



Full wwPDB EM Validation Report ⓘ

Jul 19, 2023 – 06:48 PM JST

PDB ID : 7EGB
EMDB ID : EMD-31111
Title : TFIID-based holo PIC on SCP promoter
Authors : Chen, X.; Wu, Z.; Hou, H.; Qi, Y.; Wang, X.; Li, J.; Xu, Y.
Deposited on : 2021-03-24
Resolution : 3.30 Å (reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The 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:

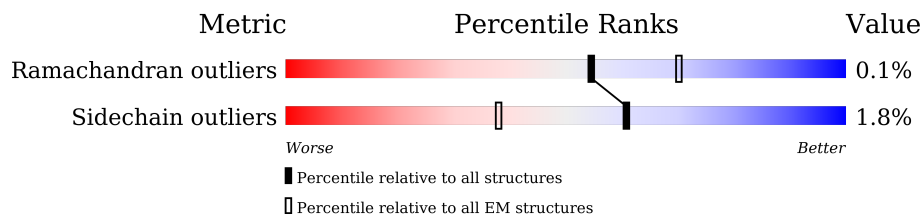
EMDB validation analysis : 0.0.1.dev50
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.34

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 3.30 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	309	69% (upper red), 74% (red), 24% (grey)
2	1	548	27% (upper red), 48% (red), 52% (grey)
3	2	395	32% (upper red), 83% (red), 17% (grey)
4	3	308	17% (upper red), 84% (red), 15% (grey)
5	4	462	36% (upper red), 83% (red), 15% (grey)
6	5	71	51% (upper red), 75% (red), 24% (grey)
7	6	782	23% (upper red), 76% (red), 23% (grey)
8	7	760	37% (upper red), 94% (red), 6% (grey)
9	8	346	74% (upper red), 86% (red), 14% (grey)

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Mol	Chain	Length	Quality of chain
10	9	323	60% 86% 13%
11	A	1872	25% 28% 70%
12	B	1199	29% 79% 20%
13	D	1085	7% 14% 85%
13	d	1085	15% 14% 85%
14	E	800	39% 66% 32%
14	e	800	67% 66% 33%
15	F	677	39% 57% 39%
15	f	677	43% 58% 40%
16	G	349	40% 39% 59%
17	H	310	22% 64% 33%
18	I	264	24% 45% 55%
18	i	264	46% 46% 54%
19	J	218	7% 38% 59%
19	j	218	44% 42% 56%
20	L	161	32% 44% 53%
20	l	161	66% 66% 34%
21	O	109	40% 89% 9%
22	P	339	9% 53% 47%
23	Q	376	11% 30% 70%
24	R	316	32% 79% 20%
25	S	517	10% 21% 79%
26	T	249	49% 88% 11%
27	U	439	20% 40% 58%
28	V	291	22% 57% 43%

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Mol	Chain	Length	Quality of chain
29	X	94	
30	Y	69	
31	c	929	
32	k	211	
33	m	124	
34	o	1970	
35	p	1174	
36	q	275	
37	r	142	
38	s	210	
39	t	127	
40	u	172	
41	v	150	
42	w	125	
43	x	67	
44	y	117	
45	z	58	

2 Entry composition [i](#)

There are 48 unique types of molecules in this entry. The entry contains 112409 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 CDK-activating kinase assembly factor MAT1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	236	1932	1211	336	373	12	0	0

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

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

- Molecule 3 is a protein called General transcription factor IIH subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	2	329	2567	1621	440	479	27	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	3	263	2066	1323	344	380	19	0	0

- Molecule 5 is a protein called General transcription factor IIH subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	4	394	3189	2068	552	557	12	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	5	54	428	277	67	82	2	0	0

- Molecule 7 is a protein called General transcription and DNA repair factor IIIH helicase subunit XPB.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	6	605	4890	3127	848	885	30	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	7	714	5751	3683	999	1040	29	0	0

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

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

- Molecule 10 is a protein called Cyclin-H.

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

- Molecule 11 is a protein called Transcription initiation factor TFIID subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	A	559	4580	2924	795	834	27	0	0

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

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

- Molecule 13 is a protein called Transcription initiation factor TFIID subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	D	160	1337	834	249	251	3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
13	d	158	Total	C	N	O	S	0	0
			1307	814	238	252	3		

- Molecule 14 is a protein called Transcription initiation factor TFIID subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	E	547	Total	C	N	O	S	0	0
			4376	2774	759	822	21		
14	e	539	Total	C	N	O	S	0	0
			4327	2746	748	814	19		

- Molecule 15 is a protein called Transcription initiation factor TFIID subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	F	412	Total	C	N	O	S	0	0
			3143	1994	548	583	18		
15	f	403	Total	C	N	O	S	0	0
			3081	1954	533	576	18		

- Molecule 16 is a protein called Transcription initiation factor TFIID subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	G	144	Total	C	N	O	S	0	0
			1171	742	215	210	4		

- Molecule 17 is a protein called Transcription initiation factor TFIID subunit 8.

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

- Molecule 18 is a protein called Transcription initiation factor TFIID subunit 9.

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

- Molecule 19 is a protein called Transcription initiation factor TFIID subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	J	90	Total	C	N	O	S	0	0
			720	466	115	135	4		
19	j	95	Total	C	N	O	S	0	0
			759	488	124	143	4		

- Molecule 20 is a protein called Transcription initiation factor TFIID subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	L	76	Total	C	N	O	S	0	0
			622	388	109	122	3		
20	l	107	Total	C	N	O	S	0	0
			876	547	158	166	5		

- Molecule 21 is a protein called Transcription initiation factor IIA subunit 2.

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

- Molecule 22 is a protein called TATA-box-binding protein.

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

- Molecule 23 is a protein called Transcription initiation factor IIA subunit 1.

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

- Molecule 24 is a protein called Transcription initiation factor IIB.

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

- Molecule 25 is a protein called General transcription factor IIF subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	S	108	Total	C	N	O	S	0	0
			872	558	153	159	2		

- Molecule 26 is a protein called General transcription factor IIF subunit 2.

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

- Molecule 27 is a protein called General transcription factor IIE subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	U	184	1520	957	272	280	11	0	0

- Molecule 28 is a protein called Transcription initiation factor IIE subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	V	165	1357	865	235	253	4	0	0

- Molecule 29 is a DNA chain called DNA (69-MER).

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

- Molecule 30 is a DNA chain called DNA (69-MER).

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

- Molecule 31 is a protein called Transcription initiation factor TFIID subunit 3.

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

- Molecule 32 is a protein called Transcription initiation factor TFIID subunit 11.

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

- Molecule 33 is a protein called Transcription initiation factor TFIID subunit 13.

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

- Molecule 34 is a protein called DNA-directed RNA polymerase II subunit RPB1.

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

- Molecule 35 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	p	1135	Total	C	N	O	S	0	0
			9068	5735	1596	1673	64		

- Molecule 36 is a protein called DNA-directed RNA polymerase II subunit RPB3.

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

- Molecule 37 is a protein called DNA-directed RNA polymerase II subunit RPB4.

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

- Molecule 38 is a protein called DNA-directed RNA polymerase II subunit E.

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

- Molecule 39 is a protein called DNA-directed RNA polymerase II subunit F.

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

- Molecule 40 is a protein called DNA-directed RNA polymerase II subunit RPB7.

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

- Molecule 41 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

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

- Molecule 42 is a protein called DNA-directed RNA polymerase II subunit RPB9.

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

- Molecule 43 is a protein called RPB10.

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

- Molecule 44 is a protein called RNA_pol_L_2 domain-containing protein.

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

- Molecule 45 is a protein called RPB12.

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

- Molecule 46 is ZINC ION (three-letter code: ZN) (formula: Zn).

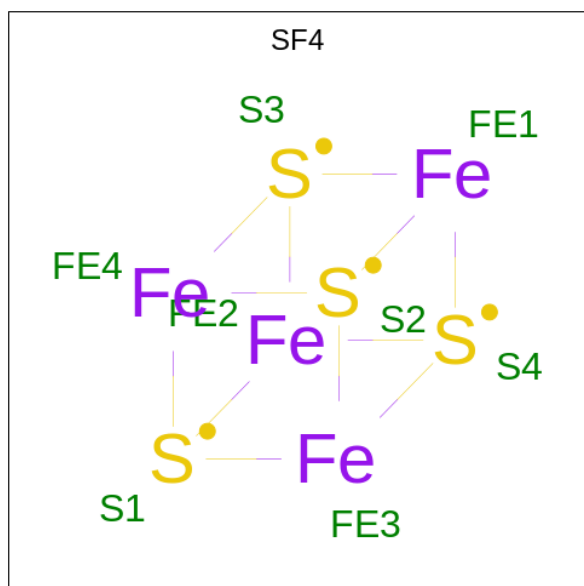
Mol	Chain	Residues	Atoms		AltConf
46	0	2	Total	Zn	0
			2	2	
46	2	3	Total	Zn	0
			3	3	
46	3	2	Total	Zn	0
			2	2	

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Mol	Chain	Residues	Atoms		AltConf
46	R	1	Total	Zn	0
			1	1	
46	U	1	Total	Zn	0
			1	1	
46	o	2	Total	Zn	0
			2	2	
46	p	1	Total	Zn	0
			1	1	
46	q	1	Total	Zn	0
			1	1	
46	w	2	Total	Zn	0
			2	2	
46	x	1	Total	Zn	0
			1	1	
46	z	1	Total	Zn	0
			1	1	

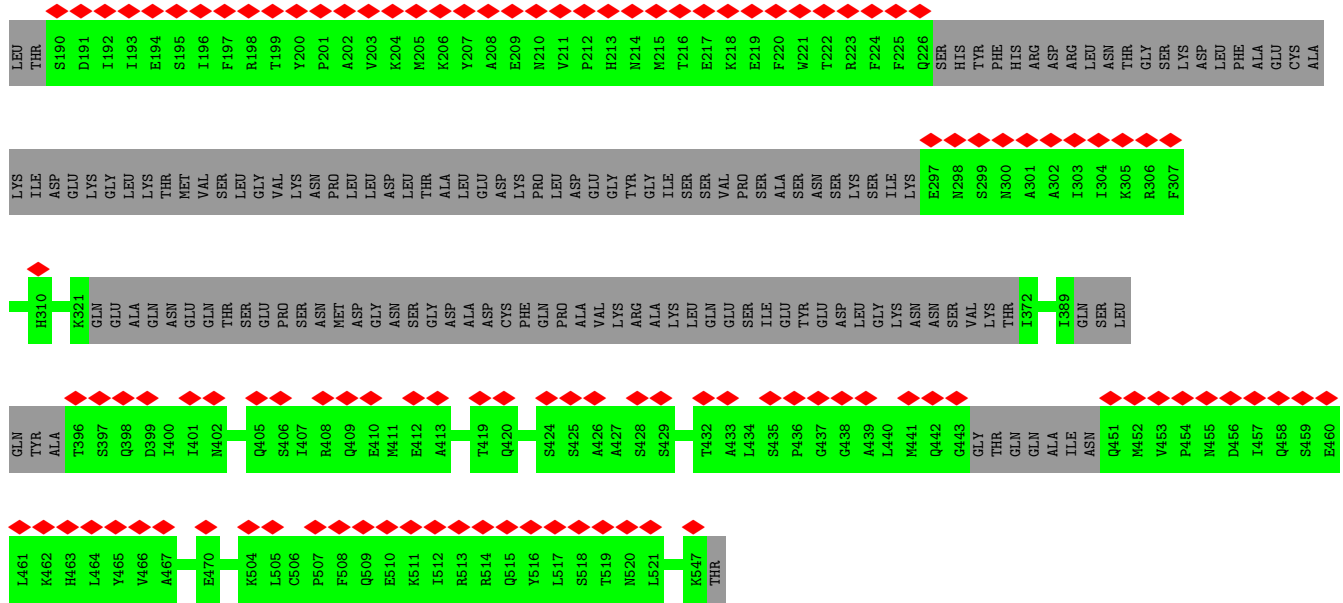
- Molecule 47 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



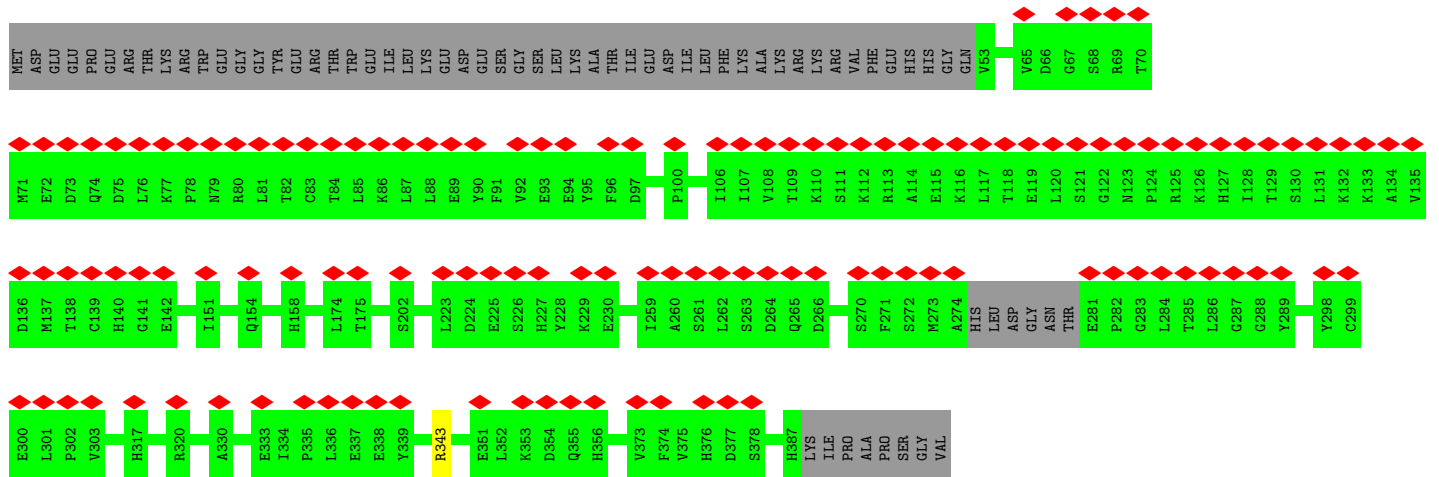
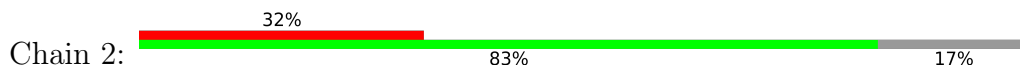
Mol	Chain	Residues	Atoms			AltConf
47	7	1	Total	Fe	S	0
			8	4	4	

- Molecule 48 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

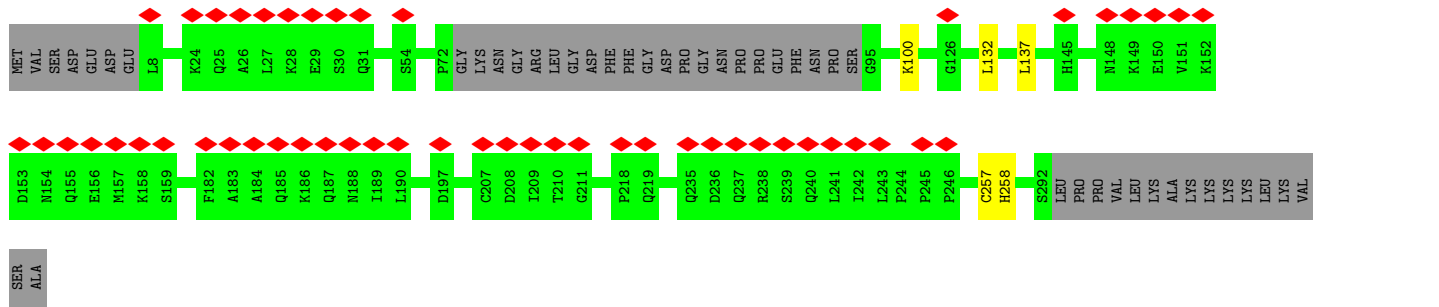
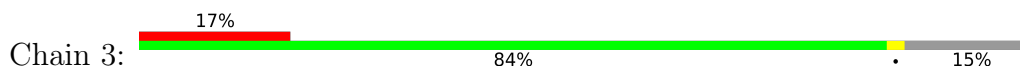
Mol	Chain	Residues	Atoms		AltConf
48	o	1	Total	Mg	0
			1	1	



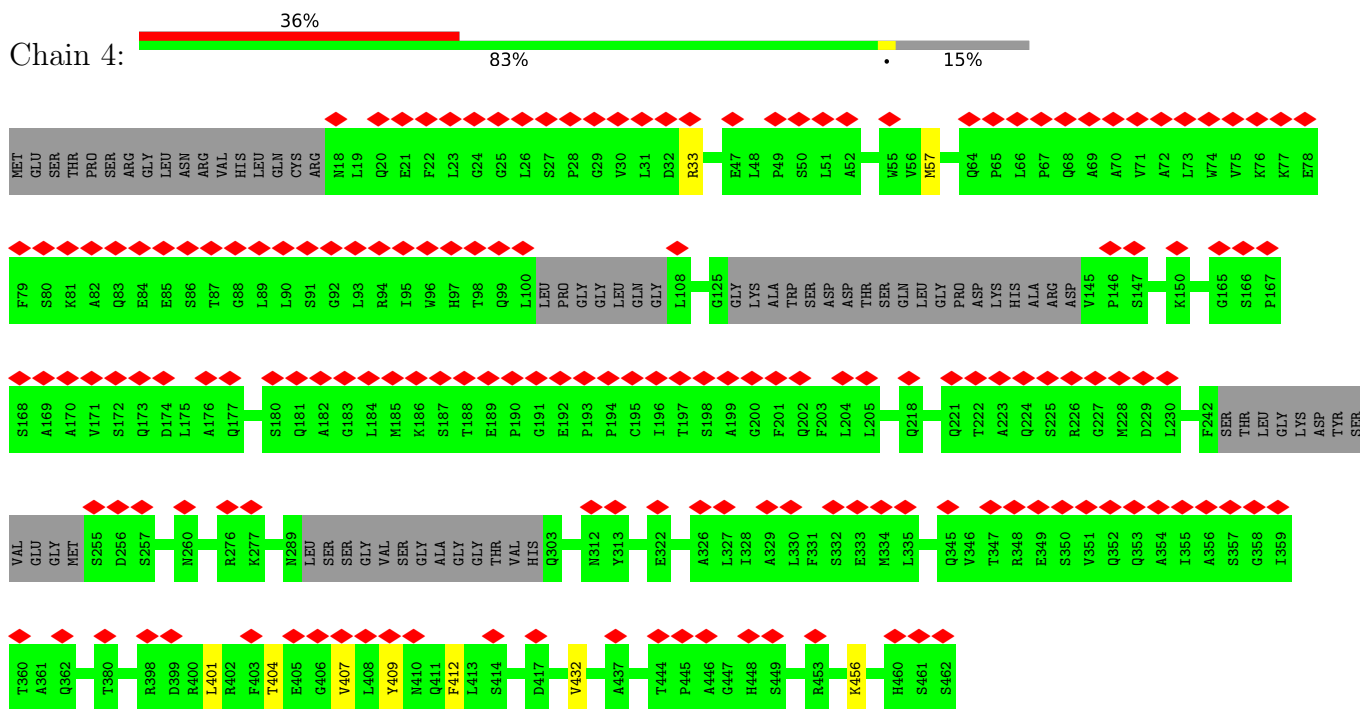
• Molecule 3: General transcription factor IIIH subunit 2



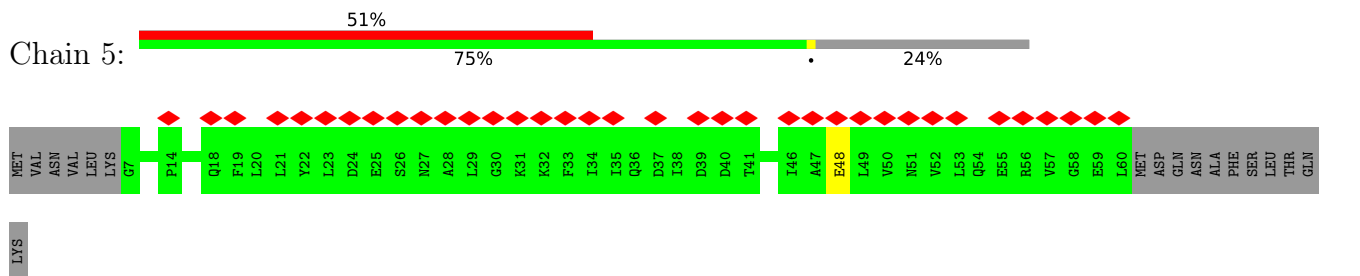
• Molecule 4: General transcription factor IIIH subunit 3



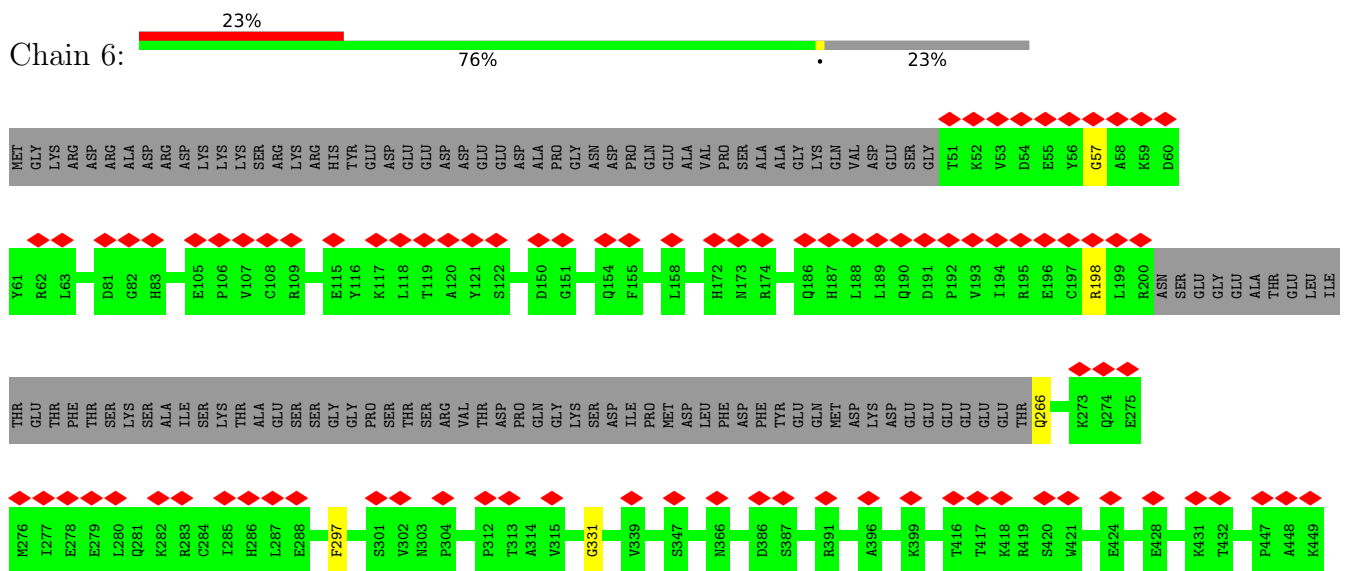
• Molecule 5: General transcription factor IIIH subunit 4

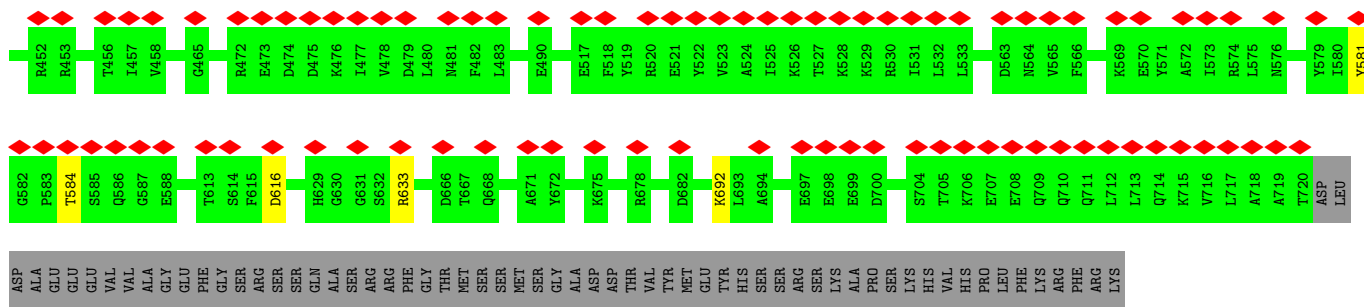


• Molecule 6: General transcription factor IIIH subunit 5

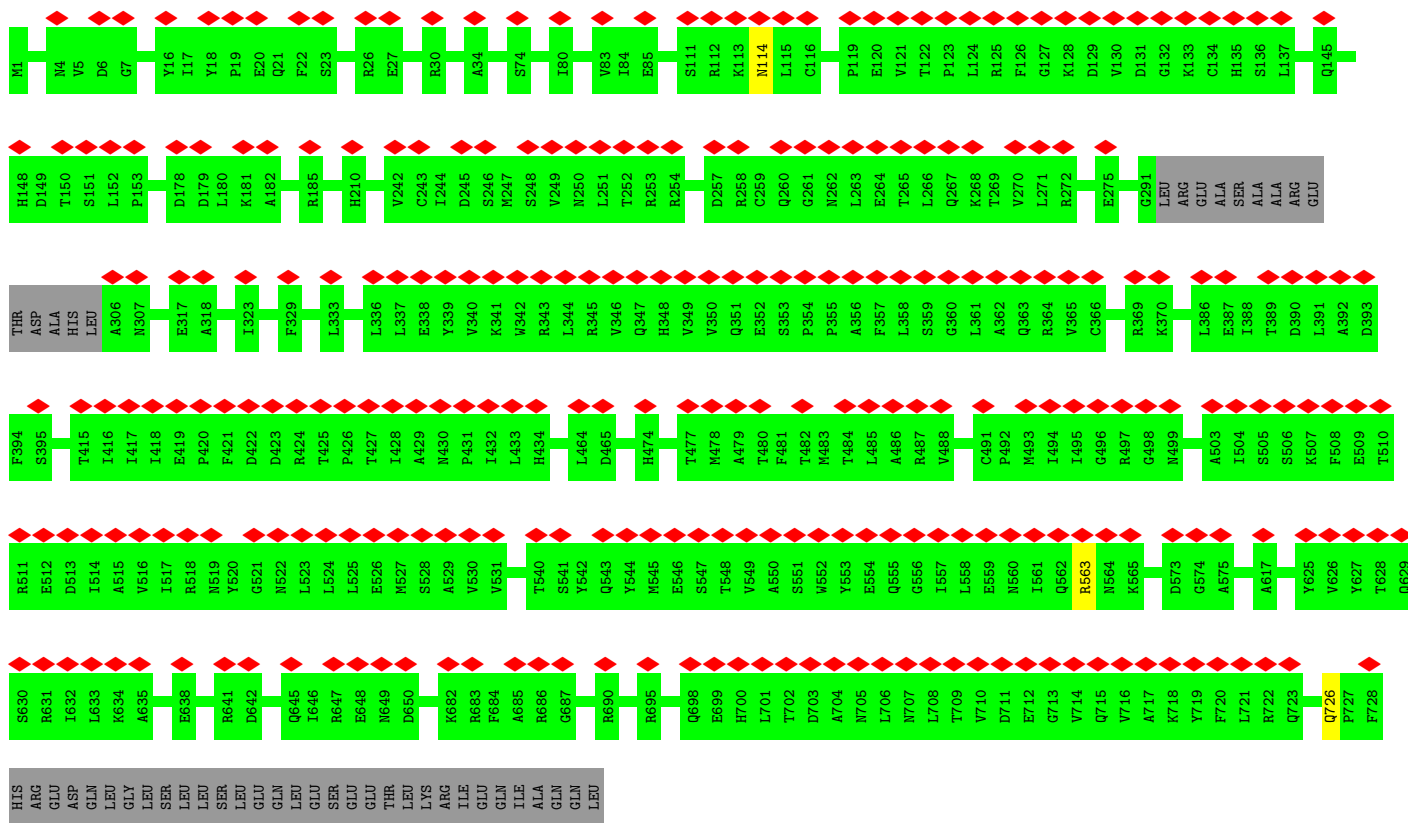
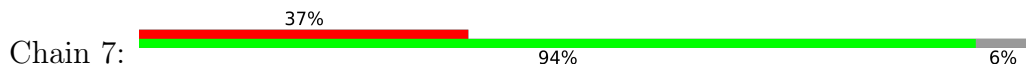


• Molecule 7: General transcription and DNA repair factor IIIH helicase subunit XPB

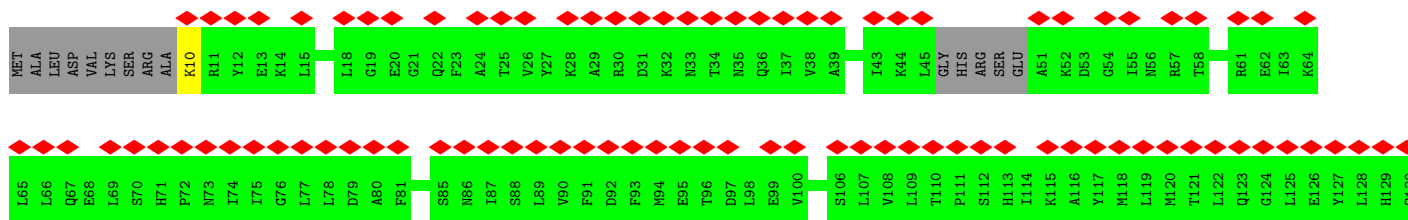
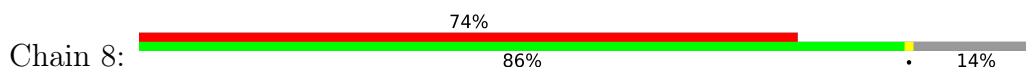


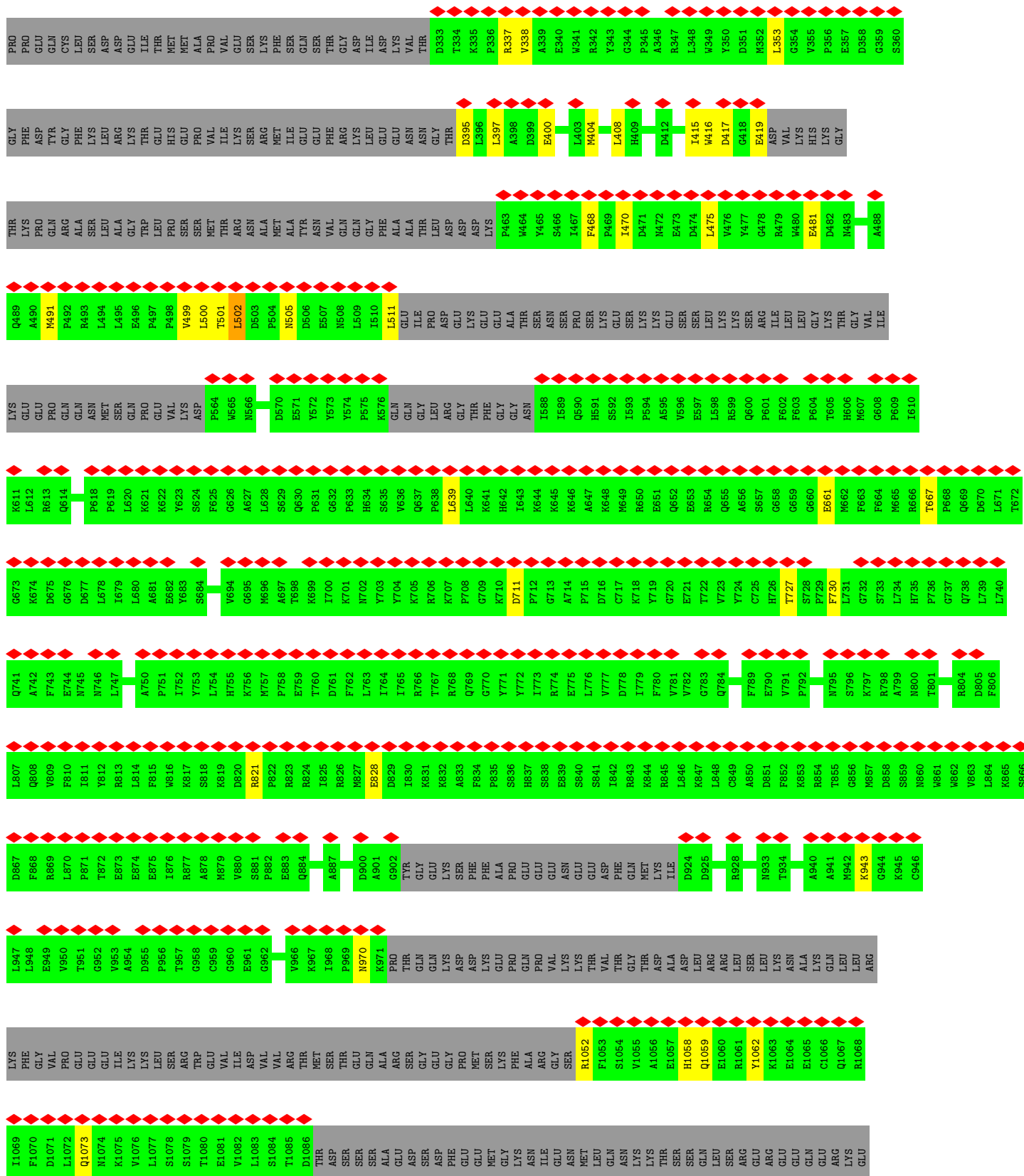


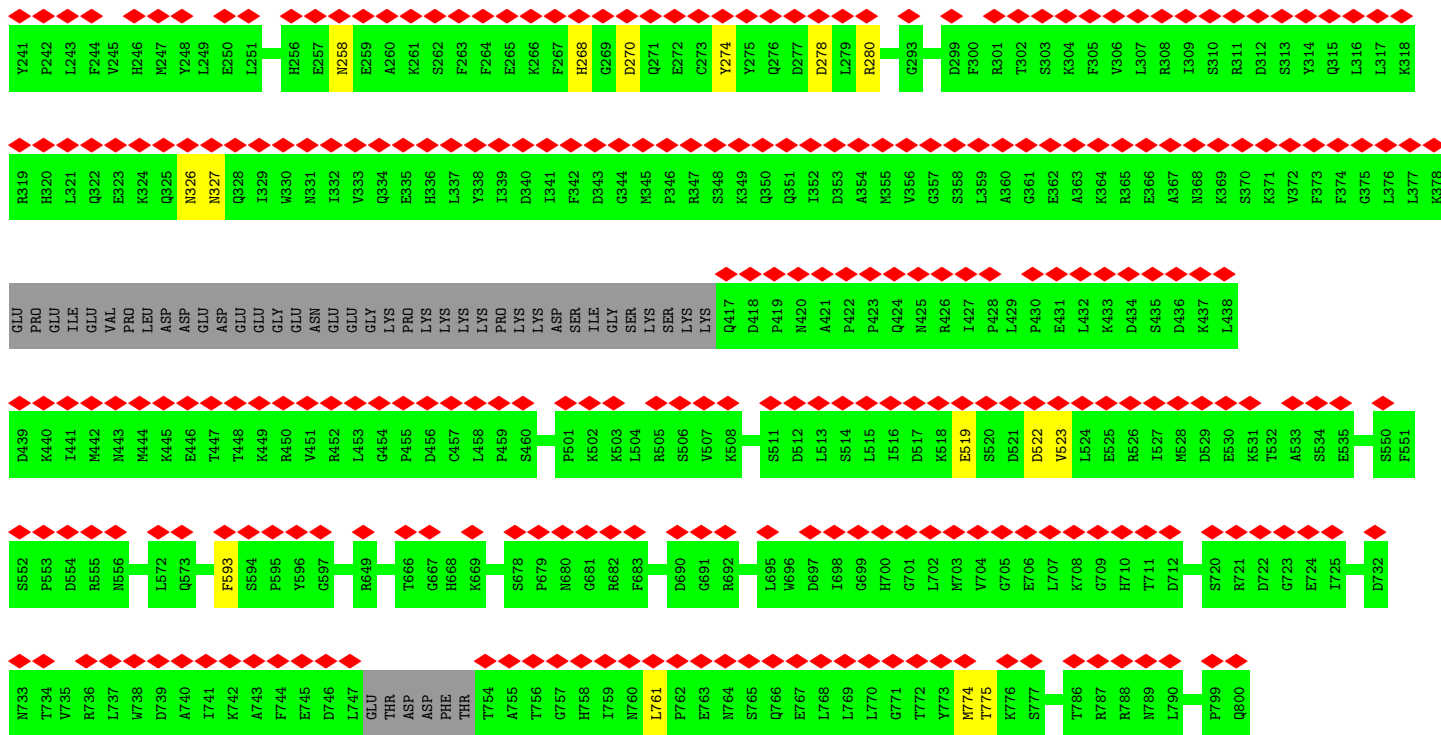
• Molecule 8: General transcription and DNA repair factor IIIH helicase subunit XPD



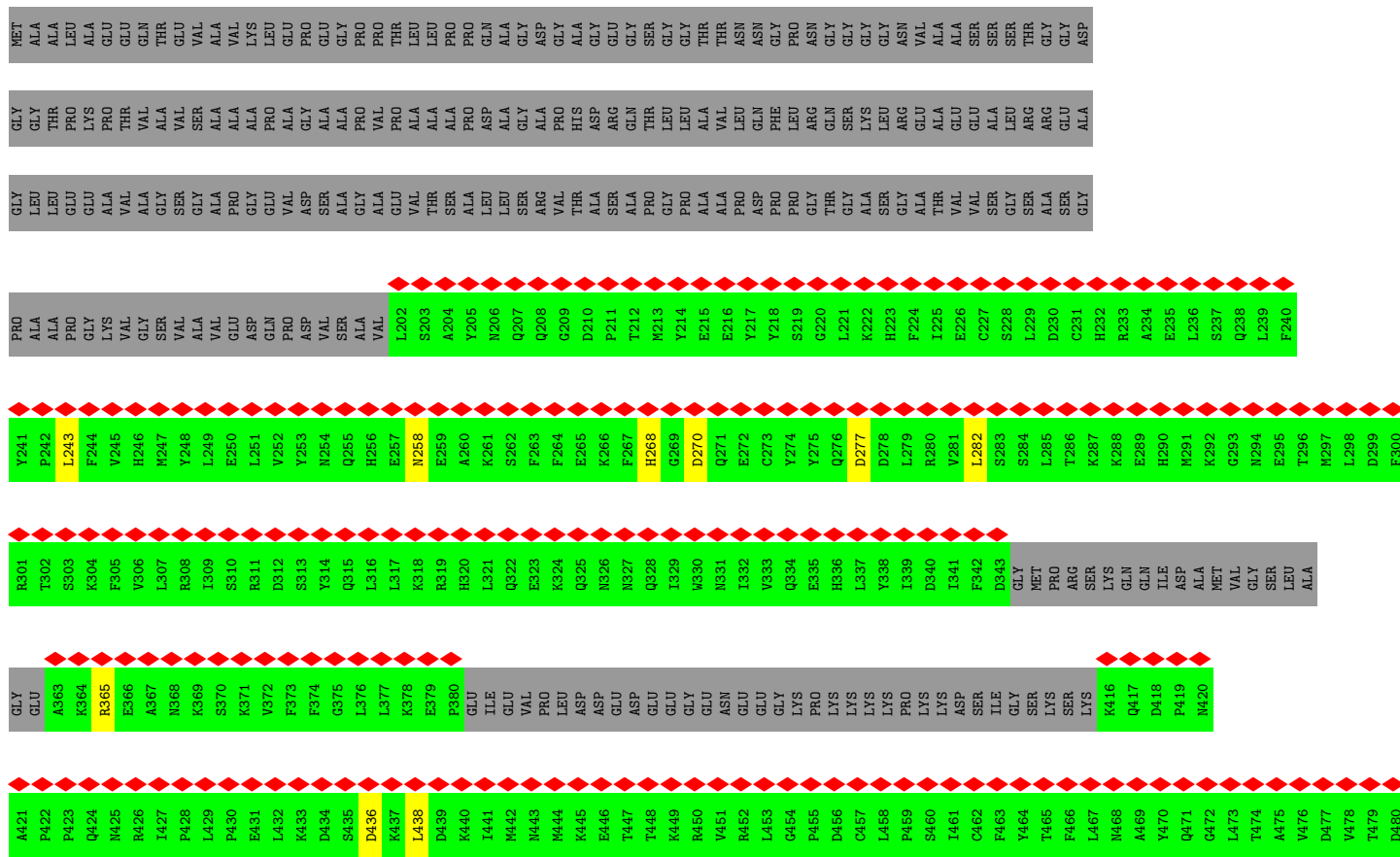
• Molecule 9: Cyclin-dependent kinase 7

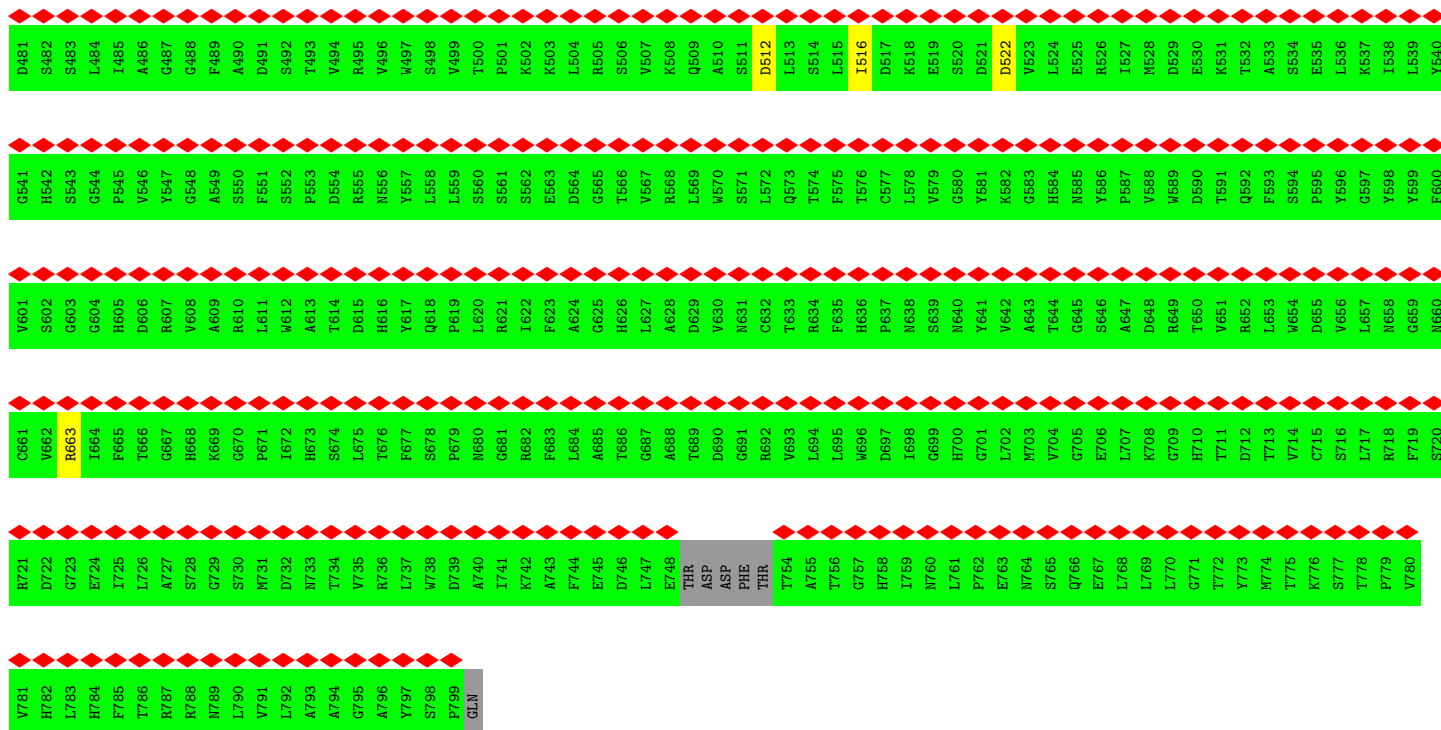




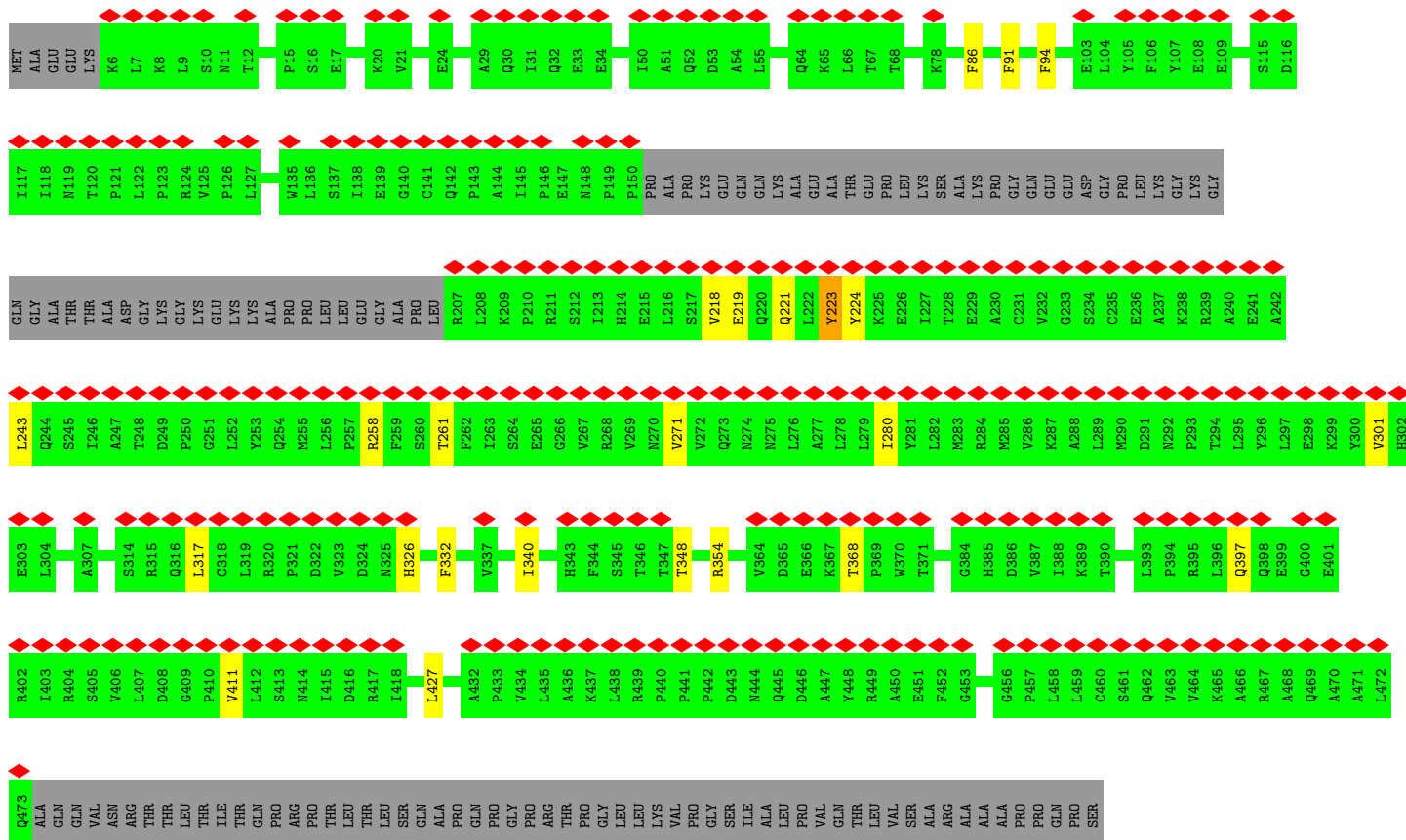
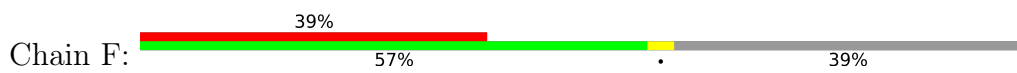


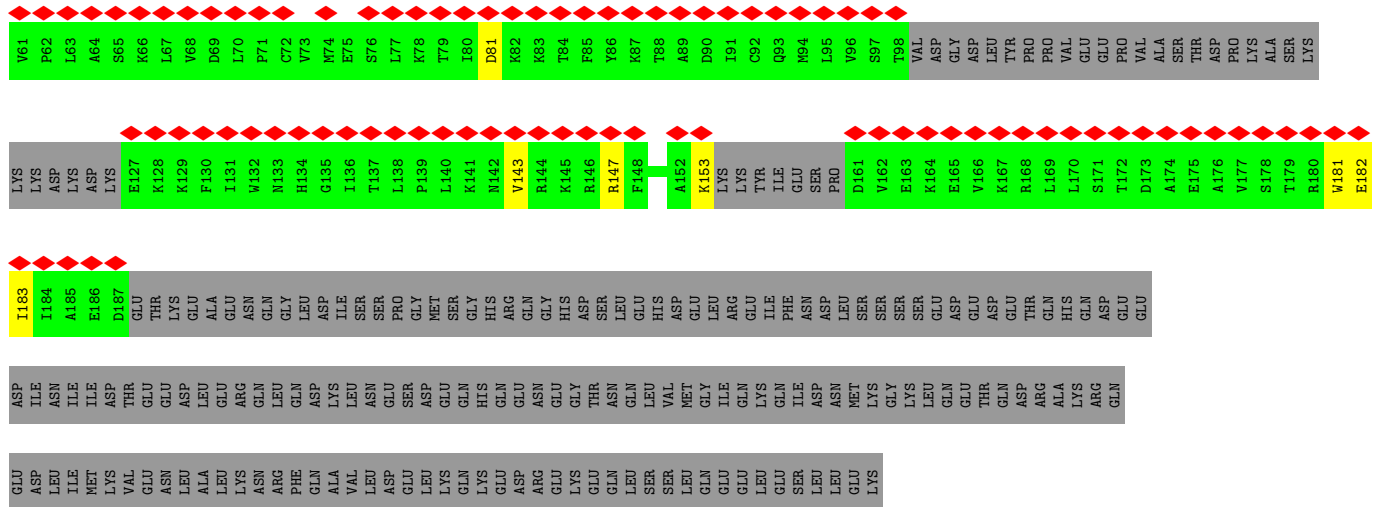
● Molecule 14: Transcription initiation factor TFIID subunit 5



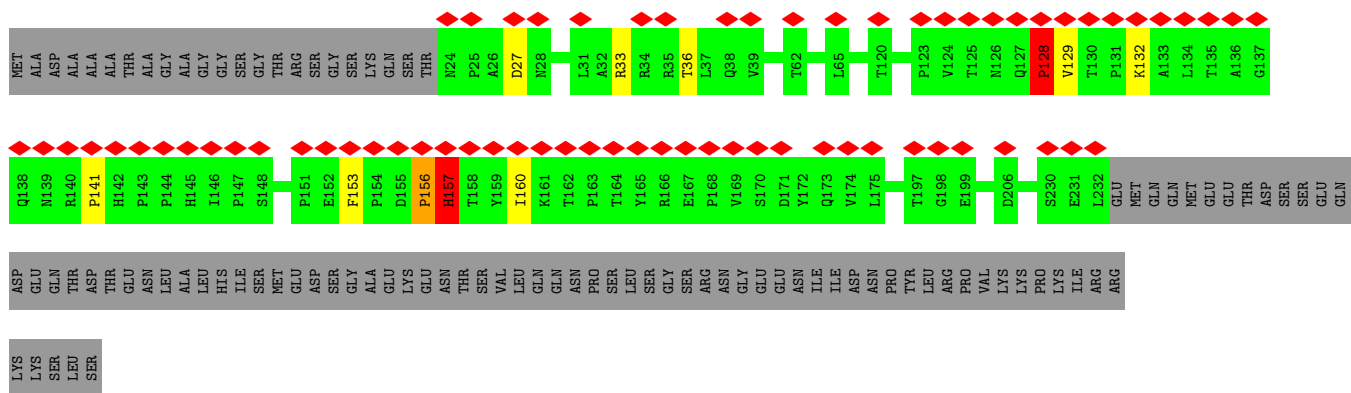


● Molecule 15: Transcription initiation factor TFIID subunit 6

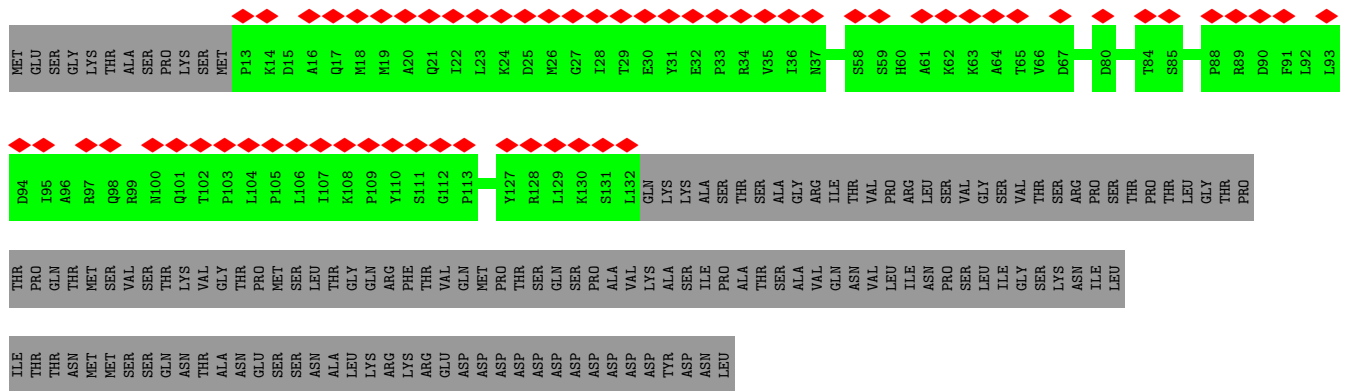




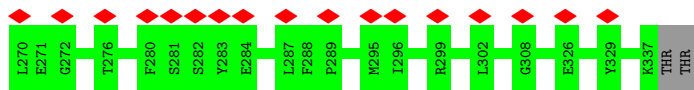
• Molecule 17: Transcription initiation factor TFIID subunit 8



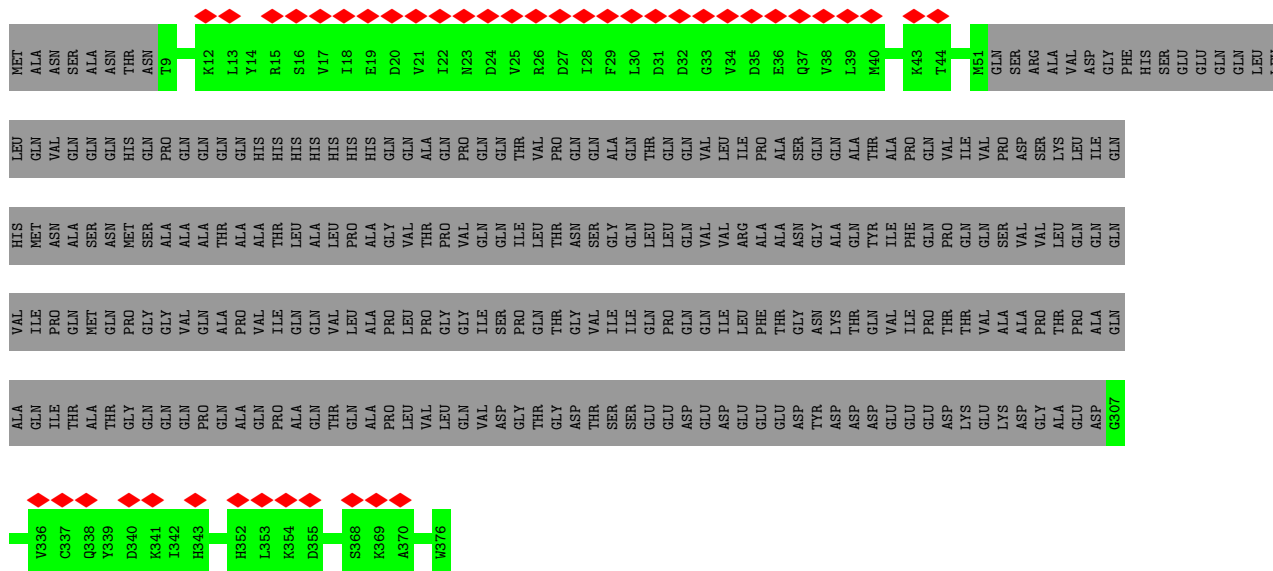
• Molecule 18: Transcription initiation factor TFIID subunit 9



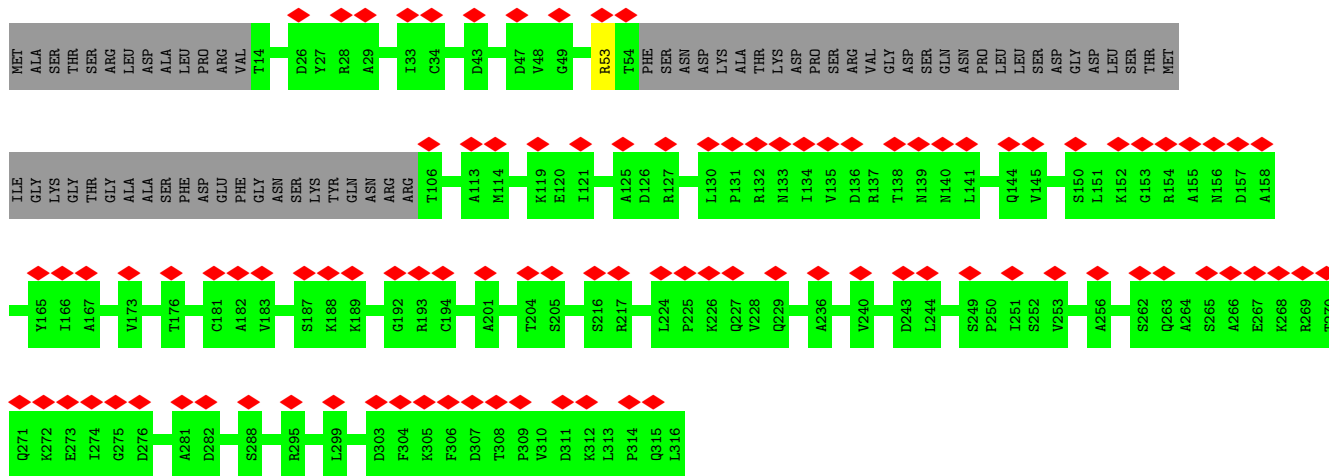
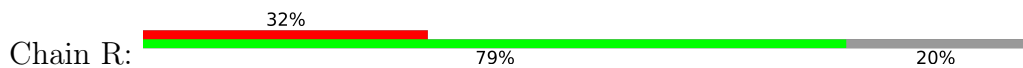
• Molecule 18: Transcription initiation factor TFIID subunit 9



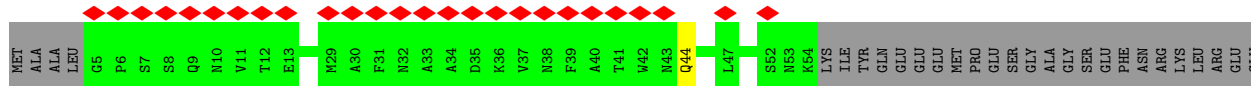
• Molecule 23: Transcription initiation factor IIA subunit 1

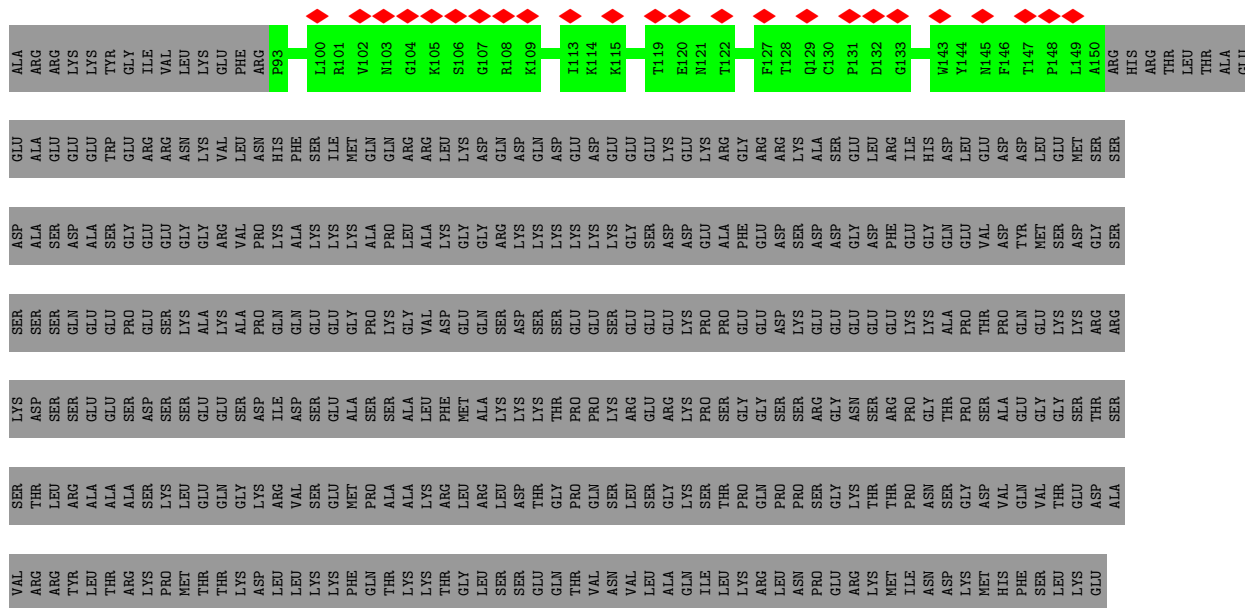


• Molecule 24: Transcription initiation factor IIB

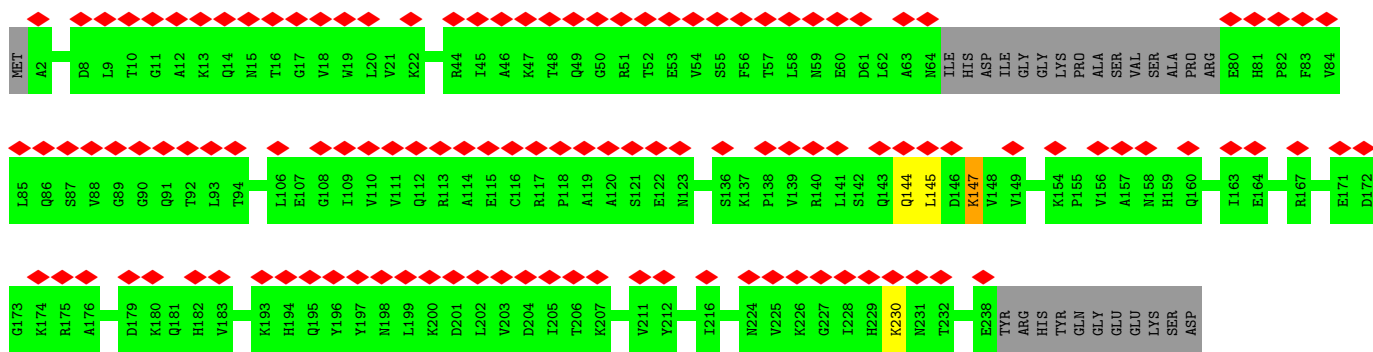
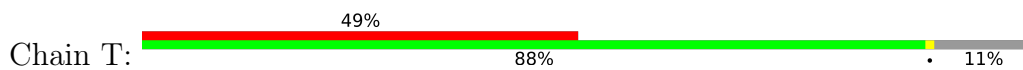


• Molecule 25: General transcription factor IIF subunit 1

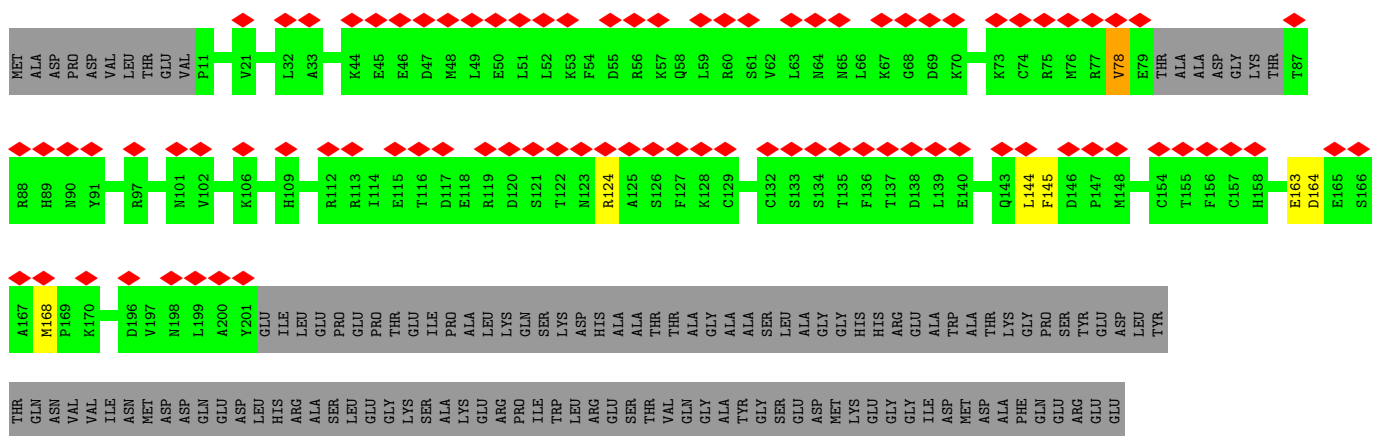


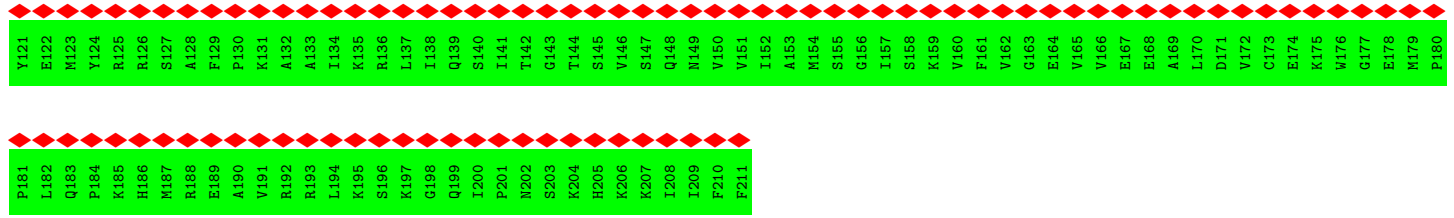


• Molecule 26: General transcription factor IIF subunit 2

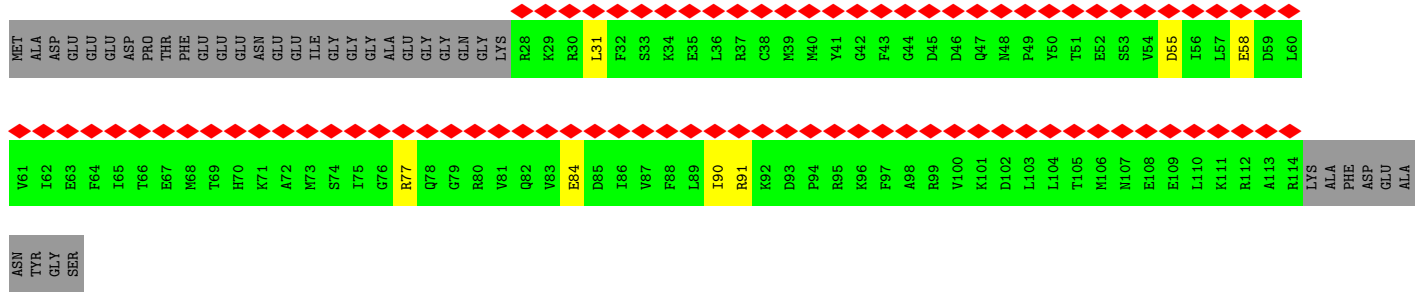


• Molecule 27: General transcription factor IIE subunit 1

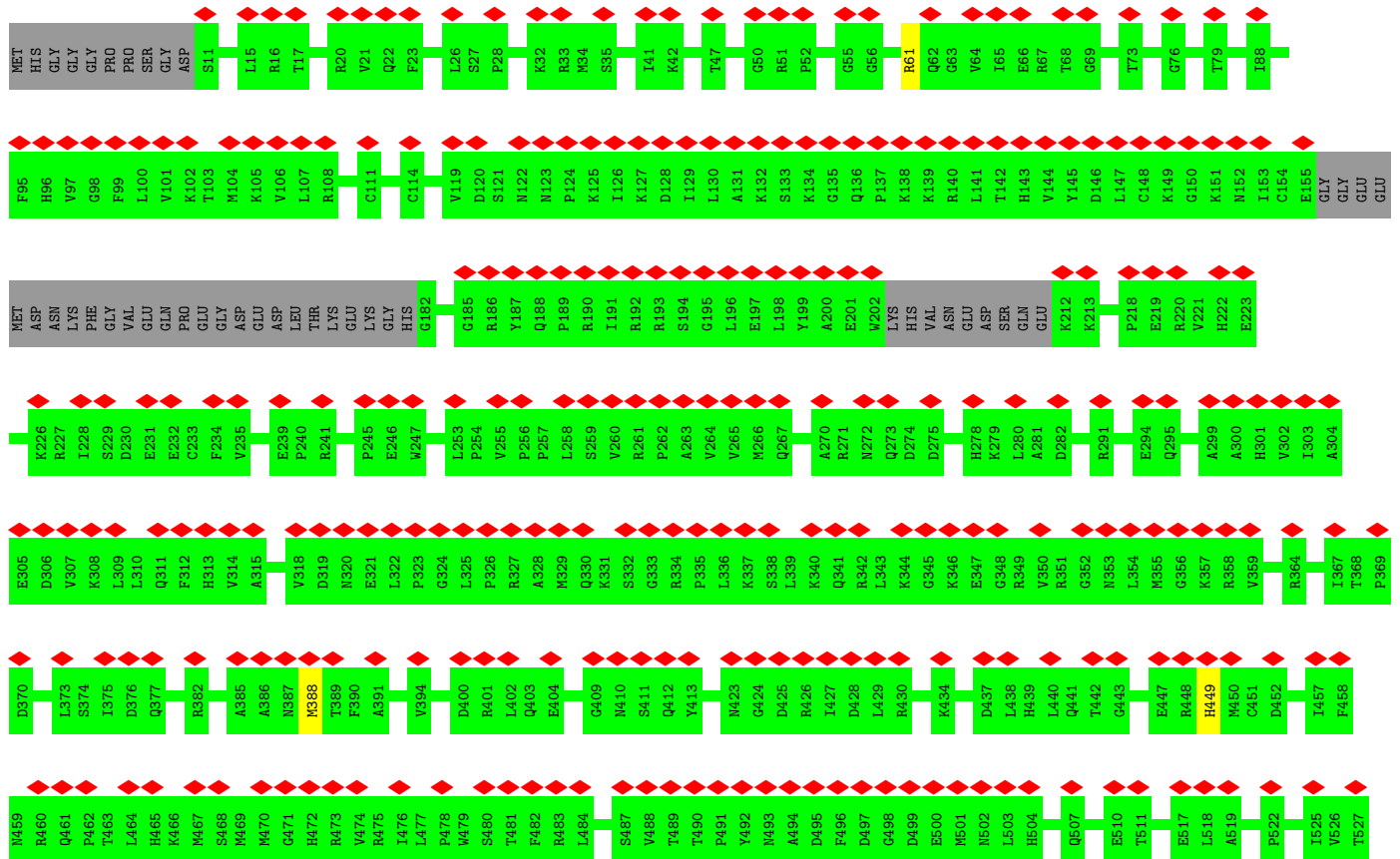


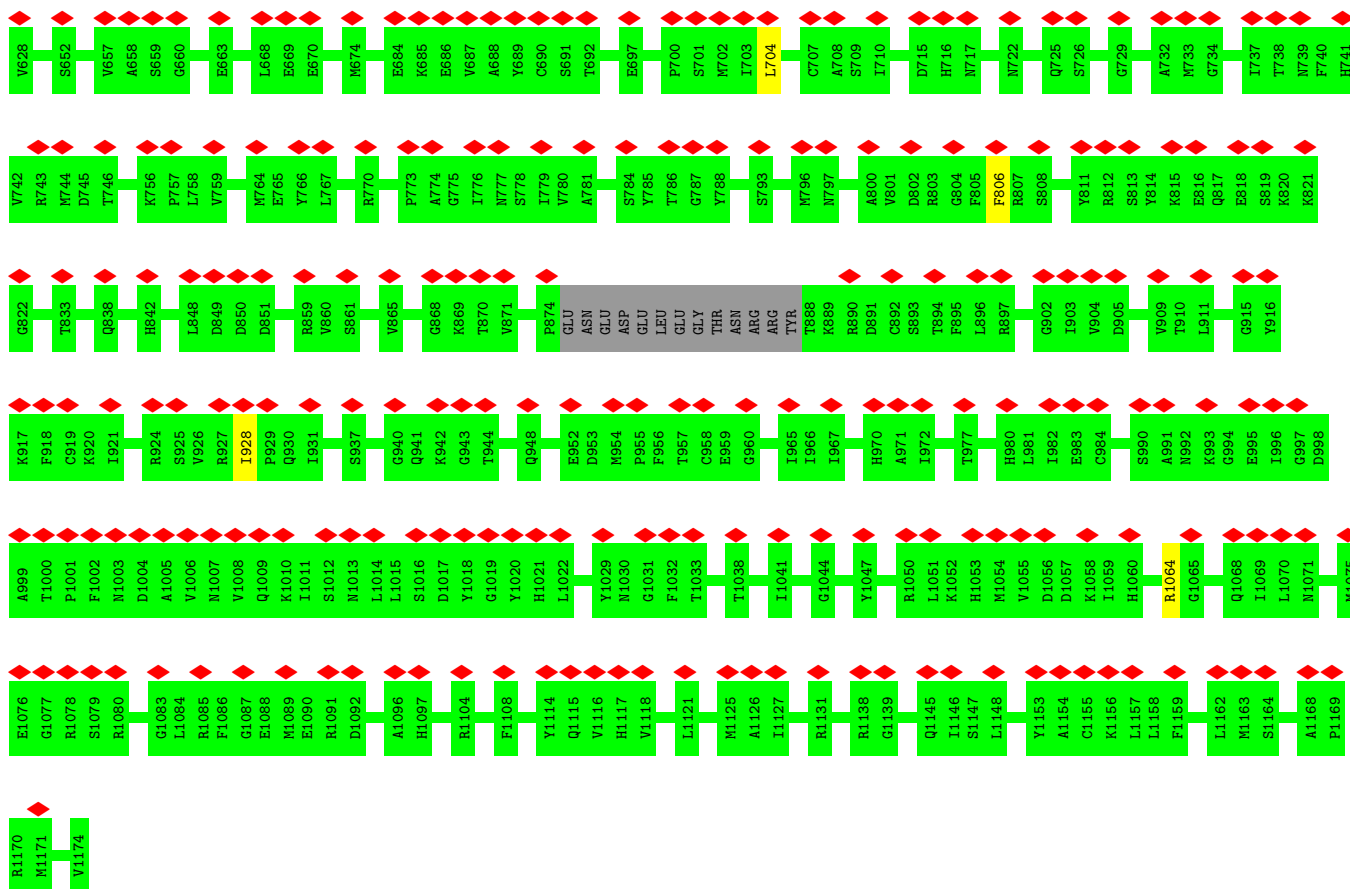


• Molecule 33: Transcription initiation factor TFIID subunit 13

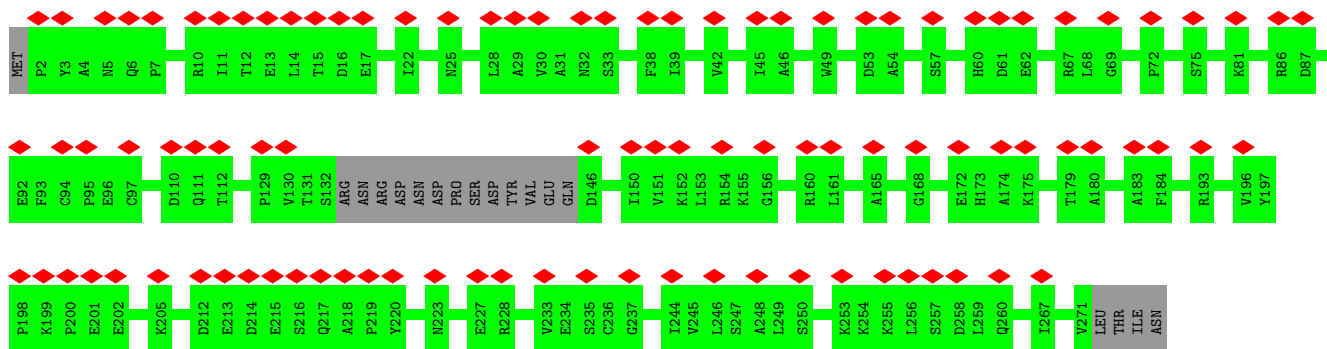


• Molecule 34: DNA-directed RNA polymerase II subunit RPB1

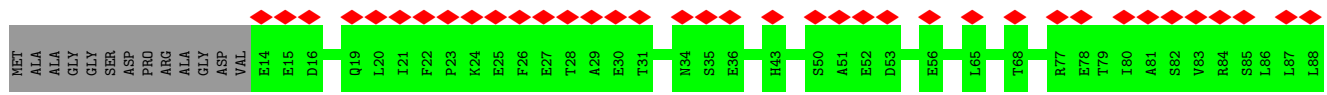
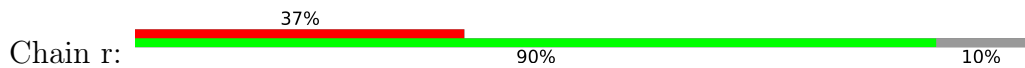




• Molecule 36: DNA-directed RNA polymerase II subunit RPB3

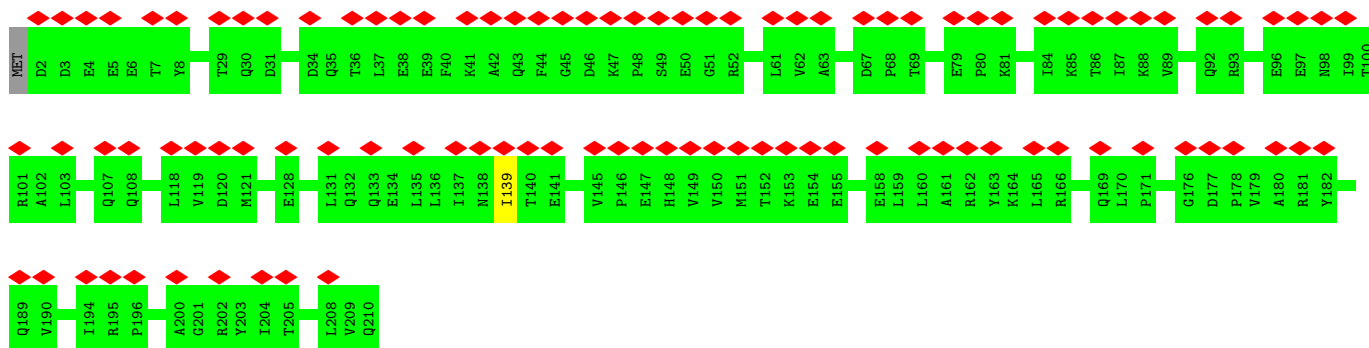


• Molecule 37: DNA-directed RNA polymerase II subunit RPB4

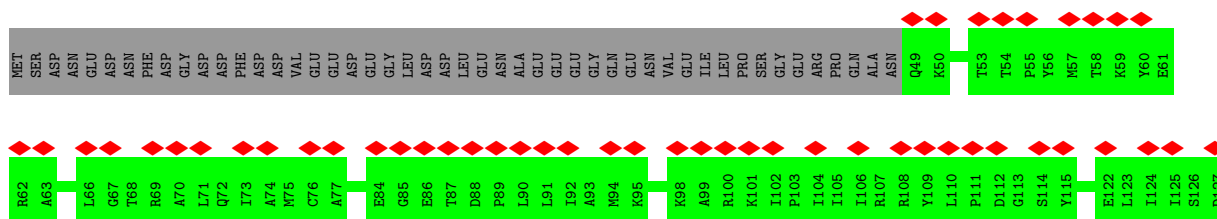
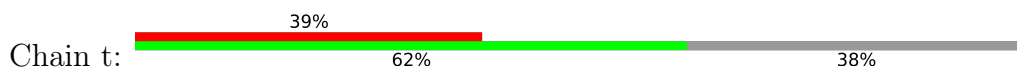




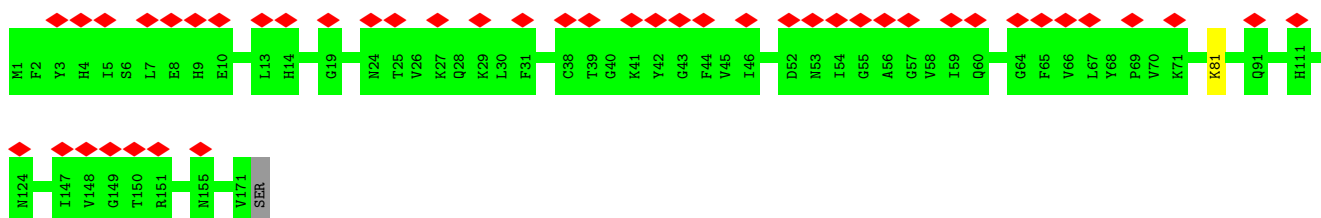
• Molecule 38: DNA-directed RNA polymerase II subunit E



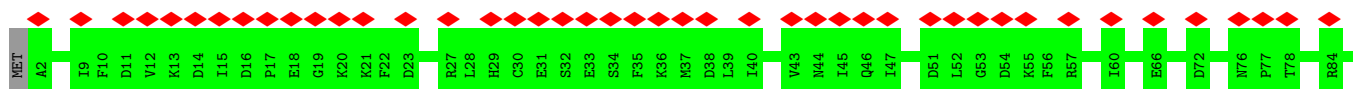
• Molecule 39: DNA-directed RNA polymerase II subunit F

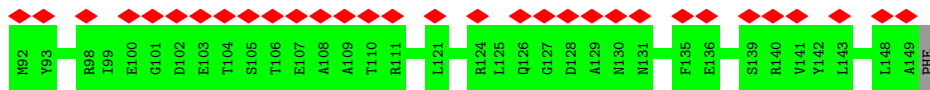


• Molecule 40: DNA-directed RNA polymerase II subunit RPB7

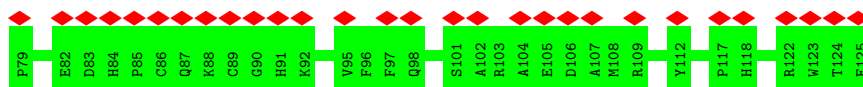
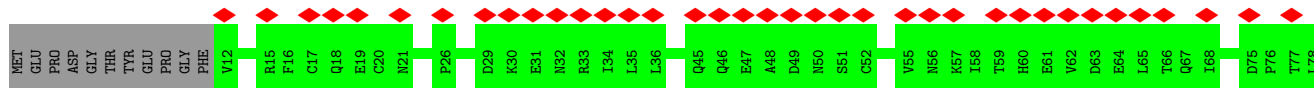
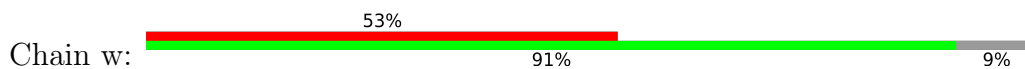


• Molecule 41: DNA-directed RNA polymerases I, II, and III subunit RPABC3

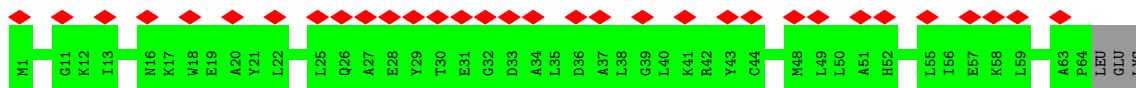




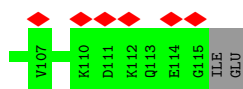
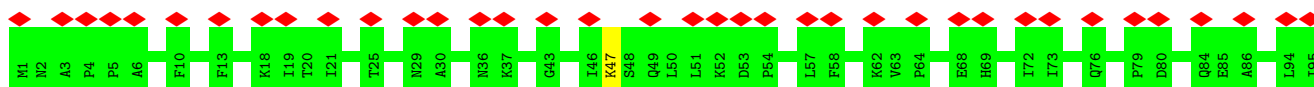
- Molecule 42: DNA-directed RNA polymerase II subunit RPB9



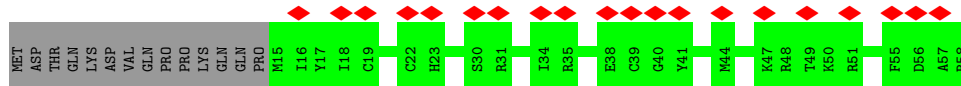
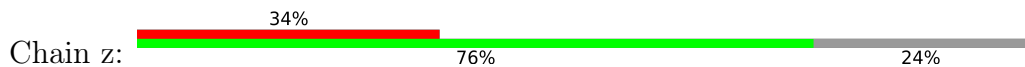
- Molecule 43: RPB10



- Molecule 44: RNA_pol_L_2 domain-containing protein



- Molecule 45: RPB12



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	92806	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.0	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	6.811	Depositor
Minimum map value	-4.382	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.084	Depositor
Recommended contour level	0.3	Depositor
Map size (\AA)	542.72, 542.72, 542.72	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.06, 1.06, 1.06	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, SF4, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	0	0.37	0/1965	0.53	0/2646
2	1	0.28	0/2210	0.42	0/2975
3	2	0.26	0/2624	0.42	0/3555
4	3	0.32	0/2103	0.49	0/2846
5	4	0.31	0/3262	0.46	1/4418 (0.0%)
6	5	0.32	0/433	0.51	0/585
7	6	0.29	0/4994	0.47	3/6745 (0.0%)
8	7	0.27	0/5875	0.43	0/7955
9	8	0.38	0/2434	0.55	0/3300
10	9	0.45	0/2342	0.58	1/3159 (0.0%)
11	A	0.50	0/4698	0.67	0/6345
12	B	0.46	0/7993	0.61	0/10836
13	D	0.41	0/1350	0.57	0/1805
13	d	0.39	0/1321	0.53	0/1772
14	E	0.39	0/4482	0.59	0/6069
14	e	0.44	0/4433	0.60	0/6004
15	F	0.49	0/3201	0.73	1/4347 (0.0%)
15	f	0.41	0/3140	0.63	0/4268
16	G	0.51	0/1190	0.62	0/1601
17	H	0.47	0/1673	0.72	3/2285 (0.1%)
18	I	0.28	0/981	0.47	0/1332
18	i	0.30	0/989	0.46	0/1343
19	J	0.57	0/736	0.69	0/998
19	j	0.54	0/775	0.63	0/1049
20	L	0.48	0/630	0.71	0/852
20	l	0.44	0/888	0.55	0/1194
21	O	0.28	0/816	0.46	0/1105
22	P	0.26	0/1448	0.42	0/1948
23	Q	0.26	0/945	0.43	0/1274
24	R	0.27	0/1983	0.43	0/2679
25	S	0.25	0/896	0.41	0/1213
26	T	0.26	0/1817	0.44	0/2445

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
27	U	0.35	0/1545	0.53	0/2075
28	V	0.28	0/1380	0.53	0/1854
29	X	0.22	0/1607	0.74	0/2481
30	Y	0.23	0/1565	0.73	0/2410
31	c	0.39	0/1035	0.54	0/1406
32	k	0.30	0/799	0.47	0/1070
33	m	0.59	0/733	0.64	0/977
34	o	0.34	5/11479 (0.0%)	0.50	14/15496 (0.1%)
35	p	0.35	4/9249 (0.0%)	0.46	3/12482 (0.0%)
36	q	0.25	0/2102	0.43	0/2857
37	r	0.26	0/1064	0.39	0/1428
38	s	0.28	1/1752 (0.1%)	0.50	3/2366 (0.1%)
39	t	0.25	0/646	0.39	0/871
40	u	0.28	0/1382	0.44	0/1874
41	v	0.25	0/1207	0.43	0/1628
42	w	0.28	0/949	0.46	0/1284
43	x	0.27	0/516	0.41	0/696
44	y	0.28	0/939	0.41	0/1271
45	z	0.28	0/378	0.41	0/500
All	All	0.37	10/114954 (0.0%)	0.54	29/155974 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	0	1
26	T	0	1
27	U	0	1
All	All	0	3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	p	704	LEU	C-N	13.21	1.56	1.33
34	o	1466	ALA	C-N	10.01	1.51	1.33
35	p	806	PHE	C-N	9.67	1.56	1.34
34	o	1424	THR	C-N	9.42	1.50	1.33
35	p	928	ILE	C-N	8.81	1.50	1.34
34	o	388	MET	C-N	7.29	1.50	1.34
35	p	534	VAL	C-N	6.82	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	o	449	HIS	C-N	6.18	1.48	1.34
38	s	139	ILE	C-N	5.98	1.47	1.34
34	o	1082	HIS	C-N	-5.03	1.24	1.34

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	s	139	ILE	O-C-N	-10.06	106.61	122.70
34	o	1082	HIS	O-C-N	-8.74	104.49	121.10
34	o	893	GLU	O-C-N	-8.54	109.04	122.70
17	H	156	PRO	N-CA-C	-8.46	90.10	112.10
34	o	1424	THR	CA-C-N	-7.29	101.61	116.20
17	H	157	HIS	CB-CA-C	-7.24	95.92	110.40
34	o	1424	THR	C-N-CA	-7.21	107.16	122.30
38	s	139	ILE	CA-C-N	7.10	132.82	117.20
34	o	1466	ALA	O-C-N	6.93	134.98	123.20
34	o	1082	HIS	CA-C-N	6.66	135.76	117.10
34	o	893	GLU	CA-C-N	6.60	131.73	117.20
34	o	1483	GLY	N-CA-C	6.45	129.23	113.10
5	4	412	PHE	CB-CA-C	6.39	123.19	110.40
17	H	128	PRO	CA-N-CD	-6.29	102.69	111.50
15	F	223	TYR	CB-CA-C	-6.24	97.92	110.40
7	6	581	TYR	CB-CA-C	-6.22	97.95	110.40
34	o	1424	THR	O-C-N	6.17	133.69	123.20
38	s	139	ILE	C-N-CA	5.97	136.63	121.70
34	o	1466	ALA	CA-C-N	-5.80	104.60	116.20
7	6	331	GLY	O-C-N	5.62	131.70	122.70
34	o	1466	ALA	C-N-CA	-5.54	110.67	122.30
7	6	616	ASP	C-N-CA	-5.46	108.06	121.70
35	p	388	TYR	C-N-CA	-5.38	111.00	122.30
34	o	893	GLU	C-N-CA	5.35	135.07	121.70
10	9	36	ALA	CB-CA-C	-5.26	102.21	110.10
34	o	1487	PRO	N-CA-CB	-5.21	96.87	102.60
34	o	1482	TYR	CA-CB-CG	5.18	123.23	113.40
35	p	199	LYS	CB-CA-C	-5.13	100.14	110.40
35	p	42	GLN	CB-CA-C	-5.01	100.39	110.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	126	GLN	Mainchain

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Mol	Chain	Res	Type	Group
26	T	144	GLN	Mainchain
27	U	78	VAL	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	232/309 (75%)	215 (93%)	17 (7%)	0	100	100
2	1	253/548 (46%)	245 (97%)	8 (3%)	0	100	100
3	2	325/395 (82%)	313 (96%)	12 (4%)	0	100	100
4	3	259/308 (84%)	251 (97%)	8 (3%)	0	100	100
5	4	384/462 (83%)	367 (96%)	17 (4%)	0	100	100
6	5	52/71 (73%)	47 (90%)	4 (8%)	1 (2%)	8	34
7	6	601/782 (77%)	576 (96%)	23 (4%)	2 (0%)	41	71
8	7	710/760 (93%)	683 (96%)	26 (4%)	1 (0%)	51	81
9	8	294/346 (85%)	277 (94%)	17 (6%)	0	100	100
10	9	277/323 (86%)	268 (97%)	9 (3%)	0	100	100
11	A	543/1872 (29%)	519 (96%)	23 (4%)	1 (0%)	47	77
12	B	959/1199 (80%)	911 (95%)	48 (5%)	0	100	100
13	D	154/1085 (14%)	148 (96%)	6 (4%)	0	100	100
13	d	154/1085 (14%)	149 (97%)	5 (3%)	0	100	100
14	E	541/800 (68%)	517 (96%)	23 (4%)	1 (0%)	47	77
14	e	531/800 (66%)	482 (91%)	48 (9%)	1 (0%)	47	77
15	F	408/677 (60%)	389 (95%)	18 (4%)	1 (0%)	47	77

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	f	399/677 (59%)	380 (95%)	19 (5%)	0	100	100
16	G	138/349 (40%)	135 (98%)	3 (2%)	0	100	100
17	H	207/310 (67%)	189 (91%)	14 (7%)	4 (2%)	8	34
18	I	118/264 (45%)	115 (98%)	3 (2%)	0	100	100
18	i	119/264 (45%)	115 (97%)	4 (3%)	0	100	100
19	J	86/218 (39%)	82 (95%)	4 (5%)	0	100	100
19	j	91/218 (42%)	85 (93%)	4 (4%)	2 (2%)	6	30
20	L	74/161 (46%)	72 (97%)	2 (3%)	0	100	100
20	l	105/161 (65%)	100 (95%)	5 (5%)	0	100	100
21	O	97/109 (89%)	97 (100%)	0	0	100	100
22	P	177/339 (52%)	175 (99%)	2 (1%)	0	100	100
23	Q	109/376 (29%)	102 (94%)	7 (6%)	0	100	100
24	R	248/316 (78%)	246 (99%)	2 (1%)	0	100	100
25	S	104/517 (20%)	104 (100%)	0	0	100	100
26	T	218/249 (88%)	211 (97%)	6 (3%)	1 (0%)	29	61
27	U	180/439 (41%)	152 (84%)	26 (14%)	2 (1%)	14	45
28	V	163/291 (56%)	139 (85%)	24 (15%)	0	100	100
31	c	125/929 (14%)	116 (93%)	9 (7%)	0	100	100
32	k	96/211 (46%)	91 (95%)	5 (5%)	0	100	100
33	m	85/124 (68%)	82 (96%)	3 (4%)	0	100	100
34	o	1413/1970 (72%)	1369 (97%)	44 (3%)	0	100	100
35	p	1129/1174 (96%)	1089 (96%)	40 (4%)	0	100	100
36	q	253/275 (92%)	241 (95%)	12 (5%)	0	100	100
37	r	126/142 (89%)	122 (97%)	4 (3%)	0	100	100
38	s	207/210 (99%)	203 (98%)	4 (2%)	0	100	100
39	t	77/127 (61%)	76 (99%)	1 (1%)	0	100	100
40	u	169/172 (98%)	166 (98%)	3 (2%)	0	100	100
41	v	146/150 (97%)	143 (98%)	3 (2%)	0	100	100
42	w	112/125 (90%)	103 (92%)	9 (8%)	0	100	100
43	x	62/67 (92%)	61 (98%)	1 (2%)	0	100	100
44	y	113/117 (97%)	112 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	z	42/58 (72%)	41 (98%)	1 (2%)	0	100	100
All	All	13465/22931 (59%)	12871 (96%)	577 (4%)	17 (0%)	54	81

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	5	48	GLU
14	E	523	VAL
17	H	128	PRO
14	e	522	ASP
19	j	124	GLU
7	6	584	THR
11	A	502	LEU
15	F	411	VAL
17	H	129	VAL
17	H	157	HIS
26	T	147	LYS
19	j	177	LYS
17	H	141	PRO
27	U	163	GLU
8	7	726	GLN
27	U	78	VAL
7	6	57	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	216/283 (76%)	211 (98%)	5 (2%)	50	73
2	1	241/484 (50%)	241 (100%)	0	100	100
3	2	295/352 (84%)	294 (100%)	1 (0%)	92	96
4	3	234/272 (86%)	229 (98%)	5 (2%)	53	75
5	4	346/399 (87%)	338 (98%)	8 (2%)	50	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	5	48/64 (75%)	48 (100%)	0	100	100
7	6	536/688 (78%)	531 (99%)	5 (1%)	78	87
8	7	624/664 (94%)	622 (100%)	2 (0%)	92	96
9	8	259/299 (87%)	257 (99%)	2 (1%)	81	89
10	9	256/296 (86%)	254 (99%)	2 (1%)	81	89
11	A	496/1665 (30%)	456 (92%)	40 (8%)	11	36
12	B	876/1083 (81%)	859 (98%)	17 (2%)	57	77
13	D	145/815 (18%)	139 (96%)	6 (4%)	30	61
13	d	146/815 (18%)	145 (99%)	1 (1%)	84	90
14	E	480/657 (73%)	466 (97%)	14 (3%)	42	69
14	e	475/657 (72%)	463 (98%)	12 (2%)	47	72
15	F	328/574 (57%)	305 (93%)	23 (7%)	15	43
15	f	322/574 (56%)	314 (98%)	8 (2%)	47	72
16	G	132/322 (41%)	124 (94%)	8 (6%)	18	48
17	H	181/270 (67%)	172 (95%)	9 (5%)	24	55
18	I	106/235 (45%)	106 (100%)	0	100	100
18	i	107/235 (46%)	107 (100%)	0	100	100
19	J	79/154 (51%)	72 (91%)	7 (9%)	9	32
19	j	83/154 (54%)	82 (99%)	1 (1%)	71	83
20	L	71/141 (50%)	66 (93%)	5 (7%)	15	43
20	l	98/141 (70%)	97 (99%)	1 (1%)	76	86
21	O	90/98 (92%)	88 (98%)	2 (2%)	52	74
22	P	154/293 (53%)	154 (100%)	0	100	100
23	Q	105/324 (32%)	105 (100%)	0	100	100
24	R	215/268 (80%)	214 (100%)	1 (0%)	88	93
25	S	93/448 (21%)	92 (99%)	1 (1%)	73	85
26	T	196/218 (90%)	193 (98%)	3 (2%)	65	81
27	U	167/373 (45%)	162 (97%)	5 (3%)	41	68
28	V	150/261 (58%)	150 (100%)	0	100	100
31	c	113/833 (14%)	111 (98%)	2 (2%)	59	78
32	k	87/182 (48%)	87 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	m	80/106 (76%)	73 (91%)	7 (9%)	10	33
34	o	1254/1748 (72%)	1247 (99%)	7 (1%)	86	91
35	p	993/1027 (97%)	990 (100%)	3 (0%)	92	96
36	q	234/252 (93%)	234 (100%)	0	100	100
37	r	118/126 (94%)	118 (100%)	0	100	100
38	s	191/192 (100%)	191 (100%)	0	100	100
39	t	69/111 (62%)	69 (100%)	0	100	100
40	u	152/153 (99%)	151 (99%)	1 (1%)	84	90
41	v	129/131 (98%)	129 (100%)	0	100	100
42	w	103/112 (92%)	103 (100%)	0	100	100
43	x	53/56 (95%)	53 (100%)	0	100	100
44	y	104/106 (98%)	103 (99%)	1 (1%)	76	86
45	z	41/55 (74%)	41 (100%)	0	100	100
All	All	12071/19766 (61%)	11856 (98%)	215 (2%)	61	78

All (215) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	10	LYS
1	0	11	THR
1	0	28	HIS
1	0	41	ARG
1	0	53	LEU
3	2	343	ARG
4	3	100	LYS
4	3	132	LEU
4	3	137	LEU
4	3	257	CYS
4	3	258	HIS
5	4	33	ARG
5	4	57	MET
5	4	401	LEU
5	4	404	THR
5	4	407	VAL
5	4	409	TYR
5	4	432	VAL
5	4	456	LYS

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Mol	Chain	Res	Type
7	6	198	ARG
7	6	266	GLN
7	6	297	PHE
7	6	633	ARG
7	6	692	LYS
8	7	114	ASN
8	7	563	ARG
9	8	10	LYS
9	8	164	SER
10	9	28	ARG
10	9	32	CYS
11	A	337	ARG
11	A	338	VAL
11	A	353	LEU
11	A	395	ASP
11	A	397	LEU
11	A	400	GLU
11	A	404	MET
11	A	408	LEU
11	A	415	ILE
11	A	416	TRP
11	A	417	ASP
11	A	419	GLU
11	A	468	PHE
11	A	470	ILE
11	A	475	LEU
11	A	481	GLU
11	A	491	MET
11	A	499	VAL
11	A	500	LEU
11	A	501	THR
11	A	502	LEU
11	A	505	ASN
11	A	511	LEU
11	A	639	LEU
11	A	661	GLU
11	A	667	THR
11	A	711	ASP
11	A	727	THR
11	A	730	PHE
11	A	821	ARG
11	A	828	GLU

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Mol	Chain	Res	Type
11	A	943	LYS
11	A	970	ASN
11	A	1052	ARG
11	A	1058	HIS
11	A	1059	GLN
11	A	1062	TYR
11	A	1073	GLN
11	A	1165	LEU
11	A	1203	GLU
12	B	21	GLU
12	B	24	ARG
12	B	71	ARG
12	B	140	GLU
12	B	184	ASN
12	B	225	TYR
12	B	262	MET
12	B	266	THR
12	B	293	GLU
12	B	431	LEU
12	B	488	PHE
12	B	559	LYS
12	B	603	LYS
12	B	638	ARG
12	B	640	VAL
12	B	771	VAL
12	B	818	THR
13	D	948	GLU
13	D	952	GLN
13	D	957	ARG
13	D	966	LEU
13	D	1006	LEU
13	D	1009	LEU
14	E	258	ASN
14	E	268	HIS
14	E	270	ASP
14	E	274	TYR
14	E	278	ASP
14	E	280	ARG
14	E	326	ASN
14	E	327	ASN
14	E	519	GLU
14	E	522	ASP

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Mol	Chain	Res	Type
14	E	593	PHE
14	E	761	LEU
14	E	774	MET
14	E	775	THR
15	F	86	PHE
15	F	91	PHE
15	F	94	PHE
15	F	218	VAL
15	F	219	GLU
15	F	221	GLN
15	F	223	TYR
15	F	224	TYR
15	F	243	LEU
15	F	258	ARG
15	F	261	THR
15	F	271	VAL
15	F	280	ILE
15	F	301	VAL
15	F	317	LEU
15	F	326	HIS
15	F	332	PHE
15	F	340	ILE
15	F	348	THR
15	F	354	ARG
15	F	368	THR
15	F	397	GLN
15	F	427	LEU
16	G	41	ASP
16	G	81	ASP
16	G	143	VAL
16	G	147	ARG
16	G	153	LYS
16	G	181	TRP
16	G	182	GLU
16	G	183	ILE
17	H	27	ASP
17	H	33	ARG
17	H	36	THR
17	H	128	PRO
17	H	132	LYS
17	H	153	PHE
17	H	156	PRO

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Mol	Chain	Res	Type
17	H	157	HIS
17	H	160	ILE
19	J	116	LEU
19	J	123	LEU
19	J	156	SER
19	J	164	SER
19	J	174	CYS
19	J	177	LYS
19	J	192	LYS
20	L	79	ASP
20	L	104	ARG
20	L	108	SER
20	L	113	VAL
20	L	114	LYS
21	O	51	ARG
21	O	82	ARG
24	R	53	ARG
25	S	44	GLN
26	T	145	LEU
26	T	147	LYS
26	T	230	LYS
27	U	124	ARG
27	U	144	LEU
27	U	145	PHE
27	U	164	ASP
27	U	168	MET
31	c	24	ASP
31	c	106	VAL
13	d	951	ASP
14	e	243	LEU
14	e	258	ASN
14	e	268	HIS
14	e	270	ASP
14	e	277	ASP
14	e	282	LEU
14	e	365	ARG
14	e	436	ASP
14	e	438	LEU
14	e	512	ASP
14	e	516	ILE
14	e	663	ARG
15	f	253	TYR

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Mol	Chain	Res	Type
15	f	261	THR
15	f	272	VAL
15	f	322	ASP
15	f	323	VAL
15	f	326	HIS
15	f	356	THR
15	f	421	ASP
19	j	114	THR
20	l	114	LYS
33	m	31	LEU
33	m	55	ASP
33	m	58	GLU
33	m	77	ARG
33	m	84	GLU
33	m	90	ILE
33	m	91	ARG
34	o	61	ARG
34	o	1289	GLU
34	o	1291	ASN
34	o	1299	GLN
34	o	1482	TYR
34	o	1486	ILE
34	o	1487	PRO
35	p	39	LEU
35	p	41	ARG
35	p	1064	ARG
40	u	81	LYS
44	y	47	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (107) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	24	ASN
1	0	45	ASN
1	0	83	ASN
1	0	136	ASN
1	0	307	GLN
3	2	227	HIS
3	2	387	HIS
4	3	240	GLN
5	4	458	GLN
5	4	460	HIS

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Mol	Chain	Res	Type
6	5	42	HIS
7	6	112	HIS
7	6	499	ASN
7	6	638	GLN
8	7	560	ASN
9	8	130	GLN
9	8	288	GLN
10	9	7	GLN
10	9	18	GLN
10	9	247	GLN
11	A	401	ASN
11	A	472	ASN
11	A	489	GLN
11	A	590	GLN
11	A	860	ASN
11	A	896	GLN
12	B	30	HIS
12	B	137	HIS
12	B	176	HIS
12	B	183	GLN
12	B	184	ASN
12	B	235	HIS
12	B	348	GLN
12	B	432	HIS
12	B	439	HIS
12	B	450	GLN
12	B	509	ASN
12	B	750	GLN
12	B	813	ASN
12	B	882	HIS
12	B	908	GLN
12	B	916	ASN
13	D	875	GLN
13	D	936	GLN
13	D	956	GLN
13	D	1001	GLN
13	D	1053	GLN
14	E	254	ASN
14	E	256	HIS
14	E	258	ASN
14	E	268	HIS
14	E	327	ASN

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Mol	Chain	Res	Type
14	E	351	GLN
14	E	616	HIS
14	E	640	ASN
14	E	758	HIS
14	E	800	GLN
15	F	59	HIS
15	F	79	ASN
15	F	89	GLN
15	F	119	ASN
15	F	244	GLN
15	F	270	ASN
15	F	273	GLN
15	F	275	ASN
16	G	48	HIS
17	H	145	HIS
18	I	21	GLN
18	I	38	GLN
18	I	98	GLN
19	J	210	ASN
20	L	117	GLN
21	O	4	GLN
22	P	189	ASN
26	T	144	GLN
27	U	64	ASN
27	U	143	GLN
27	U	183	GLN
28	V	83	ASN
28	V	90	GLN
28	V	117	GLN
28	V	157	GLN
28	V	160	GLN
13	d	912	ASN
13	d	943	GLN
13	d	1069	ASN
14	e	246	HIS
14	e	294	ASN
14	e	336	HIS
14	e	424	GLN
14	e	616	HIS
15	f	325	ASN
18	i	81	GLN
19	j	160	GLN

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Mol	Chain	Res	Type
19	j	173	HIS
32	k	186	HIS
20	l	73	ASN
20	l	105	HIS
20	l	119	HIS
33	m	70	HIS
33	m	107	ASN
34	o	671	ASN
34	o	825	ASN
34	o	1291	ASN
34	o	1445	HIS
35	p	42	GLN
44	y	89	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 18 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
47	SF4	7	1000	8	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
47	SF4	7	1000	8	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

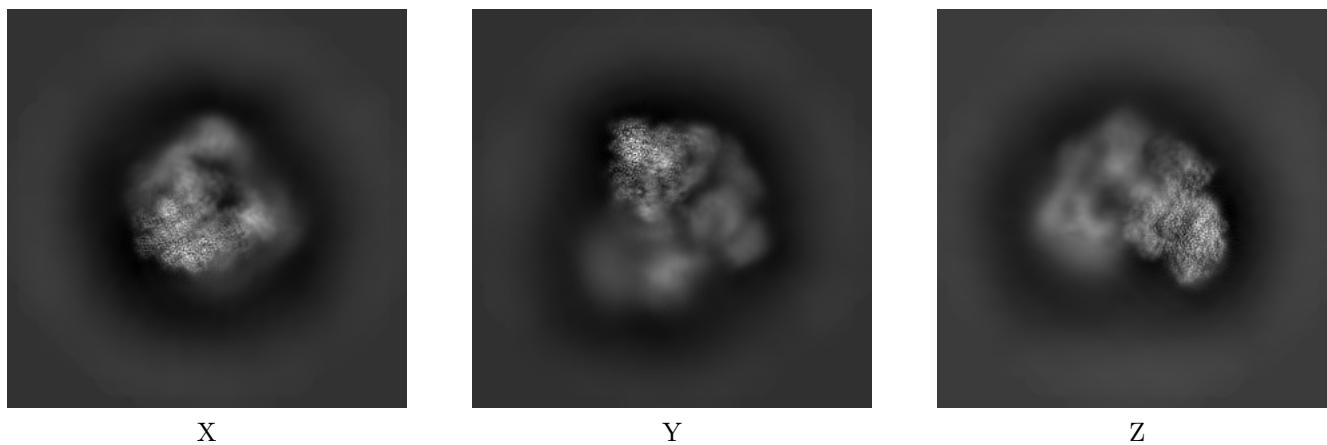
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31111. 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](#)

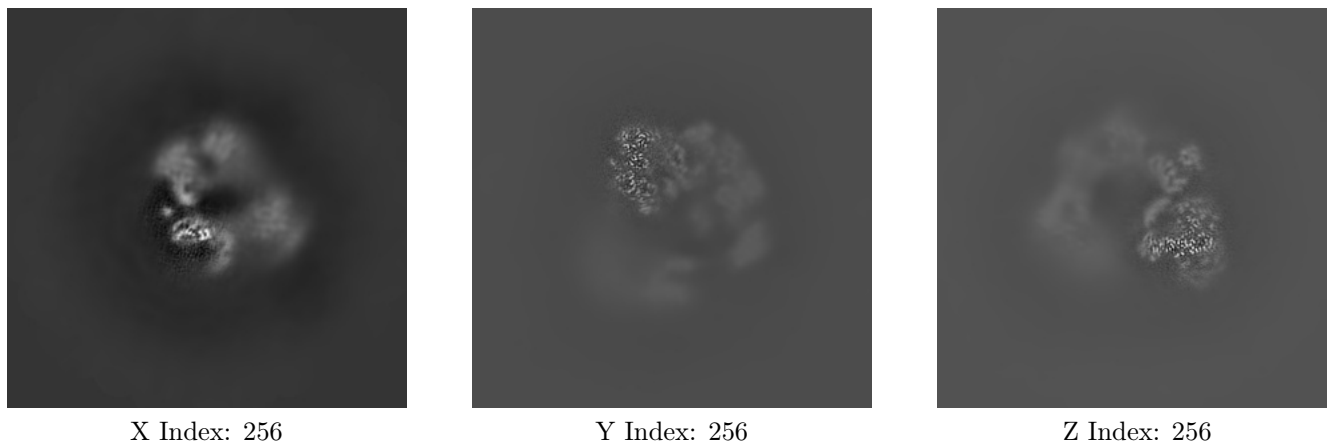
6.1.1 Primary map



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

6.2 Central slices [i](#)

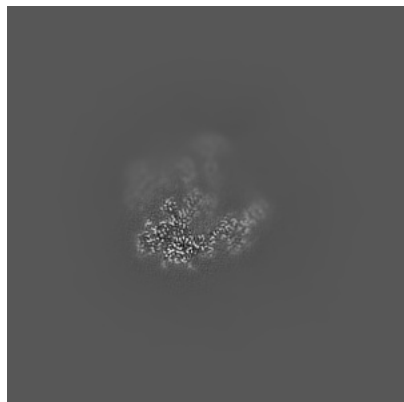
6.2.1 Primary map



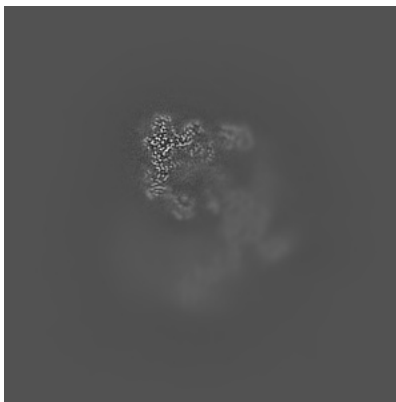
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

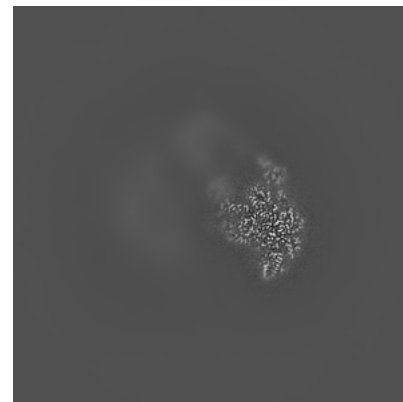
6.3.1 Primary map



X Index: 331



Y Index: 229

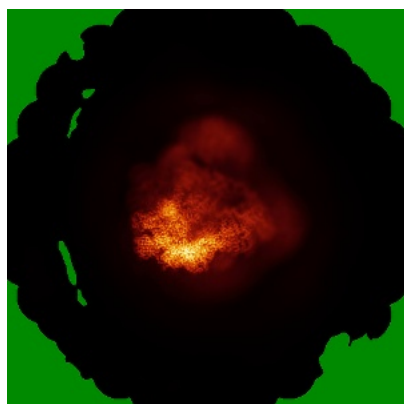


Z Index: 206

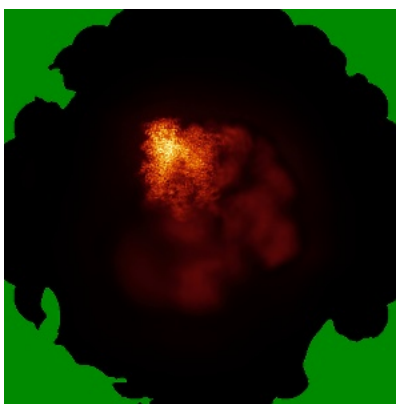
The images above show the largest variance slices of the map in three orthogonal directions.

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

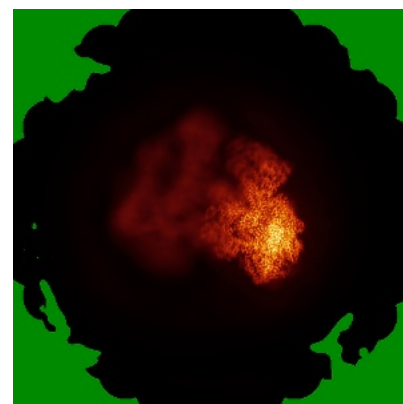
6.4.1 Primary map



X



Y

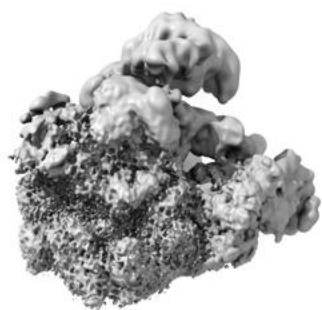


Z

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](#)

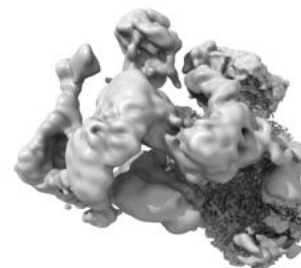
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

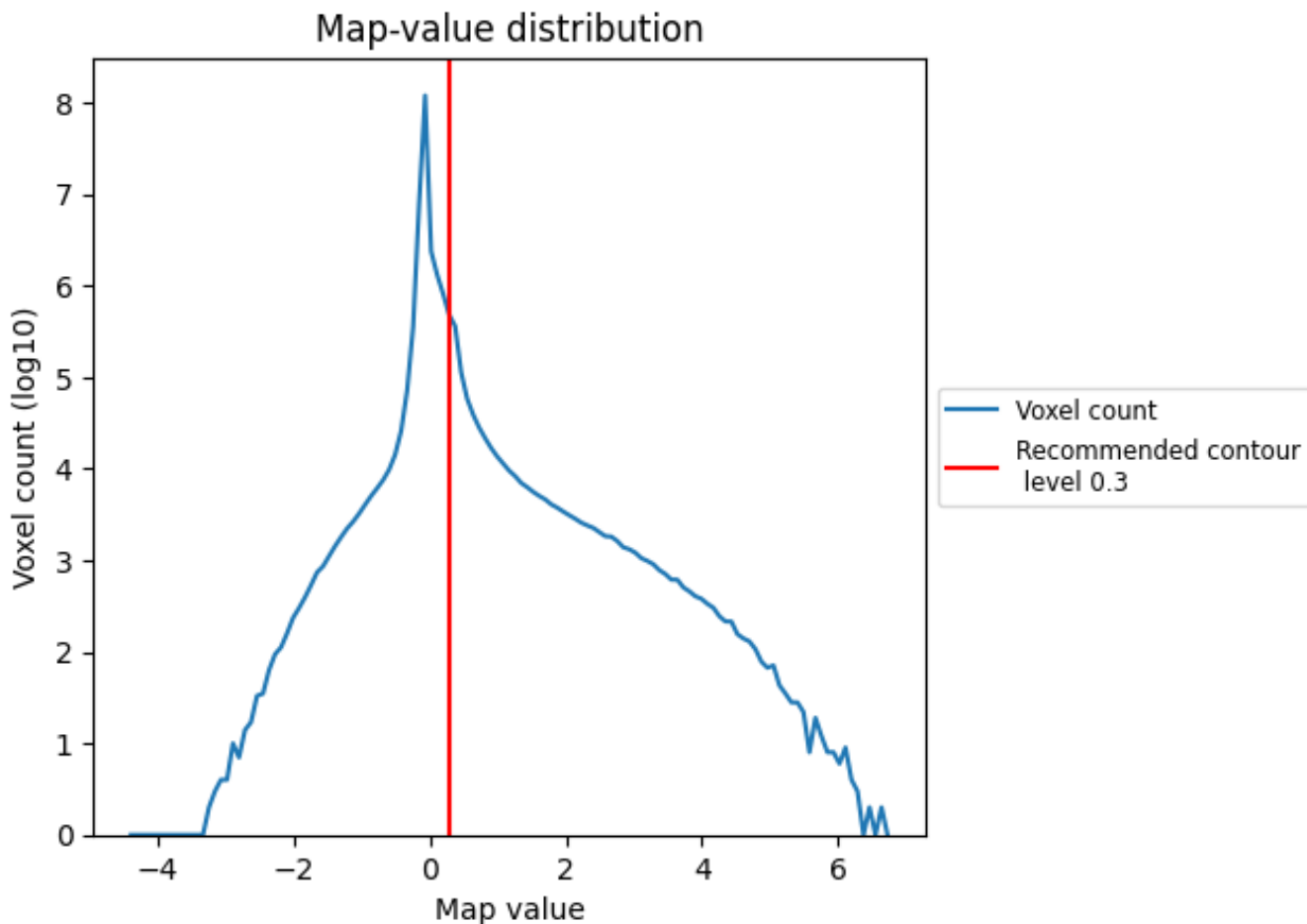
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

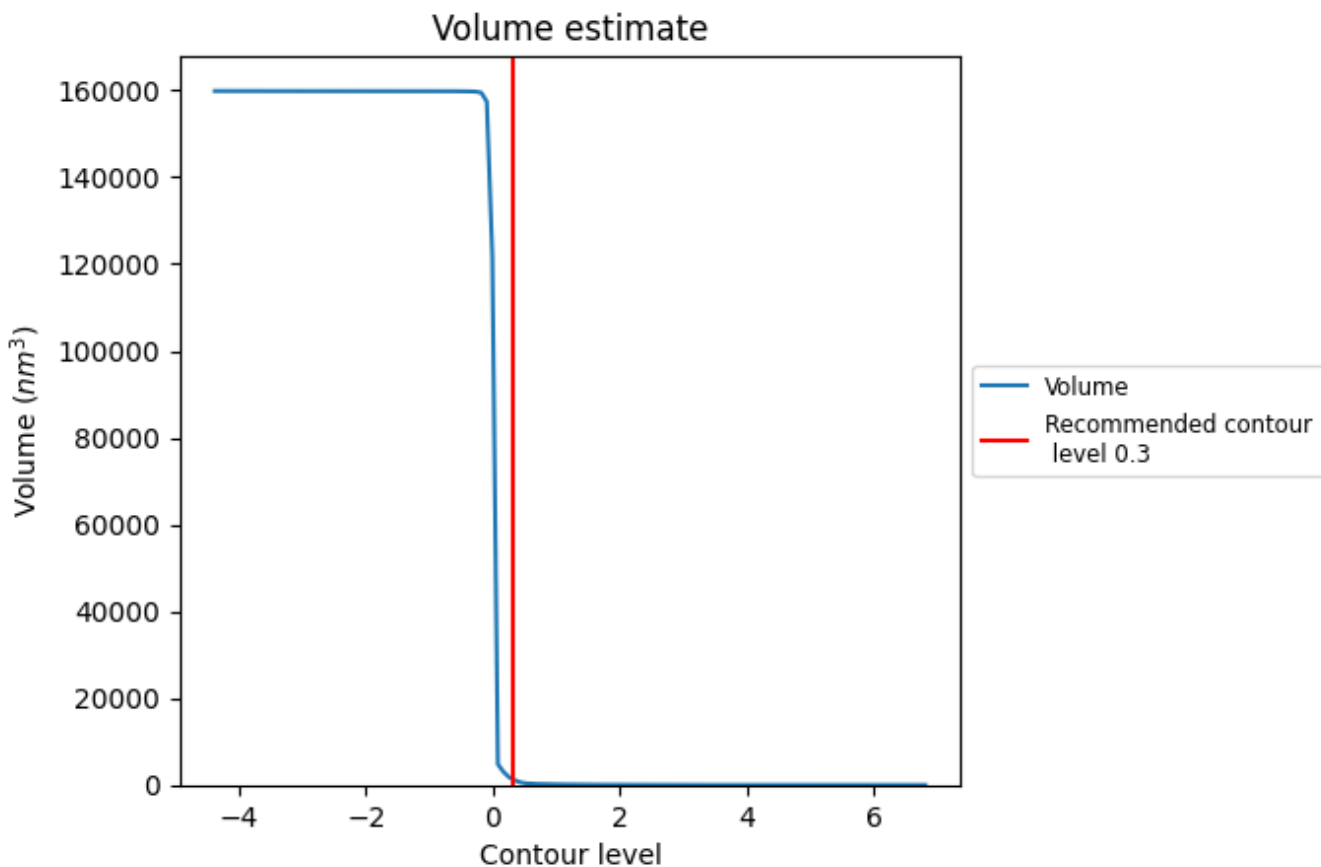
This section contains the results of statistical analysis of the map.

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.

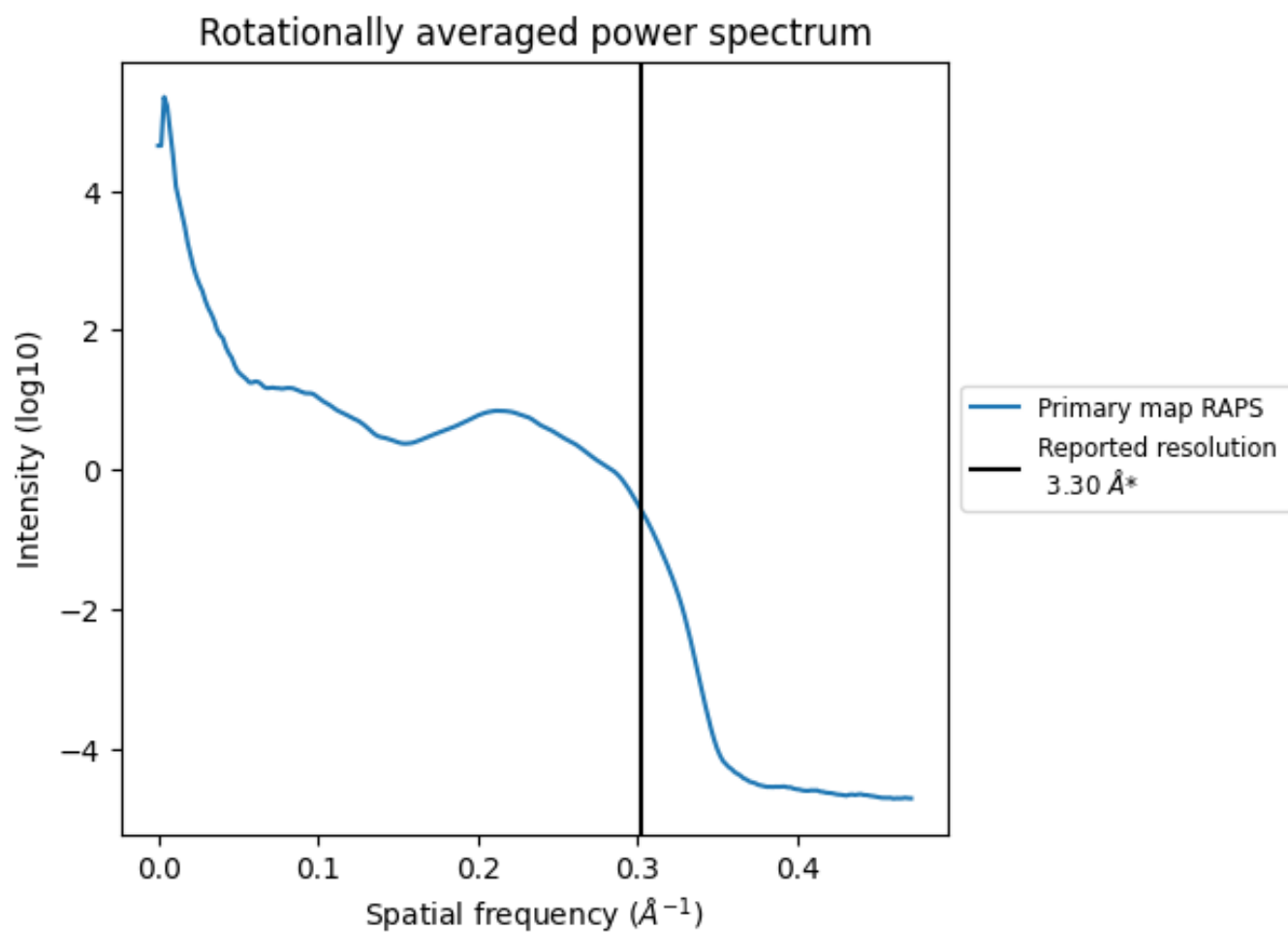
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1427 nm^3 ; this corresponds to an approximate mass of 1289 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum i



*Reported resolution corresponds to spatial frequency of 0.303\AA^{-1}

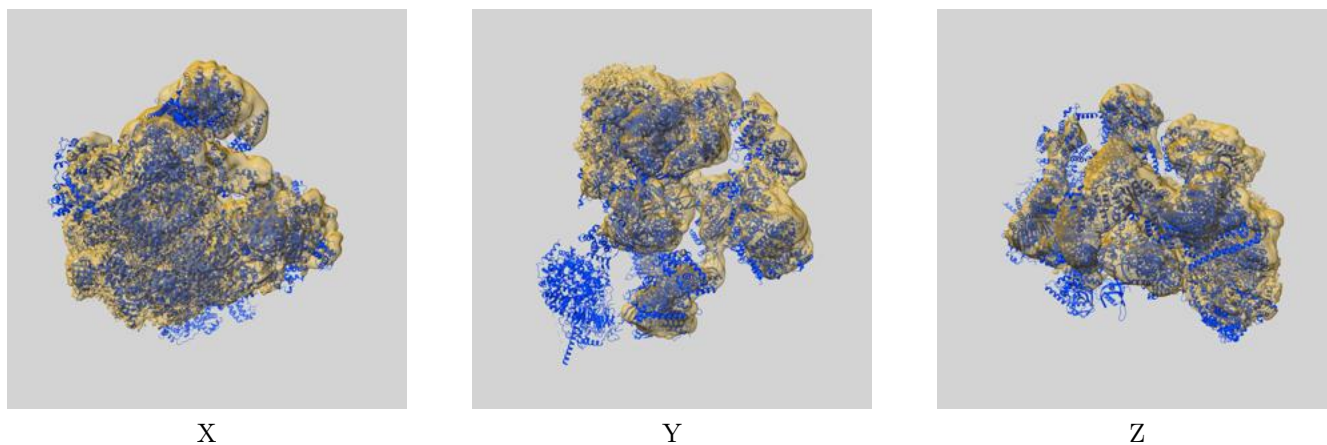
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

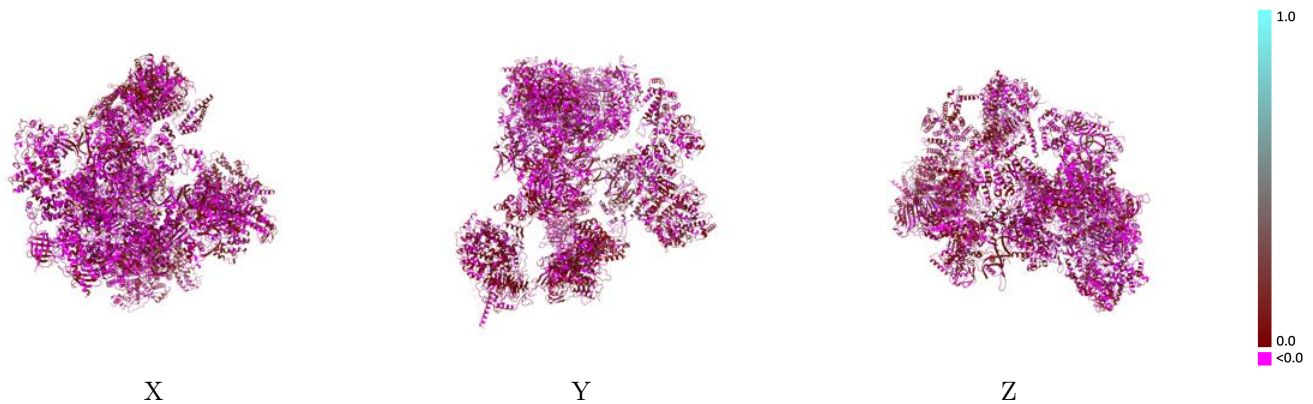
This section contains information regarding the fit between EMDB map EMD-31111 and PDB model 7EGB. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay [i](#)



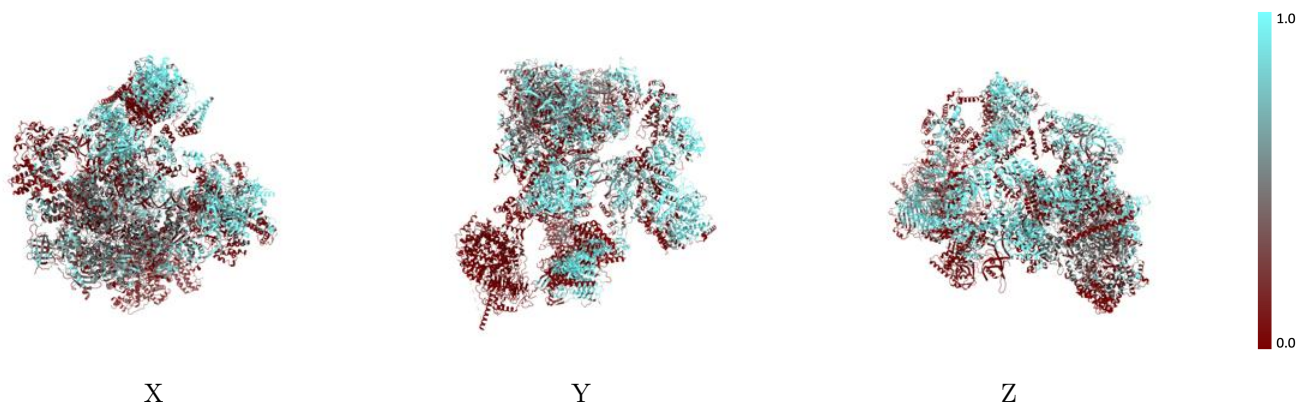
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



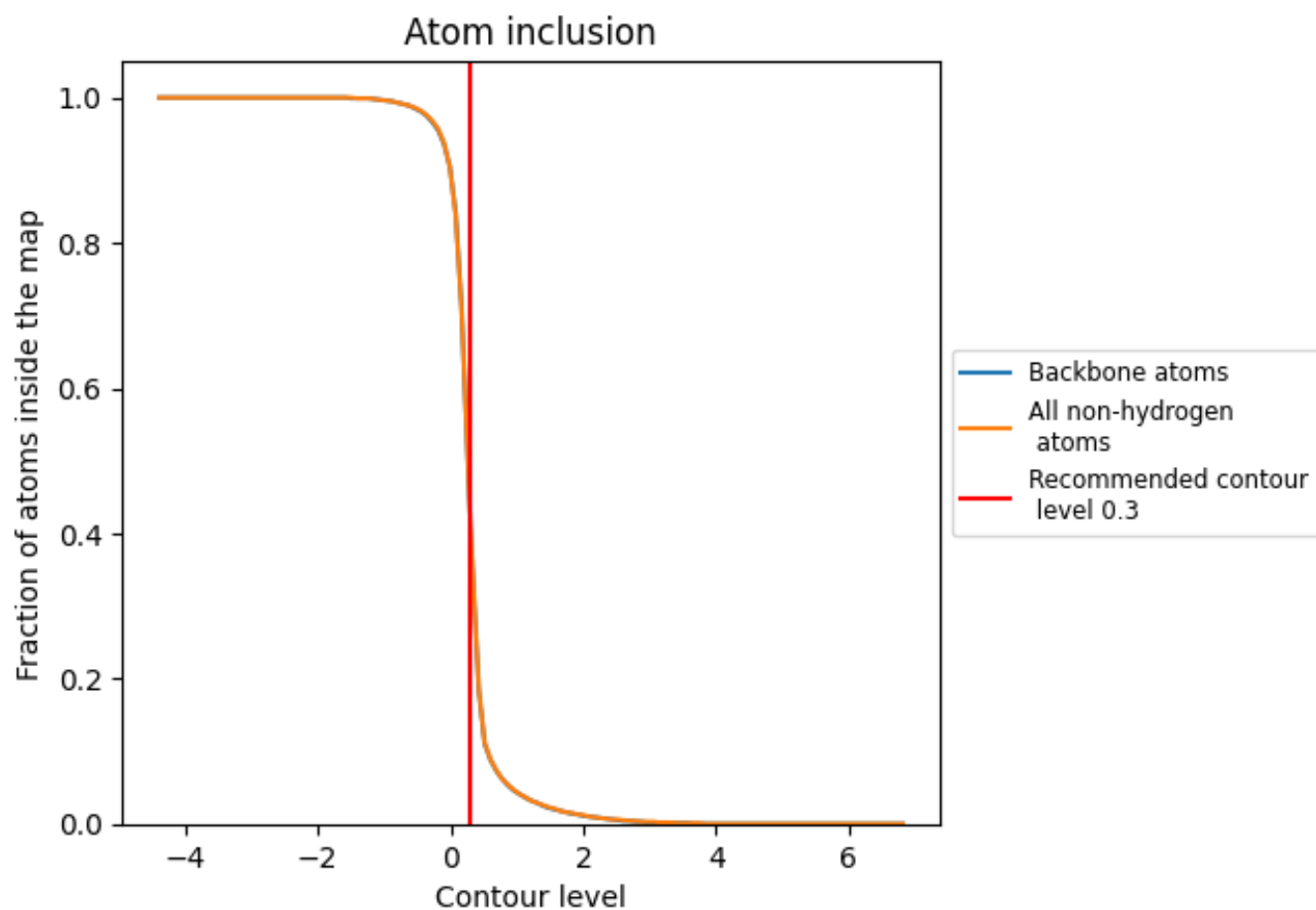
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.3).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 41% of all backbone atoms, 41% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4140	 0.0120
0	 0.0890	 -0.0020
1	 0.4320	 0.0430
2	 0.5810	 0.0260
3	 0.7830	 0.0500
4	 0.5720	 0.0510
5	 0.3110	 -0.0010
6	 0.6730	 0.0420
7	 0.5860	 0.0310
8	 0.1610	 0.0120
9	 0.2780	 0.0070
A	 0.1510	 0.0250
B	 0.6230	 0.0280
D	 0.5050	 0.0280
E	 0.4020	 0.0310
F	 0.3590	 0.0460
G	 0.0300	 0.0170
H	 0.6440	 0.0390
I	 0.4490	 -0.0180
J	 0.8020	 0.0260
L	 0.3170	 -0.0230
O	 0.5370	 -0.0150
P	 0.7170	 -0.0160
Q	 0.5570	 0.0160
R	 0.4940	 -0.0010
S	 0.5220	 0.0290
T	 0.4100	 0.0270
U	 0.4650	 -0.0380
V	 0.6180	 0.0190
X	 0.4470	 0.0500
Y	 0.4070	 0.0480
c	 0.0000	 0.0340
d	 0.0000	 0.0100
e	 0.0000	 0.0340
f	 0.2680	 0.0380



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Chain	Atom inclusion	Q-score
i	 0.0000	 0.0300
j	 0.0000	 0.0070
k	 0.0000	 0.0130
l	 0.0000	 0.0230
m	 0.0000	 0.0150
o	 0.4030	 -0.0240
p	 0.4300	 -0.0300
q	 0.4700	 0.0000
r	 0.5270	 -0.0370
s	 0.4330	 -0.0260
t	 0.3740	 -0.0310
u	 0.6640	 -0.0100
v	 0.4060	 -0.0110
w	 0.3780	 -0.0350
x	 0.4220	 0.0140
y	 0.4850	 -0.0190
z	 0.4710	 0.0040