



Full wwPDB EM Validation Report ⓘ

Jun 10, 2021 – 05:41 PM BST

PDB ID : 7NVR
EMDB ID : EMD-12610
Title : Human Mediator with RNA Polymerase II Pre-initiation complex
Authors : Rengachari, S.; Schilbach, S.; Aibara, S.; Cramer, P.
Deposited on : 2021-03-15
Resolution : 4.50 Å(reported)

This is a Full wwPDB EM Validation 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

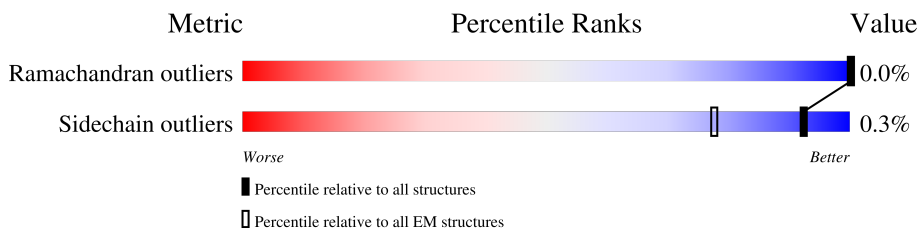
EMDB validation analysis : 0.0.0.dev75
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.20

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 4.50 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.



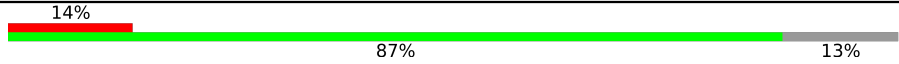

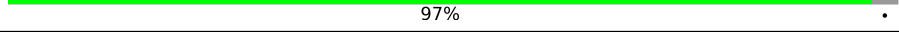
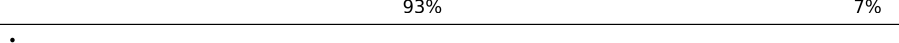
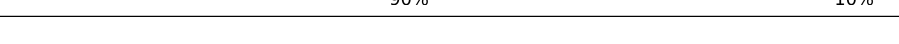
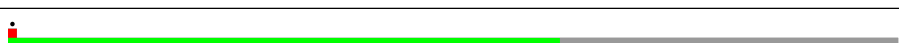


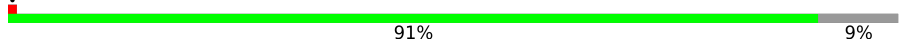
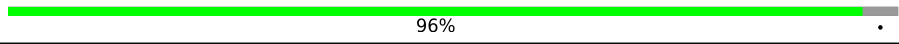
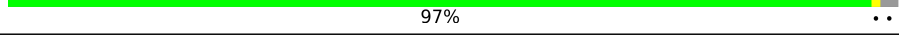
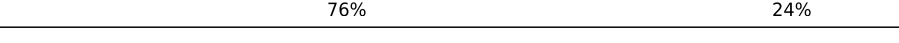
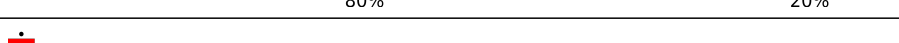







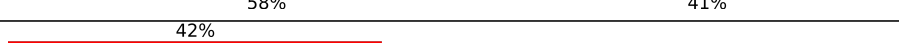
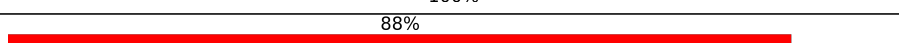



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 ≥ 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	0	760	
2	1	548	
3	2	462	
4	3	309	
5	4	308	
6	5	71	
7	6	395	
8	7	782	
9	8	346	

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Mol	Chain	Length	Quality of chain
10	9	323	
11	A	1970	
12	B	1174	
13	C	275	
14	D	142	
15	E	210	
16	F	127	
17	G	172	
18	H	150	
19	I	125	
20	J	67	
21	K	117	
22	L	58	
23	M	316	
24	N	106	
25	O	339	
26	Q	517	
27	R	249	
28	T	106	
29	U	376	
30	V	109	
31	W	439	
32	X	291	
33	Y	19	
34	Z	8	

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Mol	Chain	Length	Quality of chain
35	a	246	58% 42%
36	b	268	50% 49%
37	c	117	93% 7%
38	d	651	67% 33%
39	e	208	80% 20%
40	f	212	87% 12%
41	g	200	65% 35%
42	h	270	28% 51% 49%
43	i	233	48% 52%
44	j	146	41% 49% 51%
45	k	135	55% 99%
46	l	1454	34% 66%
47	m	244	29% 34% 66%
48	n	144	16% 92% 8%
49	o	131	69% 31%
50	p	311	50% 50%
51	q	178	39% 61%
52	r	20	100%
53	s	178	24% 75%
54	v	22	5% 100%
55	w	16	100%
56	x	11	100%
57	y	18	100%
58	z	23	100%

2 Entry composition [i](#)

There are 61 unique types of molecules in this entry. The entry contains 96126 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 TFIID basal transcription factor complex helicase XPD subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	714	5751	3683	999	1040	29	0	0

- Molecule 2 is a protein called General transcription factor IID subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1	265	2167	1382	378	395	12	0	0

- Molecule 3 is a protein called General transcription factor IID subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	2	390	3158	2050	545	551	12	0	0

- Molecule 4 is a protein called CDK-activating kinase assembly factor MAT1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	3	214	1737	1092	299	334	12	0	0

- Molecule 5 is a protein called General transcription factor IID subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	4	263	2066	1323	344	380	19	0	0

- Molecule 6 is a protein called General transcription factor IID subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	5	66	523	337	83	100	3	0	0

- Molecule 7 is a protein called General transcription factor IIIH subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	6	347	2732	1726	471	508	27	0	0

- Molecule 8 is a protein called General transcription and DNA repair factor IIIH helicase subunit XPB.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	7	605	4890	3127	848	885	30	0	0

- Molecule 9 is a protein called Cyclin-dependent kinase 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	8	298	2376	1537	404	423	12	0	0

- Molecule 10 is a protein called Cyclin-H.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	9	281	2293	1465	394	416	18	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	A	1423	11274	7092	2016	2094	72	0	0

- Molecule 12 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	B	1136	9076	5739	1597	1676	64	0	0

- Molecule 13 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	C	257	2059	1294	351	408	6	0	0

- Molecule 14 is a protein called RPOL4c domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	D	128	1050	656	178	212	4	0	0

- Molecule 15 is a protein called DNA-directed RNA polymerase II subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	E	209	1721	1089	300	324	8	0	0

- Molecule 16 is a protein called DNA-directed RNA polymerase II subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	F	79	636	406	108	117	5	0	0

- Molecule 17 is a protein called DNA-directed RNA polymerase II subunit RPB7.

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

- Molecule 18 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

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

- Molecule 19 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	I	114	928	571	166	180	11	0	0

- Molecule 20 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	J	64	507	328	86	87	6	0	0

- Molecule 21 is a protein called RNA_pol_L_2 domain-containing protein.

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

- Molecule 22 is a protein called RNA polymerase II subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	L	44	Total	C	N	O	S	0	0
			373	231	72	64	6		

- Molecule 23 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	M	252	Total	C	N	O	S	0	0
			1953	1224	346	366	17		

- Molecule 24 is a DNA chain called NT.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	N	64	Total	C	N	O	P	0	0
			1318	624	243	388	63		

- Molecule 25 is a protein called TATA-box-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	O	179	Total	C	N	O	S	0	0
			1422	923	251	241	7		

- Molecule 26 is a protein called General transcription factor IIF subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Q	138	Total	C	N	O	S	0	0
			1138	719	208	208	3		

- Molecule 27 is a protein called General transcription factor IIF subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	R	222	Total	C	N	O	S	0	0
			1788	1127	320	338	3		

- Molecule 28 is a DNA chain called TEMPLATE.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
28	T	64	1303	616	245	378	64	0	0

- Molecule 29 is a protein called Transcription initiation factor IIA subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	U	113	930	585	152	189	4	0	0

- Molecule 30 is a protein called Transcription initiation factor IIA subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	V	99	806	510	142	151	3	0	0

- Molecule 31 is a protein called General transcription factor IIE subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	W	202	1659	1042	299	307	11	0	0

- Molecule 32 is a protein called Transcription initiation factor IIE subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	X	171	1403	895	243	261	4	0	0

- Molecule 33 is a protein called Unassigned peptide, likely TFIIIE-beta.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
33	Y	19	95	57	19	19	0	0

- Molecule 34 is a protein called Unassigned peptide, likely XPB.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
34	Z	8	40	24	8	8	0	0

- Molecule 35 is a protein called Mediator of RNA polymerase II transcription subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	a	143	1167	754	198	210	5	0	0

- Molecule 36 is a protein called Mediator of RNA polymerase II transcription subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	b	136	1046	657	179	207	3	0	0

- Molecule 37 is a protein called Mediator of RNA polymerase II transcription subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	c	109	858	524	159	171	4	0	0

- Molecule 38 is a protein called Mediator of RNA polymerase II transcription subunit 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	d	439	3510	2232	627	637	14	0	0

- Molecule 39 is a protein called Mediator of RNA polymerase II transcription subunit 18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	e	167	1353	868	233	238	14	0	0

- Molecule 40 is a protein called Mediator of RNA polymerase II transcription subunit 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	f	186	1448	924	238	270	16	0	0

- Molecule 41 is a protein called Mediator of RNA polymerase II transcription subunit 22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	g	130	1063	656	181	222	4	0	0

- Molecule 42 is a protein called Mediator of RNA polymerase II transcription subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	h	138	1114	696	195	219	4	0	0

- Molecule 43 is a protein called Mediator of RNA polymerase II transcription subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	i	113	960	614	170	170	6	0	0

- Molecule 44 is a protein called Mediator of RNA polymerase II transcription subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	j	72	596	375	108	109	4	0	0

- Molecule 45 is a protein called Mediator of RNA polymerase II transcription subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	k	133	1088	690	188	206	4	0	0

- Molecule 46 is a protein called Mediator of RNA polymerase II transcription subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	l	501	4031	2591	694	722	24	0	0

- Molecule 47 is a protein called Mediator of RNA polymerase II transcription subunit 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	m	84	655	417	113	121	4	0	0

- Molecule 48 is a protein called Mediator of RNA polymerase II transcription subunit 21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	n	132	1005	621	170	210	4	0	0

- Molecule 49 is a protein called Mediator of RNA polymerase II transcription subunit 31.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	o	91	Total	C	N	O	S	0	0
			804	535	132	133	4		

- Molecule 50 is a protein called Mediator of RNA polymerase II transcription subunit 27.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	p	154	Total	C	N	O	S	0	0
			1262	813	218	222	9		

- Molecule 51 is a protein called Mediator of RNA polymerase II transcription subunit 28.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	q	69	Total	C	N	O	S	0	0
			591	373	111	106	1		

- Molecule 52 is a protein called unassigned peptide (MED29 or MED30).

Mol	Chain	Residues	Atoms				AltConf	Trace
52	r	20	Total	C	N	O	0	0
			100	60	20	20		

- Molecule 53 is a protein called Mediator of RNA polymerase II transcription subunit 30.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	s	44	Total	C	N	O	S	0	0
			369	227	72	67	3		

- Molecule 54 is a protein called unassigned peptide (MED14).

Mol	Chain	Residues	Atoms				AltConf	Trace
54	v	22	Total	C	N	O	0	0
			110	66	22	22		

- Molecule 55 is a protein called unassigned peptide (MED6).

Mol	Chain	Residues	Atoms				AltConf	Trace
55	w	16	Total	C	N	O	0	0
			80	48	16	16		

- Molecule 56 is a protein called unassigned peptide (MED17).

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
56	x	11	55	33	11	11	0	0

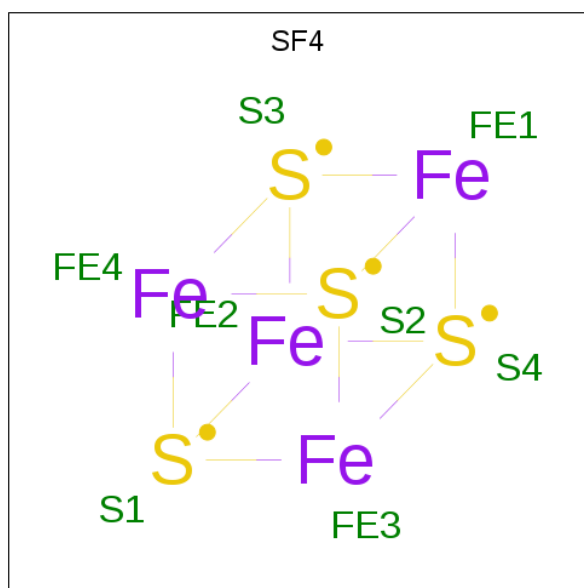
- Molecule 57 is a protein called unassigned peptide (MED29 or MED30).

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
57	y	18	90	54	18	18	0	0

- Molecule 58 is a protein called unassigned peptide (MED29 or MED30).

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
58	z	23	115	69	23	23	0	0

- Molecule 59 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
59	0	1	8	4	4	0

- Molecule 60 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
60	3	2	2	2	0

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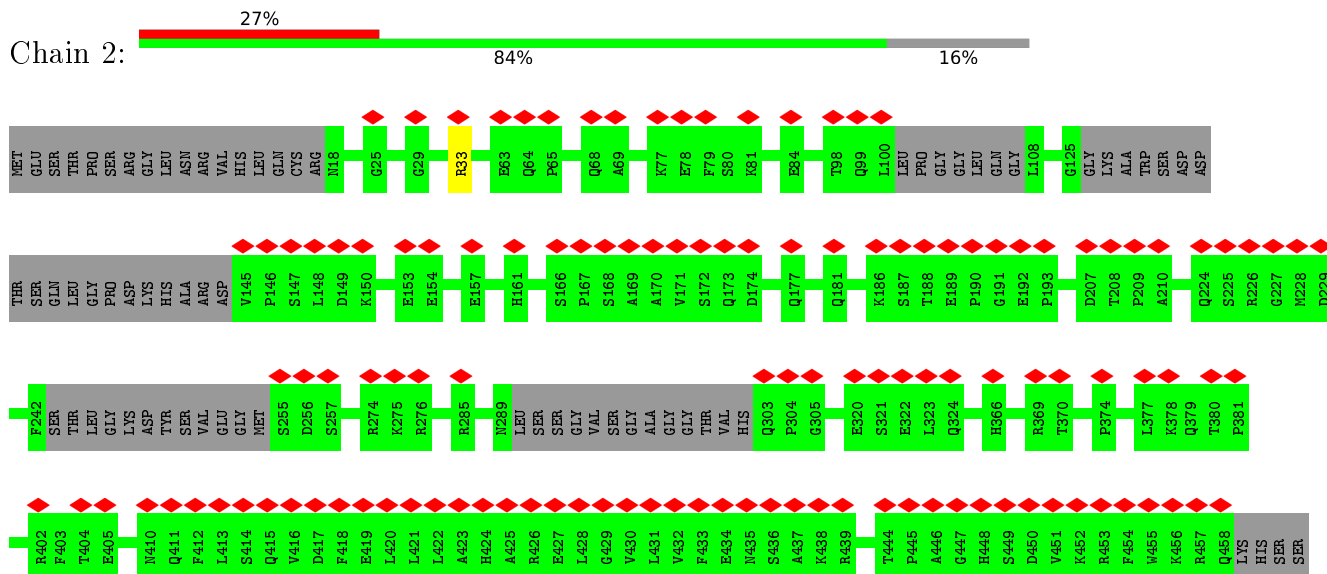
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Mol	Chain	Residues	Atoms		AltConf
60	4	2	Total 2	Zn 2	0
60	6	3	Total 3	Zn 3	0
60	A	2	Total 2	Zn 2	0
60	B	1	Total 1	Zn 1	0
60	C	1	Total 1	Zn 1	0
60	I	2	Total 2	Zn 2	0
60	J	1	Total 1	Zn 1	0
60	L	1	Total 1	Zn 1	0
60	M	1	Total 1	Zn 1	0
60	W	1	Total 1	Zn 1	0
60	p	1	Total 1	Zn 1	0

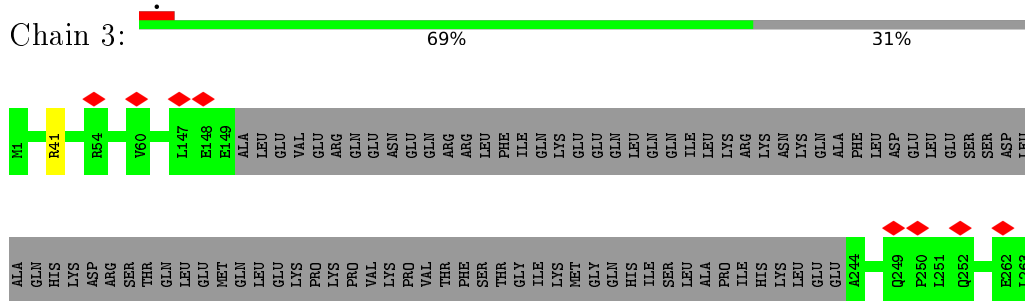
- Molecule 61 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

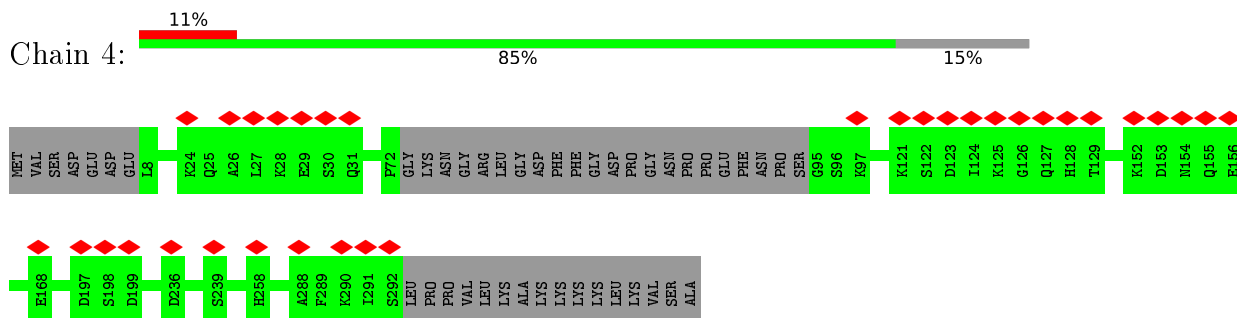
• Molecule 3: General transcription factor IIIH subunit 4



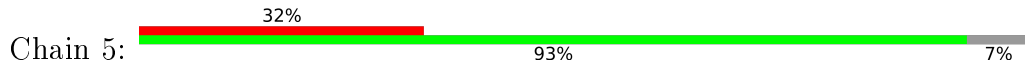
• Molecule 4: CDK-activating kinase assembly factor MAT1

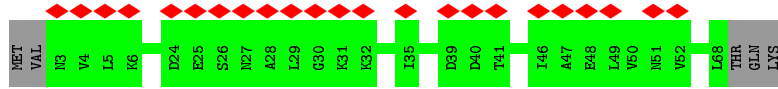


• Molecule 5: General transcription factor IIIH subunit 3

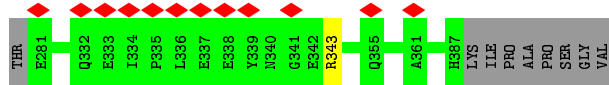
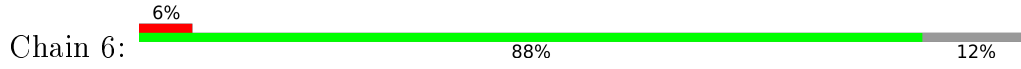


• Molecule 6: General transcription factor IIIH subunit 5

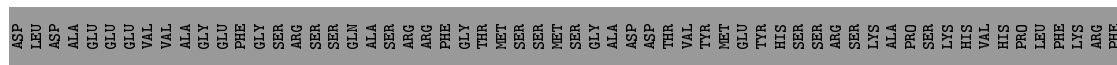
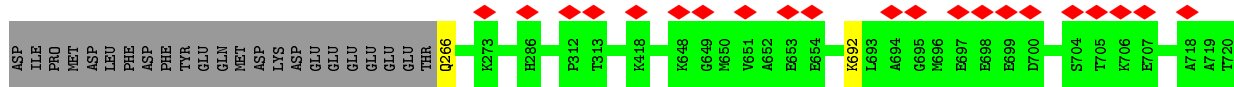
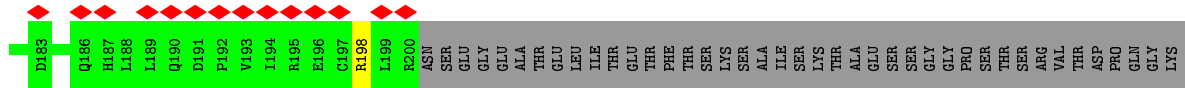
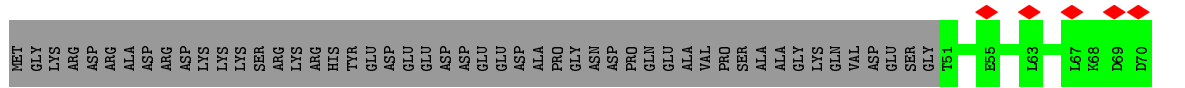
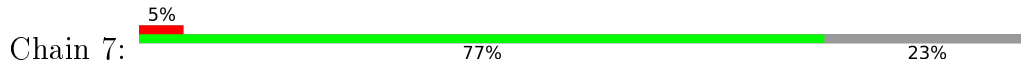




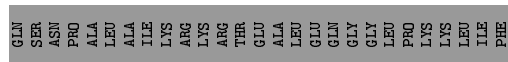
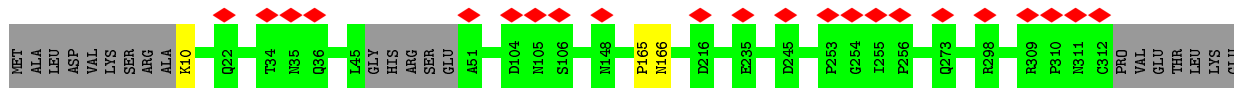
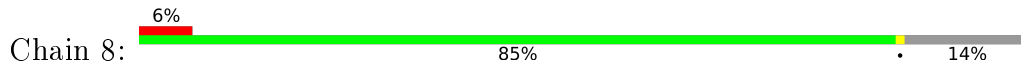
• Molecule 7: General transcription factor IIH subunit 2



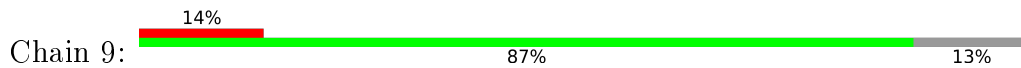
• Molecule 8: General transcription and DNA repair factor IIH helicase subunit XPB

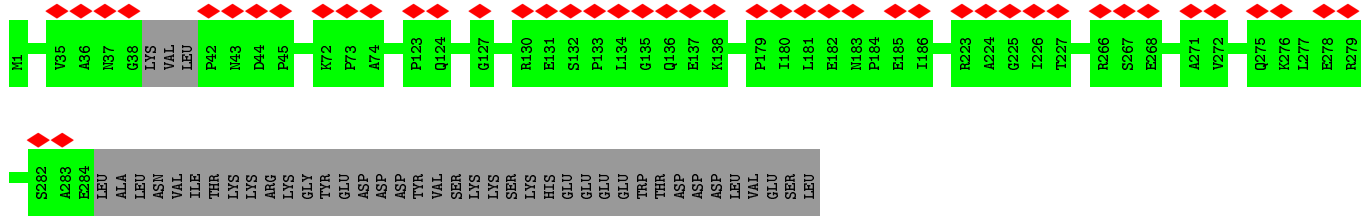


• Molecule 9: Cyclin-dependent kinase 7

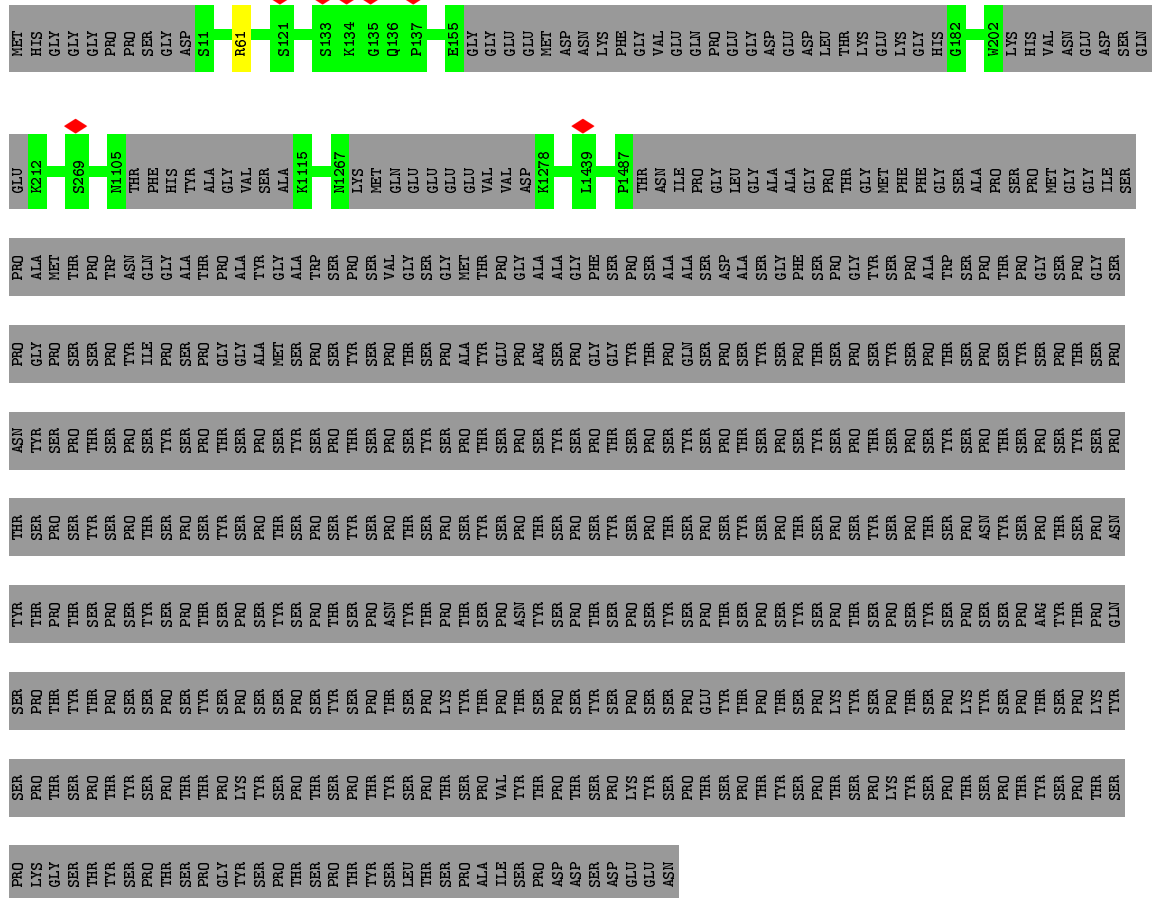


• Molecule 10: Cyclin-H

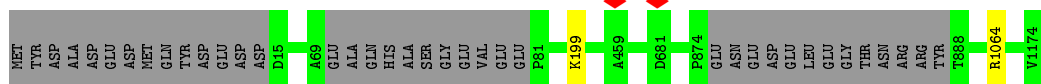




• Molecule 11: DNA-directed RNA polymerase subunit

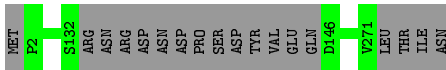


• Molecule 12: DNA-directed RNA polymerase subunit beta

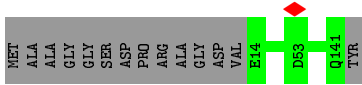


• Molecule 13: DNA-directed RNA polymerase II subunit RPB3





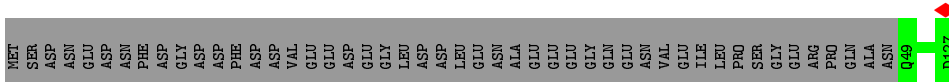
- Molecule 14: RPOL4c domain-containing protein



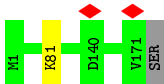
- Molecule 15: DNA-directed RNA polymerase II subunit E



- Molecule 16: DNA-directed RNA polymerase II subunit F



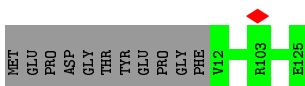
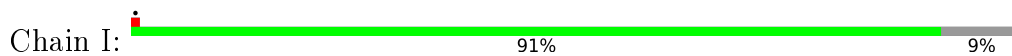
- Molecule 17: DNA-directed RNA polymerase II subunit RPB7



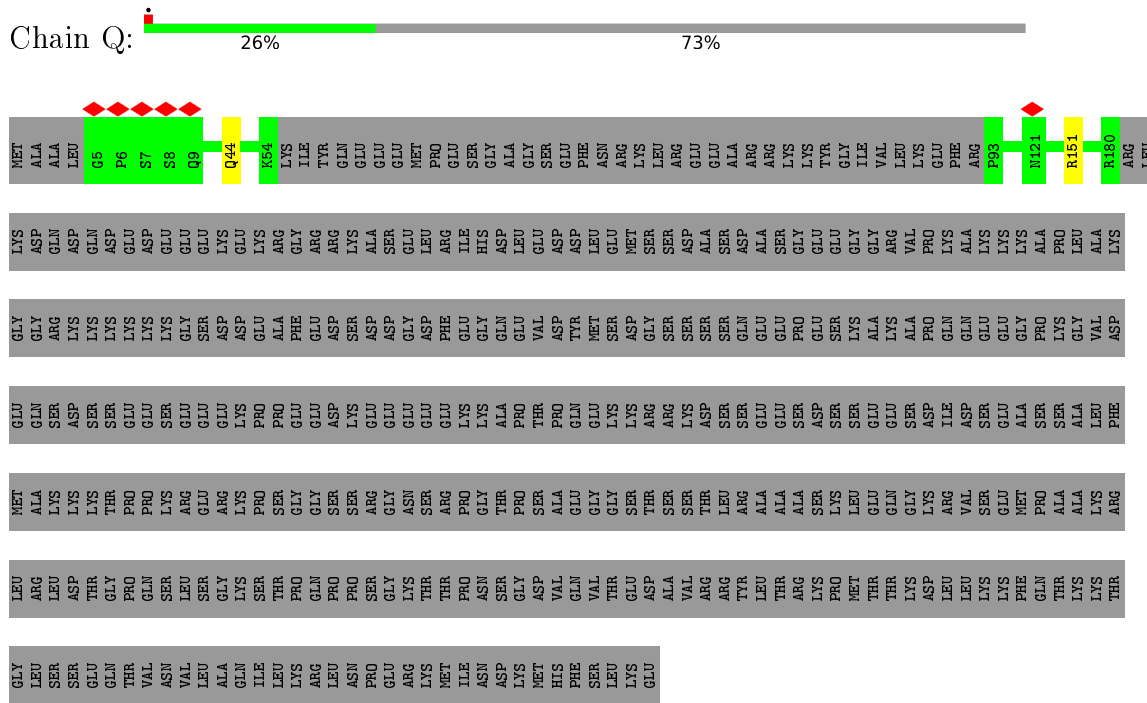
- Molecule 18: DNA-directed RNA polymerases I, II, and III subunit RPABC3



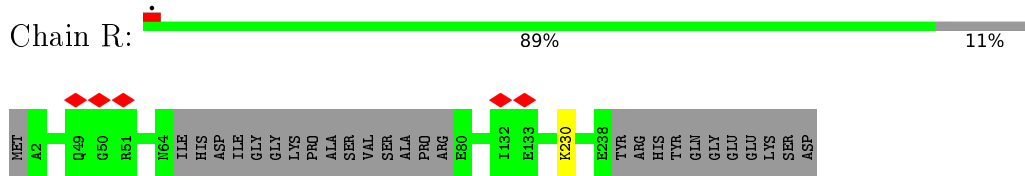
- Molecule 19: DNA-directed RNA polymerase II subunit RPB9



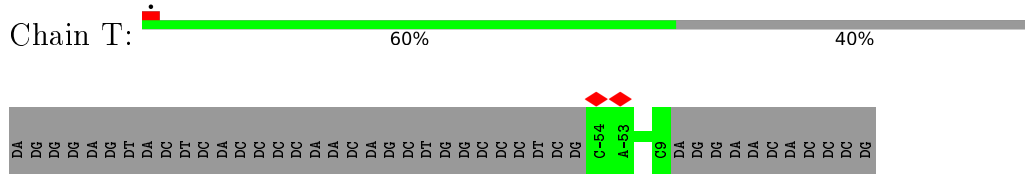
- Molecule 20: DNA-directed RNA polymerases I, II, and III subunit RPABC5



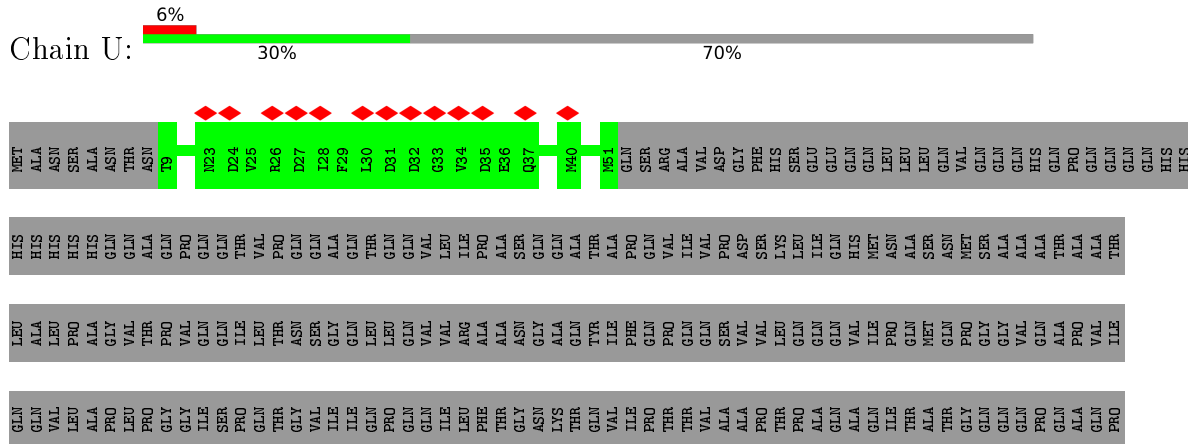
- Molecule 27: General transcription factor IIF subunit 2



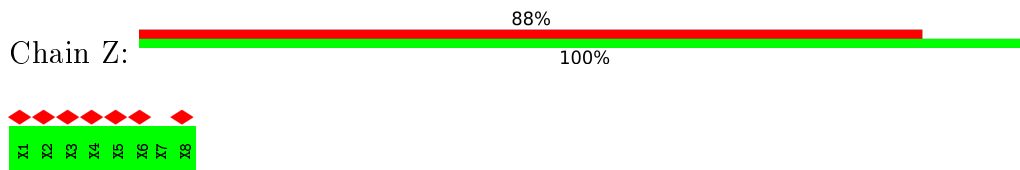
- Molecule 28: TEMPLATE



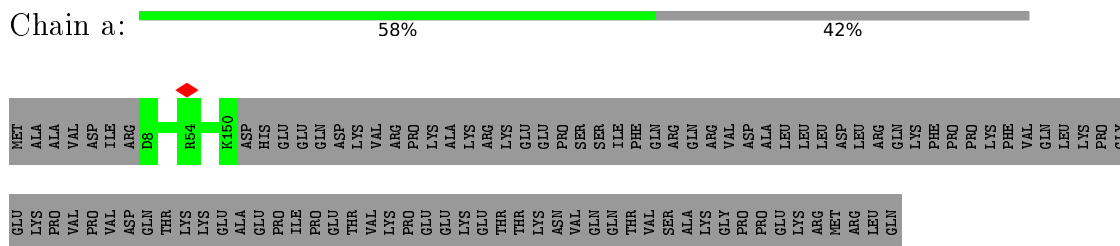
- Molecule 29: Transcription initiation factor IIA subunit 1



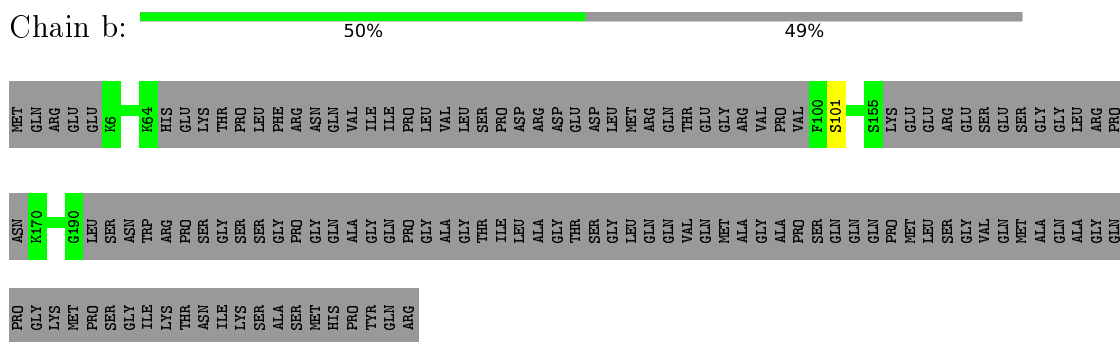
- Molecule 34: Unassigned peptide, likely XPB



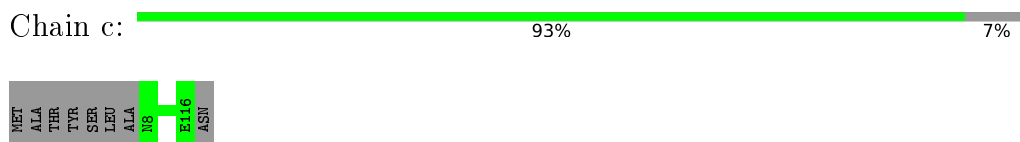
- Molecule 35: Mediator of RNA polymerase II transcription subunit 6



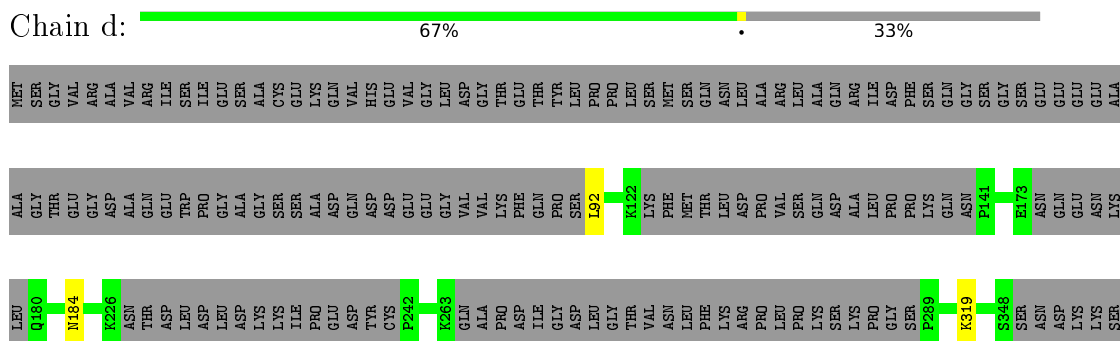
- Molecule 36: Mediator of RNA polymerase II transcription subunit 8

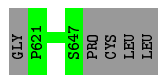
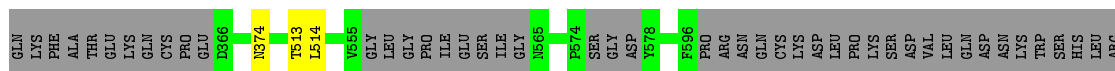


- Molecule 37: Mediator of RNA polymerase II transcription subunit 11

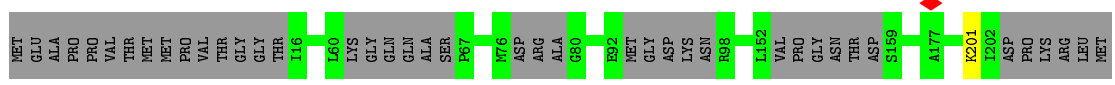
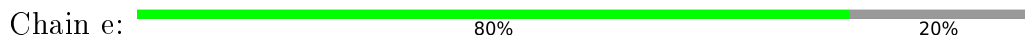


- Molecule 38: Mediator of RNA polymerase II transcription subunit 17

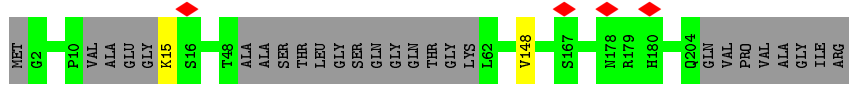
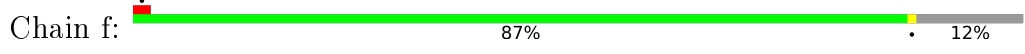




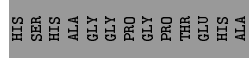
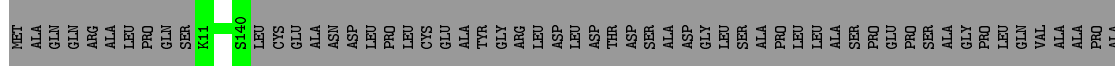
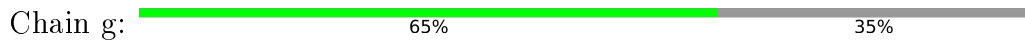
- Molecule 39: Mediator of RNA polymerase II transcription subunit 18



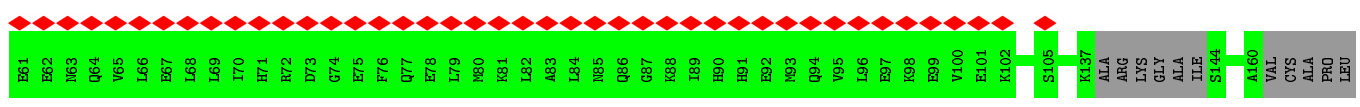
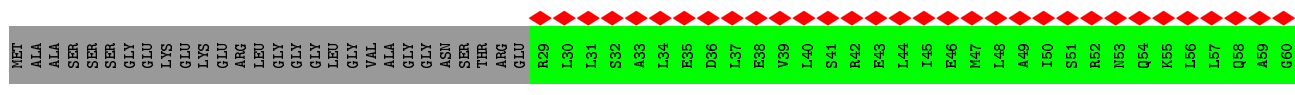
- Molecule 40: Mediator of RNA polymerase II transcription subunit 20



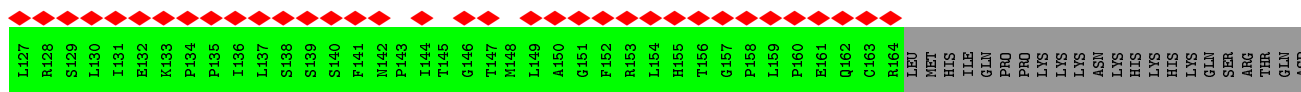
- Molecule 41: Mediator of RNA polymerase II transcription subunit 22



- Molecule 42: Mediator of RNA polymerase II transcription subunit 4

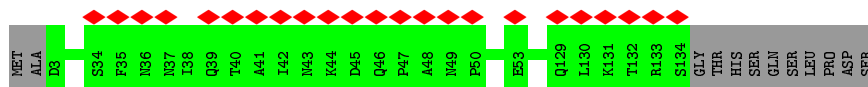


- Molecule 43: Mediator of RNA polymerase II transcription subunit 7

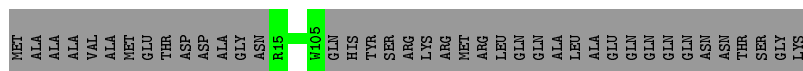


PRO VAL
PRO PRO
PRO PRO
GLU THR
PRO PRO
SER SER
ASP ASP
SER SER
HIS HIS
LYS LYS
LYS LYS
LYS LYS
LYS LYS
LYS LYS
LYS LYS
LYS LYS
GLU GLU
GLU ASP
PRO PRO
I144
T145
ASP ASP
G146
T147
M448
LYS LYS
LYS LYS
LYS LYS
G1J
LYS LYS
LYS LYS
LYS LYS
LYS LYS
H155
T156
G157
P158
L159
P160
E161
Q162
C163
R164
LEU
MET
HIS
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LYS
LYS
LYS
LYS
GLN
THR
ARG
GLN
ASP

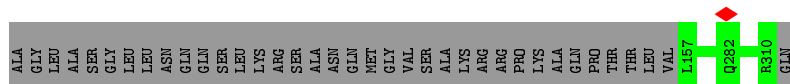
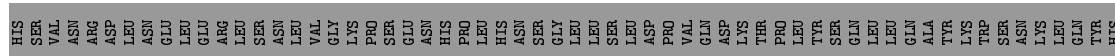
- Molecule 48: Mediator of RNA polymerase II transcription subunit 21



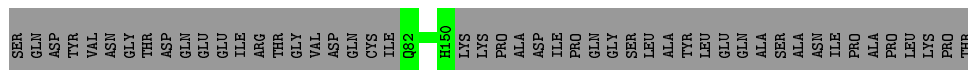
- Molecule 49: Mediator of RNA polymerase II transcription subunit 31



- Molecule 50: Mediator of RNA polymerase II transcription subunit 27



- Molecule 51: Mediator of RNA polymerase II transcription subunit 28



- Molecule 52: unassigned peptide (MED29 or MED30)



There are no outlier residues recorded for this chain.

- Molecule 53: Mediator of RNA polymerase II transcription subunit 30



MET SER THR PRO LEU ALA ALA SER MET PRO GLY PRO ALA ALA ALA ALA ALA ALA ARG VAL VAL ASN THR ALA SER LEU CYS ARG ILE GLY GLN THR VAL GLN ASP ILE VAL TYR ARG MET THR ARG PHE GLN LEU LEU LEU LEU LEU LEU LEU LEU LEU LEU LEU LEU LEU LEU LEU LEU LEU LEU

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

ASP GLY SER LYS ASN ASP ASP ARG PRO PRO ARG PHE **A134** **M152** **H177**

- Molecule 54: unassigned peptide (MED14)



- Molecule 55: unassigned peptide (MED6)



There are no outlier residues recorded for this chain.

- Molecule 56: unassigned peptide (MED17)



There are no outlier residues recorded for this chain.

- Molecule 57: unassigned peptide (MED29 or MED30)



There are no outlier residues recorded for this chain.

- Molecule 58: unassigned peptide (MED29 or MED30)



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	25967	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	58.56	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	40.088	Depositor
Minimum map value	-17.336	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	3.0	Depositor
Map size (\AA)	440.99997, 440.99997, 440.99997	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.05, 1.05, 1.05	Depositor

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, SF4, MG

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	0	0.25	0/5875	0.41	0/7955
2	1	0.25	0/2210	0.40	0/2975
3	2	0.26	0/3230	0.42	0/4376
4	3	0.33	0/1769	0.44	0/2385
5	4	0.28	0/2103	0.46	0/2846
6	5	0.25	0/529	0.40	0/714
7	6	0.24	0/2793	0.41	0/3780
8	7	0.24	0/4994	0.40	0/6745
9	8	0.38	0/2434	0.55	0/3300
10	9	0.40	0/2342	0.48	0/3159
11	A	0.24	0/11479	0.41	0/15496
12	B	0.24	0/9257	0.42	0/12493
13	C	0.24	0/2102	0.42	0/2857
14	D	0.24	0/1064	0.38	0/1428
15	E	0.24	0/1752	0.41	0/2366
16	F	0.23	0/646	0.38	0/871
17	G	0.25	0/1382	0.43	0/1874
18	H	0.24	0/1207	0.43	0/1628
19	I	0.24	0/949	0.44	0/1284
20	J	0.25	0/516	0.40	0/696
21	K	0.25	0/939	0.39	0/1271
22	L	0.26	0/378	0.41	0/500
23	M	0.24	0/1983	0.40	0/2679
24	N	0.52	0/1478	0.90	0/2283
25	O	0.25	0/1448	0.42	0/1948
26	Q	0.24	0/1167	0.41	0/1576
27	R	0.24	0/1817	0.40	0/2445
28	T	0.54	0/1461	0.85	0/2249
29	U	0.24	0/945	0.41	0/1274
30	V	0.24	0/816	0.42	0/1105
31	W	0.37	1/1686 (0.1%)	0.48	0/2266
32	X	0.28	0/1427	0.46	0/1916

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
35	a	0.24	0/1200	0.40	0/1634
36	b	0.25	0/1058	0.42	0/1427
37	c	0.24	0/864	0.41	0/1161
38	d	0.26	0/3573	0.45	1/4812 (0.0%)
39	e	0.25	0/1377	0.45	0/1846
40	f	0.28	0/1478	0.53	1/1996 (0.1%)
41	g	0.23	0/1072	0.37	0/1440
42	h	0.24	0/1121	0.37	0/1496
43	i	0.25	0/979	0.41	0/1315
44	j	0.23	0/605	0.38	0/810
45	k	0.24	0/1107	0.36	0/1487
46	l	0.24	0/4102	0.40	1/5537 (0.0%)
47	m	0.25	0/671	0.42	0/908
48	n	0.23	0/1016	0.37	0/1381
49	o	0.25	0/829	0.34	0/1119
50	p	0.29	0/1294	0.47	0/1756
51	q	0.23	0/599	0.36	0/803
53	s	0.22	0/370	0.35	0/491
All	All	0.27	1/97493 (0.0%)	0.45	3/132159 (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
38	d	0	1
46	l	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	W	105	TYR	CD2-CE2	-6.79	1.29	1.39

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	d	92	LEU	CB-CG-CD2	7.84	124.33	111.00
40	f	148	VAL	CG1-CB-CG2	6.86	121.88	110.90
46	l	470	LEU	CA-CB-CG	5.01	126.82	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
38	d	513	THR	Peptide
46	l	443	LEU	Peptide

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	710/760 (93%)	682 (96%)	28 (4%)	0	100	100
2	1	253/548 (46%)	245 (97%)	8 (3%)	0	100	100
3	2	380/462 (82%)	365 (96%)	15 (4%)	0	100	100
4	3	210/309 (68%)	195 (93%)	15 (7%)	0	100	100
5	4	259/308 (84%)	255 (98%)	4 (2%)	0	100	100
6	5	64/71 (90%)	63 (98%)	1 (2%)	0	100	100
7	6	341/395 (86%)	329 (96%)	12 (4%)	0	100	100
8	7	601/782 (77%)	576 (96%)	25 (4%)	0	100	100
9	8	294/346 (85%)	276 (94%)	16 (5%)	2 (1%)	22	62
10	9	277/323 (86%)	268 (97%)	9 (3%)	0	100	100
11	A	1413/1970 (72%)	1374 (97%)	39 (3%)	0	100	100
12	B	1130/1174 (96%)	1093 (97%)	37 (3%)	0	100	100
13	C	253/275 (92%)	241 (95%)	12 (5%)	0	100	100
14	D	126/142 (89%)	122 (97%)	4 (3%)	0	100	100
15	E	207/210 (99%)	203 (98%)	4 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	F	77/127 (61%)	76 (99%)	1 (1%)	0	100	100
17	G	169/172 (98%)	166 (98%)	3 (2%)	0	100	100
18	H	146/150 (97%)	143 (98%)	3 (2%)	0	100	100
19	I	112/125 (90%)	104 (93%)	8 (7%)	0	100	100
20	J	62/67 (92%)	61 (98%)	1 (2%)	0	100	100
21	K	113/117 (97%)	112 (99%)	1 (1%)	0	100	100
22	L	42/58 (72%)	40 (95%)	2 (5%)	0	100	100
23	M	248/316 (78%)	246 (99%)	2 (1%)	0	100	100
25	O	177/339 (52%)	175 (99%)	2 (1%)	0	100	100
26	Q	134/517 (26%)	129 (96%)	5 (4%)	0	100	100
27	R	218/249 (88%)	213 (98%)	5 (2%)	0	100	100
29	U	109/376 (29%)	102 (94%)	7 (6%)	0	100	100
30	V	97/109 (89%)	95 (98%)	2 (2%)	0	100	100
31	W	198/439 (45%)	197 (100%)	1 (0%)	0	100	100
32	X	169/291 (58%)	164 (97%)	5 (3%)	0	100	100
35	a	141/246 (57%)	132 (94%)	9 (6%)	0	100	100
36	b	130/268 (48%)	115 (88%)	15 (12%)	0	100	100
37	c	107/117 (92%)	95 (89%)	12 (11%)	0	100	100
38	d	421/651 (65%)	384 (91%)	36 (9%)	1 (0%)	47	81
39	e	157/208 (76%)	149 (95%)	8 (5%)	0	100	100
40	f	180/212 (85%)	168 (93%)	12 (7%)	0	100	100
41	g	128/200 (64%)	122 (95%)	6 (5%)	0	100	100
42	h	132/270 (49%)	128 (97%)	4 (3%)	0	100	100
43	i	107/233 (46%)	105 (98%)	2 (2%)	0	100	100
44	j	70/146 (48%)	64 (91%)	6 (9%)	0	100	100
45	k	131/135 (97%)	129 (98%)	2 (2%)	0	100	100
46	l	477/1454 (33%)	453 (95%)	24 (5%)	0	100	100
47	m	82/244 (34%)	75 (92%)	7 (8%)	0	100	100
48	n	130/144 (90%)	122 (94%)	8 (6%)	0	100	100
49	o	89/131 (68%)	88 (99%)	1 (1%)	0	100	100
50	p	152/311 (49%)	139 (91%)	13 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	q	67/178 (38%)	65 (97%)	2 (3%)	0	100	100
53	s	42/178 (24%)	41 (98%)	1 (2%)	0	100	100
All	All	11332/16853 (67%)	10884 (96%)	445 (4%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
38	d	514	LEU
9	8	166	ASN
9	8	165	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	0	624/664 (94%)	623 (100%)	1 (0%)	93	96
2	1	241/484 (50%)	241 (100%)	0	100	100
3	2	342/399 (86%)	341 (100%)	1 (0%)	92	95
4	3	195/283 (69%)	194 (100%)	1 (0%)	88	93
5	4	234/272 (86%)	234 (100%)	0	100	100
6	5	59/64 (92%)	59 (100%)	0	100	100
7	6	311/352 (88%)	310 (100%)	1 (0%)	92	95
8	7	536/688 (78%)	533 (99%)	3 (1%)	86	92
9	8	259/299 (87%)	258 (100%)	1 (0%)	91	94
10	9	256/296 (86%)	256 (100%)	0	100	100
11	A	1254/1749 (72%)	1253 (100%)	1 (0%)	93	96
12	B	994/1027 (97%)	992 (100%)	2 (0%)	93	96
13	C	234/252 (93%)	234 (100%)	0	100	100
14	D	118/126 (94%)	118 (100%)	0	100	100
15	E	191/192 (100%)	191 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	F	69/111 (62%)	69 (100%)	0	100	100
17	G	152/153 (99%)	151 (99%)	1 (1%)	84	90
18	H	129/131 (98%)	129 (100%)	0	100	100
19	I	103/112 (92%)	103 (100%)	0	100	100
20	J	53/56 (95%)	53 (100%)	0	100	100
21	K	104/106 (98%)	103 (99%)	1 (1%)	76	86
22	L	41/55 (74%)	41 (100%)	0	100	100
23	M	215/268 (80%)	215 (100%)	0	100	100
25	O	154/293 (53%)	154 (100%)	0	100	100
26	Q	121/448 (27%)	119 (98%)	2 (2%)	60	78
27	R	196/218 (90%)	195 (100%)	1 (0%)	88	93
29	U	105/324 (32%)	105 (100%)	0	100	100
30	V	90/98 (92%)	88 (98%)	2 (2%)	52	71
31	W	182/373 (49%)	182 (100%)	0	100	100
32	X	154/261 (59%)	153 (99%)	1 (1%)	86	92
35	a	128/223 (57%)	128 (100%)	0	100	100
36	b	117/225 (52%)	116 (99%)	1 (1%)	78	87
37	c	92/98 (94%)	92 (100%)	0	100	100
38	d	395/577 (68%)	392 (99%)	3 (1%)	81	89
39	e	150/183 (82%)	149 (99%)	1 (1%)	84	90
40	f	161/178 (90%)	160 (99%)	1 (1%)	86	92
41	g	122/173 (70%)	122 (100%)	0	100	100
42	h	123/230 (54%)	123 (100%)	0	100	100
43	i	109/216 (50%)	109 (100%)	0	100	100
44	j	70/133 (53%)	70 (100%)	0	100	100
45	k	122/124 (98%)	122 (100%)	0	100	100
46	l	454/1271 (36%)	453 (100%)	1 (0%)	93	96
47	m	76/208 (36%)	76 (100%)	0	100	100
48	n	109/119 (92%)	109 (100%)	0	100	100
49	o	84/115 (73%)	84 (100%)	0	100	100
50	p	143/280 (51%)	143 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
51	q	67/152 (44%)	67 (100%)	0	100	100
53	s	40/155 (26%)	39 (98%)	1 (2%)	47	68
All	All	10278/14814 (69%)	10251 (100%)	27 (0%)	92	95

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	114	ASN
3	2	33	ARG
4	3	41	ARG
7	6	343	ARG
8	7	198	ARG
8	7	266	GLN
8	7	692	LYS
9	8	10	LYS
11	A	61	ARG
12	B	199	LYS
12	B	1064	ARG
17	G	81	LYS
21	K	47	LYS
26	Q	44	GLN
26	Q	151	ARG
27	R	230	LYS
30	V	51	ARG
30	V	82	ARG
32	X	114	LYS
36	b	101	SER
38	d	184	ASN
38	d	319	LYS
38	d	374	ASN
39	e	201	LYS
40	f	15	LYS
46	l	537	LYS
53	s	152	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
10	9	7	GLN
32	X	89	HIS

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](#)

Of 20 ligands modelled in this entry, 19 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
59	SF4	0	1000	1	0,12,12	0.00	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	SF4	0	1000	1	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

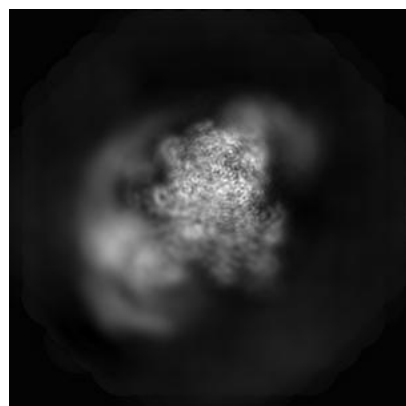
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12610. These allow visual inspection of the internal detail of the map and identification of artifacts.

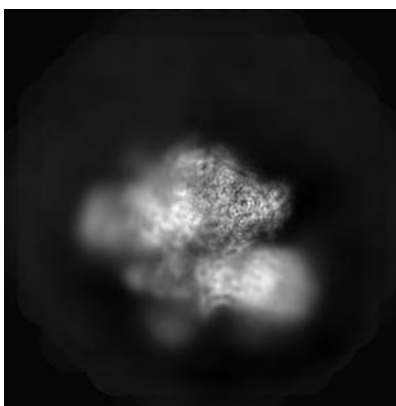
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

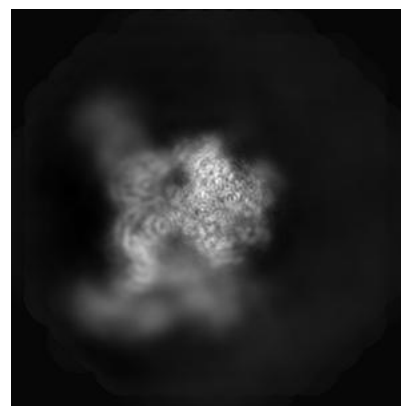
6.1.1 Primary map



X

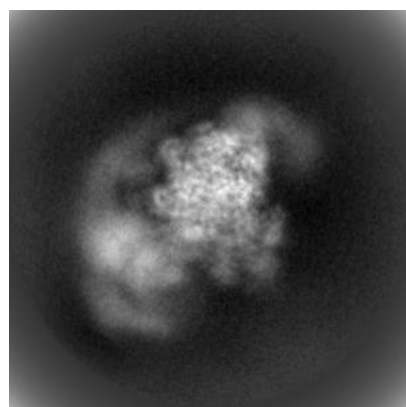


Y

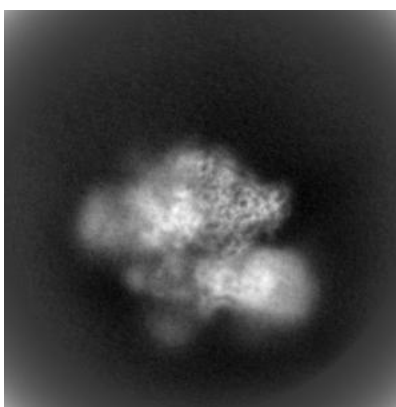


Z

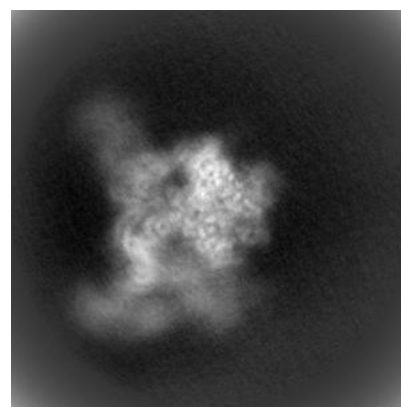
6.1.2 Raw map



X



Y

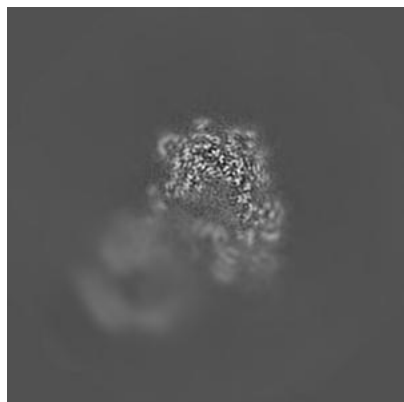


Z

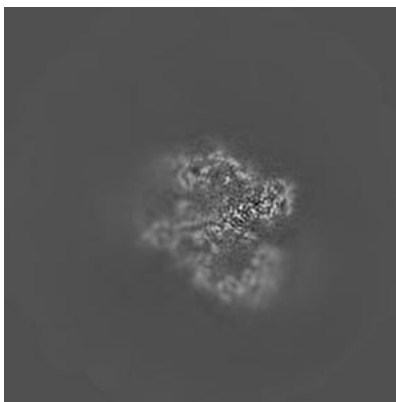
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

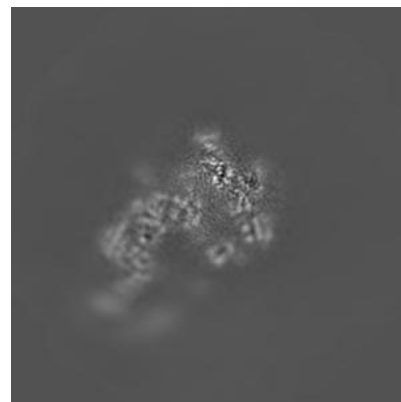
6.2.1 Primary map



X Index: 210

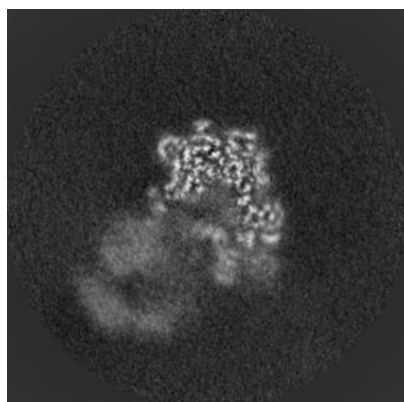


Y Index: 210

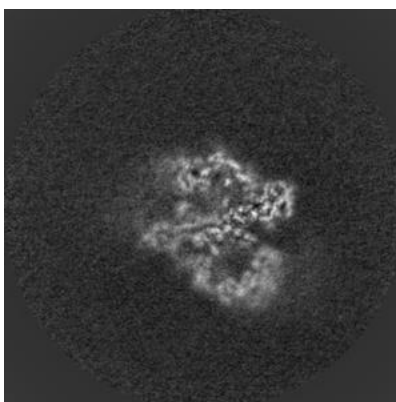


Z Index: 210

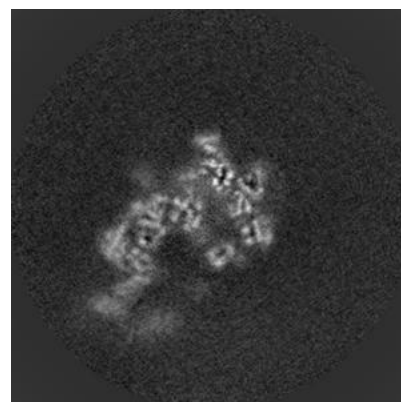
6.2.2 Raw map



X Index: 210



Y Index: 210

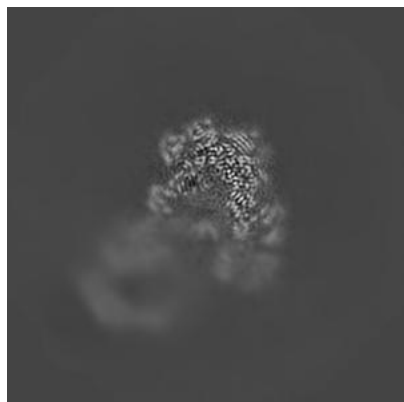


Z Index: 210

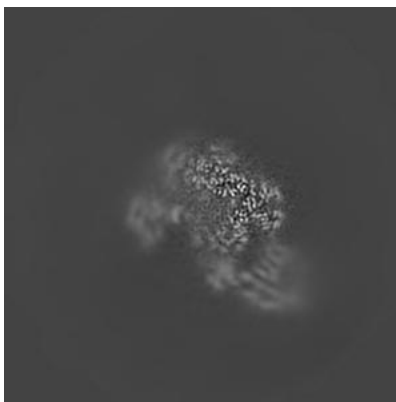
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

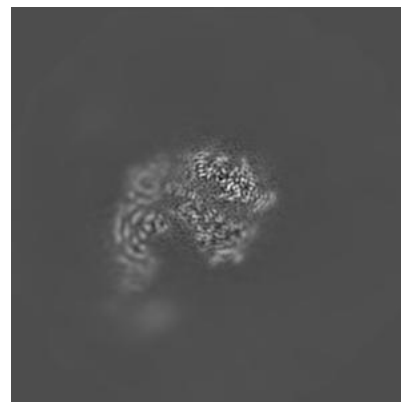
6.3.1 Primary map



X Index: 215

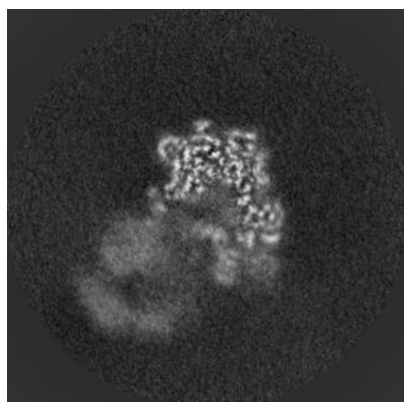


Y Index: 226

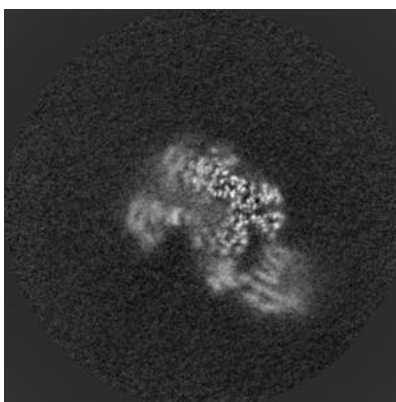


Z Index: 228

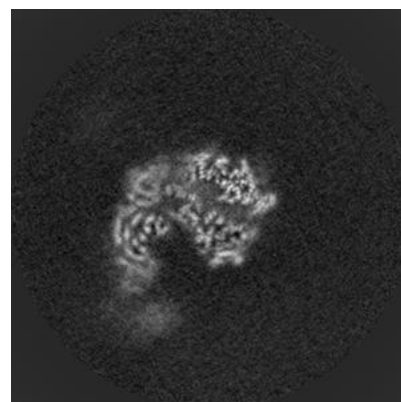
6.3.2 Raw map



X Index: 210



Y Index: 227

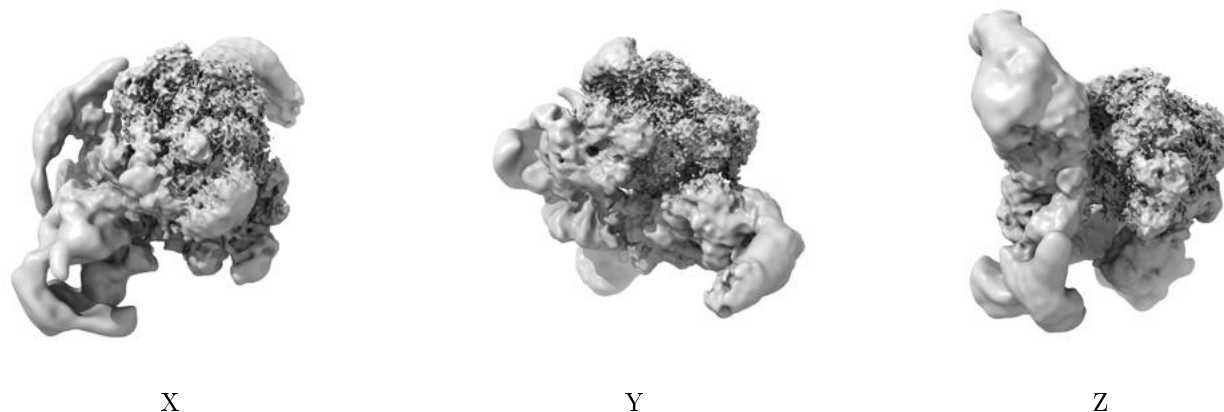


Z Index: 228

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

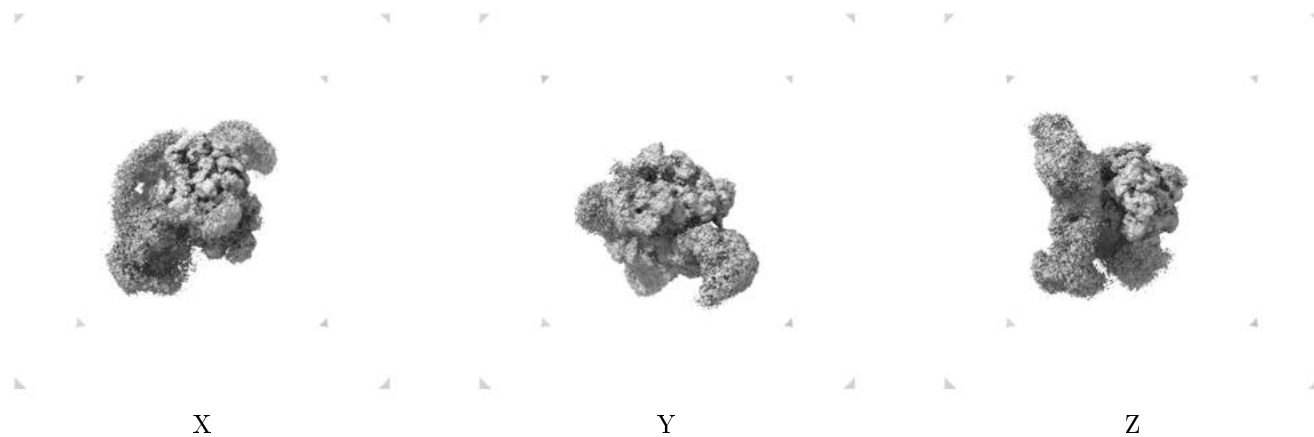
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

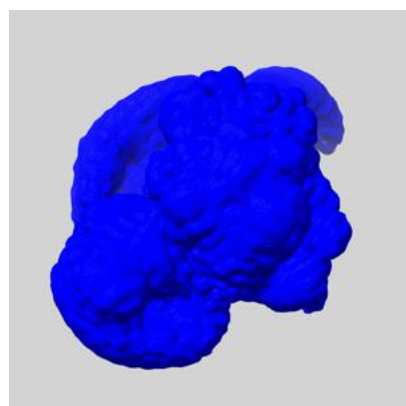
6.5 Mask visualisation [i](#)

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

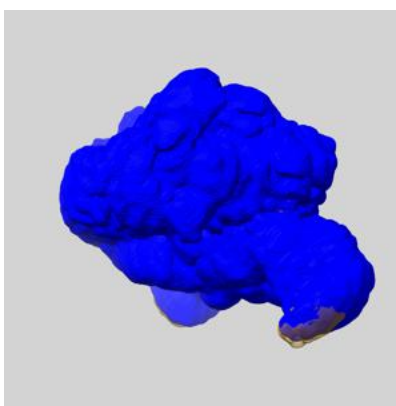
A mask typically either:

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

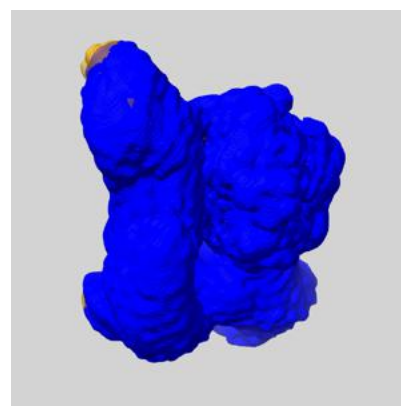
6.5.1 emd_12610_msk_1.map [i](#)



X



Y

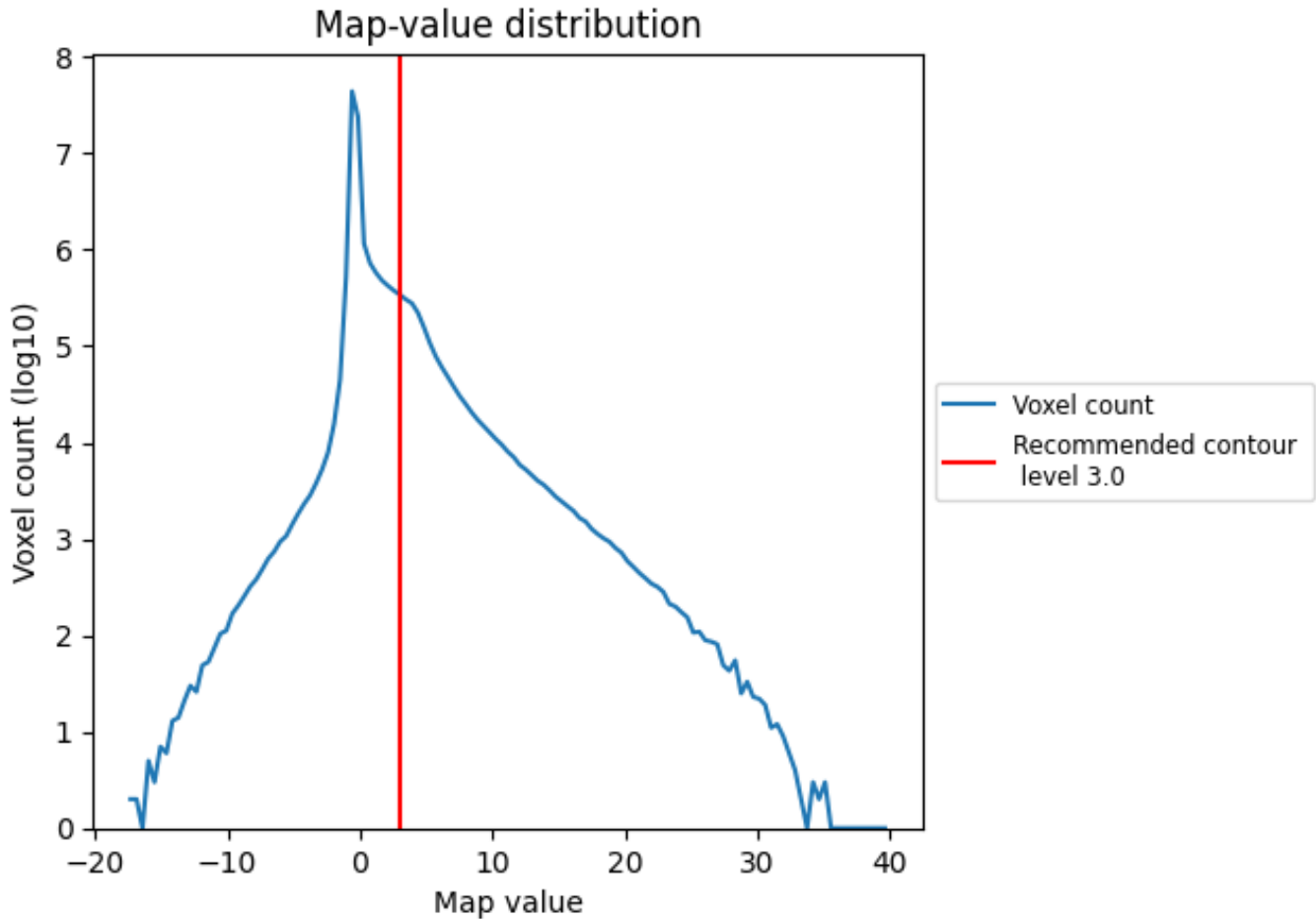


Z

7 Map analysis [i](#)

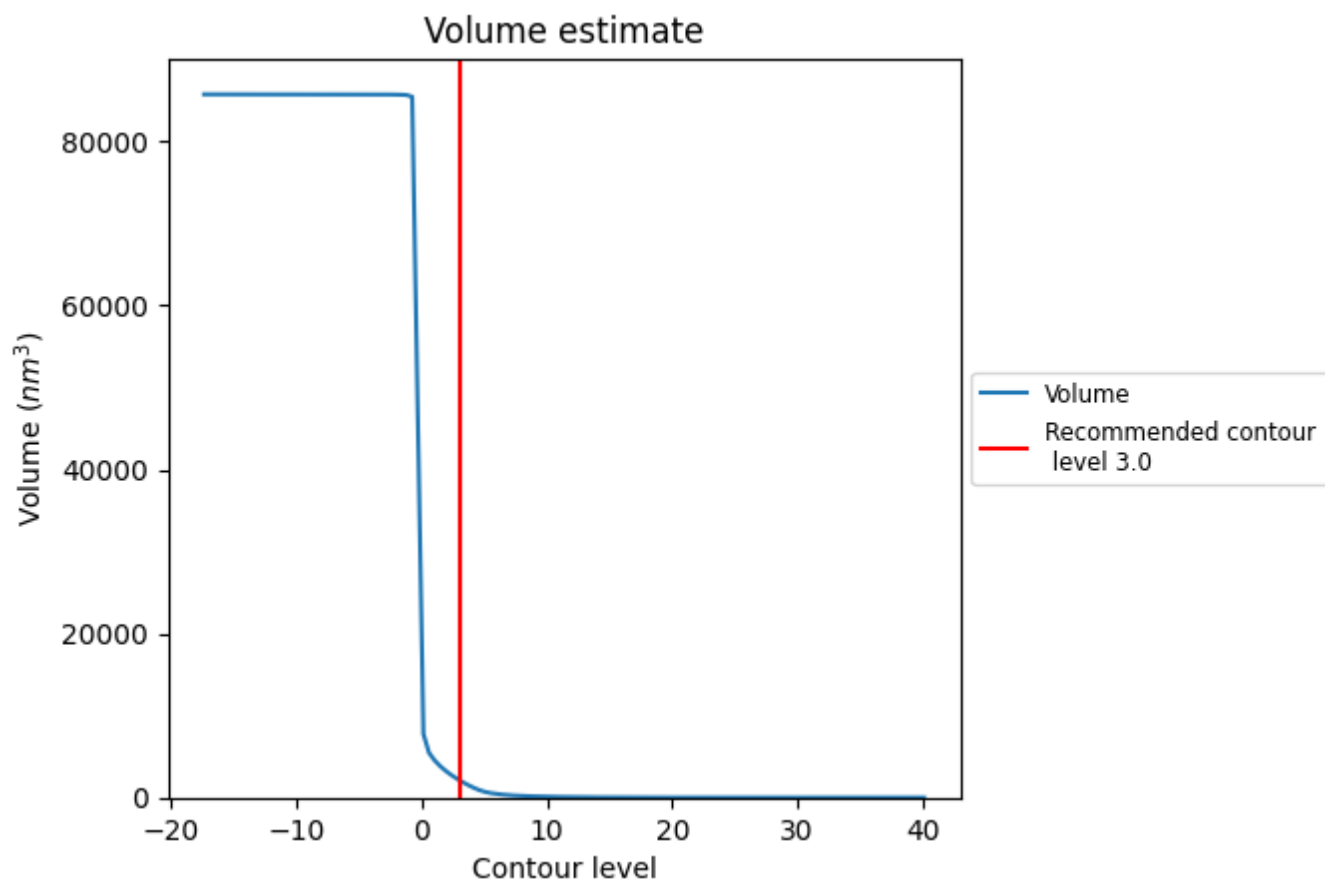
This section contains the results of statistical analysis of the map.

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.

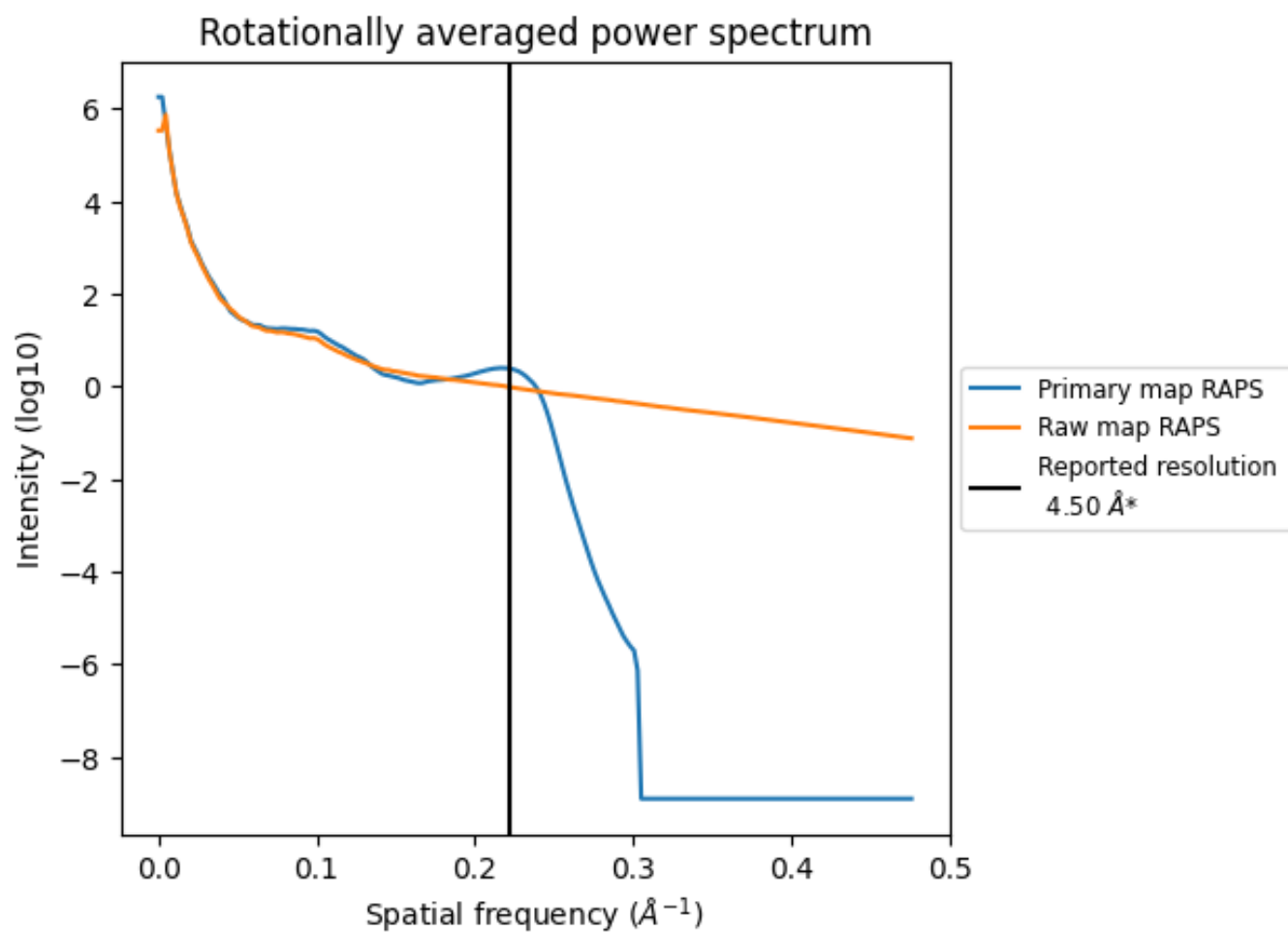
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2146 nm^3 ; this corresponds to an approximate mass of 1939 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

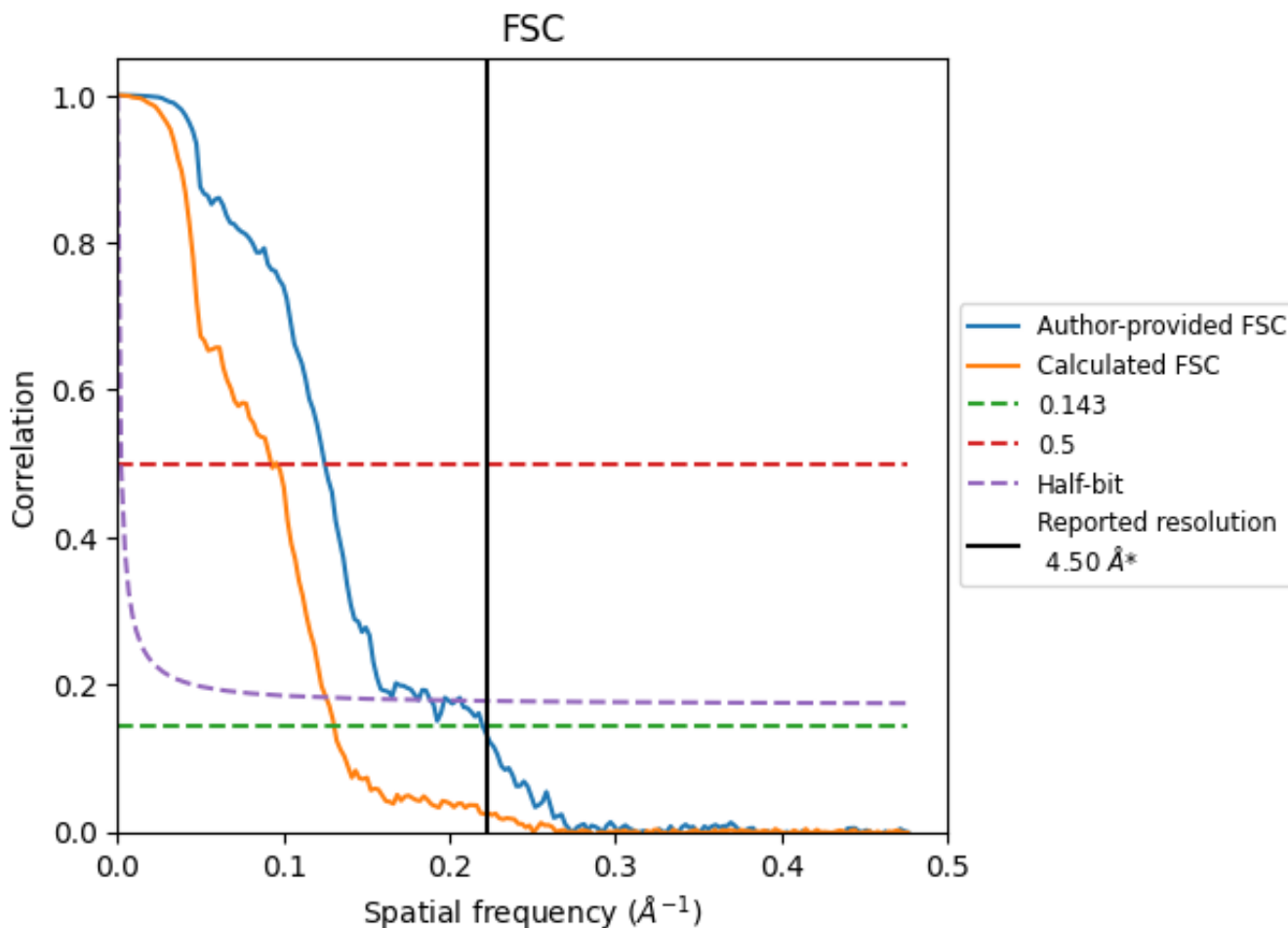


*Reported resolution corresponds to spatial frequency of 0.222 Å⁻¹

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 0.222 Å⁻¹

8.2 Resolution estimates [i](#)

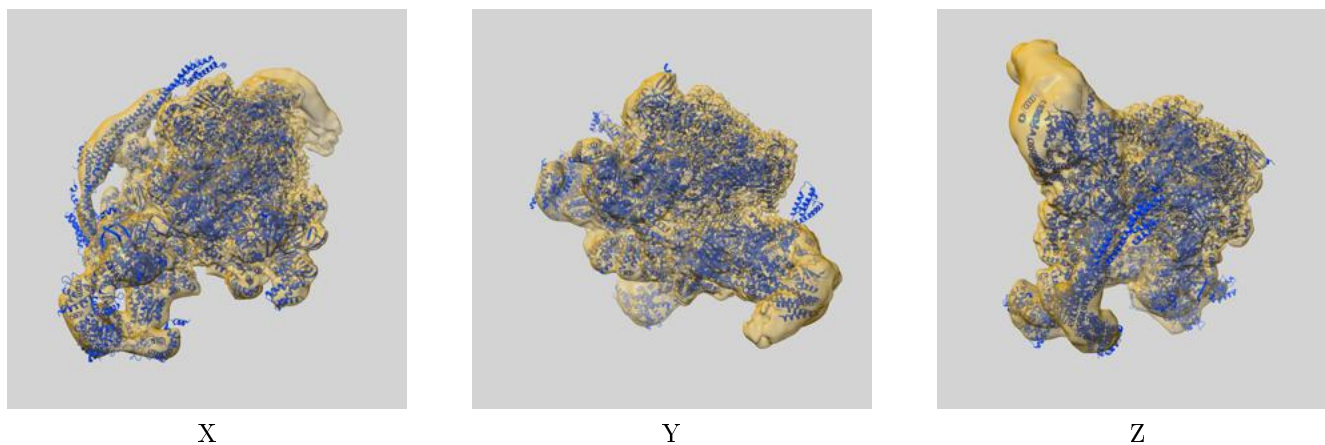
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.50	-	-
Author-provided FSC curve	4.54	8.01	5.51
Calculated*	7.66	10.79	7.95

*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 7.66 differs from the reported value 4.5 by more than 10 %

9 Map-model fit [i](#)

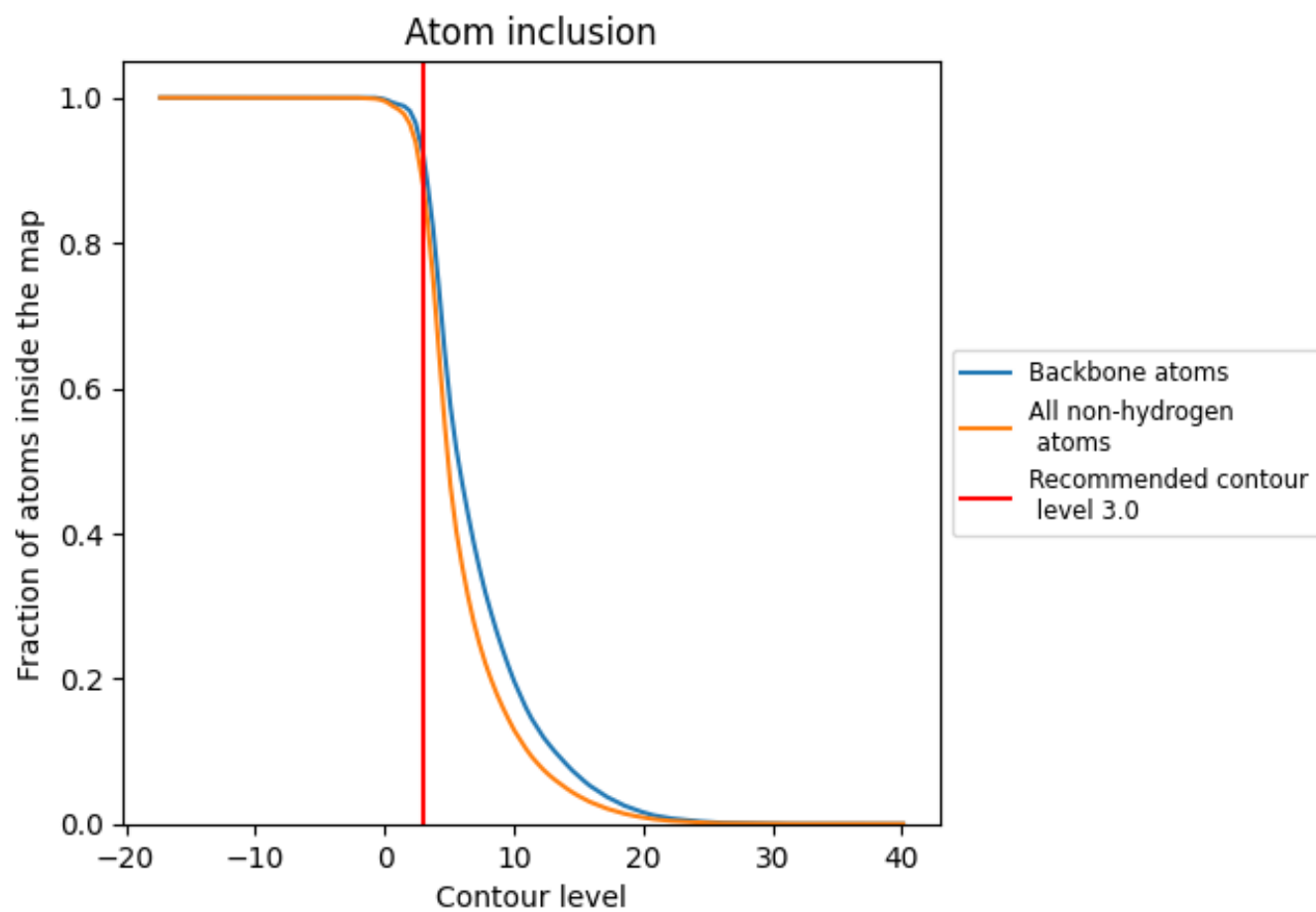
This section contains information regarding the fit between EMDB map EMD-12610 and PDB model 7NVR. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 3.0 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 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.