



## Full wwPDB EM Validation Report ⓘ

Nov 22, 2022 – 01:12 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

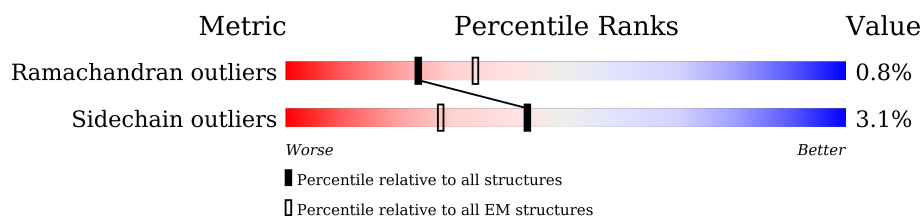
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

# 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  $\geq 3$ , 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	
2	1	548	
3	2	395	
4	3	308	
5	4	462	
6	5	71	
7	6	782	
8	7	760	
9	8	346	

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Mol	Chain	Length	Quality of chain
10	9	323	
11	A	1872	
12	B	1199	
13	D	1085	
13	d	1085	
14	E	800	
14	e	800	
15	F	677	
15	f	677	
16	G	349	
17	H	310	
18	I	264	
18	i	264	
19	J	218	
19	j	218	
20	L	161	
20	l	161	
21	O	109	
22	P	339	
23	Q	376	
24	R	316	
25	S	517	
26	T	249	
27	U	439	
28	V	291	

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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

There are 48 unique types of molecules in this entry. The entry contains 113098 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
1	0	234	Total	C	N	O	S	0	0
			1774	1108	309	347	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	405	Total	C	N	O	S	0	0
			2634	1640	486	501	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	331	Total	C	N	O	S	0	0
			2534	1597	441	470	26		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	263	Total	C	N	O	S	0	0
			2065	1323	344	379	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	449	Total	C	N	O	S	0	0
			3579	2303	624	638	14		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	606	Total	C	N	O	S	0	0
			4880	3117	849	884	30		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	734	Total	C	N	O	S	0	0
			5833	3727	1022	1055	29		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	8	298	Total	C	N	O	S	0	0
			2370	1531	404	424	11		

- Molecule 10 is a protein called Cyclin-H.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	9	287	Total	C	N	O	S	0	0
			2334	1493	402	422	17		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	D	159	Total	C	N	O	S	0	0
			1330	830	248	249	3		

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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	546	Total	C	N	O	S	0	0
			4364	2766	757	820	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	408	Total	C	N	O	S	0	0
			3109	1970	542	579	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	145	Total	C	N	O	S	0	0
			1180	748	217	211	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	74	Total	C	N	O	S	0	0
			605	379	105	118	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	97	Total	C	N	O	S	0	0
			771	491	133	145	2		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	R	250	Total	C	N	O	S	0	0
			1929	1209	343	360	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
26	T	222	Total	C	N	O	S	0	0
			1788	1127	320	338	3		

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

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

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

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

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

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

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

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

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

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

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

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

- 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	1427	Total	C	N	O	S	0	0
			11308	7114	2023	2099	72		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	p	1134	Total	C	N	O	S	0	0
			9062	5732	1595	1671	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
			1005	632	172	197	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
			1720	1089	300	323	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
			635	406	108	116	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
			927	571	166	179	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	117	Total	C	N	O	S	0	0
			937	604	154	177	2		

- Molecule 45 is a protein called RPB12.

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

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

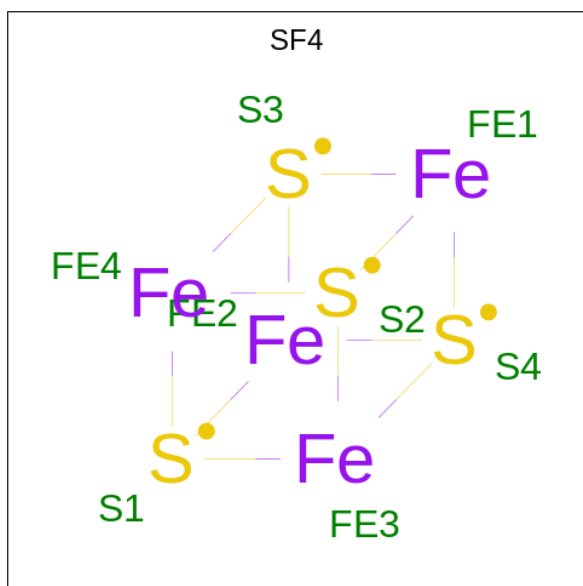
Mol	Chain	Residues	Atoms		AltConf
46	0	2	Total	Zn	0
			2	2	
46	2	3	Total	Zn	0
			3	3	
46	3	1	Total	Zn	0
			1	1	

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

- Molecule 47 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



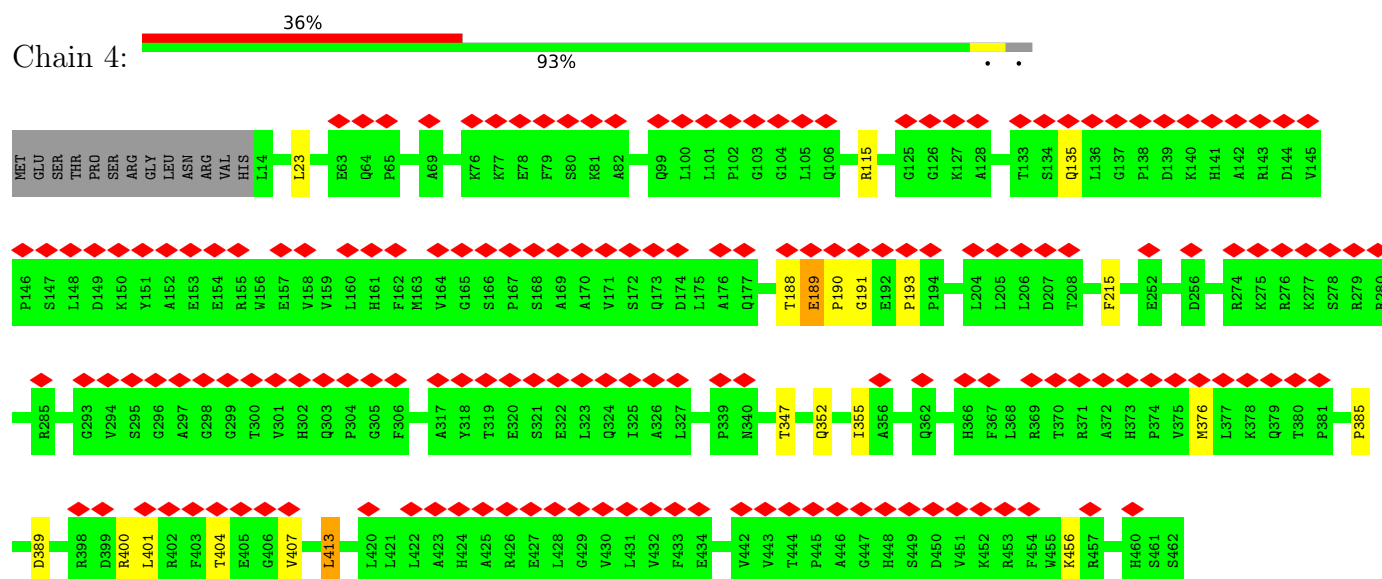
Mol	Chain	Residues	Atoms			AltConf
47	7	1	Total 8	Fe 4	S 4	0

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

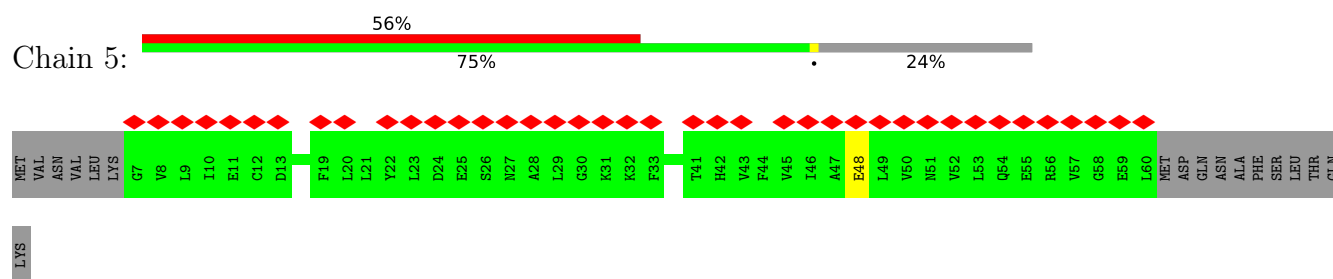
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48	o	1	Total	Mg	0
			1	1	



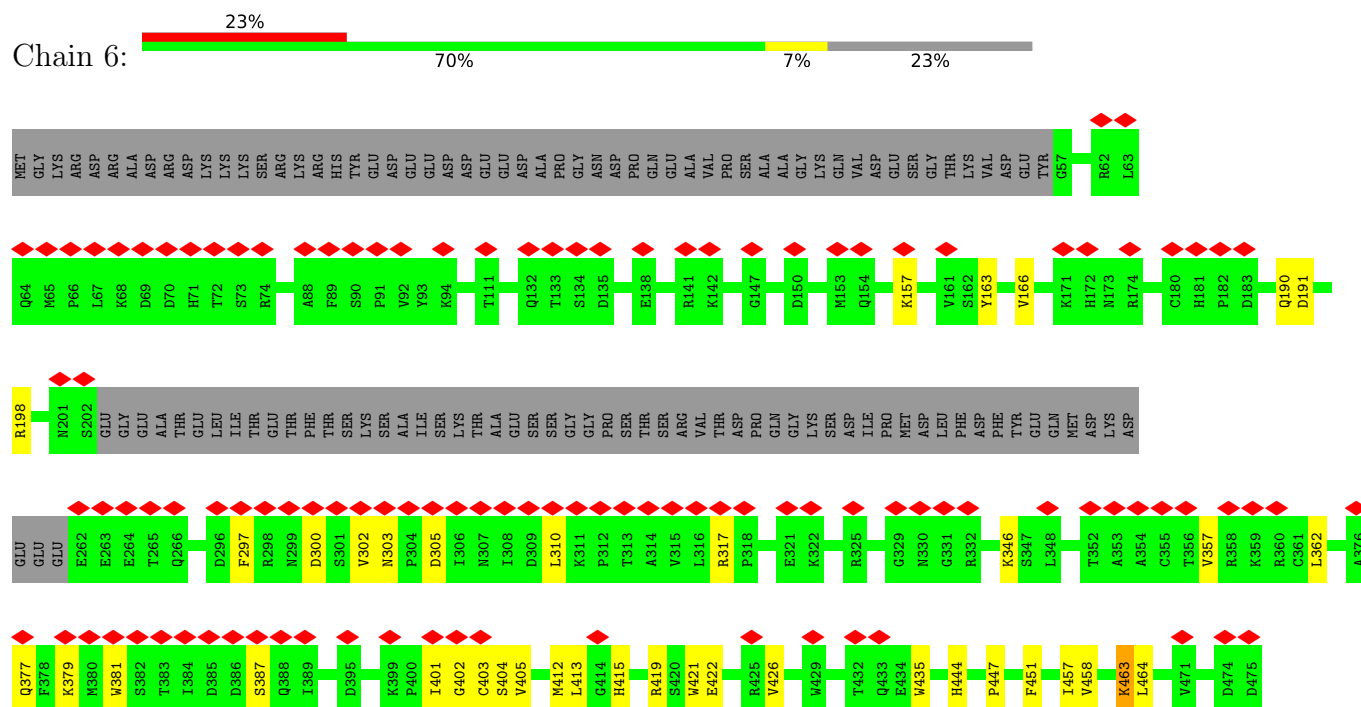


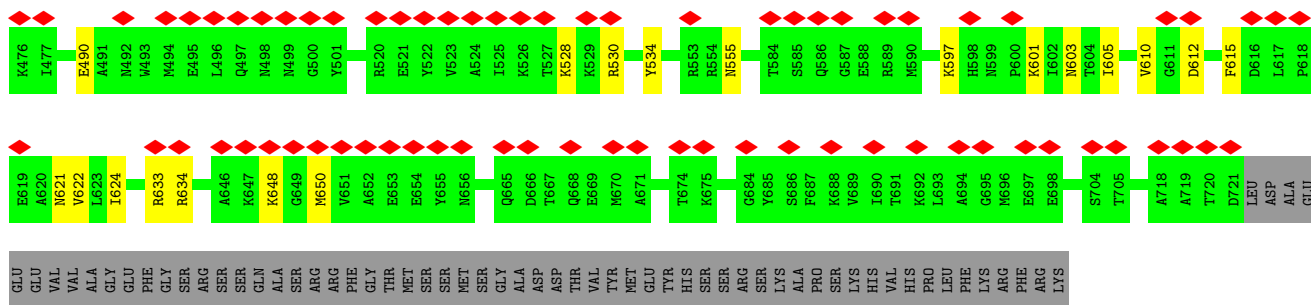


• Molecule 6: General transcription factor IIH subunit 5

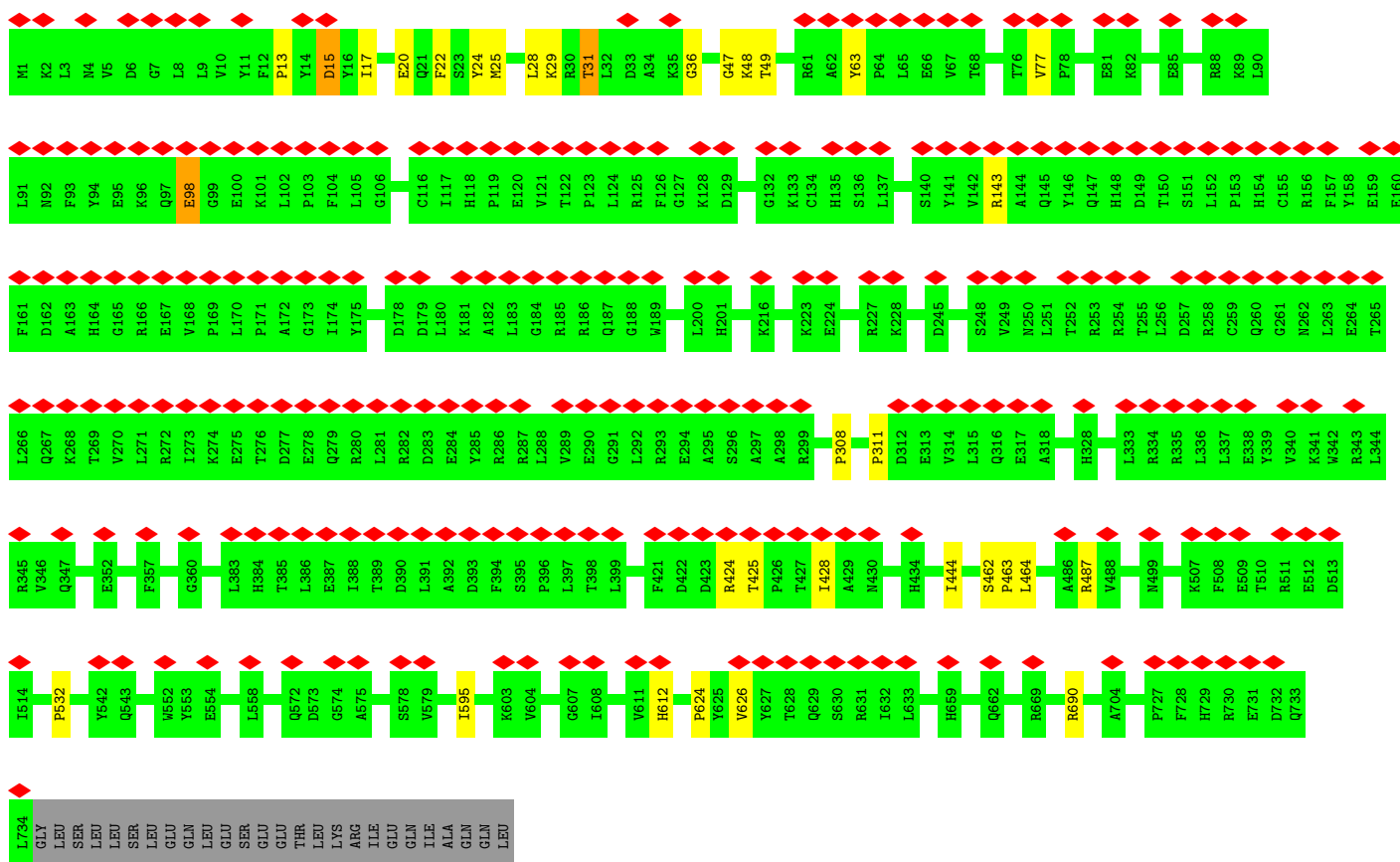


• Molecule 7: General transcription and DNA repair factor IIH helicase subunit XPB

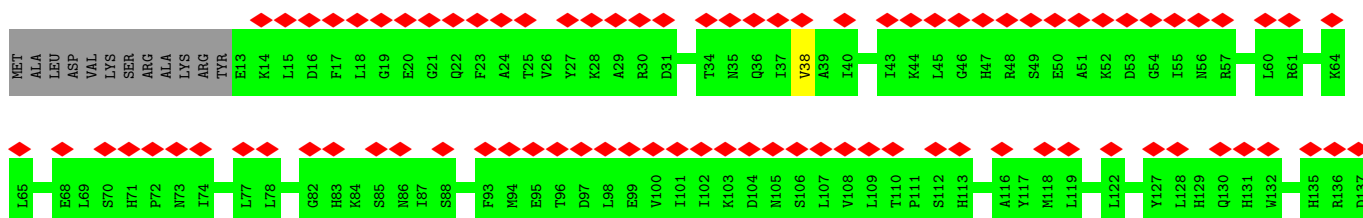
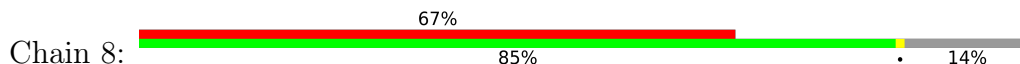


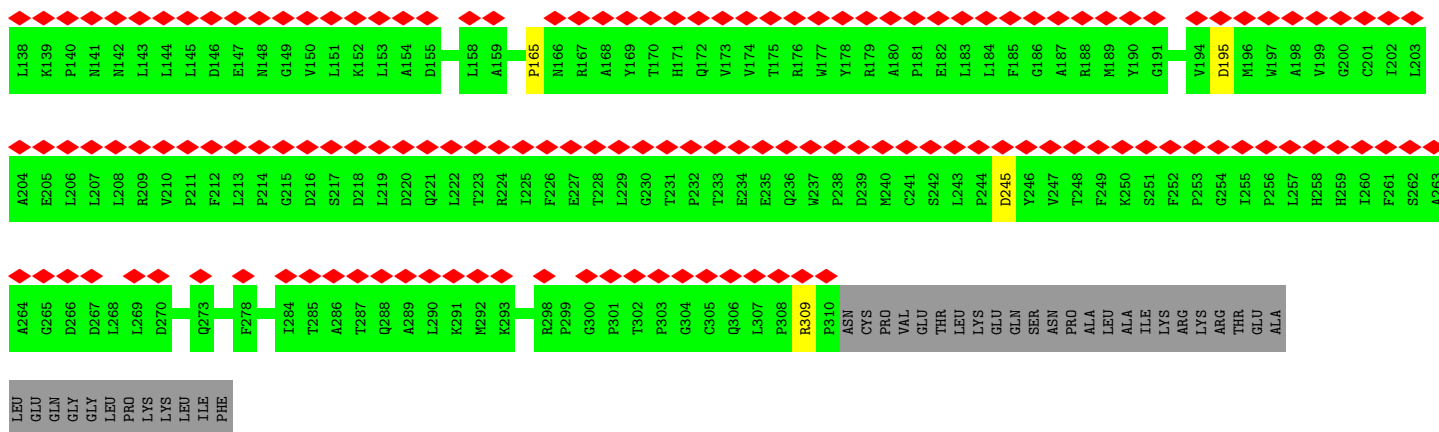


• Molecule 8: General transcription and DNA repair factor IIIH helicase subunit XPD

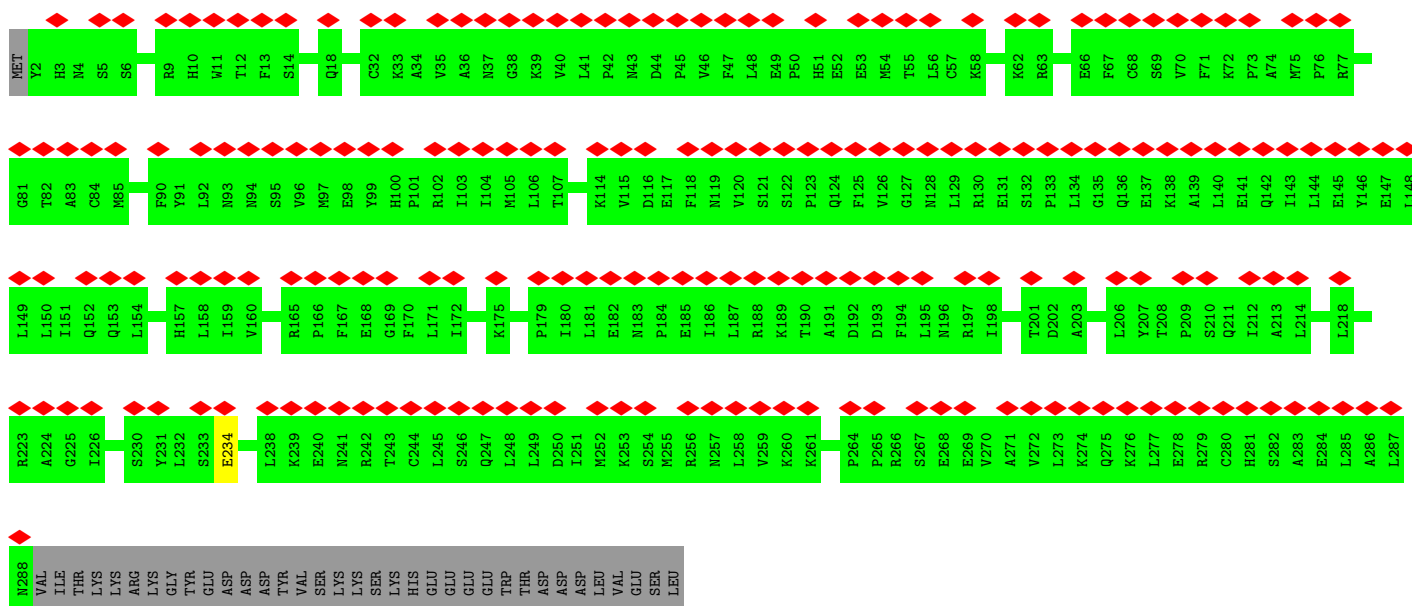
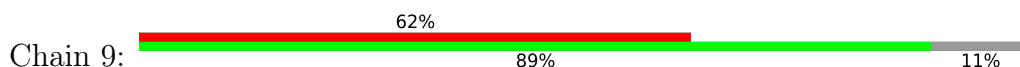


• Molecule 9: Cyclin-dependent kinase 7

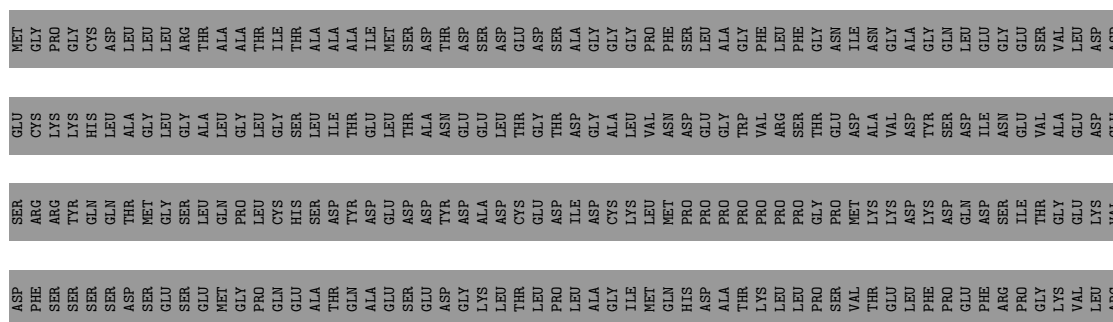




• Molecule 10: Cyclin-H



• Molecule 11: Transcription initiation factor TFIID subunit 1







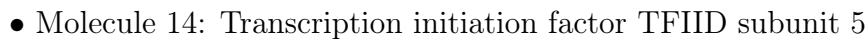


**L1078** **K1085**

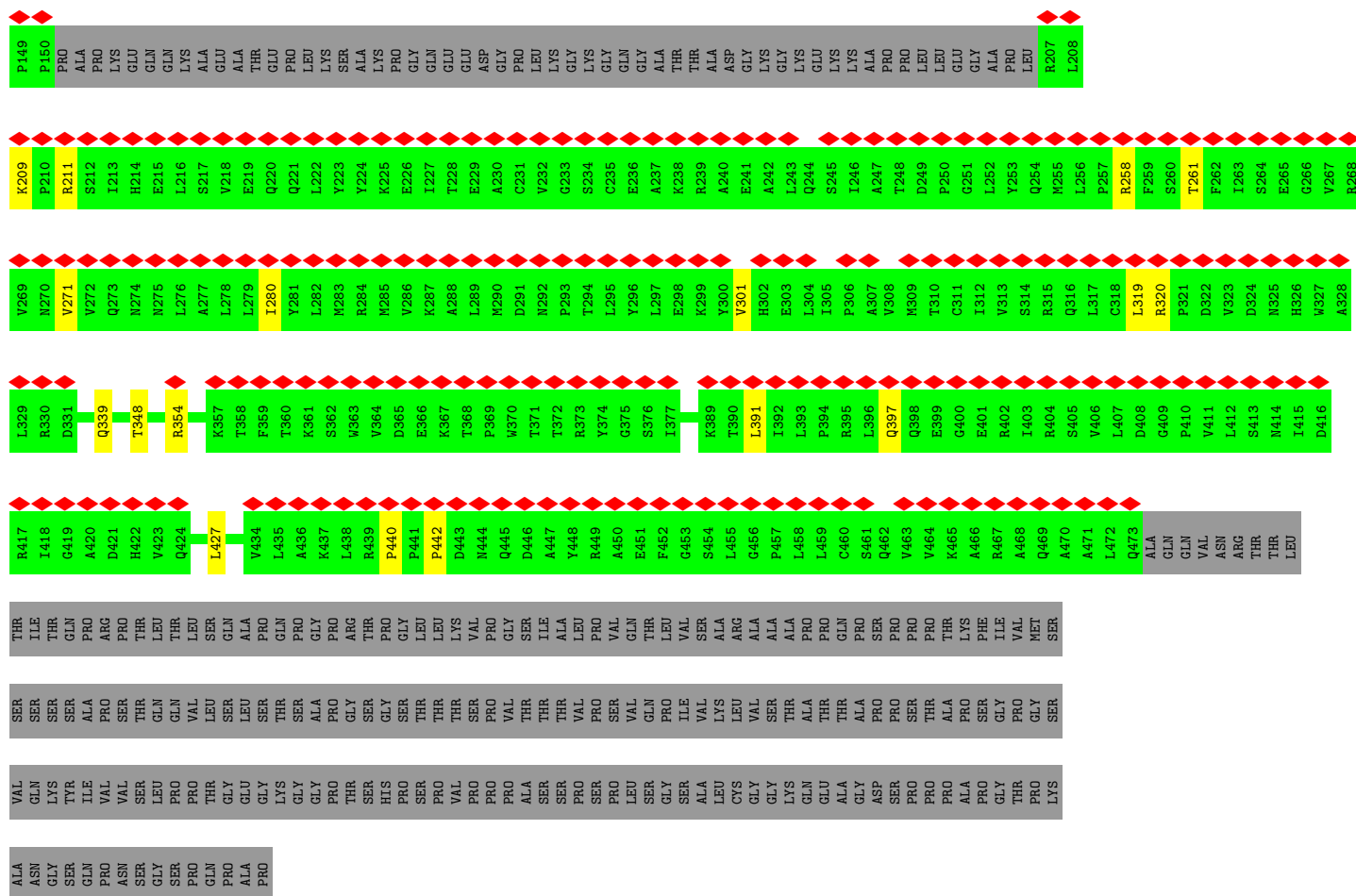
Chain d: 

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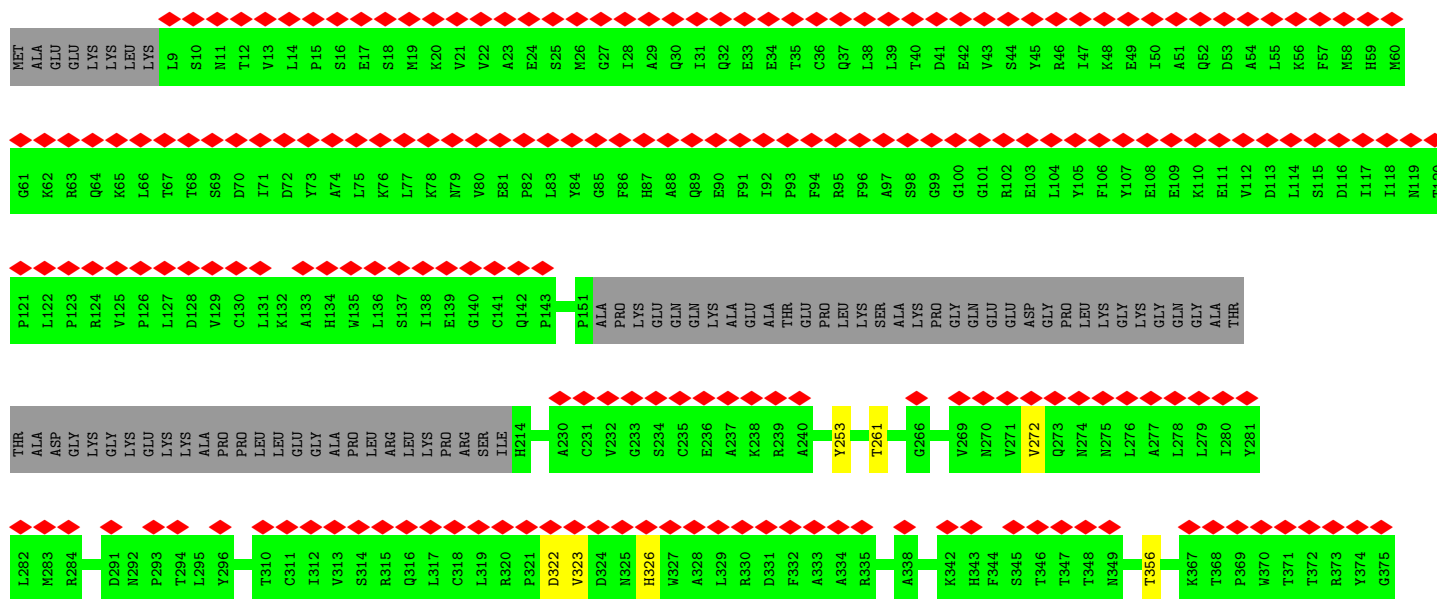
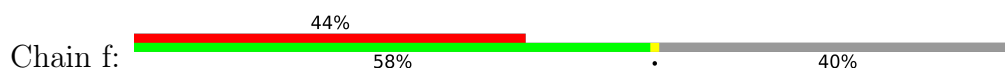


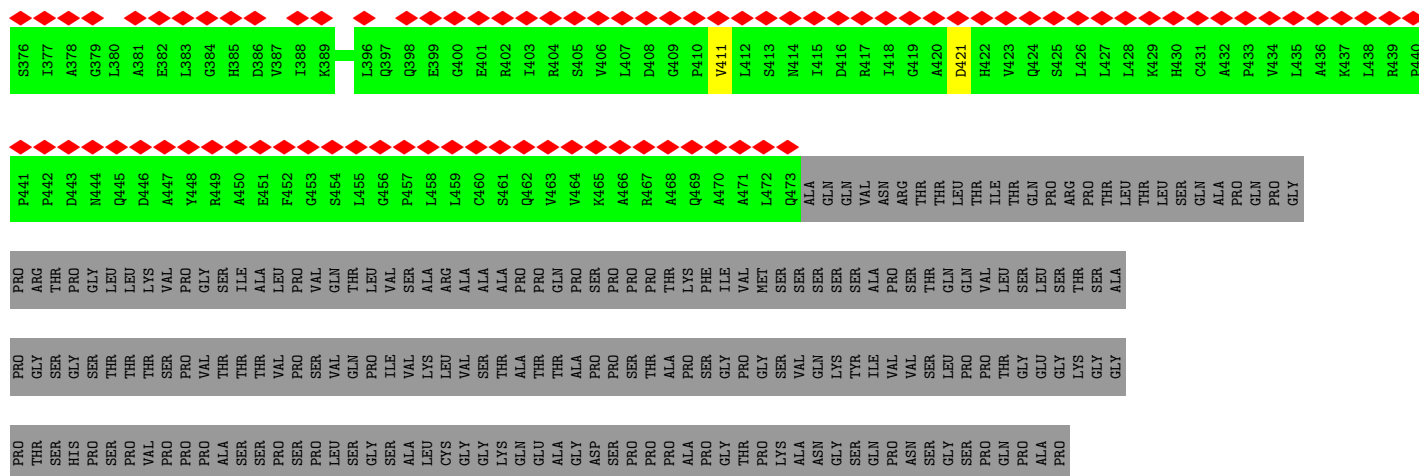
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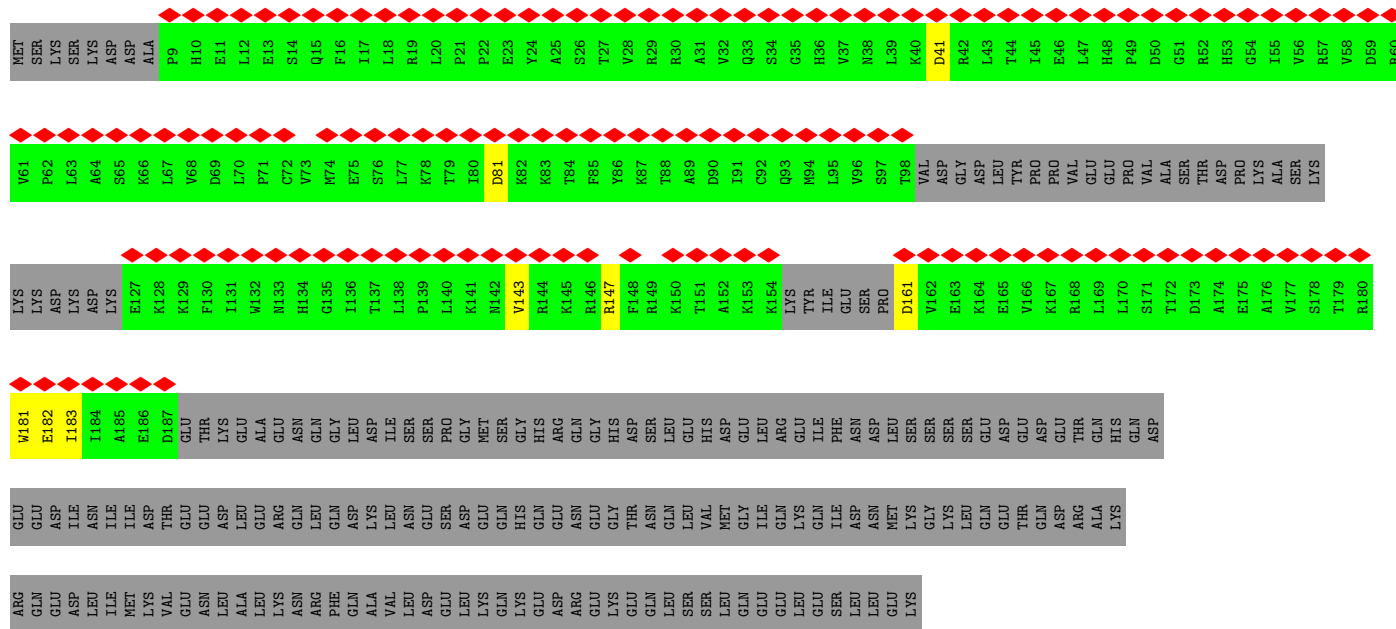


• Molecule 15: Transcription initiation factor TFIID subunit 6

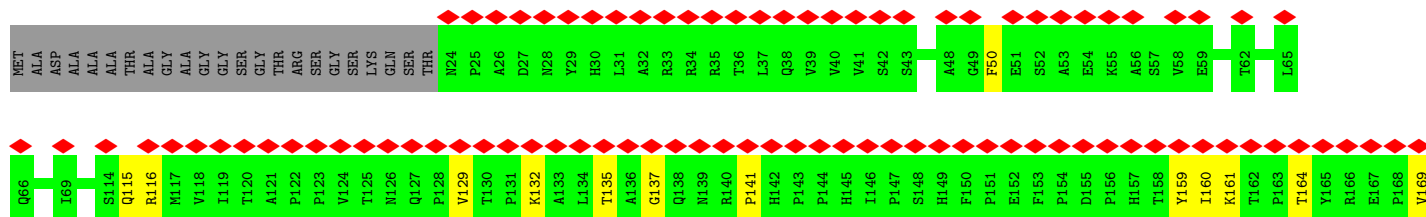


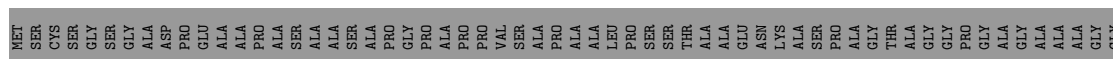


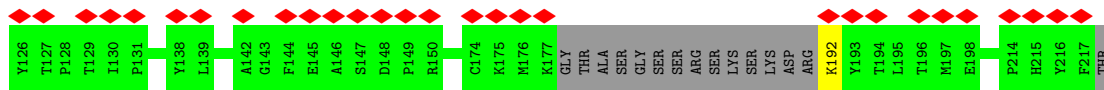
• Molecule 16: Transcription initiation factor TFIID subunit 7



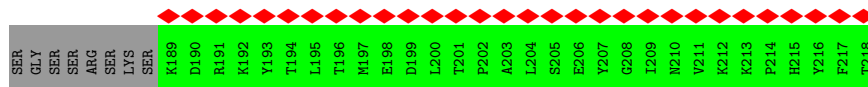
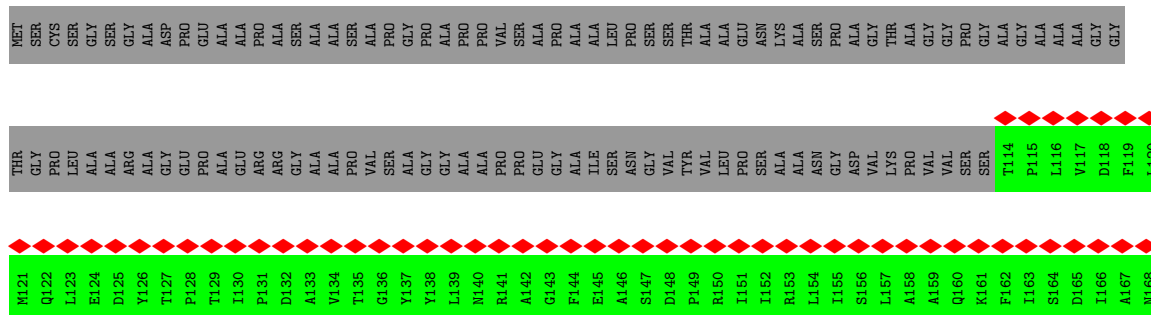
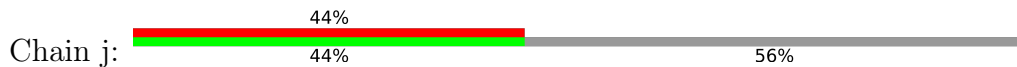
• Molecule 17: Transcription initiation factor TFIID subunit 8



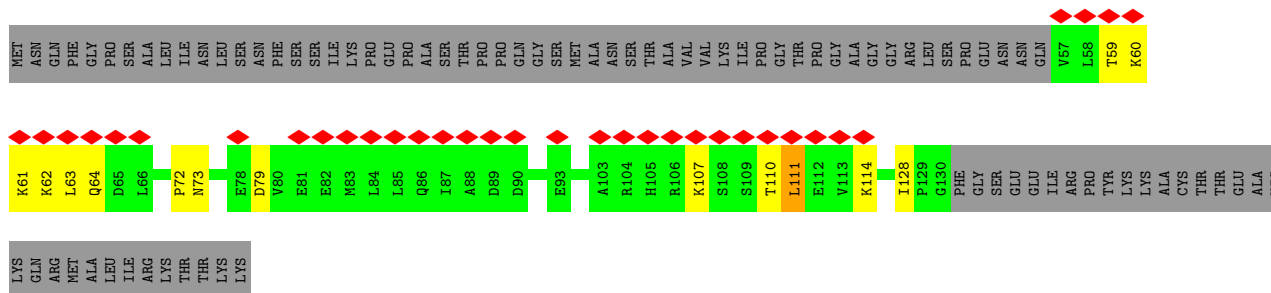
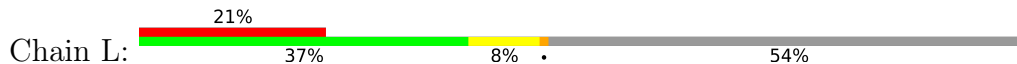




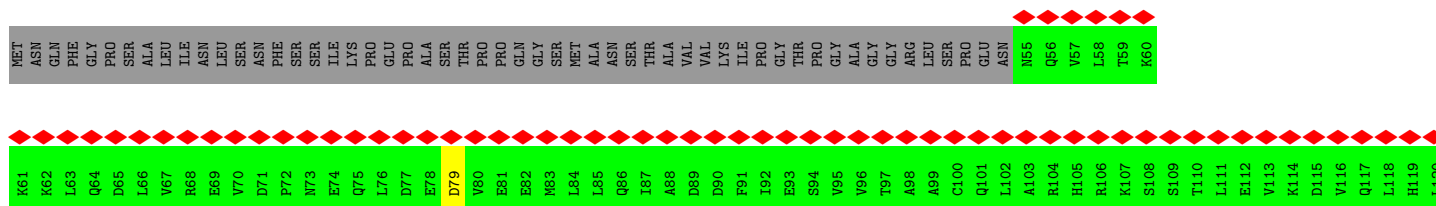
- Molecule 19: Transcription initiation factor TFIID subunit 10

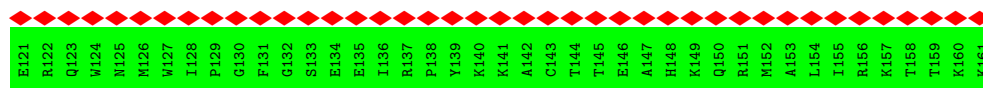


- Molecule 20: Transcription initiation factor TFIID subunit 12



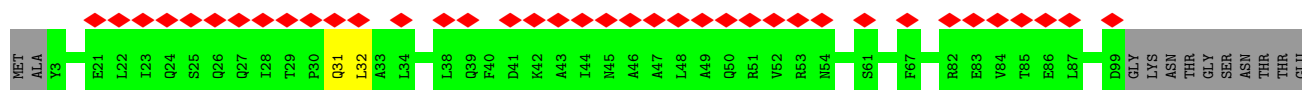
- Molecule 20: Transcription initiation factor TFIID subunit 12





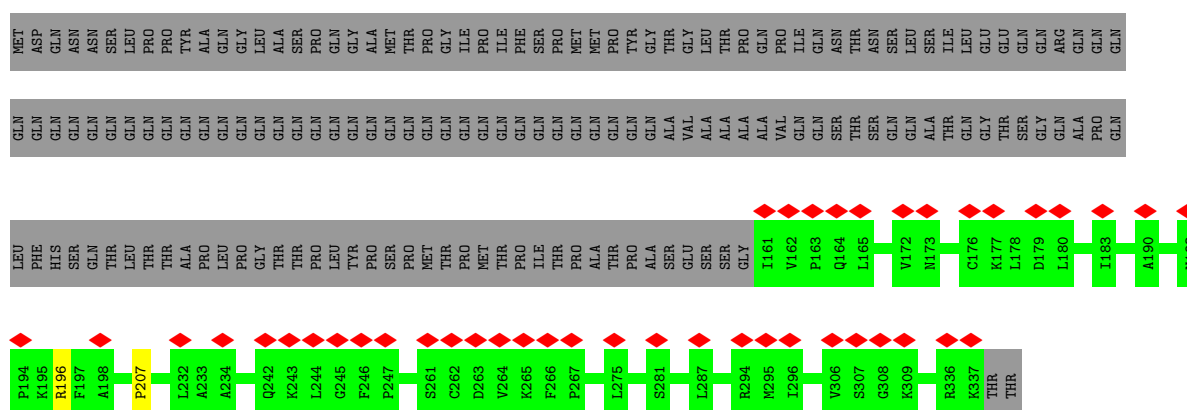
- Molecule 21: Transcription initiation factor IIA subunit 2

Chain O: 35% 87% 11%



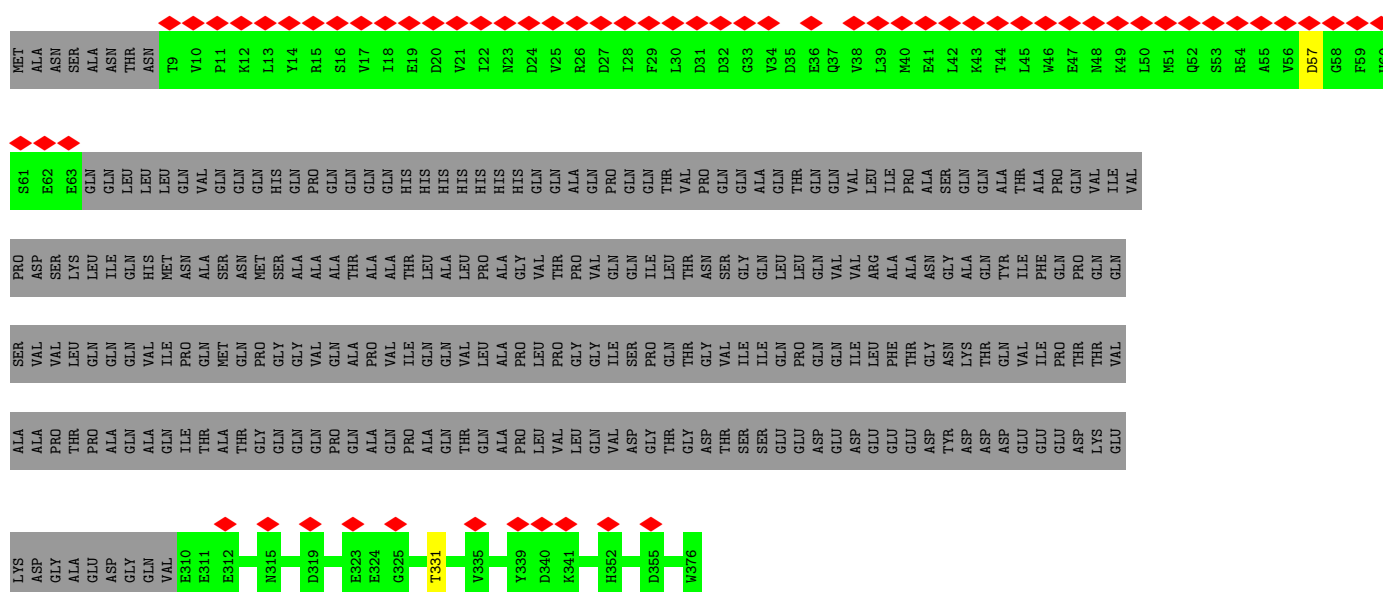
- Molecule 22: TATA-box-binding protein

Chain P: 13% 52% 48%

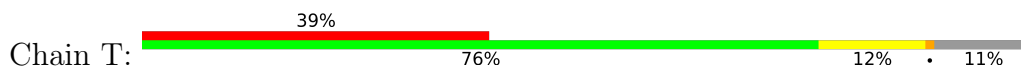


- Molecule 23: Transcription initiation factor IIA subunit 1

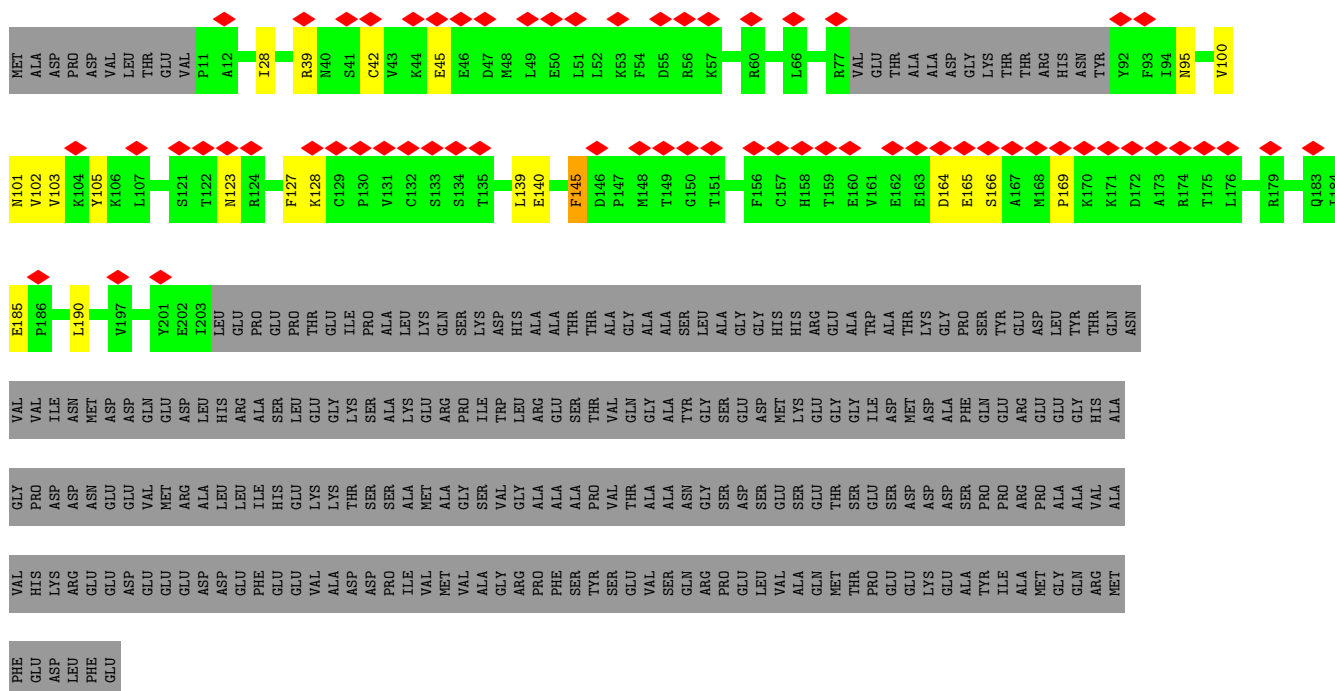
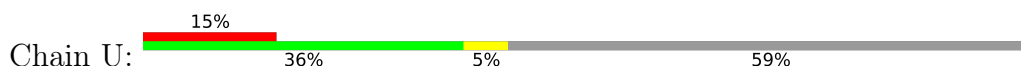
Chain Q: 17% 32% 68%



- Molecule 24: Transcription initiation factor IIB



- Molecule 27: General transcription factor IIE subunit 1



- Molecule 28: Transcription initiation factor IIE subunit beta





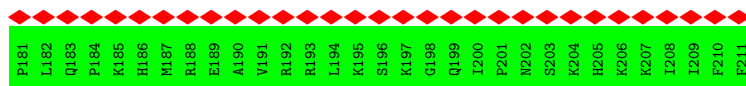
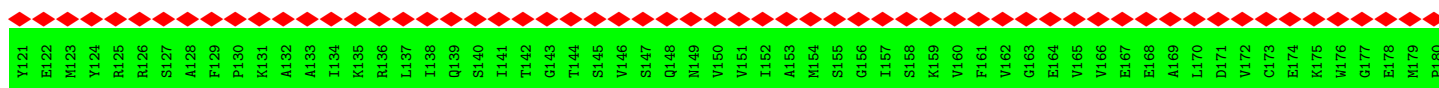
[illegible]

- Molecule 32: Transcription initiation factor TFIID subunit 11



MET	ASP	ASP	HIS	GLU	SER	PRO	SER	ASP	LYS	GLY	GLY	THR	GLU	GLY	GLU	SER	ASP	GLU	GLU	THR	ALA	ALA	VAL	PRO	PRO	GLY	ASP	ASP	PRO	GLY	ALA	ALA	THR	THR	ILE	PRO	PRO	GLU	GLU	THR	THR	LEU	LYS	GLU	ALA	ALA	ALA	ALA	GLU	GLU	GLY	GLU	LEU	GLY	GLU
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GLN	ASP	VAL	SER	ASP	LEU	THR	THR	VAL	GLU	GLU	ARG	ASP	ASP	SER	SER	LEU	LEU	LEU	ASN	PRO	ALA	ALA	LYS	LYS	LYS	LEU	LYS	ILE	ASP	THR	THR	LYS	LYS	GLU	GLU	LYS	LYS	LYS	GLN	LYS	VAL	VAL	ASP	ASP	GLU	GLU	ASP	ASP	GLU	ILE	ILE	GLN	LYS	MET	MET	GLN	ILE	ILE	LEU	VAL	SER	SER	SER	PHE	PHE	S14	E145	Q117	L118	M119	E120	E121	E122	E123	E124	E125	E126	E127	E128	E129	E130	E131	E132	E133	E134	E135	E136	E137	E138	E139	E140	E141	E142	E143	E144	E146	E147	E148	E149	E150	E151	E152	E153	E154	E155	E156	E157	E158	E159	E160	E161	E162	E163	E164	E165	E166	E167	E168	E169	E170	E171	E172	E173	E174	E175	E176	E177	E178	E179	E180	E181	E182	E183	E184	E185	E186	E187	E188	E189	E190	E191	E192	E193	E194	E195	E196	E197	E198	E199	E200	E201	E202	E203	E204	E205	E206	E207	E208	E209	E210	E211	E212	E213	E214	E215	E216	E217	E218	E219	E220	E221	E222	E223	E224	E225	E226	E227	E228	E229	E230	E231	E232	E233	E234	E235	E236	E237	E238	E239	E240	E241	E242	E243	E244	E245	E246	E247	E248	E249	E250	E251	E252	E253	E254	E255	E256	E257	E258	E259	E260	E261	E262	E263	E264	E265	E266	E267	E268	E269	E270	E271	E272	E273	E274	E275	E276	E277	E278	E279	E280	E281	E282	E283	E284	E285	E286	E287	E288	E289	E290	E291	E292	E293	E294	E295	E296	E297	E298	E299	E300	E301	E302	E303	E304	E305	E306	E307	E308	E309	E310	E311	E312	E313	E314	E315	E316	E317	E318	E319	E320	E321	E322	E323	E324	E325	E326	E327	E328	E329	E330	E331	E332	E333	E334	E335	E336	E337	E338	E339	E340	E341	E342	E343	E344	E345	E346	E347	E348	E349	E350	E351	E352	E353	E354	E355	E356	E357	E358	E359	E360	E361	E362	E363	E364	E365	E366	E367	E368	E369	E370	E371	E372	E373	E374	E375	E376	E377	E378	E379	E380	E381	E382	E383	E384	E385	E386	E387	E388	E389	E390	E391	E392	E393	E394	E395	E396	E397	E398	E399	E400	E401	E402	E403	E404	E405	E406	E407	E408	E409	E410	E411	E412	E413	E414	E415	E416	E417	E418	E419	E420	E421	E422	E423	E424	E425	E426	E427	E428	E429	E430	E431	E432	E433	E434	E435	E436	E437	E438	E439	E440	E441	E442	E443	E444	E445	E446	E447	E448	E449	E450	E451	E452	E453	E454	E455	E456	E457	E458	E459	E460	E461	E462	E463	E464	E465	E466	E467	E468	E469	E470	E471	E472	E473	E474	E475	E476	E477	E478	E479	E480	E481	E482	E483	E484	E485	E486	E487	E488	E489	E490	E491	E492	E493	E494	E495	E496	E497	E498	E499	E500	E501	E502	E503	E504	E505	E506	E507	E508	E509	E510	E511	E512	E513	E514	E515	E516	E517	E518	E519	E520	E521	E522	E523	E524	E525	E526	E527	E528	E529	E530	E531	E532	E533	E534	E535	E536	E537	E538	E539	E540	E541	E542	E543	E544	E545	E546	E547	E548	E549	E550	E551	E552	E553	E554	E555	E556	E557	E558	E559	E560	E561	E562	E563	E564	E565	E566	E567	E568	E569	E570	E571	E572	E573	E574	E575	E576	E577	E578	E579	E580	E581	E582	E583	E584	E585	E586	E587	E588	E589	E590	E591	E592	E593	E594	E595	E596	E597	E598	E599	E600	E601	E602	E603	E604	E605	E606	E607	E608	E609	E610	E611	E612	E613	E614	E615	E616	E617	E618	E619	E620	E621	E622	E623	E624	E625	E626	E627	E628	E629	E630	E631	E632	E633	E634	E635	E636	E637	E638	E639	E640	E641	E642	E643	E644	E645	E646	E647	E648	E649	E650	E651	E652	E653	E654	E655	E656	E657	E658	E659	E660	E661	E662	E663	E664	E665	E666	E667	E668	E669	E670	E671	E672	E673	E674	E675	E676	E677	E678	E679	E680	E681	E682	E683	E684	E685	E686	E687	E688	E689	E690	E691	E692	E693	E694	E695	E696	E697	E698	E699	E700	E701	E702	E703	E704	E705	E706	E707	E708	E709	E710	E711	E712	E713	E714	E715	E716	E717	E718	E719	E720	E721	E722	E723	E724	E725	E726	E727	E728	E729	E730	E731	E732	E733	E734	E735	E736	E737	E738	E739	E740	E741	E742	E743	E744	E745	E746	E747	E748	E749	E750	E751	E752	E753	E754	E755	E756	E757	E758	E759	E760	E761	E762	E763	E764	E765	E766	E767	E768	E769	E770	E771	E772	E773	E774	E775	E776	E777	E778	E779	E780	E781	E782	E783	E784	E785	E786	E787	E788	E789	E790	E791	E792	E793	E794	E795	E796	E797	E798	E799	E800	E801	E802	E803	E804	E805	E806	E807	E808	E809	E810	E811	E812	E813	E814	E815	E816	E817	E818	E819	E820	E821	E822	E823	E824	E825	E826	E827	E828	E829	E830	E831	E832	E833	E834	E835	E836	E837	E838	E839	E840	E841	E842	E843	E844	E845	E846	E847	E848	E849	E850	E851	E852	E853	E854	E855	E856	E857	E858	E859	E860	E861	E862	E863	E864	E865	E866	E867	E868	E869	E870	E871	E872	E873	E874	E875	E876	E877	E878	E879	E880	E881	E882	E883	E884	E885	E886	E887	E888	E889	E890	E891	E892	E893	E894	E895	E896	E897	E898	E899	E900	E901	E902	E903	E904	E905	E906	E907	E908	E909	E910	E911	E912	E913	E914	E915	E916	E917	E918	E919	E920	E921	E922	E923	E924	E925	E926	E927	E928	E929	E930	E931	E932	E933	E934	E935	E936	E937	E938	E939	E940	E941	E942	E943	E944	E945	E946	E947	E948	E949	E950	E951	E952	E953	E954	E955	E956	E957	E958	E959	E960	E961	E962	E963	E964	E965	E966	E967	E968	E969	E970	E971	E972	E973	E974	E975	E976	E977	E978	E979	E980	E981	E982	E983	E984	E985	E986	E987	E988	E989	E990	E991	E992	E993	E994	E995	E996	E997	E998	E999	E1000
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- Molecule 33: Transcription initiation factor TFIID subunit 13



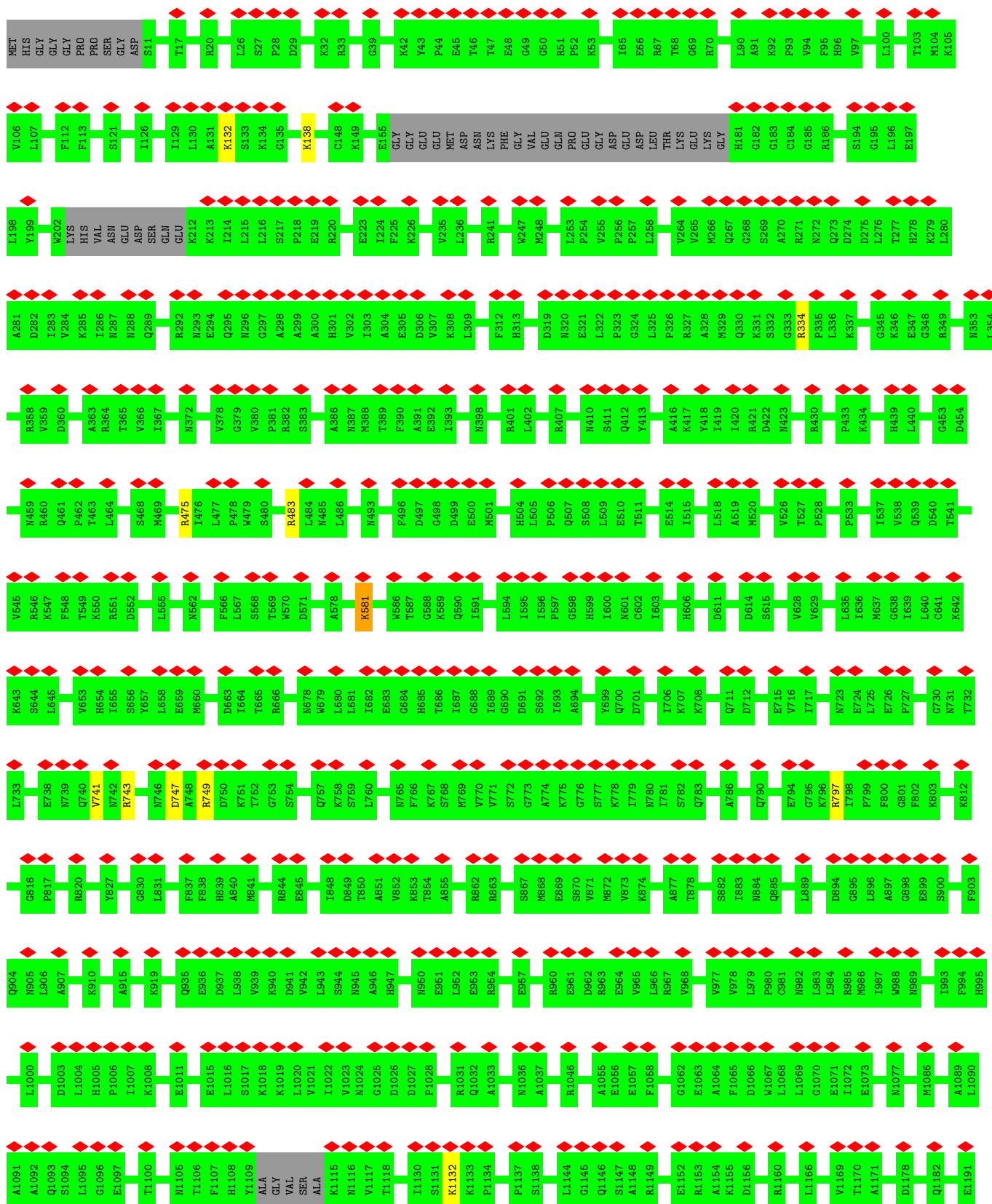
MET	ALA	ASP	GLU	GLU	GLU	ASP	PRO	THR	PHE	GLU	GLU	ASN	GLU	GLU	ILE	GLY	GLY	GLY	ALA	GLU	GLY	GLY	GLN	GLY	LYS	R28	R29	R30	L31	F32	S33	S34	E35	L36	R37	C38	N39	M40	Y41	G42	F43	G44	D45	D46	Q47	N48	P49	Y50	T51	E52	S53	V54	D55	I56	L57	E58	D59	F60	L61	L62	L63	L64	L65	L66	L67	L68	L69	L70	L71	L72	L73	L74	L75	L76	L77	L78	L79	L80	L81	L82	L83	L84	L85	L86	L87	L88	L89	L90	L91	L92	L93	L94	L95	L96	L97	L98	L99	L100	L101	L102	L103	L104	L105	L106	L107	L108	L109	L110	L111	L112	L113	L114	L115	L116	L117	L118	L119	L120	L121	L122	L123	L124	L125	L126	L127	L128	L129	L130	L131	L132	L133	L134	L135	L136	L137	L138	L139	L140	L141	L142	L143	L144	L145	L146	L147	L148	L149	L150	L151	L152	L153	L154	L155	L156	L157	L158	L159	L160	L161	L162	L163	L164	L165	L166	L167	L168	L169	L170	L171	L172	L173	L174	L175	L176	L177	L178	L179	L180	L181	L182	L183	L184	L185	L186	L187	L188	L189	L190	L191	L192	L193	L194	L195	L196	L197	L198	L199	L200	L201	L202	L203	L204	L205	L206	L207	L208	L209	L210	L211	L212	L213	L214	L215	L216	L217	L218	L219	L220	L221	L222	L223	L224	L225	L226	L227	L228	L229	L230	L231	L232	L233	L234	L235	L236	L237	L238	L239	L240	L241	L242	L243	L244	L245	L246	L247	L248	L249	L250	L251	L252	L253	L254	L255	L256	L257	L258	L259	L260	L261	L262	L263	L264	L265	L266	L267	L268	L269	L270	L271	L272	L273	L274	L275	L276	L277	L278	L279	L280	L281	L282	L283	L284	L285	L286	L287	L288	L289	L290	L291	L292	L293	L294	L295	L296	L297	L298	L299	L300	L301	L302	L303	L304	L305	L306	L307	L308	L309	L310	L311	L312	L313	L314	L315	L316	L317	L318	L319	L320	L321	L322	L323	L324	L325	L326	L327	L328	L329	L330	L331	L332	L333	L334	L335	L336	L337	L338	L339	L340	L341	L342	L343	L344	L345	L346	L347	L348	L349	L350	L351	L352	L353	L354	L355	L356	L357	L358	L359	L360	L361	L362	L363	L364	L365	L366	L367	L368	L369	L370	L371	L372	L373	L374	L375	L376	L377	L378	L379	L380	L381	L382	L383	L384	L385	L386	L387	L388	L389	L390	L391	L392	L393	L394	L395	L396	L397	L398	L399	L400	L401	L402	L403	L404	L405	L406	L407	L408	L409	L410	L411	L412	L413	L414	L415	L416	L417	L418	L419	L420	L421	L422	L423	L424	L425	L426	L427	L428	L429	L430	L431	L432	L433	L434	L435	L436	L437	L438	L439	L440	L441	L442	L443	L444	L445	L446	L447	L448	L449	L450	L451	L452	L453	L454	L455	L456	L457	L458	L459	L460	L461	L462	L463	L464	L465	L466	L467	L468	L469	L470	L471	L472	L473	L474	L475	L476	L477	L478	L479	L480	L481	L482	L483	L484	L485	L486	L487	L488	L489	L490	L491	L492	L493	L494	L495	L496	L497	L498	L499	L500	L501	L502	L503	L504	L505	L506	L507	L508	L509	L510	L511	L512	L513	L514	L515	L516	L517	L518	L519	L520	L521	L522	L523	L524	L525	L526	L527	L528	L529	L530	L531	L532	L533	L534	L535	L536	L537	L538	L539	L540	L541	L542	L543	L544	L545	L546	L547	L548	L549	L550	L551	L552	L553	L554	L555	L556	L557	L558	L559	L560	L561	L562	L563	L564	L565	L566	L567	L568	L569	L570	L571	L572	L573	L574	L575	L576	L577	L578	L579	L580	L581	L582	L583	L584	L585	L586	L587	L588	L589	L590	L591	L592	L593	L594	L595	L596	L597	L598	L599	L600	L601	L602	L603	L604	L605	L606	L607	L608	L609	L610	L611	L612	L613	L614	L615	L616	L617	L618	L619	L620	L621	L622	L623	L624	L625	L626	L627	L628	L629	L630	L631	L632	L633	L634	L635	L636	L637	L638	L639	L640	L641	L642	L643	L644	L645	L646	L647	L648	L649	L650	L651	L652	L653	L654	L655	L656	L657	L658	L659	L660	L661	L662	L663	L664	L665	L666	L667	L668	L669	L670	L671	L672	L673	L674	L675	L676	L677	L678	L679	L680	L681	L682	L683	L684	L685	L686	L687	L688	L689	L690	L691	L692	L693	L694	L695	L696	L697	L698	L699	L700	L701	L702	L703	L704	L705	L706	L707	L708	L709	L710	L711	L712	L713	L714	L715	L716	L717	L718	L719	L720	L721	L722	L723	L724	L725	L726	L727	L728	L729	L730	L731	L732	L733	L734	L735	L736	L737	L738	L739	L740	L741	L742	L743	L744	L745	L746	L747	L748	L749	L750	L751	L752	L753	L754	L755	L756	L757	L758	L759	L760	L761	L762	L763	L764	L765	L766	L767	L768	L769	L770	L771	L772	L773	L774	L775	L776	L777	L778	L779	L780	L781	L782	L783	L784	L785	L786	L787	L788	L789	L790	L791	L792	L793	L794	L795	L796	L797	L798	L799	L800	L801	L802	L803	L804	L805	L806	L807	L808	L809	L810	L811	L812	L813	L814	L815	L816	L817	L818	L819	L820	L821	L822	L823	L824	L825	L826	L827	L828	L829	L830	L831	L832	L833	L834	L835	L836	L837	L838	L839	L840	L841	L842	L843	L844	L845	L846	L847	L848	L849	L850	L851	L852	L853	L854	L855	L856	L857	L858	L859	L860	L861	L862	L863	L864	L865	L866	L867	L868	L869	L870	L871	L872	L873	L874	L875	L876	L877	L878	L879	L880	L881	L882	L883	L884	L885	L886	L887	L888	L889	L890	L891	L892	L893	L894	L895	L896	L897	L898	L899	L900	L901	L902	L903	L904	L905	L906	L907	L908	L909	L910	L911	L912	L913	L914	L915	L916	L917	L918	L919	L920	L921	L922	L923	L924	L925	L926	L927	L928	L929	L930	L931	L932	L933	L934	L935	L936	L937	L938	L939	L940	L941	L942	L943	L944	L945	L946	L947	L948	L949	L950	L951	L952	L953	L954	L955	L956	L957	L958	L959	L960	L961	L962	L963	L964	L965	L966	L967	L968	L969	L970	L971	L972	L973	L974	L975	L976	L977	L978	L979	L980	L981	L982	L983	L984	L985	L986	L987	L988	L989	L990	L991	L992	L993	L994	L995	L996	L997	L998	L999	L1000
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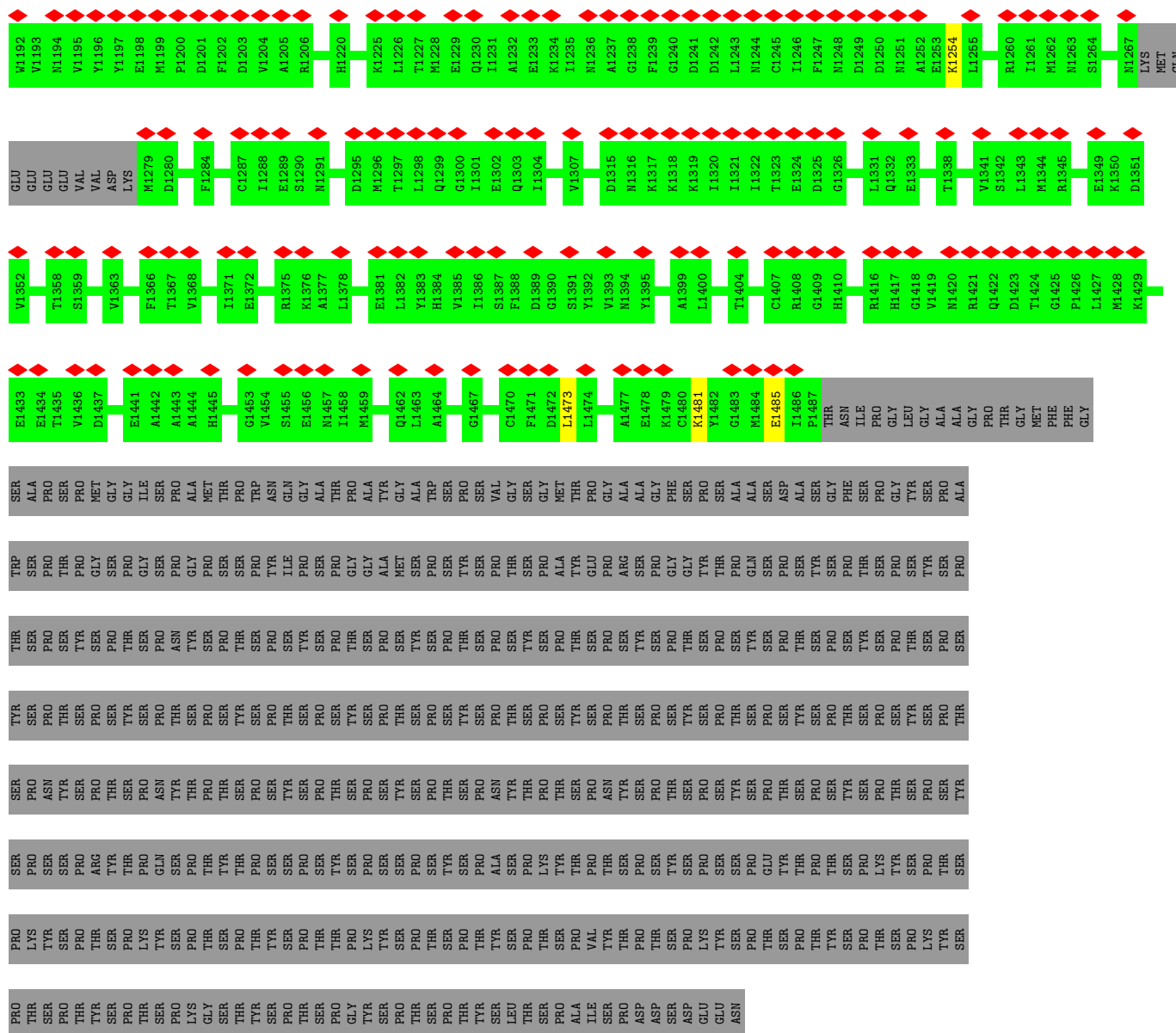
V61	I62	E63	F64	I65	T66	E67	M68	T69	H70	K71	A72	M73	S74	I75	G76	R77	Q78	G79	R80	V81	Q82	V83	E84	D85	I86	R87	F88	L89	I90	R91	K92	D93	P94	R95	K96	F97	A98	R99	V100	K101	D102	L103	L104	T105	M106	N107	E108	E109	L110	K111	A112	R113	A114	LYS	ALA	PHE	ASP	GLU
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ASN  
TYR  
GLY  
SER

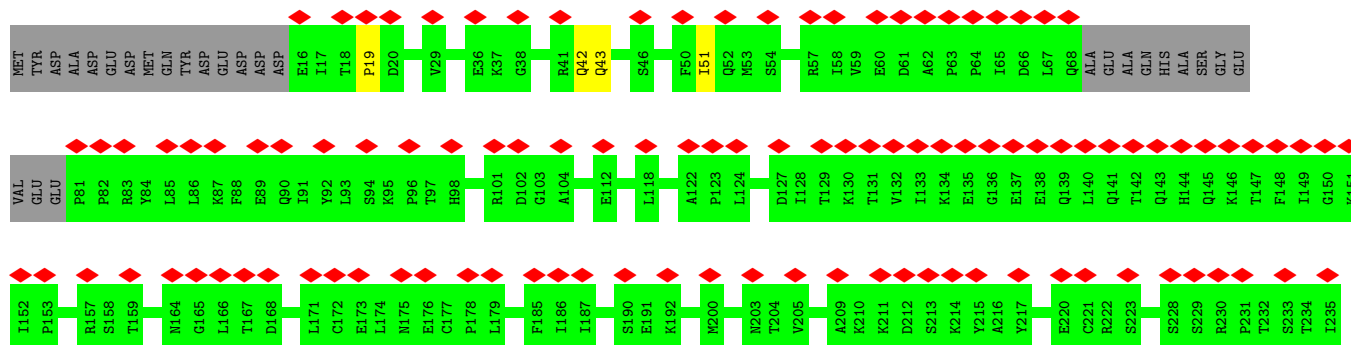
- Molecule 34: DNA-directed RNA polymerase II subunit RPB1

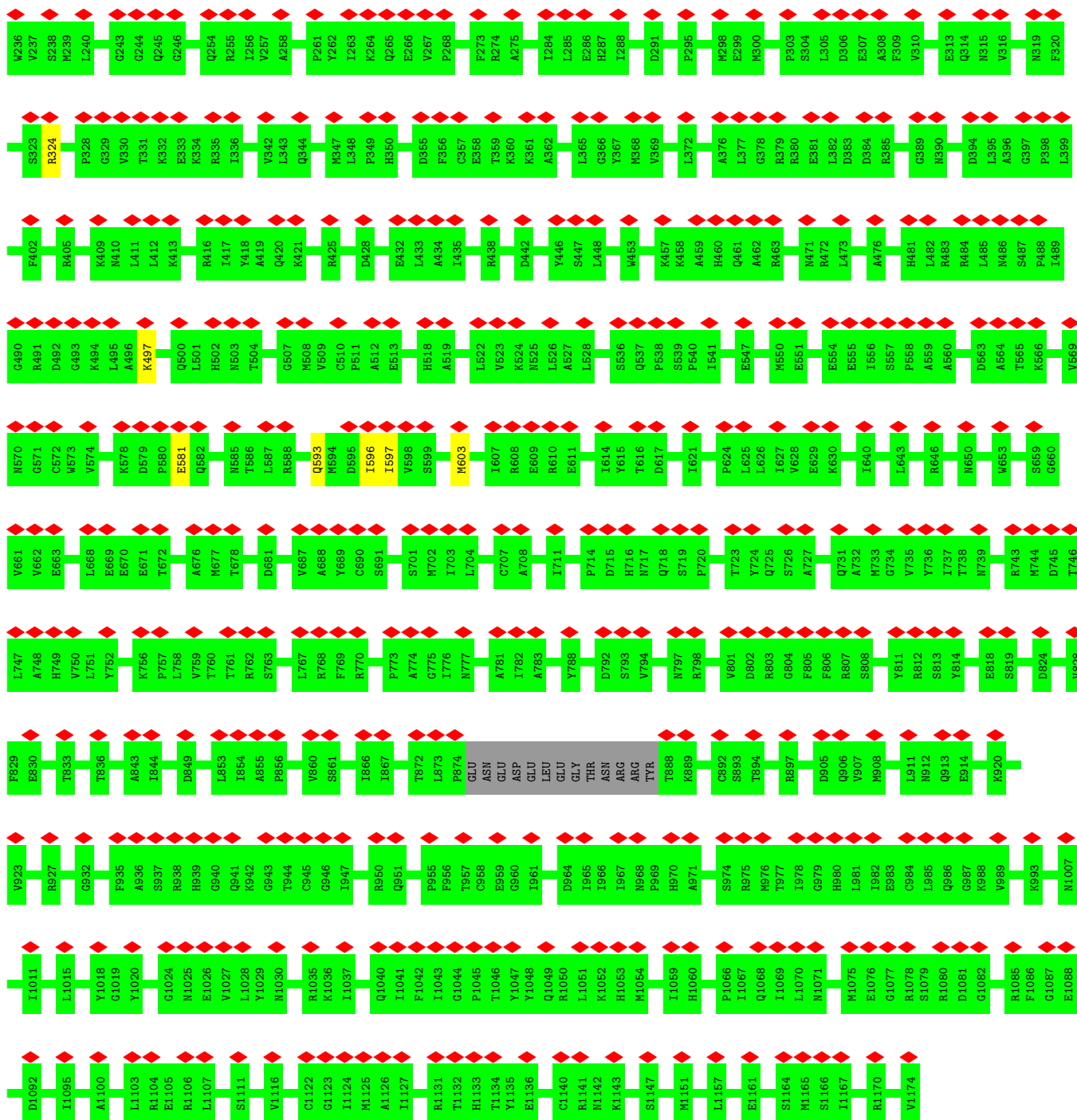




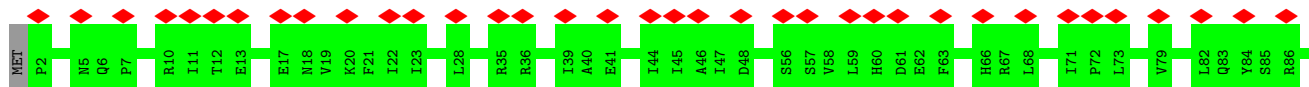
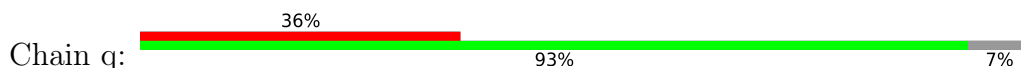


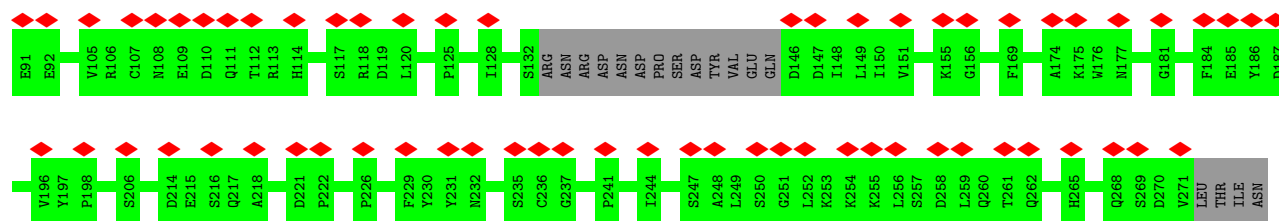
• Molecule 35: DNA-directed RNA polymerase subunit beta



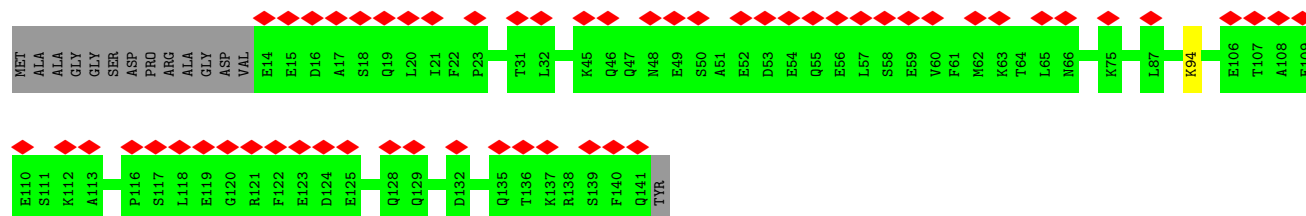
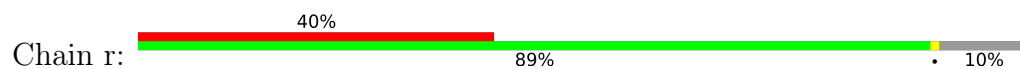


• Molecule 36: DNA-directed RNA polymerase II subunit RPB3

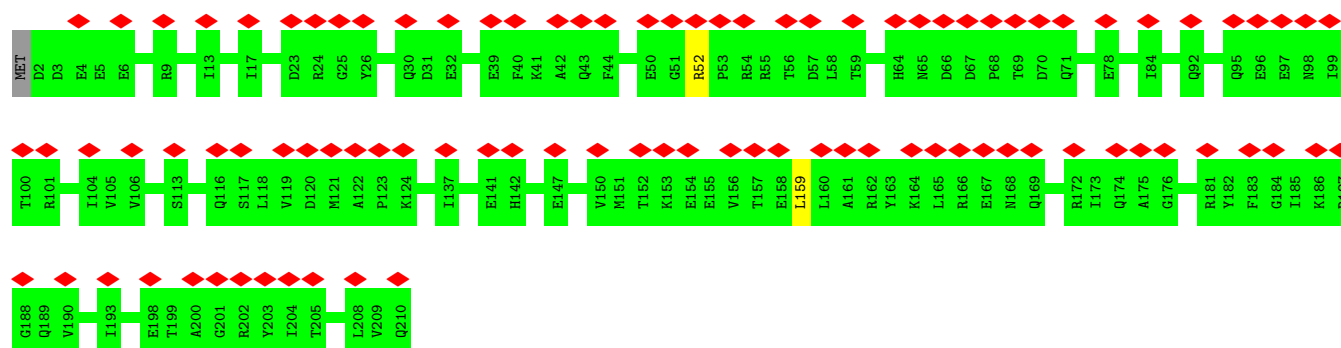




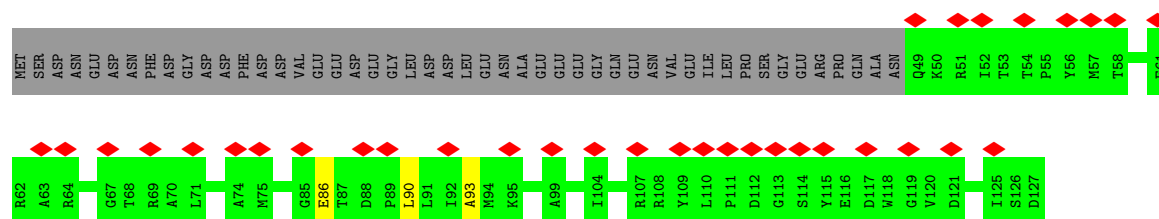
• Molecule 37: DNA-directed RNA polymerase II subunit RPB4



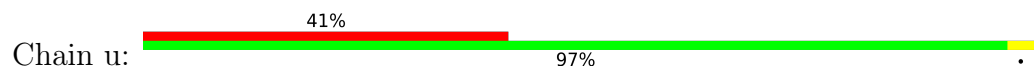
• Molecule 38: DNA-directed RNA polymerase II subunit E

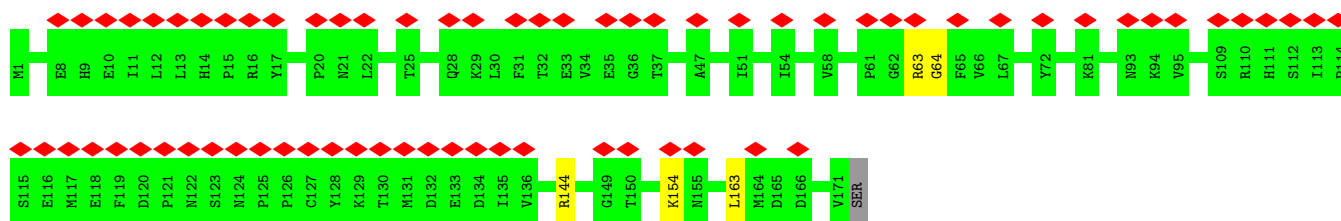


• Molecule 39: DNA-directed RNA polymerase II subunit F

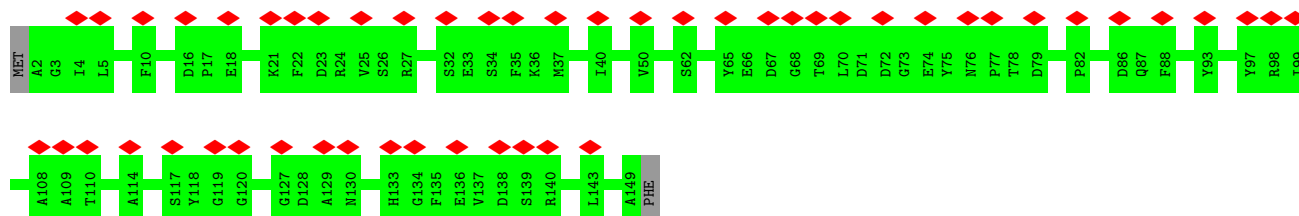


• Molecule 40: DNA-directed RNA polymerase II subunit RPB7

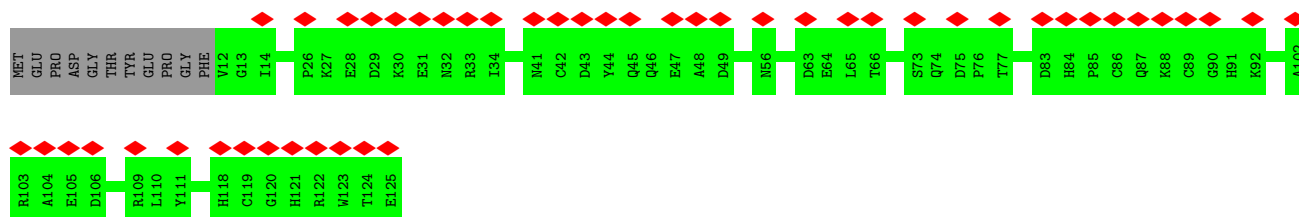




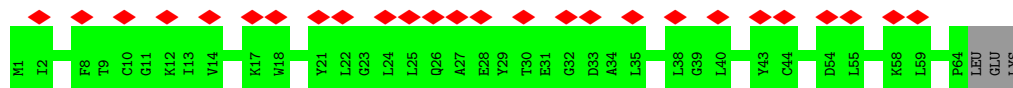
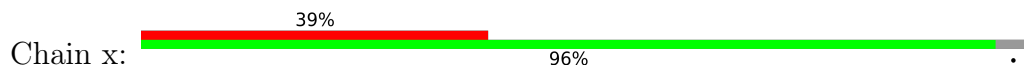
- Molecule 41: DNA-directed RNA polymerases I, II, and III subunit RPABC3



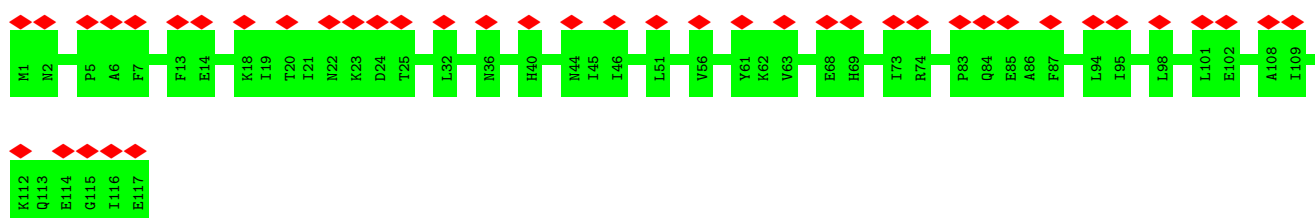
- Molecule 42: DNA-directed RNA polymerase II subunit RPB9



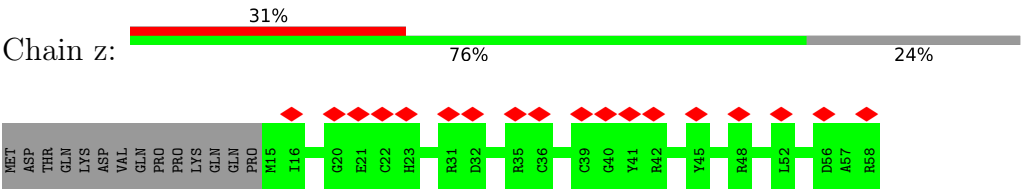
- Molecule 43: RPB10



- 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)	Not provided	
Maximum defocus (nm)	Not provided	
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 ( $\text{\AA}$ )	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 ( $\text{\AA}$ )	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	0/1804	0.59	1/2443 (0.0%)
2	1	0.45	0/2674	0.63	6/3660 (0.2%)
3	2	0.45	0/2588	0.66	2/3509 (0.1%)
4	3	0.40	0/2102	0.57	0/2844
5	4	0.44	0/3663	0.62	0/4965
6	5	0.31	0/433	0.50	0/585
7	6	0.46	0/4983	0.62	1/6731 (0.0%)
8	7	0.47	0/5957	0.67	2/8071 (0.0%)
9	8	0.54	0/2429	0.69	0/3295
10	9	0.52	0/2384	0.62	0/3220
11	A	0.51	0/4679	0.62	1/6320 (0.0%)
12	B	0.47	1/7993 (0.0%)	0.60	0/10836
13	D	0.40	0/1343	0.48	0/1795
13	d	0.28	0/1321	0.49	0/1772
14	E	0.39	0/4469	0.55	0/6050
14	e	0.33	0/4433	0.55	0/6004
15	F	0.50	0/3167	0.67	0/4303
15	f	0.41	0/3140	0.63	0/4268
16	G	0.52	0/1199	0.63	0/1612
17	H	0.36	0/1673	0.56	0/2285
18	I	0.41	0/981	0.53	0/1332
18	i	0.30	0/989	0.46	0/1343
19	J	0.30	0/736	0.49	1/998 (0.1%)
19	j	0.30	0/775	0.52	0/1049
20	L	0.41	0/613	0.63	1/829 (0.1%)
20	l	0.40	0/888	0.54	1/1194 (0.1%)
21	O	0.36	0/781	0.62	0/1061
22	P	0.43	0/1438	0.53	0/1935
23	Q	0.34	0/1013	0.65	0/1366
24	R	0.34	0/1957	0.61	0/2643
25	S	0.35	0/896	0.51	0/1213
26	T	0.48	0/1817	0.78	1/2445 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
27	U	0.40	0/1499	0.66	3/2012 (0.1%)
28	V	0.45	0/1428	0.60	0/1917
29	X	0.69	0/1607	0.91	0/2481
30	Y	0.82	0/1565	0.96	2/2410 (0.1%)
31	c	0.39	0/1035	0.54	0/1406
32	k	0.31	0/799	0.48	0/1070
33	m	0.31	0/733	0.51	0/977
34	o	0.36	0/11516	0.52	0/15548
35	p	0.39	0/9243	0.49	0/12475
36	q	0.39	0/2102	0.46	0/2857
37	r	0.27	0/1019	0.47	0/1374
38	s	0.33	0/1751	0.50	0/2366
39	t	0.49	0/645	0.65	0/871
40	u	0.33	0/1382	0.54	0/1874
41	v	0.37	0/1207	0.49	0/1628
42	w	0.30	0/948	0.46	0/1284
43	x	0.42	0/516	0.45	0/696
44	y	0.36	0/956	0.44	0/1294
45	z	0.38	0/377	0.45	0/500
All	All	0.43	1/115646 (0.0%)	0.59	22/157016 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	494	SER	CA-CB	-5.00	1.45	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	U	127	PHE	CB-CA-C	8.08	126.57	110.40
8	7	311	PRO	N-CA-CB	6.12	110.65	103.30
3	2	282	PRO	N-CA-CB	6.10	110.62	103.30
11	A	498	PRO	N-CA-CB	5.97	110.47	103.30
2	1	265	PRO	N-CA-CB	5.91	110.39	103.30
2	1	507	PRO	N-CA-CB	5.84	110.31	103.30
3	2	269	PRO	N-CA-CB	5.81	110.27	103.30
8	7	308	PRO	N-CA-CB	5.79	110.24	103.30
30	Y	21	DC	C2'-C3'-O3'	-5.78	93.54	112.60
2	1	276	PRO	N-CA-CB	5.64	110.07	103.30
2	1	484	PRO	N-CA-CB	5.49	109.88	103.30
27	U	140	GLU	CB-CA-C	-5.39	99.62	110.40
2	1	287	PRO	N-CA-CB	5.36	109.73	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	l	79	ASP	CB-CG-OD2	5.22	123.00	118.30
19	J	118	ASP	CB-CG-OD2	5.19	122.97	118.30
1	0	97	ASP	CB-CG-OD2	5.16	122.94	118.30
20	L	79	ASP	CB-CG-OD2	5.16	122.94	118.30
7	6	447	PRO	N-CA-C	5.12	125.42	112.10
2	1	480	PRO	N-CA-CB	5.08	109.39	103.30
30	Y	32	DG	P-O3'-C3'	5.03	125.73	119.70
27	U	128	LYS	N-CA-CB	5.02	119.64	110.60
26	T	229	HIS	CB-CA-C	5.01	120.42	110.40

There are no chirality outliers.

There are no planarity outliers.

## 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	230/309 (74%)	200 (87%)	29 (13%)	1 (0%)	34	66
2	1	399/548 (73%)	309 (77%)	69 (17%)	21 (5%)	2	12
3	2	327/395 (83%)	287 (88%)	38 (12%)	2 (1%)	25	57
4	3	259/308 (84%)	242 (93%)	17 (7%)	0	100	100
5	4	447/462 (97%)	402 (90%)	38 (8%)	7 (2%)	9	36
6	5	52/71 (73%)	47 (90%)	4 (8%)	1 (2%)	8	34
7	6	602/782 (77%)	511 (85%)	78 (13%)	13 (2%)	6	30
8	7	732/760 (96%)	642 (88%)	78 (11%)	12 (2%)	9	36
9	8	296/346 (86%)	261 (88%)	34 (12%)	1 (0%)	41	71

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	9	285/323 (88%)	270 (95%)	15 (5%)	0	100	100
11	A	542/1872 (29%)	523 (96%)	16 (3%)	3 (1%)	25	57
12	B	959/1199 (80%)	914 (95%)	45 (5%)	0	100	100
13	D	153/1085 (14%)	145 (95%)	5 (3%)	3 (2%)	7	32
13	d	154/1085 (14%)	150 (97%)	4 (3%)	0	100	100
14	E	540/800 (68%)	505 (94%)	33 (6%)	2 (0%)	34	66
14	e	531/800 (66%)	484 (91%)	47 (9%)	0	100	100
15	F	404/677 (60%)	379 (94%)	19 (5%)	6 (2%)	10	38
15	f	399/677 (59%)	378 (95%)	20 (5%)	1 (0%)	41	71
16	G	139/349 (40%)	135 (97%)	4 (3%)	0	100	100
17	H	207/310 (67%)	191 (92%)	12 (6%)	4 (2%)	8	34
18	I	118/264 (45%)	113 (96%)	3 (2%)	2 (2%)	9	35
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%)	89 (98%)	2 (2%)	0	100	100
20	L	72/161 (45%)	63 (88%)	4 (6%)	5 (7%)	1	8
20	l	105/161 (65%)	101 (96%)	4 (4%)	0	100	100
21	O	95/109 (87%)	86 (90%)	9 (10%)	0	100	100
22	P	175/339 (52%)	167 (95%)	7 (4%)	1 (1%)	25	57
23	Q	118/376 (31%)	105 (89%)	13 (11%)	0	100	100
24	R	246/316 (78%)	232 (94%)	12 (5%)	2 (1%)	19	51
25	S	104/517 (20%)	101 (97%)	3 (3%)	0	100	100
26	T	218/249 (88%)	202 (93%)	11 (5%)	5 (2%)	6	29
27	U	175/439 (40%)	160 (91%)	10 (6%)	5 (3%)	4	24
28	V	170/291 (58%)	139 (82%)	23 (14%)	8 (5%)	2	14
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%)	79 (93%)	6 (7%)	0	100	100
34	o	1417/1970 (72%)	1308 (92%)	107 (8%)	2 (0%)	51	81
35	p	1128/1174 (96%)	1060 (94%)	67 (6%)	1 (0%)	51	81
36	q	253/275 (92%)	225 (89%)	28 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	r	126/142 (89%)	119 (94%)	7 (6%)	0	100	100
38	s	207/210 (99%)	197 (95%)	10 (5%)	0	100	100
39	t	77/127 (61%)	73 (95%)	3 (4%)	1 (1%)	12	40
40	u	169/172 (98%)	156 (92%)	10 (6%)	3 (2%)	8	35
41	v	146/150 (97%)	132 (90%)	14 (10%)	0	100	100
42	w	112/125 (90%)	103 (92%)	9 (8%)	0	100	100
43	x	62/67 (92%)	60 (97%)	2 (3%)	0	100	100
44	y	115/117 (98%)	109 (95%)	6 (5%)	0	100	100
45	z	42/58 (72%)	38 (90%)	4 (10%)	0	100	100
All	All	13709/22931 (60%)	12596 (92%)	1001 (7%)	112 (1%)	24	51

All (112) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	1	106	LYS
2	1	108	ASN
2	1	110	GLU
2	1	114	LYS
2	1	120	GLU
2	1	237	THR
2	1	264	ASN
2	1	275	LYS
2	1	286	VAL
2	1	358	ILE
2	1	359	GLU
2	1	373	ALA
3	2	261	SER
5	4	193	PRO
6	5	48	GLU
7	6	405	VAL
7	6	421	TRP
7	6	605	ILE
7	6	622	VAL
8	7	15	ASP
8	7	612	HIS
8	7	624	PRO
11	A	498	PRO
11	A	1158	SER
13	D	876	ALA

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Mol	Chain	Res	Type
13	D	877	PRO
14	E	452	ARG
15	F	68	THR
15	F	69	SER
15	F	442	PRO
17	H	115	GLN
17	H	141	PRO
18	I	85	SER
20	L	73	ASN
20	L	107	LYS
27	U	100	VAL
39	t	93	ALA
40	u	154	LYS
2	1	113	GLU
2	1	276	PRO
2	1	287	PRO
5	4	135	GLN
7	6	379	LYS
7	6	401	ILE
7	6	458	VAL
7	6	463	LYS
7	6	555	ASN
7	6	610	VAL
8	7	31	THR
8	7	36	GLY
8	7	462	SER
8	7	464	LEU
13	D	898	VAL
14	E	704	VAL
17	H	129	VAL
20	L	111	LEU
20	L	114	LYS
22	P	207	PRO
27	U	103	VAL
28	V	79	ALA
28	V	168	LEU
28	V	178	SER
35	p	19	PRO
40	u	63	ARG
40	u	64	GLY
2	1	355	GLN
3	2	206	ARG

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Mol	Chain	Res	Type
5	4	190	PRO
7	6	387	SER
7	6	634	ARG
26	T	136	SER
27	U	165	GLU
28	V	134	ASP
34	o	1481	LYS
1	0	7	PRO
2	1	233	ASP
2	1	261	GLY
2	1	369	VAL
5	4	413	LEU
8	7	98	GLU
15	F	66	LEU
18	I	62	LYS
26	T	140	ARG
26	T	175	ARG
27	U	145	PHE
28	V	86	LYS
28	V	225	VAL
34	o	581	LYS
2	1	348	ALA
15	F	64	GLN
15	F	440	PRO
17	H	137	GLY
28	V	172	GLU
28	V	195	PRO
5	4	191	GLY
8	7	532	PRO
9	8	165	PRO
11	A	506	ASP
20	L	72	PRO
24	R	48	VAL
26	T	38	GLY
15	f	411	VAL
8	7	13	PRO
7	6	402	GLY
26	T	225	VAL
27	U	169	PRO
5	4	189	GLU
5	4	385	PRO
8	7	463	PRO

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Mol	Chain	Res	Type
24	R	30	GLY
2	1	149	VAL
8	7	47	GLY

### 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	0	173/283 (61%)	173 (100%)	0	100	100
2	1	176/484 (36%)	167 (95%)	9 (5%)	24	54
3	2	279/352 (79%)	273 (98%)	6 (2%)	52	74
4	3	234/272 (86%)	231 (99%)	3 (1%)	69	82
5	4	387/399 (97%)	371 (96%)	16 (4%)	30	61
6	5	48/64 (75%)	48 (100%)	0	100	100
7	6	533/688 (78%)	487 (91%)	46 (9%)	10	35
8	7	616/664 (93%)	593 (96%)	23 (4%)	34	63
9	8	258/299 (86%)	254 (98%)	4 (2%)	62	79
10	9	259/296 (88%)	258 (100%)	1 (0%)	91	95
11	A	495/1665 (30%)	460 (93%)	35 (7%)	14	42
12	B	876/1083 (81%)	858 (98%)	18 (2%)	53	75
13	D	144/815 (18%)	135 (94%)	9 (6%)	18	47
13	d	146/815 (18%)	146 (100%)	0	100	100
14	E	478/657 (73%)	465 (97%)	13 (3%)	44	71
14	e	475/657 (72%)	473 (100%)	2 (0%)	91	95
15	F	324/574 (56%)	300 (93%)	24 (7%)	13	40
15	f	322/574 (56%)	314 (98%)	8 (2%)	47	72
16	G	133/322 (41%)	125 (94%)	8 (6%)	19	49
17	H	181/270 (67%)	172 (95%)	9 (5%)	24	55
18	I	106/235 (45%)	99 (93%)	7 (7%)	16	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	i	107/235 (46%)	107 (100%)	0	100	100
19	J	79/154 (51%)	78 (99%)	1 (1%)	69	82
19	j	83/154 (54%)	83 (100%)	0	100	100
20	L	69/141 (49%)	60 (87%)	9 (13%)	4	17
20	l	98/141 (70%)	98 (100%)	0	100	100
21	O	84/98 (86%)	82 (98%)	2 (2%)	49	73
22	P	153/293 (52%)	152 (99%)	1 (1%)	84	90
23	Q	111/324 (34%)	109 (98%)	2 (2%)	59	78
24	R	212/268 (79%)	200 (94%)	12 (6%)	20	51
25	S	93/448 (21%)	92 (99%)	1 (1%)	73	85
26	T	196/218 (90%)	167 (85%)	29 (15%)	3	13
27	U	163/373 (44%)	148 (91%)	15 (9%)	9	31
28	V	155/261 (59%)	136 (88%)	19 (12%)	4	20
31	c	113/833 (14%)	111 (98%)	2 (2%)	59	78
32	k	87/182 (48%)	87 (100%)	0	100	100
33	m	80/106 (76%)	79 (99%)	1 (1%)	69	82
34	o	1257/1748 (72%)	1242 (99%)	15 (1%)	71	83
35	p	993/1027 (97%)	983 (99%)	10 (1%)	76	86
36	q	234/252 (93%)	234 (100%)	0	100	100
37	r	106/126 (84%)	105 (99%)	1 (1%)	78	87
38	s	191/192 (100%)	189 (99%)	2 (1%)	76	86
39	t	69/111 (62%)	67 (97%)	2 (3%)	42	69
40	u	152/153 (99%)	150 (99%)	2 (1%)	69	82
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	106/106 (100%)	106 (100%)	0	100	100
45	z	41/55 (74%)	41 (100%)	0	100	100
All	All	11960/19766 (60%)	11593 (97%)	367 (3%)	43	67

All (367) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	1	190	SER
2	1	349	VAL
2	1	353	LYS
2	1	358	ILE
2	1	362	ASP
2	1	363	LEU
2	1	372	ILE
2	1	417	LYS
2	1	434	LEU
3	2	182	ILE
3	2	185	LEU
3	2	186	ILE
3	2	195	ARG
3	2	301	LEU
3	2	313	VAL
4	3	18	ASN
4	3	146	ARG
4	3	157	MET
5	4	23	LEU
5	4	115	ARG
5	4	188	THR
5	4	189	GLU
5	4	215	PHE
5	4	347	THR
5	4	352	GLN
5	4	355	ILE
5	4	376	MET
5	4	389	ASP
5	4	400	ARG
5	4	401	LEU
5	4	404	THR
5	4	407	VAL
5	4	413	LEU
5	4	456	LYS
7	6	157	LYS
7	6	163	TYR
7	6	166	VAL
7	6	190	GLN
7	6	191	ASP
7	6	198	ARG
7	6	297	PHE
7	6	300	ASP
7	6	302	VAL

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Mol	Chain	Res	Type
7	6	303	ASN
7	6	305	ASP
7	6	310	LEU
7	6	317	ARG
7	6	346	LYS
7	6	357	VAL
7	6	362	LEU
7	6	377	GLN
7	6	381	TRP
7	6	403	CYS
7	6	404	SER
7	6	412	MET
7	6	413	LEU
7	6	415	HIS
7	6	419	ARG
7	6	422	GLU
7	6	426	VAL
7	6	435	TRP
7	6	444	HIS
7	6	451	PHE
7	6	457	ILE
7	6	463	LYS
7	6	464	LEU
7	6	490	GLU
7	6	528	LYS
7	6	530	ARG
7	6	534	TYR
7	6	597	LYS
7	6	601	LYS
7	6	603	ASN
7	6	612	ASP
7	6	615	PHE
7	6	621	ASN
7	6	624	ILE
7	6	633	ARG
7	6	648	LYS
7	6	650	MET
8	7	15	ASP
8	7	17	ILE
8	7	20	GLU
8	7	22	PHE
8	7	24	TYR

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Mol	Chain	Res	Type
8	7	25	MET
8	7	28	LEU
8	7	29	LYS
8	7	31	THR
8	7	48	LYS
8	7	49	THR
8	7	63	TYR
8	7	77	VAL
8	7	98	GLU
8	7	143	ARG
8	7	424	ARG
8	7	425	THR
8	7	428	ILE
8	7	444	ILE
8	7	487	ARG
8	7	595	ILE
8	7	626	VAL
8	7	690	ARG
9	8	38	VAL
9	8	195	ASP
9	8	245	ASP
9	8	309	ARG
10	9	234	GLU
11	A	347	ARG
11	A	353	LEU
11	A	357	GLU
11	A	396	LEU
11	A	397	LEU
11	A	401	ASN
11	A	403	LEU
11	A	405	VAL
11	A	464	TRP
11	A	468	PHE
11	A	470	ILE
11	A	474	ASP
11	A	482	ASP
11	A	491	MET
11	A	496	GLU
11	A	500	LEU
11	A	502	LEU
11	A	503	ASP
11	A	511	LEU

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Mol	Chain	Res	Type
11	A	574	TYR
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	828	GLU
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	1165	LEU
11	A	1203	GLU
12	B	21	GLU
12	B	24	ARG
12	B	71	ARG
12	B	140	GLU
12	B	159	LEU
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	877	PRO
13	D	891	ILE
13	D	894	LEU
13	D	897	ASP
13	D	924	LYS
13	D	955	LYS
13	D	958	LYS
13	D	1006	LEU

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Mol	Chain	Res	Type
13	D	1009	LEU
14	E	433	LYS
14	E	450	ARG
14	E	451	VAL
14	E	507	VAL
14	E	513	LEU
14	E	515	LEU
14	E	519	GLU
14	E	521	ASP
14	E	593	PHE
14	E	702	LEU
14	E	745	GLU
14	E	746	ASP
14	E	747	LEU
15	F	55	LEU
15	F	60	MET
15	F	62	LYS
15	F	64	GLN
15	F	66	LEU
15	F	111	GLU
15	F	114	LEU
15	F	118	ILE
15	F	120	THR
15	F	209	LYS
15	F	211	ARG
15	F	258	ARG
15	F	261	THR
15	F	271	VAL
15	F	280	ILE
15	F	301	VAL
15	F	319	LEU
15	F	320	ARG
15	F	339	GLN
15	F	348	THR
15	F	354	ARG
15	F	391	LEU
15	F	397	GLN
15	F	427	LEU
16	G	41	ASP
16	G	81	ASP
16	G	143	VAL
16	G	147	ARG

*Continued on next page...*

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Mol	Chain	Res	Type
16	G	161	ASP
16	G	181	TRP
16	G	182	GLU
16	G	183	ILE
17	H	50	PHE
17	H	116	ARG
17	H	132	LYS
17	H	135	THR
17	H	159	TYR
17	H	160	ILE
17	H	161	LYS
17	H	164	THR
17	H	169	VAL
18	I	31	TYR
18	I	32	GLU
18	I	34	ARG
18	I	63	LYS
18	I	69	ASP
18	I	82	SER
18	I	83	PHE
19	J	192	LYS
20	L	59	THR
20	L	60	LYS
20	L	61	LYS
20	L	62	LYS
20	L	63	LEU
20	L	64	GLN
20	L	110	THR
20	L	111	LEU
20	L	128	ILE
21	O	31	GLN
21	O	32	LEU
22	P	196	ARG
23	Q	57	ASP
23	Q	331	THR
24	R	27	TYR
24	R	28	ARG
24	R	39	LEU
24	R	41	VAL
24	R	44	ARG
24	R	45	VAL
24	R	46	ILE

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Mol	Chain	Res	Type
24	R	47	ASP
24	R	48	VAL
24	R	120	GLU
24	R	127	ARG
24	R	128	ILE
25	S	95	ASP
26	T	137	LYS
26	T	141	LEU
26	T	160	GLN
26	T	164	GLU
26	T	166	GLU
26	T	169	LYS
26	T	171	GLU
26	T	172	ASP
26	T	174	LYS
26	T	175	ARG
26	T	177	ARG
26	T	179	ASP
26	T	180	LYS
26	T	185	ASP
26	T	187	LEU
26	T	192	GLU
26	T	193	LYS
26	T	194	HIS
26	T	196	TYR
26	T	200	LYS
26	T	206	THR
26	T	208	GLN
26	T	211	VAL
26	T	212	TYR
26	T	226	LYS
26	T	229	HIS
26	T	231	ASN
26	T	232	THR
26	T	235	LEU
27	U	28	ILE
27	U	39	ARG
27	U	42	CYS
27	U	45	GLU
27	U	95	ASN
27	U	101	ASN
27	U	102	VAL

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Mol	Chain	Res	Type
27	U	105	TYR
27	U	123	ASN
27	U	139	LEU
27	U	145	PHE
27	U	164	ASP
27	U	166	SER
27	U	185	GLU
27	U	190	LEU
28	V	88	ARG
28	V	93	ASP
28	V	97	LEU
28	V	159	ASP
28	V	160	GLN
28	V	161	ARG
28	V	166	ILE
28	V	167	LEU
28	V	175	LEU
28	V	192	VAL
28	V	193	ASN
28	V	194	ARG
28	V	205	ASP
28	V	214	GLU
28	V	218	LYS
28	V	222	SER
28	V	229	ASP
28	V	230	GLU
28	V	234	GLU
31	c	24	ASP
31	c	106	VAL
14	e	365	ARG
14	e	663	ARG
15	f	253	TYR
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
33	m	31	LEU
34	o	132	LYS
34	o	138	LYS

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Mol	Chain	Res	Type
34	o	334	ARG
34	o	475	ARG
34	o	483	ARG
34	o	581	LYS
34	o	741	VAL
34	o	743	ARG
34	o	747	ASP
34	o	749	ARG
34	o	797	ARG
34	o	1132	LYS
34	o	1254	LYS
34	o	1473	LEU
34	o	1485	GLU
35	p	42	GLN
35	p	43	GLN
35	p	51	ILE
35	p	324	ARG
35	p	497	LYS
35	p	581	GLU
35	p	593	GLN
35	p	596	ILE
35	p	597	ILE
35	p	603	MET
37	r	94	LYS
38	s	52	ARG
38	s	159	LEU
39	t	86	GLU
39	t	90	LEU
40	u	144	ARG
40	u	163	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (168) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	117	ASN
1	0	259	HIS
2	1	384	HIS
2	1	524	HIS
3	2	235	HIS
3	2	317	HIS
3	2	340	ASN
4	3	18	ASN

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Mol	Chain	Res	Type
4	3	108	ASN
4	3	179	ASN
4	3	248	HIS
5	4	54	ASN
5	4	181	GLN
5	4	312	ASN
5	4	366	HIS
5	4	373	HIS
5	4	458	GLN
5	4	460	HIS
7	6	97	GLN
7	6	112	HIS
7	6	187	HIS
7	6	377	GLN
7	6	497	GLN
7	6	551	HIS
7	6	595	ASN
7	6	621	ASN
7	6	638	GLN
7	6	668	GLN
8	7	118	HIS
8	7	238	ASN
8	7	328	HIS
8	7	562	GLN
8	7	726	GLN
8	7	733	GLN
9	8	36	GLN
9	8	73	ASN
9	8	131	HIS
9	8	279	ASN
10	9	94	ASN
10	9	100	HIS
10	9	153	GLN
10	9	183	ASN
11	A	401	ASN
11	A	409	HIS
11	A	860	ASN
11	A	896	GLN
11	A	1073	GLN
12	B	30	HIS
12	B	137	HIS
12	B	160	HIS

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Mol	Chain	Res	Type
12	B	176	HIS
12	B	183	GLN
12	B	184	ASN
12	B	235	HIS
12	B	272	GLN
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	908	GLN
12	B	916	ASN
13	D	922	GLN
13	D	925	ASN
13	D	936	GLN
13	D	1053	GLN
13	D	1075	HIS
14	E	254	ASN
14	E	268	HIS
14	E	290	HIS
14	E	327	ASN
14	E	351	GLN
14	E	509	GLN
14	E	616	HIS
14	E	636	HIS
14	E	640	ASN
15	F	119	ASN
15	F	214	HIS
15	F	270	ASN
15	F	273	GLN
15	F	275	ASN
15	F	316	GLN
15	F	326	HIS
16	G	48	HIS
17	H	145	HIS
18	I	21	GLN
18	I	38	GLN
18	I	81	GLN
18	I	98	GLN
19	J	160	GLN

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Mol	Chain	Res	Type
19	J	173	HIS
20	L	105	HIS
20	L	117	GLN
20	L	123	GLN
21	O	4	GLN
21	O	27	GLN
22	P	167	ASN
22	P	189	ASN
22	P	193	ASN
23	Q	37	GLN
24	R	129	ASN
26	T	152	ASN
26	T	158	ASN
26	T	181	GLN
26	T	195	GLN
26	T	208	GLN
27	U	95	ASN
27	U	101	ASN
27	U	123	ASN
28	V	95	HIS
28	V	117	GLN
28	V	177	ASN
28	V	193	ASN
13	d	912	ASN
13	d	1069	ASN
14	e	294	ASN
14	e	320	HIS
14	e	336	HIS
14	e	616	HIS
15	f	325	ASN
15	f	350	ASN
18	i	81	GLN
20	l	73	ASN
20	l	105	HIS
33	m	107	ASN
34	o	123	ASN
34	o	278	HIS
34	o	289	GLN
34	o	296	ASN
34	o	301	HIS
34	o	311	GLN
34	o	330	GLN

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Mol	Chain	Res	Type
34	o	372	ASN
34	o	507	GLN
34	o	620	HIS
34	o	721	HIS
34	o	723	ASN
34	o	731	ASN
34	o	739	ASN
34	o	780	ASN
34	o	913	ASN
34	o	950	ASN
34	o	1005	HIS
34	o	1230	GLN
34	o	1248	ASN
34	o	1332	GLN
34	o	1397	HIS
34	o	1445	HIS
34	o	1462	GLN
35	p	43	GLN
35	p	111	ASN
35	p	287	HIS
35	p	370	HIS
35	p	525	ASN
35	p	570	ASN
35	p	749	HIS
35	p	1021	HIS
35	p	1094	GLN
35	p	1117	HIS
35	p	1120	ASN
37	r	19	GLN
39	t	72	GLN
40	u	60	GLN
41	v	131	ASN
44	y	2	ASN
44	y	29	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 17 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
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 ⓘ

There are no chain breaks in this entry.

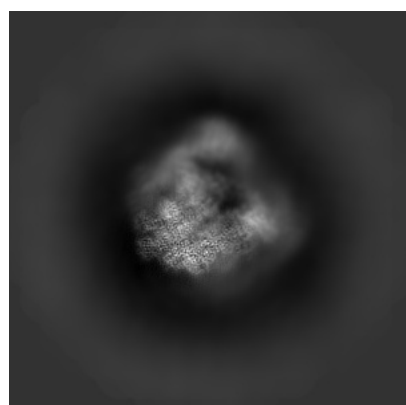
## 6 Map visualisation [i](#)

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.

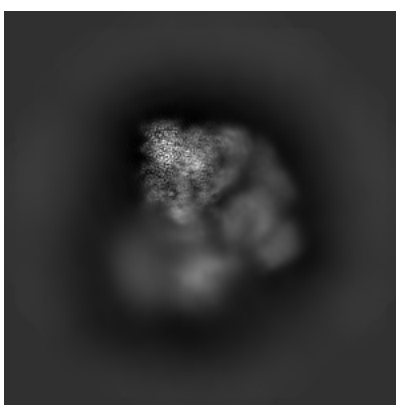
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

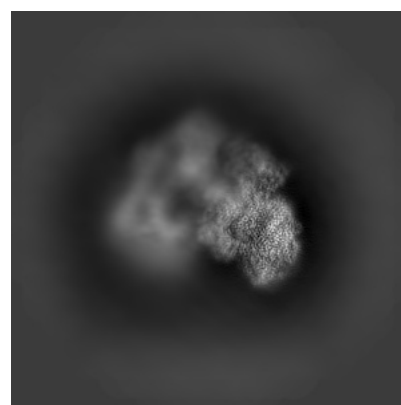
#### 6.1.1 Primary map



X



Y

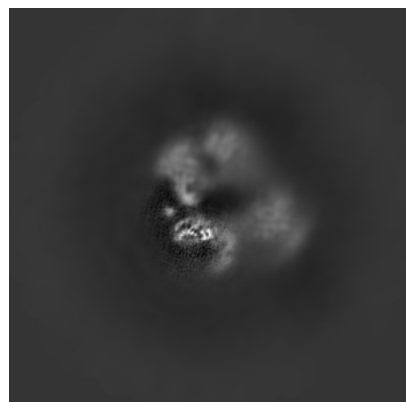


Z

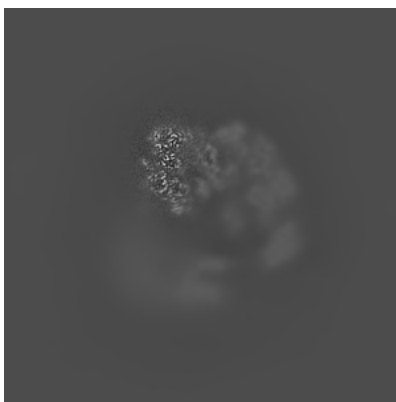
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

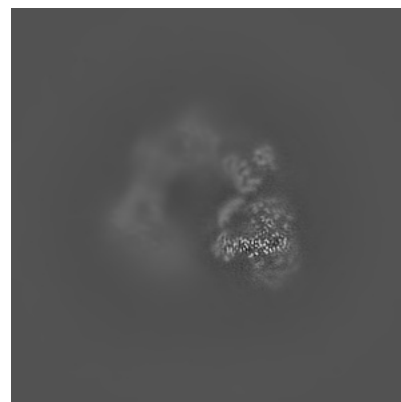
#### 6.2.1 Primary map



X Index: 256



Y Index: 256

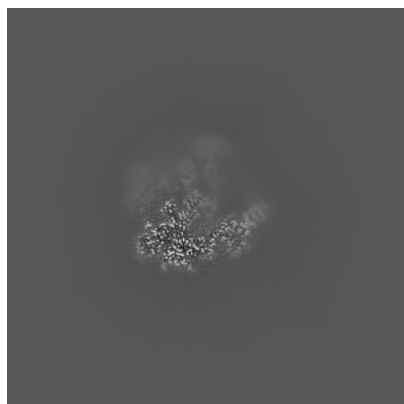


Z Index: 256

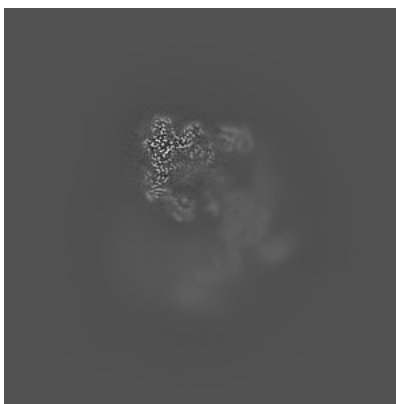
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

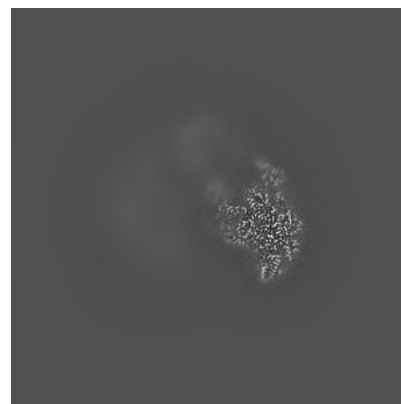
### 6.3.1 Primary map



X Index: 331



Y Index: 229

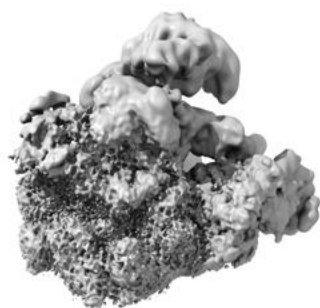


Z Index: 206

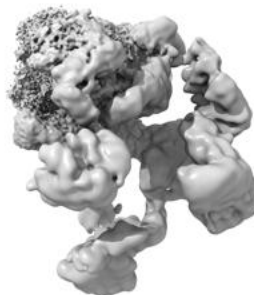
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

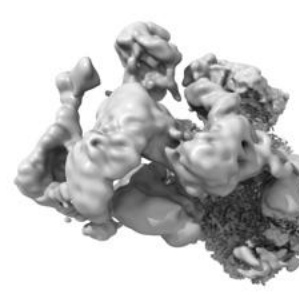
### 6.4.1 Primary map



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.

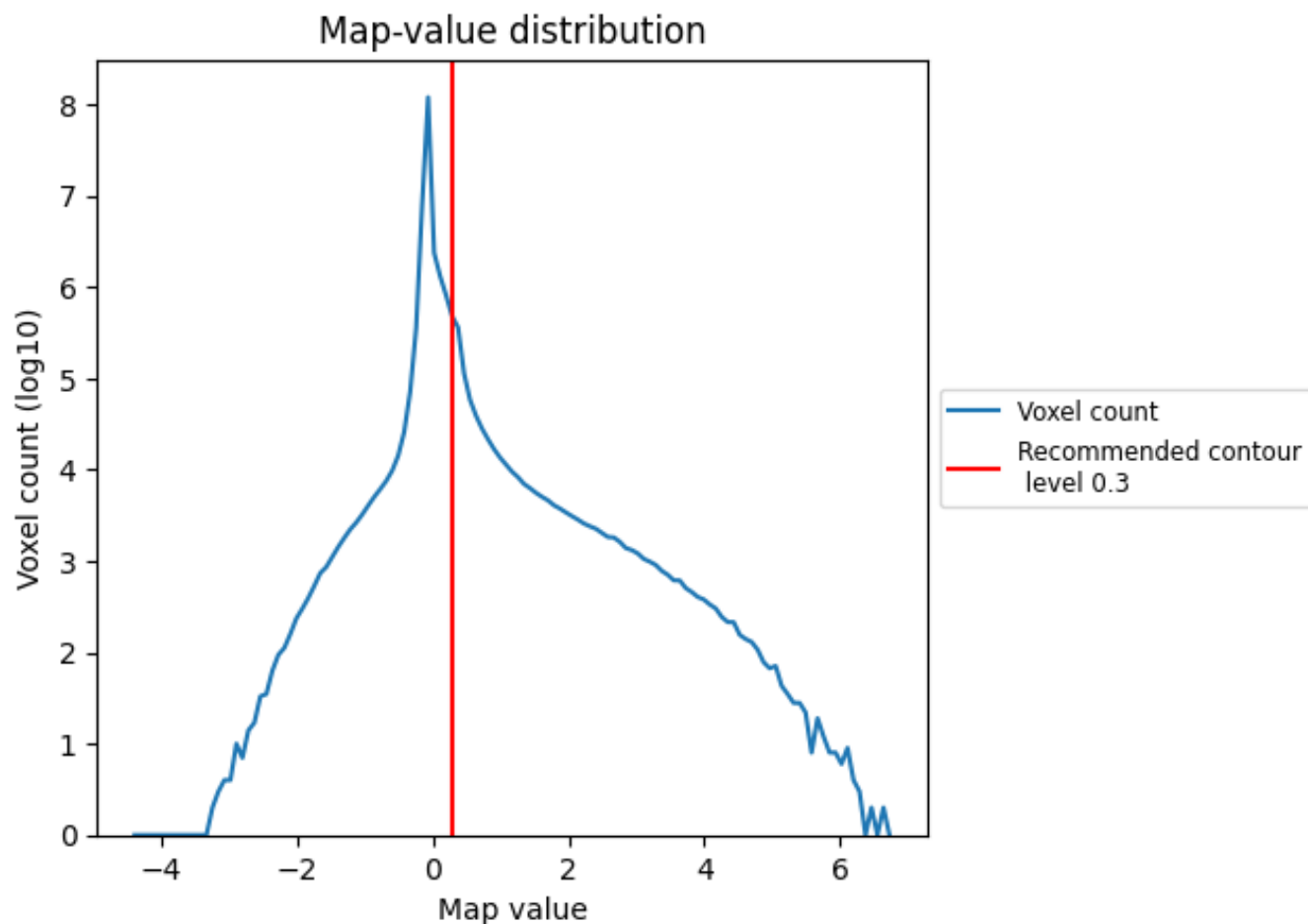
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

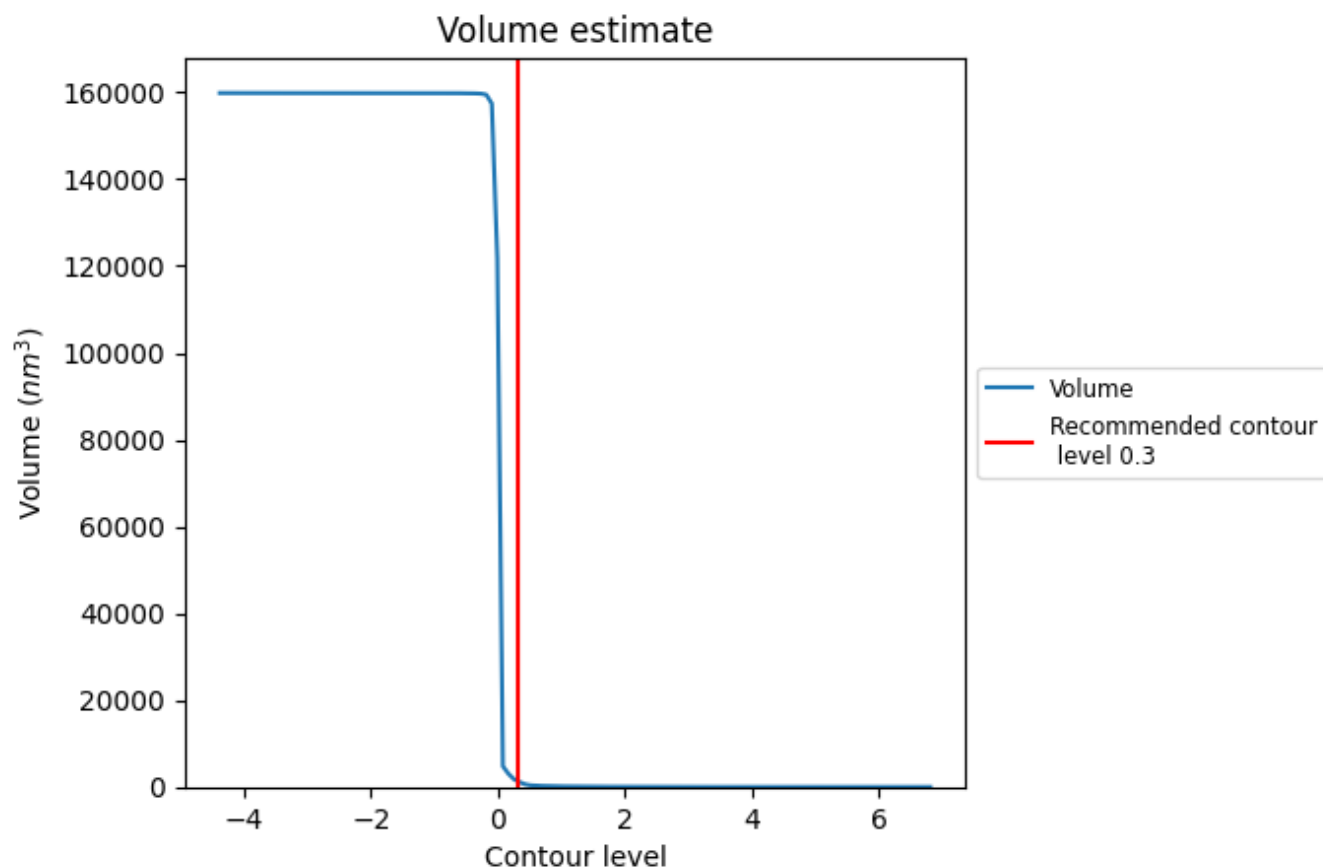
This section contains the results of statistical analysis of the map.

### 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.

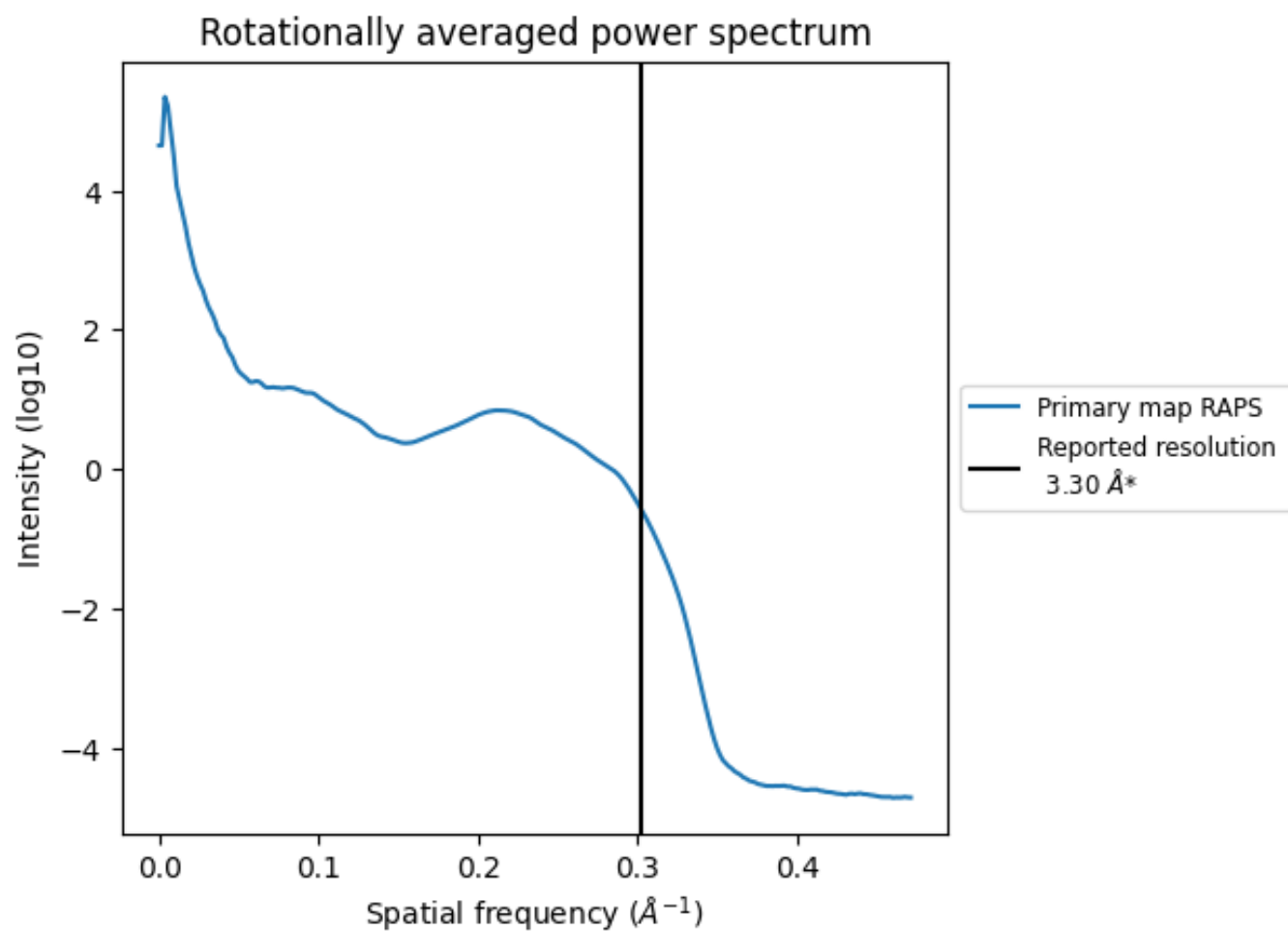
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1427 nm<sup>3</sup>; 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 ⓘ



\*Reported resolution corresponds to spatial frequency of 0.303 Å<sup>-1</sup>

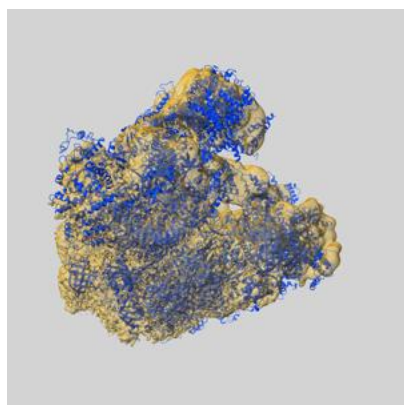
## 8 Fourier-Shell correlation

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

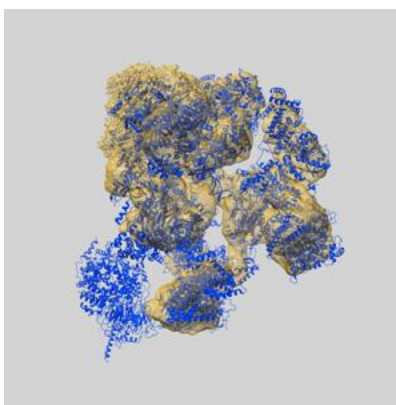
## 9 Map-model fit [i](#)

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](#).

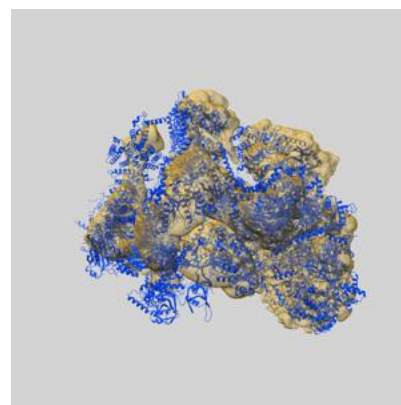
### 9.1 Map-model overlay [i](#)



X



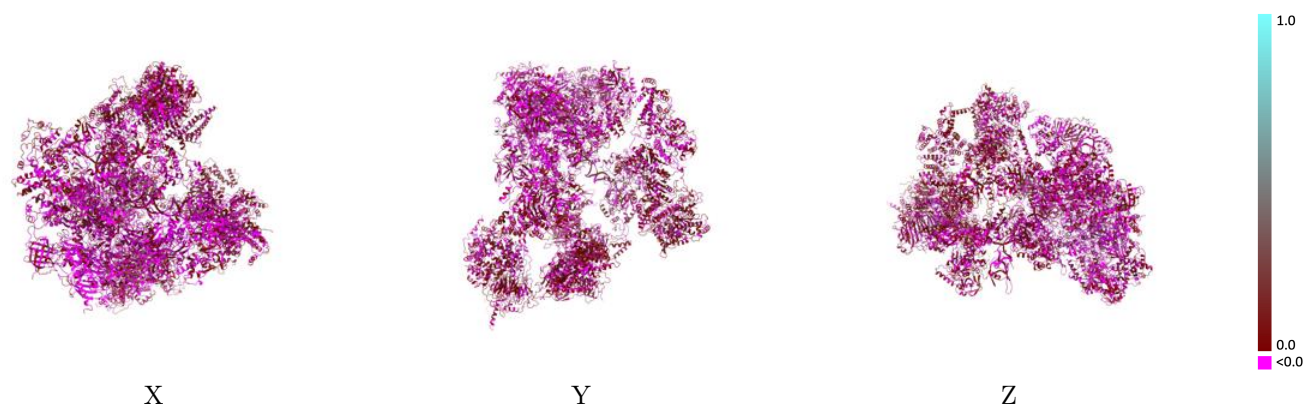
Y



Z

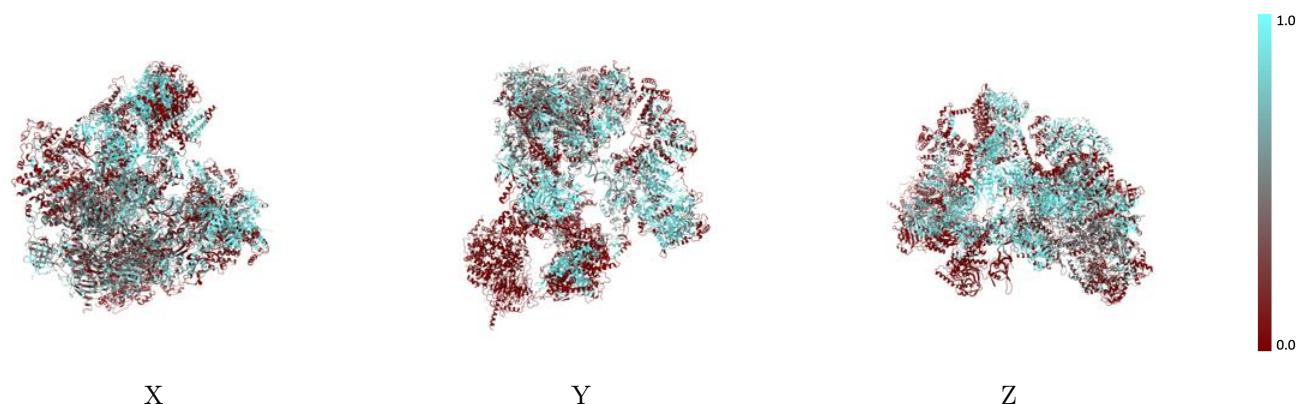
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



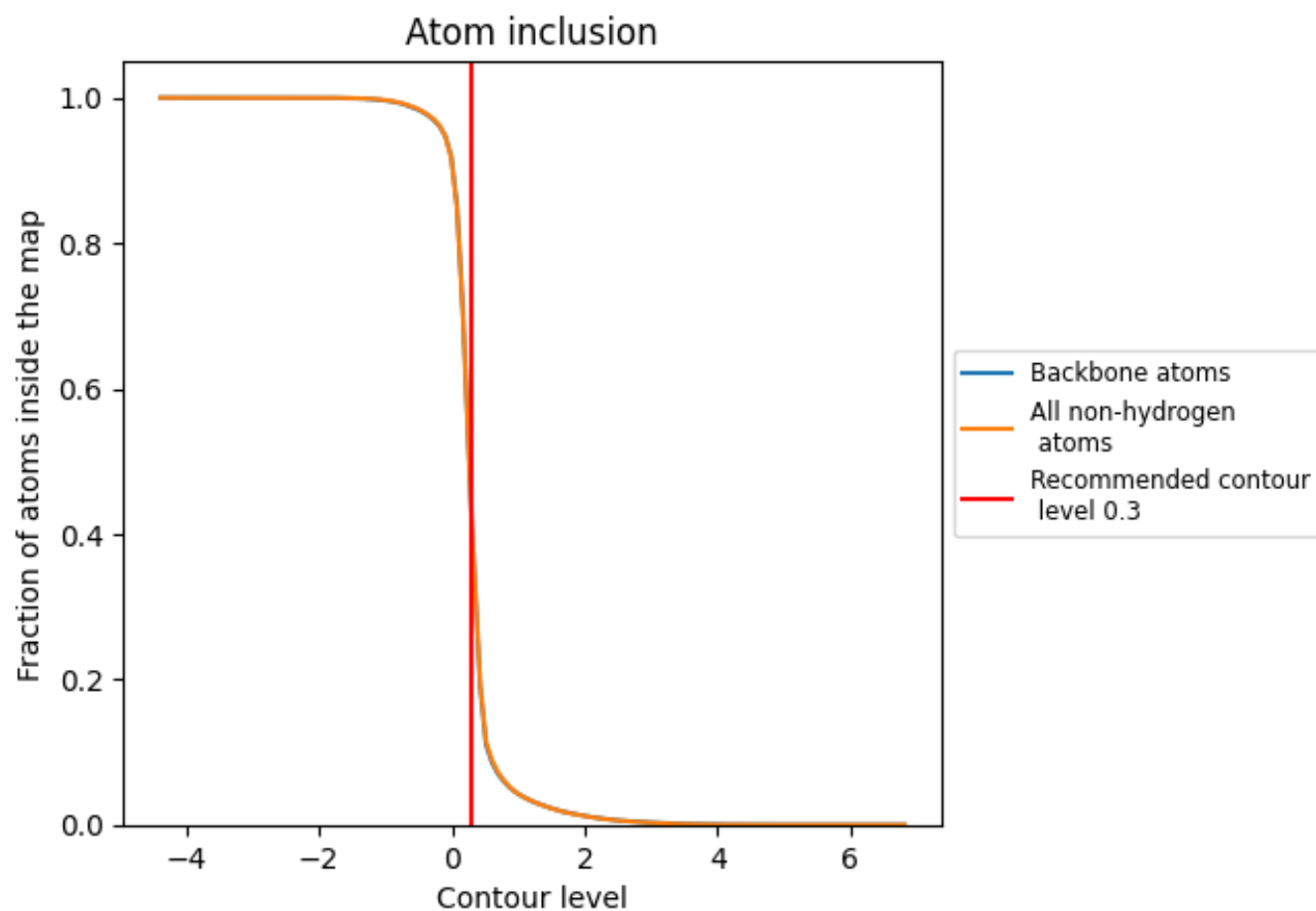
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 42% of all backbone atoms, 42% 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	 0.4164	 0.0130
0	 0.2513	 0.0190
1	 0.3080	 0.0250
2	 0.8470	 0.0610
3	 0.7085	 0.0590
4	 0.6110	 0.0570
5	 0.2753	 0.0180
6	 0.6691	 0.0300
7	 0.6094	 0.0330
8	 0.2094	 0.0200
9	 0.2879	 0.0080
A	 0.1761	 0.0280
B	 0.4666	 0.0250
D	 0.4753	 0.0070
E	 0.3713	 0.0310
F	 0.2010	 0.0330
G	 0.0270	 0.0360
H	 0.5335	 0.0340
I	 0.5091	 0.0370
J	 0.6088	 0.0390
L	 0.5261	 0.0360
O	 0.5746	 0.0150
P	 0.6669	 -0.0050
Q	 0.4287	 -0.0050
R	 0.4231	 -0.0370
S	 0.5984	 0.0440
T	 0.5077	 -0.0040
U	 0.6003	 0.0160
V	 0.6039	 0.0040
X	 0.4906	 0.0310
Y	 0.5179	 0.0320
c	 0.0000	 -0.0010
d	 0.0000	 0.0090
e	 0.0045	 0.0350
f	 0.2607	 0.0290



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Chain	Atom inclusion	Q-score
i	 0.0000	 0.0290
j	 0.0000	 0.0170
k	 0.0000	 -0.0020
l	 0.0000	 0.0190
m	 0.0000	 0.0270
o	 0.4523	 -0.0130
p	 0.4301	 -0.0390
q	 0.4916	 -0.0470
r	 0.5414	 -0.0230
s	 0.4741	 -0.0090
t	 0.4643	 -0.0060
u	 0.5518	 -0.0050
v	 0.5237	 0.0020
w	 0.5110	 0.0270
x	 0.4586	 -0.0170
y	 0.4952	 -0.0190
z	 0.5028	 -0.0130