



wwPDB EM Validation Summary Report ⓘ

Jul 9, 2025 – 02:09 pm BST

PDB ID : 9HVQ / pdb_00009hvq
EMDB ID : EMD-52443
Title : Structure of the transcribing Pol II-DSIF-PAF-SPT6-RECQL5 complex
Authors : Zhang, L.; Zhang, S.
Deposited on : 2024-12-31
Resolution : 2.00 Å(reported)

This is a wwPDB EM Validation Summary 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.dev118
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

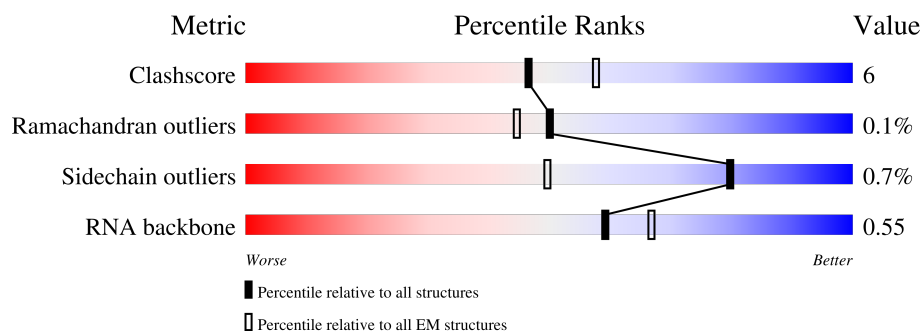
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.00 Å.

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





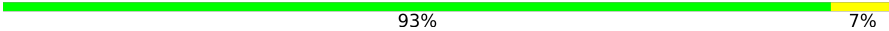



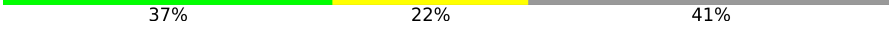




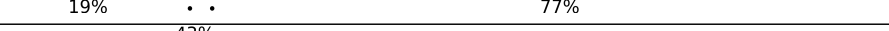
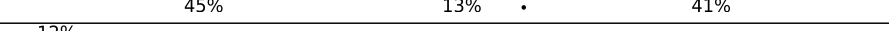




Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	1970	64% 8% 28%
2	B	1174	87% 10% .
3	C	275	87% 8% 5%
4	D	142	51% 36% . 11%
5	E	210	89% 11%
6	F	127	58% 6% 35%
7	G	172	60% 38% ..

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Mol	Chain	Length	Quality of chain
8	H	150	
9	I	125	
10	J	67	
11	K	117	
12	L	58	
13	M	1726	
14	N	63	
15	O	991	
16	P	15	
17	Q	1173	
18	T	48	
19	U	666	
20	V	531	
21	W	305	
22	X	531	
23	Y	117	
24	Z	1087	

2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 63421 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 DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1422	Total	C	N	O	S	0	0
			11266	7084	2018	2093	71		

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1131	Total	C	N	O	S	0	0
			9052	5727	1592	1669	64		

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	260	Total	C	N	O	S	0	0
			2089	1309	359	415	6		

- Molecule 4 is a protein called RNA polymerase II subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	126	Total	C	N	O	S	0	0
			1030	642	175	209	4		

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	209	Total	C	N	O	S	0	0
			1720	1089	300	323	8		

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	82	Total	C	N	O	S	0	0
			657	418	113	121	5		

- Molecule 7 is a protein called DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1351	875	219	249	8		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	148	Total	C	N	O	S	0	0
			1186	750	194	237	5		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	117	Total	C	N	O	S	0	0
			949	587	169	182	11		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	67	Total	C	N	O	S	0	0
			533	345	90	92	6		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11-a.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	115	Total	C	N	O	S	0	0
			920	593	152	173	2		

- Molecule 12 is a protein called RNA polymerase II, I and III subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	46	Total	C	N	O	S	0	0
			388	241	75	66	6		

- Molecule 13 is a protein called Transcription elongation factor SPT6.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	1120	Total	C	N	O	S	0	0
			9177	5819	1591	1725	42		

- Molecule 14 is a DNA chain called Non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	37	Total	C	N	O	P	0	0
			769	361	149	222	37		

- Molecule 15 is a protein called ATP-dependent DNA helicase Q5.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	119	Total	C	N	O	S	0	0
			969	599	186	181	3		

- Molecule 16 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	12	Total	C	N	O	P	0	0
			257	115	49	81	12		

- Molecule 17 is a protein called RNA polymerase-associated protein CTR9 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	890	Total	C	N	O	S	0	0
			7222	4574	1264	1352	32		

- Molecule 18 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	37	Total	C	N	O	P	0	0
			749	355	128	229	37		

- Molecule 19 is a protein called RNA polymerase-associated protein LEO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	154	Total	C	N	O	S	0	0
			1257	788	219	247	3		

- Molecule 20 is a protein called RNA polymerase II-associated factor 1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	311	Total	C	N	O	S	0	0
			2569	1624	435	497	13		

- Molecule 21 is a protein called WD repeat-containing protein 61.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	305	Total	C	N	O	S	0	0
			2373	1507	399	462	5		

- Molecule 22 is a protein called Parafibromin.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	X	229	Total	C	N	O	S	0	0
			1892	1213	342	332	5		

- Molecule 23 is a protein called Transcription elongation factor SPT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Y	115	Total	C	N	O	S	0	0
			906	567	158	172	9		

- Molecule 24 is a protein called Transcription elongation factor SPT5.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Z	515	Total	C	N	O	S	0	0
			4131	2626	731	756	18		

- Molecule 25 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
25	A	2	Total	Zn	0
			2	2	
25	B	1	Total	Zn	0
			1	1	
25	C	1	Total	Zn	0
			1	1	
25	I	2	Total	Zn	0
			2	2	
25	J	1	Total	Zn	0
			1	1	
25	L	1	Total	Zn	0
			1	1	

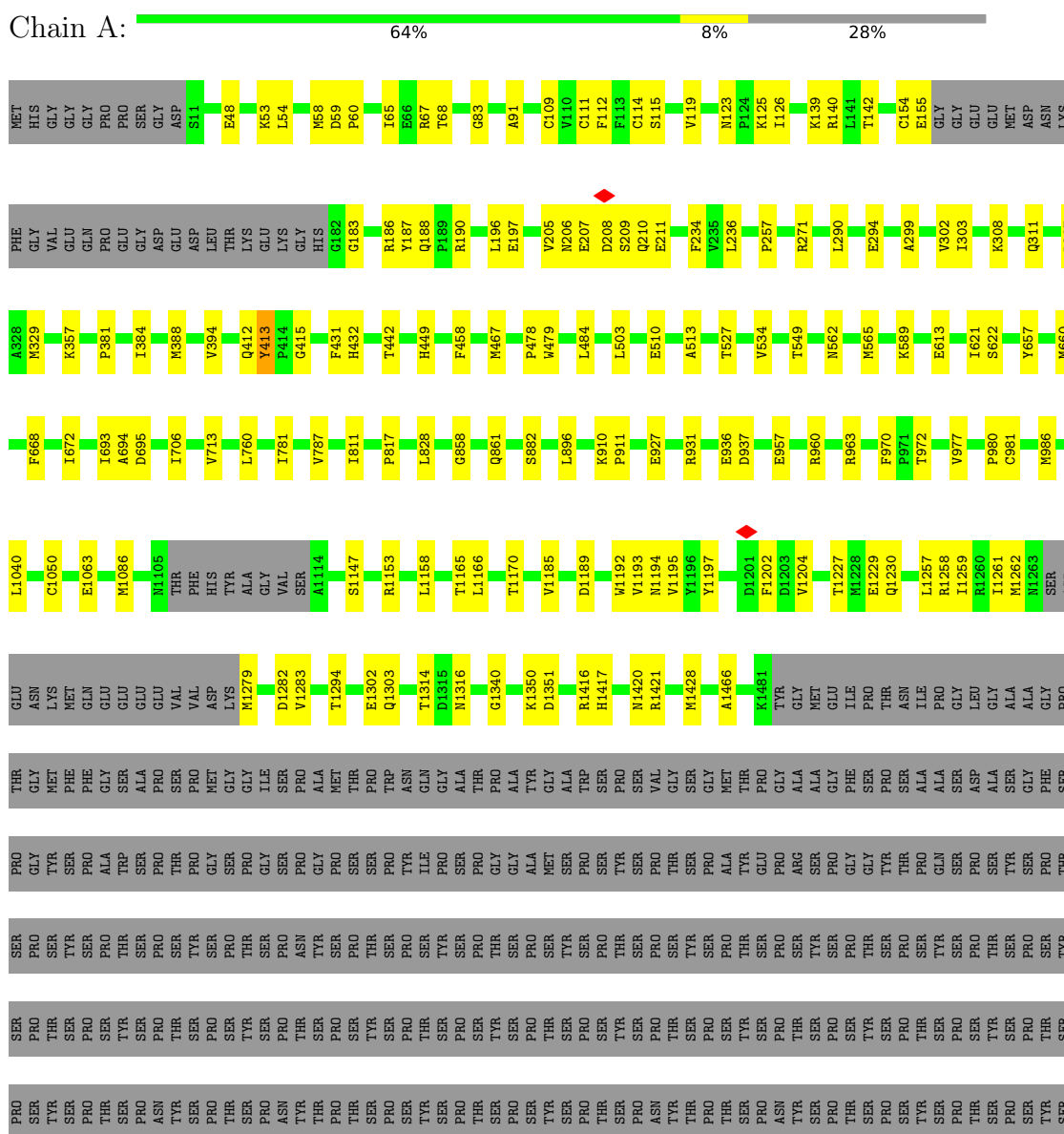
- Molecule 26 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
26	A	1	Total	Mg	0
			1	1	

3 Residue-property plots

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

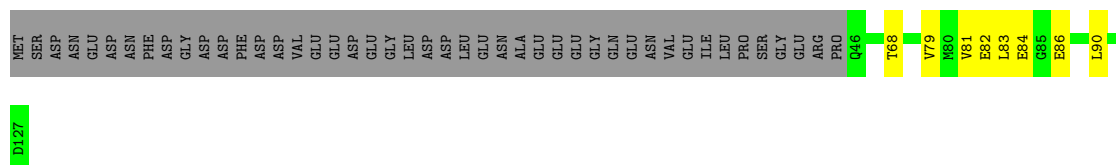
• Molecule 1: DNA-directed RNA polymerase subunit





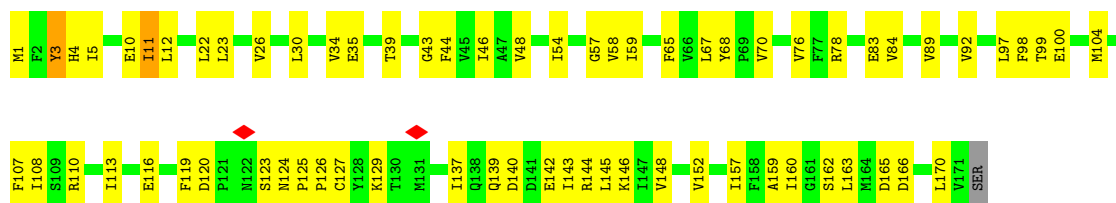
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F: 58% 6% 35%



- Molecule 7: DNA-directed RNA polymerase subunit

Chain G: 60% 38%



- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H: 87% 11%



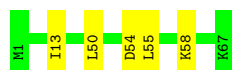
- Molecule 9: DNA-directed RNA polymerase II subunit RPB9

Chain I: 74% 18% 6%



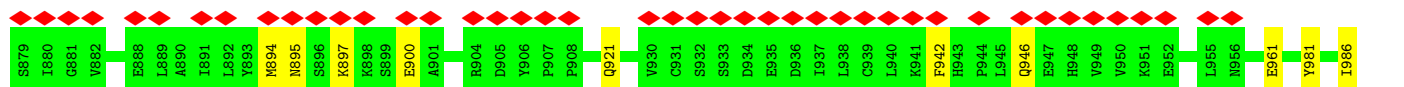
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J: 93% 7%



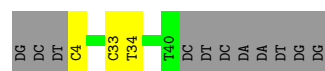
- Molecule 11: DNA-directed RNA polymerase II subunit RPB11-a

Chain K: 85% 14%

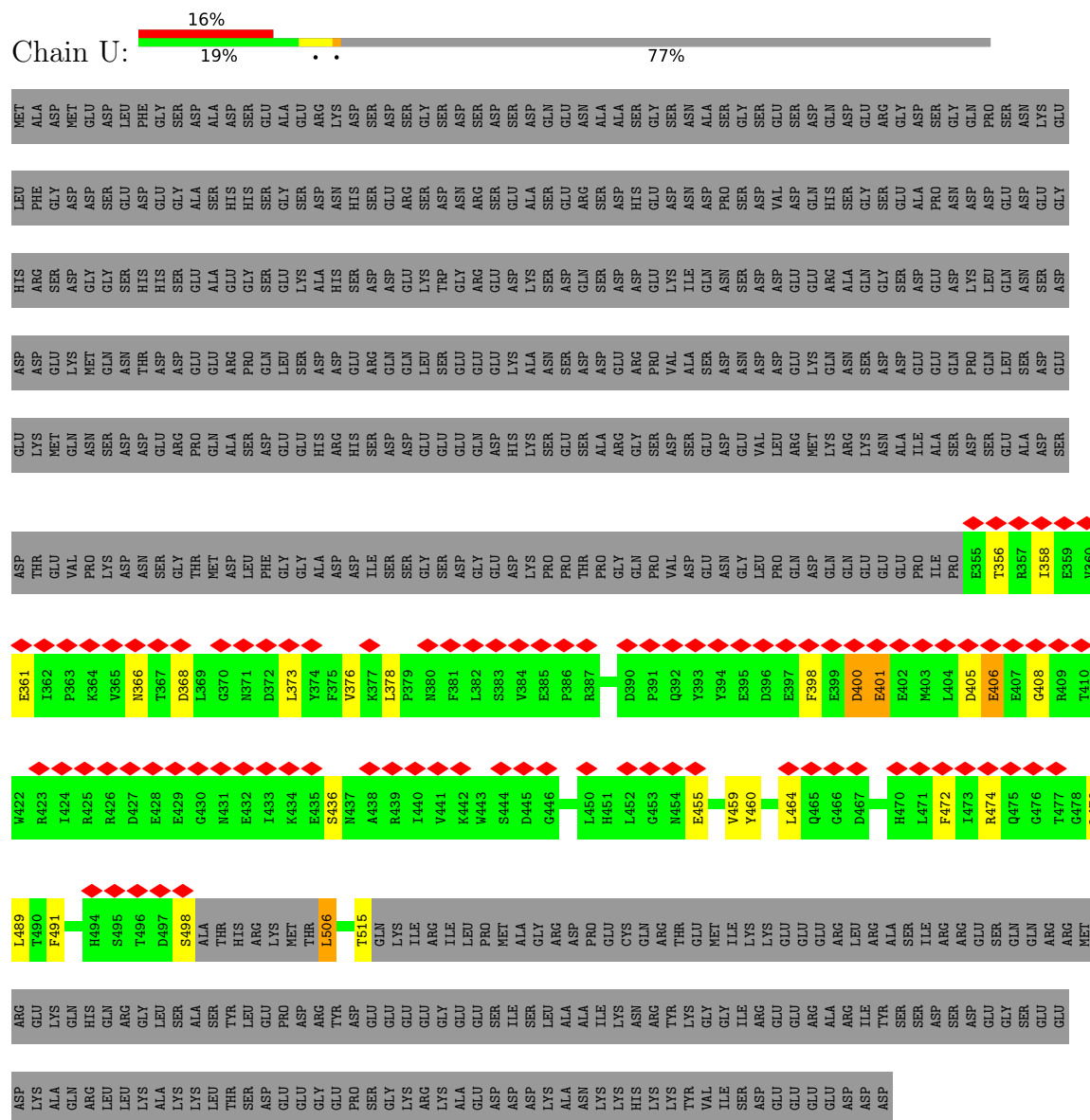




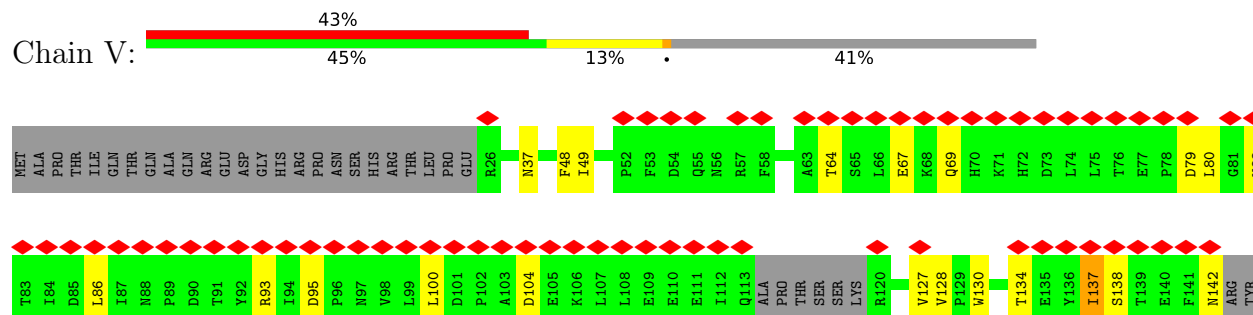


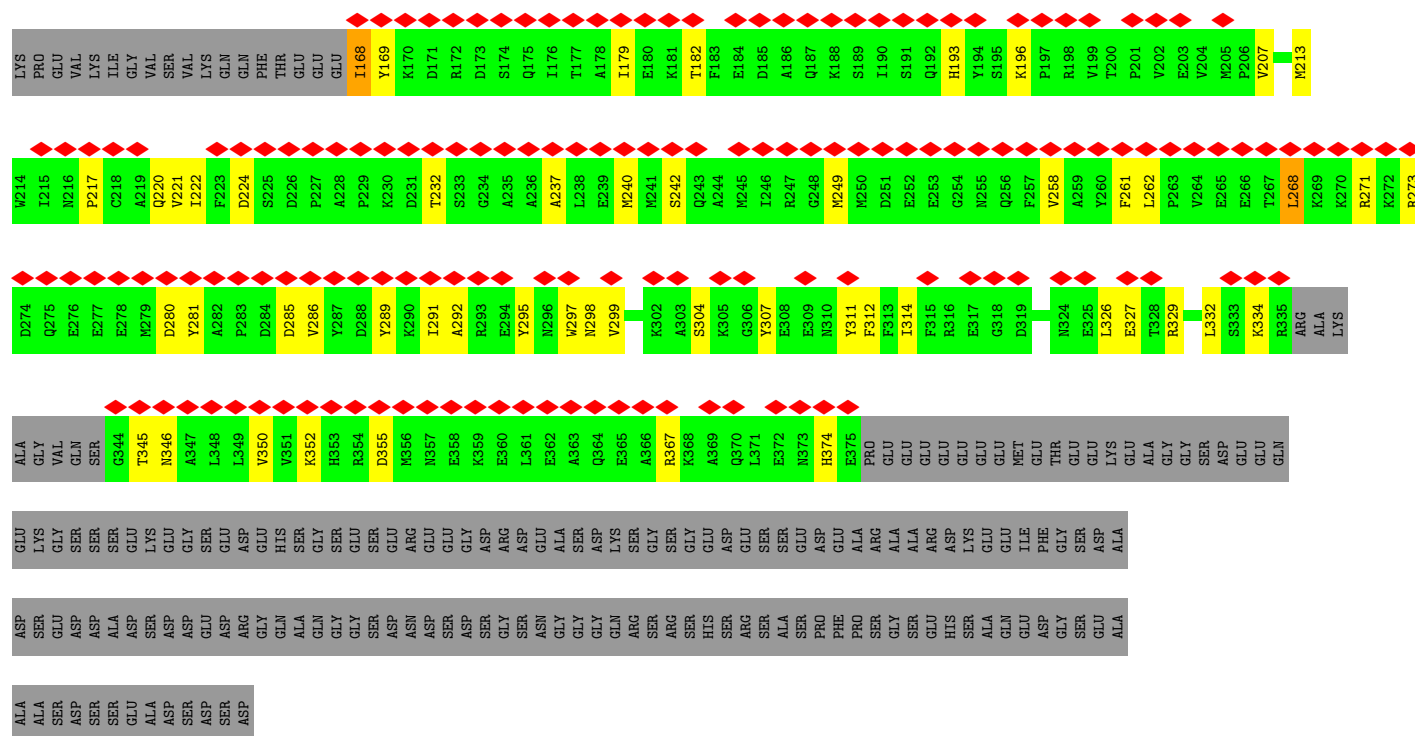


• Molecule 19: RNA polymerase-associated protein LEO1

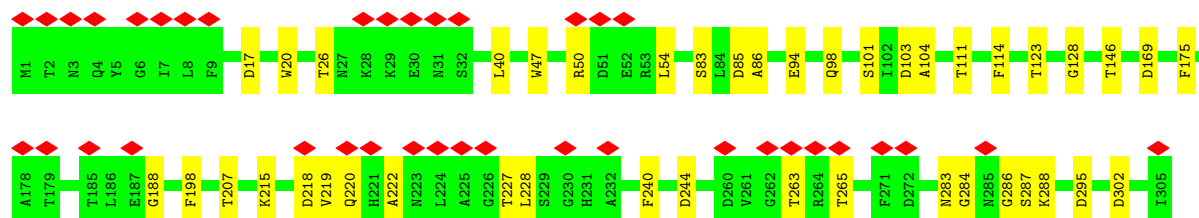
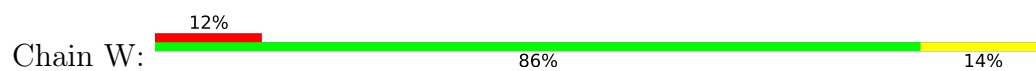


• Molecule 20: RNA polymerase II-associated factor 1 homolog

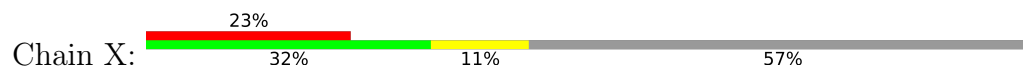


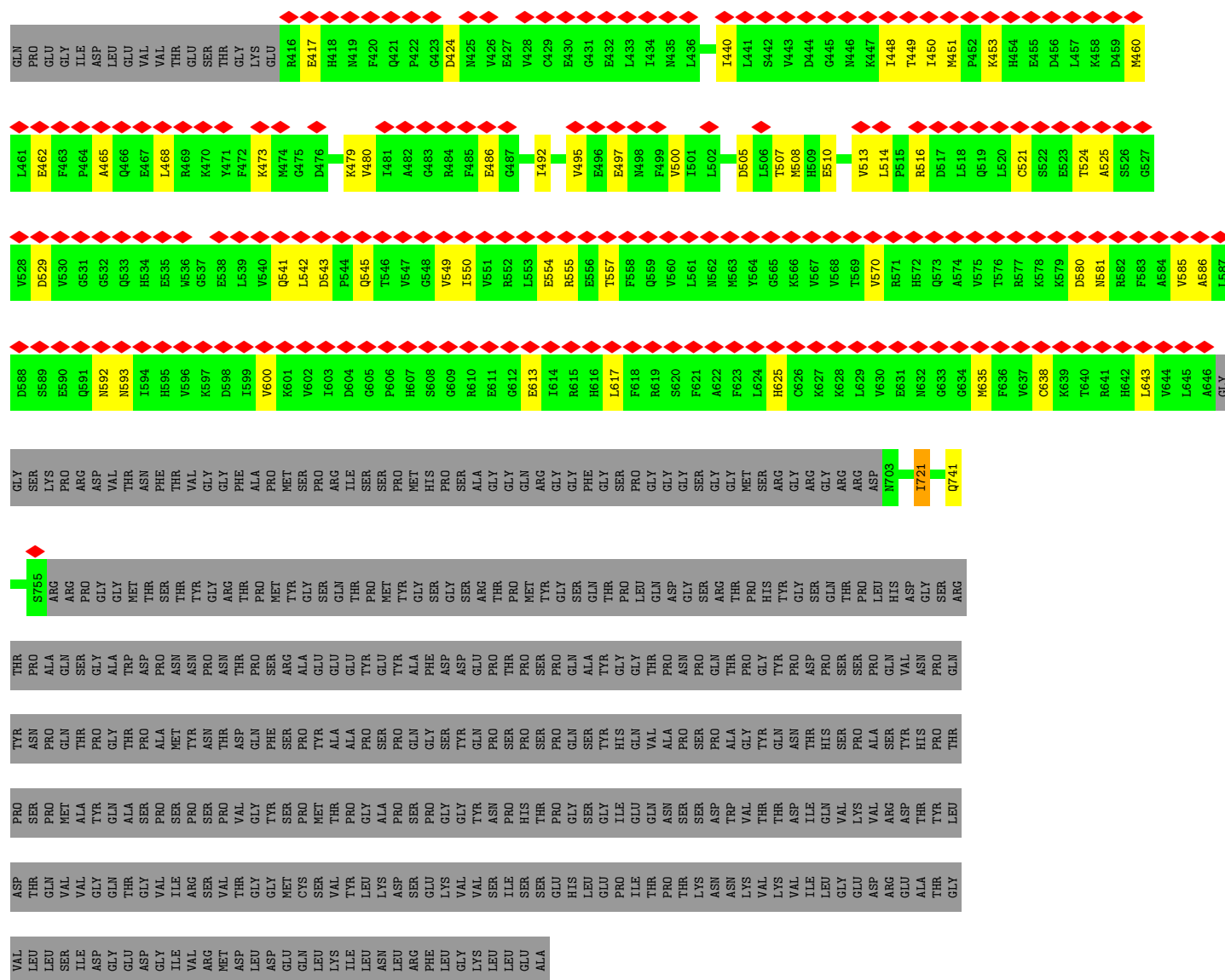


• Molecule 21: WD repeat-containing protein 61



• Molecule 22: Parafibromin





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	66771	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.067	Depositor
Minimum map value	-0.029	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.002	Depositor
Map size (Å)	391.48798, 391.48798, 391.48798	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8156, 0.8156, 0.8156	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	A	0.33	0/11471	0.41	0/15487
2	B	0.34	0/9233	0.40	0/12463
3	C	0.37	0/2132	0.41	0/2896
4	D	0.19	0/1043	0.63	0/1400
5	E	0.30	0/1751	0.33	0/2366
6	F	0.35	0/667	0.39	0/901
7	G	0.26	0/1382	0.59	0/1874
8	H	0.37	0/1207	0.36	0/1628
9	I	0.25	0/972	0.33	0/1316
10	J	0.37	0/542	0.45	0/730
11	K	0.38	0/939	0.40	0/1271
12	L	0.33	0/394	0.43	0/524
13	M	0.07	0/9369	0.21	1/12642 (0.0%)
14	N	0.21	0/864	0.43	0/1334
15	O	0.11	0/984	0.22	0/1319
16	P	0.37	0/287	0.37	0/445
17	Q	0.10	0/7360	0.27	0/9919
18	T	0.37	0/835	0.47	0/1285
19	U	0.14	0/1282	0.42	0/1730
20	V	0.11	0/2625	0.32	0/3543
21	W	0.09	0/2432	0.27	0/3311
22	X	0.12	0/1937	0.35	0/2621
23	Y	0.06	0/922	0.20	0/1243
24	Z	0.10	0/4205	0.23	0/5659
All	All	0.25	0/64835	0.35	1/87907 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
20	V	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	1052	VAL	CG1-CB-CG2	5.03	121.86	110.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
20	V	168	ILE	Peptide

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	11266	0	11398	108	0
2	B	9052	0	9087	83	0
3	C	2089	0	2031	18	0
4	D	1030	0	1016	55	0
5	E	1720	0	1737	17	0
6	F	657	0	684	7	0
7	G	1351	0	1358	63	0
8	H	1186	0	1147	11	0
9	I	949	0	879	17	0
10	J	533	0	553	6	0
11	K	920	0	942	12	0
12	L	388	0	393	8	0
13	M	9177	0	9059	67	0
14	N	769	0	414	13	0
15	O	969	0	982	15	0
16	P	257	0	131	6	0
17	Q	7222	0	7170	113	0
18	T	749	0	417	2	0
19	U	1257	0	1206	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	V	2569	0	2488	59	0
21	W	2373	0	2290	26	0
22	X	1892	0	1929	47	0
23	Y	906	0	900	6	0
24	Z	4131	0	4206	53	0
25	A	2	0	0	0	0
25	B	1	0	0	0	0
25	C	1	0	0	0	0
25	I	2	0	0	0	0
25	J	1	0	0	0	0
25	L	1	0	0	0	0
26	A	1	0	0	0	0
All	All	63421	0	62417	742	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.

The worst 5 of 742 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)
7:G:120:ASP:OD2	7:G:129:LYS:NZ	2.04	0.91
2:B:649:ASN:O	19:U:460:TYR:OH	1.87	0.90
2:B:756:LYS:NZ	20:V:134:THR:OG1	2.04	0.89
21:W:98:GLN:OE1	21:W:101:SER:OG	1.93	0.86
20:V:273:ARG:NH2	20:V:285:ASP:OD2	2.09	0.86

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	1414/1970 (72%)	1370 (97%)	44 (3%)	0	100	100
2	B	1123/1174 (96%)	1072 (96%)	51 (4%)	0	100	100
3	C	256/275 (93%)	249 (97%)	7 (3%)	0	100	100
4	D	124/142 (87%)	123 (99%)	1 (1%)	0	100	100
5	E	207/210 (99%)	201 (97%)	6 (3%)	0	100	100
6	F	80/127 (63%)	76 (95%)	4 (5%)	0	100	100
7	G	169/172 (98%)	163 (96%)	6 (4%)	0	100	100
8	H	146/150 (97%)	143 (98%)	3 (2%)	0	100	100
9	I	115/125 (92%)	109 (95%)	6 (5%)	0	100	100
10	J	65/67 (97%)	64 (98%)	1 (2%)	0	100	100
11	K	113/117 (97%)	109 (96%)	4 (4%)	0	100	100
12	L	44/58 (76%)	39 (89%)	5 (11%)	0	100	100
13	M	1106/1726 (64%)	1093 (99%)	13 (1%)	0	100	100
15	O	117/991 (12%)	113 (97%)	4 (3%)	0	100	100
17	Q	888/1173 (76%)	880 (99%)	8 (1%)	0	100	100
19	U	150/666 (22%)	140 (93%)	7 (5%)	3 (2%)	6	2
20	V	303/531 (57%)	292 (96%)	9 (3%)	2 (1%)	19	14
21	W	303/305 (99%)	289 (95%)	14 (5%)	0	100	100
22	X	225/531 (42%)	217 (96%)	8 (4%)	0	100	100
23	Y	113/117 (97%)	112 (99%)	1 (1%)	0	100	100
24	Z	507/1087 (47%)	502 (99%)	5 (1%)	0	100	100
All	All	7568/11714 (65%)	7356 (97%)	207 (3%)	5 (0%)	50	47

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
19	U	400	ASP
19	U	406	GLU
20	V	374	HIS
20	V	346	ASN
19	U	401	GLU

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	1253/1749 (72%)	1249 (100%)	4 (0%)	91	94
2	B	992/1027 (97%)	985 (99%)	7 (1%)	81	86
3	C	237/252 (94%)	237 (100%)	0	100	100
4	D	116/126 (92%)	112 (97%)	4 (3%)	32	32
5	E	191/192 (100%)	191 (100%)	0	100	100
6	F	71/111 (64%)	71 (100%)	0	100	100
7	G	152/153 (99%)	148 (97%)	4 (3%)	41	44
8	H	129/131 (98%)	128 (99%)	1 (1%)	79	84
9	I	105/112 (94%)	104 (99%)	1 (1%)	73	78
10	J	56/56 (100%)	55 (98%)	1 (2%)	54	59
11	K	104/106 (98%)	104 (100%)	0	100	100
12	L	43/55 (78%)	43 (100%)	0	100	100
13	M	993/1522 (65%)	991 (100%)	2 (0%)	92	94
15	O	104/820 (13%)	104 (100%)	0	100	100
17	Q	761/1005 (76%)	754 (99%)	7 (1%)	75	81
19	U	139/590 (24%)	135 (97%)	4 (3%)	37	39
20	V	283/462 (61%)	279 (99%)	4 (1%)	62	68
21	W	260/260 (100%)	257 (99%)	3 (1%)	67	73
22	X	209/467 (45%)	205 (98%)	4 (2%)	52	57
23	Y	102/103 (99%)	101 (99%)	1 (1%)	73	78
24	Z	455/940 (48%)	452 (99%)	3 (1%)	81	86
All	All	6755/10239 (66%)	6705 (99%)	50 (1%)	80	86

5 of 50 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	Q	352	ILE
20	V	64	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
24	Z	741	GLN
17	Q	836	GLU
19	U	464	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 64 such sidechains are listed below:

Mol	Chain	Res	Type
20	V	373	ASN
21	W	268	HIS
3	C	108	ASN
2	B	1094	GLN
21	W	285	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
16	P	11/15 (73%)	2 (18%)	2 (18%)

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
16	P	136	G
16	P	138	A

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
16	P	135	G
16	P	137	G

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

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

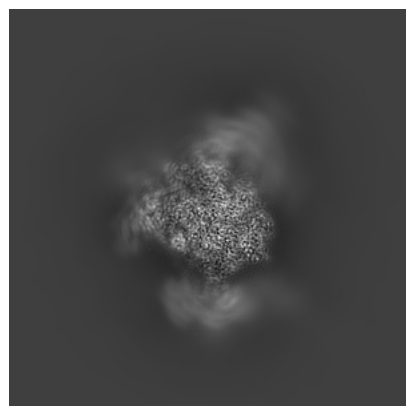
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52443. These allow visual inspection of the internal detail of the map and identification of artifacts.

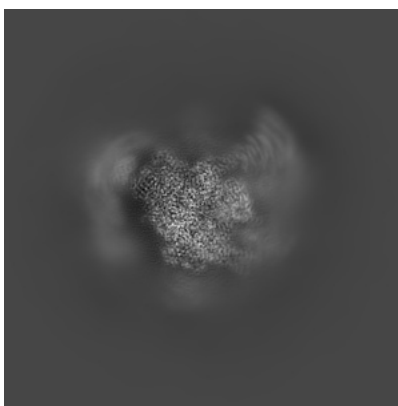
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

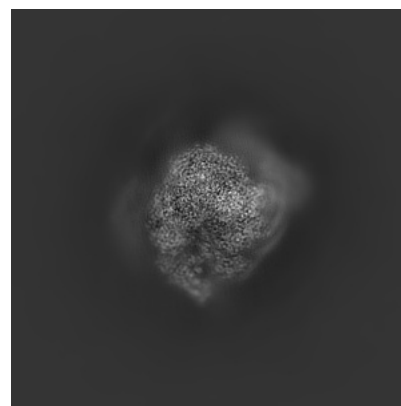
6.1.1 Primary map



X

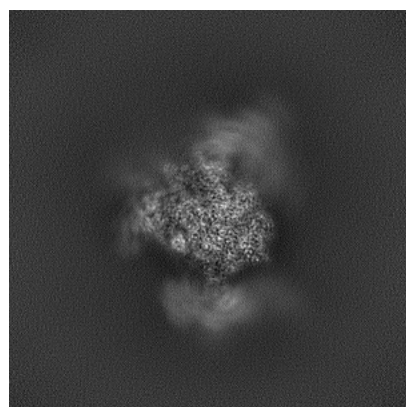


Y

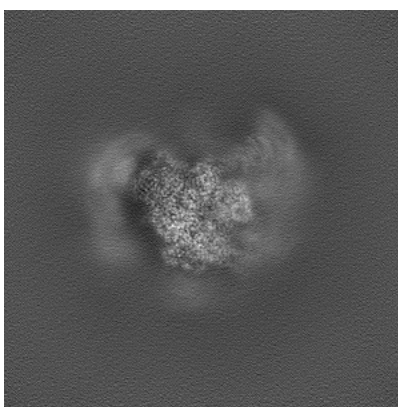


Z

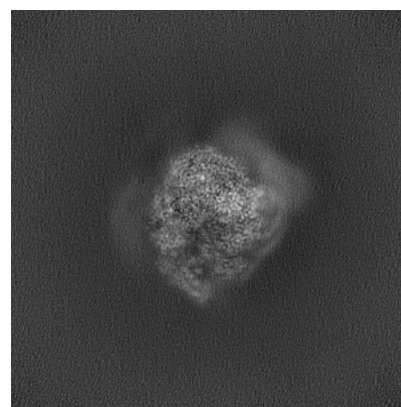
6.1.2 Raw map



X



Y

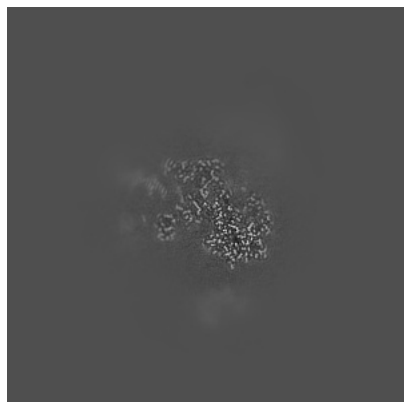


Z

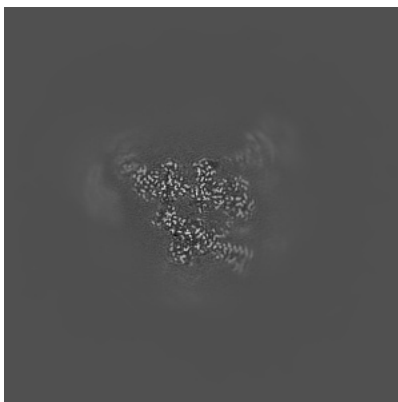
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

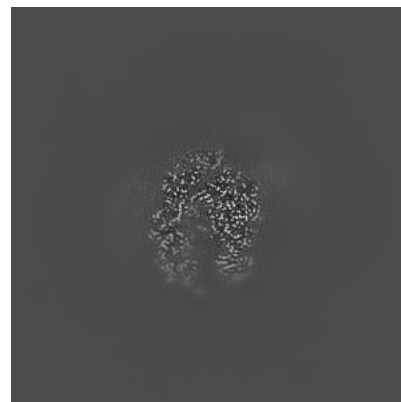
6.2.1 Primary map



X Index: 240

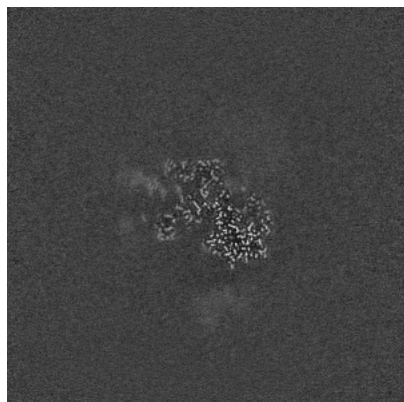


Y Index: 240

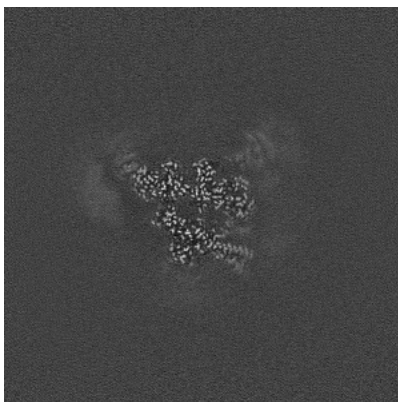


Z Index: 240

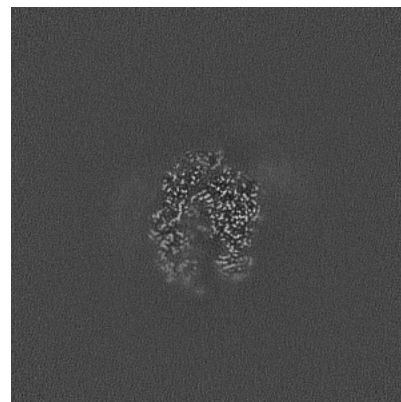
6.2.2 Raw map



X Index: 240



Y Index: 240

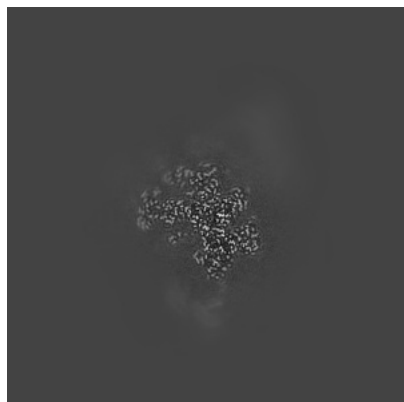


Z Index: 240

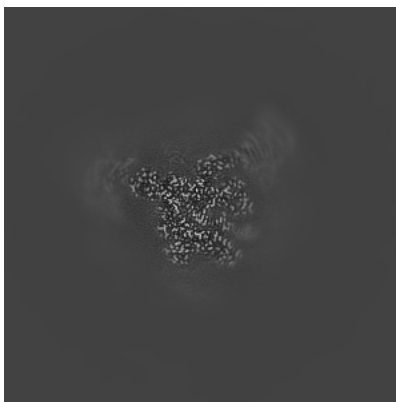
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

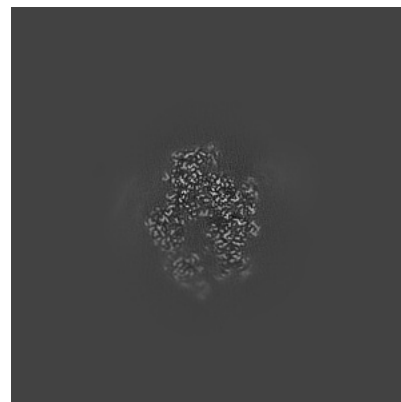
6.3.1 Primary map



X Index: 261

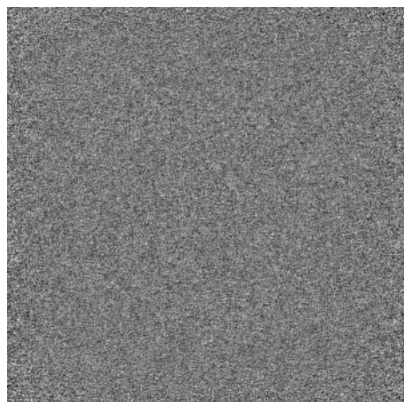


Y Index: 252

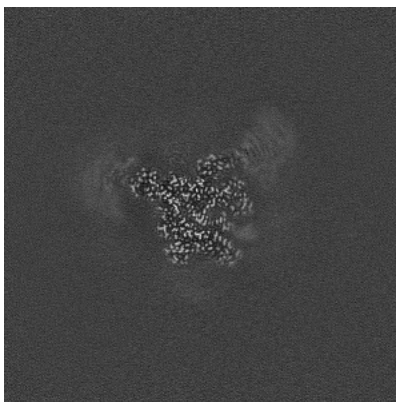


Z Index: 232

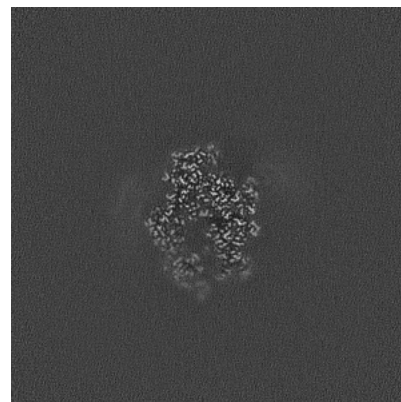
6.3.2 Raw map



X Index: 0



Y Index: 252

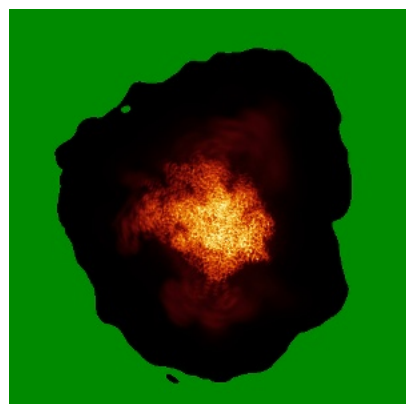


Z Index: 232

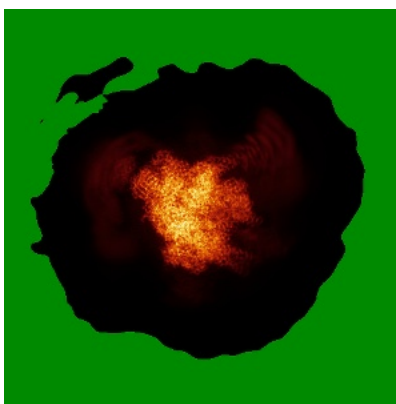
The images above show the largest variance slices of the map in three orthogonal directions.

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

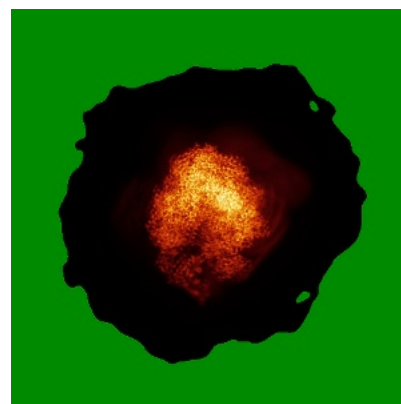
6.4.1 Primary map



X

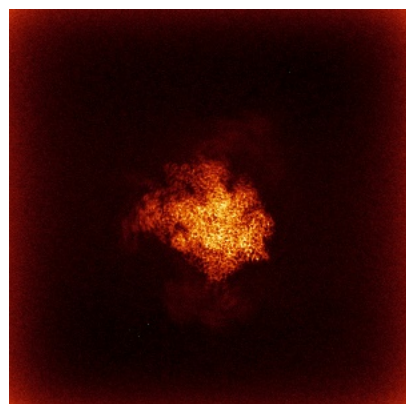


Y

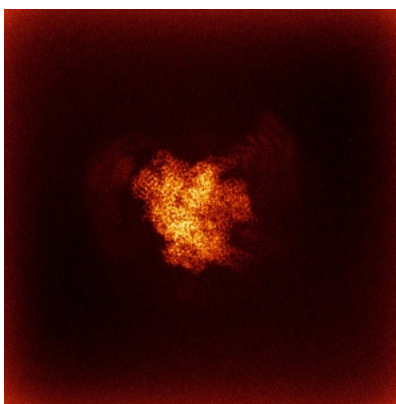


Z

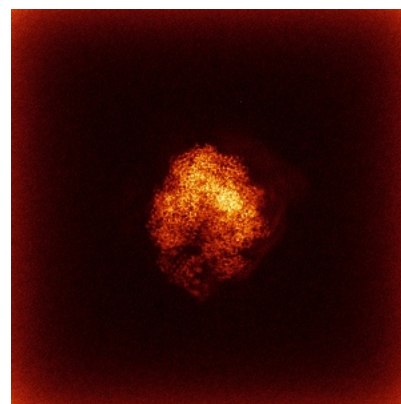
6.4.2 Raw map



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.

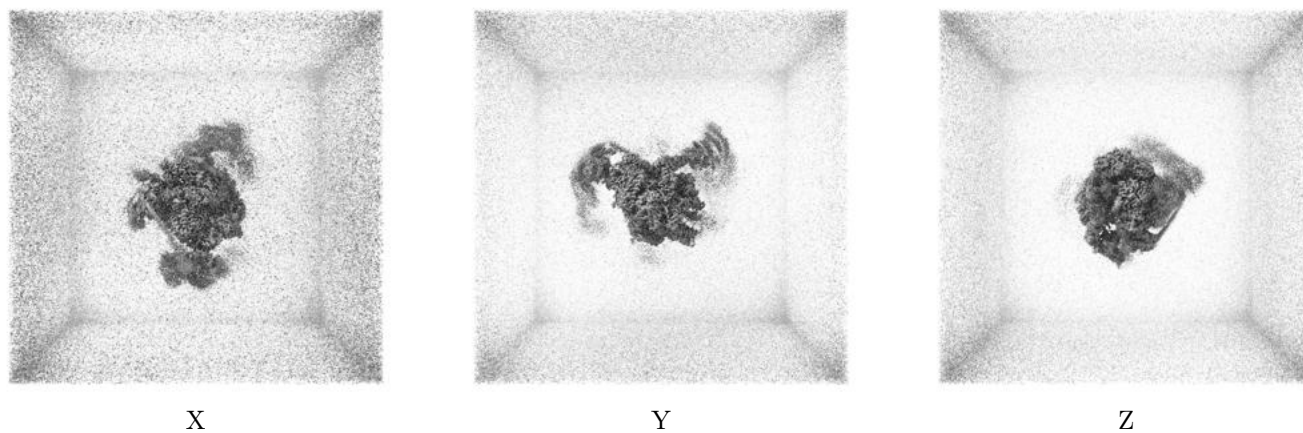
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.002. 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.

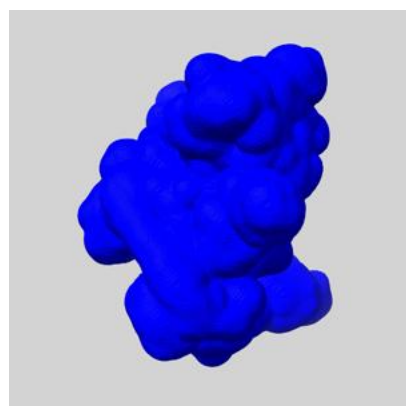
6.6 Mask visualisation [i](#)

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

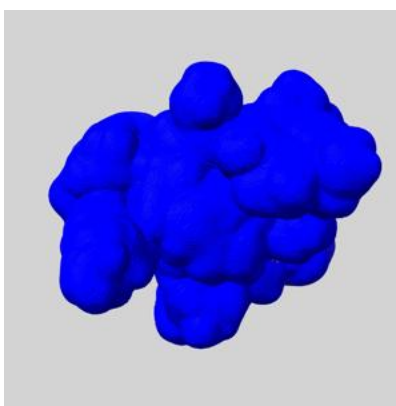
A mask typically either:

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

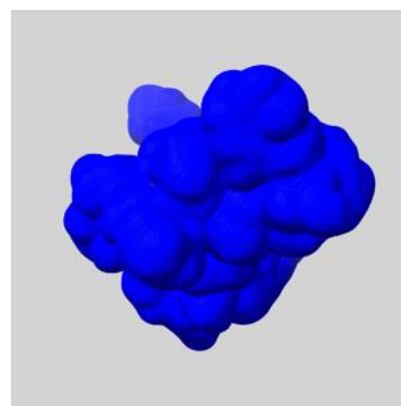
6.6.1 emd_52443_msk_1.map [i](#)



X



Y

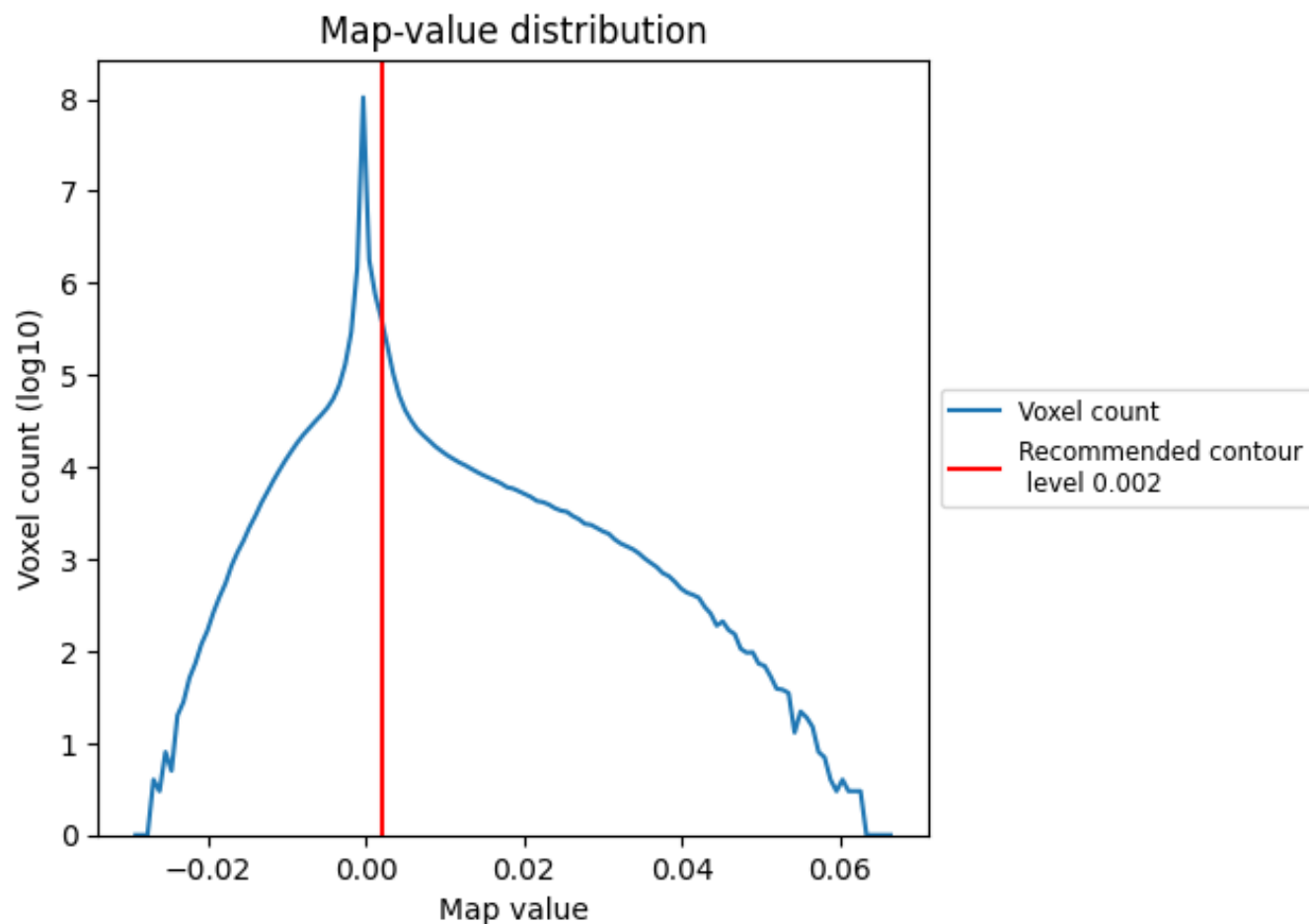


Z

7 Map analysis [i](#)

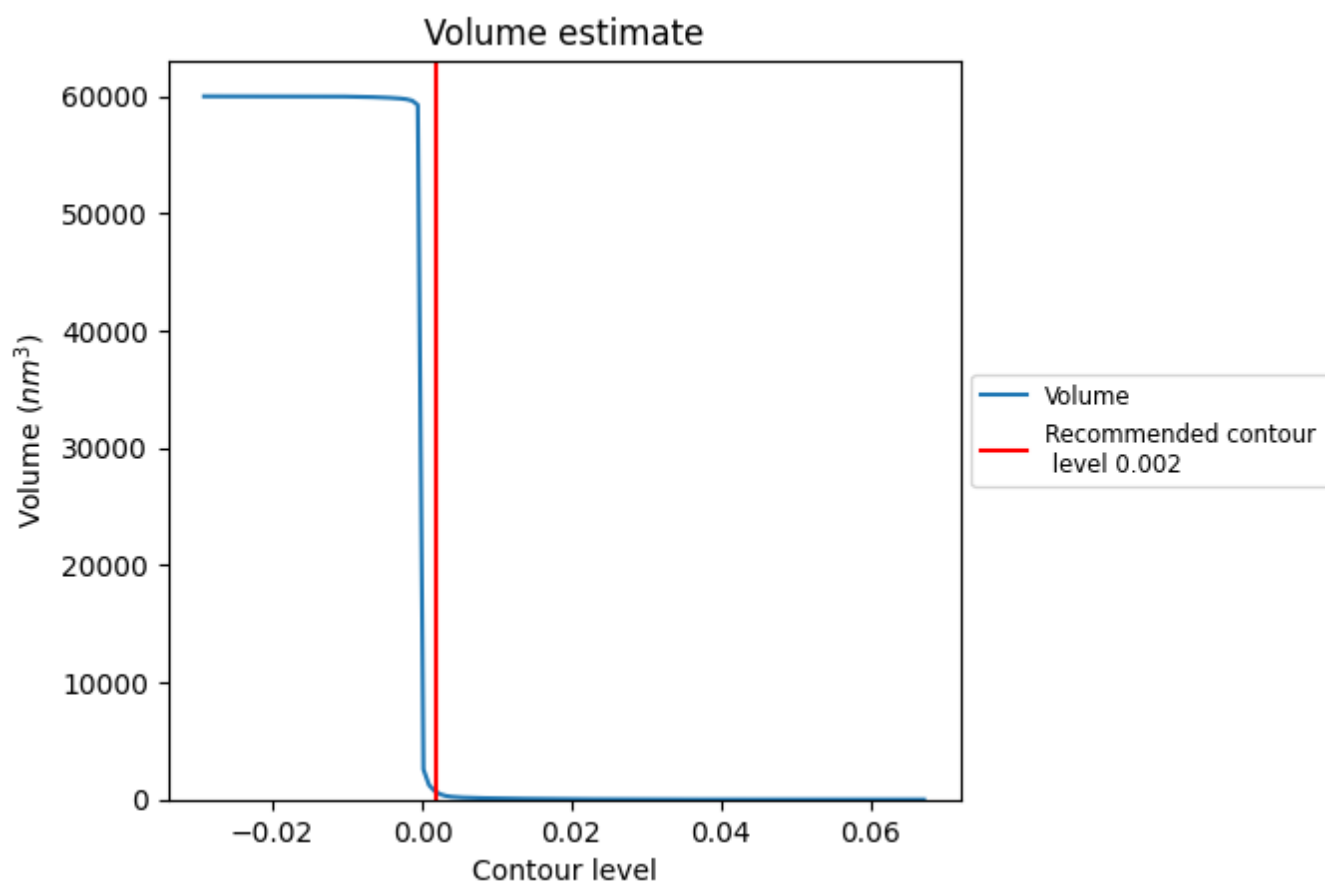
This section contains the results of statistical analysis of the map.

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.

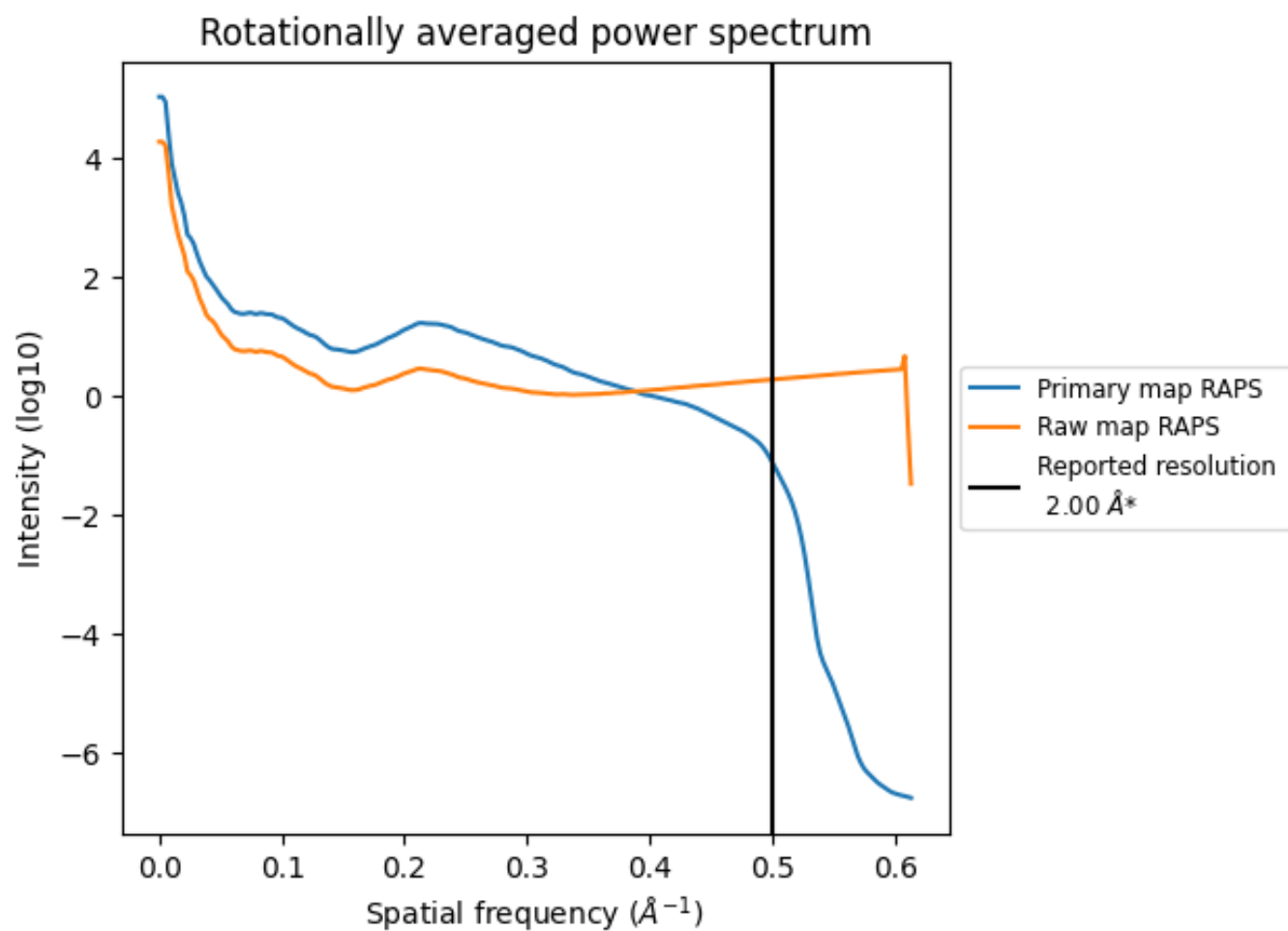
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 614 nm^3 ; this corresponds to an approximate mass of 554 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 ⓘ

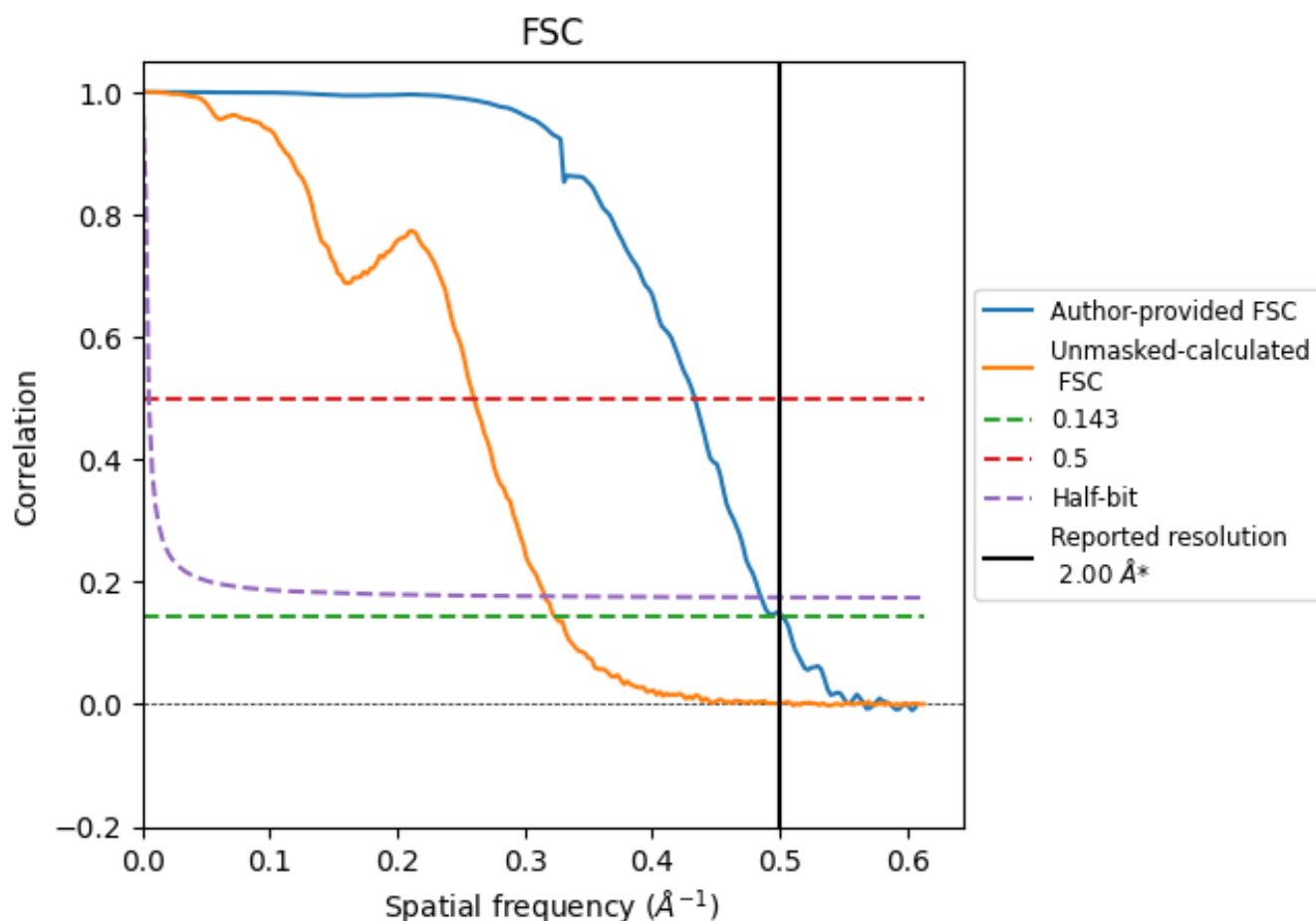


*Reported resolution corresponds to spatial frequency of 0.500 \AA^{-1}

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 0.500 \AA^{-1}

8.2 Resolution estimates [i](#)

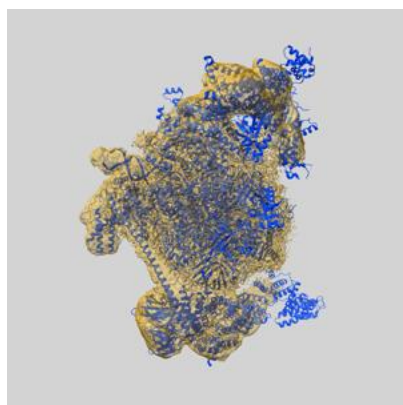
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.00	-	-
Author-provided FSC curve	1.99	2.31	2.06
Unmasked-calculated*	3.09	3.84	3.17

*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 3.09 differs from the reported value 2.0 by more than 10 %

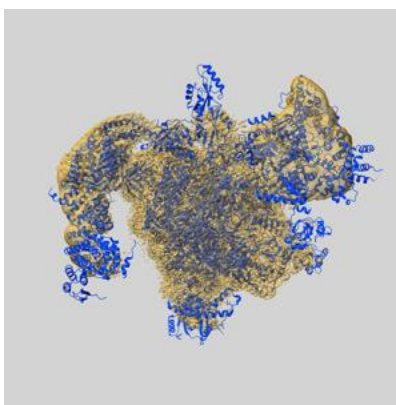
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-52443 and PDB model 9HVQ. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

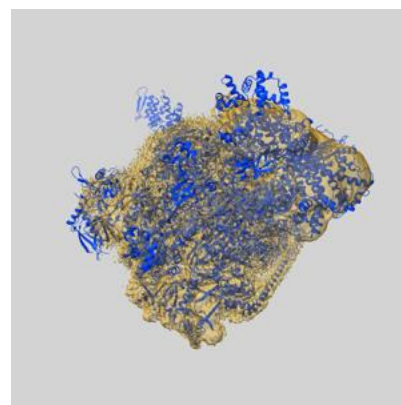
9.1 Map-model overlay [i](#)



X



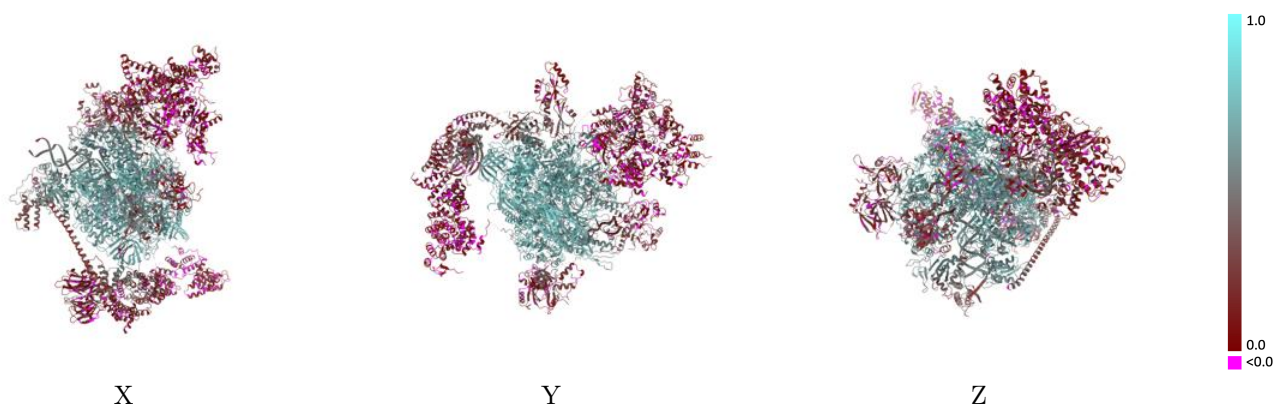
Y



Z

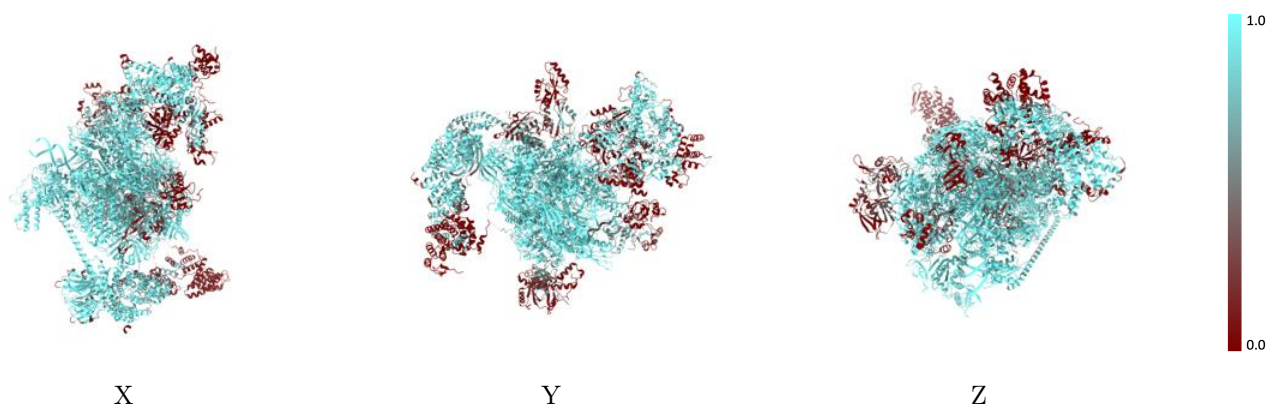
The images above show the 3D surface view of the map at the recommended contour level 0.002 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



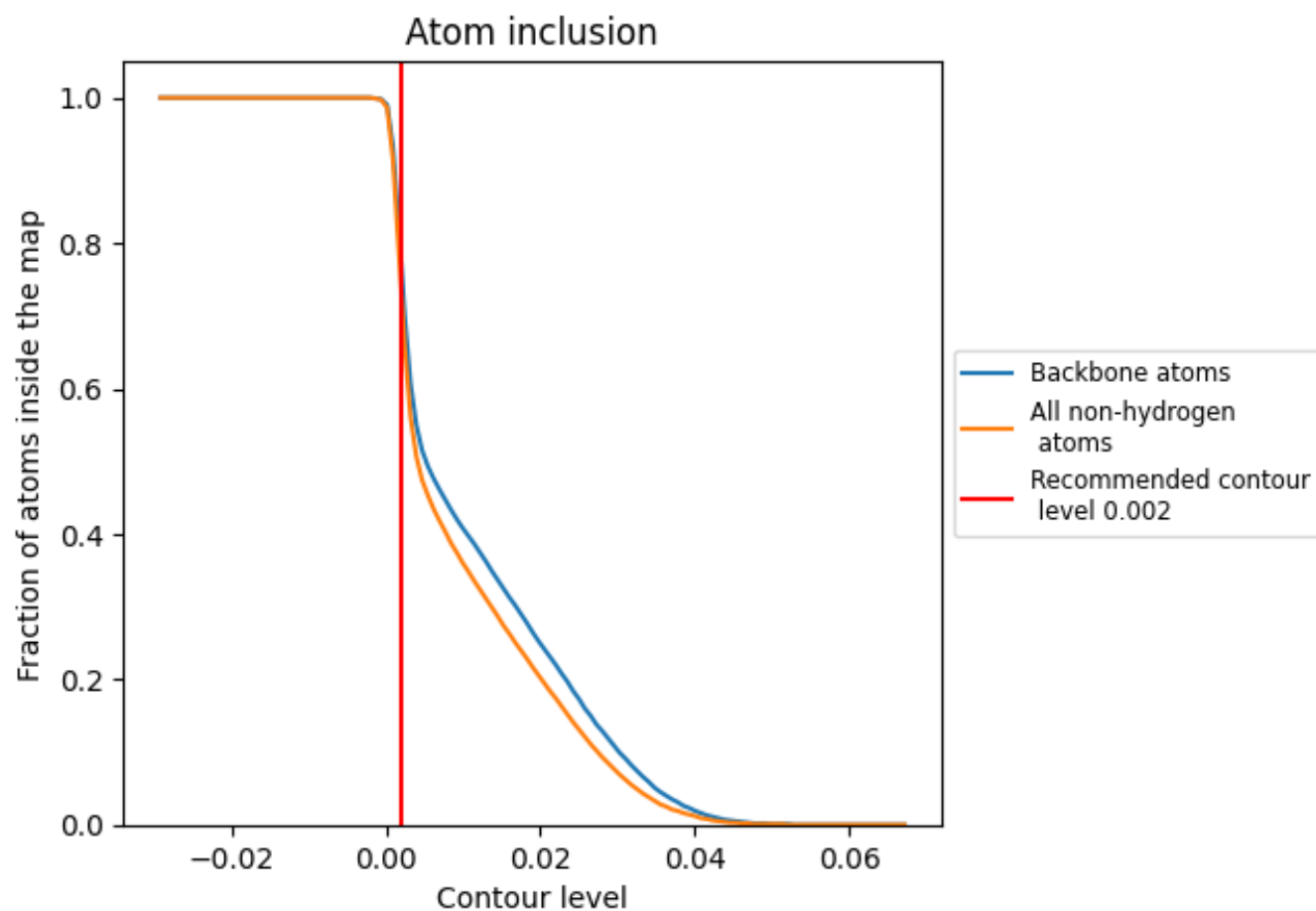
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.002).



















































9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 74% 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 (0.002) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7370	 0.4190
A	 0.9810	 0.6760
B	 0.9830	 0.6850
C	 0.9920	 0.7190
D	 0.8410	 0.2310
E	 0.9860	 0.6380
F	 0.9730	 0.6840
G	 0.8960	 0.3820
H	 0.9850	 0.6880
I	 0.9650	 0.5700
J	 0.9900	 0.7350
K	 0.9880	 0.7180
L	 0.9950	 0.6510
M	 0.4900	 0.1180
N	 0.7960	 0.3560
O	 0.9110	 0.3460
P	 0.9460	 0.6020
Q	 0.5980	 0.1720
T	 0.9650	 0.5560
U	 0.2710	 0.2310
V	 0.2470	 0.1670
W	 0.8150	 0.1500
X	 0.4260	 0.3240
Y	 0.3170	 0.1950
Z	 0.2610	 0.2160

