



# wwPDB EM Validation Summary Report ⓘ

Jul 29, 2024 – 01:53 PM EDT

PDB ID : 8T9D  
EMDB ID : EMD-41107  
Title : CryoEM structure of TR-TRAP  
Authors : Zhao, H.; Asturias, F.  
Deposited on : 2023-06-23  
Resolution : 4.66 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev92  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.37.1

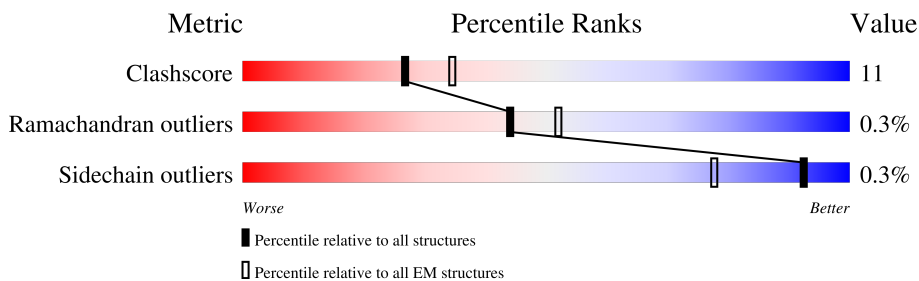
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.66 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.









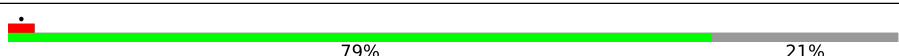










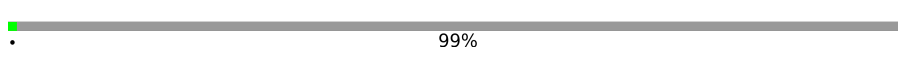
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\geq 3$ , 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	1581	29% 70%
2	B	270	57% 41%
3	C	246	49% 21% 28%
4	D	233	69% 31%
5	E	268	66% 32%
6	F	146	47% 50%
7	G	135	23% 90% 10%
8	H	117	78% 9% 10%

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Mol	Chain	Length	Quality of chain
9	I	1454	
10	J	788	
11	K	877	
12	L	651	
13	M	208	
14	O	212	
15	P	144	
16	Q	200	
17	R	1368	
18	S	989	
19	T	747	
20	V	311	
21	W	178	
22	X	200	
23	Y	178	
24	Z	131	
25	a	20	
26	9	2174	

## 2 Entry composition i

There are 26 unique types of molecules in this entry. The entry contains 49136 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
			Total	C	N	O		
1	A	467	2354	1405	476	473	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	B	158	793	475	158	160	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	C	178	931	564	185	182	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	D	161	801	479	161	161	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	181	902	537	181	183	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	73	379	228	74	76	1	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	G	122	608	362	123	123	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	105	583	354	116	112	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	1102	6855	4319	1271	1245	20	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	167	1176	753	216	203	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	732	5037	3245	903	866	23	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	543	3393	2134	632	622	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	M	180	1146	729	218	197	2	0	0

- Molecule 14 is a protein called Mediator of RNA polymerase II transcription subunit 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	O	174	1022	645	180	193	4	0	0

- Molecule 15 is a protein called Mediator of RNA polymerase II transcription subunit 21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	P	114	568	340	114	114		0	0

- Molecule 16 is a protein called Mediator of RNA polymerase II transcription subunit 22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	Q	131	759	467	145	147		0	0

- Molecule 17 is a protein called Mediator of RNA polymerase II transcription subunit 23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	R	1294	9758	6300	1684	1721	53	0	0

- Molecule 18 is a protein called Mediator of RNA polymerase II transcription subunit 24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	S	901	5888	3751	1061	1049	27	0	0

- Molecule 19 is a protein called Mediator of RNA polymerase II transcription subunit 25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	T	192	1302	837	223	237	5	0	0

- Molecule 20 is a protein called Mediator of RNA polymerase II transcription subunit 27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	V	270	1683	1067	307	306	3	0	0

- Molecule 21 is a protein called Mediator of RNA polymerase II transcription subunit 28.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	118	Total	C	N	O	S	0	0
			781	489	146	144	2		

- Molecule 22 is a protein called Mediator of RNA polymerase II transcription subunit 29.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	X	123	Total	C	N	O	S	0	0
			842	530	150	159	3		

- Molecule 23 is a protein called Mediator of RNA polymerase II transcription subunit 30.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Y	132	Total	C	N	O	S	0	0
			839	523	167	146	3		

- Molecule 24 is a protein called Mediator of RNA polymerase II transcription subunit 31.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	Z	103	Total	C	N	O	0	0
			516	308	103	105		

- Molecule 25 is a protein called Unknown Peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	a	20	Total	C	N	O	0	0
			100	60	20	20		

- Molecule 26 is a protein called Mediator of RNA polymerase II transcription subunit 13.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	9	24	Total	C	N	O	0	0
			120	72	24	24		

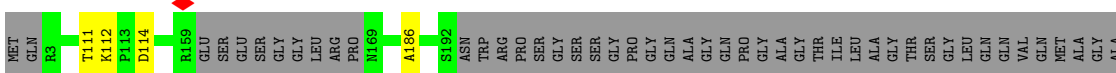






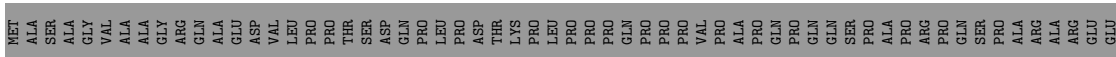
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ALA  
LEU  
CYS  
VAL  
LEU  
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ASP  
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MET  
ASN  
GLU  
ARG  
PRO

• Molecule 5: Mediator of RNA polymerase II transcription subunit 8



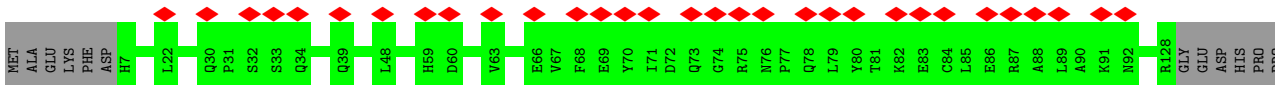
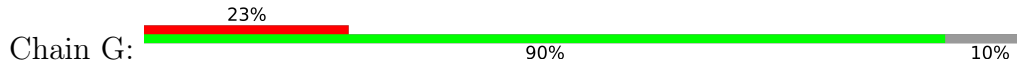
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ASN  
ILE  
LYS  
SER  
SER  
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HIS  
GLN  
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TYR  
GLN  
ARG

• Molecule 6: Mediator of RNA polymerase II transcription subunit 9



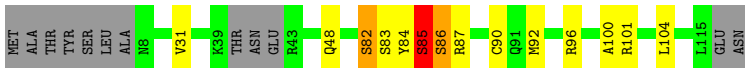
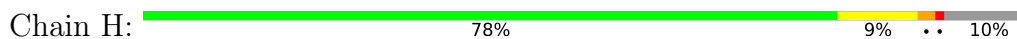
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Q115  
L118  
E142  
ILE  
PRO  
LYS  
GLU

• Molecule 7: Mediator of RNA polymerase II transcription subunit 10

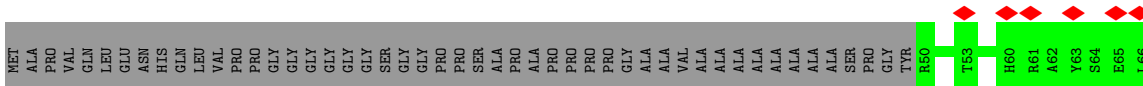


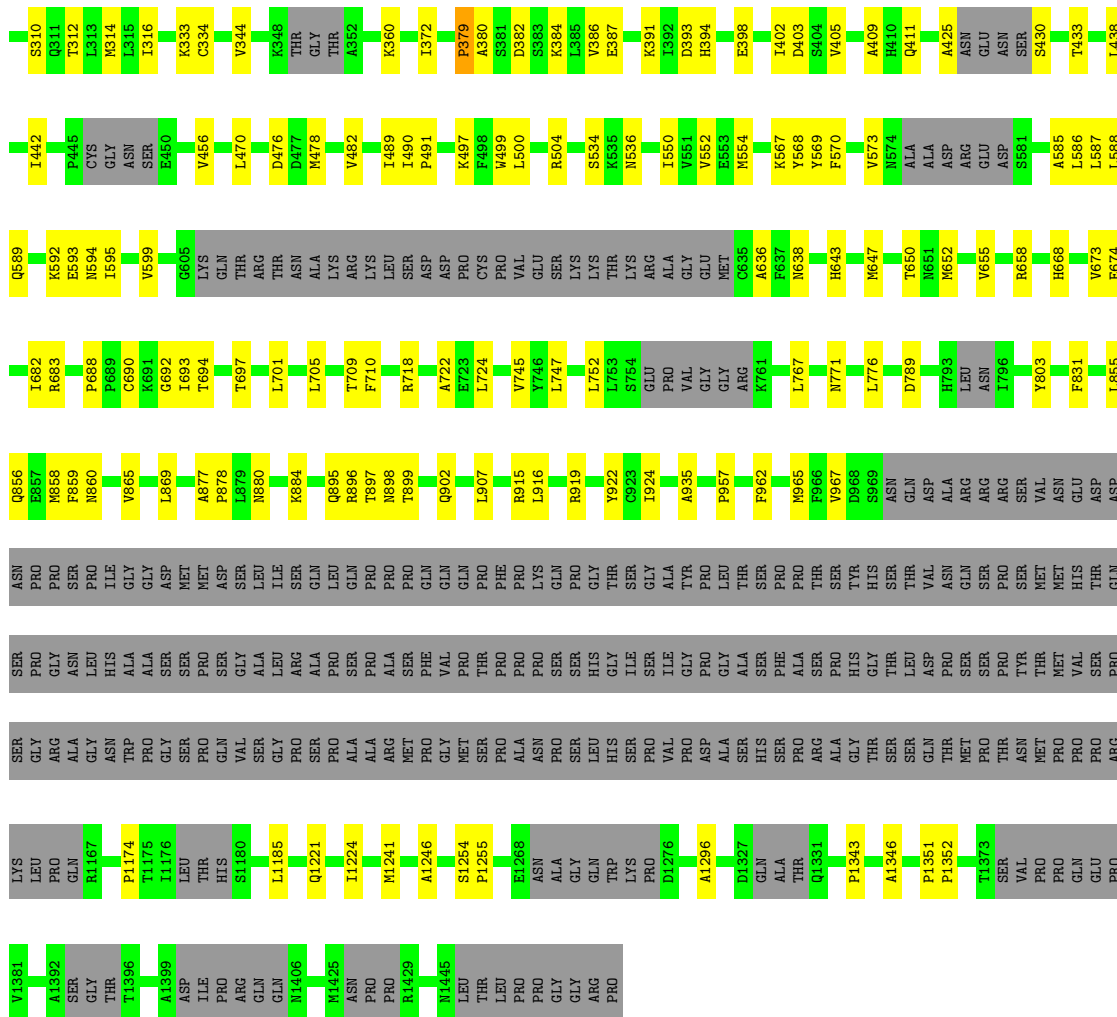
SER

• Molecule 8: Mediator of RNA polymerase II transcription subunit 11



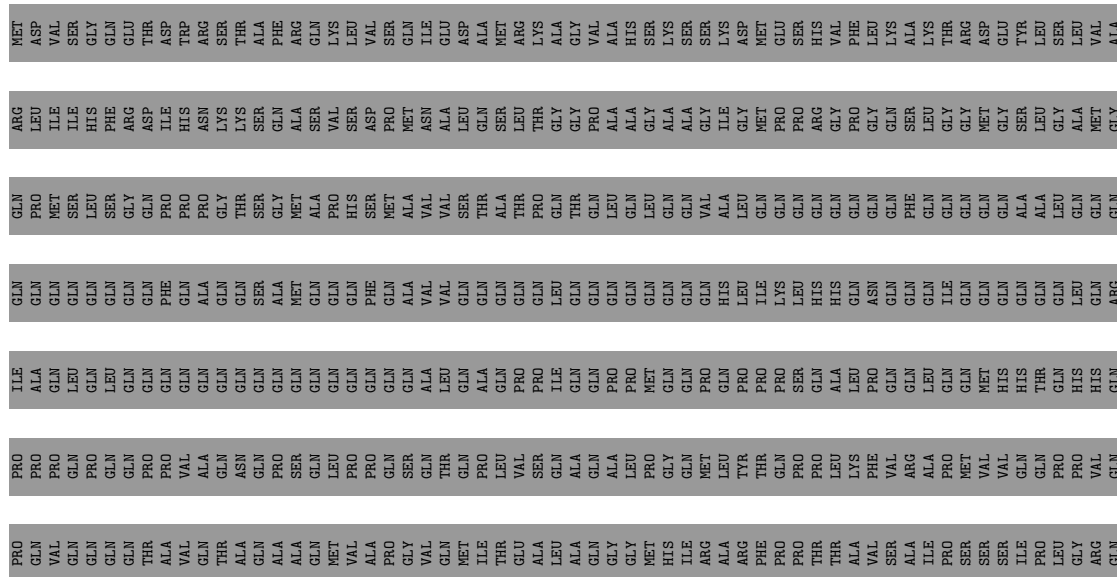
• Molecule 9: Mediator of RNA polymerase II transcription subunit 14

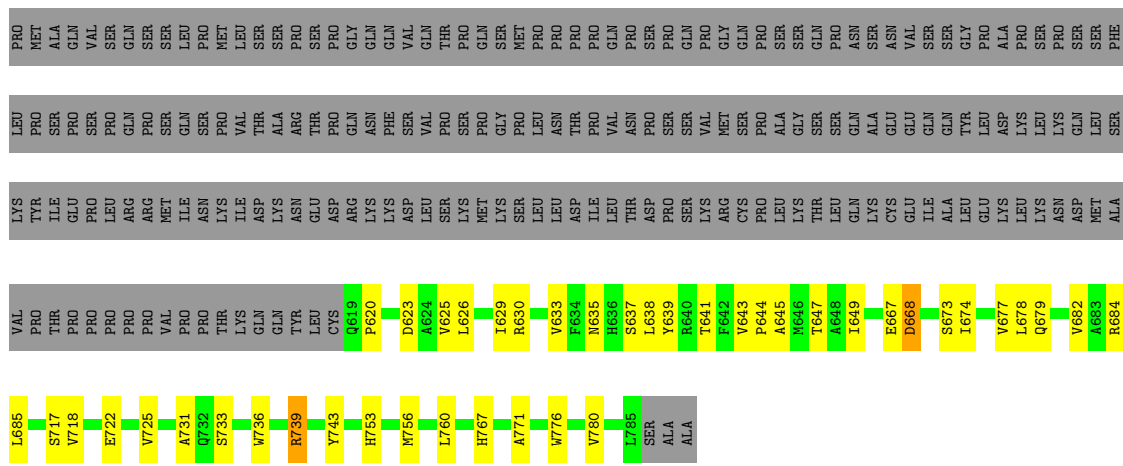




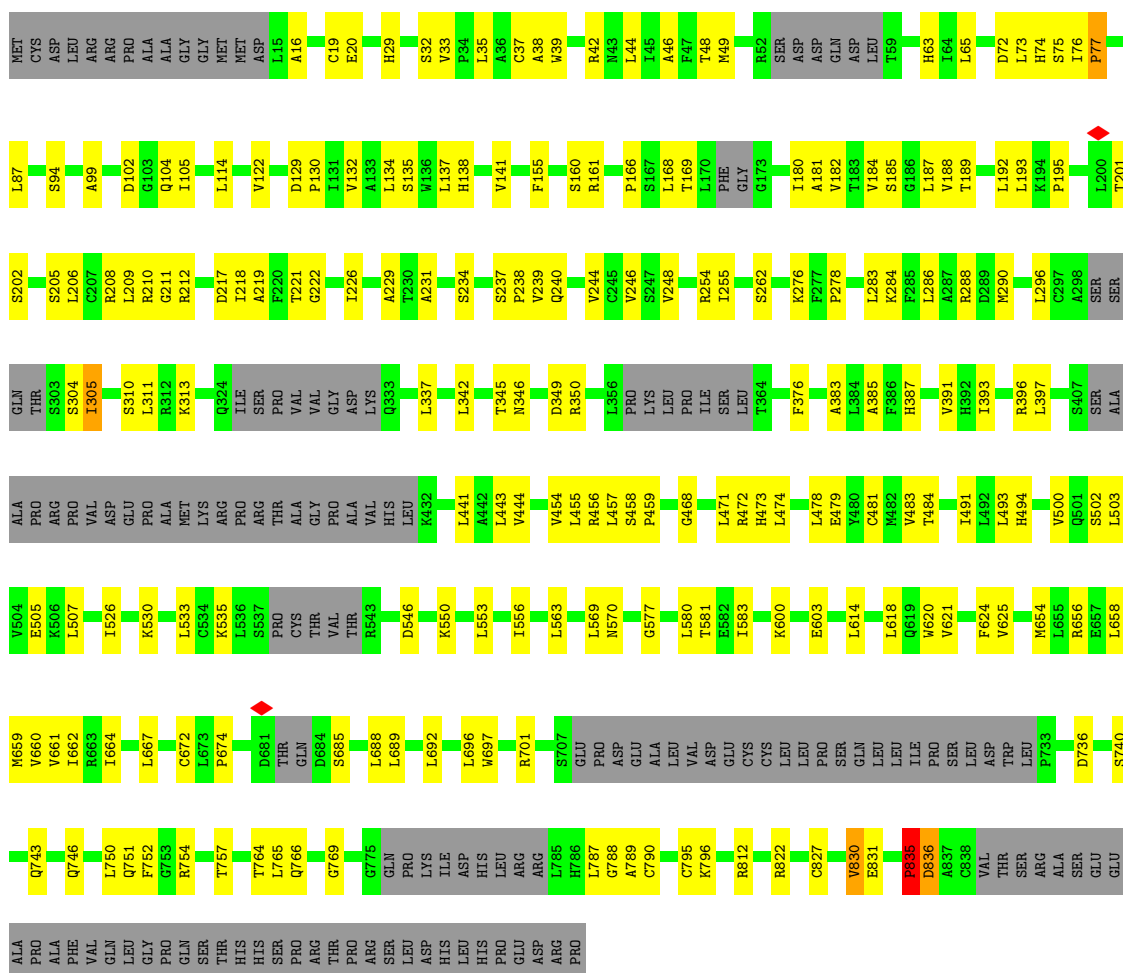
● Molecule 10: Mediator of RNA polymerase II transcription subunit 15

Chain J: 16% 5% 79%



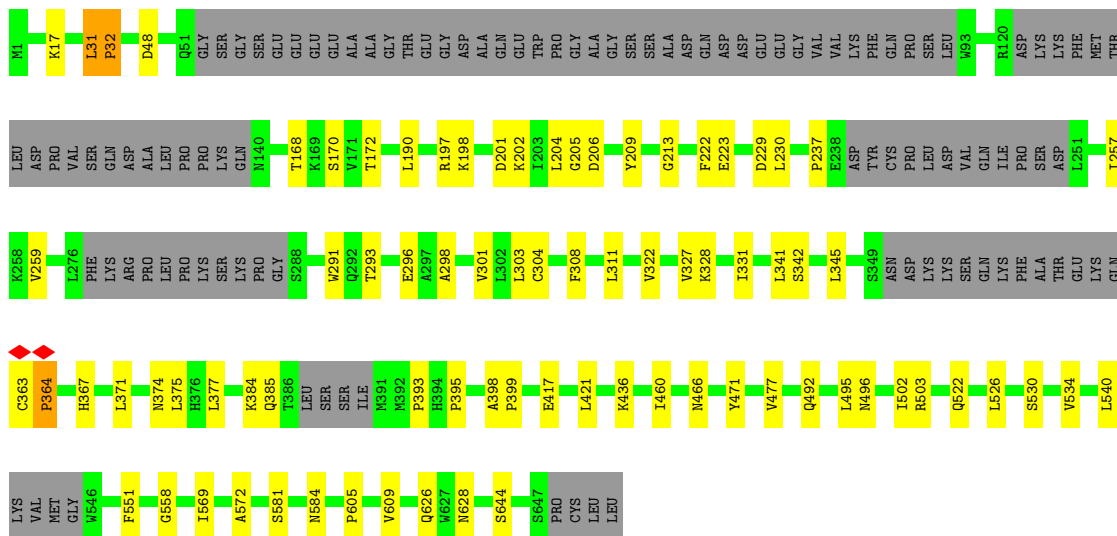


• Molecule 11: Mediator of RNA polymerase II transcription subunit 16

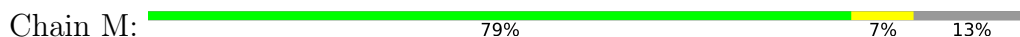


• Molecule 12: Mediator of RNA polymerase II transcription subunit 17

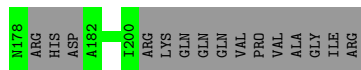
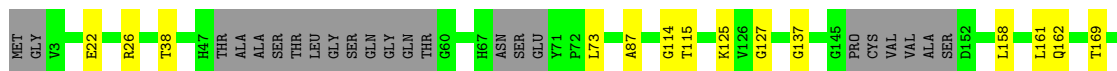




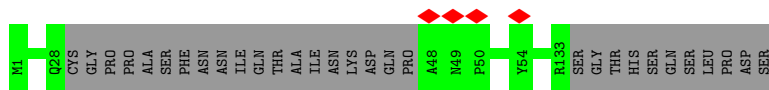
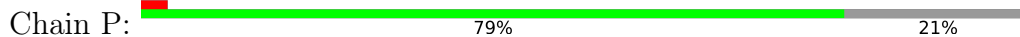
- Molecule 13: Mediator of RNA polymerase II transcription subunit 18



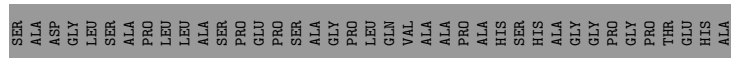
- Molecule 14: Mediator of RNA polymerase II transcription subunit 20



- Molecule 15: Mediator of RNA polymerase II transcription subunit 21

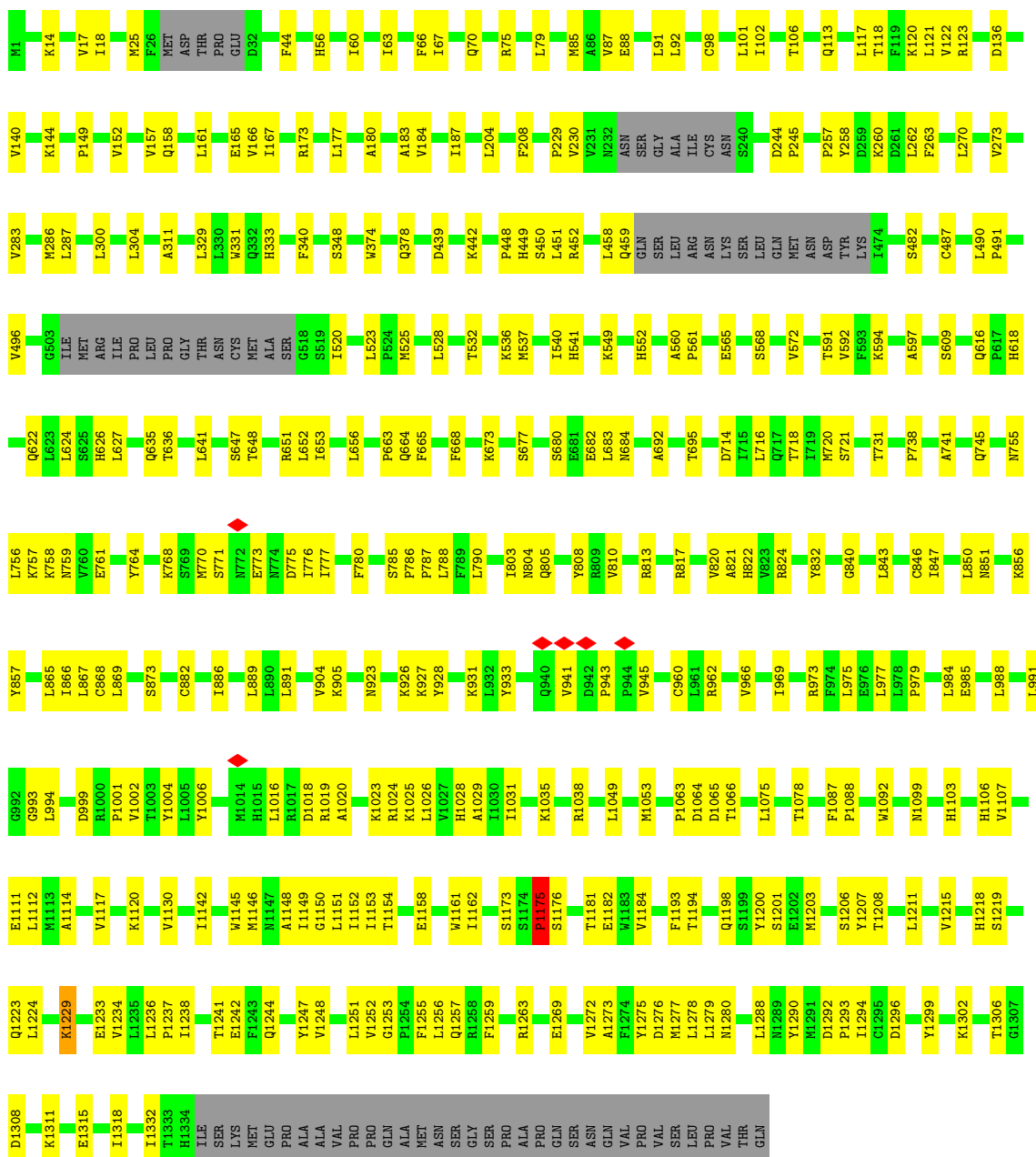


- Molecule 16: Mediator of RNA polymerase II transcription subunit 22




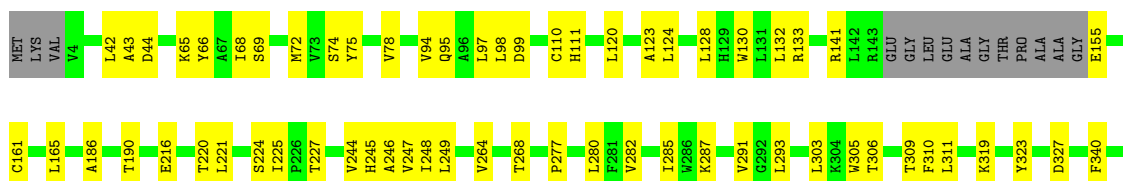
• Molecule 17: Mediator of RNA polymerase II transcription subunit 23

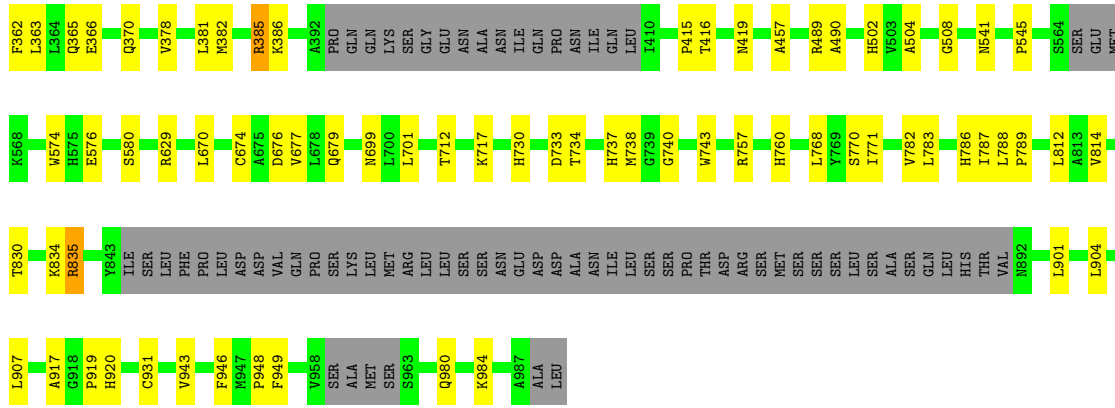
Chain R:  70% 24% 5%



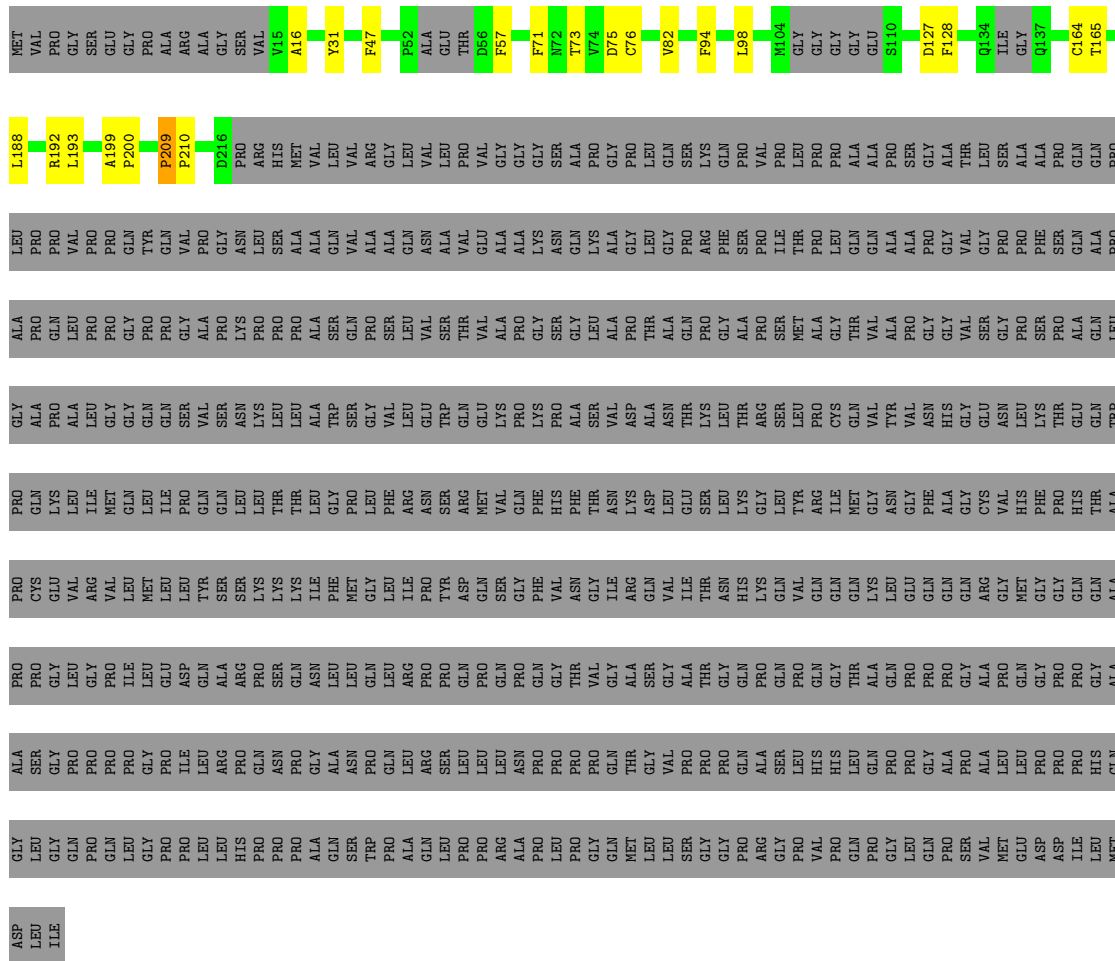
• Molecule 18: Mediator of RNA polymerase II transcription subunit 24

Chain S:  78% 13% 9%

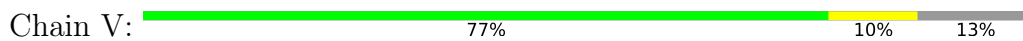


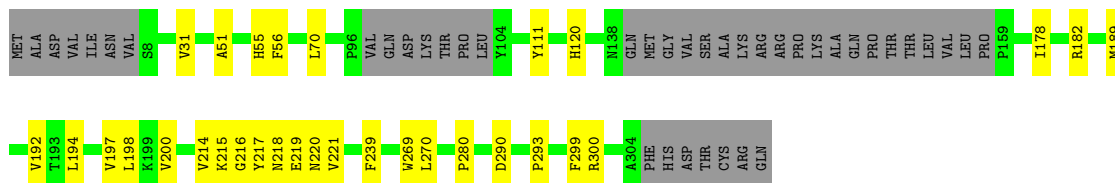


● Molecule 19: Mediator of RNA polymerase II transcription subunit 25

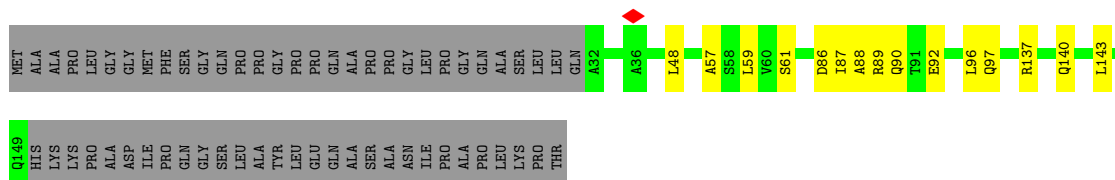


● Molecule 20: Mediator of RNA polymerase II transcription subunit 27

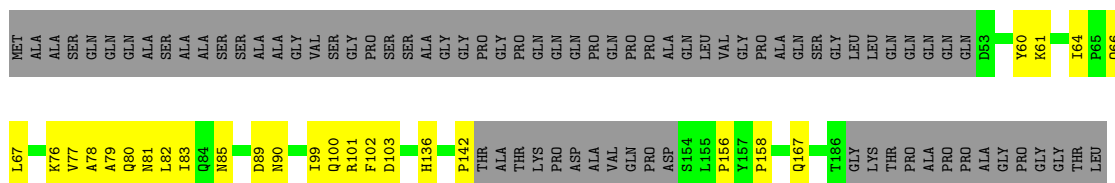




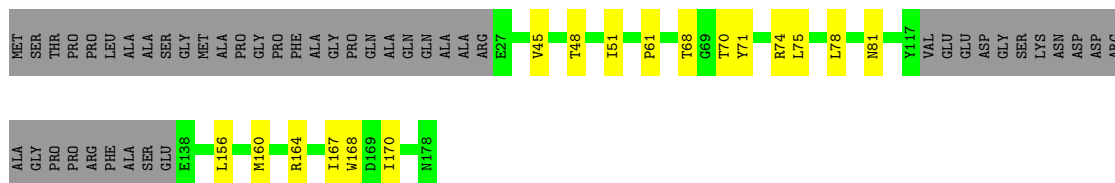
- Molecule 21: Mediator of RNA polymerase II transcription subunit 28



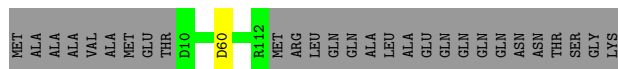
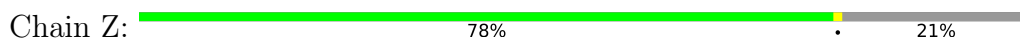
- Molecule 22: Mediator of RNA polymerase II transcription subunit 29



- Molecule 23: Mediator of RNA polymerase II transcription subunit 30



- Molecule 24: Mediator of RNA polymerase II transcription subunit 31



- Molecule 25: Unknown Peptide



There are no outlier residues recorded for this chain.

- Molecule 26: Mediator of RNA polymerase II transcription subunit 13







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	31505	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	100	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	35000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.563	Depositor
Minimum map value	-0.198	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.04	Depositor
Map size ( $\text{\AA}$ )	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 ( $\text{\AA}$ )	1.11, 1.11, 1.11	Depositor

## 5 Model quality i

### 5.1 Standard geometry i

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.23	0/2348	0.42	1/3260 (0.0%)
2	B	0.23	0/791	0.34	0/1100
3	C	0.68	2/933 (0.2%)	0.73	3/1289 (0.2%)
4	D	0.23	0/800	0.34	0/1116
5	E	0.23	0/900	0.40	0/1252
6	F	0.22	0/377	0.33	0/521
7	G	0.23	0/607	0.33	0/845
8	H	0.22	0/585	0.43	0/805
9	I	0.24	0/6977	0.43	4/9621 (0.0%)
10	J	0.24	0/1212	0.46	1/1678 (0.1%)
11	K	0.24	0/5145	0.48	4/7058 (0.1%)
12	L	0.25	0/3451	0.44	3/4749 (0.1%)
13	M	0.23	0/1169	0.42	0/1598
14	O	0.25	0/1036	0.40	0/1424
15	P	0.22	0/566	0.31	0/788
16	Q	0.22	0/763	0.38	0/1053
17	R	0.24	0/10006	0.43	5/13665 (0.0%)
18	S	0.24	0/6009	0.42	2/8258 (0.0%)
19	T	0.27	0/1340	0.48	1/1842 (0.1%)
20	V	0.23	0/1721	0.39	0/2377
21	W	0.23	0/793	0.37	0/1086
22	X	0.23	0/855	0.39	0/1172
23	Y	0.22	0/848	0.35	0/1160
24	Z	0.22	0/515	0.46	1/718 (0.1%)
26	9	0.82	0/119	1.02	3/165 (1.8%)
All	All	0.26	2/49866 (0.0%)	0.44	28/68600 (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.

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Mol	Chain	#Chirality outliers	#Planarity outliers
8	H	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	189	PRO	N-CA	13.28	1.69	1.47
3	C	188	PHE	C-N	6.00	1.45	1.34

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	168	PRO	CA-N-CD	-9.16	98.68	111.50
19	T	209	PRO	CA-N-CD	-8.76	99.24	111.50
17	R	1175	PRO	CA-N-CD	-8.64	99.41	111.50
12	L	32	PRO	CA-N-CD	-8.49	99.61	111.50
12	L	364	PRO	CA-N-CD	-8.48	99.62	111.50

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	H	82	SER	Peptide
8	H	85	SER	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	2354	0	1078	12	0
2	B	793	0	374	7	0
3	C	931	0	479	94	0
4	D	801	0	327	0	0
5	E	902	0	408	15	0
6	F	379	0	182	6	0
7	G	608	0	260	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	H	583	0	357	15	0
9	I	6855	0	5052	109	0
10	J	1176	0	1036	36	0
11	K	5037	0	4491	183	0
12	L	3393	0	2495	73	0
13	M	1146	0	845	10	0
14	O	1022	0	684	7	0
15	P	568	0	286	0	0
16	Q	759	0	459	30	0
17	R	9758	0	9145	239	0
18	S	5888	0	4727	105	0
19	T	1302	0	1025	20	0
20	V	1683	0	1190	23	0
21	W	781	0	618	10	0
22	X	842	0	710	31	0
23	Y	839	0	637	17	0
24	Z	516	0	227	0	0
25	a	100	0	23	0	0
26	9	120	0	43	8	0
All	All	49136	0	37158	949	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 11.

The worst 5 of 949 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:130:PHE:CE2	16:Q:62:HIS:CB	1.82	1.57
19:T:209:PRO:CD	19:T:210:PRO:HD2	1.19	1.57
3:C:189:PRO:N	3:C:189:PRO:CA	1.69	1.53
19:T:209:PRO:HD2	19:T:210:PRO:CD	1.08	1.53
3:C:118:ARG:HA	5:E:112:LYS:CB	1.03	1.50

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	455/1581 (29%)	430 (94%)	25 (6%)	0	100	100
2	B	154/270 (57%)	151 (98%)	3 (2%)	0	100	100
3	C	174/246 (71%)	118 (68%)	51 (29%)	5 (3%)	4	32
4	D	159/233 (68%)	153 (96%)	6 (4%)	0	100	100
5	E	177/268 (66%)	161 (91%)	16 (9%)	0	100	100
6	F	69/146 (47%)	67 (97%)	2 (3%)	0	100	100
7	G	120/135 (89%)	119 (99%)	1 (1%)	0	100	100
8	H	101/117 (86%)	92 (91%)	6 (6%)	3 (3%)	4	31
9	I	1068/1454 (74%)	958 (90%)	110 (10%)	0	100	100
10	J	165/788 (21%)	144 (87%)	21 (13%)	0	100	100
11	K	710/877 (81%)	598 (84%)	109 (15%)	3 (0%)	34	72
12	L	527/651 (81%)	460 (87%)	66 (12%)	1 (0%)	47	81
13	M	176/208 (85%)	162 (92%)	14 (8%)	0	100	100
14	O	164/212 (77%)	145 (88%)	19 (12%)	0	100	100
15	P	110/144 (76%)	108 (98%)	2 (2%)	0	100	100
16	Q	129/200 (64%)	123 (95%)	6 (5%)	0	100	100
17	R	1284/1368 (94%)	1127 (88%)	155 (12%)	2 (0%)	47	81
18	S	889/989 (90%)	802 (90%)	86 (10%)	1 (0%)	51	85
19	T	184/747 (25%)	171 (93%)	13 (7%)	0	100	100
20	V	264/311 (85%)	226 (86%)	37 (14%)	1 (0%)	34	72
21	W	116/178 (65%)	113 (97%)	3 (3%)	0	100	100
22	X	119/200 (60%)	115 (97%)	4 (3%)	0	100	100
23	Y	128/178 (72%)	120 (94%)	8 (6%)	0	100	100
24	Z	101/131 (77%)	100 (99%)	1 (1%)	0	100	100
26	9	22/2174 (1%)	6 (27%)	7 (32%)	9 (41%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	7565/13806 (55%)	6769 (90%)	771 (10%)	25 (0%)	44 76

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	168	PRO
3	C	176	ARG
8	H	86	SER
11	K	835	PRO
26	9	621	PRO

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	13/1391 (1%)	13 (100%)	0	100 100
2	B	3/230 (1%)	3 (100%)	0	100 100
3	C	12/223 (5%)	11 (92%)	1 (8%)	11 36
5	E	3/225 (1%)	3 (100%)	0	100 100
6	F	6/133 (4%)	6 (100%)	0	100 100
7	G	1/124 (1%)	1 (100%)	0	100 100
8	H	14/98 (14%)	14 (100%)	0	100 100
9	I	401/1271 (32%)	400 (100%)	1 (0%)	93 96
10	J	104/697 (15%)	103 (99%)	1 (1%)	76 86
11	K	418/766 (55%)	417 (100%)	1 (0%)	93 96
12	L	199/577 (34%)	199 (100%)	0	100 100
13	M	62/183 (34%)	62 (100%)	0	100 100
14	O	47/178 (26%)	47 (100%)	0	100 100
16	Q	25/173 (14%)	25 (100%)	0	100 100
17	R	956/1232 (78%)	954 (100%)	2 (0%)	93 96
18	S	402/864 (46%)	399 (99%)	3 (1%)	84 90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	T	96/601 (16%)	96 (100%)	0	100	100
20	V	95/280 (34%)	95 (100%)	0	100	100
21	W	55/152 (36%)	55 (100%)	0	100	100
22	X	67/163 (41%)	67 (100%)	0	100	100
23	Y	47/155 (30%)	47 (100%)	0	100	100
24	Z	1/115 (1%)	1 (100%)	0	100	100
All	All	3027/9831 (31%)	3018 (100%)	9 (0%)	92	95

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	S	489	ARG
18	S	835	ARG
11	K	754	ARG
17	R	536	LYS
17	R	1229	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
18	S	747	ASN
20	V	252	HIS
18	S	760	HIS
20	V	55	HIS
21	W	140	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

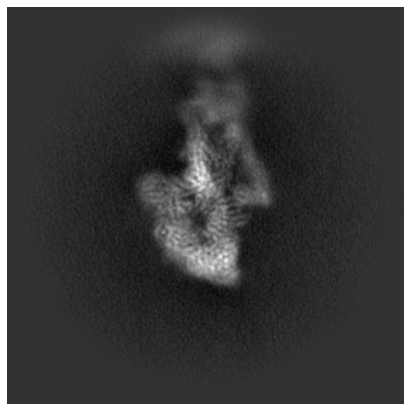
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41107. These allow visual inspection of the internal detail of the map and identification of artifacts.

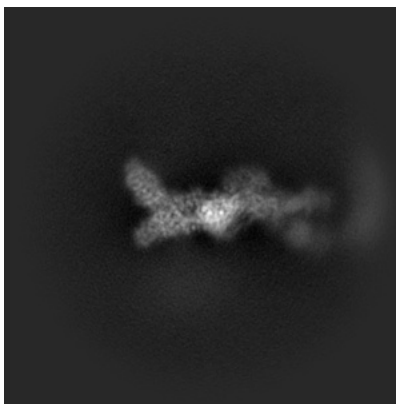
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

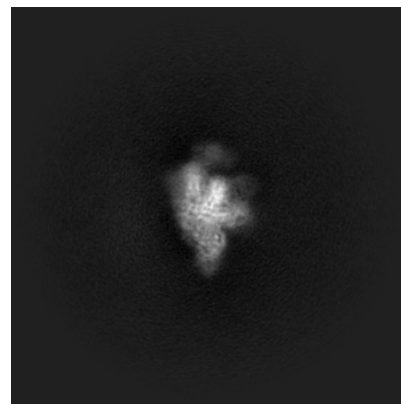
#### 6.1.1 Primary map



X

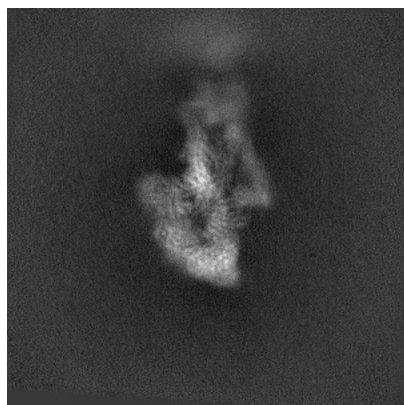


Y

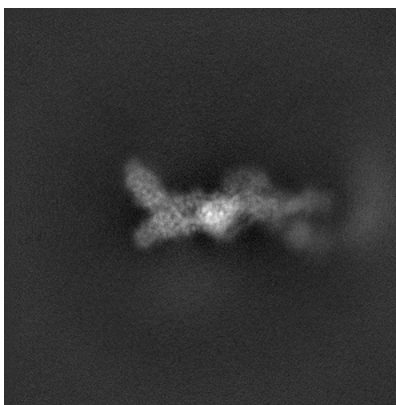


Z

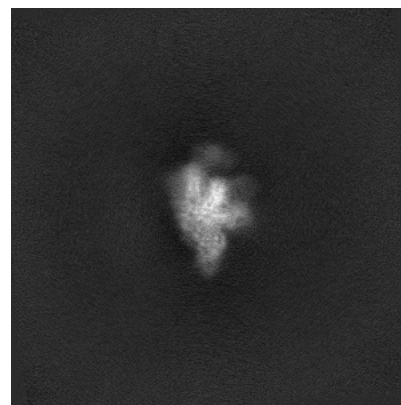
#### 6.1.2 Raw map



X



Y

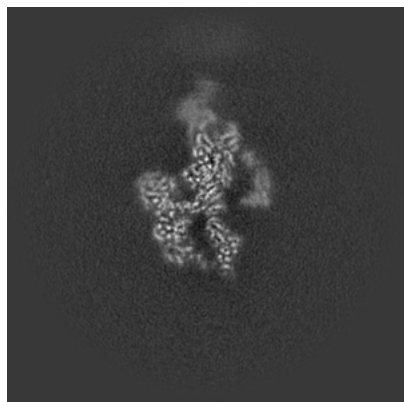


Z

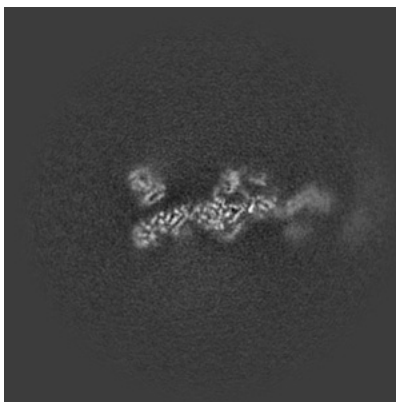
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

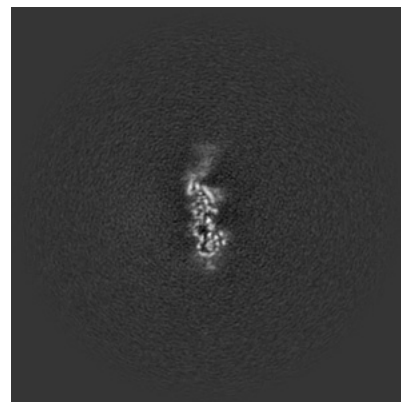
### 6.2.1 Primary map



X Index: 280

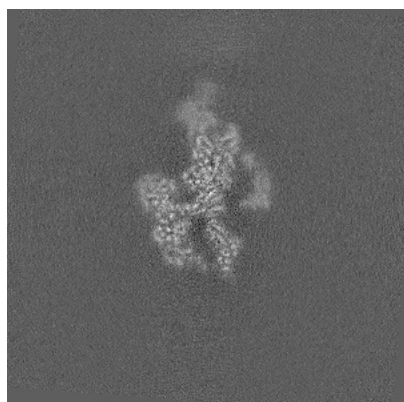


Y Index: 280



Z Index: 280

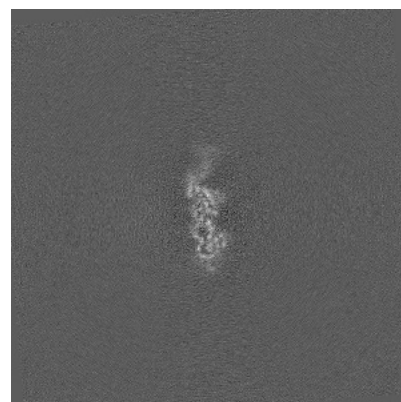
### 6.2.2 Raw map



X Index: 280



Y Index: 280

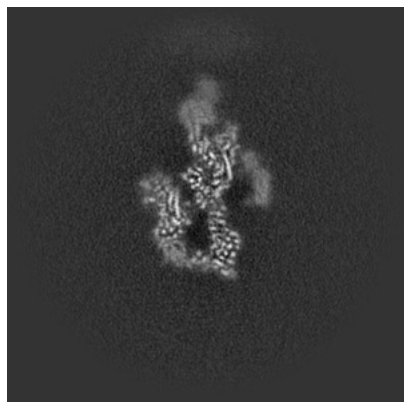


Z Index: 280

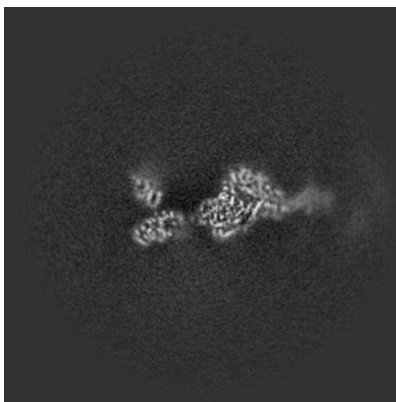
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

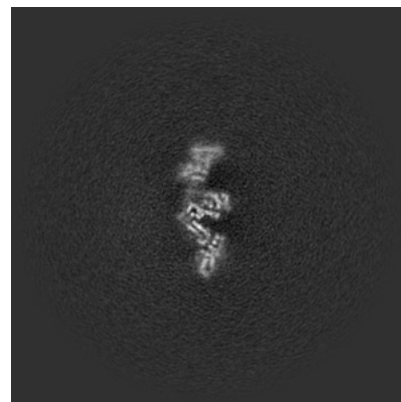
### 6.3.1 Primary map



X Index: 286

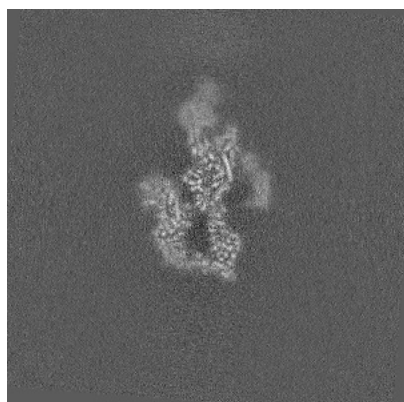


Y Index: 270

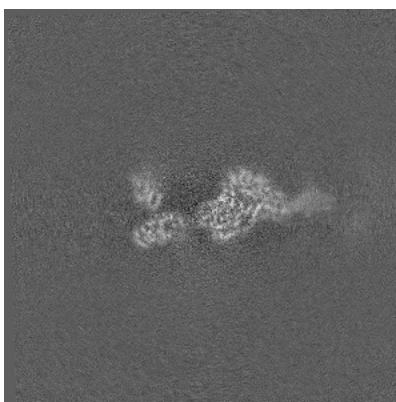


Z Index: 297

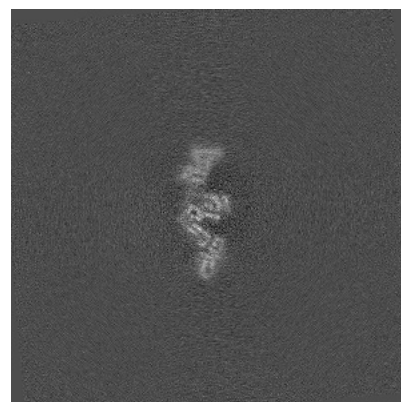
### 6.3.2 Raw map



X Index: 285



Y Index: 270

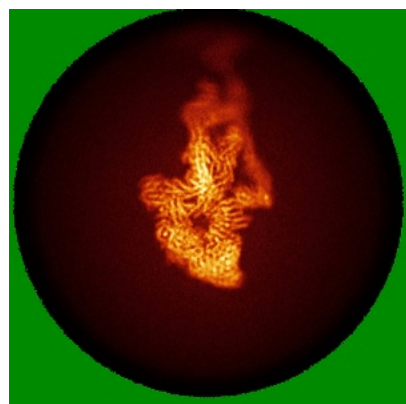


Z Index: 297

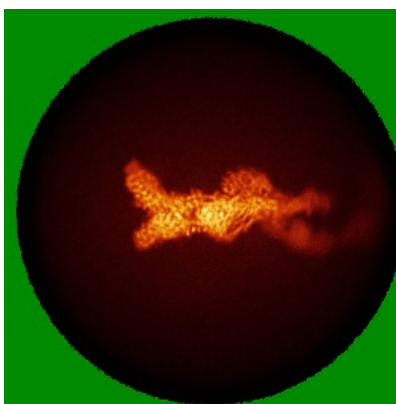
The images above show the largest variance slices of the map in three orthogonal directions.

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

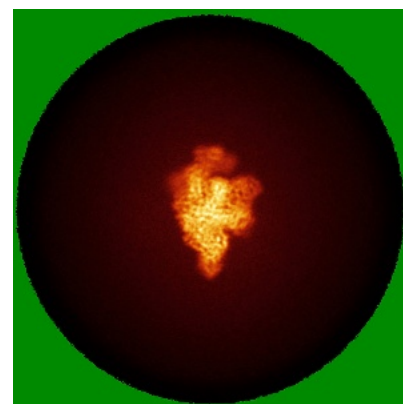
### 6.4.1 Primary map



X

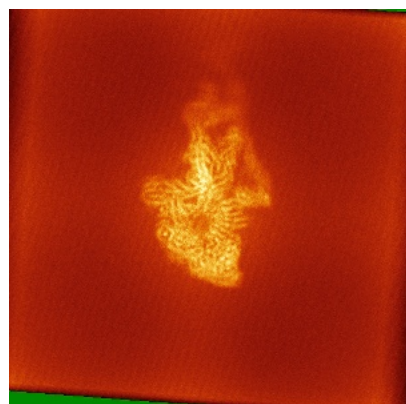


Y

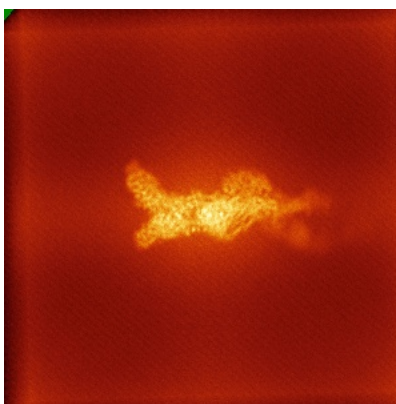


Z

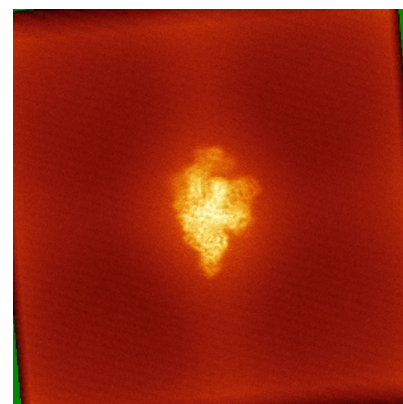
### 6.4.2 Raw map



X



Y

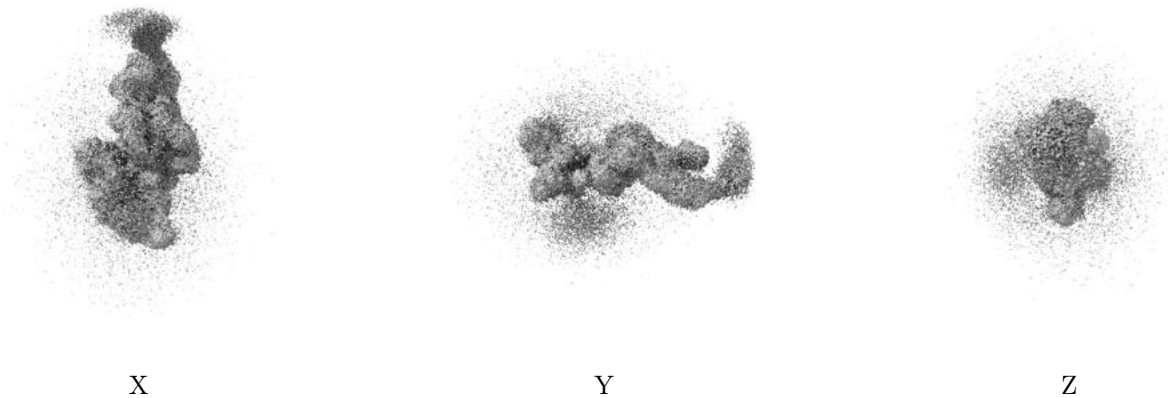


Z

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.

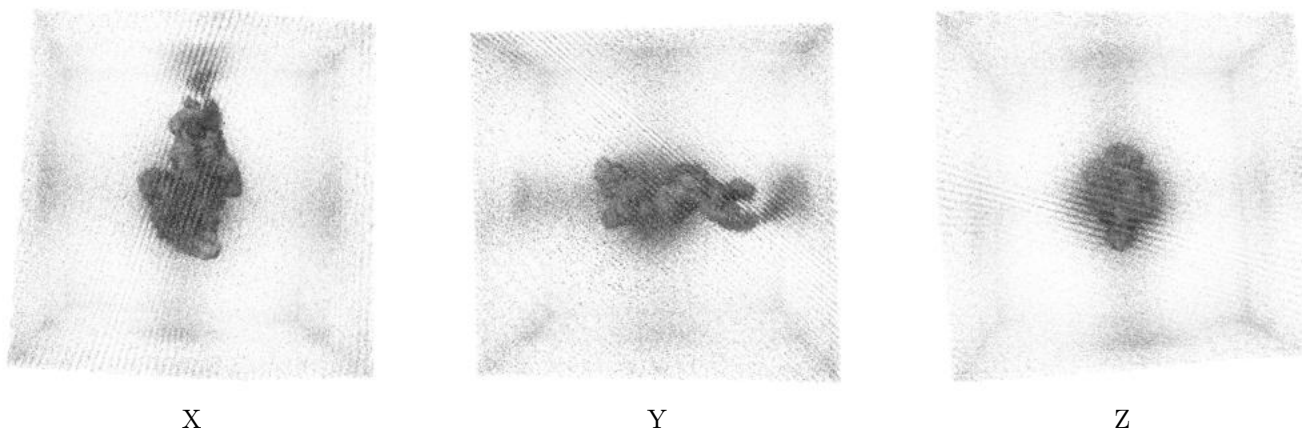
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

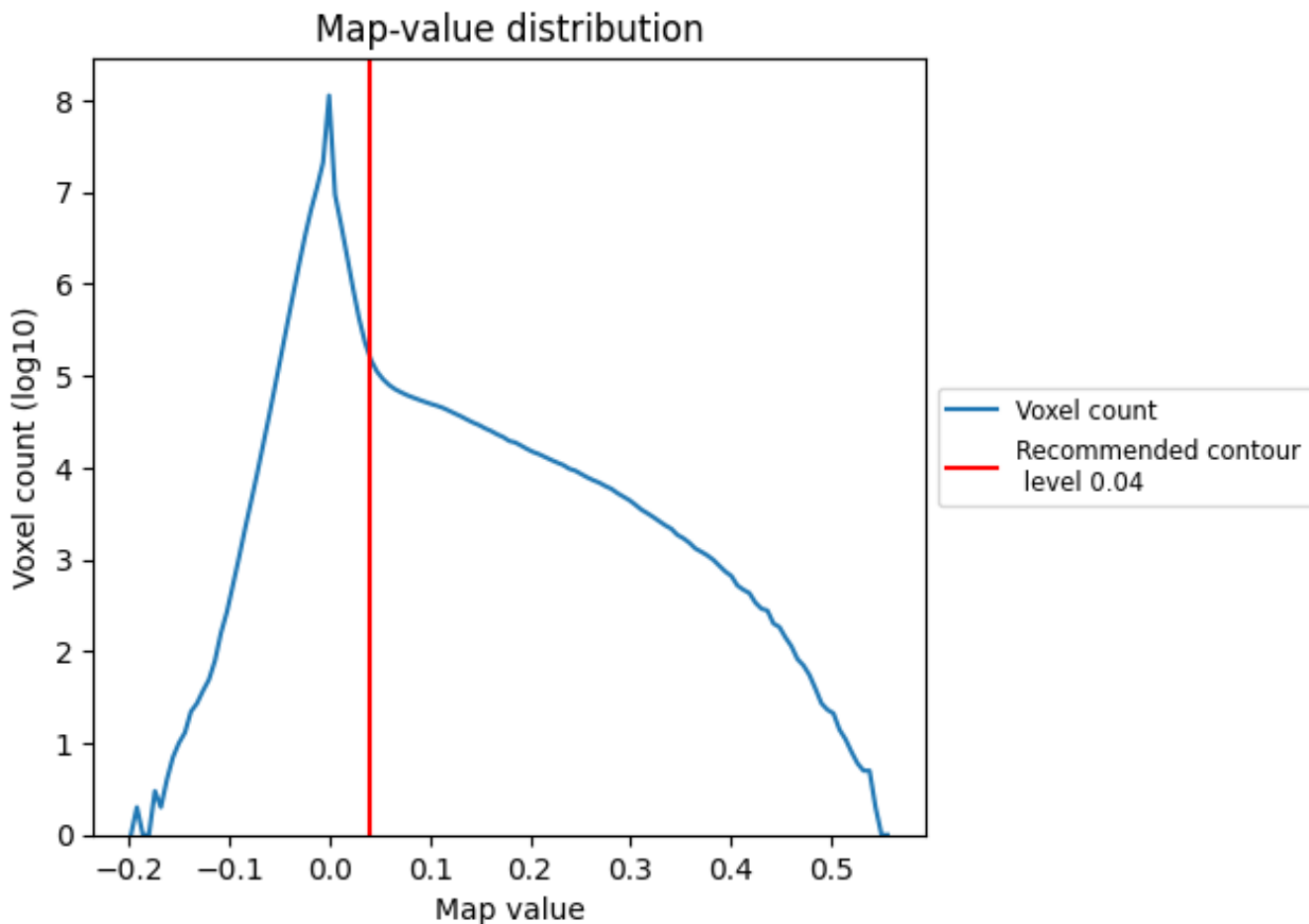
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

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

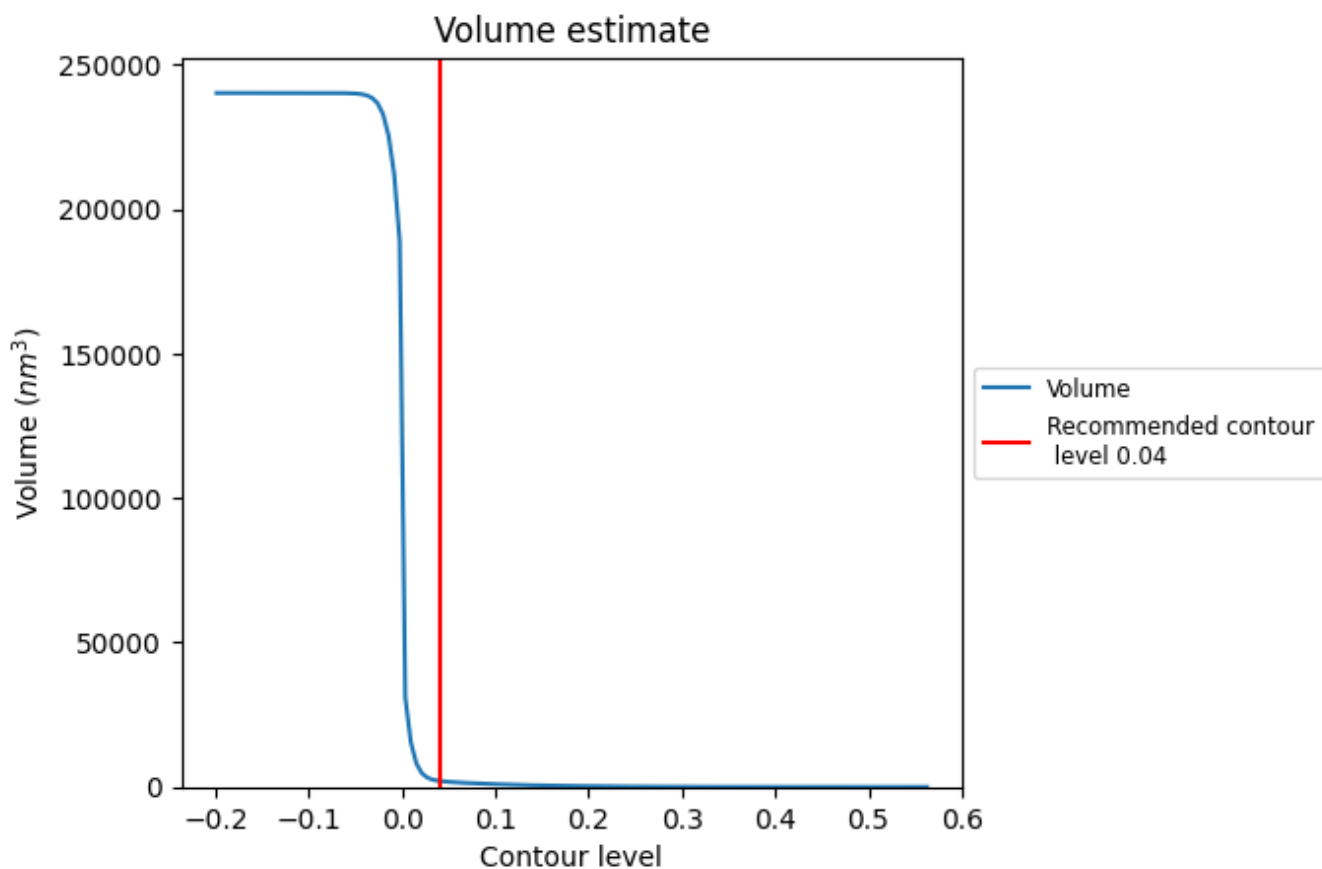
### 7.1 Map-value distribution [i](#)



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



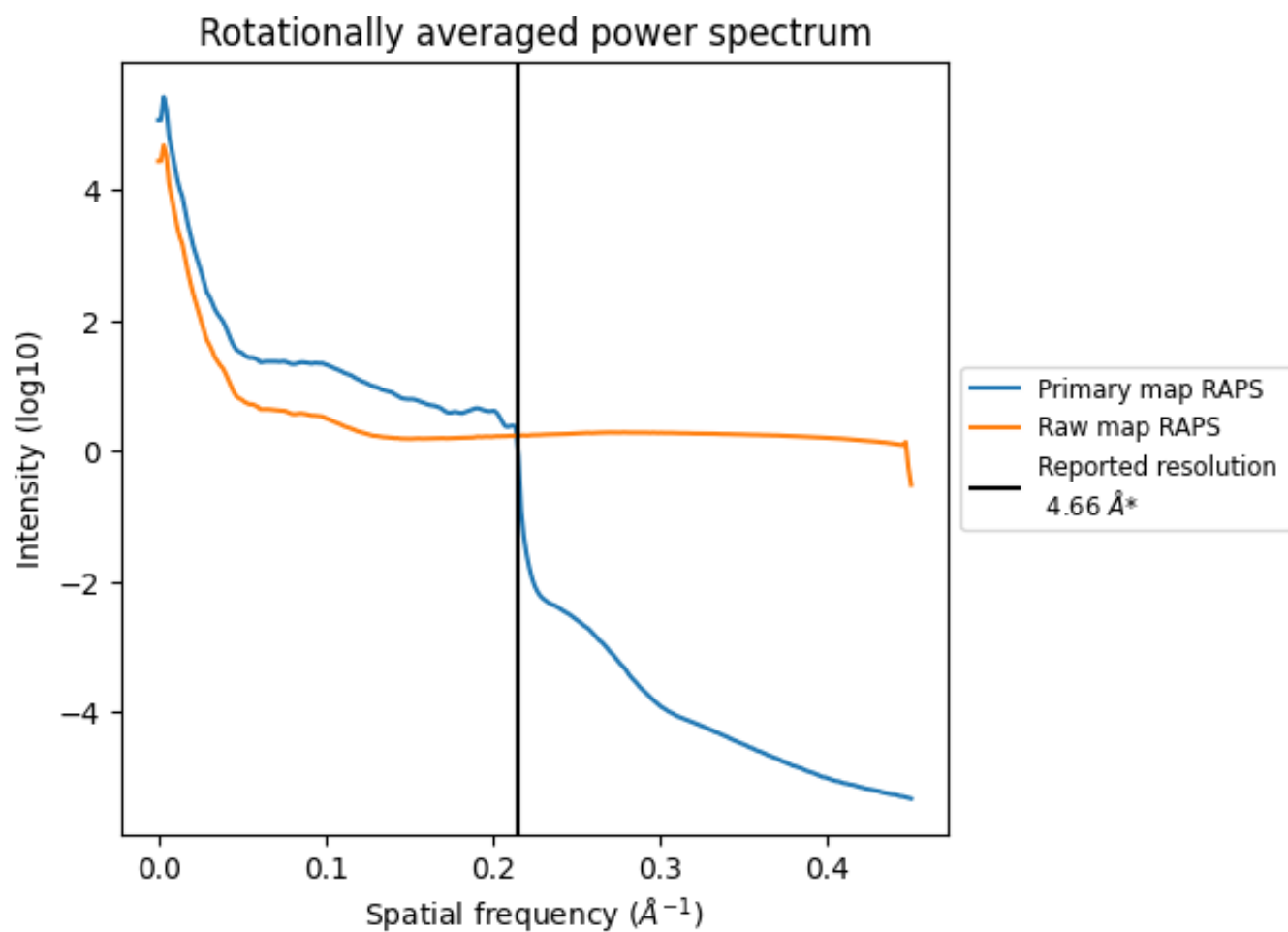
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 2101  $\text{nm}^3$ ; this corresponds to an approximate mass of 1898 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 [i](#)

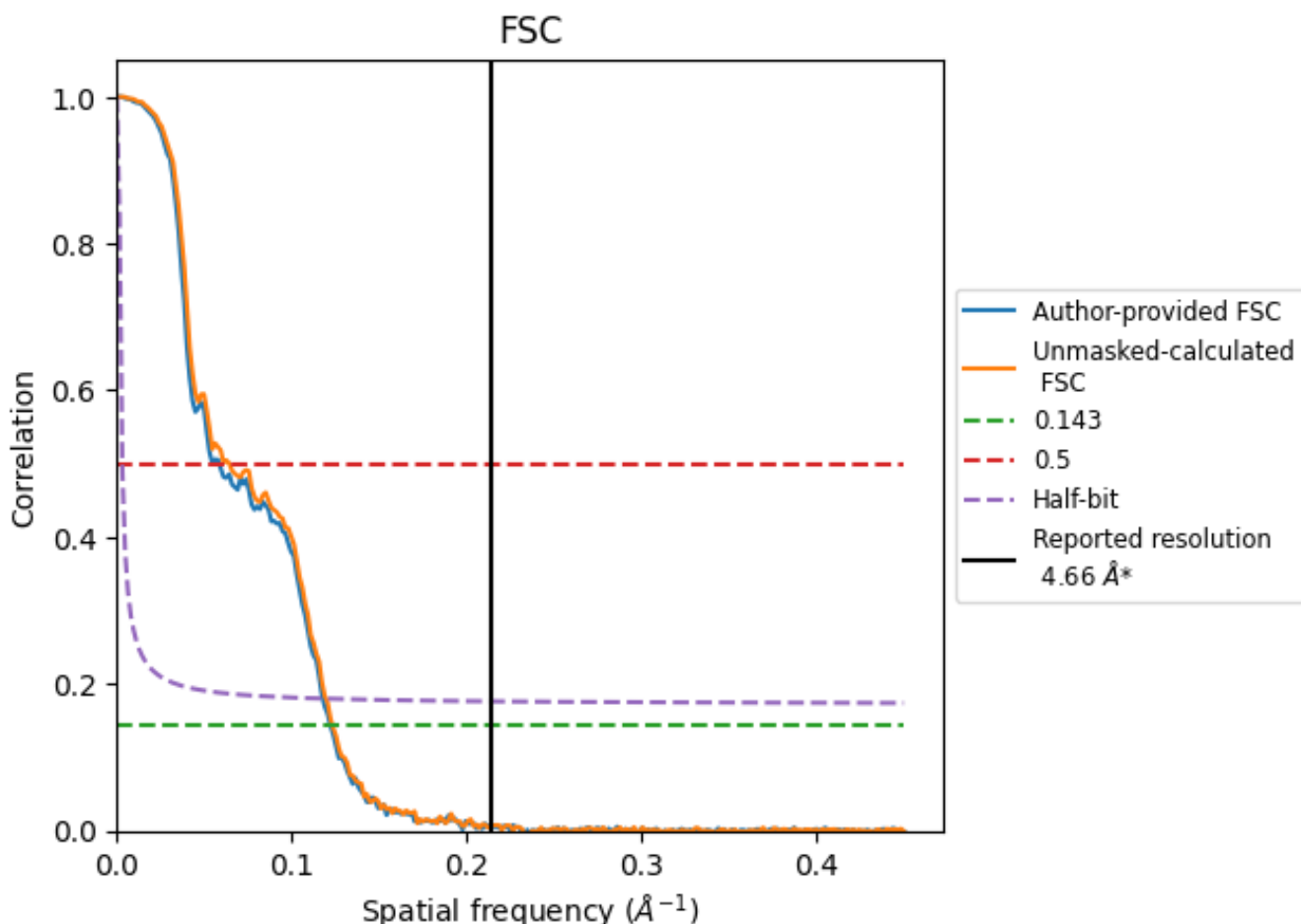


\*Reported resolution corresponds to spatial frequency of  $0.215 \text{ \AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.215 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.66	-	-
Author-provided FSC curve	8.18	17.06	8.47
Unmasked-calculated*	8.10	15.55	8.35

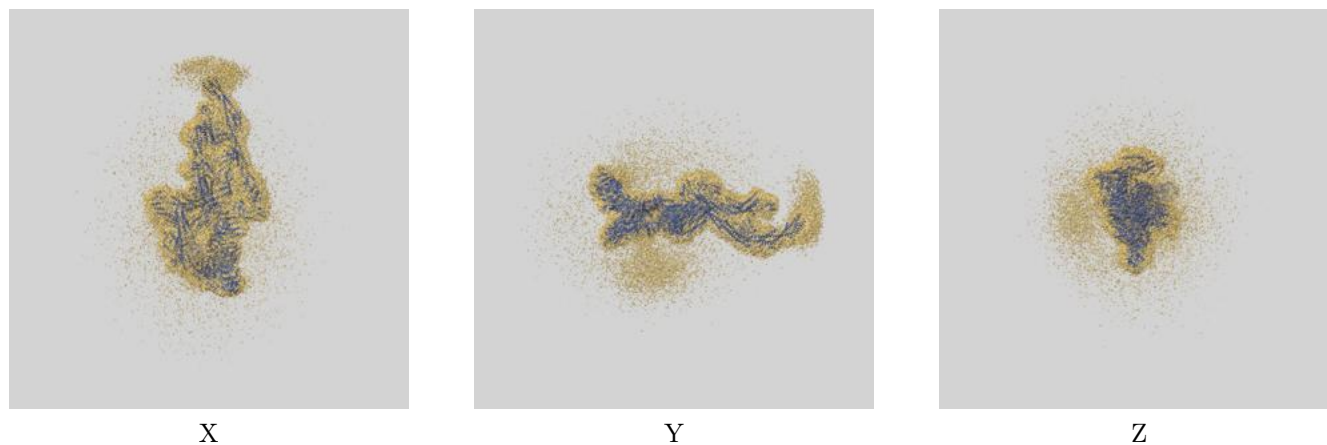
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 8.18 differs from the reported value 4.66 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.10 differs from the reported value 4.66 by more than 10 %

## 9 Map-model fit [i](#)

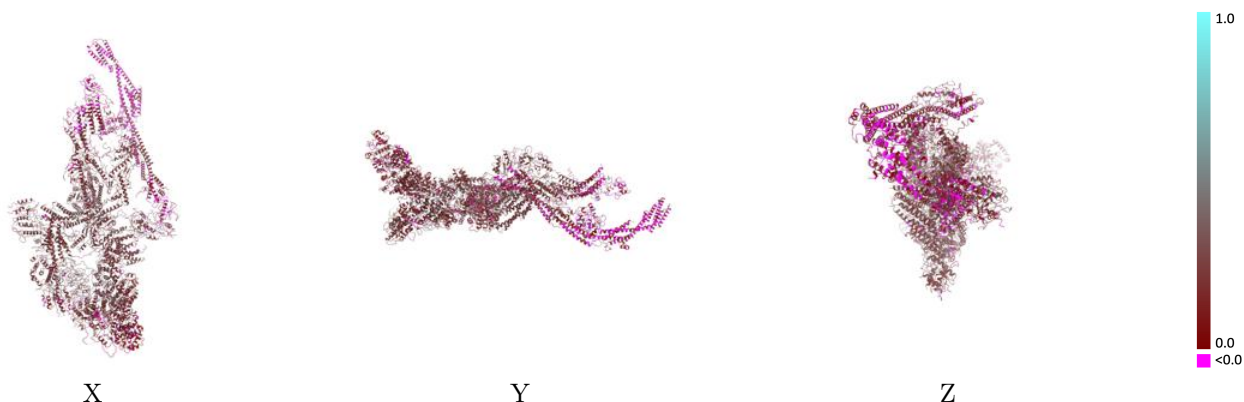
This section contains information regarding the fit between EMDB map EMD-41107 and PDB model 8T9D. Per-residue inclusion information can be found in section [3](#) on page [8](#).

### 9.1 Map-model overlay [i](#)



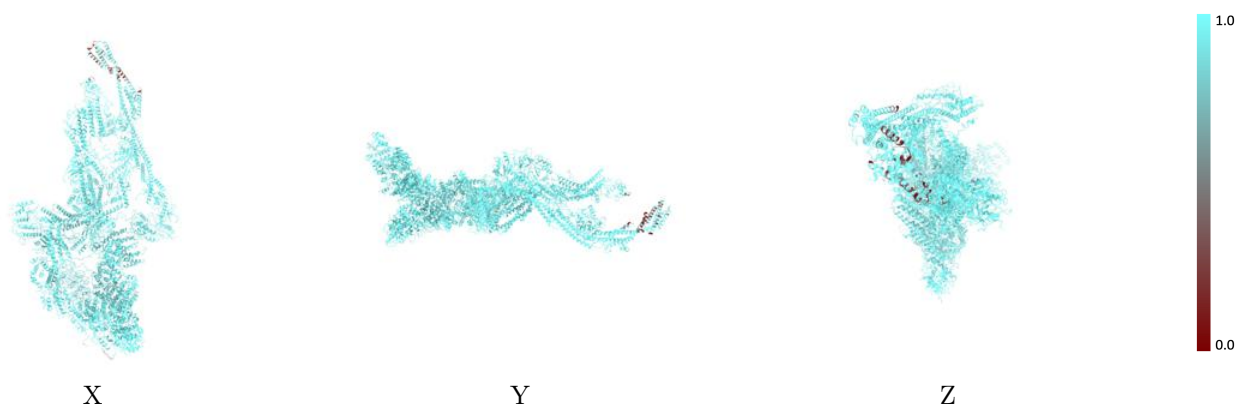
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



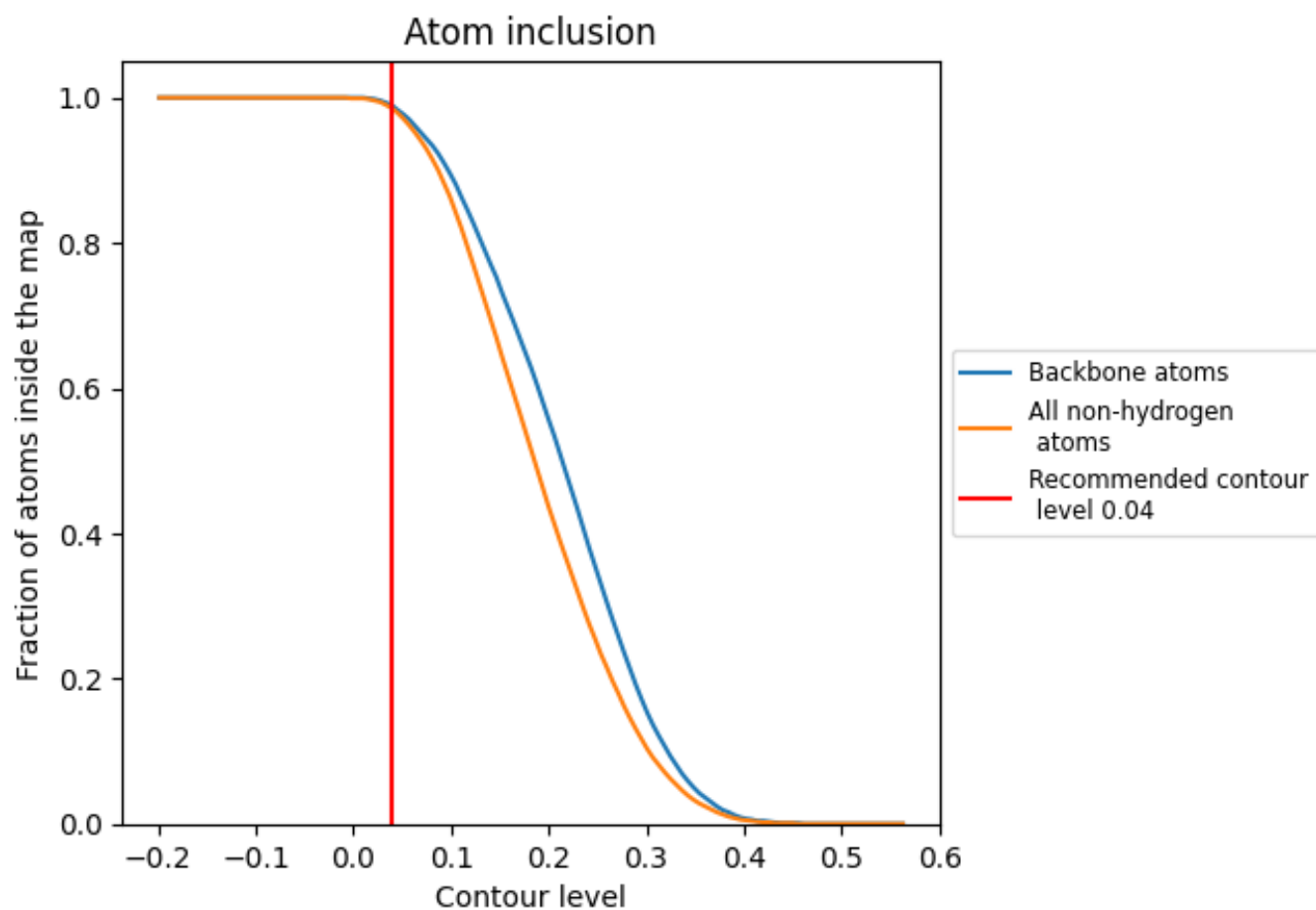
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).























































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 98% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9850	 0.2150
9	 1.0000	 0.2220
A	 0.9970	 0.1740
B	 0.9950	 0.1190
C	 0.9630	 0.1290
D	 0.9950	 0.0790
E	 0.9950	 0.1370
F	 1.0000	 0.1670
G	 0.7220	 0.0500
H	 0.9970	 0.1930
I	 0.9800	 0.2420
J	 0.9910	 0.2480
K	 0.9890	 0.2450
L	 0.9880	 0.2410
M	 0.9990	 0.2300
O	 1.0000	 0.2760
P	 0.9600	 0.0750
Q	 0.9930	 0.1920
R	 0.9840	 0.1950
S	 0.9920	 0.2380
T	 0.9950	 0.2050
V	 0.9960	 0.3020
W	 0.9910	 0.2380
X	 1.0000	 0.2500
Y	 0.9990	 0.2570
Z	 0.9940	 0.0880
a	 1.0000	 0.2080

