



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 06:00 PM UTC

PDB ID : 6V8O / pdb_00006v8o
EMDB ID : EMD-21107
Title : RSC core
Authors : Patel, A.B.; Moore, C.M.; Greber, B.J.; Nogales, E.
Deposited on : 2019-12-11
Resolution : 3.07 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:

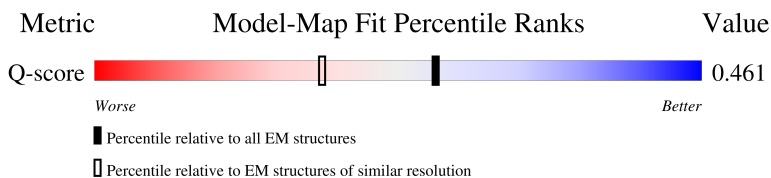
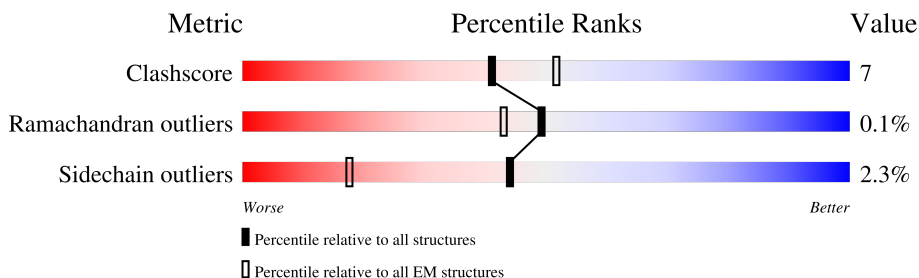
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.07 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.



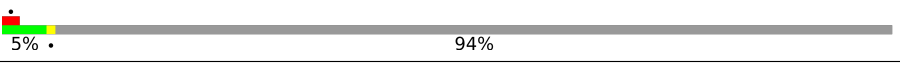
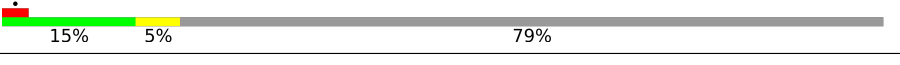
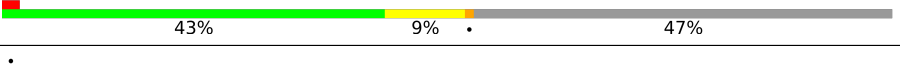
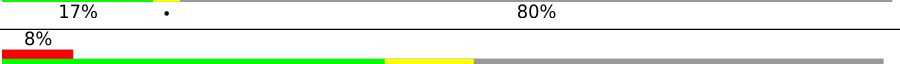
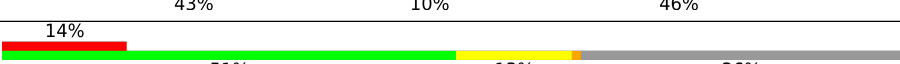
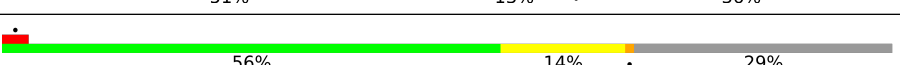
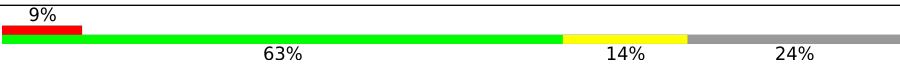
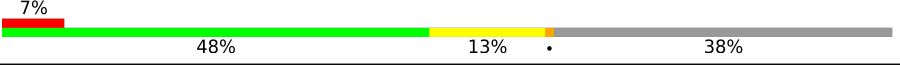
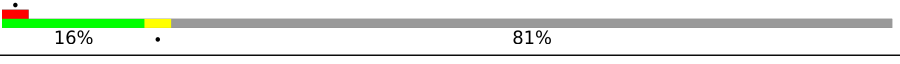
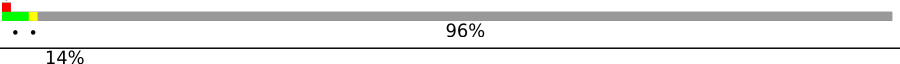
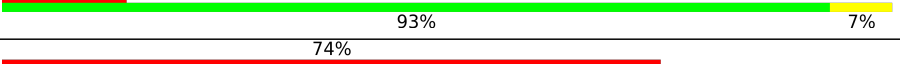
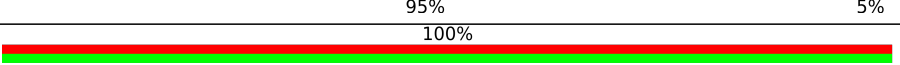
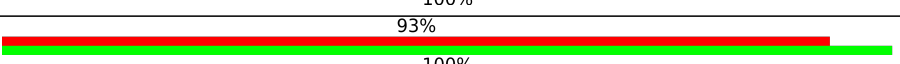
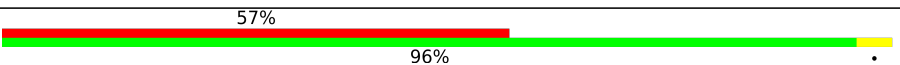
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13977 (2.57 - 3.57)

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	C	78	
2	D	180	
3	E	435	
4	F	889	

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Mol	Chain	Length	Quality of chain
5	G	885	
6	H	625	
7	I	557	
7	J	557	
7	K	557	
7	L	557	
8	M	483	
9	N	581	
10	O	502	
11	Q	426	
12	R	1359	
13	S	883	
14	2	28	
15	3	19	
15	4	19	
16	5	14	
17	6	15	
18	7	49	

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 25103 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 High temperature lethal protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	60	Total	C	N	O	S	0	0
			493	301	92	96	4		

- Molecule 2 is a protein called Chromatin structure-remodeling complex protein RSC14.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	100	Total	C	N	O	S	0	0
			772	490	132	148	2		

- Molecule 3 is a protein called Chromatin structure-remodeling complex subunit RSC7.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	120	Total	C	N	O	S	0	0
			978	610	166	200	2		

- Molecule 4 is a protein called Chromatin structure-remodeling complex subunit RSC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	67	Total	C	N	O	S	0	0
			536	346	94	95	1		

- Molecule 5 is a protein called Chromatin structure-remodeling complex protein RSC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	53	Total	C	N	O	S	0	0
			422	270	71	79	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	767	SER	THR	conflict	UNP Q06639

- Molecule 6 is a protein called Chromatin structure-remodeling complex subunit RSC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	131	Total	C	N	O	S	0	0
			1083	696	175	205	7		

- Molecule 7 is a protein called Chromatin structure-remodeling complex protein RSC8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	293	Total	C	N	O	S	0	0
			2416	1537	423	448	8		
7	J	115	Total	C	N	O	S	0	0
			924	579	149	190	6		
7	K	109	Total	C	N	O	S	0	0
			878	554	139	179	6		
7	L	298	Total	C	N	O	S	0	0
			2445	1557	428	452	8		

- Molecule 8 is a protein called Chromatin structure-remodeling complex protein RSC6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	M	310	Total	C	N	O	S	0	0
			2474	1558	414	496	6		

- Molecule 9 is a protein called Chromatin structure-remodeling complex subunit RSC9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	N	412	Total	C	N	O	S	0	0
			3275	2105	540	612	18		

- Molecule 10 is a protein called Chromatin structure-remodeling complex protein RSC58.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	O	384	Total	C	N	O	S	0	0
			3145	2025	529	581	10		

- Molecule 11 is a protein called Chromatin structure-remodeling complex subunit SFH1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Q	264	Total	C	N	O	S	0	0
			2137	1349	362	418	8		

- Molecule 12 is a protein called Nuclear protein STH1/NPS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	R	262	Total	C	N	O	S	0	0
			2126	1339	378	407	2		

- Molecule 13 is a protein called Chromatin structure-remodeling complex protein RSC30.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	S	34	Total	C	N	O	S	0	0
			278	182	41	54	1		

- Molecule 14 is a protein called Unknown protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	2	28	Total	C	N	O	0	0
			140	84	28	28		

- Molecule 15 is a protein called Unknown Protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	3	19	Total	C	N	O	0	0
			95	57	19	19		
15	4	19	Total	C	N	O	0	0
			95	57	19	19		

- Molecule 16 is a protein called Unknown protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	5	14	Total	C	N	O	0	0
			70	42	14	14		

- Molecule 17 is a protein called Unknown Protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	6	15	Total	C	N	O	0	0
			75	45	15	15		

- Molecule 18 is a protein called Unknown Protein.

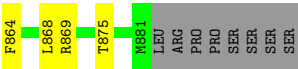
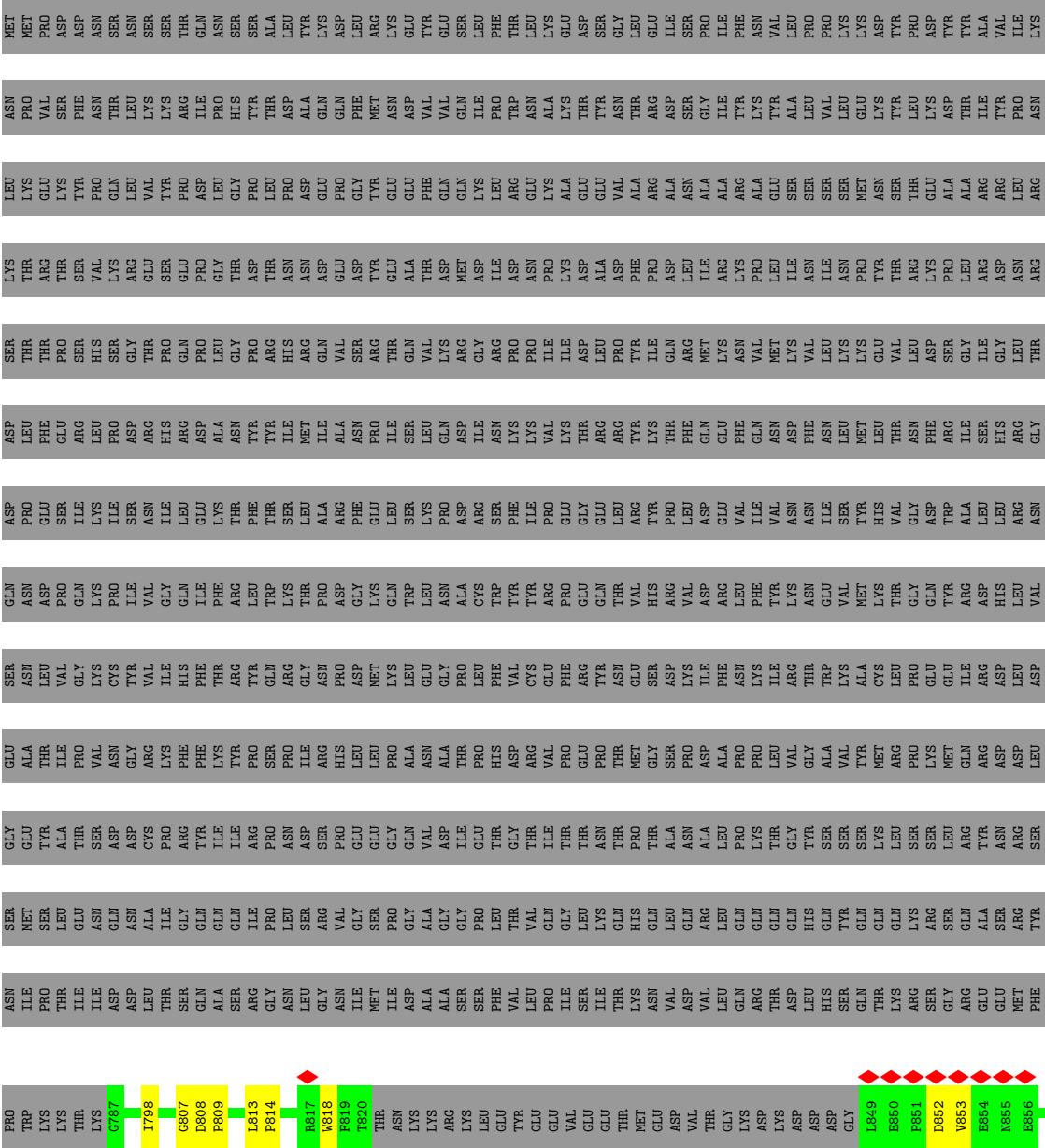
Mol	Chain	Residues	Atoms				AltConf	Trace
18	7	49	Total	C	N	O	0	0
			245	147	49	49		

- Molecule 19 is ZINC ION (CCD ID: ZN) (formula: Zn).

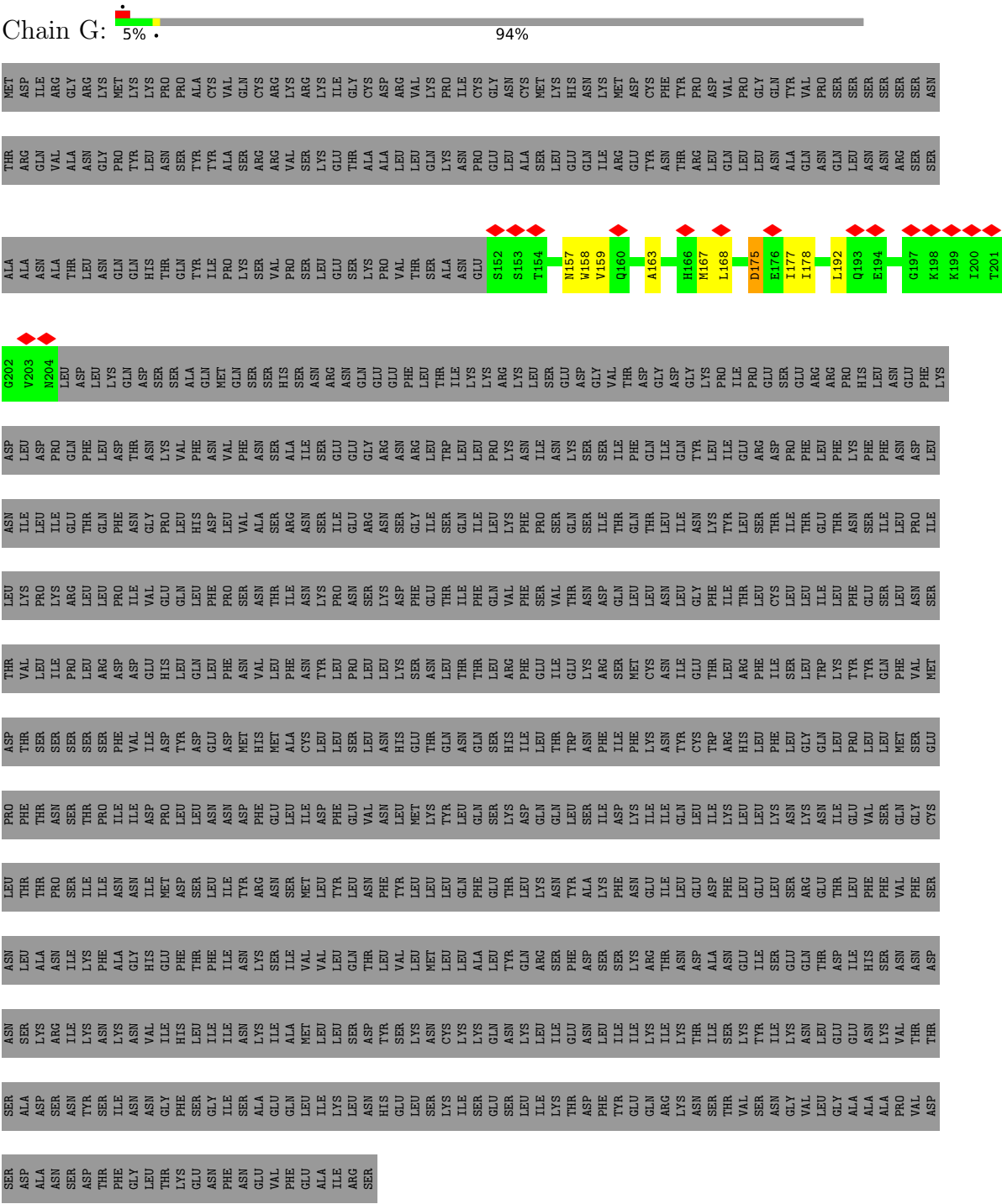
Mol	Chain	Residues	Atoms		AltConf
19	I	1	Total	Zn	0
			1	1	



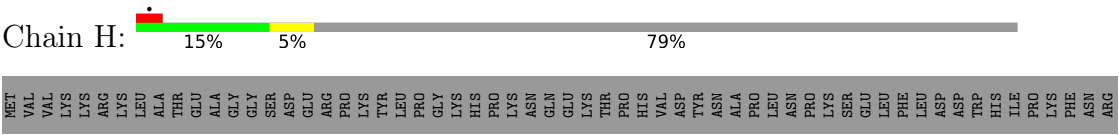
• Molecule 4: Chromatin structure-remodeling complex subunit RSC2

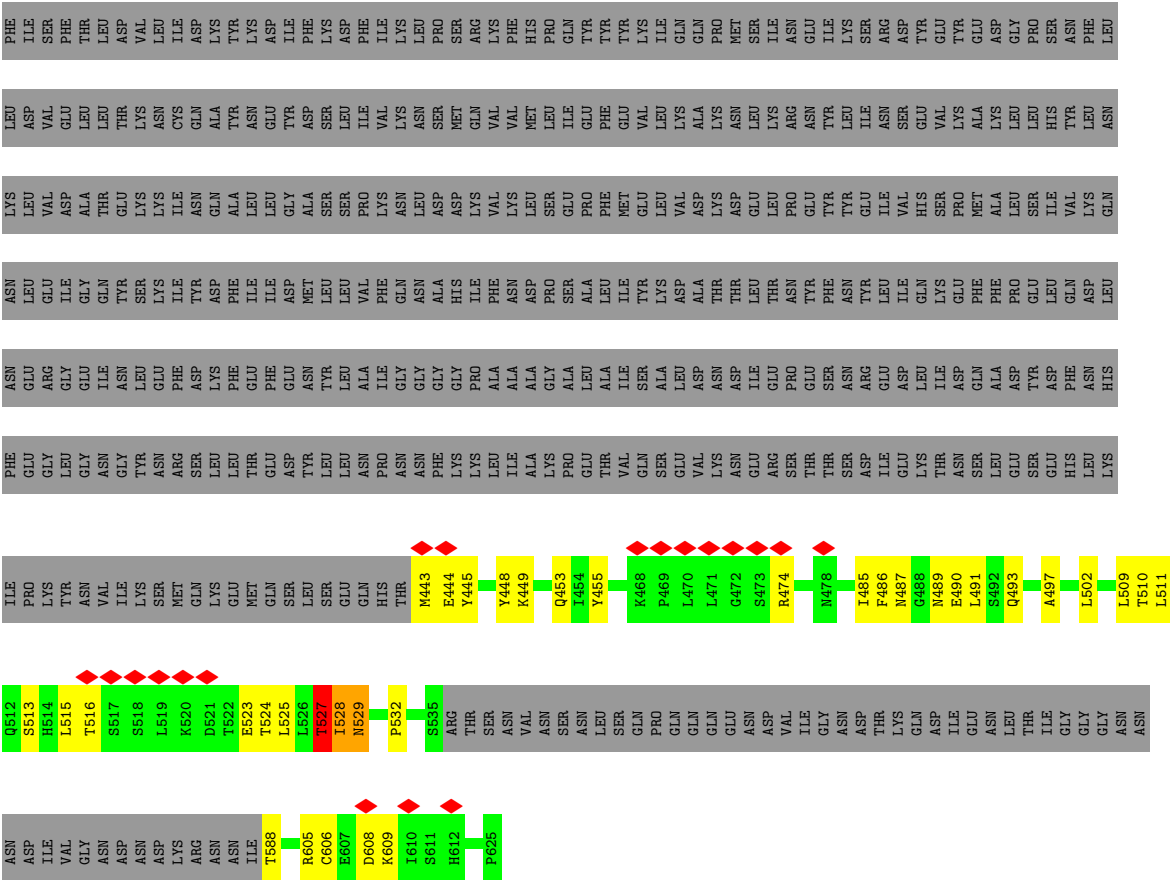


● Molecule 5: Chromatin structure-remodeling complex protein RSC3

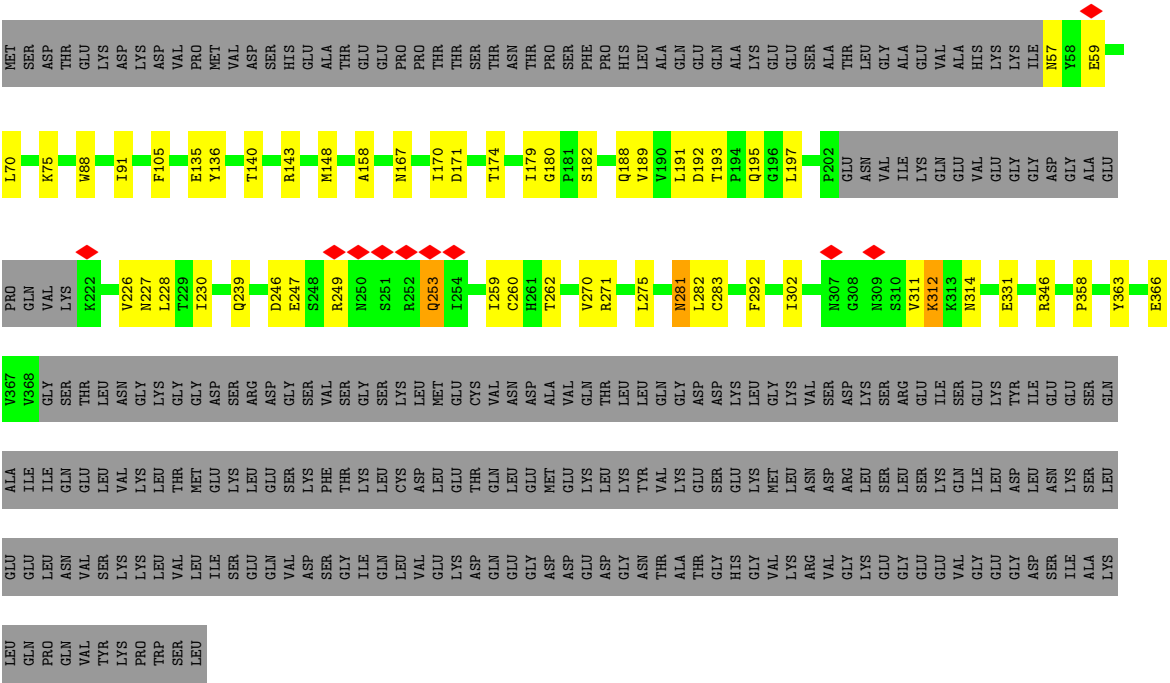


● Molecule 6: Chromatin structure-remodeling complex subunit RSC4

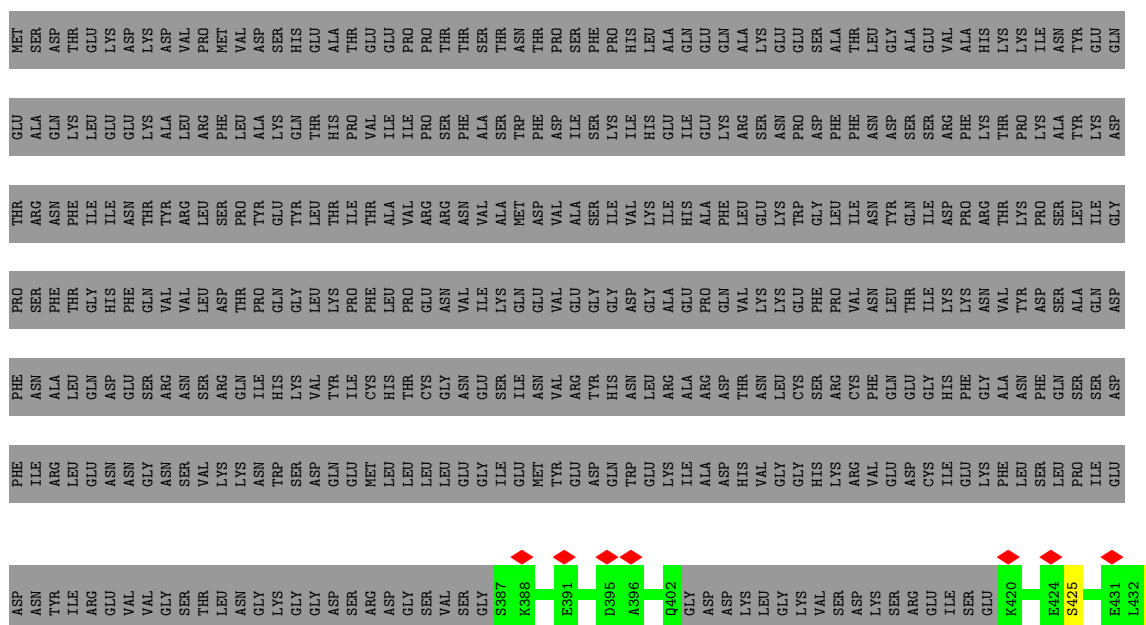
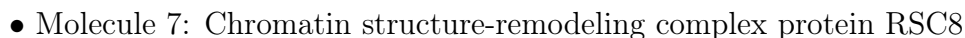


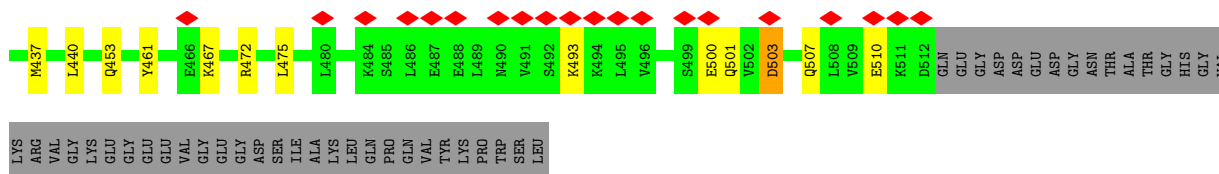


● Molecule 7: Chromatin structure-remodeling complex protein RSC8

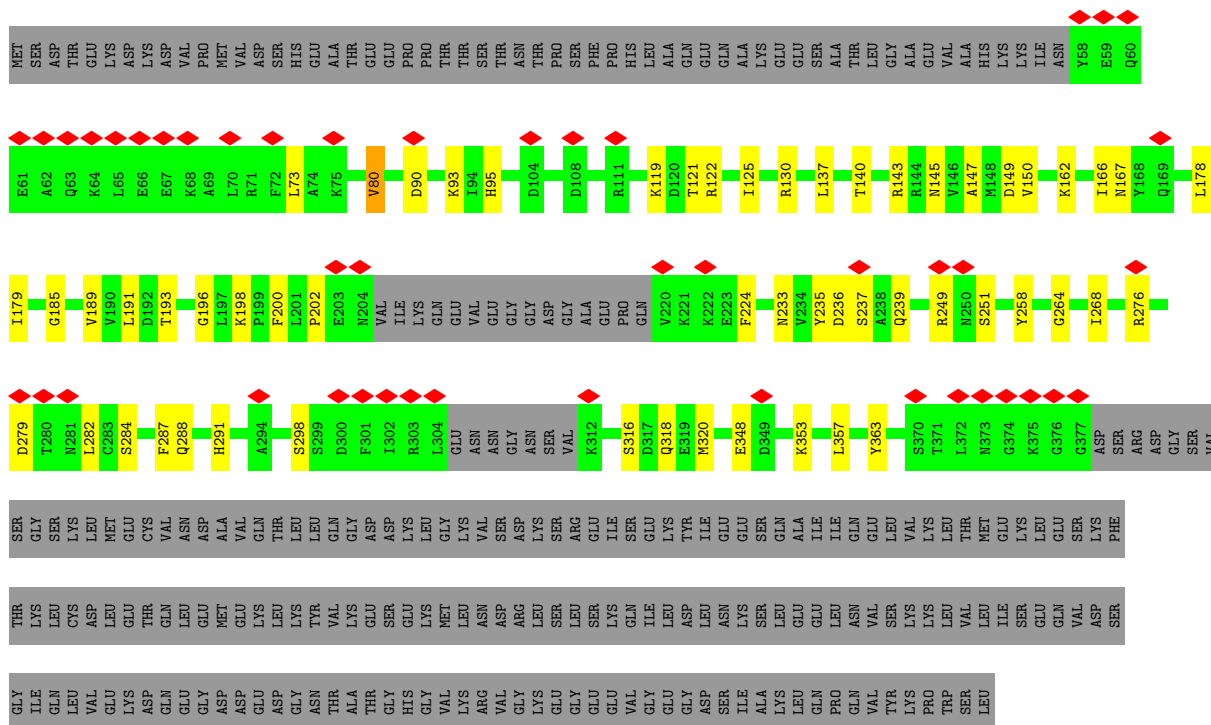
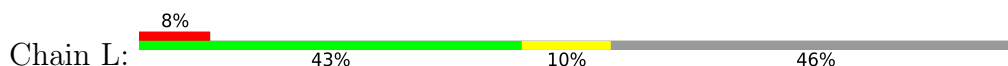


Chain J: 18% 79%

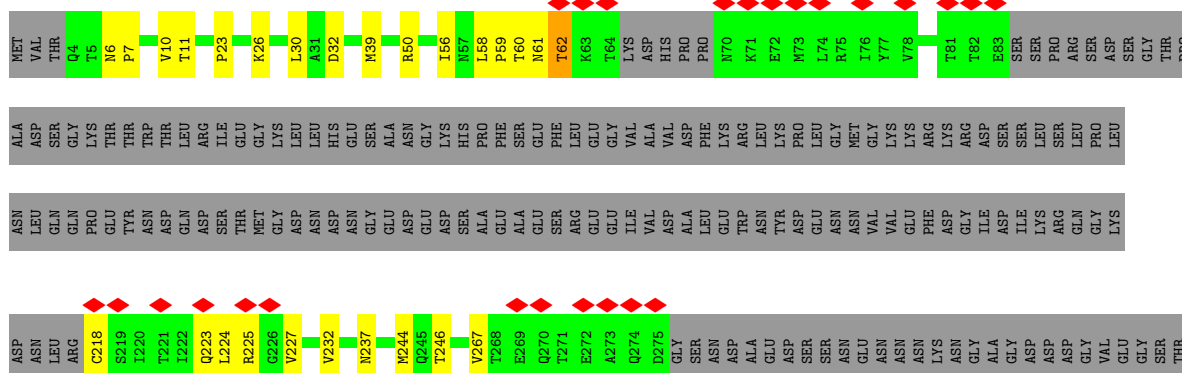


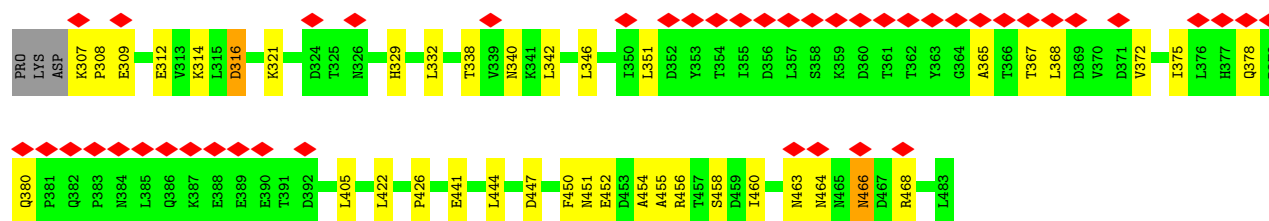


• Molecule 7: Chromatin structure-remodeling complex protein RSC8



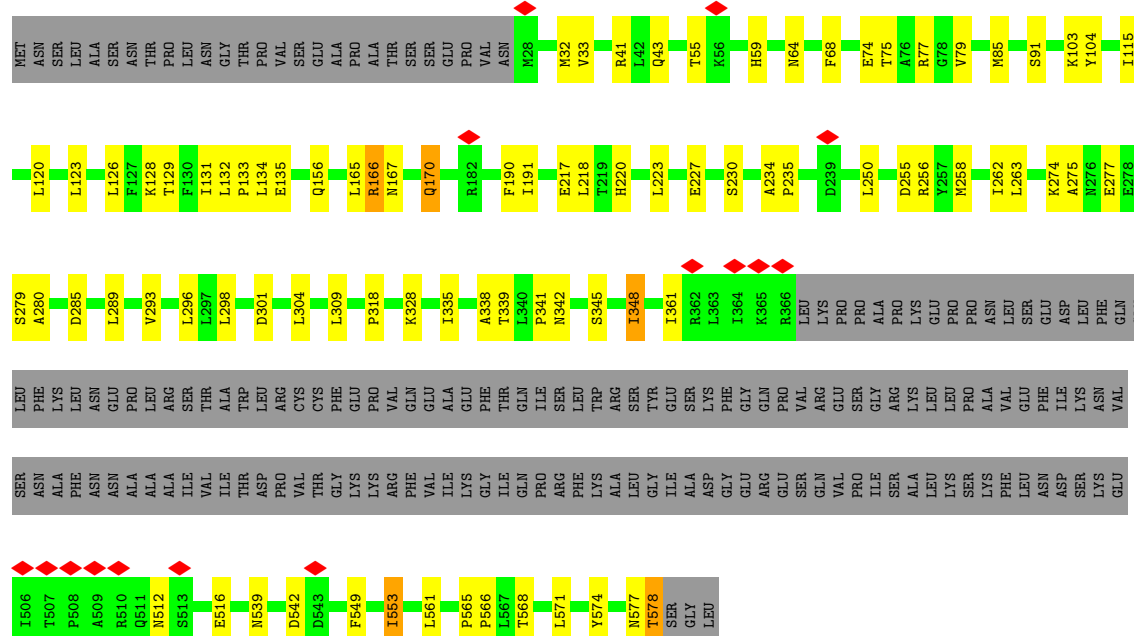
• Molecule 8: Chromatin structure-remodeling complex protein RSC6





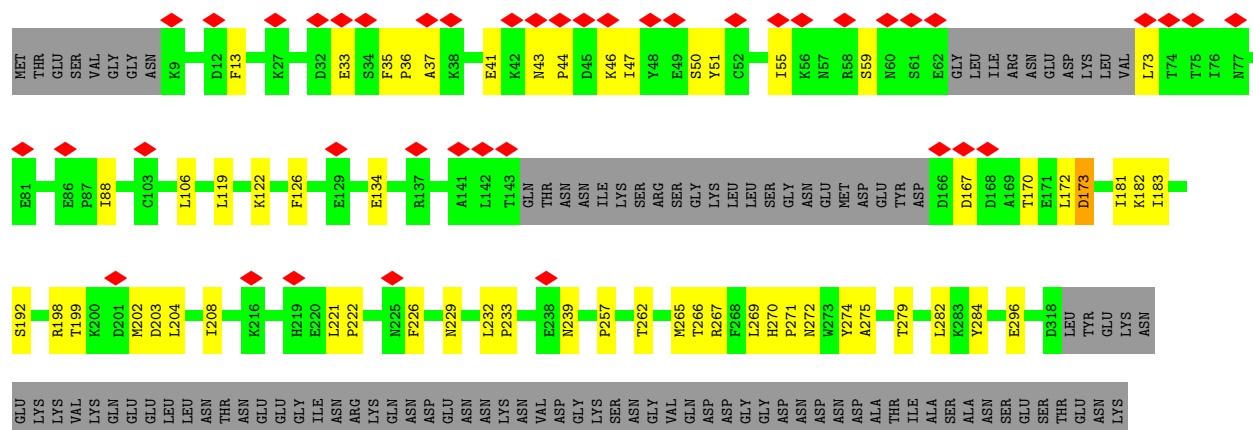
• Molecule 9: Chromatin structure-remodeling complex subunit RSC9

Chain N: 56% 14% 29%



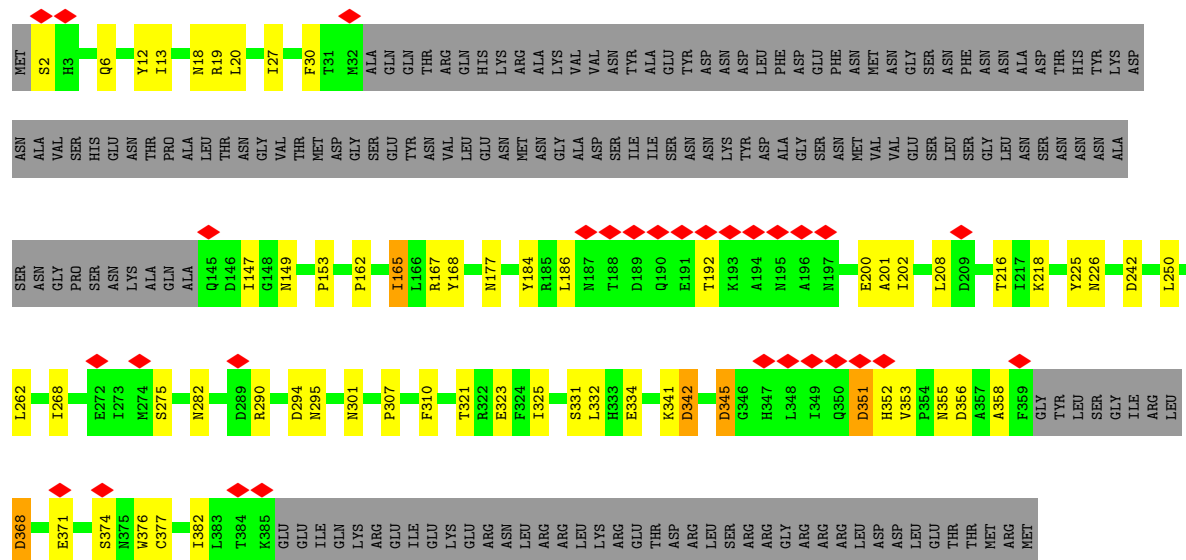
• Molecule 10: Chromatin structure-remodeling complex protein RSC58

Chain O: 9% 63% 14% 24%

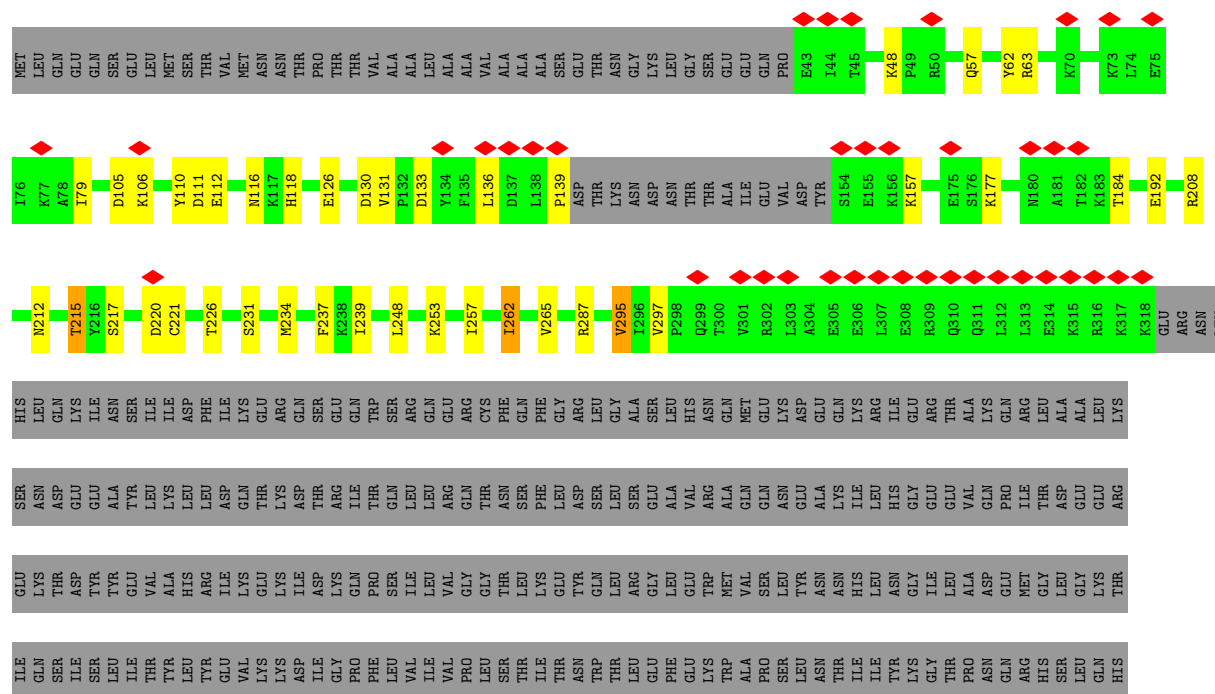




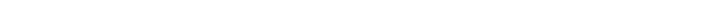
• Molecule 11: Chromatin structure-remodeling complex subunit SFH1

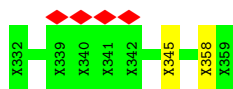


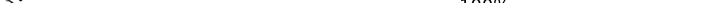
• Molecule 12: Nuclear protein STH1/NPS1

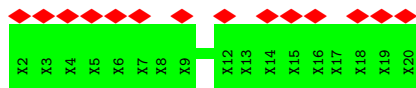


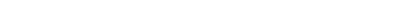
[illegible]

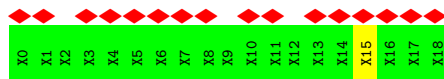
Chain 2:  14% 93% 7%

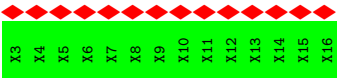


Chain 3:  74% 100%

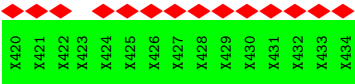
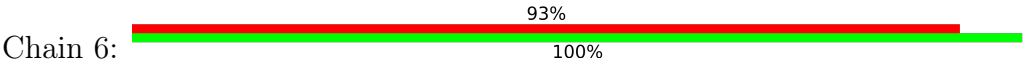


Chain 4:  84% 95% 5%

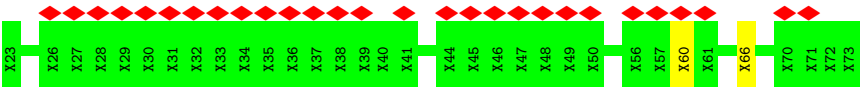
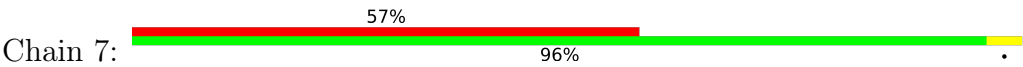




• Molecule 17: Unknown Protein



• Molecule 18: Unknown Protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	1920066	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.231	Depositor
Minimum map value	-0.121	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.03	Depositor
Map size ($\text{\AA}$)	414.432, 414.432, 414.432	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.439, 1.439, 1.439	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	C	0.17	0/495	0.27	0/662
2	D	0.14	0/786	0.25	0/1062
3	E	0.17	0/997	0.31	0/1356
4	F	0.18	0/551	0.27	0/748
5	G	0.13	0/431	0.24	0/584
6	H	0.18	0/1108	0.35	0/1497
7	I	0.22	0/2474	0.31	0/3343
7	J	0.21	0/926	0.31	0/1233
7	K	0.17	0/879	0.26	0/1172
7	L	0.18	0/2502	0.29	0/3376
8	M	0.17	0/2515	0.29	0/3423
9	N	0.21	0/3334	0.34	0/4515
10	O	0.19	0/3216	0.32	0/4358
11	Q	0.18	0/2181	0.36	0/2964
12	R	0.19	0/2154	0.32	0/2897
13	S	0.10	0/281	0.17	0/378
All	All	0.19	0/24830	0.31	0/33568

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

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	C	493	0	507	7	0
2	D	772	0	754	11	0
3	E	978	0	935	27	0
4	F	536	0	533	14	0
5	G	422	0	423	10	0
6	H	1083	0	1062	24	0
7	I	2416	0	2358	40	0
7	J	924	0	976	11	0
7	K	878	0	930	14	0
7	L	2445	0	2402	49	0
8	M	2474	0	2465	52	0
9	N	3275	0	3373	55	0
10	O	3145	0	3168	53	0
11	Q	2137	0	2069	41	0
12	R	2126	0	2205	35	0
13	S	278	0	287	6	0
14	2	140	0	34	2	0
15	3	95	0	21	0	0
15	4	95	0	21	1	0
16	5	70	0	16	0	0
17	6	75	0	17	0	0
18	7	245	0	63	2	0
19	I	1	0	0	0	0
All	All	25103	0	24619	342	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 7.

All (342) 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)
11:Q:282:ASN:OD1	11:Q:295:ASN:ND2	2.20	0.75
9:N:217:GLU:OE1	12:R:287:ARG:NH1	2.21	0.74
6:H:443:MET:HE2	10:O:221:LEU:HD11	1.72	0.72
2:D:96:GLN:NE2	15:4:15:UNK:O	2.22	0.72
4:F:813:LEU:HD11	10:O:183:ILE:HD12	1.73	0.71
7:L:268:ILE:HD11	10:O:232:LEU:HD22	1.73	0.70
6:H:527:THR:C	6:H:529:ASN:H	1.97	0.70
7:I:136:TYR:O	7:I:167:ASN:ND2	2.26	0.69
9:N:345:SER:HA	9:N:348:ILE:HD11	1.75	0.68
10:O:35:PHE:O	10:O:73:LEU:N	2.26	0.68
12:R:231:SER:HB3	12:R:234:MET:HG2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:135:GLU:OE2	11:Q:19:ARG:NH2	2.27	0.68
9:N:220:HIS:NE2	10:O:296:GLU:O	2.27	0.68
1:C:20:THR:HG22	10:O:275:ALA:H	1.58	0.68
3:E:376:ASN:ND2	3:E:381:ASP:O	2.27	0.67
7:L:178:LEU:HD21	11:Q:325:ILE:HD11	1.76	0.67
8:M:218:CYS:SG	18:7:60:UNK:N	2.68	0.67
8:M:456:ARG:NH2	10:O:262:THR:O	2.28	0.66
10:O:126:PHE:HB2	12:R:226:THR:HG22	1.78	0.66
11:Q:18:ASN:ND2	11:Q:177:ASN:O	2.29	0.66
9:N:55:THR:O	9:N:64:ASN:ND2	2.28	0.65
7:L:363:TYR:OH	12:R:116:ASN:ND2	2.29	0.65
10:O:401:TYR:OH	12:R:48:LYS:NZ	2.21	0.65
10:O:33:GLU:HG3	10:O:106:LEU:HD11	1.79	0.65
4:F:813:LEU:HD22	7:L:276:ARG:HH21	1.62	0.65
7:J:426:GLN:NE2	8:M:26:LYS:O	2.30	0.64
11:Q:184:TYR:OH	11:Q:242:ASP:OD1	2.15	0.64
3:E:392:ASP:HB3	7:I:226:VAL:HB	1.80	0.64
7:K:501:GLN:HG2	8:M:244:MET:HB3	1.79	0.63
10:O:430:ARG:NH2	12:R:130:ASP:OD1	2.31	0.63
10:O:41:GLU:OE2	10:O:50:SER:OG	2.16	0.62
4:F:875:THR:HG22	12:R:221:CYS:HB3	1.81	0.62
6:H:449:LYS:O	6:H:516:THR:OG1	2.16	0.61
7:I:260:CYS:HB2	7:I:283:CYS:SG	2.40	0.61
3:E:405:ILE:HD11	7:L:162:LYS:HD3	1.82	0.61
9:N:296:LEU:HD21	9:N:309:LEU:HG	1.83	0.61
7:I:282:LEU:HD21	7:I:292:PHE:HB3	1.83	0.61
7:L:95:HIS:O	7:L:95:HIS:ND1	2.34	0.61
9:N:75:THR:HG1	11:Q:12:TYR:HH	1.47	0.61
2:D:64:HIS:HD2	2:D:66:TYR:H	1.47	0.60
8:M:463:ASN:HA	8:M:468:ARG:HH21	1.66	0.60
7:L:237:SER:OG	7:L:249:ARG:NH1	2.35	0.60
7:I:312:LYS:H	7:I:312:LYS:HD3	1.66	0.60
10:O:265:MET:HE3	12:R:262:ILE:HD13	1.83	0.60
7:L:288:GLN:HB2	7:L:291:HIS:CE1	2.37	0.60
11:Q:368:ASP:OD1	11:Q:368:ASP:N	2.35	0.59
11:Q:351:ASP:OD1	11:Q:351:ASP:N	2.35	0.59
7:I:239:GLN:OE1	7:I:346:ARG:NH1	2.35	0.59
8:M:378:GLN:OE1	8:M:380:GLN:NE2	2.36	0.59
10:O:170:THR:HG22	10:O:172:LEU:H	1.68	0.59
11:Q:2:SER:N	11:Q:6:GLN:OE1	2.35	0.58
3:E:408:GLU:N	3:E:408:GLU:OE1	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:167:MET:HE1	5:G:177:ILE:HA	1.86	0.58
10:O:167:ASP:OD2	10:O:182:LYS:NZ	2.36	0.58
4:F:852:ASP:OD1	4:F:853:VAL:N	2.36	0.57
7:J:434:LYS:NZ	7:J:438:GLU:OE2	2.37	0.57
9:N:574:TYR:O	9:N:578:THR:OG1	2.21	0.57
7:I:271:ARG:HD2	7:I:281:ASN:HD22	1.68	0.57
1:C:33:ARG:NH2	8:M:441:GLU:OE2	2.36	0.56
3:E:380:SER:HB2	8:M:464:ASN:HA	1.85	0.56
1:C:68:MET:HE1	7:J:437:MET:HB3	1.87	0.56
7:I:57:ASN:N	7:I:59:GLU:OE1	2.38	0.56
10:O:266:THR:HG23	10:O:267:ARG:HG3	1.87	0.56
6:H:527:THR:O	6:H:529:ASN:N	2.33	0.56
9:N:156:GLN:OE1	12:R:287:ARG:NH2	2.38	0.56
8:M:227:VAL:HG12	9:N:361:ILE:HD12	1.88	0.55
6:H:489:ASN:O	6:H:490:GLU:HG2	2.06	0.55
7:I:226:VAL:HG13	7:I:228:LEU:HG	1.88	0.55
3:E:372:ARG:HB2	7:I:188:GLN:HB2	1.89	0.55
4:F:814:PRO:O	7:L:276:ARG:NH2	2.39	0.55
6:H:513:SER:O	6:H:588:THR:HA	2.07	0.55
11:Q:202:ILE:HG12	11:Q:226:ASN:HB2	1.87	0.55
7:L:179:ILE:HD11	11:Q:321:THR:HA	1.89	0.55
12:R:111:ASP:OD1	12:R:111:ASP:N	2.38	0.55
4:F:813:LEU:HD23	4:F:814:PRO:HD2	1.90	0.54
7:L:268:ILE:HD12	10:O:233:PRO:HD2	1.88	0.54
10:O:198:ARG:NH2	10:O:199:THR:O	2.41	0.54
7:L:251:SER:OG	12:R:57:GLN:NE2	2.41	0.54
12:R:105:ASP:OD1	12:R:106:LYS:N	2.40	0.54
12:R:253:LYS:HE3	12:R:257:ILE:HD11	1.90	0.54
6:H:448:TYR:HA	6:H:493:GLN:HE21	1.73	0.54
7:I:302:ILE:HD11	12:R:239:ILE:HG12	1.89	0.54
10:O:35:PHE:HB2	10:O:36:PRO:HD2	1.89	0.54
7:L:193:THR:OG1	7:L:196:GLY:O	2.26	0.54
2:D:98:GLU:OE2	9:N:41:ARG:NH2	2.29	0.54
7:L:191:LEU:HG	7:L:200:PHE:HB2	1.90	0.54
9:N:227:GLU:O	9:N:230:SER:OG	2.15	0.54
9:N:335:ILE:O	9:N:339:THR:OG1	2.24	0.53
7:I:363:TYR:HA	7:I:366:GLU:HG2	1.91	0.53
10:O:167:ASP:HB3	10:O:173:ASP:HB3	1.89	0.53
7:J:430:GLN:NE2	7:K:425:SER:OG	2.41	0.53
7:J:458:LYS:NZ	7:K:453:GLN:OE1	2.42	0.53
7:L:80:VAL:HG21	7:L:130:ARG:HG2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:431:CYS:HA	3:E:434:TYR:HD2	1.72	0.53
8:M:451:ASN:OD1	8:M:451:ASN:N	2.42	0.53
9:N:170:GLN:HG3	12:R:295:VAL:HG12	1.90	0.53
8:M:225:ARG:HB3	18:7:66:UNK:HA	1.90	0.53
8:M:267:VAL:HG22	8:M:314:LYS:HE3	1.89	0.53
3:E:327:CYS:SG	7:L:145:ASN:ND2	2.82	0.52
5:G:159:VAL:HG11	13:S:208:VAL:HG21	1.91	0.52
6:H:453:GLN:HA	6:H:486:PHE:O	2.09	0.52
7:I:70:LEU:O	7:I:75:LYS:NZ	2.39	0.52
7:L:233:ASN:ND2	12:R:126:GLU:OE2	2.42	0.52
8:M:456:ARG:NH1	12:R:192:GLU:OE2	2.42	0.52
3:E:319:TRP:H	3:E:319:TRP:CD1	2.27	0.52
11:Q:342:ASP:N	11:Q:342:ASP:OD1	2.42	0.52
4:F:798:ILE:HD11	10:O:192:SER:HB2	1.92	0.52
7:I:91:ILE:HD12	7:L:185:GLY:HA2	1.91	0.52
10:O:491:ARG:HG2	14:2:358:UNK:HA	1.91	0.52
3:E:402:LEU:HD12	3:E:405:ILE:HD13	1.92	0.52
7:L:235:TYR:O	10:O:446:ARG:NH1	2.41	0.52
11:Q:147:ILE:HD11	11:Q:167:ARG:HB3	1.90	0.52
8:M:351:LEU:HD11	8:M:368:LEU:HD11	1.90	0.52
3:E:380:SER:OG	8:M:463:ASN:ND2	2.43	0.52
6:H:497:ALA:HB3	10:O:229:ASN:HA	1.92	0.52
7:K:433:VAL:HG21	8:M:32:ASP:HB3	1.90	0.52
8:M:466:ASN:OD1	8:M:466:ASN:N	2.42	0.52
9:N:250:LEU:HB2	9:N:262:ILE:HG21	1.92	0.51
11:Q:358:ALA:H	11:Q:371:GLU:HB2	1.75	0.51
12:R:62:TYR:HB2	12:R:79:ILE:HG21	1.91	0.51
11:Q:268:ILE:HD13	11:Q:341:LYS:HG2	1.93	0.51
3:E:417:ASP:N	3:E:417:ASP:OD1	2.42	0.51
11:Q:200:GLU:HG3	11:Q:201:ALA:H	1.76	0.51
10:O:122:LYS:HG3	12:R:226:THR:HG21	1.93	0.51
6:H:527:THR:C	6:H:529:ASN:N	2.68	0.51
9:N:255:ASP:OD1	9:N:256:ARG:N	2.44	0.51
8:M:60:THR:O	8:M:61:ASN:ND2	2.44	0.51
9:N:285:ASP:OD1	9:N:285:ASP:N	2.36	0.51
11:Q:345:ASP:OD1	11:Q:345:ASP:N	2.43	0.50
7:L:348:GLU:HB3	10:O:457:LYS:HE3	1.92	0.50
5:G:175:ASP:OD1	5:G:175:ASP:N	2.43	0.50
10:O:270:HIS:HD2	10:O:272:ASN:HB2	1.77	0.50
7:I:249:ARG:NH2	7:I:253:GLN:HE21	2.09	0.50
7:I:105:PHE:HE1	7:I:148:MET:HE1	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Q:275:SER:O	11:Q:301:ASN:ND2	2.41	0.50
6:H:511:LEU:HD23	6:H:525:LEU:HD11	1.94	0.49
7:L:147:ALA:HB1	11:Q:355:ASN:HD22	1.76	0.49
4:F:869:ARG:H	7:L:318:GLN:NE2	2.09	0.49
7:I:358:PRO:HB2	7:L:224:PHE:HB2	1.95	0.49
5:G:163:ALA:HB1	13:S:194:ALA:HB1	1.94	0.49
11:Q:153:PRO:HB3	11:Q:168:TYR:CE1	2.47	0.49
2:D:66:TYR:OH	7:I:331:GLU:OE2	2.20	0.49
7:L:236:ASP:OD2	7:L:239:GLN:NE2	2.45	0.49
7:L:284:SER:HB2	10:O:181:ILE:HD11	1.95	0.49
7:I:192:ASP:OD1	7:I:193:THR:N	2.45	0.49
8:M:454:ALA:HB1	8:M:460:ILE:HG21	1.93	0.49
9:N:75:THR:OG1	11:Q:12:TYR:OH	2.20	0.49
11:Q:208:LEU:O	11:Q:218:LYS:HA	2.13	0.49
12:R:110:TYR:HH	12:R:118:HIS:HD1	1.60	0.49
7:L:282:LEU:HD22	7:L:291:HIS:CD2	2.48	0.49
7:J:419:GLU:O	7:J:422:ILE:HG12	2.13	0.49
3:E:345:ASP:O	11:Q:149:ASN:ND2	2.45	0.49
11:Q:30:PHE:HA	11:Q:216:THR:O	2.11	0.49
11:Q:294:ASP:OD1	11:Q:295:ASN:N	2.46	0.49
2:D:62:ALA:HB3	2:D:71:VAL:HG23	1.94	0.48
7:I:249:ARG:HH21	7:I:253:GLN:HE21	1.61	0.48
8:M:308:PRO:HB3	8:M:329:HIS:CD2	2.48	0.48
12:R:217:SER:OG	12:R:220:ASP:OD1	2.32	0.48
3:E:331:ASN:HD21	7:L:137:LEU:HA	1.78	0.48
3:E:353:TYR:OH	11:Q:323:GLU:OE2	2.24	0.48
7:L:140:THR:HG22	7:L:143:ARG:HH22	1.79	0.48
7:J:467:LYS:NZ	8:M:62:THR:O	2.42	0.48
11:Q:202:ILE:HB	11:Q:225:TYR:HB3	1.96	0.48
9:N:191:ILE:HD12	9:N:218:LEU:HD21	1.96	0.47
8:M:237:ASN:ND2	8:M:321:LYS:O	2.47	0.47
8:M:23:PRO:HB2	8:M:26:LYS:HG2	1.97	0.47
9:N:115:ILE:HA	9:N:120:LEU:HD12	1.96	0.47
11:Q:307:PRO:HB3	11:Q:332:LEU:HD23	1.97	0.47
9:N:341:PRO:HD3	9:N:553:ILE:HD11	1.95	0.47
9:N:68:PHE:CZ	11:Q:13:ILE:HD11	2.49	0.47
7:L:320:MET:HE3	7:L:357:LEU:HD21	1.95	0.47
10:O:198:ARG:HD3	10:O:203:ASP:OD1	2.14	0.47
2:D:64:HIS:CD2	2:D:66:TYR:H	2.29	0.47
7:L:258:TYR:OH	10:O:173:ASP:OD1	2.33	0.47
6:H:444:GLU:HG2	6:H:445:TYR:H	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:O:427:LYS:HZ1	12:R:133:ASP:HA	1.80	0.47
5:G:175:ASP:O	5:G:178:ILE:HG22	2.15	0.47
9:N:223:LEU:HD12	9:N:258:MET:HE2	1.98	0.47
7:L:147:ALA:HB3	11:Q:371:GLU:H	1.80	0.46
7:L:298:SER:HB3	10:O:390:LEU:HG	1.98	0.46
3:E:372:ARG:HH12	7:I:227:ASN:HD21	1.62	0.46
7:K:493:LYS:HE2	7:K:510:GLU:HG2	1.97	0.46
12:R:215:THR:HG21	12:R:237:PHE:H	1.79	0.46
2:D:64:HIS:HD2	2:D:66:TYR:HB2	1.81	0.46
3:E:331:ASN:ND2	7:L:137:LEU:HA	2.31	0.46
7:I:195:GLN:C	7:I:197:LEU:H	2.23	0.46
9:N:279:SER:OG	9:N:280:ALA:N	2.48	0.46
12:R:136:LEU:C	12:R:139:PRO:HD2	2.40	0.46
7:I:311:VAL:HB	7:I:314:ASN:HD22	1.79	0.46
8:M:444:LEU:HD13	12:R:177:LYS:HG2	1.98	0.46
11:Q:331:SER:O	11:Q:334:GLU:HB2	2.15	0.46
6:H:524:THR:HG23	6:H:605:ARG:HB3	1.97	0.46
1:C:44:GLU:HB2	12:R:157:LYS:HD3	1.98	0.46
5:G:192:LEU:HD11	13:S:209:LEU:HD22	1.97	0.46
7:I:246:ASP:OD1	7:I:247:GLU:N	2.49	0.46
7:J:472:ARG:HH22	7:K:467:LYS:HB2	1.81	0.46
10:O:55:ILE:O	10:O:59:SER:N	2.48	0.46
11:Q:162:PRO:O	11:Q:165:ILE:HB	2.16	0.46
4:F:818:TRP:HA	7:L:287:PHE:CD2	2.51	0.45
9:N:561:LEU:HD21	9:N:571:LEU:HD12	1.98	0.45
6:H:490:GLU:HG3	7:L:264:GLY:O	2.15	0.45
8:M:309:GLU:N	8:M:312:GLU:OE1	2.47	0.45
3:E:414:VAL:HG22	3:E:418:VAL:HB	1.98	0.45
7:J:482:LEU:HD11	7:K:507:GLN:HA	1.99	0.45
8:M:452:GLU:HA	8:M:455:ALA:HB3	1.98	0.45
7:L:150:VAL:HG11	11:Q:310:PHE:CE1	2.51	0.45
2:D:123:ASP:OD2	6:H:474:ARG:NH2	2.50	0.45
8:M:227:VAL:HG13	8:M:346:LEU:HD12	1.99	0.45
10:O:466:SER:OG	12:R:112:GLU:OE2	2.29	0.45
7:I:171:ASP:O	7:I:174:THR:HG22	2.17	0.45
8:M:450:PHE:HA	10:O:265:MET:HE1	1.98	0.45
2:D:85:HIS:O	12:R:208:ARG:NH1	2.48	0.45
8:M:59:PRO:HB2	8:M:244:MET:HE1	1.99	0.45
8:M:372:VAL:HG12	8:M:375:ILE:HB	1.98	0.45
9:N:59:HIS:O	9:N:59:HIS:ND1	2.49	0.45
9:N:234:ALA:HB3	9:N:235:PRO:HD3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Q:20:LEU:HA	11:Q:27:ILE:HD12	1.99	0.45
6:H:525:LEU:O	6:H:532:PRO:HD2	2.16	0.45
7:I:59:GLU:H	7:I:59:GLU:CD	2.25	0.45
7:L:353:LYS:HD2	7:L:353:LYS:HA	1.86	0.44
9:N:77:ARG:NH1	13:S:198:LEU:H	2.15	0.44
10:O:173:ASP:OD1	10:O:173:ASP:N	2.48	0.44
3:E:392:ASP:OD2	3:E:395:LEU:HD13	2.16	0.44
7:K:500:GLU:OE1	8:M:246:THR:OG1	2.33	0.44
8:M:447:ASP:HB3	10:O:270:HIS:CD2	2.52	0.44
10:O:257:PRO:HG2	12:R:248:LEU:O	2.18	0.44
8:M:30:LEU:HD23	8:M:30:LEU:HA	1.85	0.44
9:N:301:ASP:OD2	10:O:284:TYR:OH	2.33	0.44
6:H:608:ASP:O	6:H:609:LYS:HG2	2.16	0.44
7:I:180:GLY:HA3	7:L:198:LYS:HE3	2.00	0.44
8:M:372:VAL:HG13	8:M:375:ILE:HD12	1.99	0.44
9:N:32:MET:HE2	14:2:345:UNK:HA	1.99	0.44
2:D:64:HIS:CD2	2:D:66:TYR:HB2	2.52	0.44
3:E:388:THR:HG23	7:I:230:ILE:HB	1.99	0.44
3:E:371:TRP:CD2	7:L:202:PRO:HG3	2.53	0.44
3:E:372:ARG:HH22	7:I:227:ASN:HD21	1.64	0.44
7:K:433:VAL:O	7:K:437:MET:HG2	2.17	0.44
7:L:166:ILE:HG22	7:L:167:ASN:CG	2.41	0.44
10:O:202:MET:HG3	10:O:204:LEU:HD11	2.00	0.44
7:I:281:ASN:OD1	7:I:281:ASN:N	2.50	0.43
8:M:50:ARG:HA	8:M:50:ARG:HD3	1.78	0.43
3:E:394:ASP:HB2	3:E:428:PHE:HE1	1.84	0.43
8:M:458:SER:O	8:M:458:SER:OG	2.35	0.43
1:C:36:ILE:HD13	1:C:36:ILE:HA	1.89	0.43
5:G:158:TRP:CD1	9:N:74:GLU:HG3	2.54	0.43
9:N:539:ASN:OD1	9:N:577:ASN:ND2	2.51	0.43
9:N:338:ALA:O	9:N:342:ASN:ND2	2.52	0.43
7:I:135:GLU:HG2	7:I:136:TYR:H	1.84	0.43
7:I:140:THR:HG23	7:I:143:ARG:HH21	1.83	0.43
6:H:491:LEU:HD23	6:H:491:LEU:HA	1.90	0.43
7:J:479:ILE:HD11	7:K:475:LEU:HD21	2.01	0.43
8:M:378:GLN:HG2	8:M:380:GLN:HG3	2.00	0.43
7:I:148:MET:HE2	7:I:148:MET:HB3	1.95	0.43
8:M:332:LEU:HD23	9:N:565:PRO:HB3	2.00	0.43
10:O:51:TYR:CE2	10:O:55:ILE:HD11	2.53	0.43
6:H:523:GLU:HG2	6:H:606:CYS:SG	2.59	0.43
9:N:132:LEU:N	9:N:133:PRO:HD2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:N:85:MET:SD	9:N:103:LYS:HB3	2.59	0.42
10:O:44:PRO:HA	10:O:47:ILE:HG13	2.00	0.42
11:Q:356:ASP:O	11:Q:374:SER:N	2.37	0.42
5:G:178:ILE:HD12	13:S:226:LEU:HD23	2.01	0.42
10:O:433:ARG:NH1	10:O:441:PRO:HB3	2.34	0.42
3:E:320:LEU:HB3	7:L:73:LEU:HD11	2.02	0.42
7:L:121:THR:O	7:L:125:ILE:HG13	2.20	0.42
9:N:328:LYS:HE2	9:N:328:LYS:HB3	1.87	0.42
7:I:158:ALA:HB2	11:Q:186:LEU:HD12	2.01	0.42
8:M:10:VAL:HG22	8:M:11:THR:H	1.84	0.42
9:N:126:LEU:O	9:N:129:THR:OG1	2.26	0.42
11:Q:20:LEU:HD23	11:Q:27:ILE:HG21	2.01	0.42
11:Q:358:ALA:H	11:Q:371:GLU:CB	2.32	0.42
5:G:168:LEU:HD23	5:G:168:LEU:HA	1.93	0.42
7:I:260:CYS:SG	7:I:262:THR:OG1	2.76	0.42
10:O:427:LYS:NZ	12:R:133:ASP:HA	2.34	0.42
12:R:212:ASN:OD1	12:R:212:ASN:N	2.48	0.42
7:I:88:TRP:H	7:I:88:TRP:CD1	2.34	0.42
7:L:119:LYS:HG3	7:L:122:ARG:NH2	2.34	0.42
9:N:542:ASP:OD1	9:N:542:ASP:N	2.50	0.42
8:M:7:PRO:HB2	10:O:282:LEU:HB3	2.02	0.42
10:O:13:PHE:CE1	10:O:134:GLU:HB3	2.55	0.42
3:E:407:LYS:HA	3:E:410:TYR:CZ	2.55	0.42
4:F:808:ASP:OD1	4:F:809:PRO:HD2	2.19	0.42
10:O:119:LEU:HD23	10:O:119:LEU:HA	1.91	0.42
1:C:61:SER:O	1:C:65:MET:HG2	2.20	0.41
4:F:818:TRP:HA	7:L:287:PHE:HD2	1.85	0.41
9:N:165:LEU:HD23	9:N:165:LEU:HA	1.79	0.41
2:D:110:HIS:NE2	2:D:115:CYS:SG	2.93	0.41
7:L:287:PHE:HA	12:R:63:ARG:HH21	1.85	0.41
9:N:298:LEU:HD12	9:N:304:LEU:HD23	2.01	0.41
4:F:862:GLY:HA3	4:F:864:PHE:CE2	2.56	0.41
7:K:472:ARG:NH2	7:K:503:ASP:OD2	2.37	0.41
10:O:222:PRO:HG2	10:O:226:PHE:CE2	2.55	0.41
10:O:270:HIS:ND1	10:O:271:PRO:HD2	2.34	0.41
12:R:248:LEU:HA	12:R:248:LEU:HD23	1.85	0.41
8:M:340:ASN:HD21	9:N:516:GLU:HG3	1.86	0.41
8:M:405:LEU:HD12	8:M:405:LEU:HA	1.92	0.41
9:N:275:ALA:HB2	9:N:318:PRO:O	2.20	0.41
9:N:361:ILE:HA	9:N:512:ASN:HD21	1.85	0.41
10:O:37:ALA:HB3	10:O:73:LEU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:320:MET:HE1	7:L:353:LYS:HE3	2.03	0.41
9:N:561:LEU:HD22	9:N:568:THR:HA	2.03	0.41
9:N:166:ARG:HG3	9:N:167:ASN:N	2.34	0.41
9:N:274:LYS:HB2	9:N:277:GLU:HB3	2.02	0.41
10:O:239:ASN:ND2	10:O:482:ASN:O	2.53	0.41
1:C:52:ILE:O	1:C:57:ARG:NH2	2.54	0.41
5:G:157:ASN:ND2	13:S:203:PHE:O	2.46	0.41
6:H:455:TYR:CD2	6:H:485:ILE:HG12	2.56	0.41
6:H:502:LEU:HD11	6:H:509:LEU:HD11	2.03	0.41
7:K:440:LEU:HD13	8:M:39:MET:HE2	2.02	0.41
7:K:461:TYR:HE2	8:M:56:ILE:HG22	1.86	0.41
7:K:493:LYS:HG3	7:K:510:GLU:HG2	2.02	0.41
8:M:223:GLN:HG3	8:M:224:LEU:H	1.86	0.41
8:M:422:LEU:HD12	8:M:426:PRO:HA	2.03	0.41
8:M:451:ASN:O	12:R:184:THR:HG21	2.21	0.41
9:N:289:LEU:O	9:N:293:VAL:HG23	2.21	0.41
9:N:549:PHE:CZ	9:N:553:ILE:HD12	2.56	0.41
10:O:43:ASN:HD21	10:O:46:LYS:HD2	1.86	0.41
11:Q:356:ASP:N	11:Q:374:SER:HA	2.35	0.41
11:Q:376:TRP:CG	11:Q:377:CYS:H	2.37	0.41
3:E:373:ARG:HH22	7:I:182:SER:HA	1.86	0.41
9:N:128:LYS:O	9:N:132:LEU:HG	2.22	0.41
9:N:131:ILE:O	9:N:134:LEU:HB3	2.21	0.41
8:M:6:ASN:HA	8:M:7:PRO:HD3	1.86	0.40
9:N:565:PRO:N	9:N:566:PRO:HD2	2.36	0.40
4:F:868:LEU:HD23	4:F:868:LEU:HA	1.94	0.40
6:H:487:ASN:ND2	6:H:490:GLU:OE2	2.43	0.40
6:H:489:ASN:OD1	6:H:489:ASN:N	2.54	0.40
7:J:418:SER:O	7:J:422:ILE:HG23	2.21	0.40
7:L:90:ASP:HB3	7:L:93:LYS:HB2	2.02	0.40
8:M:338:THR:O	8:M:342:LEU:HG	2.21	0.40
8:M:365:ALA:O	8:M:367:THR:HG23	2.21	0.40
11:Q:290:ARG:HG2	11:Q:382:ILE:HG12	2.04	0.40
4:F:807:GLY:O	7:L:316:SER:HB2	2.21	0.40
6:H:515:LEU:HD11	6:H:523:GLU:CD	2.47	0.40
7:L:149:ASP:OD1	7:L:149:ASP:N	2.54	0.40
8:M:307:LYS:HA	8:M:308:PRO:HD3	1.96	0.40
3:E:392:ASP:CG	7:I:193:THR:HG21	2.46	0.40
7:I:259:ILE:HD12	9:N:43:GLN:HG2	2.03	0.40
8:M:316:ASP:OD1	8:M:316:ASP:N	2.53	0.40
9:N:135:GLU:HG3	9:N:190:PHE:CD1	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:N:223:LEU:HD23	9:N:223:LEU:HA	1.82	0.40
9:N:263:LEU:HD23	9:N:263:LEU:HA	1.88	0.40
10:O:427:LYS:NZ	12:R:131:VAL:O	2.52	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	C	58/78 (74%)	56 (97%)	2 (3%)	0	100	100
2	D	96/180 (53%)	90 (94%)	6 (6%)	0	100	100
3	E	118/435 (27%)	108 (92%)	10 (8%)	0	100	100
4	F	63/889 (7%)	56 (89%)	7 (11%)	0	100	100
5	G	51/885 (6%)	49 (96%)	2 (4%)	0	100	100
6	H	127/625 (20%)	114 (90%)	10 (8%)	3 (2%)	4	20
7	I	289/557 (52%)	274 (95%)	15 (5%)	0	100	100
7	J	113/557 (20%)	109 (96%)	4 (4%)	0	100	100
7	K	105/557 (19%)	101 (96%)	4 (4%)	0	100	100
7	L	292/557 (52%)	278 (95%)	14 (5%)	0	100	100
8	M	302/483 (62%)	281 (93%)	21 (7%)	0	100	100
9	N	408/581 (70%)	380 (93%)	28 (7%)	0	100	100
10	O	376/502 (75%)	352 (94%)	24 (6%)	0	100	100
11	Q	258/426 (61%)	224 (87%)	34 (13%)	0	100	100
12	R	258/1359 (19%)	236 (92%)	22 (8%)	0	100	100
13	S	32/883 (4%)	32 (100%)	0	0	100	100
All	All	2946/9554 (31%)	2740 (93%)	203 (7%)	3 (0%)	49	76

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	H	528	ILE
6	H	529	ASN
6	H	527	THR

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	C	58/75 (77%)	58 (100%)	0	100	100
2	D	82/151 (54%)	82 (100%)	0	100	100
3	E	113/388 (29%)	105 (93%)	8 (7%)	13	39
4	F	60/810 (7%)	60 (100%)	0	100	100
5	G	48/832 (6%)	47 (98%)	1 (2%)	47	68
6	H	126/578 (22%)	123 (98%)	3 (2%)	43	66
7	I	268/500 (54%)	259 (97%)	9 (3%)	32	60
7	J	111/500 (22%)	110 (99%)	1 (1%)	70	78
7	K	106/500 (21%)	105 (99%)	1 (1%)	70	78
7	L	270/500 (54%)	267 (99%)	3 (1%)	65	76
8	M	286/435 (66%)	281 (98%)	5 (2%)	53	71
9	N	374/521 (72%)	364 (97%)	10 (3%)	39	64
10	O	358/462 (78%)	351 (98%)	7 (2%)	48	69
11	Q	243/384 (63%)	233 (96%)	10 (4%)	27	56
12	R	240/1228 (20%)	235 (98%)	5 (2%)	47	68
13	S	33/824 (4%)	32 (97%)	1 (3%)	36	62
All	All	2776/8688 (32%)	2712 (98%)	64 (2%)	44	67

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	E	327	CYS

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Mol	Chain	Res	Type
3	E	351	ASP
3	E	356	ILE
3	E	359	ILE
3	E	384	ILE
3	E	413	VAL
3	E	414	VAL
3	E	417	ASP
5	G	175	ASP
6	H	510	THR
6	H	527	THR
6	H	528	ILE
7	I	170	ILE
7	I	179	ILE
7	I	189	VAL
7	I	191	LEU
7	I	253	GLN
7	I	270	VAL
7	I	275	LEU
7	I	281	ASN
7	I	312	LYS
7	J	459	LEU
7	K	503	ASP
7	L	80	VAL
7	L	189	VAL
7	L	279	ASP
8	M	58	LEU
8	M	62	THR
8	M	232	VAL
8	M	316	ASP
8	M	466	ASN
9	N	33	VAL
9	N	79	VAL
9	N	91	SER
9	N	104	TYR
9	N	123	LEU
9	N	166	ARG
9	N	170	GLN
9	N	348	ILE
9	N	553	ILE
9	N	578	THR
10	O	88	ILE
10	O	173	ASP

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Mol	Chain	Res	Type
10	O	208	ILE
10	O	269	LEU
10	O	274	TYR
10	O	279	THR
10	O	490	VAL
11	Q	165	ILE
11	Q	192	THR
11	Q	250	LEU
11	Q	262	LEU
11	Q	342	ASP
11	Q	345	ASP
11	Q	351	ASP
11	Q	352	HIS
11	Q	353	VAL
11	Q	368	ASP
12	R	215	THR
12	R	262	ILE
12	R	265	VAL
12	R	295	VAL
12	R	297	VAL
13	S	198	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	64	HIS
2	D	108	HIS
3	E	331	ASN
3	E	396	ASN
4	F	800	ASN
4	F	877	HIS
6	H	465	GLN
6	H	478	ASN
6	H	493	GLN
6	H	506	GLN
6	H	512	GLN
6	H	601	HIS
7	I	60	GLN
7	I	63	GLN
7	I	167	ASN
7	I	227	ASN
7	I	253	GLN

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Mol	Chain	Res	Type
7	I	314	ASN
7	J	430	GLN
7	J	478	GLN
7	K	426	GLN
7	L	145	ASN
7	L	188	GLN
7	L	291	HIS
8	M	233	GLN
8	M	329	HIS
8	M	340	ASN
8	M	378	GLN
8	M	380	GLN
8	M	432	HIS
9	N	43	GLN
9	N	512	ASN
9	N	559	HIS
9	N	577	ASN
10	O	22	ASN
10	O	97	HIS
10	O	270	HIS
10	O	272	ASN
10	O	391	GLN
10	O	484	ASN
11	Q	158	GLN
11	Q	261	GLN
12	R	116	ASN
12	R	201	ASN
12	R	270	HIS
12	R	290	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
18	7	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	7	57:UNK	C	60:UNK	N	4.98

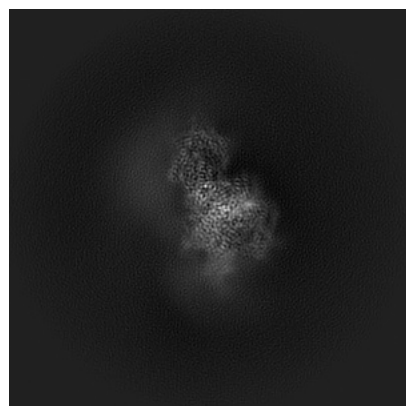
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21107. These allow visual inspection of the internal detail of the map and identification of artifacts.

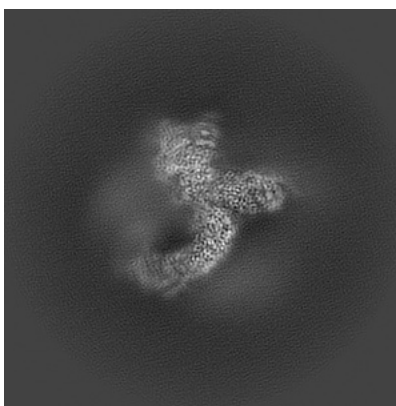
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

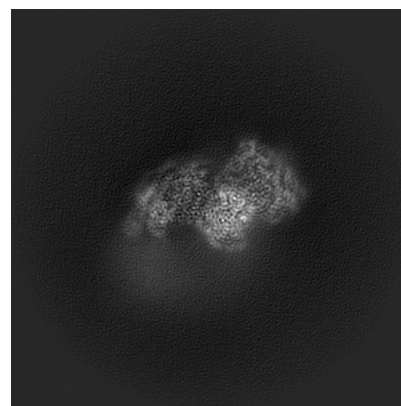
6.1.1 Primary map



X

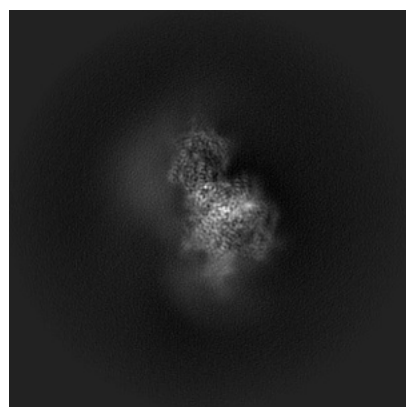


Y

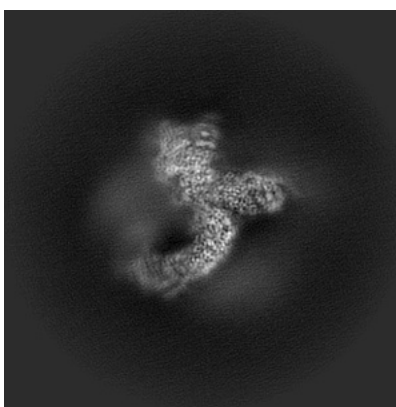


Z

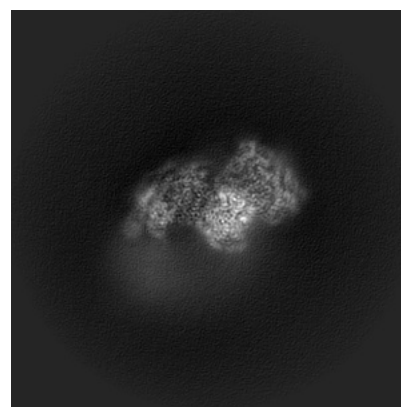
6.1.2 Raw map



X



Y

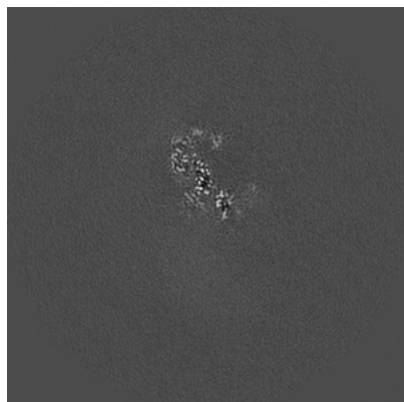


Z

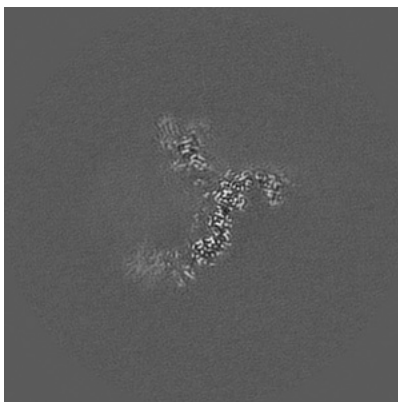
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

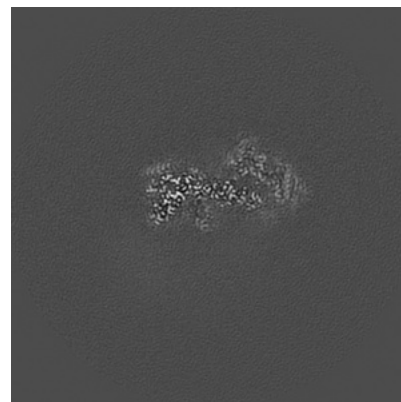
6.2.1 Primary map



X Index: 144

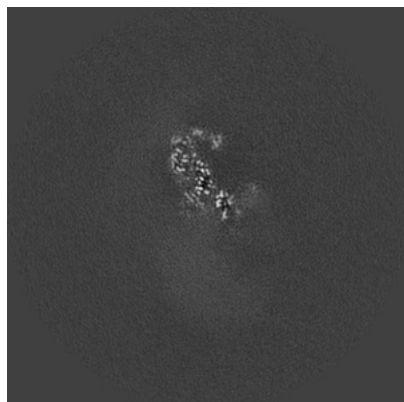


Y Index: 144

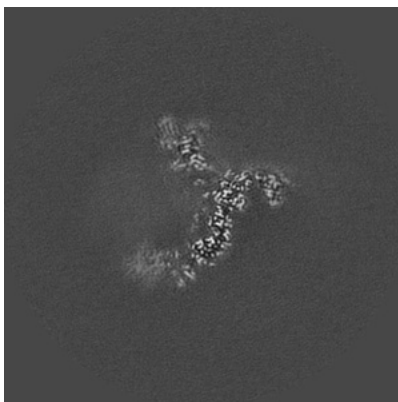


Z Index: 144

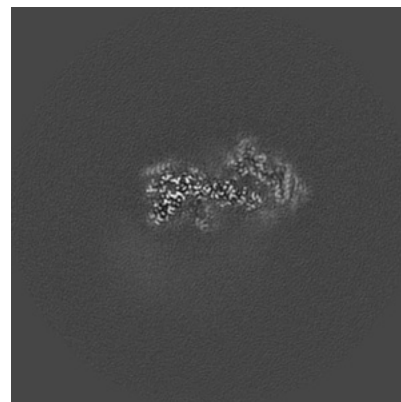
6.2.2 Raw map



X Index: 144



Y Index: 144

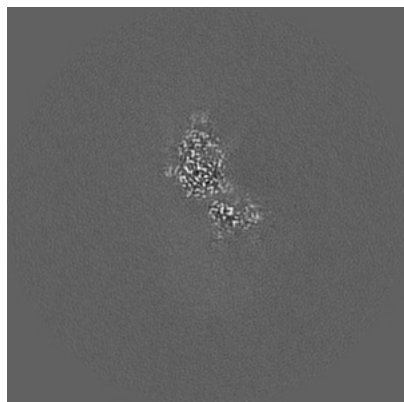


Z Index: 144

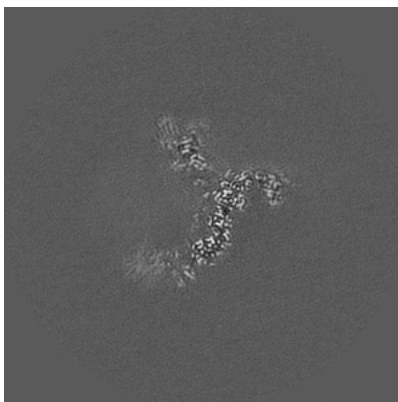
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

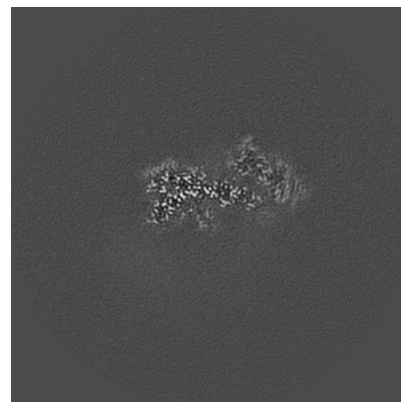
6.3.1 Primary map



X Index: 159

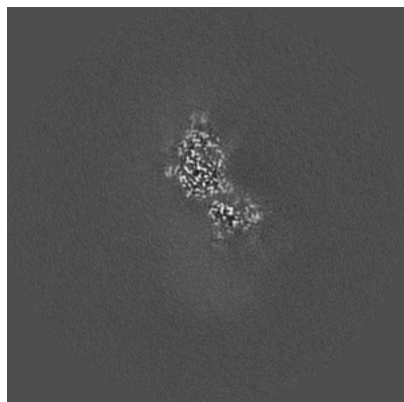


Y Index: 144

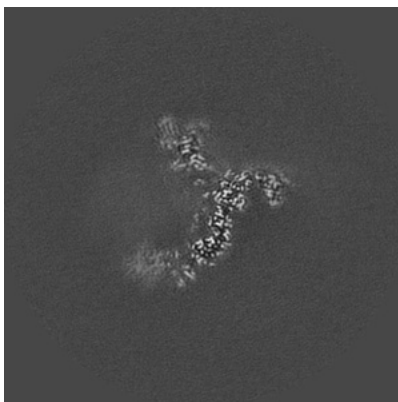


Z Index: 145

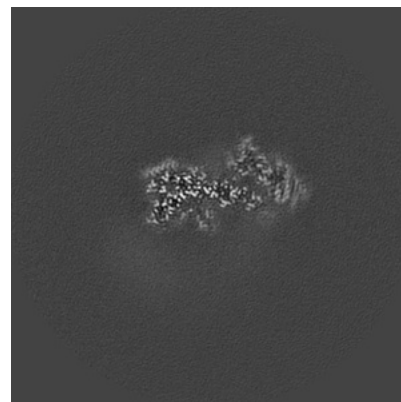
6.3.2 Raw map



X Index: 159



Y Index: 144

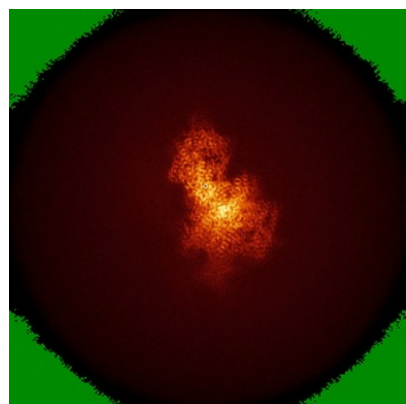


Z Index: 145

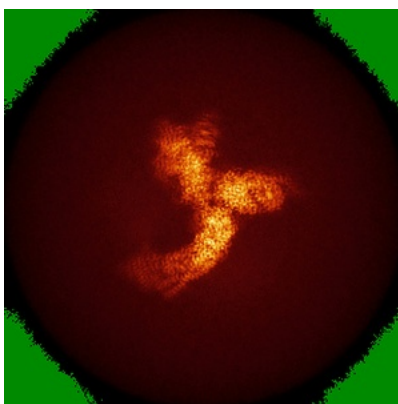
The images above show the largest variance slices of the map in three orthogonal directions.

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

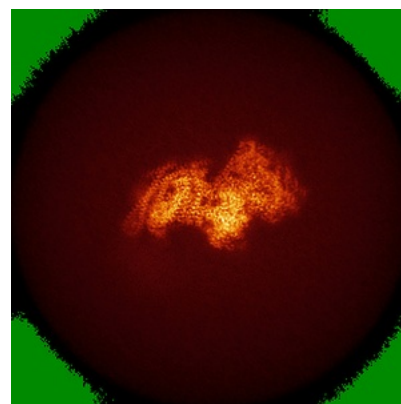
6.4.1 Primary map



X

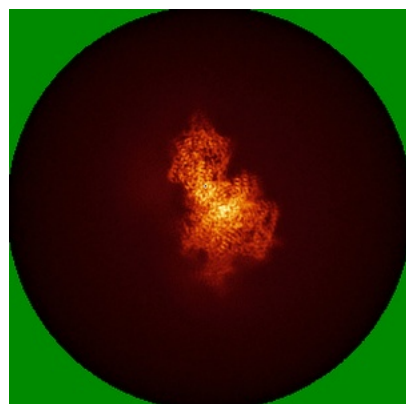


Y



Z

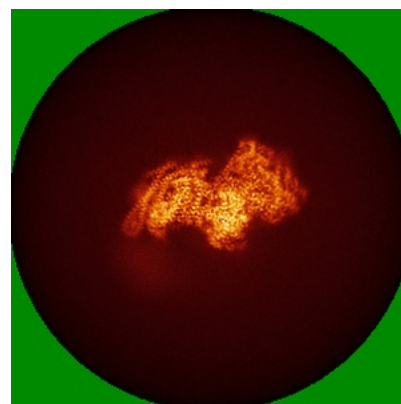
6.4.2 Raw map



X



Y

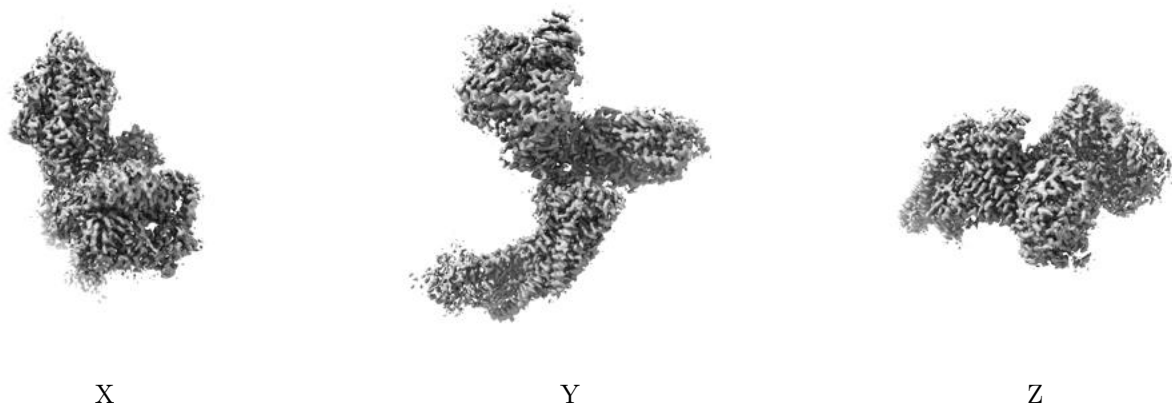


Z

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.

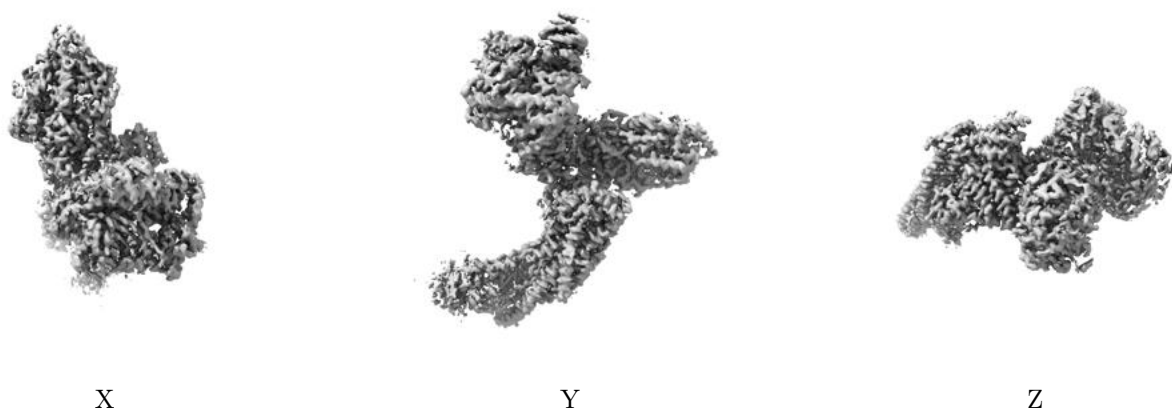
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. 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.

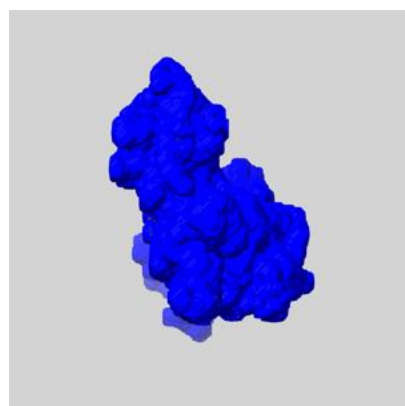
6.6 Mask visualisation [i](#)

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

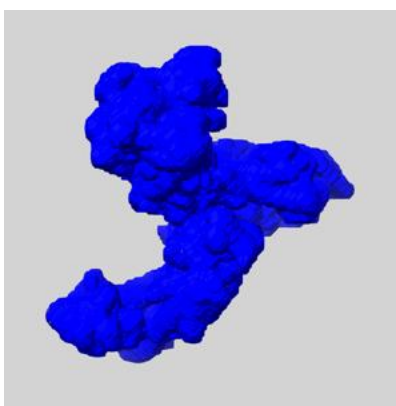
A mask typically either:

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

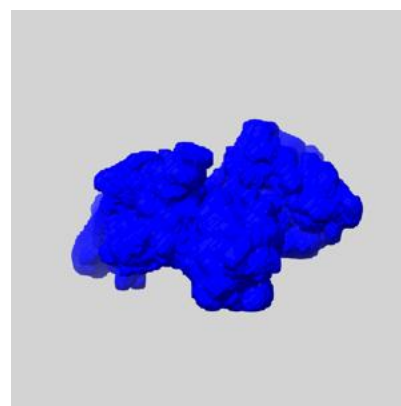
6.6.1 emd_21107_msk_1.map [i](#)



X



Y

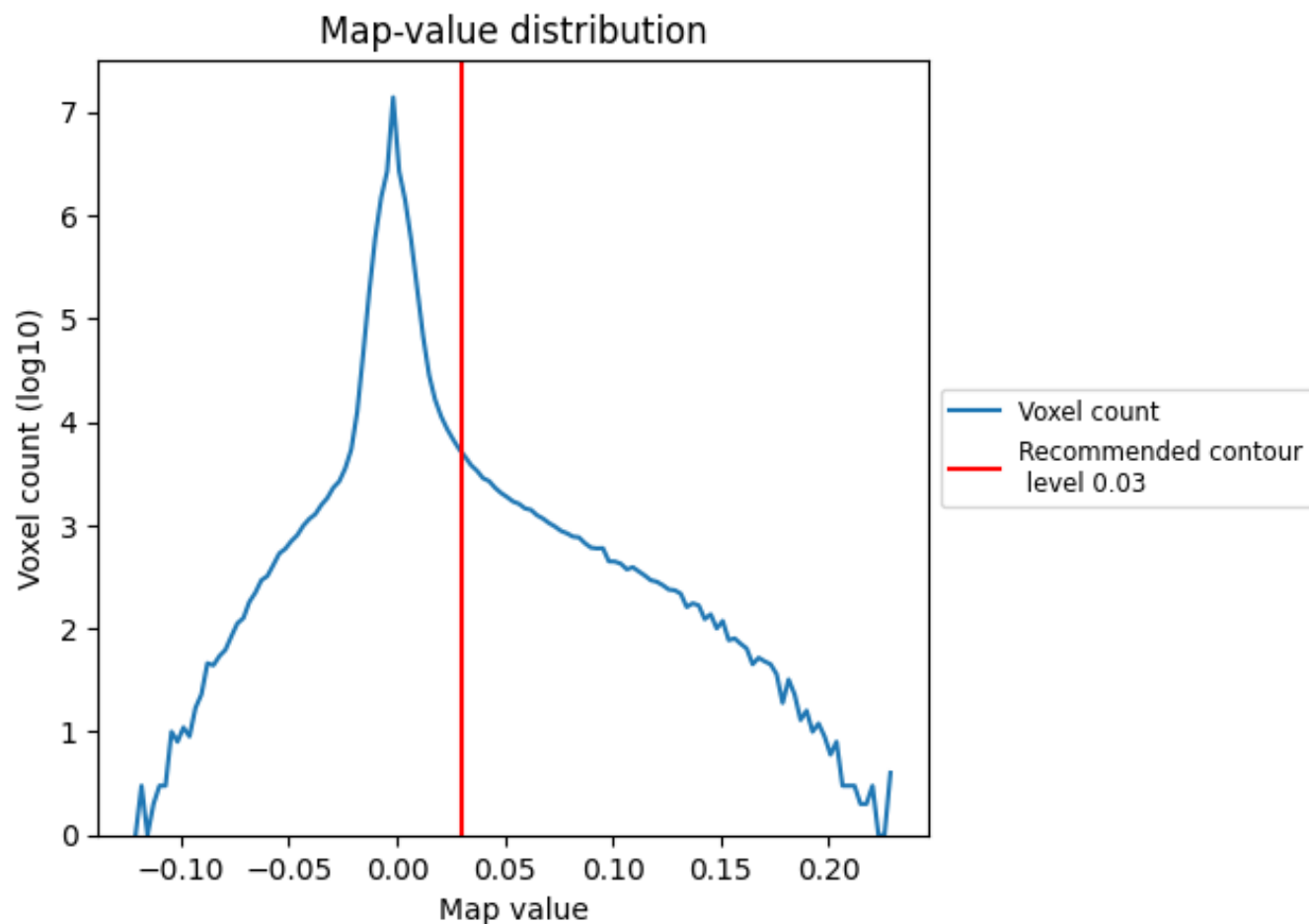


Z

7 Map analysis [i](#)

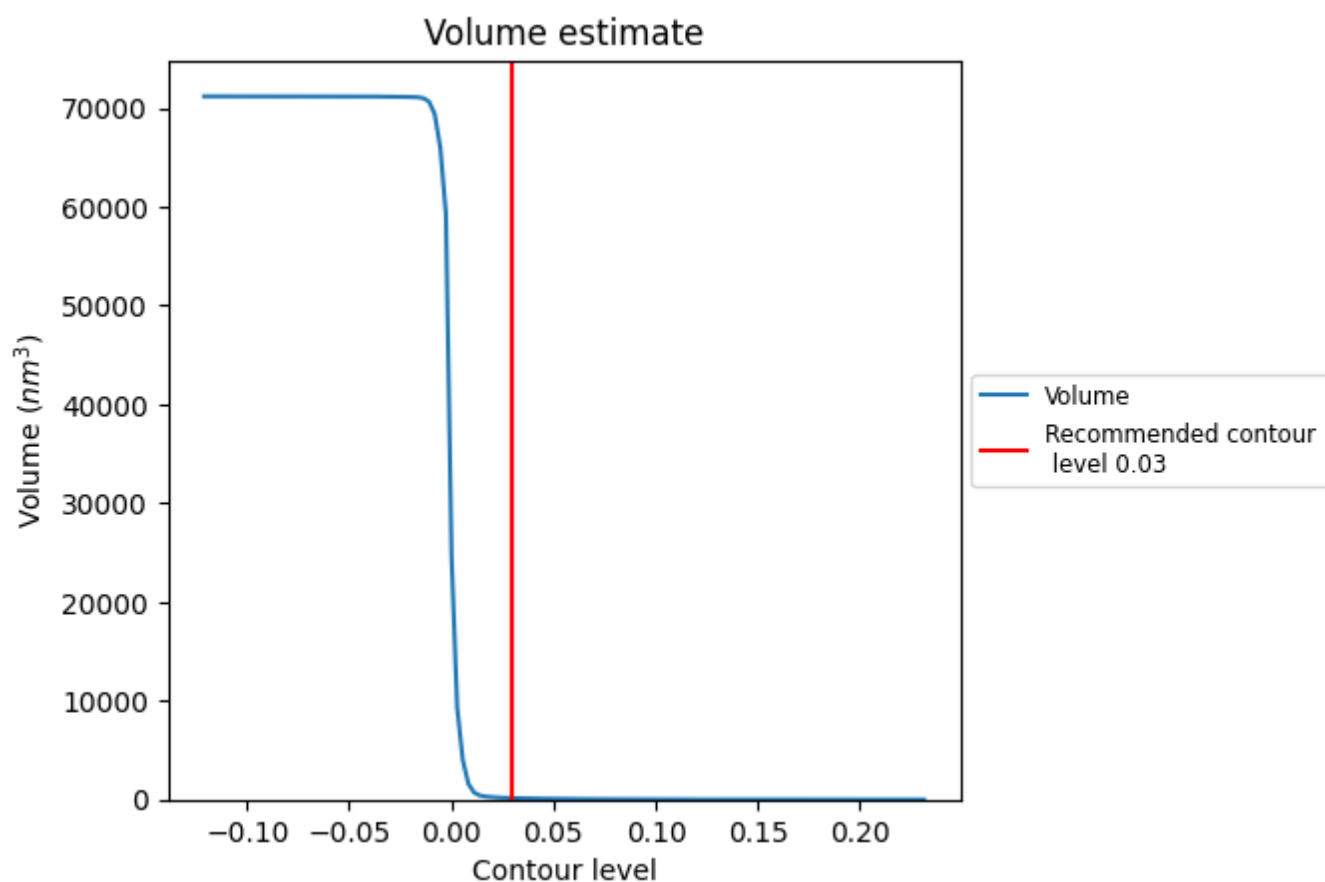
This section contains the results of statistical analysis of the map.

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.

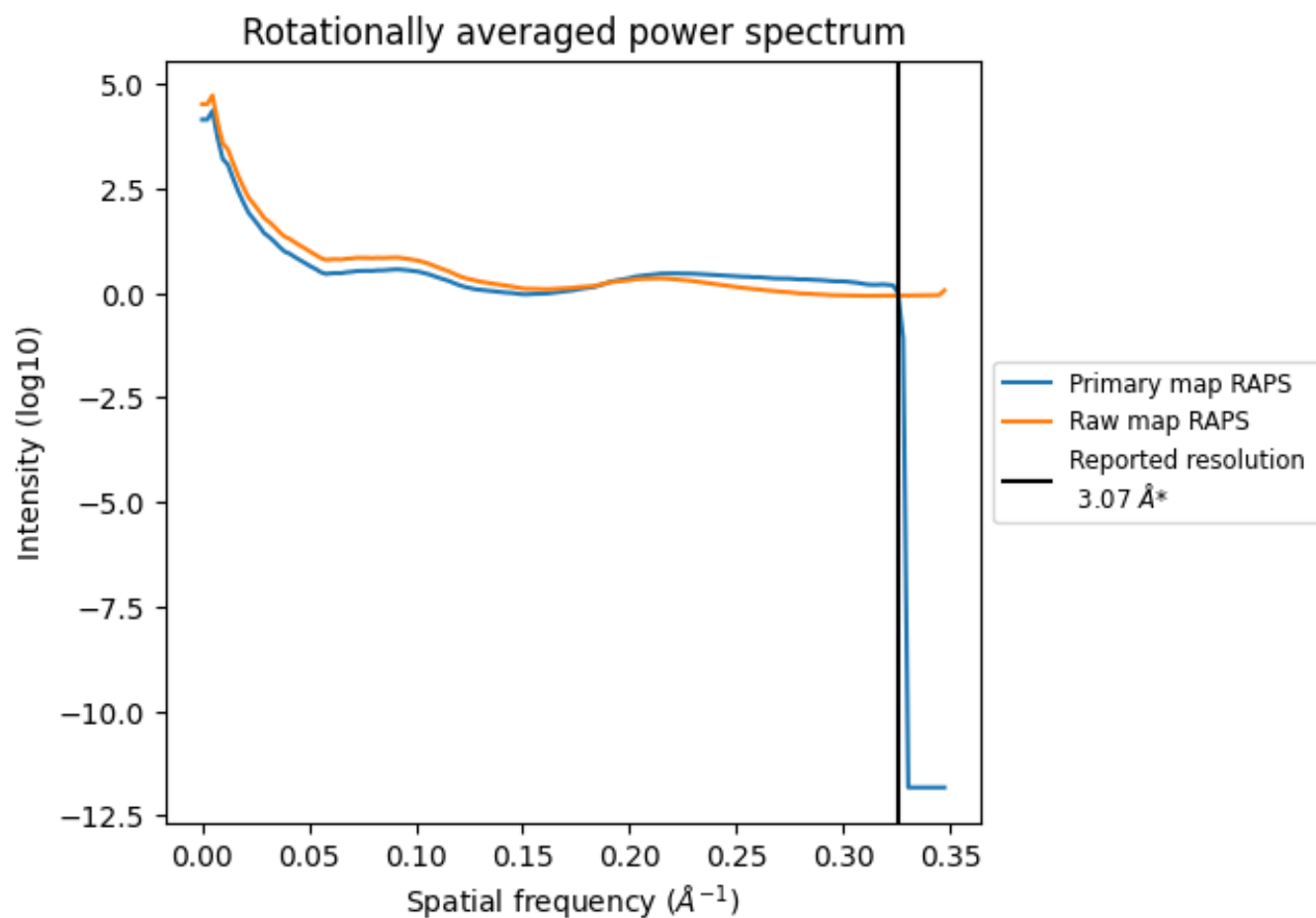
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 146 nm³; this corresponds to an approximate mass of 132 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 ⓘ

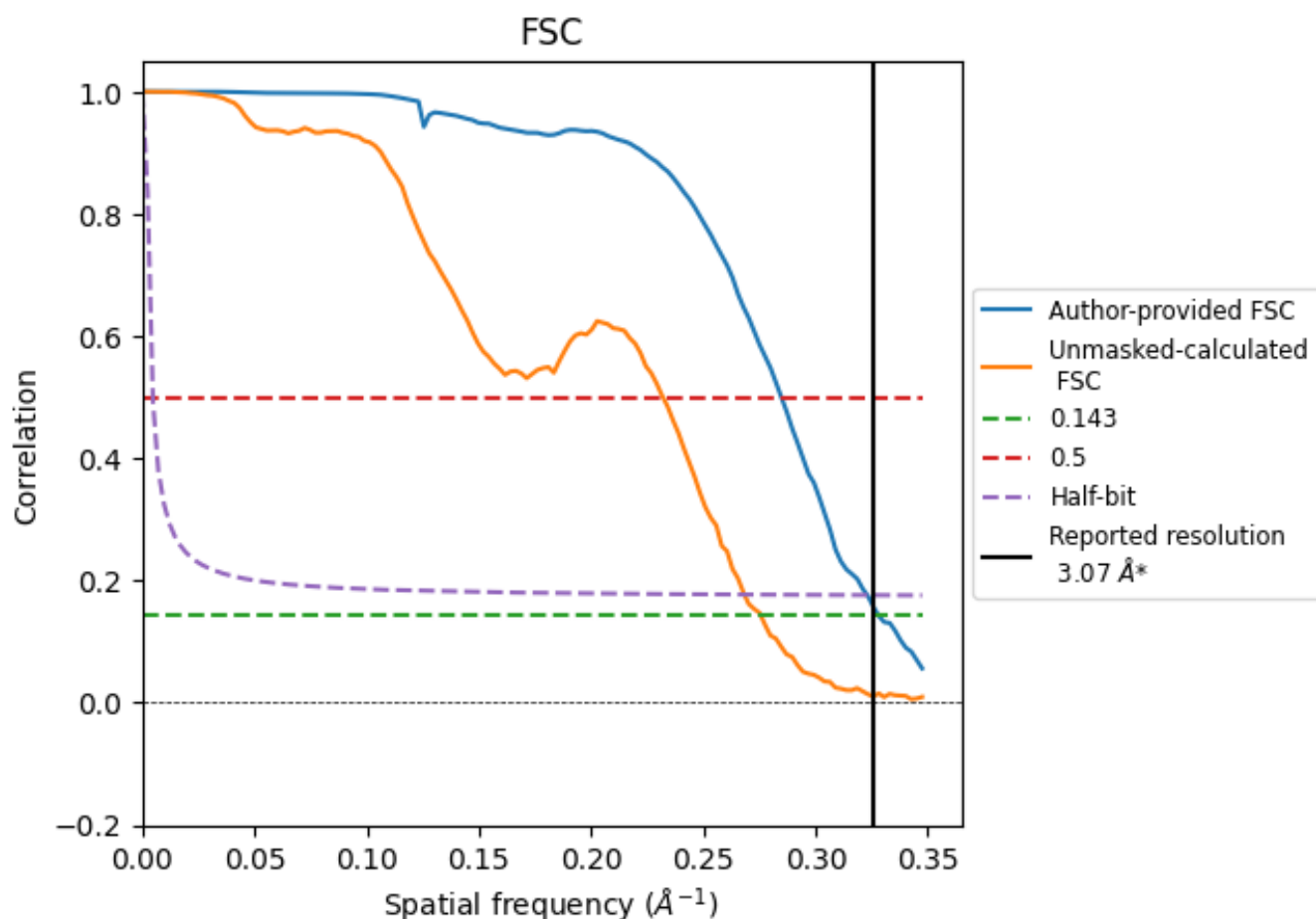


*Reported resolution corresponds to spatial frequency of 0.326 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.326 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.07	-	-
Author-provided FSC curve	3.05	3.51	3.10
Unmasked-calculated*	3.63	4.31	3.73

*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 3.63 differs from the reported value 3.07 by more than 10 %

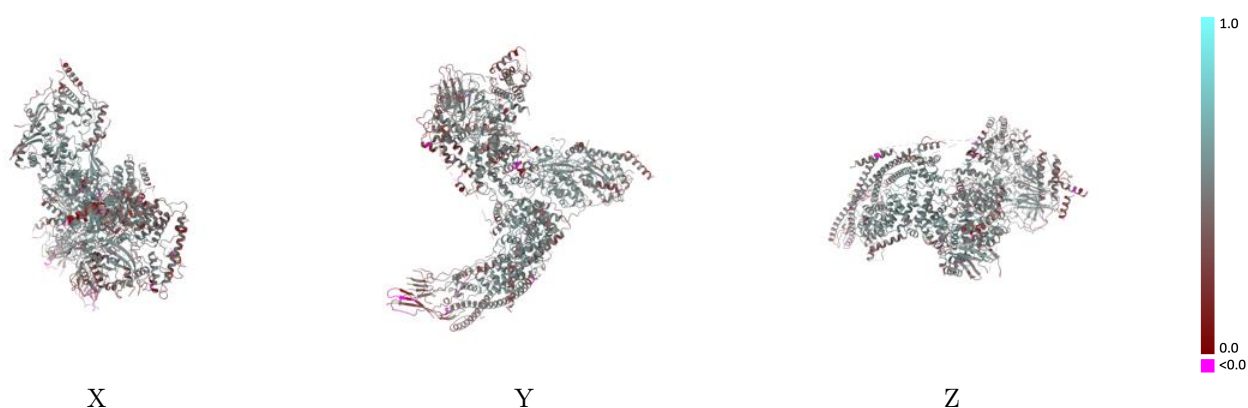
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-21107 and PDB model 6V8O. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)

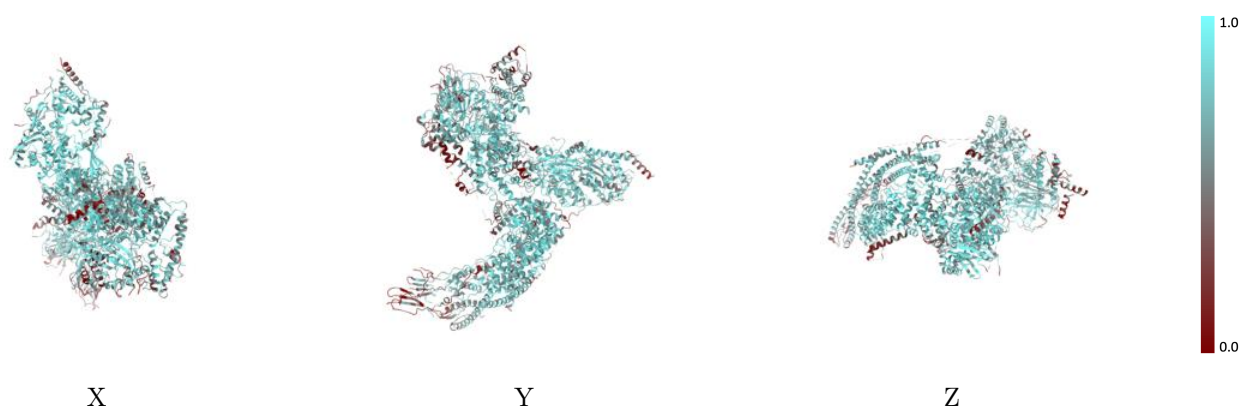
This section was not generated.

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



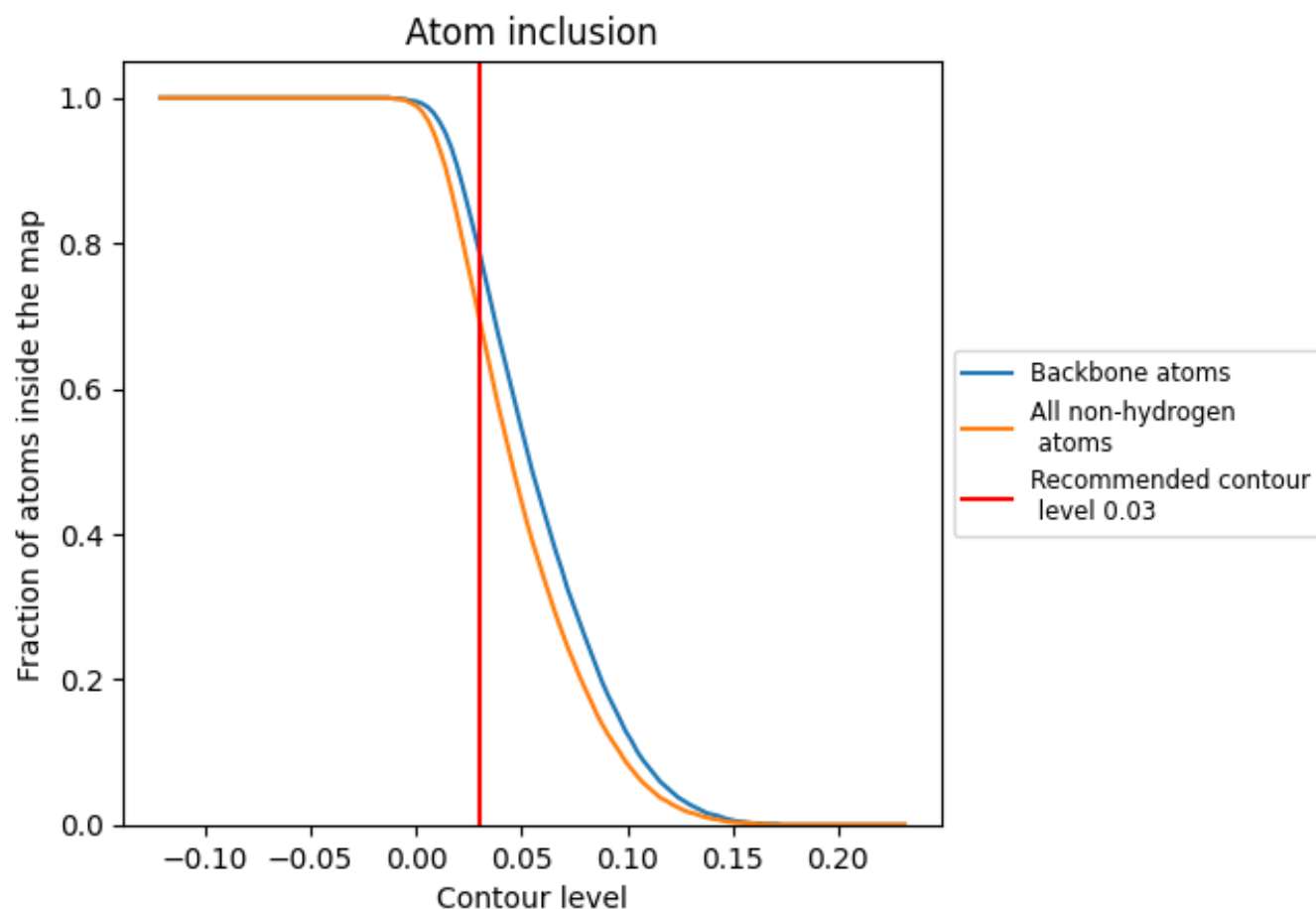
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6970	 0.4610
2	 0.7290	 0.4070
3	 0.3370	 0.3100
4	 0.2320	 0.3290
5	 0.0290	 0.3260
6	 0.1330	 0.2050
7	 0.3800	 0.2310
C	 0.7310	 0.4690
D	 0.5730	 0.3970
E	 0.7350	 0.4600
F	 0.6760	 0.4780
G	 0.4860	 0.4360
H	 0.6530	 0.4340
I	 0.8270	 0.5300
J	 0.6490	 0.4340
K	 0.5760	 0.3920
L	 0.6970	 0.4570
M	 0.6470	 0.4410
N	 0.8150	 0.5190
O	 0.7010	 0.4490
Q	 0.7220	 0.4640
R	 0.6910	 0.4630
S	 0.5180	 0.4750

