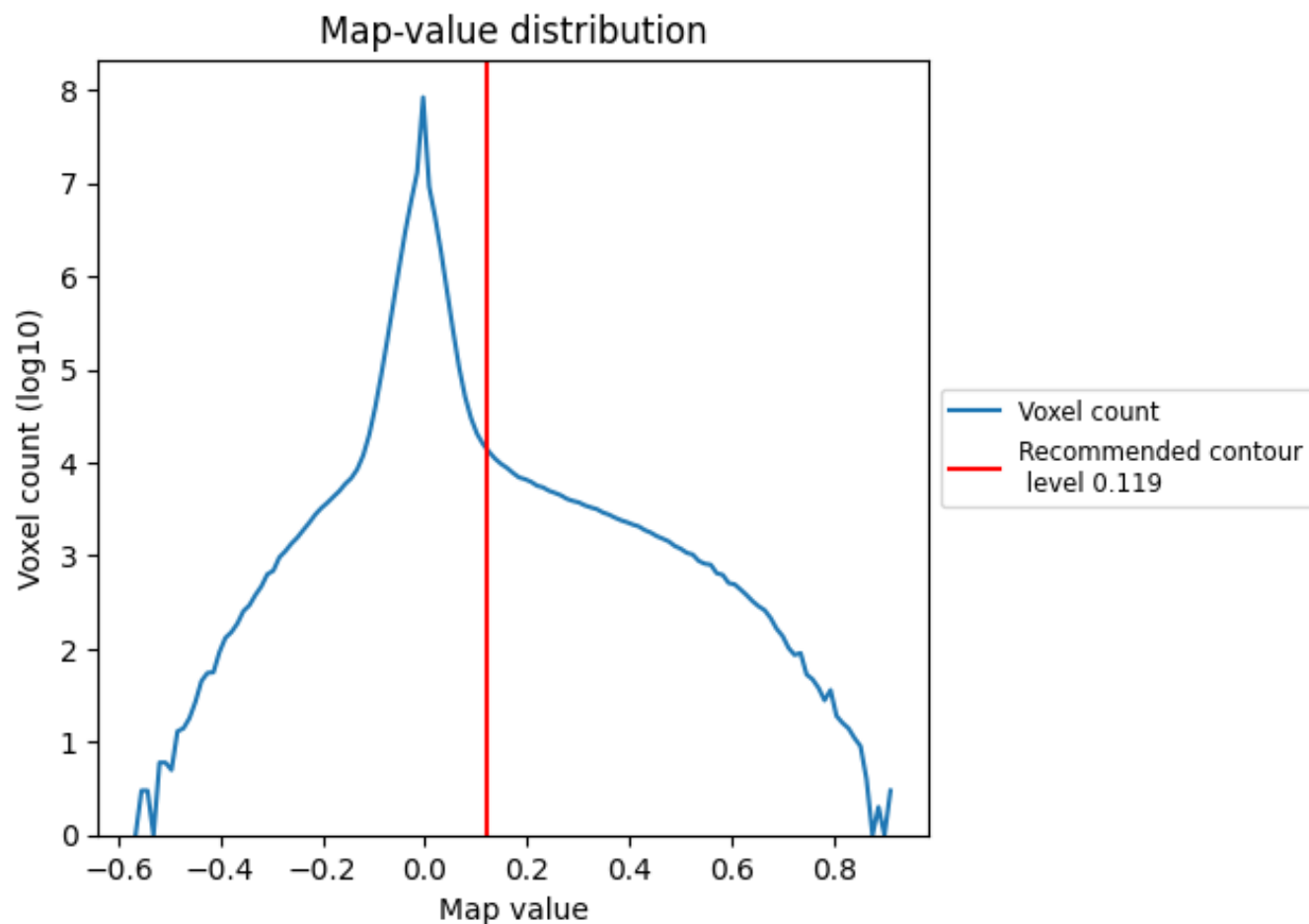


Z

7 Map analysis [i](#)

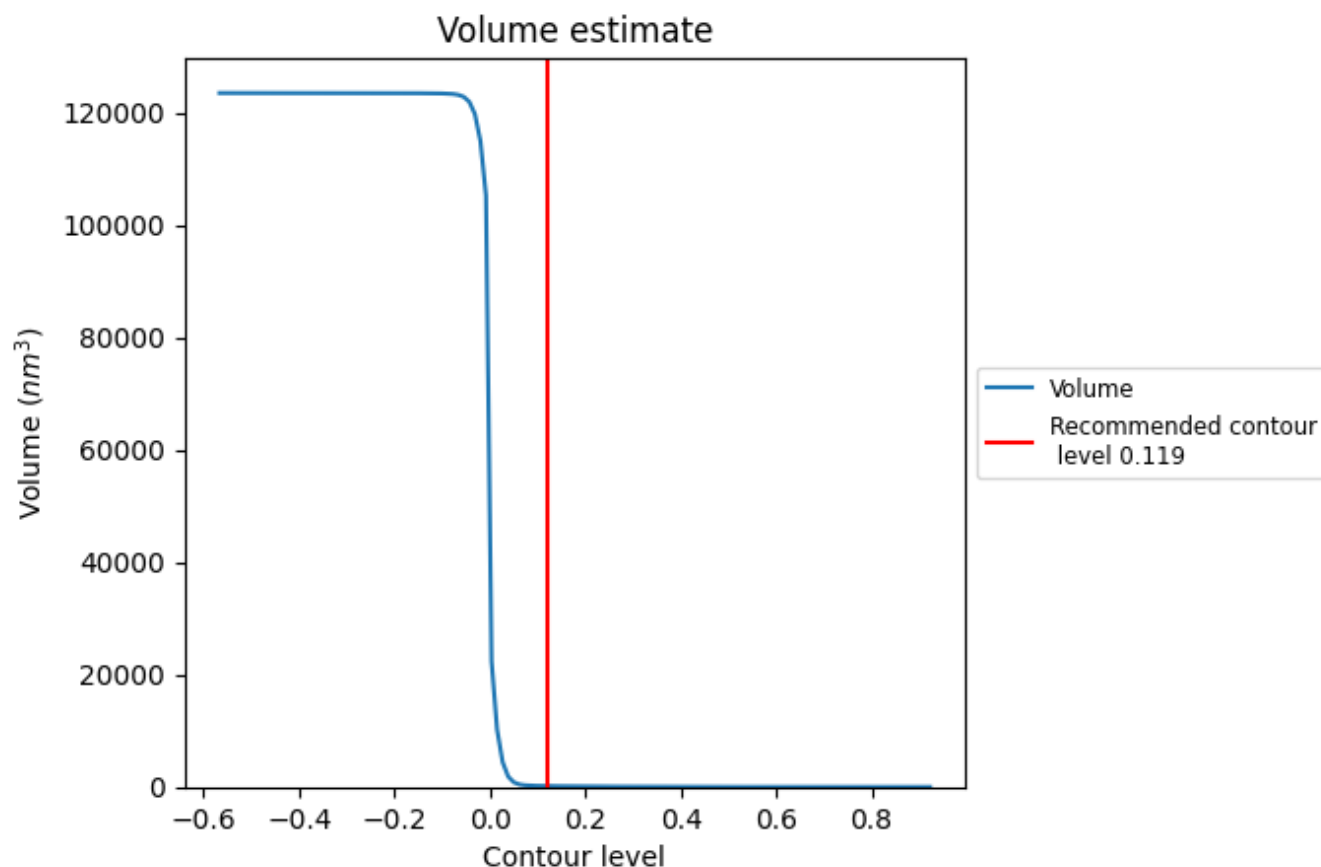
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

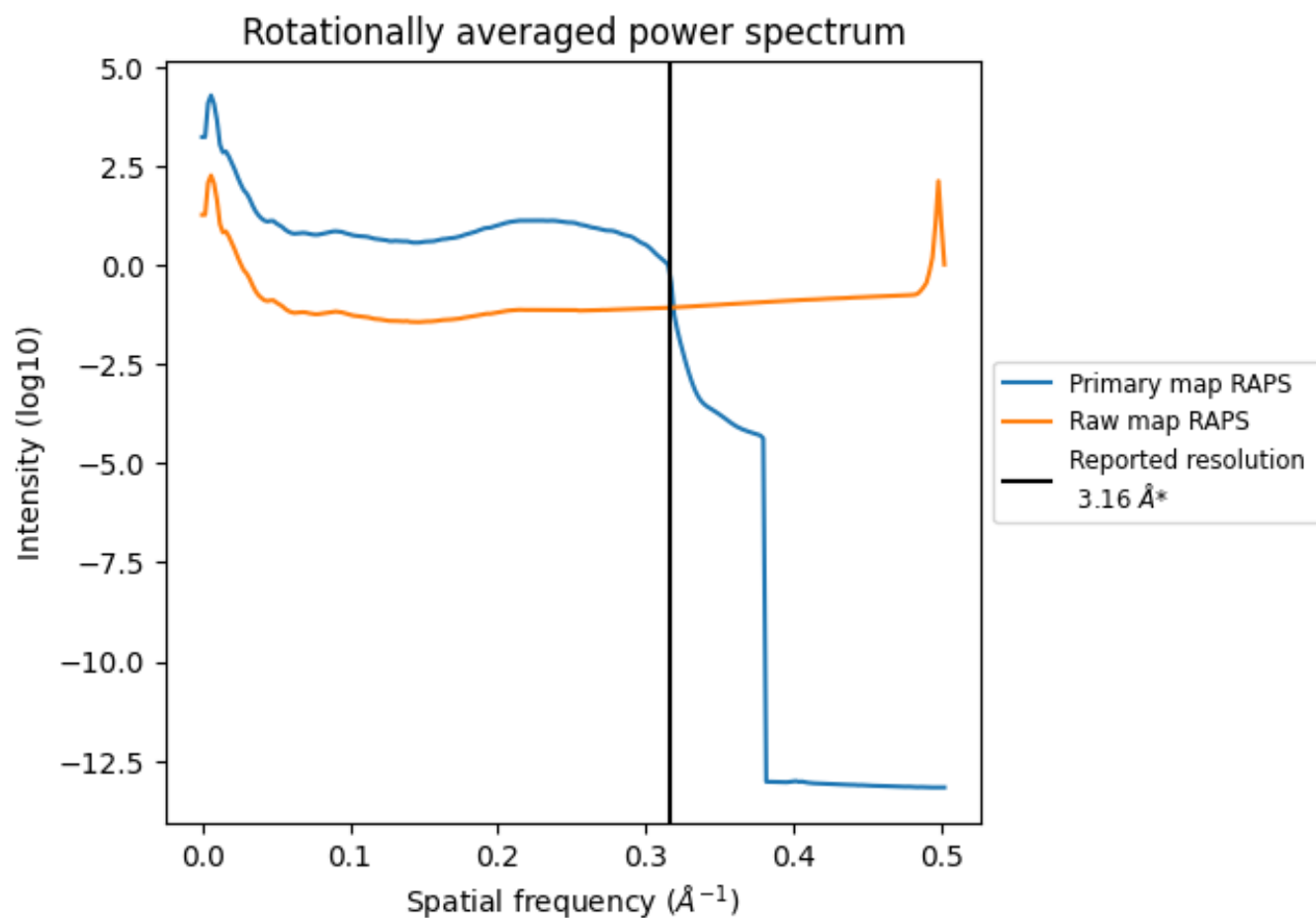
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 161 nm³; this corresponds to an approximate mass of 145 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 ⓘ

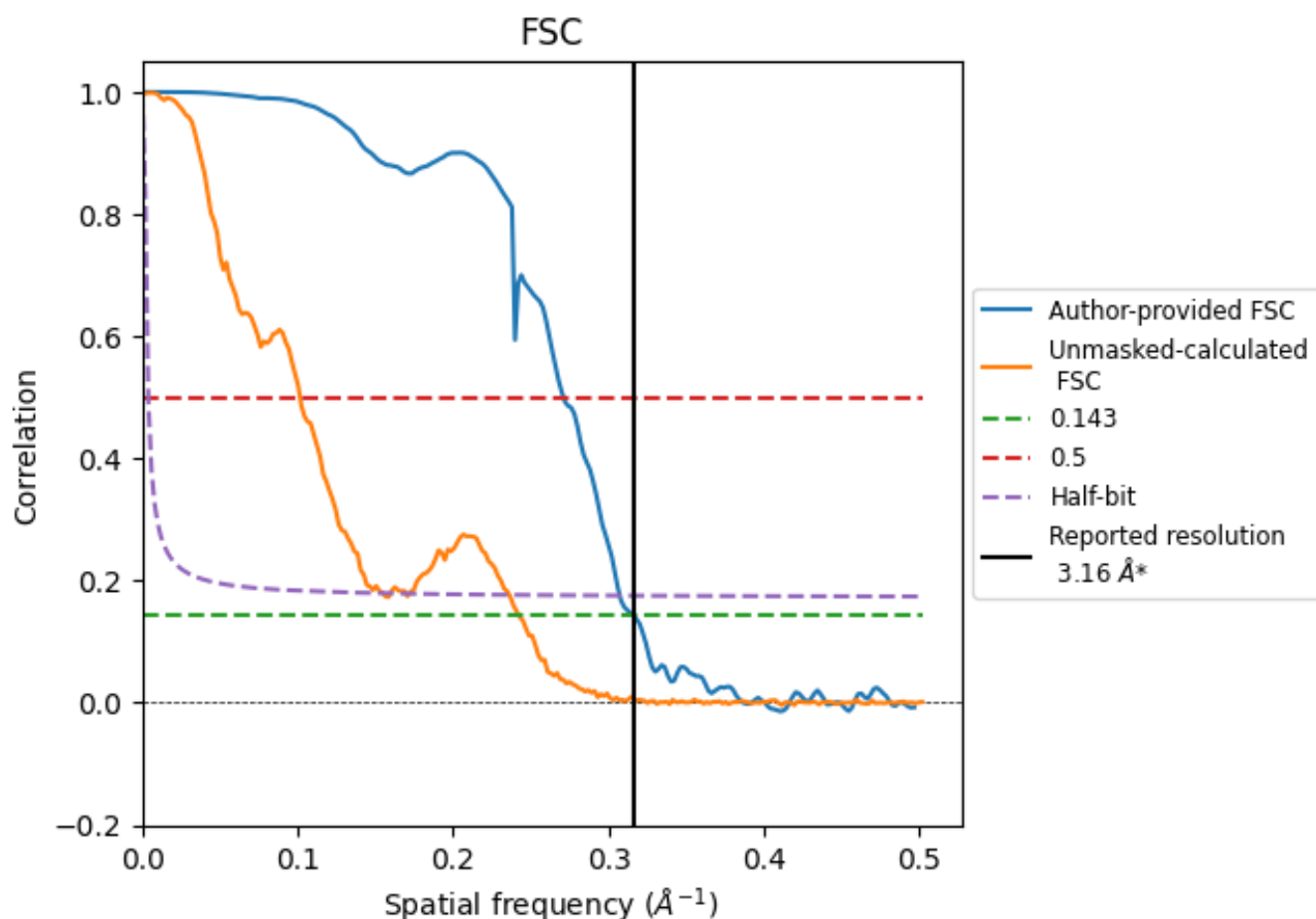


*Reported resolution corresponds to spatial frequency of 0.316 \AA^{-1}

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 0.316 \AA^{-1}

8.2 Resolution estimates [i](#)

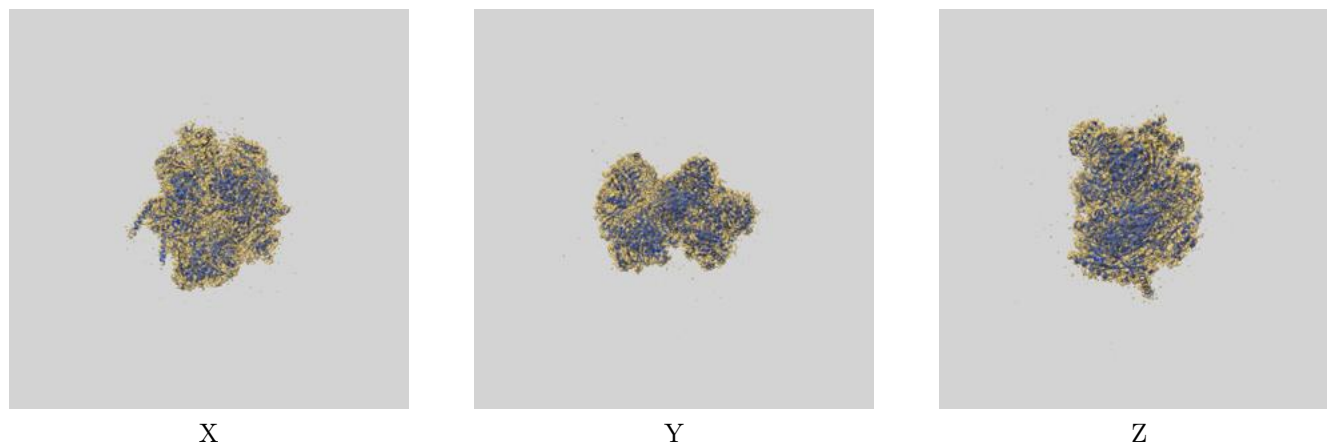
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.16	-	-
Author-provided FSC curve	3.16	3.69	3.25
Unmasked-calculated*	4.13	9.84	6.45

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.13 differs from the reported value 3.16 by more than 10 %

9 Map-model fit [i](#)

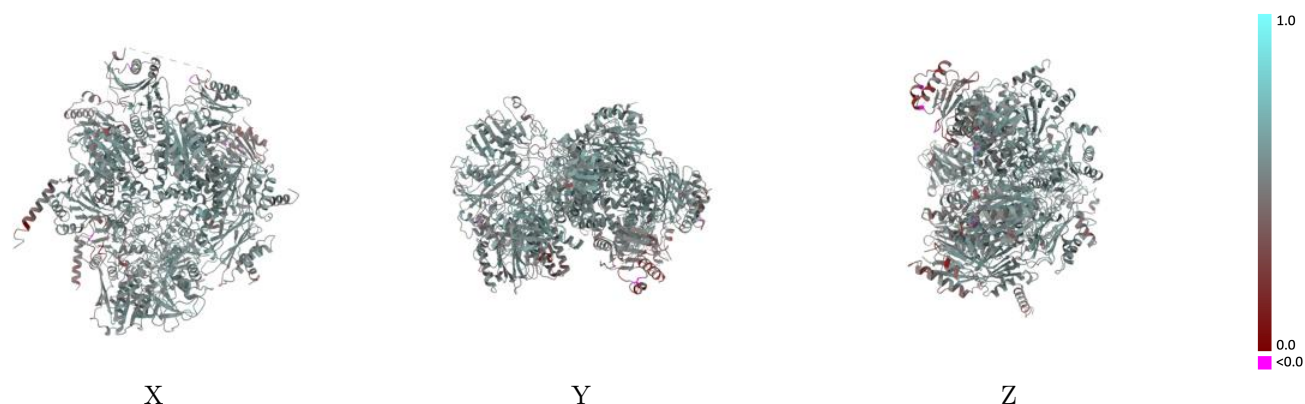
This section contains information regarding the fit between EMDB map EMD-54032 and PDB model 9RLA. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



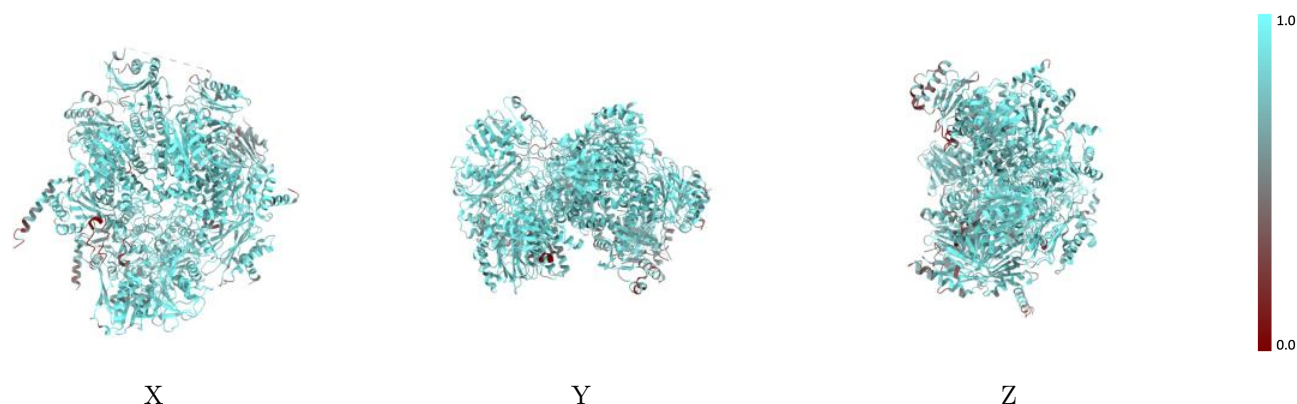
The images above show the 3D surface view of the map at the recommended contour level 0.119 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



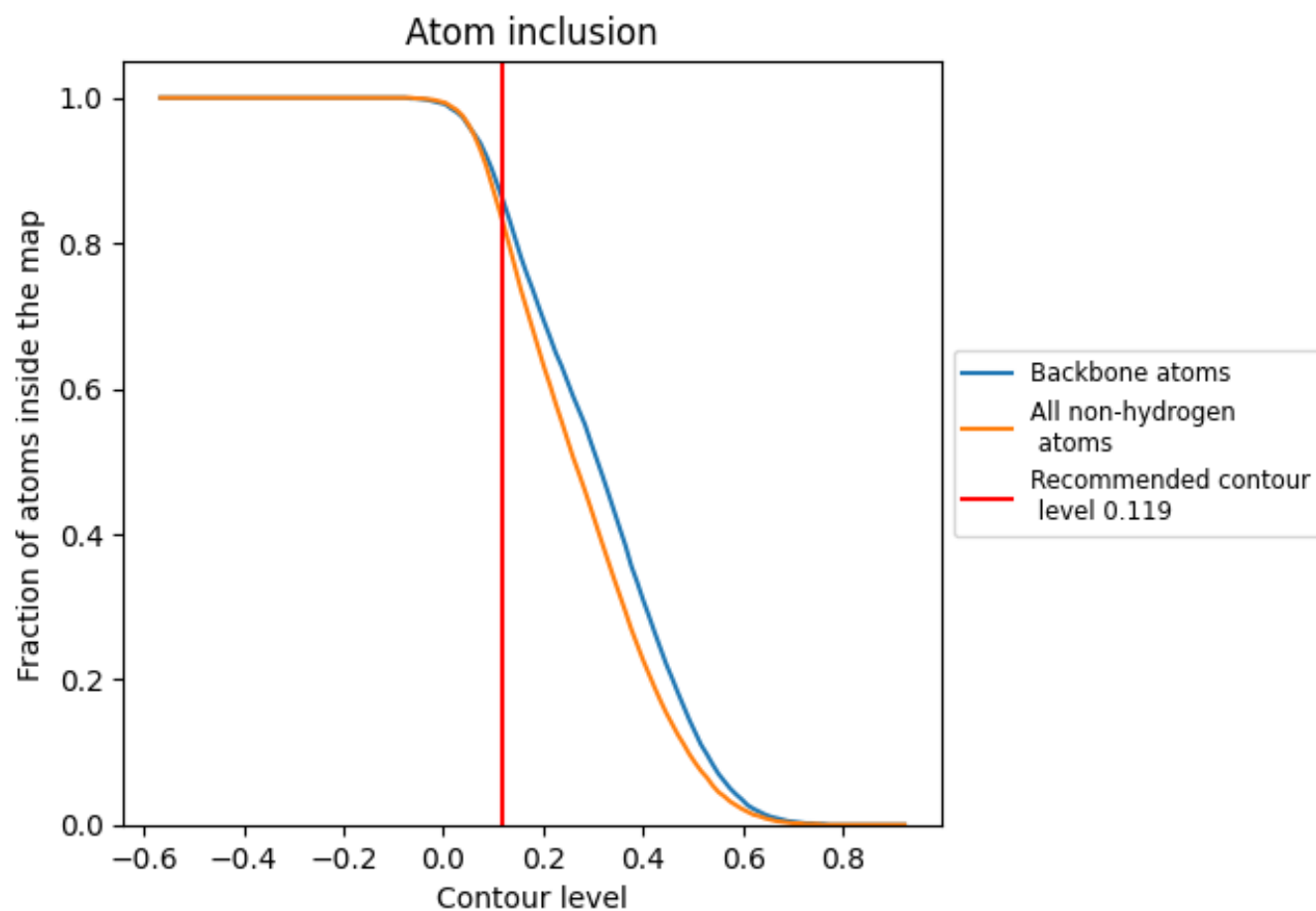
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.119).































9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 83% 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 (0.119) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8290	 0.5290
3	 0.7210	 0.5190
4	 0.8100	 0.5240
5	 0.8600	 0.5390
A	 0.8870	 0.5610
B	 0.8890	 0.5640
C	 0.8780	 0.5510
D	 0.8130	 0.5250
E	 0.7990	 0.5080
F	 0.8660	 0.5440
G	 0.8740	 0.5460
H	 0.6670	 0.4180
I	 0.8280	 0.5300
J	 0.8310	 0.5300
K	 0.7580	 0.5000

