



wwPDB EM Validation Summary Report ⓘ

Aug 6, 2026 – 08:05 PM JST

PDB ID : 8GXS / pdb_00008gxs
EMDB ID : EMD-34360
Title : PIC-Mediator in complex with +1 nucleosome (T40N) in H-binding state
Authors : Chen, X.; Wang, X.; Liu, W.; Ren, Y.; Qu, X.; Li, J.; Yin, X.
Deposited on : 2022-09-21
Resolution : 4.16 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.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
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) : 2.50

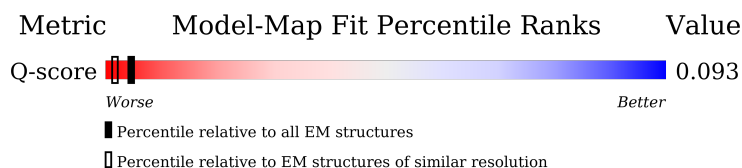
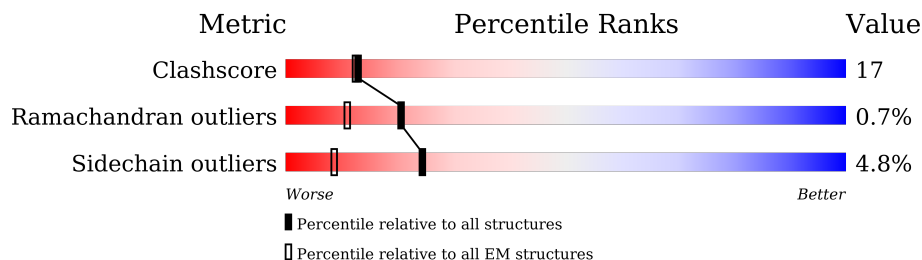
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.16 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	5480 (3.66 - 4.66)

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	X	228	
2	Y	228	
3	NX	162	
4	NY	162	

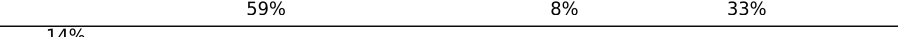
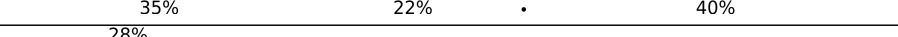
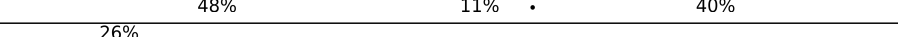
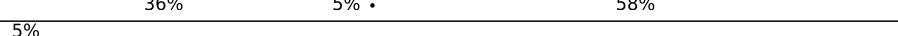
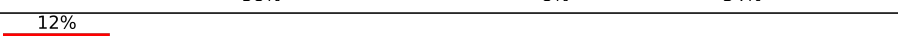
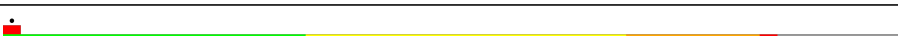
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Mol	Chain	Length	Quality of chain
5	BA	316	
6	DA	1872	
7	EA	439	
8	FA	517	
9	HA	760	
10	NA	136	
10	NE	136	
11	PA	1970	
12	DB	1199	
13	EB	291	
14	FB	249	
15	HB	548	
16	NB	103	
16	NF	103	
17	PB	1174	
18	HC	462	
19	DO	109	
20	DP	339	
21	DQ	376	
22	PC	275	
23	PE	210	
24	PF	127	
25	PH	150	
26	PI	125	
27	PJ	67	

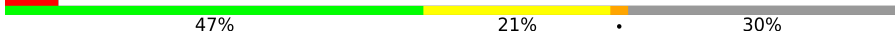
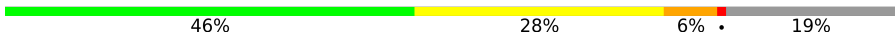
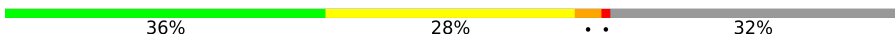
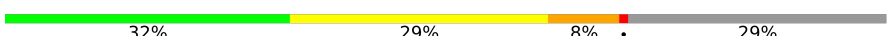
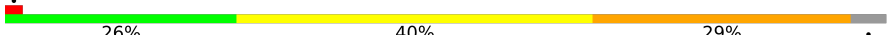
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Mol	Chain	Length	Quality of chain
28	PK	117	
29	PL	58	
30	HD	309	
31	HG	395	
32	HE	308	
33	HF	71	
34	HH	782	
35	DD	1085	
35	Dd	1085	
36	DE	800	
36	De	800	
37	DF	677	
37	Df	677	
38	DG	349	
39	DH	310	
40	DI	264	
40	Di	264	
41	DL	161	
41	Dl	161	
42	Dc	929	
43	DJ	218	
43	Dj	218	
44	Dk	211	
45	Dm	124	
46	HI	346	

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Mol	Chain	Length	Quality of chain
47	HJ	323	
48	PD	142	
49	PG	172	
50	g	233	
51	j	135	
52	n	1454	
53	s	244	
54	u	144	
55	a	1581	
56	d	270	
57	f	246	
58	i	146	
59	m	131	
60	q	651	
61	z	600	
62	b	200	
63	c	311	
64	e	178	
65	l	178	
66	o	788	
67	h	268	
68	k	117	
69	r	208	
70	t	212	
71	v	200	

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Mol	Chain	Length	Quality of chain
72	p	841	
73	w	1368	
74	x	989	
75	y	747	
76	NC	128	
76	NG	128	
77	ND	126	
77	NH	126	

2 Entry composition

There are 80 unique types of molecules in this entry. The entry contains 185972 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 DNA chain called DNA (228-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	X	67	Total	C	N	O	P	0	0
			1387	652	275	394	66		

- Molecule 2 is a DNA chain called DNA (228-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Y	67	Total	C	N	O	P	0	0
			1357	643	239	408	67		

- Molecule 3 is a DNA chain called DNA (162-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	NX	162	Total	C	N	O	P	0	0
			3078	1458	486	972	162		

- Molecule 4 is a DNA chain called DNA (162-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	NY	162	Total	C	N	O	P	0	0
			3561	1620	810	970	161		

- Molecule 5 is a protein called Transcription initiation factor IIB.

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

- Molecule 6 is a protein called Transcription initiation factor TFIID subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	DA	558	Total	C	N	O	S	0	0
			4563	2913	791	832	27		

- Molecule 7 is a protein called General transcription factor IIE subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	EA	187	Total	C	N	O	S	0	0
			1535	964	275	285	11		

- Molecule 8 is a protein called General transcription factor IIF subunit 1.

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

- Molecule 9 is a protein called General transcription and DNA repair factor IIH helicase subunit XPD.

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

- Molecule 10 is a protein called Histone H3.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	NA	100	Total	C	N	O	0	0
			498	298	100	100		
10	NE	103	Total	C	N	O	0	0
			511	305	103	103		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	PA	1471	Total	C	N	O	S	0	0
			11628	7314	2064	2178	72		

- Molecule 12 is a protein called Transcription initiation factor TFIID subunit 2.

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

- Molecule 13 is a protein called Transcription initiation factor IIE subunit beta.

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

- Molecule 14 is a protein called General transcription factor IIF subunit 2.

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

- Molecule 15 is a protein called General transcription factor IIH subunit 1.

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

- Molecule 16 is a protein called Histone H4.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	NB	80	Total	C	N	O	0	0
			391	231	80	80		
16	NF	86	Total	C	N	O	0	0
			421	249	86	86		

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

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

- Molecule 18 is a protein called General transcription factor IIH subunit 4.

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

- Molecule 19 is a protein called Transcription initiation factor IIA subunit 2.

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

- Molecule 20 is a protein called TATA-box-binding protein.

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

- Molecule 21 is a protein called Transcription initiation factor IIA subunit 1.

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

- Molecule 22 is a protein called DNA-directed RNA polymerase II subunit RPB3.

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

- Molecule 23 is a protein called DNA-directed RNA polymerase II subunit E.

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

- Molecule 24 is a protein called DNA-directed RNA polymerase II subunit F.

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

- Molecule 25 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

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

- Molecule 26 is a protein called DNA-directed RNA polymerase II subunit RPB9.

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

- Molecule 27 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

- Molecule 28 is a protein called RNA_pol_L_2 domain-containing protein.

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

- Molecule 29 is a protein called RPB12.

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

- Molecule 30 is a protein called CDK-activating kinase assembly factor MAT1.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	HD	306	Total	C	N	O	S	0	0
			2400	1498	424	465	13		

- Molecule 31 is a protein called General transcription factor IIH subunit 2.

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

- Molecule 32 is a protein called General transcription factor IIH subunit 3.

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

- Molecule 33 is a protein called General transcription factor IIH subunit 5.

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

- Molecule 34 is a protein called General transcription and DNA repair factor IIH helicase subunit XPB.

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

- Molecule 35 is a protein called Transcription initiation factor TFIID subunit 4.

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

- Molecule 36 is a protein called Transcription initiation factor TFIID subunit 5.

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

- Molecule 37 is a protein called Transcription initiation factor TFIID subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	DF	408	Total	C	N	O	S	0	0
			3109	1970	542	579	18		
37	Df	403	Total	C	N	O	S	0	0
			3081	1954	533	576	18		

- Molecule 38 is a protein called Transcription initiation factor TFIID subunit 7.

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

- Molecule 39 is a protein called Transcription initiation factor TFIID subunit 8.

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

- Molecule 40 is a protein called Transcription initiation factor TFIID subunit 9.

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

- Molecule 41 is a protein called Transcription initiation factor TFIID subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	DL	74	Total	C	N	O	S	0	0
			605	379	105	118	3		
41	Dl	107	Total	C	N	O	S	0	0
			876	547	158	166	5		

- Molecule 42 is a protein called Transcription initiation factor TFIID subunit 3.

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

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

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

- Molecule 44 is a protein called Transcription initiation factor TFIID subunit 11.

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

- Molecule 45 is a protein called Transcription initiation factor TFIID subunit 13.

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

- Molecule 46 is a protein called Cyclin-dependent kinase 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	HI	299	Total	C	N	O	S	0	0
			2374	1532	405	426	11		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
HI	41	ALA	LYS	engineered mutation	UNP P50613

- Molecule 47 is a protein called Cyclin-H.

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

- Molecule 48 is a protein called DNA-directed RNA polymerase II subunit RPB4.

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

- Molecule 49 is a protein called DNA-directed RNA polymerase II subunit RPB7.

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

- Molecule 50 is a protein called Mediator of RNA polymerase II transcription subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	g	106	Total	C	N	O	S	0	0
			898	569	166	157	6		

- Molecule 51 is a protein called Mediator of RNA polymerase II transcription subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	j	122	Total	C	N	O	S	0	0
			840	527	151	159	3		

- Molecule 52 is a protein called Mediator of RNA polymerase II transcription subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	n	1015	Total	C	N	O	S	0	0
			7751	4941	1363	1405	42		

- Molecule 53 is a protein called Mediator of RNA polymerase II transcription subunit 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	s	93	Total	C	N	O	S	0	0
			723	463	121	135	4		

- Molecule 54 is a protein called Mediator of RNA polymerase II transcription subunit 21.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	u	117	Total	C	N	O	S	0	0
			886	552	146	184	4		

- Molecule 55 is a protein called Mediator of RNA polymerase II transcription subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	a	438	Total	C	N	O	S	0	0
			3430	2190	584	632	24		

- Molecule 56 is a protein called Mediator of RNA polymerase II transcription subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	d	158	Total	C	N	O	S	0	0
			1268	791	228	243	6		

- Molecule 57 is a protein called Mediator of RNA polymerase II transcription subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	f	167	Total	C	N	O	S	0	0
			1365	882	235	243	5		

- Molecule 58 is a protein called Mediator of RNA polymerase II transcription subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	i	73	Total	C	N	O	S	0	0
			605	382	107	110	6		

- Molecule 59 is a protein called Mediator of RNA polymerase II transcription subunit 31.

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

- Molecule 60 is a protein called Mediator of RNA polymerase II transcription subunit 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	q	555	Total	C	N	O	S	0	0
			4373	2765	783	805	20		

- Molecule 61 is a protein called Mediator of RNA polymerase II transcription subunit 26.

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

- Molecule 62 is a protein called Mediator of RNA polymerase II transcription subunit 29.

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

- Molecule 63 is a protein called Mediator of RNA polymerase II transcription subunit 27.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	c	263	Total	C	N	O	S	0	0
			2131	1356	379	385	11		

- Molecule 64 is a protein called Mediator of RNA polymerase II transcription subunit 28.

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

- Molecule 65 is a protein called Mediator of RNA polymerase II transcription subunit 30.

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

- Molecule 66 is a protein called Mediator of RNA polymerase II transcription subunit 15.

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

- Molecule 67 is a protein called Isoform 2 of Mediator of RNA polymerase II transcription subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	h	190	Total	C	N	O	S	0	0
			1465	913	259	289	4		

- Molecule 68 is a protein called Mediator of RNA polymerase II transcription subunit 11.

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

- Molecule 69 is a protein called Mediator of RNA polymerase II transcription subunit 18.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	r	192	Total	C	N	O	S	0	0
			1535	973	271	276	15		

- Molecule 70 is a protein called Mediator of RNA polymerase II transcription subunit 20.

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

- Molecule 71 is a protein called Mediator of RNA polymerase II transcription subunit 22.

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

- Molecule 72 is a protein called Isoform 2 of Mediator of RNA polymerase II transcription subunit 16.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	p	766	Total	C	N	O	S	0	0
			5983	3816	1026	1092	49		

- Molecule 73 is a protein called Mediator of RNA polymerase II transcription subunit 23.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	w	1334	Total	C	N	O	S	0	0
			10774	6967	1827	1909	71		

- Molecule 74 is a protein called Mediator of RNA polymerase II transcription subunit 24.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	x	897	Total	C	N	O	S	0	0
			7061	4524	1190	1293	54		

- Molecule 75 is a protein called Mediator of RNA polymerase II transcription subunit 25.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	y	210	Total	C	N	O	S	0	0
			1605	1030	264	302	9		

- Molecule 76 is a protein called HISTONE H2A.Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	NC	103	Total	C	N	O		0	0
			506	300	103	103			
76	NG	107	Total	C	N	O		0	0
			524	310	107	107			

- Molecule 77 is a protein called Histone H2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	ND	95	Total	C	N	O		0	0
			471	281	95	95			
77	NH	95	Total	C	N	O		0	0
			471	281	95	95			

- Molecule 78 is ZINC ION (CCD ID: ZN) (formula: Zn).

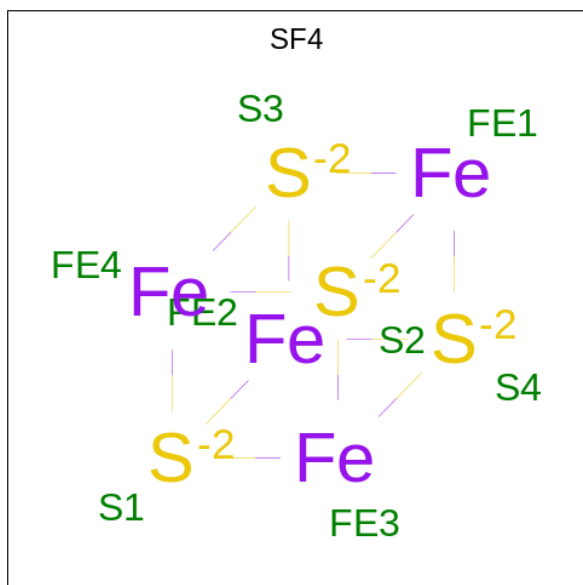
Mol	Chain	Residues	Atoms		AltConf
78	BA	1	Total	Zn	0
			1	1	
78	EA	1	Total	Zn	0
			1	1	
78	PA	2	Total	Zn	0
			2	2	
78	PB	1	Total	Zn	0
			1	1	
78	PC	1	Total	Zn	0
			1	1	
78	PI	2	Total	Zn	0
			2	2	
78	PJ	1	Total	Zn	0
			1	1	
78	PL	1	Total	Zn	0
			1	1	
78	HD	2	Total	Zn	0
			2	2	
78	HG	3	Total	Zn	0
			3	3	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
78	HE	2	Total	Zn	0
			2	2	
78	c	1	Total	Zn	0
			1	1	
78	p	1	Total	Zn	0
			1	1	

- Molecule 79 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

- Molecule 80 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

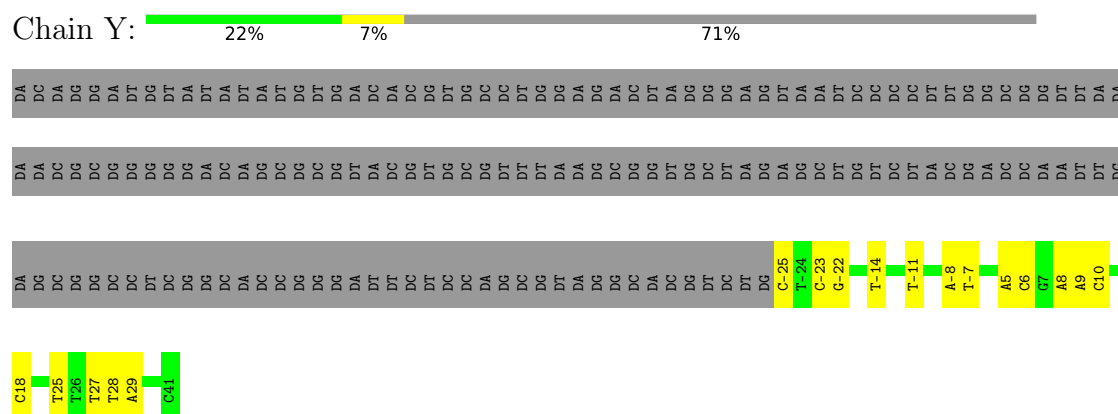
3 Residue-property plots [i](#)

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

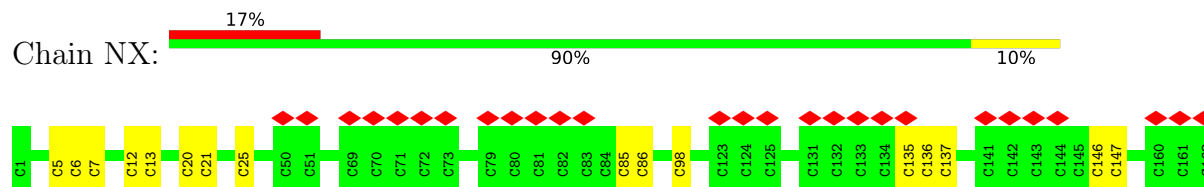
• Molecule 1: DNA (228-mer)



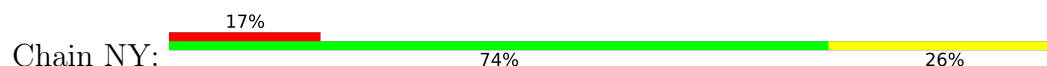
• Molecule 2: DNA (228-mer)



• Molecule 3: DNA (162-mer)

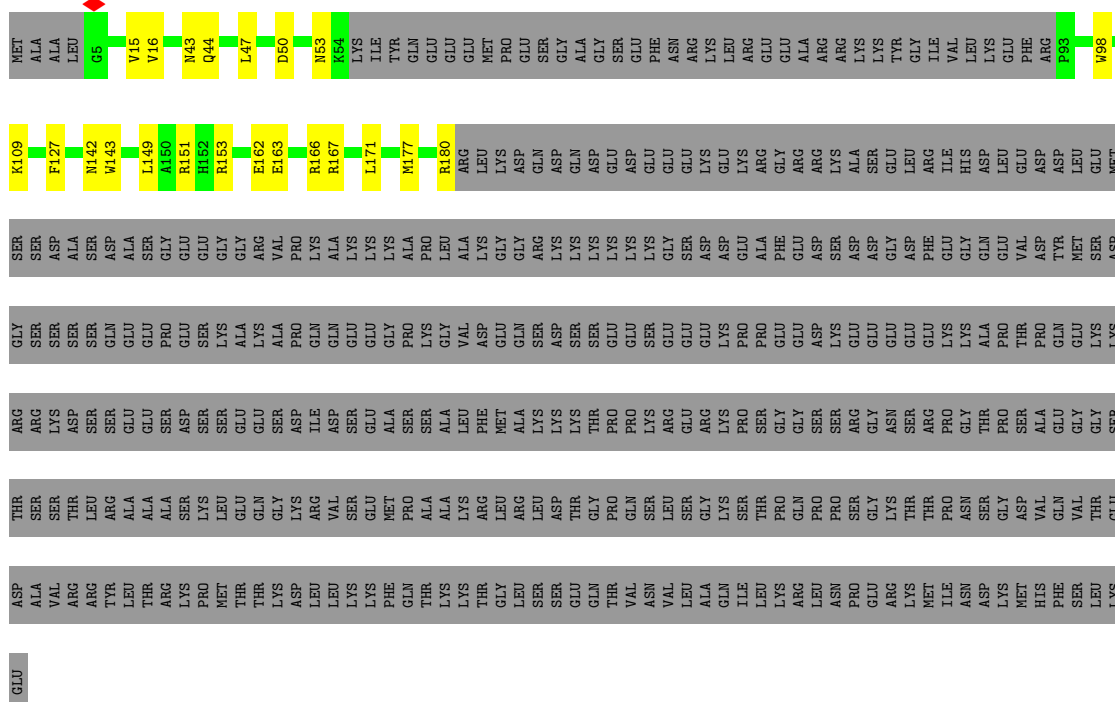


• Molecule 4: DNA (162-mer)

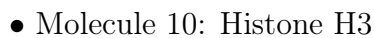
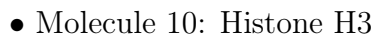


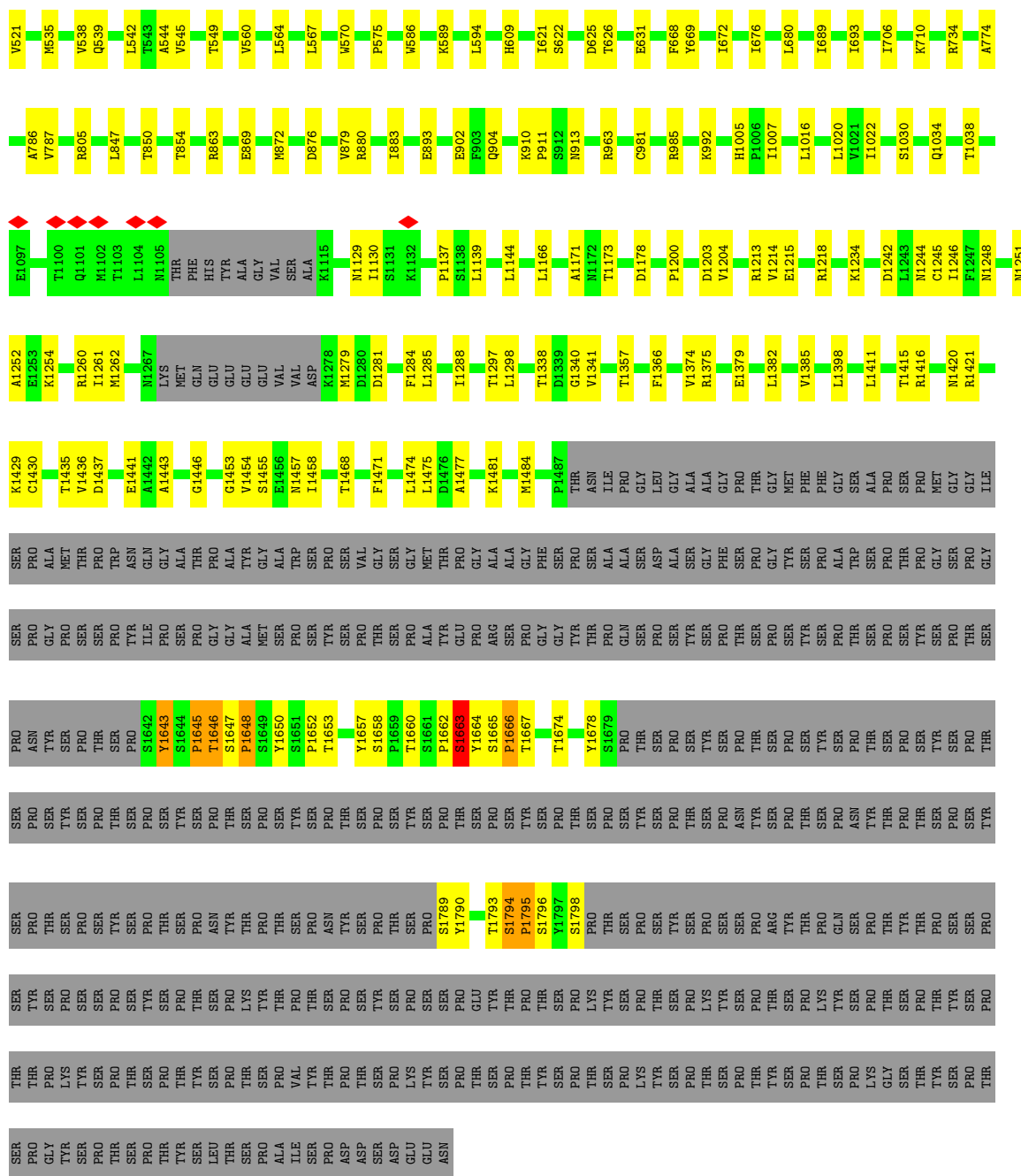






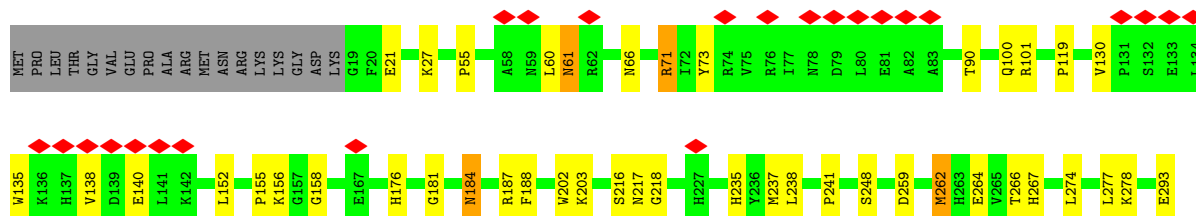
- Chain HA:



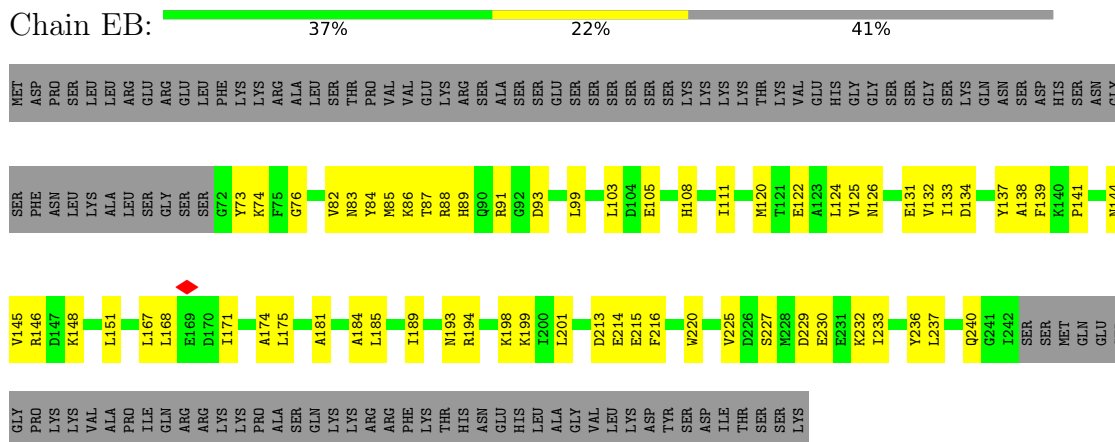


• Molecule 12: Transcription initiation factor TFIID subunit 2

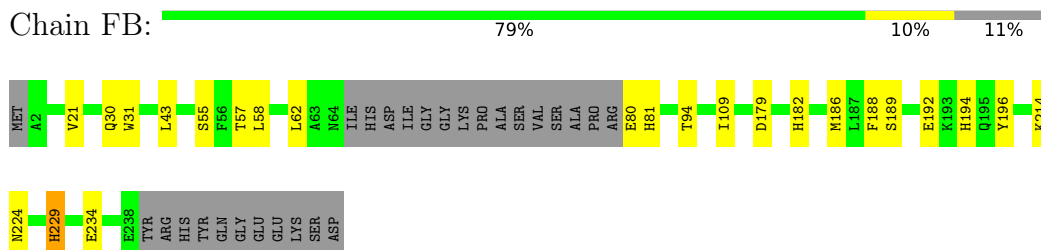
Chain DB:



- Molecule 13: Transcription initiation factor IIE subunit beta



- Molecule 14: General transcription factor IIF subunit 2

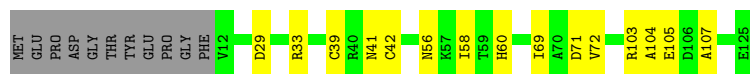


Chain PH:  91% 8%



- Molecule 26: DNA-directed RNA polymerase II subunit RPB9

Chain PI:  79% 12% 9%



- Molecule 27: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain PJ:  78% 18%



- Molecule 28: RNA_pol_L_2 domain-containing protein

Chain PK:  89% 9%



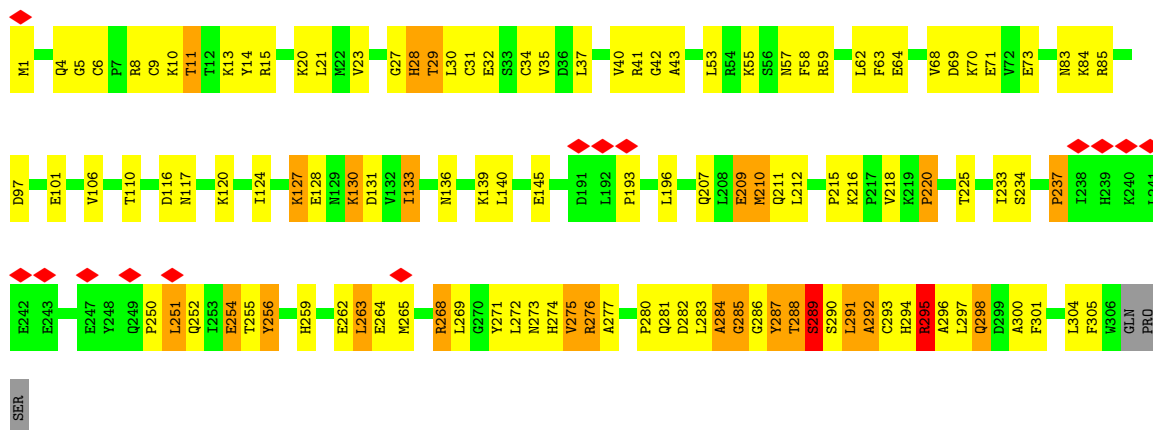
- Molecule 29: RPB12

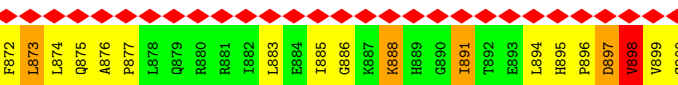
Chain PL:  60% 16% 24%

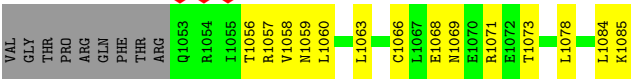
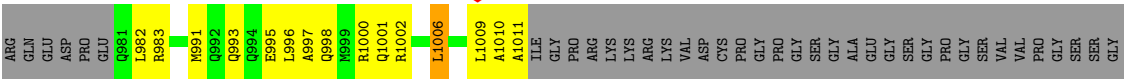


- Molecule 30: CDK-activating kinase assembly factor MAT1

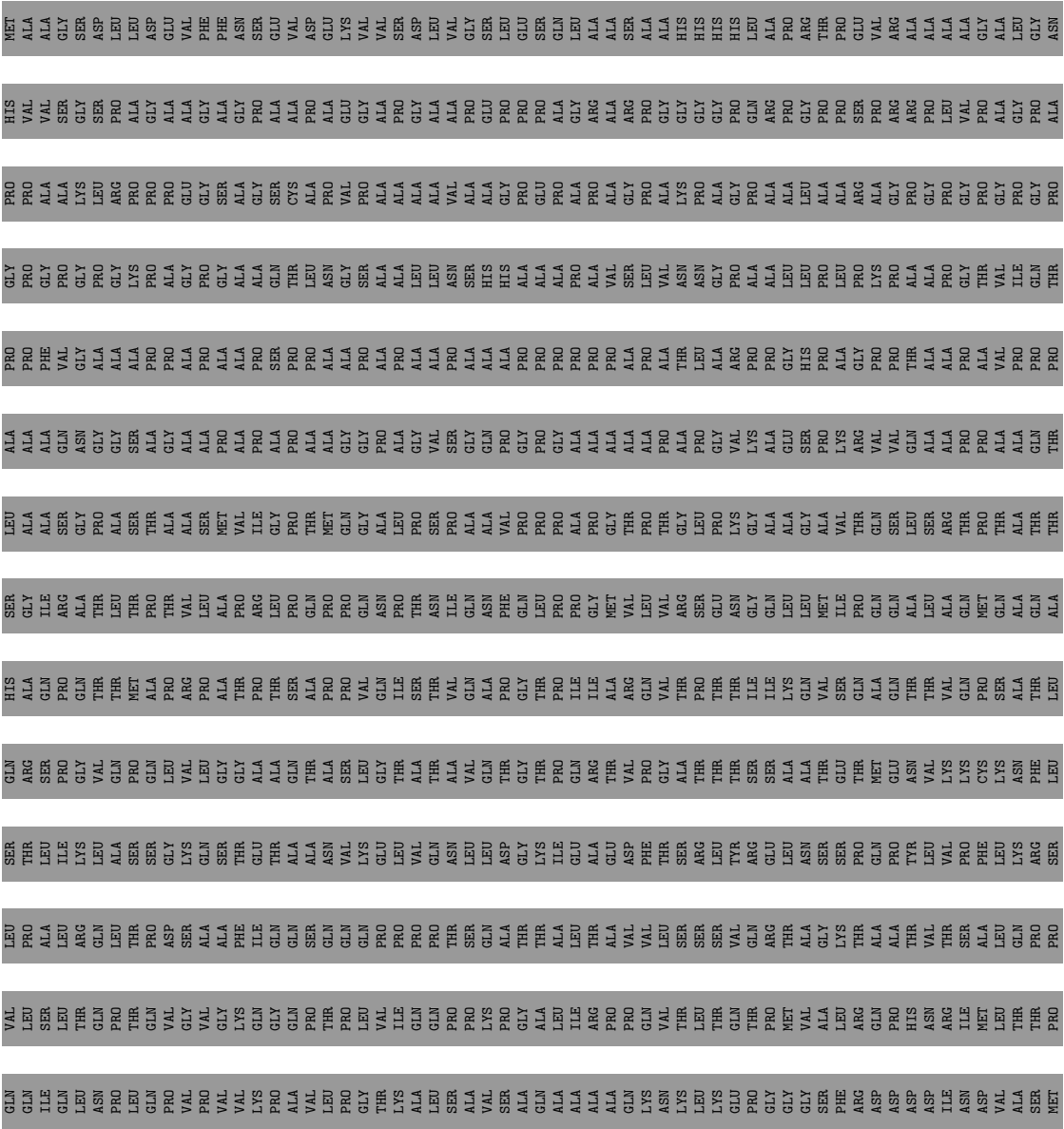
Chain HD:  5% 61% 30% 8%





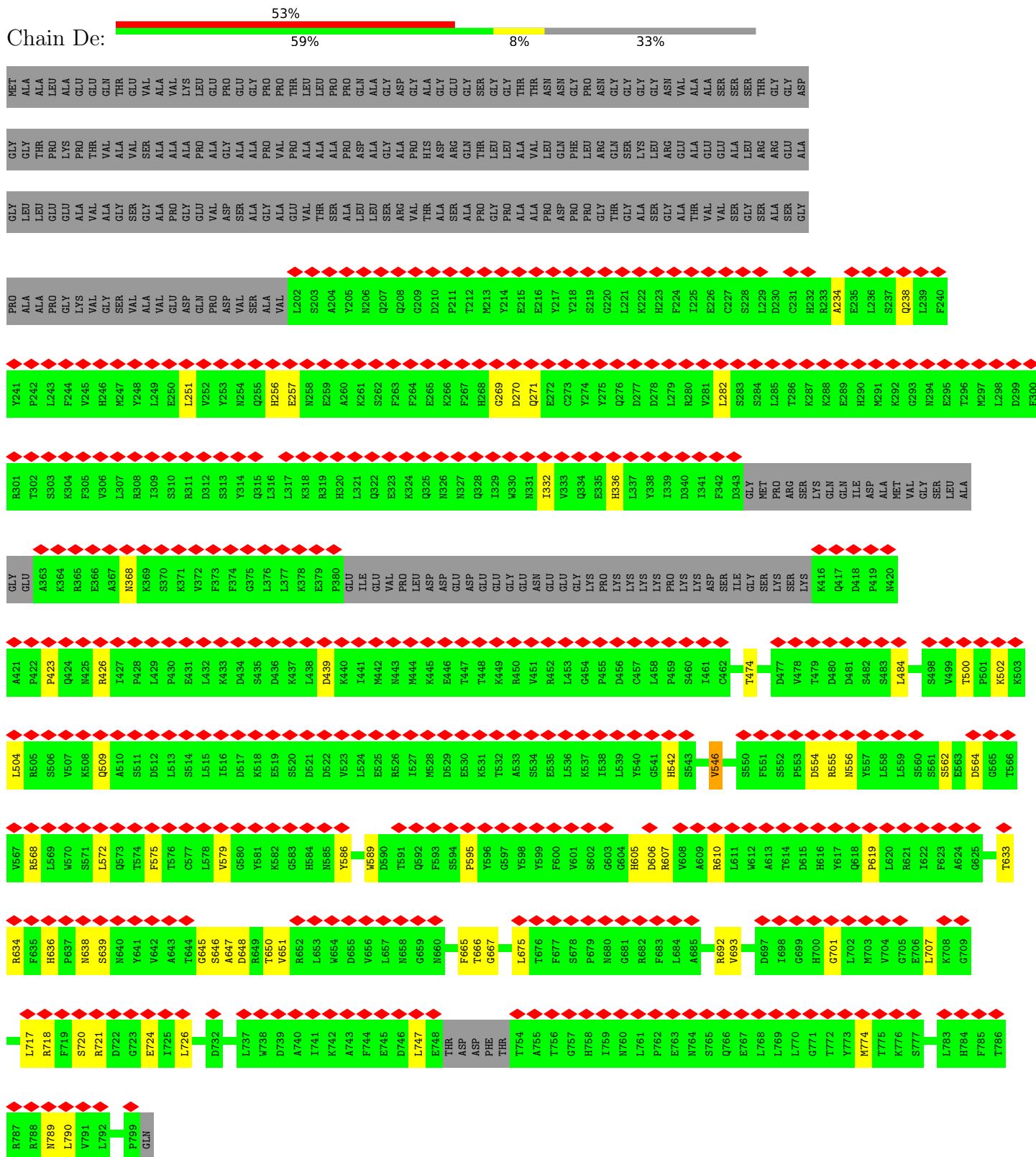


● Molecule 35: Transcription initiation factor TFIID subunit 4

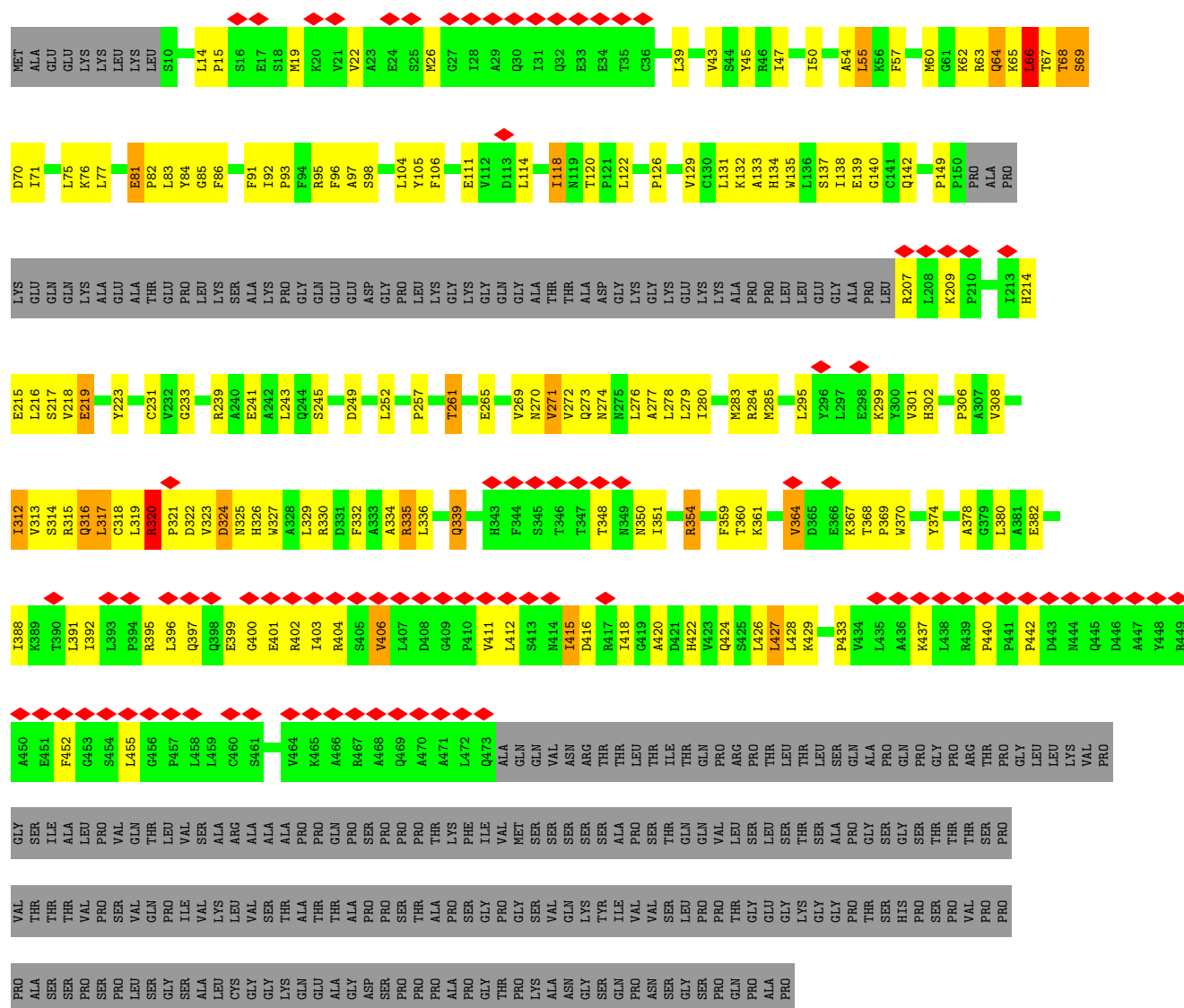
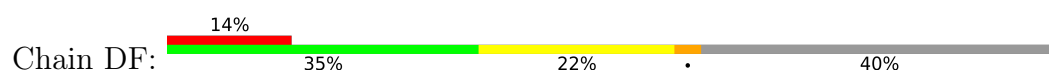




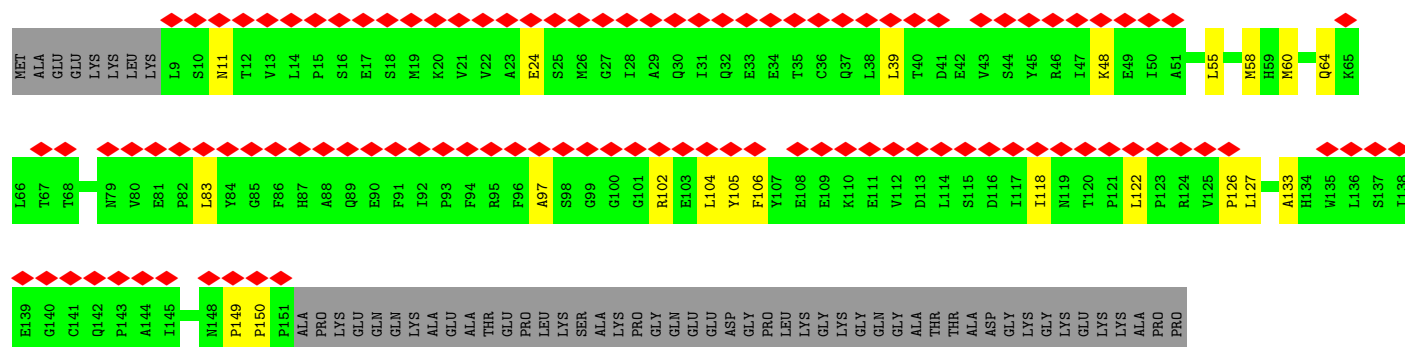
- Molecule 36: Transcription initiation factor TFIID subunit 5



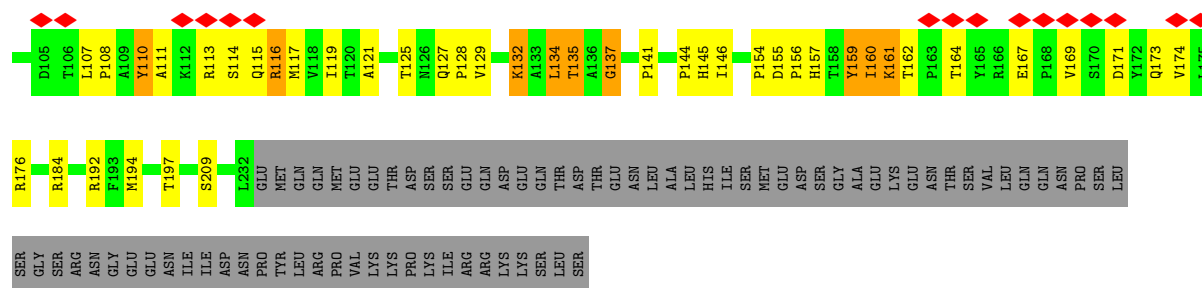
- Molecule 37: Transcription initiation factor TFIID subunit 6



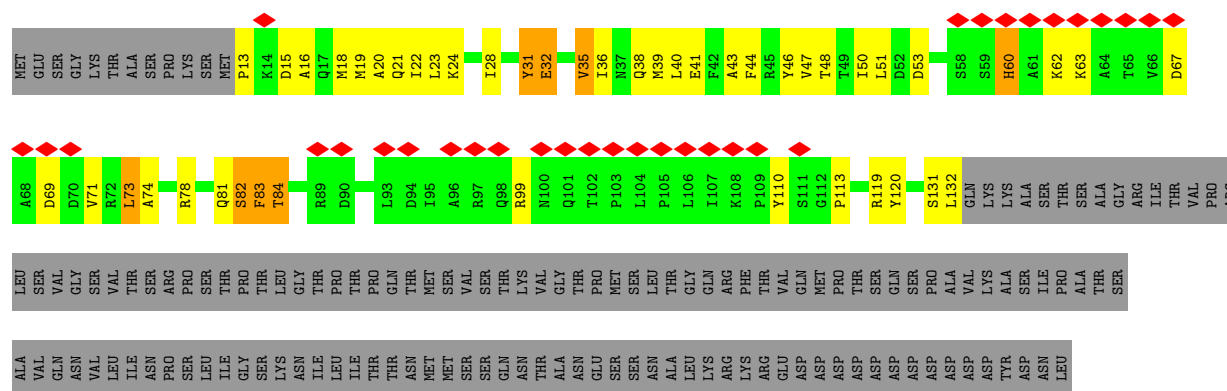
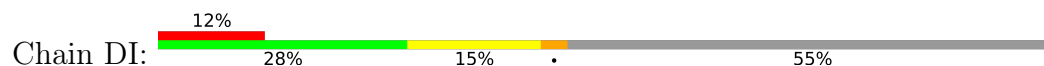
• Molecule 37: Transcription initiation factor TFIID subunit 6



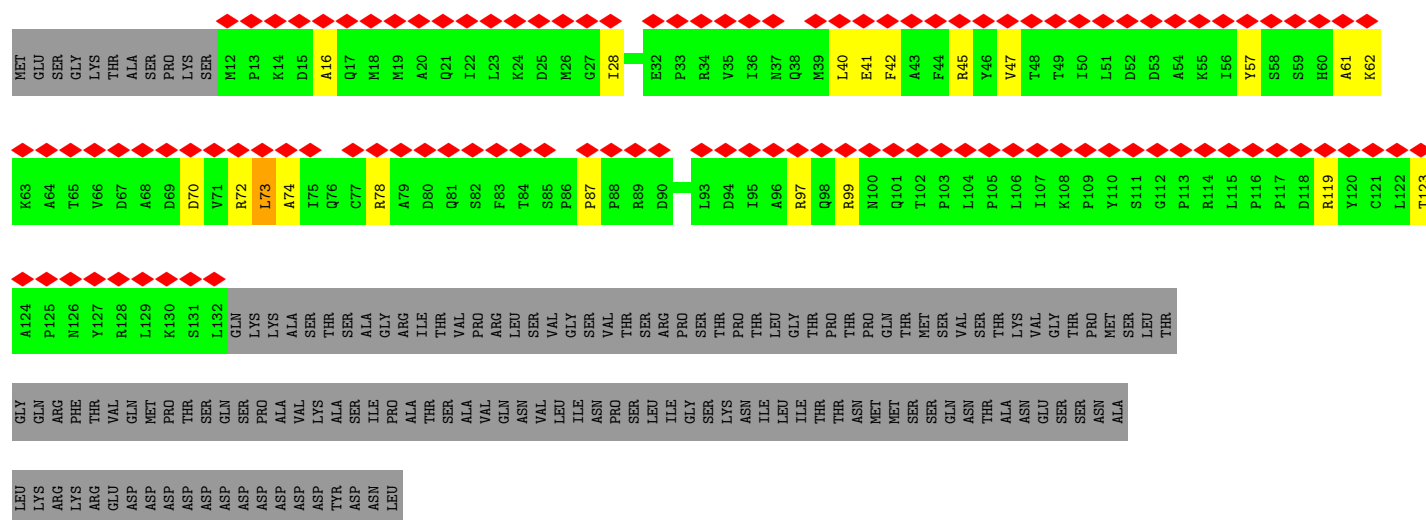
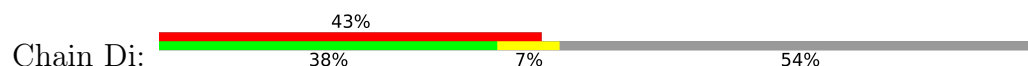




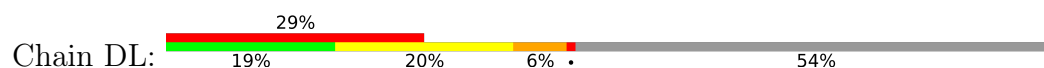
• Molecule 40: Transcription initiation factor TFIID subunit 9



• Molecule 40: Transcription initiation factor TFIID subunit 9

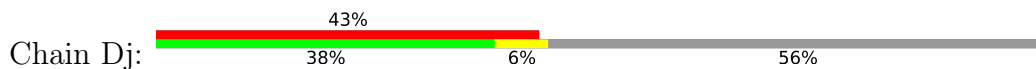


• Molecule 41: Transcription initiation factor TFIID subunit 12



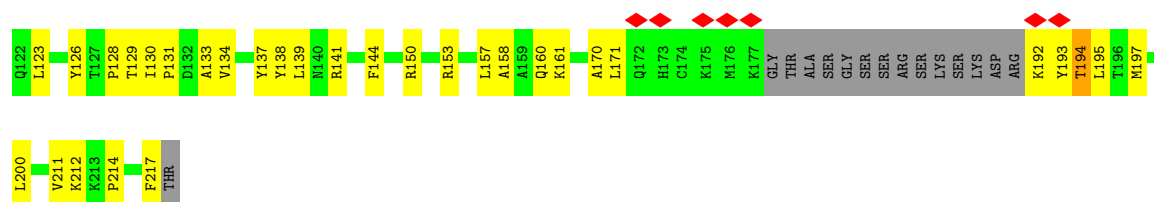
[illegible]

- Molecule 43: Transcription initiation factor TFIID subunit 10

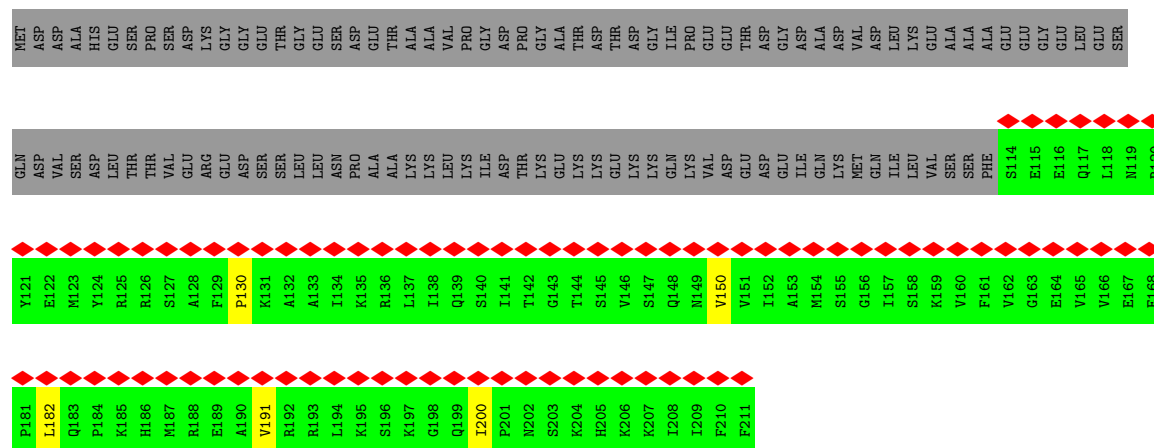
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- Molecule 43: Transcription initiation factor TFIID subunit 10

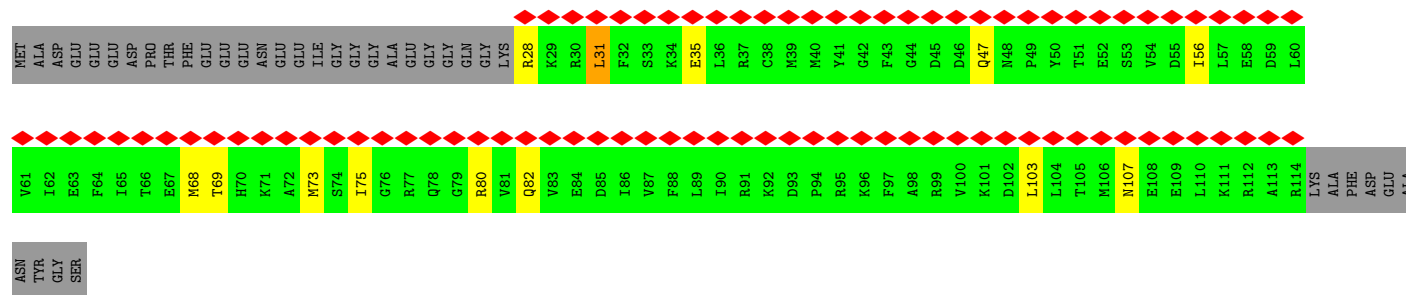
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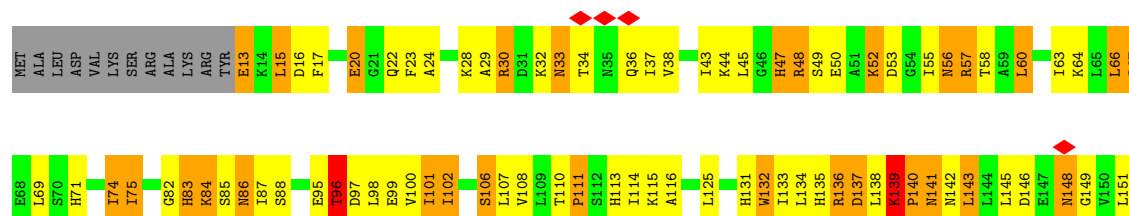
• Molecule 44: Transcription initiation factor TFIID subunit 11

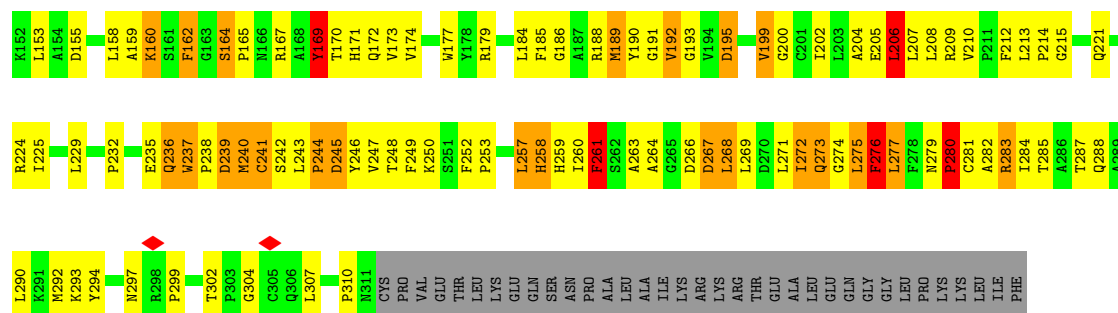


• Molecule 45: Transcription initiation factor TFIID subunit 13

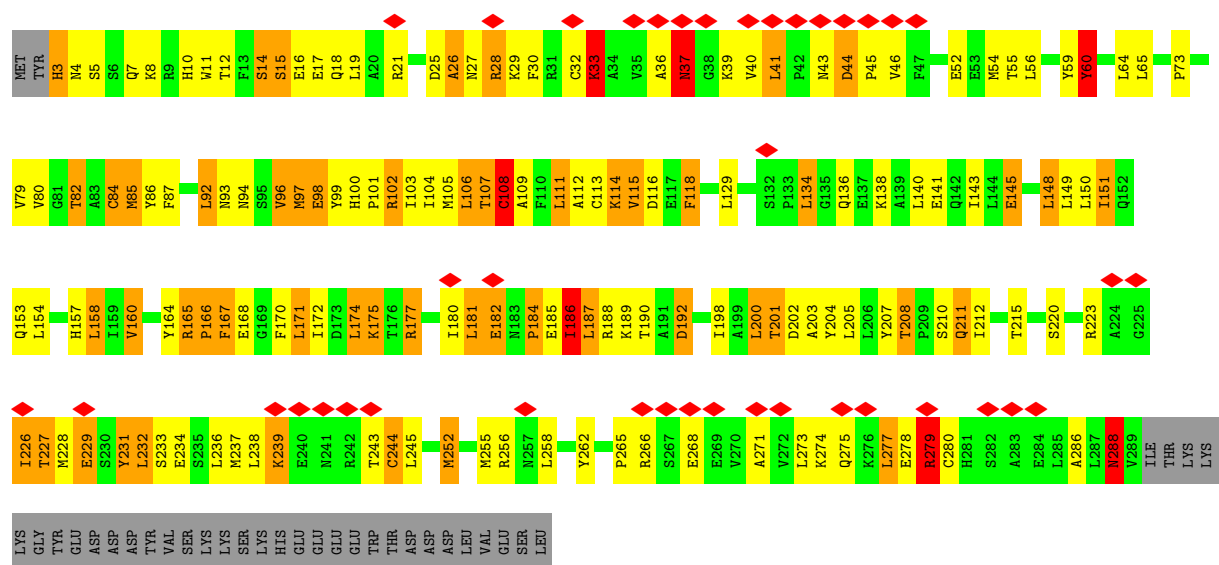
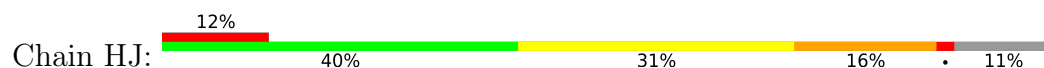


• Molecule 46: Cyclin-dependent kinase 7





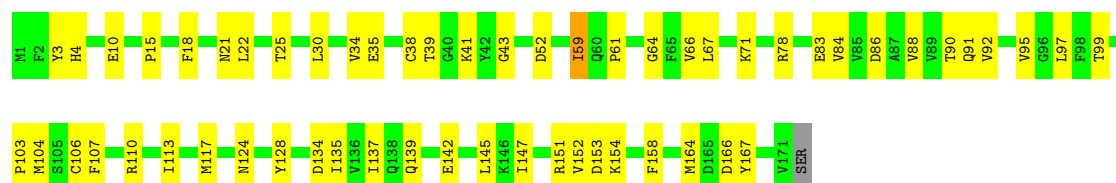
• Molecule 47: Cyclin-H



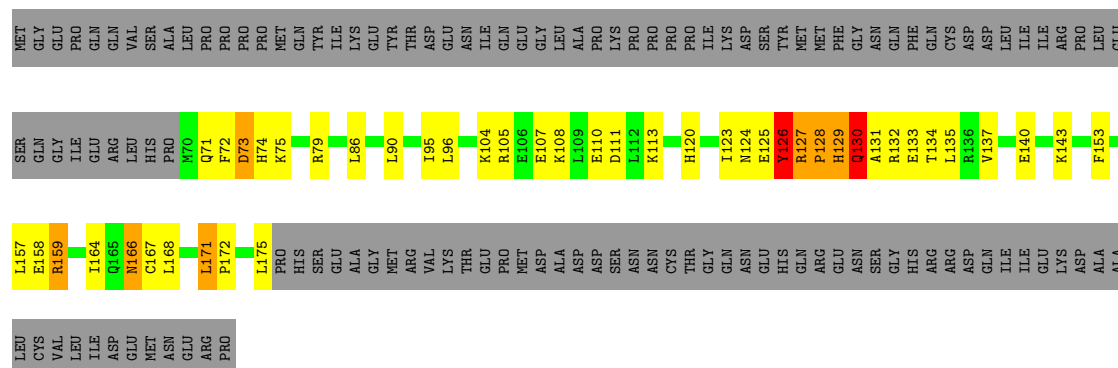
• Molecule 48: DNA-directed RNA polymerase II subunit RPB4



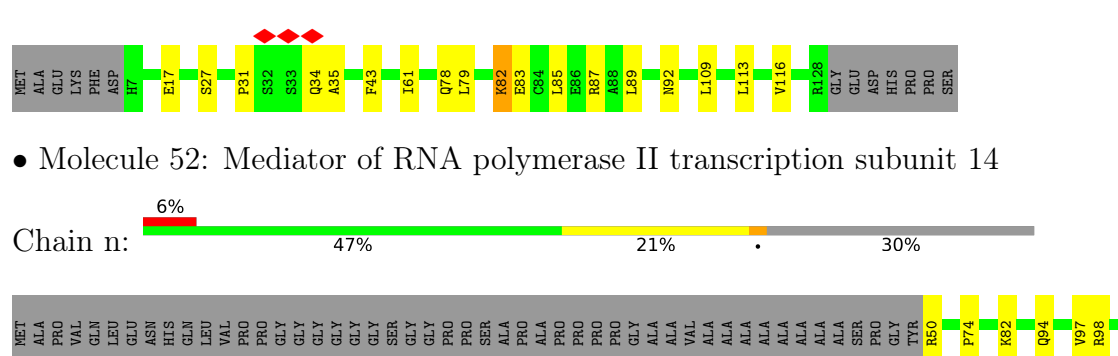
• Molecule 49: DNA-directed RNA polymerase II subunit RPB7



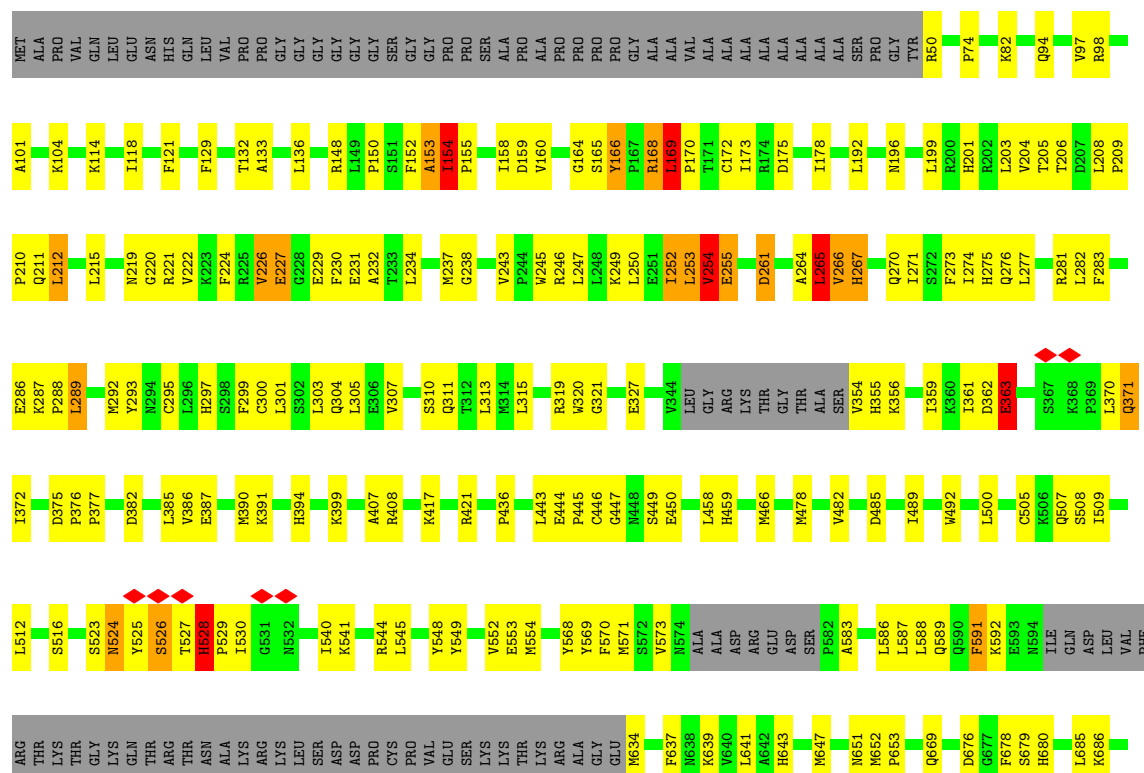
Chain g: 26% 15% .. 55%



Chain j: 77% 13% • 10%



Chain n:





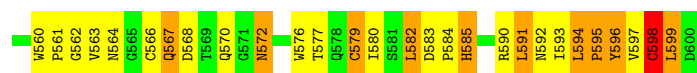
WORLD WIDE
PDB
PROTEIN DATA BANK

L90	L93	E96	E99	T102	C103	L104	D106	V107	V108	V109	R110	G111	L115	E116	K117	I118	L122	A123	D124	I125	S128	Q129	T132	ARG	SER	GLY	HIS	THR	SER	GLN	SER	LEU	PRO	ASP	SER																											
■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■																											
MET	ALA	ASP	R4	L5	T6	Q7	L8	Q9					T23		Q27	Q28	C29	G30	P31	P32			F35	ASN	ASN	TLE	GLN	THR	ALA	ALA	LLE	LYS	ASP	GLN	PRO	A48	M49	P50		A60	L61		R64		K67		V71	L72	I73	D74	S75	L76	P77	S78	E80	S81	I82	A83	A84	L85	O86	A87

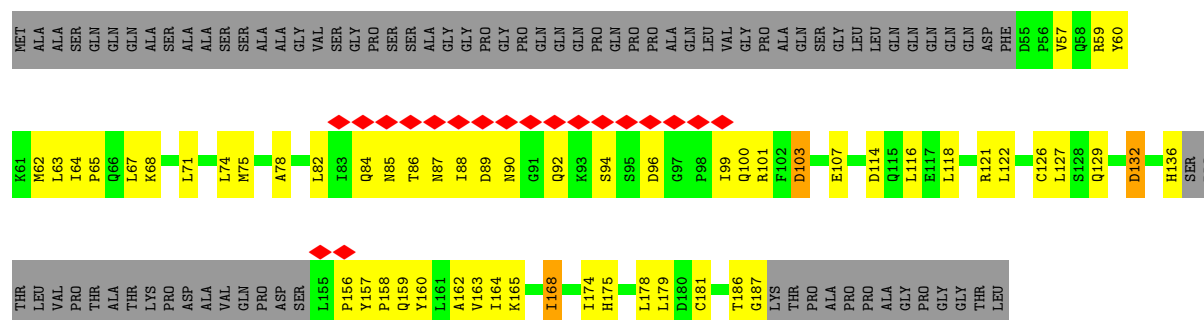
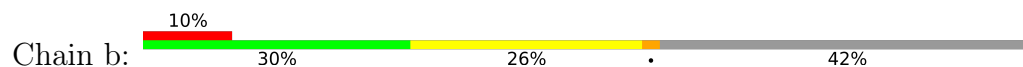
Chain a:



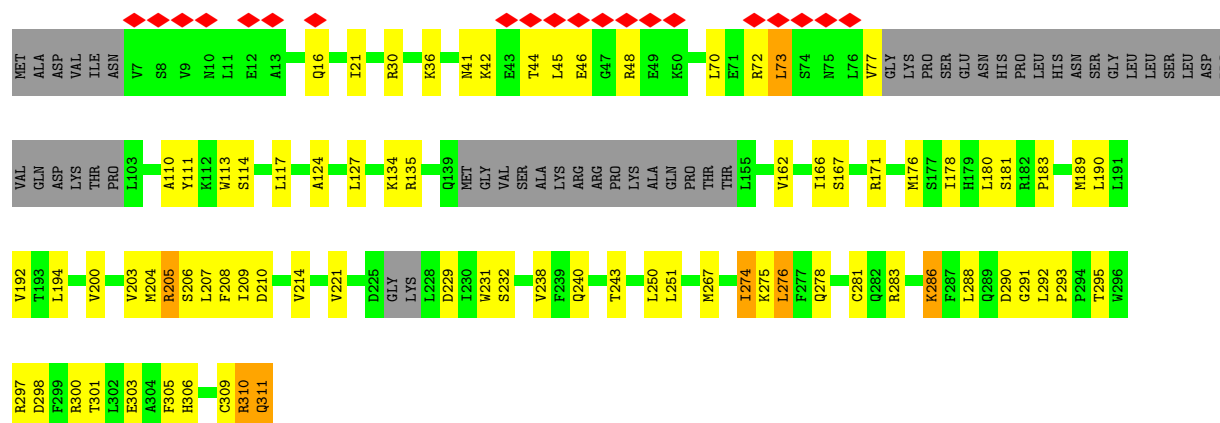




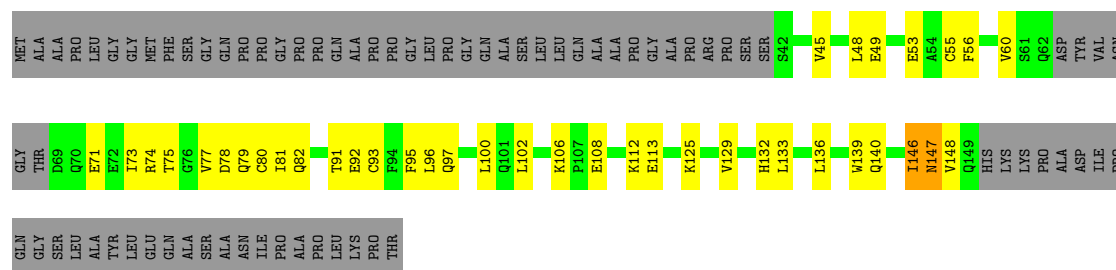
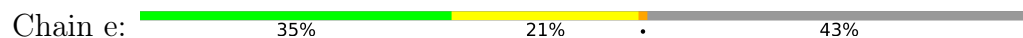
• Molecule 62: Mediator of RNA polymerase II transcription subunit 29



• Molecule 63: Mediator of RNA polymerase II transcription subunit 27

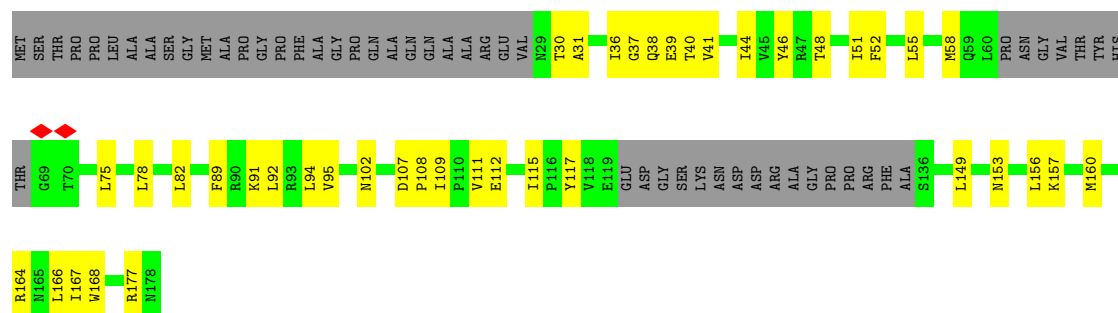


• Molecule 64: Mediator of RNA polymerase II transcription subunit 28



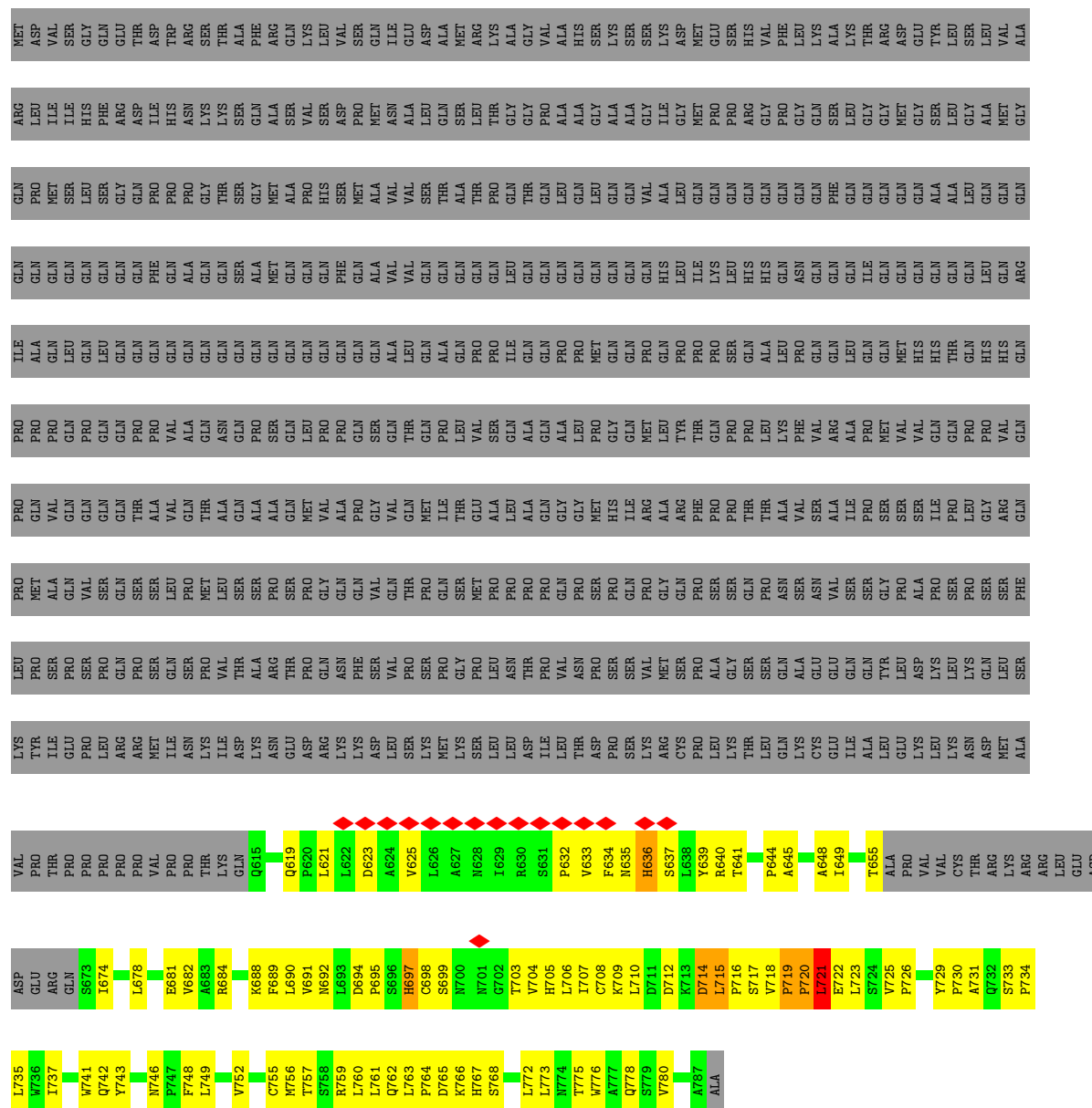
• Molecule 65: Mediator of RNA polymerase II transcription subunit 30



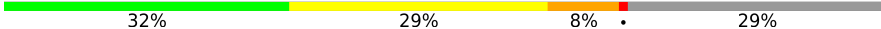


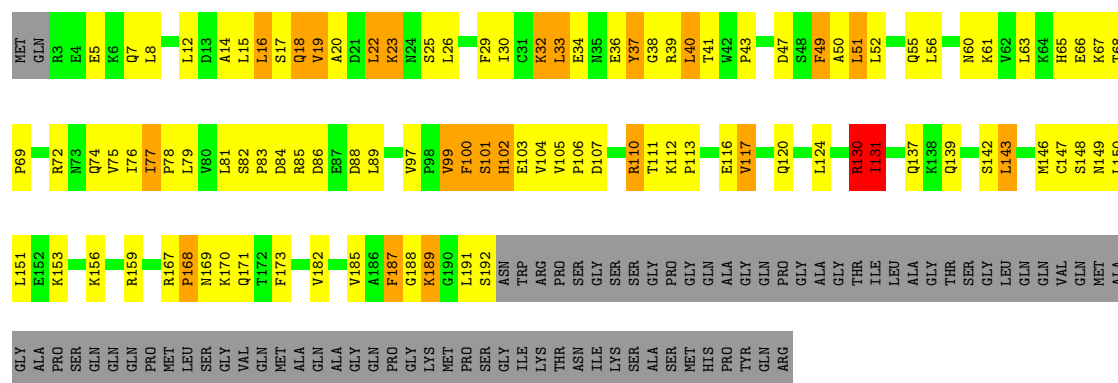
- Molecule 66: Mediator of RNA polymerase II transcription subunit 15

Chain o: 9% 10% 80%

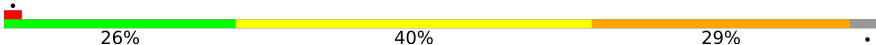


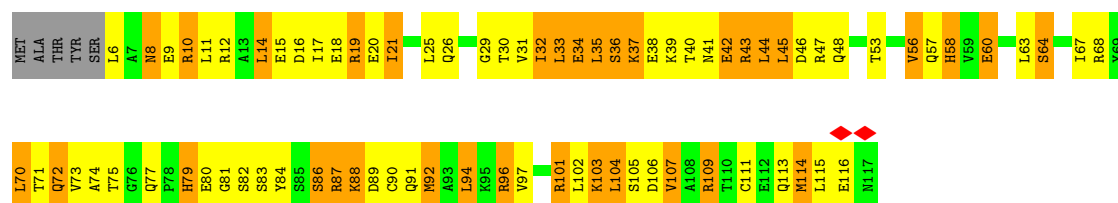
- Molecule 67: Isoform 2 of Mediator of RNA polymerase II transcription subunit 8

Chain h: 



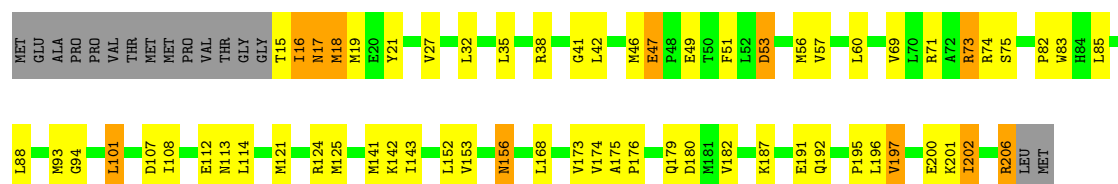
- Molecule 68: Mediator of RNA polymerase II transcription subunit 11

Chain k: 



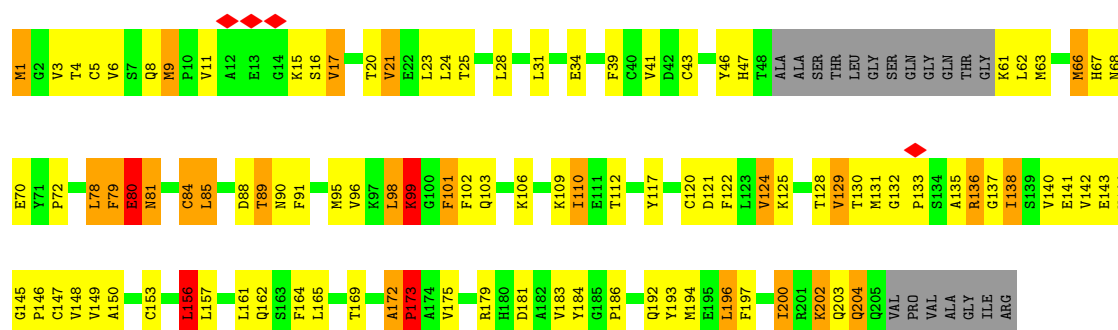
- Molecule 69: Mediator of RNA polymerase II transcription subunit 18

Chain r: 



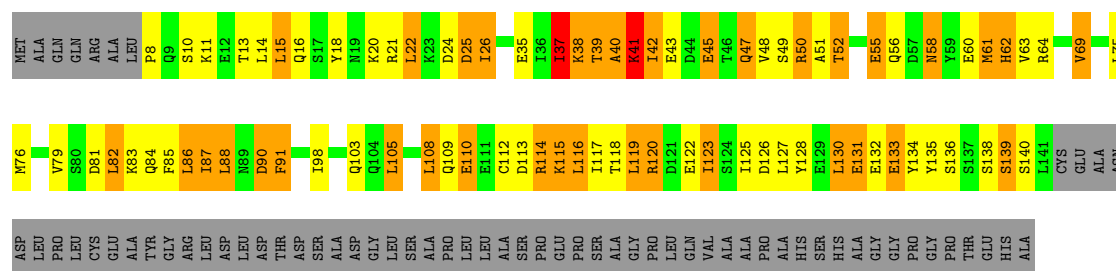
- Molecule 70: Mediator of RNA polymerase II transcription subunit 20

Chain t: 



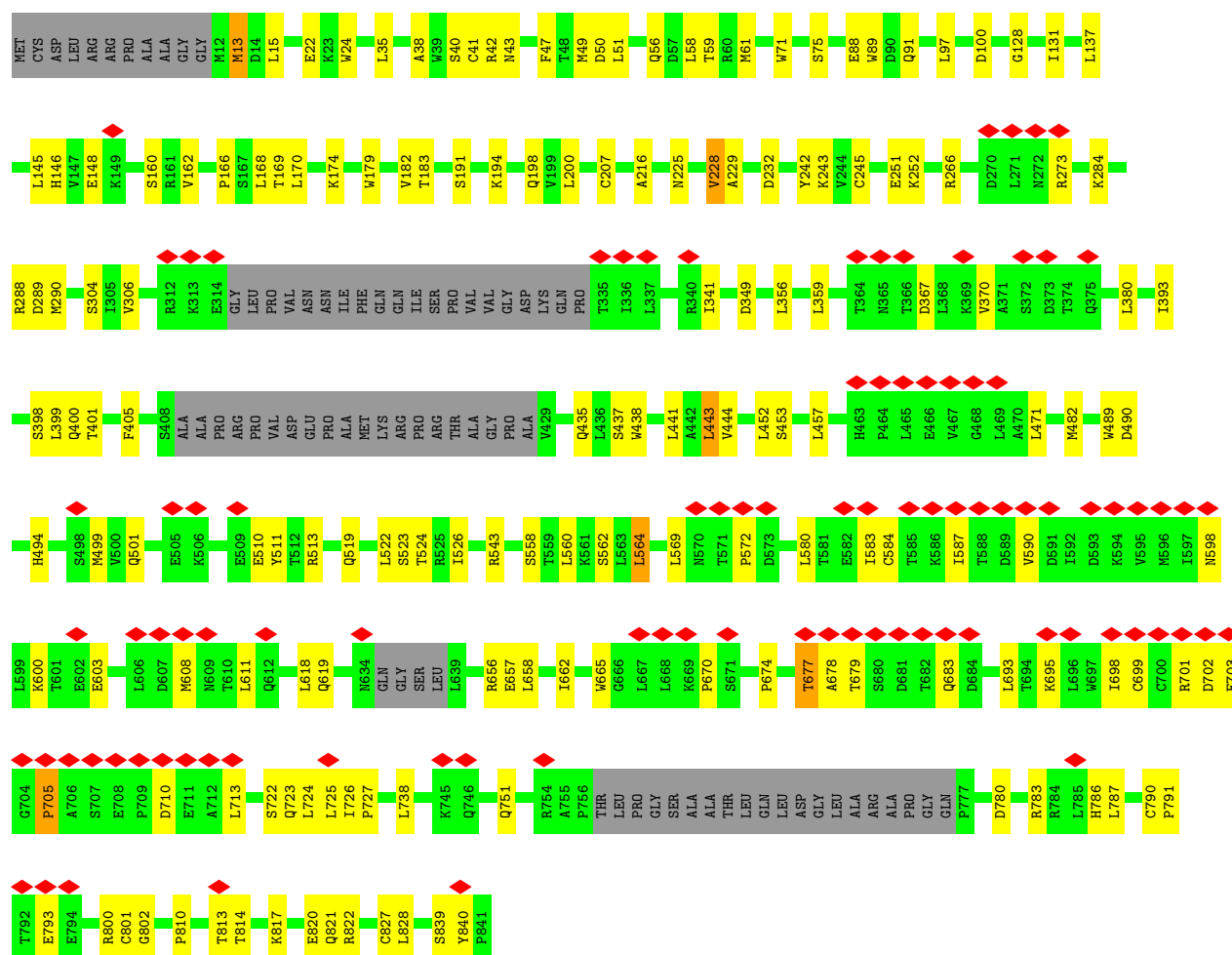
- Molecule 71: Mediator of RNA polymerase II transcription subunit 22

Chain v: 



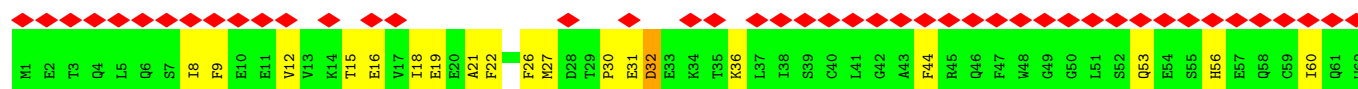
- Molecule 72: Isoform 2 of Mediator of RNA polymerase II transcription subunit 16

Chain p: 

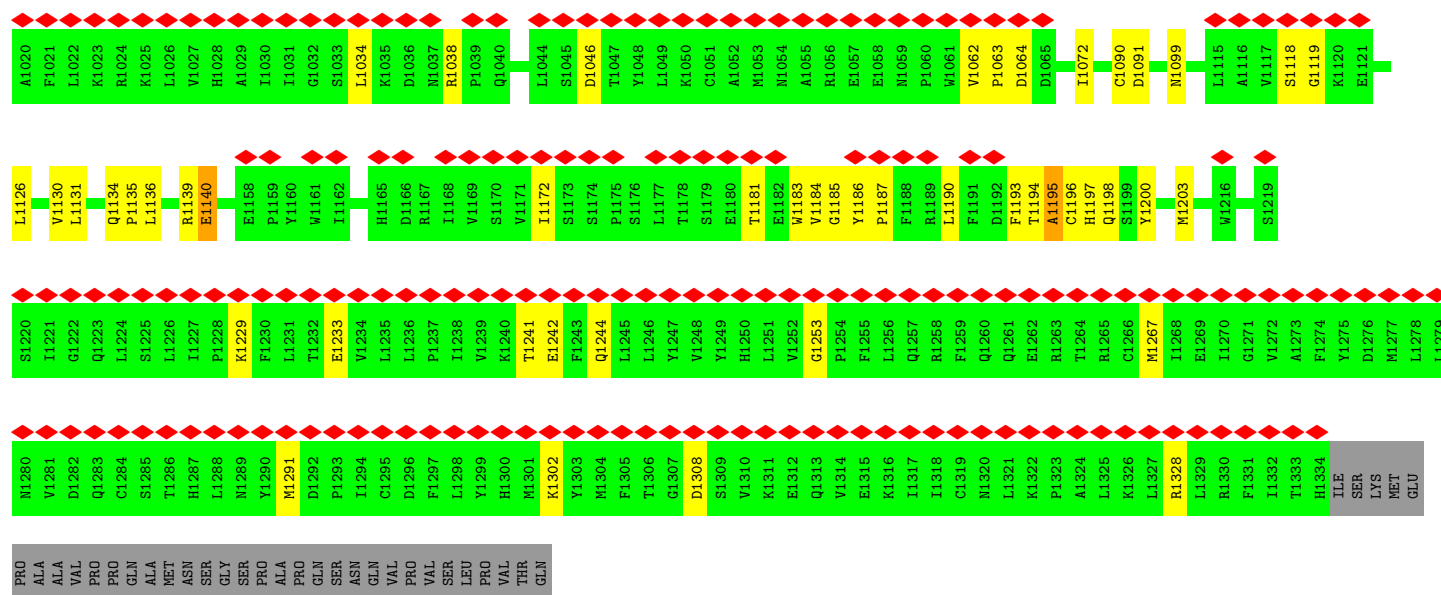


- Molecule 73: Mediator of RNA polymerase II transcription subunit 23

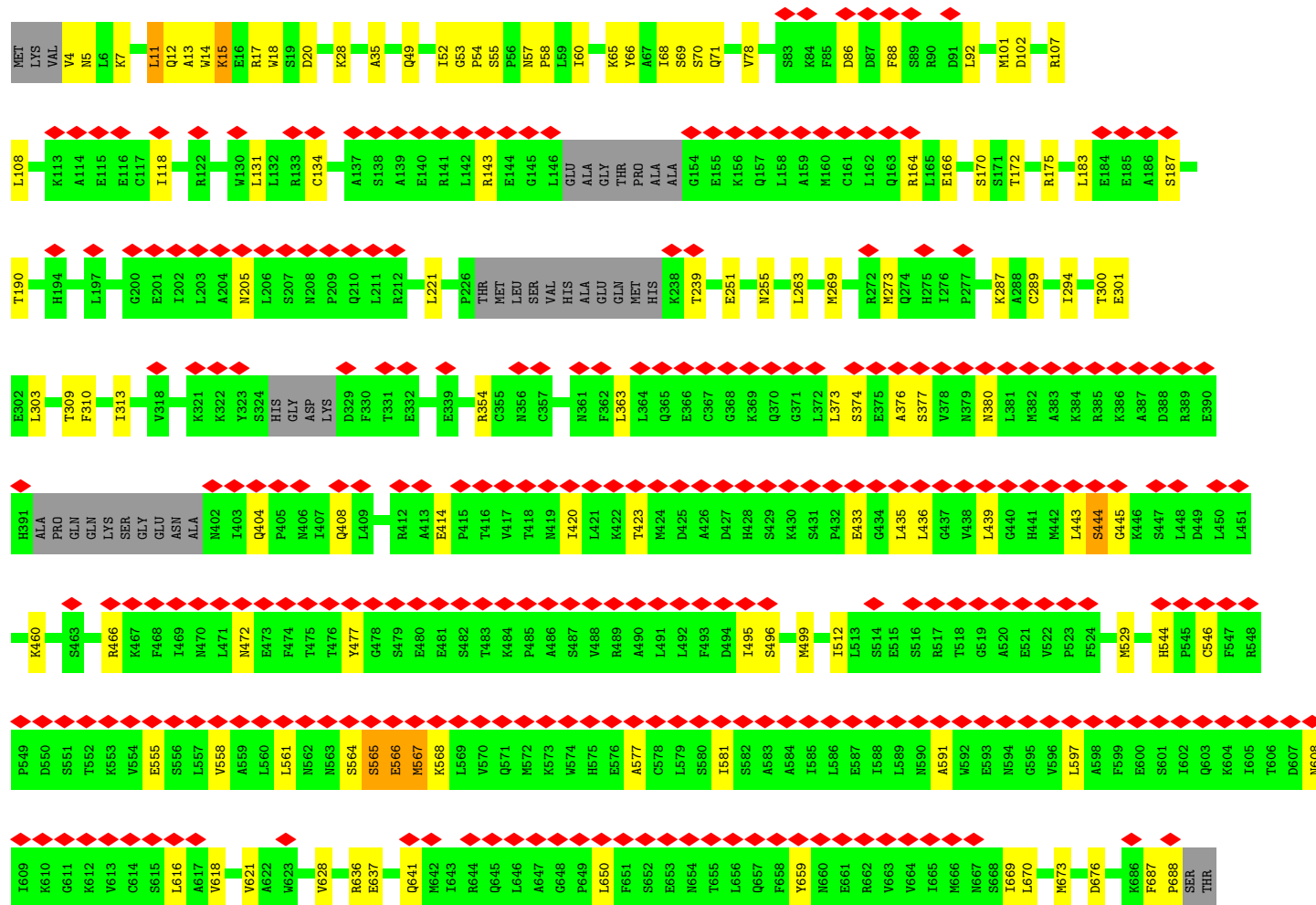
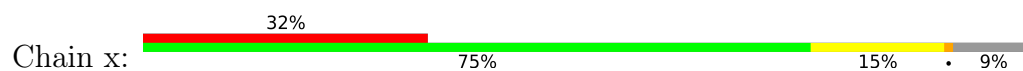
Chain w: 

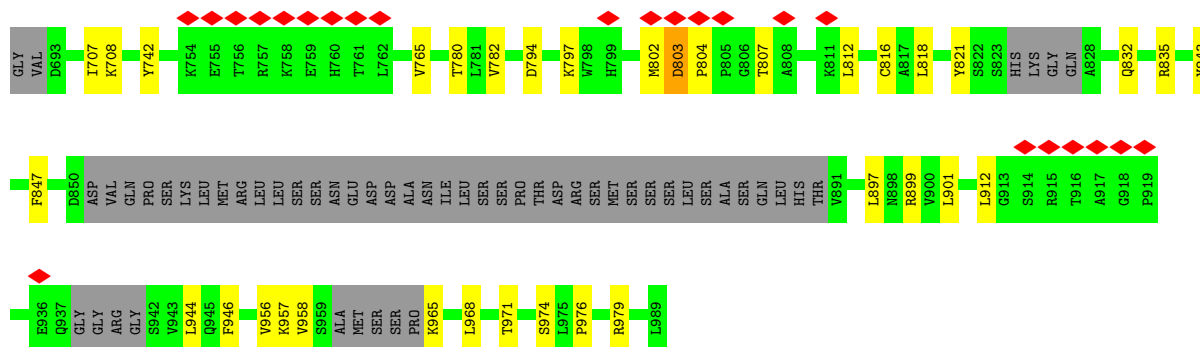


P950	Y951	L952	P953	I954	Y955	F956	G957	N958	V959	C960	L961	R962	F963	L964	P965	V966	F967	D968	I969	V970	I971	H972	R973	F974	L975	E976	L977	L978	P979	V980	K981	K982	S983	L984	E985	T986	L987	L988	D989	H990	L991	G992	G993	L994	Y995	K996	F997	H998	D999	Y1011	Y1012	E1013	M1014	H1015	L1016	L1017	D1018	R1019																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
Q887	L888	L889	L890	L891	K892	P893	P894	G895	F896	T897	S898	R899	G900	Q901	P902	F903	Q904	K905	C906	N907	S908	P909		Q914	N915	D916	W917	H918	T919	K920	L921	M922	N923	Y924	H925	K926	K927	Y928	P929	E930	K931	L932	F933	Y934	E935	G936	L937	H938	D939	Y940	Y1011	Y1012	E1013	M1014	H1015	L1016	L1017	D1018	R1019																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
A827	D828	F829	L830	W831	Y832	E833	F834	S835	T836	S837	A838	G839	C840	Q841	Q842	L843	N844	R845	C846	I847	E848	H849	L850	N851	D852	M853	W854	W855	K856	Y857	N858	L859	N860	T861	L862	D863	R864	L865	T866	L867	C868	L869	A870	M871	R872	S873	H874	E875	G876	N877	E878	A879	Q880	W881	C882	H883	F884	I885	L886																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
W767	K768	S769	W770	S771	W772	E773	W774	D775	L776	I777	T778	F779	F780	S781	W782	Q783	G784	S785	P786	P787	L788	F789	L790	C791	L792	L793	W794	K795	W796	L797	L798	E799	T800	D801	H802	L803	N804	Q805	I806	G807	Y808	R809	V810	L811	E812	R813	T814	G815	A816	R817	A818	L819	W820	A821	W822	H823	R824	T825	F826																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
Q638	N639	Q640	L641	H642	L643	C644	V645	E646	L650		I653		E660	V661	Q662	P663	Q664	F665	T666	R667	F668	L669	S670	D671	P672	K673	T674	V675	L676	S677	A678	E679	S680	E681	E682	L683	M684	R685	A686	L687	L688	L689	T690	L691	A692		T695	H696	V697	T698	D699	F700	F701	T702	G703	S704	D705	S706																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
I707	Q708	G709	T710	W711	C712	K713	C714	W715	L716	Q717	T718	I719	W720	S721	F722	T723	P724	H725	N726	W727	A728	S729	H730	T731	L732	S733	C734	F735	P736	G737	P738	L739	Q740	A741	F742	F743	K744	Q745	W746	W747	W748	F749	Q750	E751	S752	R753	F754	W755	L756	K757	K758	W759	V760	E761	E762	E763	Y764	R765	K766																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
V547	I548	K549	L550	A551	H552	A553	K554	S555	S556	V557	A558	L559	P561	E565	L571	S586	P590	T591	V592	F593	K594	S595	H596	A597	W598	G599	I600	M612	L615	Q616	P617	H618	V619	R620	V621	Q622	L623	L624	S625	H626	L627	H628	T629	L630	A631	A632	V633	A634	Q635	T636	N637																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
L453		E456	F457	L458	Q459	Q460	S461	L462	R463	M464	K465	S466	L467	Q468	M469	M470	D471	Y472	K473	L474	L477		S485	E486		G493	A494	L495	V496	E497	T498		G501	N502	G503	I504	M505	R506	I507	P508	L509	P510	G511	T512	N513	C514	M515	A516	S517	G518	S519	I520	P522		T532	V533	H534																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
L343	F344	Q345	F346	A347	S348	H351	L356	R363	G364	L365	I366	R369	D370	H371	L372	Q378	S381	N387	A388	L389	A390	D391	F392	L402		Y408	I409	P410	V411	P412	D413	I414	M415	K416	P417	Q418	S419	T420	H421	M425	T426	C427	H431	L432	M433	T445		R452																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							



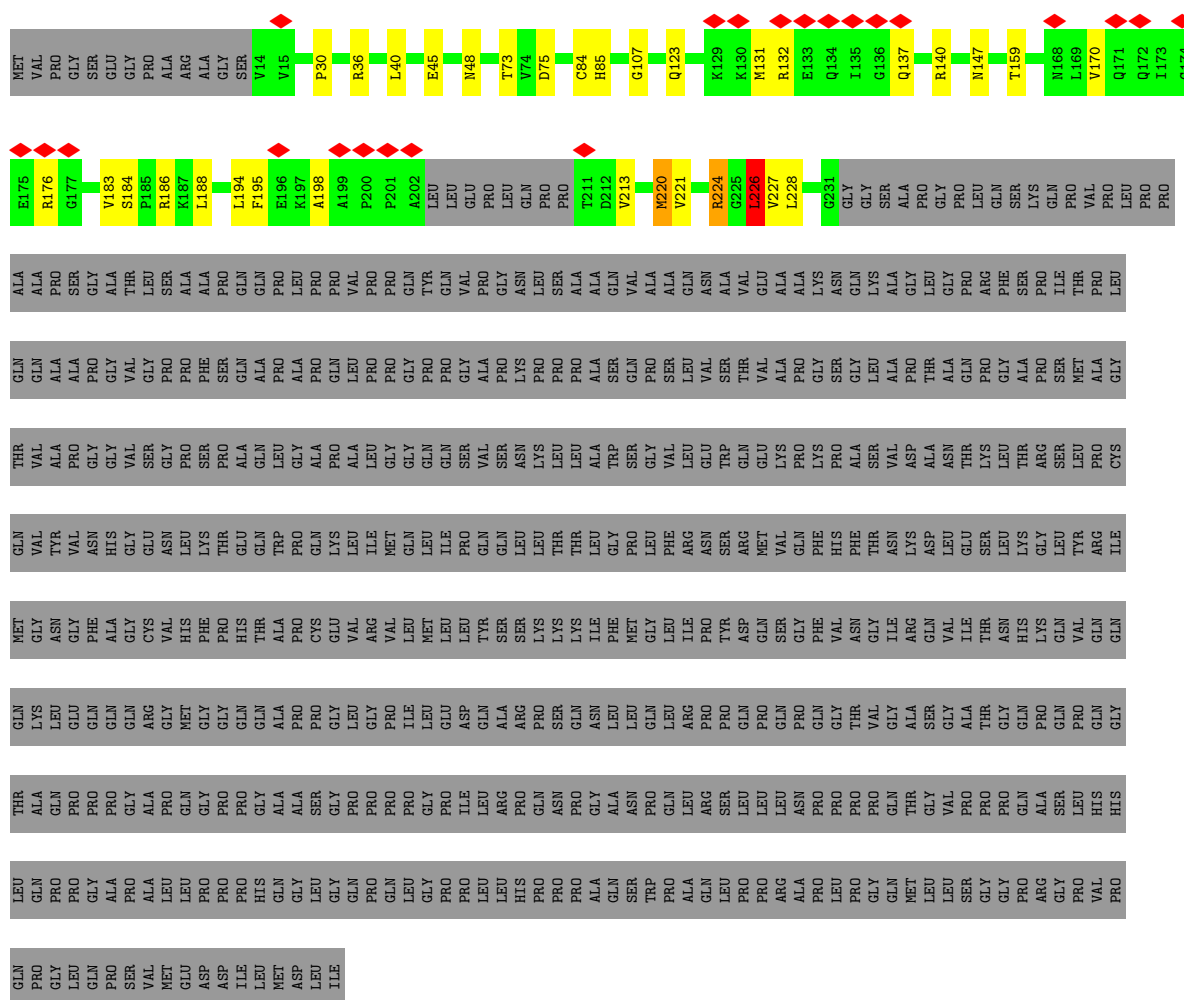
• Molecule 74: Mediator of RNA polymerase II transcription subunit 24





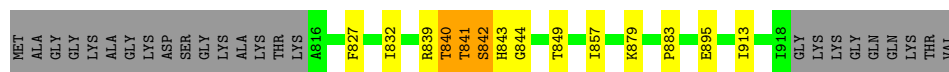
• Molecule 75: Mediator of RNA polymerase II transcription subunit 25

Chain y: 24% 72%

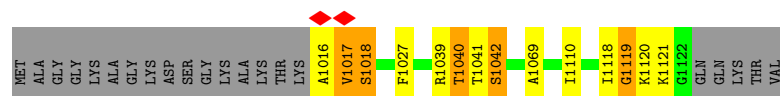


• Molecule 76: HISTONE H2A.Z

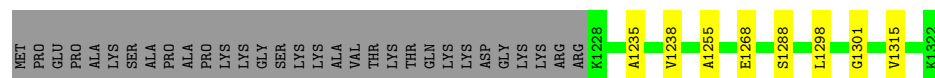
Chain NC: 70% 9% 20%



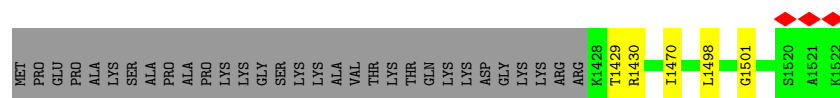
Chain NG:



Chain ND:



Chain NH:



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	29473	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)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.762	Depositor
Minimum map value	-1.277	Depositor
Average map value	0.015	Depositor
Map value standard deviation	0.075	Depositor
Recommended contour level	0.205	Depositor
Map size ($\text{\AA}$)	560.27997, 560.27997, 560.27997	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.3339999, 1.3339999, 1.3339999	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, ZN, 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	X	0.47	0/1561	0.64	2/2411 (0.1%)
2	Y	0.47	0/1516	0.63	1/2334 (0.0%)
3	NX	0.37	0/3401	0.65	1/5180 (0.0%)
4	NY	0.33	0/4046	0.55	0/6310
5	BA	0.14	0/1983	0.27	0/2679
6	DA	0.66	0/4679	0.90	6/6320 (0.1%)
7	EA	0.33	0/1560	0.58	1/2097 (0.0%)
8	FA	0.11	0/1167	0.27	0/1576
9	HA	0.16	0/5875	0.31	0/7955
10	NA	1.12	1/497 (0.2%)	1.44	2/693 (0.3%)
10	NE	1.27	0/510	1.54	6/710 (0.8%)
11	PA	0.24	0/11851	0.38	1/16014 (0.0%)
12	DB	0.49	1/7993 (0.0%)	0.71	8/10836 (0.1%)
13	EB	0.23	0/1427	0.44	0/1916
14	FB	0.20	0/1817	0.35	0/2445
15	HB	0.15	0/2210	0.31	0/2975
16	NB	1.23	0/390	1.46	5/539 (0.9%)
16	NF	1.40	5/420 (1.2%)	1.49	6/581 (1.0%)
17	PB	0.14	0/9257	0.29	0/12493
18	HC	0.21	0/3230	0.37	0/4376
19	DO	0.15	0/816	0.29	0/1105
20	DP	0.14	0/1448	0.28	0/1948
21	DQ	0.16	0/945	0.35	0/1274
22	PC	0.13	0/2102	0.29	0/2857
23	PE	0.16	0/1752	0.30	0/2366
24	PF	0.25	0/646	0.42	0/871
25	PH	0.12	0/1207	0.28	0/1628
26	PI	0.13	0/949	0.29	0/1284
27	PJ	0.14	0/516	0.25	0/696
28	PK	0.15	0/939	0.27	0/1271
29	PL	0.14	0/378	0.28	0/500
30	HD	0.70	0/2436	1.03	18/3286 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	HG	0.13	0/2793	0.28	0/3780
32	HE	0.25	0/2103	0.39	0/2846
33	HF	0.20	0/529	0.43	1/714 (0.1%)
34	HH	0.16	0/4994	0.31	1/6745 (0.0%)
35	DD	0.56	0/1343	0.83	2/1795 (0.1%)
35	Dd	0.23	0/1321	0.44	0/1772
36	DE	0.43	0/4469	0.64	1/6050 (0.0%)
36	De	0.30	0/4433	0.53	0/6004
37	DF	0.70	1/3167 (0.0%)	1.08	10/4303 (0.2%)
37	Df	0.48	0/3140	0.81	6/4268 (0.1%)
38	DG	0.71	0/1199	0.95	1/1612 (0.1%)
39	DH	0.46	0/1673	0.75	2/2285 (0.1%)
40	DI	0.58	0/981	0.90	5/1332 (0.4%)
40	Di	0.24	0/989	0.48	2/1343 (0.1%)
41	DL	0.65	0/613	1.03	1/829 (0.1%)
41	DI	0.54	0/888	0.80	0/1194
42	Dc	0.48	0/1035	0.67	0/1406
43	DJ	0.24	0/736	0.46	0/998
43	Dj	0.23	0/775	0.45	0/1049
44	Dk	0.30	0/799	0.53	1/1070 (0.1%)
45	Dm	0.31	0/733	0.55	0/977
46	HI	1.02	0/2433	1.64	45/3302 (1.4%)
47	HJ	1.10	3/2356 (0.1%)	1.72	54/3185 (1.7%)
48	PD	0.26	0/1064	0.43	1/1428 (0.1%)
49	PG	0.18	0/1382	0.28	0/1874
50	g	0.79	1/911 (0.1%)	1.40	8/1219 (0.7%)
51	j	0.38	0/849	0.61	0/1150
52	n	0.43	0/7901	0.73	17/10731 (0.2%)
53	s	0.93	0/741	1.26	6/1002 (0.6%)
54	u	0.75	1/895 (0.1%)	1.09	9/1215 (0.7%)
55	a	0.93	0/3507	1.34	11/4760 (0.2%)
56	d	0.92	0/1281	1.30	1/1718 (0.1%)
57	f	0.76	1/1402 (0.1%)	1.07	6/1905 (0.3%)
58	i	0.99	1/612 (0.2%)	1.35	1/815 (0.1%)
59	m	0.21	0/1010	0.39	0/1359
60	q	0.66	1/4456 (0.0%)	0.87	0/6019
61	z	0.95	0/781	1.41	6/1067 (0.6%)
62	b	0.75	0/911	1.13	1/1229 (0.1%)
63	c	0.58	0/2172	0.90	5/2935 (0.2%)
64	e	0.25	0/840	0.44	0/1128
65	l	0.20	0/1048	0.41	0/1405
66	o	0.53	0/1256	0.86	3/1724 (0.2%)
67	h	0.94	0/1485	1.33	4/2008 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
68	k	0.98	0/885	1.31	1/1190 (0.1%)
69	r	0.91	0/1565	1.26	3/2106 (0.1%)
70	t	1.05	2/1530 (0.1%)	1.49	11/2066 (0.5%)
71	v	0.98	0/1092	1.43	5/1468 (0.3%)
72	p	0.65	0/6116	0.76	3/8311 (0.0%)
73	w	0.52	0/11056	0.65	5/15023 (0.0%)
74	x	0.59	0/7191	0.78	11/9728 (0.1%)
75	y	0.63	0/1645	0.83	0/2240
76	NC	1.27	2/505 (0.4%)	1.53	9/700 (1.3%)
76	NG	1.08	1/523 (0.2%)	1.43	10/724 (1.4%)
77	ND	1.22	2/470 (0.4%)	1.46	5/654 (0.8%)
77	NH	1.09	0/470	1.44	4/654 (0.6%)
All	All	0.53	23/190578 (0.0%)	0.77	335/259940 (0.1%)

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	q	452	ALA	C-N	9.12	1.47	1.33
57	f	110	ASP	C-N	-8.20	1.22	1.33
47	HJ	244	CYS	C-O	7.08	1.32	1.24
70	t	136	ARG	C-O	-6.88	1.15	1.23
70	t	89	THR	C-O	6.60	1.32	1.24

The worst 5 of 335 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	g	128	PRO	N-CA-C	-13.22	92.27	114.75
10	NA	464	LYS	N-CA-C	12.63	124.58	111.07
50	g	130	GLN	N-CA-C	-12.41	97.80	111.07
74	x	12	GLN	N-CA-C	-11.51	99.19	113.01
10	NE	635	VAL	N-CA-C	-10.85	102.26	111.91

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	X	1387	0	747	14	0
2	Y	1357	0	752	14	0
3	NX	3078	0	1783	11	0
4	NY	3561	0	1784	26	0
5	BA	1953	0	1987	20	0
6	DA	4563	0	4485	99	0
7	EA	1535	0	1539	140	0
8	FA	1138	0	1103	15	0
9	HA	5751	0	5794	105	0
10	NA	498	0	230	2	0
10	NE	511	0	238	5	0
11	PA	11628	0	11712	210	0
12	DB	7796	0	7751	148	0
13	EB	1403	0	1428	57	0
14	FB	1788	0	1819	32	0
15	HB	2167	0	2175	34	0
16	NB	391	0	185	0	0
16	NF	421	0	197	1	0
17	PB	9076	0	9116	130	0
18	HC	3158	0	3213	130	0
19	DO	806	0	818	31	0
20	DP	1422	0	1514	17	0
21	DQ	930	0	888	15	0
22	PC	2059	0	2007	22	0
23	PE	1721	0	1737	16	0
24	PF	636	0	665	11	0
25	PH	1186	0	1147	8	0
26	PI	928	0	859	11	0
27	PJ	507	0	523	14	0
28	PK	920	0	942	12	0
29	PL	373	0	378	8	0
30	HD	2400	0	2295	225	0
31	HG	2732	0	2698	42	0
32	HE	2066	0	2097	51	0
33	HF	523	0	530	52	0
34	HH	4890	0	4949	66	0
35	DD	1330	0	1351	138	0
35	Dd	1307	0	1318	13	0
36	DE	4364	0	4244	150	0
36	De	4327	0	4197	44	0
37	DF	3109	0	3045	310	0
37	Df	3081	0	3012	66	0
38	DG	1180	0	1235	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	DH	1633	0	1621	165	0
40	DI	959	0	969	135	0
40	Di	967	0	977	31	0
41	DL	605	0	606	76	0
41	Dl	876	0	893	25	0
42	Dc	1011	0	975	25	0
43	DJ	720	0	719	136	0
43	Dj	759	0	759	18	0
44	Dk	785	0	818	8	0
45	Dm	724	0	744	13	0
46	HI	2374	0	2389	172	0
47	HJ	2307	0	2314	148	0
48	PD	1050	0	1033	76	0
49	PG	1351	0	1358	139	0
50	g	898	0	936	77	0
51	j	840	0	718	37	0
52	n	7751	0	7530	593	0
53	s	723	0	727	57	0
54	u	886	0	871	138	0
55	a	3430	0	3461	423	0
56	d	1268	0	1305	279	0
57	f	1365	0	1337	153	0
58	i	605	0	628	210	0
59	m	983	0	968	91	0
60	q	4373	0	4433	546	0
61	z	765	0	728	79	0
62	b	899	0	908	114	0
63	c	2131	0	2140	133	0
64	e	832	0	824	101	0
65	l	1040	0	1065	85	0
66	o	1221	0	1212	120	0
67	h	1465	0	1460	213	0
68	k	879	0	886	197	0
69	r	1535	0	1545	54	0
70	t	1499	0	1482	105	0
71	v	1083	0	1059	196	0
72	p	5983	0	6071	134	0
73	w	10774	0	10838	146	0
74	x	7061	0	7223	226	0
75	y	1605	0	1576	24	0
76	NC	506	0	250	4	0
76	NG	524	0	260	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
77	ND	471	0	221	0	0
77	NH	471	0	221	0	0
78	BA	1	0	0	0	0
78	EA	1	0	0	0	0
78	HD	2	0	0	0	0
78	HE	2	0	0	0	0
78	HG	3	0	0	0	0
78	PA	2	0	0	0	0
78	PB	1	0	0	0	0
78	PC	1	0	0	0	0
78	PI	2	0	0	0	0
78	PJ	1	0	0	0	0
78	PL	1	0	0	0	0
78	c	1	0	0	0	0
78	p	1	0	0	0	0
79	HA	8	0	0	0	0
80	PA	1	0	0	0	0
All	All	185972	0	179545	6043	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 6043 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)
56:d:49:ALA:HB2	58:i:76:MET:SD	1.21	1.70
12:DB:672:PHE:CD1	18:HC:414:SER:HB3	1.22	1.69
11:PA:1795:PRO:HD2	56:d:169:PRO:CB	1.24	1.63
7:EA:139:LEU:HD11	49:PG:151:ARG:CD	1.25	1.61
48:PD:79:THR:HG22	67:h:51:LEU:CD2	1.29	1.61

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	
5	BA	248/316 (78%)	246 (99%)	2 (1%)	0	100	100
6	DA	542/1872 (29%)	524 (97%)	15 (3%)	3 (1%)	21	58
7	EA	185/439 (42%)	183 (99%)	1 (0%)	1 (0%)	24	61
8	FA	134/517 (26%)	129 (96%)	5 (4%)	0	100	100
9	HA	710/760 (93%)	682 (96%)	28 (4%)	0	100	100
10	NA	98/136 (72%)	94 (96%)	2 (2%)	2 (2%)	6	31
10	NE	101/136 (74%)	96 (95%)	3 (3%)	2 (2%)	6	31
11	PA	1457/1970 (74%)	1406 (96%)	47 (3%)	4 (0%)	36	70
12	DB	959/1199 (80%)	910 (95%)	49 (5%)	0	100	100
13	EB	169/291 (58%)	164 (97%)	5 (3%)	0	100	100
14	FB	218/249 (88%)	213 (98%)	4 (2%)	1 (0%)	24	61
15	HB	253/548 (46%)	245 (97%)	8 (3%)	0	100	100
16	NB	78/103 (76%)	78 (100%)	0	0	100	100
16	NF	84/103 (82%)	77 (92%)	4 (5%)	3 (4%)	2	20
17	PB	1130/1174 (96%)	1093 (97%)	37 (3%)	0	100	100
18	HC	380/462 (82%)	363 (96%)	17 (4%)	0	100	100
19	DO	97/109 (89%)	95 (98%)	2 (2%)	0	100	100
20	DP	177/339 (52%)	175 (99%)	2 (1%)	0	100	100
21	DQ	109/376 (29%)	102 (94%)	7 (6%)	0	100	100
22	PC	253/275 (92%)	241 (95%)	12 (5%)	0	100	100
23	PE	207/210 (99%)	203 (98%)	4 (2%)	0	100	100
24	PF	77/127 (61%)	76 (99%)	1 (1%)	0	100	100
25	PH	146/150 (97%)	143 (98%)	3 (2%)	0	100	100
26	PI	112/125 (90%)	104 (93%)	8 (7%)	0	100	100
27	PJ	62/67 (92%)	60 (97%)	2 (3%)	0	100	100
28	PK	113/117 (97%)	112 (99%)	1 (1%)	0	100	100
29	PL	42/58 (72%)	40 (95%)	2 (5%)	0	100	100
30	HD	304/309 (98%)	265 (87%)	29 (10%)	10 (3%)	3	21
31	HG	341/395 (86%)	329 (96%)	12 (4%)	0	100	100
32	HE	259/308 (84%)	253 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	HF	64/71 (90%)	62 (97%)	2 (3%)	0	100	100
34	HH	601/782 (77%)	573 (95%)	27 (4%)	1 (0%)	43	76
35	DD	153/1085 (14%)	146 (95%)	5 (3%)	2 (1%)	9	41
35	Dd	154/1085 (14%)	150 (97%)	4 (3%)	0	100	100
36	DE	540/800 (68%)	506 (94%)	32 (6%)	2 (0%)	30	65
36	De	531/800 (66%)	484 (91%)	47 (9%)	0	100	100
37	DF	404/677 (60%)	377 (93%)	20 (5%)	7 (2%)	7	35
37	Df	399/677 (59%)	378 (95%)	20 (5%)	1 (0%)	36	70
38	DG	139/349 (40%)	135 (97%)	4 (3%)	0	100	100
39	DH	207/310 (67%)	191 (92%)	12 (6%)	4 (2%)	6	32
40	DI	118/264 (45%)	113 (96%)	4 (3%)	1 (1%)	16	52
40	Di	119/264 (45%)	115 (97%)	4 (3%)	0	100	100
41	DL	72/161 (45%)	62 (86%)	6 (8%)	4 (6%)	1	15
41	DI	105/161 (65%)	101 (96%)	4 (4%)	0	100	100
42	Dc	125/929 (14%)	116 (93%)	9 (7%)	0	100	100
43	DJ	86/218 (39%)	82 (95%)	4 (5%)	0	100	100
43	Dj	91/218 (42%)	89 (98%)	2 (2%)	0	100	100
44	Dk	96/211 (46%)	91 (95%)	5 (5%)	0	100	100
45	Dm	85/124 (68%)	79 (93%)	6 (7%)	0	100	100
46	HI	297/346 (86%)	265 (89%)	20 (7%)	12 (4%)	2	19
47	HJ	285/323 (88%)	268 (94%)	14 (5%)	3 (1%)	11	44
48	PD	126/142 (89%)	122 (97%)	4 (3%)	0	100	100
49	PG	169/172 (98%)	166 (98%)	3 (2%)	0	100	100
50	g	104/233 (45%)	99 (95%)	4 (4%)	1 (1%)	12	46
51	j	120/135 (89%)	117 (98%)	1 (1%)	2 (2%)	7	35
52	n	993/1454 (68%)	894 (90%)	80 (8%)	19 (2%)	6	32
53	s	91/244 (37%)	81 (89%)	8 (9%)	2 (2%)	5	29
54	u	113/144 (78%)	104 (92%)	5 (4%)	4 (4%)	3	21
55	a	430/1581 (27%)	387 (90%)	38 (9%)	5 (1%)	10	42
56	d	154/270 (57%)	143 (93%)	9 (6%)	2 (1%)	9	41
57	f	163/246 (66%)	150 (92%)	12 (7%)	1 (1%)	21	58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
58	i	69/146 (47%)	65 (94%)	2 (3%)	2 (3%)	3	24
59	m	110/131 (84%)	106 (96%)	4 (4%)	0	100	100
60	q	543/651 (83%)	486 (90%)	50 (9%)	7 (1%)	9	41
61	z	93/600 (16%)	83 (89%)	7 (8%)	3 (3%)	3	22
62	b	111/200 (56%)	109 (98%)	1 (1%)	1 (1%)	14	48
63	c	255/311 (82%)	239 (94%)	15 (6%)	1 (0%)	30	65
64	e	98/178 (55%)	92 (94%)	4 (4%)	2 (2%)	6	31
65	l	120/178 (67%)	115 (96%)	5 (4%)	0	100	100
66	o	152/788 (19%)	135 (89%)	13 (9%)	4 (3%)	4	26
67	h	188/268 (70%)	165 (88%)	15 (8%)	8 (4%)	2	18
68	k	110/117 (94%)	96 (87%)	12 (11%)	2 (2%)	6	33
69	r	190/208 (91%)	180 (95%)	6 (3%)	4 (2%)	5	30
70	t	189/212 (89%)	169 (89%)	16 (8%)	4 (2%)	5	30
71	v	132/200 (66%)	116 (88%)	10 (8%)	6 (4%)	2	17
72	p	756/841 (90%)	707 (94%)	47 (6%)	2 (0%)	36	70
73	w	1332/1368 (97%)	1262 (95%)	66 (5%)	4 (0%)	36	70
74	x	877/989 (89%)	828 (94%)	44 (5%)	5 (1%)	21	58
75	y	206/747 (28%)	196 (95%)	9 (4%)	1 (0%)	24	61
76	NC	101/128 (79%)	93 (92%)	5 (5%)	3 (3%)	3	23
76	NG	105/128 (82%)	94 (90%)	8 (8%)	3 (3%)	3	24
77	ND	93/126 (74%)	91 (98%)	1 (1%)	1 (1%)	11	44
77	NH	93/126 (74%)	89 (96%)	3 (3%)	1 (1%)	11	44
All	All	22102/36357 (61%)	20863 (94%)	1076 (5%)	163 (1%)	20	54

5 of 163 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	DA	498	PRO
6	DA	1158	SER
10	NA	534	ARG
11	PA	1666	PRO
14	FB	229	HIS

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	
5	BA	215/268 (80%)	215 (100%)	0	100	100
6	DA	495/1665 (30%)	461 (93%)	34 (7%)	14	37
7	EA	169/373 (45%)	166 (98%)	3 (2%)	51	66
8	FA	121/448 (27%)	121 (100%)	0	100	100
9	HA	624/664 (94%)	623 (100%)	1 (0%)	87	85
11	PA	1302/1749 (74%)	1296 (100%)	6 (0%)	81	81
12	DB	876/1083 (81%)	861 (98%)	15 (2%)	53	67
13	EB	154/261 (59%)	154 (100%)	0	100	100
14	FB	196/218 (90%)	196 (100%)	0	100	100
15	HB	241/484 (50%)	241 (100%)	0	100	100
17	PB	994/1027 (97%)	994 (100%)	0	100	100
18	HC	342/399 (86%)	342 (100%)	0	100	100
19	DO	90/98 (92%)	90 (100%)	0	100	100
20	DP	154/293 (53%)	154 (100%)	0	100	100
21	DQ	105/324 (32%)	105 (100%)	0	100	100
22	PC	234/252 (93%)	234 (100%)	0	100	100
23	PE	191/192 (100%)	190 (100%)	1 (0%)	81	81
24	PF	69/111 (62%)	68 (99%)	1 (1%)	59	70
25	PH	129/131 (98%)	129 (100%)	0	100	100
26	PI	103/112 (92%)	103 (100%)	0	100	100
27	PJ	53/56 (95%)	53 (100%)	0	100	100
28	PK	104/106 (98%)	104 (100%)	0	100	100
29	PL	41/55 (74%)	41 (100%)	0	100	100
30	HD	251/283 (89%)	227 (90%)	24 (10%)	8	26
31	HG	311/352 (88%)	311 (100%)	0	100	100
32	HE	234/272 (86%)	230 (98%)	4 (2%)	53	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	HF	59/64 (92%)	59 (100%)	0	100	100
34	HH	536/688 (78%)	533 (99%)	3 (1%)	78	80
35	DD	144/815 (18%)	131 (91%)	13 (9%)	9	29
35	Dd	146/815 (18%)	146 (100%)	0	100	100
36	DE	478/657 (73%)	465 (97%)	13 (3%)	39	60
36	De	475/657 (72%)	473 (100%)	2 (0%)	84	82
37	DF	324/574 (56%)	292 (90%)	32 (10%)	7	25
37	Df	322/574 (56%)	312 (97%)	10 (3%)	35	56
38	DG	133/322 (41%)	125 (94%)	8 (6%)	17	41
39	DH	181/270 (67%)	171 (94%)	10 (6%)	19	43
40	DI	106/235 (45%)	97 (92%)	9 (8%)	10	30
40	Di	107/235 (46%)	106 (99%)	1 (1%)	70	75
41	DL	69/141 (49%)	58 (84%)	11 (16%)	2	13
41	DI	98/141 (70%)	98 (100%)	0	100	100
42	Dc	113/833 (14%)	111 (98%)	2 (2%)	51	66
43	DJ	79/154 (51%)	77 (98%)	2 (2%)	42	62
43	Dj	83/154 (54%)	83 (100%)	0	100	100
44	Dk	87/182 (48%)	87 (100%)	0	100	100
45	Dm	80/106 (76%)	79 (99%)	1 (1%)	61	71
46	HI	258/298 (87%)	183 (71%)	75 (29%)	0	2
47	HJ	252/296 (85%)	173 (69%)	79 (31%)	0	2
48	PD	118/126 (94%)	116 (98%)	2 (2%)	53	67
49	PG	152/153 (99%)	151 (99%)	1 (1%)	76	78
50	g	102/216 (47%)	94 (92%)	8 (8%)	11	33
51	j	66/124 (53%)	65 (98%)	1 (2%)	57	70
52	n	807/1271 (64%)	785 (97%)	22 (3%)	39	60
53	s	83/208 (40%)	74 (89%)	9 (11%)	6	22
54	u	95/119 (80%)	91 (96%)	4 (4%)	26	49
55	a	393/1391 (28%)	316 (80%)	77 (20%)	1	9
56	d	139/230 (60%)	93 (67%)	46 (33%)	0	2
57	f	149/223 (67%)	131 (88%)	18 (12%)	5	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
58	i	71/133 (53%)	61 (86%)	10 (14%)	3	16
59	m	102/115 (89%)	101 (99%)	1 (1%)	68	75
60	q	491/577 (85%)	405 (82%)	86 (18%)	2	11
61	z	89/512 (17%)	74 (83%)	15 (17%)	2	12
62	b	102/163 (63%)	91 (89%)	11 (11%)	6	22
63	c	238/280 (85%)	225 (94%)	13 (6%)	19	43
64	e	94/152 (62%)	94 (100%)	0	100	100
65	l	116/155 (75%)	116 (100%)	0	100	100
66	o	141/697 (20%)	136 (96%)	5 (4%)	32	54
67	h	161/225 (72%)	125 (78%)	36 (22%)	1	6
68	k	94/98 (96%)	43 (46%)	51 (54%)	0	0
69	r	169/183 (92%)	140 (83%)	29 (17%)	2	12
70	t	166/178 (93%)	124 (75%)	42 (25%)	0	4
71	v	122/173 (70%)	76 (62%)	46 (38%)	0	1
72	p	681/736 (92%)	670 (98%)	11 (2%)	55	68
73	w	1203/1232 (98%)	1198 (100%)	5 (0%)	84	82
74	x	789/864 (91%)	779 (99%)	10 (1%)	61	71
75	y	175/601 (29%)	171 (98%)	4 (2%)	44	64
All	All	19036/30622 (62%)	18113 (95%)	923 (5%)	24	46

5 of 923 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
55	a	376	LEU
71	v	130	LEU
60	q	100	ASN
71	v	114	ARG
69	r	200	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 361 such sidechains are listed below:

Mol	Chain	Res	Type
59	m	80	GLN
68	k	66	GLN
60	q	321	GLN

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Mol	Chain	Res	Type
61	z	567	GLN
72	p	63	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 21 ligands modelled in this entry, 20 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	$\# Z > 2$
79	SF4	HA	1000	9	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
79	SF4	HA	1000	9	-	-	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.

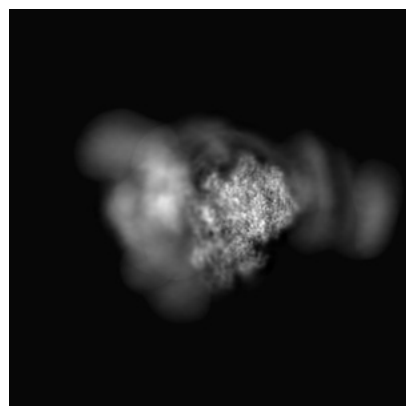
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34360. These allow visual inspection of the internal detail of the map and identification of artifacts.

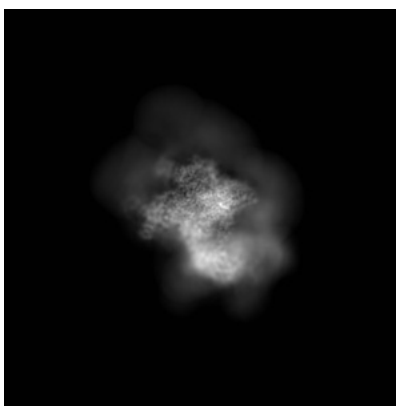
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

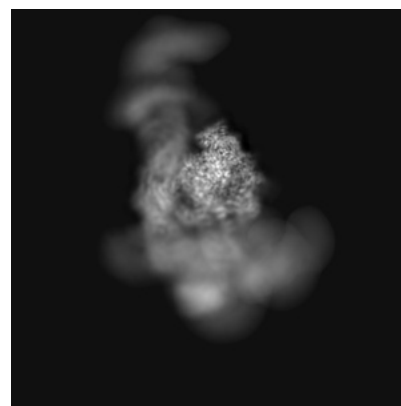
6.1.1 Primary map



X

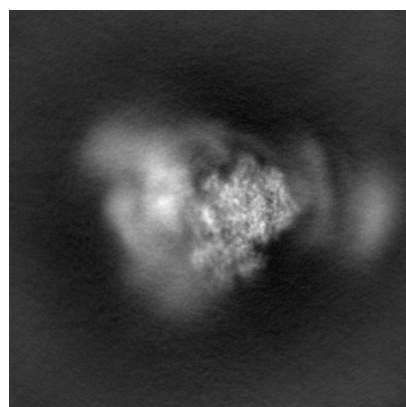


Y

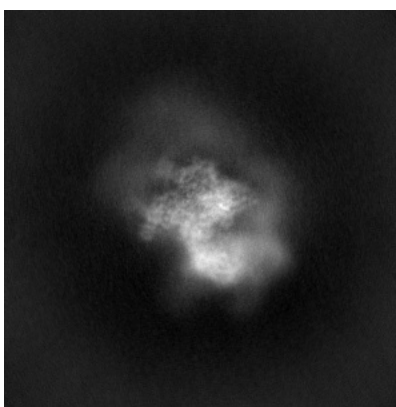


Z

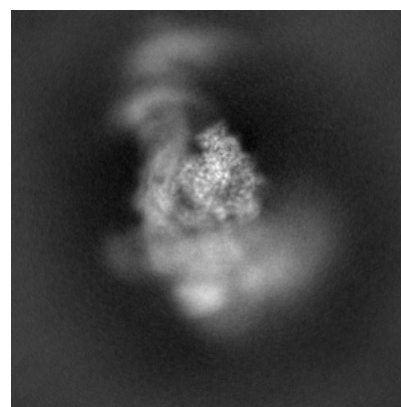
6.1.2 Raw map



X



Y

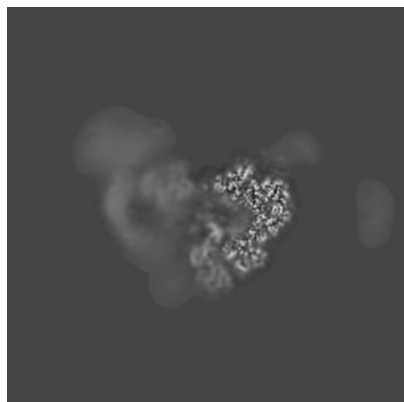


Z

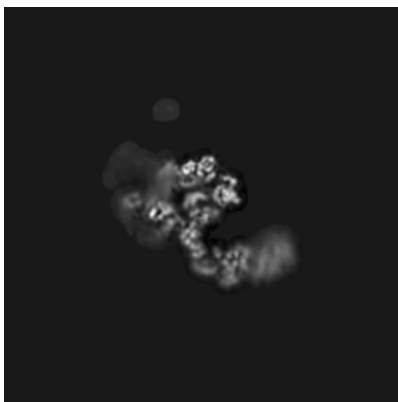
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

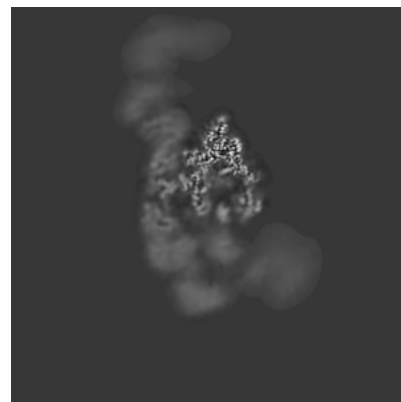
6.2.1 Primary map



X Index: 210

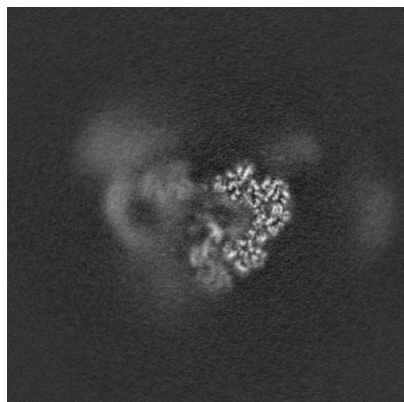


Y Index: 210

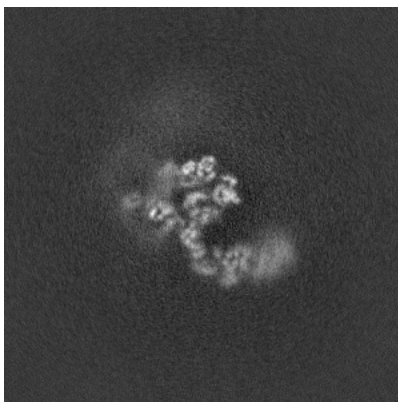


Z Index: 210

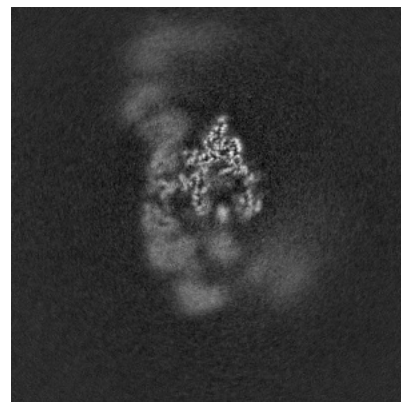
6.2.2 Raw map



X Index: 210



Y Index: 210

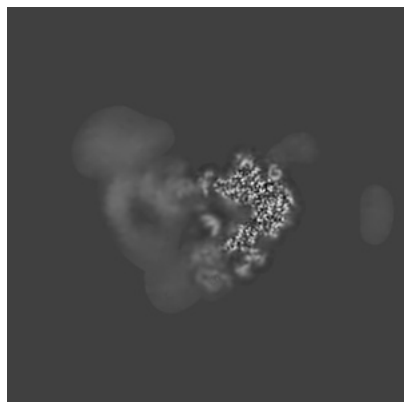


Z Index: 210

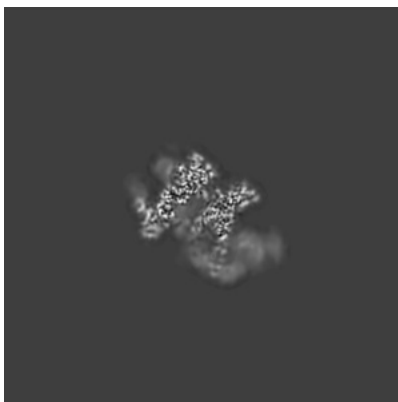
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

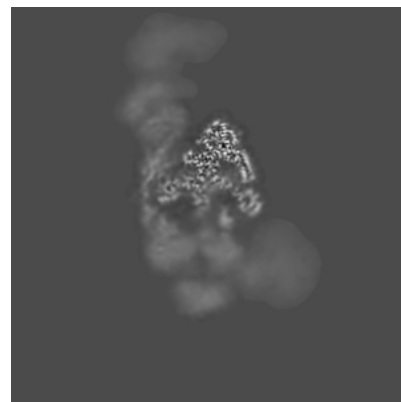
6.3.1 Primary map



X Index: 215

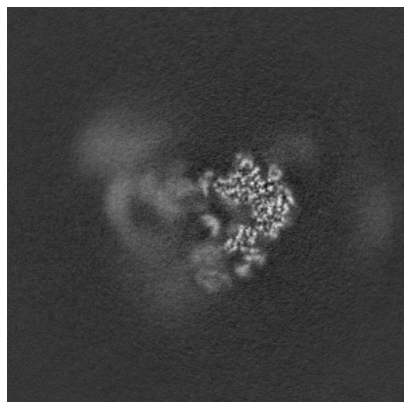


Y Index: 246

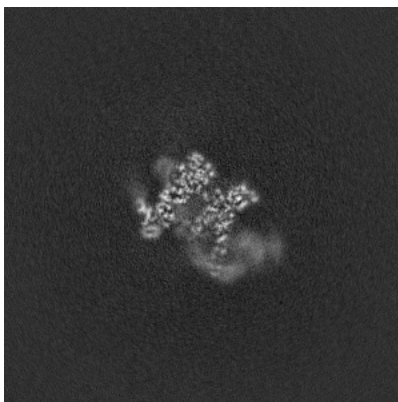


Z Index: 217

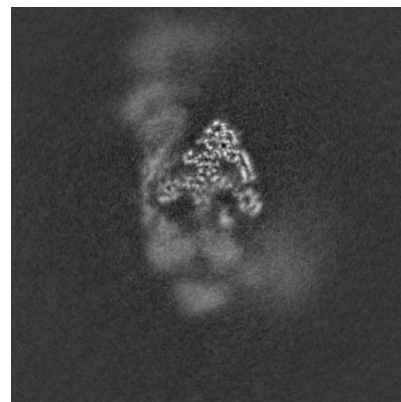
6.3.2 Raw map



X Index: 215



Y Index: 245

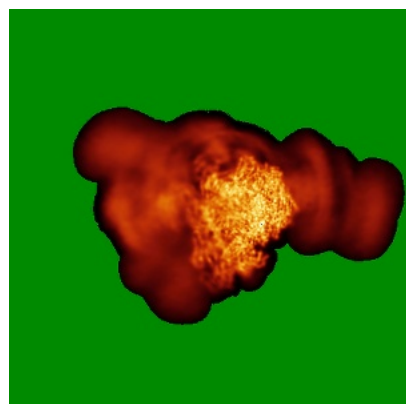


Z Index: 217

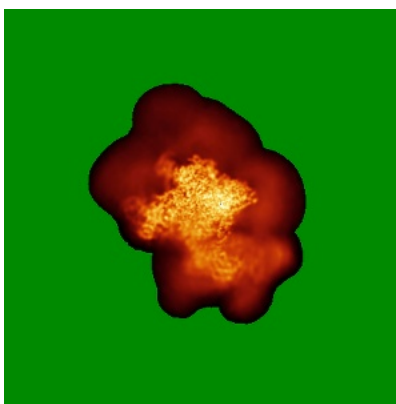
The images above show the largest variance slices of the map in three orthogonal directions.

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

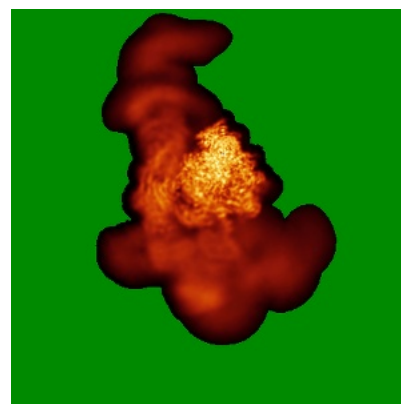
6.4.1 Primary map



X

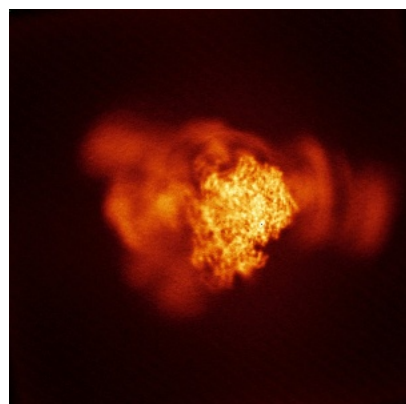


Y

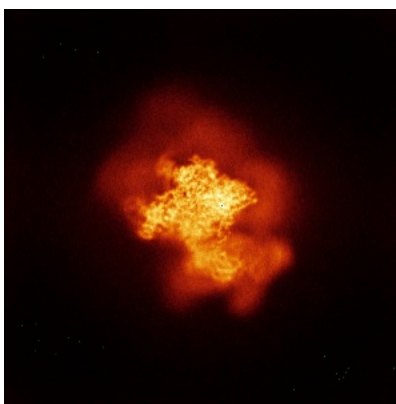


Z

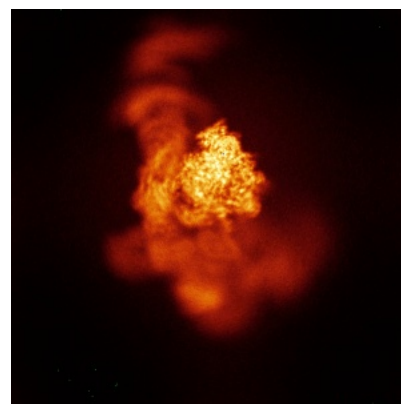
6.4.2 Raw map



X



Y

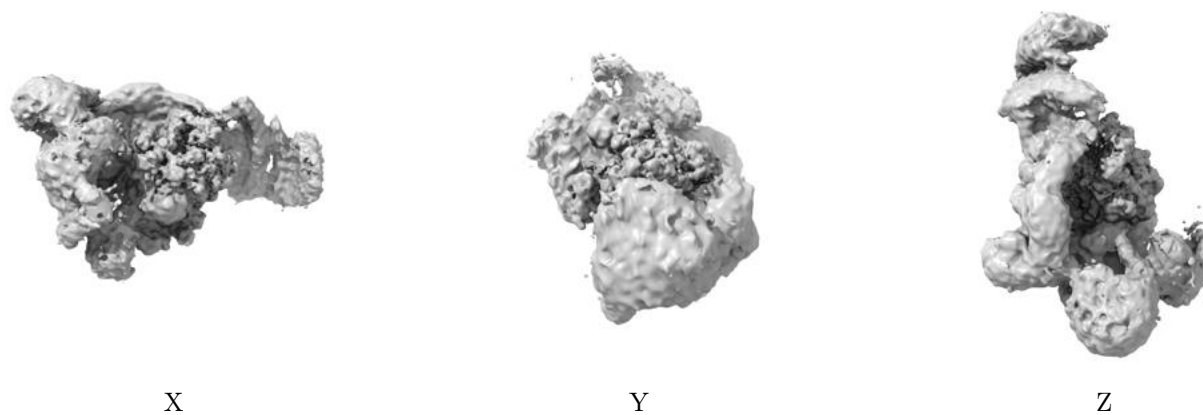


Z

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

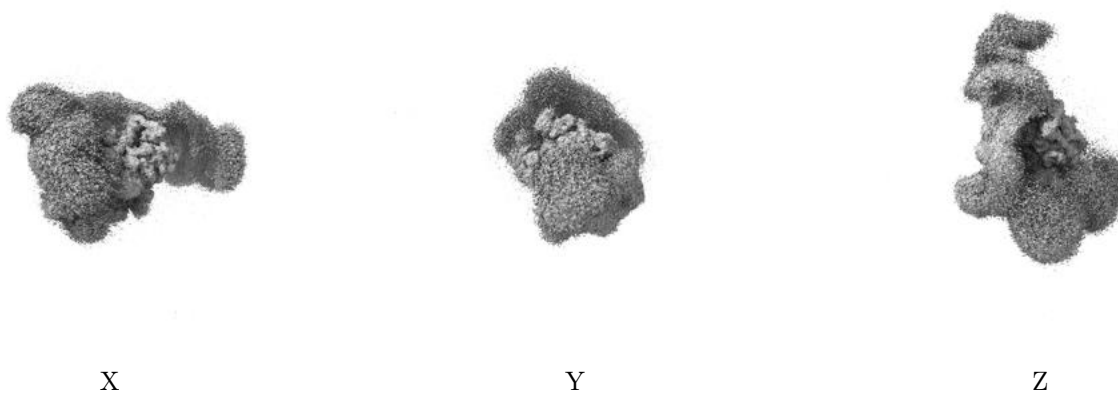
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.205. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

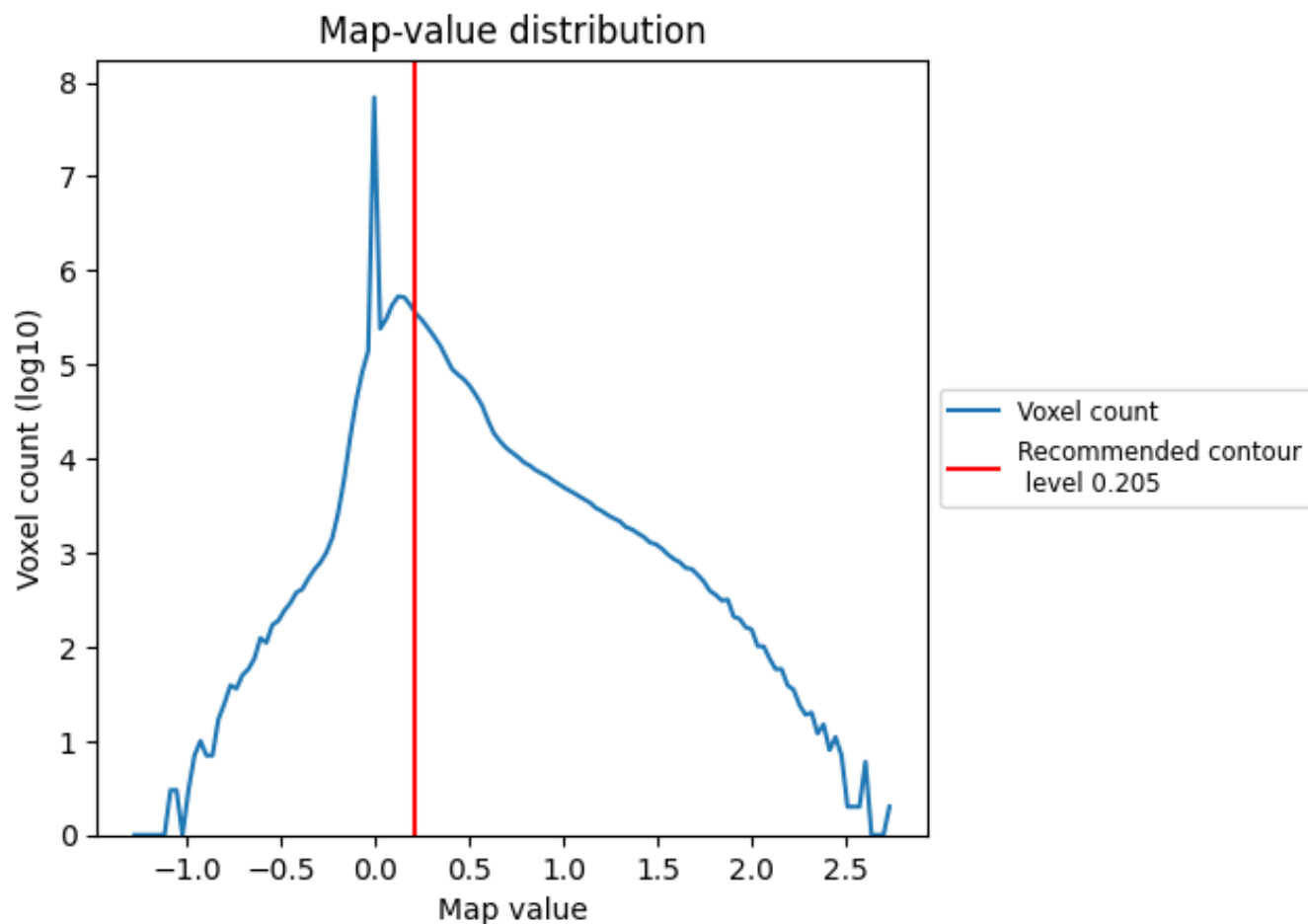
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

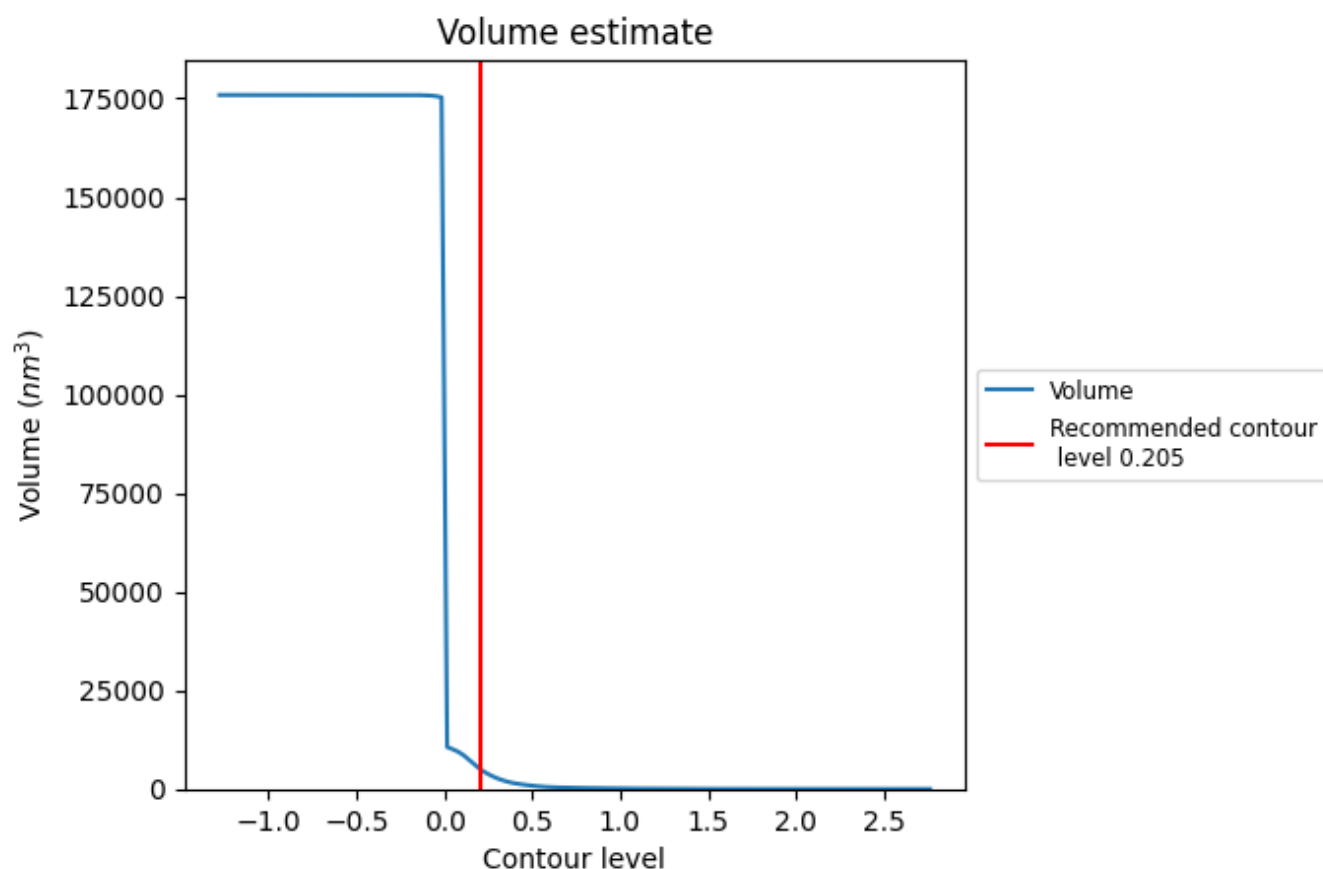
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

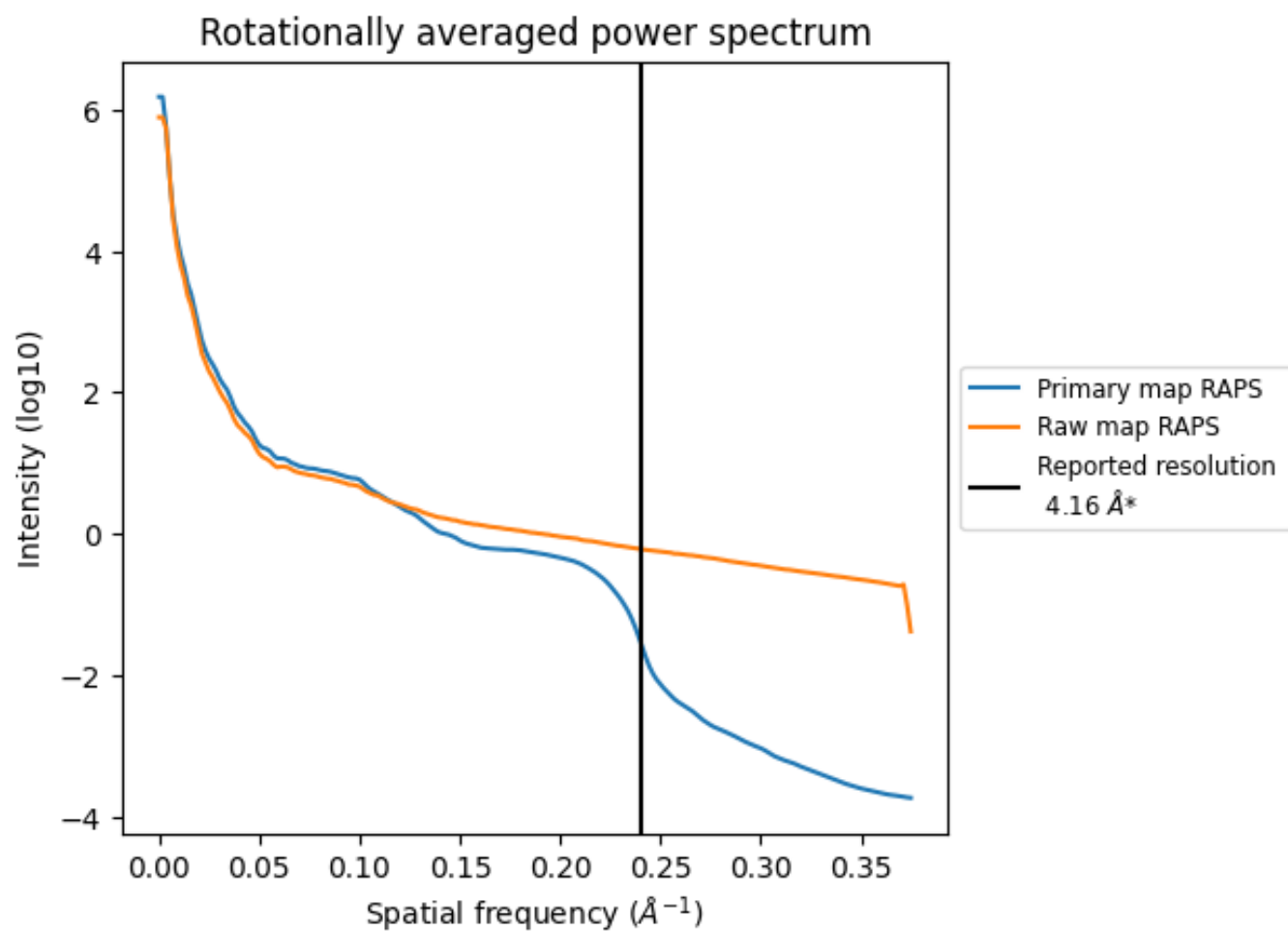
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 4986 nm^3 ; this corresponds to an approximate mass of 4504 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 ⓘ

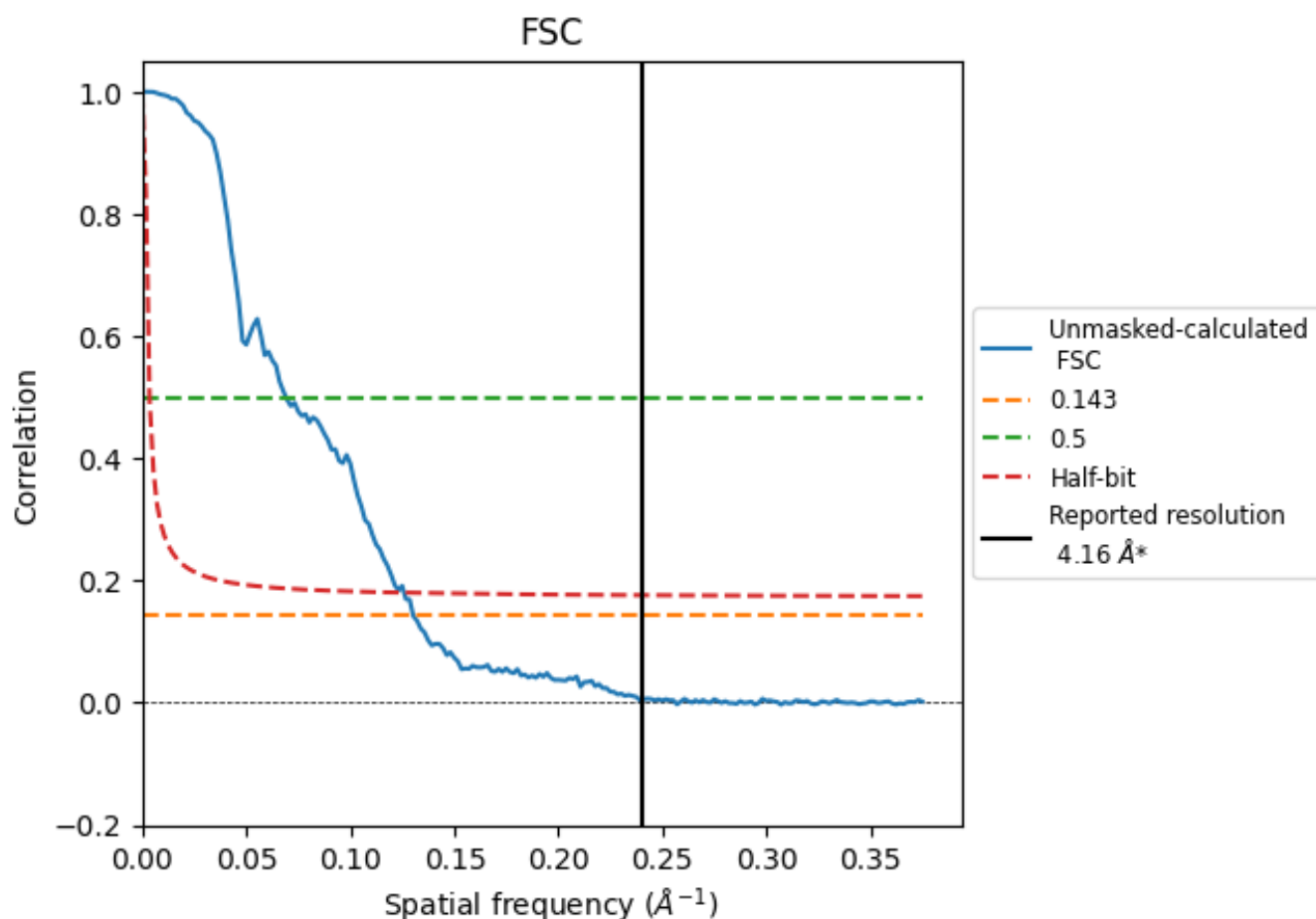


*Reported resolution corresponds to spatial frequency of $0.240 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.240 Å⁻¹

8.2 Resolution estimates [i](#)

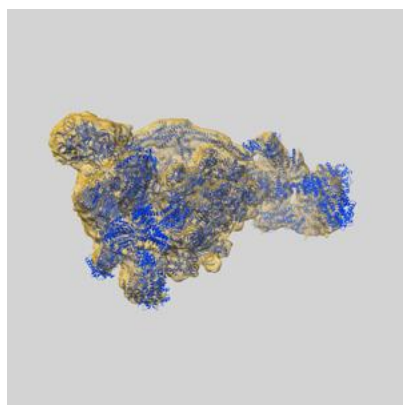
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.16	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.68	14.47	7.94

*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 7.68 differs from the reported value 4.16 by more than 10 %

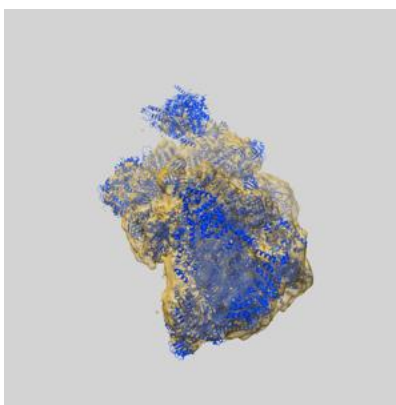
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-34360 and PDB model 8GXS. Per-residue inclusion information can be found in section 3 on page 20.

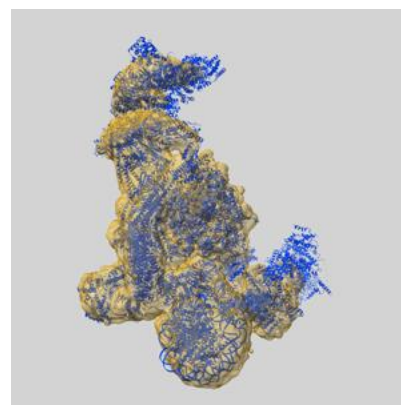
9.1 Map-model overlay [i](#)



X



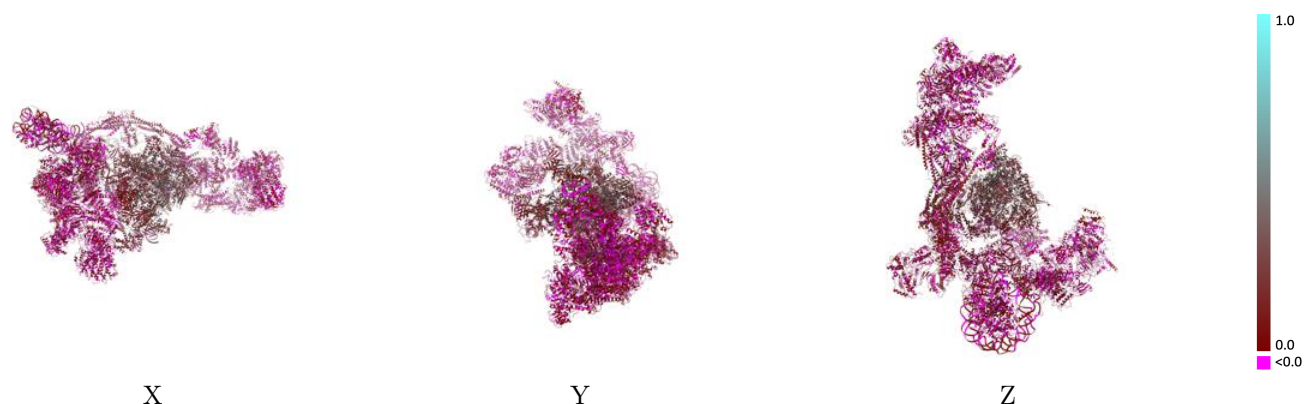
Y



Z

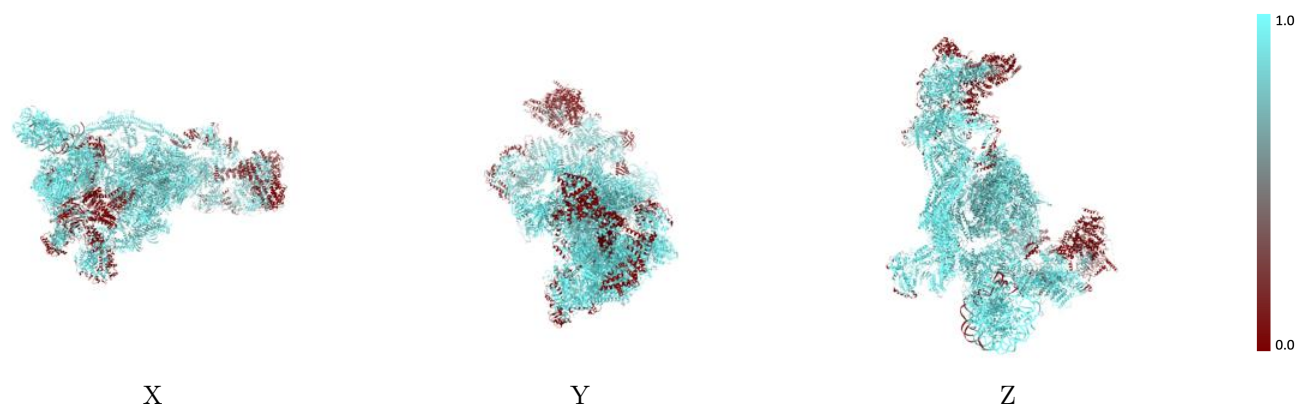
The images above show the 3D surface view of the map at the recommended contour level 0.205 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



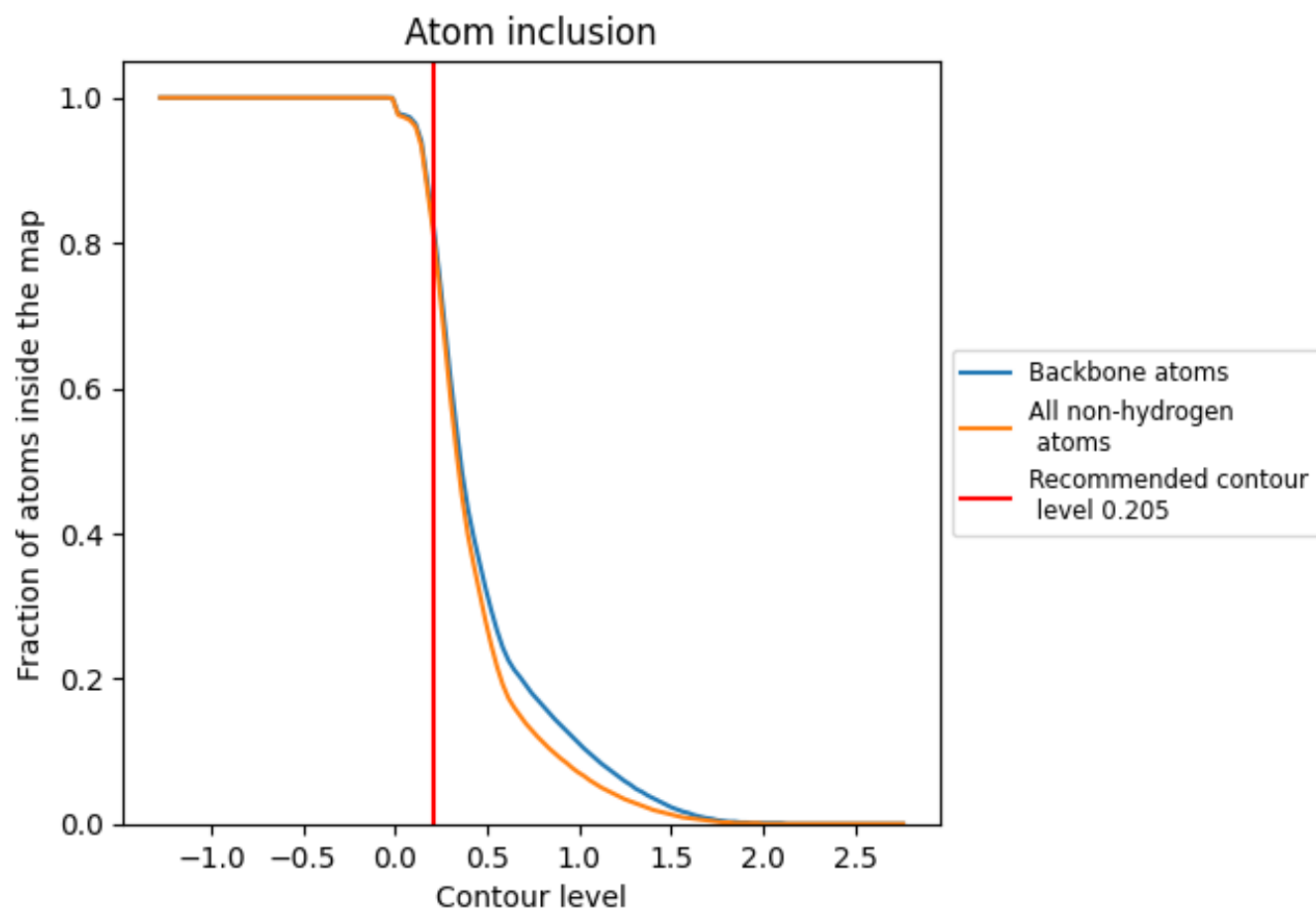
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.205).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 82% 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 (0.205) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8180	 0.0930
BA	 0.9700	 0.2280
DA	 0.7100	 0.0220
DB	 0.9430	 0.0400
DD	 0.6540	 0.0380
DE	 0.8400	 0.0360
DF	 0.7870	 0.0420
DG	 0.3760	 0.0250
DH	 0.9100	 0.0420
DI	 0.7220	 0.0330
DJ	 0.8810	 0.0270
DL	 0.3730	 0.0400
DO	 0.9520	 0.1340
DP	 0.9860	 0.1680
DQ	 0.9410	 0.1180
Dc	 0.0650	 0.0310
Dd	 0.0020	 0.0010
De	 0.1900	 0.0150
Df	 0.5500	 0.0330
Di	 0.0590	 0.0290
Dj	 0.0170	 0.0500
Dk	 0.0000	 -0.0140
DI	 0.0000	 -0.0070
Dm	 0.0000	 -0.0090
EA	 0.9340	 0.1170
EB	 0.9760	 0.1150
FA	 0.9710	 0.1500
FB	 0.9780	 0.1680
HA	 0.9890	 0.0880
HB	 0.9870	 0.0480
HC	 0.9830	 0.0680
HD	 0.9190	 0.1020
HE	 0.9820	 0.0530
HF	 1.0000	 0.0510
HG	 0.9890	 0.0560



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Chain	Atom inclusion	Q-score
HH	 0.9900	 0.0720
HI	 0.9670	 0.0600
HJ	 0.8510	 0.0620
NA	 0.9420	 0.0310
NB	 1.0000	 0.0490
NC	 1.0000	 0.0050
ND	 1.0000	 0.0090
NE	 0.9770	 0.0330
NF	 0.9720	 0.0480
NG	 0.9850	 0.0410
NH	 0.9640	 0.0380
NX	 0.8070	 0.0300
NY	 0.7950	 0.0250
PA	 0.9580	 0.2510
PB	 0.9670	 0.3080
PC	 0.9740	 0.3060
PD	 0.9710	 0.1790
PE	 0.9610	 0.2250
PF	 0.9290	 0.2910
PG	 0.9770	 0.1770
PH	 0.9740	 0.2790
PI	 0.9770	 0.2320
PJ	 0.9720	 0.3180
PK	 0.9570	 0.3000
PL	 0.9640	 0.3100
X	 0.9990	 0.1960
Y	 0.9970	 0.2010
a	 0.6860	 0.0430
b	 0.8340	 0.0330
c	 0.9130	 0.0440
d	 0.8600	 0.0710
e	 0.9870	 0.0840
f	 0.9930	 0.1270
g	 1.0000	 0.0910
h	 0.9850	 0.1250
i	 0.6570	 0.0630
j	 0.9780	 0.0830
k	 0.9760	 0.1280
l	 0.9910	 0.0600
m	 1.0000	 0.0720
n	 0.9280	 0.0510
o	 0.8830	 0.0320

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Chain	Atom inclusion	Q-score
p	 0.8590	 0.0390
q	 0.9980	 0.0750
r	 0.9910	 0.0850
s	 0.9920	 0.0460
t	 0.9650	 0.0660
u	 1.0000	 0.0740
v	 0.9850	 0.1190
w	 0.3200	 0.0150
x	 0.6380	 0.0290
y	 0.8770	 0.0350
z	 0.9320	 0.0350