



wwPDB EM Validation Summary Report ⓘ

Mar 29, 2026 – 04:32 PM UTC

PDB ID : 7UIF / pdb_00007uif
EMDB ID : EMD-26544
Title : Mediator-PIC Early (Core B)
Authors : Gorbea Colon, J.J.; Chen, S.-F.; Tsai, K.L.; Murakami, K.
Deposited on : 2022-03-29
Resolution : 4.60 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:

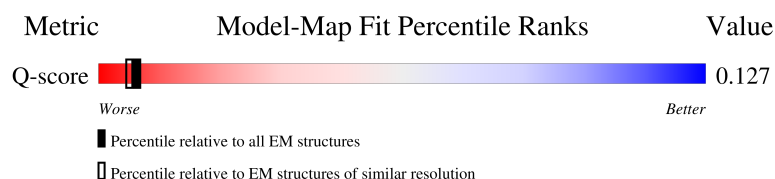
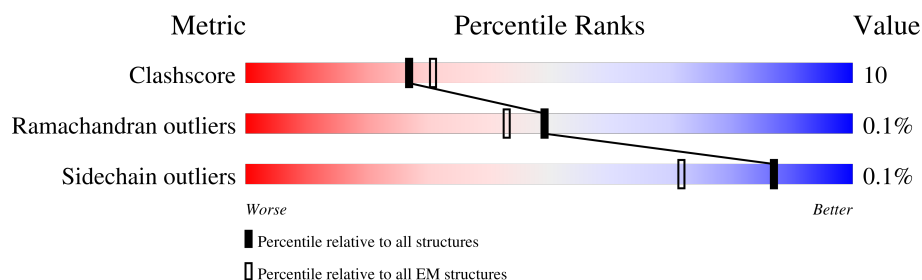
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 4.60 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2407 (4.10 - 5.10)

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	1733	
1	z	1733	
2	B	1224	
3	C	318	

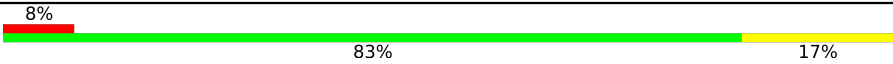
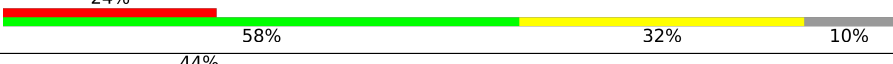
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Mol	Chain	Length	Quality of chain
4	D	221	
5	E	215	
6	F	155	
7	G	171	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	M	345	
14	P	735	
15	Q	400	
16	S	309	
17	a	566	
18	d	284	
19	f	295	
20	g	222	
21	h	223	
22	i	149	
23	j	157	
24	k	115	
25	n	1082	
26	q	687	
27	r	307	
28	s	220	

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Mol	Chain	Length	Quality of chain
29	t	210	
30	u	140	
31	v	121	
32	w	127	

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 63137 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1453	Total	C	N	O	S	0	0
			11425	7192	1995	2176	62		
1	z	25	Total	C	N	O		0	0
			184	116	25	43			

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1172	Total	C	N	O	S	0	0
			9336	5895	1637	1748	56		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	271	Total	C	N	O	S	0	0
			2133	1340	355	424	14		

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	169	Total	C	N	O	S	0	0
			1353	838	237	275	3		

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	215	Total	C	N	O	S	0	0
			1760	1116	310	322	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	86	Total	C	N	O	S	0	0
			697	445	118	131	3		

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1340	861	222	249	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	141	Total	C	N	O	S	0	0
			1126	706	189	226	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	116	Total	C	N	O	S	0	0
			943	580	171	181	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	70	Total	C	N	O	S	0	0
			578	366	102	104	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	116	Total	C	N	O	S	0	0
			929	596	158	173	2		

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	43	Total	C	N	O	S	0	0
			344	211	69	60	4		

- Molecule 13 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	35	Total	C	N	O	S	0	0
			263	169	41	49	4		

- Molecule 14 is a protein called Transcription initiation factor IIF subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	P	103	Total	C	N	O	S	0	0
			861	554	142	162	3		

- Molecule 15 is a protein called Transcription initiation factor IIF subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Q	125	Total	C	N	O	S	0	0
			1033	644	189	195	5		

- Molecule 16 is a protein called Transcription elongation factor S-II.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	S	181	Total	C	N	O	S	0	0
			1436	893	256	279	8		

- Molecule 17 is a protein called Mediator of RNA polymerase II transcription subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	a	365	Total	C	N	O	S	0	0
			3008	1932	478	588	10		

- Molecule 18 is a protein called Mediator of RNA polymerase II transcription subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	d	171	Total	C	N	O	S	0	0
			1388	875	233	276	4		

- Molecule 19 is a protein called Mediator of RNA polymerase II transcription subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	f	169	Total	C	N	O	S	0	0
			1407	905	234	262	6		

- Molecule 20 is a protein called Mediator of RNA polymerase II transcription subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	g	169	Total	C	N	O	S	0	0
			1409	903	238	263	5		

- Molecule 21 is a protein called Mediator of RNA polymerase II transcription subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	h	136	Total	C	N	O	S	0	0
			1126	709	199	215	3		

- Molecule 22 is a protein called Mediator of RNA polymerase II transcription subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	i	83	Total	C	N	O	S	0	0
			709	444	130	134	1		

- Molecule 23 is a protein called Mediator of RNA polymerase II transcription subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	j	146	Total	C	N	O	S	0	0
			1173	725	206	239	3		

- Molecule 24 is a protein called Mediator of RNA polymerase II transcription subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	k	108	Total	C	N	O	S	0	0
			876	546	149	177	4		

- Molecule 25 is a protein called Mediator of RNA polymerase II transcription subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	n	625	Total	C	N	O	S	0	0
			5139	3318	884	913	24		

- Molecule 26 is a protein called Mediator of RNA polymerase II transcription subunit 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	q	515	Total	C	N	O	S	0	0
			4182	2674	707	788	13		

- Molecule 27 is a protein called Mediator of RNA polymerase II transcription subunit 18.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	r	253	Total	C	N	O	S	0	0
			1995	1271	331	383	10		

- Molecule 28 is a protein called Mediator of RNA polymerase II transcription subunit 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	s	81	Total	C	N	O	S	0	0
			657	415	109	132	1		

- Molecule 29 is a protein called Mediator of RNA polymerase II transcription subunit 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	t	210	Total	C	N	O	S	0	0
			1609	1016	270	317	6		

- Molecule 30 is a protein called Mediator of RNA polymerase II transcription subunit 21.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	u	122	Total	C	N	O	S	0	0
			978	611	163	199	5		

- Molecule 31 is a protein called Mediator of RNA polymerase II transcription subunit 22.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	v	109	Total	C	N	O	S	0	0
			869	540	143	180	6		

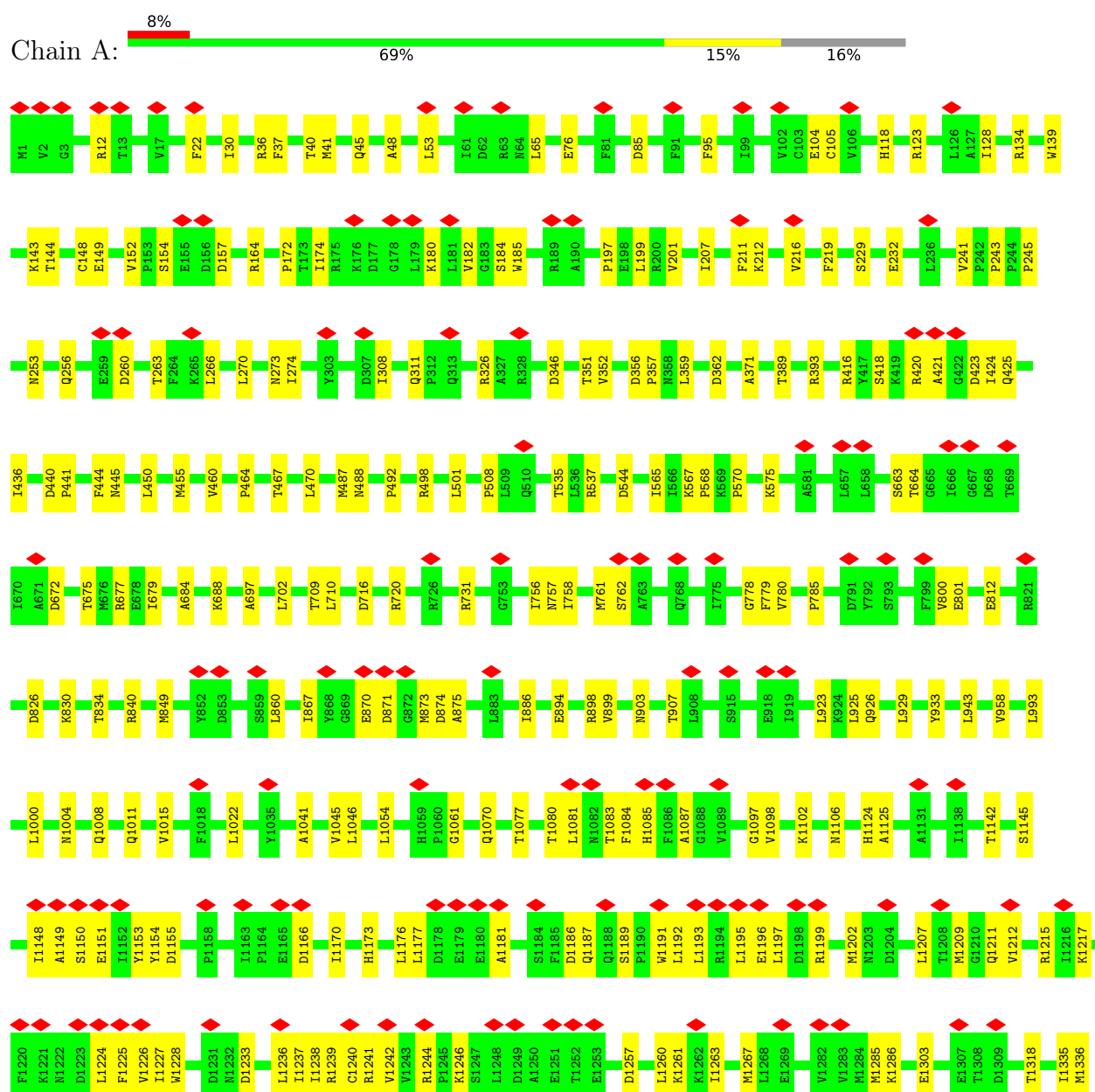
- Molecule 32 is a protein called Mediator of RNA polymerase II transcription subunit 31.

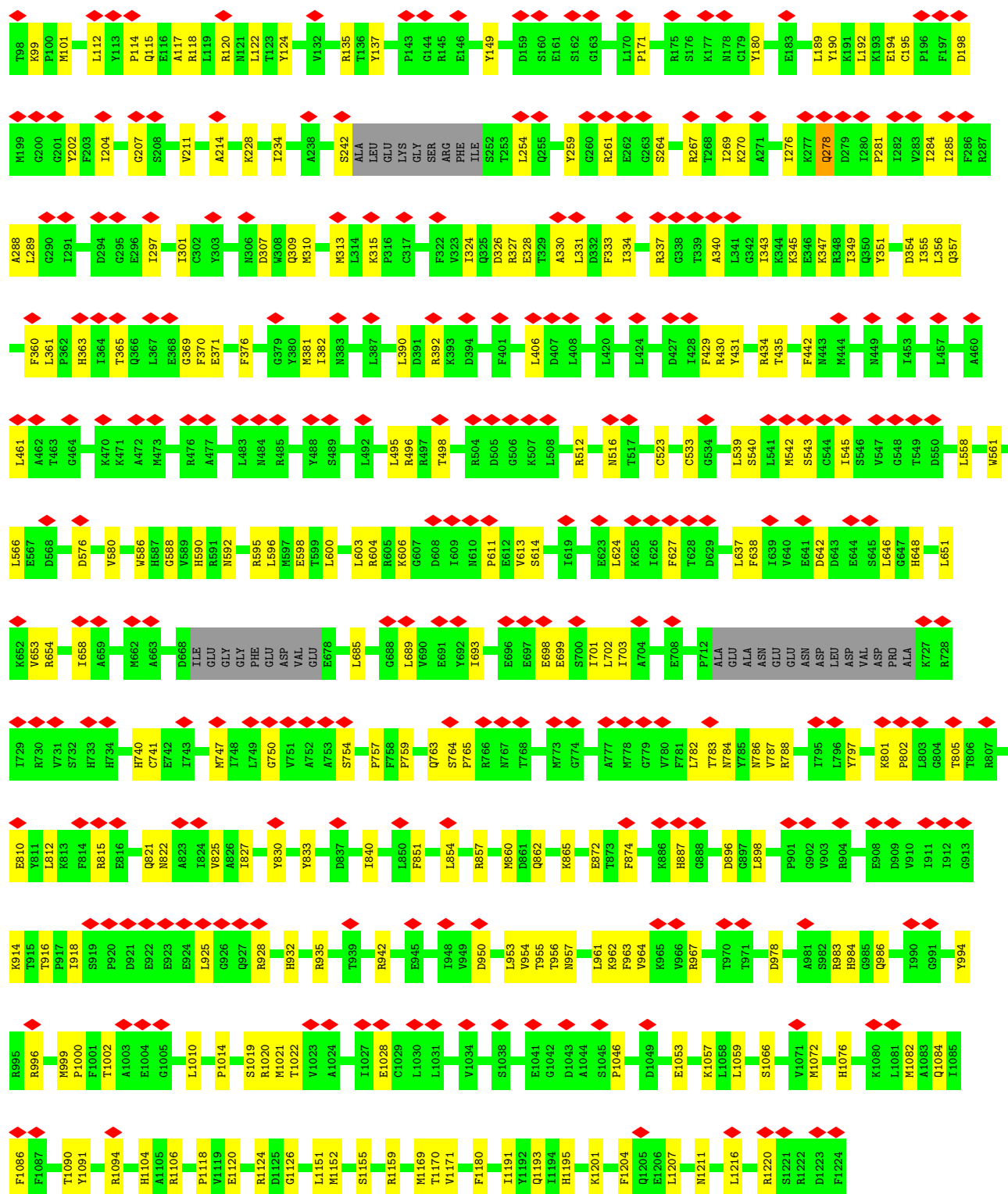
Mol	Chain	Residues	Atoms					AltConf	Trace
32	w	103	Total	C	N	O	S	0	0
			871	575	135	155	6		

3 Residue-property plots

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

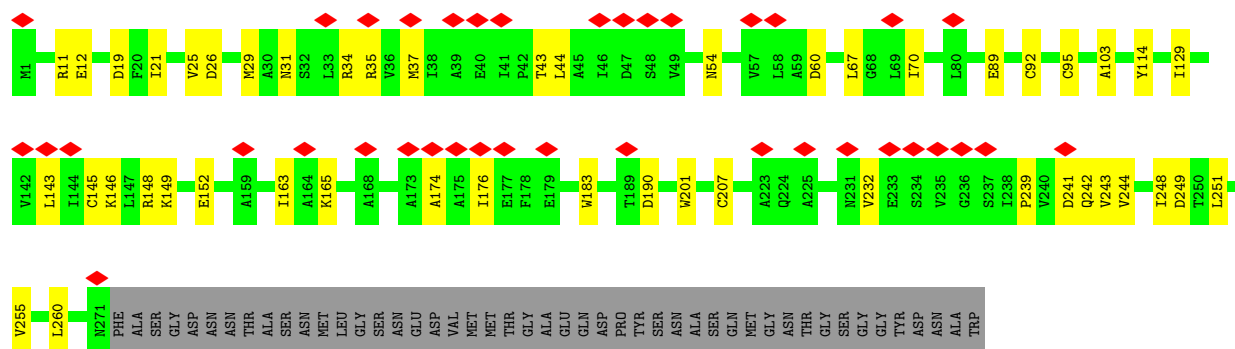
- Molecule 1: DNA-directed RNA polymerase II subunit RPB1



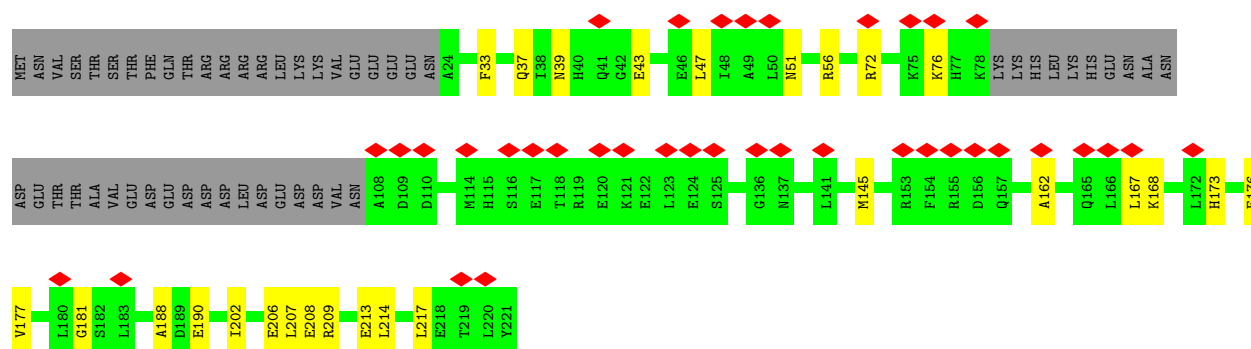


• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

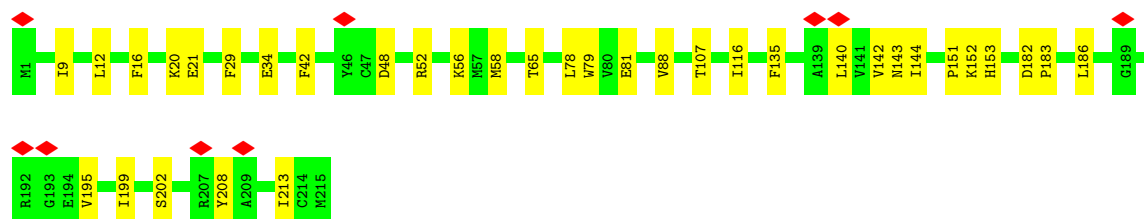
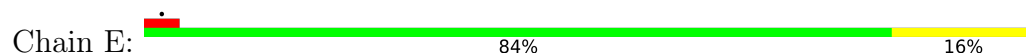




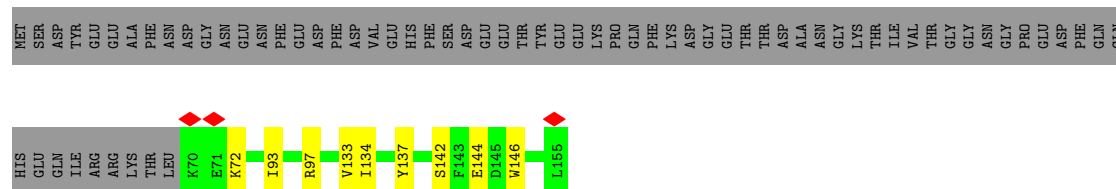
• Molecule 4: DNA-directed RNA polymerase II subunit RPB4



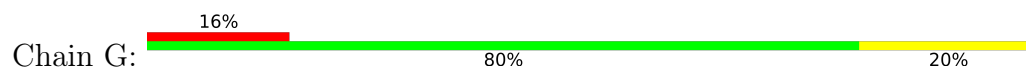
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

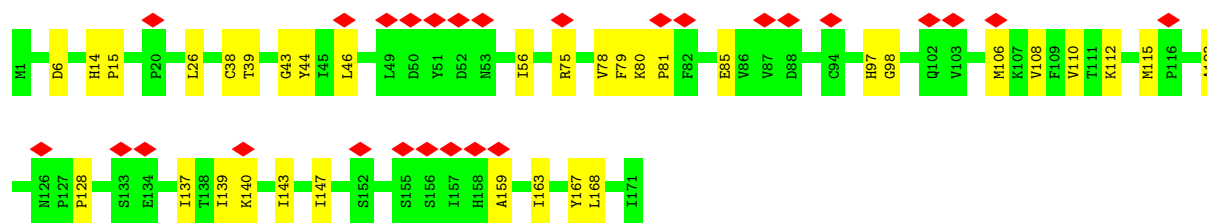


• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

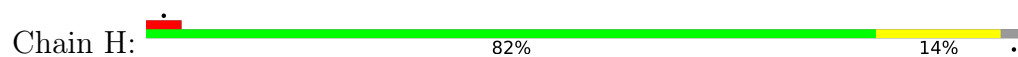


• Molecule 7: DNA-directed RNA polymerase II subunit RPB7

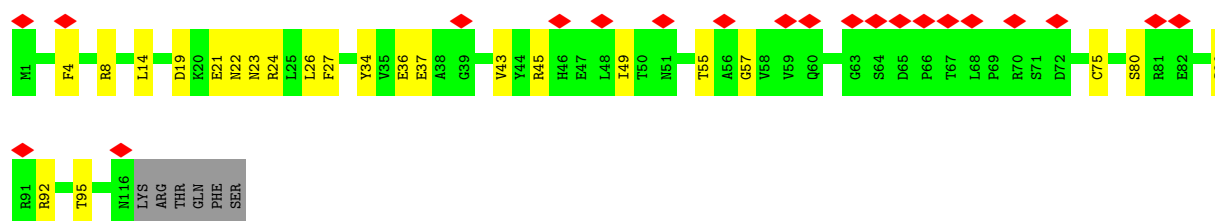
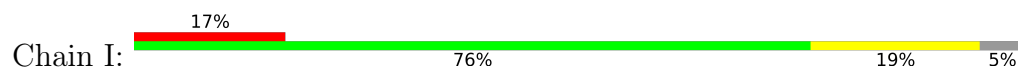




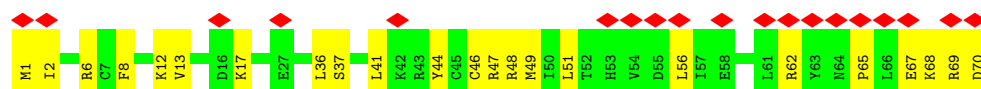
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



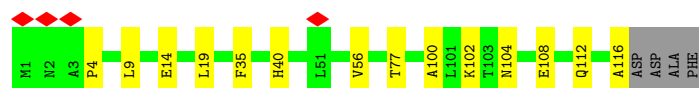
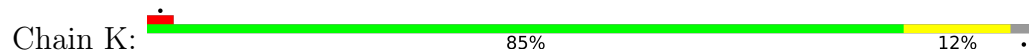
- Molecule 9: DNA-directed RNA polymerase II subunit RPB9



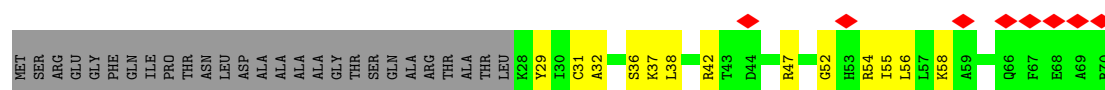
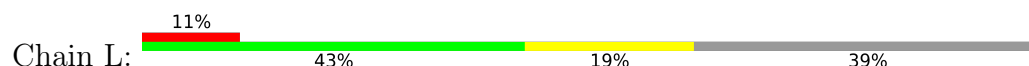
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



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



- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

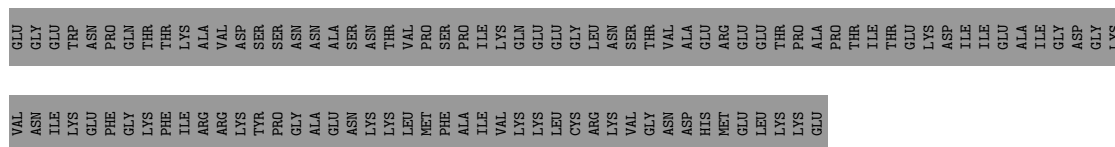


- Molecule 13: Transcription initiation factor IIB

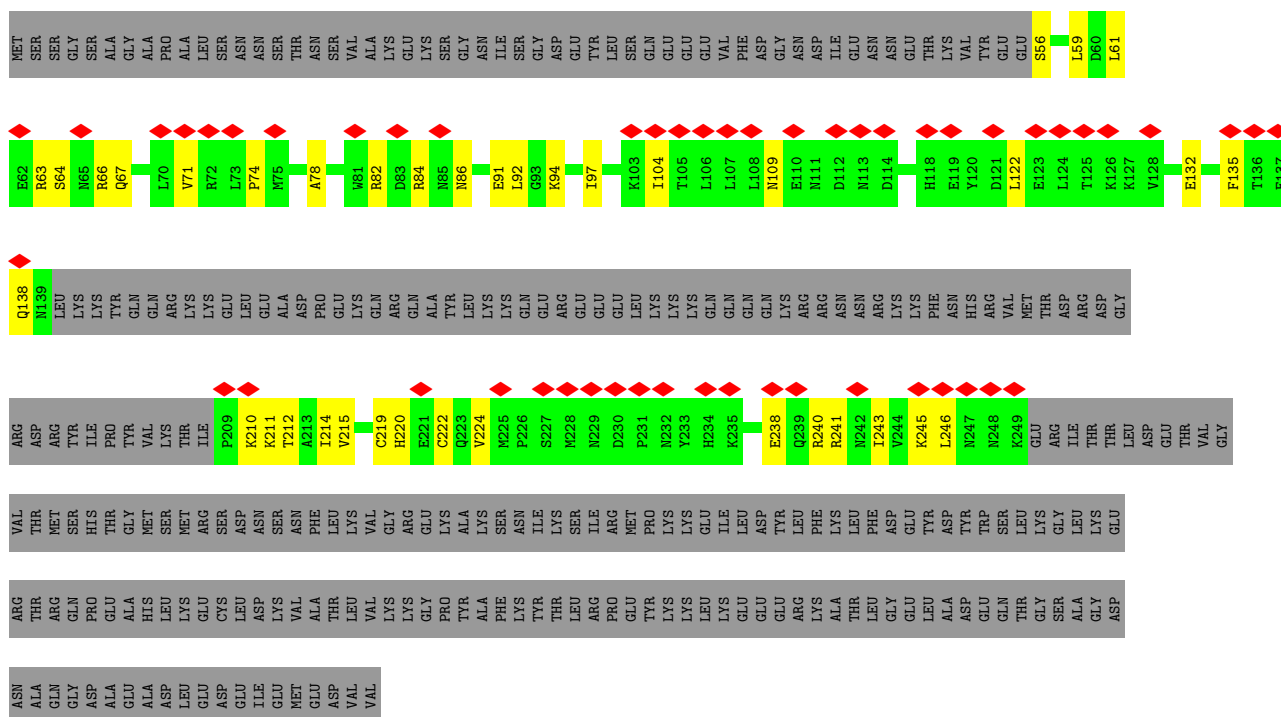
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Chain P: 10% 86%

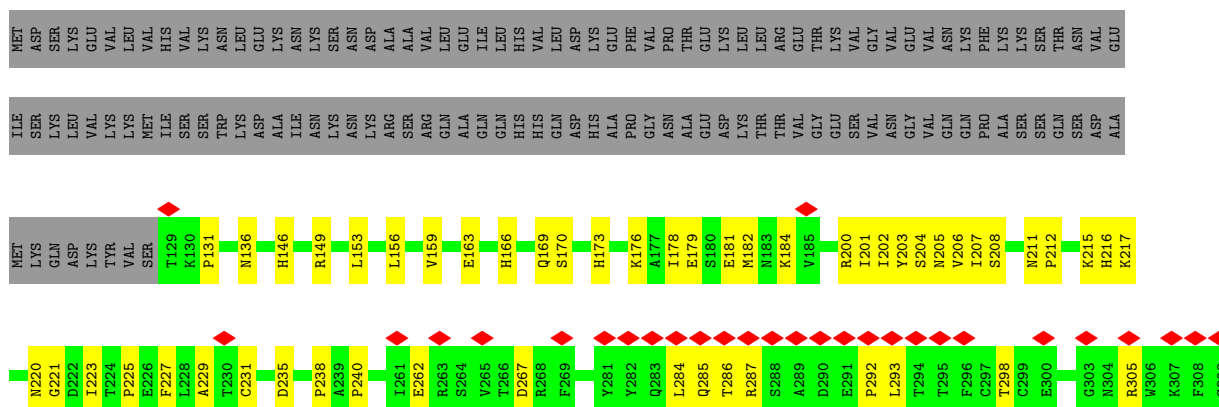
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VAL	ALA	ALA	Y393	ASN	ALA	ASP	THR	THR	ASP	THR
LYS	PRO	MET	K394	LEU	ASN	ASP	ARG	ARG	ASP	ARG
GLY	GLU	GLU	F395	ARG	GLY	VAL	THR	LEU	PRO	ASN
ASN	ASN	ASP	T396	LYS	PRO	LYS	LYS	GLN	TYR	PRO
GLU	GLU	ASP	A397	THR	LEU	ASP	THR	PHE	ALA	PRO
ASP	ASP	ASP	R398	ARG	VAL	VAL	ARG	GLN	ALA	GLY
ASP	ASP	ASP	H399	GLN	THR	THR	THR	LEU	GLU	SER
THR	GLU	ASP	LYS	LEU	LYS	LYS	ALA	THR	ARG	THR
LEU	LEU	ASN	TYR	VAL	GLU	GLY	ASN	ARG	GLY	ASN
SER	PHE	SER	ALA	VAL	ASP	VAL	GLY	ALA	LYS	GLY
LYS	GLY	GLU	THR	LEU	ASP	VAL	THR	ILE	MET	GLY
SER	GLU	VAL	THR	ASP	ALA	ASN	GLY	ILE	LEU	GLY
LYS	GLU	GLU	THR	GLU	GLY	SER	SER	GLN	LEU	PRO
ARG	LYS	LEU	ILE	PRO	PRO	ILE	ILE	ARG	ILE	THR
SER	ASP	TYR	ASP	GLU	GLU	PRO	GLY	GLN	GLY	ASN
PRO	GLU	ASP	ALA	LYS	ASP	THR	VAL	LYS	VAL	ALA
LYS	ASP	GLU	ALA	LYS	MET	ASP	SER	GLY	ARG	SER
GLN	GLY	PHE	PHE	PHE	VAL	SER	GLY	SER	TYR	LYS
GLN	ARG	ALA	E346	E346	VAL	SER	SER	LYS	LYS	ASP
ALA	LYS	ASP	F347	F347	MET	VAL	VAL	ASP	ASP	ARG
LYS	ALA	GLY	Y348	Y348	GLY	VAL	PRO	LYS	SER	ARG
THR	ALA	GLU	SER	SER	LYS	PRO	ALA	LYS	THR	THR
ASN	LEU	ALA	GLY	GLY	TYR	ALA	ALA	VAL	ALA	PRO
ALA	GLN	PRO	GLU	ASP	ASP	ASP	ASP	GLY	GLY	LYS
HIS	LYS	ILE	VAL	VAL	GLY	PRO	PRO	GLN	VAL	VAL
VAL	THR	ILE	VAL	K352	GLY	THR	THR	GLY	LYS	PHE
HIS	GLU	ASP	PRO	E353	GLU	THR	THR	ARG	ASP	LEU
LYS	LEU	GLY	TRP	D354	VAL	VAL	VAL	SER	GLU	ARG
GLU	ALA	ASN	F355	F355	THR	THR	VAL	THR	ASP	MET
PRO	ALA	GLU	MET	M359	ASN	VAL	VAL	PRO	ASP	ARG
THR	LEU	GLN	LYS	LYS	GLU	VAL	GLU	ASN	GLY	GLY
LEU	TYR	GLU	HIS	LEU	PRO	GLU	SER	GLY	SER	GLN
ARG	SER	ASN	LEU	K361	PHE	GLU	ASN	GLY	GLY	ASN
VAL	SER	LYS	ASP	V362	GLU	GLY	GLY	MET	GLY	LYS
LYS	ASP	GLU	ASN	ASN	GLU	GLU	LEU	LYS	ASN	SER
ILE	ASN	GLU	ILE	G363	GLY	GLY	GLY	SER	LYS	SER
LYS	GLU	GLN	THR	K364	THR	THR	THR	LYS	GLY	ASN
ASN	ILE	ARG	THR	Y365	MET	MET	MET	GLY	GLY	SER
CYS	ASN	ILE	THR	E366	ASP	ASP	ASP	THR	L118	SER
VAL	PRO	LYS	THR	A367	PRO	PRO	THR	VAL	L119	SER
ILE	TYR	LEU	THR	G368	LEU	SER	LEU	VAL	K120	PRO
ILE	ILE	GLU	ARG	C368	ALA	ALA	LEU	SER	K124	GLY
LEU	SER	MET	TYR	H369	ASP	ASP	ASN	ASN	K125	PRO
LYS	GLU	LEU	ARG	S370	VAL	VAL	ASN	ASN	K126	GLY
GLY	SER	GLN	THR	D371	ALA	GLY	THR	THR	I127	ASN
ASP	ASP	ALA	THR	S372	PRO	LEU	VAL	VAL	I128	GLY
LYS	ILE	ASN	ARG	Y373	GLY	GLY	LYS	LYS	P129	ASN
GLU	GLU	ALA	ARG	LYS	GLY	ASN	ASP	ASP	V130	SER
ILE	ASN	MET	LYS	Y374	GLY	GLY	GLY	GLY	T131	ARG
LEU	LYS	GLY	LYS	L375	GLY	ALA	SER	SER	D132	GLY
LYS	GLU	LEU	ALA	L376	ARG	ARG	GLN	GLN	F133	LEU
SER	ASN	ARG	VAL	S377	ALA	THR	THR	THR	H134	SER
PHE	GLU	ASP	VAL	GLY	LYS	ALA	PRO	PRO	R141	LEU



- Molecule 15: Transcription initiation factor IIF subunit beta

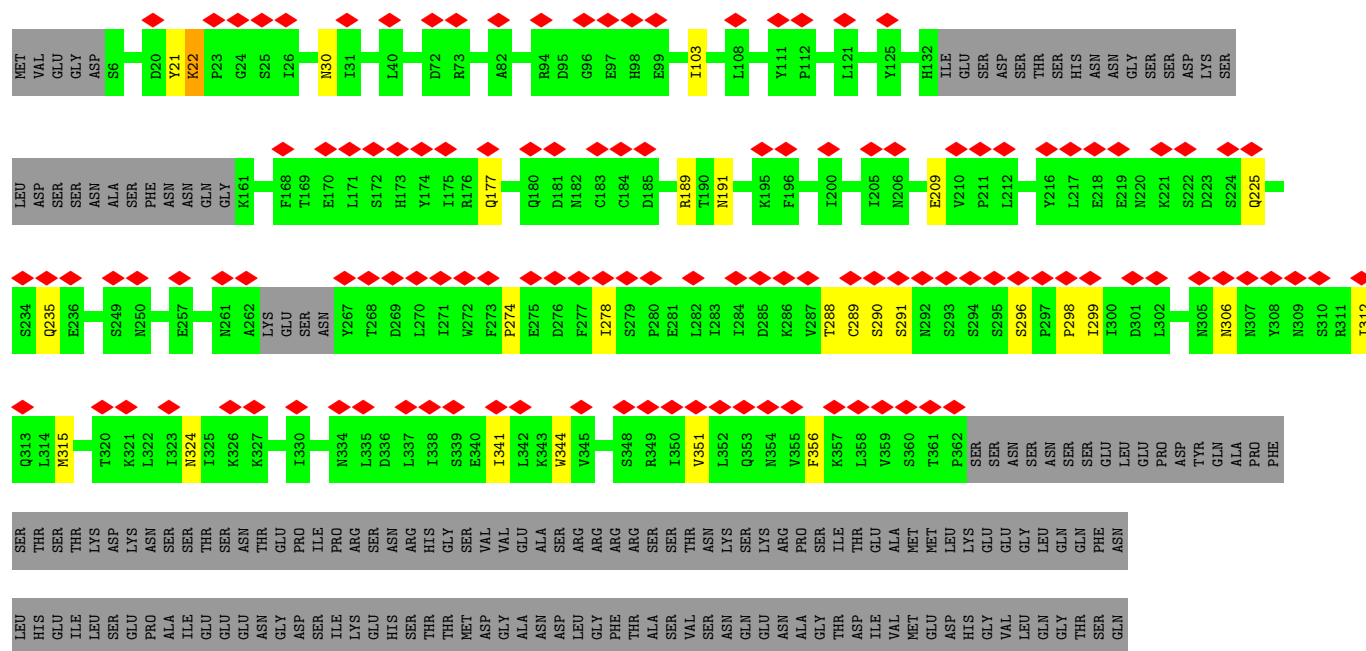


- Molecule 16: Transcription elongation factor S-II

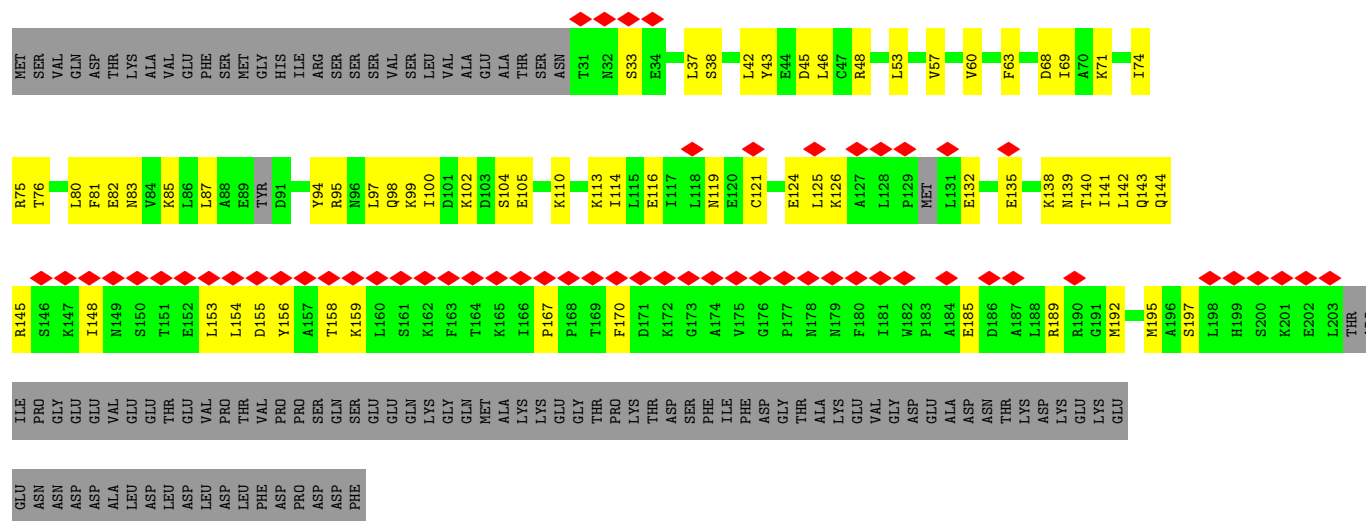


- Molecule 17: Mediator of RNA polymerase II transcription subunit 1

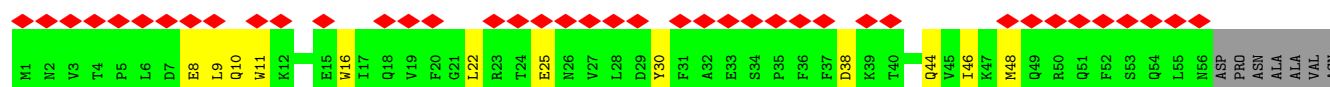


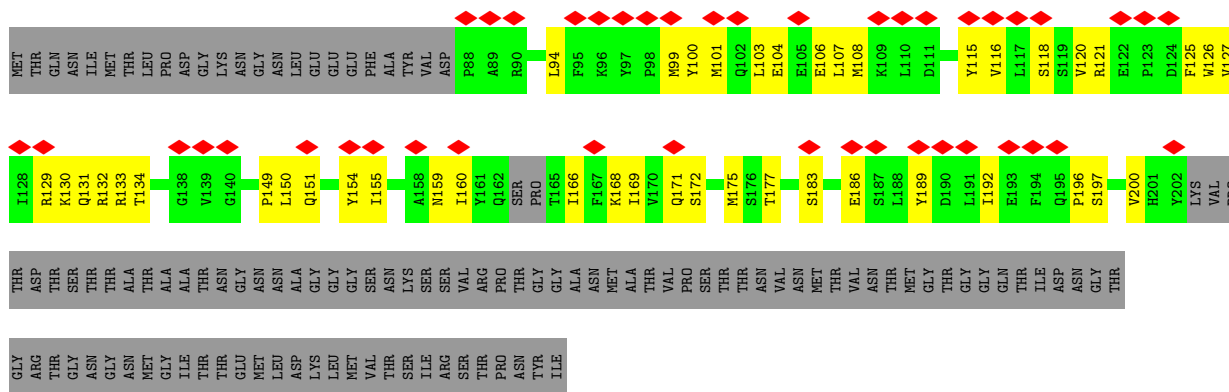


• Molecule 18: Mediator of RNA polymerase II transcription subunit 4

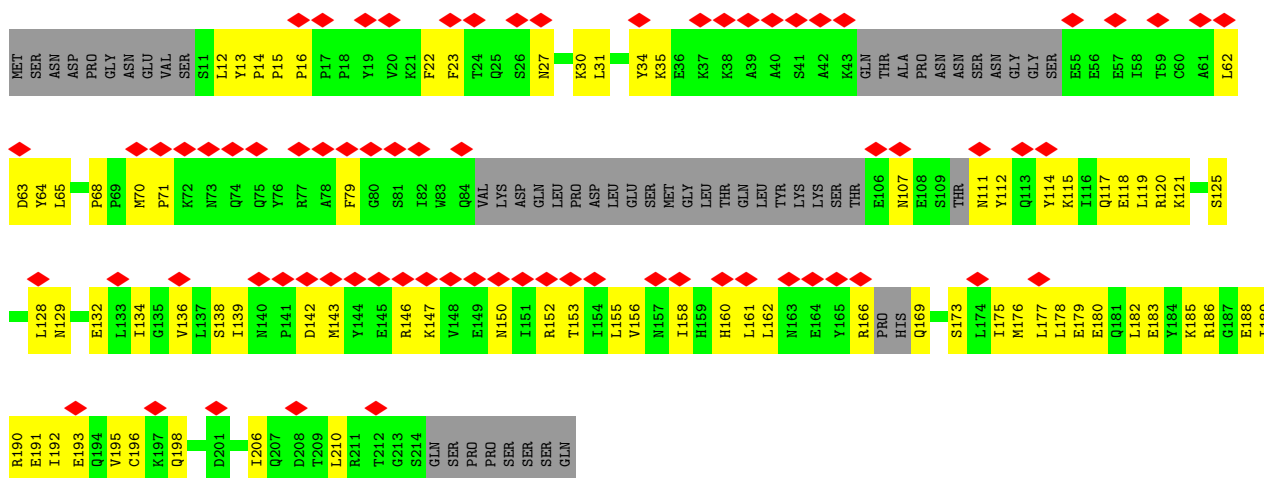


• Molecule 19: Mediator of RNA polymerase II transcription subunit 6

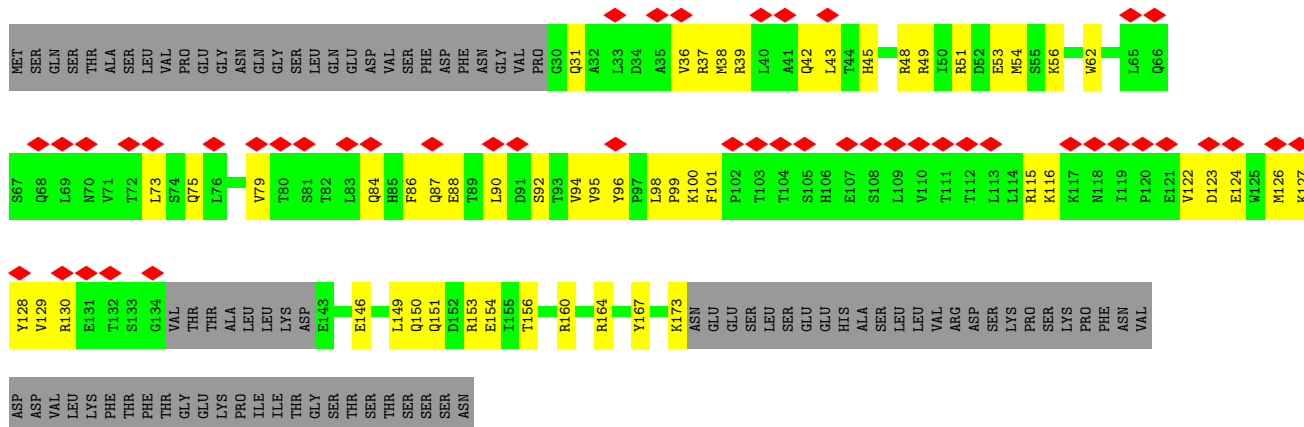




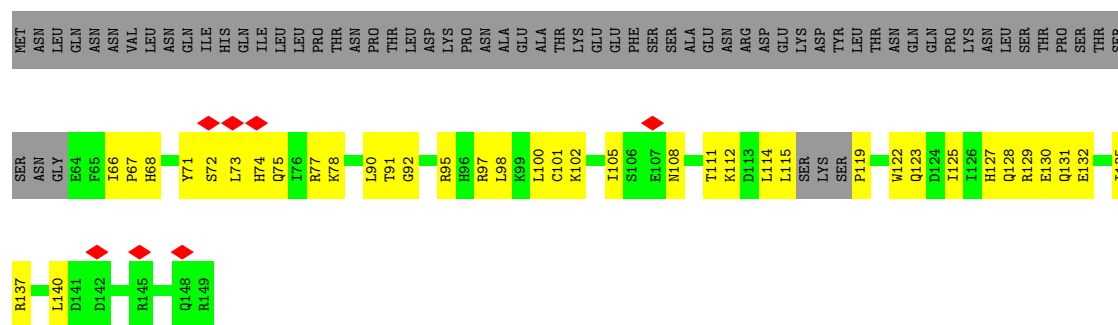
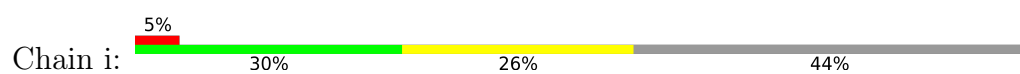
- Molecule 20: Mediator of RNA polymerase II transcription subunit 7



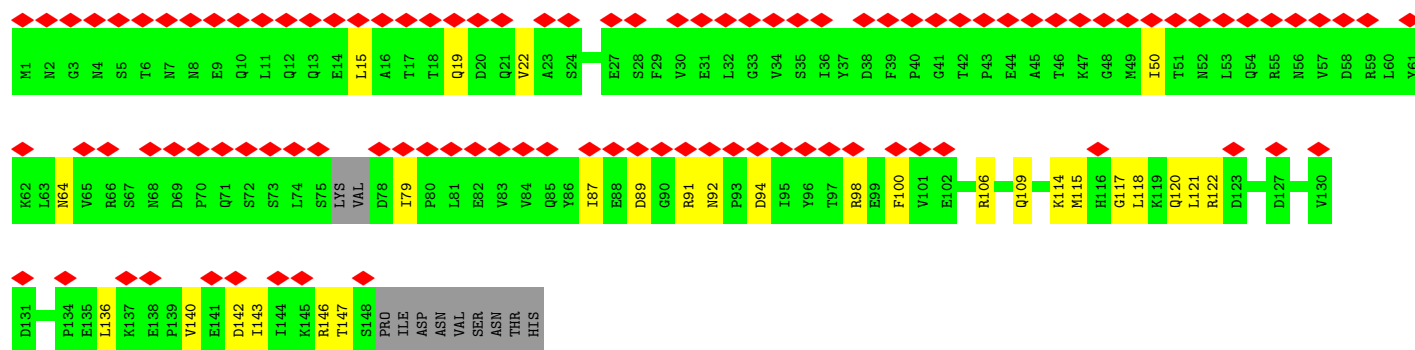
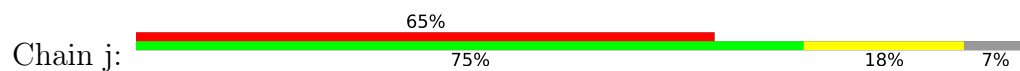
- Molecule 21: Mediator of RNA polymerase II transcription subunit 8



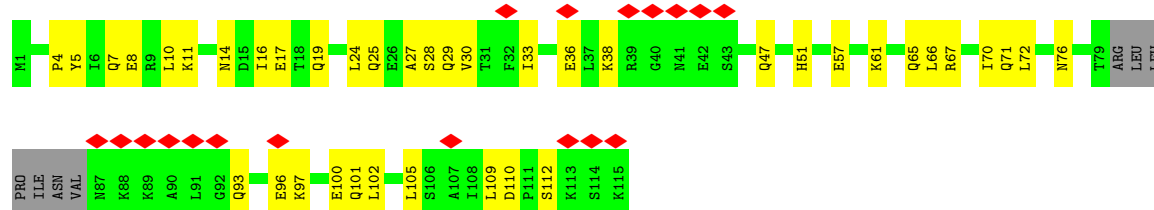
- Molecule 22: Mediator of RNA polymerase II transcription subunit 9



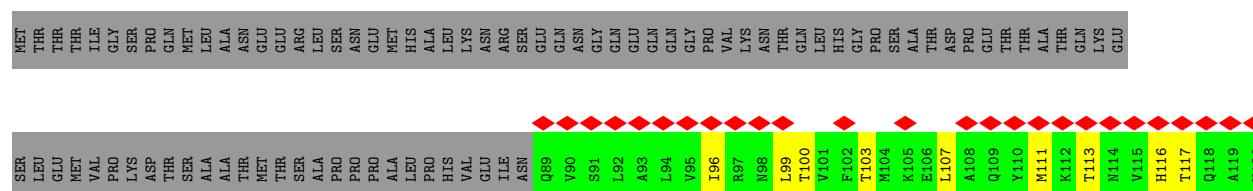
• Molecule 23: Mediator of RNA polymerase II transcription subunit 10

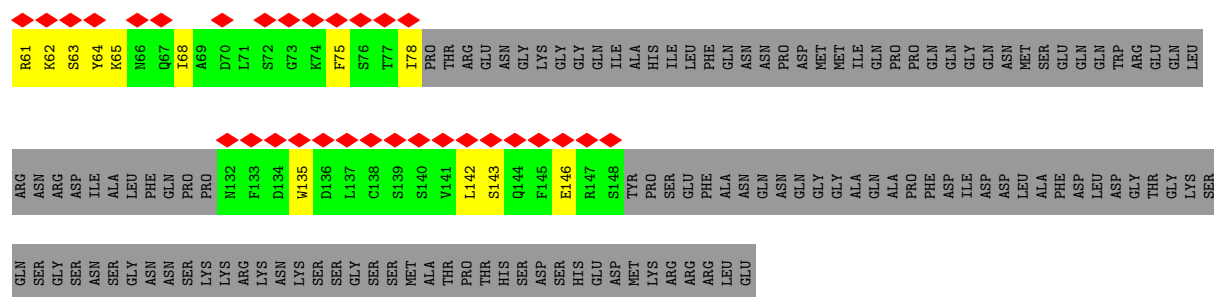


• Molecule 24: Mediator of RNA polymerase II transcription subunit 11

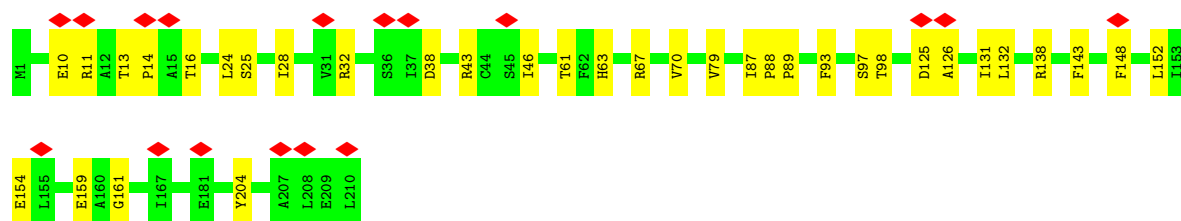
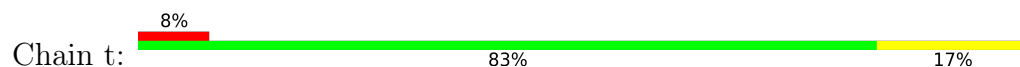


• Molecule 25: Mediator of RNA polymerase II transcription subunit 14

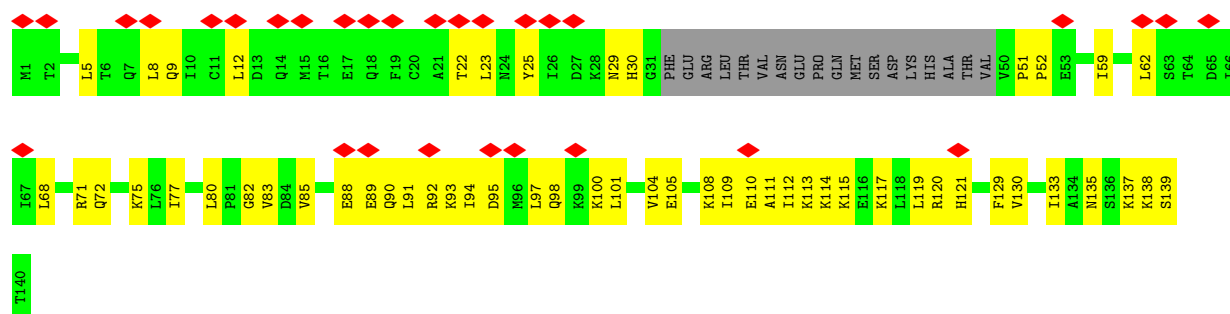




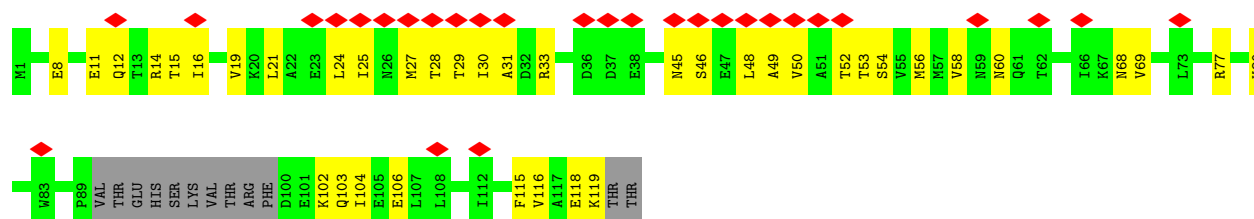
- Molecule 29: Mediator of RNA polymerase II transcription subunit 20



- Molecule 30: Mediator of RNA polymerase II transcription subunit 21

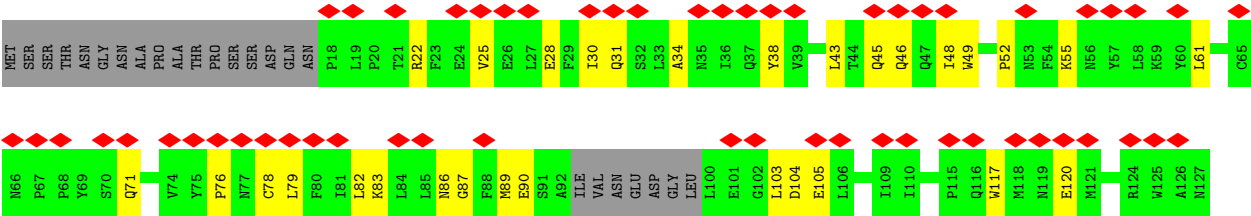


- Molecule 31: Mediator of RNA polymerase II transcription subunit 22



- Molecule 32: 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	91293	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	42	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.051	Depositor
Minimum map value	-0.036	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.004	Depositor
Map size ($\text{\AA}$)	496.8, 496.8, 496.8	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.38, 1.38, 1.38	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	0.18	0/11632	0.35	0/15735
1	z	0.15	0/194	0.36	0/270
2	B	0.17	0/9520	0.35	2/12839 (0.0%)
3	C	0.17	0/2171	0.35	0/2941
4	D	0.10	0/1365	0.21	0/1831
5	E	0.13	0/1796	0.28	0/2416
6	F	0.16	0/709	0.31	0/956
7	G	0.13	0/1368	0.30	0/1844
8	H	0.15	0/1144	0.32	0/1548
9	I	0.13	0/961	0.35	0/1294
10	J	0.19	0/587	0.45	0/786
11	K	0.18	0/947	0.35	0/1279
12	L	0.12	0/346	0.27	0/457
13	M	0.14	0/267	0.27	0/362
14	P	0.11	0/886	0.24	0/1198
15	Q	0.11	0/1049	0.28	0/1413
16	S	0.13	0/1462	0.31	0/1973
17	a	0.67	0/3067	1.13	7/4148 (0.2%)
18	d	0.18	0/1405	0.51	0/1889
19	f	0.15	0/1440	0.35	0/1946
20	g	0.17	0/1434	0.41	1/1930 (0.1%)
21	h	0.16	0/1147	0.44	0/1552
22	i	0.21	0/720	0.54	0/965
23	j	0.13	0/1188	0.25	0/1604
24	k	0.17	0/885	0.44	0/1183
25	n	0.11	0/5226	0.28	0/7051
26	q	0.13	0/4245	0.33	0/5702
27	r	0.16	0/2030	0.33	0/2747
28	s	0.11	0/669	0.22	0/906
29	t	0.15	0/1635	0.32	0/2215
30	u	0.19	0/984	0.54	0/1317
31	v	0.18	0/873	0.46	0/1177
32	w	0.13	0/897	0.32	0/1219
All	All	0.21	0/64249	0.42	10/86693 (0.0%)

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	278	GLN	CA-C-N	5.83	132.68	121.54
2	B	278	GLN	C-N-CA	5.83	132.68	121.54
20	g	16	PRO	CA-N-CD	-5.60	104.16	112.00
17	a	298	PRO	CA-C-N	5.45	127.43	120.56
17	a	298	PRO	C-N-CA	5.45	127.43	120.56

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11425	0	11482	211	0
1	z	184	0	163	6	0
2	B	9336	0	9341	213	0
3	C	2133	0	2096	37	0
4	D	1353	0	1352	21	0
5	E	1760	0	1788	23	0
6	F	697	0	720	7	0
7	G	1340	0	1357	23	0
8	H	1126	0	1094	13	0
9	I	943	0	906	17	0
10	J	578	0	593	31	0
11	K	929	0	939	12	0
12	L	344	0	367	11	0
13	M	263	0	273	3	0
14	P	861	0	819	22	0
15	Q	1033	0	1036	28	0
16	S	1436	0	1428	37	0
17	a	3008	0	2953	35	0
18	d	1388	0	1400	71	0
19	f	1407	0	1385	48	0
20	g	1409	0	1434	68	0
21	h	1126	0	1125	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	i	709	0	712	51	0
23	j	1173	0	1156	36	0
24	k	876	0	885	29	0
25	n	5139	0	5375	94	0
26	q	4182	0	4324	109	0
27	r	1995	0	2018	29	0
28	s	657	0	636	24	0
29	t	1609	0	1626	23	0
30	u	978	0	1005	52	0
31	v	869	0	881	43	0
32	w	871	0	857	20	0
All	All	63137	0	63526	1250	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 10.

The worst 5 of 1250 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)
17:a:21:TYR:CE1	18:d:74:ILE:HG21	1.49	1.44
17:a:21:TYR:HE1	18:d:74:ILE:CG2	1.46	1.26
17:a:22:LYS:NZ	22:i:73:LEU:HD22	1.56	1.19
17:a:22:LYS:NZ	22:i:73:LEU:CD2	2.11	1.13
17:a:22:LYS:HD2	18:d:74:ILE:HD12	1.35	1.09

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	1451/1733 (84%)	1407 (97%)	43 (3%)	1 (0%)	48 83

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	z	23/1733 (1%)	21 (91%)	1 (4%)	1 (4%)	2	17
2	B	1164/1224 (95%)	1132 (97%)	32 (3%)	0	100	100
3	C	269/318 (85%)	261 (97%)	8 (3%)	0	100	100
4	D	165/221 (75%)	163 (99%)	2 (1%)	0	100	100
5	E	213/215 (99%)	210 (99%)	3 (1%)	0	100	100
6	F	84/155 (54%)	83 (99%)	1 (1%)	0	100	100
7	G	169/171 (99%)	166 (98%)	3 (2%)	0	100	100
8	H	137/146 (94%)	134 (98%)	3 (2%)	0	100	100
9	I	114/122 (93%)	113 (99%)	1 (1%)	0	100	100
10	J	68/70 (97%)	65 (96%)	3 (4%)	0	100	100
11	K	114/120 (95%)	112 (98%)	2 (2%)	0	100	100
12	L	41/70 (59%)	39 (95%)	2 (5%)	0	100	100
13	M	33/345 (10%)	33 (100%)	0	0	100	100
14	P	99/735 (14%)	98 (99%)	1 (1%)	0	100	100
15	Q	121/400 (30%)	121 (100%)	0	0	100	100
16	S	179/309 (58%)	177 (99%)	2 (1%)	0	100	100
17	a	357/566 (63%)	343 (96%)	11 (3%)	3 (1%)	16	53
18	d	165/284 (58%)	164 (99%)	1 (1%)	0	100	100
19	f	163/295 (55%)	161 (99%)	2 (1%)	0	100	100
20	g	159/222 (72%)	158 (99%)	1 (1%)	0	100	100
21	h	132/223 (59%)	129 (98%)	3 (2%)	0	100	100
22	i	79/149 (53%)	79 (100%)	0	0	100	100
23	j	142/157 (90%)	137 (96%)	5 (4%)	0	100	100
24	k	104/115 (90%)	104 (100%)	0	0	100	100
25	n	611/1082 (56%)	607 (99%)	4 (1%)	0	100	100
26	q	505/687 (74%)	500 (99%)	5 (1%)	0	100	100
27	r	249/307 (81%)	244 (98%)	5 (2%)	0	100	100
28	s	77/220 (35%)	76 (99%)	1 (1%)	0	100	100
29	t	208/210 (99%)	206 (99%)	2 (1%)	0	100	100
30	u	116/140 (83%)	115 (99%)	1 (1%)	0	100	100
31	v	105/121 (87%)	105 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	w	99/127 (78%)	97 (98%)	2 (2%)	0	100	100
All	All	7715/12992 (59%)	7560 (98%)	150 (2%)	5 (0%)	49	83

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	z	21	SER
17	a	291	SER
17	a	306	ASN
17	a	289	CYS
1	A	958	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	
1	A	1268/1520 (83%)	1267 (100%)	1 (0%)	88	88
1	z	25/1520 (2%)	25 (100%)	0	100	100
2	B	1018/1061 (96%)	1018 (100%)	0	100	100
3	C	239/274 (87%)	239 (100%)	0	100	100
4	D	150/200 (75%)	150 (100%)	0	100	100
5	E	197/197 (100%)	197 (100%)	0	100	100
6	F	76/137 (56%)	76 (100%)	0	100	100
7	G	152/152 (100%)	152 (100%)	0	100	100
8	H	124/128 (97%)	124 (100%)	0	100	100
9	I	110/116 (95%)	110 (100%)	0	100	100
10	J	65/65 (100%)	65 (100%)	0	100	100
11	K	99/102 (97%)	99 (100%)	0	100	100
12	L	38/57 (67%)	38 (100%)	0	100	100
13	M	32/299 (11%)	32 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	P	95/641 (15%)	95 (100%)	0	100	100
15	Q	119/363 (33%)	119 (100%)	0	100	100
16	S	158/274 (58%)	158 (100%)	0	100	100
17	a	350/528 (66%)	347 (99%)	3 (1%)	70	76
18	d	158/258 (61%)	158 (100%)	0	100	100
19	f	158/259 (61%)	158 (100%)	0	100	100
20	g	160/208 (77%)	160 (100%)	0	100	100
21	h	128/207 (62%)	128 (100%)	0	100	100
22	i	82/144 (57%)	82 (100%)	0	100	100
23	j	134/145 (92%)	134 (100%)	0	100	100
24	k	101/108 (94%)	101 (100%)	0	100	100
25	n	591/1001 (59%)	591 (100%)	0	100	100
26	q	482/642 (75%)	482 (100%)	0	100	100
27	r	228/280 (81%)	228 (100%)	0	100	100
28	s	75/195 (38%)	75 (100%)	0	100	100
29	t	178/178 (100%)	178 (100%)	0	100	100
30	u	115/132 (87%)	115 (100%)	0	100	100
31	v	101/113 (89%)	101 (100%)	0	100	100
32	w	97/117 (83%)	97 (100%)	0	100	100
All	All	7103/11621 (61%)	7099 (100%)	4 (0%)	87	88

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1124	HIS
17	a	288	THR
17	a	290	SER
17	a	296	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 61 such sidechains are listed below:

Mol	Chain	Res	Type
16	S	304	ASN
30	u	98	GLN

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Mol	Chain	Res	Type
18	d	144	GLN
30	u	9	GLN
31	v	86	ASN

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
26	q	1
30	u	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	q	318:ASN	C	319:LYS	N	5.82
1	u	80:LEU	C	81:PRO	N	3.17

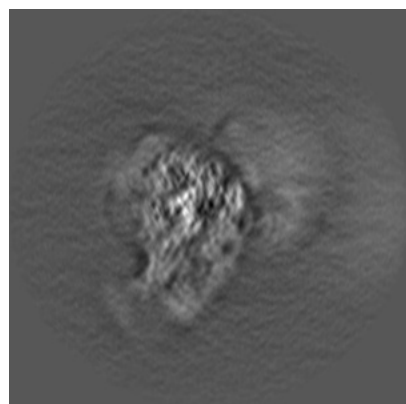
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26544. These allow visual inspection of the internal detail of the map and identification of artifacts.

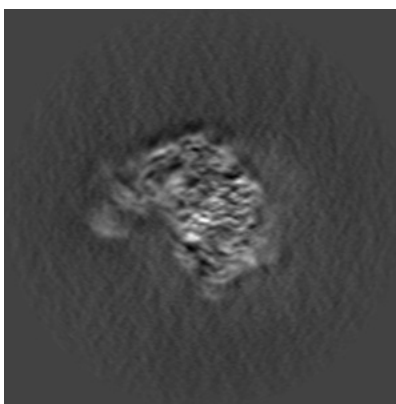
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

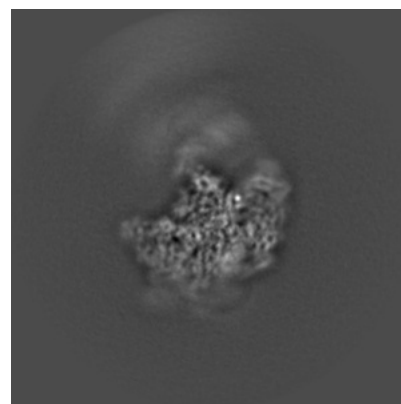
6.1.1 Primary map



X

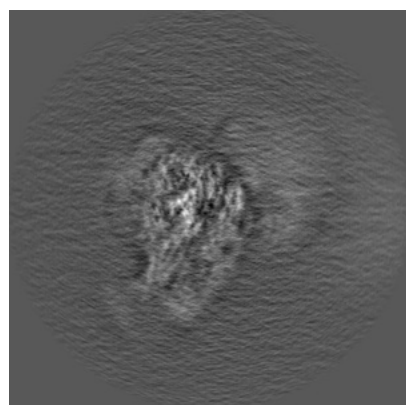


Y

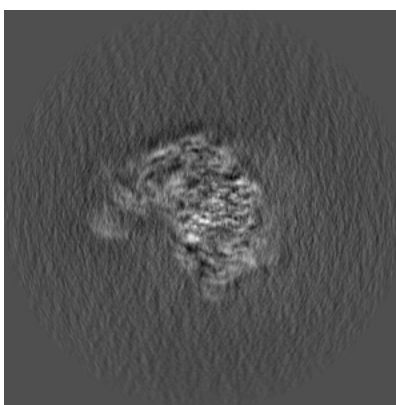


Z

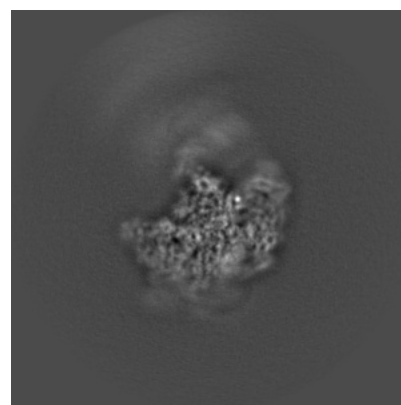
6.1.2 Raw map



X



Y

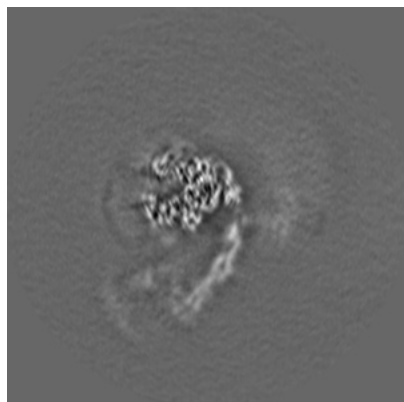


Z

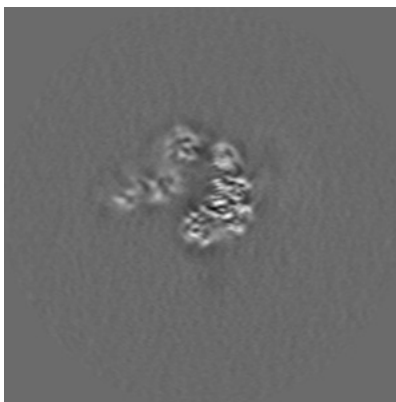
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

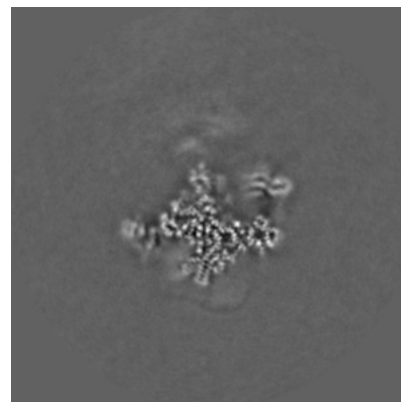
6.2.1 Primary map



X Index: 180

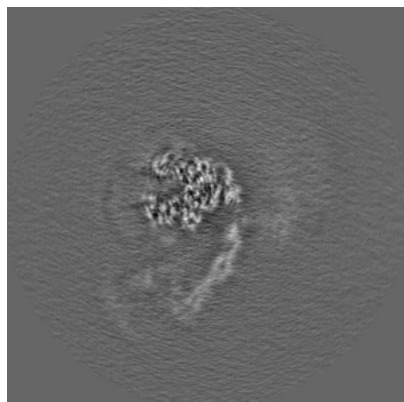


Y Index: 180

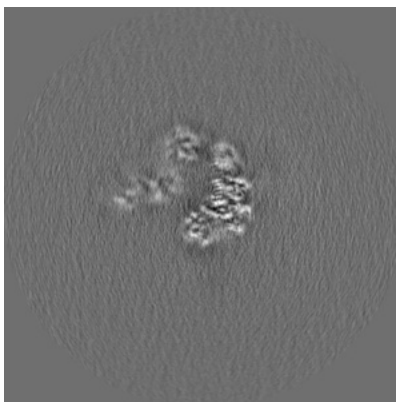


Z Index: 180

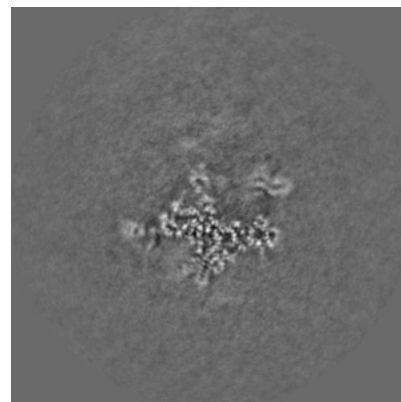
6.2.2 Raw map



X Index: 180



Y Index: 180

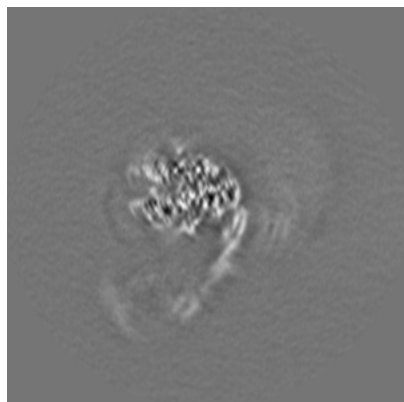


Z Index: 180

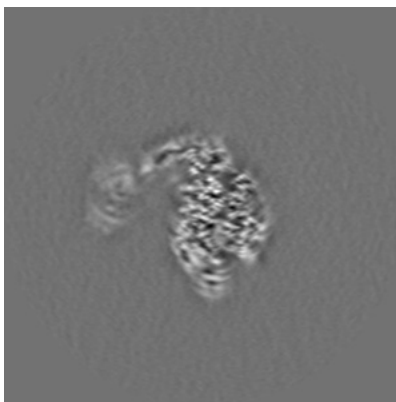
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

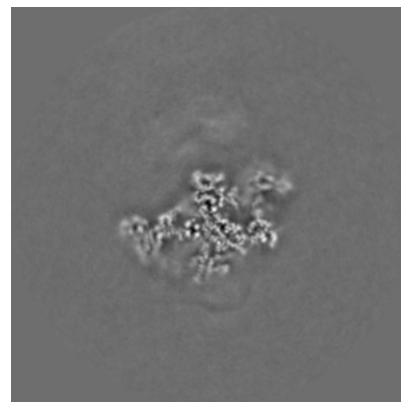
6.3.1 Primary map



X Index: 176

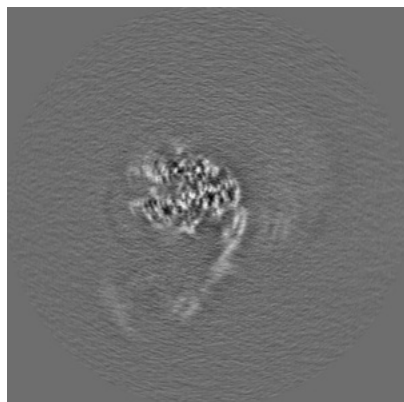


Y Index: 160

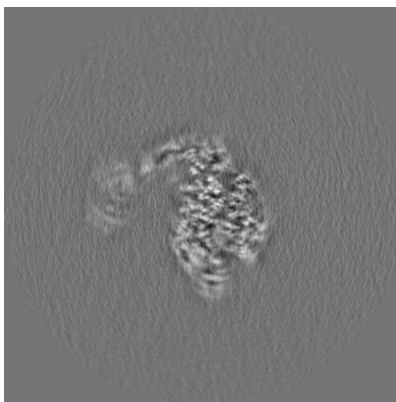


Z Index: 187

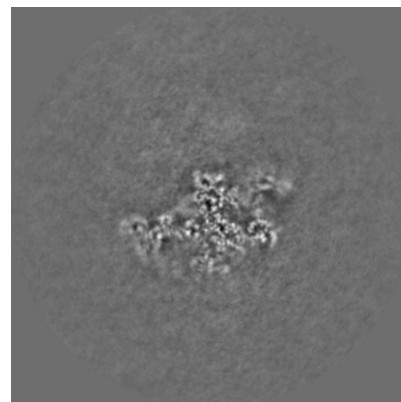
6.3.2 Raw map



X Index: 176



Y Index: 160

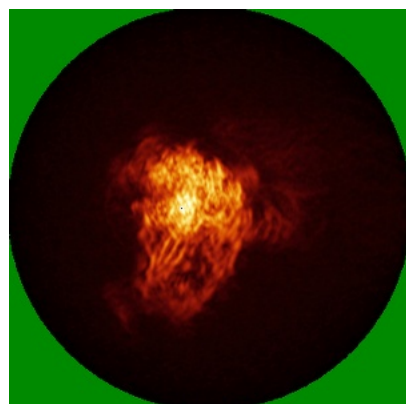


Z Index: 188

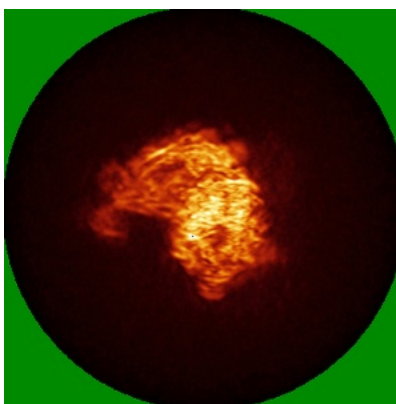
The images above show the largest variance slices of the map in three orthogonal directions.

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

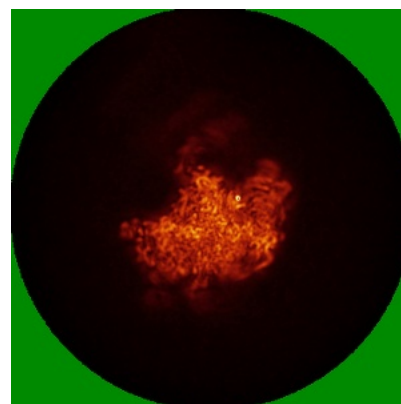
6.4.1 Primary map



X

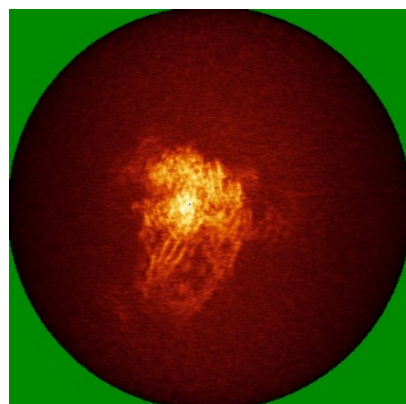


Y

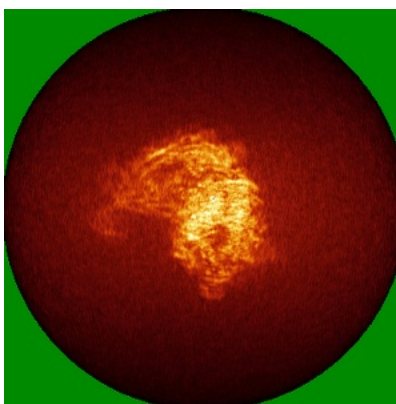


Z

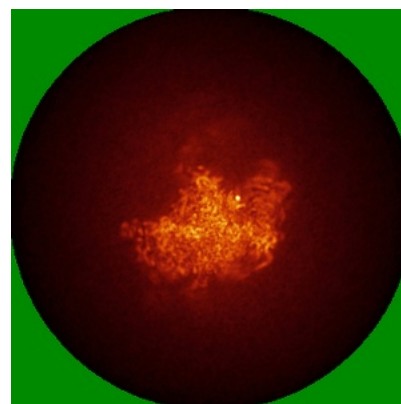
6.4.2 Raw map



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.

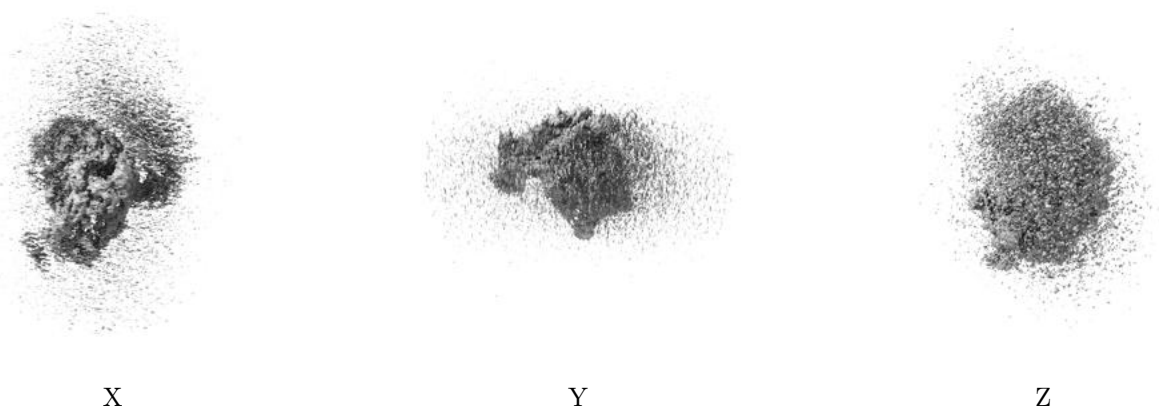
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.004. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

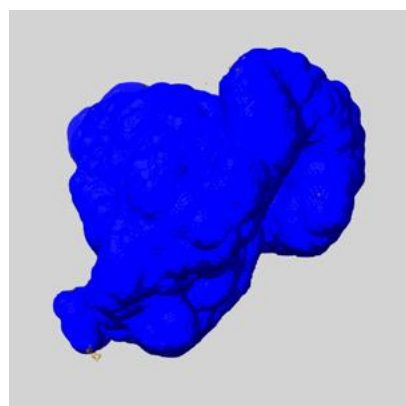
6.6 Mask visualisation [i](#)

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

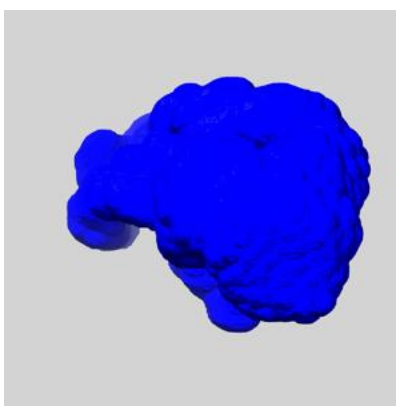
A mask typically either:

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

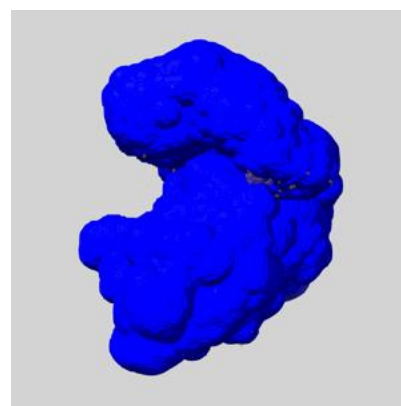
6.6.1 emd_26544_msk_1.map [i](#)



X



Y

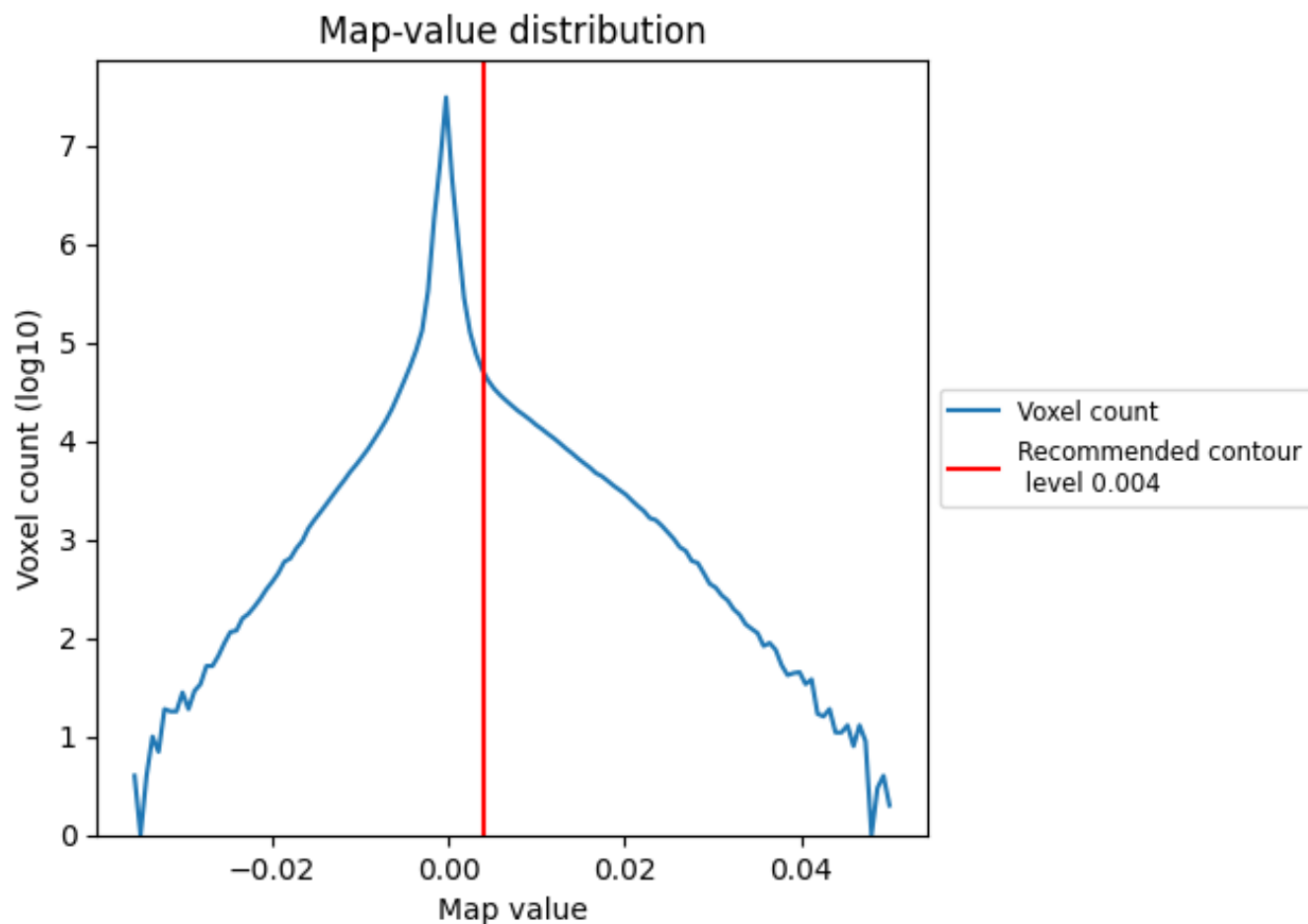


Z

7 Map analysis [i](#)

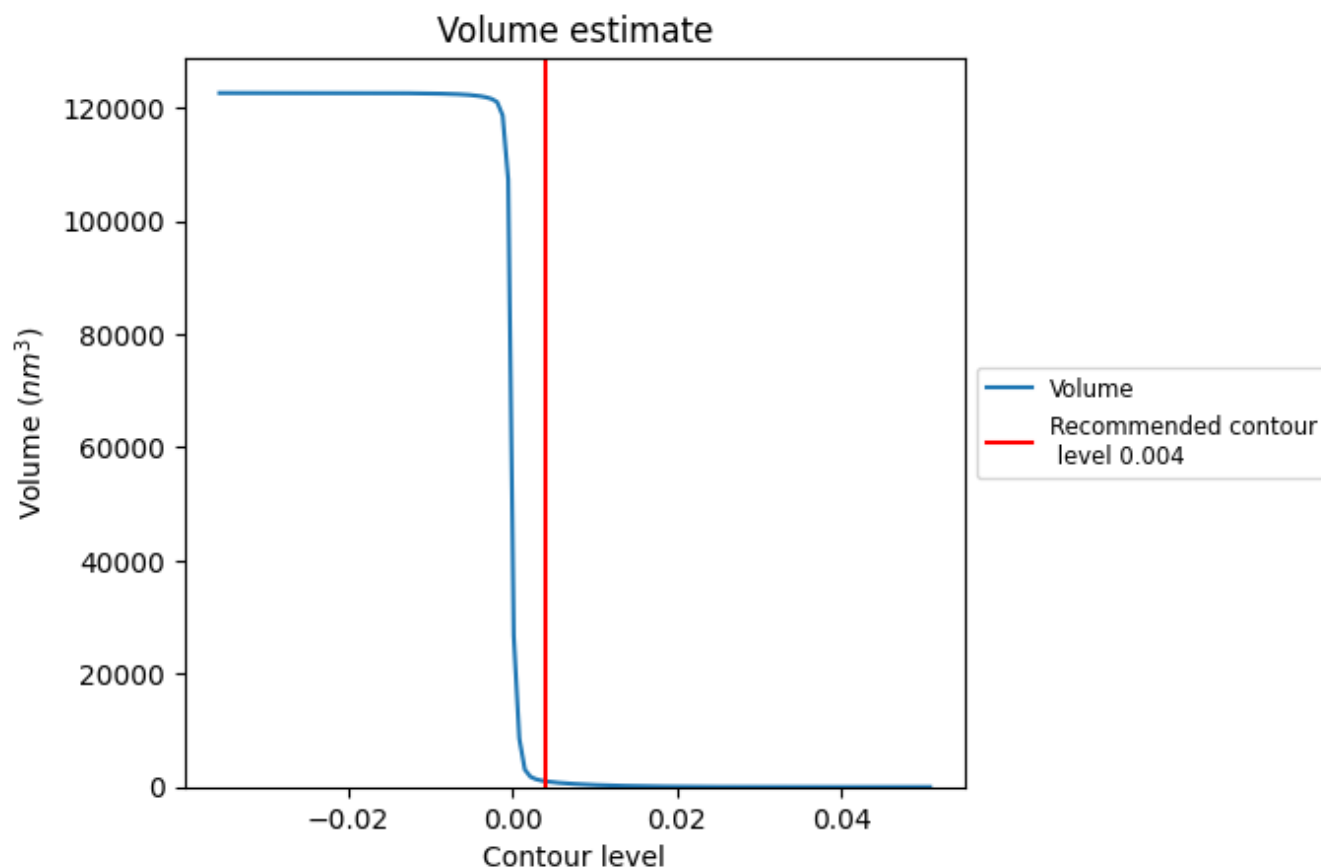
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

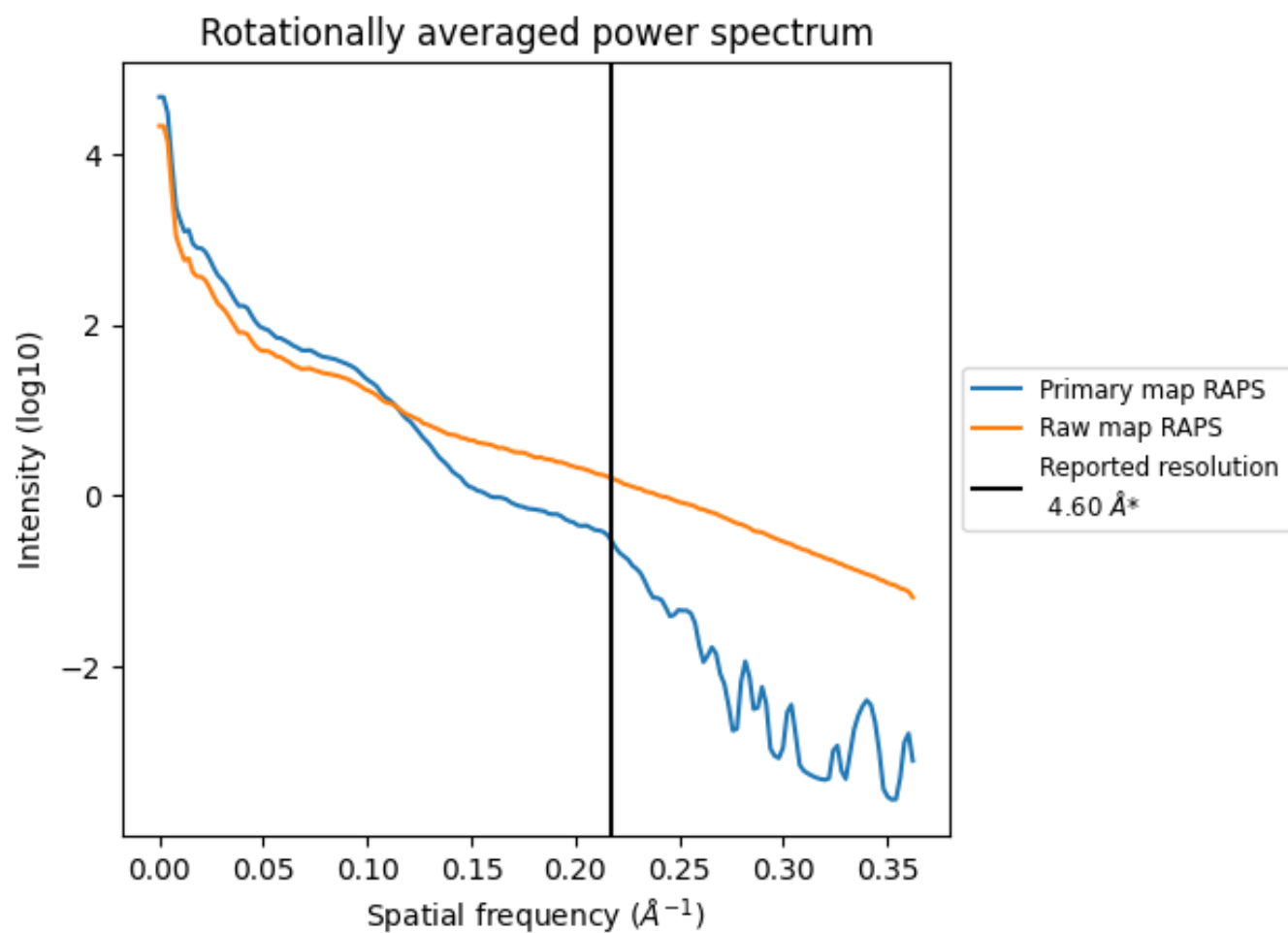
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1005 nm³; this corresponds to an approximate mass of 908 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 ⓘ

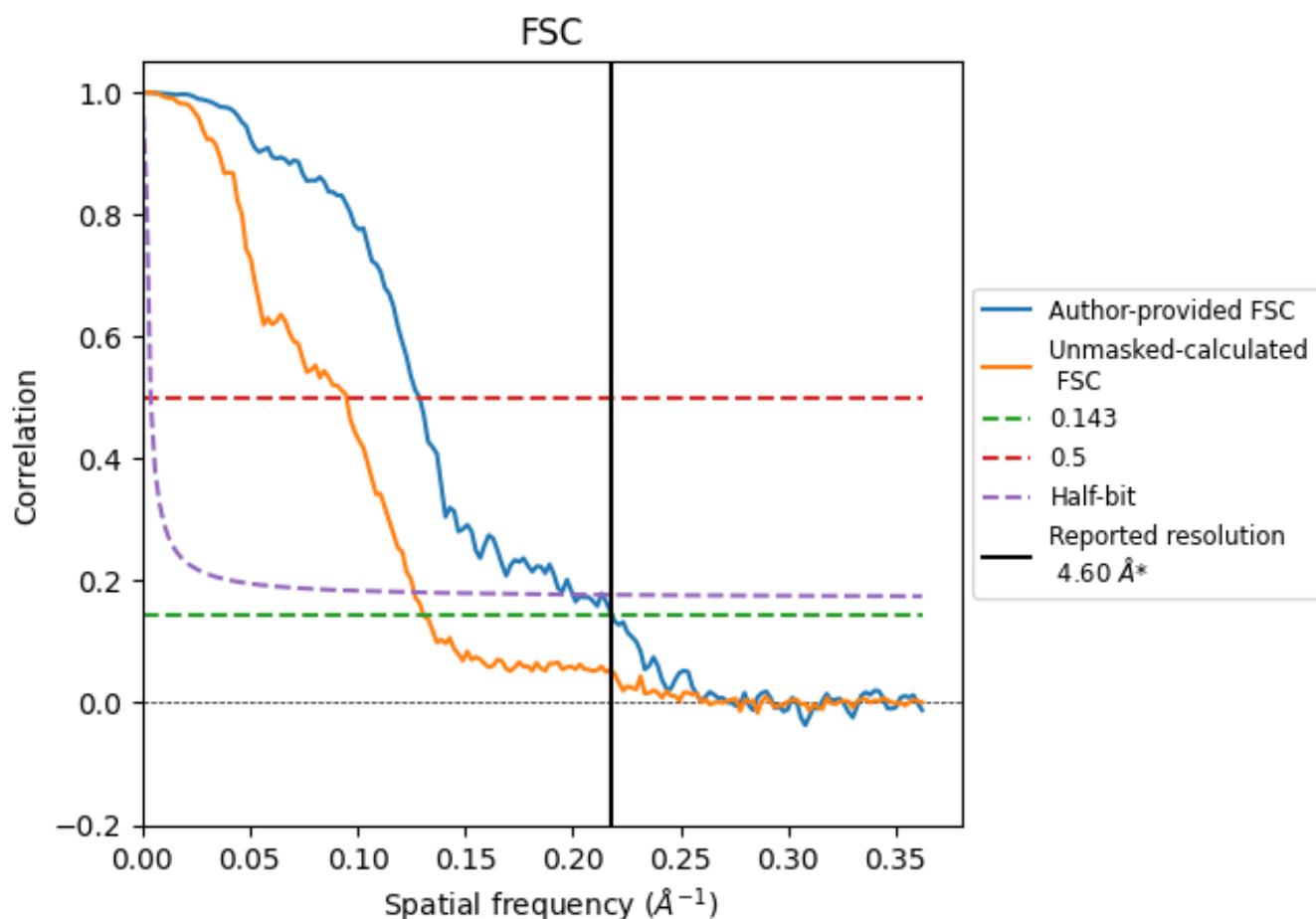


*Reported resolution corresponds to spatial frequency of 0.217 Å⁻¹

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 0.217 Å⁻¹

8.2 Resolution estimates [i](#)

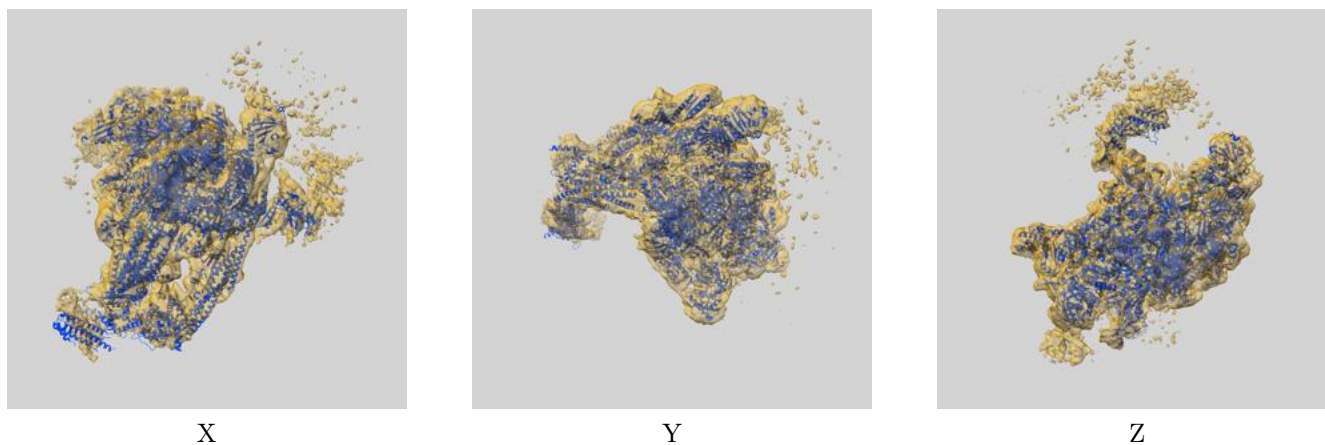
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.60	-	-
Author-provided FSC curve	4.58	7.76	5.00
Unmasked-calculated*	7.65	10.54	7.92

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.65 differs from the reported value 4.6 by more than 10 %

9 Map-model fit [i](#)

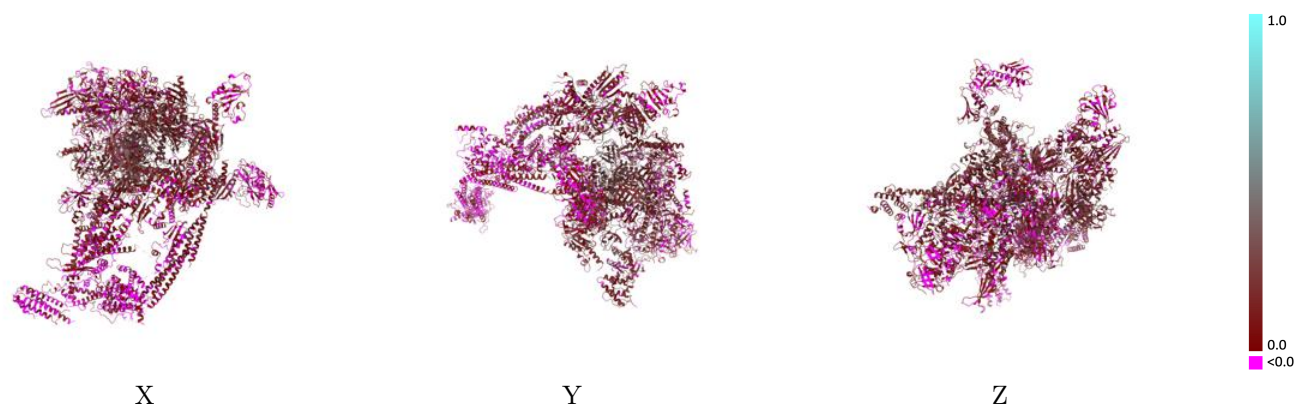
This section contains information regarding the fit between EMDB map EMD-26544 and PDB model 7UIF. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

9.1 Map-model overlay [i](#)



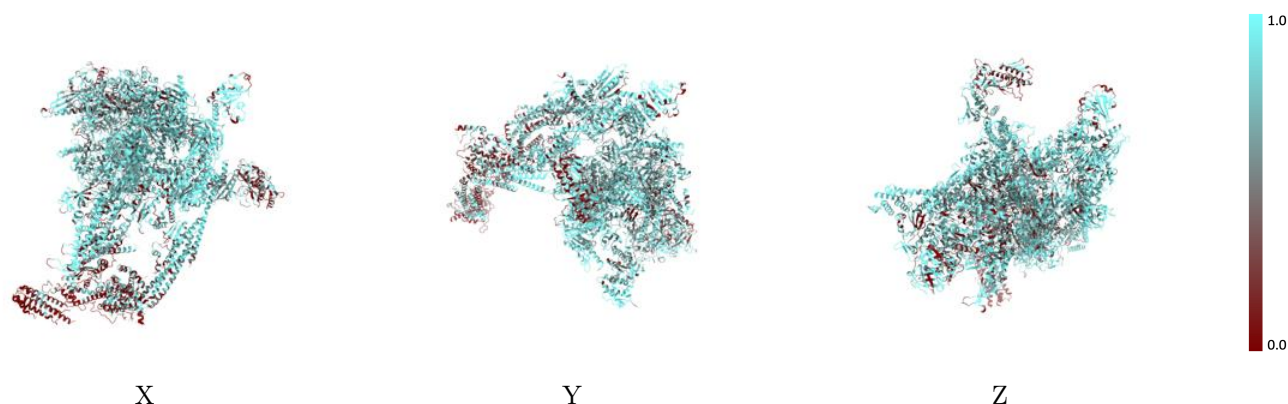
The images above show the 3D surface view of the map at the recommended contour level 0.004 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



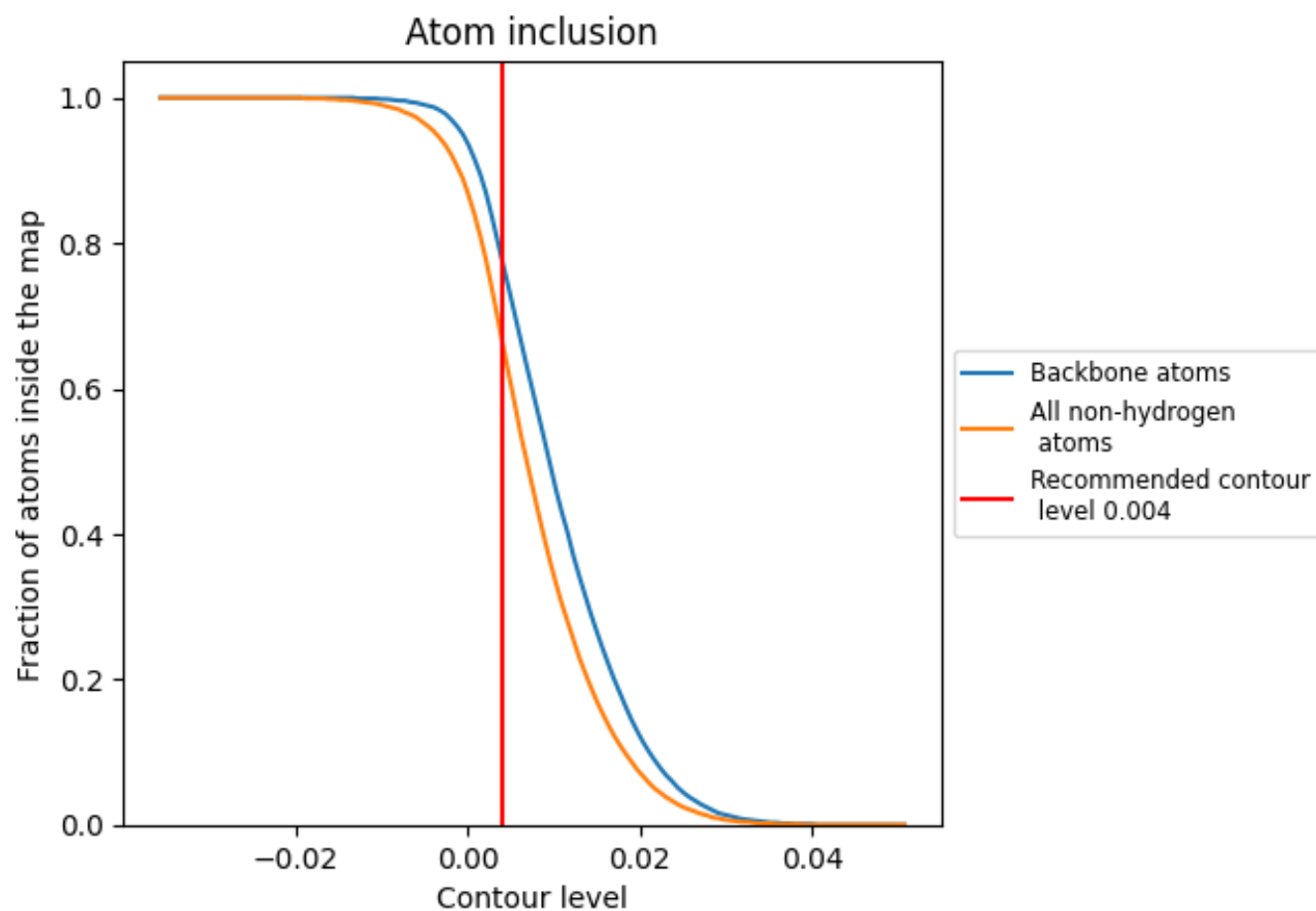
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.004).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 67% 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 (0.004) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6660	 0.1270
A	 0.7460	 0.2120
B	 0.6400	 0.1190
C	 0.7500	 0.1590
D	 0.6820	 0.0850
E	 0.8280	 0.1850
F	 0.7780	 0.2120
G	 0.7350	 0.1250
H	 0.8210	 0.2300
I	 0.7460	 0.1490
J	 0.5930	 0.0660
K	 0.7780	 0.2310
L	 0.6830	 0.0900
M	 0.7960	 0.2840
P	 0.6520	 0.0890
Q	 0.5050	 0.0270
S	 0.7260	 0.1410
a	 0.5300	 0.0480
d	 0.5980	 0.0650
f	 0.4640	 0.0360
g	 0.5340	 0.0110
h	 0.5950	 0.0450
i	 0.7770	 0.1330
j	 0.2830	 0.0210
k	 0.7530	 0.1220
n	 0.6590	 0.0750
q	 0.6910	 0.1120
r	 0.7730	 0.2220
s	 0.0890	 0.0160
t	 0.7820	 0.2000
u	 0.6690	 0.0670
v	 0.6410	 0.0800
w	 0.4040	 -0.0340
z	 0.3330	 0.0140

