



wwPDB EM Validation Summary Report ⓘ

Mar 19, 2026 – 10:45 PM UTC

PDB ID : 8T1I / pdb_00008t1i
EMDB ID : EMD-40968
Title : Atomic model of the mammalian Mediator complex with MED26 subunit
Authors : Zhao, H.; Asturias, F.
Deposited on : 2023-06-02
Resolution : 4.68 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.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

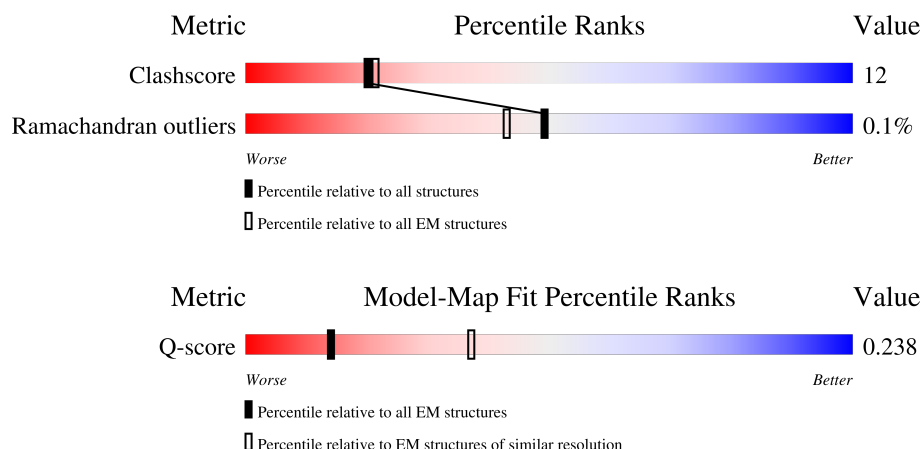
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.68 Å.

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



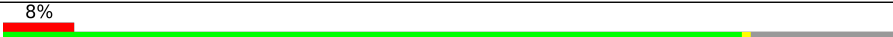
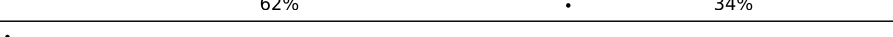
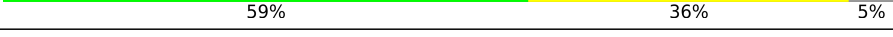
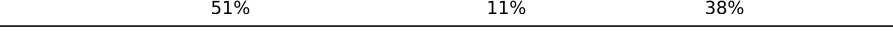
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Q-score	-	25397	1991 (4.18 - 5.18)

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	1575	 27% 70%
2	B	270	 58% 41%
3	C	246	 23% 59% 5% 36%
4	D	233	 66% 31%
5	E	268	 6% 62% 38%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
6	F	142	
7	G	135	
8	H	117	
9	I	1459	
10	J	789	
11	K	828	
12	L	649	
13	M	208	
14	N	240	
15	O	212	
16	P	144	
17	Q	200	
18	R	1367	
19	S	987	
20	T	745	
21	U	588	
22	V	311	
23	W	178	
24	X	199	
25	Y	178	
26	Z	131	
27	a	20	

2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 49568 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	467	Total	C	N	O	0	0
			2314	1380	467	467		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	158	Total	C	N	O	0	0
			784	468	158	158		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	157	Total	C	N	O	0	0
			785	471	157	157		

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

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

- 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	73	Total	C	N	O	0	0
			363	217	73	73		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	122	Total	C	N	O	0	0
			605	361	122	122		

- 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	1086	Total	C	N	O	S	0	0
			6772	4287	1254	1211	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	738	Total	C	N	O	S	0	0
			5085	3283	912	867	23		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	544	Total	C	N	O	S	0	0
			3335	2093	628	611	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	75	Total	C	N	O	S	0	0
			475	293	85	95	2		

- 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	121	Total	C	N	O		0	0
			602	360	121	121			

- 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 26.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	U	97	Total	C	N	O	0	0
			481	287	97	97		

- Molecule 22 is a protein called Mediator of RNA polymerase II transcription subunit 27.

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

- Molecule 23 is a protein called Mediator of RNA polymerase II transcription subunit 28.

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

- Molecule 24 is a protein called Mediator of RNA polymerase II transcription subunit 29.

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

- Molecule 25 is a protein called Mediator of RNA polymerase II transcription subunit 30.

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

- Molecule 26 is a protein called Mediator of RNA polymerase II transcription subunit 31.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	Z	109	Total	C	N	O	0	0
			543	325	109	109		

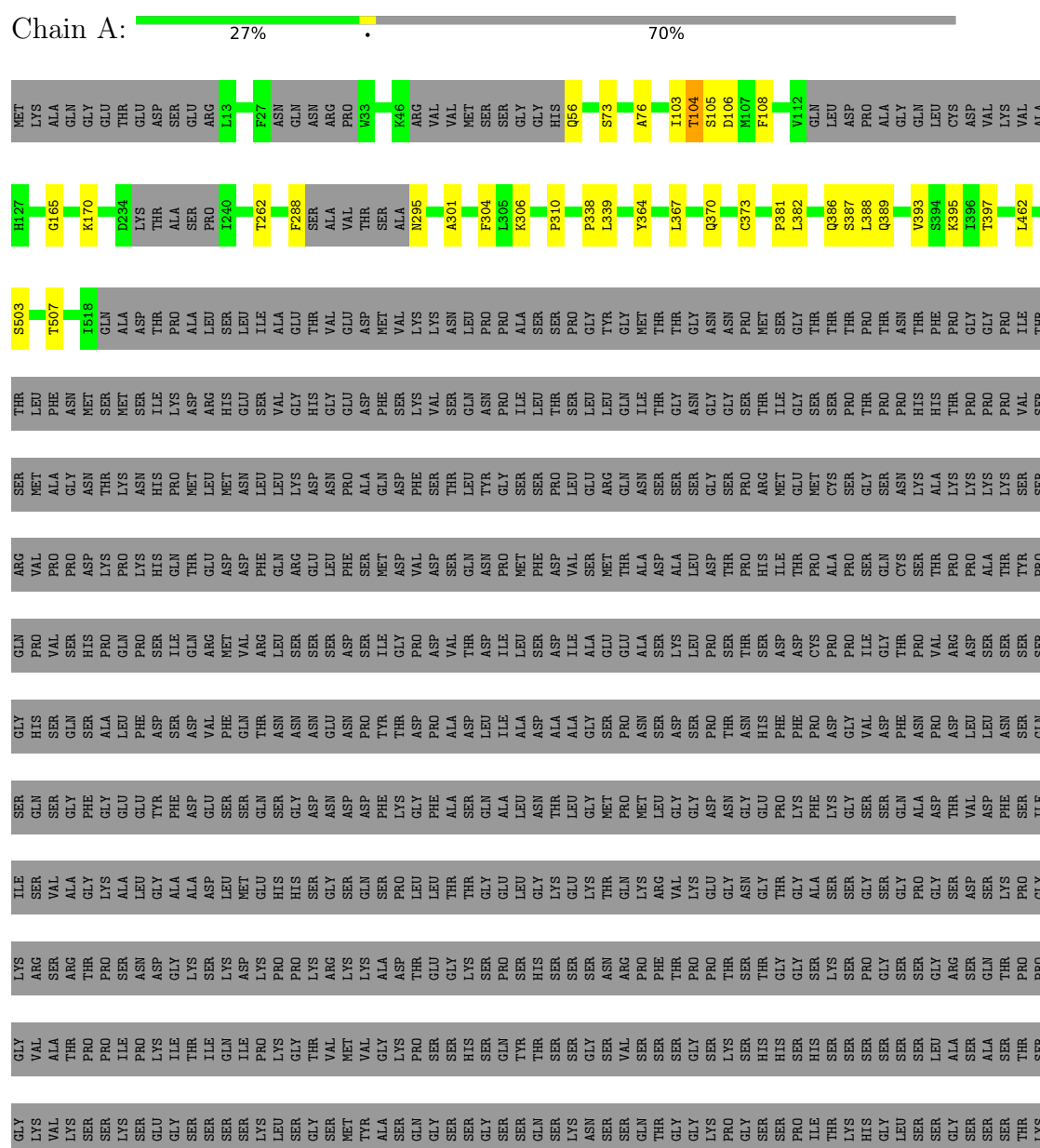
- Molecule 27 is a protein called Unknown Peptide.

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

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: Mediator of RNA polymerase II transcription subunit 1



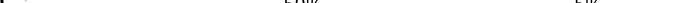
SER	ASP	GLU	ALA	LYS	GLN	GLY	LYS	SER	GLN	GLY	SER	MET
THR	PRO	ARG	GLU	GLY	LYS	SER	GLY	VAL	LYS	HIS	PRO	LYS
ALA	THR	SER	SER	GLU	ARG	GLN	TYR	ARG	GLY	SER	GLY	GLY
SER	VAL	GLN	ASN	GLY	LYS	SER	LYS	ARG	ASN	THR	LYS	LYS
THR	THR	SER	SER	ASP	ASP	ASP	LYS	SER	LYS	SER	SER	PRO
ASN	ASN	PRO	PRO	GLY	LYS	LEU	ASP	PRO	LYS	SER	SER	SER
PRO	PRO	SER	ARG	ARG	LYS	SER	ARG	LYS	LYS	MET	ASN	ASN
ILE	ILE	GLU	GLU	PRO	SER	LYS	GLN	LEU	THR	LYS	PRO	PRO
LEU	LEU	ASP	ASP	GLN	LYS	ILE	VAL	ALA	ALA	SER	SER	ILE
SER	SER	ILE	ILE	ILE	VAL	SER	VAL	SER	VAL	SER	SER	ILE
ALA	ALA	GLY	ARG	SER	ALA	SER	ALA	ILE	ILE	SER	SER	ILE
ASP	ASP	PRO	PRO	SER	SER	SER	PRO	ASP	PRO	GLY	LYS	LYS
ARG	ARG	LEU	LEU	ASN	GLY	GLY	LYS	GLY	GLY	SER	PRO	LYS
LEU	LEU	GLU	GLU	TYR	VAL	GLY	TYR	HIS	HIS	THR	GLN	PRO
THR	THR	THR	THR	SER	ASP	VAL	PRO	LYS	LYS	SER	ASN	ILE
PRO	PRO	GLU	GLU	PRO	SER	SER	LEU	VAL	VAL	VAL	ASN	THR
ASP	ASP	GLU	LYS	ILE	LYS	ILE	LEU	SER	LYS	THR	GLN	GLY
PHE	PHE	LYS	LYS	ILE	LYS	LYS	ILE	LYS	LYS	THR	ASN	GLY
ILE	ILE	HIS	HIS	SER	LYS	SER	GLY	THR	GLY	SER	GLN	SER
GLY	GLY	LYS	LYS	GLY	GLY	GLY	GLY	THR	GLY	PRO	ASN	SER
GLU	GLU	HIS	HIS	THR	GLU	SER	THR	GLU	GLY	THR	ASN	GLY
GLU	GLU	LYS	LYS	PRO	SER	SER	PRO	GLY	GLY	PRO	ASN	GLY
ASP	ASP	LYS	LYS	LYS	LYS	LYS	LYS	GLU	GLU	ALA	ASN	GLY
ASP	ASP	GLU	GLU	HIS	ASN	ASN	ASN	ASP	ASP	SER	SER	GLY
ASP	ASP	GLU	LYS	GLU	VAL	VAL	VAL	PRO	PRO	ASN	LYS	GLY
LEU	LEU	LYS	ARG	GLY	GLY	GLY	ILE	ILE	ILE	SER	SER	GLY
LEU	LEU	LYS	ASP	GLY	LYS	LYS	LYS	SER	ALA	SER	VAL	GLY
ILE	ILE	ARG	ARG	LYS	ILE	ILE	ILE	SER	ALA	SER	VAL	GLY
GLY	GLY	ASP	ASP	SER	THR	SER	SER	THR	PHE	THR	ASN	GLY
ASN	ASN	LYS	LYS	PRO	ILE	ASN	PRO	GLN	GLY	THR	ASN	GLY
		LYS	ALA	ALA	ILE	ASN	ALA	SER	SER	SER	GLN	LYS
		LYS	LYS	LYS	LYS	LYS	LYS	VAL	SER	SER	GLN	LYS
		THR	THR	THR	HIS	HIS	THR	THR	SER	SER	ASN	LYS
		THR	THR	THR	LYS	LYS	THR	THR	THR	SER	GLN	LYS
		THR	THR	THR	ASP	ASP	THR	THR	THR	SER	ASN	LYS
		HIS	HIS	PRO	GLY	GLY	GLY	GLY	THR	SER	ASN	LYS
		SER	SER	GLN	THR	THR	THR	THR	THR	SER	ASN	LYS
		MET	MET	ASN	GLY	GLY	ASN	MET	MET	MET	ASN	LYS
		LYS	LYS	VAL	SER	SER	SER	SER	SER	LYS	ASN	LYS
		PRO	PRO	ASP	PRO	PRO	PRO	PRO	PRO	VAL	ASN	LYS
		ASN	ASN	GLU	ILE	ASN	ASN	ASN	ASN	ASN	ASN	LYS
		THR	THR	SER	THR	THR	THR	THR	THR	THR	THR	LYS
		SER	SER	SER	THR	THR	THR	THR	THR	THR	THR	LYS
		GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	LYS
		THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	LYS
		ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	LYS
		GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	LYS
		ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	LYS
		LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LYS

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

Chain B: 58% 41%

[illegible]

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

Chain C: 

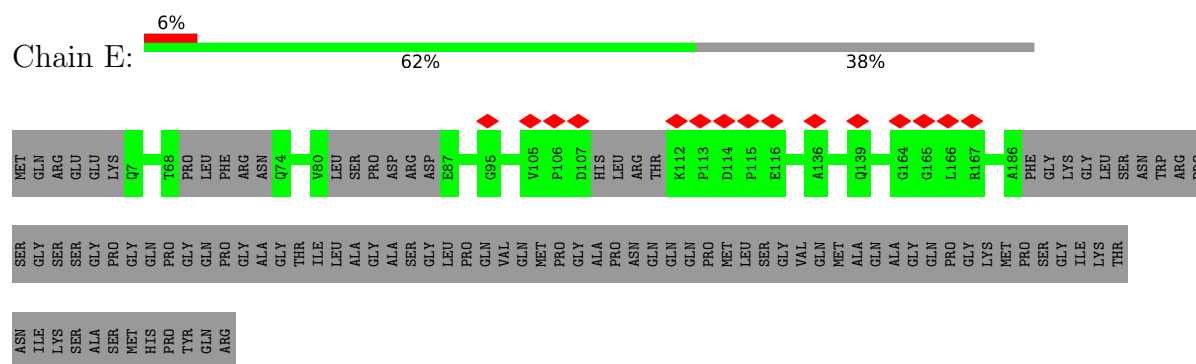
GLU	ALA	GLU	PRO	LEU	PRO	GLU	THR	VAL	LYS	SER	GLU	GLU	LYS	GLU	SER	THR	ASN	ILE	GLN	THR	VAL	SER	THR	LYS	GLY	PRO	GLU	LYS	ARG	LEU	GLN
161	162	163	164	165	166	167	168	169	170	171	172	173	174	175	176	177	178	179	180	181	182	183	184	185	186	187	188	189	190	191	192
ALA	ALA	VAL	ASP	ILE	ARG	ASP	193	194	195	196	197	198	199	200	201	202	203	204	205	206	207	208	209	210	211	212	213	214	215	216	217
193	194	195	196	197	198	199	200	201	202	203	204	205	206	207	208	209	210	211	212	213	214	215	216	217	218	219	220	221	222	223	224
225	226	227	228	229	230	231	232	233	234	235	236	237	238	239	240	241	242	243	244	245	246	247	248	249	250	251	252	253	254	255	256
257	258	259	260	261	262	263	264	265	266	267	268	269	270	271	272	273	274	275	276	277	278	279	280	281	282	283	284	285	286	287	288
289	290	291	292	293	294	295	296	297	298	299	300	301	302	303	304	305	306	307	308	309	310	311	312	313	314	315	316	317	318	319	320
321	322	323	324	325	326	327	328	329	330	331	332	333	334	335	336	337	338	339	340	341	342	343	344	345	346	347	348	349	350	351	352
353	354	355	356	357	358	359	360	361	362	363	364	365	366	367	368	369	370	371	372	373	374	375	376	377	378	379	380	381	382	383	384
385	386	387	388	389	390	391	392	393	394	395	396	397	398	399	400	401	402	403	404	405	406	407	408	409	410	411	412	413	414	415	416
417	418	419	420	421	422	423	424	425	426	427	428	429	430	431	432	433	434	435	436	437	438	439	440	441	442	443	444	445	446	447	448
449	450	451	452	453	454	455	456	457	458	459	460	461	462	463	464	465	466	467	468	469	470	471	472	473	474	475	476	477	478	479	480
481	482	483	484	485	486	487	488	489	490	491	492	493	494	495	496	497	498	499	500	501	502	503	504	505	506	507	508	509	510	511	512
513	514	515	516	517	518	519	520	521	522	523	524	525	526	527	528	529	530	531	532	533	534	535	536	537	538	539	540	541	542	543	544
545	546	547	548	549	550	551	552	553	554	555	556	557	558	559	560	561	562	563	564	565	566	567	568	569	570	571	572	573	574	575	576
577	578	579	580	581	582	583	584	585	586	587	588	589	590	591	592	593	594	595	596	597	598	599	600	601	602	603	604	605	606	607	608

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

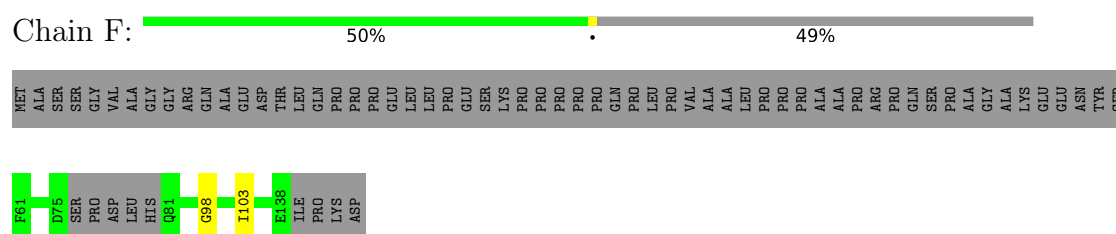
Chain D: 66% 31%

[illegible]

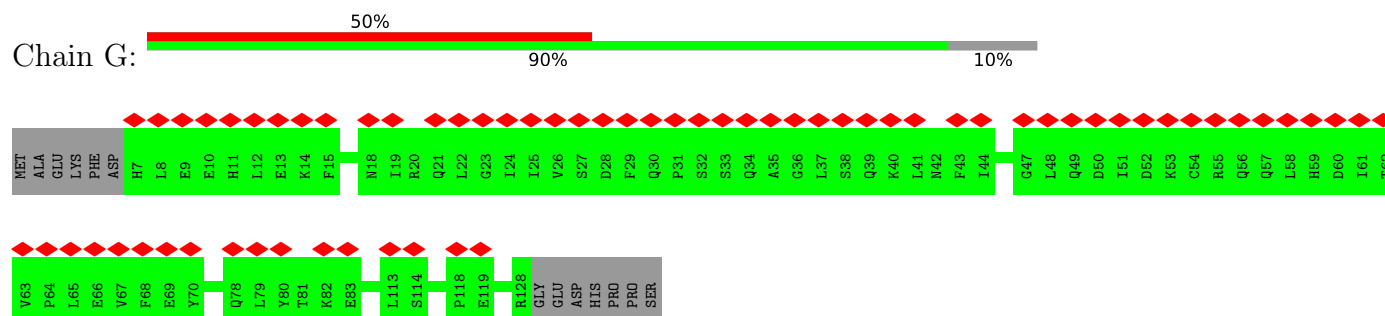
- Molecule 5: Mediator of RNA polymerase II transcription subunit 8



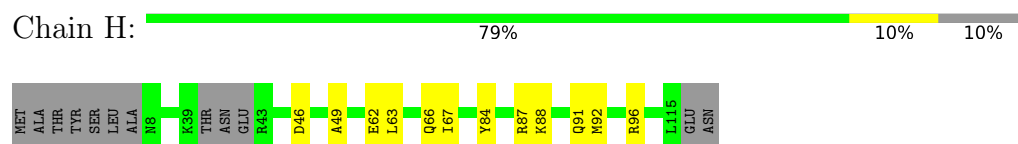
- Molecule 6: Mediator of RNA polymerase II transcription subunit 9



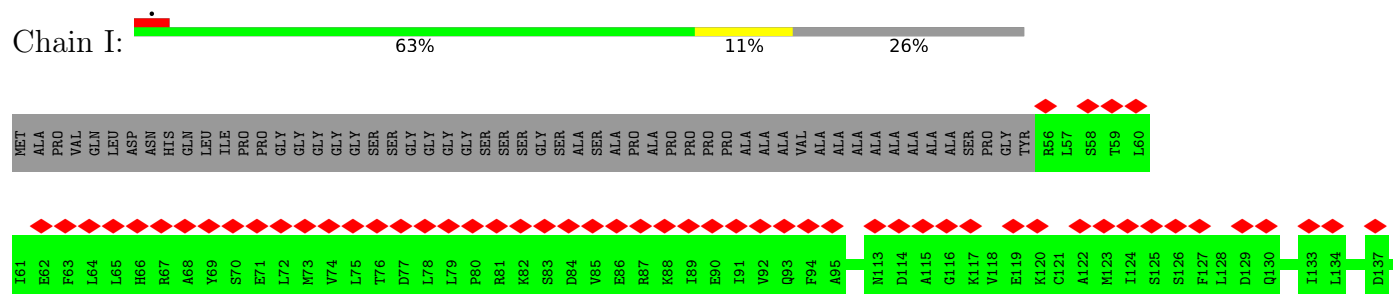
- Molecule 7: Mediator of RNA polymerase II transcription subunit 10



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



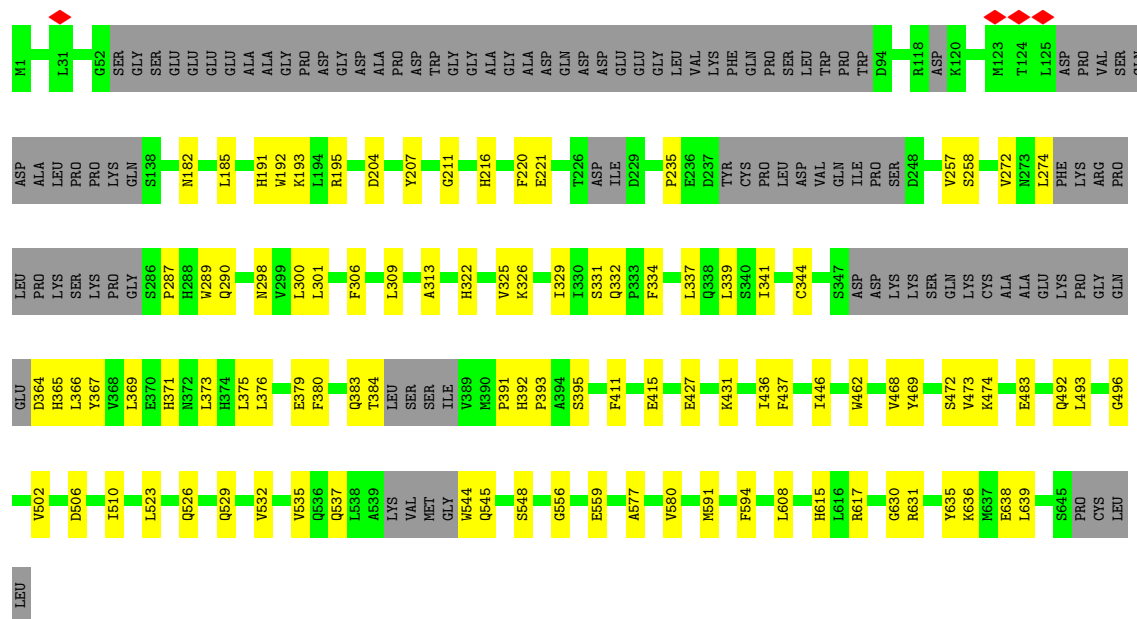
- Molecule 9: Mediator of RNA polymerase II transcription subunit 14



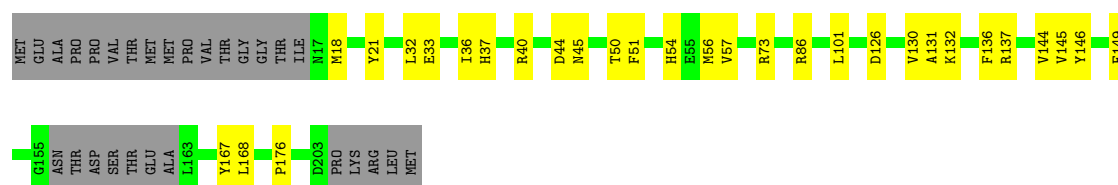


5828

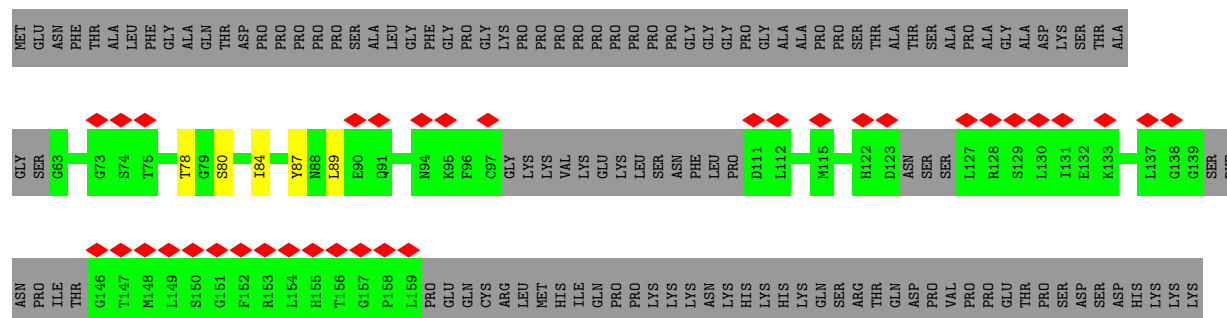
- Molecule 12: Mediator of RNA polymerase II transcription subunit 17

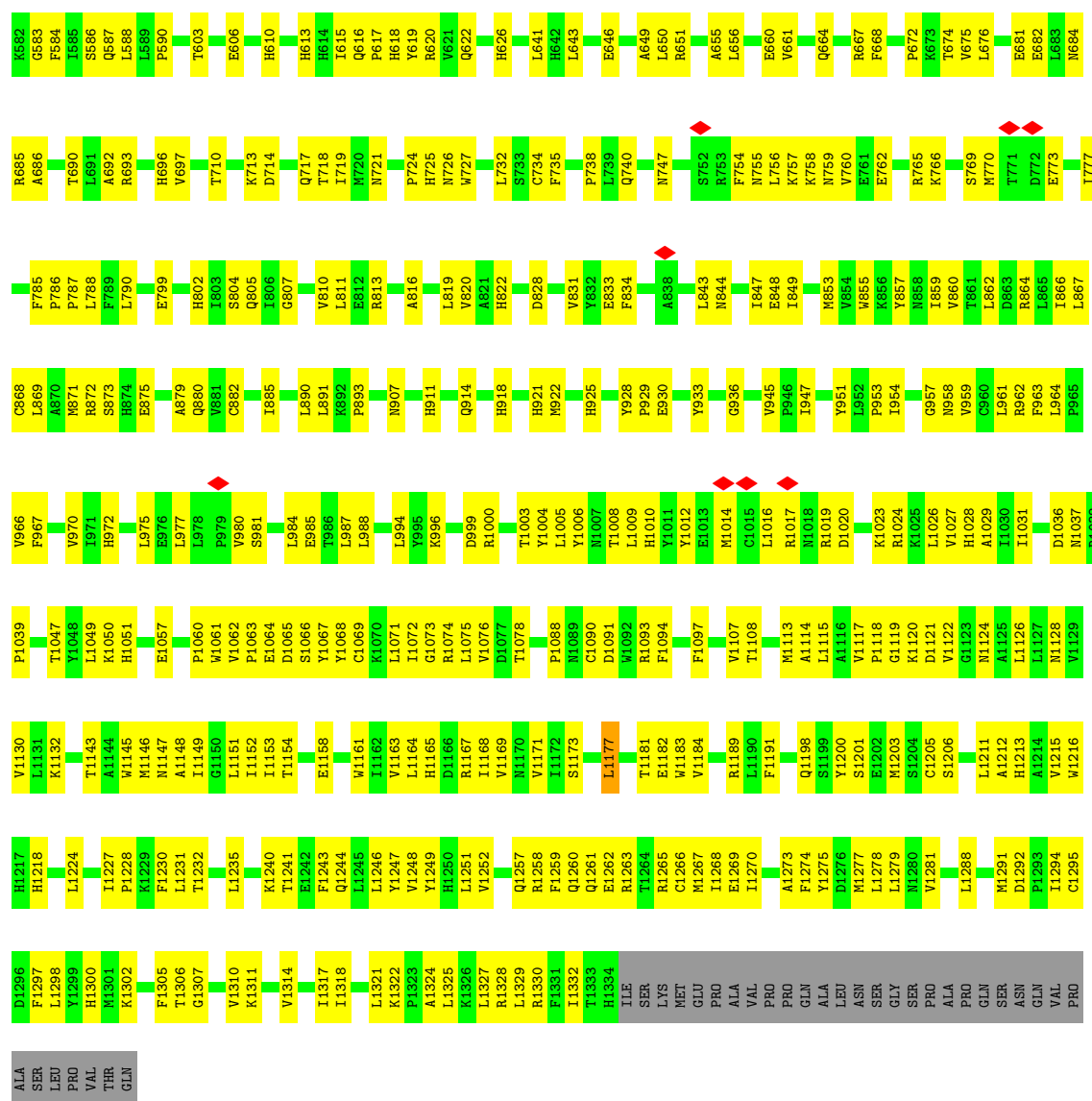
Chain L: 

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

Chain M: 

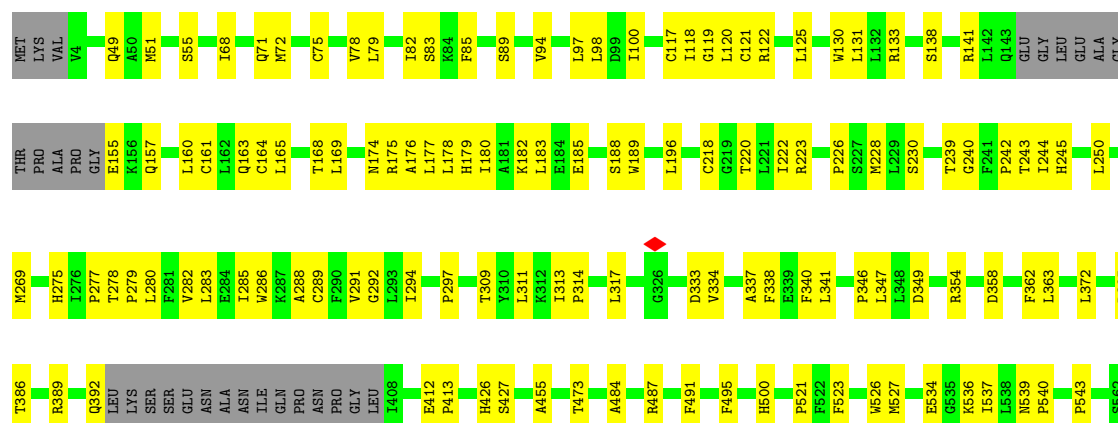
- Molecule 14: Mediator of RNA polymerase II transcription subunit 19

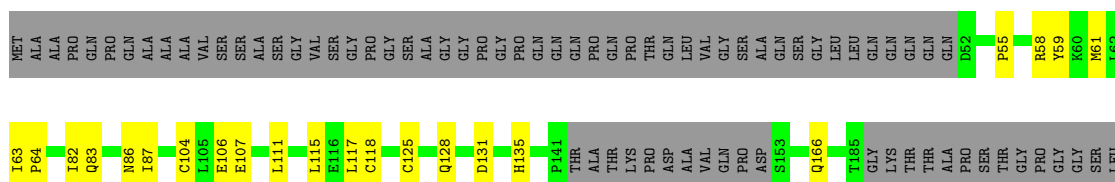
Chain N: 



- Molecule 19: Mediator of RNA polymerase II transcription subunit 24

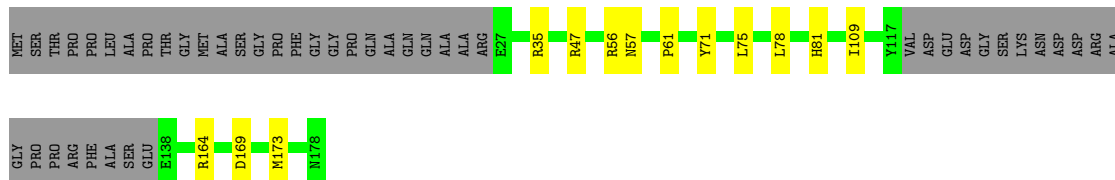
Chain S: 71% 21% 9%





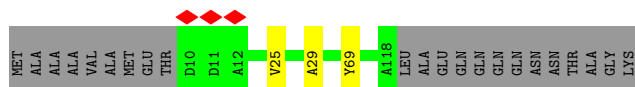
- Molecule 25: Mediator of RNA polymerase II transcription subunit 30

Chain Y: 67% 7% 26%



- Molecule 26: Mediator of RNA polymerase II transcription subunit 31

Chain Z: 81% 17%



- Molecule 27: Unknown Peptide

Chain a: 100%

There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	199078	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)	700	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.308	Depositor
Minimum map value	-0.071	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.054	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 ⓘ

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	$\# Z > 5$
1	A	0.11	0/2308	0.28	0/3209
2	B	0.12	0/782	0.23	0/1088
3	C	0.13	0/784	0.47	0/1090
4	D	0.12	0/800	0.39	0/1116
5	E	0.10	0/840	0.26	0/1170
6	F	0.09	0/361	0.22	0/501
7	G	0.08	0/604	0.21	0/841
8	H	0.12	0/580	0.30	0/798
9	I	0.13	0/6899	0.36	0/9516
10	J	0.16	0/1207	0.41	0/1668
11	K	0.15	0/5202	0.44	2/7144 (0.0%)
12	L	0.13	0/3385	0.33	0/4658
13	M	0.12	0/1163	0.31	0/1593
14	N	0.09	0/479	0.28	0/648
15	O	1.49	7/1026 (0.7%)	0.44	1/1409 (0.1%)
16	P	0.10	0/600	0.26	0/835
17	Q	0.11	0/758	0.26	0/1046
18	R	0.14	0/9995	0.39	0/13654
19	S	0.14	0/6000	0.34	0/8250
20	T	0.12	0/1336	0.34	0/1836
21	U	0.42	0/480	0.48	0/666
22	V	0.13	0/1694	0.36	0/2338
23	W	0.13	0/785	0.34	0/1076
24	X	0.12	0/852	0.32	0/1169
25	Y	0.13	0/853	0.30	0/1167
26	Z	0.11	0/542	0.36	0/756
All	All	0.25	7/50315 (0.0%)	0.36	3/69242 (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
1	A	0	1
3	C	0	3
All	All	0	4

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	O	46	TYR	CD2-CE2	24.93	2.13	1.38
15	O	46	TYR	CD1-CE1	23.92	2.10	1.38
15	O	46	TYR	CE1-CZ	17.01	1.79	1.38
15	O	46	TYR	CE2-CZ	16.99	1.79	1.38
15	O	46	TYR	CG-CD2	15.24	1.71	1.39

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	286	ALA	CA-C-N	8.64	137.26	121.70
11	K	286	ALA	C-N-CA	8.64	137.26	121.70
15	O	104	SER	CA-C-O	-7.46	111.42	120.89

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	104	THR	Peptide
3	C	46	ASN	Peptide
3	C	50	VAL	Peptide
3	C	58	GLU	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	2314	0	992	19	0
2	B	784	0	357	1	0
3	C	785	0	344	10	0
4	D	801	0	327	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	837	0	402	0	0
6	F	363	0	146	1	0
7	G	605	0	256	0	0
8	H	578	0	341	8	0
9	I	6772	0	4972	113	0
10	J	1171	0	1010	34	0
11	K	5085	0	4509	164	0
12	L	3335	0	2395	74	0
13	M	1140	0	832	22	0
14	N	475	0	349	4	0
15	O	1013	0	662	36	0
16	P	602	0	302	7	0
17	Q	754	0	448	4	0
18	R	9744	0	9105	382	0
19	S	5875	0	4690	150	0
20	T	1299	0	1022	12	0
21	U	481	0	202	0	0
22	V	1657	0	1170	25	0
23	W	773	0	607	16	0
24	X	839	0	700	18	0
25	Y	843	0	639	11	0
26	Z	543	0	240	2	0
27	a	100	0	23	0	0
All	All	49568	0	37042	1063	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 12.

The worst 5 of 1063 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)
15:O:46:TYR:CZ	15:O:46:TYR:CE1	1.79	1.66
15:O:46:TYR:CZ	15:O:46:TYR:CE2	1.79	1.63
15:O:46:TYR:CE1	15:O:46:TYR:CD1	2.10	1.39
15:O:46:TYR:CE2	15:O:46:TYR:CD2	2.13	1.35
15:O:46:TYR:CD1	15:O:105:ALA:N	1.97	1.33

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	455/1575 (29%)	426 (94%)	28 (6%)	1 (0%)	43	78
2	B	154/270 (57%)	150 (97%)	4 (3%)	0	100	100
3	C	153/246 (62%)	123 (80%)	30 (20%)	0	100	100
4	D	159/233 (68%)	147 (92%)	12 (8%)	0	100	100
5	E	157/268 (59%)	144 (92%)	13 (8%)	0	100	100
6	F	69/142 (49%)	66 (96%)	3 (4%)	0	100	100
7	G	120/135 (89%)	119 (99%)	1 (1%)	0	100	100
8	H	101/117 (86%)	94 (93%)	7 (7%)	0	100	100
9	I	1050/1459 (72%)	901 (86%)	149 (14%)	0	100	100
10	J	165/789 (21%)	135 (82%)	30 (18%)	0	100	100
11	K	718/828 (87%)	574 (80%)	143 (20%)	1 (0%)	48	83
12	L	524/649 (81%)	457 (87%)	67 (13%)	0	100	100
13	M	176/208 (85%)	160 (91%)	16 (9%)	0	100	100
14	N	67/240 (28%)	63 (94%)	4 (6%)	0	100	100
15	O	162/212 (76%)	134 (83%)	28 (17%)	0	100	100
16	P	117/144 (81%)	107 (92%)	10 (8%)	0	100	100
17	Q	129/200 (64%)	126 (98%)	3 (2%)	0	100	100
18	R	1285/1367 (94%)	1105 (86%)	179 (14%)	1 (0%)	48	83
19	S	889/987 (90%)	790 (89%)	99 (11%)	0	100	100
20	T	184/745 (25%)	163 (89%)	21 (11%)	0	100	100
21	U	93/588 (16%)	84 (90%)	8 (9%)	1 (1%)	11	45
22	V	258/311 (83%)	216 (84%)	42 (16%)	0	100	100
23	W	116/178 (65%)	109 (94%)	7 (6%)	0	100	100
24	X	119/199 (60%)	116 (98%)	3 (2%)	0	100	100
25	Y	128/178 (72%)	112 (88%)	16 (12%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	Z	107/131 (82%)	96 (90%)	11 (10%)	0	100	100
All	All	7655/12399 (62%)	6717 (88%)	934 (12%)	4 (0%)	49	83

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	105	SER
18	R	1177	LEU
21	U	528	LEU
11	K	97	SER

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
15	O	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	O	104:SER	C	105:ALA	N	2.41

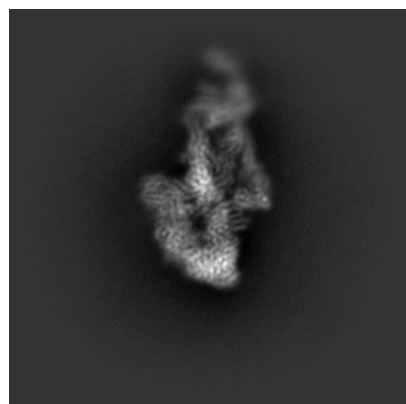
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40968. These allow visual inspection of the internal detail of the map and identification of artifacts.

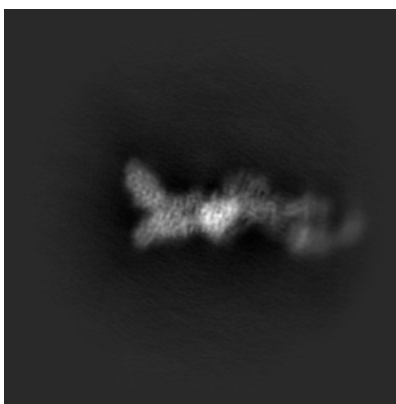
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

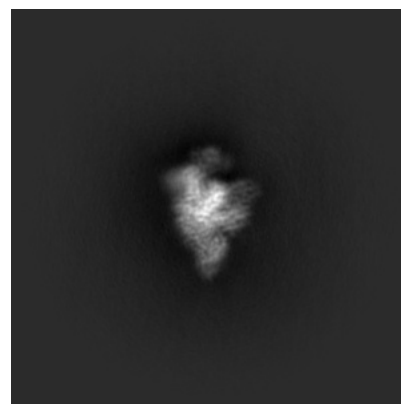
6.1.1 Primary map



X

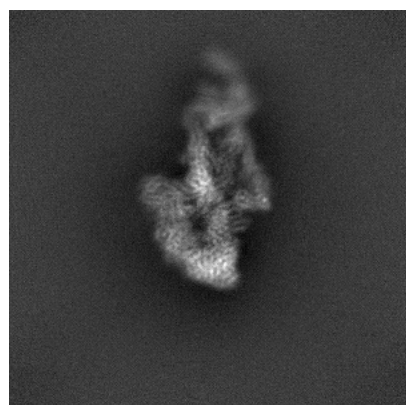


Y

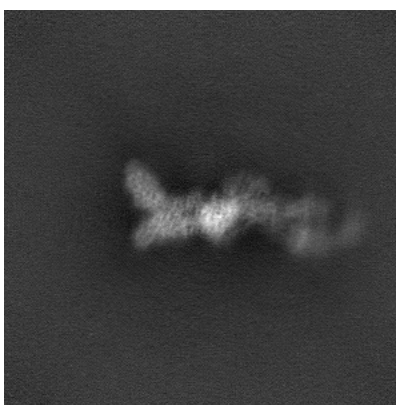


Z

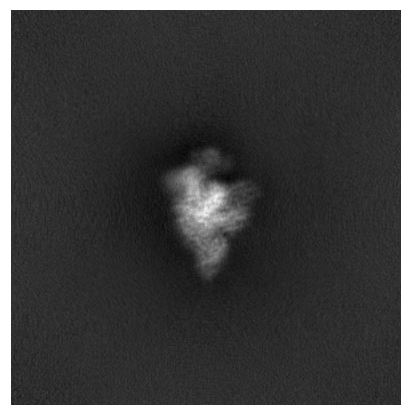
6.1.2 Raw map



X



Y

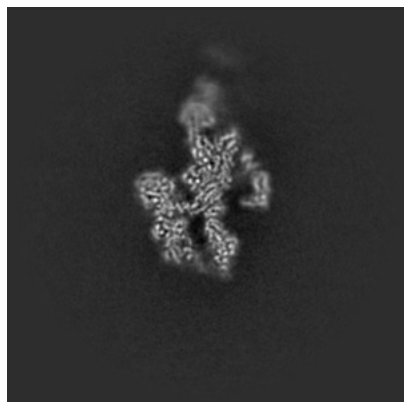


Z

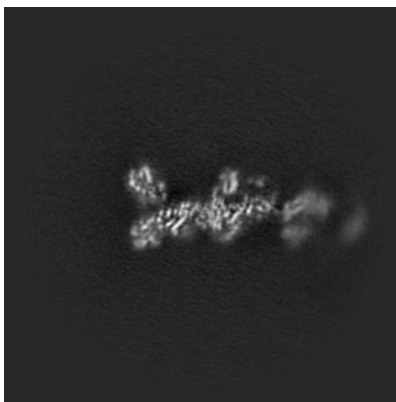
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

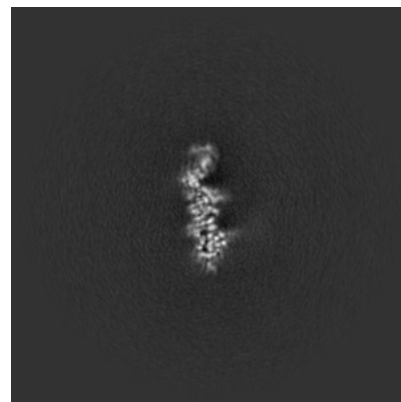
6.2.1 Primary map



X Index: 280

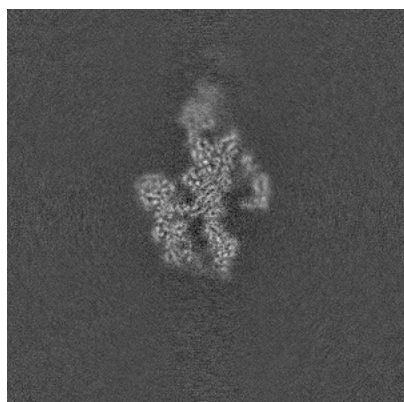


Y Index: 280

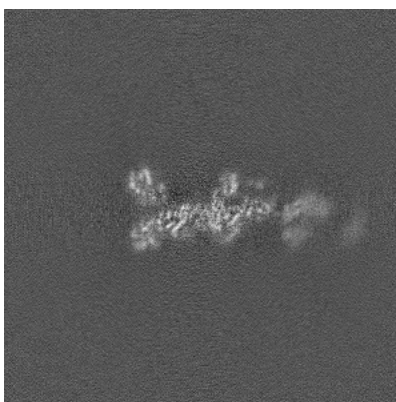


Z Index: 280

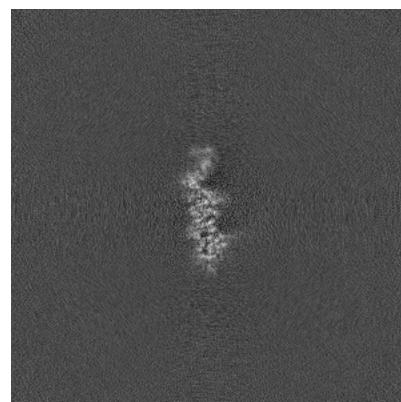
6.2.2 Raw map



X Index: 280



Y Index: 280

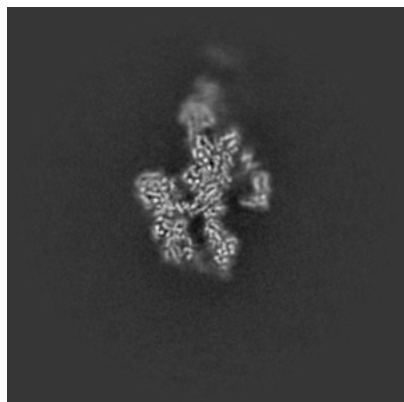


Z Index: 280

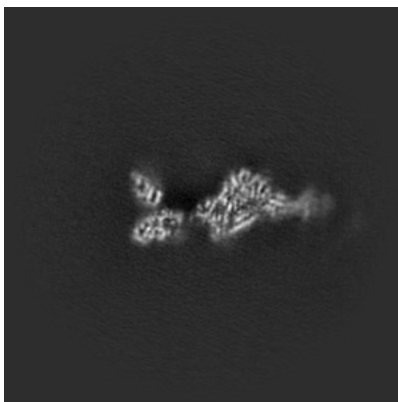
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

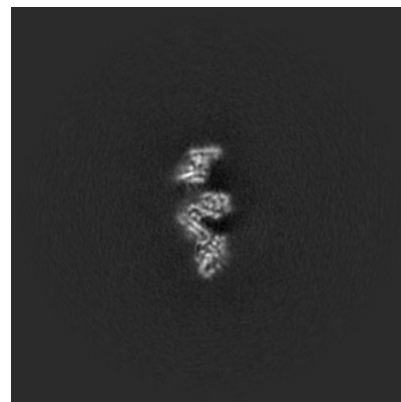
6.3.1 Primary map



X Index: 279

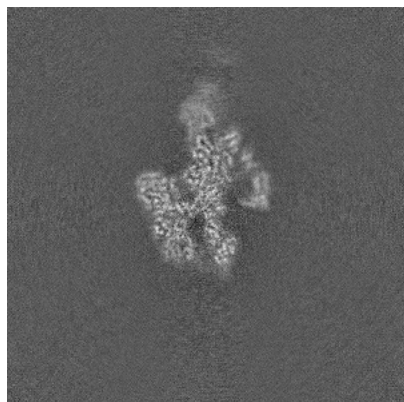


Y Index: 266



Z Index: 296

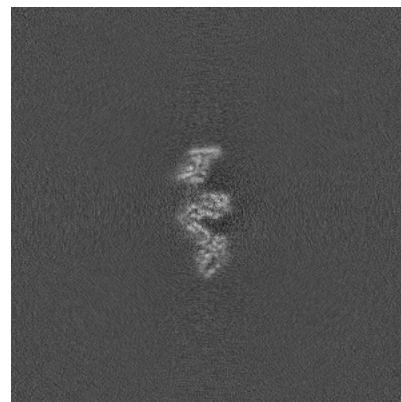
6.3.2 Raw map



X Index: 278



Y Index: 267



Z Index: 295

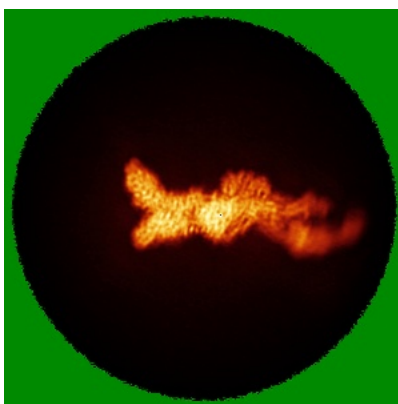
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X

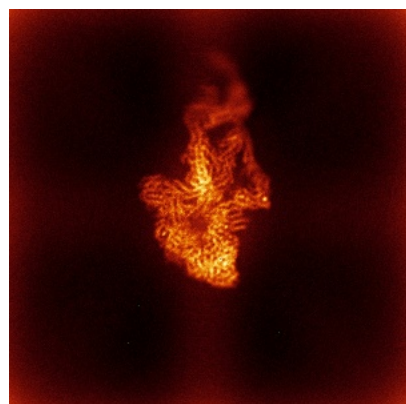


Y

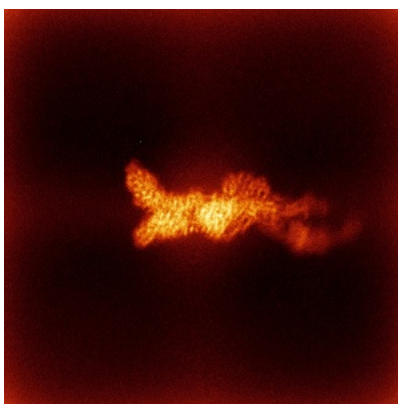


Z

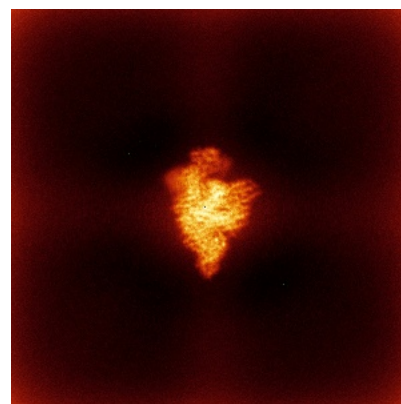
6.4.2 Raw map



X



Y

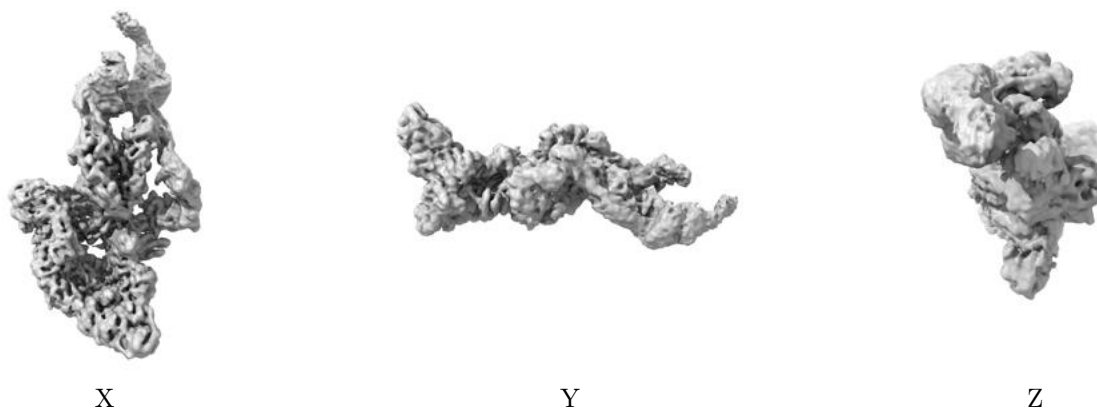


Z

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.

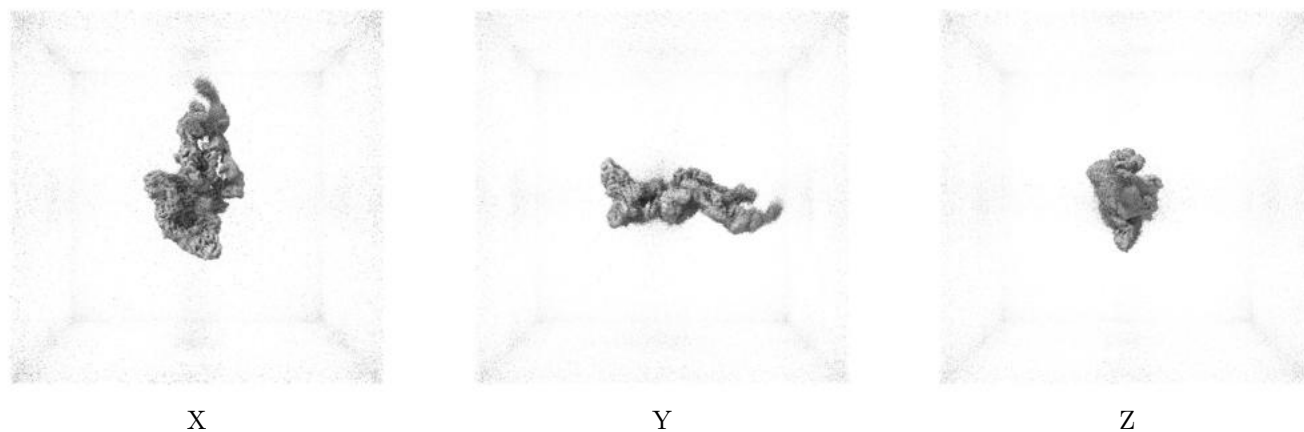
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.054. 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.

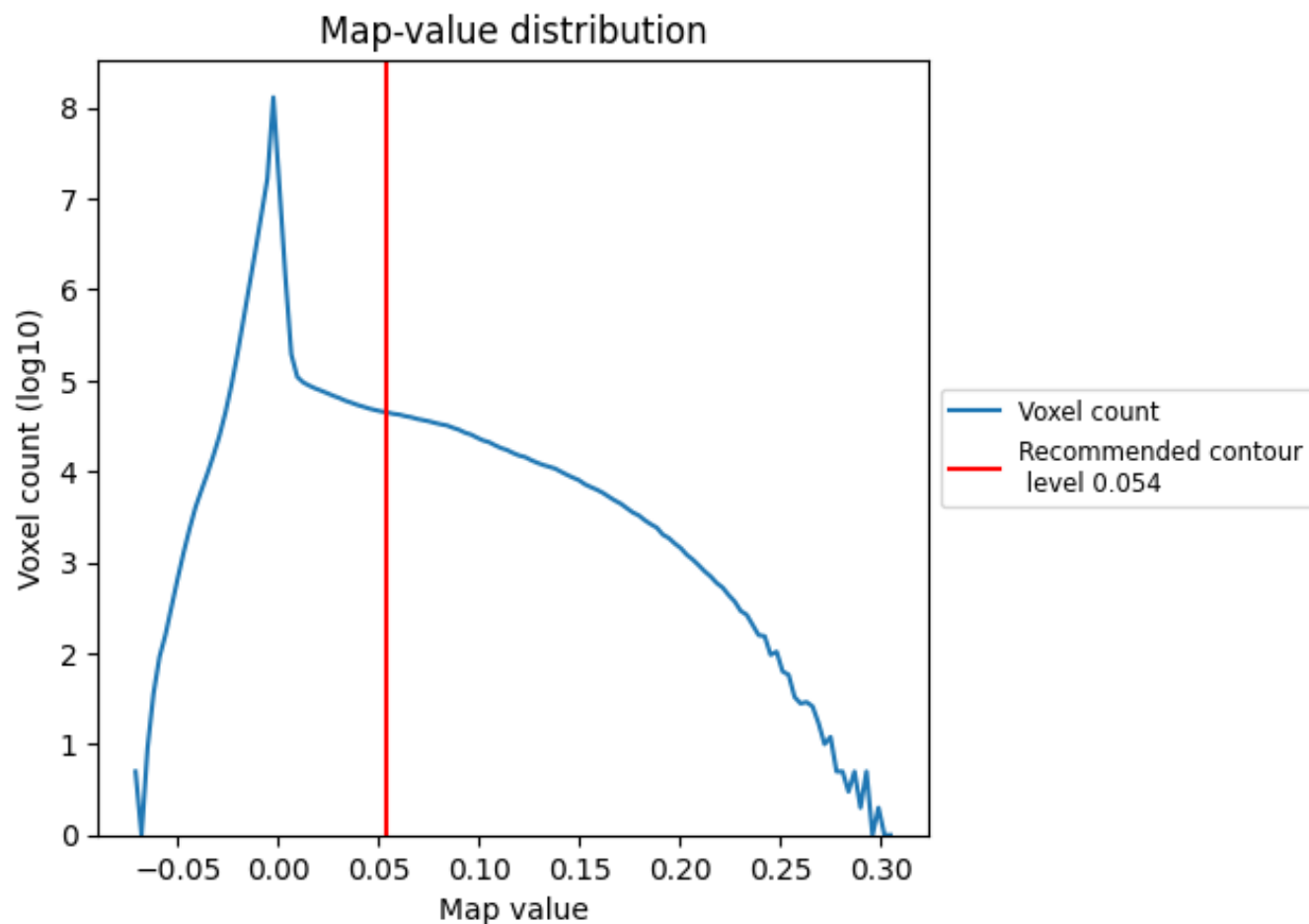
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

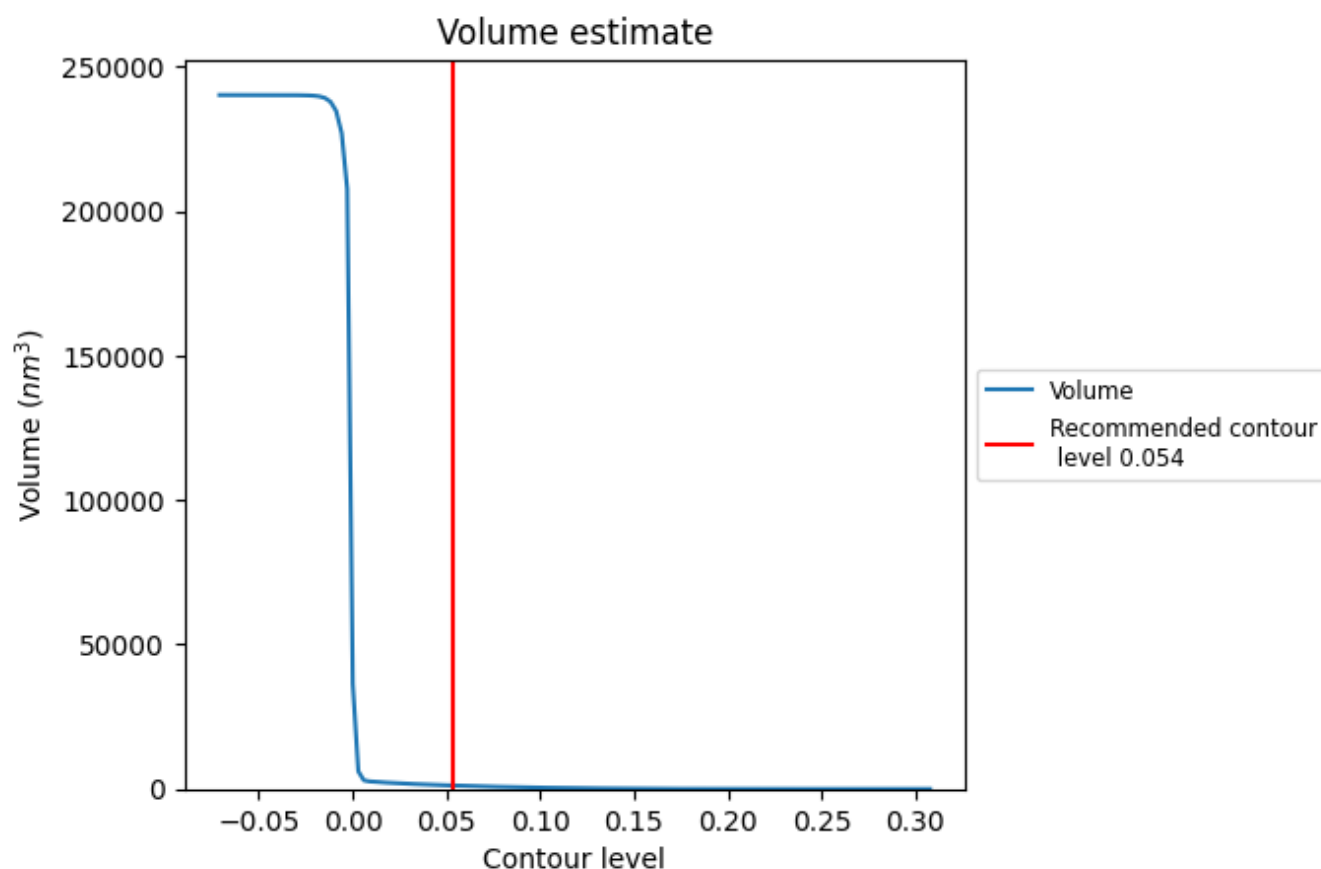
This section contains the results of statistical analysis of the map.

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.

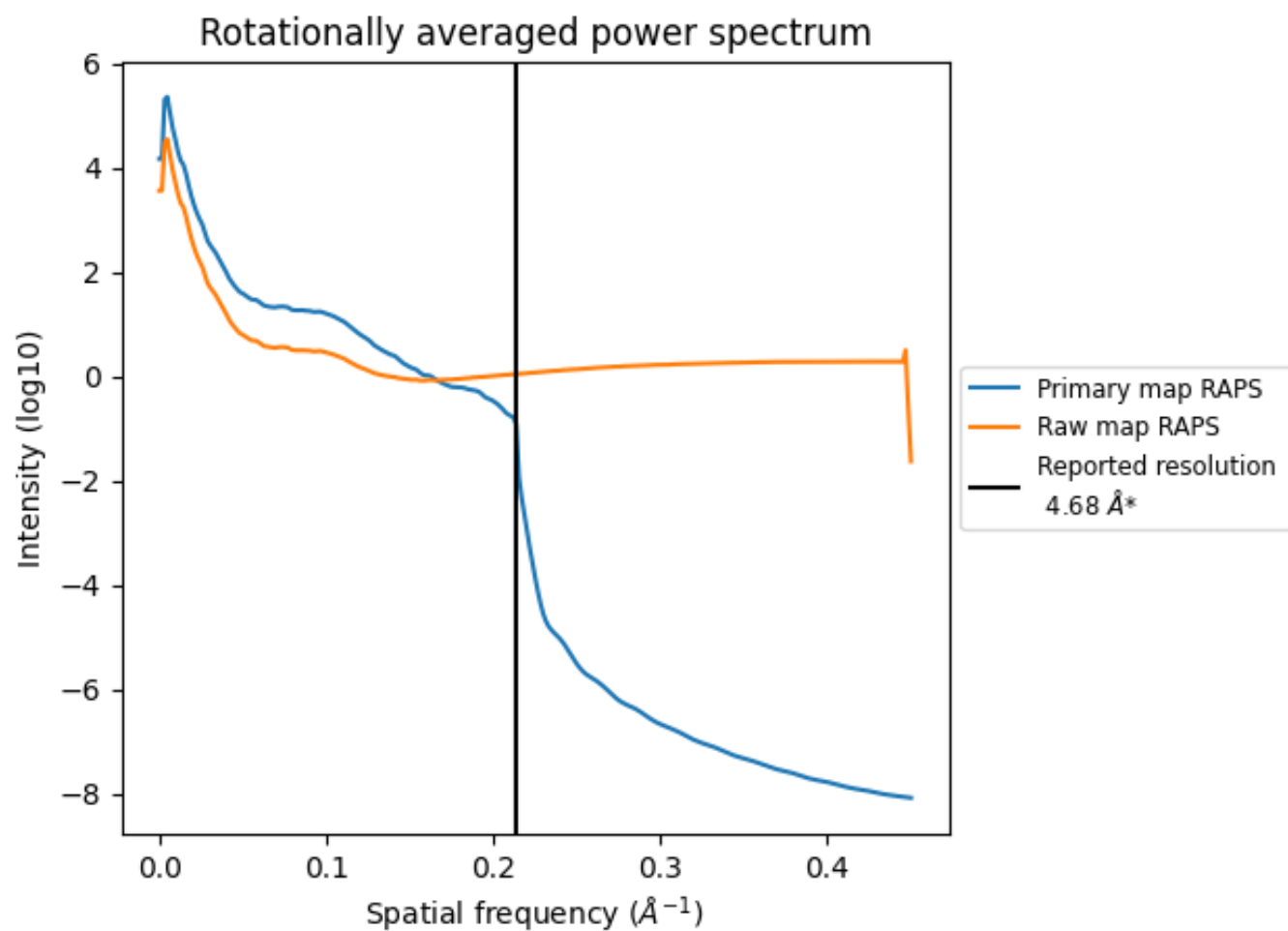
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1192 nm^3 ; this corresponds to an approximate mass of 1076 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 ⓘ

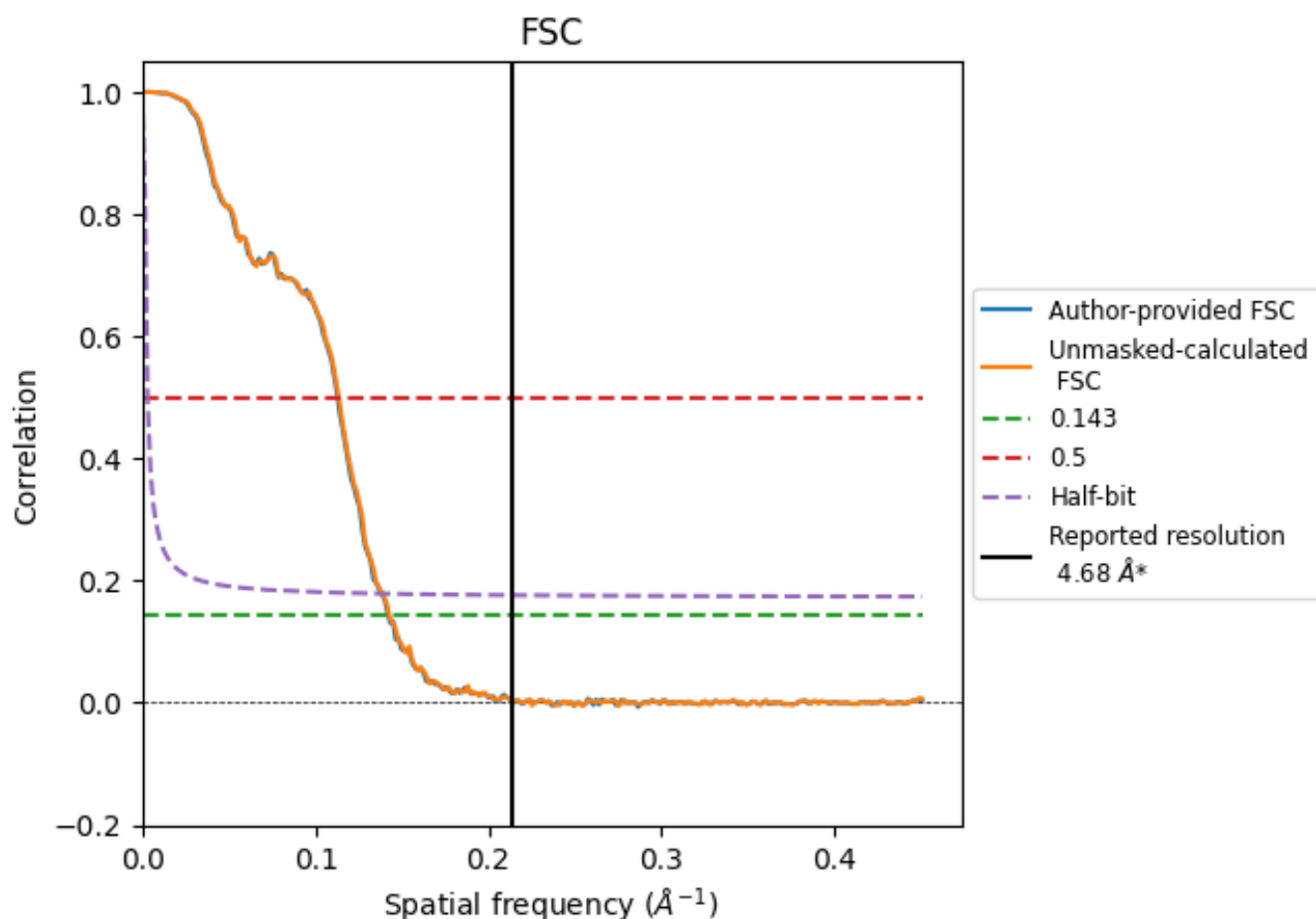


*Reported resolution corresponds to spatial frequency of 0.214 $\text{\AA}^{-1}$

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 $0.214 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.68	-	-
Author-provided FSC curve	7.04	8.87	7.24
Unmasked-calculated*	7.00	8.80	7.20

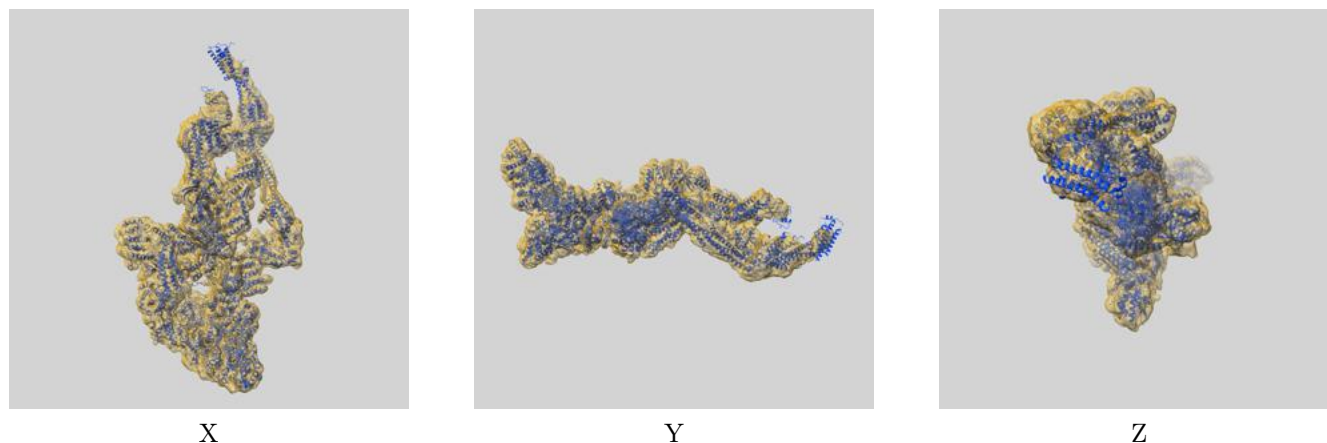
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 7.04 differs from the reported value 4.68 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.00 differs from the reported value 4.68 by more than 10 %

9 Map-model fit [i](#)

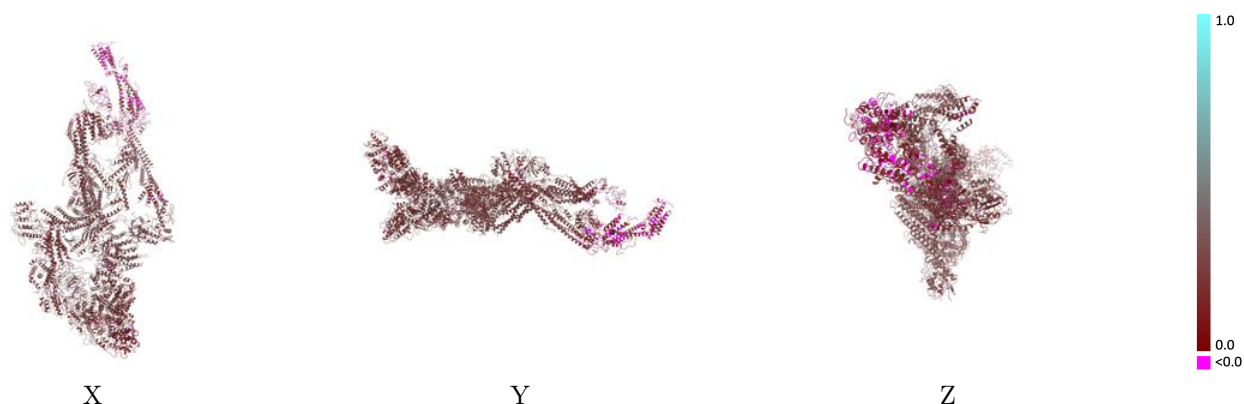
This section contains information regarding the fit between EMDB map EMD-40968 and PDB model 8T1I. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



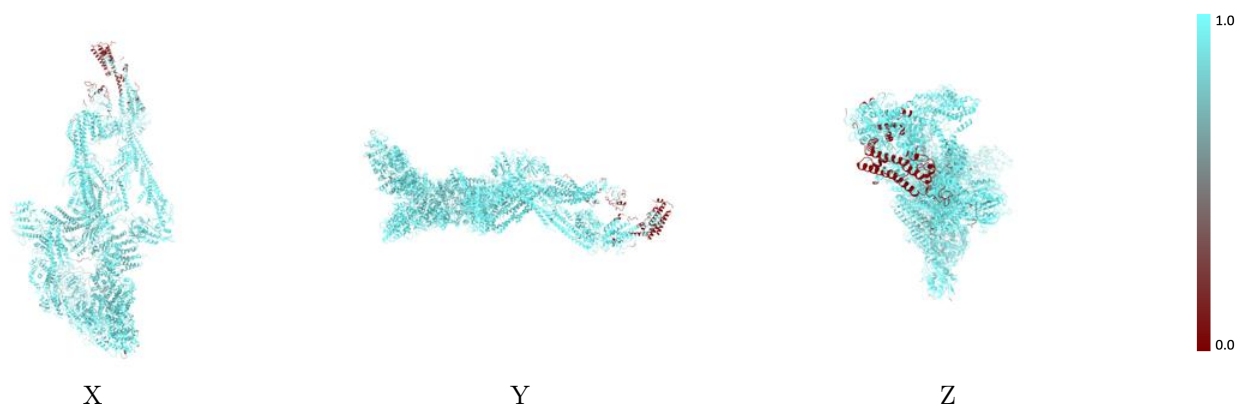
The images above show the 3D surface view of the map at the recommended contour level 0.054 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



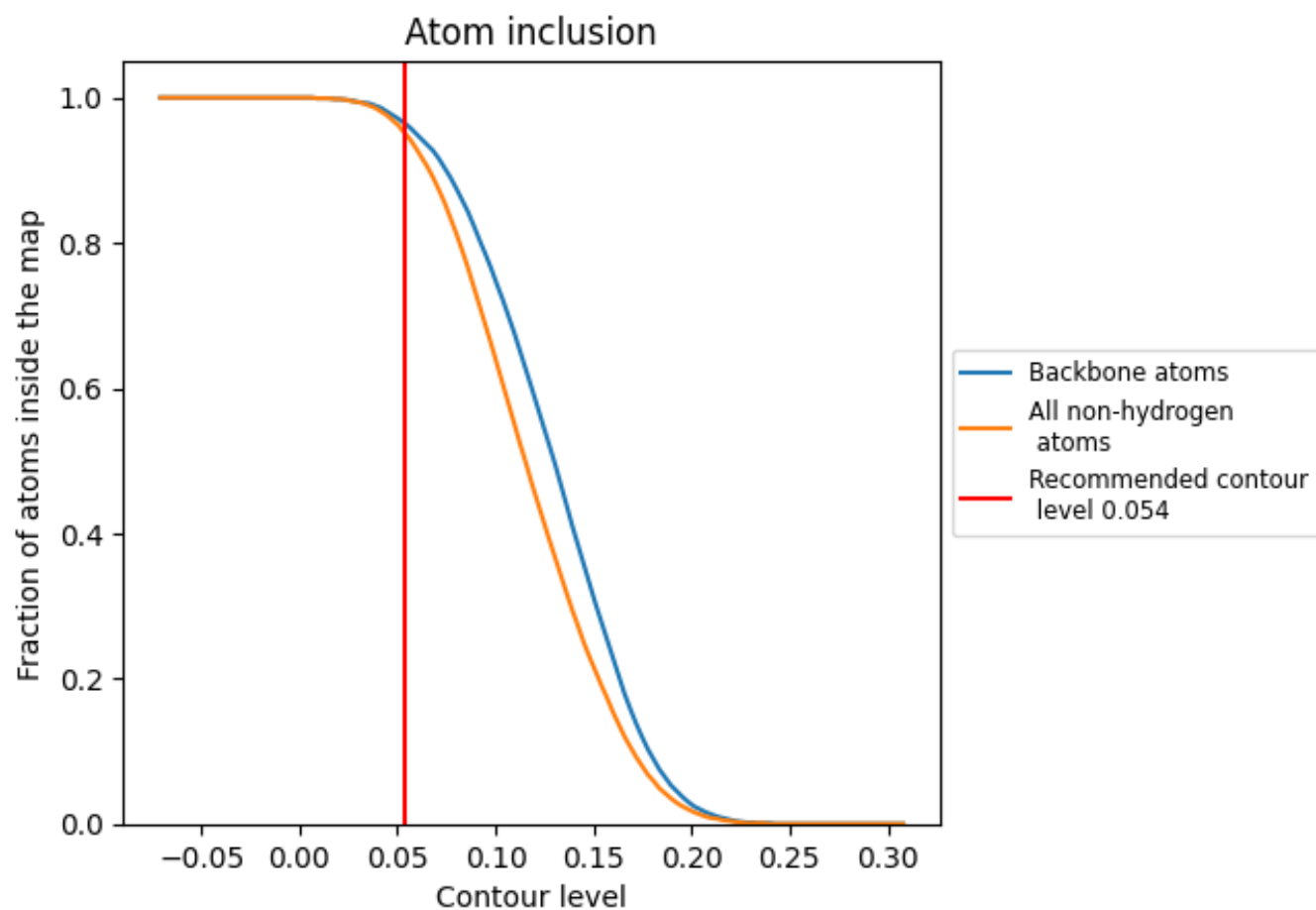
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.054).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 95% 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 (0.054) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9500	 0.2380
A	 0.9950	 0.2750
B	 0.9940	 0.1950
C	 0.6480	 0.1630
D	 0.9760	 0.1820
E	 0.8900	 0.2080
F	 0.9970	 0.2470
G	 0.4300	 0.0860
H	 0.9970	 0.2420
I	 0.9340	 0.2580
J	 0.9390	 0.2720
K	 0.9820	 0.2550
L	 0.9700	 0.2640
M	 0.9900	 0.2400
N	 0.5570	 0.0880
O	 0.9940	 0.2680
P	 0.9000	 0.1290
Q	 0.9840	 0.2220
R	 0.9650	 0.2220
S	 0.9760	 0.2530
T	 0.9200	 0.2340
U	 0.9540	 0.1250
V	 0.9880	 0.2870
W	 0.9670	 0.2440
X	 0.9890	 0.2470
Y	 0.9820	 0.2480
Z	 0.9760	 0.1780
a	 1.0000	 0.3010

