



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 11:20 PM UTC

PDB ID : 7ENC / pdb_00007enc
EMDB ID : EMD-31207
Title : TFIID-based PIC-Mediator holo-complex in fully-assembled state (hPIC-MED)
Authors : Chen, X.; Qi, Y.; Wang, X.; Wu, Z.; Yin, X.; Li, J.; Liu, W.; Xu, Y.
Deposited on : 2021-04-16
Resolution : 4.13 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
Mogul : 2022.3.0, CSD as543be (2022)
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

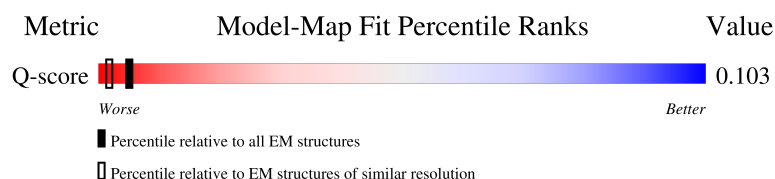
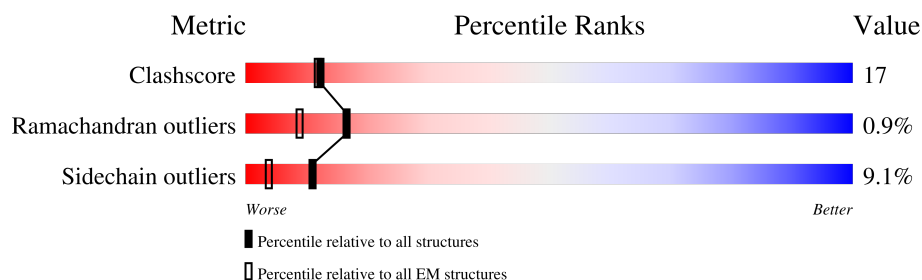
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.13 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.



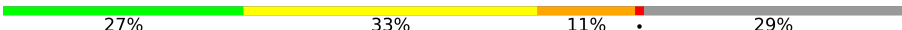
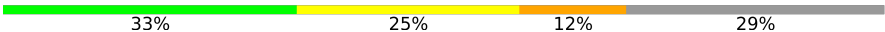
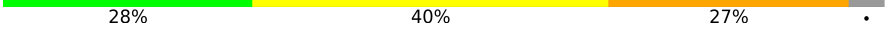
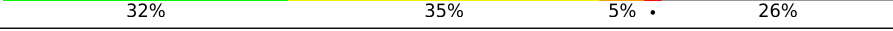
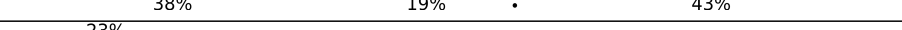
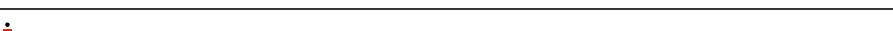
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5607 (3.63 - 4.63)

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	1581	30% 17% 9% . 70%
2	m	131	47% 38% 15%
3	d	270	14% 24% 24% 10% 41%
4	f	246	32% 28% 6% . 32%

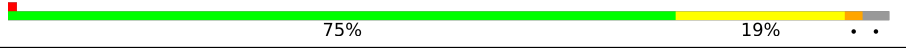
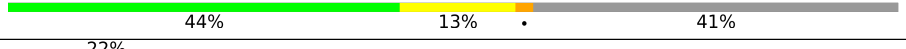
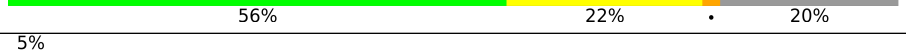
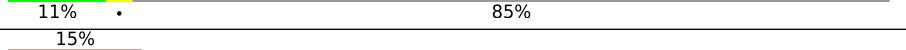
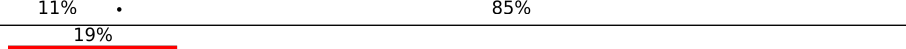
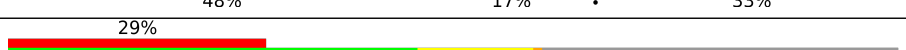
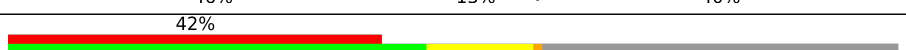
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	g	233	
6	h	268	
7	r	208	
8	t	212	
9	j	135	
10	k	117	
11	n	1454	
12	q	651	
13	s	244	
14	u	144	
15	v	200	
16	z	600	
17	c	311	
18	e	178	
19	b	200	
20	l	178	
21	o	788	
22	i	146	
23	0	309	
24	8	346	
25	9	323	
26	1	548	
27	2	395	
28	3	308	
29	4	462	

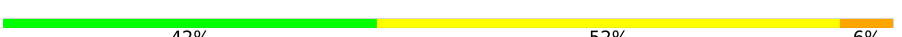
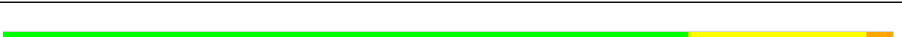
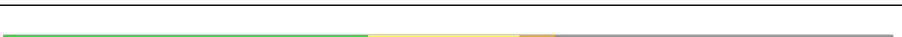
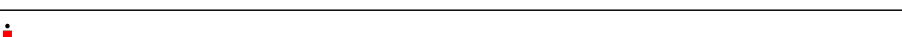
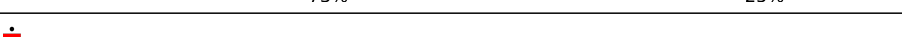
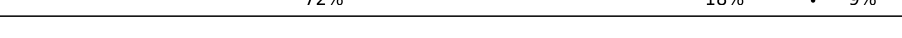
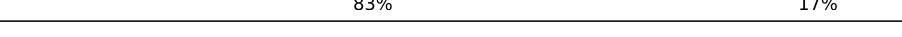
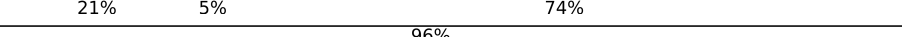
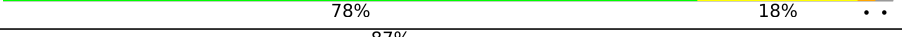
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
30	5	71	
31	6	782	
32	7	760	
33	EA	439	
34	EB	291	
35	DA	1872	
36	DB	1199	
37	DD	1085	
37	Dd	1085	
38	DE	800	
38	De	800	
39	DF	677	
39	Df	677	
40	DG	349	
41	DH	310	
42	DI	264	
42	Di	264	
43	DJ	218	
43	Dj	218	
44	DL	161	
44	DI	161	
45	Dc	929	
46	Dk	211	
47	Dm	124	
48	DO	109	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
49	DP	339	
50	DQ	307	
51	BA	316	
52	FB	249	
53	X	69	
54	Y	69	
55	PA	1970	
56	PB	1174	
57	PC	275	
58	PD	142	
59	PE	210	
60	PF	127	
61	PG	172	
62	PH	150	
63	PI	125	
64	PJ	67	
65	PK	117	
66	PL	58	
67	FA	517	
68	w	1368	
69	x	989	
70	p	841	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
71	ZN	0	401	-	-	X	-

2 Entry composition

There are 73 unique types of molecules in this entry. The entry contains 171177 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	469	Total	C	N	O	S	0	0
			3570	2271	614	661	24		

- Molecule 2 is a protein called Mediator of RNA polymerase II transcription subunit 31.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	m	112	Total	C	N	O	S	0	0
			983	641	172	165	5		

- Molecule 3 is a protein called Mediator of RNA polymerase II transcription subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	d	158	Total	C	N	O	S	0	0
			1264	788	227	243	6		

- Molecule 4 is a protein called Mediator of RNA polymerase II transcription subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	f	167	Total	C	N	O	S	0	0
			1329	851	231	242	5		

- Molecule 5 is a protein called Mediator of RNA polymerase II transcription subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	g	166	Total	C	N	O	S	0	0
			1382	880	244	248	10		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
g	10	ALA	LEU	conflict	UNP O43513
g	11	LEU	PRO	conflict	UNP O43513

- Molecule 6 is a protein called Isoform 2 of Mediator of RNA polymerase II transcription subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	h	190	Total	C	N	O	S	0	0
			1486	925	262	295	4		

- Molecule 7 is a protein called Mediator of RNA polymerase II transcription subunit 18.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	r	191	Total	C	N	O	S	0	0
			1528	969	270	274	15		

- Molecule 8 is a protein called Mediator of RNA polymerase II transcription subunit 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	t	193	Total	C	N	O	S	0	0
			1499	955	247	280	17		

- Molecule 9 is a protein called Mediator of RNA polymerase II transcription subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	j	122	Total	C	N	O	S	0	0
			1001	636	174	187	4		

- Molecule 10 is a protein called Mediator of RNA polymerase II transcription subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	k	112	Total	C	N	O	S	0	0
			879	537	163	175	4		

- Molecule 11 is a protein called Mediator of RNA polymerase II transcription subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	n	994	Total	C	N	O	S	0	0
			7241	4576	1293	1334	38		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	133	LEU	ALA	conflict	UNP O60244

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	q	552	Total	C	N	O	S	0	0
			4261	2691	764	789	17		

- Molecule 13 is a protein called Mediator of RNA polymerase II transcription subunit 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	s	77	Total	C	N	O	S	0	0
			485	300	87	96	2		

- Molecule 14 is a protein called Mediator of RNA polymerase II transcription subunit 21.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	u	107	Total	C	N	O	S	0	0
			792	492	132	165	3		

- Molecule 15 is a protein called Mediator of RNA polymerase II transcription subunit 22.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	v	134	Total	C	N	O	S	0	0
			1083	668	185	226	4		

- Molecule 16 is a protein called Mediator of RNA polymerase II transcription subunit 26.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	z	97	Total	C	N	O	S	0	0
			765	472	136	154	3		

- Molecule 17 is a protein called Mediator of RNA polymerase II transcription subunit 27.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	c	255	Total	C	N	O	S	0	0
			2069	1314	370	374	11		

- Molecule 18 is a protein called Mediator of RNA polymerase II transcription subunit 28.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	e	102	Total	C	N	O	S	0	0
			832	520	146	163	3		

- Molecule 19 is a protein called Mediator of RNA polymerase II transcription subunit 29.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	b	115	Total	C	N	O	S	0	0
			899	563	155	172	9		

- Molecule 20 is a protein called Mediator of RNA polymerase II transcription subunit 30.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	l	126	Total	C	N	O	S	0	0
			1040	649	191	193	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	o	156	Total	C	N	O	S	0	0
			1221	780	212	222	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	i	62	Total	C	N	O	S	0	0
			520	329	92	94	5		

- Molecule 23 is a protein called CDK-activating kinase assembly factor MAT1.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	0	306	Total	C	N	O	S	0	0
			2255	1404	399	441	11		

- Molecule 24 is a protein called Cyclin-dependent kinase 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	8	299	Total	C	N	O	S	0	0
			2378	1535	406	426	11		

- Molecule 25 is a protein called Cyclin-H.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	9	287	Total	C	N	O	S	0	0
			2307	1477	398	417	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	1	405	Total	C	N	O	S	0	0
			2634	1640	486	501	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	2	331	Total	C	N	O	S	0	0
			2534	1597	441	470	26		

- Molecule 28 is a protein called General transcription factor IIH subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	3	263	Total	C	N	O	S	0	0
			2065	1323	344	379	19		

- Molecule 29 is a protein called General transcription factor IIH subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	4	449	Total	C	N	O	S	0	0
			3579	2303	624	638	14		

- Molecule 30 is a protein called General transcription factor IIH subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	5	54	Total	C	N	O	S	0	0
			428	277	67	82	2		

- Molecule 31 is a protein called General transcription and DNA repair factor IIH helicase subunit XPB.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	6	606	Total	C	N	O	S	0	0
			4880	3117	849	884	30		

- Molecule 32 is a protein called General transcription and DNA repair factor IIH helicase subunit XPD.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	7	734	Total	C	N	O	S	0	0
			5833	3727	1022	1055	29		

- Molecule 33 is a protein called General transcription factor IIE subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	EA	179	Total	C	N	O	S	0	0
			1476	932	261	272	11		

- Molecule 34 is a protein called Transcription initiation factor IIE subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	EB	172	Total	C	N	O	S	0	0
			1404	893	243	264	4		

- Molecule 35 is a protein called Transcription initiation factor TFIID subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	DA	550	Total	C	N	O	S	0	0
			4511	2882	782	820	27		

- Molecule 36 is a protein called Transcription initiation factor TFIID subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	DB	963	Total	C	N	O	S	0	0
			7796	5011	1315	1412	58		

- Molecule 37 is a protein called Transcription initiation factor TFIID subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	DD	159	Total	C	N	O	S	0	0
			1330	830	248	249	3		
37	Dd	158	Total	C	N	O	S	0	0
			1307	814	238	252	3		

- Molecule 38 is a protein called Transcription initiation factor TFIID subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	DE	546	Total	C	N	O	S	0	0
			4364	2766	757	820	21		
38	De	539	Total	C	N	O	S	0	0
			4327	2746	748	814	19		

- Molecule 39 is a protein called Transcription initiation factor TFIID subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	DF	408	Total	C	N	O	S	0	0
			3109	1970	542	579	18		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Df	403	Total	C	N	O	S	0	0
			3081	1954	533	576	18		

- Molecule 40 is a protein called Transcription initiation factor TFIID subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	DG	145	Total	C	N	O	S	0	0
			1180	748	217	211	4		

- Molecule 41 is a protein called Transcription initiation factor TFIID subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	DH	209	Total	C	N	O	S	0	0
			1633	1034	283	311	5		

- Molecule 42 is a protein called Transcription initiation factor TFIID subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	DI	120	Total	C	N	O	S	0	0
			959	610	166	177	6		
42	Di	121	Total	C	N	O	S	0	0
			967	615	167	178	7		

- Molecule 43 is a protein called Transcription initiation factor TFIID subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	DJ	90	Total	C	N	O	S	0	0
			720	466	115	135	4		
43	Dj	95	Total	C	N	O	S	0	0
			759	488	124	143	4		

- Molecule 44 is a protein called Transcription initiation factor TFIID subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	DL	75	Total	C	N	O	S	0	0
			614	384	107	120	3		
44	DI	107	Total	C	N	O	S	0	0
			876	547	158	166	5		

- Molecule 45 is a protein called Transcription initiation factor TFIID subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Dc	127	Total	C	N	O	S	0	0
			1011	638	174	193	6		

- Molecule 46 is a protein called Transcription initiation factor TFIID subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Dk	98	Total	C	N	O	S	0	0
			785	499	142	139	5		

- Molecule 47 is a protein called Transcription initiation factor TFIID subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Dm	87	Total	C	N	O	S	0	0
			724	456	131	131	6		

- Molecule 48 is a protein called Transcription initiation factor IIA subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	DO	97	Total	C	N	O	S	0	0
			771	491	133	145	2		

- Molecule 49 is a protein called TATA-box-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	DP	177	Total	C	N	O	S	0	0
			1412	918	249	238	7		

- Molecule 50 is a protein called TFIIA-a.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	DQ	122	Total	C	N	O	S	0	0
			996	623	162	207	4		

- Molecule 51 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	BA	251	Total	C	N	O	S	0	0
			1939	1214	344	364	17		

- Molecule 52 is a protein called General transcription factor IIF subunit 2.

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

- Molecule 53 is a DNA chain called DNA (69-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
53	X	69	Total	C	N	O	P	0	0
			1429	672	279	409	69		

- Molecule 54 is a DNA chain called DNA (69-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
54	Y	69	Total	C	N	O	P	0	0
			1400	664	248	419	69		

- Molecule 55 is a protein called RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	PA	1474	Total	C	N	O	S	0	0
			11655	7333	2070	2180	72		

- Molecule 56 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	PB	1134	Total	C	N	O	S	0	0
			9062	5732	1595	1671	64		

- Molecule 57 is a protein called DNA-directed RNA polymerase II subunit RPB3.

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

- Molecule 58 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	PD	129	Total	C	N	O	S	0	0
			1021	643	174	200	4		

- Molecule 59 is a protein called DNA-directed RNA polymerase II subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	PE	209	Total	C	N	O	S	0	0
			1720	1089	300	323	8		

- Molecule 60 is a protein called DNA-directed RNA polymerase II subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	PF	79	Total	C	N	O	S	0	0
			635	406	108	116	5		

- Molecule 61 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	PG	171	Total	C	N	O	S	0	0
			1334	867	216	243	8		

- Molecule 62 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

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

- Molecule 63 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	PI	114	Total	C	N	O	S	0	0
			927	571	166	179	11		

- Molecule 64 is a protein called RPB10.

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

- Molecule 65 is a protein called RNA_pol_L_2 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	PK	117	Total	C	N	O	S	0	0
			937	604	154	177	2		

- Molecule 66 is a protein called RPB12.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	PL	44	Total	C	N	O	S	0	0
			372	231	72	63	6		

- Molecule 67 is a protein called General transcription factor IIF subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	FA	134	Total	C	N	O	S	0	0
			1101	698	199	202	2		

- Molecule 68 is a protein called Mediator of RNA polymerase II transcription subunit 23.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	w	1334	Total	C	N	O	S	0	0
			10772	6965	1827	1909	71		

- Molecule 69 is a protein called Mediator of RNA polymerase II transcription subunit 24.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	x	896	Total	C	N	O	S	0	0
			7050	4516	1188	1292	54		

- Molecule 70 is a protein called Isoform 2 of Mediator of RNA polymerase II transcription subunit 16.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	p	406	Total	C	N	O	S	0	0
			3124	1982	536	585	21		

- Molecule 71 is ZINC ION (CCD ID: ZN) (formula: Zn).

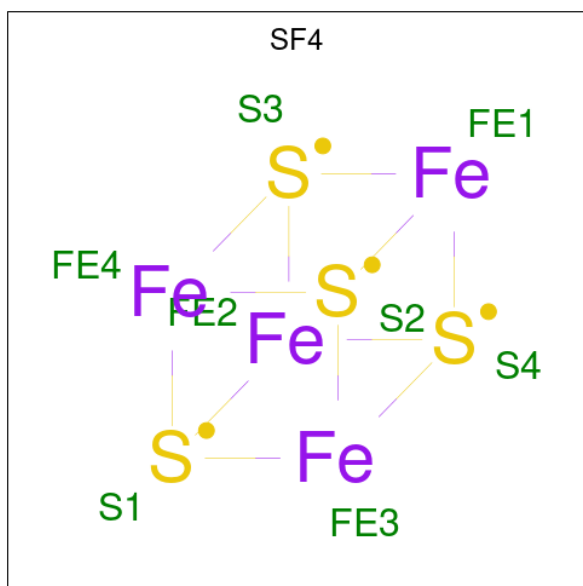
Mol	Chain	Residues	Atoms		AltConf
71	0	2	Total	Zn	0
			2	2	
71	2	3	Total	Zn	0
			3	3	
71	3	1	Total	Zn	0
			1	1	
71	EA	1	Total	Zn	0
			1	1	
71	BA	1	Total	Zn	0
			1	1	
71	PA	2	Total	Zn	0
			2	2	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
71	PB	1	Total	Zn	0
			1	1	
71	PC	1	Total	Zn	0
			1	1	
71	PI	2	Total	Zn	0
			2	2	
71	PJ	1	Total	Zn	0
			1	1	
71	PL	1	Total	Zn	0
			1	1	

- Molecule 72 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
72	7	1	Total	Fe	S	0
			8	4	4	

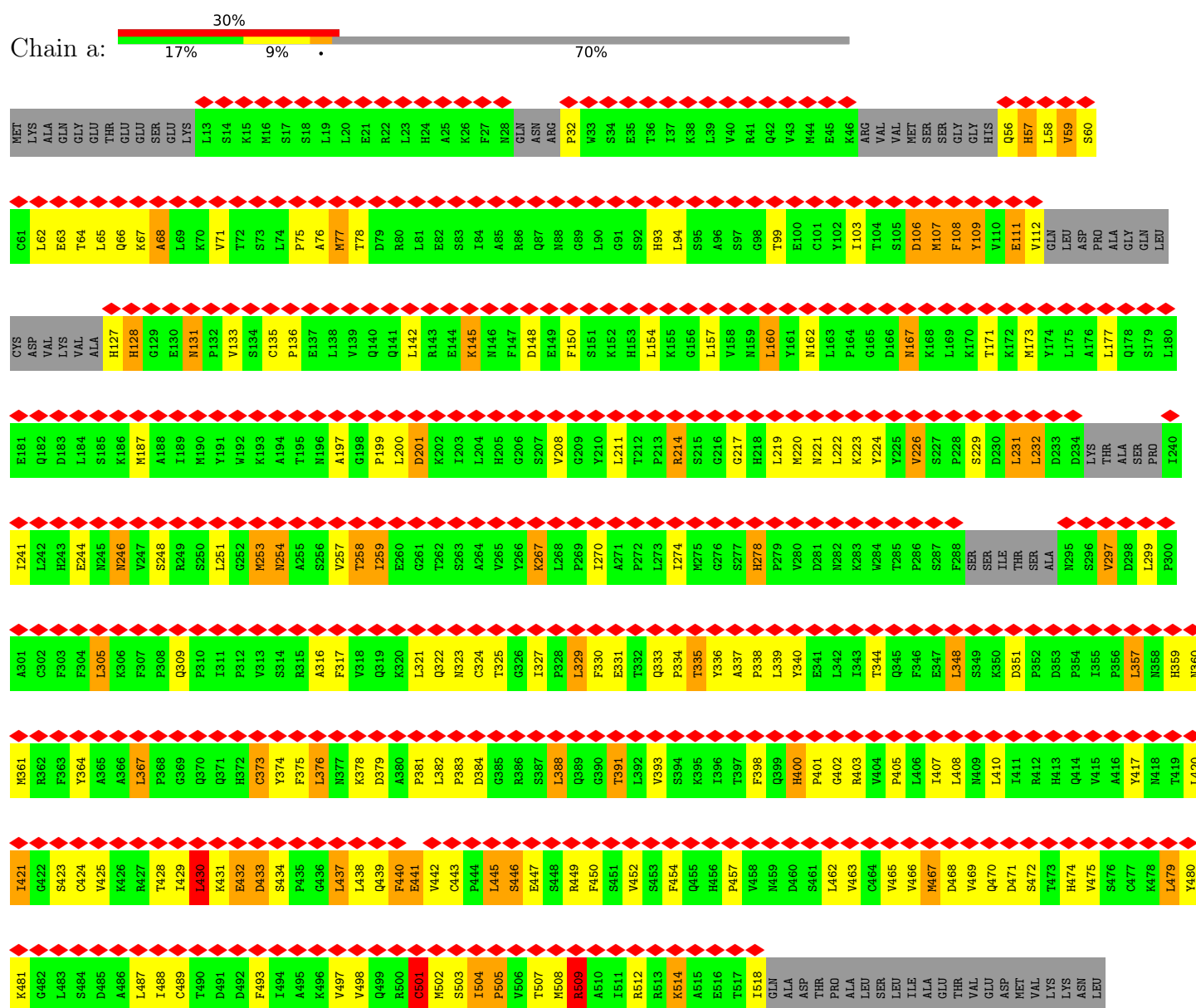
- Molecule 73 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
73	PA	1	Total	Mg	0
			1	1	

3 Residue-property plots

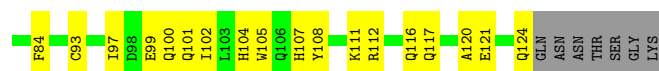
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

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

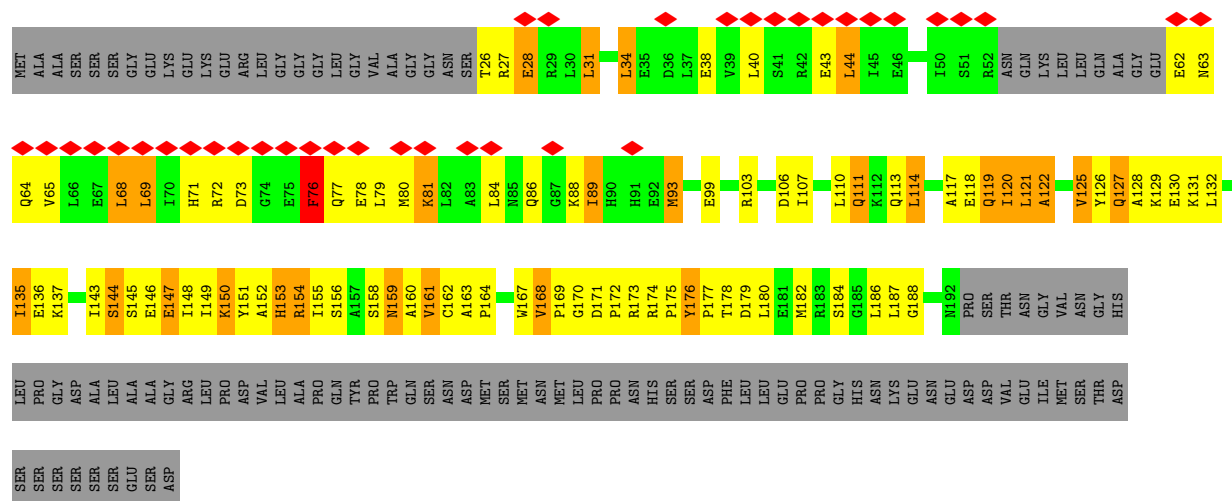
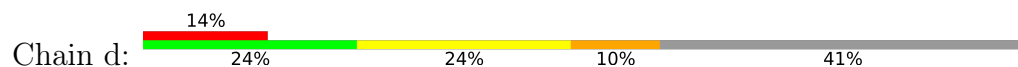


- Molecule 2: Mediator of RNA polymerase II transcription subunit 31

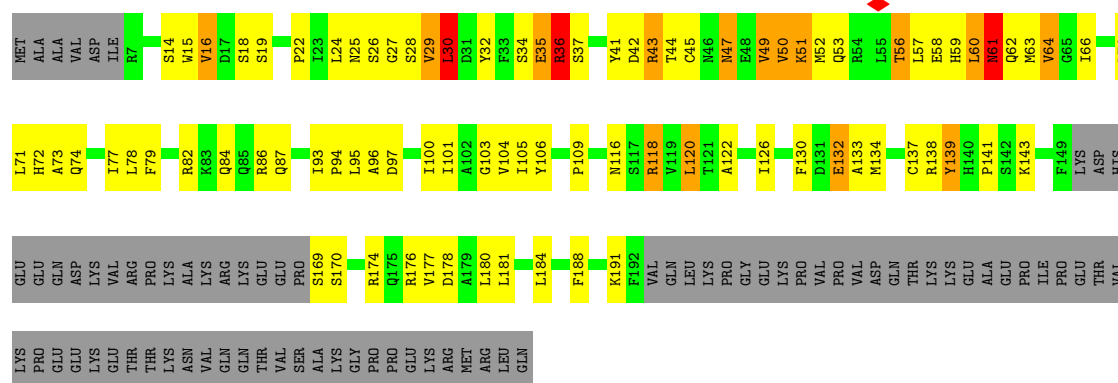




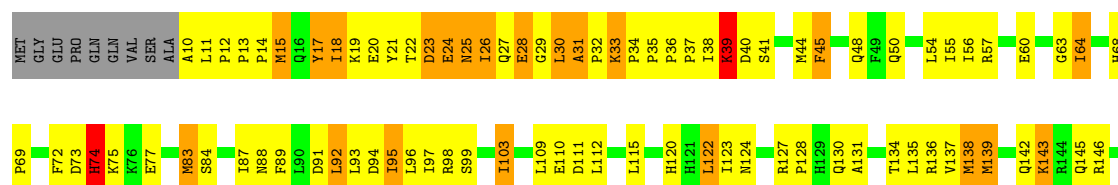
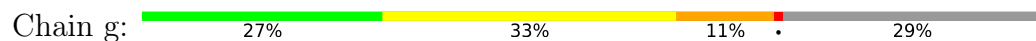
• Molecule 3: Mediator of RNA polymerase II transcription subunit 4

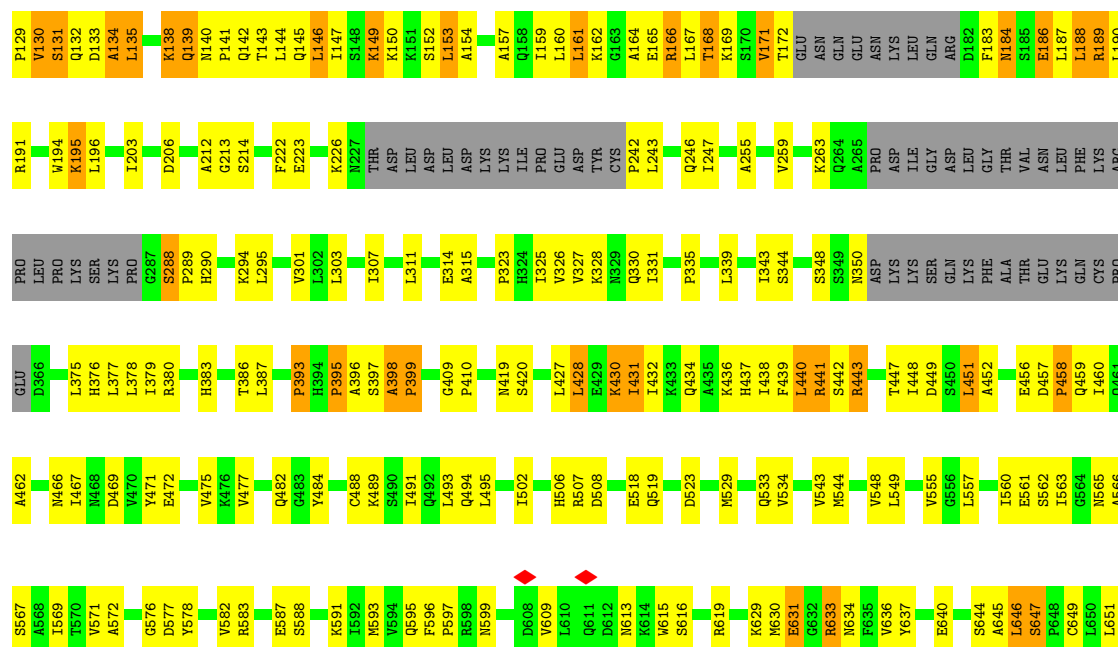


• Molecule 4: Mediator of RNA polymerase II transcription subunit 6

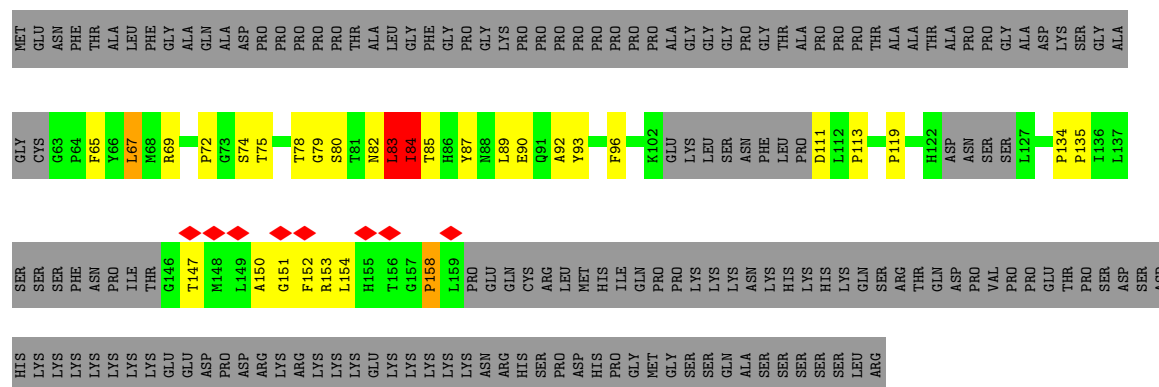


• Molecule 5: Mediator of RNA polymerase II transcription subunit 7

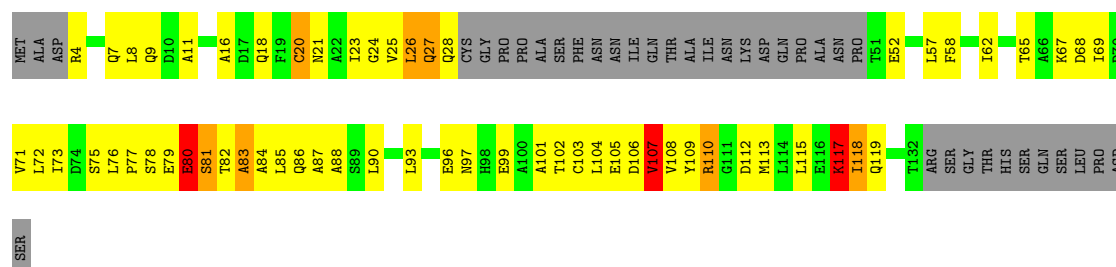




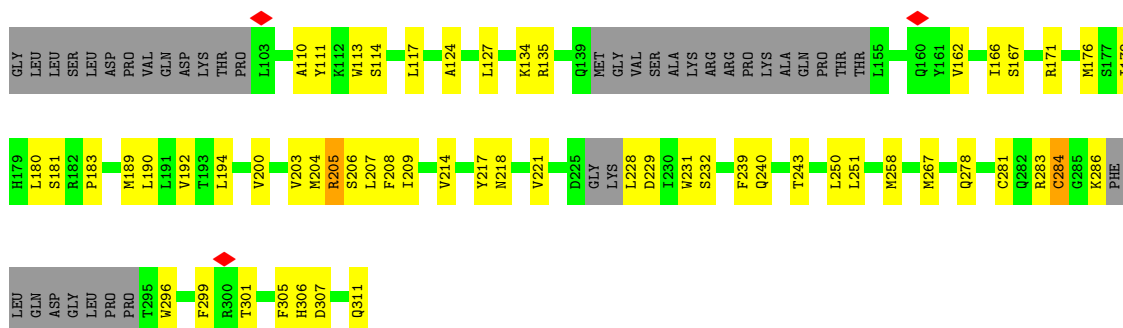
• Molecule 13: Mediator of RNA polymerase II transcription subunit 19



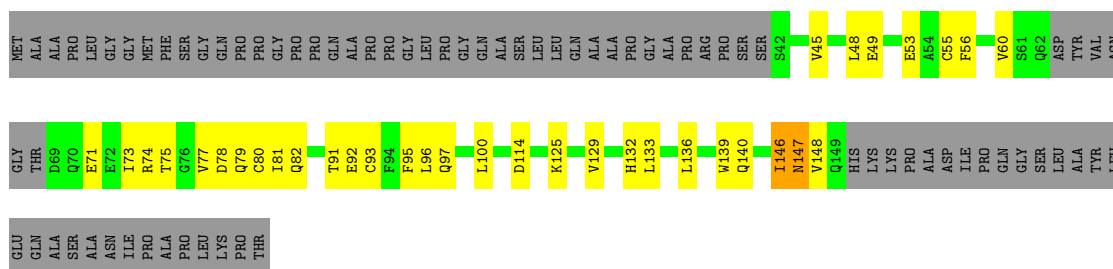
• Molecule 14: Mediator of RNA polymerase II transcription subunit 21



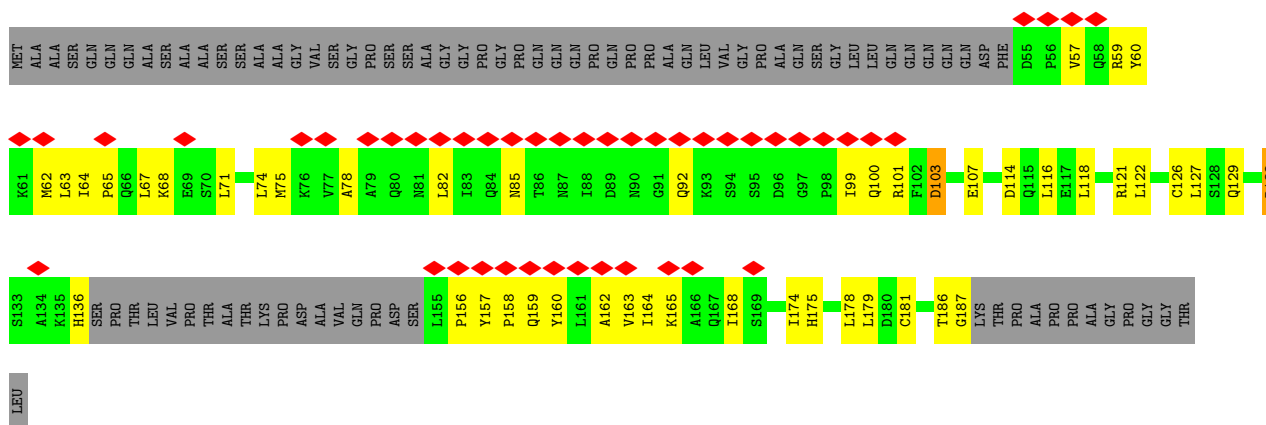
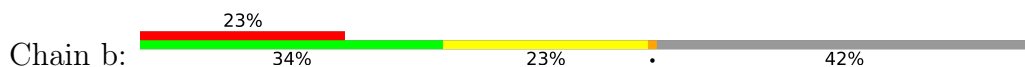
• Molecule 15: Mediator of RNA polymerase II transcription subunit 22



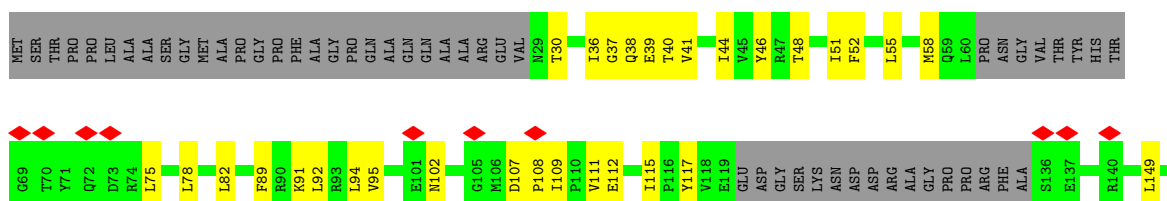
- Molecule 18: Mediator of RNA polymerase II transcription subunit 28

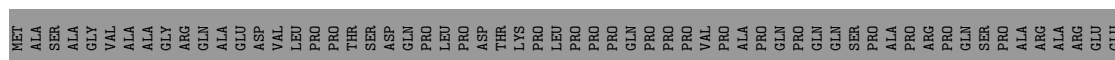


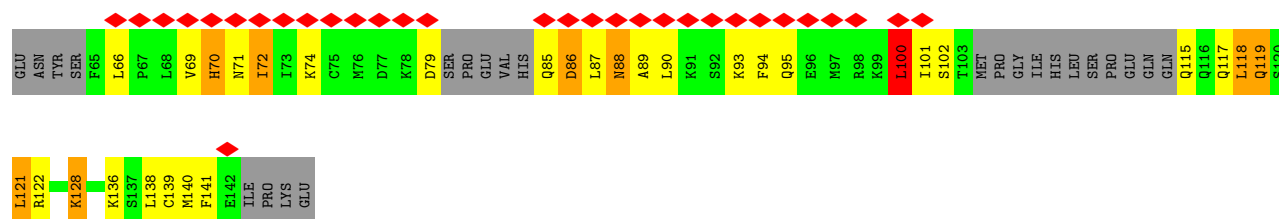
- Molecule 19: Mediator of RNA polymerase II transcription subunit 29



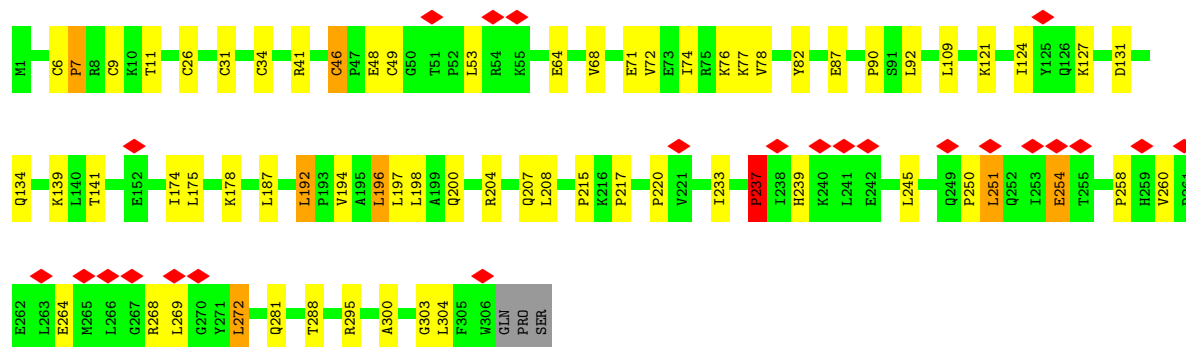
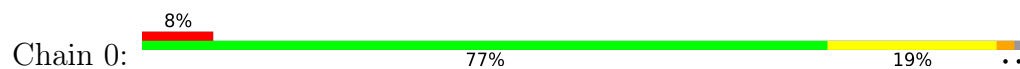
- Molecule 20: Mediator of RNA polymerase II transcription subunit 30



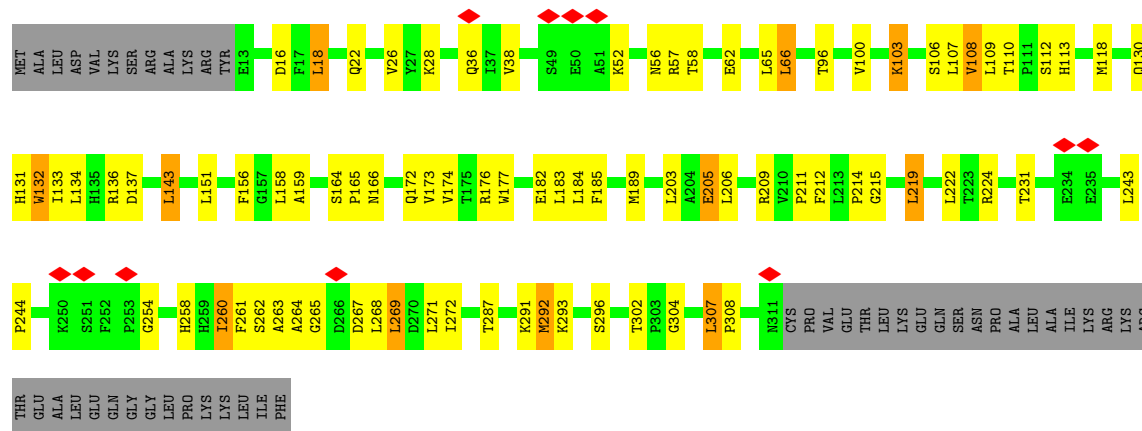




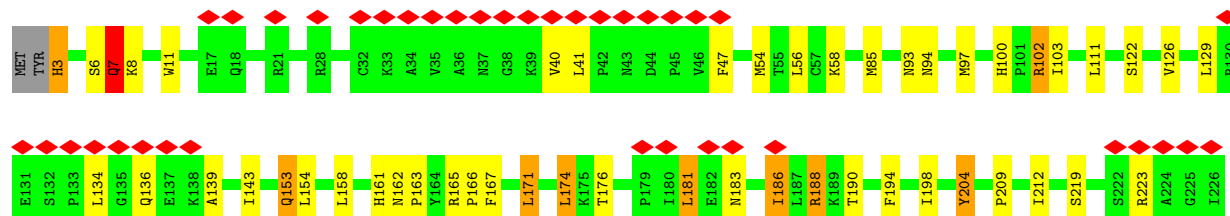
• Molecule 23: CDK-activating kinase assembly factor MAT1

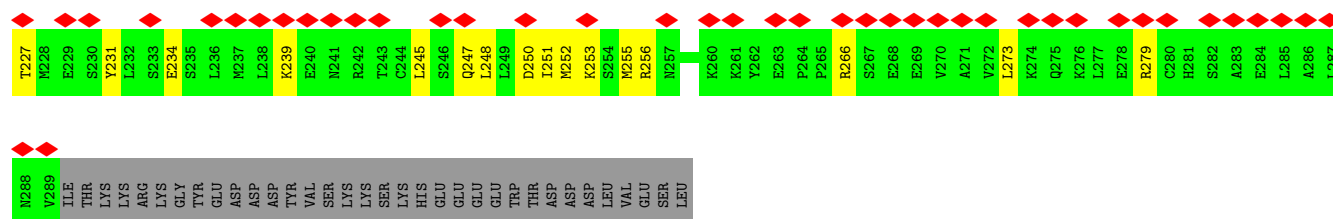


• Molecule 24: Cyclin-dependent kinase 7

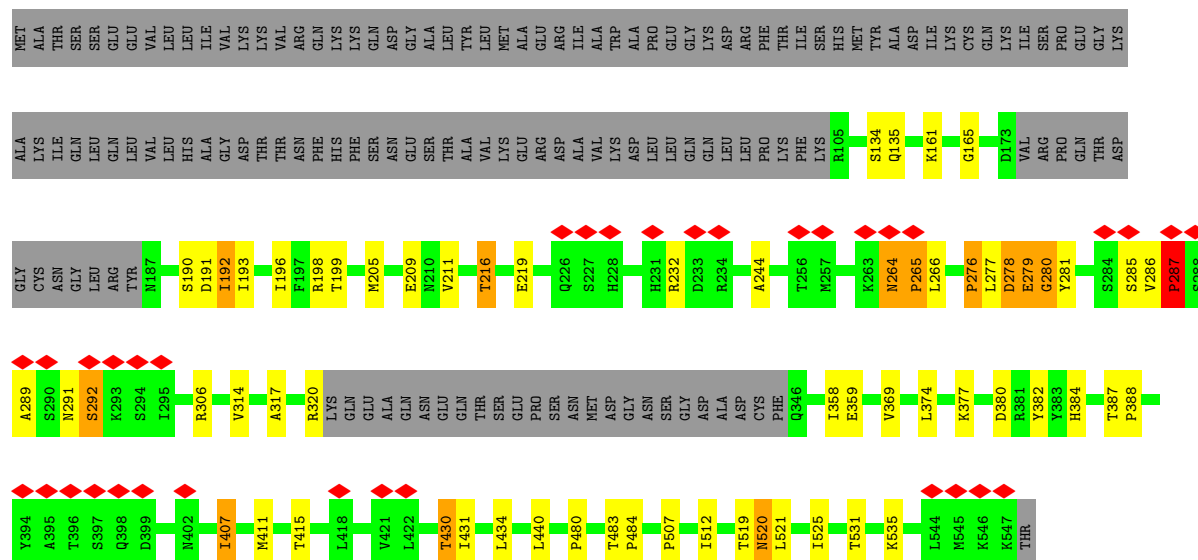


• Molecule 25: Cyclin-H

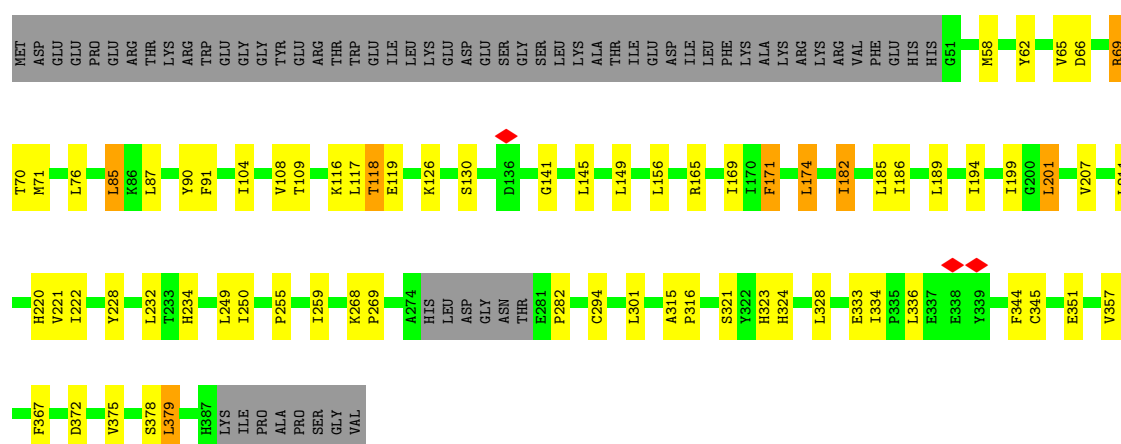




• Molecule 26: General transcription factor IIH subunit 1

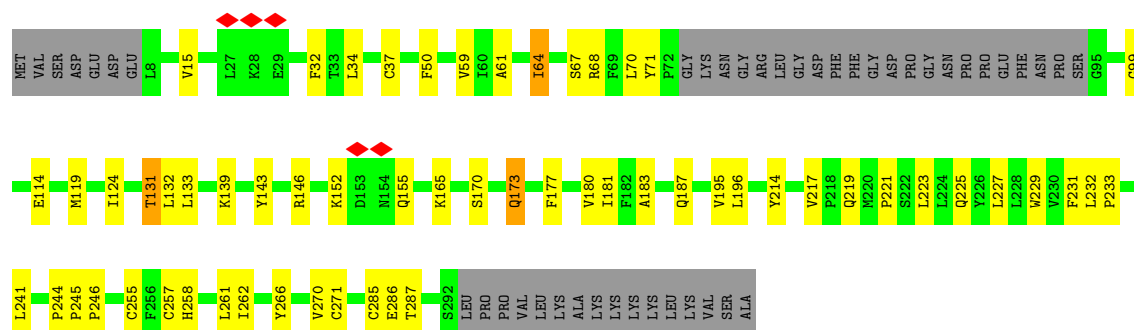


• Molecule 27: General transcription factor IIH subunit 2



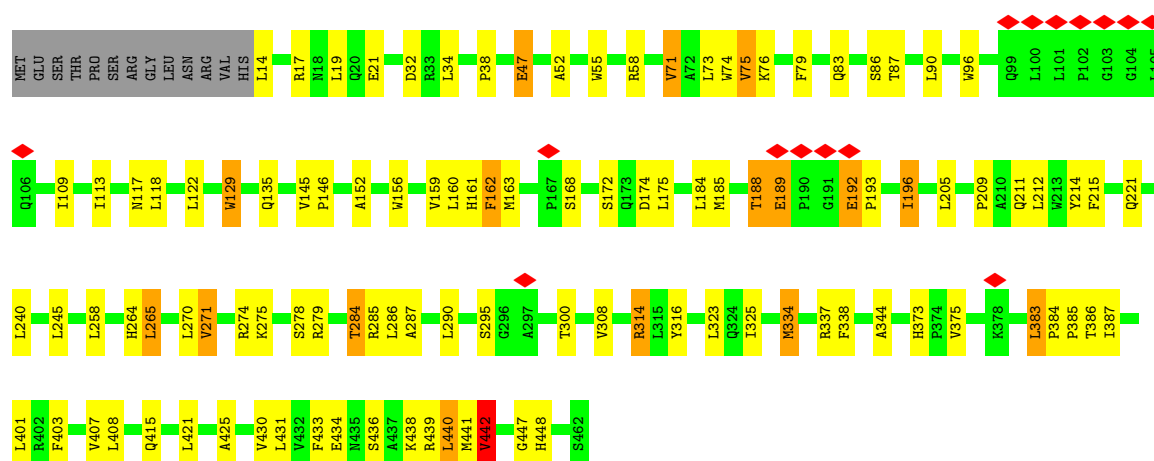
• Molecule 28: General transcription factor IIH subunit 3





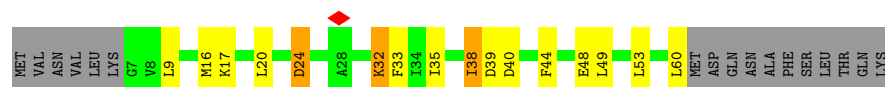
- Molecule 29: General transcription factor IIH subunit 4

Chain 4: 74% 20%



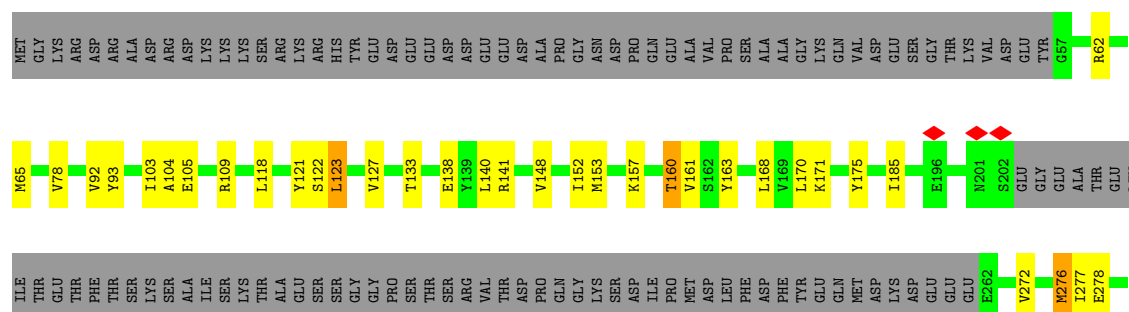
- Molecule 30: General transcription factor IIH subunit 5

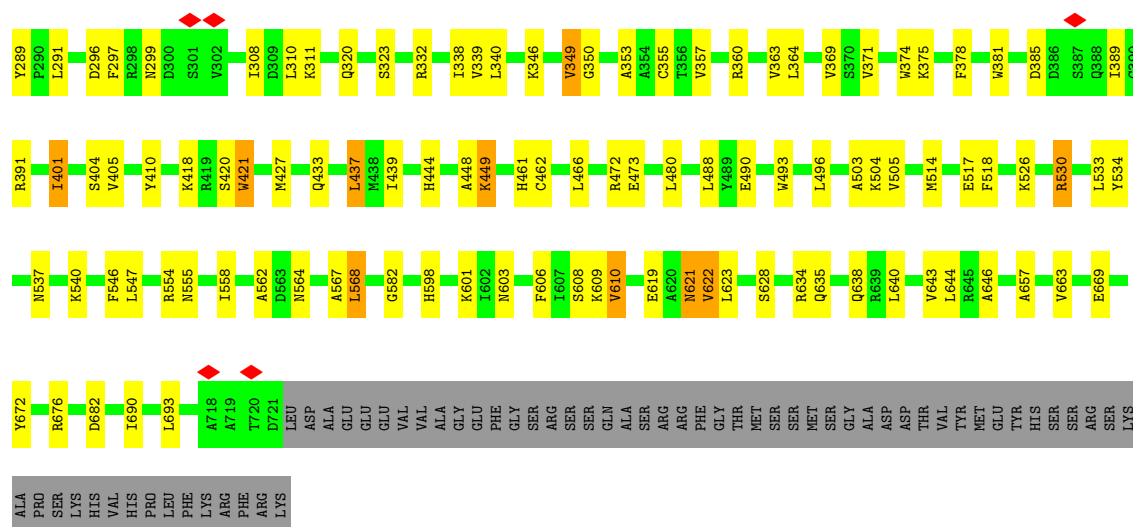
Chain 5: 54% 18% 24%



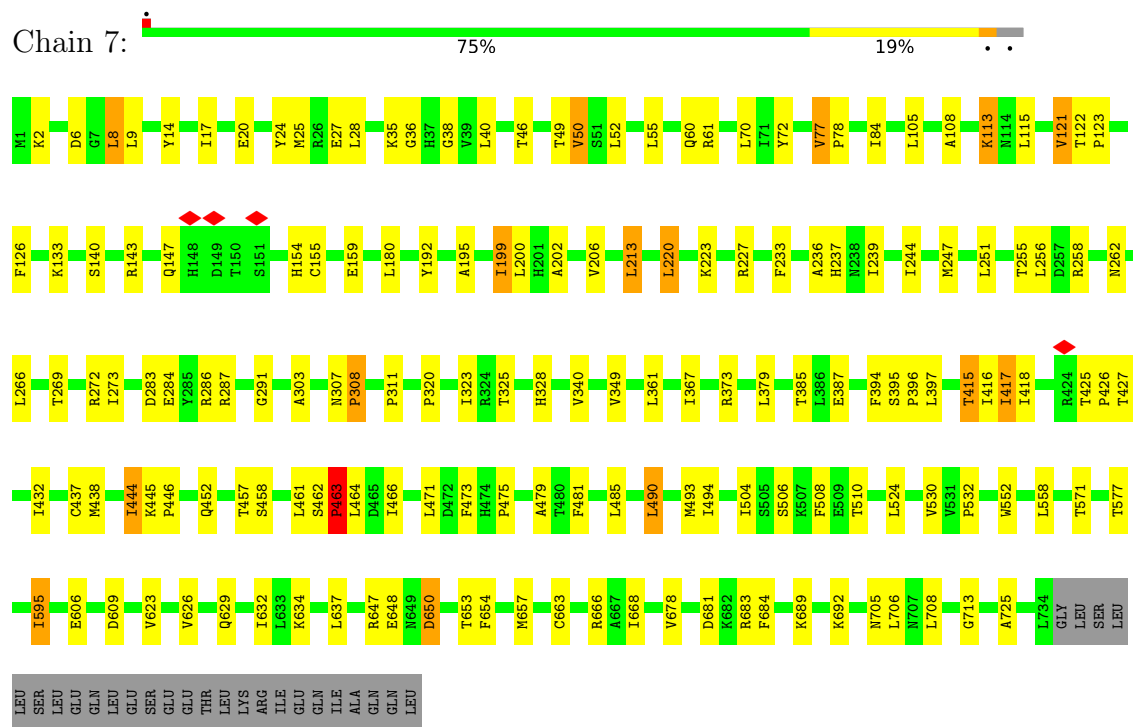
- Molecule 31: General transcription and DNA repair factor IIH helicase subunit XPB

Chain 6: 60% 16% 23%

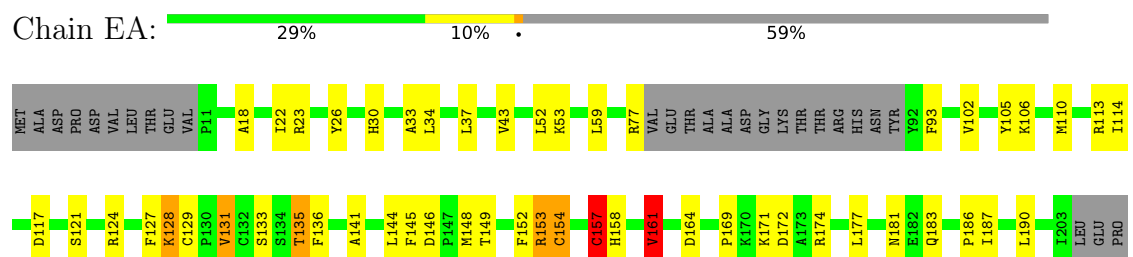


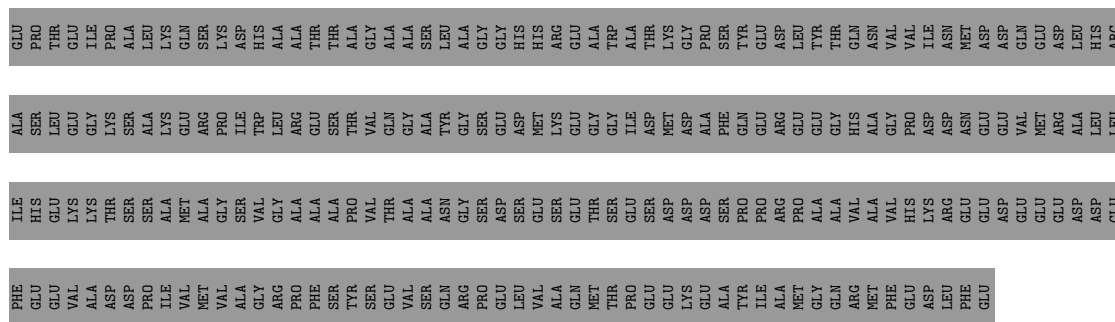


• Molecule 32: General transcription and DNA repair factor IIH helicase subunit XPD

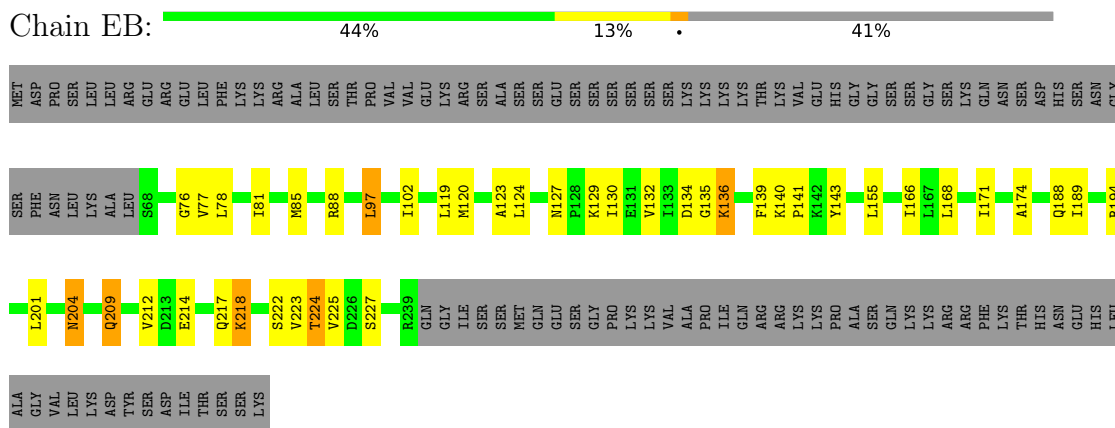


• Molecule 33: General transcription factor IIE subunit 1

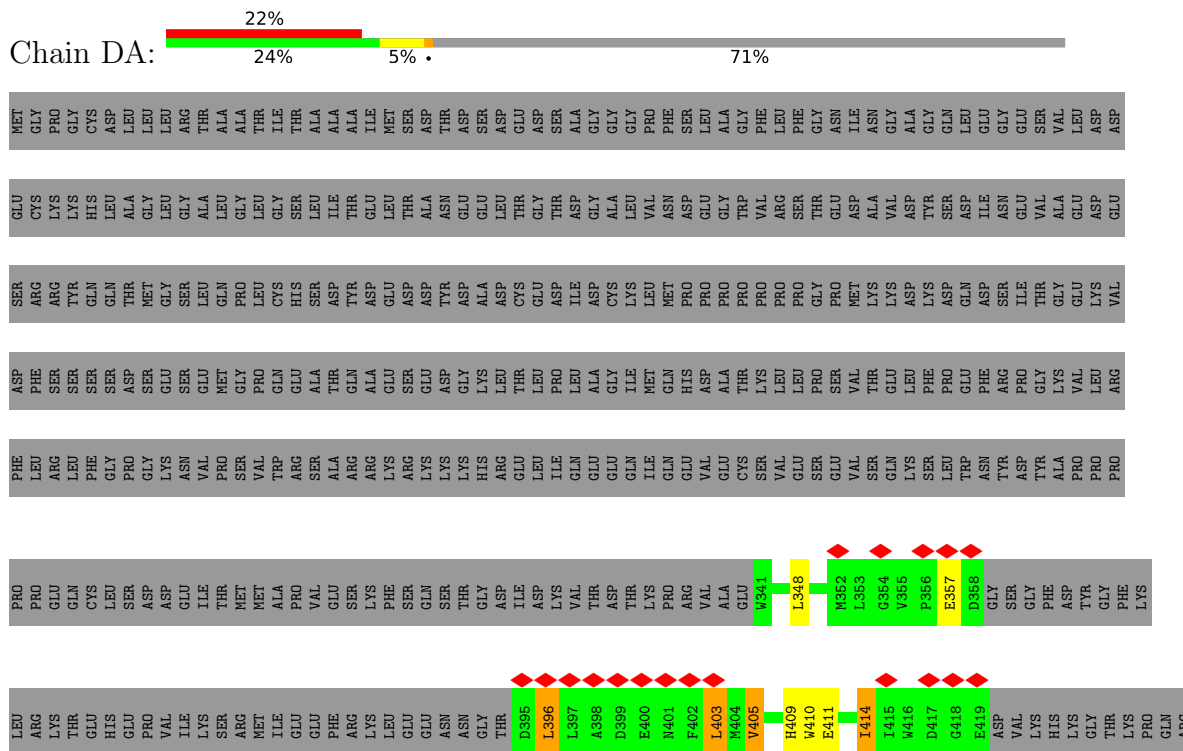




- Molecule 34: Transcription initiation factor IIE subunit beta

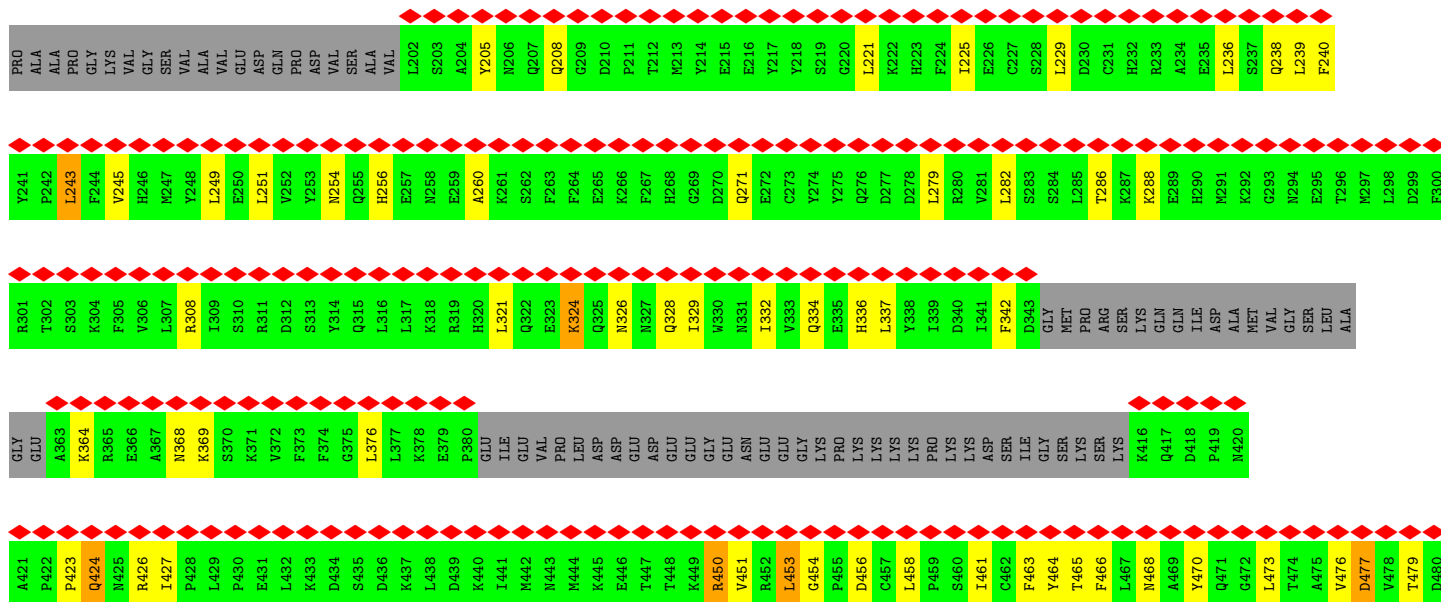


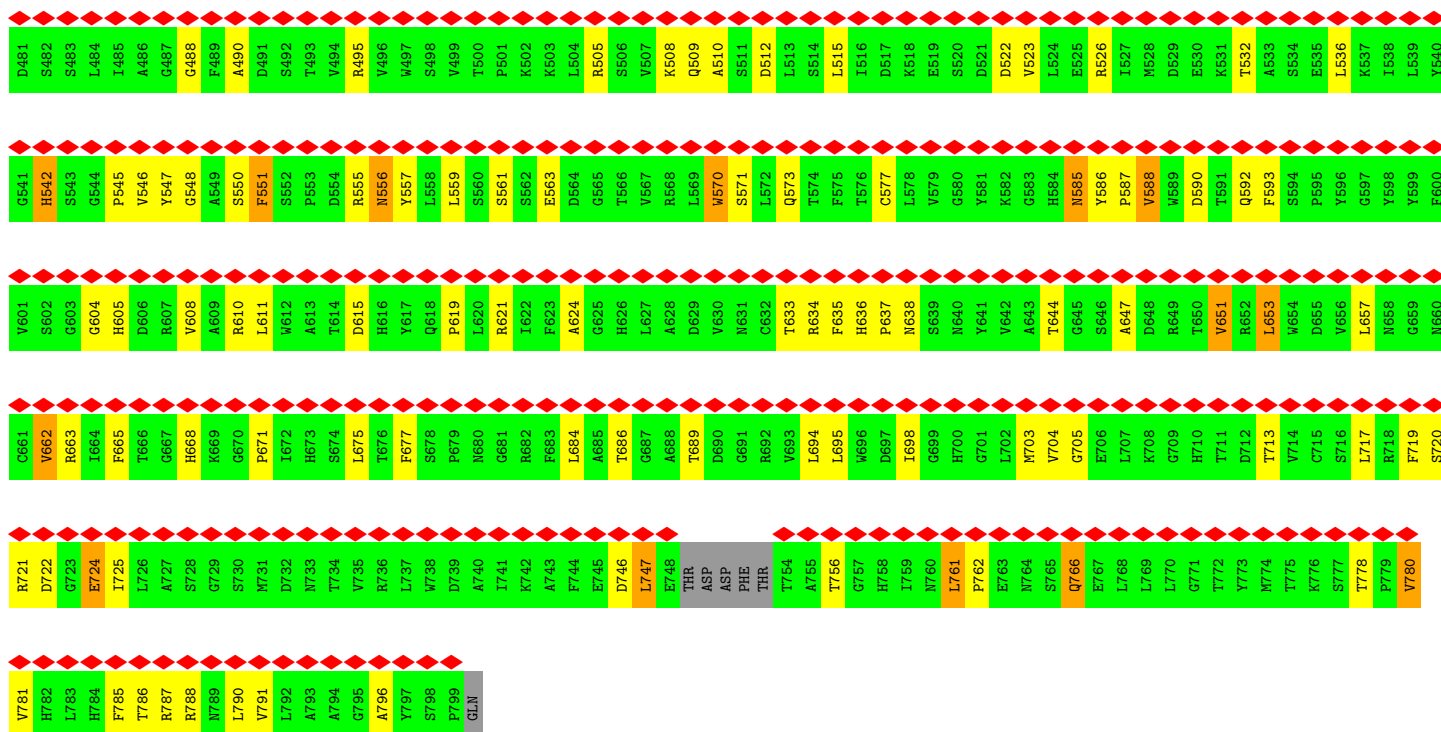
- Molecule 35: Transcription initiation factor TFIID subunit 1



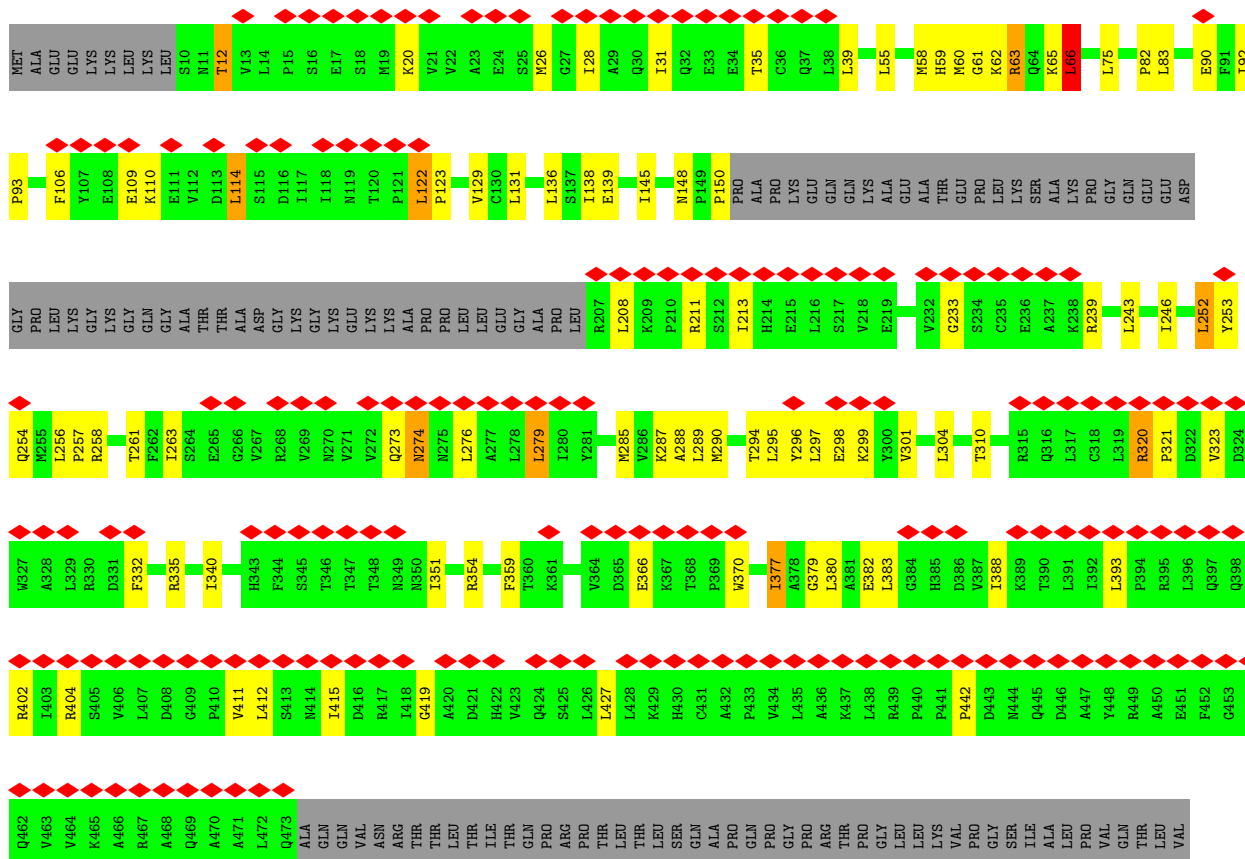








• Molecule 39: Transcription initiation factor TFIID subunit 6



PRO	SER	LEU	ILE	GLY	SER	LYS	ASN	ILE	LEU	ILE	THR	THR	ASN	MET	SER	SER	GLN	ASN	THR	ALA	ALA	GLU	SER	SER	ASN	ASN	ALA	LEU	LYS	ARG	LYS	ARG	ARG	GLU	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	TYR	ASP	ASN	LEU
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

Chain Di:

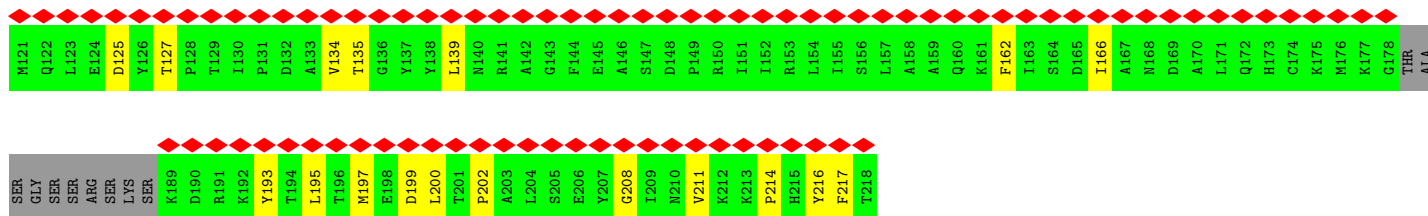
[illegible]

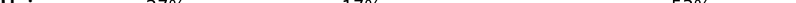
Chain DJ:

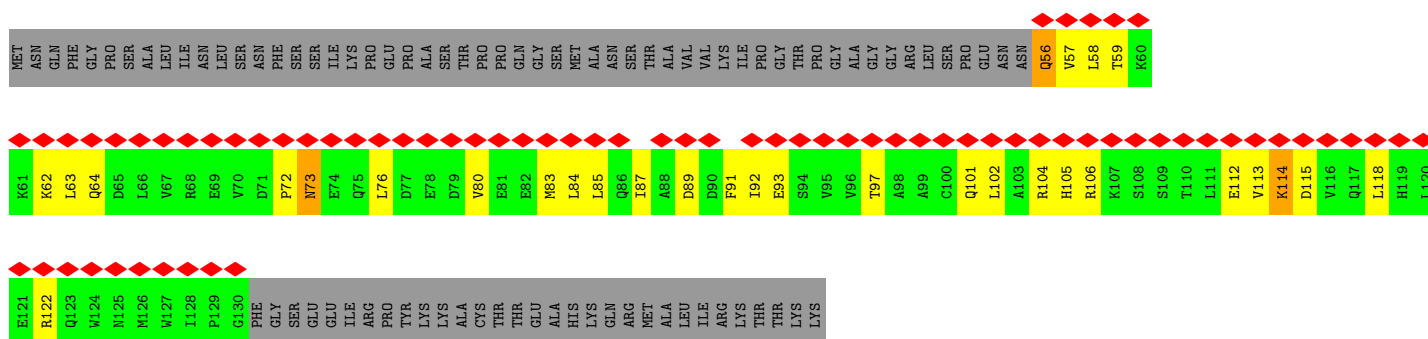
[illegible]

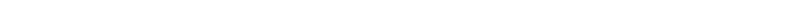
Chain Dj:

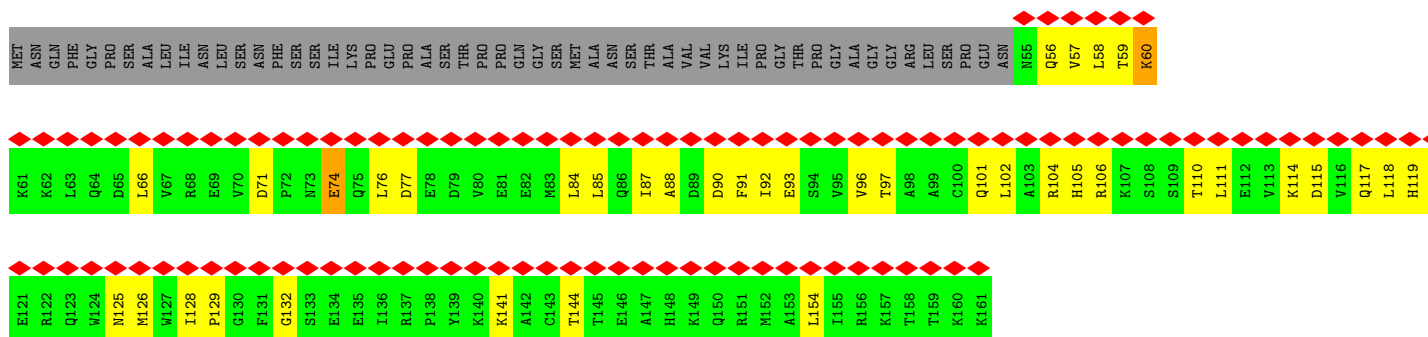
MET	SER	CYS	SER	GLY	SER	GLY	ALA	ASP	PRO	GLU	ALA	ALA	ALA	ALA	ALA	SER	SER	GLY	PRO	VAL	SER	SER	THR	ALA	ALA	ALA	GLU	ASN	LYS	ALA	SER	PRO	ALA	GLY	THR	ALA	GLY	PRO	GLY	ALA	ALA	ALA	ALA	GLY
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

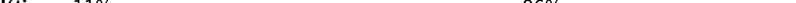


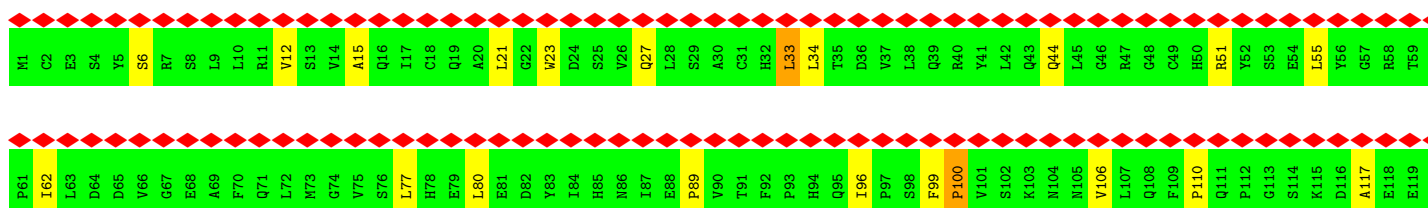
Chain DL: 

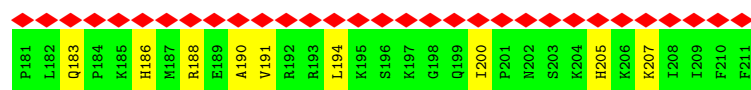


Chain DI: 

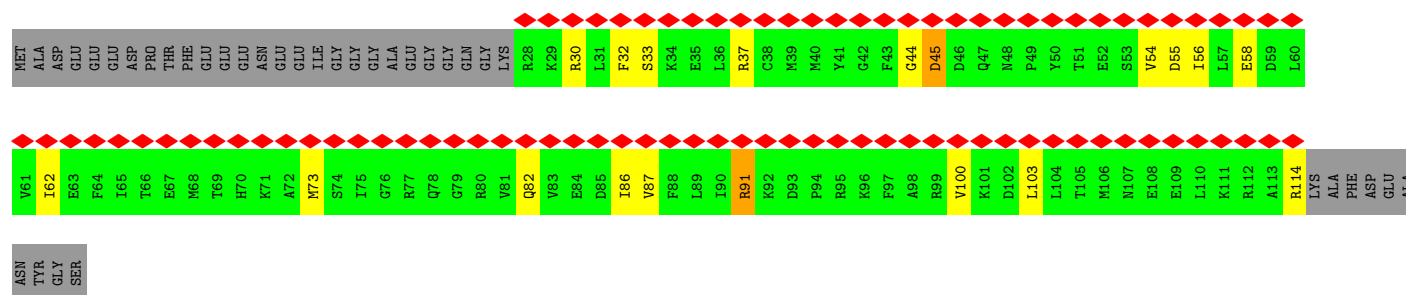


Chain Dc:  14% 11% 86%





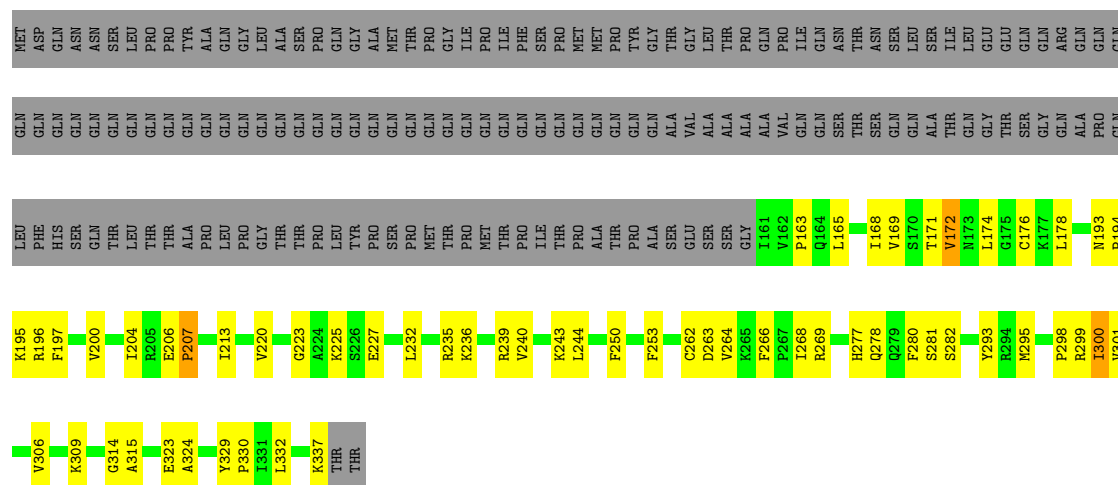
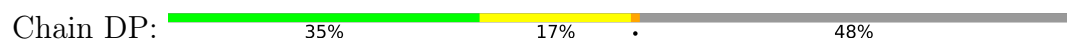
- Molecule 47: Transcription initiation factor TFIID subunit 13



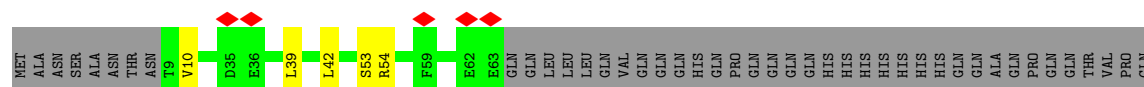
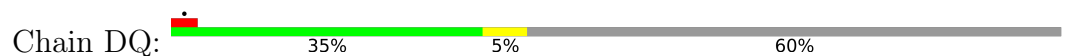
- Molecule 48: Transcription initiation factor IIA subunit 2

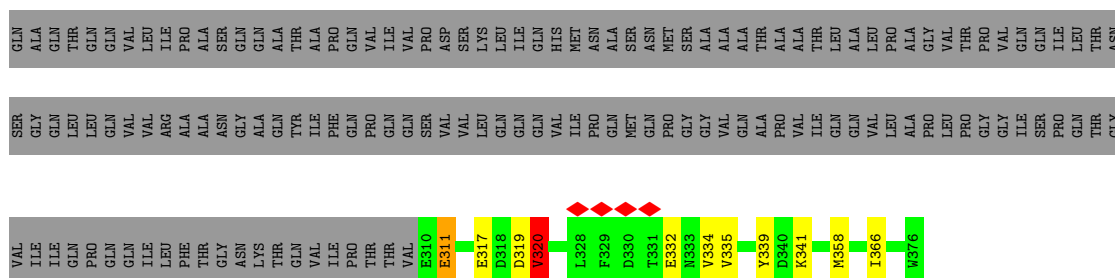


- Molecule 49: TATA-box-binding protein

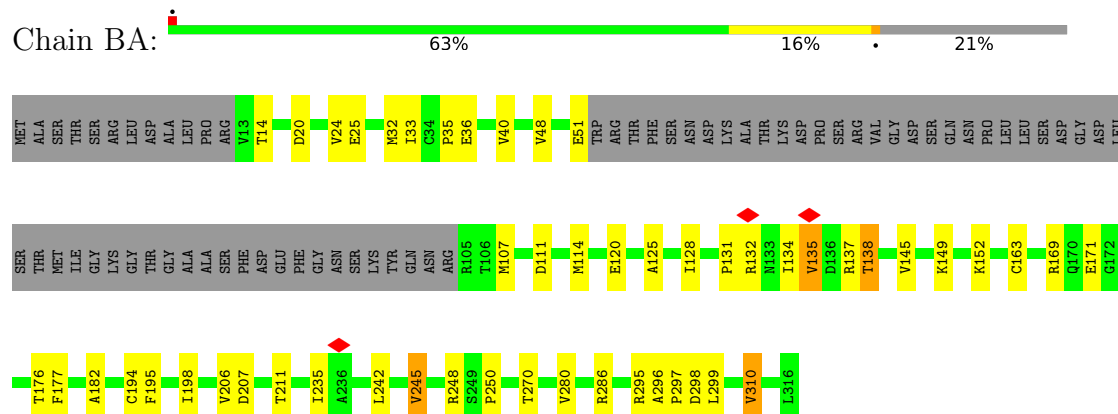


- Molecule 50: TFIIA-a

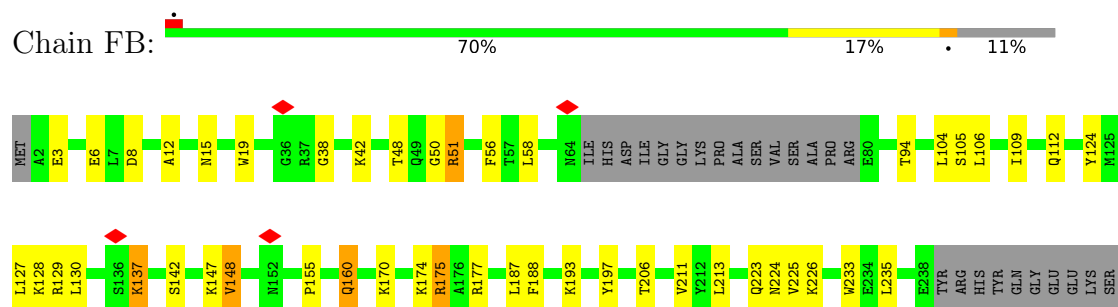




• Molecule 51: Transcription initiation factor IIB



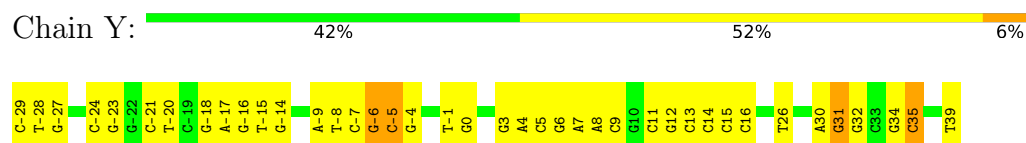
• Molecule 52: General transcription factor IIF subunit 2



• Molecule 53: DNA (69-MER)

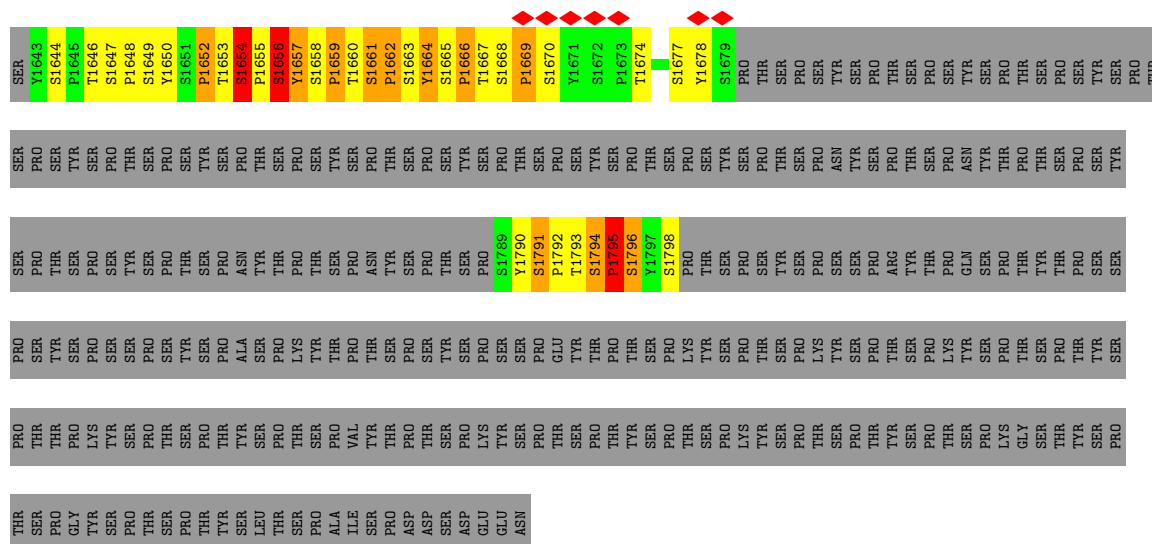


• Molecule 54: DNA (69-MER)



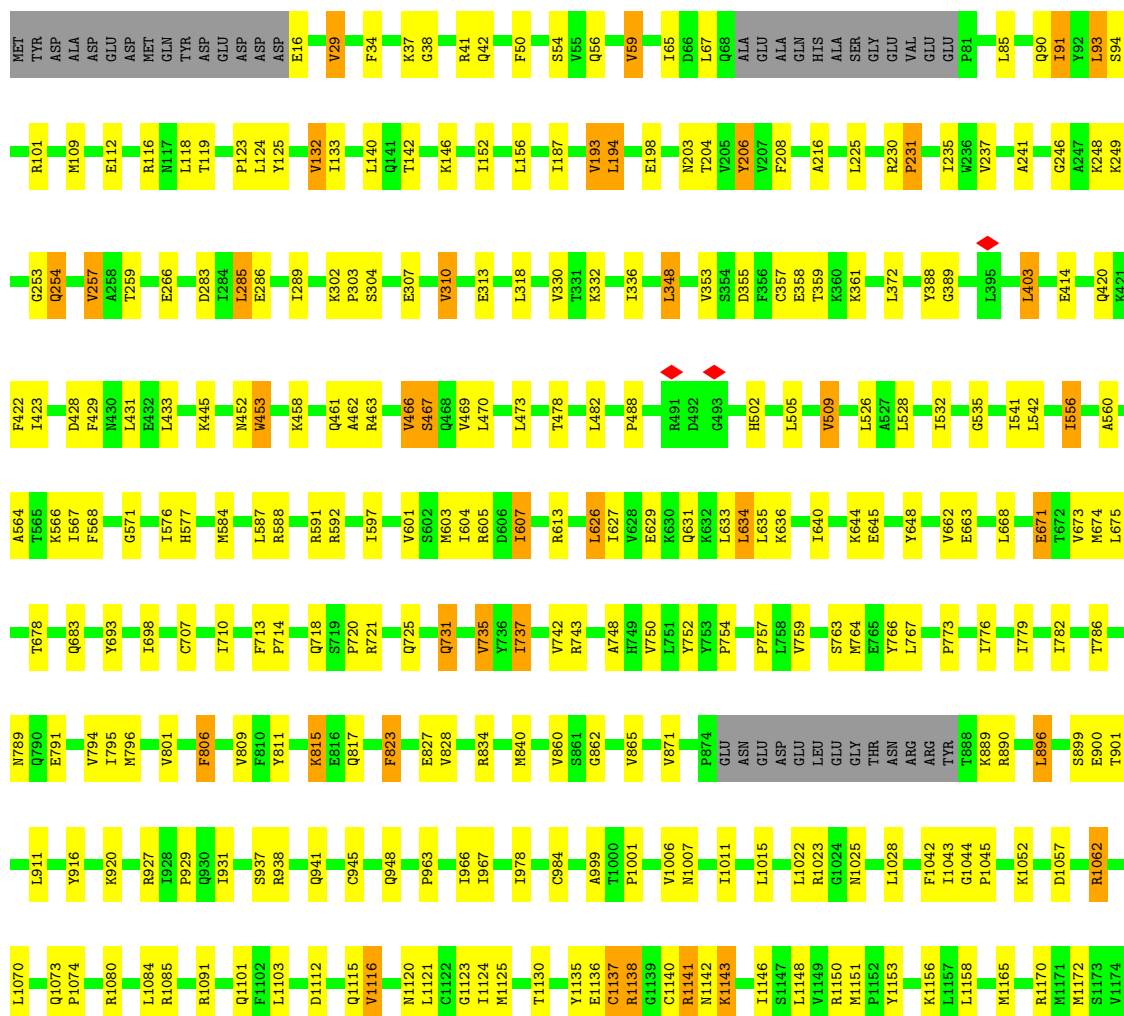
• Molecule 55: RPB1



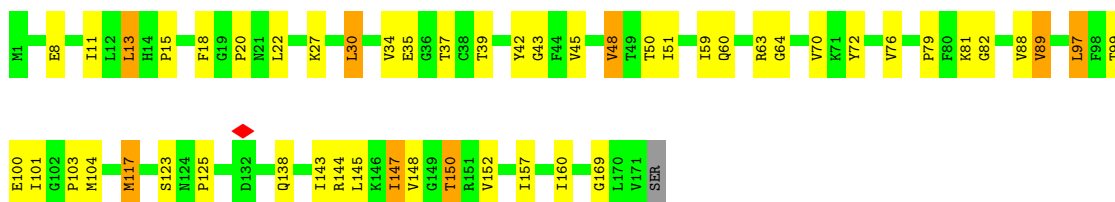


• Molecule 56: DNA-directed RNA polymerase subunit beta

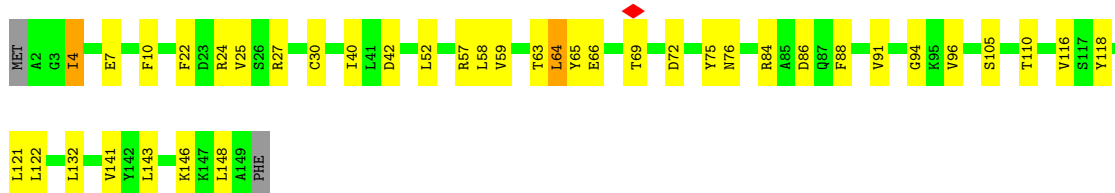
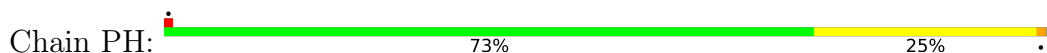
Chain PB: 73% 21%



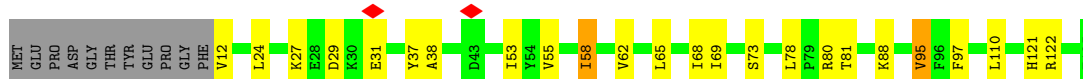




- Molecule 62: DNA-directed RNA polymerases I, II, and III subunit RPABC3



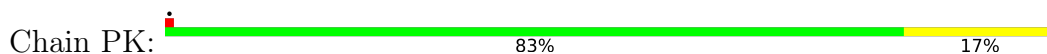
- Molecule 63: DNA-directed RNA polymerase II subunit RPB9



- Molecule 64: RPB10



- Molecule 65: RNA_pol_L_2 domain-containing protein



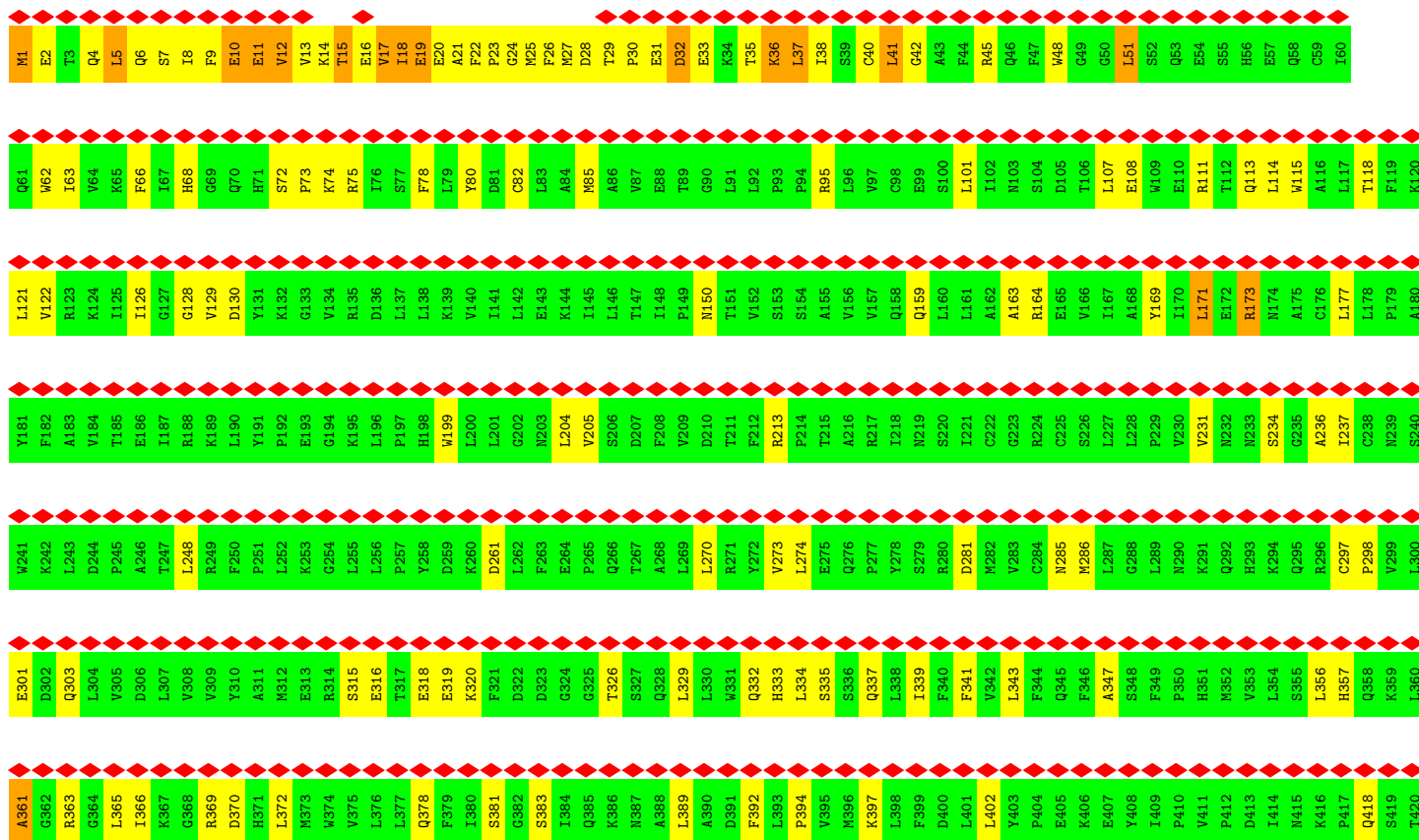
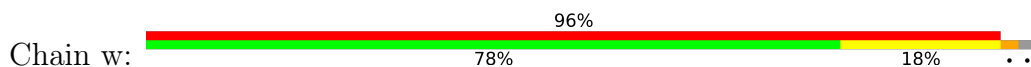
- Molecule 66: RPB12



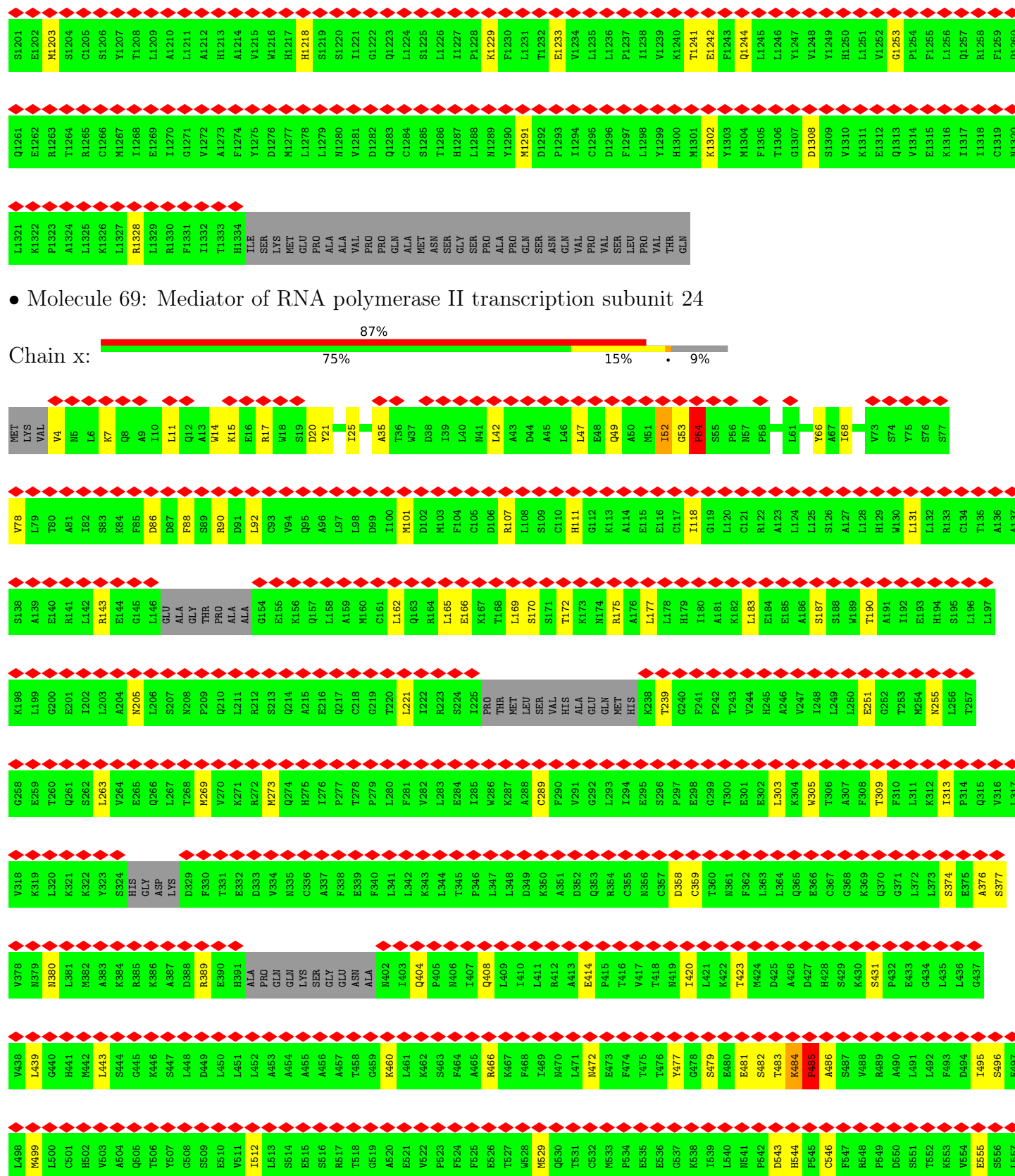
- Molecule 67: General transcription factor IIF subunit 1

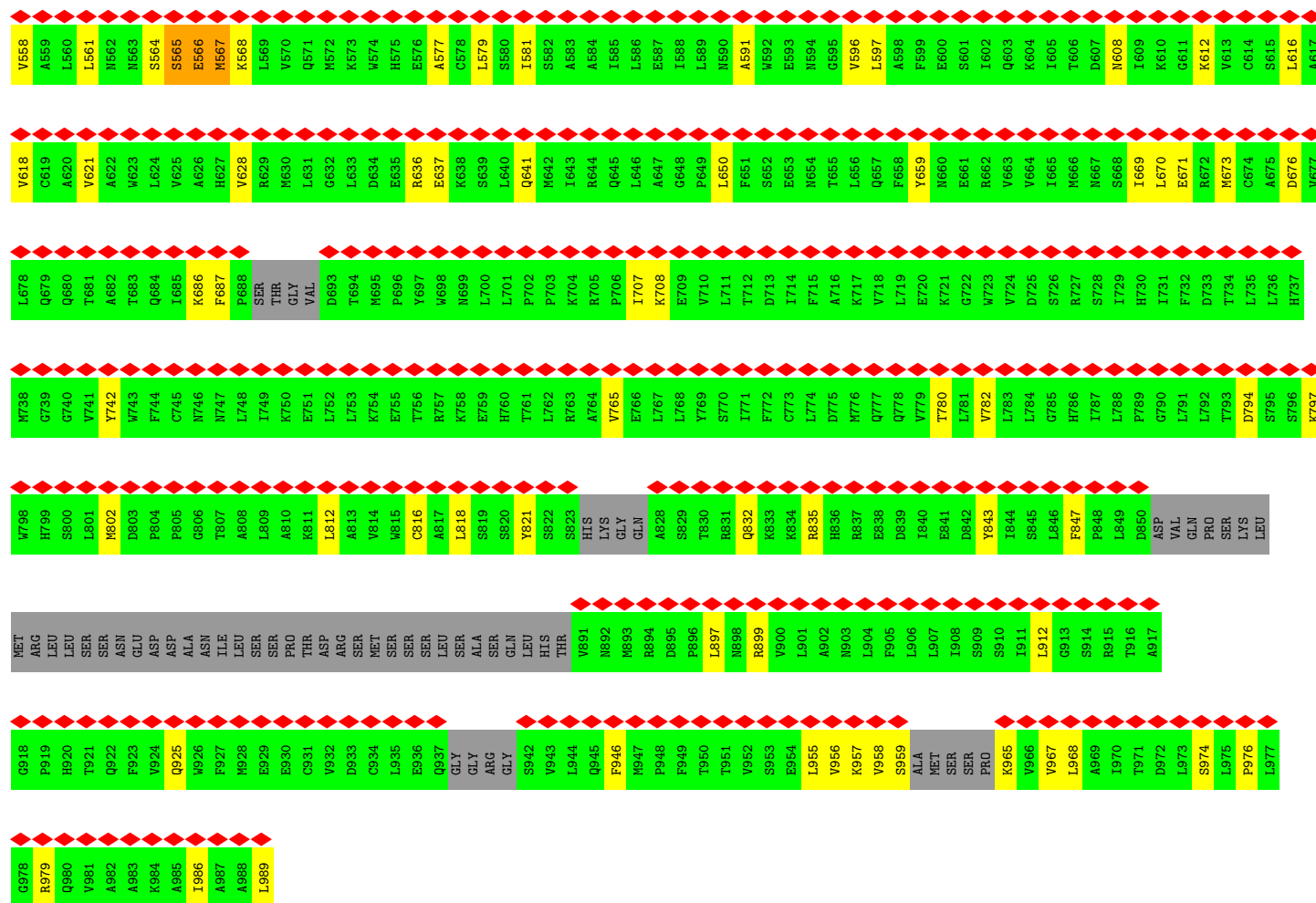


- Molecule 68: Mediator of RNA polymerase II transcription subunit 23

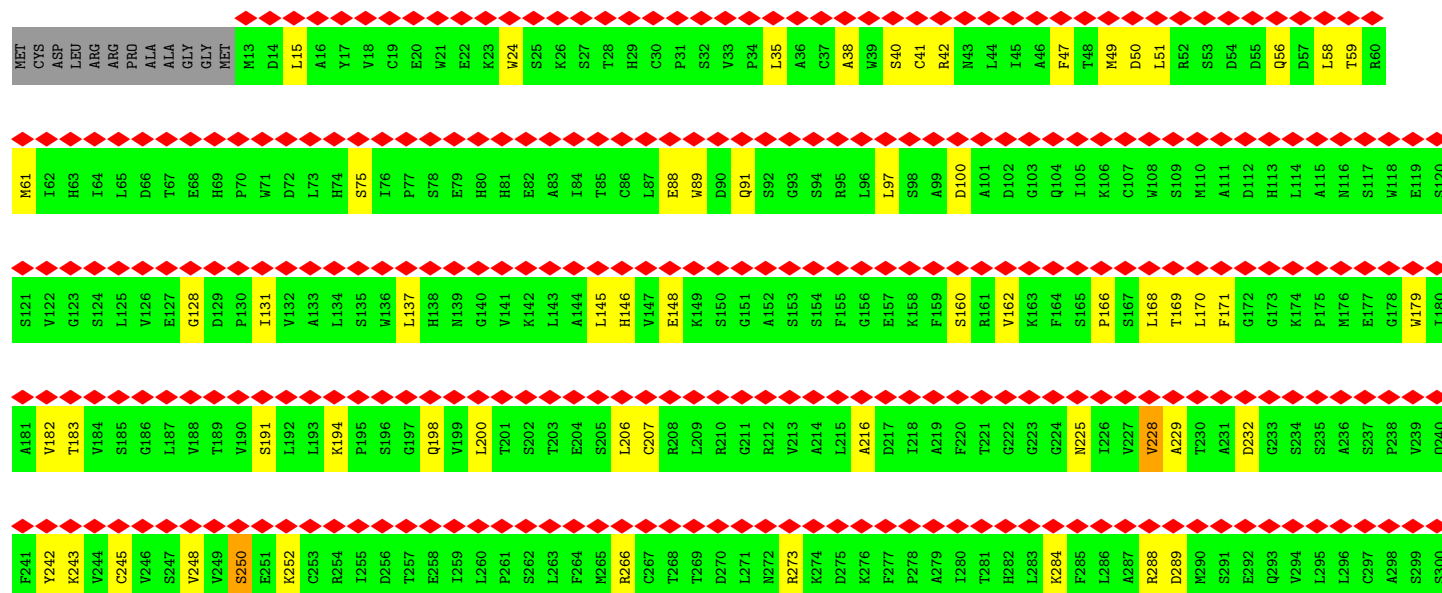
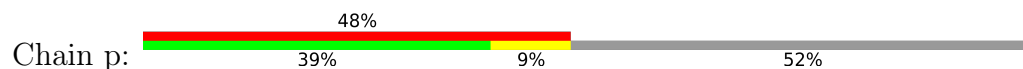


M141	G1081	F1021	S901	Q841	S781	S721	V661	L601	H541	Y481	H421
I1142	K1082	L1022	D902	Q842	M782	F722	Q662	H602	S542	S482	A422
T1143	S1083	K1023	F903	L843	Q783	T723	P663	T603	I543	T483	F423
A1144	P1084	R1024	V904	N844	G784	P724	Q664	L604	A544	N484	A424
M1145	G1085	K1025	X905	K845	S785	H725	F665	L605	T545	S485	M425
M1146	P1086	L1026	E906	C846	P786	N726	T666	E906	R546	E486	T426
N1147	F1087	V1027	N907	L847	P787	W727	R667	M607	V547	C487	C427
A1148	P1088	H1028	S908	E848	L788	A728	F668	F608	I548	F488	I428
I1149	N1089	A1029	P909	L849	F789	S729	L669	S609	K549	T489	W429
G1150	C1090	I1030	E910	L850	L790	H730	S670	Y610	A550	L490	I430
L1151	D1091	I1031	H911	N851	C791	T731	D871	R611	A551	P491	H431
I1152	W1092	G1032	Y912	D852	L792	L732	P672	M612	H552	M492	L432
T1153	R1093	L1033	L913	M853	L793	S733	K673	H613	A553	G493	N433
T1154	F1094	L1034	Q914	V854	W794	C734	T674	H614	K554	A494	R434
A1155	N1095	K1035	Y915	N855	K795	F735	V675	I615	S555	L495	K435
L1156	E1096	D1036	D916	K856	M796	P736	L676	Q616	S556	V496	A436
P1157	F1097	M1037	Y917	E857	L797	G737	S677	P617	V557	E497	Q437
E1158	P1098	R1038	H918	N858	L798	P738	A678	H618	A558	T498	N438
P1159	N1099	P1039	T919	L859	E799	L739	E579	Y619	L559	I499	D439
Y1160	P1100	Q1040	K920	V860	T800	Q740	S680	R620	A560	Y500	N440
W1161	A1101	G1041	H921	T861	D801	A741	E881	R621	P661	G501	S441
I1162	A1102	W1042	Y922	L862	H802	F742	E682	Q622	A562	N502	K442
V1163	H1103	C1043	N923	D863	L803	F743	L683	L623	L563	G503	L443
L1164	A1104	L1044	Y924	R864	N804	K744	N684	L624	V564	I504	Q444
H1165	L1105	S1045	H925	L865	Q805	Q745	R685	S625	E565	M505	I445
D1166	H1106	D1046	K926	T866	L806	N746	A686	H626	T566	R506	P446
A1167	V1107	T1047	X927	L867	G807	N747	L687	L627	Y567	I507	I447
T1168	T1108	Y1048	Y928	C868	Y808	V748	I688	H628	S568	P508	P448
V1169	C1109	L1049	P929	L869	R809	P749	L689	T629	R569	H449	H449
S1170	V1110	K1050	E930	A870	V610	Q750	T690	L630	L570	P510	S450
V1171	E1111	C1051	X931	M871	L811	E751	L691	A631	L571	G511	L451
I1172	L1112	A1052	L932	R872	E812	S752	A692	A632	V572	T512	R452
S1173	M1113	M1053	Y833	S873	R613	R753	R693	V633	Y573	N513	L453
T1174	A1114	L1054	F934	H874	L814	F754	A694	A634	M574	C514	H454
P1175	L1115	A1055	E935	E875	G815	N755	T695	Q635	E575	M515	H455
S1176	V1116	R1056	G936	G876	A816	L756	H696	T636	I576	A516	E456
L1177	E1057	E1057	L937	N877	R617	K757	V697	M637	E577	S517	F457
T1178	S1118	E1058	A938	E878	A818	K758	T698	Q638	S578	G518	L458
S1179	G1119	M1059	E939	A879	L819	N759	D699	M639	L579	S519	Q459
E1180	K1120	P1060	Q940	Q880	V620	V760	F700	Q640	G580	I520	Q460
T1181	E1121	W1061	Y941	V881	A821	E761	F701	L641	I581	T521	S461
I1182	V1122	V1062	D942	C882	H822	E762	T702	H642	K582	P522	L462
W1183	G1123	P1063	P943	Y883	V623	E763	G703	L643	G583	L523	R463
V1184	N1124	D1064	P944	F884	R624	W764	S704	C644	F584	P524	N464
K1185	A1125	L1065	Y945	L885	T625	R765	D705	V645	I585	M525	K465
Y1186	L1126	Y1066	Q946	T886	R626	K766	S706	E546	S586	M526	K466
P1187	L1127	Y1067	I947	Q887	A827	W767	T707	S947	Q587	L527	L467
F1188	N1128	Y1068	Q948	L888	D828	K768	Q708	T648	L588	L528	Q468
A1189	V1129	C1069	S949	L889	F829	S769	G709	A649	L589	D529	M469
L1190	H1070	R1070	P950	L890	L830	M770	T710	L650	P590	S530	N470
F1191	L1131	L1071	Y951	L891	V631	S771	W711	R651	T591	L531	D471
D1192	K1132	I1072	L952	K892	Y832	N772	C712	L652	V592	T532	Y472
F1193	G1073	G1073	P953	P893	E833	E773	K713	I653	F993	V533	K473
T1194	T1074	R1074	L954	N894	F834	N774	D714	T654	K594	H534	I474
A1195	P1135	L1075	Y955	D895	S835	D775	I715	A655	S595	A535	A475
C1196	H1076	V1076	F956	F896	T636	L776	L716	L656	H596	K536	L476
L1197	V1137	D1077	G957	R897	S837	I777	Q717	G657	A597	M537	L477
Q1198	P1138	T1078	N958	R898	A838	T778	T718	S658	W598	L539	C478
S1199	R1139	M1079	Y959	R899	G839	H779	I719	S659	G599	I540	N479
Y1200	E1140	A1080	C960	V900	G840	F780	M720	E560	I600		A480





• Molecule 70: Isoform 2 of Mediator of RNA polymerase II transcription subunit 16



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	67732	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	7.867	Depositor
Minimum map value	-3.734	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.101	Depositor
Recommended contour level	0.41	Depositor
Map size ($\text{\AA}$)	674.39996, 674.39996, 674.39996	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.405, 1.405, 1.405	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	a	0.98	3/3645 (0.1%)	1.37	15/4952 (0.3%)
2	m	0.19	0/1010	0.38	0/1359
3	d	0.97	0/1277	1.50	11/1714 (0.6%)
4	f	0.76	0/1359	1.04	4/1845 (0.2%)
5	g	0.94	0/1411	1.38	2/1901 (0.1%)
6	h	0.94	1/1507 (0.1%)	1.31	2/2036 (0.1%)
7	r	0.94	1/1558 (0.1%)	1.27	5/2096 (0.2%)
8	t	1.05	2/1530 (0.1%)	1.54	20/2066 (1.0%)
9	j	0.55	1/1016 (0.1%)	0.91	6/1363 (0.4%)
10	k	0.96	0/885	1.26	0/1190
11	n	0.45	2/7371 (0.0%)	0.73	20/10037 (0.2%)
12	q	0.67	2/4336 (0.0%)	0.89	4/5865 (0.1%)
13	s	0.73	0/489	1.27	8/663 (1.2%)
14	u	0.68	0/797	1.12	5/1082 (0.5%)
15	v	1.00	2/1092 (0.2%)	1.58	8/1468 (0.5%)
16	z	0.92	0/781	1.39	5/1067 (0.5%)
17	c	0.51	0/2106	0.79	3/2842 (0.1%)
18	e	0.18	0/840	0.34	0/1128
19	b	0.75	0/911	1.08	0/1229
20	l	0.18	0/1048	0.36	0/1405
21	o	0.39	0/1256	0.76	2/1724 (0.1%)
22	i	0.98	1/523 (0.2%)	1.25	0/692
23	0	0.99	0/2288	1.27	4/3101 (0.1%)
24	8	0.97	0/2437	1.19	1/3306 (0.0%)
25	9	0.95	0/2356	1.23	1/3185 (0.0%)
26	1	1.06	0/2674	1.28	7/3660 (0.2%)
27	2	1.00	0/2588	1.18	2/3509 (0.1%)
28	3	0.99	0/2102	1.17	0/2844
29	4	0.97	0/3663	1.18	2/4965 (0.0%)
30	5	0.99	0/433	1.22	0/585
31	6	0.97	0/4983	1.18	1/6731 (0.0%)
32	7	0.97	0/5957	1.19	3/8071 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	EA	0.95	1/1499 (0.1%)	1.21	2/2012 (0.1%)
34	EB	0.96	0/1428	1.21	0/1917
35	DA	0.96	0/4627	1.17	3/6248 (0.0%)
36	DB	0.97	0/7993	1.16	5/10836 (0.0%)
37	DD	0.94	0/1343	1.22	2/1795 (0.1%)
37	Dd	0.95	0/1321	1.17	0/1772
38	DE	0.98	0/4469	1.19	3/6050 (0.0%)
38	De	0.98	0/4433	1.18	2/6004 (0.0%)
39	DF	1.00	0/3167	1.22	1/4303 (0.0%)
39	Df	1.00	0/3140	1.21	1/4268 (0.0%)
40	DG	1.00	0/1199	1.15	0/1612
41	DH	0.99	0/1673	1.18	0/2285
42	DI	0.98	0/981	1.20	0/1332
42	Di	0.95	0/989	1.18	0/1343
43	DJ	0.94	0/736	1.18	0/998
43	Dj	0.93	0/775	1.19	0/1049
44	DL	0.94	0/622	1.23	0/841
44	DI	0.95	0/888	1.22	1/1194 (0.1%)
45	Dc	0.98	0/1035	1.16	0/1406
46	Dk	0.96	0/799	1.19	1/1070 (0.1%)
47	Dm	0.94	0/733	1.20	0/977
48	DO	1.00	0/781	1.20	0/1061
49	DP	0.98	0/1438	1.14	0/1935
50	DQ	0.96	0/1013	1.19	0/1366
51	BA	0.98	0/1967	1.21	0/2656
52	FB	0.98	0/1817	1.17	1/2445 (0.0%)
53	X	0.73	4/1607 (0.2%)	0.69	6/2481 (0.2%)
54	Y	0.57	0/1565	0.73	5/2410 (0.2%)
55	PA	0.99	0/11881	1.21	8/16057 (0.0%)
56	PB	0.99	0/9243	1.17	4/12475 (0.0%)
57	PC	1.00	0/2102	1.17	0/2857
58	PD	0.97	0/1036	1.20	0/1397
59	PE	0.97	0/1751	1.18	0/2366
60	PF	0.95	0/645	1.20	1/871 (0.1%)
61	PG	1.02	0/1365	1.18	1/1853 (0.1%)
62	PH	0.99	0/1207	1.14	0/1628
63	PI	0.99	0/948	1.15	1/1284 (0.1%)
64	PJ	0.96	0/516	1.19	0/696
65	PK	0.96	0/956	1.16	0/1294
66	PL	0.98	0/377	1.07	0/500
67	FA	0.96	0/1130	1.13	0/1528
68	w	0.56	0/11053	0.73	8/15018 (0.1%)
69	x	0.57	0/7179	0.72	5/9712 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
70	p	0.72	0/3191	0.78	0/4333
All	All	0.89	20/174847 (0.0%)	1.11	202/237216 (0.1%)

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	X	-39	DA	O3'-P	-13.42	1.41	1.61
12	q	452	ALA	C-N	9.04	1.46	1.33
7	r	174	VAL	C-O	-8.00	1.15	1.24
9	j	94	GLN	C-N	-7.89	1.24	1.33
1	a	57	HIS	C-O	7.62	1.32	1.24

The worst 5 of 202 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	d	161	VAL	N-CA-C	-12.81	100.00	112.17
3	d	130	GLU	N-CA-C	-11.44	98.89	111.36
54	Y	35	DC	C2'-C3'-O3'	-10.79	95.32	111.50
8	t	11	VAL	N-CA-C	-9.86	100.96	110.42
9	j	77	PRO	CA-N-CD	-9.34	98.92	112.00

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	3570	0	3480	309	0
2	m	983	0	967	231	0
3	d	1264	0	1293	227	0
4	f	1329	0	1302	173	0
5	g	1382	0	1410	307	0
6	h	1486	0	1500	230	0
7	r	1528	0	1538	139	0
8	t	1499	0	1482	132	0
9	j	1001	0	1021	364	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	k	879	0	886	200	0
11	n	7241	0	6673	623	0
12	q	4261	0	4237	508	0
13	s	485	0	352	101	0
14	u	792	0	749	231	0
15	v	1083	0	1059	169	0
16	z	765	0	727	162	0
17	c	2069	0	2079	101	0
18	e	832	0	824	112	0
19	b	899	0	908	110	0
20	l	1040	0	1065	81	0
21	o	1221	0	1212	125	0
22	i	520	0	545	46	0
23	0	2255	0	2007	81	0
24	8	2378	0	2397	79	0
25	9	2307	0	2314	34	0
26	1	2634	0	2042	38	0
27	2	2534	0	2455	33	0
28	3	2065	0	2098	33	0
29	4	3579	0	3620	67	0
30	5	428	0	434	11	0
31	6	4880	0	4924	66	0
32	7	5833	0	5798	72	0
33	EA	1476	0	1489	41	0
34	EB	1404	0	1424	26	0
35	DA	4511	0	4429	44	0
36	DB	7796	0	7751	213	0
37	DD	1330	0	1351	27	0
37	Dd	1307	0	1318	51	0
38	DE	4364	0	4244	86	0
38	De	4327	0	4197	77	0
39	DF	3109	0	3045	57	0
39	Df	3081	0	3012	58	0
40	DG	1180	0	1235	19	0
41	DH	1633	0	1621	27	0
42	DI	959	0	969	28	0
42	Di	967	0	977	25	0
43	DJ	720	0	719	12	0
43	Dj	759	0	759	19	0
44	DL	614	0	614	86	0
44	DI	876	0	893	91	0
45	Dc	1011	0	975	19	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	Dk	785	0	818	18	0
47	Dm	724	0	744	14	0
48	DO	771	0	764	9	0
49	DP	1412	0	1506	42	0
50	DQ	996	0	926	8	0
51	BA	1939	0	1979	29	0
52	FB	1788	0	1819	27	0
53	X	1429	0	770	120	0
54	Y	1400	0	775	90	0
55	PA	11655	0	11726	248	0
56	PB	9062	0	9107	131	0
57	PC	2059	0	2008	33	0
58	PD	1021	0	979	33	0
59	PE	1720	0	1737	25	0
60	PF	635	0	665	16	0
61	PG	1334	0	1333	39	0
62	PH	1186	0	1147	19	0
63	PI	927	0	859	9	0
64	PJ	507	0	523	4	0
65	PK	937	0	959	13	0
66	PL	372	0	379	4	0
67	FA	1101	0	1065	20	0
68	w	10772	0	10832	335	0
69	x	7050	0	7203	154	0
70	p	3124	0	3133	62	0
71	0	2	0	0	2	0
71	2	3	0	0	0	0
71	3	1	0	0	0	0
71	BA	1	0	0	0	0
71	EA	1	0	0	0	0
71	PA	2	0	0	0	0
71	PB	1	0	0	0	0
71	PC	1	0	0	0	0
71	PI	2	0	0	0	0
71	PJ	1	0	0	0	0
71	PL	1	0	0	0	0
72	7	8	0	0	0	0
73	PA	1	0	0	0	0
All	All	171177	0	168176	5753	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 17.

The worst 5 of 5753 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)
33:EA:129:CYS:SG	33:EA:131:VAL:HG23	1.29	1.73
3:d:121:LEU:CD1	5:g:160:VAL:HG21	1.18	1.64
68:w:394:PRO:HA	70:p:171:PHE:CZ	1.29	1.63
3:d:121:LEU:HD11	5:g:160:VAL:CG2	1.21	1.62
9:j:82:LYS:HG2	13:s:96:PHE:CD1	1.17	1.62

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a	457/1581 (29%)	421 (92%)	29 (6%)	7 (2%)	8	38
2	m	110/131 (84%)	106 (96%)	4 (4%)	0	100	100
3	d	154/270 (57%)	143 (93%)	6 (4%)	5 (3%)	3	24
4	f	163/246 (66%)	142 (87%)	15 (9%)	6 (4%)	2	22
5	g	164/233 (70%)	145 (88%)	10 (6%)	9 (6%)	1	17
6	h	188/268 (70%)	167 (89%)	12 (6%)	9 (5%)	2	18
7	r	189/208 (91%)	176 (93%)	10 (5%)	3 (2%)	7	37
8	t	189/212 (89%)	166 (88%)	15 (8%)	8 (4%)	2	20
9	j	120/135 (89%)	110 (92%)	6 (5%)	4 (3%)	3	24
10	k	110/117 (94%)	99 (90%)	9 (8%)	2 (2%)	6	34
11	n	980/1454 (67%)	877 (90%)	86 (9%)	17 (2%)	7	36
12	q	540/651 (83%)	474 (88%)	53 (10%)	13 (2%)	4	29
13	s	69/244 (28%)	60 (87%)	7 (10%)	2 (3%)	3	26
14	u	103/144 (72%)	93 (90%)	8 (8%)	2 (2%)	6	33

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	v	132/200 (66%)	119 (90%)	10 (8%)	3 (2%)	5	30
16	z	93/600 (16%)	84 (90%)	7 (8%)	2 (2%)	5	31
17	c	245/311 (79%)	232 (95%)	13 (5%)	0	100	100
18	e	98/178 (55%)	92 (94%)	4 (4%)	2 (2%)	6	33
19	b	111/200 (56%)	109 (98%)	1 (1%)	1 (1%)	14	48
20	l	120/178 (67%)	115 (96%)	5 (4%)	0	100	100
21	o	152/788 (19%)	138 (91%)	10 (7%)	4 (3%)	4	28
22	i	56/146 (38%)	54 (96%)	1 (2%)	1 (2%)	6	34
23	0	304/309 (98%)	285 (94%)	15 (5%)	4 (1%)	9	41
24	8	297/346 (86%)	290 (98%)	7 (2%)	0	100	100
25	9	285/323 (88%)	279 (98%)	6 (2%)	0	100	100
26	1	399/548 (73%)	336 (84%)	53 (13%)	10 (2%)	4	29
27	2	327/395 (83%)	315 (96%)	10 (3%)	2 (1%)	21	58
28	3	259/308 (84%)	257 (99%)	2 (1%)	0	100	100
29	4	447/462 (97%)	431 (96%)	12 (3%)	4 (1%)	14	48
30	5	52/71 (73%)	50 (96%)	2 (4%)	0	100	100
31	6	602/782 (77%)	585 (97%)	14 (2%)	3 (0%)	24	61
32	7	732/760 (96%)	704 (96%)	23 (3%)	5 (1%)	18	54
33	EA	175/439 (40%)	163 (93%)	12 (7%)	0	100	100
34	EB	170/291 (58%)	161 (95%)	4 (2%)	5 (3%)	3	26
35	DA	534/1872 (28%)	523 (98%)	9 (2%)	2 (0%)	30	65
36	DB	959/1199 (80%)	932 (97%)	25 (3%)	2 (0%)	43	76
37	DD	153/1085 (14%)	148 (97%)	4 (3%)	1 (1%)	18	54
37	Dd	154/1085 (14%)	152 (99%)	2 (1%)	0	100	100
38	DE	540/800 (68%)	524 (97%)	16 (3%)	0	100	100
38	De	531/800 (66%)	514 (97%)	16 (3%)	1 (0%)	43	76
39	DF	404/677 (60%)	393 (97%)	9 (2%)	2 (0%)	24	61
39	Df	399/677 (59%)	394 (99%)	4 (1%)	1 (0%)	36	70
40	DG	139/349 (40%)	137 (99%)	2 (1%)	0	100	100
41	DH	207/310 (67%)	199 (96%)	5 (2%)	3 (1%)	9	39
42	DI	118/264 (45%)	116 (98%)	1 (1%)	1 (1%)	16	52

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	Di	119/264 (45%)	118 (99%)	1 (1%)	0	100	100
43	DJ	86/218 (39%)	84 (98%)	2 (2%)	0	100	100
43	Dj	91/218 (42%)	90 (99%)	1 (1%)	0	100	100
44	DL	73/161 (45%)	68 (93%)	2 (3%)	3 (4%)	2	20
44	DI	105/161 (65%)	104 (99%)	0	1 (1%)	12	46
45	Dc	125/929 (14%)	122 (98%)	1 (1%)	2 (2%)	7	37
46	Dk	96/211 (46%)	93 (97%)	3 (3%)	0	100	100
47	Dm	85/124 (68%)	82 (96%)	3 (4%)	0	100	100
48	DO	95/109 (87%)	91 (96%)	2 (2%)	2 (2%)	5	32
49	DP	175/339 (52%)	170 (97%)	4 (2%)	1 (1%)	21	58
50	DQ	118/307 (38%)	115 (98%)	2 (2%)	1 (1%)	16	52
51	BA	247/316 (78%)	244 (99%)	3 (1%)	0	100	100
52	FB	218/249 (88%)	210 (96%)	7 (3%)	1 (0%)	24	61
55	PA	1460/1970 (74%)	1415 (97%)	38 (3%)	7 (0%)	24	61
56	PB	1128/1174 (96%)	1104 (98%)	22 (2%)	2 (0%)	43	76
57	PC	253/275 (92%)	252 (100%)	1 (0%)	0	100	100
58	PD	127/142 (89%)	127 (100%)	0	0	100	100
59	PE	207/210 (99%)	204 (99%)	2 (1%)	1 (0%)	24	61
60	PF	77/127 (61%)	76 (99%)	0	1 (1%)	9	41
61	PG	169/172 (98%)	165 (98%)	4 (2%)	0	100	100
62	PH	146/150 (97%)	144 (99%)	2 (1%)	0	100	100
63	PI	112/125 (90%)	111 (99%)	1 (1%)	0	100	100
64	PJ	62/67 (92%)	61 (98%)	1 (2%)	0	100	100
65	PK	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
66	PL	42/58 (72%)	42 (100%)	0	0	100	100
67	FA	130/517 (25%)	126 (97%)	4 (3%)	0	100	100
68	w	1332/1368 (97%)	1261 (95%)	65 (5%)	6 (0%)	24	61
69	x	876/989 (89%)	820 (94%)	51 (6%)	5 (1%)	21	58
70	p	400/841 (48%)	367 (92%)	32 (8%)	1 (0%)	36	70
All	All	20999/34555 (61%)	19990 (95%)	829 (4%)	180 (1%)	16	48

5 of 180 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	a	67	LYS
1	a	331	GLU
4	f	25	ASN
4	f	35	GLU
4	f	36	ARG

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	387/1391 (28%)	322 (83%)	65 (17%)	2	12
2	m	102/115 (89%)	102 (100%)	0	100	100
3	d	138/230 (60%)	98 (71%)	40 (29%)	0	3
4	f	144/223 (65%)	122 (85%)	22 (15%)	3	14
5	g	157/215 (73%)	126 (80%)	31 (20%)	1	9
6	h	168/225 (75%)	126 (75%)	42 (25%)	0	4
7	r	168/183 (92%)	126 (75%)	42 (25%)	0	4
8	t	166/178 (93%)	136 (82%)	30 (18%)	2	11
9	j	113/124 (91%)	108 (96%)	5 (4%)	25	48
10	k	94/98 (96%)	45 (48%)	49 (52%)	0	0
11	n	689/1272 (54%)	654 (95%)	35 (5%)	21	44
12	q	461/577 (80%)	383 (83%)	78 (17%)	2	12
13	s	31/208 (15%)	27 (87%)	4 (13%)	4	18
14	u	78/119 (66%)	66 (85%)	12 (15%)	2	14
15	v	122/173 (70%)	88 (72%)	34 (28%)	0	3
16	z	89/512 (17%)	74 (83%)	15 (17%)	2	12
17	c	231/280 (82%)	225 (97%)	6 (3%)	40	60
18	e	94/152 (62%)	94 (100%)	0	100	100
19	b	102/163 (63%)	92 (90%)	10 (10%)	7	26
20	l	116/155 (75%)	116 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	o	141/697 (20%)	139 (99%)	2 (1%)	59	71
22	i	61/133 (46%)	42 (69%)	19 (31%)	0	2
23	0	209/283 (74%)	194 (93%)	15 (7%)	13	36
24	8	259/299 (87%)	225 (87%)	34 (13%)	4	18
25	9	252/296 (85%)	224 (89%)	28 (11%)	6	22
26	1	176/484 (36%)	162 (92%)	14 (8%)	11	33
27	2	279/352 (79%)	251 (90%)	28 (10%)	7	25
28	3	234/272 (86%)	219 (94%)	15 (6%)	16	40
29	4	387/399 (97%)	355 (92%)	32 (8%)	10	32
30	5	48/64 (75%)	42 (88%)	6 (12%)	4	19
31	6	533/688 (78%)	487 (91%)	46 (9%)	10	31
32	7	616/664 (93%)	565 (92%)	51 (8%)	10	32
33	EA	163/373 (44%)	148 (91%)	15 (9%)	8	29
34	EB	155/261 (59%)	143 (92%)	12 (8%)	12	34
35	DA	488/1665 (29%)	441 (90%)	47 (10%)	8	27
36	DB	876/1083 (81%)	790 (90%)	86 (10%)	7	26
37	DD	144/815 (18%)	134 (93%)	10 (7%)	14	38
37	Dd	146/815 (18%)	138 (94%)	8 (6%)	19	43
38	DE	478/657 (73%)	435 (91%)	43 (9%)	9	30
38	De	475/657 (72%)	420 (88%)	55 (12%)	5	21
39	DF	324/574 (56%)	295 (91%)	29 (9%)	9	30
39	Df	322/574 (56%)	307 (95%)	15 (5%)	23	46
40	DG	133/322 (41%)	117 (88%)	16 (12%)	5	20
41	DH	181/270 (67%)	170 (94%)	11 (6%)	17	41
42	DI	106/235 (45%)	101 (95%)	5 (5%)	23	46
42	Di	107/235 (46%)	104 (97%)	3 (3%)	38	59
43	DJ	79/154 (51%)	76 (96%)	3 (4%)	29	51
43	Dj	83/154 (54%)	82 (99%)	1 (1%)	63	73
44	DL	70/141 (50%)	64 (91%)	6 (9%)	10	31
44	Dl	98/141 (70%)	94 (96%)	4 (4%)	27	49
45	Dc	113/833 (14%)	106 (94%)	7 (6%)	16	40

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	Dk	87/182 (48%)	84 (97%)	3 (3%)	32	55
47	Dm	80/106 (76%)	75 (94%)	5 (6%)	16	40
48	DO	84/98 (86%)	75 (89%)	9 (11%)	6	23
49	DP	153/293 (52%)	143 (94%)	10 (6%)	15	40
50	DQ	111/269 (41%)	105 (95%)	6 (5%)	20	44
51	BA	214/268 (80%)	197 (92%)	17 (8%)	11	33
52	FB	196/218 (90%)	179 (91%)	17 (9%)	9	31
55	PA	1303/1748 (74%)	1163 (89%)	140 (11%)	6	23
56	PB	993/1027 (97%)	887 (89%)	106 (11%)	6	23
57	PC	234/252 (93%)	218 (93%)	16 (7%)	14	38
58	PD	108/126 (86%)	91 (84%)	17 (16%)	2	14
59	PE	191/192 (100%)	174 (91%)	17 (9%)	9	30
60	PF	69/111 (62%)	60 (87%)	9 (13%)	4	18
61	PG	147/153 (96%)	125 (85%)	22 (15%)	3	15
62	PH	129/131 (98%)	118 (92%)	11 (8%)	10	31
63	PI	103/112 (92%)	93 (90%)	10 (10%)	8	26
64	PJ	53/56 (95%)	51 (96%)	2 (4%)	29	51
65	PK	106/106 (100%)	101 (95%)	5 (5%)	23	46
66	PL	41/55 (74%)	38 (93%)	3 (7%)	13	36
67	FA	117/448 (26%)	115 (98%)	2 (2%)	53	68
68	w	1202/1232 (98%)	1181 (98%)	21 (2%)	53	68
69	x	787/864 (91%)	769 (98%)	18 (2%)	44	63
70	p	353/736 (48%)	347 (98%)	6 (2%)	53	68
All	All	18247/29966 (61%)	16589 (91%)	1658 (9%)	11	29

5 of 1658 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
36	DB	487	LYS
38	De	675	LEU
63	PI	81	THR
36	DB	784	ASN
36	DB	486	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 486 such sidechains are listed below:

Mol	Chain	Res	Type
36	DB	450	GLN
68	w	358	GLN
44	DL	117	GLN
67	FA	141	HIS
69	x	402	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](#)

Of 18 ligands modelled in this entry, 17 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	$\# Z > 2$
72	SF4	7	1000	32	0,12,12	-	-	-		

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
72	SF4	7	1000	32	-	-	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.

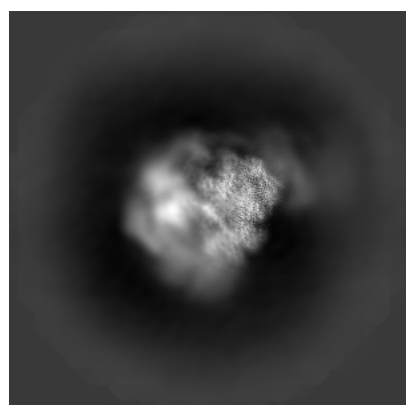
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31207. These allow visual inspection of the internal detail of the map and identification of artifacts.

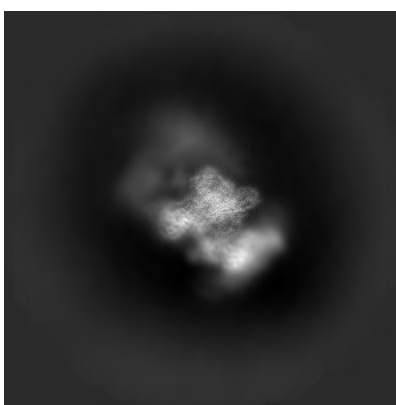
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

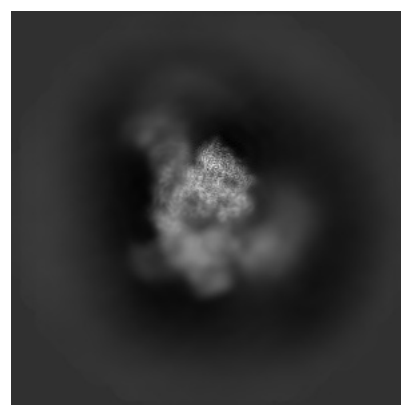
6.1.1 Primary map



X



Y

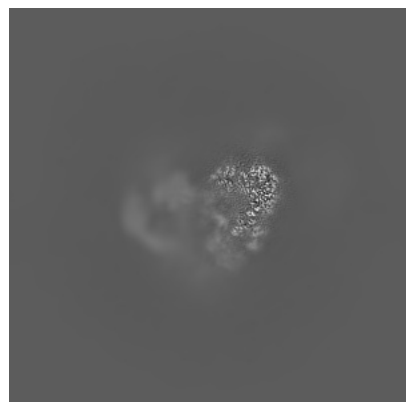


Z

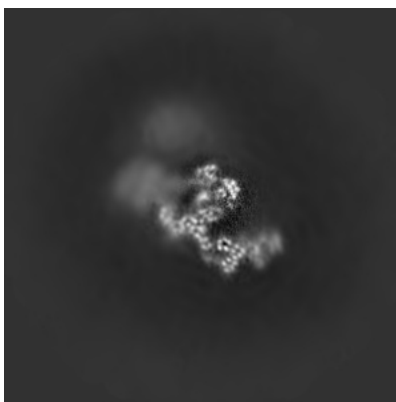
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

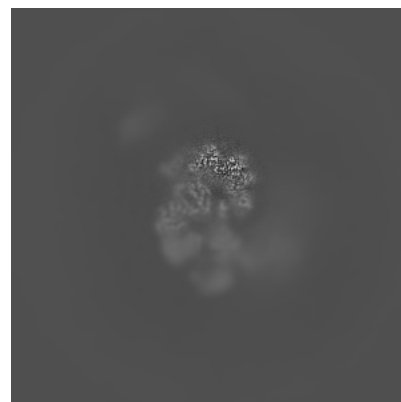
6.2.1 Primary map



X Index: 240



Y Index: 240

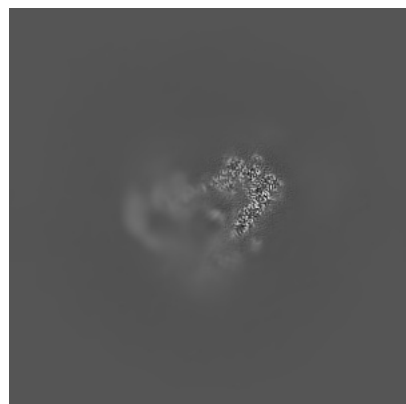


Z Index: 240

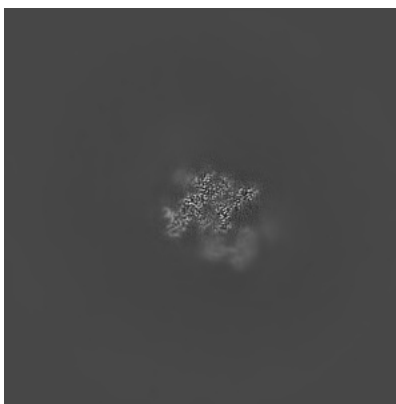
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

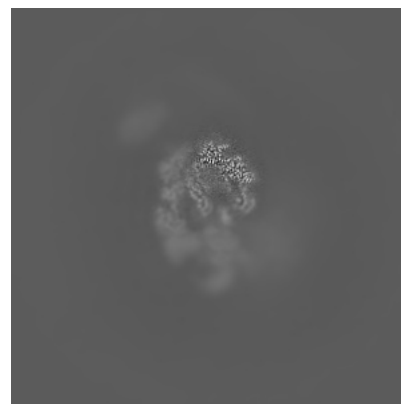
6.3.1 Primary map



X Index: 246



Y Index: 287

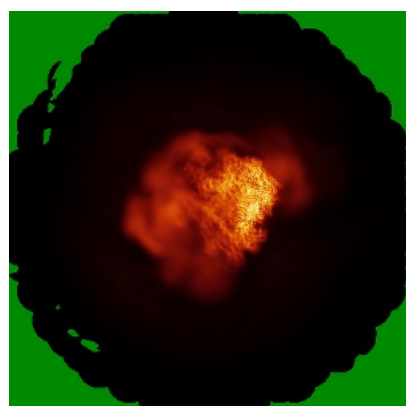


Z Index: 247

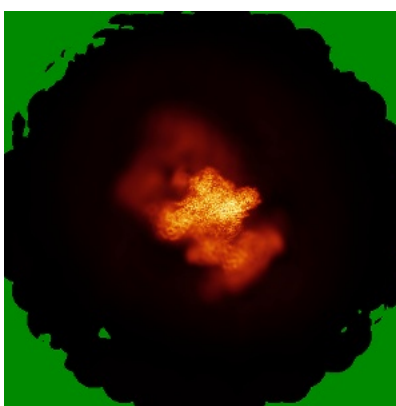
The images above show the largest variance slices of the map in three orthogonal directions.

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

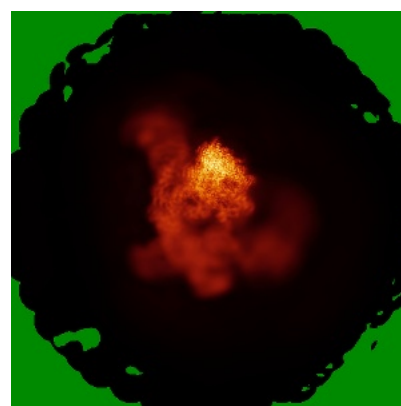
6.4.1 Primary map



X



Y

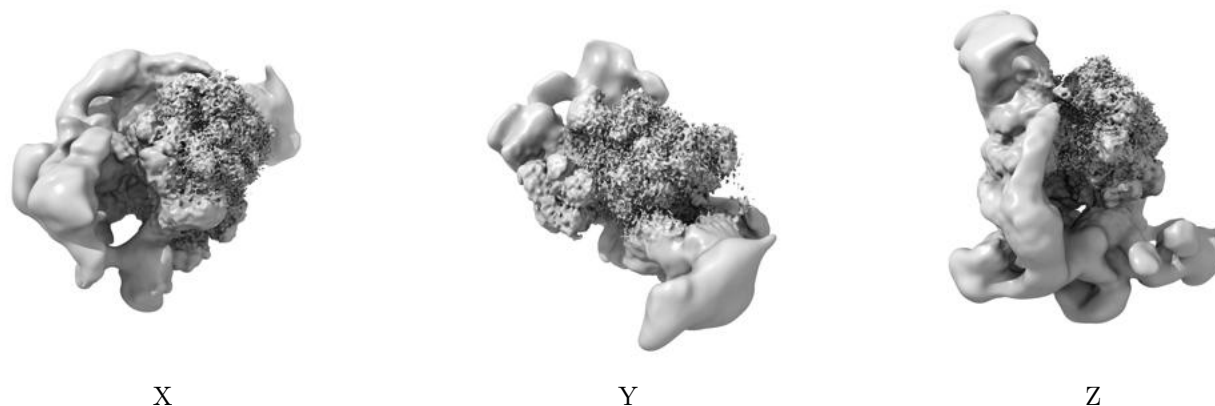


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.41. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

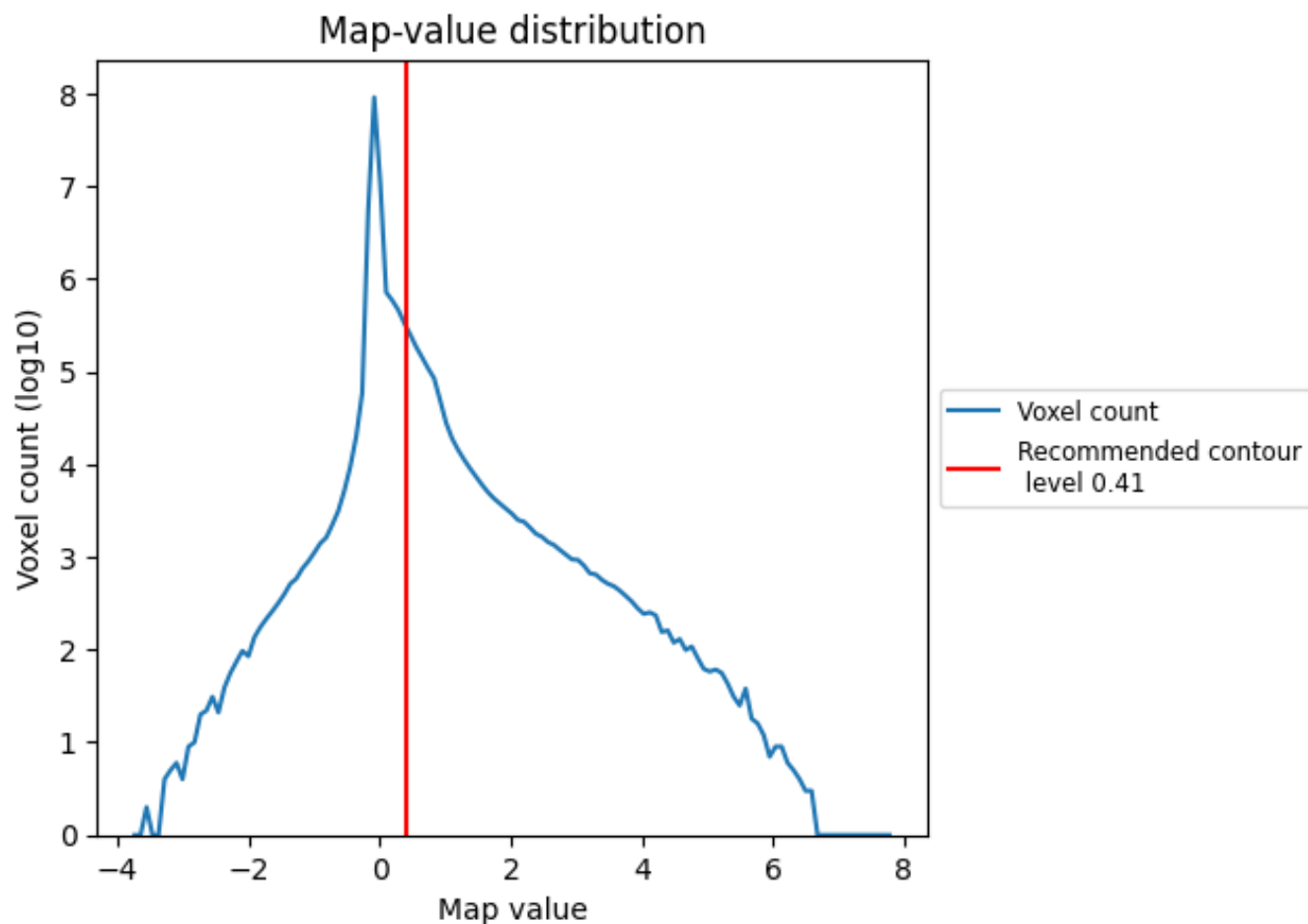
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

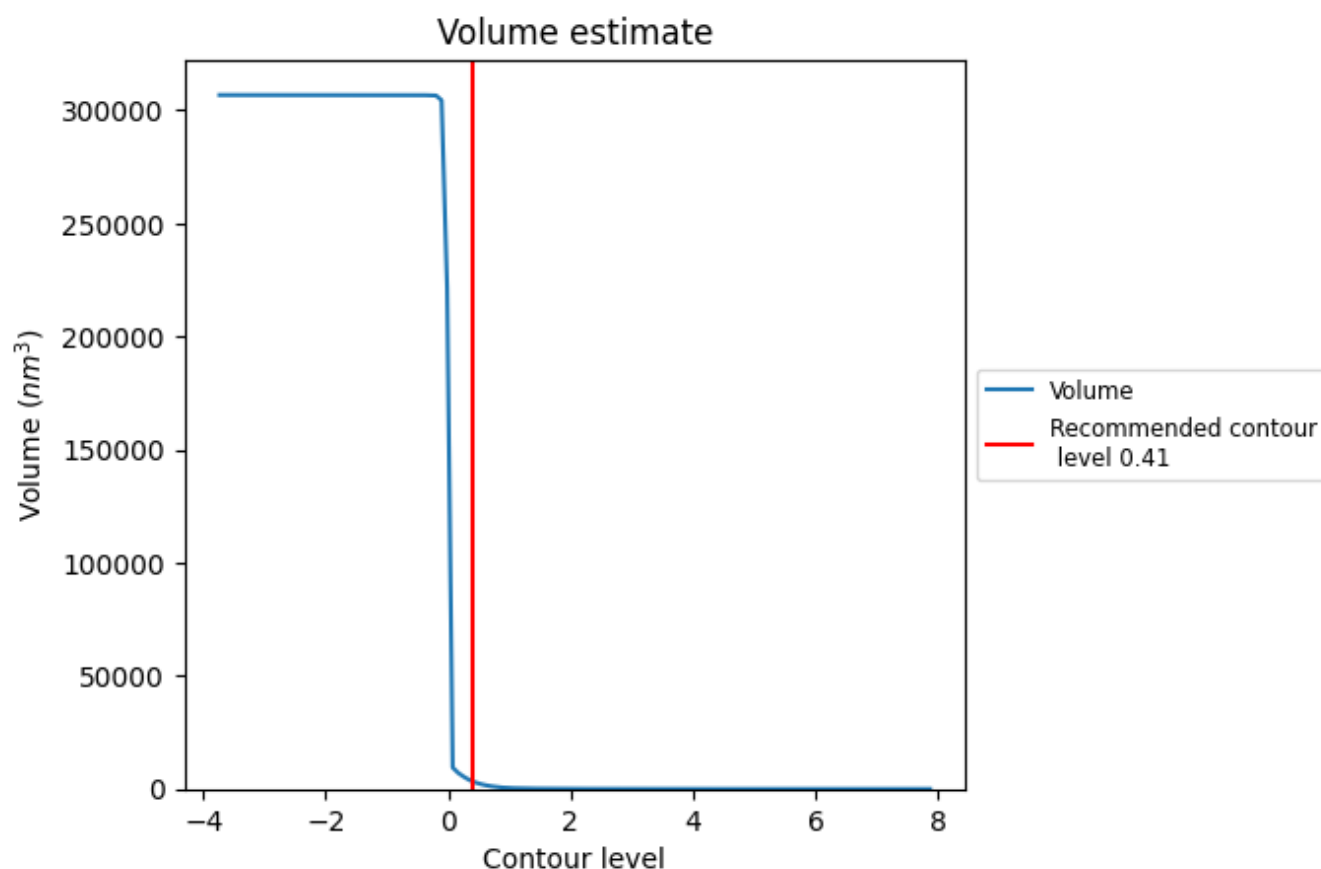
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

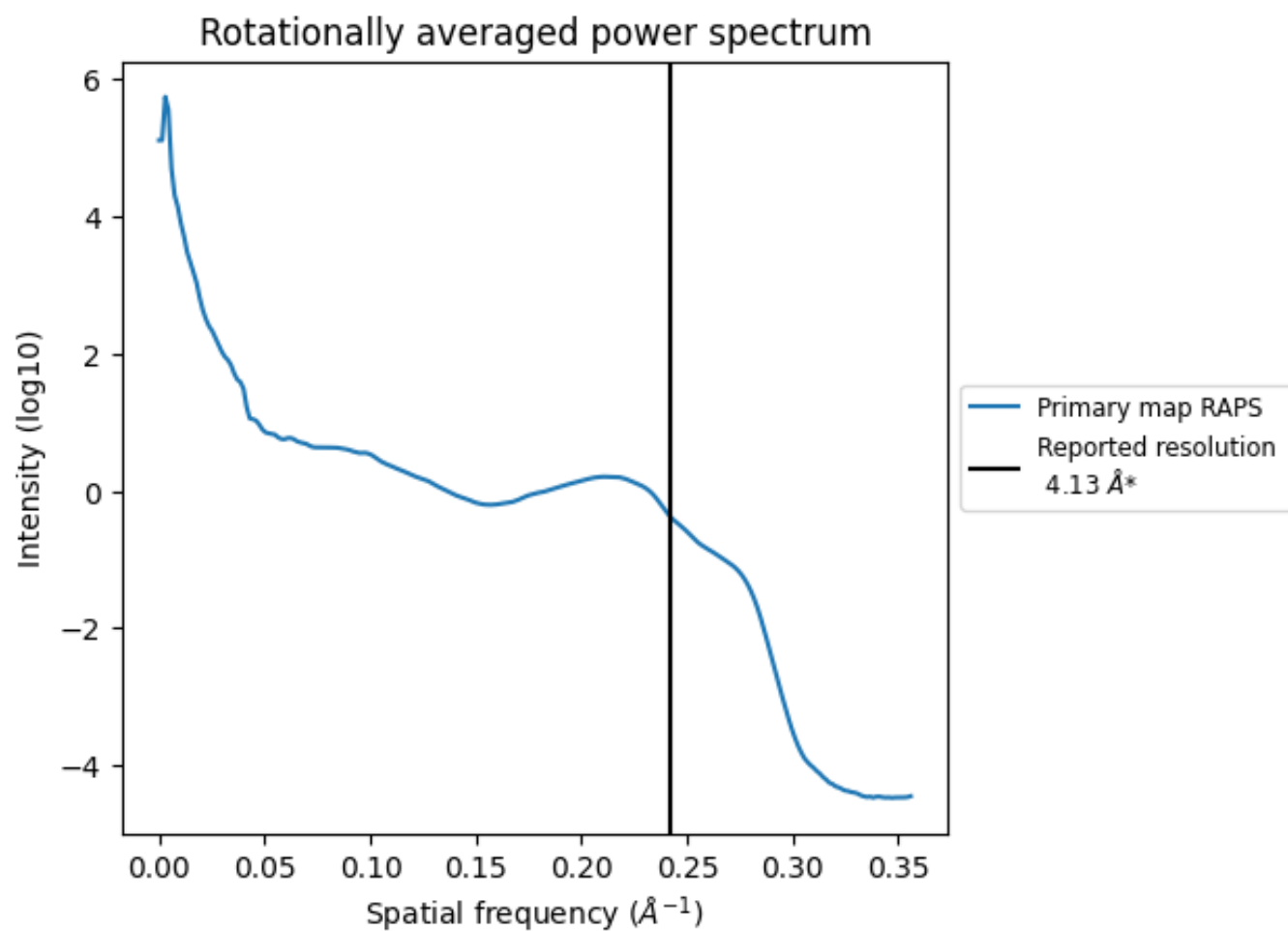
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3240 nm³; this corresponds to an approximate mass of 2927 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 0.242 Å⁻¹

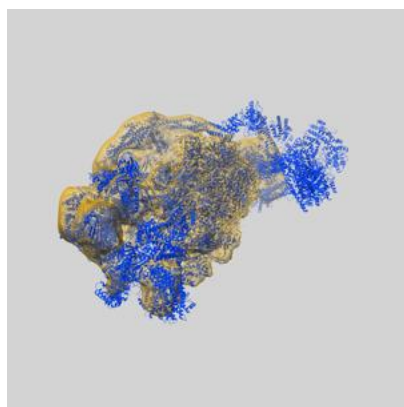
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

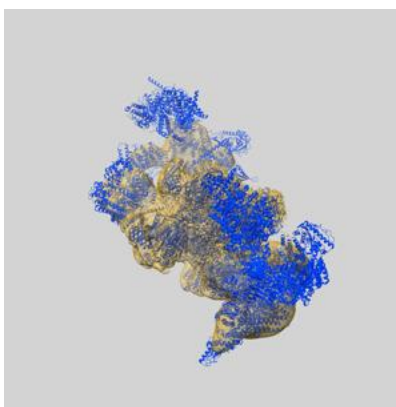
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-31207 and PDB model 7ENC. Per-residue inclusion information can be found in section 3 on page 19.

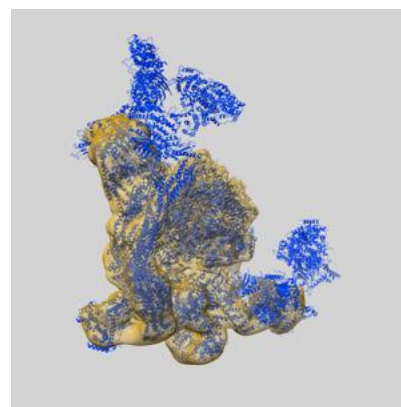
9.1 Map-model overlay [i](#)



X



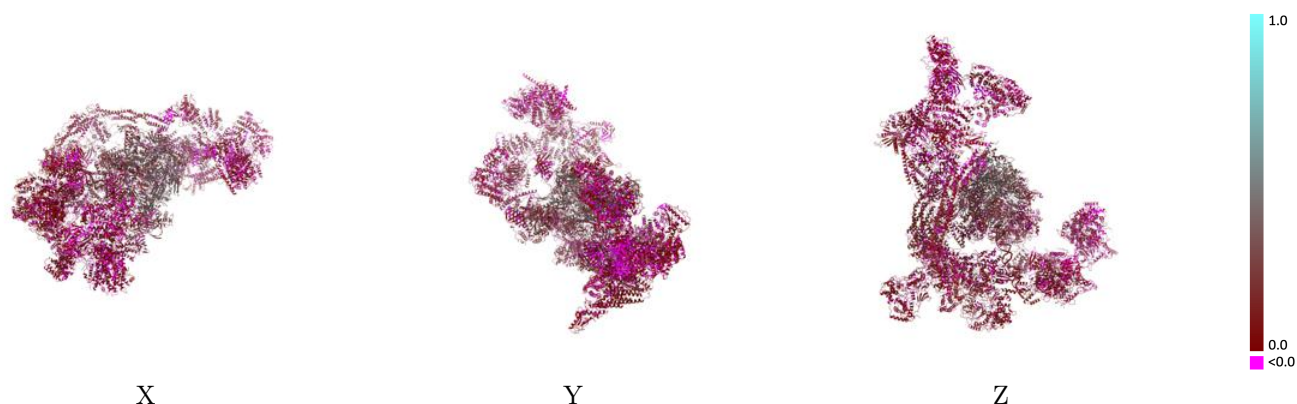
Y



Z

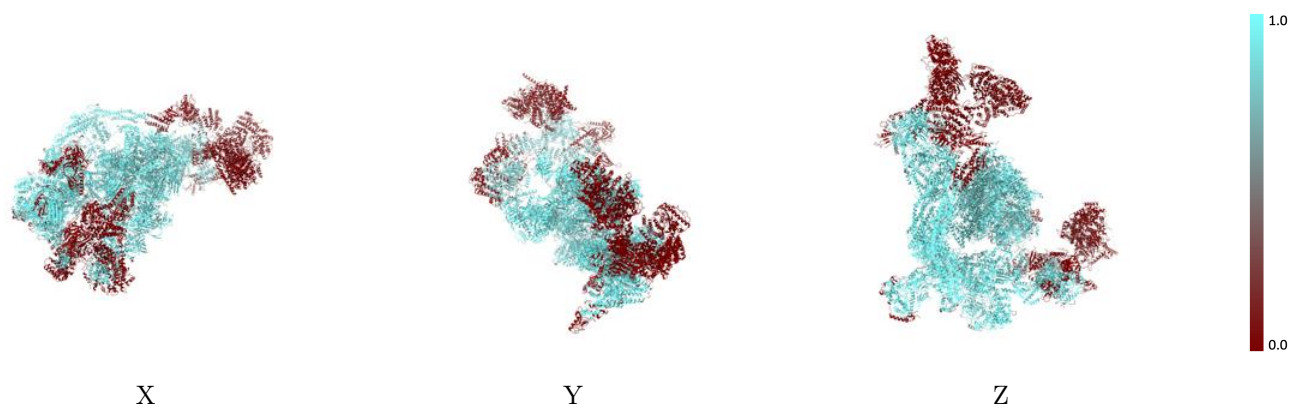
The images above show the 3D surface view of the map at the recommended contour level 0.41 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



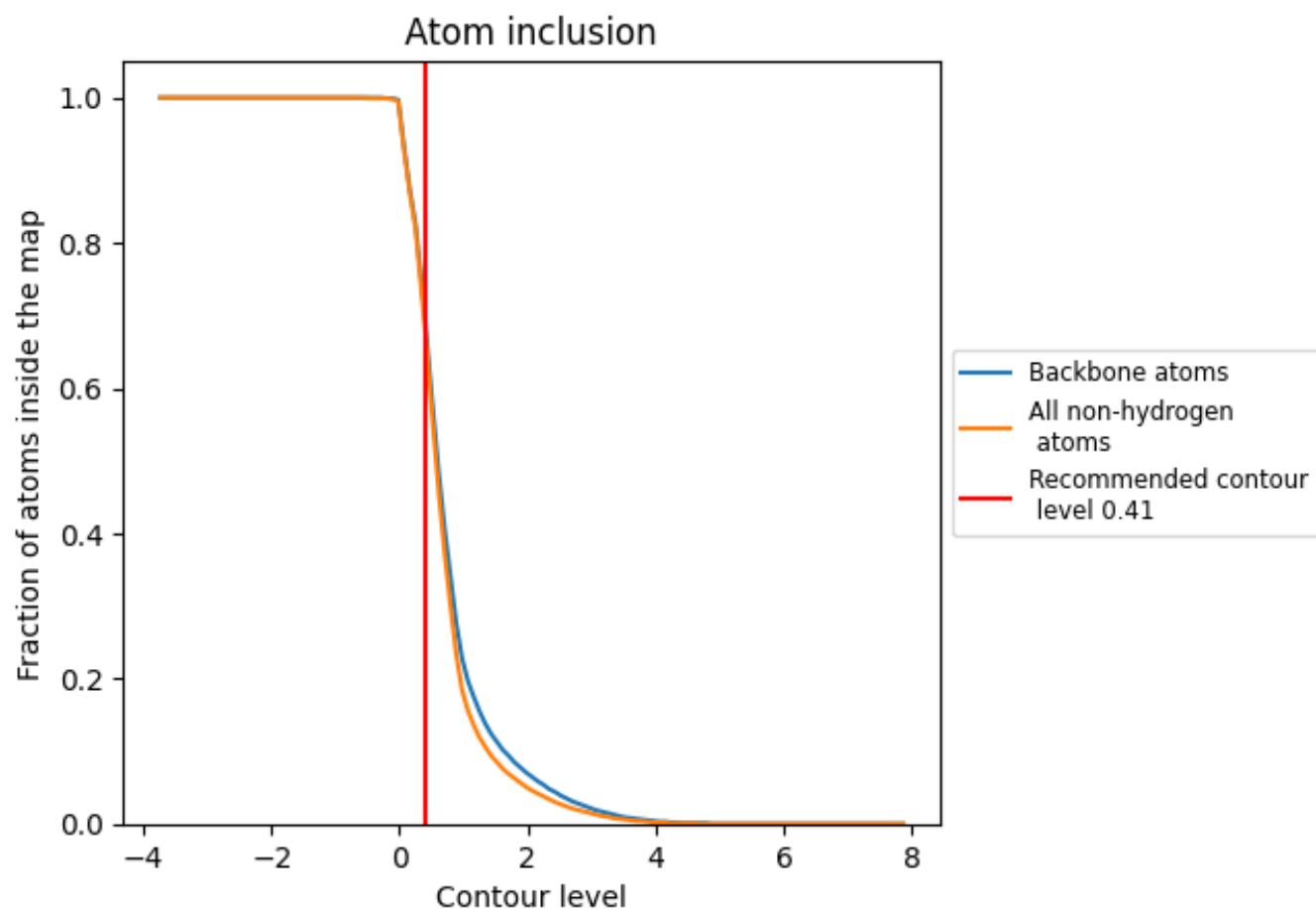
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.41).

9.4 Atom inclusion [i](#)



At the recommended contour level, 69% 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 (0.41) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6730	 0.1030
0	 0.8870	 0.0830
1	 0.9000	 0.0380
2	 0.9830	 0.0690
3	 0.9750	 0.0630
4	 0.9620	 0.0740
5	 0.9790	 0.0560
6	 0.9800	 0.0700
7	 0.9840	 0.0970
8	 0.9410	 0.0760
9	 0.7290	 0.0650
BA	 0.9130	 0.2020
DA	 0.2540	 0.0410
DB	 0.8240	 0.0560
DD	 0.6080	 0.0580
DE	 0.6890	 0.0520
DF	 0.5060	 0.0580
DG	 0.0200	 0.0240
DH	 0.6950	 0.0550
DI	 0.5240	 0.0260
DJ	 0.5820	 0.0500
DL	 0.0280	 0.0310
DO	 0.9350	 0.1010
DP	 0.9670	 0.1650
DQ	 0.8710	 0.0990
Dc	 0.0000	 0.0330
Dd	 0.0000	 0.0140
De	 0.0000	 0.0180
Df	 0.2940	 0.0470
Di	 0.0000	 0.0440
Dj	 0.0000	 0.0320
Dk	 0.0000	 -0.0020
Dl	 0.0000	 0.0200
Dm	 0.0000	 0.0190
EA	 0.9800	 0.1020



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
EB	 0.9870	 0.1230
FA	 0.9480	 0.0680
FB	 0.9520	 0.1150
PA	 0.9230	 0.2390
PB	 0.9390	 0.3370
PC	 0.9300	 0.3250
PD	 0.9370	 0.1590
PE	 0.9560	 0.2170
PF	 0.8880	 0.2560
PG	 0.9480	 0.1770
PH	 0.9240	 0.3110
PI	 0.9260	 0.1450
PJ	 0.9090	 0.3050
PK	 0.8800	 0.2840
PL	 0.9180	 0.2750
X	 0.9990	 0.1760
Y	 0.9950	 0.2000
a	 0.0030	 0.0340
b	 0.5510	 0.0380
c	 0.8450	 0.0550
d	 0.7480	 0.0840
e	 0.9600	 0.0930
f	 0.9870	 0.1340
g	 0.9810	 0.1050
h	 0.9870	 0.1610
i	 0.5010	 0.0850
j	 0.9190	 0.0640
k	 0.9560	 0.1540
l	 0.9170	 0.0710
m	 0.9990	 0.0910
n	 0.8740	 0.0690
o	 0.6690	 0.0440
p	 0.0000	 -0.0260
q	 0.9870	 0.0940
r	 0.9750	 0.0870
s	 0.9040	 0.0620
t	 0.9280	 0.0540
u	 0.9920	 0.0930
v	 0.9890	 0.1300
w	 0.0110	 0.0280
x	 0.0360	 0.0360
z	 0.8980	 0.0450