



wwPDB EM Validation Summary Report ⓘ

Oct 13, 2024 – 09:05 AM EDT

PDB ID : 6W1S
EMDB ID : EMD-21514
Title : Atomic model of the mammalian Mediator complex
Authors : Zhao, H.; Young, N.; Asturias, F.
Deposited on : 2020-03-04
Resolution : 4.02 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.dev113
MolProbity : 4.02b-467
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) : 2.39

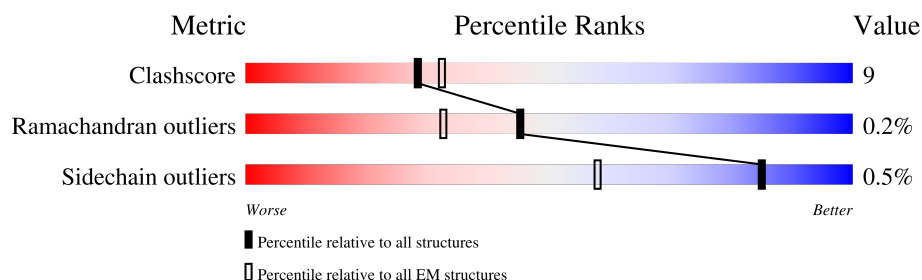
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.02 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

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	382	
2	B	100	
3	C	246	
4	D	157	
5	E	180	
6	F	76	
7	G	155	
8	H	108	

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Mol	Chain	Length	Quality of chain
9	I	1548	
10	J	167	
11	K	828	
12	L	631	
13	M	187	
14	N	243	
15	O	198	
16	P	126	
17	Q	131	
18	R	1367	
19	S	982	
20	T	202	
21	V	297	
22	W	118	
23	X	134	
24	Y	152	
25	Z	93	

2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 47275 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 Mediator of RNA polymerase II transcription subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	381	Total	C	N	O	0	0
			1905	1143	381	381		

- Molecule 2 is a protein called Mediator of RNA polymerase II transcription subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	94	Total	C	N	O	0	0
			468	280	94	94		

- Molecule 3 is a protein called Mediator of RNA polymerase II transcription subunit 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	149	Total	C	N	O	0	0
			744	446	149	149		

- Molecule 4 is a protein called Mediator of RNA polymerase II transcription subunit 7.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	157	Total	C	N	O	0	0
			781	467	157	157		

- Molecule 5 is a protein called Mediator of RNA polymerase II transcription subunit 8.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	165	Total	C	N	O	0	0
			837	506	166	165		

- Molecule 6 is a protein called Mediator of RNA polymerase II transcription subunit 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	F	68	Total	C	N	O	0	0
			339	203	68	68		

- Molecule 7 is a protein called Mediator of RNA polymerase II transcription subunit 10.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	70	Total	C	N	O	0	0
			350	210	70	70		

- Molecule 8 is a protein called Mediator of RNA polymerase II transcription subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	105	Total	C	N	O	S	0	0
			578	349	116	112	1		

- Molecule 9 is a protein called Mediator of RNA polymerase II transcription subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	1077	Total	C	N	O	S	0	0
			6731	4263	1245	1203	20		

- Molecule 10 is a protein called Mediator of RNA polymerase II transcription subunit 15.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	167	Total	C	N	O	S	0	0
			1171	748	217	200	6		

- Molecule 11 is a protein called Mediator of RNA polymerase II transcription subunit 16.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	735	Total	C	N	O	S	0	0
			5070	3274	909	864	23		

- Molecule 12 is a protein called Mediator of RNA polymerase II transcription subunit 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	524	Total	C	N	O	S	0	0
			3243	2041	608	591	3		

- Molecule 13 is a protein called Mediator of RNA polymerase II transcription subunit 18.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	180	Total	C	N	O	S	0	0
			1140	725	217	197	1		

- Molecule 14 is a protein called Mediator of RNA polymerase II transcription subunit 19.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	N	27	Total	C	N	O	0	0
			135	81	27	27		

- Molecule 15 is a protein called Mediator of RNA polymerase II transcription subunit 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	174	Total	C	N	O	S	0	0
			1013	640	177	192	4		

- Molecule 16 is a protein called Mediator of RNA polymerase II transcription subunit 21.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	P	105	Total	C	N	O	0	0
			523	313	105	105		

- Molecule 17 is a protein called Mediator of RNA polymerase II transcription subunit 22.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	Q	131	Total	C	N	O	0	0
			754	463	145	146		

- Molecule 18 is a protein called Mediator of RNA polymerase II transcription subunit 23.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	1295	Total	C	N	O	S	0	0
			9744	6296	1680	1715	53		

- Molecule 19 is a protein called Mediator of RNA polymerase II transcription subunit 24.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	901	Total	C	N	O	S	0	0
			5875	3750	1062	1036	27		

- Molecule 20 is a protein called Mediator of RNA polymerase II transcription subunit 25.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	192	Total	C	N	O	S	0	0
			1299	837	222	235	5		

- Molecule 21 is a protein called Mediator of RNA polymerase II transcription subunit 27.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	266	Total	C	N	O	S	0	0
			1657	1053	301	300	3		

- Molecule 22 is a protein called Mediator of RNA polymerase II transcription subunit 28.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	118	Total	C	N	O	S	0	0
			773	486	145	140	2		

- Molecule 23 is a protein called Mediator of RNA polymerase II transcription subunit 29.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	123	Total	C	N	O	S	0	0
			839	528	150	158	3		

- Molecule 24 is a protein called Mediator of RNA polymerase II transcription subunit 30.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	132	Total	C	N	O	S	0	0
			843	527	168	145	3		

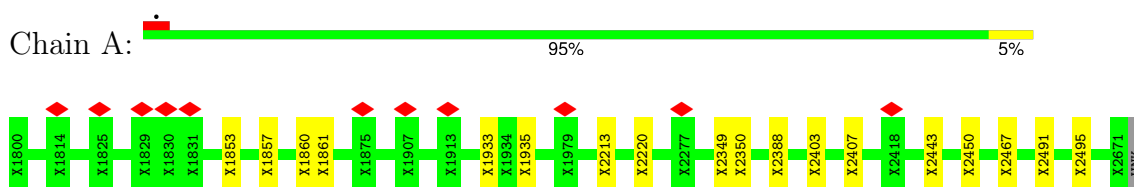
- Molecule 25 is a protein called Mediator of RNA polymerase II transcription subunit 31.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	Z	93	Total	C	N	O	0	0
			463	277	93	93		

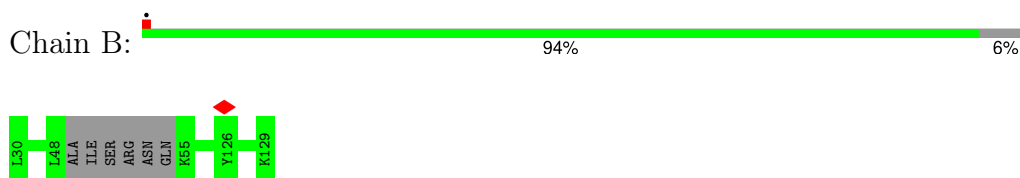
3 Residue-property plots [i](#)

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

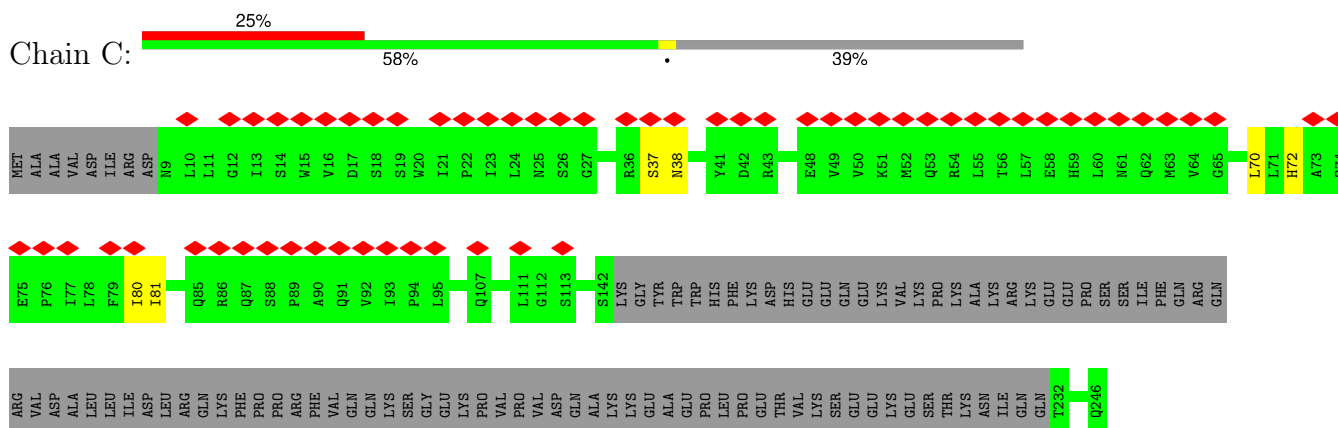
- Molecule 1: Mediator of RNA polymerase II transcription subunit 1



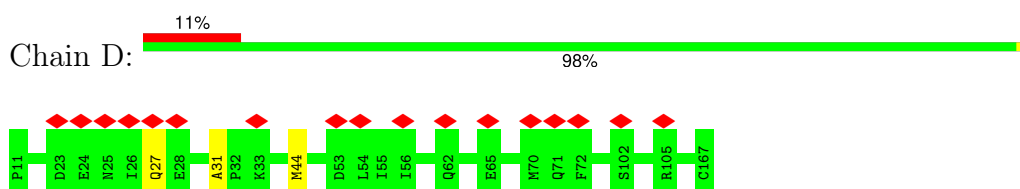
- Molecule 2: Mediator of RNA polymerase II transcription subunit 4

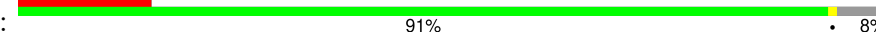


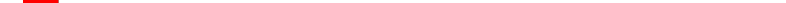

- Molecule 3: Mediator of RNA polymerase II transcription subunit 6



- Molecule 4: Mediator of RNA polymerase II transcription subunit 7



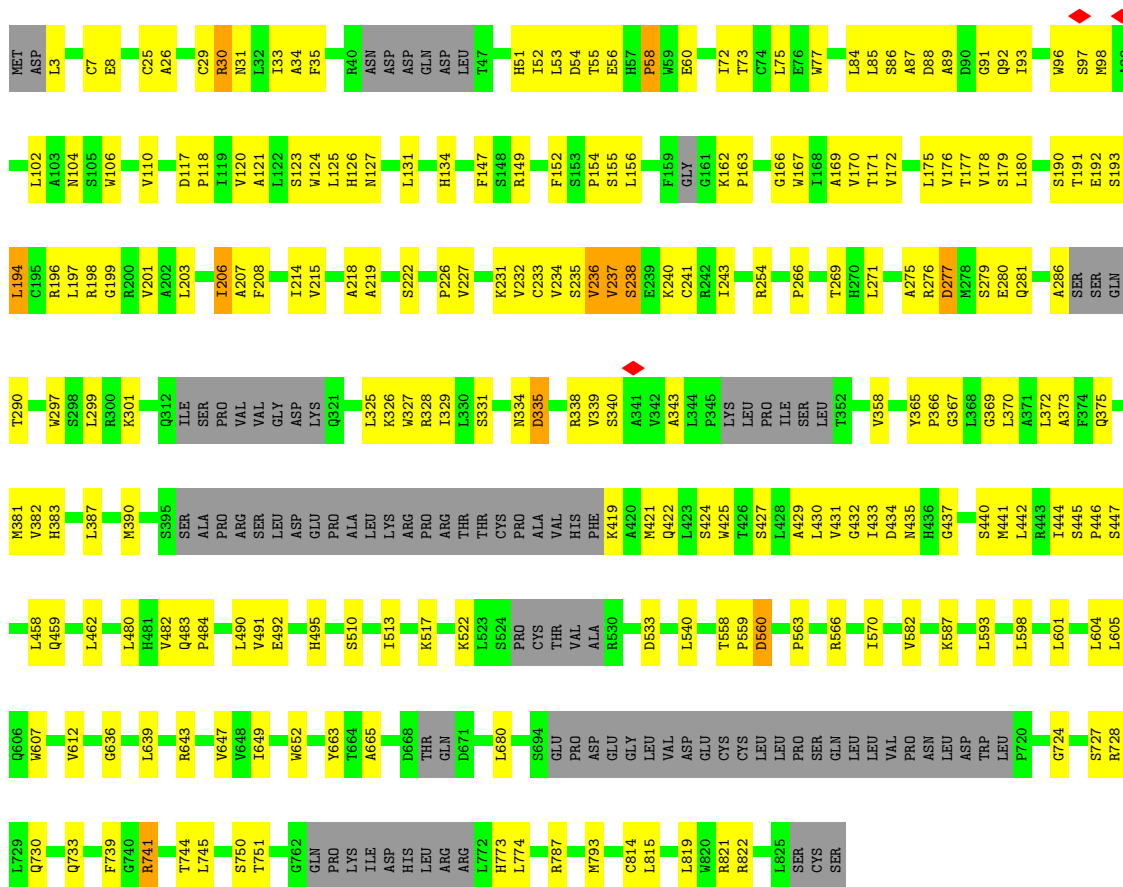
- Chain E: 

- Chain F:  89% 11%
- 

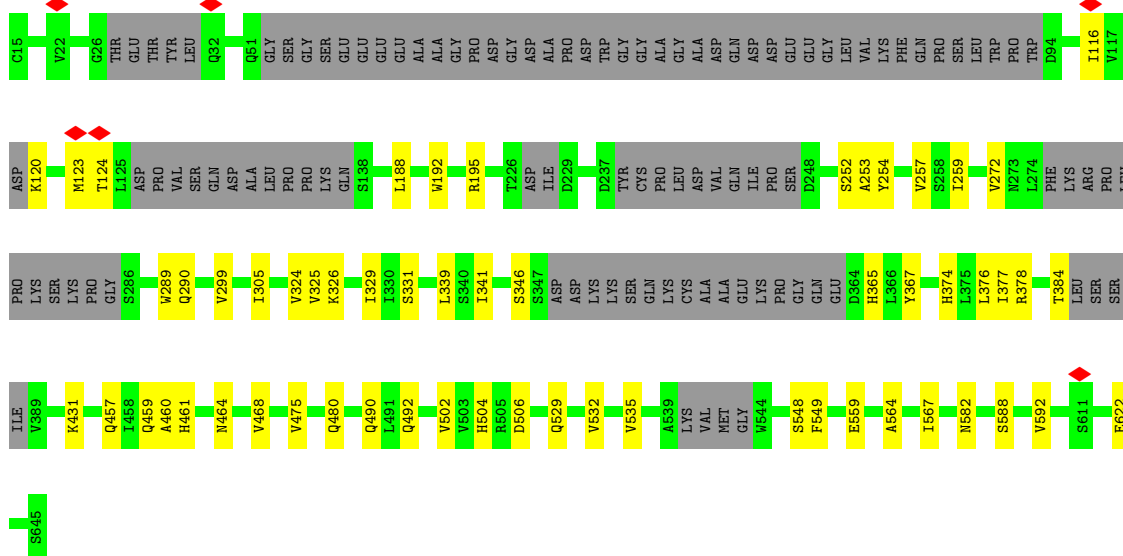
- Chain G:
-
- Sequence logo for Chain G. The y-axis represents information content in bits (0.00 to 0.25). The x-axis shows positions 200 to 267. A bar at the top indicates the percentage of positions with conservation: 34% (red), 43% (green), and 55% (grey).
- | Position | Residue |
|----------|---------|
| 200 | LEU |
| 201 | LEU |
| 202 | LEU |
| 203 | ILE |
| 204 | GLN |
| 205 | LEU |
| 206 | SER |
| 207 | SER |
| 208 | VAL |
| 209 | PHE |
| 210 | PRO |
| 211 | GLU |
| 212 | ASP |
| 213 | MET |
| 214 | ALA |
| 215 | ILE |
| 216 | ARG |
| 217 | GLY |
| 218 | GLU |
| 219 | GLY |
| 220 | ASP |
| 221 | HIS |
| 222 | PRO |
| 223 | PRO |
| 224 | PRO |
| 225 | GLN |
| 226 | LEU |
| 227 | TYR |
| 228 | THR |
| 229 | LYS |
| 230 | GLU |
| 231 | LEU |
| 232 | ARG |
| 233 | ALA |
| 234 | LEU |
| 235 | ALA |
| 236 | LYS |
| 237 | ASN |
| 238 | GLU |
| 239 | GLN |
| 240 | VAL |
| 241 | LYS |
| 242 | ILE |
| 243 | ASP |
| 244 | THR |
| 245 | NET |
| 246 | LYS |
| 247 | LYS |
| 248 | PHE |
| 249 | LYS |
| 250 | LYS |
| 251 | LYS |
| 252 | LYS |
| 253 | LYS |
| 254 | LYS |
| 255 | LYS |
| 256 | LYS |
| 257 | LYS |
| 258 | LYS |
| 259 | LYS |
| 260 | LYS |
| 261 | LYS |
| 262 | LYS |
| 263 | LYS |
| 264 | LYS |
| 265 | LYS |
| 266 | LYS |
| 267 | LYS |

- [illegible]

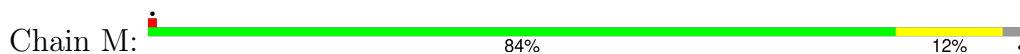
- [illegible]

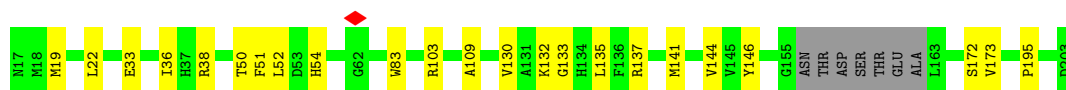


- Molecule 12: Mediator of RNA polymerase II transcription subunit 17

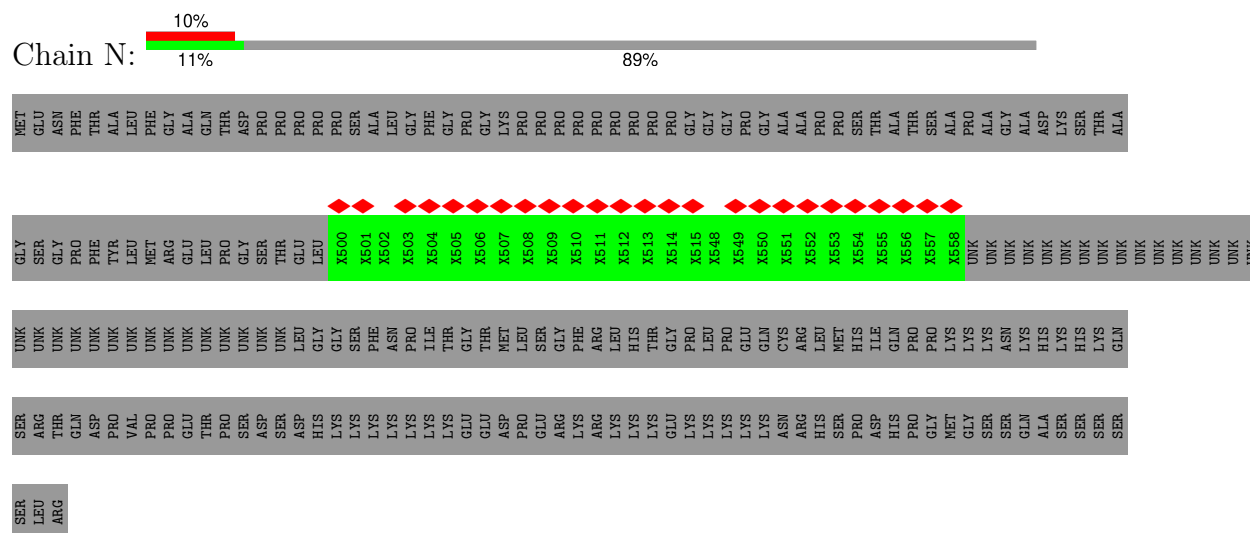


- Molecule 13: Mediator of RNA polymerase II transcription subunit 18

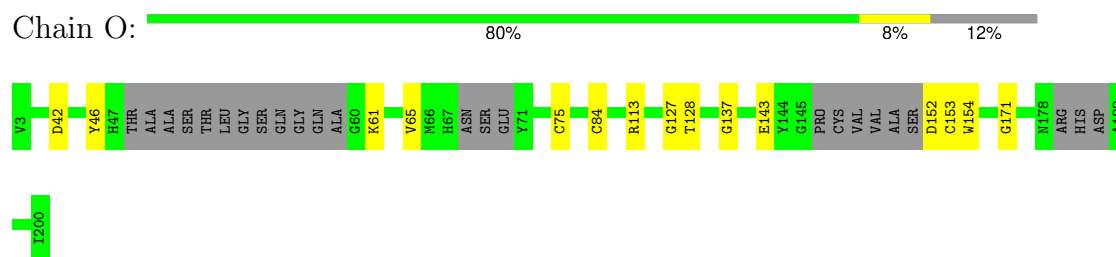




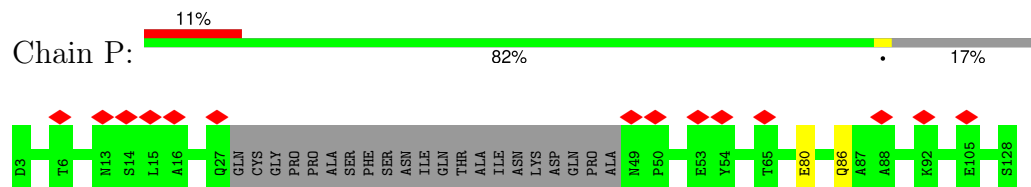
- Molecule 14: Mediator of RNA polymerase II transcription subunit 19



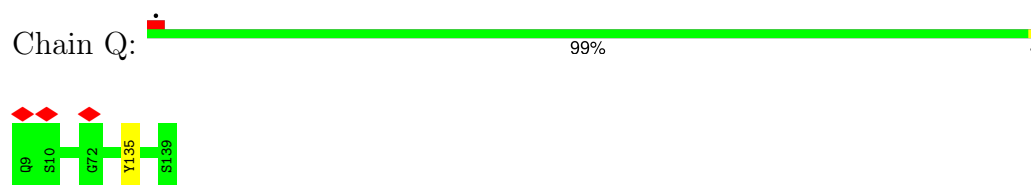
- Molecule 15: Mediator of RNA polymerase II transcription subunit 20



- Molecule 16: Mediator of RNA polymerase II transcription subunit 21

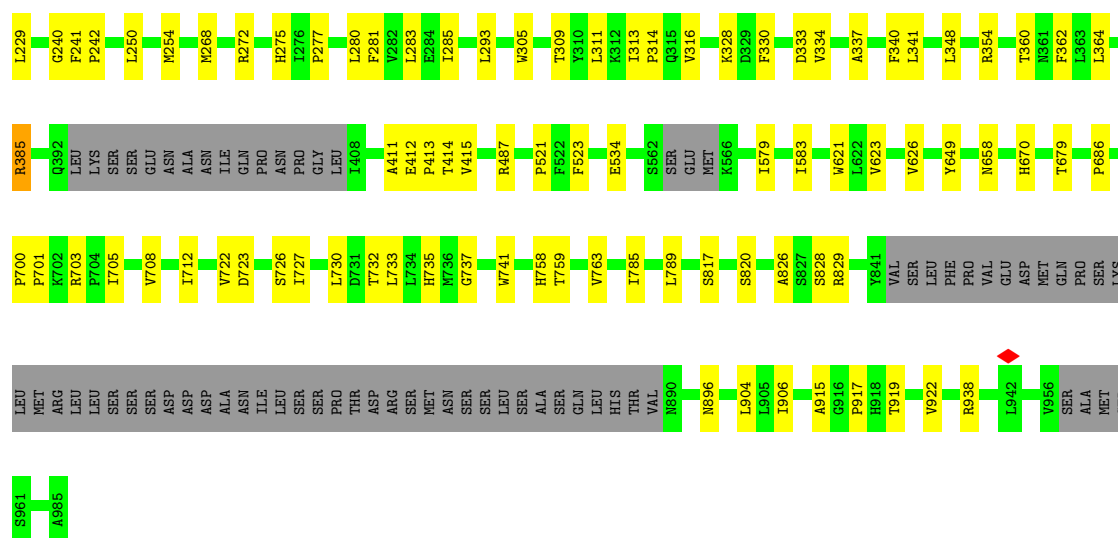


- Molecule 17: Mediator of RNA polymerase II transcription subunit 22

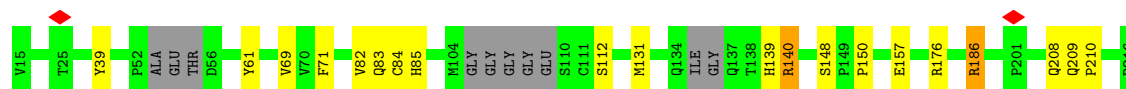
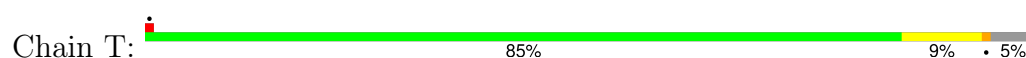


- Molecule 18: Mediator of RNA polymerase II transcription subunit 23

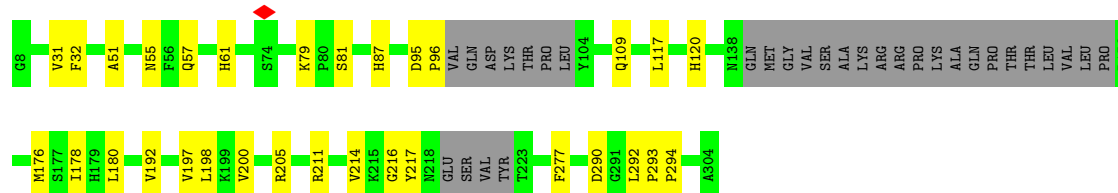
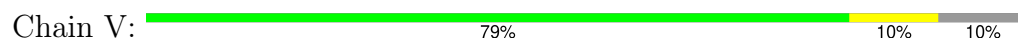




- Molecule 20: Mediator of RNA polymerase II transcription subunit 25



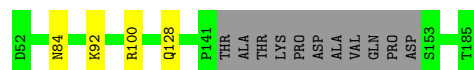
- Molecule 21: Mediator of RNA polymerase II transcription subunit 27



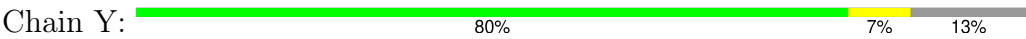
- Molecule 22: Mediator of RNA polymerase II transcription subunit 28



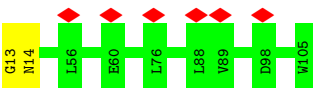
- Molecule 23: Mediator of RNA polymerase II transcription subunit 29



- Molecule 24: Mediator of RNA polymerase II transcription subunit 30



● Molecule 25: Mediator of RNA polymerase II transcription subunit 31



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	217557	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	22.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.669	Depositor
Minimum map value	-0.398	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.1	Depositor
Map size (\AA)	621.60004, 621.60004, 621.60004	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.11, 1.11, 1.11	Depositor

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	B	0.23	0/466	0.31	0/648
3	C	0.24	0/743	0.40	0/1032
4	D	0.24	0/780	0.37	0/1088
5	E	0.23	0/840	0.39	0/1170
6	F	0.22	0/337	0.33	0/468
8	H	0.23	0/580	0.35	0/798
9	I	0.25	0/6411	0.43	0/8831
10	J	0.26	0/1207	0.45	0/1668
11	K	0.25	0/5186	0.51	3/7120 (0.0%)
12	L	0.24	0/3293	0.42	0/4528
13	M	0.24	0/1163	0.43	0/1593
15	O	0.26	0/1027	0.45	0/1412
16	P	0.23	0/521	0.36	0/725
17	Q	0.23	0/758	0.35	0/1046
18	R	0.25	0/9995	0.43	0/13654
19	S	0.24	0/6000	0.41	1/8250 (0.0%)
20	T	0.26	0/1336	0.44	0/1836
21	V	0.25	0/1694	0.43	0/2338
22	W	0.25	0/785	0.37	0/1076
23	X	0.24	0/852	0.38	0/1169
24	Y	0.23	0/853	0.35	0/1167
25	Z	0.22	0/462	0.31	0/644
All	All	0.24	0/45289	0.43	4/62261 (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
4	D	0	1
10	J	0	1
11	K	0	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
18	R	0	4
All	All	0	11

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	S	59	LEU	CA-CB-CG	5.26	127.40	115.30
11	K	335	ASP	CB-CG-OD2	5.21	122.99	118.30
11	K	277	ASP	CB-CG-OD2	5.18	122.96	118.30
11	K	560	ASP	CB-CG-OD2	5.18	122.96	118.30

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	44	MET	Peptide
10	J	734	SER	Peptide
11	K	194	LEU	Peptide
11	K	206	ILE	Peptide
11	K	58	PRO	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	1905	0	460	9	0
2	B	468	0	209	0	0
3	C	744	0	325	3	0
4	D	781	0	314	1	0
5	E	837	0	402	2	0
6	F	339	0	136	0	0
7	G	350	0	74	2	0
8	H	578	0	341	3	0
9	I	6731	0	4840	62	0
10	J	1171	0	1010	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	K	5070	0	4502	251	0
12	L	3243	0	2350	47	0
13	M	1140	0	832	13	0
14	N	135	0	31	0	0
15	O	1013	0	663	10	0
16	P	523	0	259	1	0
17	Q	754	0	448	1	0
18	R	9744	0	9105	242	0
19	S	5875	0	4690	80	0
20	T	1299	0	1022	12	0
21	V	1657	0	1170	21	0
22	W	773	0	607	4	0
23	X	839	0	700	4	0
24	Y	843	0	639	8	0
25	Z	463	0	202	1	0
All	All	47275	0	35331	767	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 9.

The worst 5 of 767 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:K:446:PRO:CB	11:K:480:LEU:HD21	1.17	1.62
11:K:271:LEU:CD2	11:K:279:SER:HA	1.24	1.59
11:K:175:LEU:CD2	11:K:201:VAL:CG1	1.82	1.57
11:K:271:LEU:HD22	11:K:279:SER:CA	1.10	1.56
11:K:446:PRO:HG2	11:K:480:LEU:CD2	1.37	1.51

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	
2	B	90/100 (90%)	90 (100%)	0	0	100	100
3	C	145/246 (59%)	133 (92%)	12 (8%)	0	100	100
4	D	155/157 (99%)	135 (87%)	20 (13%)	0	100	100
5	E	157/180 (87%)	137 (87%)	20 (13%)	0	100	100
6	F	64/76 (84%)	61 (95%)	3 (5%)	0	100	100
8	H	101/108 (94%)	98 (97%)	3 (3%)	0	100	100
9	I	948/1548 (61%)	793 (84%)	155 (16%)	0	100	100
10	J	165/167 (99%)	129 (78%)	36 (22%)	0	100	100
11	K	713/828 (86%)	560 (78%)	148 (21%)	5 (1%)	19	55
12	L	502/631 (80%)	436 (87%)	66 (13%)	0	100	100
13	M	176/187 (94%)	164 (93%)	12 (7%)	0	100	100
15	O	164/198 (83%)	140 (85%)	24 (15%)	0	100	100
16	P	101/126 (80%)	96 (95%)	5 (5%)	0	100	100
17	Q	129/131 (98%)	121 (94%)	8 (6%)	0	100	100
18	R	1285/1367 (94%)	1082 (84%)	200 (16%)	3 (0%)	44	76
19	S	889/982 (90%)	795 (89%)	92 (10%)	2 (0%)	44	76
20	T	184/202 (91%)	150 (82%)	34 (18%)	0	100	100
21	V	258/297 (87%)	219 (85%)	38 (15%)	1 (0%)	30	66
22	W	116/118 (98%)	109 (94%)	7 (6%)	0	100	100
23	X	119/134 (89%)	118 (99%)	1 (1%)	0	100	100
24	Y	128/152 (84%)	116 (91%)	12 (9%)	0	100	100
25	Z	91/93 (98%)	91 (100%)	0	0	100	100
All	All	6680/8028 (83%)	5773 (86%)	896 (13%)	11 (0%)	45	76

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	K	563	PRO
19	S	722	VAL
18	R	1182	GLU
19	S	41	ASN
11	K	237	VAL

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	
3	C	1/223 (0%)	1 (100%)	0	100	100
5	E	6/160 (4%)	6 (100%)	0	100	100
8	H	12/91 (13%)	12 (100%)	0	100	100
9	I	388/1276 (30%)	387 (100%)	1 (0%)	91	92
10	J	100/153 (65%)	100 (100%)	0	100	100
11	K	418/729 (57%)	416 (100%)	2 (0%)	86	90
12	L	181/557 (32%)	181 (100%)	0	100	100
13	M	61/165 (37%)	61 (100%)	0	100	100
15	O	44/166 (26%)	44 (100%)	0	100	100
17	Q	23/122 (19%)	23 (100%)	0	100	100
18	R	949/1231 (77%)	944 (100%)	5 (0%)	86	90
19	S	395/863 (46%)	391 (99%)	4 (1%)	73	81
20	T	94/169 (56%)	92 (98%)	2 (2%)	48	67
21	V	92/266 (35%)	92 (100%)	0	100	100
22	W	52/108 (48%)	52 (100%)	0	100	100
23	X	65/120 (54%)	65 (100%)	0	100	100
24	Y	47/140 (34%)	47 (100%)	0	100	100
All	All	2928/6539 (45%)	2914 (100%)	14 (0%)	85	90

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	R	1328	ARG
19	S	164	CYS
20	T	186	ARG
19	S	487	ARG
20	T	140	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37

such sidechains are listed below:

Mol	Chain	Res	Type
19	S	111	HIS
22	W	90	GLN
19	S	370	GLN
21	V	41	ASN
12	L	290	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	24
9	I	2
14	N	1
7	G	1

The worst 5 of 28 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	2468:UNK	C	2489:UNK	N	30.97
1	I	2096:UNK	C	2097:UNK	N	23.72
1	N	515:UNK	C	548:UNK	N	23.17
1	A	2377:UNK	C	2388:UNK	N	22.68
1	A	2628:UNK	C	2656:UNK	N	22.03

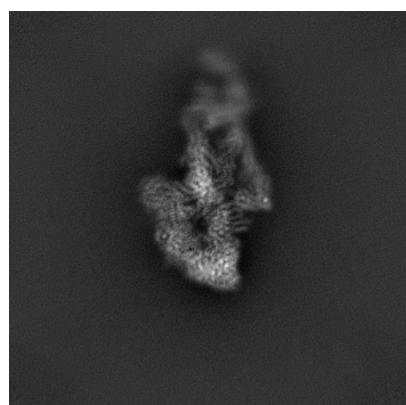
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21514. These allow visual inspection of the internal detail of the map and identification of artifacts.

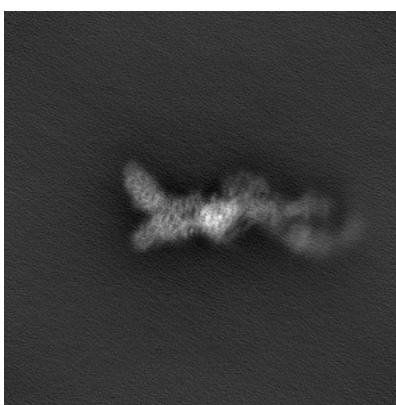
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

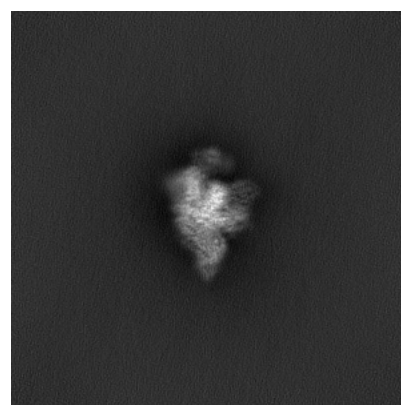
6.1.1 Primary map



X



Y

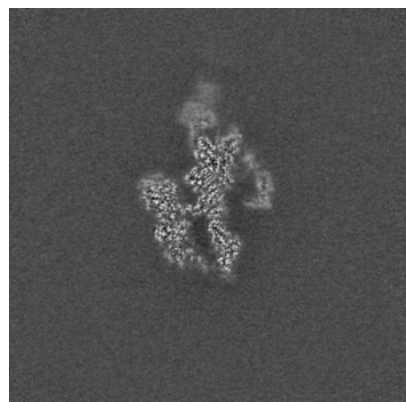


Z

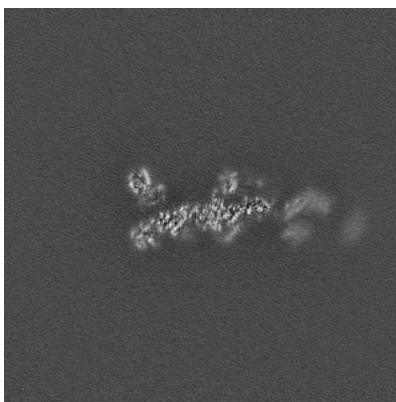
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

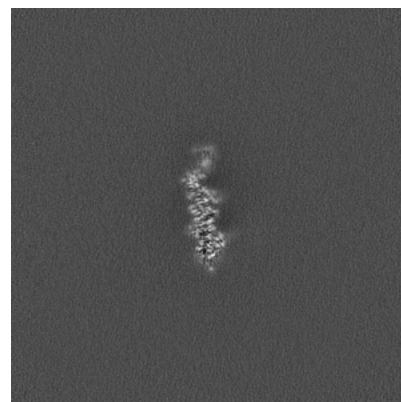
6.2.1 Primary map



X Index: 280



Y Index: 280

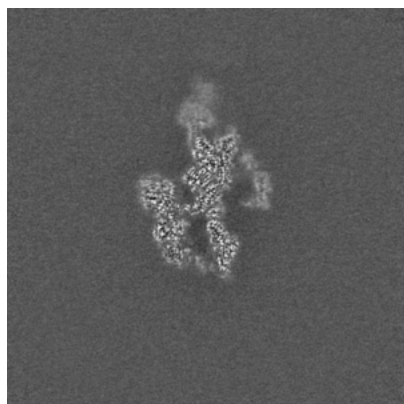


Z Index: 280

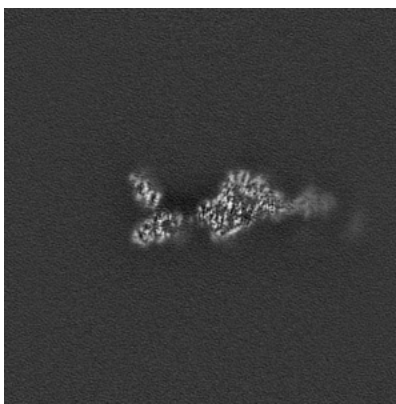
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

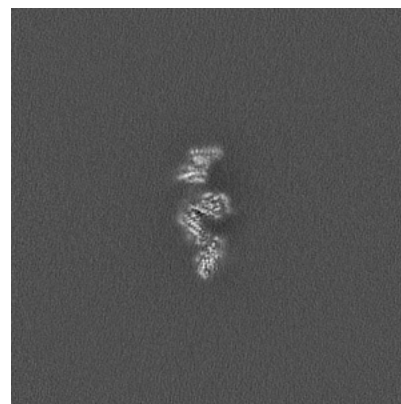
6.3.1 Primary map



X Index: 281



Y Index: 268

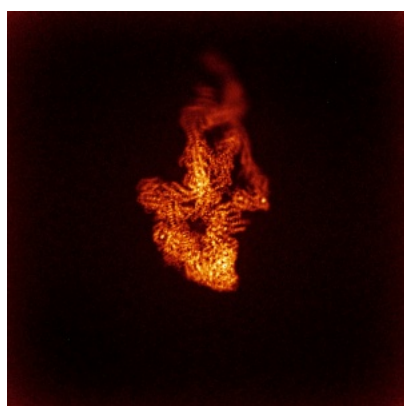


Z Index: 297

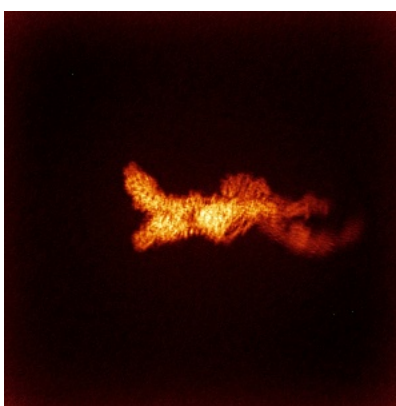
The images above show the largest variance slices of the map in three orthogonal directions.

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

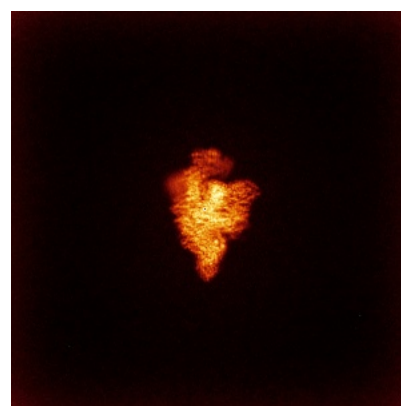
6.4.1 Primary map



X



Y

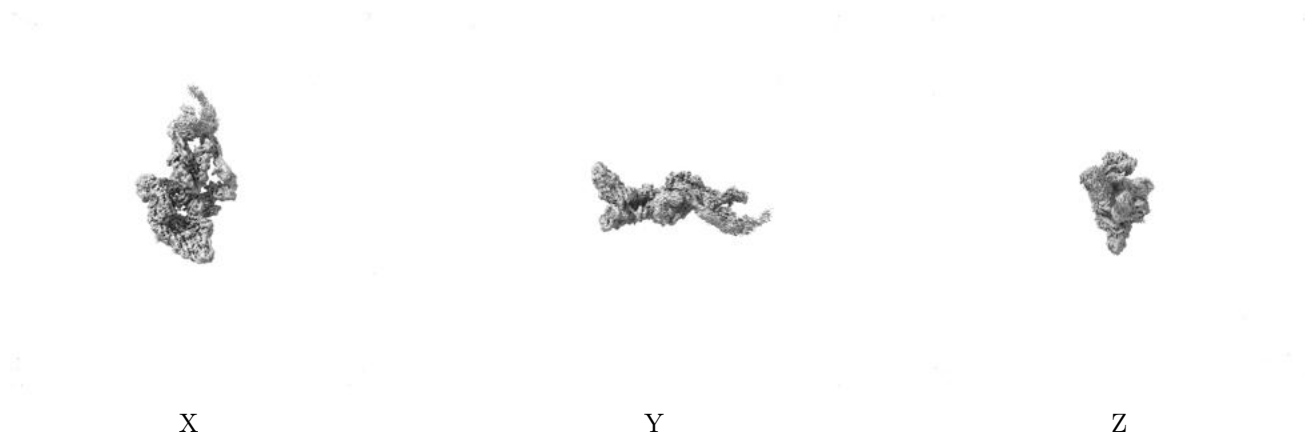


Z

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 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

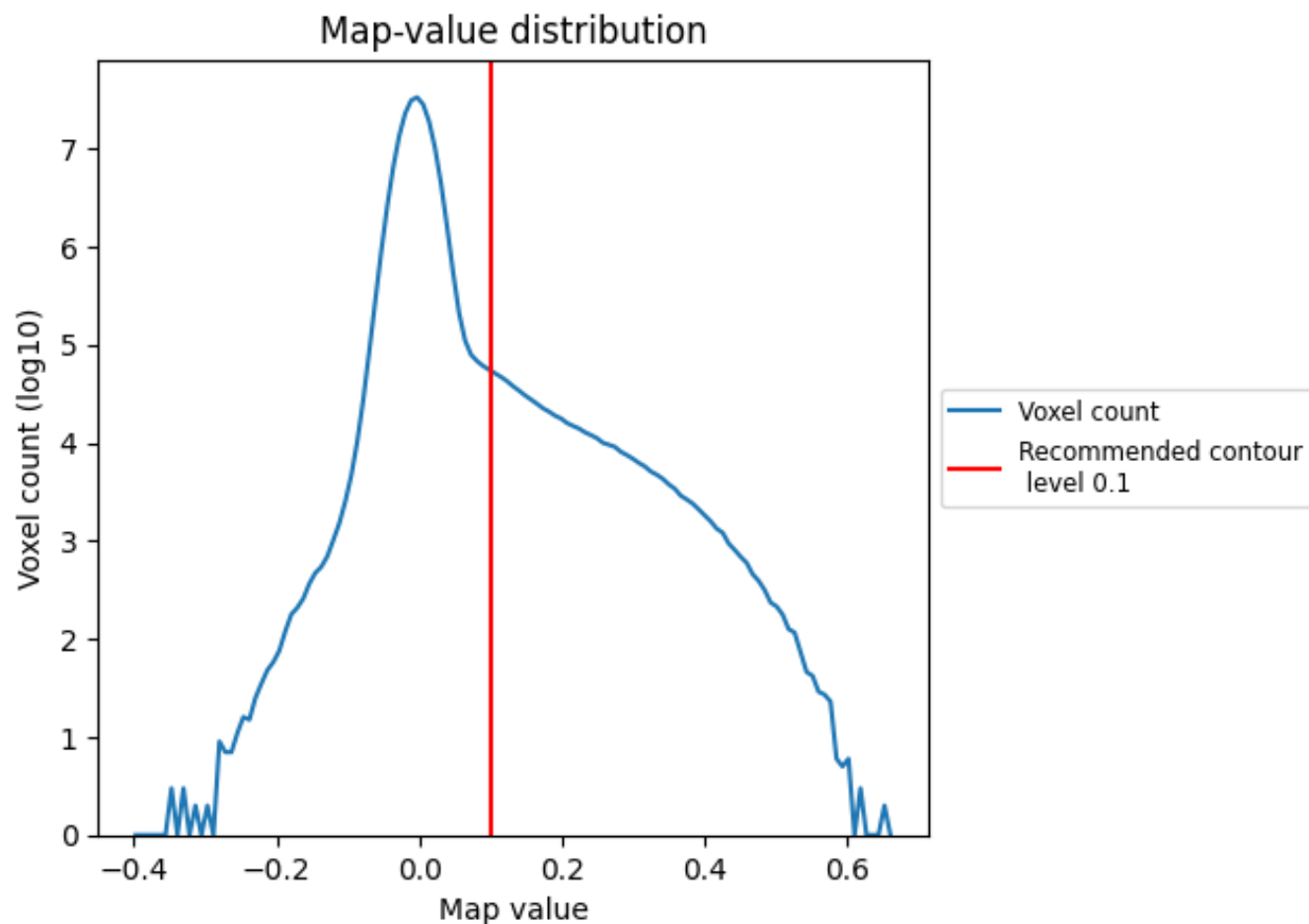
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

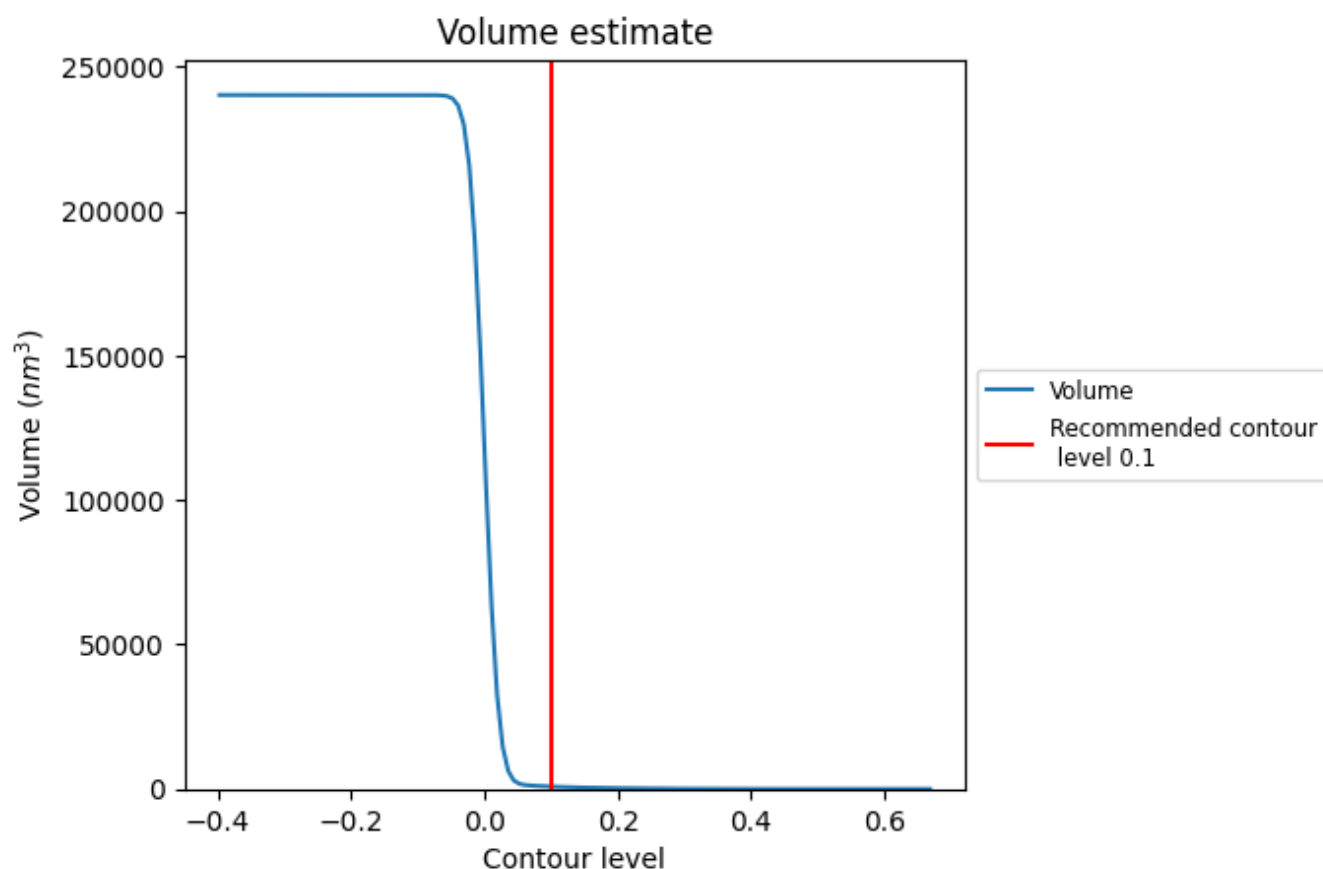
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

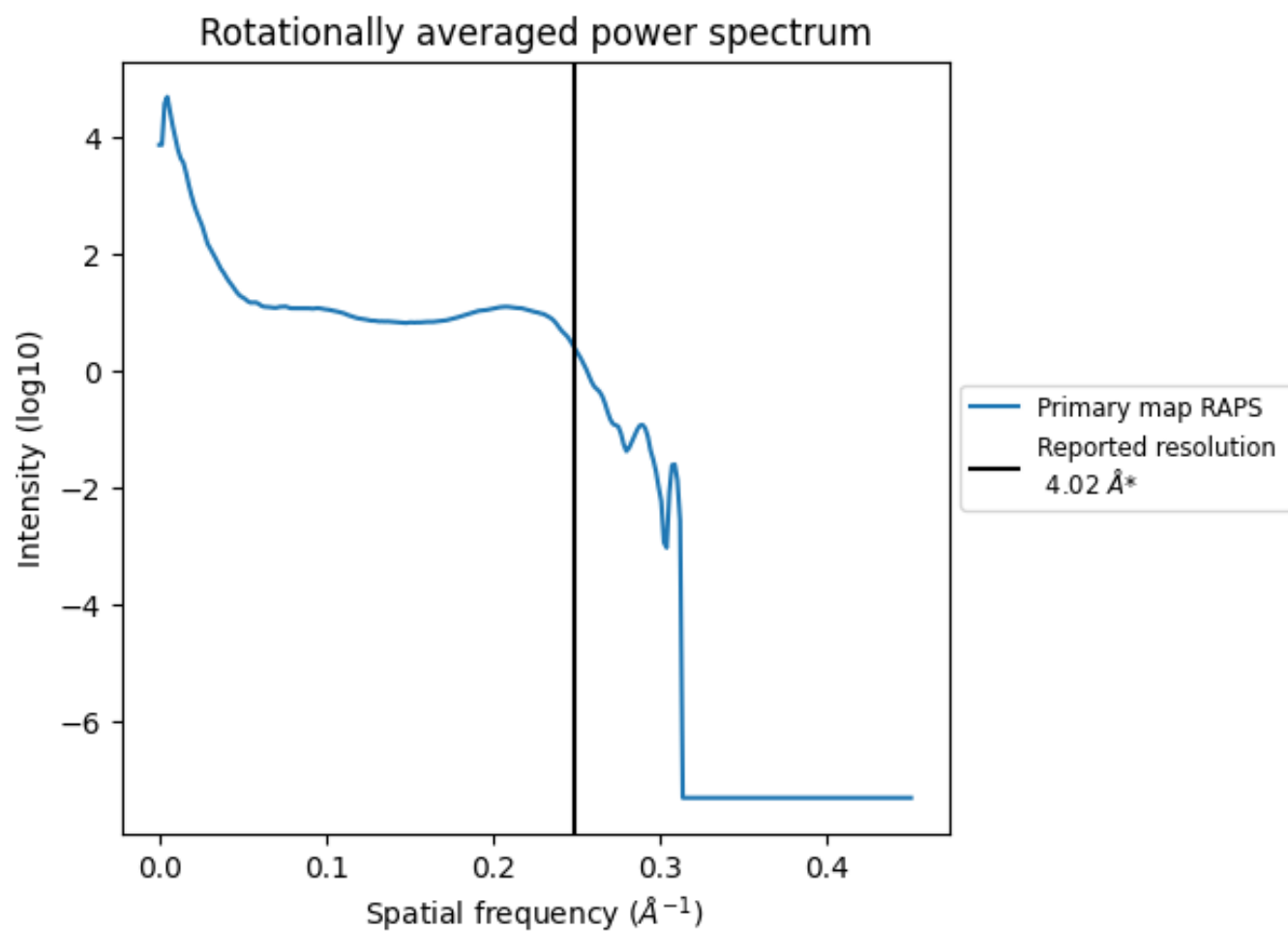
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 824 nm³; this corresponds to an approximate mass of 744 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 ⓘ

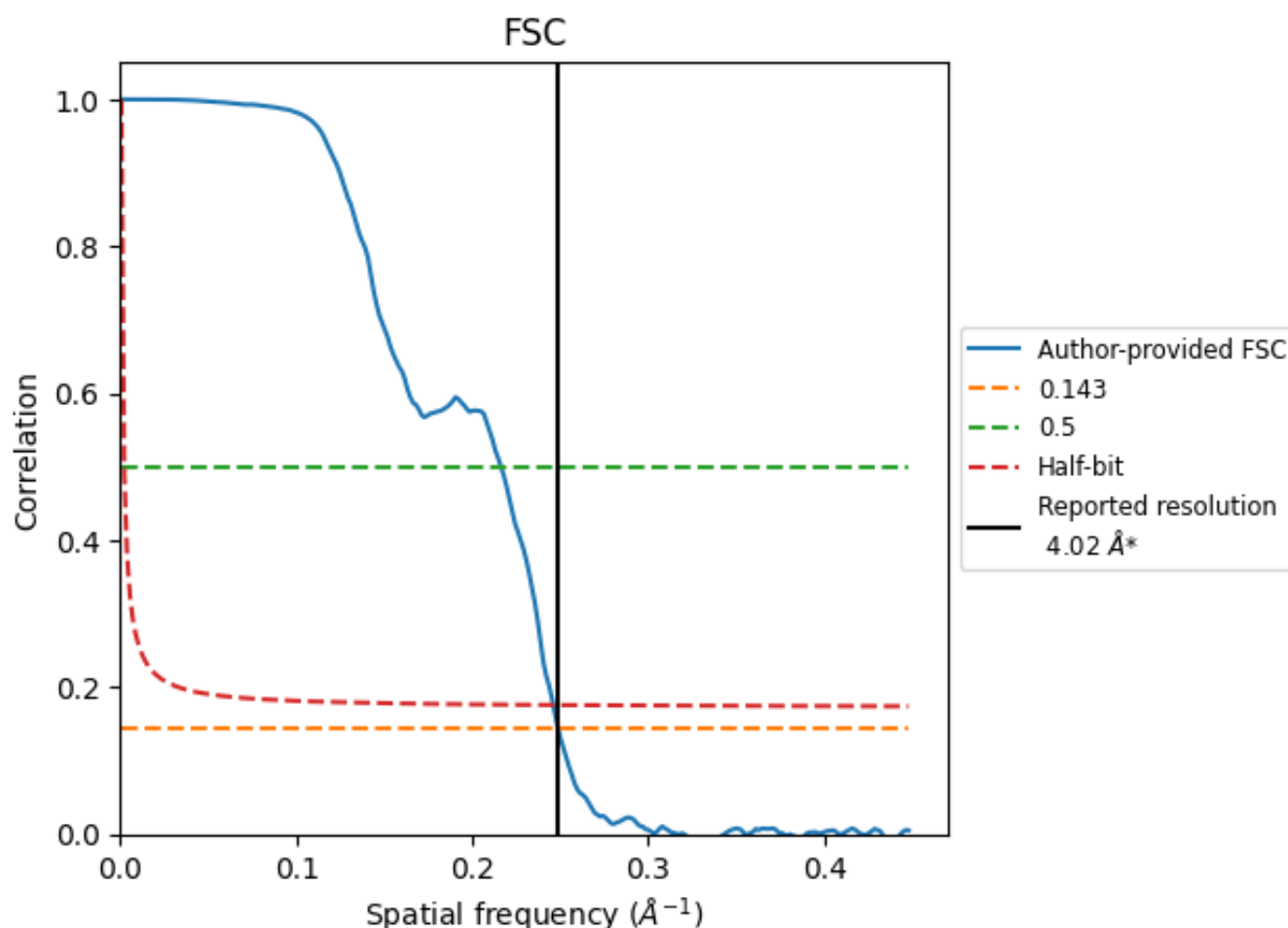


*Reported resolution corresponds to spatial frequency of 0.249 Å⁻¹

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 0.249 Å⁻¹

8.2 Resolution estimates [i](#)

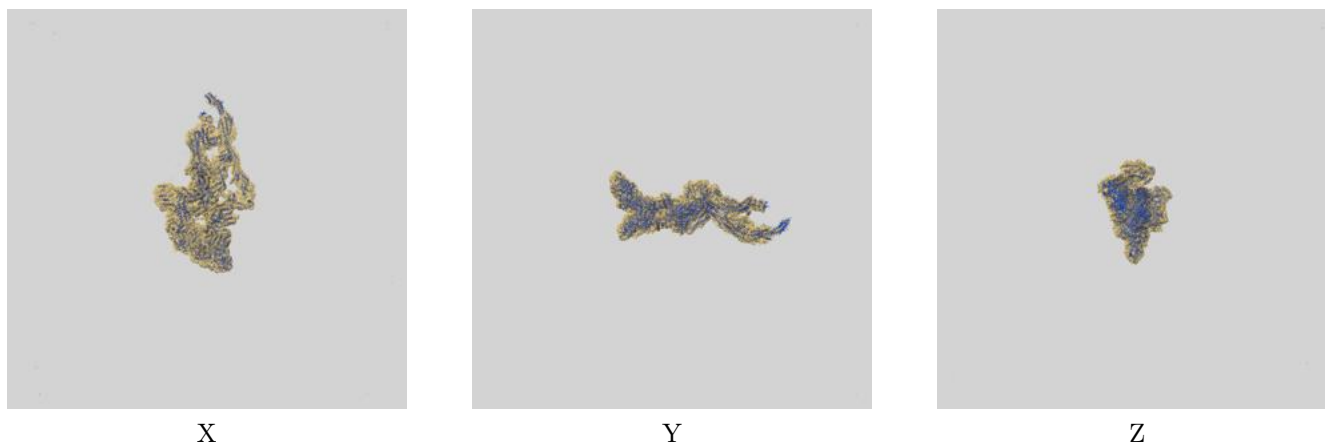
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.02	-	-
Author-provided FSC curve	4.02	4.62	4.06
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

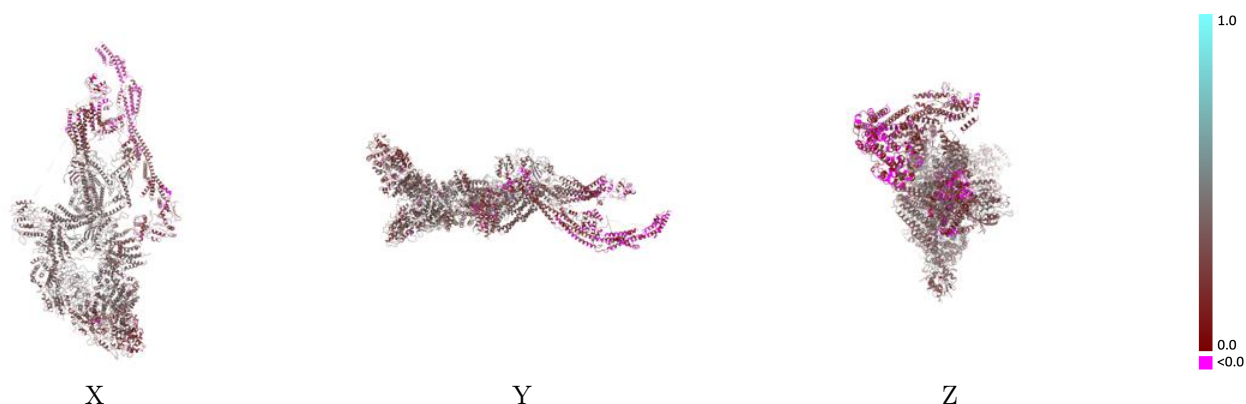
This section contains information regarding the fit between EMDB map EMD-21514 and PDB model 6W1S. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



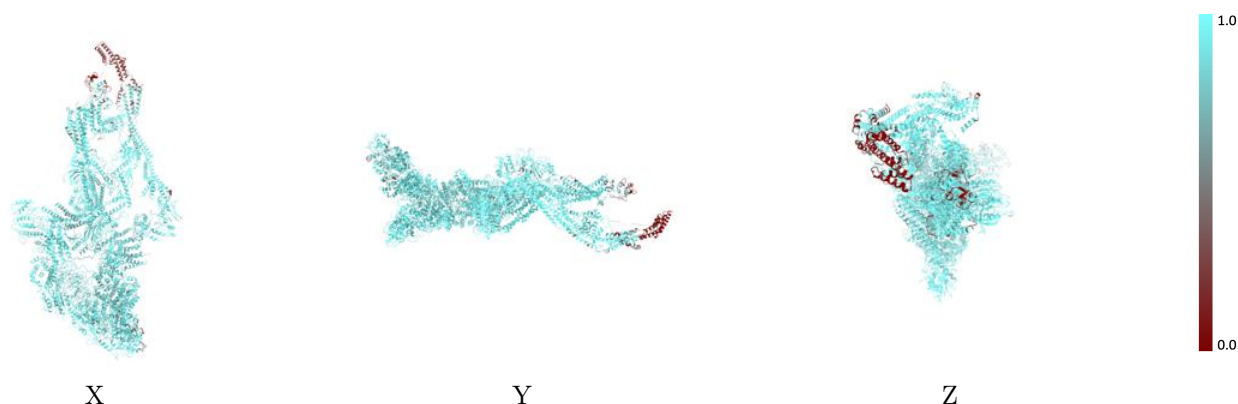
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



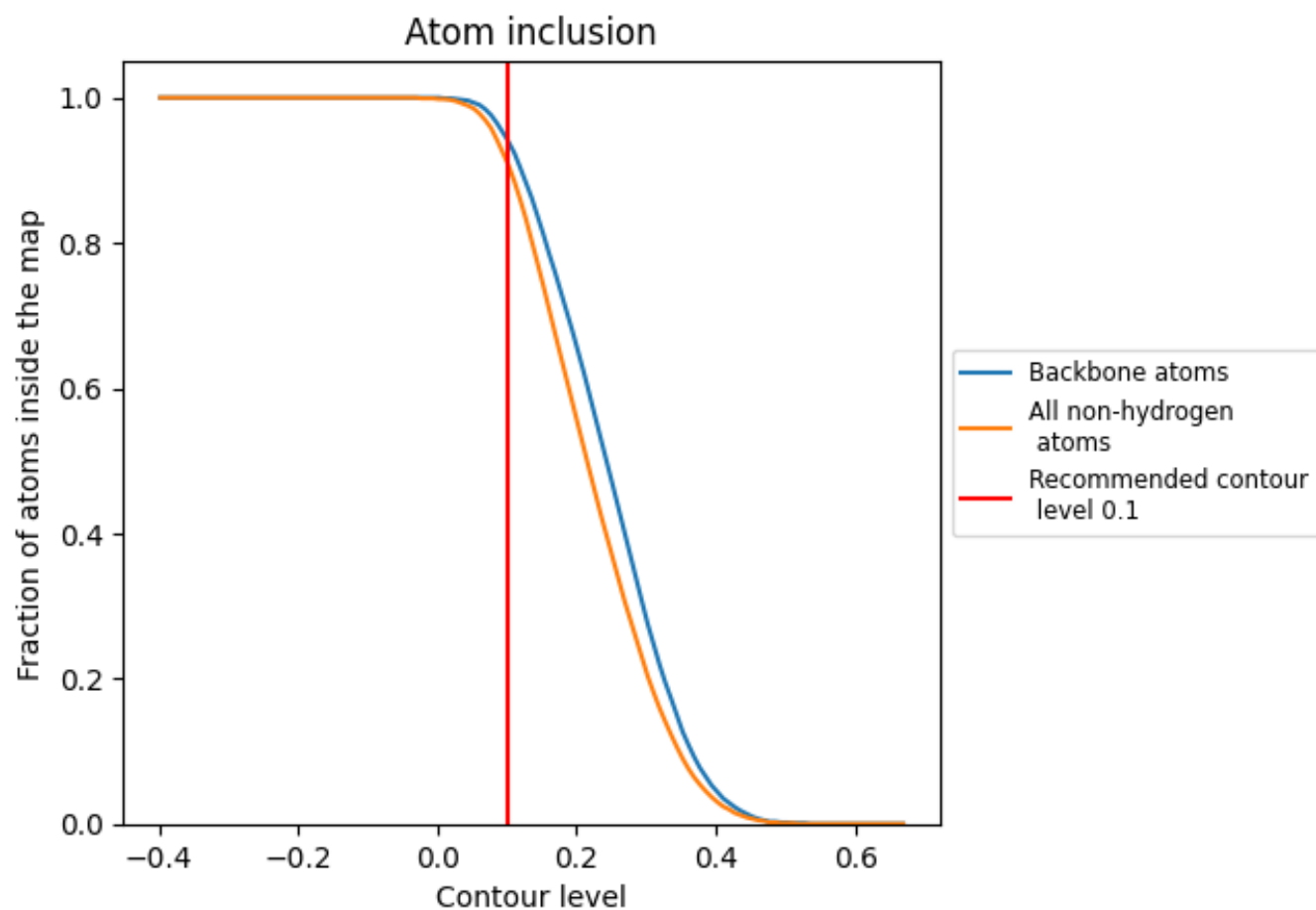
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).





















































9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 91% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9120	 0.3210
A	 0.9300	 0.2030
B	 0.9660	 0.2110
C	 0.5940	 0.1670
D	 0.8570	 0.1280
E	 0.8250	 0.1820
F	 0.9440	 0.2180
G	 0.3060	 0.0530
H	 0.9650	 0.3020
I	 0.9020	 0.3480
J	 0.8890	 0.3520
K	 0.9390	 0.3650
L	 0.9400	 0.3670
M	 0.9660	 0.3710
N	 0.0960	 0.0320
O	 0.9840	 0.3760
P	 0.8160	 0.0910
Q	 0.9570	 0.2970
R	 0.9040	 0.3100
S	 0.9480	 0.3540
T	 0.8900	 0.3580
V	 0.9760	 0.4070
W	 0.9490	 0.3680
X	 0.9650	 0.3750
Y	 0.9580	 0.3410
Z	 0.9290	 0.1410

