



wwPDB EM Validation Summary Report ⓘ

Oct 8, 2026 – 04:36 PM EDT

PDB ID : 9PDK / pdb_00009pdk
EMDB ID : EMD-71536
Title : Composite map of closed form of PIC-Med-SWI/SNF
Authors : Yang, C.; Nagai, S.; Chen, D.-H.
Deposited on : 2025-06-30
Resolution : 2.80 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:

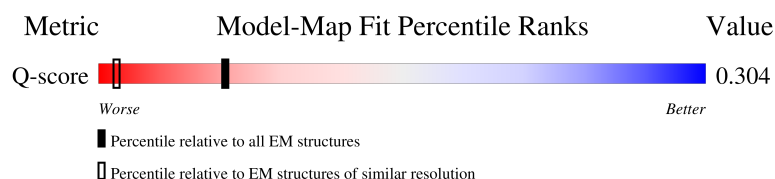
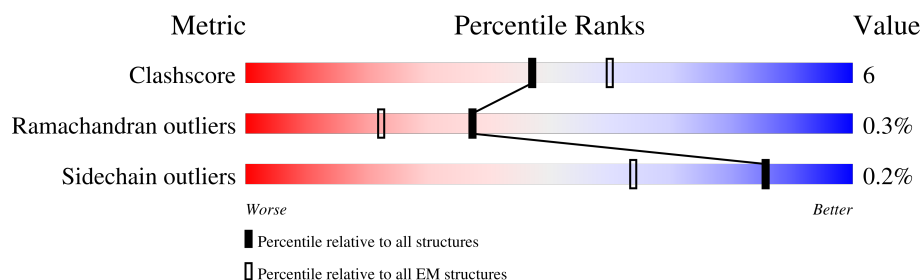
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.2
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.51

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 2.80 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.



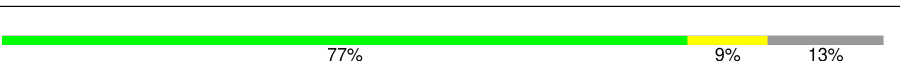
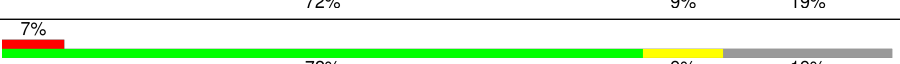
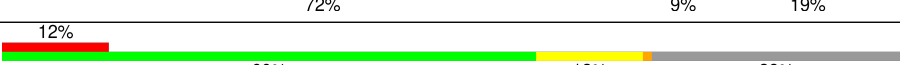
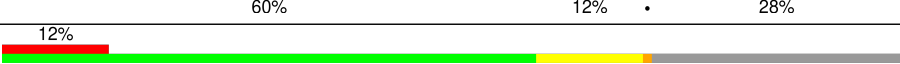
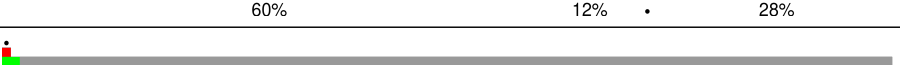
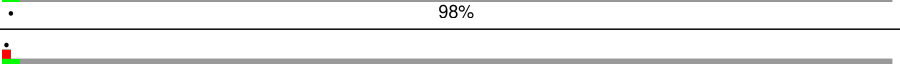
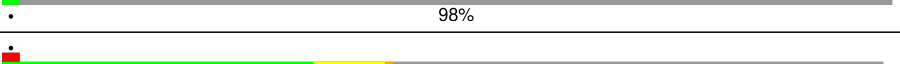
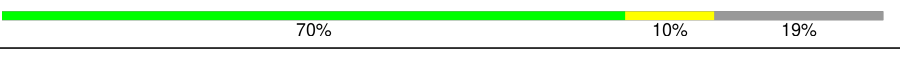
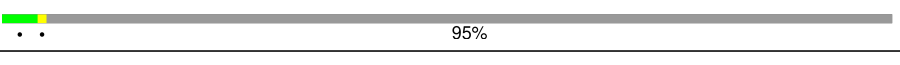
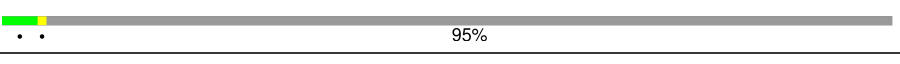
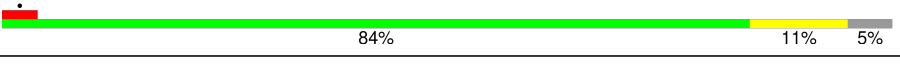
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11806 (2.30 - 3.30)

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	A0	778	
1	B0	778	
2	A1	642	
2	B1	642	

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Mol	Chain	Length	Quality of chain
3	A2	513	
3	B2	513	
4	A3	321	
4	B3	321	
5	A4	338	
5	B4	338	
6	A5	72	
6	B5	72	
7	A6	461	
7	B6	461	
8	A7	843	
8	B7	843	
9	A8	905	
9	B8	905	
9	SF	905	
9	sF	905	
10	A9	244	
10	B9	244	
11	AA	1733	
11	BA	1733	
11	MA	1733	
11	mA	1733	
12	AB	1224	
12	BB	1224	
13	AC	318	

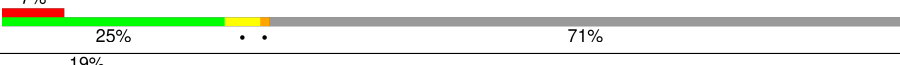
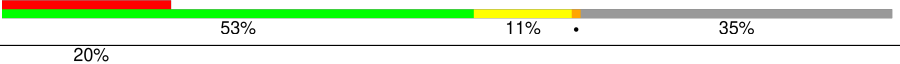
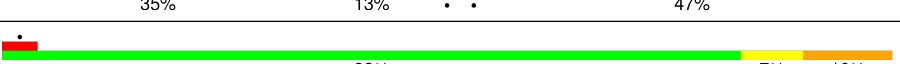
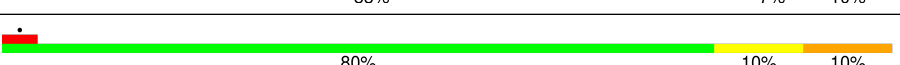
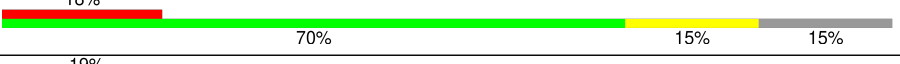
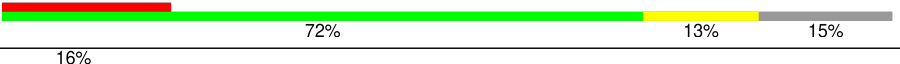
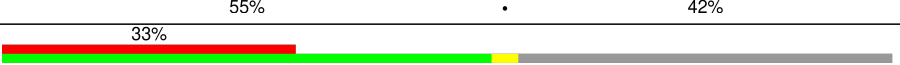
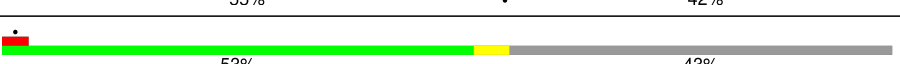
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Mol	Chain	Length	Quality of chain
13	BC	318	
14	AD	221	
14	BD	221	
15	AE	215	
15	BE	215	
16	AF	155	
16	BF	155	
17	AG	171	
17	BG	171	
18	AH	146	
18	BH	146	
19	AI	122	
19	BI	122	
20	AJ	70	
20	BJ	70	
21	AK	120	
21	BK	120	
22	AL	70	
22	BL	70	
23	AM	345	
23	BM	345	
24	AN	69	
24	BN	69	
25	AO	240	
25	BO	240	

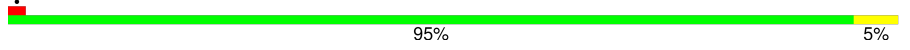
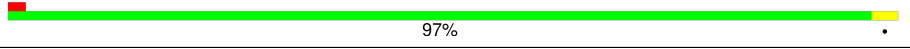
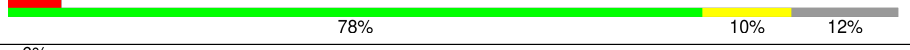
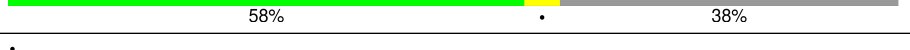
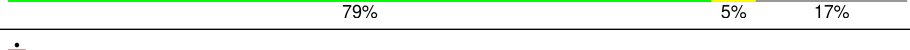
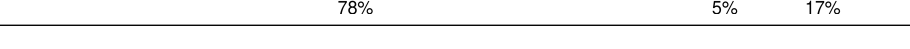
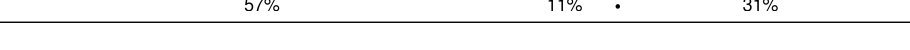
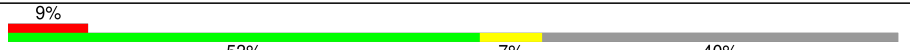
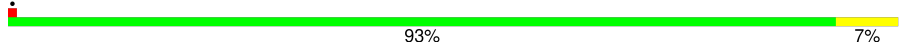
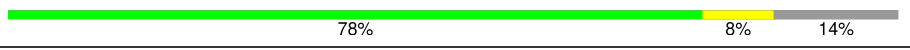
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Mol	Chain	Length	Quality of chain
26	AQ	735	
26	BQ	735	
27	AR	400	
27	BR	400	
28	AS	309	
28	BS	309	
29	AT	69	
29	BT	69	
30	AU	286	
30	BU	286	
31	AV	122	
31	BV	122	
32	AW	482	
32	BW	482	
33	AX	328	
33	BX	328	
34	Ma	295	
34	ma	295	
35	Mb	223	
35	mb	223	
36	Mc	115	
36	mc	115	
37	Md	687	
37	md	687	
38	Me	307	

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Mol	Chain	Length	Quality of chain
38	me	307	
39	Mf	210	
39	mf	210	
40	Mg	121	
40	mg	121	
41	Mh	284	
41	mh	284	
42	Mi	222	
42	mi	222	
43	Mj	149	
43	mj	149	
44	Mk	157	
44	mk	157	
45	MI	1082	
45	T4	1082	
45	ml	1082	
45	t4	1082	
46	Mm	220	
46	mm	220	
47	Mn	140	
47	mn	140	
48	Mo	127	
48	mo	127	
49	Mp	566	
49	mp	566	

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Mol	Chain	Length	Quality of chain
50	SA	566	
50	sA	566	
51	SB	825	
51	SD	825	
51	sB	825	
51	sD	825	
52	SC	332	
52	sC	332	
53	SE	623	
53	sE	623	
54	SG	47	
54	sG	47	
55	SH	1703	
55	sH	1703	
56	SI	1314	
56	sI	1314	
57	SJ	157	
57	sJ	157	
58	SK	477	
58	sK	477	
59	SL	467	
59	sL	467	
60	T1	431	
60	t1	431	
61	T2	397	

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Mol	Chain	Length	Quality of chain
61	t2	397	
62	T3	1132	
62	t3	1132	
63	T5	1081	
63	t5	1081	
64	T6	974	
64	t6	974	

2 Entry composition

There are 67 unique types of molecules in this entry. The entry contains 305572 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 General transcription and DNA repair factor IIIH helicase subunit XPD/RAD3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B0	752	Total	C	N	O	S	0	0
			6091	3882	1029	1142	38		
1	A0	752	Total	C	N	O	S	0	0
			6091	3882	1029	1142	38		

- Molecule 2 is a protein called General transcription and DNA repair factor IIIH subunit TFB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B1	416	Total	C	N	O	S	0	0
			3374	2133	586	639	16		
2	A1	416	Total	C	N	O	S	0	0
			3374	2133	586	639	16		

- Molecule 3 is a protein called General transcription and DNA repair factor IIIH subunit TFB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B2	445	Total	C	N	O	S	0	0
			3597	2327	591	663	16		
3	A2	445	Total	C	N	O	S	0	0
			3597	2327	591	663	16		

- Molecule 4 is a protein called RNA polymerase II transcription factor B subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B3	131	Total	C	N	O	S	0	0
			1089	692	180	209	8		
4	A3	131	Total	C	N	O	S	0	0
			1089	692	180	209	8		

- Molecule 5 is a protein called General transcription and DNA repair factor IIIH subunit TFB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B4	293	Total	C	N	O	S	0	0
			2274	1454	377	429	14		
5	A4	293	Total	C	N	O	S	0	0
			2274	1454	377	429	14		

- Molecule 6 is a protein called General transcription and DNA repair factor IIH subunit TFB5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B5	65	Total	C	N	O	S	0	0
			514	326	90	95	3		
6	A5	65	Total	C	N	O	S	0	0
			514	326	90	95	3		

- Molecule 7 is a protein called General transcription and DNA repair factor IIH subunit SSL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B6	374	Total	C	N	O	S	0	0
			2946	1870	507	541	28		
7	A6	374	Total	C	N	O	S	0	0
			2946	1870	507	541	28		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B7	607	Total	C	N	O	S	0	0
			4881	3104	846	905	26		
8	A7	607	Total	C	N	O	S	0	0
			4881	3104	846	905	26		

- Molecule 9 is a protein called SWI/SNF chromatin-remodeling complex subunit SNF5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B8	17	Total	C	N	O	S	0	0
			134	89	22	22	1		
9	sF	411	Total	C	N	O	S	0	0
			3374	2130	571	663	10		
9	A8	17	Total	C	N	O	S	0	0
			134	89	22	22	1		
9	SF	411	Total	C	N	O	S	0	0
			3374	2130	571	663	10		

- Molecule 10 is a protein called Transcription initiation factor TFIID subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	B9	68	Total	C	N	O	S	0	0
			542	345	82	113	2		
10	A9	68	Total	C	N	O	S	0	0
			542	345	82	113	2		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	BA	1398	Total	C	N	O	S	0	0
			10996	6931	1926	2078	61		
11	mA	79	Total	C	N	O		0	0
			575	361	79	135			
11	AA	1398	Total	C	N	O	S	0	0
			10996	6931	1926	2078	61		
11	MA	79	Total	C	N	O		0	0
			575	361	79	135			

- Molecule 12 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	BB	1161	Total	C	N	O	S	0	0
			9249	5848	1619	1726	56		
12	AB	1161	Total	C	N	O	S	0	0
			9249	5848	1619	1726	56		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	BC	262	Total	C	N	O	S	0	0
			2061	1299	343	406	13		
13	AC	262	Total	C	N	O	S	0	0
			2061	1299	343	406	13		

- Molecule 14 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	BD	157	Total	C	N	O	S	0	0
			1253	779	220	252	2		
14	AD	157	Total	C	N	O	S	0	0
			1253	779	220	252	2		

- Molecule 15 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	BE	213	Total	C	N	O	S	0	0
			1744	1107	308	318	11		
15	AE	213	Total	C	N	O	S	0	0
			1744	1107	308	318	11		

- Molecule 16 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	BF	83	Total	C	N	O	S	0	0
			670	428	114	125	3		
16	AF	83	Total	C	N	O	S	0	0
			670	428	114	125	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	BG	171	Total	C	N	O	S	0	0
			1340	861	222	249	8		
17	AG	171	Total	C	N	O	S	0	0
			1340	861	222	249	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	BH	136	Total	C	N	O	S	0	0
			1089	686	184	215	4		
18	AH	136	Total	C	N	O	S	0	0
			1089	686	184	215	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	BI	116	Total	C	N	O	S	0	0
			944	581	172	181	10		
19	AI	116	Total	C	N	O	S	0	0
			944	581	172	181	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	BJ	69	Total	C	N	O	S	0	0
			569	362	101	100	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
20	AJ	69	Total	C	N	O	S	0	0
			569	362	101	100	6		

- Molecule 21 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	BK	115	Total	C	N	O	S	0	0
			924	593	157	172	2		
21	AK	115	Total	C	N	O	S	0	0
			924	593	157	172	2		

- Molecule 22 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	BL	45	Total	C	N	O	S	0	0
			359	221	71	63	4		
22	AL	45	Total	C	N	O	S	0	0
			359	221	71	63	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	BM	276	Total	C	N	O	S	0	0
			2097	1328	359	393	17		
23	AM	276	Total	C	N	O	S	0	0
			2097	1328	359	393	17		

- Molecule 24 is a DNA chain called promoter DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	BN	69	Total	C	N	O	P	0	0
			1413	679	248	417	69		
24	AN	69	Total	C	N	O	P	0	0
			1413	679	248	417	69		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	BO	181	Total	C	N	O	S	0	0
			1422	925	243	248	6		
25	AO	181	Total	C	N	O	S	0	0
			1422	925	243	248	6		

- Molecule 26 is a protein called Transcription initiation factor IIF subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	BQ	214	Total	C	N	O	S	0	0
			1817	1149	337	324	7		
26	AQ	214	Total	C	N	O	S	0	0
			1817	1149	337	324	7		

- Molecule 27 is a protein called Transcription initiation factor IIF subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	BR	261	Total	C	N	O	S	0	0
			2173	1369	383	411	10		
27	AR	261	Total	C	N	O	S	0	0
			2173	1369	383	411	10		

- Molecule 28 is a protein called Transcription elongation factor S-II.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	BS	164	Total	C	N	O	S	0	0
			1301	812	230	251	8		
28	AS	164	Total	C	N	O	S	0	0
			1301	812	230	251	8		

- Molecule 29 is a DNA chain called promoter DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	BT	69	Total	C	N	O	P	0	0
			1416	679	257	411	69		
29	AT	69	Total	C	N	O	P	0	0
			1416	679	257	411	69		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	BU	102	Total	C	N	O	S	0	0
			843	531	142	167	3		
30	AU	102	Total	C	N	O	S	0	0
			843	531	142	167	3		

- Molecule 31 is a protein called Transcription initiation factor IIA subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	BV	104	Total	C	N	O	S	0	0
			815	511	136	164	4		
31	AV	104	Total	C	N	O	S	0	0
			815	511	136	164	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	BW	226	Total	C	N	O	S	0	0
			1836	1168	317	344	7		
32	AW	226	Total	C	N	O	S	0	0
			1836	1168	317	344	7		

- Molecule 33 is a protein called Transcription initiation factor IIE subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	BX	191	Total	C	N	O	S	0	0
			1530	980	256	289	5		
33	AX	191	Total	C	N	O	S	0	0
			1530	980	256	289	5		

- Molecule 34 is a protein called Mediator of RNA polymerase II transcription subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	ma	169	Total	C	N	O	S	0	0
			1407	905	234	262	6		
34	Ma	169	Total	C	N	O	S	0	0
			1407	905	234	262	6		

- Molecule 35 is a protein called Mediator of RNA polymerase II transcription subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	mb	157	Total	C	N	O	S	0	0
			1295	822	224	246	3		
35	Mb	157	Total	C	N	O	S	0	0
			1295	822	224	246	3		

- Molecule 36 is a protein called Mediator of RNA polymerase II transcription subunit 11.

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

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

- Molecule 37 is a protein called Mediator of RNA polymerase II transcription subunit 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	md	535	Total	C	N	O	S	0	0
			4325	2766	730	816	13		
37	Md	535	Total	C	N	O	S	0	0
			4325	2766	730	816	13		

- Molecule 38 is a protein called Mediator of RNA polymerase II transcription subunit 18.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	me	248	Total	C	N	O	S	0	0
			1958	1247	325	376	10		
38	Me	248	Total	C	N	O	S	0	0
			1958	1247	325	376	10		

- Molecule 39 is a protein called Mediator of RNA polymerase II transcription subunit 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	mf	210	Total	C	N	O	S	0	0
			1609	1016	270	317	6		
39	Mf	210	Total	C	N	O	S	0	0
			1609	1016	270	317	6		

- Molecule 40 is a protein called Mediator of RNA polymerase II transcription subunit 22.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	mg	106	Total	C	N	O	S	0	0
			847	528	139	175	5		
40	Mg	106	Total	C	N	O	S	0	0
			847	528	139	175	5		

- Molecule 41 is a protein called Mediator of RNA polymerase II transcription subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	mh	177	Total	C	N	O	S	0	0
			1441	910	242	284	5		
41	Mh	177	Total	C	N	O	S	0	0
			1441	910	242	284	5		

- Molecule 42 is a protein called Mediator of RNA polymerase II transcription subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	mi	185	Total	C	N	O	S	0	0
			1538	989	259	284	6		
42	Mi	185	Total	C	N	O	S	0	0
			1538	989	259	284	6		

- Molecule 43 is a protein called Mediator of RNA polymerase II transcription subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	mj	103	Total	C	N	O	S	0	0
			864	539	160	164	1		
43	Mj	103	Total	C	N	O	S	0	0
			864	539	160	164	1		

- Molecule 44 is a protein called Mediator of RNA polymerase II transcription subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	mk	144	Total	C	N	O	S	0	0
			1157	715	204	235	3		
44	Mk	144	Total	C	N	O	S	0	0
			1157	715	204	235	3		

- Molecule 45 is a protein called Mediator of RNA polymerase II transcription subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	ml	654	Total	C	N	O	S	0	0
			5367	3465	924	954	24		
45	Ml	654	Total	C	N	O	S	0	0
			5367	3465	924	954	24		
45	T4	220	Total	C	N	O	S	0	0
			1780	1136	302	333	9		
45	t4	220	Total	C	N	O	S	0	0
			1780	1136	302	333	9		

- Molecule 46 is a protein called Mediator of RNA polymerase II transcription subunit 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	mm	83	Total	C	N	O	S	0	0
			671	424	111	135	1		
46	Mm	83	Total	C	N	O	S	0	0
			671	424	111	135	1		

- Molecule 47 is a protein called Mediator of RNA polymerase II transcription subunit 21.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	mn	140	Total	C	N	O	S	0	0
			1124	701	189	228	6		
47	Mn	140	Total	C	N	O	S	0	0
			1124	701	189	228	6		

- Molecule 48 is a protein called Mediator of RNA polymerase II transcription subunit 31.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	mo	109	Total	C	N	O	S	0	0
			914	603	141	164	6		
48	Mo	109	Total	C	N	O	S	0	0
			914	603	141	164	6		

- Molecule 49 is a protein called Mediator of RNA polymerase II transcription subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	mp	409	Total	C	N	O	S	0	0
			3330	2115	535	669	11		
49	Mp	409	Total	C	N	O	S	0	0
			3330	2115	535	669	11		

- Molecule 50 is a protein called Transcription regulatory protein SNF12.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	sA	442	Total	C	N	O	S	0	0
			3552	2231	608	698	15		
50	SA	442	Total	C	N	O	S	0	0
			3552	2231	608	698	15		

- Molecule 51 is a protein called SWI/SNF complex subunit SWI3.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	sB	395	Total	C	N	O	S	0	0
			3250	2082	560	597	11		
51	sD	421	Total	C	N	O	S	0	0
			3445	2203	592	638	12		
51	SB	395	Total	C	N	O	S	0	0
			3250	2082	560	597	11		
51	SD	421	Total	C	N	O	S	0	0
			3445	2203	592	638	12		

- Molecule 52 is a protein called Transcription regulatory protein SNF6.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	sC	154	Total	C	N	O	S	0	0
			1266	793	232	236	5		
52	SC	154	Total	C	N	O	S	0	0
			1266	793	232	236	5		

- Molecule 53 is a protein called SWI/SNF global transcription activator complex subunit SWP82.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	sE	411	Total	C	N	O	S	0	0
			3333	2142	569	617	5		
53	SE	411	Total	C	N	O	S	0	0
			3333	2142	569	617	5		

- Molecule 54 is a protein called unsigned peptide of SWISNF.

Mol	Chain	Residues	Atoms				AltConf	Trace
54	sG	47	Total	C	N	O	0	0
			271	166	56	49		
54	SG	47	Total	C	N	O	0	0
			271	166	56	49		

- Molecule 55 is a protein called Transcription regulatory protein SNF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	sH	241	Total	C	N	O	S	0	0
			1958	1227	353	372	6		
55	SH	241	Total	C	N	O	S	0	0
			1958	1227	353	372	6		

- Molecule 56 is a protein called SWI/SNF chromatin-remodeling complex subunit SWI1.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	sI	552	Total	C	N	O	S	0	0
			4474	2894	749	820	11		
56	SI	552	Total	C	N	O	S	0	0
			4474	2894	749	820	11		

- Molecule 57 is a protein called Regulator of Ty1 transposition protein 102.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	sJ	82	Total	C	N	O	S	0	0
			711	450	123	135	3		
57	SJ	82	Total	C	N	O	S	0	0
			711	450	123	135	3		

- Molecule 58 is a protein called Actin-related protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	sK	431	Total	C	N	O	S	0	0
			3453	2213	563	658	19		
58	SK	431	Total	C	N	O	S	0	0
			3453	2213	563	658	19		

- Molecule 59 is a protein called Actin-like protein ARP9.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	sL	406	Total	C	N	O	S	0	0
			3266	2095	533	630	8		
59	SL	406	Total	C	N	O	S	0	0
			3266	2095	533	630	8		

- Molecule 60 is a protein called Mediator of RNA polymerase II transcription subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	T1	65	Total	C	N	O	S	0	0
			516	328	82	102	4		
60	t1	65	Total	C	N	O	S	0	0
			516	328	82	102	4		

- Molecule 61 is a protein called Mediator of RNA polymerase II transcription subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	T2	110	Total	C	N	O	S	0	0
			891	560	155	172	4		
61	t2	110	Total	C	N	O	S	0	0
			891	560	155	172	4		

- Molecule 62 is a protein called Mediator of RNA polymerase II transcription subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	T3	761	Total	C	N	O	S	0	0
			6173	3979	999	1181	14		

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Mol	Chain	Residues	Atoms					AltConf	Trace
62	t3	761	Total	C	N	O	S	0	0
			6173	3979	999	1181	14		

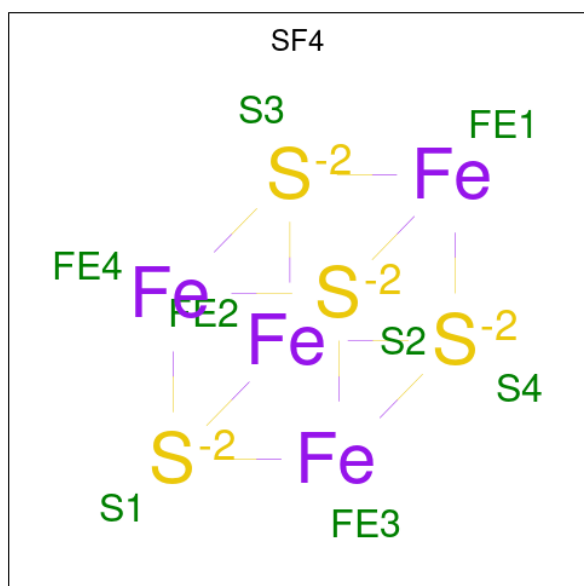
- Molecule 63 is a protein called Mediator of RNA polymerase II transcription subunit 15.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	T5	111	Total	C	N	O	S	0	0
			894	558	161	169	6		
63	t5	111	Total	C	N	O	S	0	0
			894	558	161	169	6		

- Molecule 64 is a protein called Mediator of RNA polymerase II transcription subunit 16.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	T6	932	Total	C	N	O	S	0	0
			7551	4859	1258	1399	35		
64	t6	932	Total	C	N	O	S	0	0
			7551	4859	1258	1399	35		

- Molecule 65 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			AltConf
65	B0	1	Total	Fe	S	0
			8	4	4	
65	A0	1	Total	Fe	S	0
			8	4	4	

- Molecule 66 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
66	B3	2	Total 2	Zn 2	0
66	B4	1	Total 1	Zn 1	0
66	B6	4	Total 4	Zn 4	0
66	BA	2	Total 2	Zn 2	0
66	BB	1	Total 1	Zn 1	0
66	BC	1	Total 1	Zn 1	0
66	BI	2	Total 2	Zn 2	0
66	BJ	1	Total 1	Zn 1	0
66	BL	1	Total 1	Zn 1	0
66	BM	1	Total 1	Zn 1	0
66	BS	1	Total 1	Zn 1	0
66	BW	1	Total 1	Zn 1	0
66	A3	2	Total 2	Zn 2	0
66	A4	1	Total 1	Zn 1	0
66	A6	4	Total 4	Zn 4	0
66	AA	2	Total 2	Zn 2	0
66	AB	1	Total 1	Zn 1	0
66	AC	1	Total 1	Zn 1	0
66	AI	2	Total 2	Zn 2	0
66	AJ	1	Total 1	Zn 1	0
66	AL	1	Total 1	Zn 1	0

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Mol	Chain	Residues	Atoms		AltConf
66	AM	1	Total 1	Zn 1	0
66	AS	1	Total 1	Zn 1	0
66	AW	1	Total 1	Zn 1	0

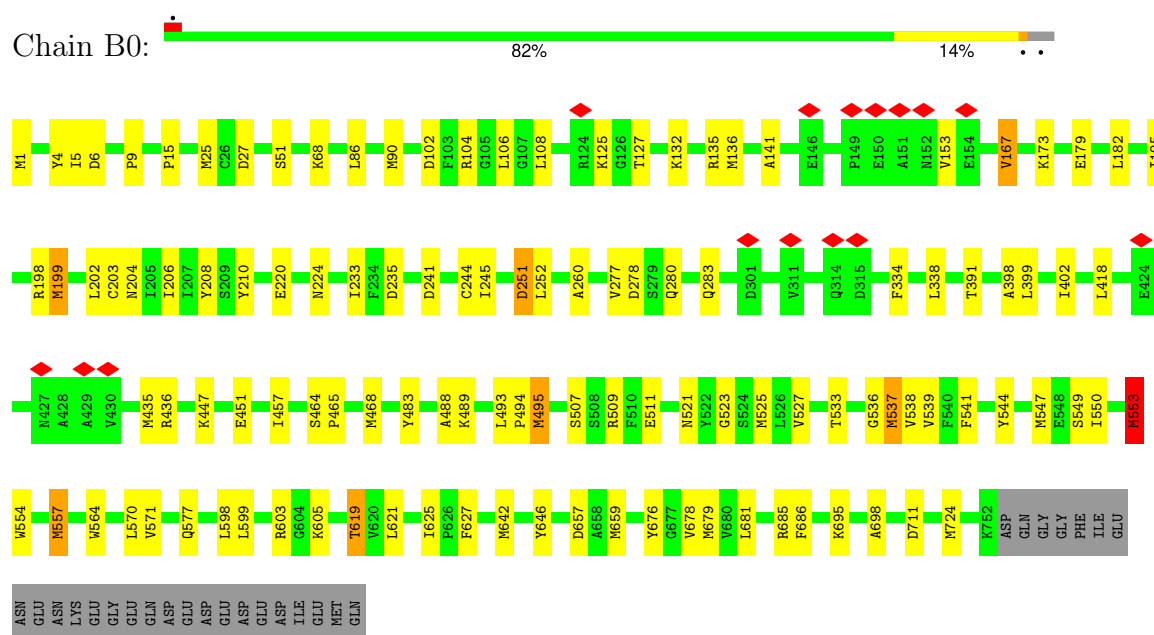
- Molecule 67 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
67	BA	1	Total 1	Mg 1	0
67	AA	1	Total 1	Mg 1	0

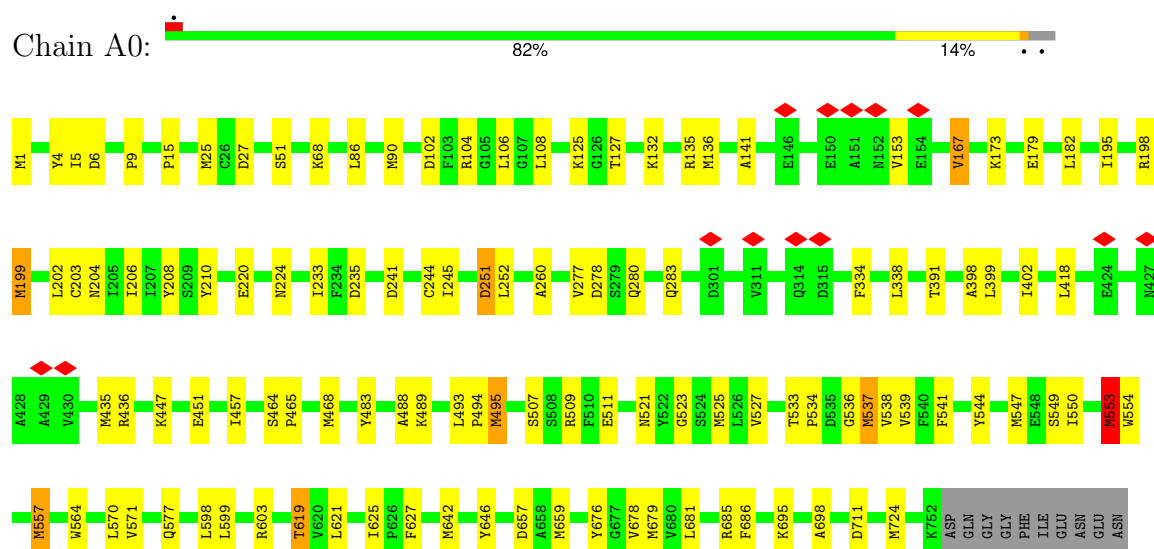
3 Residue-property plots

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: General transcription and DNA repair factor IIH helicase subunit XPD/RAD3



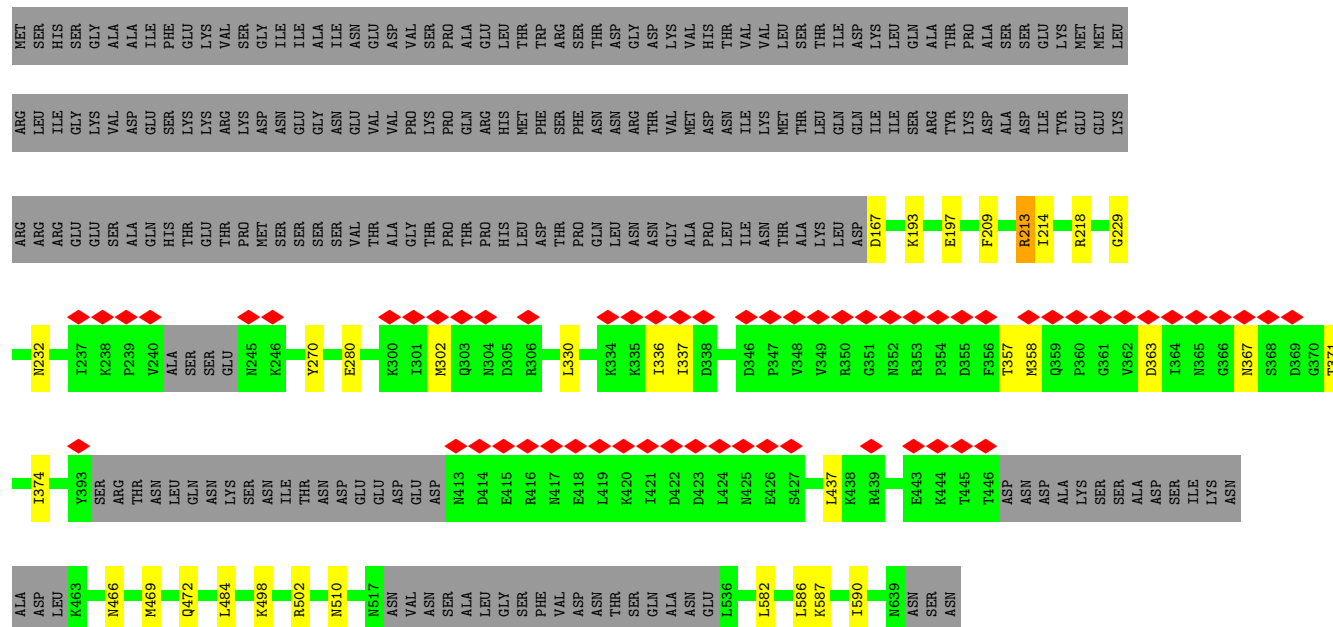
- Molecule 1: General transcription and DNA repair factor IIH helicase subunit XPD/RAD3



LYS
GLY
GLY
GLY
GLN
ASP
GLU
GLU
ASP
GLU
GLU
ASP
GLU
TLE
GLU
MET
GLN

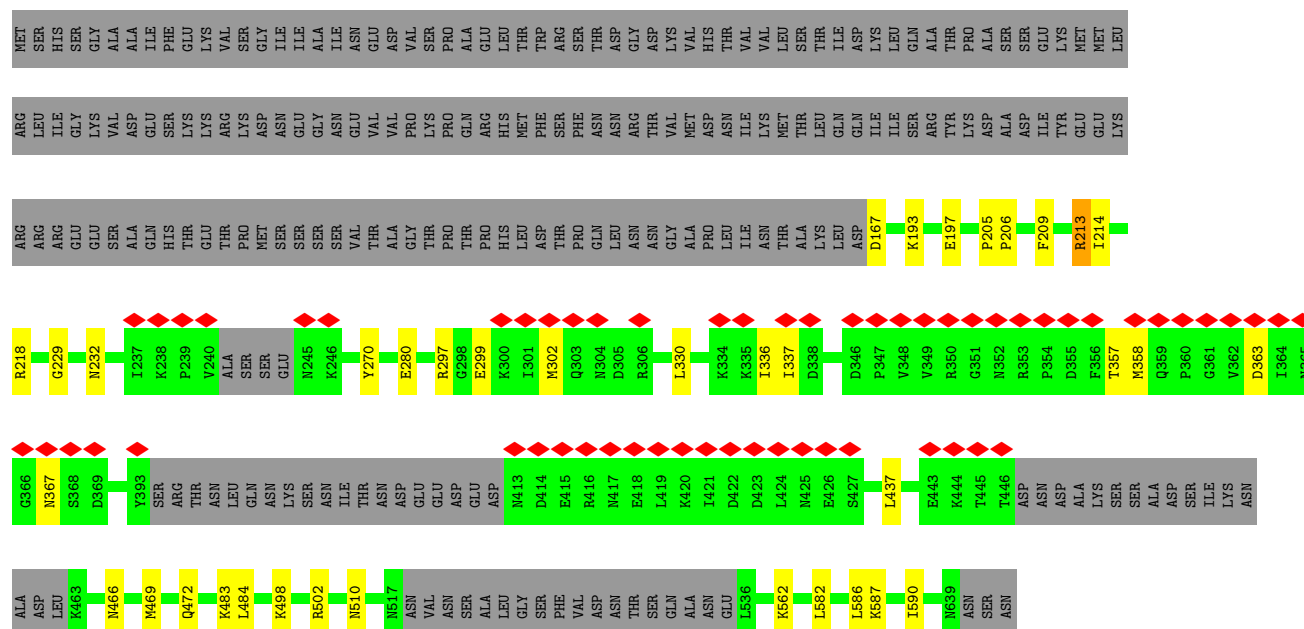
• Molecule 2: General transcription and DNA repair factor IIH subunit TFB1

Chain B1: 



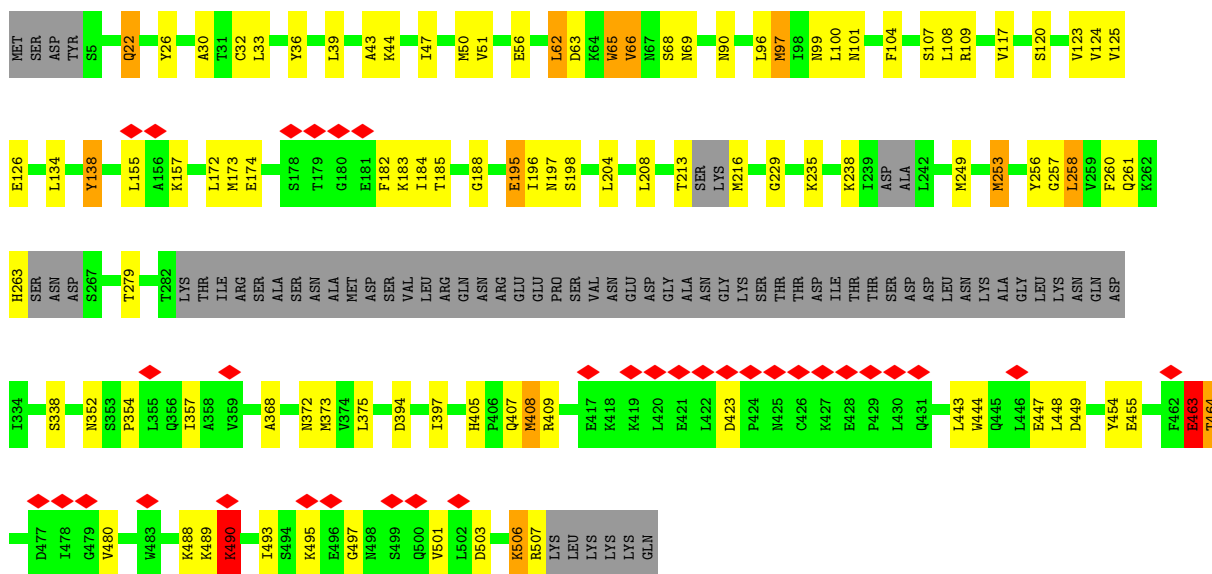
• Molecule 2: General transcription and DNA repair factor IIH subunit TFB1

Chain A1: 

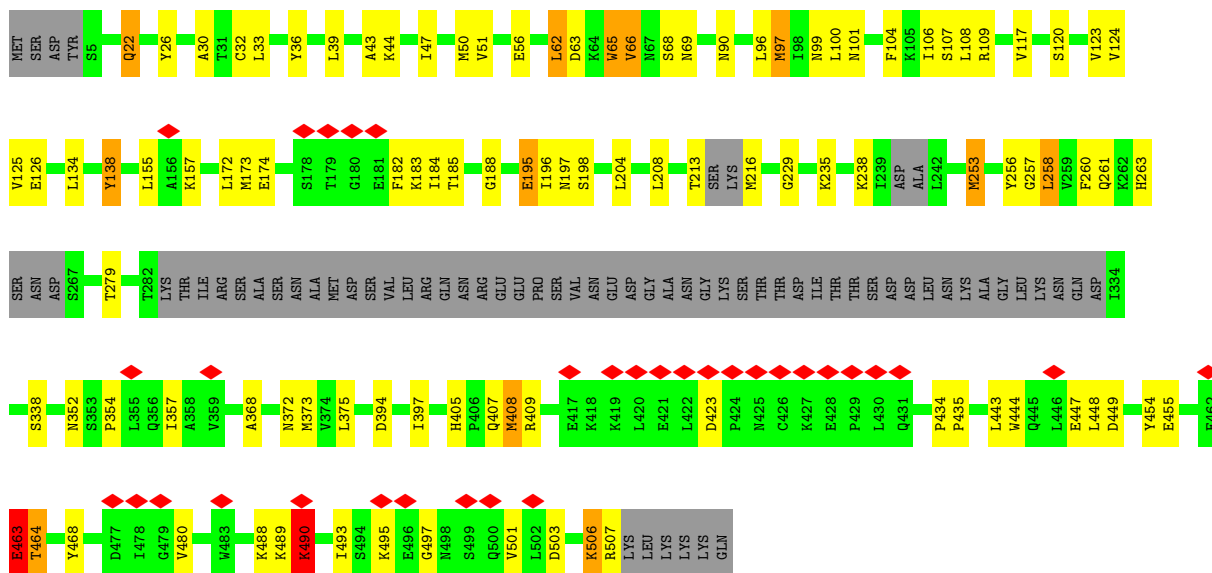


• Molecule 3: General transcription and DNA repair factor IIH subunit TFB2

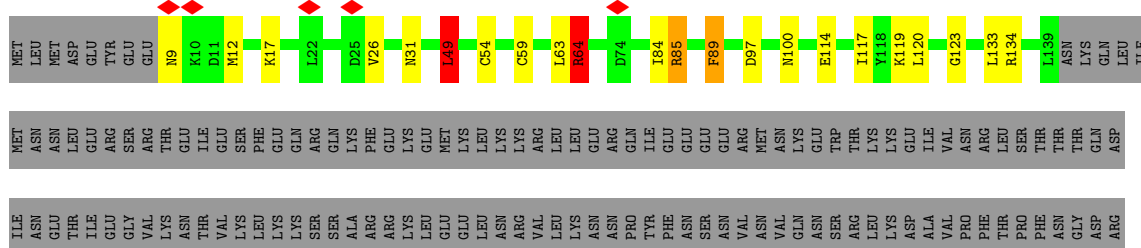
Chain B2: 



• Molecule 3: General transcription and DNA repair factor IIH subunit TFB2



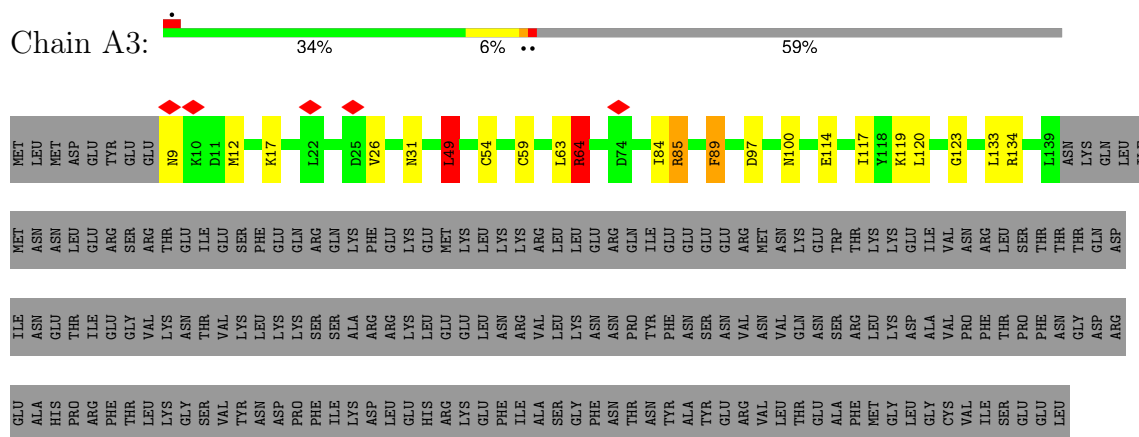
• Molecule 4: RNA polymerase II transcription factor B subunit 3



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

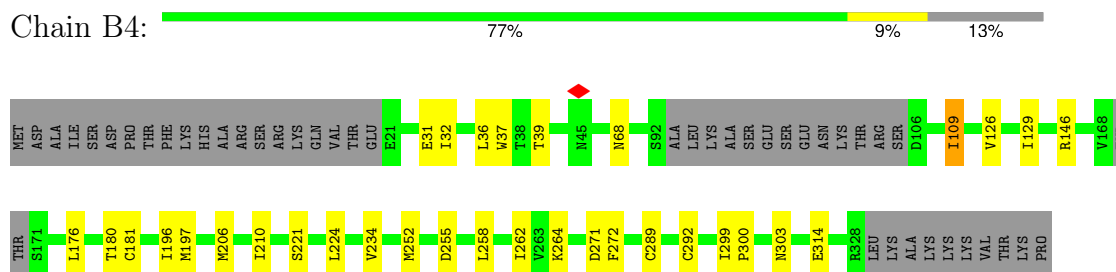
- Molecule 4: RNA polymerase II transcription factor B subunit 3

Chain A3:



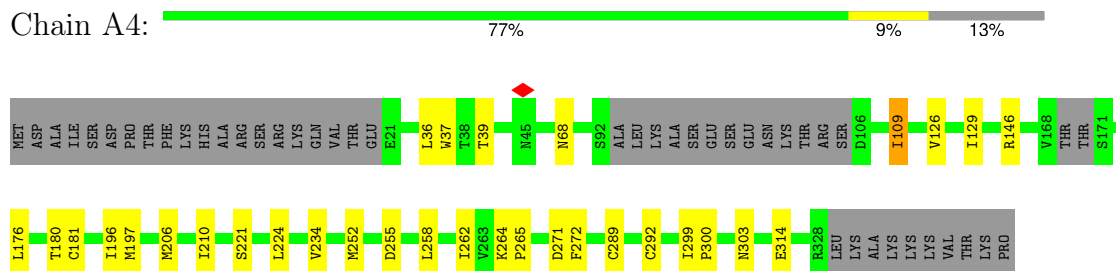
- Molecule 5: General transcription and DNA repair factor IIH subunit TFB4

Chain B4:



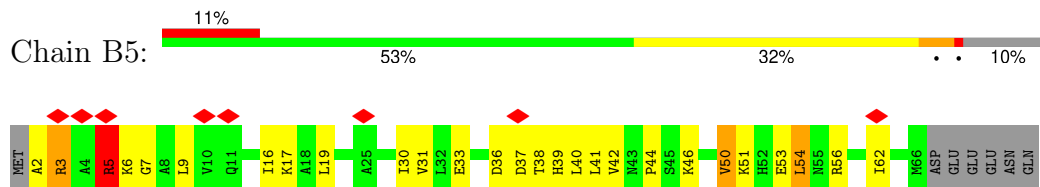
- Molecule 5: General transcription and DNA repair factor IIH subunit TFB4

Chain A4:



- Molecule 6: General transcription and DNA repair factor IIH subunit TFB5

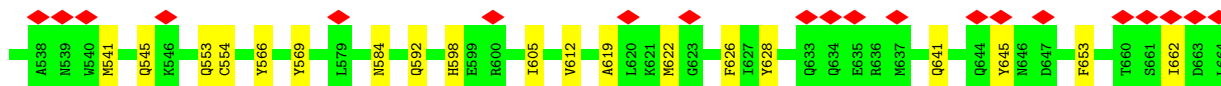
Chain B5:

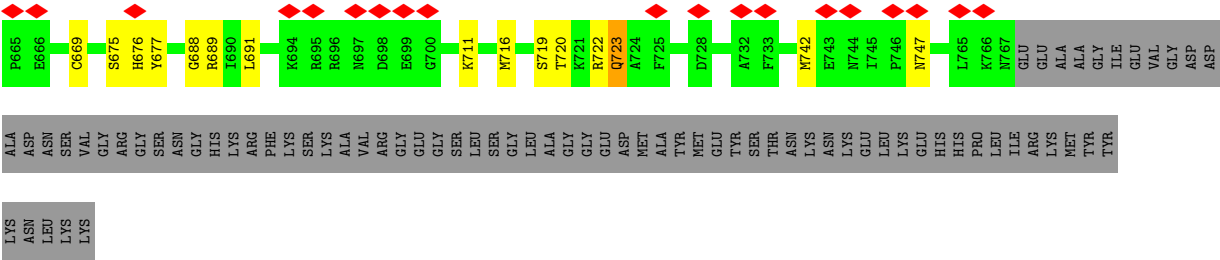


- Molecule 6: General transcription and DNA repair factor IIH subunit TFB5

Chain A5:

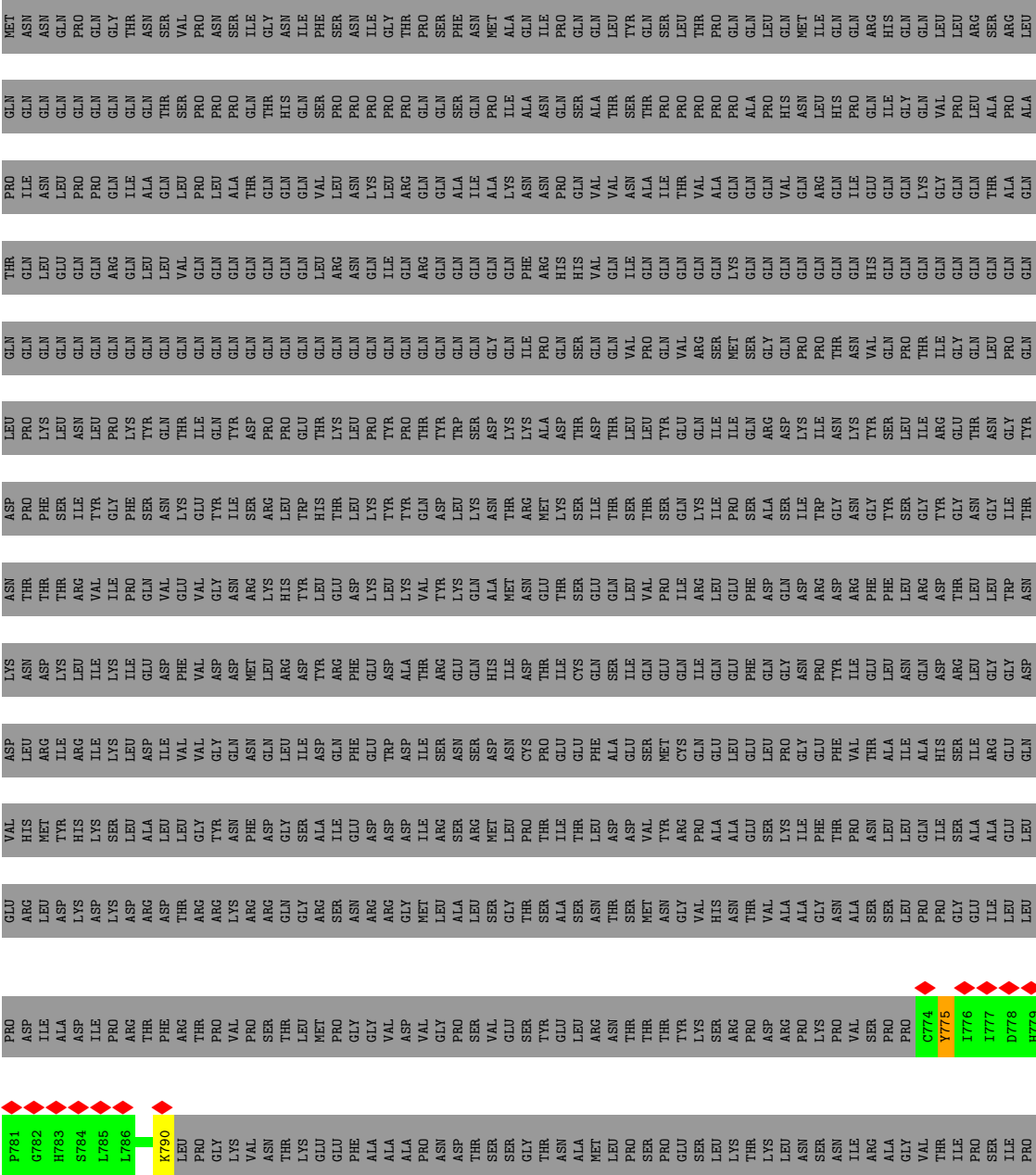






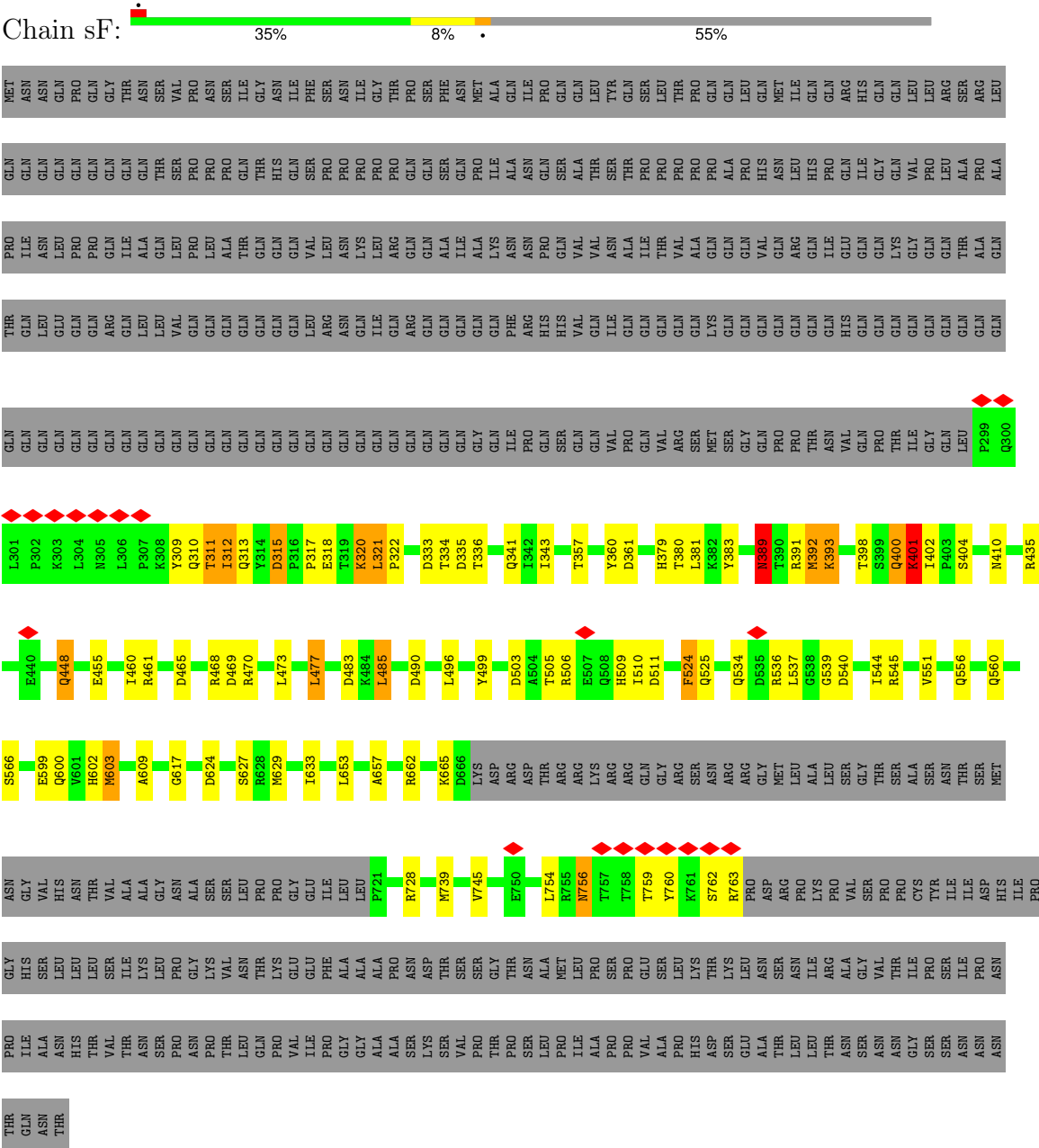
● Molecule 9: SWI/SNF chromatin-remodeling complex subunit SNF5

Chain B8: 98%

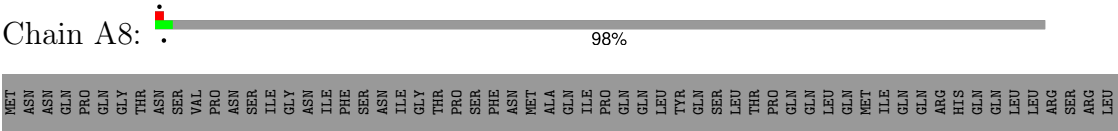


ILE	ALA	ASN	HIS	THR	VAL	THR	THR	ASN	SER	PRO	ASN	PRO	THR	LEU	GLN	PRO	VAL	ILE	PRO	GLY	GLY	ALA	ALA	ALA	LYS	SER	VAL	PRO	THR	PRO	THR	ALA	ALA	ASP	SER	GLU	ALA	THR	THR	LEU	LEU	GLN	GLY	SER	ASN	ASN	ASN	THR
GLN	ASN	THR																																														

● Molecule 9: SWI/SNF chromatin-remodeling complex subunit SNF5



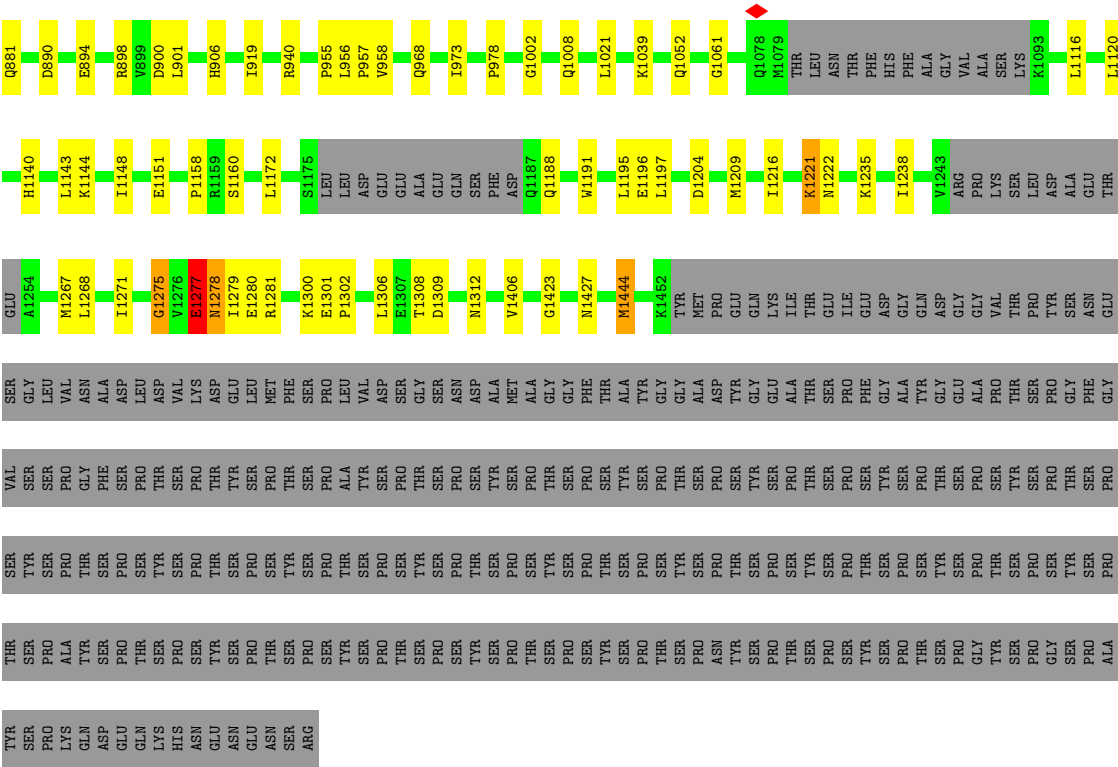
● Molecule 9: SWI/SNF chromatin-remodeling complex subunit SNF5



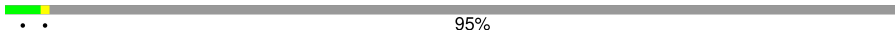
- Molecule 9: SWI/SNF chromatin-remodeling complex subunit SNF5

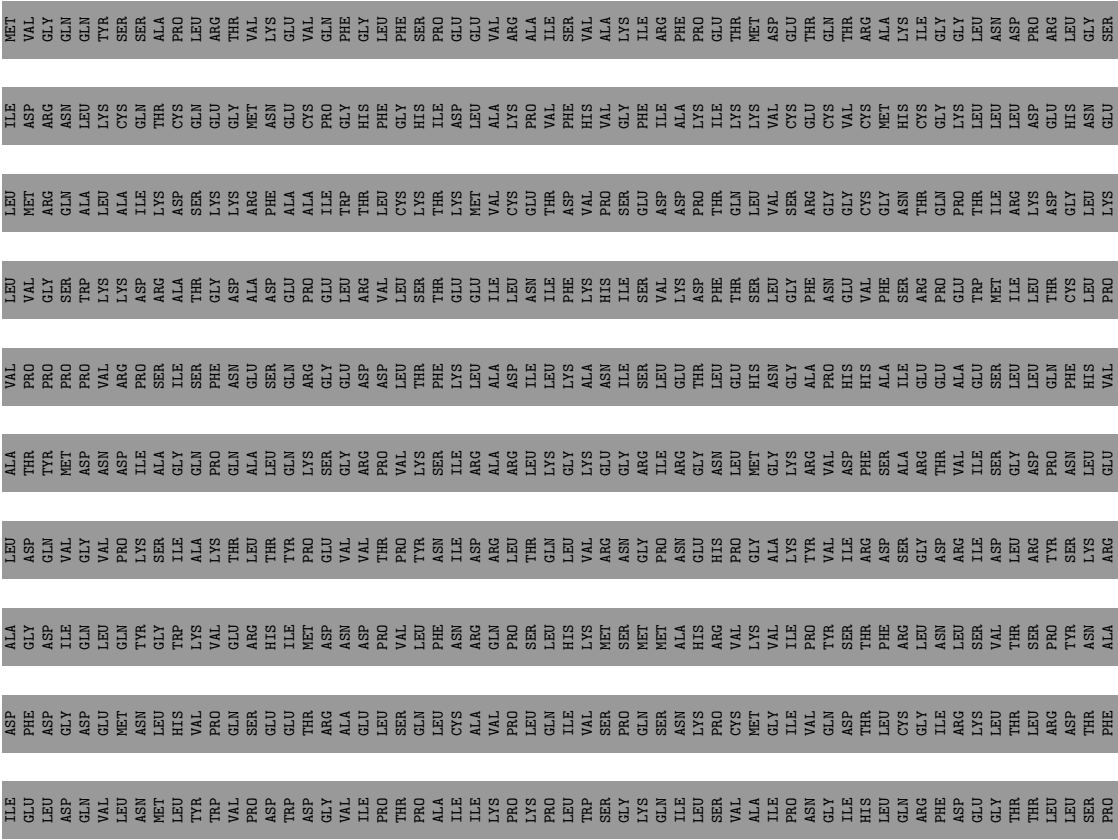
- Molecule 11: DNA-directed RNA polymerase II subunit RPB1

[illegible]



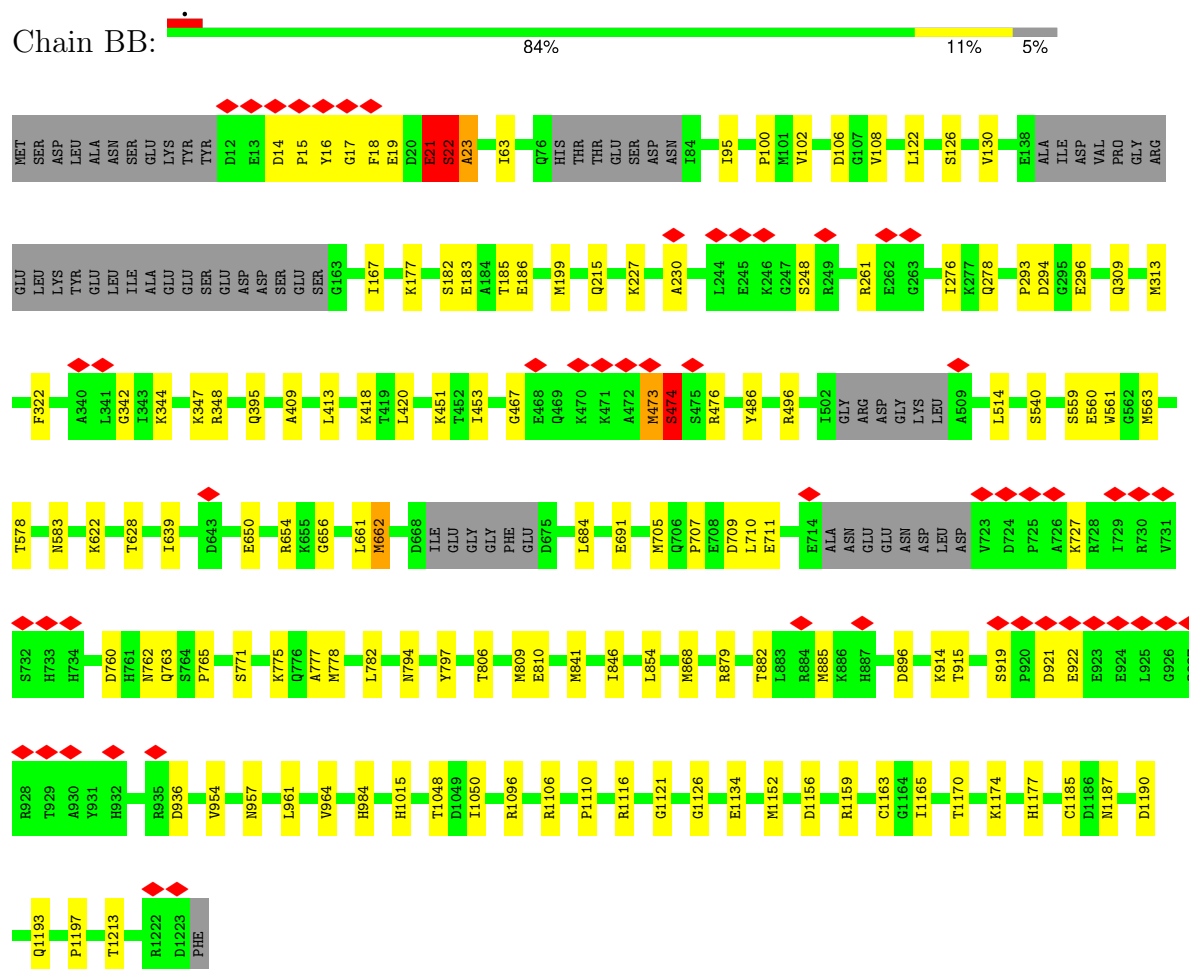
● Molecule 11: DNA-directed RNA polymerase II subunit RPB1

Chain MA:  95%



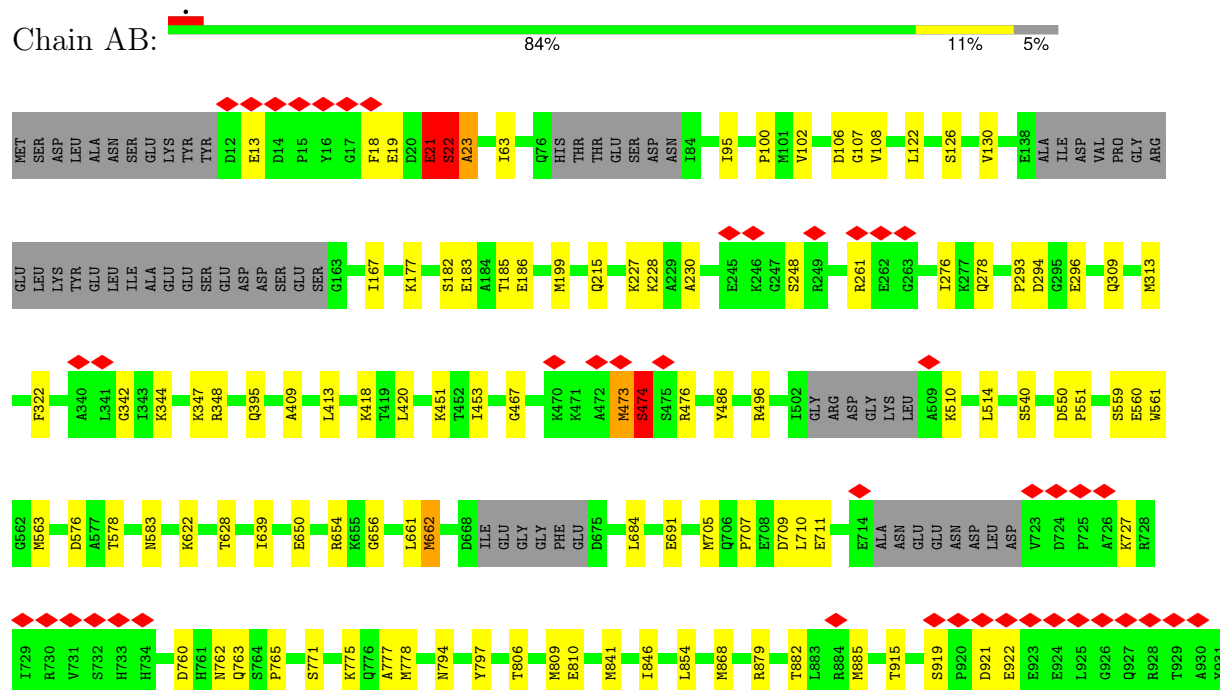
- Molecule 12: DNA-directed RNA polymerase II subunit RPB2

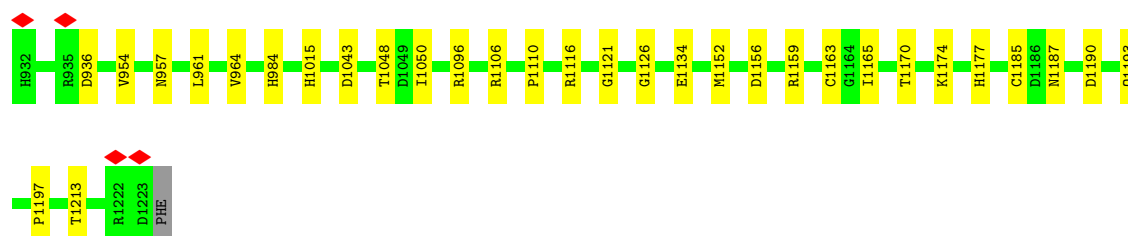
Chain BB:



- Molecule 12: DNA-directed RNA polymerase II subunit RPB2

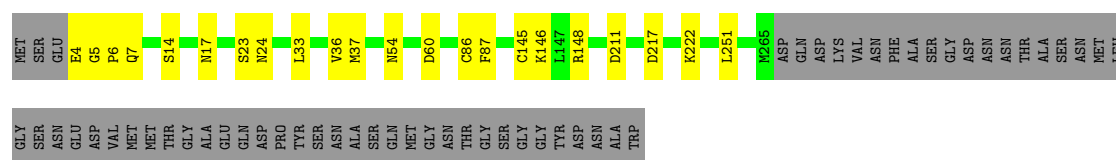
Chain AB:





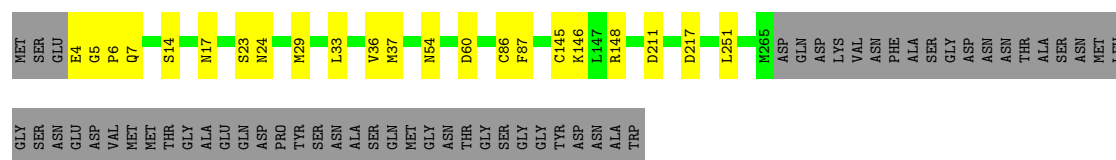
• Molecule 13: DNA-directed RNA polymerase II subunit RPB3

Chain BC: 75% 7% 18%



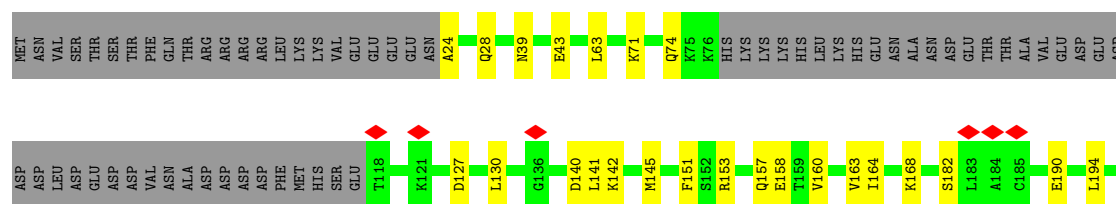
• Molecule 13: DNA-directed RNA polymerase II subunit RPB3

Chain AC: 75% 7% 18%



• Molecule 14: DNA-directed RNA polymerase II subunit RPB4

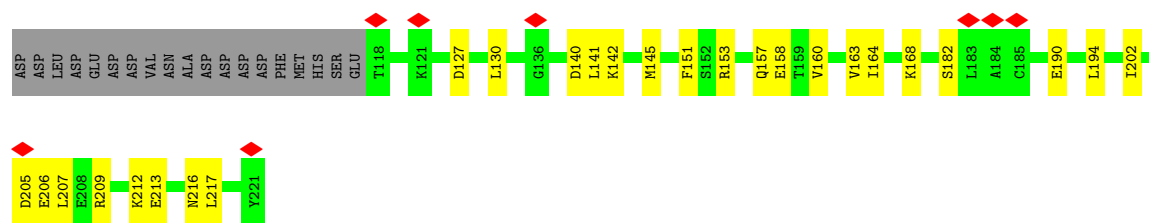
Chain BD: 56% 15% 29%



• Molecule 14: DNA-directed RNA polymerase II subunit RPB4

Chain AD: 56% 15% 29%





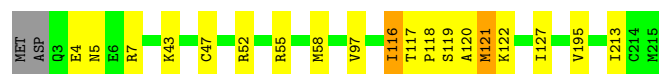
- Molecule 15: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain BE: 90% 8% ..



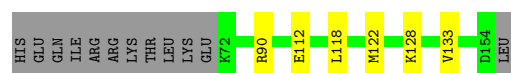
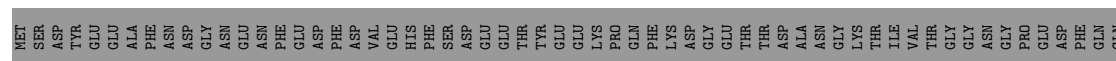
- Molecule 15: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain AE: 90% 8% ..



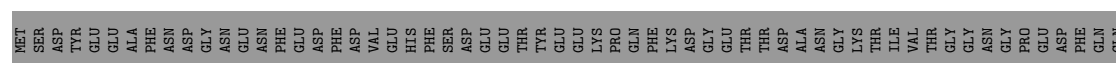
- Molecule 16: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain BF: 50% 46%



- Molecule 16: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain AF: 49% 5% 46%

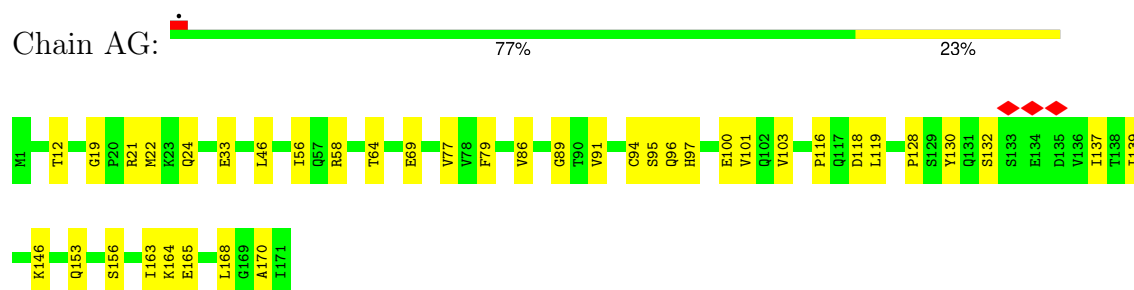


- Molecule 17: DNA-directed RNA polymerase II subunit RPB7

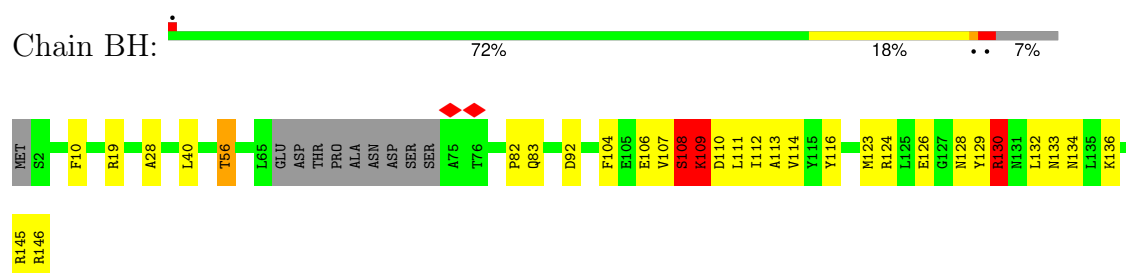
Chain BG: 75% 25%



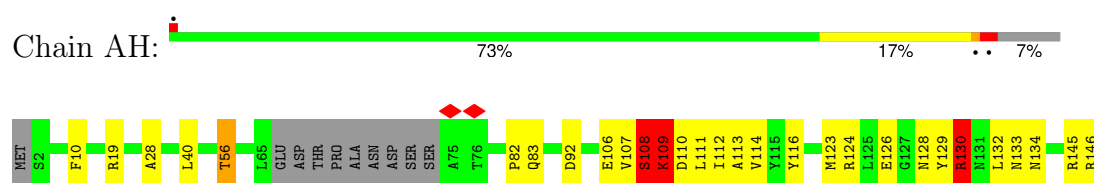
- Molecule 17: DNA-directed RNA polymerase II subunit RPB7



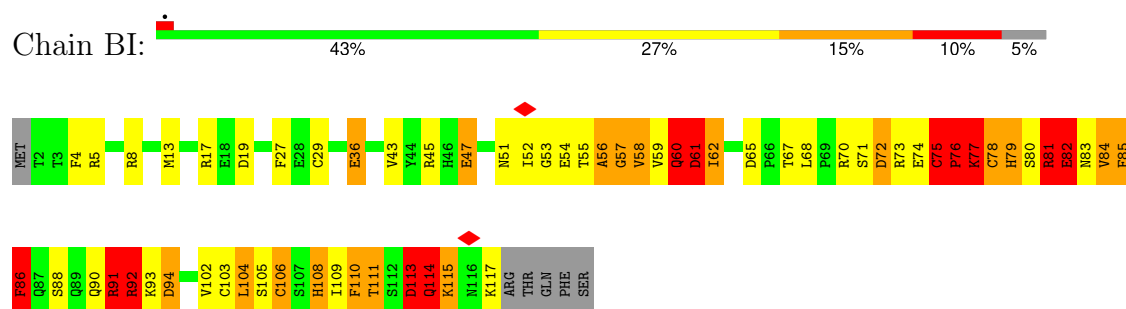
- Molecule 18: DNA-directed RNA polymerases I, II, and III subunit RPABC3



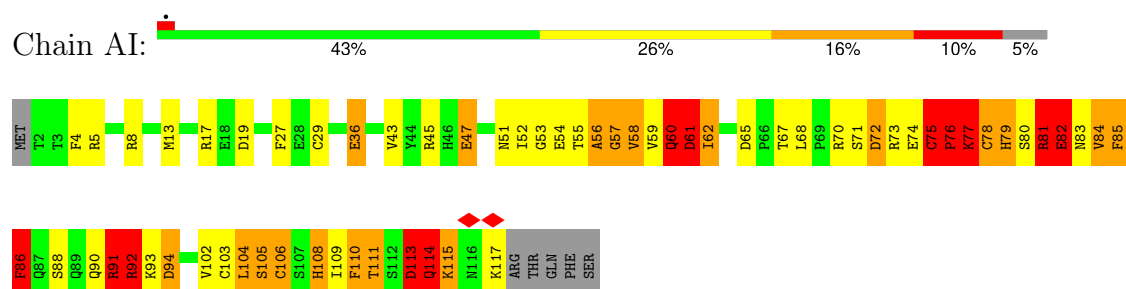
- Molecule 18: DNA-directed RNA polymerases I, II, and III subunit RPABC3



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



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



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

Chain BJ:  79% 19% ..



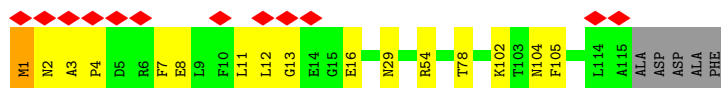
- Molecule 20: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain AJ:  79% 19% ..



- Molecule 21: DNA-directed RNA polymerase II subunit RPB11

Chain BK:  10% 82% 12% ..



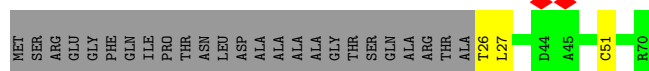
- Molecule 21: DNA-directed RNA polymerase II subunit RPB11

Chain AK:  7% 82% 13% ..



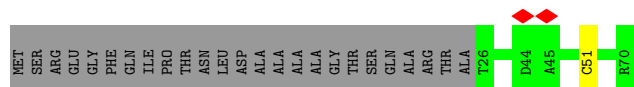
- Molecule 22: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain BL:  60% 36%



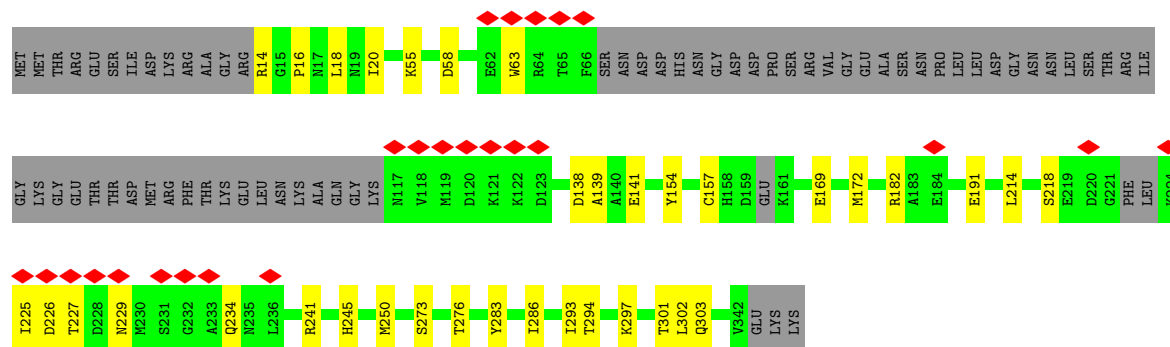
- Molecule 22: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain AL:  63% 36%

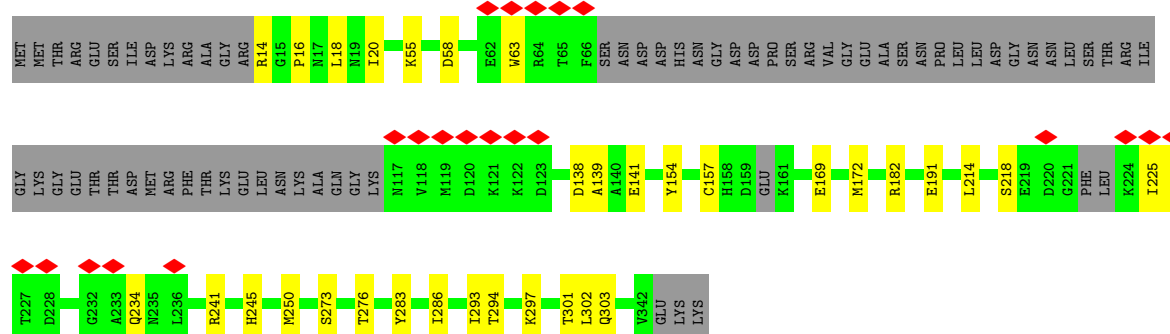


- Molecule 23: Transcription initiation factor IIB

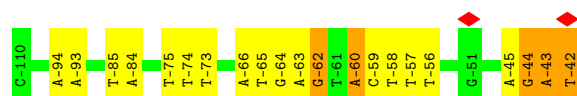
Chain BM:  7% 70% 10% 20%



• Molecule 23: Transcription initiation factor IIB



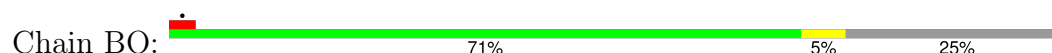
• Molecule 24: promoter DNA



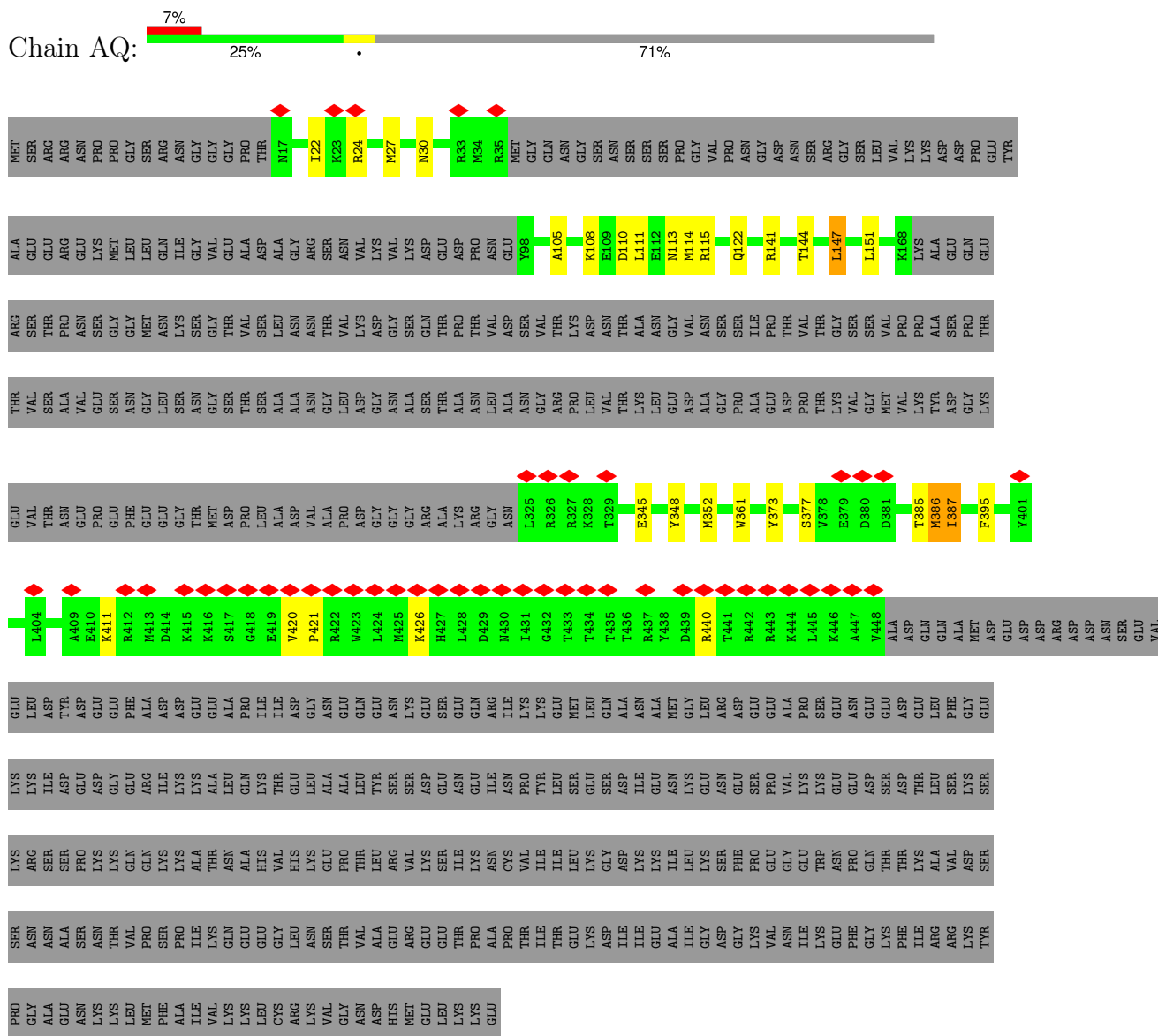
• Molecule 24: promoter DNA



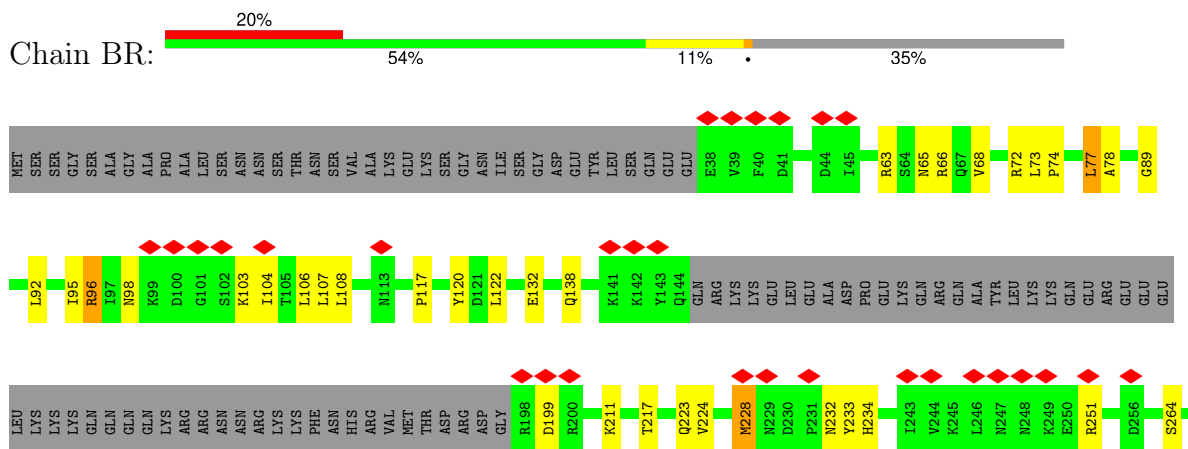
• Molecule 25: TATA-box-binding protein

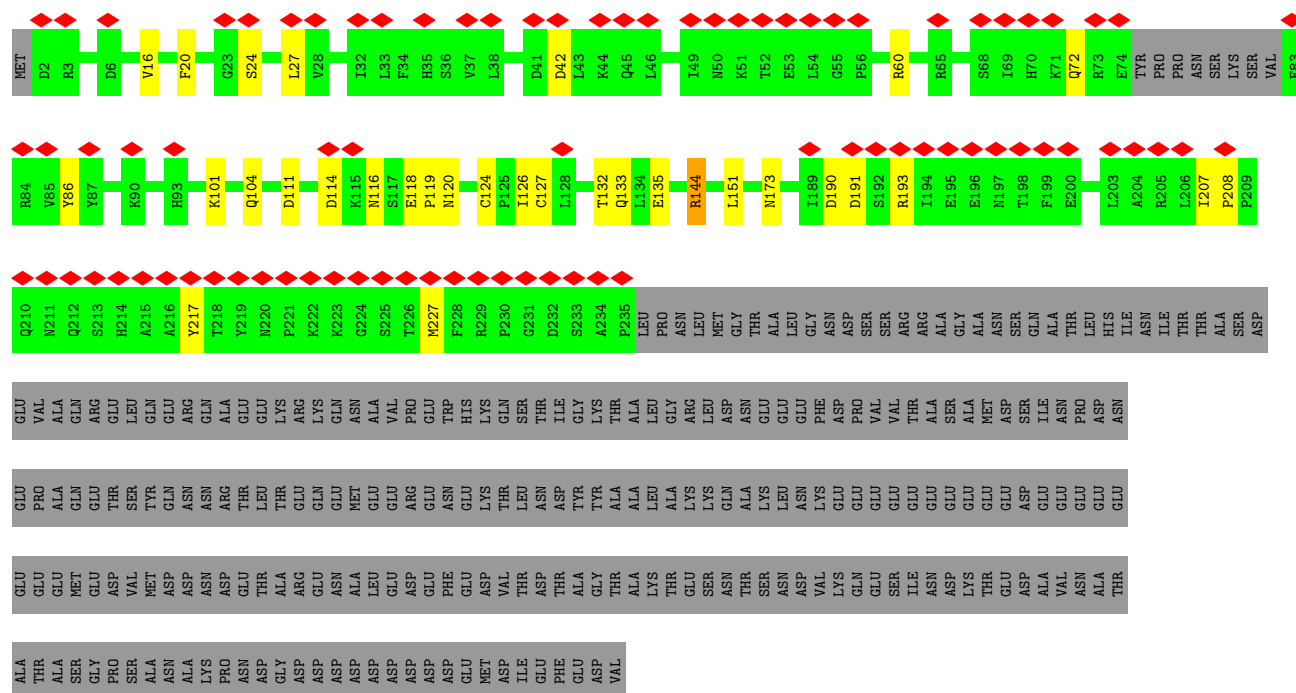




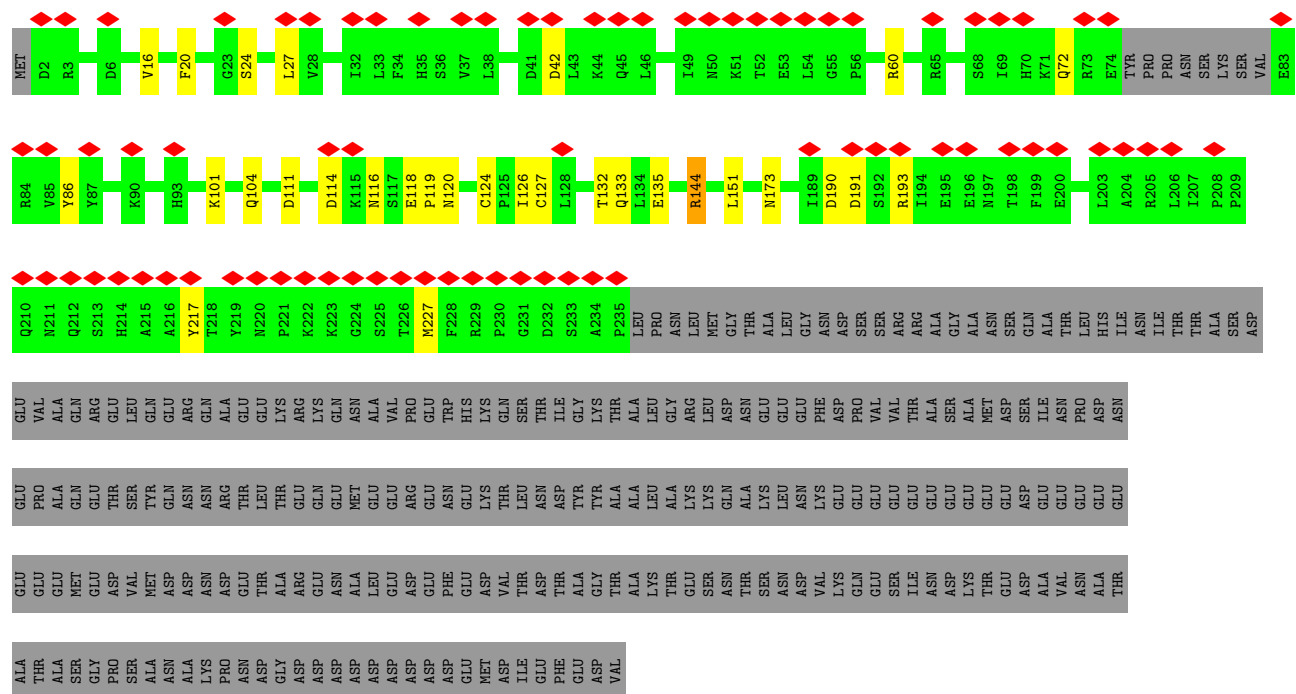
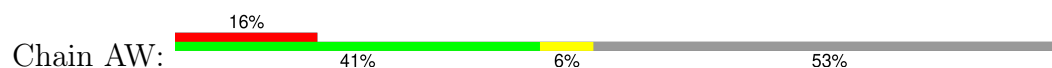


- Molecule 27: Transcription initiation factor IIF subunit beta





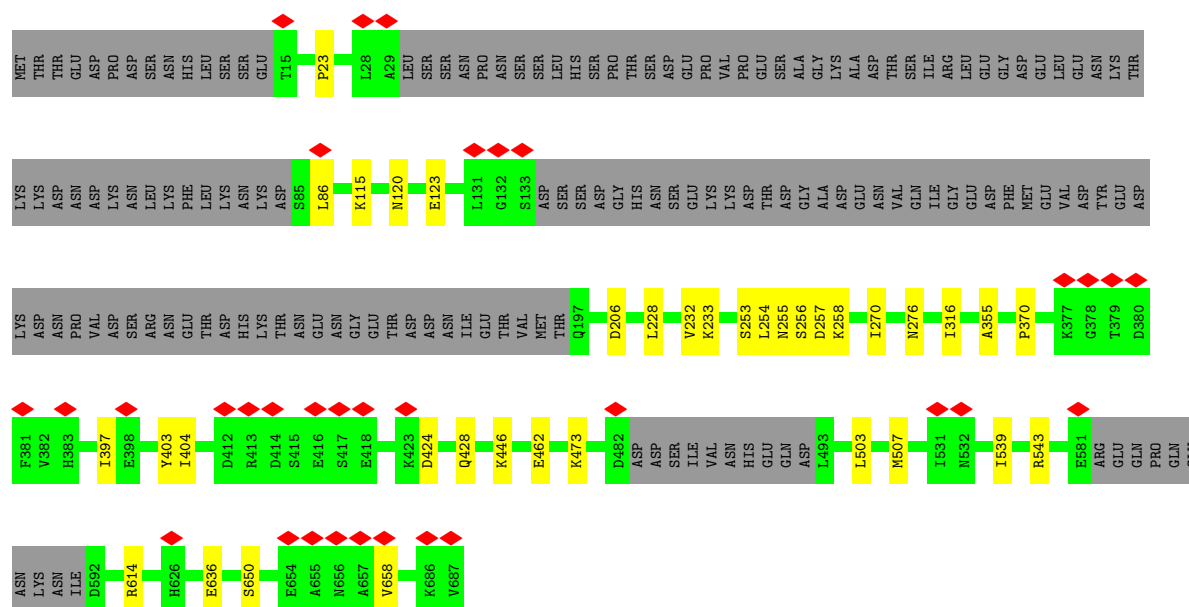
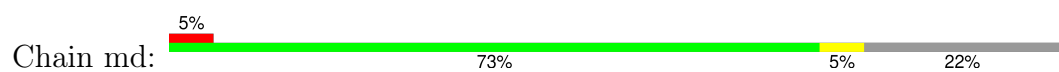
• Molecule 32: Transcription initiation factor IIE subunit alpha



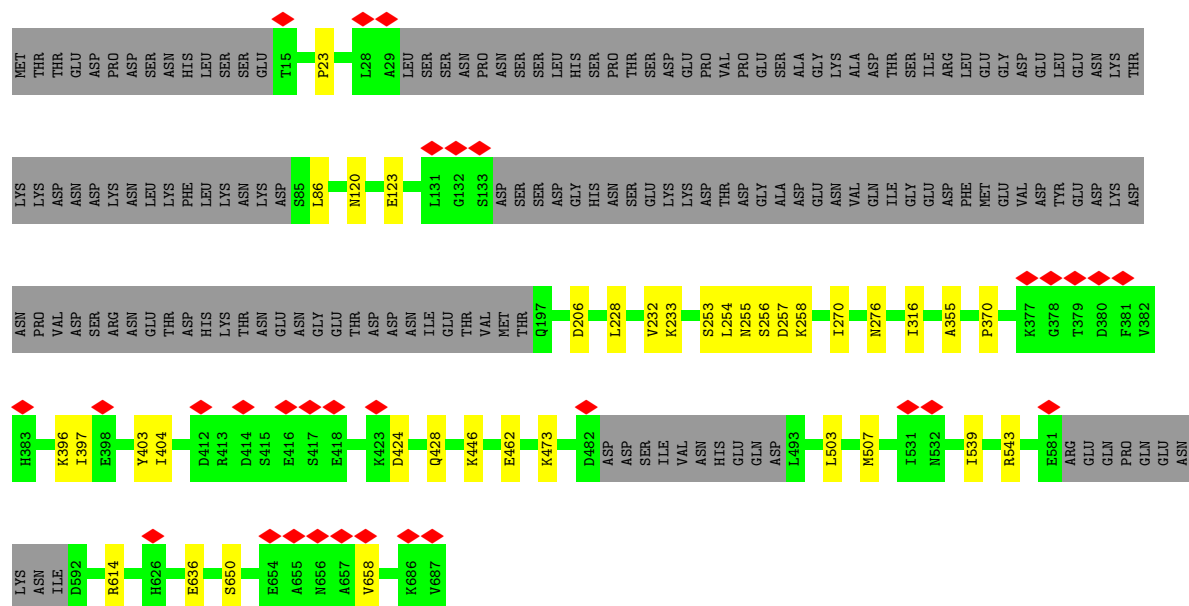
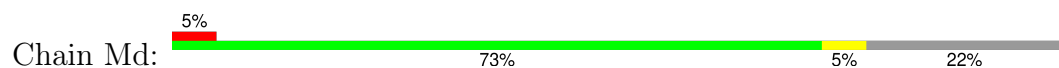
• Molecule 33: Transcription initiation factor IIE subunit beta



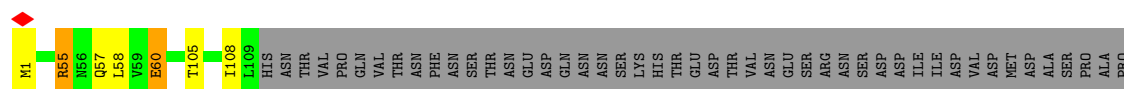
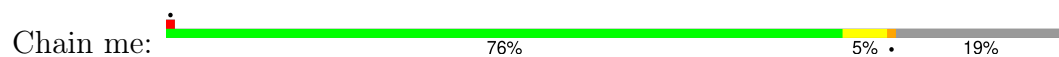




• Molecule 37: Mediator of RNA polymerase II transcription subunit 17

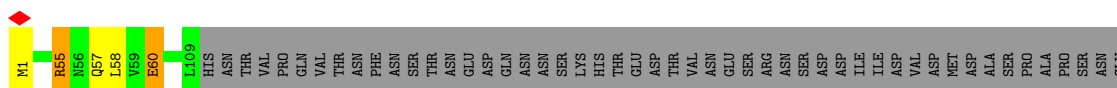
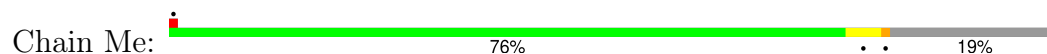


• Molecule 38: Mediator of RNA polymerase II transcription subunit 18

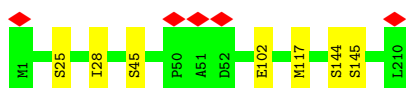




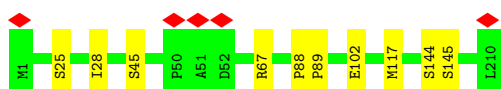
- Molecule 38: Mediator of RNA polymerase II transcription subunit 18



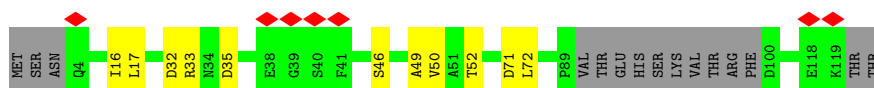
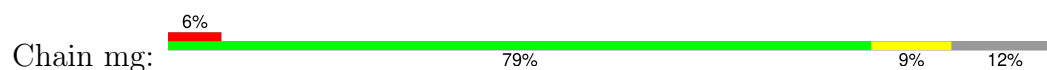
- Molecule 39: Mediator of RNA polymerase II transcription subunit 20



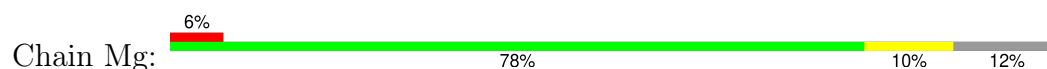
- Molecule 39: Mediator of RNA polymerase II transcription subunit 20



- Molecule 40: Mediator of RNA polymerase II transcription subunit 22

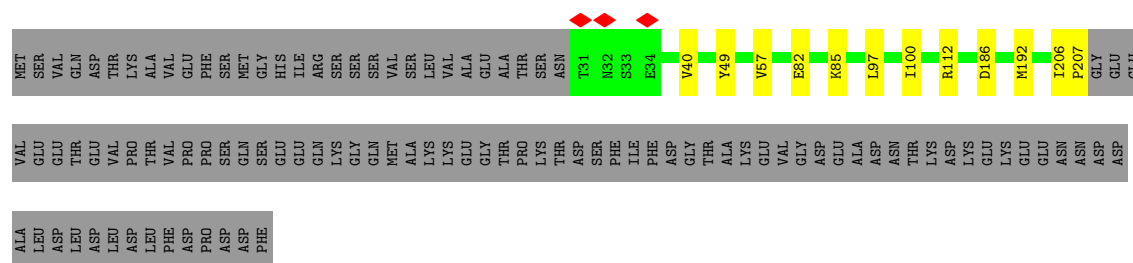


- Molecule 40: Mediator of RNA polymerase II transcription subunit 22

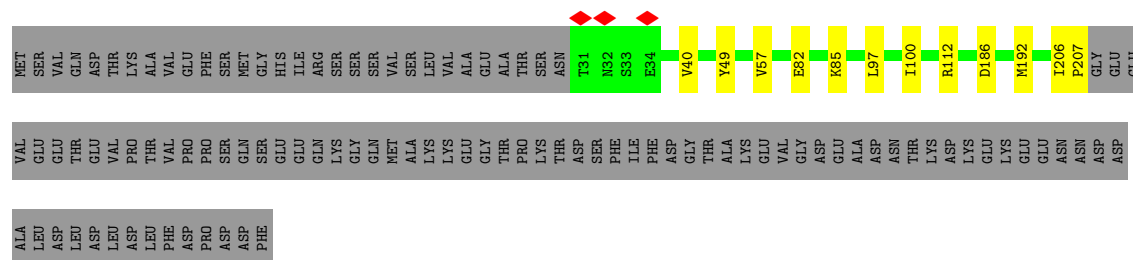


- Molecule 41: Mediator of RNA polymerase II transcription subunit 4

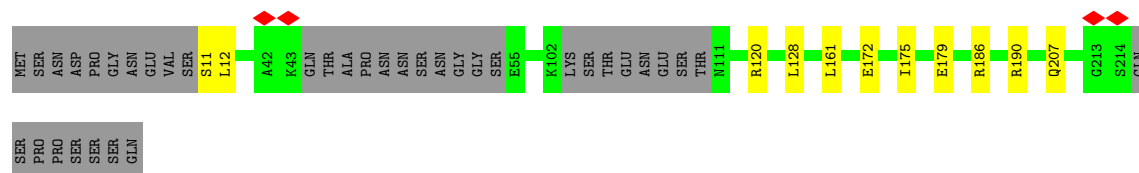
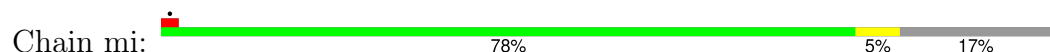




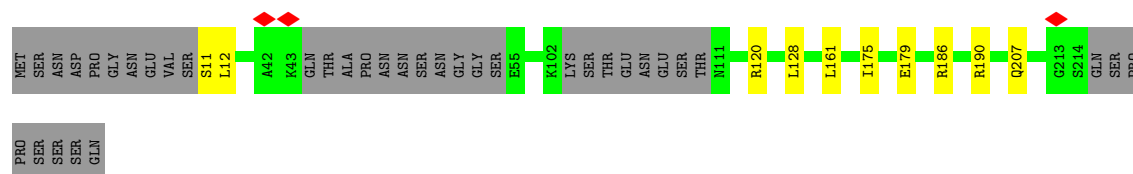
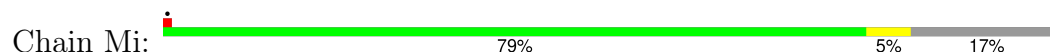
- Molecule 41: Mediator of RNA polymerase II transcription subunit 4



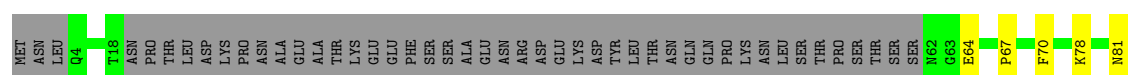
- Molecule 42: Mediator of RNA polymerase II transcription subunit 7



- Molecule 42: Mediator of RNA polymerase II transcription subunit 7

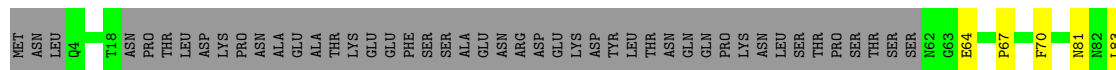


- Molecule 43: Mediator of RNA polymerase II transcription subunit 9

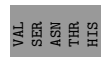
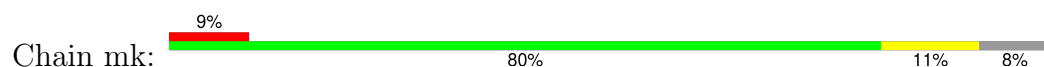




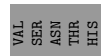
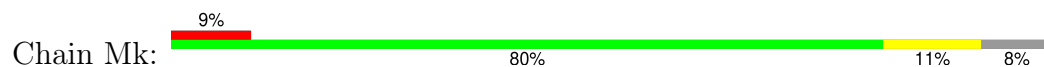
- Molecule 43: Mediator of RNA polymerase II transcription subunit 9



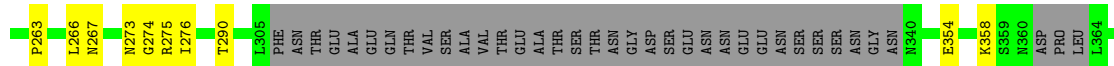
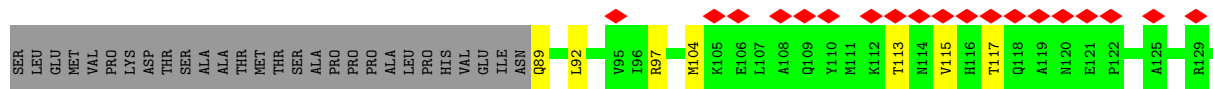
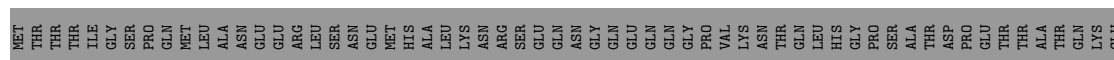
- Molecule 44: Mediator of RNA polymerase II transcription subunit 10

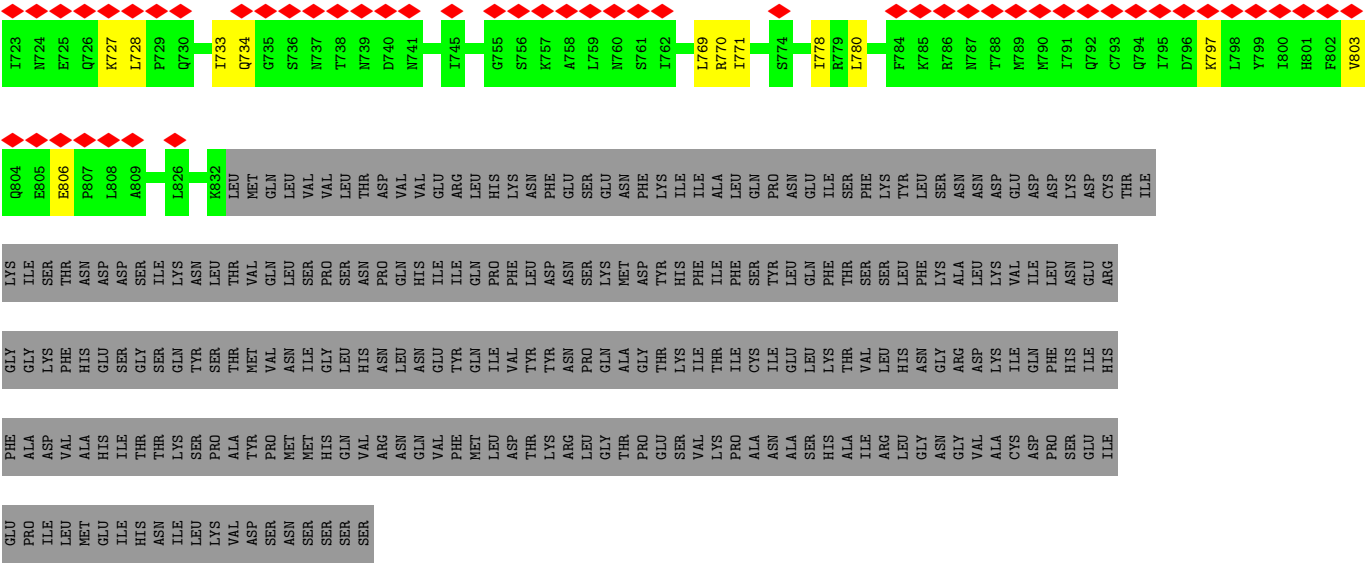


- Molecule 44: Mediator of RNA polymerase II transcription subunit 10

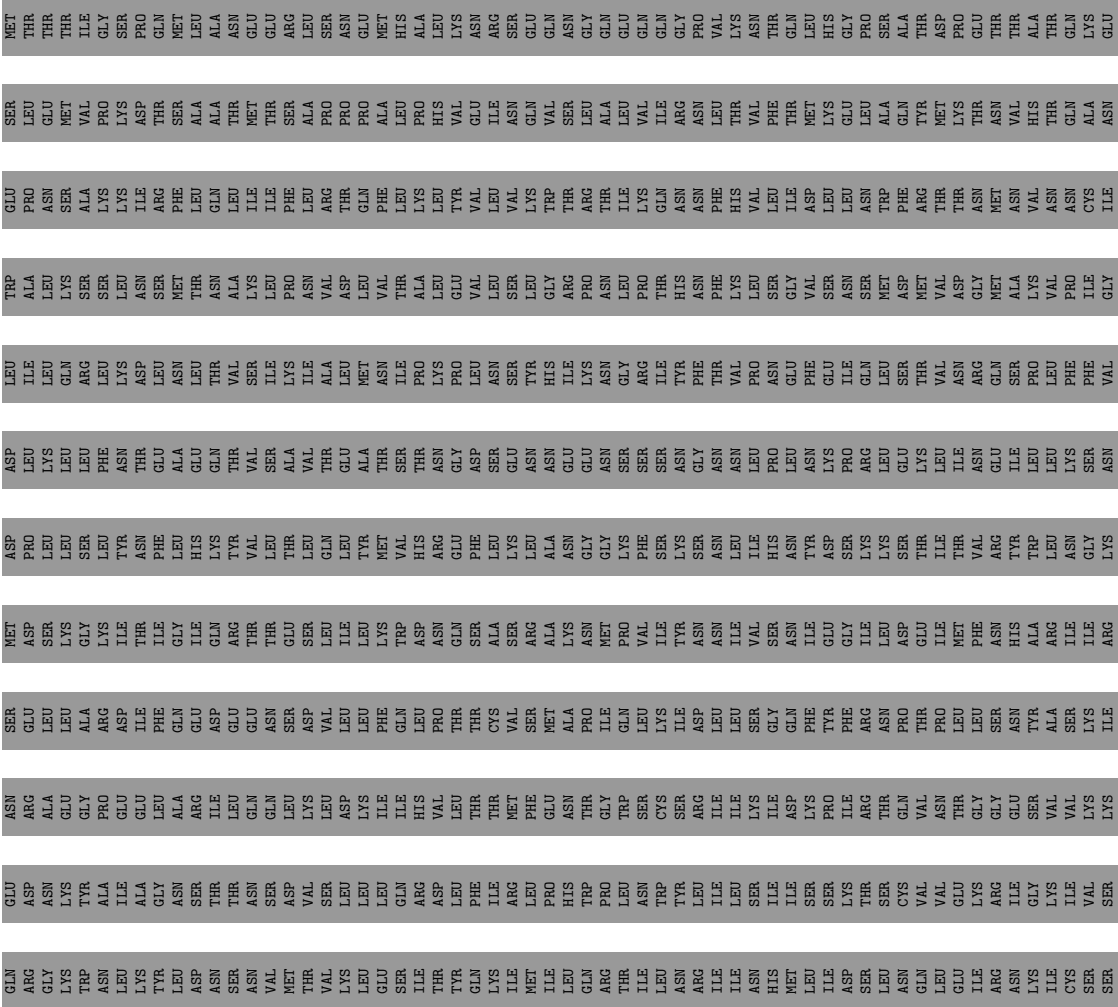


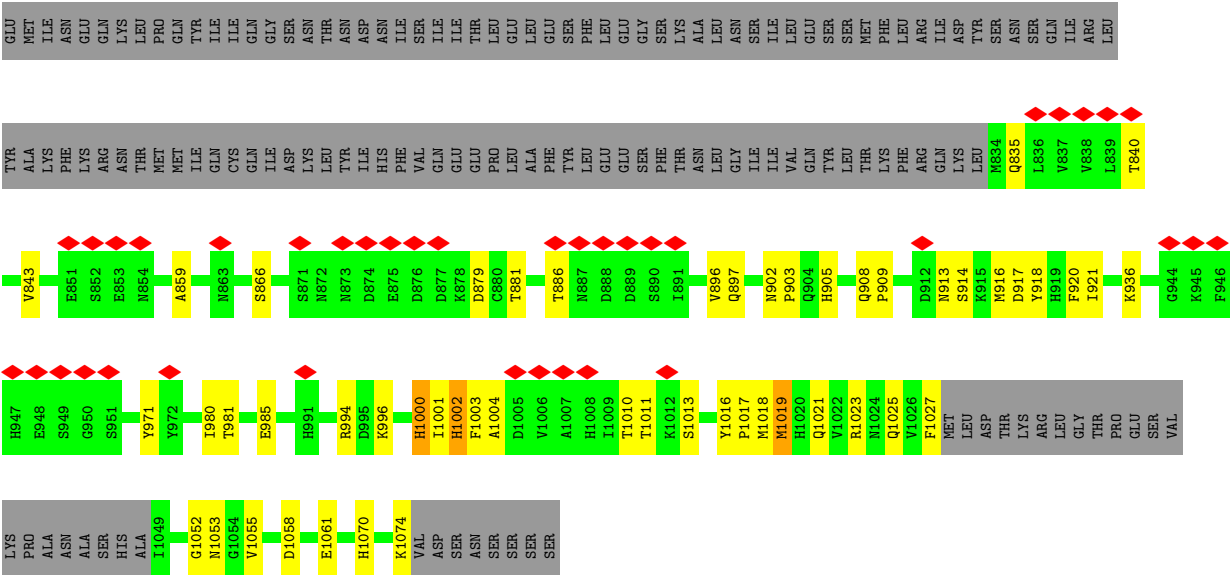
- Molecule 45: Mediator of RNA polymerase II transcription subunit 14



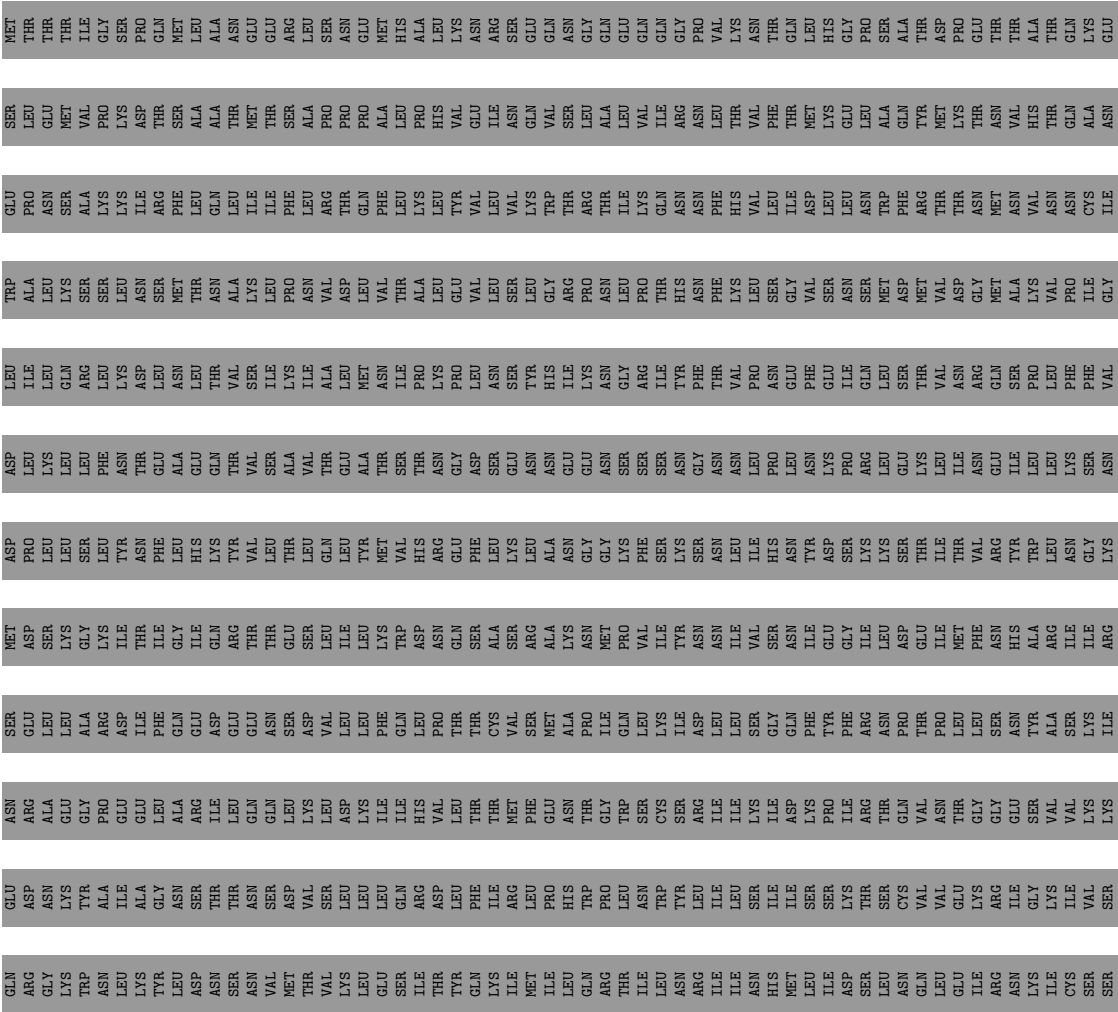


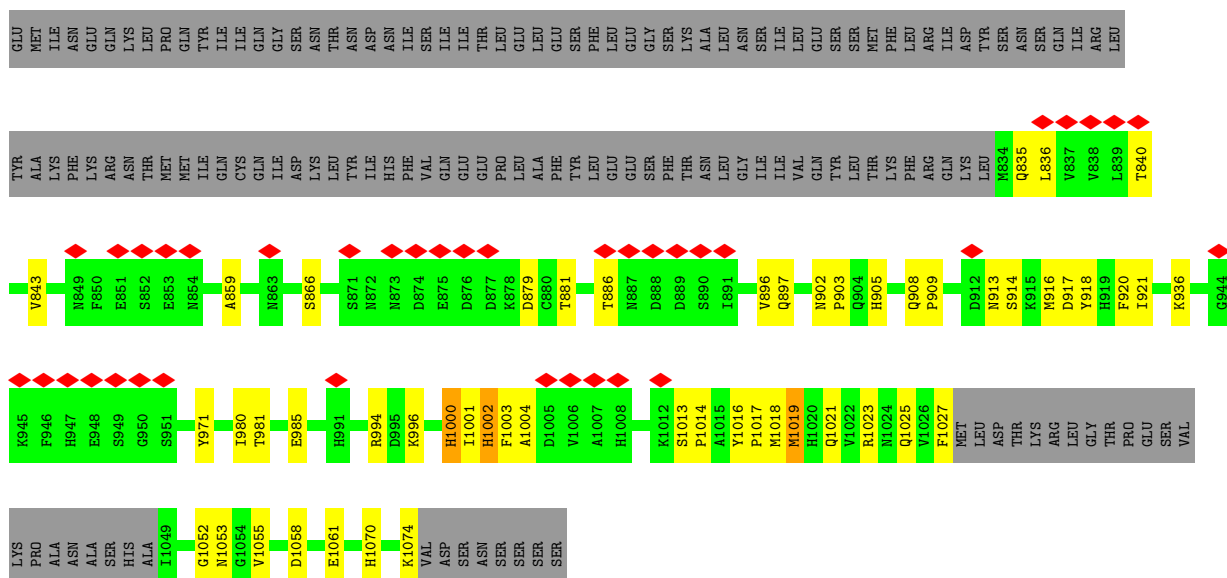
● Molecule 45: Mediator of RNA polymerase II transcription subunit 14



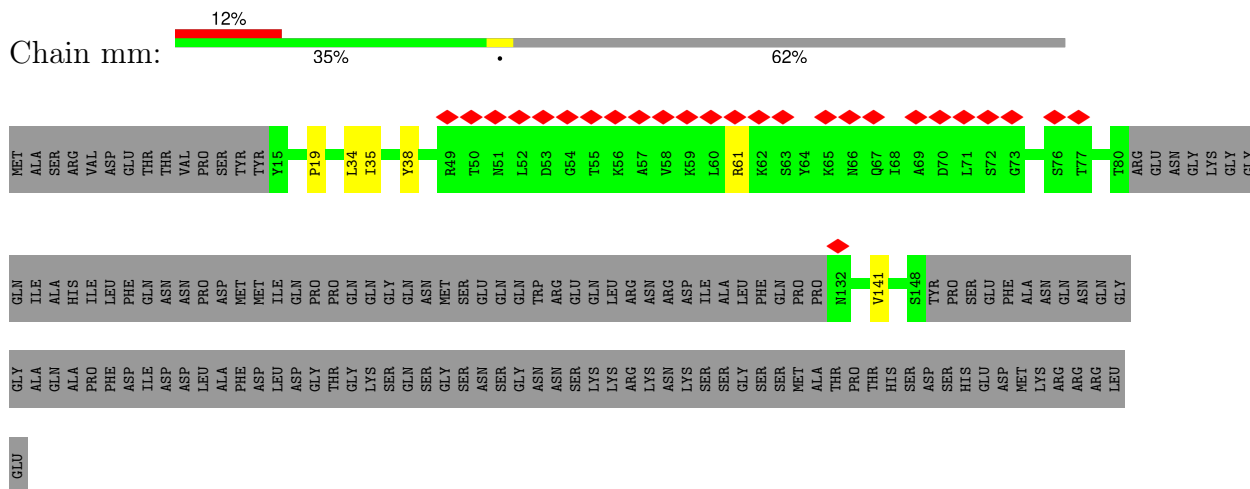


• Molecule 45: Mediator of RNA polymerase II transcription subunit 14

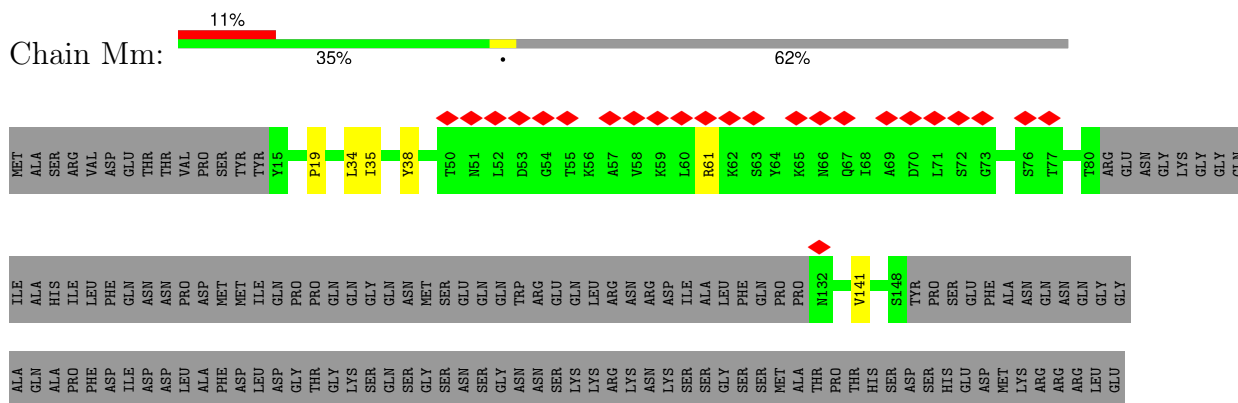




- Molecule 46: Mediator of RNA polymerase II transcription subunit 19



- Molecule 46: Mediator of RNA polymerase II transcription subunit 19

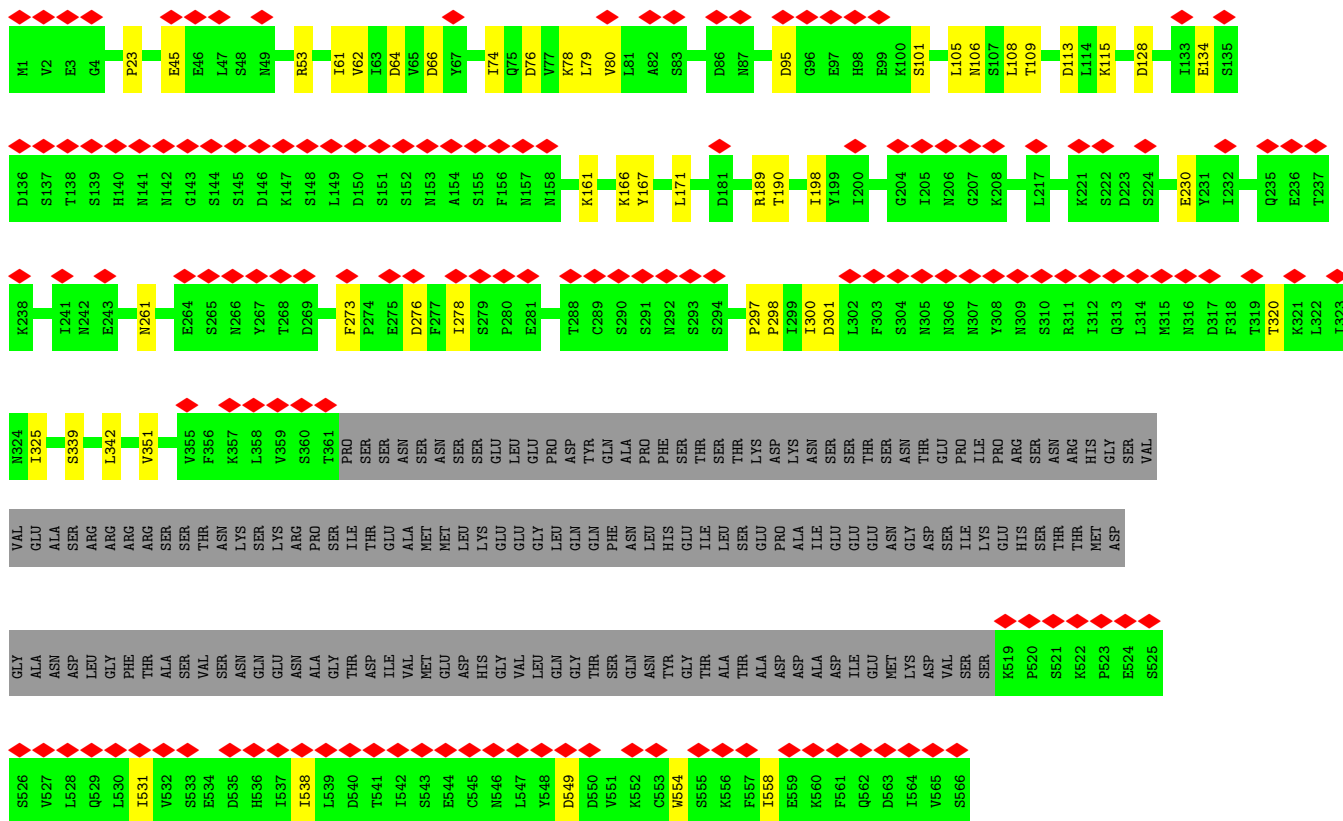


- Molecule 47: Mediator of RNA polymerase II transcription subunit 21

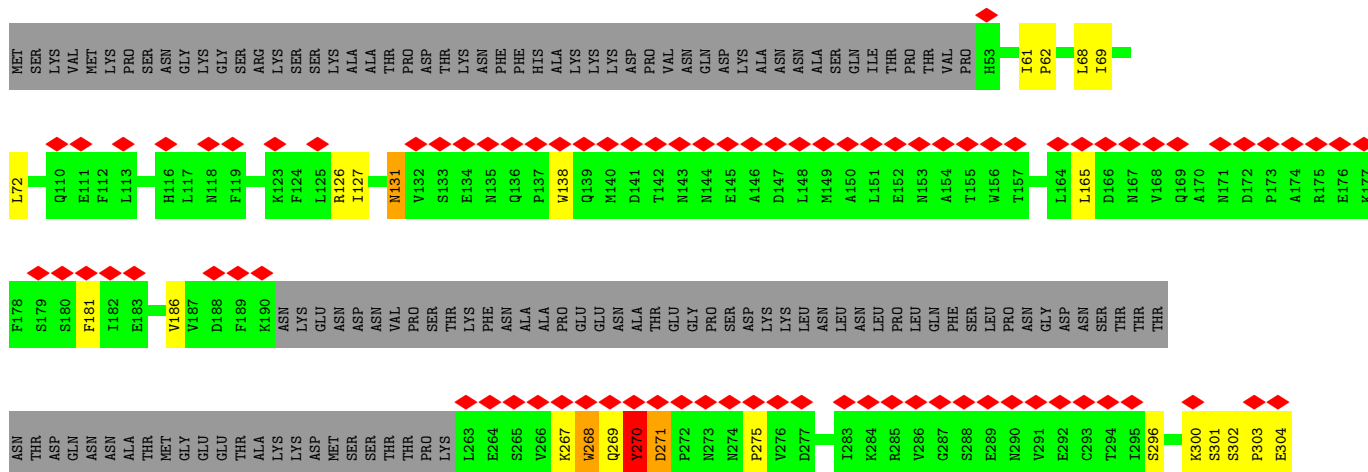


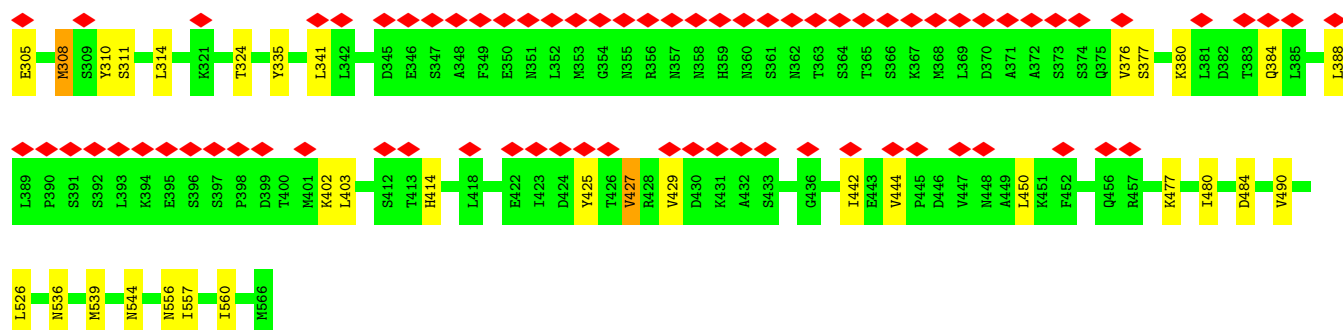


• Molecule 49: Mediator of RNA polymerase II transcription subunit 1

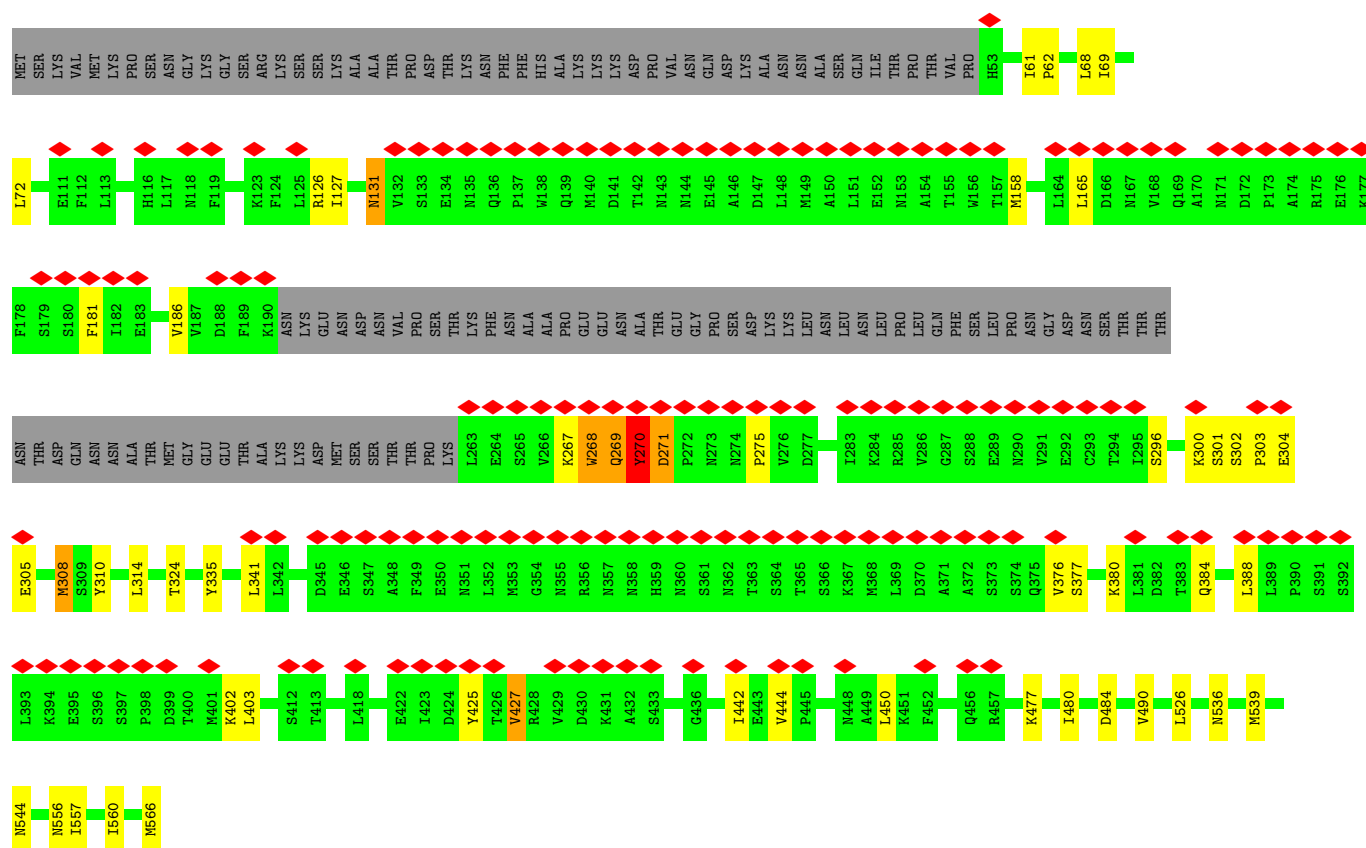


• Molecule 50: Transcription regulatory protein SNF12

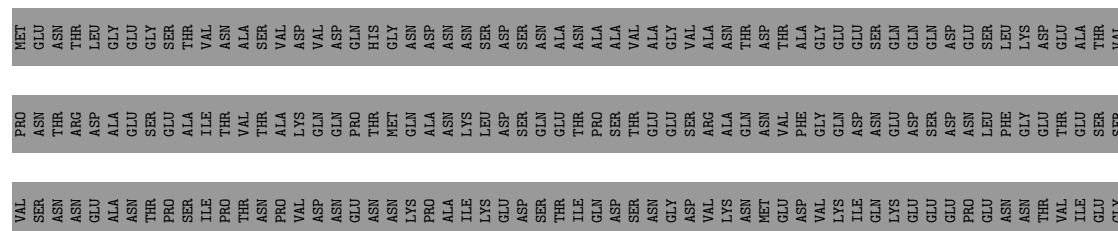


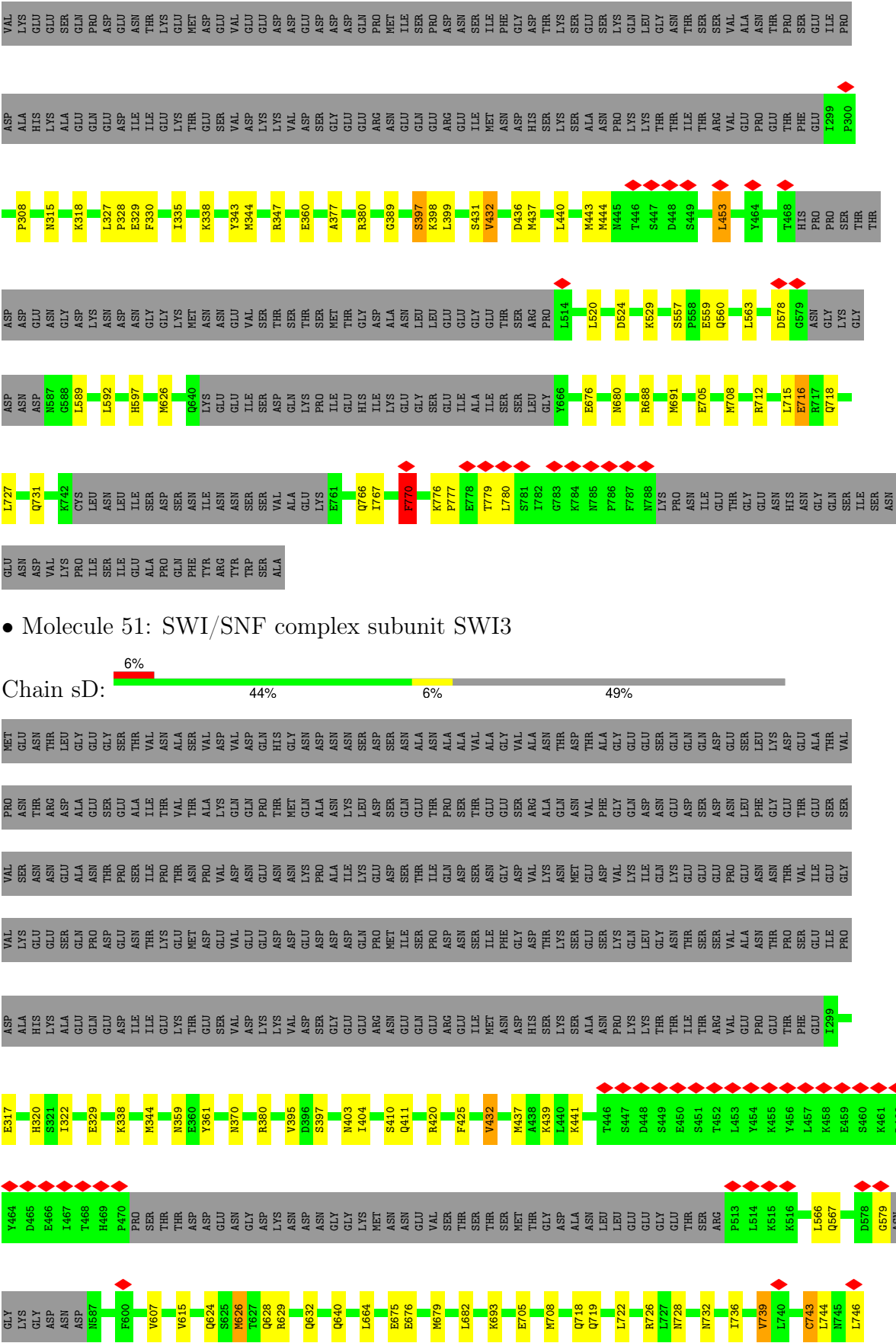


• Molecule 50: Transcription regulatory protein SNF12

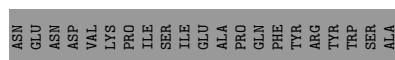
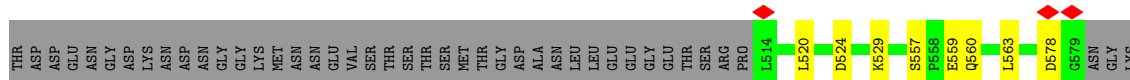
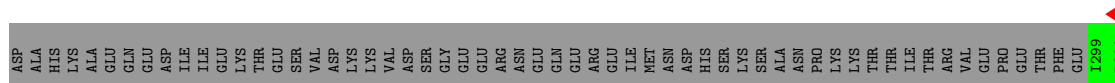


• Molecule 51: SWI/SNF complex subunit SWI3

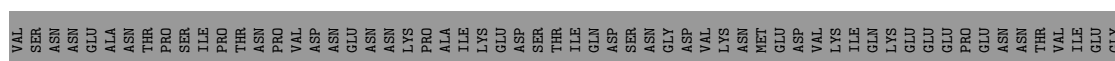


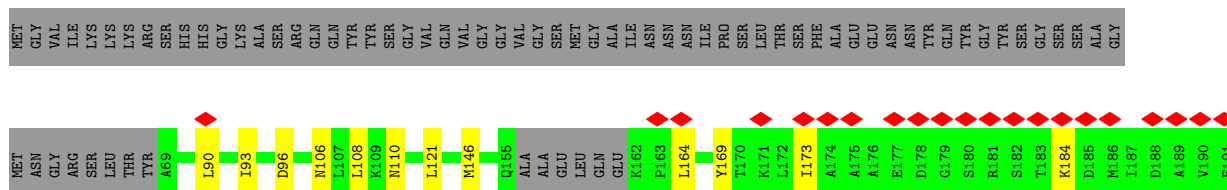


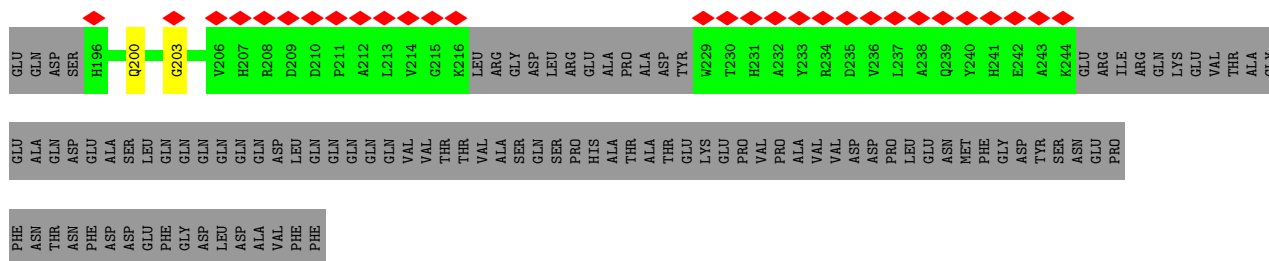
- Molecule 51: SWI/SNF complex subunit SWI3



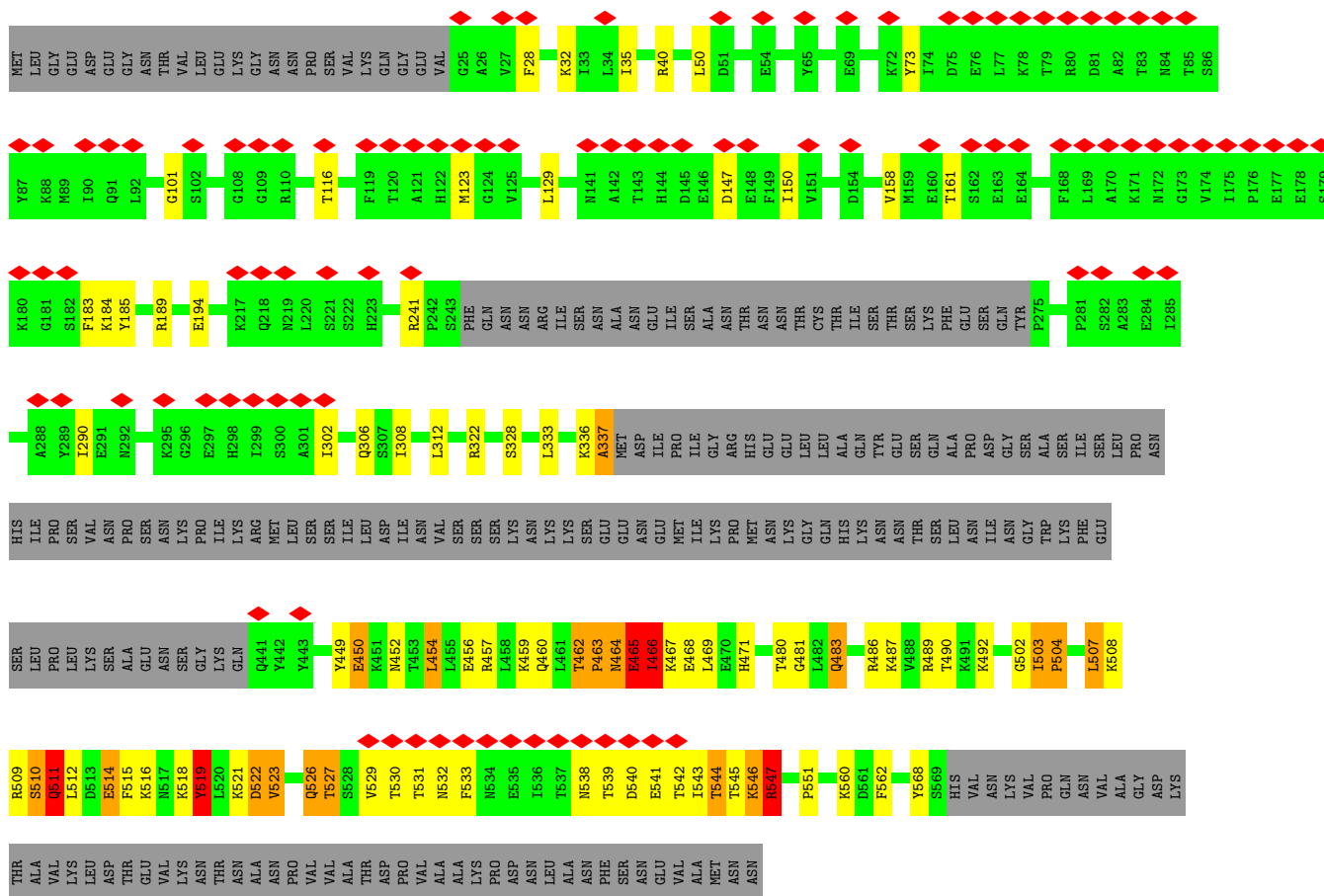
- Molecule 51: SWI/SNF complex subunit SWI3



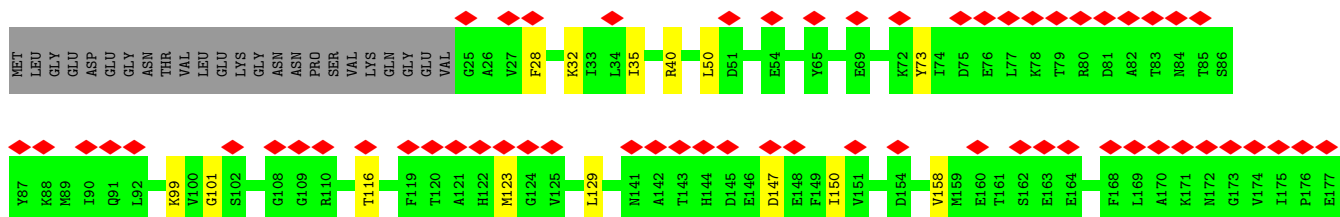




- Molecule 53: SWI/SNF global transcription activator complex subunit SWP82



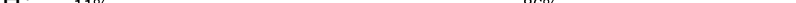
- Molecule 53: SWI/SNF global transcription activator complex subunit SWP82





[illegible]

- Molecule 55: Transcription regulatory protein SNF2

Chain SH:  11% 86%

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

GLN	NET	PRO	PRO	LEU	ASN	SER	ASN	GLY	ASN	ASN	MET	LEU	PRO	GLN	GLN	SER	SER	VAL	GLY	SER	LEU	ASN	ALA	ALA	THR	ASN	ASN	PHE	SER	SER	PRO	PRO	THR	PRO	ALA	ALA	ASN	ASN	GLY	GLY	GLU	LYS	GLU	ASN	ASN	ALA	ALA	GLU	GLU	LYS	PRO	PRO	ASP	ASN	ASN	SER	SER	ASN	HIS	ASN	ASN	LEU	LEU	ASN	ASN	LEU	LEU	GLU	SER	SER	GLN	PRO
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[illegible][illegible][illegible]

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Year	Category	Value
2013	Category 1	432
2013	Category 2	435
2014	Category 1	439
2014	Category 2	443
2015	Category 1	447
2015	Category 2	448
2016	Category 1	449
2016	Category 2	453
2017	Category 1	454
2017	Category 2	455
2018	Category 1	468
2019	Category 1	472
2019	Category 2	475
2020	Category 1	482
2020	Category 2	505
2021	Category 1	517
2021	Category 2	518
2022	Category 1	526
2022	Category 2	534
2023	Category 1	535
2023	Category 2	536
2024	Category 1	537
2024	Category 2	538
2025	Category 1	539
2025	Category 2	553
2026	Category 1	562
2026	Category 2	584
2027	Category 1	585
2027	Category 2	586
2028	Category 1	587
2028	Category 2	588
2029	Category 1	590
2029	Category 2	591
2030	Category 1	592
2030	Category 2	593
2031	Category 1	594
2031	Category 2	595
2032	Category 1	596
2032	Category 2	597
2033	Category 1	598
2033	Category 2	599

Residue	Number of Mutations
A601	1
L605	1
M608	2
N609	2
K610	2
I613	1
K623	1
L627	2
K628	2
F629	2
L633	1
K646	6
K653	6
E654	6
R655	6
L656	6
Q657	6
A658	6
LEU	0
LYS	0
ALA	0
ASN	0
ASP	0
GLU	0
GLU	0
ALA	0
TYR	0
ILE	0
LYS	0
LEU	0
LEU	0
ASP	0
GLN	0
THR	0
LYS	0
ASP	0
THR	0
ARG	0
ARG	0
ILE	0
THR	0
HIS	0
LEU	0
LEU	0
ARG	0
GLN	0
THR	0
ASN	0
ALA	0
PHE	0
LEU	0

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

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

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

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

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

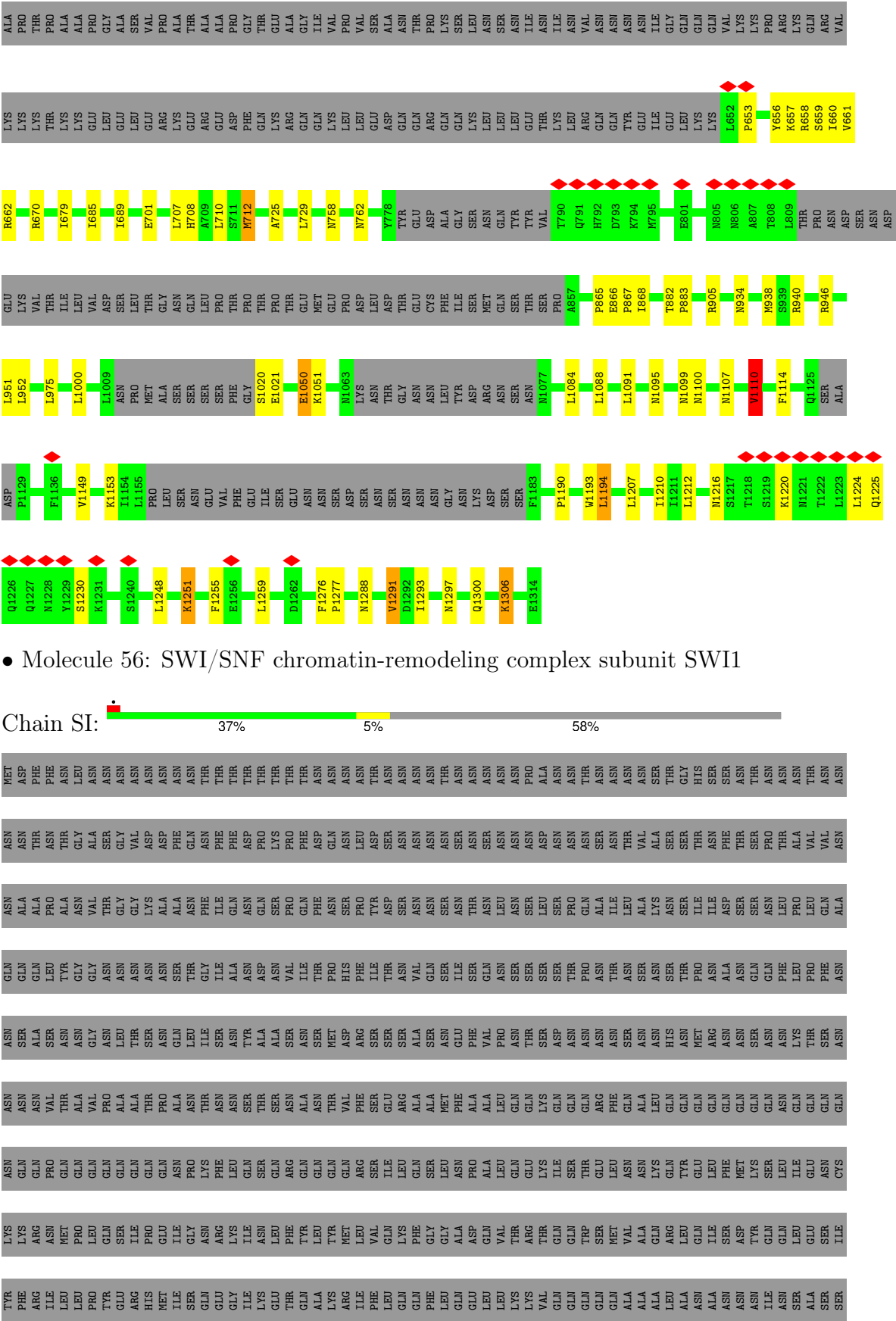
MET	GLN	LEU	LYS	LYS	ILE	CYS	ASN	HIS	PRO	PHE	VAL	PHE	GLU	GLU	VAL	GLU	ASP	GLN	ILE	ASN	PRO	THR	ARG	GLU	THR	ASN	ASP	ASP	ILE	TRP	TRP	VAL	ALA	ALA	LYS	LYS	ALA	THR	GLY	HIS	ARG	VAL	LEU	ILE	PHE	PHE	GLN	MET
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[illegible]

- Molecule 56: SWI/SNF chromatin-remodeling complex subunit SWI1

Chain sI:

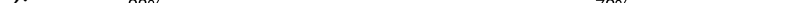
[illegible]

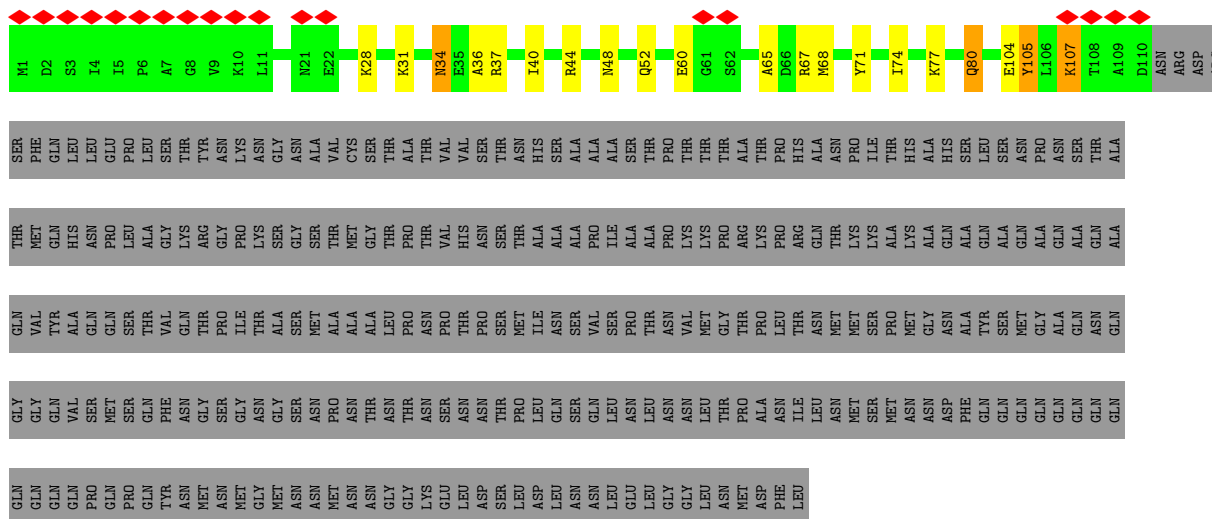


Chain t1: 12% . 85%

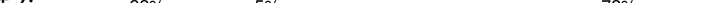


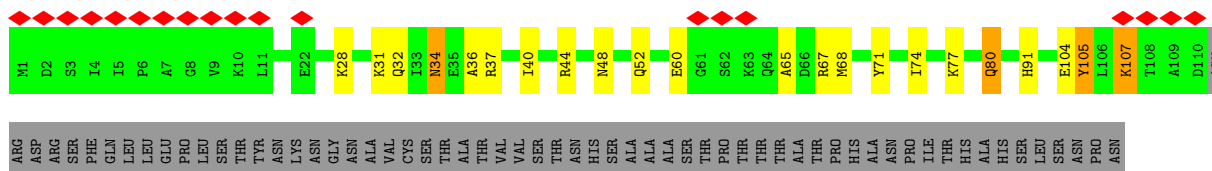
- Molecule 61: Mediator of RNA polymerase II transcription subunit 3

Chain T2:  5% 23% 72%



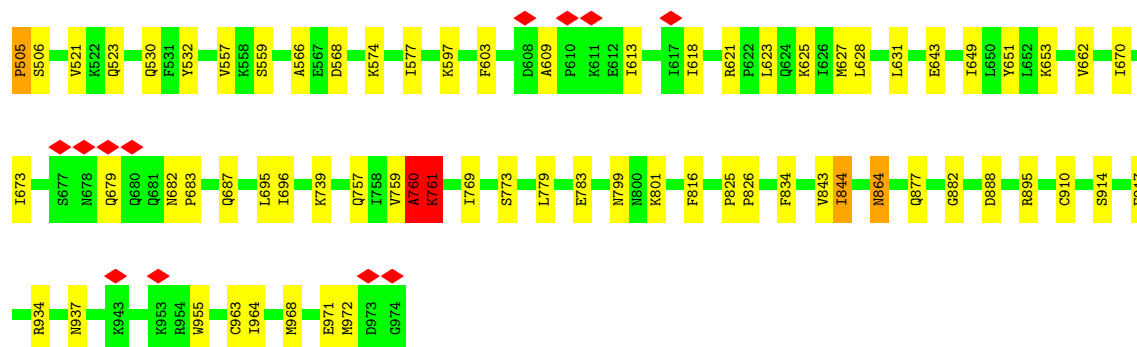
- Molecule 61: Mediator of RNA polymerase II transcription subunit 3

Chain t2:  5% 22% 5% 72%

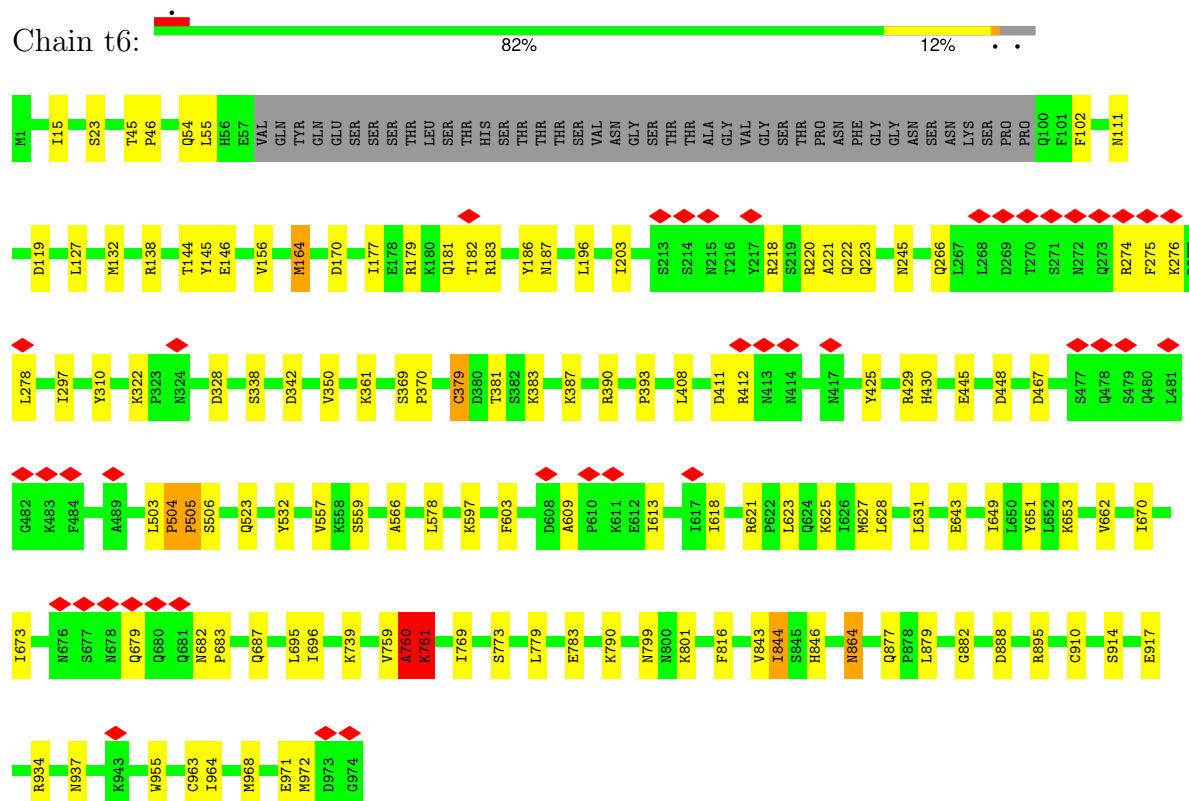








- Molecule 64: Mediator of RNA polymerase II transcription subunit 16



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	3090211	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40.8	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.713	Depositor
Minimum map value	0.000	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.054	Depositor
Recommended contour level	0.407	Depositor
Map size (Å)	896.0, 896.0, 896.0	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4, 1.4, 1.4	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	A0	0.52	10/6209 (0.2%)	0.63	6/8384 (0.1%)
1	B0	0.52	10/6209 (0.2%)	0.63	6/8384 (0.1%)
2	A1	0.35	2/3426 (0.1%)	0.63	5/4613 (0.1%)
2	B1	0.35	2/3426 (0.1%)	0.64	5/4613 (0.1%)
3	A2	0.76	20/3664 (0.5%)	1.51	37/4952 (0.7%)
3	B2	0.76	20/3664 (0.5%)	1.51	37/4952 (0.7%)
4	A3	0.86	6/1109 (0.5%)	1.30	13/1492 (0.9%)
4	B3	0.86	6/1109 (0.5%)	1.30	13/1492 (0.9%)
5	A4	0.31	1/2312 (0.0%)	0.58	0/3127
5	B4	0.32	1/2312 (0.0%)	0.58	0/3127
6	A5	1.29	9/520 (1.7%)	2.38	15/701 (2.1%)
6	B5	1.29	9/520 (1.7%)	2.38	15/701 (2.1%)
7	A6	0.43	4/3007 (0.1%)	0.60	0/4066
7	B6	0.43	4/3007 (0.1%)	0.60	0/4066
8	A7	0.43	5/4985 (0.1%)	0.67	2/6745 (0.0%)
8	B7	0.43	5/4985 (0.1%)	0.67	2/6745 (0.0%)
9	A8	0.72	0/137	1.19	0/185
9	B8	0.72	0/137	1.19	0/185
9	SF	0.85	17/3447 (0.5%)	1.30	40/4671 (0.9%)
9	sF	0.86	17/3447 (0.5%)	1.30	40/4671 (0.9%)
10	A9	1.65	8/549 (1.5%)	2.59	23/743 (3.1%)
10	B9	1.65	8/549 (1.5%)	2.59	23/743 (3.1%)
11	AA	0.43	13/11191 (0.1%)	0.75	34/15127 (0.2%)
11	BA	0.43	13/11191 (0.1%)	0.76	33/15127 (0.2%)
11	MA	0.23	0/606	0.70	0/848
11	mA	0.23	0/606	0.70	0/848
12	AB	0.34	4/9431 (0.0%)	0.58	18/12718 (0.1%)
12	BB	0.34	4/9431 (0.0%)	0.58	18/12718 (0.1%)
13	AC	0.19	0/2099	0.40	0/2845
13	BC	0.19	0/2099	0.40	0/2845
14	AD	0.23	0/1262	0.51	0/1693
14	BD	0.24	0/1262	0.51	0/1693

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
15	AE	0.29	1/1780 (0.1%)	0.45	1/2395 (0.0%)
15	BE	0.29	1/1780 (0.1%)	0.45	1/2395 (0.0%)
16	AF	0.31	0/682	0.61	1/922 (0.1%)
16	BF	0.31	0/682	0.61	1/922 (0.1%)
17	AG	0.35	0/1368	0.74	4/1844 (0.2%)
17	BG	0.36	0/1368	0.74	4/1844 (0.2%)
18	AH	0.80	3/1107 (0.3%)	1.15	12/1499 (0.8%)
18	BH	0.80	3/1107 (0.3%)	1.15	12/1499 (0.8%)
19	AI	2.04	31/962 (3.2%)	3.30	102/1295 (7.9%)
19	BI	2.04	32/962 (3.3%)	3.30	102/1295 (7.9%)
20	AJ	0.70	3/578 (0.5%)	0.93	3/775 (0.4%)
20	BJ	0.70	3/578 (0.5%)	0.93	3/775 (0.4%)
21	AK	0.29	0/942	0.58	1/1272 (0.1%)
21	BK	0.29	0/942	0.58	1/1272 (0.1%)
22	AL	0.29	0/361	0.51	0/478
22	BL	0.29	0/361	0.51	0/478
23	AM	0.31	0/2120	0.68	5/2849 (0.2%)
23	BM	0.31	0/2120	0.68	5/2849 (0.2%)
24	AN	1.09	7/1583 (0.4%)	1.23	11/2441 (0.5%)
24	BN	1.09	7/1583 (0.4%)	1.23	11/2441 (0.5%)
25	AO	0.25	0/1449	0.60	0/1952
25	BO	0.26	0/1449	0.60	0/1952
26	AQ	0.42	4/1852 (0.2%)	0.55	1/2480 (0.0%)
26	BQ	0.42	4/1852 (0.2%)	0.55	1/2480 (0.0%)
27	AR	0.51	2/2207 (0.1%)	0.76	11/2963 (0.4%)
27	BR	0.51	2/2207 (0.1%)	0.76	11/2963 (0.4%)
28	AS	1.15	14/1324 (1.1%)	1.69	35/1787 (2.0%)
28	BS	1.15	14/1324 (1.1%)	1.69	35/1787 (2.0%)
29	AT	1.10	5/1589 (0.3%)	1.23	14/2450 (0.6%)
29	BT	1.10	5/1589 (0.3%)	1.23	14/2450 (0.6%)
30	AU	0.31	0/856	0.82	4/1156 (0.3%)
30	BU	0.31	0/856	0.82	4/1156 (0.3%)
31	AV	0.30	0/822	0.83	2/1109 (0.2%)
31	BV	0.30	0/822	0.83	2/1109 (0.2%)
32	AW	0.30	0/1870	0.66	0/2524
32	BW	0.30	0/1870	0.66	0/2524
33	AX	0.20	0/1559	0.51	0/2102
33	BX	0.21	0/1559	0.51	0/2102
34	Ma	0.19	0/1440	0.46	0/1946
34	ma	0.19	0/1440	0.46	0/1946
35	Mb	0.23	0/1320	0.58	3/1785 (0.2%)
35	mb	0.23	0/1320	0.58	3/1785 (0.2%)
36	Mc	0.42	1/885 (0.1%)	0.80	2/1183 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
36	mc	0.42	1/885 (0.1%)	0.80	2/1183 (0.2%)
37	Md	0.19	0/4389	0.49	3/5901 (0.1%)
37	md	0.20	0/4389	0.49	3/5901 (0.1%)
38	Me	0.20	0/1993	0.59	4/2698 (0.1%)
38	me	0.20	0/1993	0.59	4/2698 (0.1%)
39	Mf	0.19	0/1635	0.49	0/2215
39	mf	0.19	0/1635	0.49	0/2215
40	Mg	0.28	0/851	0.65	0/1148
40	mg	0.28	0/851	0.64	0/1148
41	Mh	0.30	0/1462	0.62	2/1970 (0.1%)
41	mh	0.30	0/1462	0.62	2/1970 (0.1%)
42	Mi	0.28	0/1569	0.59	0/2117
42	mi	0.28	0/1569	0.59	0/2117
43	Mj	0.37	0/877	0.92	8/1180 (0.7%)
43	mj	0.37	0/877	0.92	8/1180 (0.7%)
44	Mk	0.28	0/1172	0.62	1/1581 (0.1%)
44	mk	0.28	0/1172	0.62	1/1581 (0.1%)
45	Ml	0.22	0/5460	0.52	0/7373
45	T4	0.55	5/1817 (0.3%)	0.86	9/2456 (0.4%)
45	ml	0.22	0/5460	0.52	0/7373
45	t4	0.56	5/1817 (0.3%)	0.86	9/2456 (0.4%)
46	Mm	0.24	0/684	0.67	3/928 (0.3%)
46	mm	0.24	0/684	0.68	3/928 (0.3%)
47	Mn	0.30	0/1135	0.63	0/1526
47	mn	0.30	0/1135	0.63	0/1526
48	Mo	0.36	0/941	0.71	3/1282 (0.2%)
48	mo	0.36	0/941	0.70	3/1282 (0.2%)
49	Mp	0.15	0/3394	0.40	0/4589
49	mp	0.16	0/3394	0.40	0/4589
50	SA	0.59	10/3617 (0.3%)	0.90	13/4895 (0.3%)
50	sA	0.59	10/3617 (0.3%)	0.90	13/4895 (0.3%)
51	SB	0.56	5/3318 (0.2%)	0.73	9/4465 (0.2%)
51	SD	0.40	2/3517 (0.1%)	0.69	5/4735 (0.1%)
51	sB	0.56	5/3318 (0.2%)	0.73	9/4465 (0.2%)
51	sD	0.41	2/3517 (0.1%)	0.69	5/4735 (0.1%)
52	SC	0.37	0/1287	0.74	1/1729 (0.1%)
52	sC	0.37	0/1287	0.74	1/1729 (0.1%)
53	SE	1.05	24/3399 (0.7%)	1.21	42/4584 (0.9%)
53	sE	1.05	24/3399 (0.7%)	1.21	42/4584 (0.9%)
54	SG	0.20	0/101	0.50	0/123
54	sG	0.20	0/101	0.50	0/123
55	SH	1.16	21/1991 (1.1%)	1.36	26/2692 (1.0%)
55	sH	1.16	21/1991 (1.1%)	1.36	26/2692 (1.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
56	SI	0.53	6/4552 (0.1%)	0.70	11/6163 (0.2%)
56	sI	0.53	6/4552 (0.1%)	0.70	11/6163 (0.2%)
57	SJ	0.52	1/728 (0.1%)	0.64	0/978
57	sJ	0.52	1/728 (0.1%)	0.64	0/978
58	SK	0.59	9/3525 (0.3%)	0.74	9/4769 (0.2%)
58	sK	0.59	10/3525 (0.3%)	0.74	9/4769 (0.2%)
59	SL	0.33	2/3333 (0.1%)	0.55	1/4517 (0.0%)
59	sL	0.33	2/3333 (0.1%)	0.55	1/4517 (0.0%)
60	T1	0.68	2/520 (0.4%)	0.79	0/693
60	t1	0.68	2/520 (0.4%)	0.79	0/693
61	T2	0.85	2/902 (0.2%)	1.06	6/1215 (0.5%)
61	t2	0.85	2/902 (0.2%)	1.06	6/1215 (0.5%)
62	T3	0.64	17/6293 (0.3%)	0.97	36/8534 (0.4%)
62	t3	0.64	17/6293 (0.3%)	0.97	38/8534 (0.4%)
63	T5	1.28	16/904 (1.8%)	2.16	31/1202 (2.6%)
63	t5	1.29	16/904 (1.8%)	2.16	31/1202 (2.6%)
64	T6	0.46	9/7725 (0.1%)	0.71	10/10461 (0.1%)
64	t6	0.46	9/7725 (0.1%)	0.71	10/10461 (0.1%)
All	All	0.56	604/311402 (0.2%)	0.87	1277/421672 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A0	0	1
1	B0	0	1
2	A1	0	1
2	B1	0	1
3	A2	0	5
3	B2	0	5
4	A3	0	2
4	B3	0	2
5	A4	0	1
5	B4	0	1
6	A5	0	2
6	B5	0	2
8	A7	0	4
8	B7	0	4
9	A8	0	1
9	B8	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
9	SF	1	6
9	sF	1	6
10	A9	1	2
10	B9	1	2
11	AA	0	7
11	BA	0	7
12	AB	0	3
12	BB	0	3
17	AG	0	1
17	BG	0	1
18	AH	0	3
18	BH	0	3
19	AI	0	13
19	BI	0	13
20	AJ	0	1
20	BJ	0	1
28	AS	1	4
28	BS	1	4
31	AV	0	1
31	BV	0	1
32	AW	0	1
32	BW	0	1
37	Md	0	1
37	md	0	1
38	Me	0	2
38	me	0	2
45	T4	0	1
45	t4	0	1
47	Mn	0	1
47	mn	0	1
50	SA	1	2
50	sA	1	2
51	SB	0	1
51	sB	0	1
53	SE	0	10
53	sE	0	10
55	SH	0	2
55	sH	0	2
56	SI	0	4
56	sI	0	4
58	SK	0	3
58	sK	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
61	T2	0	1
61	t2	0	1
62	T3	1	6
62	t3	1	6
63	T5	1	2
63	t5	1	2
64	T6	0	1
64	t6	0	1
All	All	12	192

The worst 5 of 604 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	SE	547	ARG	CZ-NH1	-29.68	0.91	1.32
53	sE	547	ARG	CZ-NH1	-29.66	0.91	1.32
19	BI	86	PHE	CG-CD2	21.75	1.84	1.38
19	AI	86	PHE	CG-CD2	21.73	1.84	1.38
55	SH	608	MET	SD-CE	-19.93	1.29	1.79

The worst 5 of 1277 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A2	69	ASN	CA-CB-CG	54.96	167.56	112.60
3	B2	69	ASN	CA-CB-CG	54.95	167.56	112.60
50	sA	269	GLN	CA-CB-CG	32.94	179.98	114.10
50	SA	269	GLN	CA-CB-CG	32.94	179.97	114.10
10	A9	199	GLN	CA-CB-CG	32.92	179.93	114.10

5 of 12 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	B9	199	GLN	CA
28	BS	206	VAL	CA
50	sA	269	GLN	CA
9	sF	398	THR	CB
10	A9	199	GLN	CA

5 of 192 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B0	553	MET	Mainchain
2	B1	193	LYS	Mainchain

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Mol	Chain	Res	Type	Group
3	B2	182	PHE	Peptide
3	B2	257	GLY	Peptide
3	B2	449	ASP	Peptide

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	A0	6091	0	6155	77	0
1	B0	6091	0	6155	77	0
2	A1	3374	0	3425	26	0
2	B1	3374	0	3425	22	0
3	A2	3597	0	3687	78	0
3	B2	3597	0	3687	74	0
4	A3	1089	0	1069	56	0
4	B3	1089	0	1069	55	0
5	A4	2274	0	2332	21	0
5	B4	2274	0	2332	21	0
6	A5	514	0	541	20	0
6	B5	514	0	541	19	0
7	A6	2946	0	2958	31	0
7	B6	2946	0	2958	31	0
8	A7	4881	0	4868	63	0
8	B7	4881	0	4868	61	0
9	A8	134	0	141	5	0
9	B8	134	0	141	5	0
9	SF	3374	0	3292	76	0
9	sF	3374	0	3292	80	0
10	A9	542	0	537	10	0
10	B9	542	0	537	10	0
11	AA	10996	0	11079	143	0
11	BA	10996	0	11079	143	0
11	MA	575	0	507	6	0
11	mA	575	0	507	5	0
12	AB	9249	0	9247	96	0
12	BB	9249	0	9247	108	0
13	AC	2061	0	2029	15	0
13	BC	2061	0	2029	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	AD	1253	0	1275	38	0
14	BD	1253	0	1275	38	0
15	AE	1744	0	1772	13	0
15	BE	1744	0	1772	14	0
16	AF	670	0	690	5	0
16	BF	670	0	690	4	0
17	AG	1340	0	1357	60	0
17	BG	1340	0	1357	60	0
18	AH	1089	0	1062	37	0
18	BH	1089	0	1062	38	0
19	AI	944	0	901	49	0
19	BI	944	0	901	69	0
20	AJ	569	0	585	10	0
20	BJ	569	0	585	10	0
21	AK	924	0	934	15	0
21	BK	924	0	934	15	0
22	AL	359	0	381	1	0
22	BL	359	0	381	2	0
23	AM	2097	0	2182	88	0
23	BM	2097	0	2182	86	0
24	AN	1413	0	785	14	0
24	BN	1413	0	785	14	0
25	AO	1422	0	1500	7	0
25	BO	1422	0	1500	7	0
26	AQ	1817	0	1843	26	0
26	BQ	1817	0	1843	25	0
27	AR	2173	0	2192	73	0
27	BR	2173	0	2192	71	0
28	AS	1301	0	1294	45	0
28	BS	1301	0	1294	47	0
29	AT	1416	0	782	11	0
29	BT	1416	0	782	11	0
30	AU	843	0	827	11	0
30	BU	843	0	827	11	0
31	AV	815	0	822	13	0
31	BV	815	0	822	12	0
32	AW	1836	0	1854	55	0
32	BW	1836	0	1854	54	0
33	AX	1530	0	1565	6	0
33	BX	1530	0	1565	6	0
34	Ma	1407	0	1385	23	0
34	ma	1407	0	1385	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	Mb	1295	0	1297	32	0
35	mb	1295	0	1297	32	0
36	Mc	876	0	885	7	0
36	mc	876	0	885	7	0
37	Md	4325	0	4482	22	0
37	md	4325	0	4482	22	0
38	Me	1958	0	1976	17	0
38	me	1958	0	1976	18	0
39	Mf	1609	0	1626	6	0
39	mf	1609	0	1626	4	0
40	Mg	847	0	858	10	0
40	mg	847	0	858	10	0
41	Mh	1441	0	1461	7	0
41	mh	1441	0	1461	7	0
42	Mi	1538	0	1576	8	0
42	mi	1538	0	1576	8	0
43	Mj	864	0	870	28	0
43	mj	864	0	870	27	0
44	Mk	1157	0	1142	13	0
44	mk	1157	0	1142	13	0
45	Ml	5367	0	5607	55	0
45	T4	1780	0	1765	31	0
45	ml	5367	0	5607	47	0
45	t4	1780	0	1765	37	0
46	Mm	671	0	650	2	0
46	mm	671	0	650	2	0
47	Mn	1124	0	1147	7	0
47	mn	1124	0	1147	8	0
48	Mo	914	0	902	5	0
48	mo	914	0	902	5	0
49	Mp	3330	0	3243	27	0
49	mp	3330	0	3243	46	0
50	SA	3552	0	3509	34	0
50	sA	3552	0	3509	34	0
51	SB	3250	0	3302	45	0
51	SD	3445	0	3505	38	0
51	sB	3250	0	3302	44	0
51	sD	3445	0	3505	40	0
52	SC	1266	0	1264	10	0
52	sC	1266	0	1264	9	0
53	SE	3333	0	3375	76	0
53	sE	3333	0	3375	75	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	SG	271	0	131	5	0
54	sG	271	0	131	5	0
55	SH	1958	0	1976	55	0
55	sH	1958	0	1976	54	0
56	SI	4474	0	4633	47	0
56	sI	4474	0	4633	50	0
57	SJ	711	0	695	14	0
57	sJ	711	0	695	14	0
58	SK	3453	0	3449	45	0
58	sK	3453	0	3449	42	0
59	SL	3266	0	3264	22	0
59	sL	3266	0	3264	22	0
60	T1	516	0	527	9	0
60	t1	516	0	527	10	0
61	T2	891	0	907	14	0
61	t2	891	0	907	15	0
62	T3	6173	0	6169	73	0
62	t3	6173	0	6169	90	0
63	T5	894	0	930	23	0
63	t5	894	0	928	36	0
64	T6	7551	0	7605	86	0
64	t6	7551	0	7605	101	0
65	A0	8	0	0	0	0
65	B0	8	0	0	0	0
66	A3	2	0	0	0	0
66	A4	1	0	0	0	0
66	A6	4	0	0	0	0
66	AA	2	0	0	0	0
66	AB	1	0	0	0	0
66	AC	1	0	0	0	0
66	AI	2	0	0	0	0
66	AJ	1	0	0	0	0
66	AL	1	0	0	0	0
66	AM	1	0	0	0	0
66	AS	1	0	0	0	0
66	AW	1	0	0	0	0
66	B3	2	0	0	0	0
66	B4	1	0	0	0	0
66	B6	4	0	0	0	0
66	BA	2	0	0	0	0
66	BB	1	0	0	0	0
66	BC	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
66	BI	2	0	0	0	0
66	BJ	1	0	0	0	0
66	BL	1	0	0	0	0
66	BM	1	0	0	0	0
66	BS	1	0	0	0	0
66	BW	1	0	0	0	0
67	AA	1	0	0	0	0
67	BA	1	0	0	0	0
All	All	305572	0	305164	3655	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 6.

The worst 5 of 3655 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)
62:T3:837:TYR:CD2	62:T3:837:TYR:CG	1.80	1.68
19:BI:86:PHE:CD2	19:BI:86:PHE:CG	1.84	1.64
19:AI:86:PHE:CD2	19:AI:86:PHE:CG	1.84	1.64
62:t3:837:TYR:CD2	62:t3:837:TYR:CG	1.80	1.64
4:A3:100:ASN:HB3	34:Ma:140:GLY:CA	1.26	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	A0	750/778 (96%)	731 (98%)	19 (2%)	0	100	100
1	B0	750/778 (96%)	731 (98%)	19 (2%)	0	100	100
2	A1	406/642 (63%)	389 (96%)	17 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B1	406/642 (63%)	389 (96%)	17 (4%)	0	100	100
3	A2	435/513 (85%)	418 (96%)	13 (3%)	4 (1%)	14	41
3	B2	435/513 (85%)	418 (96%)	13 (3%)	4 (1%)	14	41
4	A3	129/321 (40%)	126 (98%)	3 (2%)	0	100	100
4	B3	129/321 (40%)	126 (98%)	3 (2%)	0	100	100
5	A4	287/338 (85%)	281 (98%)	6 (2%)	0	100	100
5	B4	287/338 (85%)	281 (98%)	6 (2%)	0	100	100
6	A5	63/72 (88%)	62 (98%)	1 (2%)	0	100	100
6	B5	63/72 (88%)	62 (98%)	1 (2%)	0	100	100
7	A6	368/461 (80%)	354 (96%)	14 (4%)	0	100	100
7	B6	368/461 (80%)	354 (96%)	14 (4%)	0	100	100
8	A7	605/843 (72%)	572 (94%)	32 (5%)	1 (0%)	43	72
8	B7	605/843 (72%)	572 (94%)	32 (5%)	1 (0%)	43	72
9	A8	15/905 (2%)	12 (80%)	3 (20%)	0	100	100
9	B8	15/905 (2%)	12 (80%)	3 (20%)	0	100	100
9	SF	407/905 (45%)	366 (90%)	36 (9%)	5 (1%)	10	34
9	sF	407/905 (45%)	366 (90%)	36 (9%)	5 (1%)	10	34
10	A9	66/244 (27%)	65 (98%)	1 (2%)	0	100	100
10	B9	66/244 (27%)	65 (98%)	1 (2%)	0	100	100
11	AA	1386/1733 (80%)	1315 (95%)	69 (5%)	2 (0%)	48	77
11	BA	1386/1733 (80%)	1316 (95%)	68 (5%)	2 (0%)	48	77
11	MA	73/1733 (4%)	64 (88%)	7 (10%)	2 (3%)	4	15
11	mA	73/1733 (4%)	64 (88%)	7 (10%)	2 (3%)	4	15
12	AB	1147/1224 (94%)	1103 (96%)	42 (4%)	2 (0%)	43	72
12	BB	1147/1224 (94%)	1102 (96%)	43 (4%)	2 (0%)	43	72
13	AC	260/318 (82%)	251 (96%)	9 (4%)	0	100	100
13	BC	260/318 (82%)	252 (97%)	8 (3%)	0	100	100
14	AD	153/221 (69%)	148 (97%)	5 (3%)	0	100	100
14	BD	153/221 (69%)	148 (97%)	5 (3%)	0	100	100
15	AE	211/215 (98%)	208 (99%)	3 (1%)	0	100	100
15	BE	211/215 (98%)	208 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	AF	81/155 (52%)	78 (96%)	3 (4%)	0	100	100
16	BF	81/155 (52%)	78 (96%)	3 (4%)	0	100	100
17	AG	169/171 (99%)	163 (96%)	6 (4%)	0	100	100
17	BG	169/171 (99%)	163 (96%)	6 (4%)	0	100	100
18	AH	132/146 (90%)	122 (92%)	10 (8%)	0	100	100
18	BH	132/146 (90%)	122 (92%)	10 (8%)	0	100	100
19	AI	114/122 (93%)	88 (77%)	18 (16%)	8 (7%)	1	2
19	BI	114/122 (93%)	88 (77%)	18 (16%)	8 (7%)	1	2
20	AJ	67/70 (96%)	66 (98%)	1 (2%)	0	100	100
20	BJ	67/70 (96%)	66 (98%)	1 (2%)	0	100	100
21	AK	113/120 (94%)	108 (96%)	5 (4%)	0	100	100
21	BK	113/120 (94%)	108 (96%)	5 (4%)	0	100	100
22	AL	43/70 (61%)	42 (98%)	1 (2%)	0	100	100
22	BL	43/70 (61%)	42 (98%)	1 (2%)	0	100	100
23	AM	267/345 (77%)	255 (96%)	12 (4%)	0	100	100
23	BM	267/345 (77%)	255 (96%)	12 (4%)	0	100	100
25	AO	179/240 (75%)	166 (93%)	12 (7%)	1 (1%)	21	51
25	BO	179/240 (75%)	166 (93%)	12 (7%)	1 (1%)	21	51
26	AQ	208/735 (28%)	199 (96%)	9 (4%)	0	100	100
26	BQ	208/735 (28%)	200 (96%)	8 (4%)	0	100	100
27	AR	251/400 (63%)	241 (96%)	10 (4%)	0	100	100
27	BR	251/400 (63%)	241 (96%)	10 (4%)	0	100	100
28	AS	162/309 (52%)	139 (86%)	19 (12%)	4 (2%)	4	16
28	BS	162/309 (52%)	139 (86%)	19 (12%)	4 (2%)	4	16
30	AU	98/286 (34%)	91 (93%)	6 (6%)	1 (1%)	12	38
30	BU	98/286 (34%)	91 (93%)	6 (6%)	1 (1%)	12	38
31	AV	100/122 (82%)	93 (93%)	6 (6%)	1 (1%)	12	38
31	BV	100/122 (82%)	93 (93%)	6 (6%)	1 (1%)	12	38
32	AW	222/482 (46%)	212 (96%)	9 (4%)	1 (0%)	24	55
32	BW	222/482 (46%)	212 (96%)	9 (4%)	1 (0%)	24	55
33	AX	189/328 (58%)	180 (95%)	9 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	BX	189/328 (58%)	180 (95%)	9 (5%)	0	100	100
34	Ma	163/295 (55%)	153 (94%)	10 (6%)	0	100	100
34	ma	163/295 (55%)	153 (94%)	10 (6%)	0	100	100
35	Mb	151/223 (68%)	145 (96%)	5 (3%)	1 (1%)	18	47
35	mb	151/223 (68%)	145 (96%)	5 (3%)	1 (1%)	18	47
36	Mc	104/115 (90%)	99 (95%)	4 (4%)	1 (1%)	12	38
36	mc	104/115 (90%)	99 (95%)	4 (4%)	1 (1%)	12	38
37	Md	525/687 (76%)	511 (97%)	13 (2%)	1 (0%)	43	72
37	md	525/687 (76%)	511 (97%)	13 (2%)	1 (0%)	43	72
38	Me	244/307 (80%)	234 (96%)	10 (4%)	0	100	100
38	me	244/307 (80%)	234 (96%)	10 (4%)	0	100	100
39	Mf	208/210 (99%)	192 (92%)	16 (8%)	0	100	100
39	mf	208/210 (99%)	192 (92%)	16 (8%)	0	100	100
40	Mg	102/121 (84%)	89 (87%)	13 (13%)	0	100	100
40	mg	102/121 (84%)	89 (87%)	13 (13%)	0	100	100
41	Mh	175/284 (62%)	164 (94%)	10 (6%)	1 (1%)	21	51
41	mh	175/284 (62%)	164 (94%)	10 (6%)	1 (1%)	21	51
42	Mi	179/222 (81%)	175 (98%)	4 (2%)	0	100	100
42	mi	179/222 (81%)	175 (98%)	4 (2%)	0	100	100
43	Mj	99/149 (66%)	91 (92%)	7 (7%)	1 (1%)	12	38
43	mj	99/149 (66%)	91 (92%)	7 (7%)	1 (1%)	12	38
44	Mk	140/157 (89%)	139 (99%)	1 (1%)	0	100	100
44	mk	140/157 (89%)	139 (99%)	1 (1%)	0	100	100
45	Ml	640/1082 (59%)	607 (95%)	32 (5%)	1 (0%)	43	72
45	T4	214/1082 (20%)	203 (95%)	10 (5%)	1 (0%)	24	55
45	ml	640/1082 (59%)	607 (95%)	32 (5%)	1 (0%)	43	72
45	t4	214/1082 (20%)	203 (95%)	10 (5%)	1 (0%)	24	55
46	Mm	79/220 (36%)	69 (87%)	8 (10%)	2 (2%)	4	16
46	mm	79/220 (36%)	69 (87%)	8 (10%)	2 (2%)	4	16
47	Mn	138/140 (99%)	130 (94%)	8 (6%)	0	100	100
47	mn	138/140 (99%)	130 (94%)	8 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	Mo	107/127 (84%)	101 (94%)	6 (6%)	0	100	100
48	mo	107/127 (84%)	101 (94%)	6 (6%)	0	100	100
49	Mp	405/566 (72%)	385 (95%)	20 (5%)	0	100	100
49	mp	405/566 (72%)	385 (95%)	20 (5%)	0	100	100
50	SA	438/566 (77%)	413 (94%)	23 (5%)	2 (0%)	24	55
50	sA	438/566 (77%)	413 (94%)	23 (5%)	2 (0%)	24	55
51	SB	385/825 (47%)	370 (96%)	15 (4%)	0	100	100
51	SD	413/825 (50%)	391 (95%)	22 (5%)	0	100	100
51	sB	385/825 (47%)	370 (96%)	15 (4%)	0	100	100
51	sD	413/825 (50%)	391 (95%)	22 (5%)	0	100	100
52	SC	146/332 (44%)	141 (97%)	5 (3%)	0	100	100
52	sC	146/332 (44%)	141 (97%)	5 (3%)	0	100	100
53	SE	401/623 (64%)	359 (90%)	37 (9%)	5 (1%)	10	34
53	sE	401/623 (64%)	359 (90%)	37 (9%)	5 (1%)	10	34
54	SG	13/47 (28%)	11 (85%)	1 (8%)	1 (8%)	1	2
54	sG	13/47 (28%)	11 (85%)	1 (8%)	1 (8%)	1	2
55	SH	237/1703 (14%)	228 (96%)	8 (3%)	1 (0%)	30	60
55	sH	237/1703 (14%)	228 (96%)	8 (3%)	1 (0%)	30	60
56	SI	536/1314 (41%)	517 (96%)	17 (3%)	2 (0%)	30	60
56	sI	536/1314 (41%)	517 (96%)	17 (3%)	2 (0%)	30	60
57	SJ	78/157 (50%)	72 (92%)	6 (8%)	0	100	100
57	sJ	78/157 (50%)	72 (92%)	6 (8%)	0	100	100
58	SK	427/477 (90%)	403 (94%)	24 (6%)	0	100	100
58	sK	427/477 (90%)	403 (94%)	24 (6%)	0	100	100
59	SL	400/467 (86%)	386 (96%)	12 (3%)	2 (0%)	24	55
59	sL	400/467 (86%)	386 (96%)	12 (3%)	2 (0%)	24	55
60	T1	61/431 (14%)	61 (100%)	0	0	100	100
60	t1	61/431 (14%)	61 (100%)	0	0	100	100
61	T2	108/397 (27%)	105 (97%)	3 (3%)	0	100	100
61	t2	108/397 (27%)	105 (97%)	3 (3%)	0	100	100
62	T3	749/1132 (66%)	705 (94%)	40 (5%)	4 (0%)	24	55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
62	t3	749/1132 (66%)	705 (94%)	40 (5%)	4 (0%)	24	55
63	T5	109/1081 (10%)	98 (90%)	9 (8%)	2 (2%)	6	23
63	t5	109/1081 (10%)	98 (90%)	9 (8%)	2 (2%)	6	23
64	T6	928/974 (95%)	889 (96%)	36 (4%)	3 (0%)	36	66
64	t6	928/974 (95%)	889 (96%)	36 (4%)	3 (0%)	36	66
All	All	36516/65810 (56%)	34690 (95%)	1700 (5%)	126 (0%)	37	66

5 of 126 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	BB	22	SER
12	BB	474	SER
19	BI	76	PRO
19	BI	113	ASP
28	BS	238	PRO

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	A0	684/707 (97%)	684 (100%)	0	100	100
1	B0	684/707 (97%)	684 (100%)	0	100	100
2	A1	388/589 (66%)	388 (100%)	0	100	100
2	B1	388/589 (66%)	388 (100%)	0	100	100
3	A2	408/468 (87%)	406 (100%)	2 (0%)	81	93
3	B2	408/468 (87%)	406 (100%)	2 (0%)	81	93
4	A3	125/303 (41%)	123 (98%)	2 (2%)	55	83
4	B3	125/303 (41%)	123 (98%)	2 (2%)	55	83
5	A4	260/300 (87%)	260 (100%)	0	100	100
5	B4	260/300 (87%)	260 (100%)	0	100	100
6	A5	59/66 (89%)	59 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	B5	59/66 (89%)	59 (100%)	0	100	100
7	A6	338/418 (81%)	338 (100%)	0	100	100
7	B6	338/418 (81%)	338 (100%)	0	100	100
8	A7	539/737 (73%)	539 (100%)	0	100	100
8	B7	539/737 (73%)	539 (100%)	0	100	100
9	A8	16/823 (2%)	16 (100%)	0	100	100
9	B8	16/823 (2%)	16 (100%)	0	100	100
9	SF	379/823 (46%)	377 (100%)	2 (0%)	81	93
9	sF	379/823 (46%)	377 (100%)	2 (0%)	81	93
10	A9	63/219 (29%)	62 (98%)	1 (2%)	55	83
10	B9	63/219 (29%)	63 (100%)	0	100	100
11	AA	1221/1520 (80%)	1218 (100%)	3 (0%)	87	96
11	BA	1221/1520 (80%)	1218 (100%)	3 (0%)	87	96
11	MA	79/1520 (5%)	79 (100%)	0	100	100
11	mA	79/1520 (5%)	79 (100%)	0	100	100
12	AB	1007/1061 (95%)	1006 (100%)	1 (0%)	88	97
12	BB	1007/1061 (95%)	1006 (100%)	1 (0%)	88	97
13	AC	230/274 (84%)	230 (100%)	0	100	100
13	BC	230/274 (84%)	230 (100%)	0	100	100
14	AD	139/200 (70%)	139 (100%)	0	100	100
14	BD	139/200 (70%)	139 (100%)	0	100	100
15	AE	195/197 (99%)	195 (100%)	0	100	100
15	BE	195/197 (99%)	195 (100%)	0	100	100
16	AF	73/137 (53%)	73 (100%)	0	100	100
16	BF	73/137 (53%)	73 (100%)	0	100	100
17	AG	152/152 (100%)	152 (100%)	0	100	100
17	BG	152/152 (100%)	152 (100%)	0	100	100
18	AH	119/128 (93%)	117 (98%)	2 (2%)	53	83
18	BH	119/128 (93%)	117 (98%)	2 (2%)	53	83
19	AI	110/116 (95%)	101 (92%)	9 (8%)	10	33
19	BI	110/116 (95%)	101 (92%)	9 (8%)	10	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	AJ	64/65 (98%)	64 (100%)	0	100	100
20	BJ	64/65 (98%)	64 (100%)	0	100	100
21	AK	99/102 (97%)	99 (100%)	0	100	100
21	BK	99/102 (97%)	99 (100%)	0	100	100
22	AL	40/57 (70%)	40 (100%)	0	100	100
22	BL	40/57 (70%)	40 (100%)	0	100	100
23	AM	234/299 (78%)	234 (100%)	0	100	100
23	BM	234/299 (78%)	234 (100%)	0	100	100
25	AO	153/205 (75%)	153 (100%)	0	100	100
25	BO	153/205 (75%)	153 (100%)	0	100	100
26	AQ	198/641 (31%)	198 (100%)	0	100	100
26	BQ	198/641 (31%)	198 (100%)	0	100	100
27	AR	247/363 (68%)	247 (100%)	0	100	100
27	BR	247/363 (68%)	247 (100%)	0	100	100
28	AS	143/274 (52%)	140 (98%)	3 (2%)	47	79
28	BS	143/274 (52%)	140 (98%)	3 (2%)	47	79
30	AU	94/260 (36%)	94 (100%)	0	100	100
30	BU	94/260 (36%)	94 (100%)	0	100	100
31	AV	94/108 (87%)	94 (100%)	0	100	100
31	BV	94/108 (87%)	94 (100%)	0	100	100
32	AW	207/429 (48%)	207 (100%)	0	100	100
32	BW	207/429 (48%)	207 (100%)	0	100	100
33	AX	171/295 (58%)	171 (100%)	0	100	100
33	BX	171/295 (58%)	171 (100%)	0	100	100
34	Ma	158/259 (61%)	158 (100%)	0	100	100
34	ma	158/259 (61%)	158 (100%)	0	100	100
35	Mb	148/207 (72%)	148 (100%)	0	100	100
35	mb	148/207 (72%)	148 (100%)	0	100	100
36	Mc	101/108 (94%)	101 (100%)	0	100	100
36	mc	101/108 (94%)	101 (100%)	0	100	100
37	Md	499/642 (78%)	499 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	md	499/642 (78%)	499 (100%)	0	100	100
38	Me	224/280 (80%)	224 (100%)	0	100	100
38	me	224/280 (80%)	224 (100%)	0	100	100
39	Mf	178/178 (100%)	178 (100%)	0	100	100
39	mf	178/178 (100%)	178 (100%)	0	100	100
40	Mg	98/113 (87%)	98 (100%)	0	100	100
40	mg	98/113 (87%)	98 (100%)	0	100	100
41	Mh	164/258 (64%)	164 (100%)	0	100	100
41	mh	164/258 (64%)	164 (100%)	0	100	100
42	Mi	175/208 (84%)	175 (100%)	0	100	100
42	mi	175/208 (84%)	175 (100%)	0	100	100
43	Mj	101/144 (70%)	101 (100%)	0	100	100
43	mj	101/144 (70%)	101 (100%)	0	100	100
44	Mk	132/145 (91%)	132 (100%)	0	100	100
44	mk	132/145 (91%)	132 (100%)	0	100	100
45	MI	618/1001 (62%)	618 (100%)	0	100	100
45	T4	205/1001 (20%)	205 (100%)	0	100	100
45	ml	618/1001 (62%)	618 (100%)	0	100	100
45	t4	205/1001 (20%)	205 (100%)	0	100	100
46	Mm	77/195 (40%)	77 (100%)	0	100	100
46	mm	77/195 (40%)	77 (100%)	0	100	100
47	Mn	132/132 (100%)	132 (100%)	0	100	100
47	mn	132/132 (100%)	132 (100%)	0	100	100
48	Mo	102/117 (87%)	102 (100%)	0	100	100
48	mo	102/117 (87%)	102 (100%)	0	100	100
49	Mp	390/528 (74%)	390 (100%)	0	100	100
49	mp	390/528 (74%)	390 (100%)	0	100	100
50	SA	408/517 (79%)	406 (100%)	2 (0%)	81	93
50	sA	408/517 (79%)	407 (100%)	1 (0%)	87	96
51	SB	368/751 (49%)	368 (100%)	0	100	100
51	SD	392/751 (52%)	392 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
51	sB	368/751 (49%)	368 (100%)	0	100	100
51	sD	392/751 (52%)	392 (100%)	0	100	100
52	SC	141/288 (49%)	141 (100%)	0	100	100
52	sC	141/288 (49%)	141 (100%)	0	100	100
53	SE	368/558 (66%)	368 (100%)	0	100	100
53	sE	368/558 (66%)	368 (100%)	0	100	100
54	SG	7/13 (54%)	7 (100%)	0	100	100
54	sG	7/13 (54%)	7 (100%)	0	100	100
55	SH	221/1520 (14%)	221 (100%)	0	100	100
55	sH	221/1520 (14%)	221 (100%)	0	100	100
56	SI	528/1218 (43%)	528 (100%)	0	100	100
56	sI	528/1218 (43%)	528 (100%)	0	100	100
57	SJ	80/140 (57%)	80 (100%)	0	100	100
57	sJ	80/140 (57%)	80 (100%)	0	100	100
58	SK	381/420 (91%)	381 (100%)	0	100	100
58	sK	381/420 (91%)	381 (100%)	0	100	100
59	SL	370/423 (88%)	370 (100%)	0	100	100
59	sL	370/423 (88%)	370 (100%)	0	100	100
60	T1	60/389 (15%)	60 (100%)	0	100	100
60	t1	60/389 (15%)	60 (100%)	0	100	100
61	T2	100/339 (30%)	100 (100%)	0	100	100
61	t2	100/339 (30%)	100 (100%)	0	100	100
62	T3	713/1053 (68%)	709 (99%)	4 (1%)	78	92
62	t3	713/1053 (68%)	709 (99%)	4 (1%)	78	92
63	T5	103/944 (11%)	99 (96%)	4 (4%)	28	64
63	t5	103/944 (11%)	99 (96%)	4 (4%)	28	64
64	T6	861/897 (96%)	860 (100%)	1 (0%)	88	97
64	t6	861/897 (96%)	860 (100%)	1 (0%)	88	97
All	All	33862/59186 (57%)	33792 (100%)	70 (0%)	85	96

5 of 70 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
63	T5	919	ARG
63	T5	931	GLN
63	t5	877	LYS
9	sF	401	LYS
9	sF	379	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 617 such sidechains are listed below:

Mol	Chain	Res	Type
53	SE	280	GLN
62	t3	537	GLN
9	SF	556	GLN
51	SD	769	HIS
62	T3	702	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 40 ligands modelled in this entry, 38 are monoatomic - leaving 2 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
65	SF4	A0	801	1	0,12,12	-	-	-		
65	SF4	B0	801	1	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
65	SF4	A0	801	1	-	-	0/6/5/5
65	SF4	B0	801	1	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
62	T3	4
62	t3	4
53	sE	3
53	SE	3
54	sG	2
54	SG	2
11	mA	2
11	MA	2
27	BR	2
27	AR	2

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Mol	Chain	Number of breaks
56	sI	1
56	SI	1
45	T4	1
45	t4	1
23	BM	1
23	AM	1
12	BB	1
12	AB	1
55	sH	1
55	SH	1

The worst 5 of 36 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	sG	95:UNK	C	118:ARG	N	72.09
1	SG	95:UNK	C	118:ARG	N	72.09
1	sG	66:UNK	C	82:UNK	N	34.38
1	SG	66:UNK	C	82:UNK	N	34.38
1	mA	1652:PRO	C	1667:SER	N	32.61

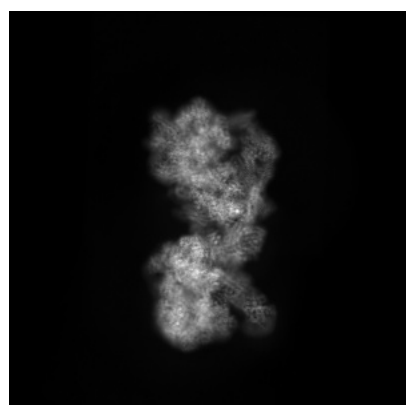
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71536. These allow visual inspection of the internal detail of the map and identification of artifacts.

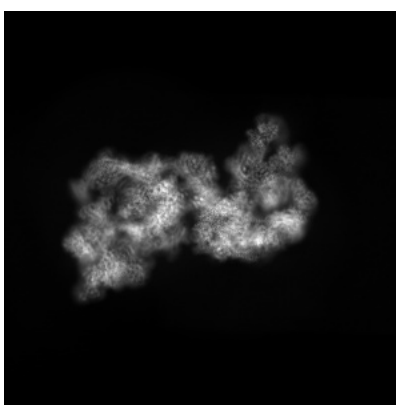
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X



Y

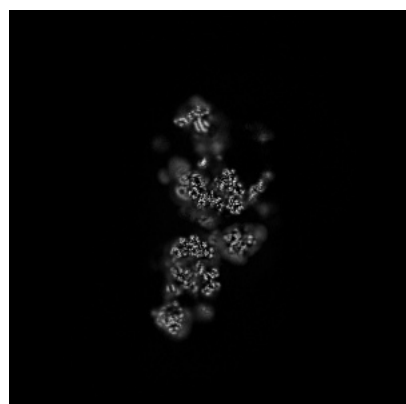


Z

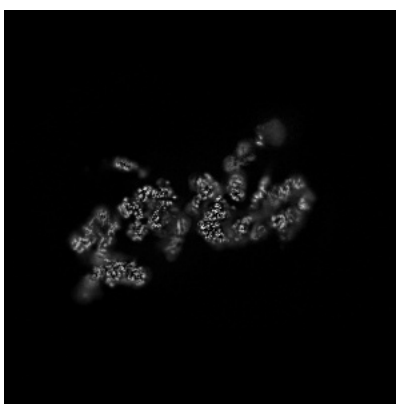
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

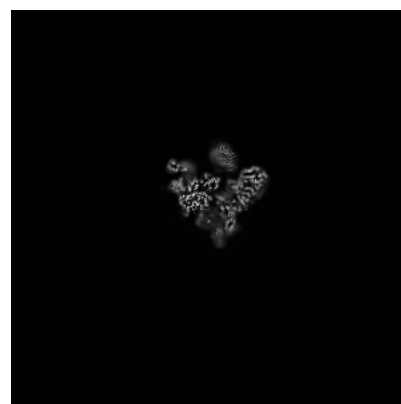
6.2.1 Primary map



X Index: 320



Y Index: 320

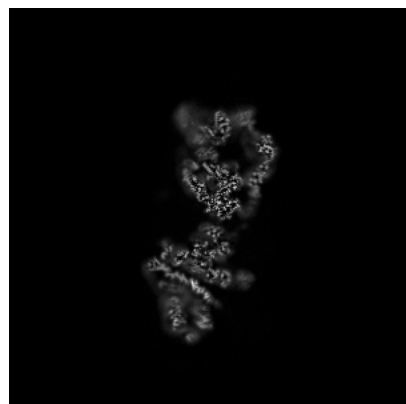


Z Index: 320

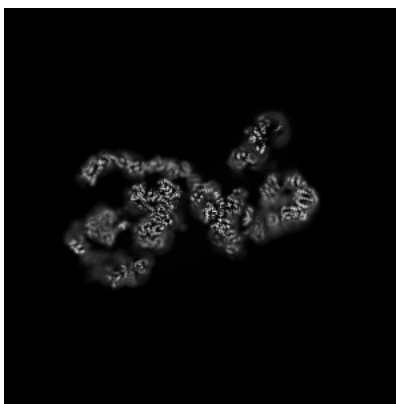
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

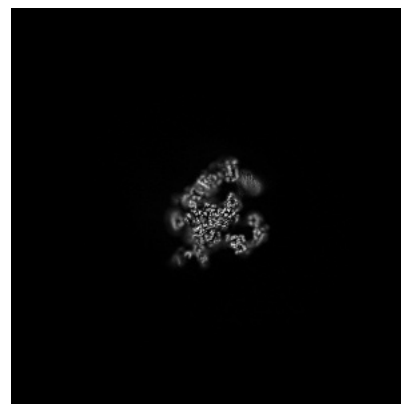
6.3.1 Primary map



X Index: 292



Y Index: 303

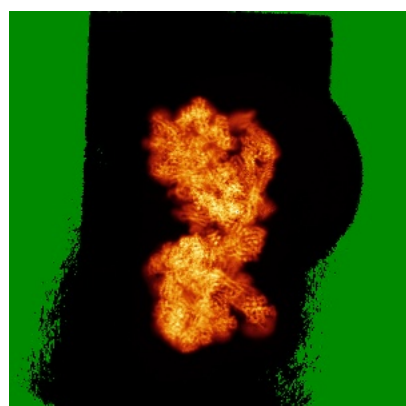


Z Index: 249

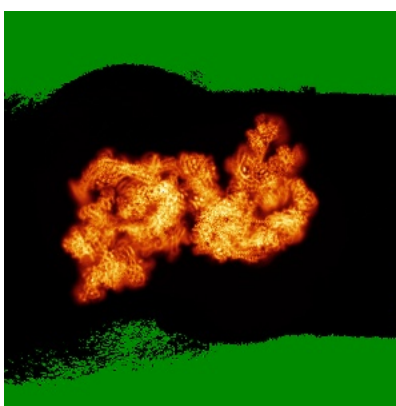
The images above show the largest variance slices of the map in three orthogonal directions.

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

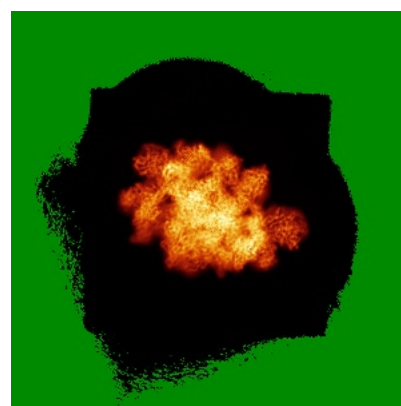
6.4.1 Primary map



X



Y



Z

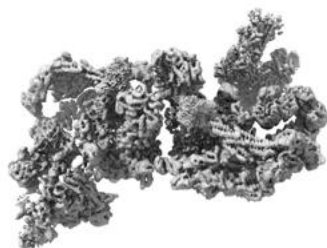
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

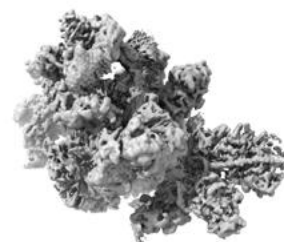
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.407. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

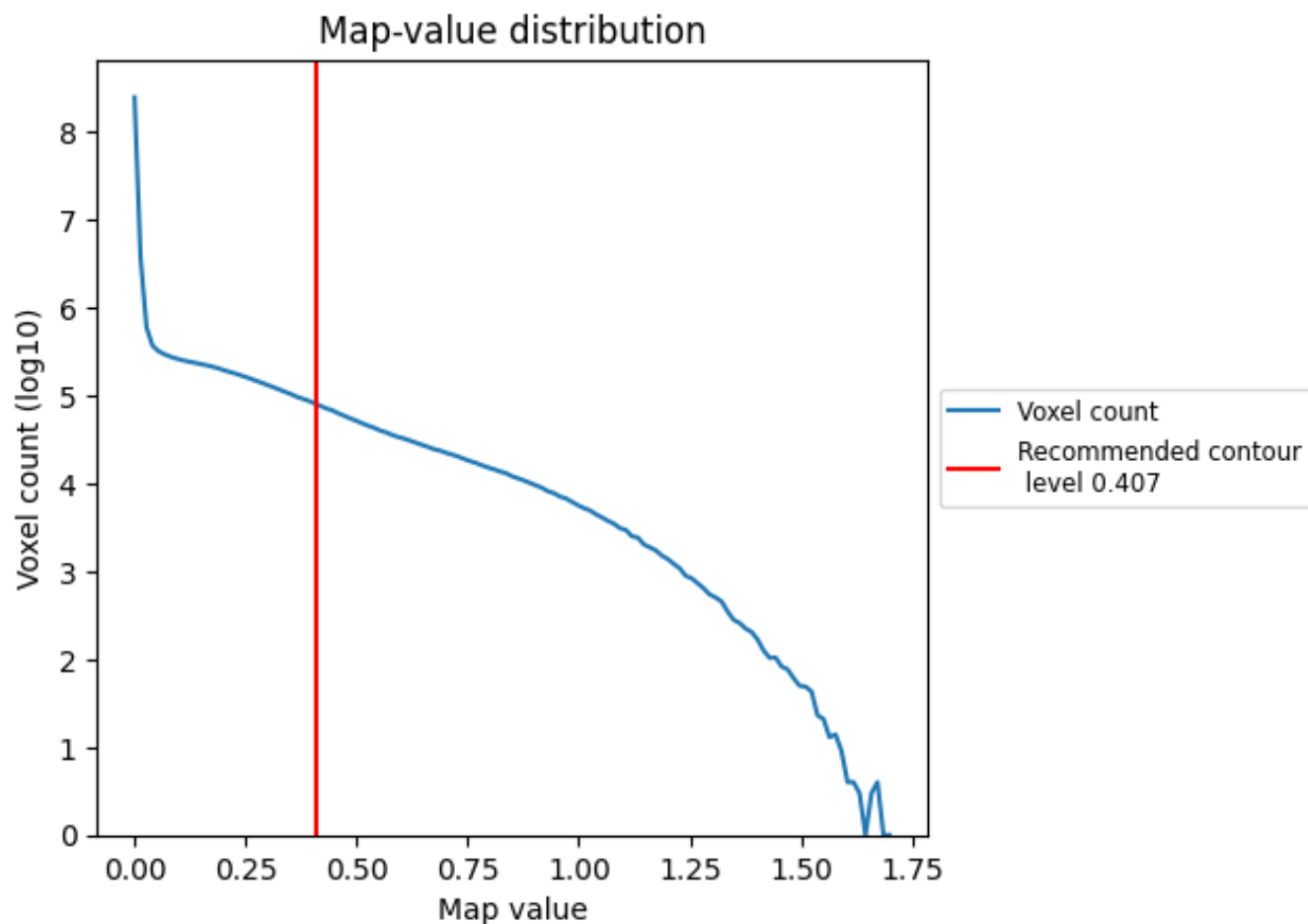
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

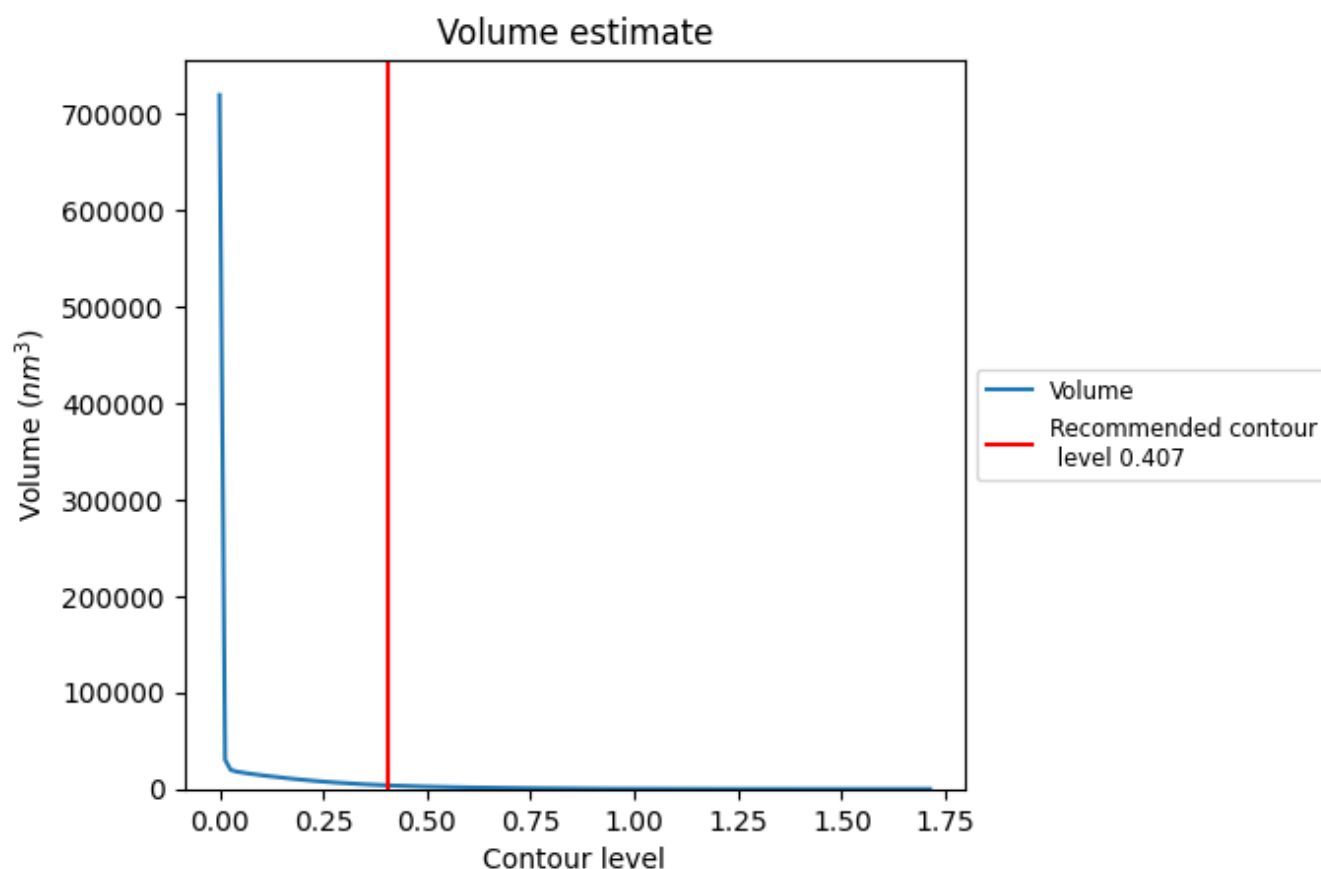
This section contains the results of statistical analysis of the map.

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.

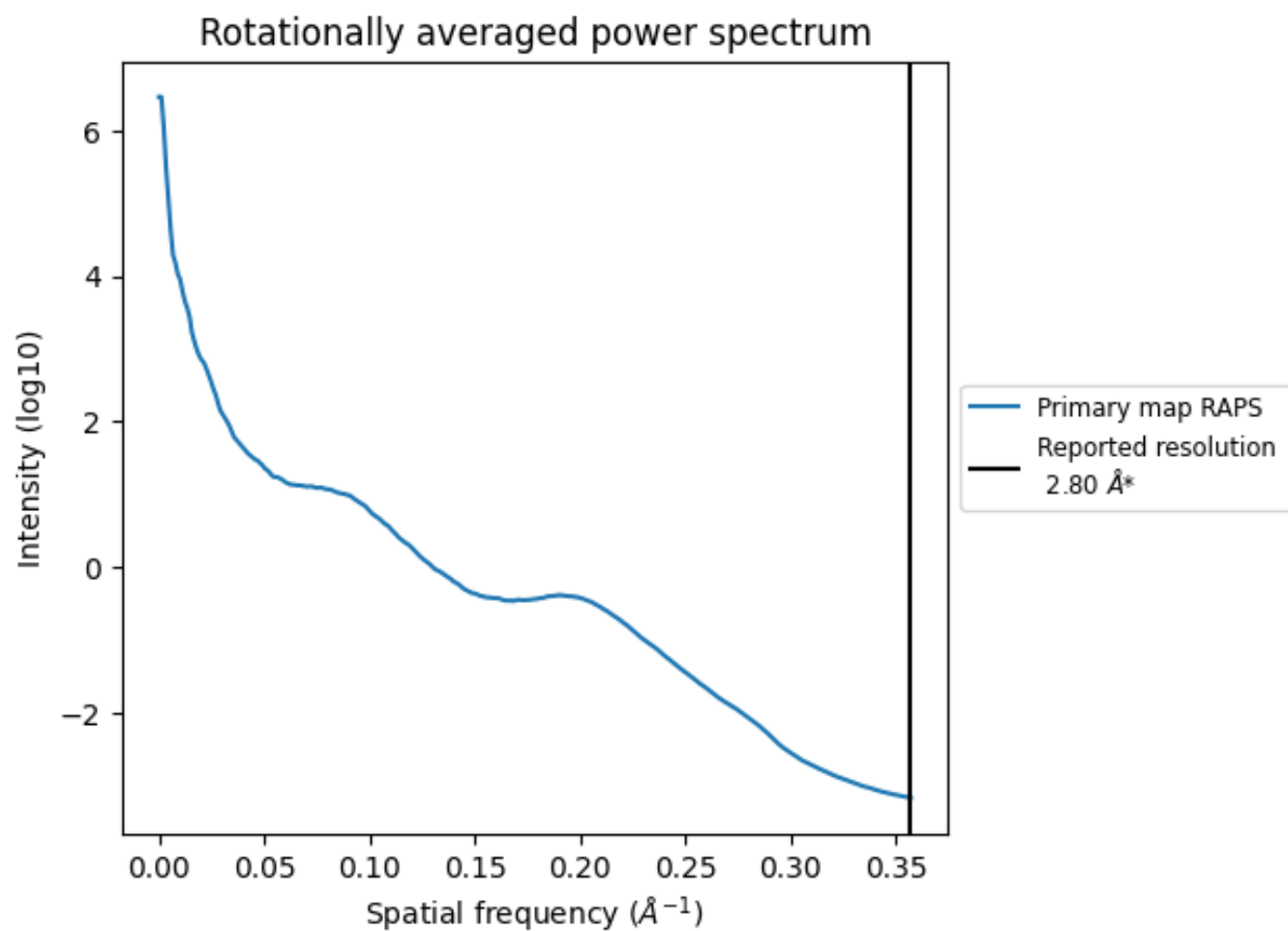
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3703 nm³; this corresponds to an approximate mass of 3345 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 0.357 Å⁻¹

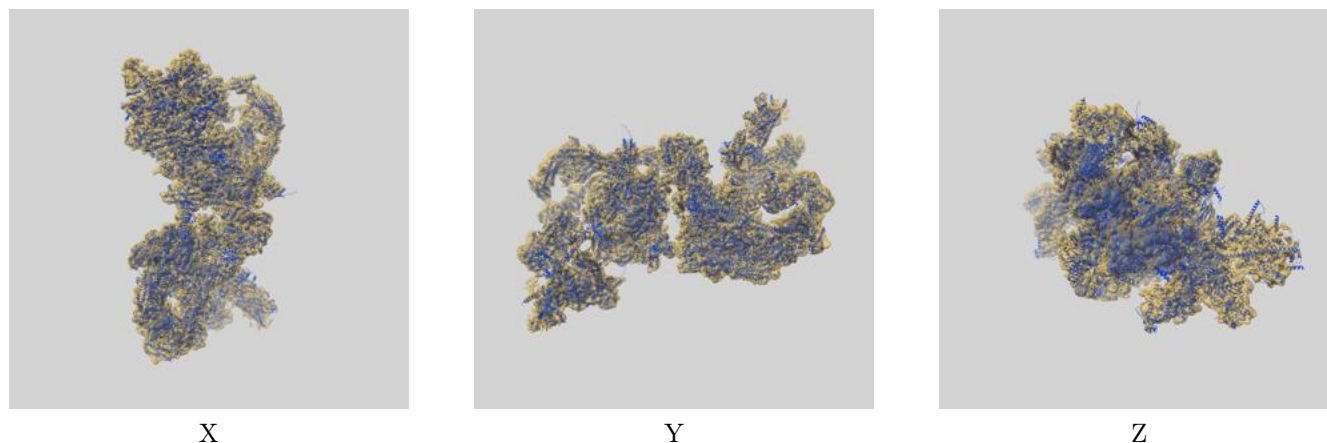
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

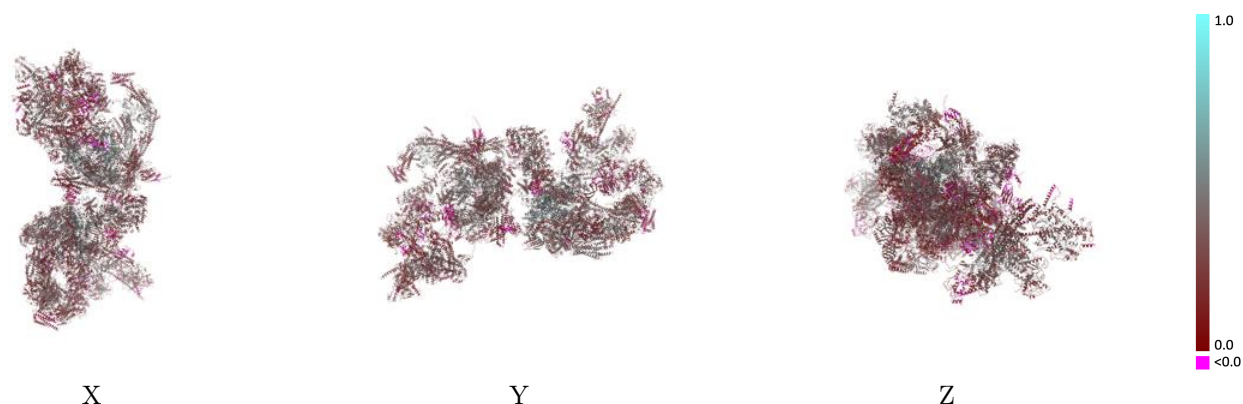
This section contains information regarding the fit between EMDB map EMD-71536 and PDB model 9PDK. Per-residue inclusion information can be found in [section 3](#) on [page 24](#).

9.1 Map-model overlay [i](#)



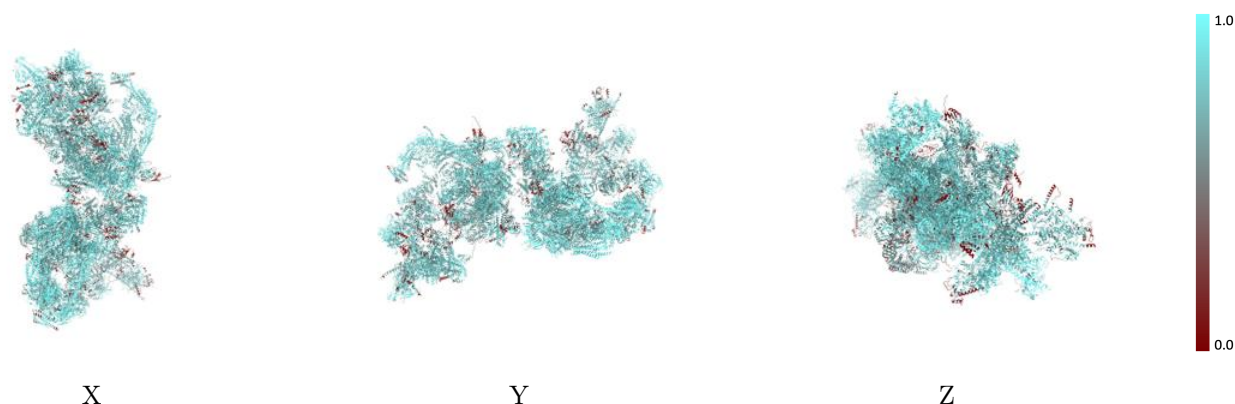
The images above show the 3D surface view of the map at the recommended contour level 0.407 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



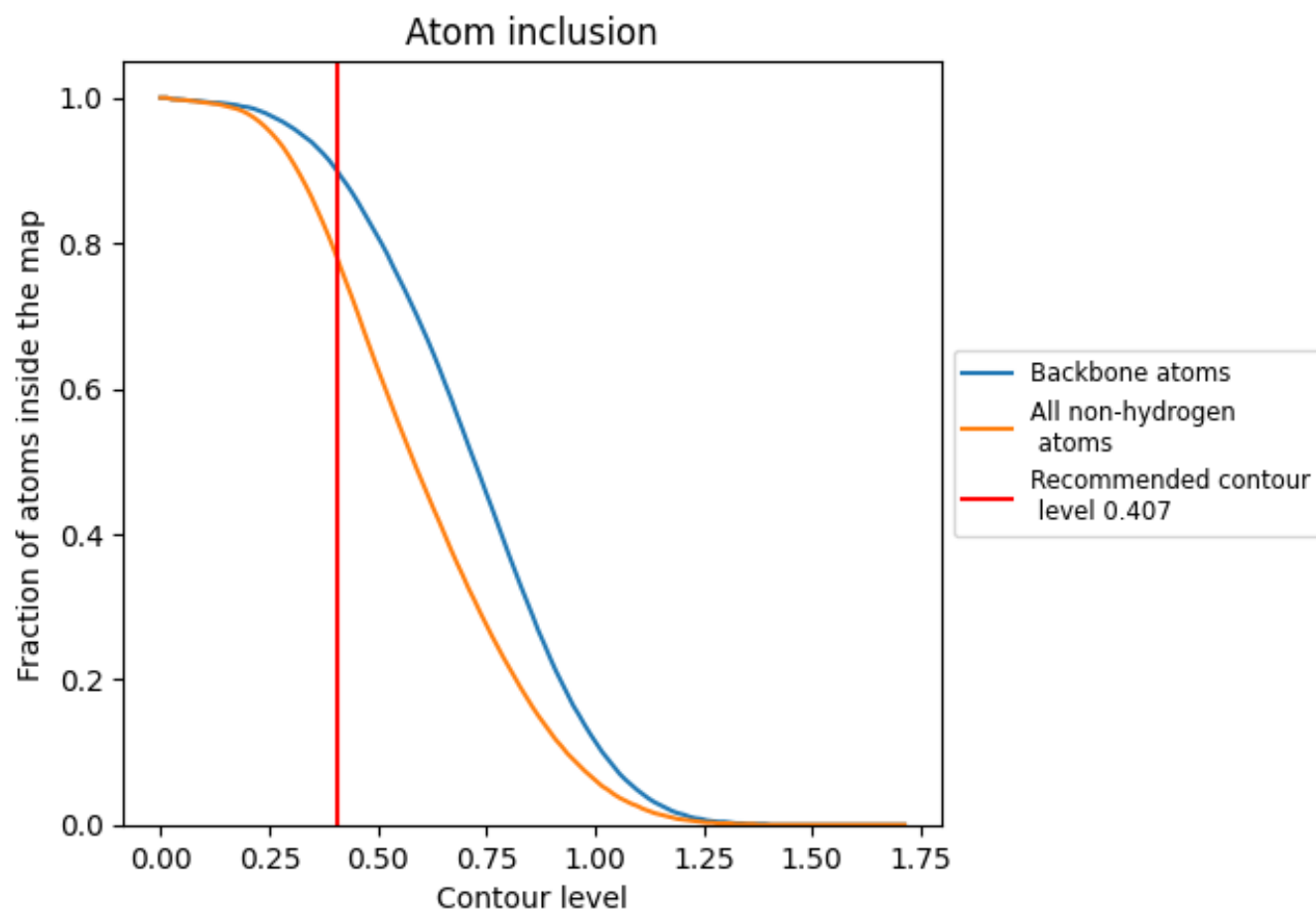
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.407).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 78% 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 (0.407) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7790	 0.3040
A0	 0.8460	 0.2820
A1	 0.7670	 0.2400
A2	 0.8150	 0.2150
A3	 0.8120	 0.2280
A4	 0.9190	 0.3290
A5	 0.7260	 0.1310
A6	 0.8290	 0.3040
A7	 0.7210	 0.1860
A8	 0.2860	 -0.0200
A9	 0.0330	 0.0170
AA	 0.8970	 0.4490
AB	 0.8640	 0.4460
AC	 0.9440	 0.5110
AD	 0.7660	 0.2210
AE	 0.9230	 0.4330
AF	 0.9280	 0.4830
AG	 0.8860	 0.3400
AH	 0.9170	 0.4550
AI	 0.8820	 0.4080
AJ	 0.9040	 0.4740
AK	 0.8620	 0.4620
AL	 0.8990	 0.4220
AM	 0.7610	 0.3120
AN	 0.8520	 0.2410
AO	 0.7130	 0.3130
AQ	 0.6370	 0.2250
AR	 0.5880	 0.1870
AS	 0.6090	 0.2400
AT	 0.8510	 0.2440
AU	 0.5360	 0.2420
AV	 0.5710	 0.2430
AW	 0.5420	 0.1510
AX	 0.3750	 0.2020
B0	 0.8460	 0.2700



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Chain	Atom inclusion	Q-score
B1	 0.7610	 0.2280
B2	 0.8150	 0.2080
B3	 0.8150	 0.2190
B4	 0.9170	 0.3120
B5	 0.7300	 0.1310
B6	 0.8270	 0.2870
B7	 0.7190	 0.1780
B8	 0.2780	 -0.0210
B9	 0.0330	 0.0380
BA	 0.8800	 0.4200
BB	 0.8450	 0.4210
BC	 0.9280	 0.4830
BD	 0.7640	 0.2100
BE	 0.9120	 0.4070
BF	 0.9160	 0.4550
BG	 0.8800	 0.3220
BH	 0.8960	 0.4310
BI	 0.8630	 0.3900
BJ	 0.8970	 0.4460
BK	 0.8340	 0.4270
BL	 0.8900	 0.4070
BM	 0.7410	 0.2980
BN	 0.8480	 0.2400
BO	 0.6980	 0.2980
BQ	 0.6250	 0.2100
BR	 0.5770	 0.1830
BS	 0.6030	 0.2320
BT	 0.8450	 0.2430
BU	 0.5190	 0.2370
BV	 0.5500	 0.2370
BW	 0.5320	 0.1500
BX	 0.3470	 0.1950
MA	 0.8640	 0.4180
Ma	 0.8990	 0.3970
Mb	 0.9160	 0.3680
Mc	 0.8960	 0.3620
Md	 0.8550	 0.3330
Me	 0.9140	 0.4380
Mf	 0.9010	 0.4190
Mg	 0.8440	 0.3400
Mh	 0.8840	 0.3670
Mi	 0.9180	 0.3830

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Chain	Atom inclusion	Q-score
Mj	 0.9100	 0.3250
Mk	 0.8240	 0.1930
MI	 0.7650	 0.2320
Mm	 0.6940	 0.1900
Mn	 0.8810	 0.3180
Mo	 0.8990	 0.4110
Mp	 0.5570	 0.2010
SA	 0.5400	 0.1880
SB	 0.8160	 0.2980
SC	 0.5890	 0.2480
SD	 0.7650	 0.3050
SE	 0.6530	 0.1930
SF	 0.8290	 0.3390
SG	 0.9320	 0.3550
SH	 0.8070	 0.3230
SI	 0.7890	 0.3550
SJ	 0.6150	 0.2250
SK	 0.7180	 0.2880
SL	 0.6790	 0.3040
T1	 0.8050	 0.2380
T2	 0.7070	 0.2030
T3	 0.7820	 0.3130
T4	 0.7170	 0.2140
T5	 0.5920	 0.2240
T6	 0.8220	 0.3420
mA	 0.8580	 0.4040
ma	 0.8900	 0.3760
mb	 0.9120	 0.3450
mc	 0.8890	 0.3430
md	 0.8460	 0.3120
me	 0.9030	 0.4140
mf	 0.8900	 0.3990
mg	 0.8300	 0.3190
mh	 0.8740	 0.3470
mi	 0.9050	 0.3610
mj	 0.9070	 0.3100
mk	 0.8220	 0.1840
ml	 0.7600	 0.2240
mm	 0.6880	 0.1840
mn	 0.8720	 0.3010
mo	 0.8910	 0.3880
mp	 0.5480	 0.1910

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Chain	Atom inclusion	Q-score
sA	 0.5240	 0.1800
sB	 0.8070	 0.2850
sC	 0.5700	 0.2390
sD	 0.7540	 0.2920
sE	 0.6480	 0.1870
sF	 0.8160	 0.3210
sG	 0.9280	 0.3460
sH	 0.7950	 0.3070
sI	 0.7650	 0.3360
sJ	 0.6090	 0.2190
sK	 0.7080	 0.2740
sL	 0.6640	 0.2870
t1	 0.7980	 0.2280
t2	 0.7020	 0.1940
t3	 0.7700	 0.2990
t4	 0.7030	 0.2070
t5	 0.5670	 0.2070
t6	 0.8080	 0.3240