



wwPDB EM Validation Summary Report ⓘ

Nov 4, 2024 – 05:23 AM JST

PDB ID : 7EG8
EMDB ID : EMD-31108
Title : TFIID-based core PIC on PUMA promoter
Authors : Chen, X.; Qi, Y.; Hou, H.; Wang, X.; Wu, Z.; Li, J.; Xu, Y.
Deposited on : 2021-03-24
Resolution : 7.40 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:

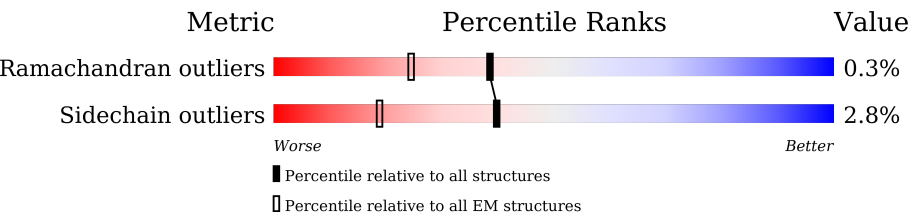
EMDB validation analysis : 0.0.1.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 7.40 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	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	1872	
2	B	1199	
3	D	1085	
3	d	1085	
4	E	800	
4	e	800	
5	F	677	
5	f	677	
6	G	349	

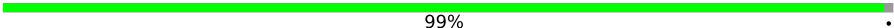

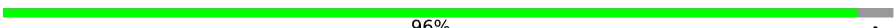
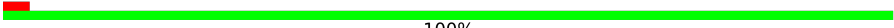

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Mol	Chain	Length	Quality of chain
7	H	310	
8	I	264	
8	i	264	
9	J	218	
9	j	218	
10	L	161	
10	l	161	
11	O	109	
12	P	339	
13	Q	376	
14	R	316	
15	S	517	
16	T	249	
17	X	85	
18	Y	85	
19	c	929	
20	k	211	
21	m	124	
22	o	1970	
23	p	1174	
24	q	275	
25	r	142	
26	s	210	
27	t	127	
28	u	172	

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Mol	Chain	Length	Quality of chain
29	v	150	 99%.
30	w	125	 91%9%
31	x	67	 96%.
32	y	117	 100%
33	z	58	 76%24%

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 82798 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 Transcription initiation factor TFIID subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	602	Total	C	N	O	S	0	0
			4927	3142	858	899	28		

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

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

- Molecule 3 is a protein called Transcription initiation factor TFIID subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	164	Total	C	N	O	S	0	0
			1366	851	256	255	4		
3	d	158	Total	C	N	O	S	0	0
			1307	814	238	252	3		

- Molecule 4 is a protein called Transcription initiation factor TFIID subunit 5.

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

- Molecule 5 is a protein called Transcription initiation factor TFIID subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	404	Total	C	N	O	S	0	0
			3081	1954	537	572	18		
5	f	403	Total	C	N	O	S	0	0
			3081	1954	533	576	18		

- Molecule 6 is a protein called Transcription initiation factor TFIID subunit 7.

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

- Molecule 7 is a protein called Transcription initiation factor TFIID subunit 8.

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

- Molecule 8 is a protein called Transcription initiation factor TFIID subunit 9.

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

- Molecule 9 is a protein called Transcription initiation factor TFIID subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	89	Total	C	N	O	S	0	0
			709	457	114	134	4		
9	j	95	Total	C	N	O	S	0	0
			759	488	124	143	4		

- Molecule 10 is a protein called Transcription initiation factor TFIID subunit 12.

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

- Molecule 11 is a protein called Transcription initiation factor IIA subunit 2.

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

- Molecule 12 is a protein called TATA-box-binding protein.

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

- Molecule 13 is a protein called Transcription initiation factor IIA subunit 1.

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

- Molecule 14 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	R	251	Total	C	N	O	S	0	0
			1938	1214	344	363	17		

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

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

- Molecule 16 is a protein called General transcription factor IIF subunit 2.

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

- Molecule 17 is a DNA chain called DNA (85-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
17	X	85	Total	C	N	O	P	0	0
			1751	829	329	508	85		

- Molecule 18 is a DNA chain called DNA (85-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Y	85	Total	C	N	O	P	0	0
			1734	824	313	512	85		

- Molecule 19 is a protein called Transcription initiation factor TFIID subunit 3.

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

- Molecule 20 is a protein called Transcription initiation factor TFIID subunit 11.

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

- Molecule 21 is a protein called Transcription initiation factor TFIID subunit 13.

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

- Molecule 22 is a protein called RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	o	1427	Total	C	N	O	S	0	0
			11308	7114	2023	2099	72		

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

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

- Molecule 24 is a protein called DNA-directed RNA polymerase II subunit RPB3.

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

- Molecule 25 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	r	128	Total	C	N	O	S	0	0
			1005	632	172	197	4		

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

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

- Molecule 27 is a protein called DNA-directed RNA polymerase II subunit F.

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

- Molecule 28 is a protein called DNA-directed RNA polymerase II subunit RPB7.

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

- Molecule 29 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

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

- Molecule 30 is a protein called DNA-directed RNA polymerase II subunit RPB9.

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

- Molecule 31 is a protein called RPB10.

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

- Molecule 32 is a protein called RNA_pol_L_2 domain-containing protein.

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

- Molecule 33 is a protein called RPB12.

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

- Molecule 34 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

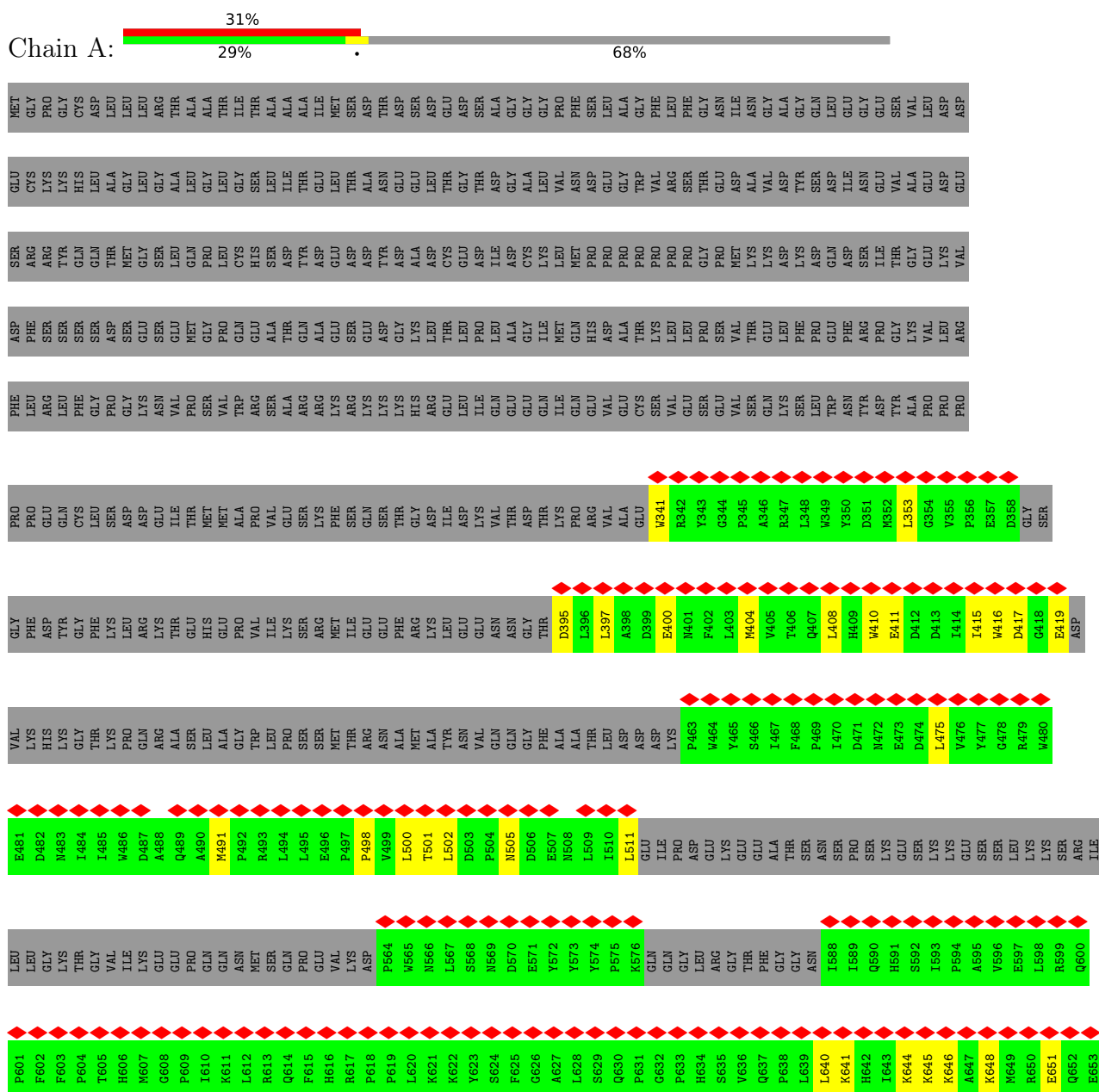
- Molecule 35 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

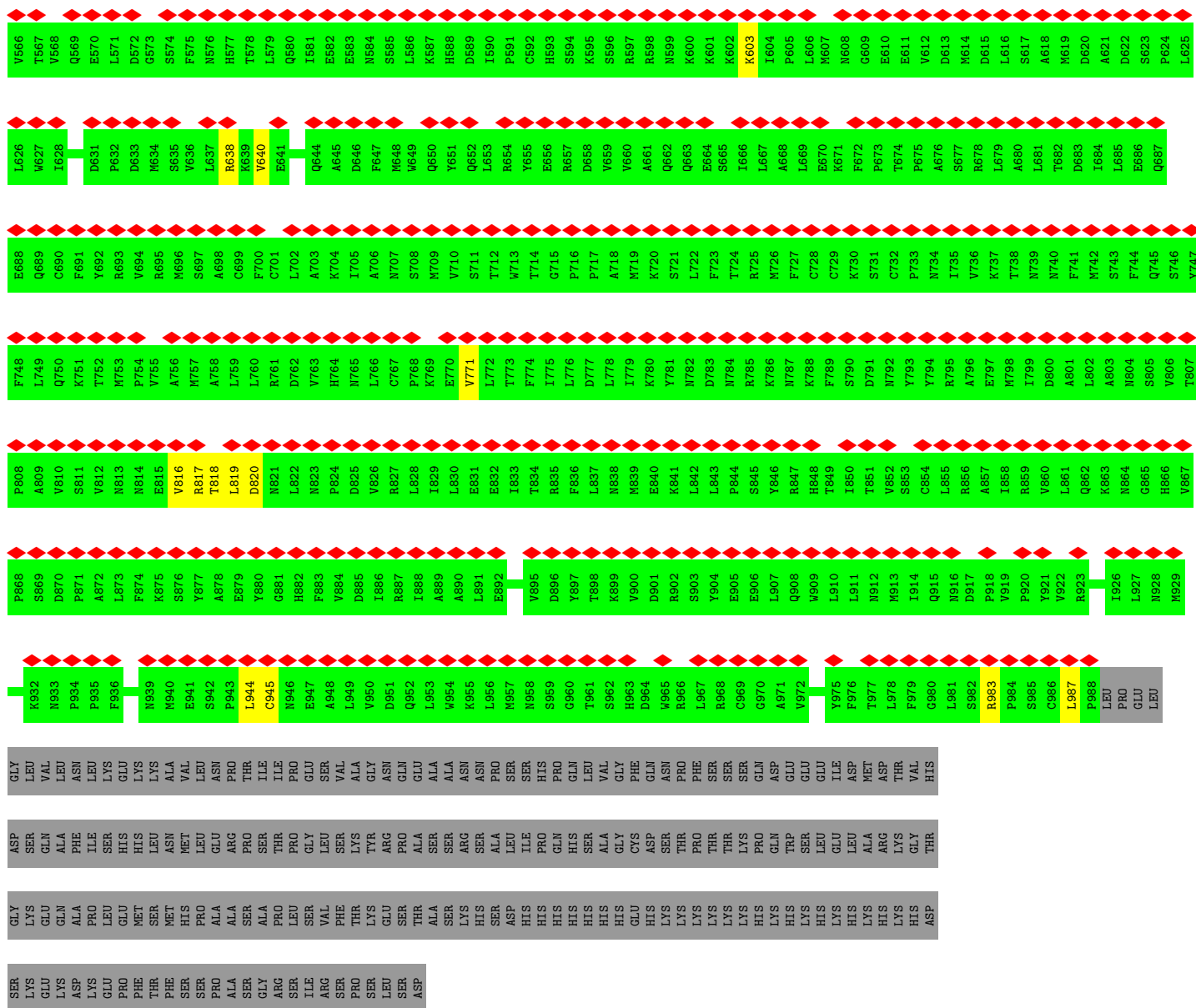
3 Residue-property plots

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

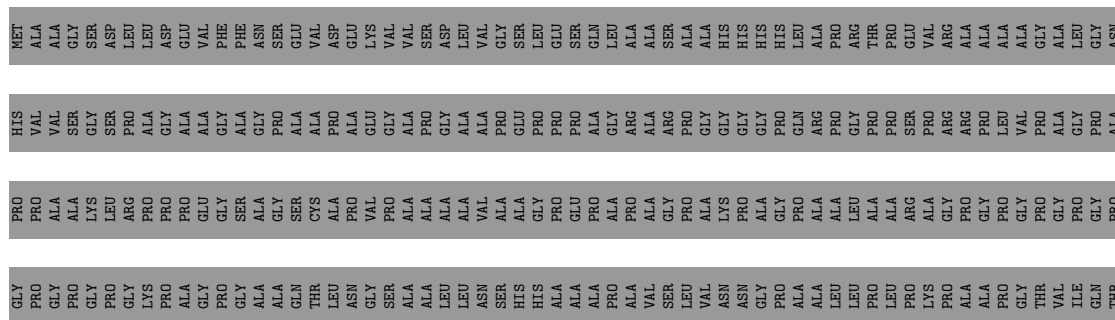
• Molecule 1: Transcription initiation factor TFIID subunit 1



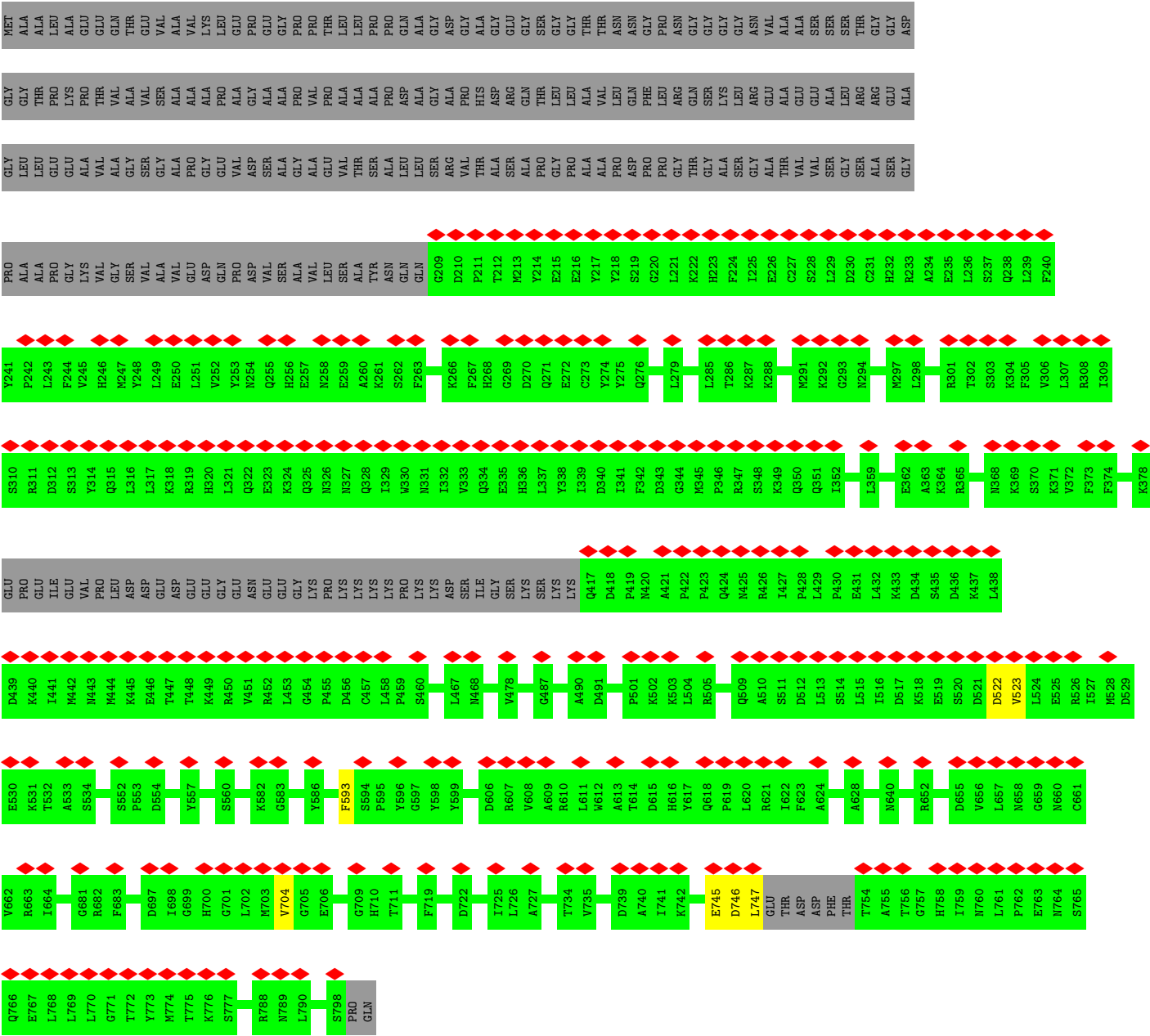




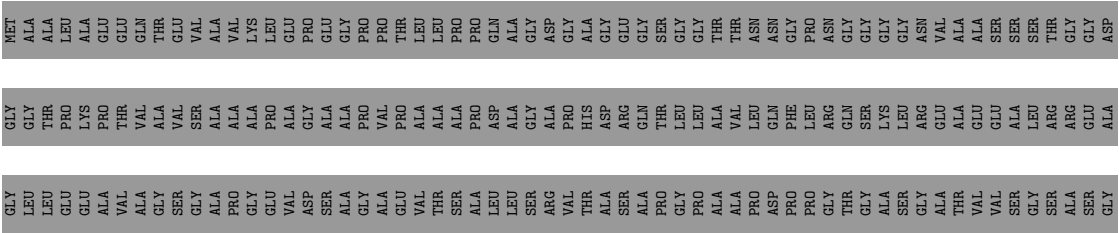
• Molecule 3: Transcription initiation factor TFIID subunit 4



- Molecule 3: Transcription initiation factor TFIID subunit 4



● Molecule 4: Transcription initiation factor TFIID subunit 5



V781	H782	L783	H784	F785	T786	R787	R788	R789	L790	V791	L792	A793	A794	G795	A796	Y797	S798	F799	GLN	L202	S203	A204	Y205	N206	Q207	Q208	G209	D210	P211	T212	M213	Y214	E215	E216	Y217	Y218	S219	G220	L221	K222	H223	F224	I225	E226	C227	S228	L229	D230	C231	H232	R233	A234	E235	L236	S237	Q238	L239	F240		
R721	D722	G723	E724	L725	L726	A727	S728	G729	S730	M731	D732	M733	T734	V735	R736	L737	W738	D739	A740	I741	K742	A743	F744	E745	D746	L747	E748	THR	ASP	ASP	PHE	THR	T754	A755	T756	G757	H758	L759	N760	L761	P762	E763	N764	S765	Q766	E767	L768	L769	L770	G771	T772	W773	M774	T775	K776	S777	T778	P779	V780	
C661	V662	R663	I664	F665	T666	G667	H668	K669	G670	P671	L672	H673	S674	L675	T676	F677	S678	P679	N680	G681	R682	F683	L684	A685	T686	G687	A688	T689	D690	G691	R692	V693	L694	L695	W696	D697	T698	G699	H700	G701	L702	M703	V704	G705	E706	L707	K708	G709	H710	T711	D712	T713	V714	C715	S716	L717	R718	F719	S720	
G541	H542	S543	G544	P545	V546	Y547	G548	A549	S550	F551	S552	P553	D554	R555	N556	Y557	L558	L559	S560	S561	S562	E563	D564	G565	T566	V567	R568	L569	W570	S571	L572	Q573	T574	F575	T576	C577	L578	V579	G580	Y581	K582	G583	H584	N585	Y586	P587	V588	W589	D590	T591	Q592	F593	S594	P595	Y596	G597	Y598	Y599	F600	
D481	S482	S483	L484	I485	A486	G487	G488	F489	A490	D491	S492	T493	V494	R495	V496	W497	S498	V499	T500	P501	K502	K503	L504	R505	S506	V507	K508	Q509	A510	S511	D512	L513	S514	L515	I516	D517	K518	E519	S520	D521	D522	V523	L524	E525	N526	I527	M528	D529	E530	K531	A533	S534	F535	L536	K537	I538	L539	Y540		
A421	P422	P423	Q424	M425	R426	I427	P428	L429	P430	E431	L432	K433	D434	S435	D436	K437	L438	D439	K440	I441	M442	M443	M444	K445	E446	T447	T448	K449	R450	V451	R452	L453	G454	P455	D456	C457	L458	P459	S460	I461	C462	F463	Y464	T465	F466	L467	M468	A469	Y470	Q471	G472	L473	T474	A475	V476	D477	T479	D480		
R301	T302	S303	K304	F305	V306	L307	R308	I309	S310	R311	D312	S313	Y314	Q315	L316	L317	K318	R319	H320	L321	Q322	E323	K324	Q325	N326	N327	Q328	I329	W330	N331	I332	V333	Q334	E335	H336	L337	Y338	I339	D340	I341	S342	D343	GLY	MET	PRO	ARG	SER	LYS	GLN	R289	TLE	ASP	ALA	MET	VAL	GLY	SER	LEU	ALA	
GLY	GLU	A363	K364	R365	E366	A367	N368	K369	S370	K371	V372	F373	F374	G375	L376	L377	K378	E379	F380	GLU	TLE	GLU	VAL	PRO	LEU	ASP	GLU	ASP	GLU	GLU	GLY	ASN	GLU	GLU	GLY	LYS	PRO	LYS	LYS	LYS	LYS	ASP	SER	TLE	GLY	SER	LYS	LYS	SER	LYS	K416	Q417	D418	P419	M420					
Y241	P242	L243	F244	V245	H246	M247	Y248	L249	I250	E251	V252	Y253	Y254	Q255	H256	E257	N258	E259	A260	K261	S262	F263	F264	G265	K266	F267	H268	G269	D270	Q271	E272	C273	Y274	Y275	Q276	D277	D278	L279	R280	V281	L282	C227	S283	S284	L285	T286	K287	K288	E289	H290	M291	K292	G293	N294	E295	T296	M297	L298	D299	F300

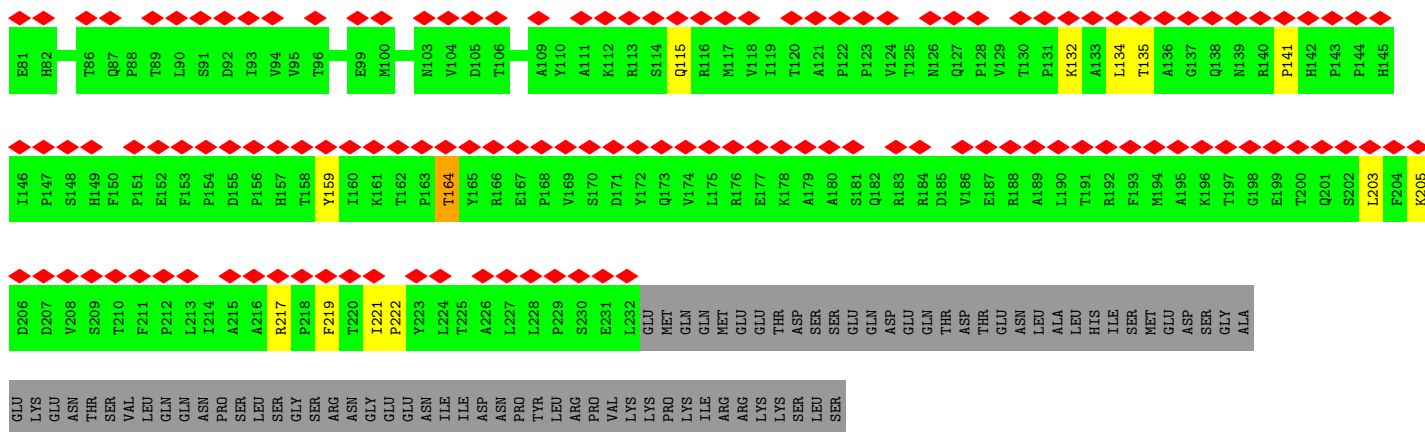
• Molecule 5: Transcription initiation factor TFIID subunit 6

Chain F: 

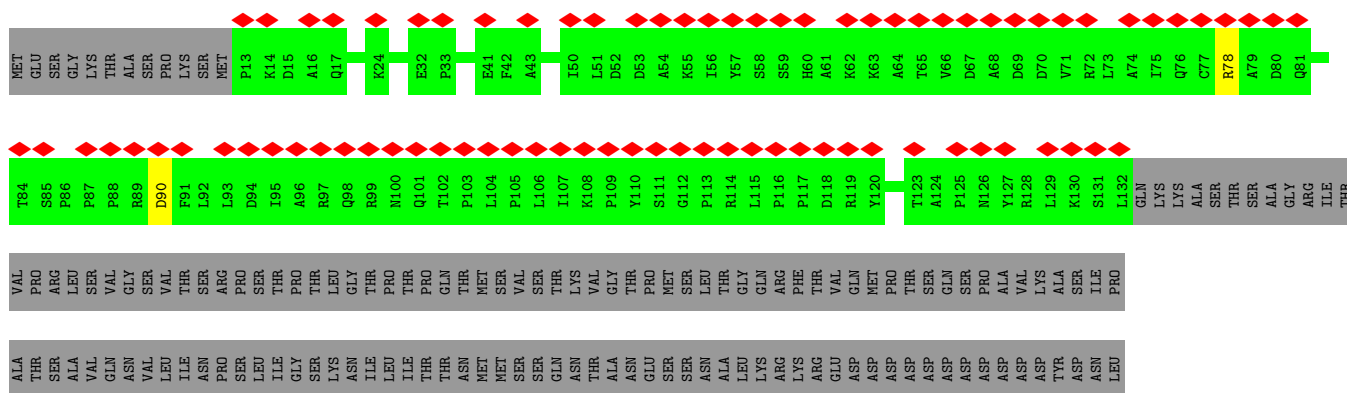
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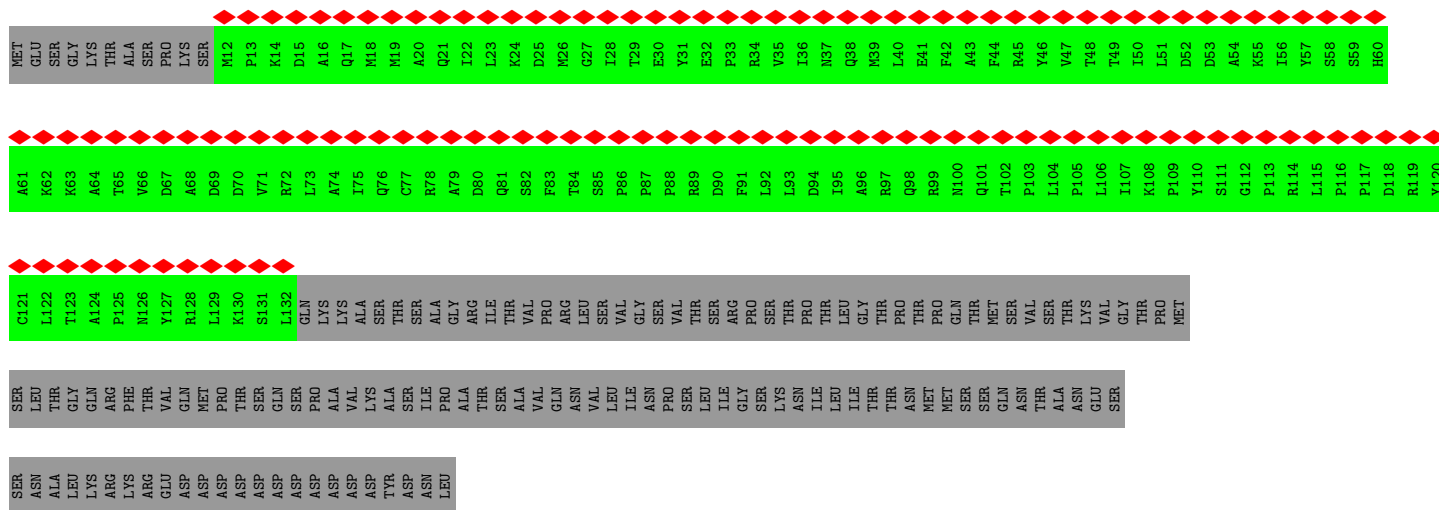




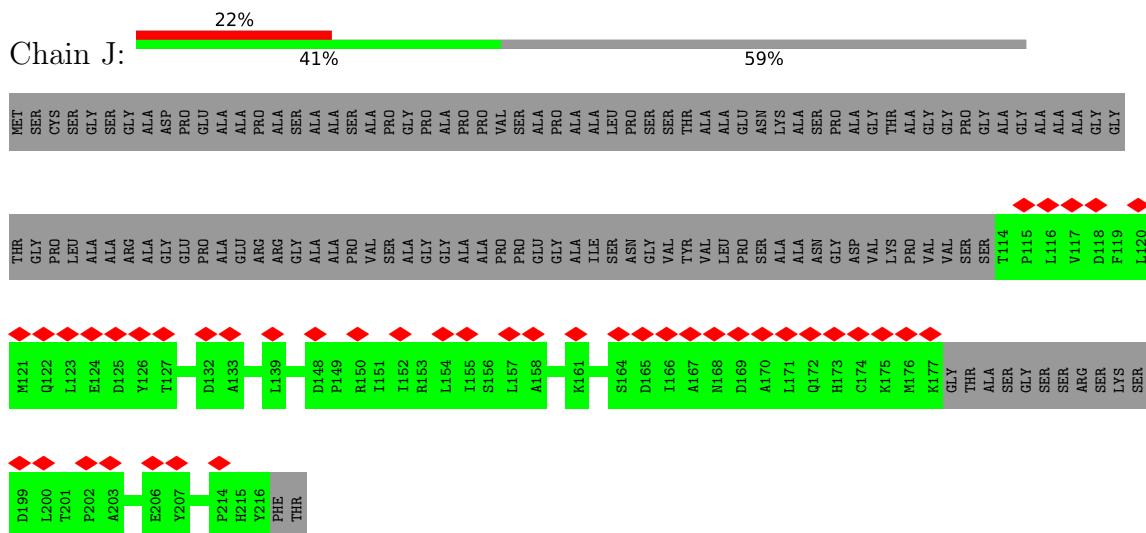
• Molecule 8: Transcription initiation factor TFIID subunit 9



• Molecule 8: Transcription initiation factor TFIID subunit 9



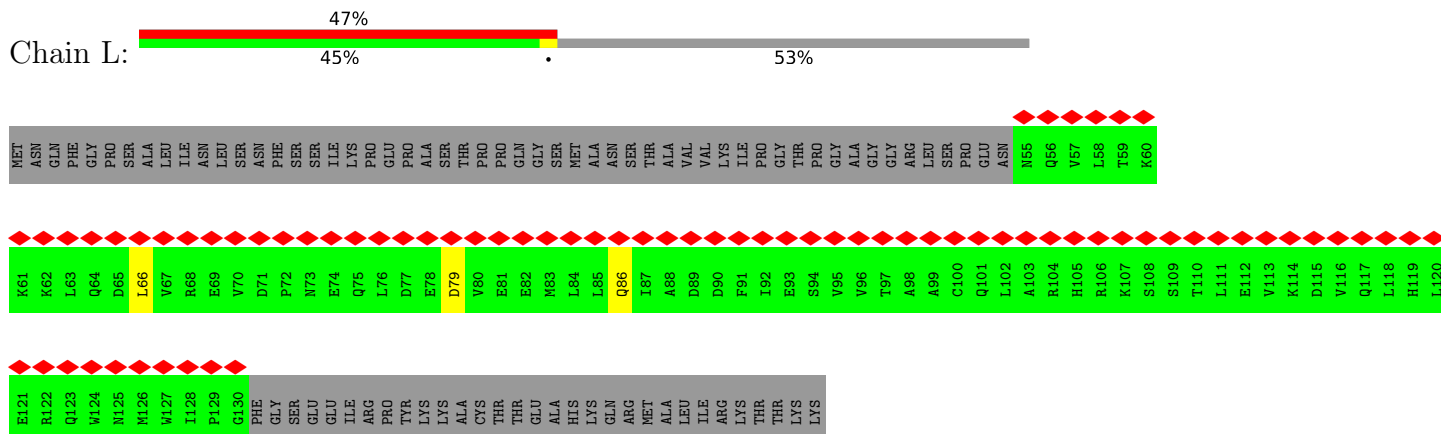
• Molecule 9: Transcription initiation factor TFIID subunit 10



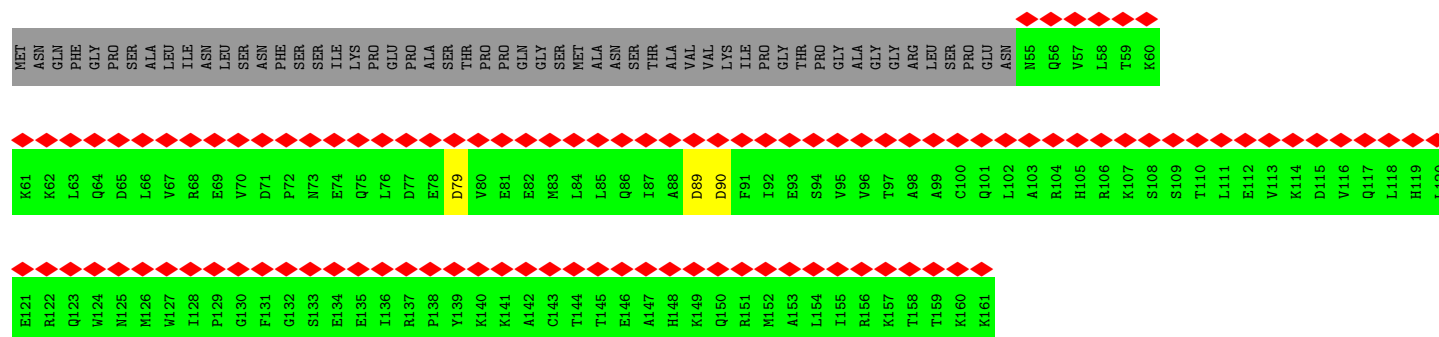
- Molecule 9: Transcription initiation factor TFIID subunit 10



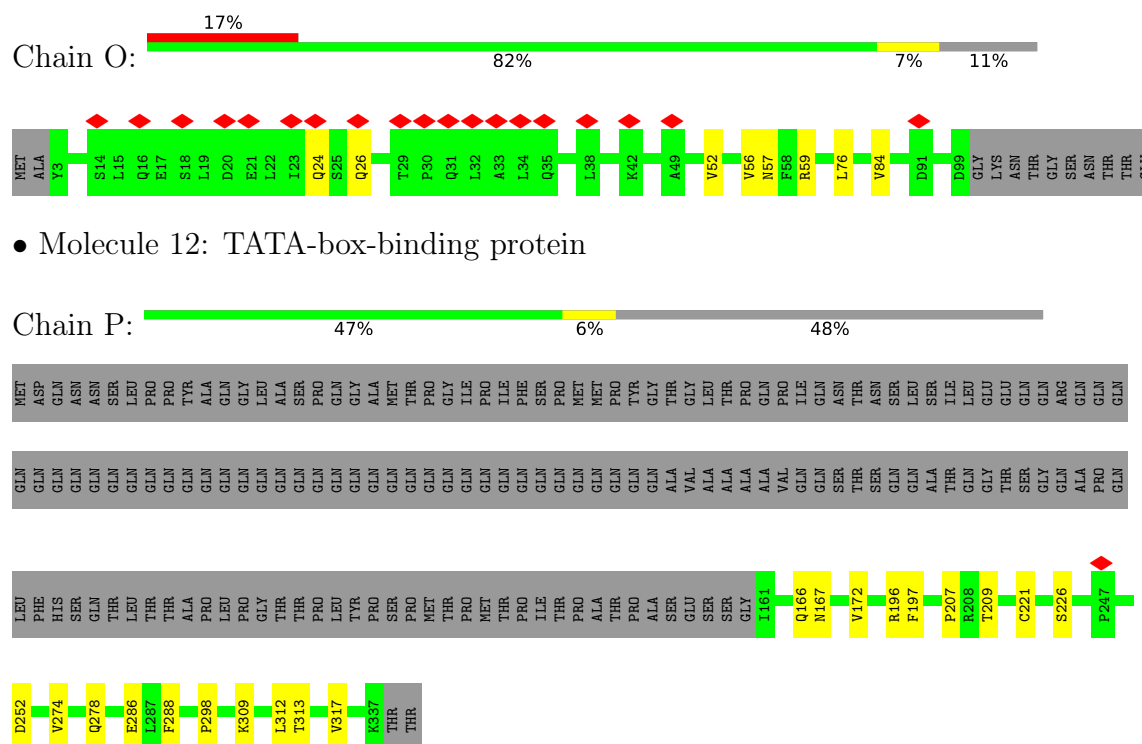
- Molecule 10: Transcription initiation factor TFIID subunit 12



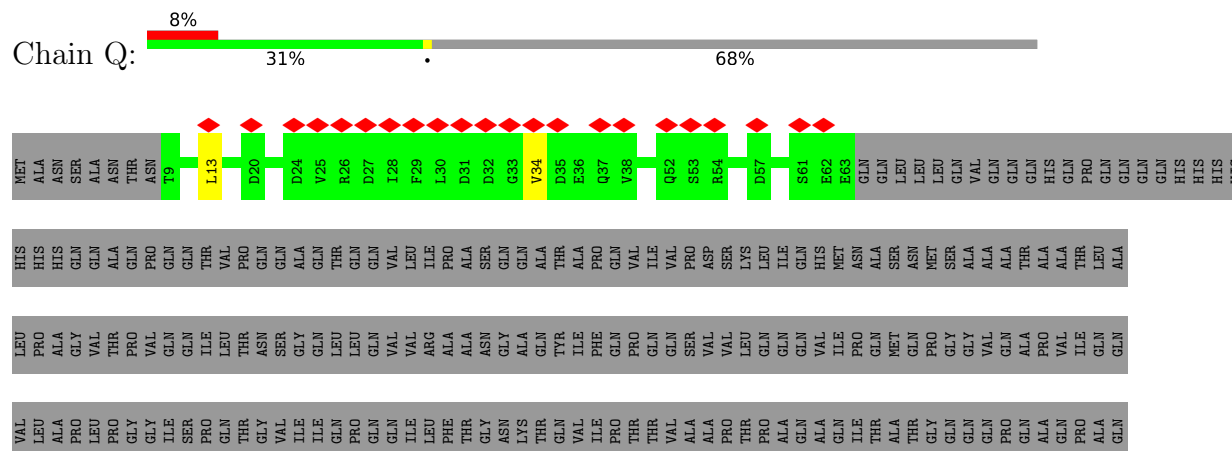
- Molecule 10: Transcription initiation factor TFIID subunit 12



- Molecule 11: Transcription initiation factor IIA subunit 2

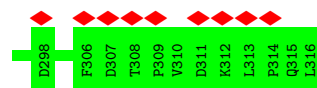
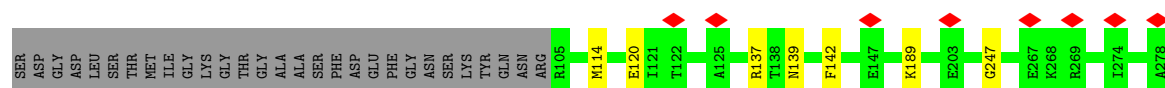
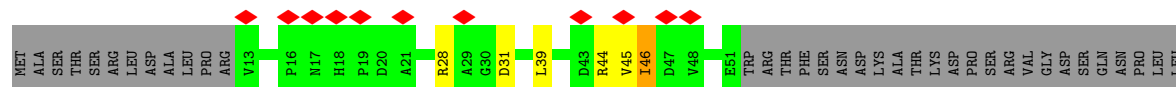


- Molecule 13: Transcription initiation factor IIA subunit 1

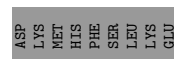
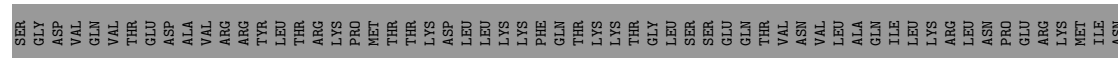
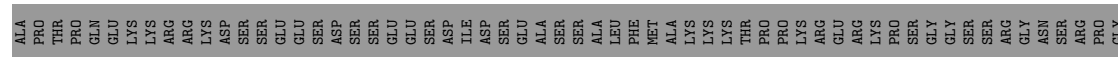
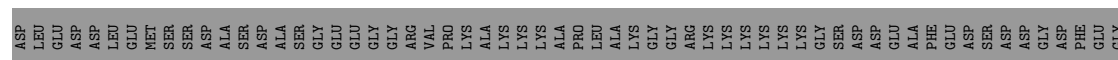
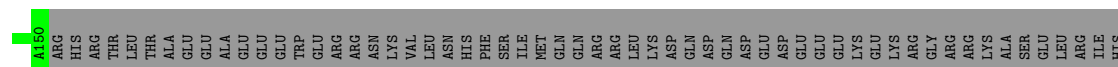
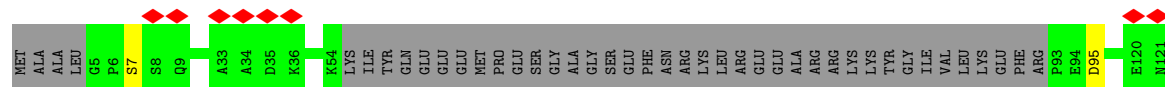




- Molecule 14: Transcription initiation factor IIB

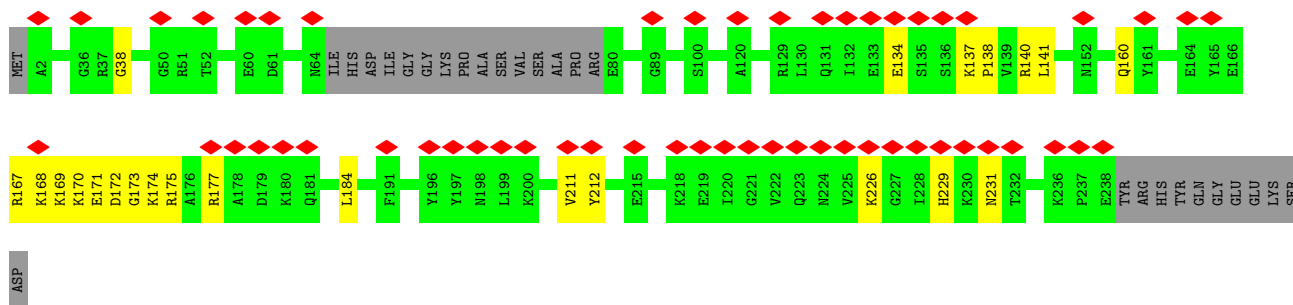


- Molecule 15: General transcription factor IIF subunit 1

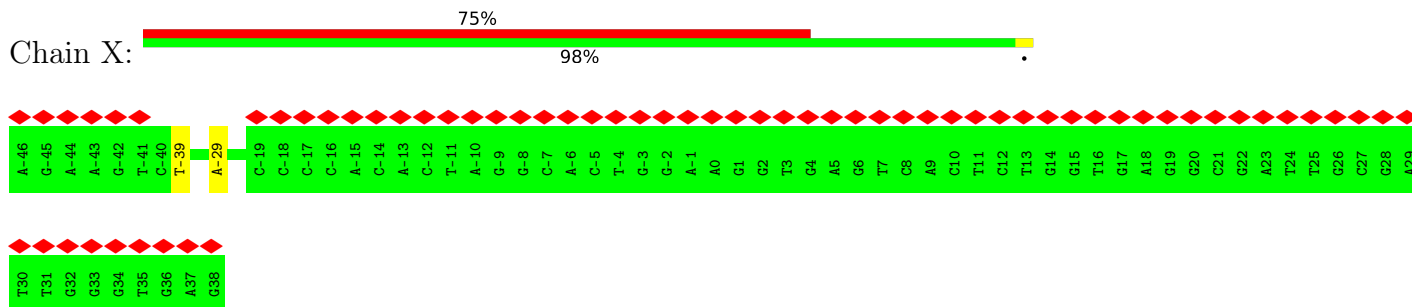


- Molecule 16: General transcription factor IIF subunit 2

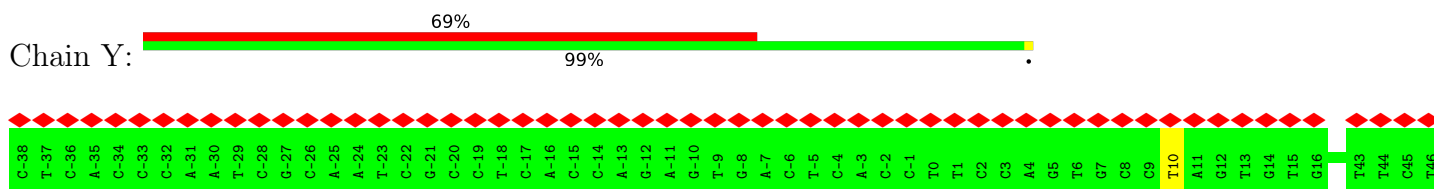




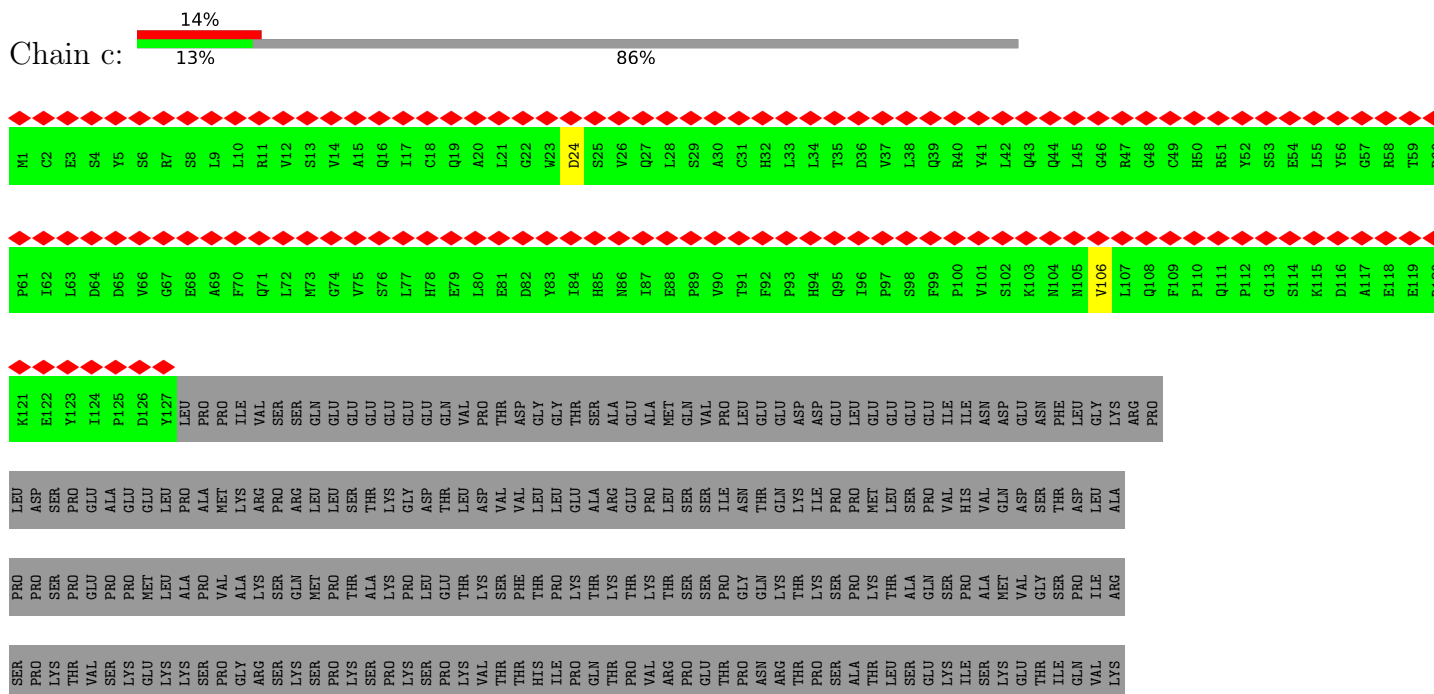
• Molecule 17: DNA (85-MER)



• Molecule 18: DNA (85-MER)



• Molecule 19: Transcription initiation factor TFIID subunit 3



[illegible]

- Molecule 20: Transcription initiation factor TFIID subunit 11

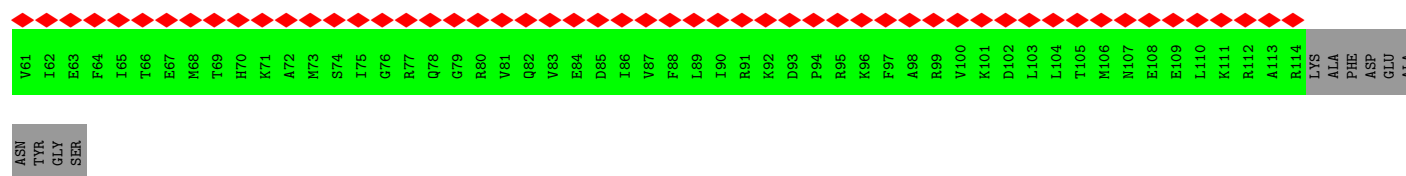


P181	L182	Q183	P184	K185	H186	M187	R188	E189	A190	V191	R192	L193	L194	K195	S196	K197	G198	Q199	I200	P201	N202	S203	K204	H205	K206	K207	I208	I209	F210	F211																							
Y121	E122	M123	Y124	R125	R126	S127	A128	F129	P130	K131	A132	A133	I134	K135	R136	L137	I138	Q139	S140	I141	T142	G143	T144	S145	V146	S147	Q148	M149	V150	V151	I152	A153	M154	S155	G156	I157	S158	K159	V160	F161	V162	G163	E164	V165	V166								
GLN	ASP	VAL	SER	ASP	LEU	THR	VAL	GLU	ARG	LYS	GLY	GLY	ASP	PRO	ALA	ALA	LYS	LYS	ILE	ASP	THR	LYS	GLU	LYS	GLU	LYS	GLN	LYS	VAL	ASP	GLU	ASP	GLU	ILE	GLN	LYS	MET	GLN	ILE	LEU	VAL	SER	SER	ALA	ALA	PHE	S114	E115	E116	Q117	L118		
MET	ASP	ASP	ALA	HIS	GLU	SER	PRO	SER	ASP	LYS	GLY	GLY	GLY	GLU	THR	THR	GLY	GLY	GLY	ASP	PRO	ALA	ALA	THR	THR	ASP	GLY	ILE	PRO	GLU	GLU	THR	THR	ASP	GLY	ASP	ASP	VAL	ASP	LEU	LYS	GLU	ALA	GLA	ALA	ALA	GLU	GLY	GLY	LEU	LEU	SER	SER

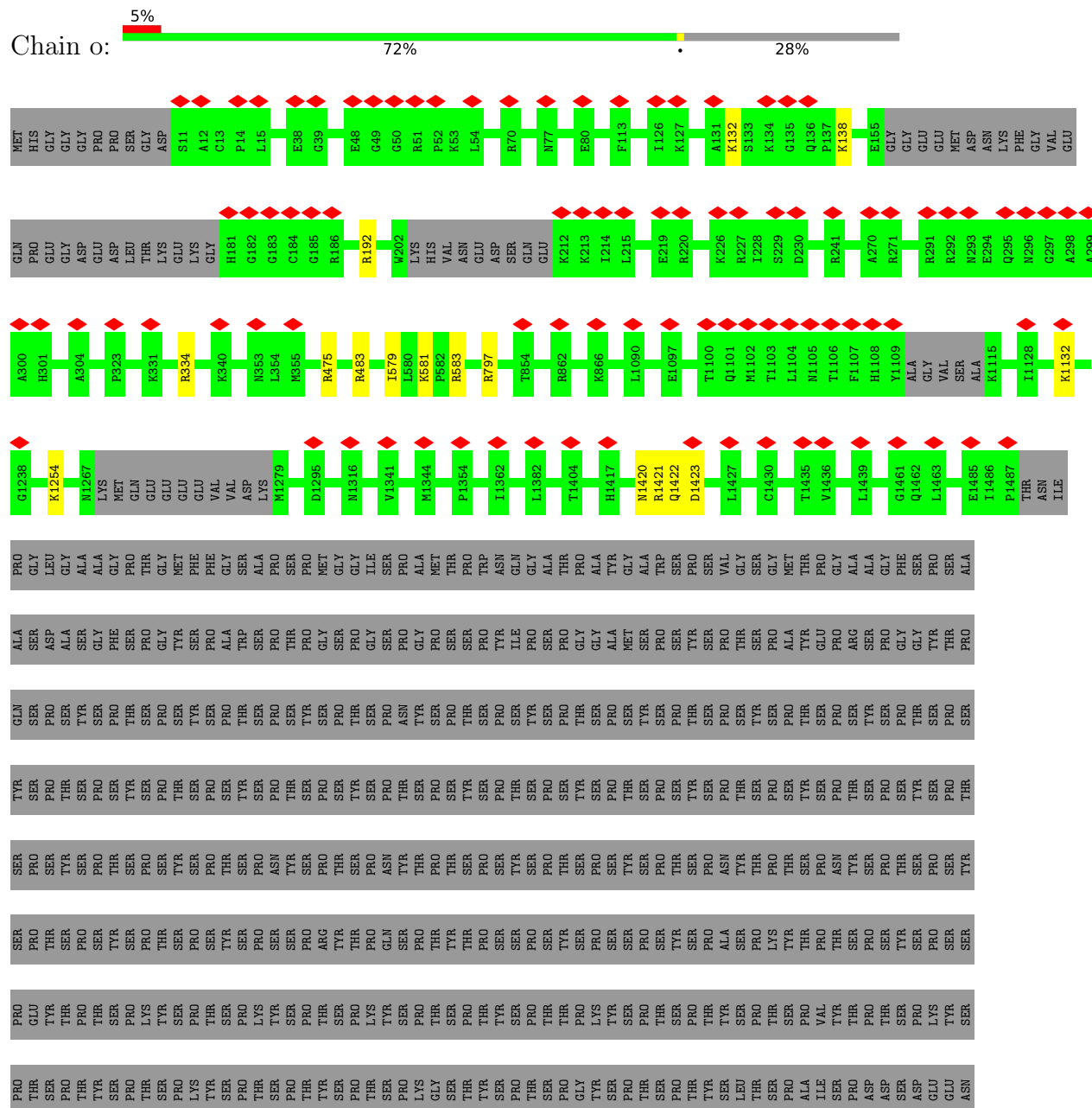
- Molecule 21: Transcription initiation factor TFIID subunit 13



MET	ALA	ASP	GLU	GLU	ASP	PRO	THR	PHE	GLU	GLU	GLU	ASN	GLU	GLU	ILE	GLY	GLY	GLY	ALA	GLU	GLY	GLY	GLN	GLY	LYS								
	R28	K29	R30	L31	F32	S33	K34	S35	L36	R37	C38	N39	M40	Y41	G42	F43	G44	D45	D46	Q47	N48	P49	Y50	T51	E52	S53	V54	D55	L56	L57	E58	D59	L60

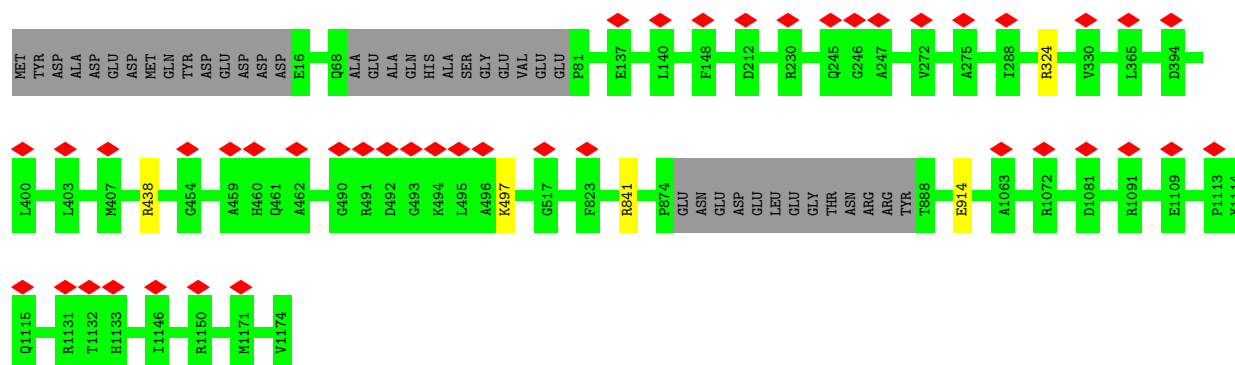


• Molecule 22: RPB1



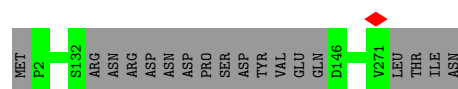
• Molecule 23: DNA-directed RNA polymerase subunit beta





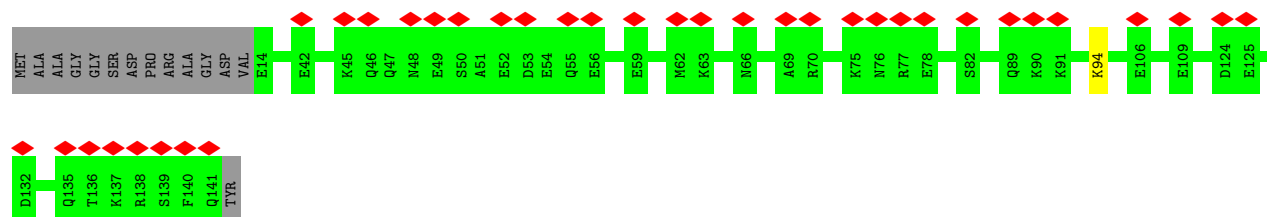
- Molecule 24: DNA-directed RNA polymerase II subunit RPB3

Chain q: 93% 7%



- Molecule 25: DNA-directed RNA polymerase II subunit RPB4

Chain r: 25% 89% 10%



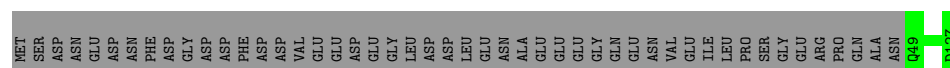
- Molecule 26: DNA-directed RNA polymerase II subunit E

Chain s: 99%



- Molecule 27: DNA-directed RNA polymerase II subunit F

Chain t: 62% 38%



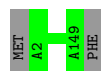
- Molecule 28: DNA-directed RNA polymerase II subunit RPB7

Chain u: 15% 99%



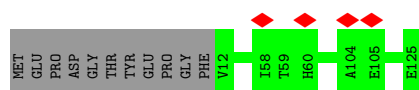
- Molecule 29: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain v: 99%



- Molecule 30: DNA-directed RNA polymerase II subunit RPB9

Chain w: 91% 9%



- Molecule 31: RPB10

Chain x: 96%



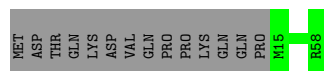
- Molecule 32: RNA_pol_L_2 domain-containing protein

Chain y: 100%



- Molecule 33: RPB12

Chain z: 76% 24%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	7186	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)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.689	Depositor
Minimum map value	-0.746	Depositor
Average map value	-0.003	Depositor
Map value standard deviation	0.049	Depositor
Recommended contour level	0.19	Depositor
Map size (\AA)	496.8, 496.8, 496.8	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.38, 1.38, 1.38	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	A	0.52	0/5046	0.65	0/6810
2	B	0.47	0/7993	0.60	0/10836
3	D	0.45	0/1379	0.58	0/1843
3	d	0.29	0/1321	0.49	0/1772
4	E	0.35	0/4469	0.55	0/6050
4	e	0.33	0/4433	0.55	0/6004
5	F	0.50	0/3139	0.67	0/4264
5	f	0.40	0/3140	0.63	0/4268
6	G	0.51	0/1199	0.63	0/1612
7	H	0.41	0/1673	0.60	0/2285
8	I	0.32	0/981	0.50	0/1332
8	i	0.30	0/989	0.46	0/1343
9	J	0.31	0/724	0.50	0/982
9	j	0.30	0/775	0.52	0/1049
10	L	0.36	0/630	0.57	0/852
10	l	0.29	0/888	0.55	3/1194 (0.3%)
11	O	0.50	0/781	0.74	0/1061
12	P	0.61	0/1438	0.75	1/1935 (0.1%)
13	Q	0.44	0/1013	0.60	0/1366
14	R	0.33	0/1966	0.56	0/2655
15	S	0.32	0/896	0.49	0/1213
16	T	0.49	0/1817	0.67	0/2445
17	X	0.77	1/1966 (0.1%)	1.00	1/3034 (0.0%)
18	Y	0.67	1/1942 (0.1%)	0.90	0/2993
19	c	0.39	0/1035	0.54	0/1406
20	k	0.30	0/799	0.47	0/1070
21	m	0.31	0/733	0.51	0/977
22	o	0.34	0/11516	0.50	0/15548
23	p	0.37	0/9243	0.47	0/12475
24	q	0.39	0/2102	0.46	0/2857
25	r	0.26	0/1019	0.47	0/1374
26	s	0.30	0/1751	0.46	0/2366

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
27	t	0.37	0/645	0.47	0/871
28	u	0.29	0/1365	0.47	0/1853
29	v	0.37	0/1207	0.49	0/1628
30	w	0.30	0/948	0.46	0/1284
31	x	0.43	0/516	0.45	0/696
32	y	0.35	0/956	0.44	0/1294
33	z	0.38	0/377	0.44	0/500
All	All	0.42	2/84810 (0.0%)	0.58	5/115397 (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	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	X	-39	DT	C1'-N1	5.03	1.55	1.49
18	Y	10	DT	C1'-N1	5.02	1.55	1.49

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	P	167	ASN	CB-CA-C	-6.91	96.59	110.40
17	X	-29	DA	C1'-O4'-C4'	-6.06	104.04	110.10
10	l	79	ASP	CB-CG-OD2	5.21	122.98	118.30
10	l	89	ASP	CB-CG-OD2	5.18	122.96	118.30
10	l	90	ASP	CB-CG-OD2	5.16	122.95	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	821	ARG	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	A	584/1872 (31%)	544 (93%)	35 (6%)	5 (1%)	14	52
2	B	959/1199 (80%)	913 (95%)	46 (5%)	0	100	100
3	D	158/1085 (15%)	141 (89%)	17 (11%)	0	100	100
3	d	154/1085 (14%)	150 (97%)	4 (3%)	0	100	100
4	E	540/800 (68%)	503 (93%)	34 (6%)	3 (1%)	22	60
4	e	531/800 (66%)	484 (91%)	47 (9%)	0	100	100
5	F	400/677 (59%)	373 (93%)	23 (6%)	4 (1%)	13	49
5	f	399/677 (59%)	377 (94%)	22 (6%)	0	100	100
6	G	139/349 (40%)	135 (97%)	4 (3%)	0	100	100
7	H	207/310 (67%)	184 (89%)	19 (9%)	4 (2%)	6	32
8	I	118/264 (45%)	114 (97%)	4 (3%)	0	100	100
8	i	119/264 (45%)	115 (97%)	4 (3%)	0	100	100
9	J	85/218 (39%)	82 (96%)	3 (4%)	0	100	100
9	j	91/218 (42%)	89 (98%)	2 (2%)	0	100	100
10	L	74/161 (46%)	67 (90%)	7 (10%)	0	100	100
10	l	105/161 (65%)	101 (96%)	4 (4%)	0	100	100
11	O	95/109 (87%)	85 (90%)	7 (7%)	3 (3%)	3	21
12	P	175/339 (52%)	162 (93%)	11 (6%)	2 (1%)	12	47
13	Q	118/376 (31%)	110 (93%)	7 (6%)	1 (1%)	16	55
14	R	247/316 (78%)	235 (95%)	10 (4%)	2 (1%)	16	55
15	S	104/517 (20%)	102 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	T	218/249 (88%)	198 (91%)	15 (7%)	5 (2%)	5	28
19	c	125/929 (14%)	116 (93%)	9 (7%)	0	100	100
20	k	96/211 (46%)	91 (95%)	5 (5%)	0	100	100
21	m	85/124 (68%)	79 (93%)	6 (7%)	0	100	100
22	o	1417/1970 (72%)	1306 (92%)	110 (8%)	1 (0%)	48	83
23	p	1128/1174 (96%)	1054 (93%)	74 (7%)	0	100	100
24	q	253/275 (92%)	226 (89%)	27 (11%)	0	100	100
25	r	126/142 (89%)	119 (94%)	7 (6%)	0	100	100
26	s	207/210 (99%)	196 (95%)	11 (5%)	0	100	100
27	t	77/127 (61%)	73 (95%)	4 (5%)	0	100	100
28	u	169/172 (98%)	156 (92%)	13 (8%)	0	100	100
29	v	146/150 (97%)	133 (91%)	13 (9%)	0	100	100
30	w	112/125 (90%)	103 (92%)	9 (8%)	0	100	100
31	x	62/67 (92%)	59 (95%)	3 (5%)	0	100	100
32	y	115/117 (98%)	109 (95%)	6 (5%)	0	100	100
33	z	42/58 (72%)	38 (90%)	4 (10%)	0	100	100
All	All	9780/17897 (55%)	9122 (93%)	628 (6%)	30 (0%)	38	73

5 of 30 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1000	LEU
1	A	1158	SER
5	F	323	VAL
7	H	141	PRO
7	H	222	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	A	536/1665 (32%)	484 (90%)	52 (10%)	6	22
2	B	876/1083 (81%)	851 (97%)	25 (3%)	37	56
3	D	147/815 (18%)	117 (80%)	30 (20%)	1	6
3	d	146/815 (18%)	145 (99%)	1 (1%)	81	87
4	E	478/657 (73%)	474 (99%)	4 (1%)	79	85
4	e	475/657 (72%)	473 (100%)	2 (0%)	89	91
5	F	320/574 (56%)	304 (95%)	16 (5%)	20	41
5	f	322/574 (56%)	312 (97%)	10 (3%)	35	54
6	G	133/322 (41%)	126 (95%)	7 (5%)	19	40
7	H	181/270 (67%)	171 (94%)	10 (6%)	18	39
8	I	106/235 (45%)	104 (98%)	2 (2%)	52	69
8	i	107/235 (46%)	107 (100%)	0	100	100
9	J	78/154 (51%)	78 (100%)	0	100	100
9	j	83/154 (54%)	83 (100%)	0	100	100
10	L	71/141 (50%)	68 (96%)	3 (4%)	25	46
10	l	98/141 (70%)	98 (100%)	0	100	100
11	O	84/98 (86%)	79 (94%)	5 (6%)	16	37
12	P	153/293 (52%)	137 (90%)	16 (10%)	5	19
13	Q	111/324 (34%)	108 (97%)	3 (3%)	40	58
14	R	213/268 (80%)	201 (94%)	12 (6%)	17	38
15	S	93/448 (21%)	91 (98%)	2 (2%)	47	65
16	T	196/218 (90%)	178 (91%)	18 (9%)	7	23
19	c	113/833 (14%)	111 (98%)	2 (2%)	54	71
20	k	87/182 (48%)	87 (100%)	0	100	100
21	m	80/106 (76%)	79 (99%)	1 (1%)	65	77
22	o	1257/1748 (72%)	1242 (99%)	15 (1%)	67	78
23	p	993/1027 (97%)	988 (100%)	5 (0%)	86	89
24	q	234/252 (93%)	234 (100%)	0	100	100
25	r	106/126 (84%)	105 (99%)	1 (1%)	75	83
26	s	191/192 (100%)	190 (100%)	1 (0%)	86	89
27	t	69/111 (62%)	69 (100%)	0	100	100
28	u	147/153 (96%)	147 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	v	129/131 (98%)	129 (100%)	0	100	100
30	w	103/112 (92%)	103 (100%)	0	100	100
31	x	53/56 (95%)	53 (100%)	0	100	100
32	y	106/106 (100%)	106 (100%)	0	100	100
33	z	41/55 (74%)	41 (100%)	0	100	100
All	All	8716/15331 (57%)	8473 (97%)	243 (3%)	40	57

5 of 243 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	F	261	THR
22	o	132	LYS
7	H	221	ILE
5	f	421	ASP
23	p	324	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 123 such sidechains are listed below:

Mol	Chain	Res	Type
10	L	117	GLN
23	p	570	ASN
16	T	208	GLN
23	p	525	ASN
26	s	133	GLN

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

Of 10 ligands modelled in this entry, 10 are monoatomic - leaving 0 for Mogul analysis.

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

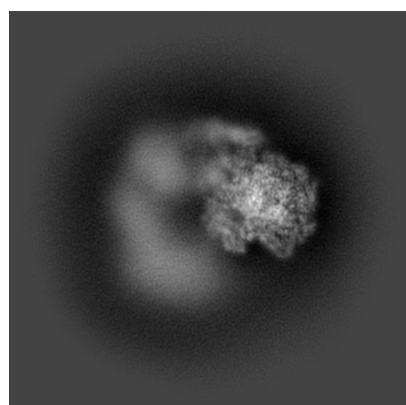
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31108. These allow visual inspection of the internal detail of the map and identification of artifacts.

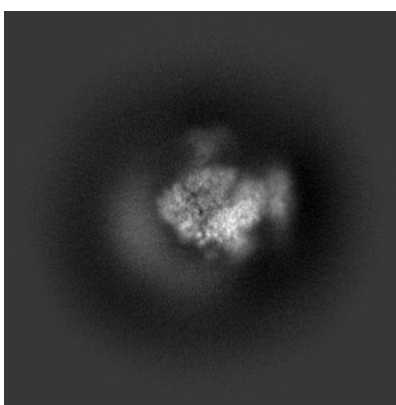
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

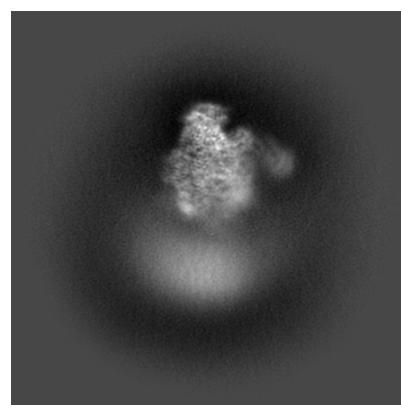
6.1.1 Primary map



X



Y

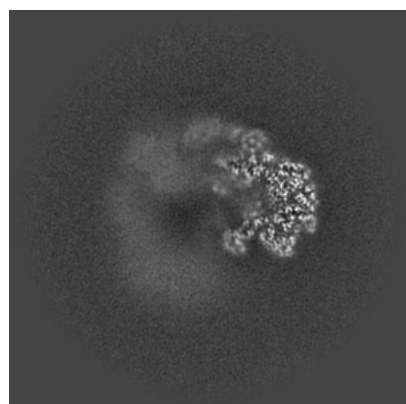


Z

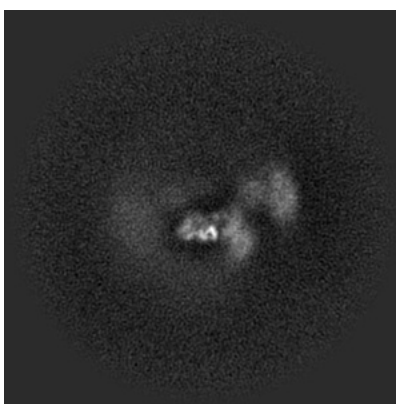
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

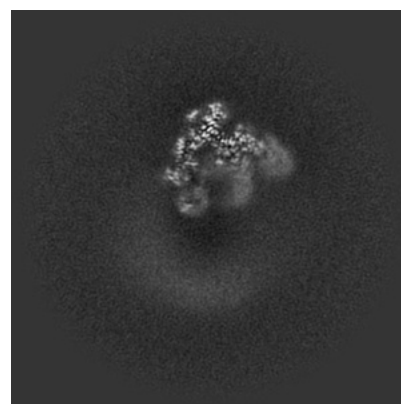
6.2.1 Primary map



X Index: 180



Y Index: 180

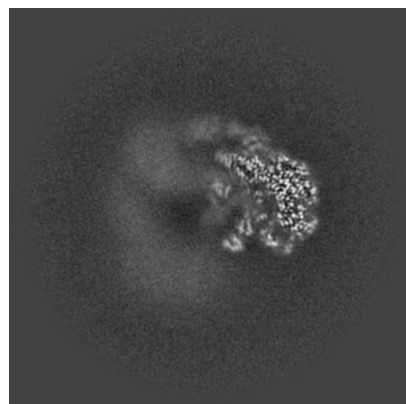


Z Index: 180

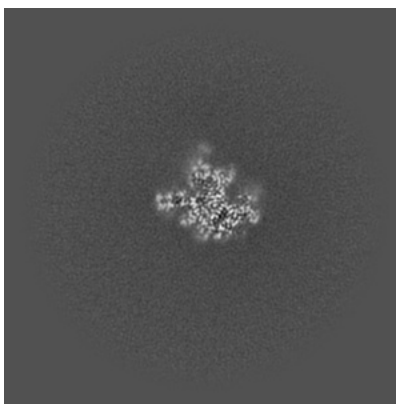
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

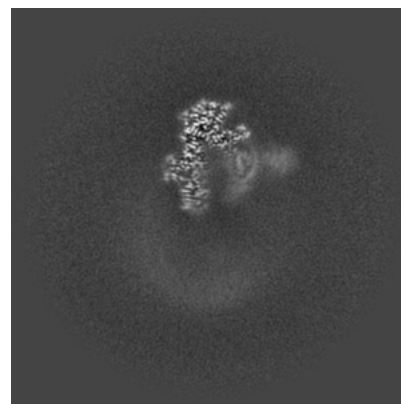
6.3.1 Primary map



X Index: 176



Y Index: 244

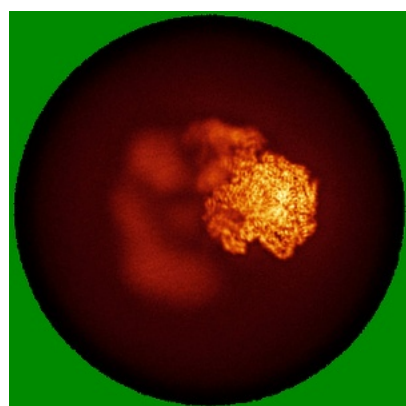


Z Index: 190

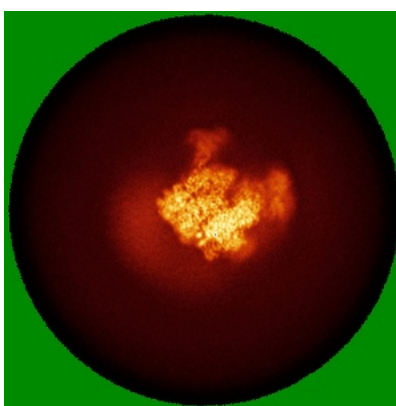
The images above show the largest variance slices of the map in three orthogonal directions.

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

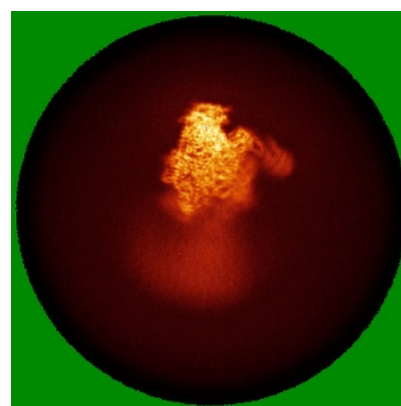
6.4.1 Primary map



X



Y

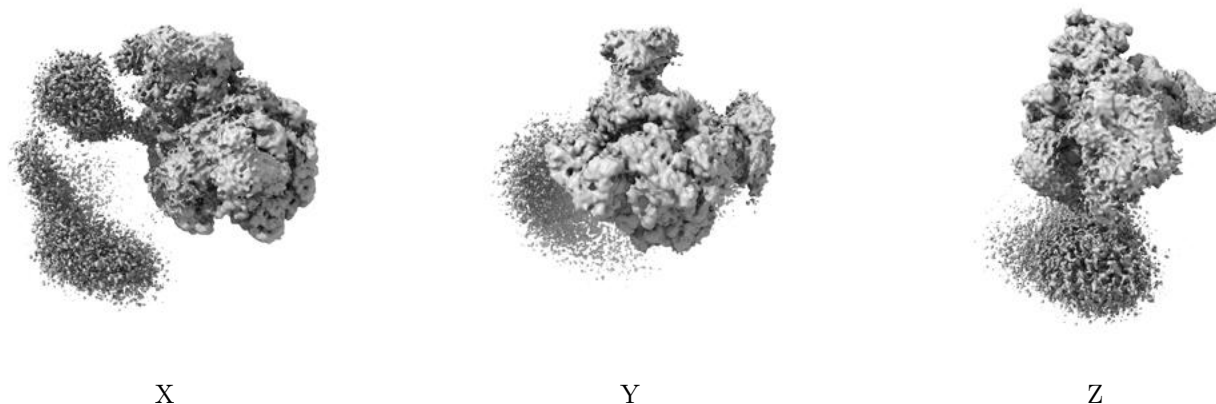


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.19. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

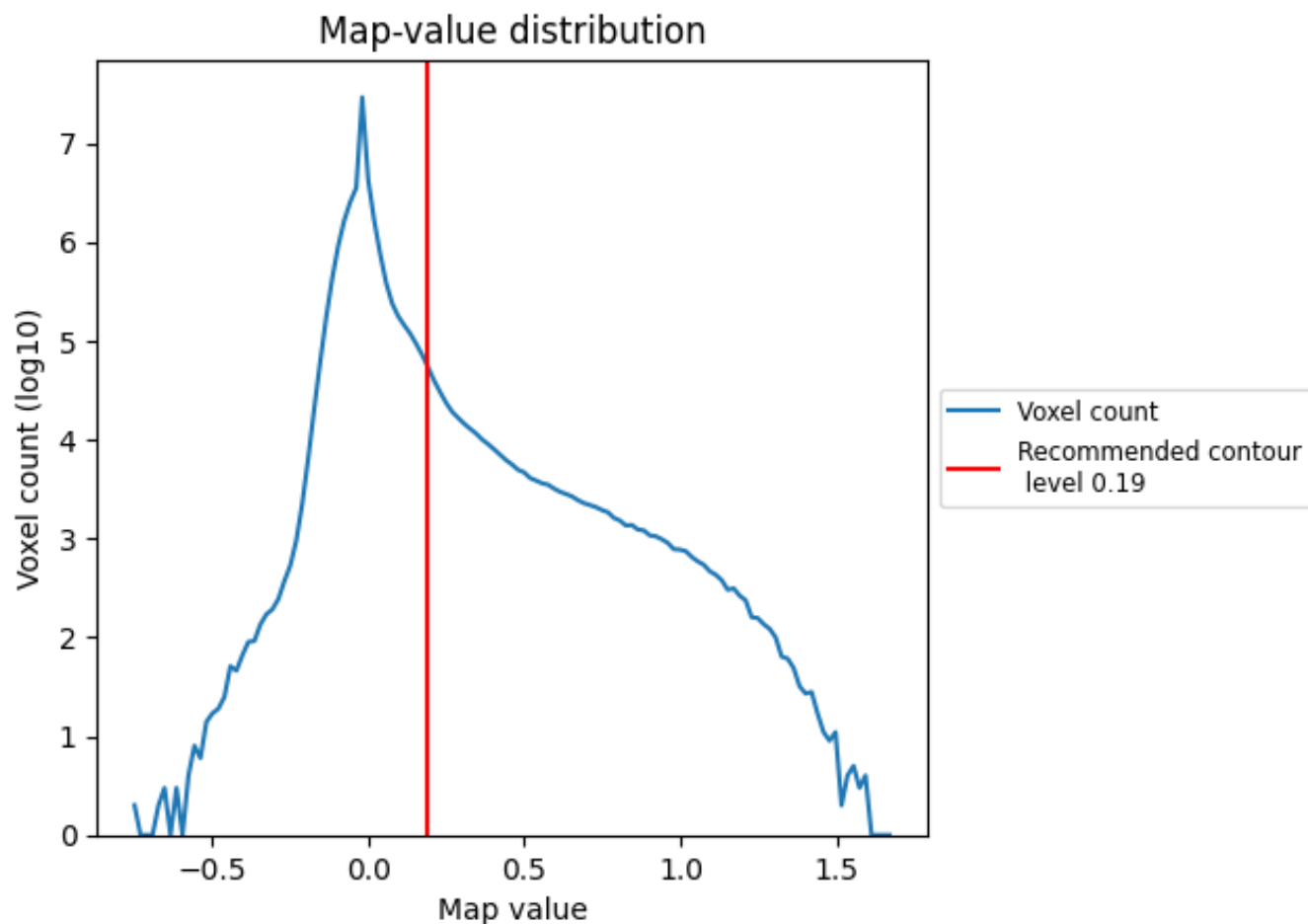
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

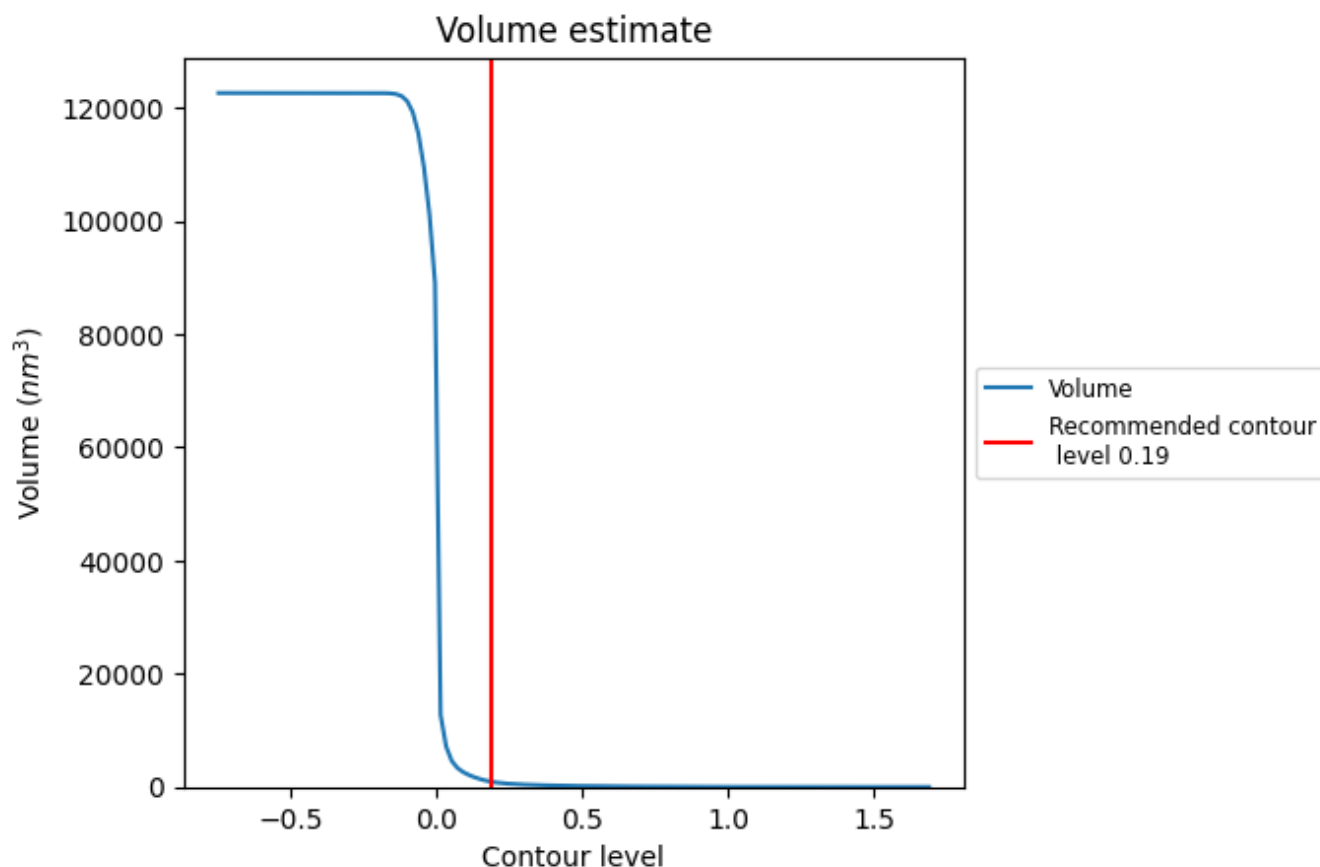
This section contains the results of statistical analysis of the map.

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.

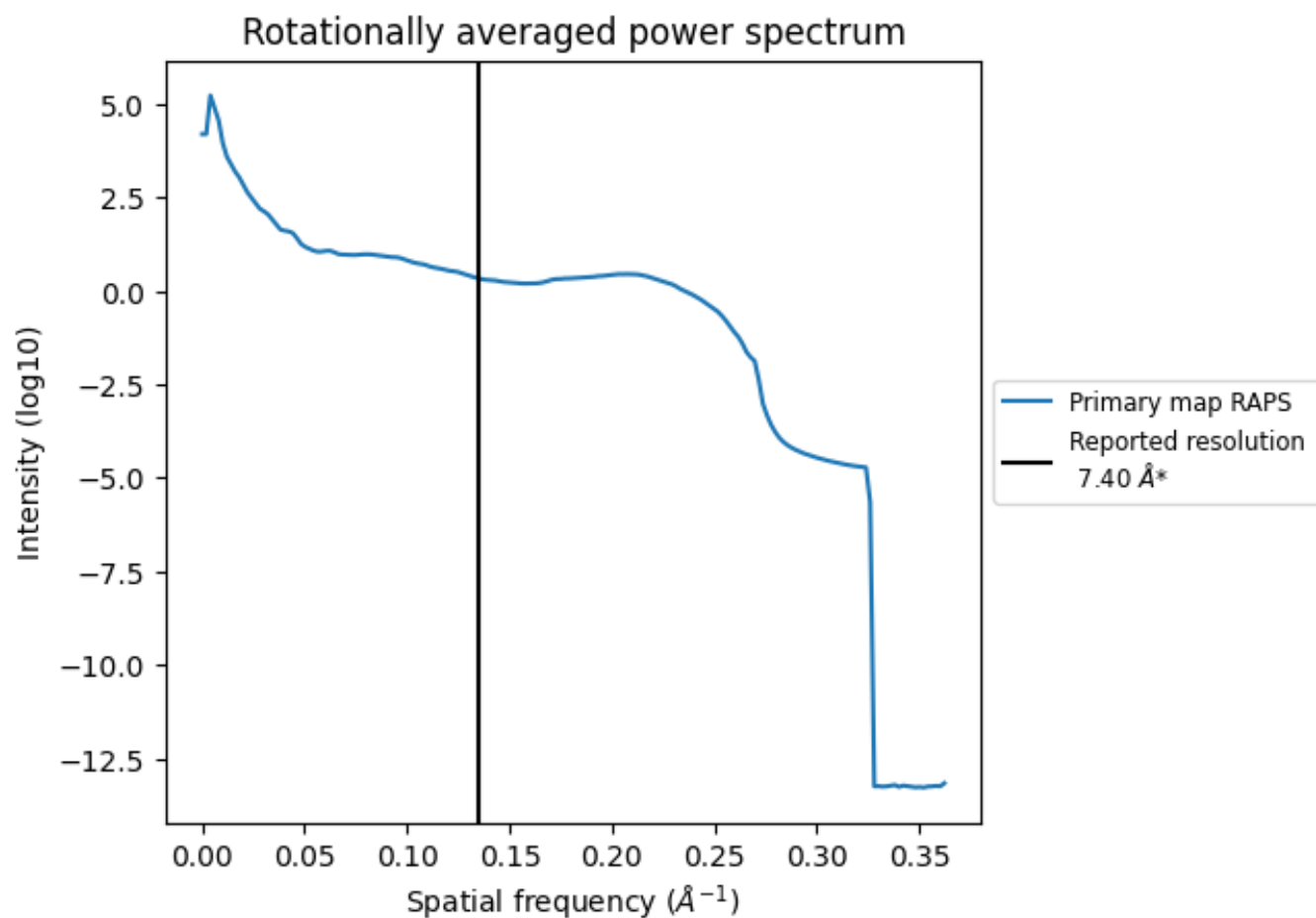
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 917 nm^3 ; this corresponds to an approximate mass of 828 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 0.135 Å⁻¹

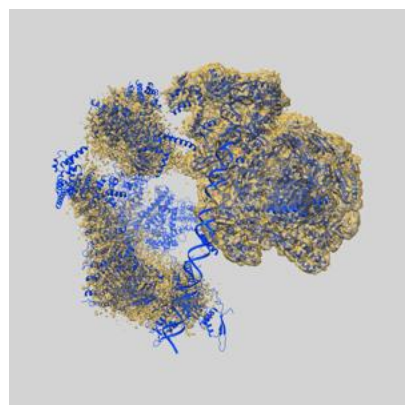
8 Fourier-Shell correlation

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

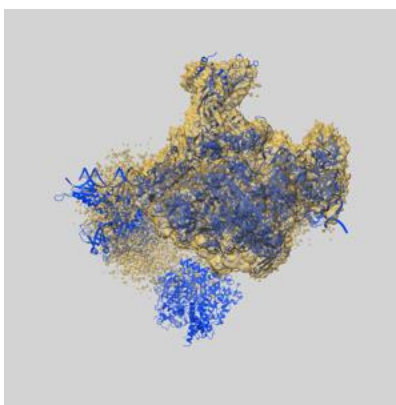
9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-31108 and PDB model 7EG8. Per-residue inclusion information can be found in section 3 on page 11.

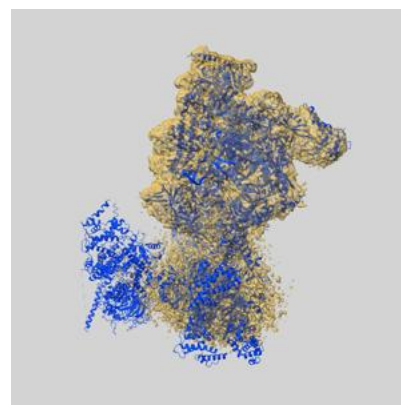
9.1 Map-model overlay ⓘ



X



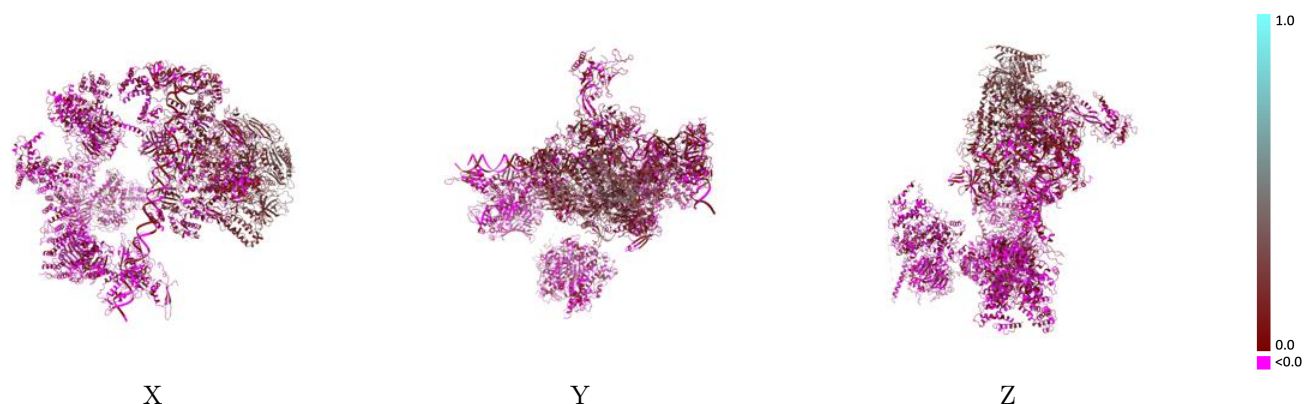
Y



Z

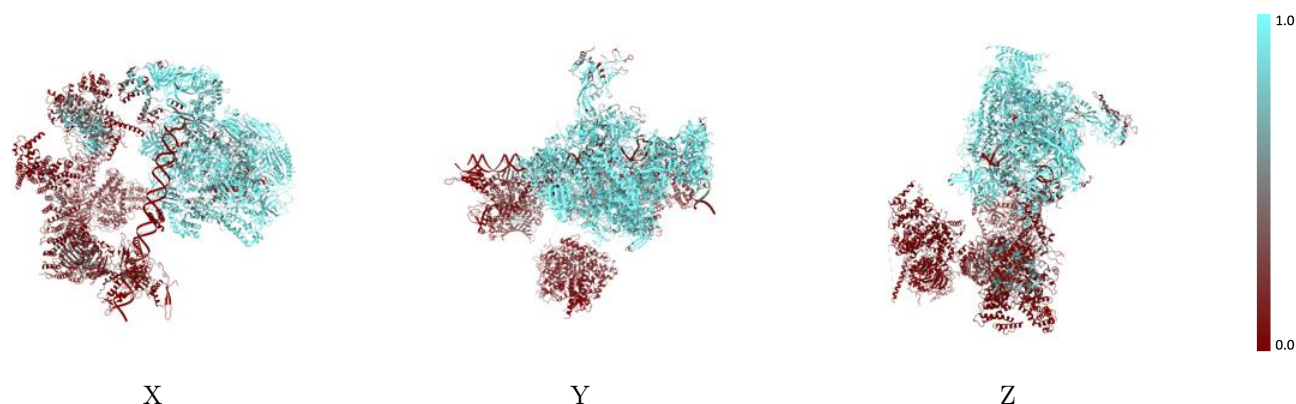
The images above show the 3D surface view of the map at the recommended contour level 0.19 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



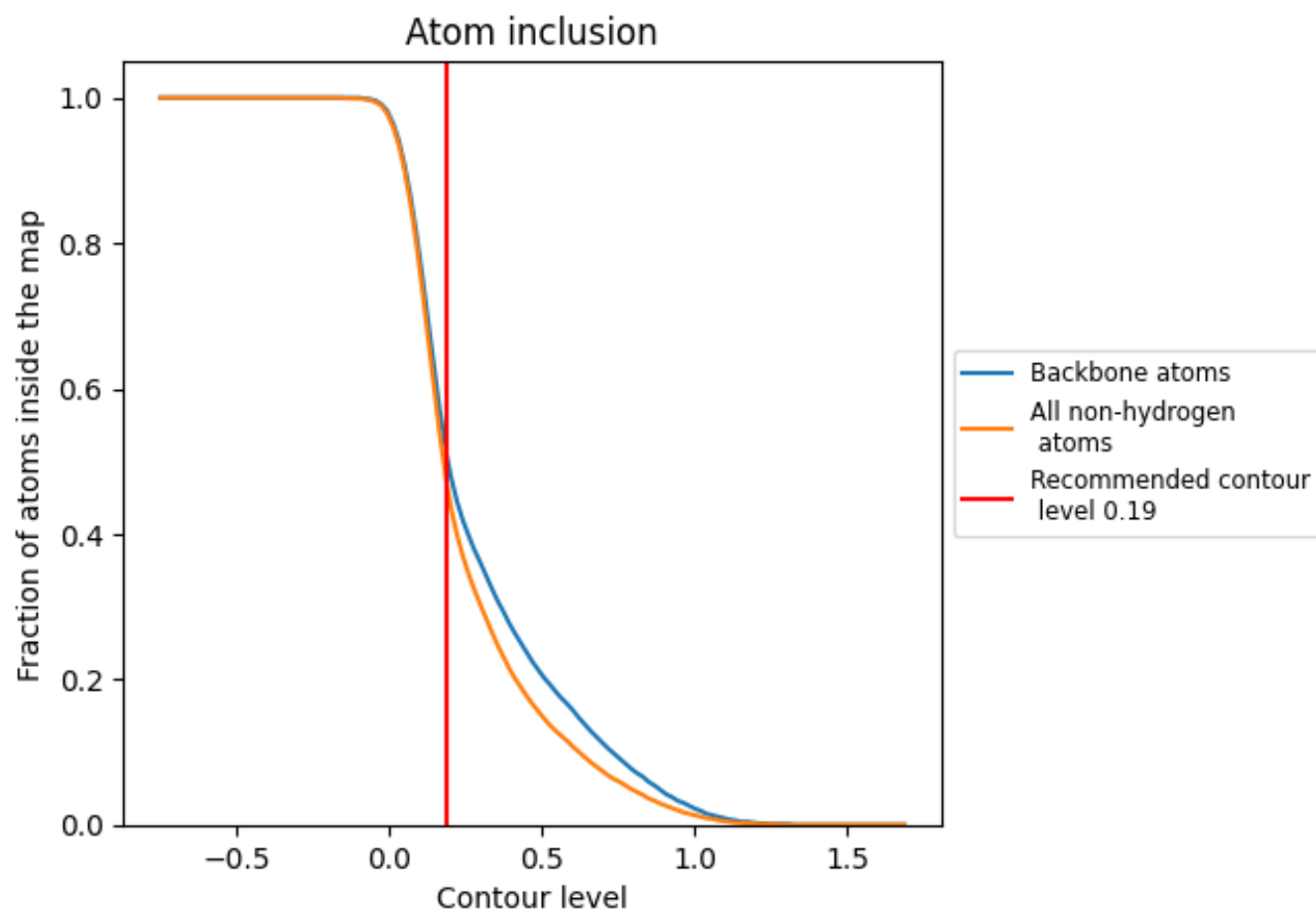
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.19).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 51% of all backbone atoms, 47% 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 (0.19) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4700	 0.0740
A	 0.0570	 -0.0030
B	 0.1580	 -0.0020
D	 0.1770	 0.0200
E	 0.4080	 0.0150
F	 0.1710	 0.0150
G	 0.0380	 0.0120
H	 0.2120	 0.0060
I	 0.3090	 0.0320
J	 0.3760	 0.0080
L	 0.0410	 0.0510
O	 0.7370	 0.0280
P	 0.9270	 0.0760
Q	 0.7070	 0.0260
R	 0.7950	 0.0950
S	 0.9090	 0.0710
T	 0.6790	 0.0610
X	 0.2470	 0.0420
Y	 0.2990	 0.0290
c	 0.0030	 -0.0170
d	 0.0000	 0.0130
e	 0.0070	 -0.0070
f	 0.0560	 0.0020
i	 0.0030	 0.0160
j	 0.0000	 0.0210
k	 0.0000	 -0.0100
l	 0.0010	 -0.0020
m	 0.0000	 -0.0130
o	 0.8420	 0.1510
p	 0.8460	 0.1660
q	 0.9570	 0.3080
r	 0.6830	 0.0570
s	 0.8600	 0.1060
t	 0.9290	 0.1960
u	 0.7780	 0.0630



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Chain	Atom inclusion	Q-score
v	 0.9500	 0.2600
w	 0.8880	 0.1830
x	 0.9310	 0.2950
y	 0.9290	 0.2800
z	 0.9580	 0.2160