



## wwPDB EM Validation Summary Report ⓘ

Dec 17, 2024 – 04:33 pm GMT

PDB ID : 9ESH  
EMDB ID : EMD-19941  
Title : Structure of a B-state intermediate committed to discard (Bd-I state)  
Authors : Soni, K.; Wild, K.; Sinning, I.  
Deposited on : 2024-03-26  
Resolution : 3.20 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](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>.

---

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

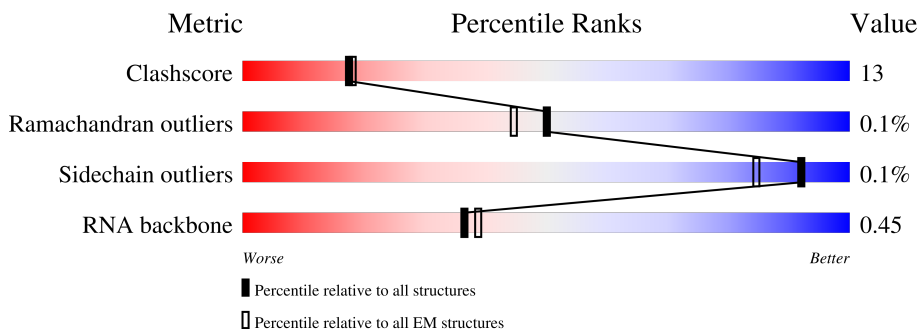
EMDB validation analysis : 0.0.1.dev113  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.40

# 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 3.20 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.





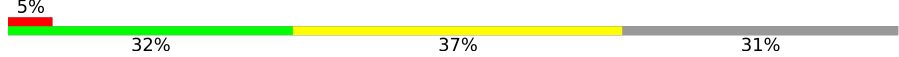









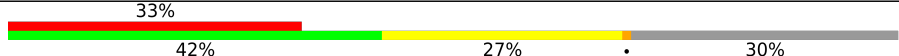
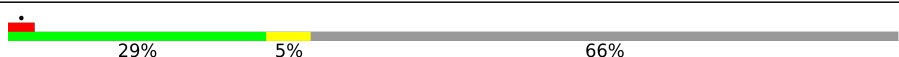

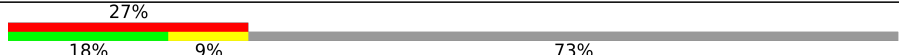
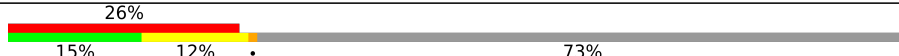


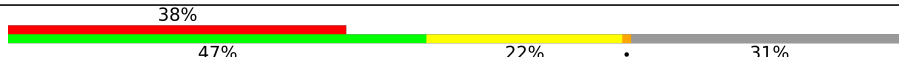

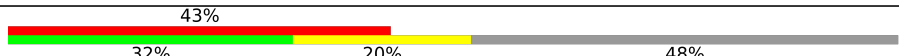


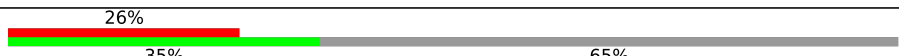
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	1	29	
2	2	186	
3	5	120	
4	6	99	
5	A	2363	
6	B	984	
7	C	340	


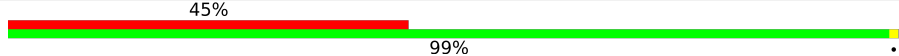

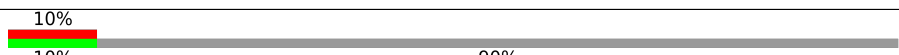

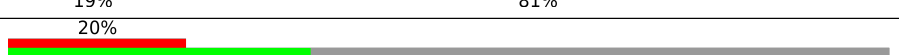

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	D	97	
9	E	147	
10	F	117	
11	G	115	
12	H	84	
13	I	78	
14	J	77	
15	K	473	
16	L	557	
17	M	354	
18	N	1284	
19	O	146	
20	P	388	
21	Q	265	
22	R	674	
23	S	488	
23	T	488	
23	U	488	
23	V	488	
24	W	757	
25	X	790	
26	Y	229	
27	Z	187	
28	a	558	
29	b	293	

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
30	c	887	 23% 77%
31	d	155	 45% 99%
32	f	22	 86% 100%
33	m	797	 10% 90%
34	r	346	 17% 81%
35	y	534	 20% 34% 65%
36	z	647	 80% 96%

## 2 Entry composition [i](#)

There are 41 unique types of molecules in this entry. The entry contains 90868 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 RNA chain called pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	1	29	605	272	91	213	29	0	0

- Molecule 2 is a RNA chain called U2snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	2	24	500	224	79	173	24	0	0

- Molecule 3 is a RNA chain called U5snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	5	102	2149	963	358	726	102	0	0

- Molecule 4 is a RNA chain called U6snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	6	92	1970	882	365	631	92	0	0

- Molecule 5 is a protein called Pre-mRNA-splicing factor spp42.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	A	1737	14402	9229	2543	2565	65	0	0

- Molecule 6 is a protein called Pre-mRNA-splicing factor cwf10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	B	918	7298	4650	1251	1362	35	0	0

- Molecule 7 is a protein called Pre-mRNA-splicing factor cwf17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	C	301	2328	1460	415	442	11	0	0

- Molecule 8 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	D	96	760	470	147	136	7	0	0

- Molecule 9 is a protein called Small nuclear ribonucleoprotein-associated protein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	E	97	726	462	129	130	5	0	0

- Molecule 10 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	F	81	638	407	109	118	4	0	0

- Molecule 11 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	G	102	819	516	150	149	4	0	0

- Molecule 12 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	H	80	652	422	113	115	2	0	0

- Molecule 13 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	I	73	574	373	95	104	2	0	0

- Molecule 14 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	73	Total	C	N	O	S	0	0
			573	366	98	108	1		

- Molecule 15 is a protein called Pre-mRNA-splicing factor prp5.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	391	Total	C	N	O	S	0	0
			3053	1925	551	563	14		

- Molecule 16 is a protein called Pre-mRNA-processing protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	234	Total	C	N	O	S	0	0
			1849	1154	345	345	5		

- Molecule 17 is a protein called Pre-mRNA-splicing factor cwf5.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	M	234	Total	C	N	O	S	0	0
			1818	1131	329	343	15		

- Molecule 18 is a protein called Pre-mRNA-splicing factor cwf11.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	N	1284	Total	C	N	O	S	0	0
			10461	6715	1732	1969	45		

- Molecule 19 is a protein called Pre-mRNA-splicing factor cwf14.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	O	144	Total	C	N	O	S	0	0
			1176	733	216	214	13		

- Molecule 20 is a protein called Pre-mRNA-splicing factor cwf2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	P	271	Total	C	N	O	S	0	0
			2178	1354	397	416	11		

- Molecule 21 is a protein called Pre-mRNA-splicing factor cwf15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	Q	90	752	467	146	138	1	0	0

- Molecule 22 is a protein called Pre-mRNA-splicing factor cwf4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	R	603	5108	3280	892	913	23	0	0

- Molecule 23 is a protein called Pre-mRNA-processing factor 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	S	132	1055	664	181	207	3	0	0
23	T	134	1069	671	183	212	3	0	0
23	U	430	2870	1806	492	563	9	0	0
23	V	131	1044	655	180	206	3	0	0

- Molecule 24 is a protein called Pre-mRNA-splicing factor cdc5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	W	526	4346	2710	792	832	12	0	0

- Molecule 25 is a protein called Pre-mRNA-splicing factor cwf3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	X	654	5467	3534	918	996	19	0	0

- Molecule 26 is a protein called Pre-mRNA-splicing factor syf2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
26	Y	120	1049	656	195	198	0	0

- Molecule 27 is a protein called Pre-mRNA-splicing factor cwf7.



Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	Z	155	1232	766	220	243	3	0	0

- Molecule 28 is a protein called Pre-mRNA-processing factor 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	a	152	1035	644	185	205	1	0	0

- Molecule 29 is a protein called Pre-mRNA-splicing factor cwf21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	b	104	822	503	148	169	2	0	0

- Molecule 30 is a protein called Pre-mRNA-splicing factor cwf22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	c	204	1678	1071	280	315	12	0	0

- Molecule 31 is a protein called Peptidyl-prolyl cis-trans isomerase ppl1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	d	154	1179	750	202	223	4	0	0

- Molecule 32 is a protein called UNK1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
32	f	22	110	66	22	22	0	0

- Molecule 33 is a protein called G-patch domain-containing protein C1486.03.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	m	81	649	413	112	122	2	0	0

- Molecule 34 is a protein called UNK2.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	r	67	Total	C	N	O	0	0
			335	201	67	67		

- Molecule 35 is a protein called Uncharacterized protein C20H4.06c.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	y	185	Total	C	N	O	S	0	0
			1480	921	257	298	4		

- Molecule 36 is a protein called Putative pre-mRNA-splicing factor ATP-dependent RNA helicase C20H4.09.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	z	626	Total	C	N	O	S	0	0
			4980	3193	835	933	19		

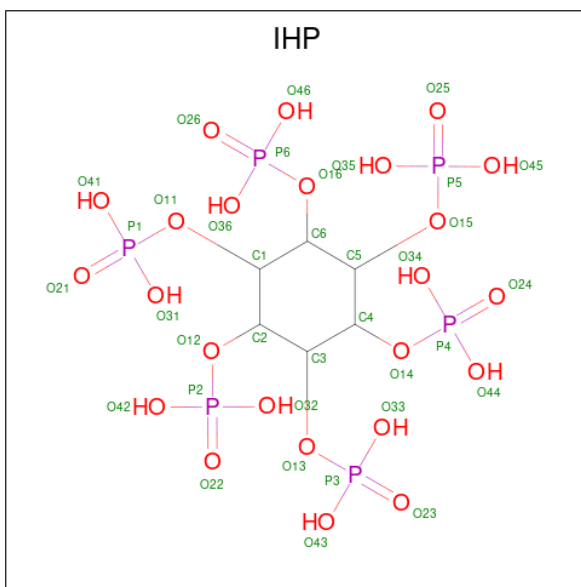
- Molecule 37 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
37	6	3	Total	Mg	0
			3	3	
37	B	1	Total	Mg	0
			1	1	

- Molecule 38 is POTASSIUM ION (three-letter code: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

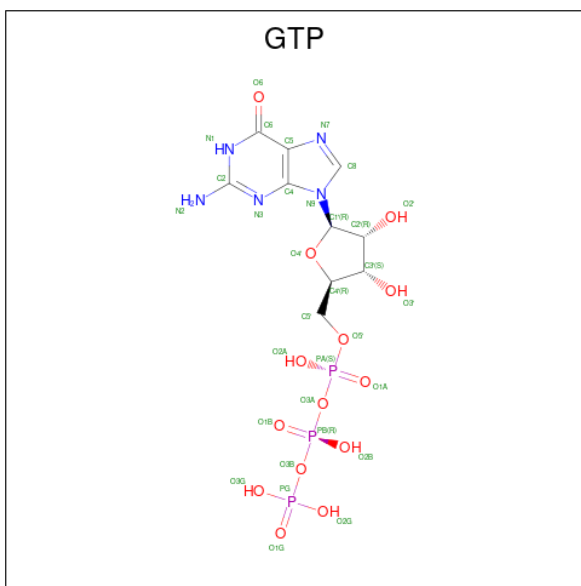
Mol	Chain	Residues	Atoms		AltConf
38	6	1	Total	K	0
			1	1	

- Molecule 39 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: C<sub>6</sub>H<sub>18</sub>O<sub>24</sub>P<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
39	A	1	36	6	24	6	0

- Molecule 40 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ) (labeled as "Ligand of Interest" by depositor).

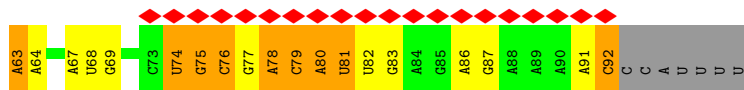


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
40	B	1	32	10	5	14	3	0

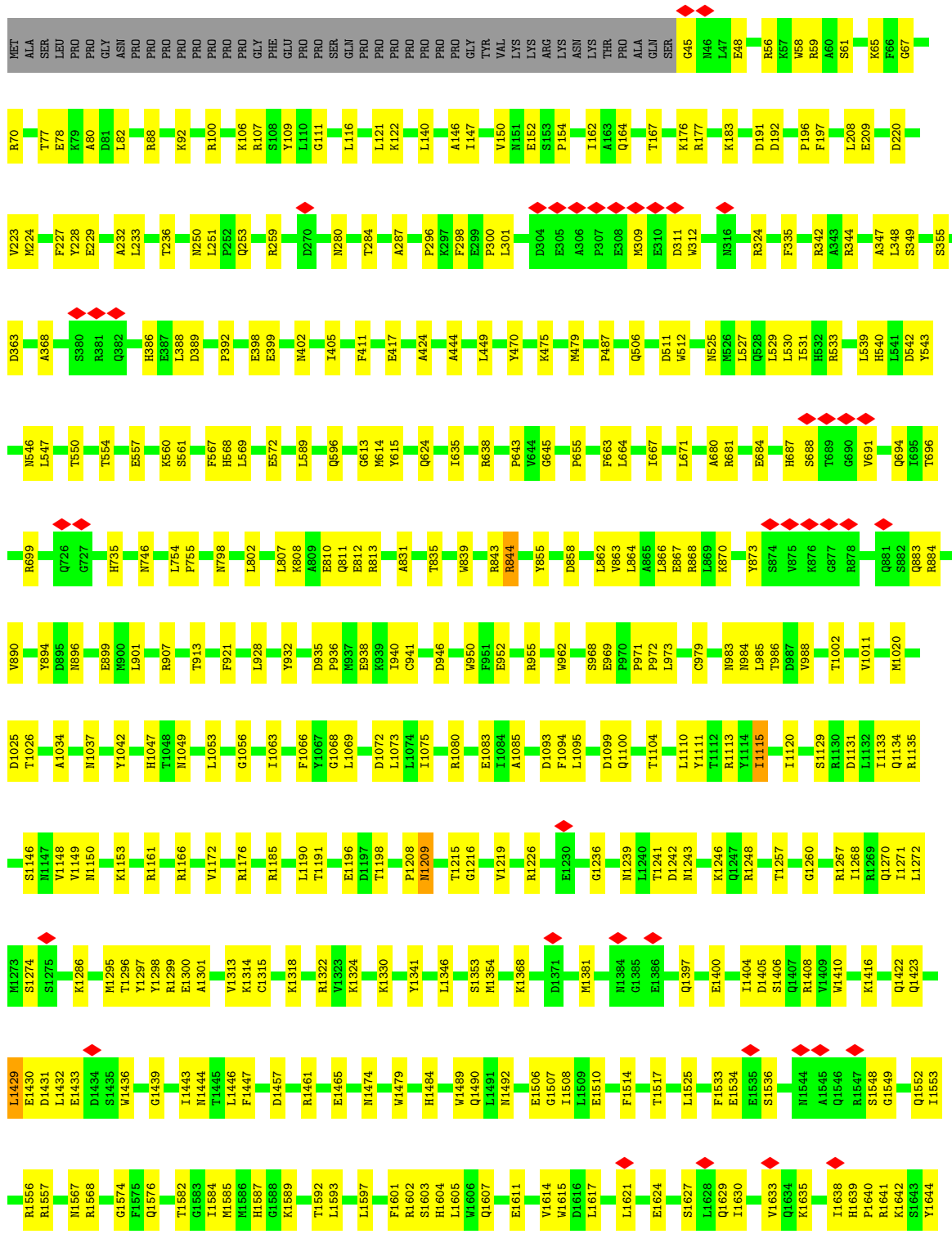
- Molecule 41 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>AltConf</b>
41	M	2	Total 2	Zn 2	0
41	O	3	Total 3	Zn 3	0
41	P	1	Total 1	Zn 1	0

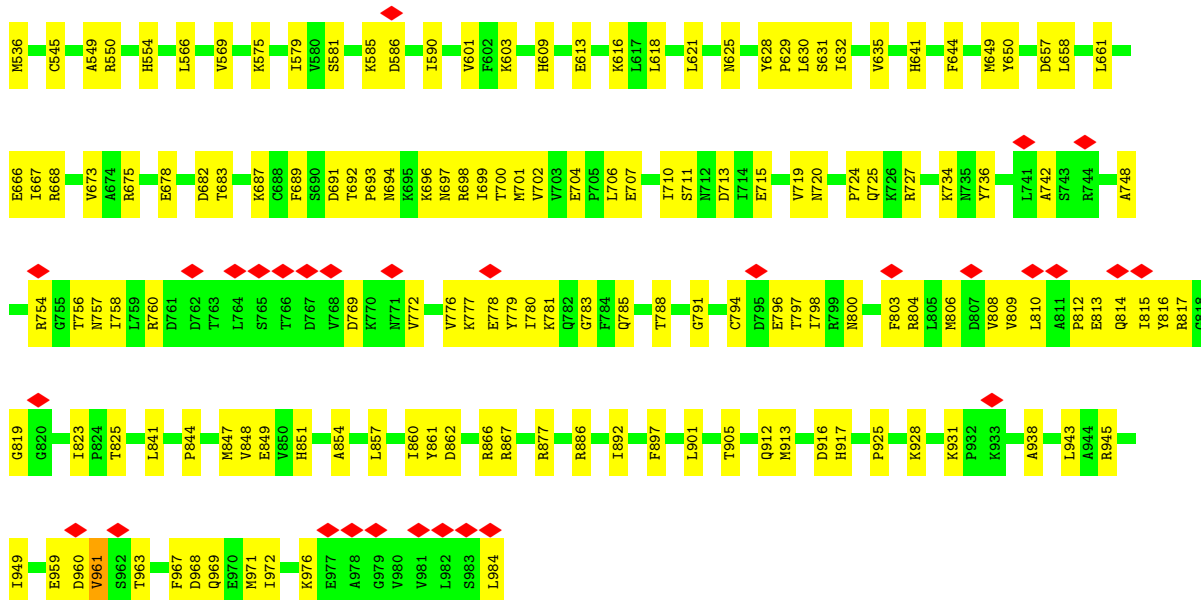




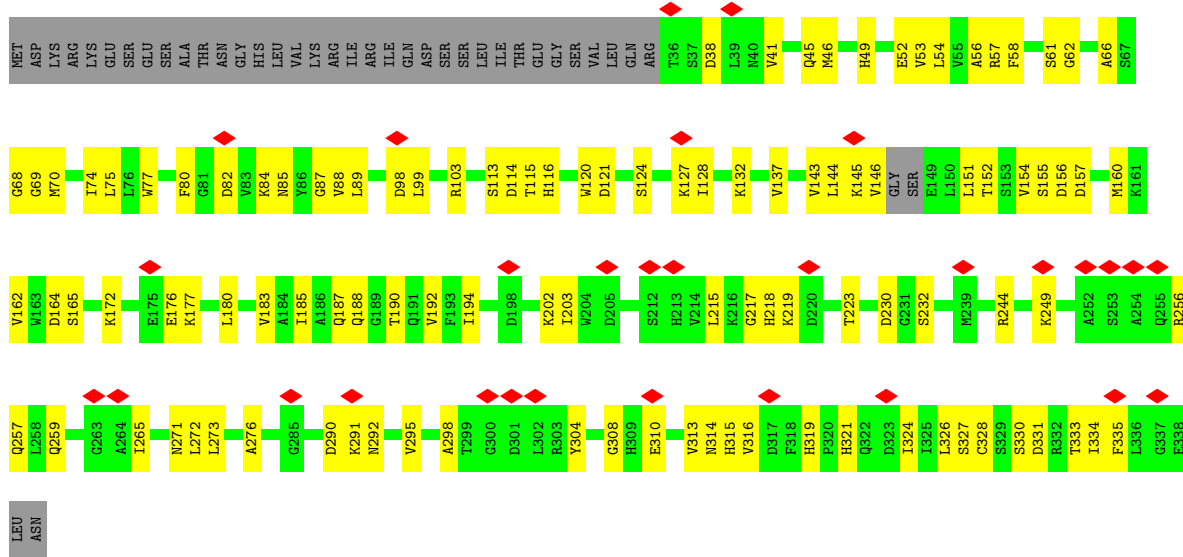
• Molecule 5: Pre-mRNA-splicing factor spp42







• Molecule 7: Pre-mRNA-splicing factor cwf17



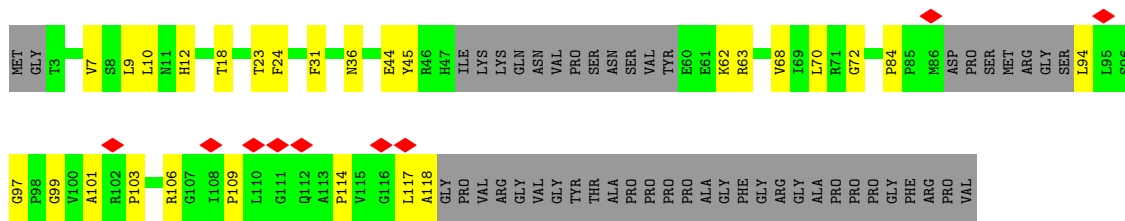
• Molecule 8: Small nuclear ribonucleoprotein Sm D3



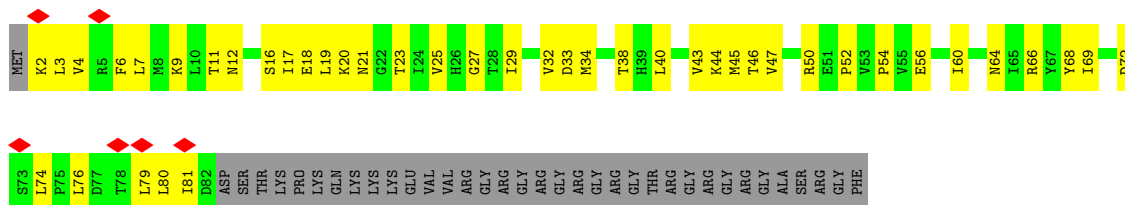
• Molecule 9: Small nuclear ribonucleoprotein-associated protein B



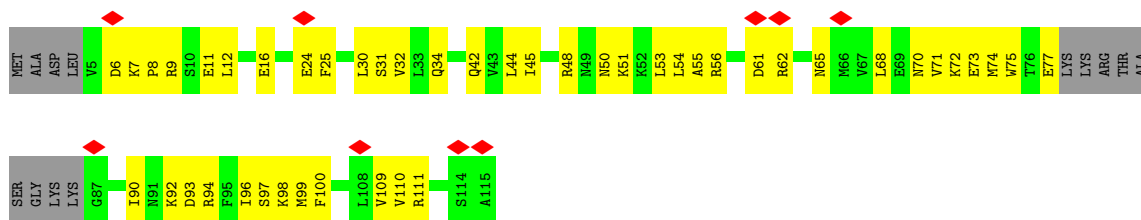




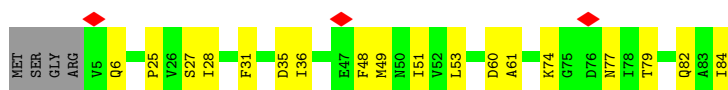
• Molecule 10: Small nuclear ribonucleoprotein Sm D1



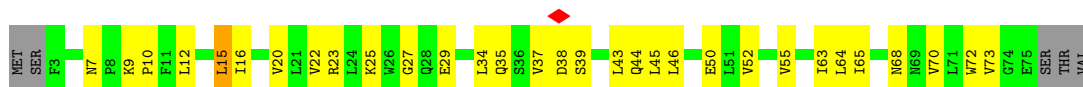
• Molecule 11: Small nuclear ribonucleoprotein Sm D2



• Molecule 12: Small nuclear ribonucleoprotein E



• Molecule 13: Small nuclear ribonucleoprotein F

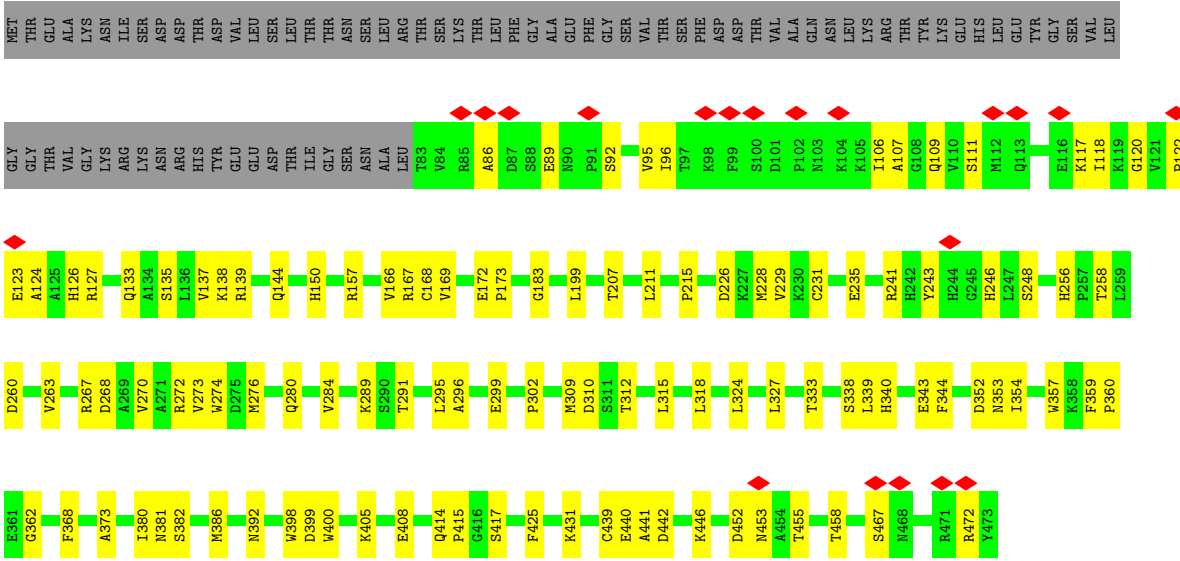


• Molecule 14: Small nuclear ribonucleoprotein G

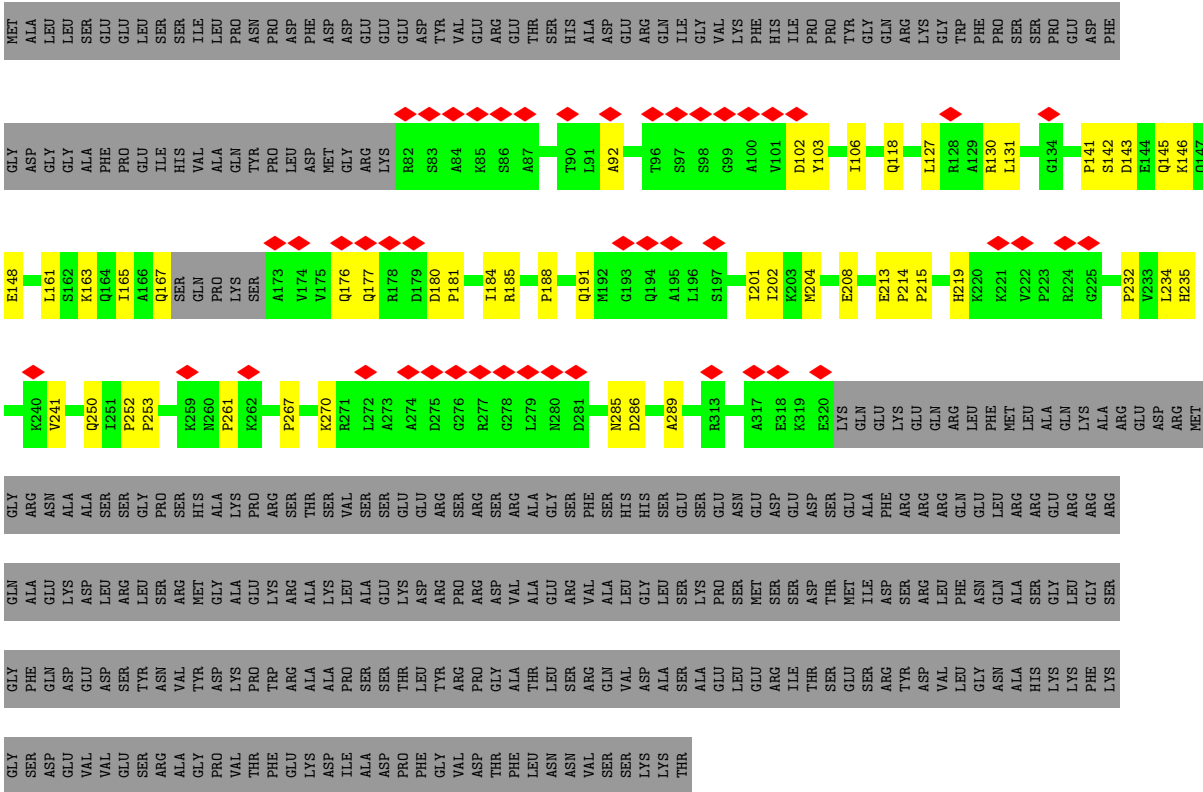
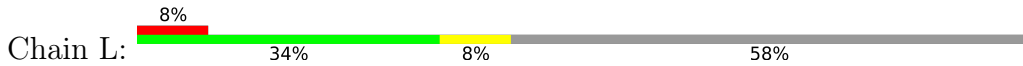




● Molecule 15: Pre-mRNA-splicing factor prp5

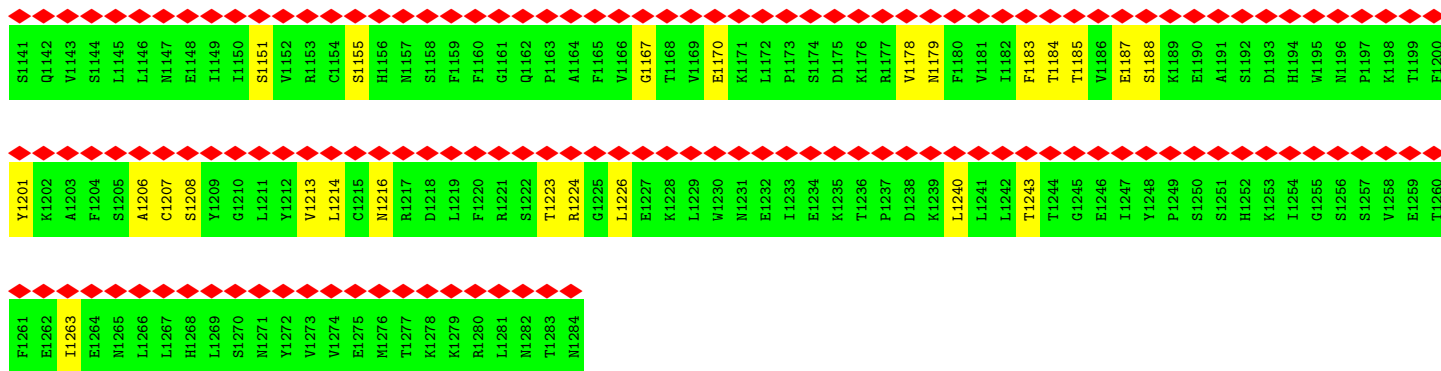


● Molecule 16: Pre-mRNA-processing protein 45

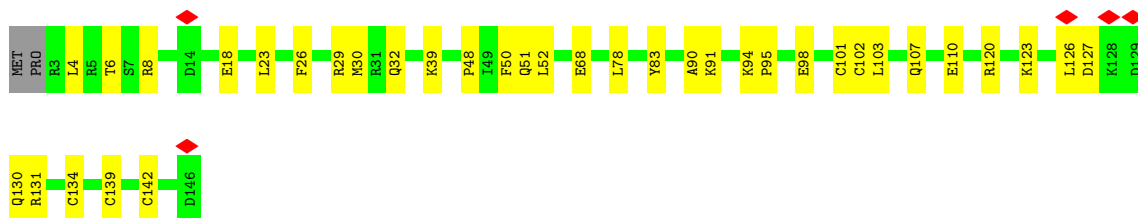




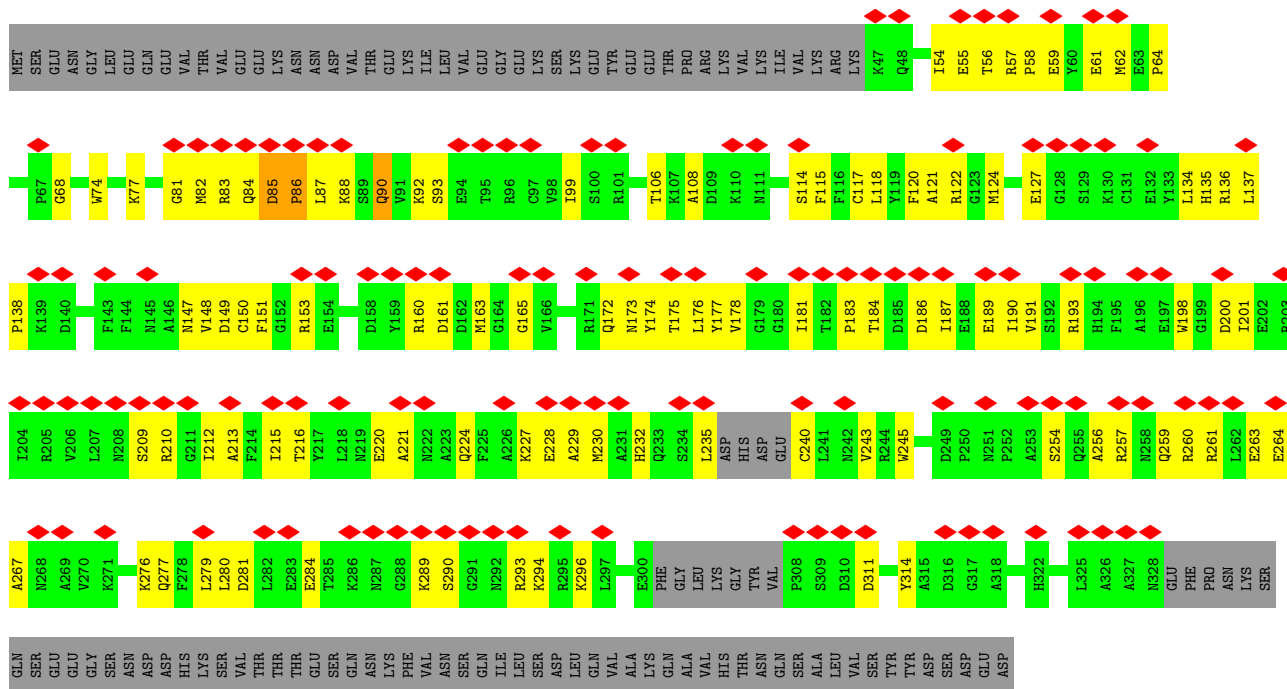
G1081	F1082	A1083	H1084	E1085	V1086	Q1087	F1088	I1089	N1090	V1091	G1092	A1093	F1094	K1095	G1096	S1097	Q1098	E1099	T1100	E1101	P1102	V1103	S1104	G1105	Y1106	K1107	Q1108	N1109	L1110	G1111	A1112	E1113	A1114	Y1115	A1116	V1117	A1118	L1119	F1120	Q1121	L1122	M1123	R1124	M1125	L1126	G1127	Y1128	P1129	T1130	N1131	E1132	I1133	L1134	I1135	C1136	T1137	L1138	Y1139	E1140	
T961	R962	L963	G964	T965	L966	K967	E968	K969	G970	F971	C972	F973	N974	N975	L976	I977	V978	M979	N980	S981	Q982	N983	I984	S985	E986	S987	S988	I989	T990	S991	I992	L993	L994	S995	N996	C997	E998	P999	T1000	G1001	F1002	D1003	R1004	L1005	V1006	L1007	L1008	G1009	M1010	Q1011	I1012	L1013	T1014	S1015	G1016	M1017	Q1018	D1019	I1020	
M1021	N1022	T1023	S1024	G1025	M1026	S1027	L1028	F1029	K1030	R1031	L1032	R1033	Y1034	L1035	K1036	S1037	R1038	I1039	I1040	D1041	L1042	M1043	T1044	Q1045	M1047	V1048	R1049	E1050	S1051	I1052	S1053	L1054	L1055	C1056	S1057	S1058	I1059	Y1060	P1061	L1062	D1063	I1064	K1065	T1066	V1067	D1068	S1069	S1070	P1071	M1072	K1073	R1074	L1075	D1076	Y1077	G1078	M1079	S1080		
I841	Q842	A843	P844	G845	S846	H847	D848	A849	S850	P851	D852	T853	A854	L855	Y856	F857	R858	D859	A860	Y861	T862	K863	R864	L865	R866	E867	K868	Y869	L870	H871	T872	H873	D874	D875	K876	D877	S878	Y879	D880	A881	Y882	H883	R884	F885	P886	F887	H888	S889	Y890	F891	G892	D893	K894	S895	K896	R897	L898	E900		
M781	F782	S783	M784	N785	T786	L787	F788	T789	L790	L791	E792	K793	A794	R795	C796	F797	H798	Q799	G800	H801	L802	L803	Y804	L805	S806	D807	E808	G809	K810	D811	E812	T813	L814	E815	R816	Y817	G818	T819	L820	S821	S822	M823	L824	S825	K826	L827	P828	G829	L830	L831	R832	E833	L834	G835	R836	L837	A838	A839	S840	
S721	N722	R723	L724	Q725	T726	Y727	N728	D729	K730	F731	L732	T733	E734	I735	L736	R737	G738	S739	Q740	L881	G742	L743	T744	M745	V746	M747	G748	P749	T750	R751	G752	G753	K754	H755	V756	L757	L758	C759	K760	L761	N762	E763	V764	L765	K766	D767	T768	S769	P770	M771	D772	R773	T774	V775	V776	L777	D778	D779	S780	
G661	L662	M663	S664	I665	Y666	A667	R668	N669	L670	F671	N672	T673	V674	E675	Q676	L677	Q678	S679	V680	L681	M682	N683	C684	H685	V686	P687	S688	M689	L690	S691	T692	E693	S694	L695	L696	I697	K698	F699	Y700	T701	N702	Q703	N704	L705	K706	S707	A708	D709	F710	T711	A712	S713	D714	R715	H716	F717	L718	L719	P720	
Y601	R602	P603	K604	Q605	L606	K607	F608	N609	F610	A611	L612	V613	L614	S615	P616	E617	A618	N619	K620	Y621	V622	L623	D624	L625	N626	I627	L628	V629	S630	L631	L632	N633	R634	A635	K636	E637	F638	P639	K640	M641	S642	E643	D644	V645	L646	L647	G648	F649	G650	T651	P652	H653	I654	G655	A656	G657	M658	N659	A660	
N481	F482	K483	K484	V485	L486	S487	V488	A489	P490	P491	Q492	I493	G494	Q495	V496	L497	P498	Q499	F500	V501	K502	C503	Q504	M505	G506	L507	S508	R509	P510	G511	P512	F513	L514	H515	S516	A516	L517	R518	D519	L520	K521	N522	S523	I524	K525	S526	P527	F528	L529	C530	L531	I532	Y533	K534	D535	K536	M537	F538	E539	Y540
Q421	N422	T423	A424	I425	Q426	Y427	L428	S429	I430	S431	F432	F433	M434	R435	Q436	Q437	S438	K439	A440	Y441	K442	K443	L444	L445	L446	R447	S448	L449	Y450	A451	A452	L453	L454	N455	F456	S457	A458	K459	Y460	R461	R462	L463	S464	L465	K466	N467	A468	L469	K470	M471	L472	T473	K474	L475	D476	N477	F478	M479	S479	L480
P361	E362	K363	Y364	A365	L366	K367	V368	D369	F370	E371	F372	L373	K374	N375	V376	F377	I378	N379	T380	Y381	D382	R383	T384	R385	L386	V387	N388	D389	Y390	D391	E392	I393	I394	N395	F396	T397	L398	K399	D400	V401	L402	G403	E404	R405	S406	V407	M408	D409	Q410	E411	N412	S413	L414	T415	N416	Y417	F418	L419	L420	



• Molecule 19: Pre-mRNA-splicing factor cwf14

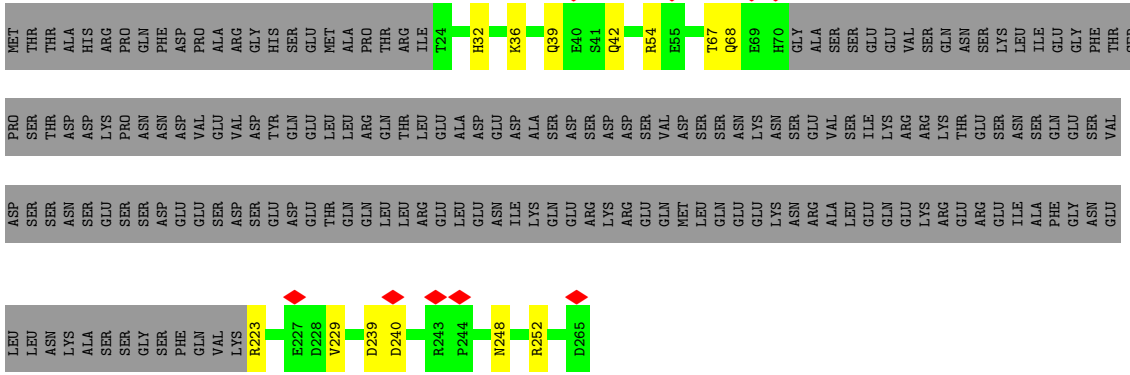


• Molecule 20: Pre-mRNA-splicing factor cwf2

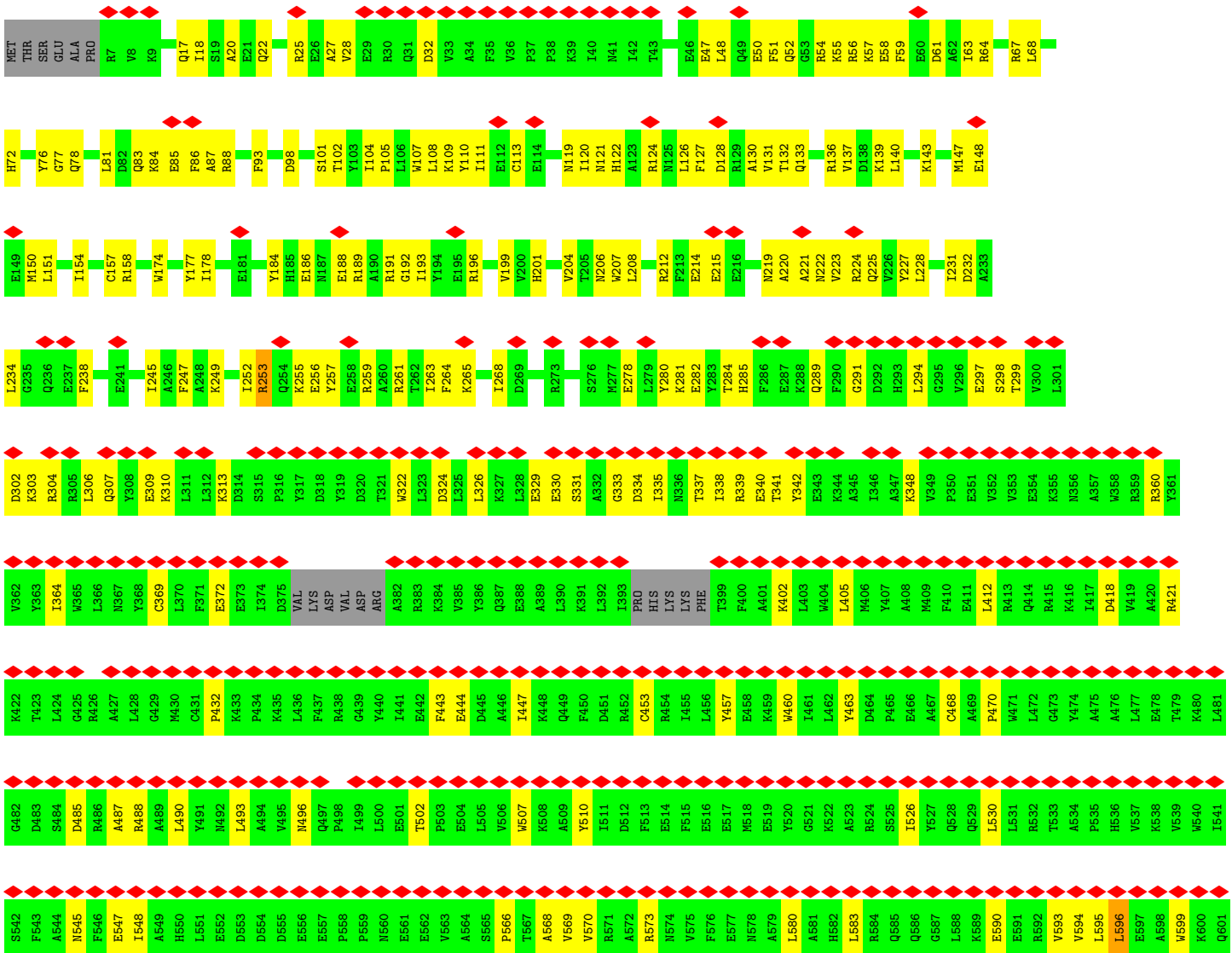


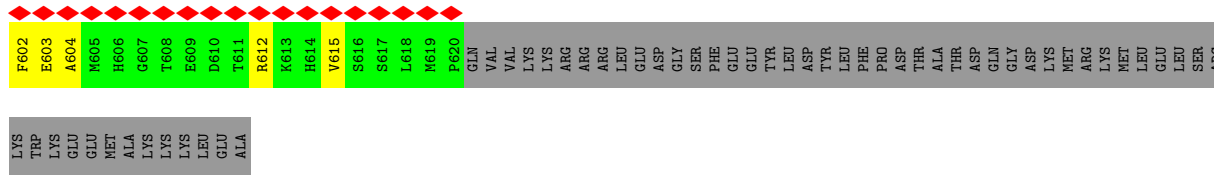
• Molecule 21: Pre-mRNA-splicing factor cwf15



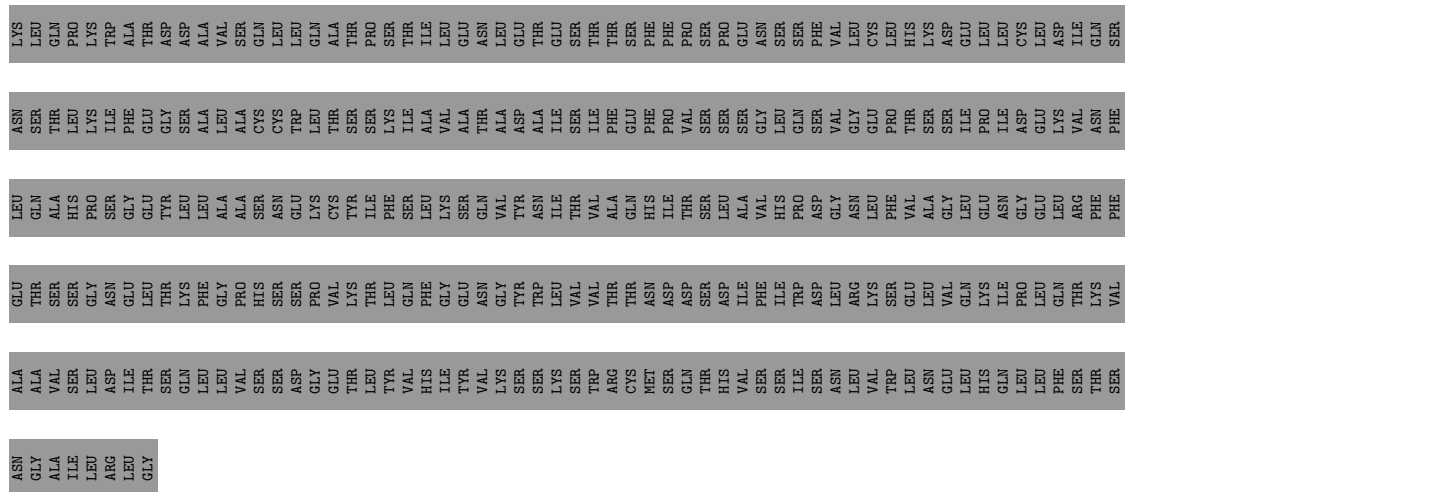
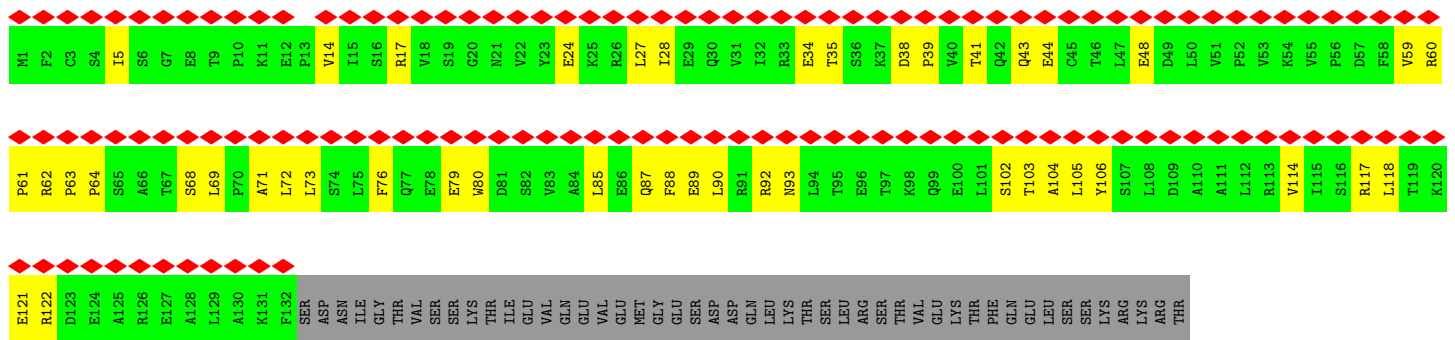


● Molecule 22: Pre-mRNA-splicing factor cwf4

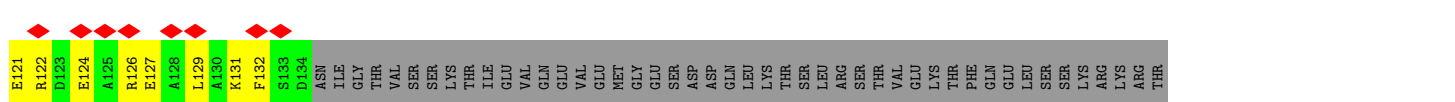




● Molecule 23: Pre-mRNA-processing factor 19



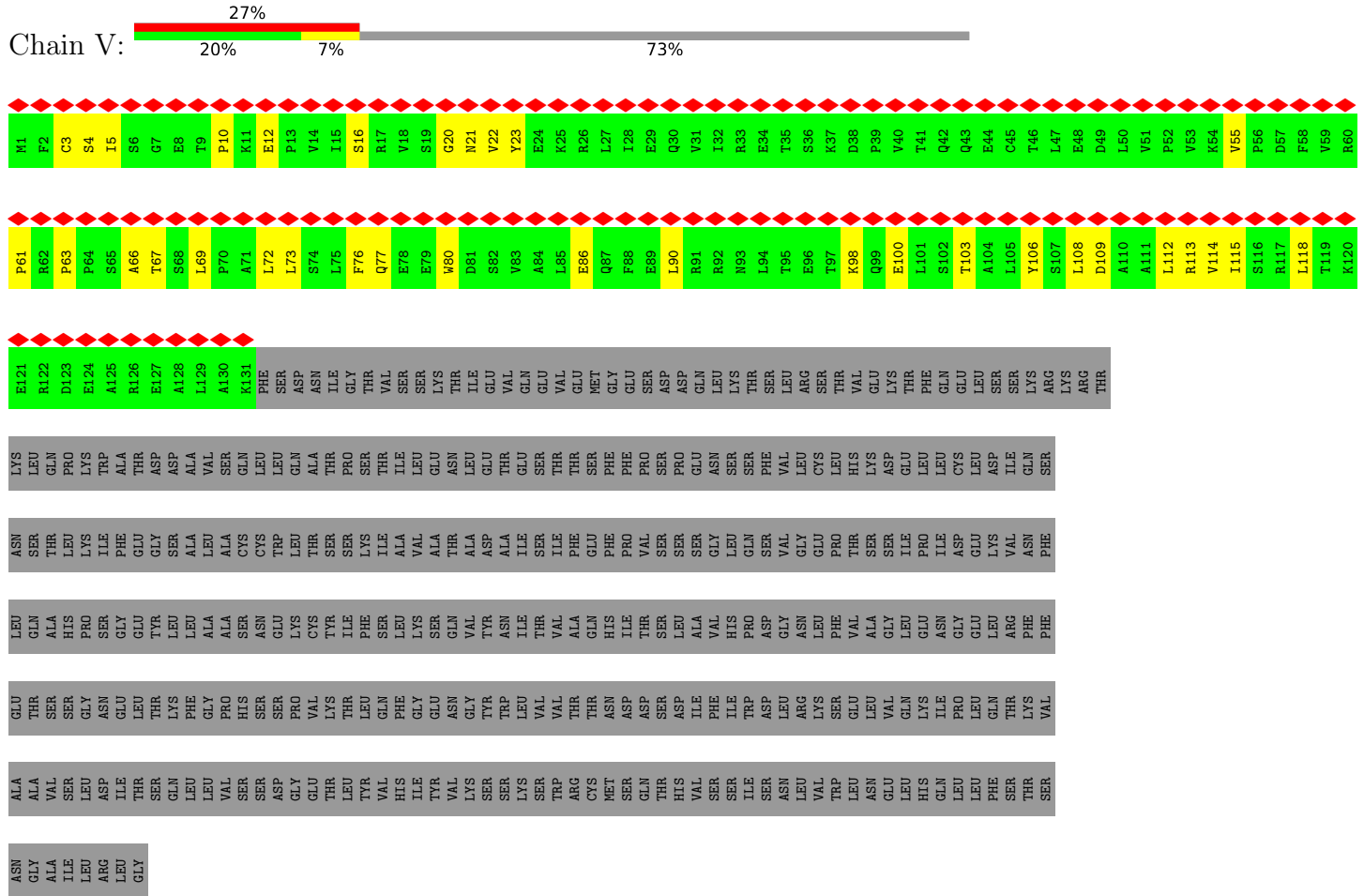
● Molecule 23: Pre-mRNA-processing factor 19



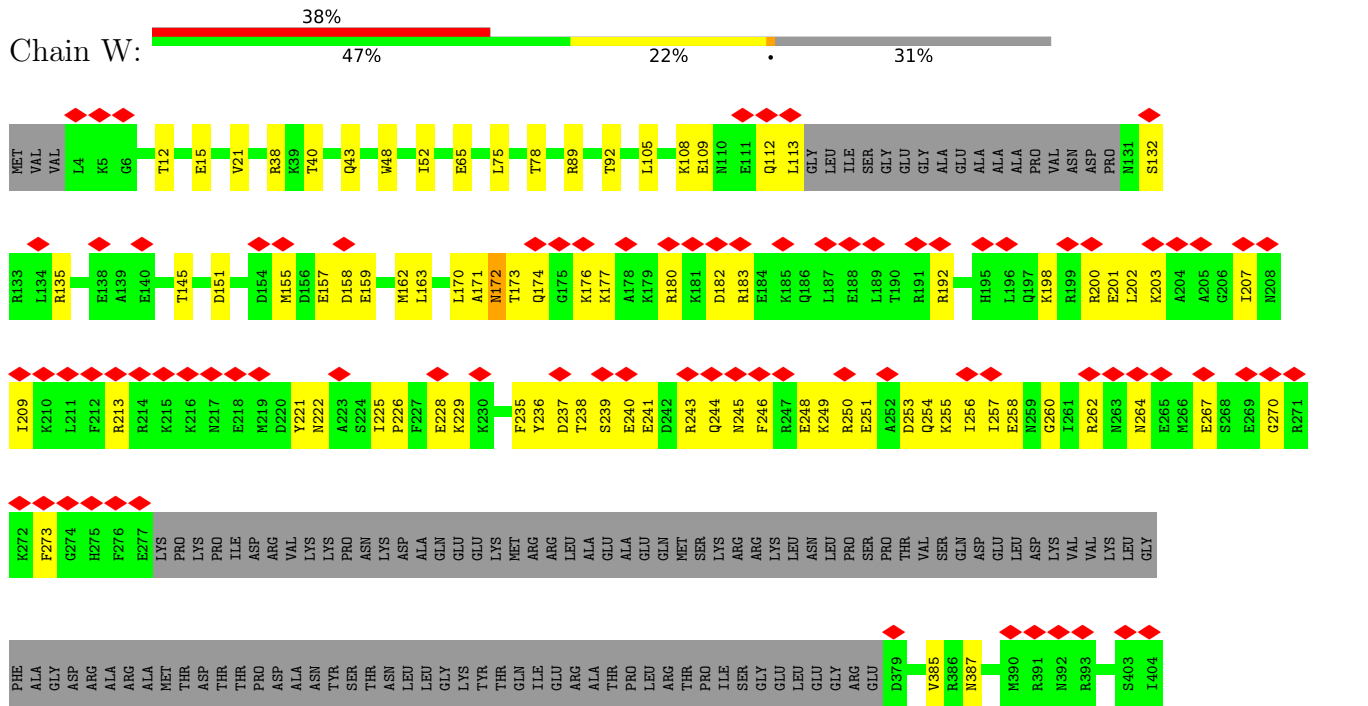


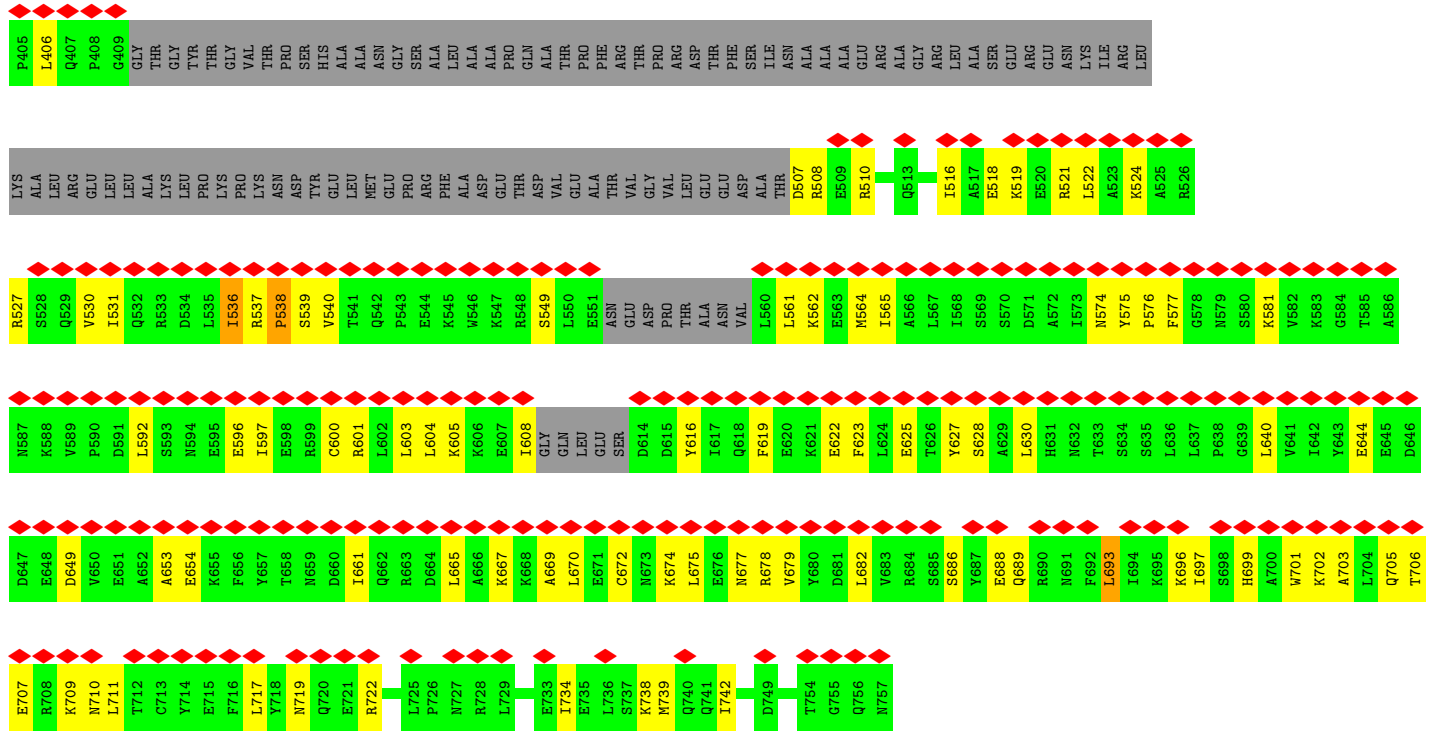


• Molecule 23: Pre-mRNA-processing factor 19

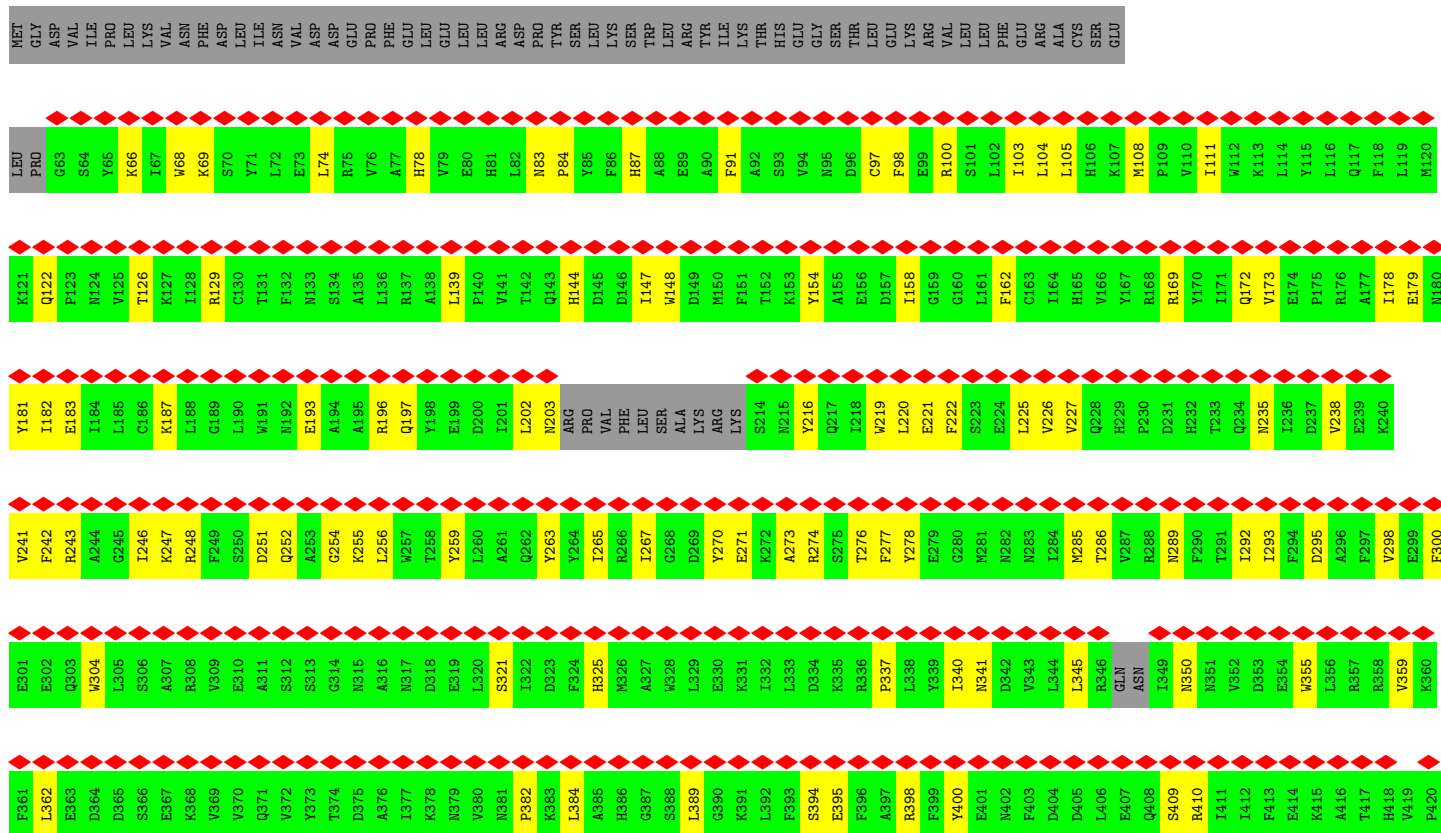
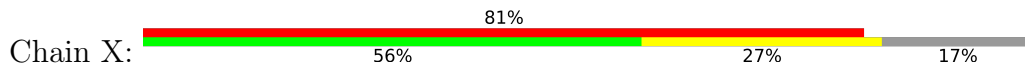


• Molecule 24: Pre-mRNA-splicing factor cdc5

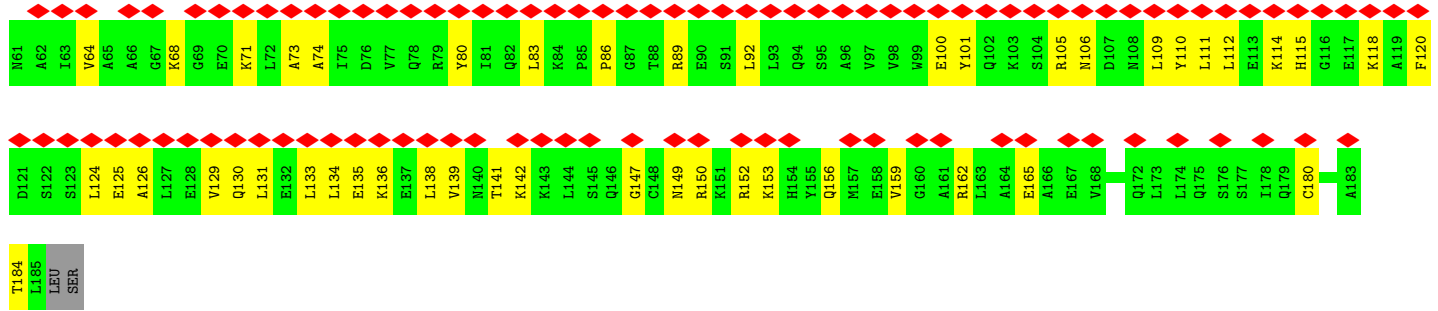




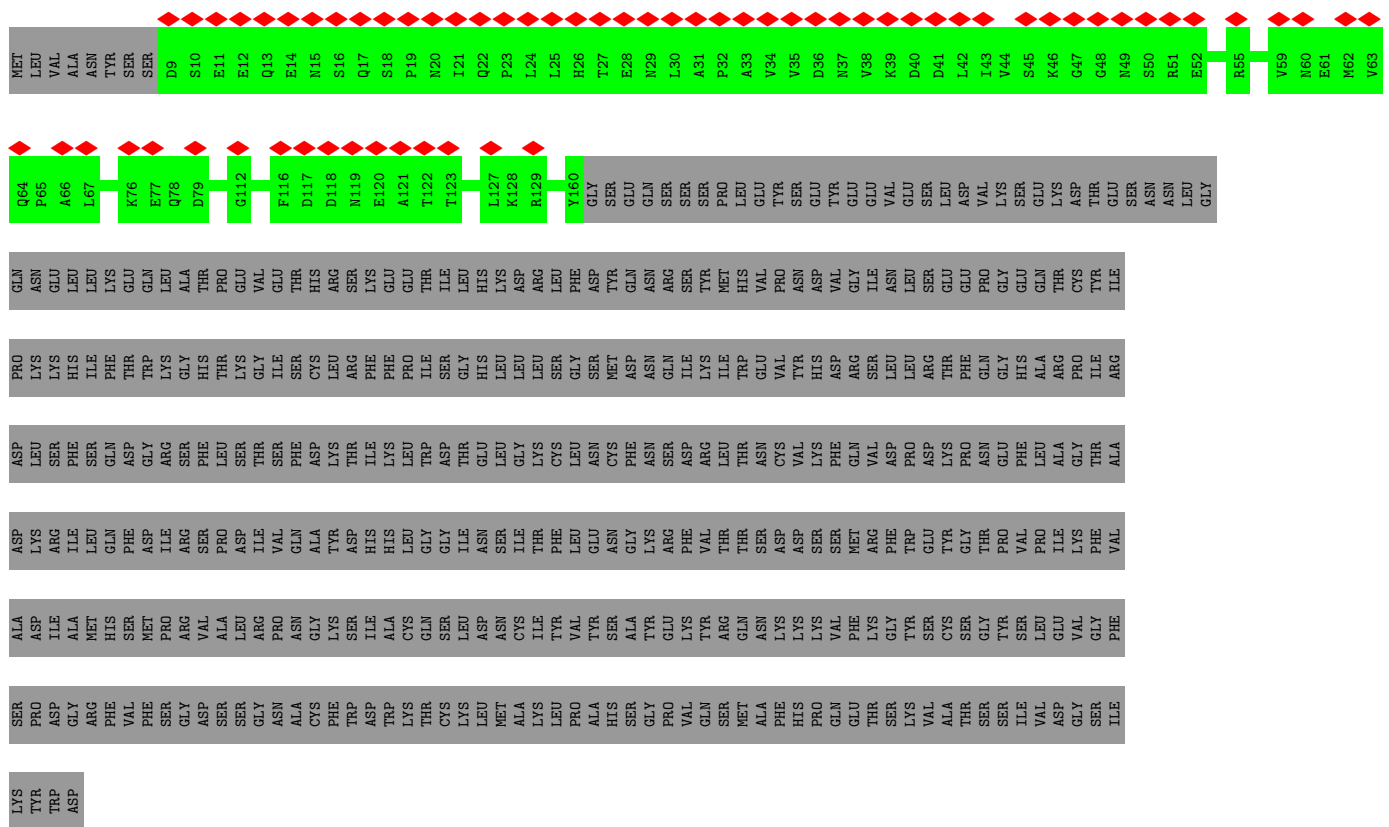
• Molecule 25: Pre-mRNA-splicing factor cwf3



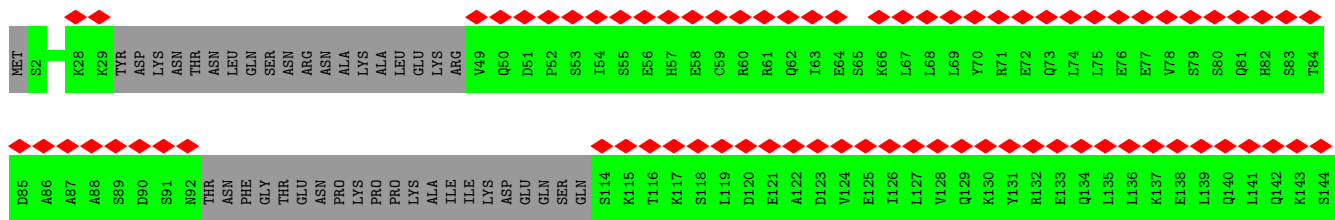




● Molecule 28: Pre-mRNA-processing factor 17

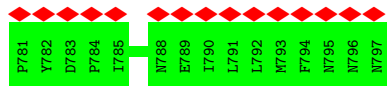


● Molecule 29: Pre-mRNA-splicing factor cwf21

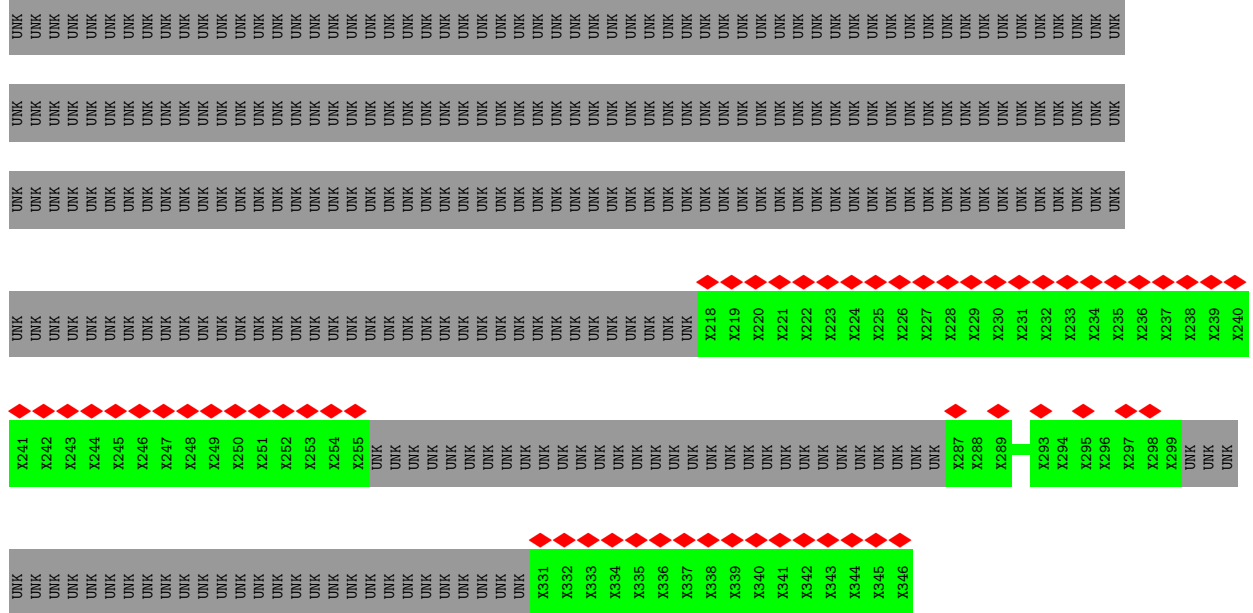




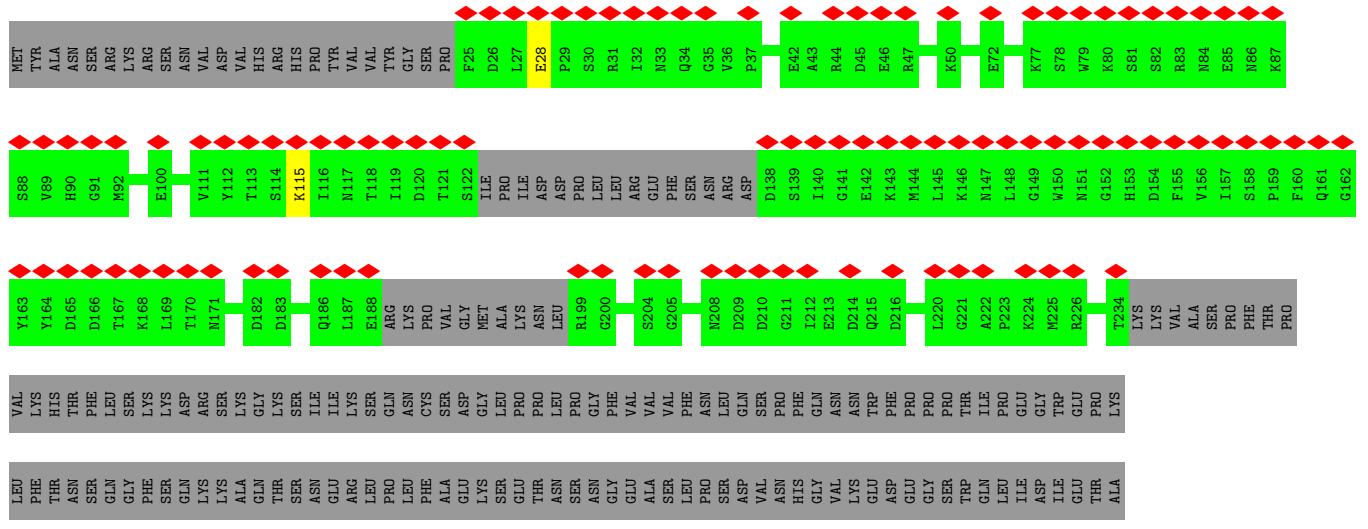




• Molecule 34: UNK2



• Molecule 35: Uncharacterized protein C20H4.06c







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	61423	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	49.4	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	37.729	Depositor
Minimum map value	-20.085	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.902	Depositor
Recommended contour level	3.55	Depositor
Map size (Å)	460.32, 460.32, 460.32	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.822, 0.822, 0.822	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: IHP, ZN, K, GTP, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	1	0.30	0/673	0.78	0/1043
2	2	0.23	0/554	0.74	0/856
3	5	0.36	0/2397	0.76	4/3727 (0.1%)
4	6	0.26	0/2207	0.78	0/3438
5	A	0.32	0/14793	0.56	1/20040 (0.0%)
6	B	0.31	0/7459	0.56	0/10117
7	C	0.28	0/2376	0.59	0/3216
8	D	0.30	0/772	0.63	0/1038
9	E	0.29	0/737	0.62	0/993
10	F	0.33	0/646	0.69	0/875
11	G	0.30	0/829	0.72	0/1111
12	H	0.26	0/662	0.57	0/894
13	I	0.28	0/585	0.59	1/794 (0.1%)
14	J	0.31	0/578	0.56	0/774
15	K	0.32	0/3130	0.58	0/4251
16	L	0.29	0/1885	0.57	0/2545
17	M	0.30	0/1841	0.61	0/2468
18	N	0.25	0/10690	0.47	1/14463 (0.0%)
19	O	0.33	0/1199	0.63	0/1609
20	P	0.33	0/2222	0.65	1/2991 (0.0%)
21	Q	0.28	0/767	0.57	0/1028
22	R	0.30	0/5235	0.60	1/7067 (0.0%)
23	S	0.29	0/1072	0.59	0/1453
23	T	0.31	0/1086	0.71	3/1472 (0.2%)
23	U	0.25	0/2897	0.56	1/3914 (0.0%)
23	V	0.27	0/1060	0.60	0/1437
24	W	0.28	0/4407	0.59	1/5907 (0.0%)
25	X	0.27	0/5599	0.54	2/7566 (0.0%)
26	Y	0.26	0/1065	0.60	0/1413
27	Z	0.27	0/1244	0.56	0/1667
28	a	0.31	0/1055	0.54	0/1443
29	b	0.30	0/829	0.51	0/1111

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
30	c	0.31	0/1711	0.56	0/2312
31	d	0.29	0/1206	0.62	1/1636 (0.1%)
33	m	0.27	0/663	0.55	0/895
35	y	0.29	0/1511	0.61	0/2032
36	z	0.27	0/5079	0.53	1/6875 (0.0%)
All	All	0.29	0/92721	0.58	18/126471 (0.0%)

There are no bond length outliers.

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	U	118	LEU	CA-CB-CG	9.08	136.19	115.30
22	R	596	LEU	CA-CB-CG	8.87	135.71	115.30
3	5	32	C	C2-N1-C1'	7.93	127.52	118.80
3	5	32	C	N1-C2-O2	7.66	123.50	118.90
23	T	72	LEU	CA-CB-CG	6.72	130.76	115.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	605	0	302	10	0
2	2	500	0	257	12	0
3	5	2149	0	1085	23	0
4	6	1970	0	994	52	0
5	A	14402	0	14306	312	0
6	B	7298	0	7336	178	0
7	C	2328	0	2276	84	0
8	D	760	0	776	26	0
9	E	726	0	750	23	0
10	F	638	0	682	37	0
11	G	819	0	845	46	0
12	H	652	0	680	13	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	I	574	0	591	27	0
14	J	573	0	602	12	0
15	K	3053	0	3011	88	0
16	L	1849	0	1879	47	0
17	M	1818	0	1822	67	0
18	N	10461	0	10412	189	0
19	O	1176	0	1167	31	0
20	P	2178	0	2101	105	0
21	Q	752	0	729	15	0
22	R	5108	0	5024	179	0
23	S	1055	0	1075	61	0
23	T	1069	0	1084	72	0
23	U	2870	0	2403	82	0
23	V	1044	0	1066	44	0
24	W	4346	0	4375	176	0
25	X	5467	0	5372	160	0
26	Y	1049	0	1052	46	0
27	Z	1232	0	1242	56	0
28	a	1035	0	837	0	0
29	b	822	0	820	0	0
30	c	1678	0	1659	0	0
31	d	1179	0	1169	0	0
32	f	110	0	29	0	0
33	m	649	0	641	0	0
34	r	335	0	77	0	0
35	y	1480	0	1379	0	0
36	z	4980	0	5047	0	0
37	6	3	0	0	0	0
37	B	1	0	0	0	0
38	6	1	0	0	0	0
39	A	36	0	6	0	0
40	B	32	0	12	3	0
41	M	2	0	0	0	0
41	O	3	0	0	0	0
41	P	1	0	0	0	0
All	All	90868	0	86972	1981	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

The worst 5 of 1981 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1642:LYS:HD3	5:A:1650:CYS:SG	1.36	1.62
5:A:1642:LYS:CD	5:A:1650:CYS:SG	2.14	1.34
5:A:1638:ILE:CD1	5:A:1642:LYS:HE3	1.73	1.18
4:6:32:G:N2	20:P:82:MET:HG2	1.57	1.17
4:6:32:G:N2	20:P:82:MET:CG	2.07	1.16

There are no symmetry-related clashes.

## 5.3 Torsion angles [\(i\)](#)

### 5.3.1 Protein backbone [\(i\)](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	A	1735/2363 (73%)	1635 (94%)	99 (6%)	1 (0%)	48	80
6	B	916/984 (93%)	866 (94%)	49 (5%)	1 (0%)	48	80
7	C	297/340 (87%)	274 (92%)	23 (8%)	0	100	100
8	D	94/97 (97%)	92 (98%)	2 (2%)	0	100	100
9	E	91/147 (62%)	85 (93%)	6 (7%)	0	100	100
10	F	79/117 (68%)	73 (92%)	6 (8%)	0	100	100
11	G	98/115 (85%)	93 (95%)	5 (5%)	0	100	100
12	H	78/84 (93%)	77 (99%)	1 (1%)	0	100	100
13	I	71/78 (91%)	70 (99%)	1 (1%)	0	100	100
14	J	71/77 (92%)	66 (93%)	5 (7%)	0	100	100
15	K	389/473 (82%)	357 (92%)	32 (8%)	0	100	100
16	L	230/557 (41%)	211 (92%)	19 (8%)	0	100	100
17	M	222/354 (63%)	214 (96%)	8 (4%)	0	100	100
18	N	1282/1284 (100%)	1260 (98%)	22 (2%)	0	100	100
19	O	142/146 (97%)	135 (95%)	7 (5%)	0	100	100
20	P	265/388 (68%)	244 (92%)	19 (7%)	2 (1%)	16	51

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	Q	86/265 (32%)	77 (90%)	9 (10%)	0	100	100
22	R	597/674 (89%)	588 (98%)	9 (2%)	0	100	100
23	S	130/488 (27%)	122 (94%)	8 (6%)	0	100	100
23	T	132/488 (27%)	123 (93%)	9 (7%)	0	100	100
23	U	414/488 (85%)	394 (95%)	20 (5%)	0	100	100
23	V	129/488 (26%)	118 (92%)	11 (8%)	0	100	100
24	W	514/757 (68%)	479 (93%)	32 (6%)	3 (1%)	22	57
25	X	642/790 (81%)	610 (95%)	31 (5%)	1 (0%)	44	75
26	Y	114/229 (50%)	108 (95%)	5 (4%)	1 (1%)	14	49
27	Z	151/187 (81%)	144 (95%)	7 (5%)	0	100	100
28	a	150/558 (27%)	140 (93%)	10 (7%)	0	100	100
29	b	98/293 (33%)	94 (96%)	4 (4%)	0	100	100
30	c	202/887 (23%)	192 (95%)	10 (5%)	0	100	100
31	d	152/155 (98%)	137 (90%)	15 (10%)	0	100	100
33	m	79/797 (10%)	78 (99%)	1 (1%)	0	100	100
35	y	179/534 (34%)	154 (86%)	23 (13%)	2 (1%)	12	44
36	z	624/647 (96%)	611 (98%)	12 (2%)	1 (0%)	44	75
All	All	10453/16329 (64%)	9921 (95%)	520 (5%)	12 (0%)	50	80

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
20	P	90	GLN
24	W	536	ILE
35	y	115	LYS
5	A	1115	ILE
26	Y	144	VAL

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	A	1570/2138 (73%)	1568 (100%)	2 (0%)	92	98
6	B	821/881 (93%)	821 (100%)	0	100	100
7	C	257/292 (88%)	257 (100%)	0	100	100
8	D	85/86 (99%)	85 (100%)	0	100	100
9	E	80/118 (68%)	80 (100%)	0	100	100
10	F	76/102 (74%)	76 (100%)	0	100	100
11	G	91/101 (90%)	91 (100%)	0	100	100
12	H	73/76 (96%)	73 (100%)	0	100	100
13	I	64/69 (93%)	64 (100%)	0	100	100
14	J	63/67 (94%)	63 (100%)	0	100	100
15	K	333/405 (82%)	333 (100%)	0	100	100
16	L	200/477 (42%)	200 (100%)	0	100	100
17	M	198/306 (65%)	198 (100%)	0	100	100
18	N	1188/1188 (100%)	1188 (100%)	0	100	100
19	O	130/132 (98%)	130 (100%)	0	100	100
20	P	231/340 (68%)	231 (100%)	0	100	100
21	Q	79/240 (33%)	79 (100%)	0	100	100
22	R	532/597 (89%)	531 (100%)	1 (0%)	92	97
23	S	121/443 (27%)	121 (100%)	0	100	100
23	T	123/443 (28%)	123 (100%)	0	100	100
23	U	223/443 (50%)	223 (100%)	0	100	100
23	V	120/443 (27%)	120 (100%)	0	100	100
24	W	469/656 (72%)	468 (100%)	1 (0%)	92	97
25	X	586/707 (83%)	585 (100%)	1 (0%)	92	97
26	Y	116/214 (54%)	116 (100%)	0	100	100
27	Z	132/163 (81%)	132 (100%)	0	100	100
28	a	79/496 (16%)	79 (100%)	0	100	100
29	b	95/275 (34%)	95 (100%)	0	100	100
30	c	188/816 (23%)	188 (100%)	0	100	100
31	d	128/129 (99%)	128 (100%)	0	100	100
33	m	72/719 (10%)	72 (100%)	0	100	100
35	y	158/478 (33%)	158 (100%)	0	100	100

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	z	564/585 (96%)	564 (100%)	0	100	100
All	All	9245/14625 (63%)	9240 (100%)	5 (0%)	92	98

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	A	844	ARG
5	A	1209	ASN
22	R	253	ARG
24	W	155	MET
25	X	410	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	Res	Type
24	W	245	ASN
27	Z	130	GLN
24	W	387	ASN
26	Y	111	GLN
28	a	101	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	28/29 (96%)	19 (67%)	2 (7%)
2	2	22/186 (11%)	4 (18%)	0
3	5	101/120 (84%)	23 (22%)	2 (1%)
4	6	91/99 (91%)	44 (48%)	7 (7%)
All	All	242/434 (55%)	90 (37%)	11 (4%)

5 of 90 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	-14	U
1	1	-13	U
1	1	-12	U
1	1	-8	U
1	1	-4	A



5 of 11 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	6	30	A
4	6	37	A
4	6	74	U
4	6	52	G
4	6	13	A

#### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

#### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

#### 5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 11 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
40	GTP	B	1001	37	26,34,34	1.22	2 (7%)	32,54,54	1.69	7 (21%)
39	IHP	A	2401	-	36,36,36	1.39	13 (36%)	54,60,60	1.47	9 (16%)

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
40	GTP	B	1001	37	-	0/18/38/38	0/3/3/3
39	IHP	A	2401	-	-	5/30/54/54	0/1/1/1

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	B	1001	GTP	C5-C6	-4.21	1.38	1.47
39	A	2401	IHP	P6-O46	-2.42	1.45	1.54
39	A	2401	IHP	P1-O31	-2.19	1.46	1.54
39	A	2401	IHP	P1-O11	2.18	1.63	1.59
39	A	2401	IHP	P5-O45	-2.11	1.46	1.54

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	B	1001	GTP	PB-O3B-PG	-4.73	116.59	132.83
40	B	1001	GTP	C5-C6-N1	3.36	119.88	113.95
40	B	1001	GTP	O4'-C1'-C2'	-3.25	102.18	106.93
39	A	2401	IHP	O11-P1-O21	-3.17	97.15	109.39
39	A	2401	IHP	C5-C6-C1	3.15	117.30	110.41

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
39	A	2401	IHP	C6-O16-P6-O26
39	A	2401	IHP	C1-O11-P1-O41
39	A	2401	IHP	C6-O16-P6-O36
39	A	2401	IHP	C5-O15-P5-O35
39	A	2401	IHP	C5-O15-P5-O45

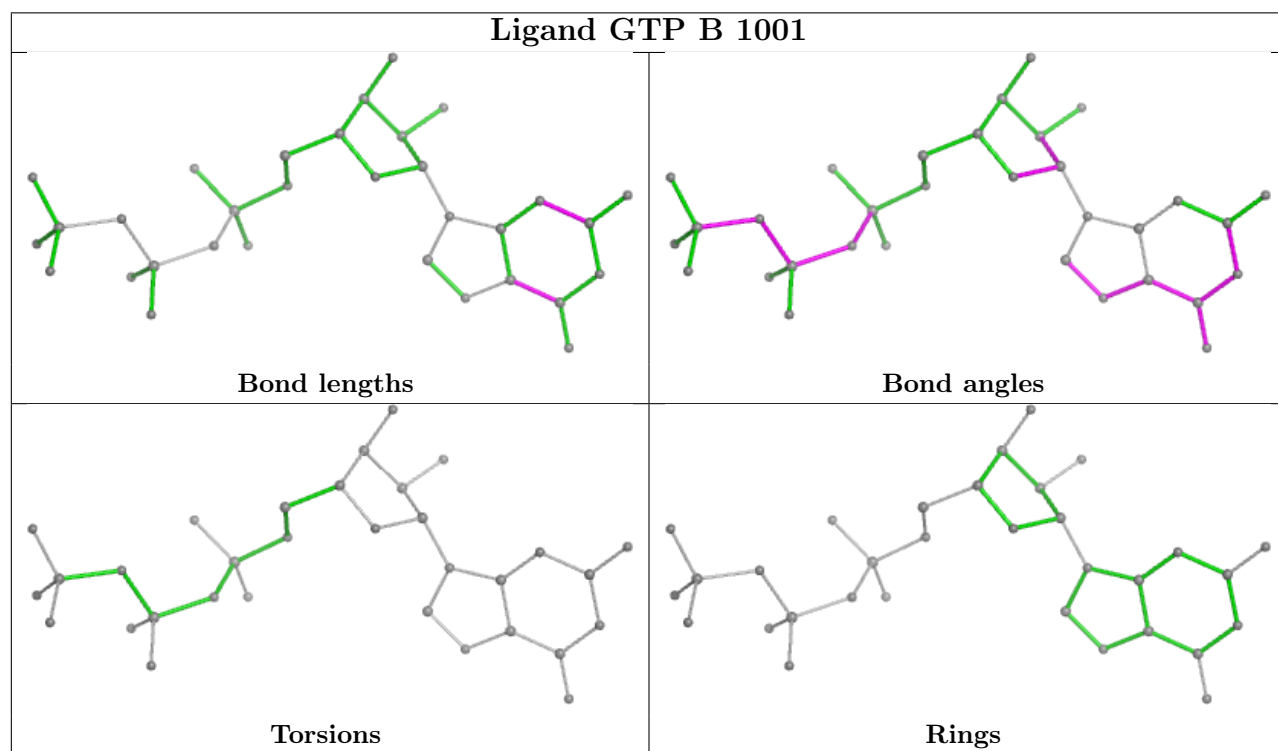
There are no ring outliers.

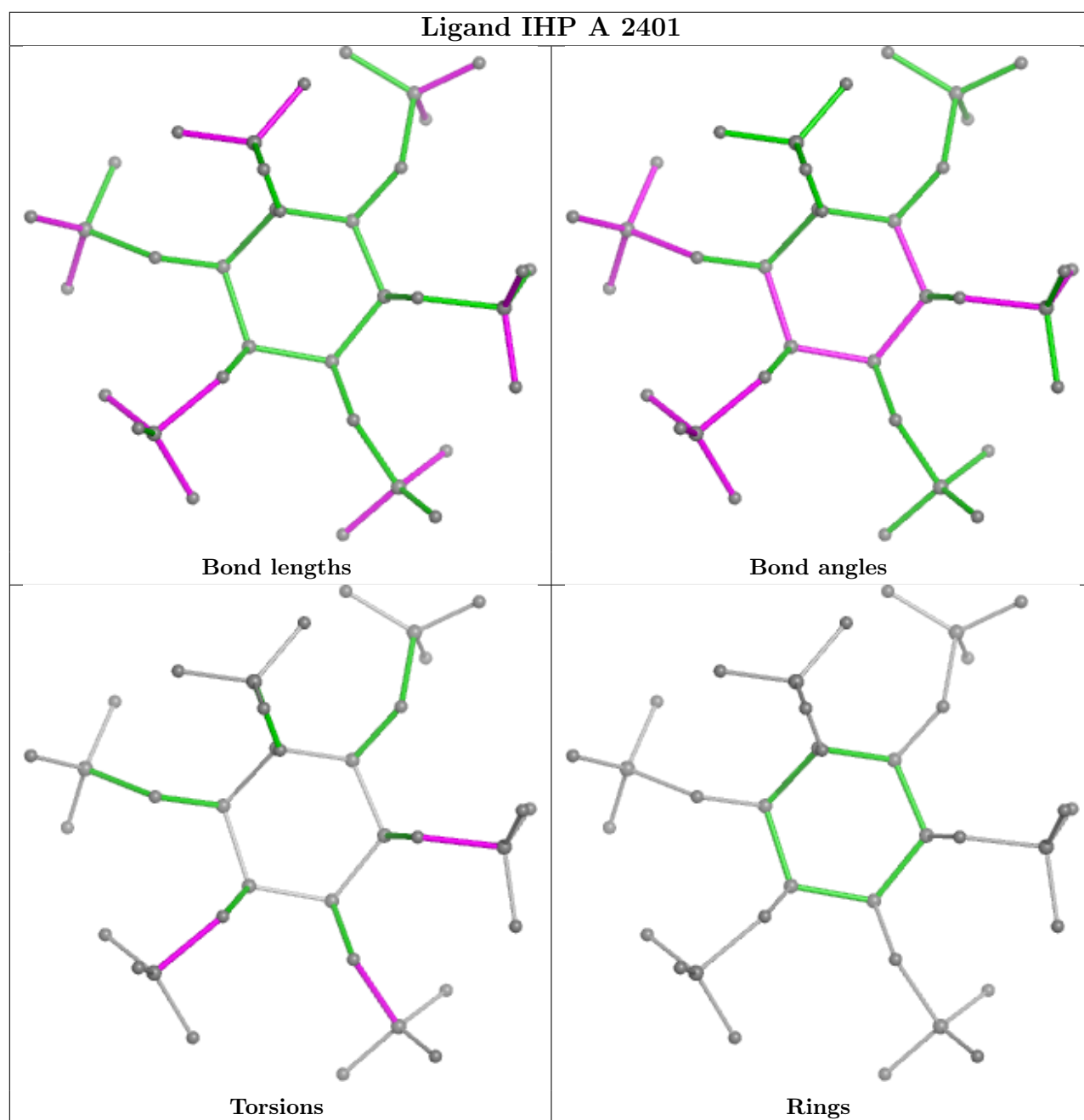
1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
40	B	1001	GTP	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

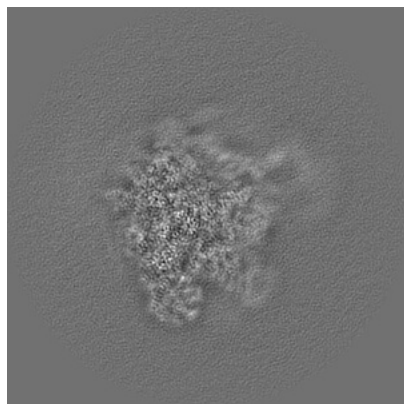
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19941. These allow visual inspection of the internal detail of the map and identification of artifacts.

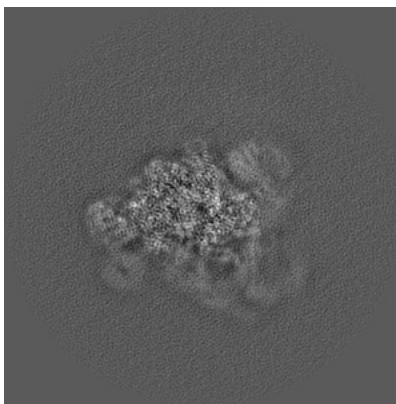
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

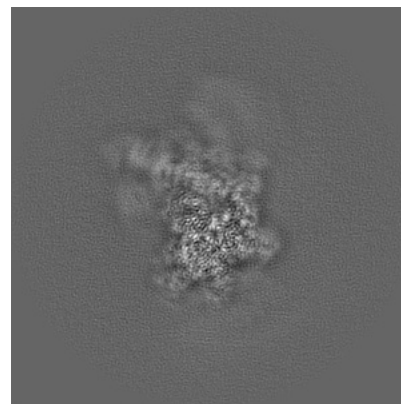
#### 6.1.1 Primary map



X

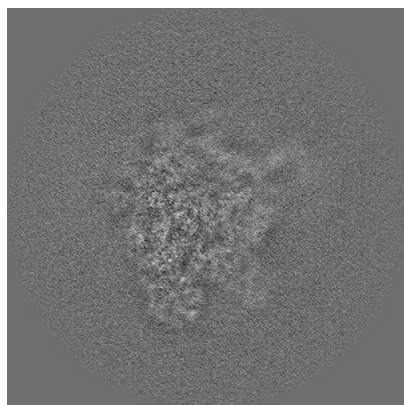


Y

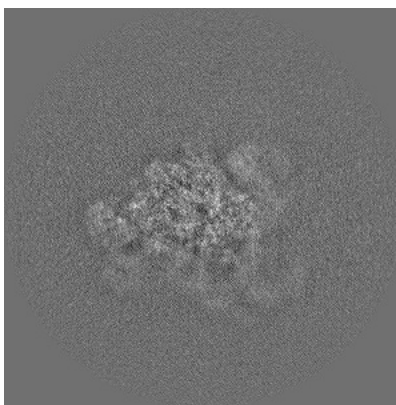


Z

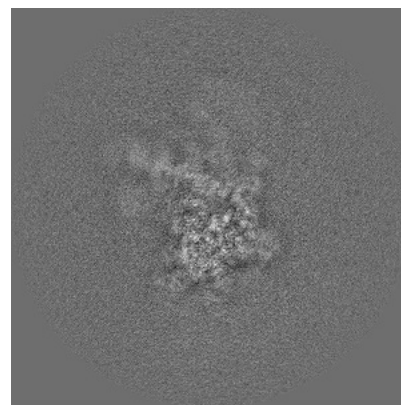
#### 6.1.2 Raw map



X



Y

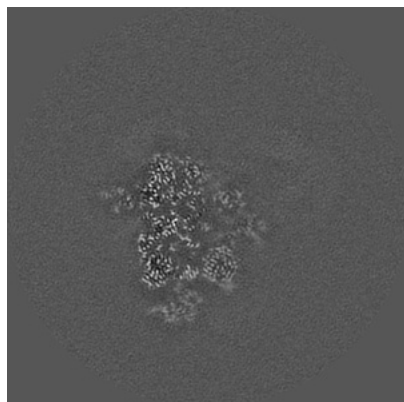


Z

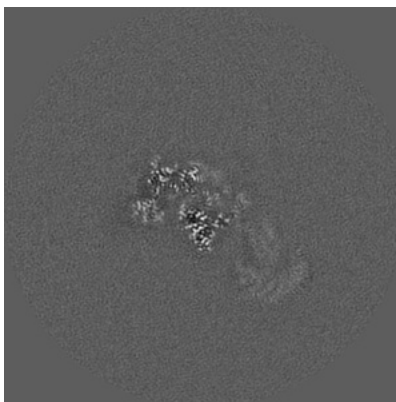
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

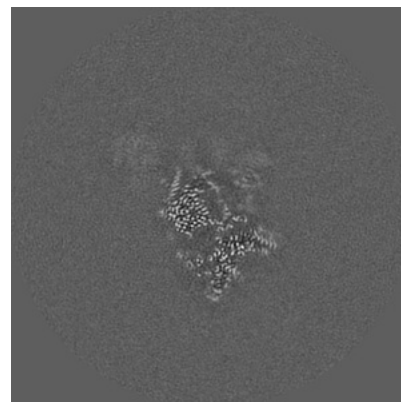
### 6.2.1 Primary map



X Index: 280

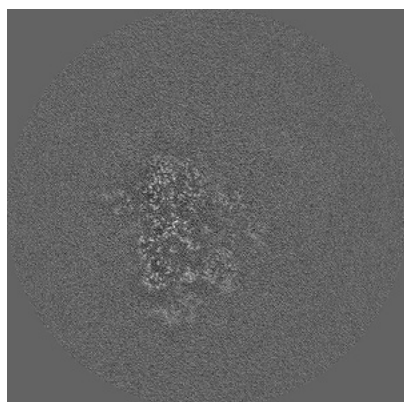


Y Index: 280

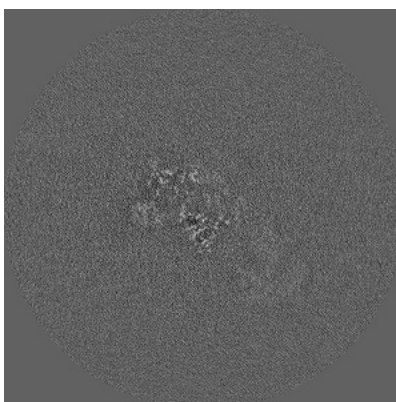


Z Index: 280

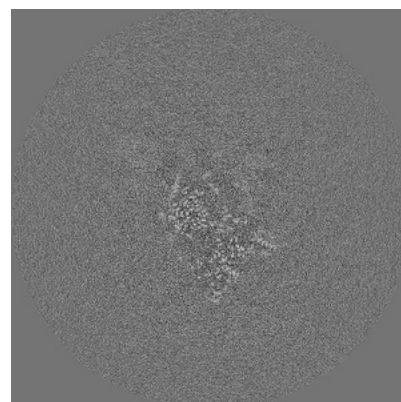
### 6.2.2 Raw map



X Index: 280



Y Index: 280

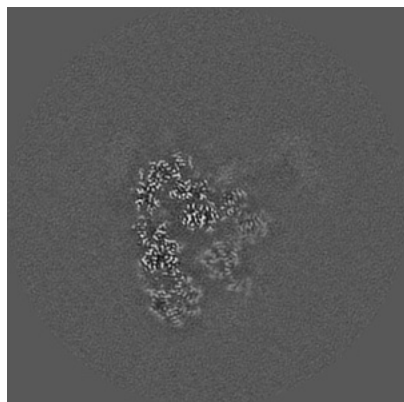


Z Index: 280

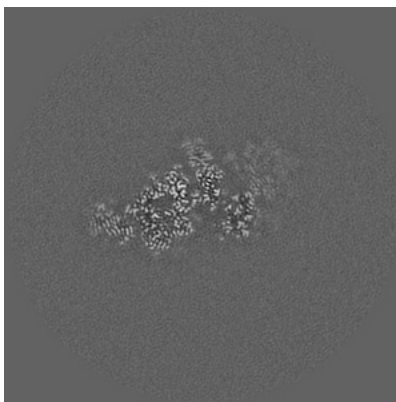
The images above show central slices of the map in three orthogonal directions.

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

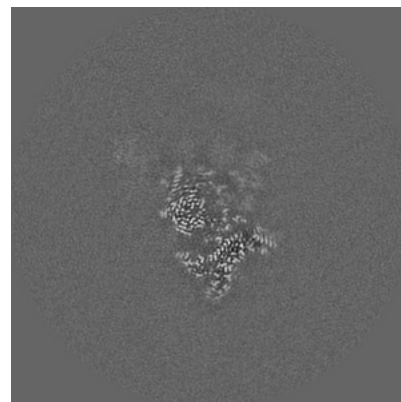
### 6.3.1 Primary map



X Index: 263

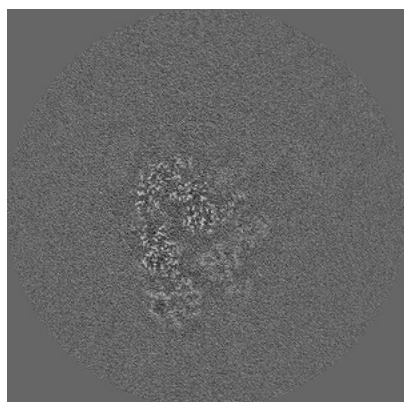


Y Index: 220

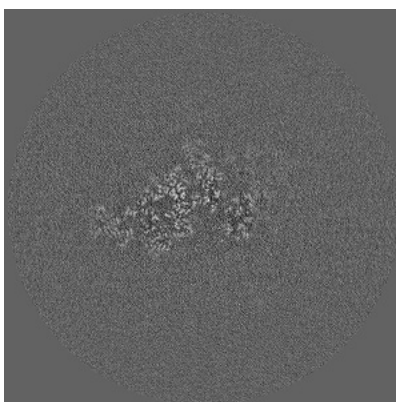


Z Index: 282

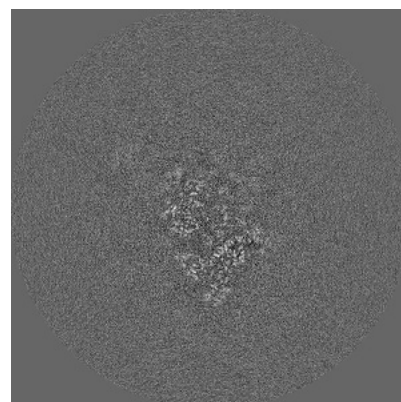
### 6.3.2 Raw map



X Index: 263



Y Index: 220

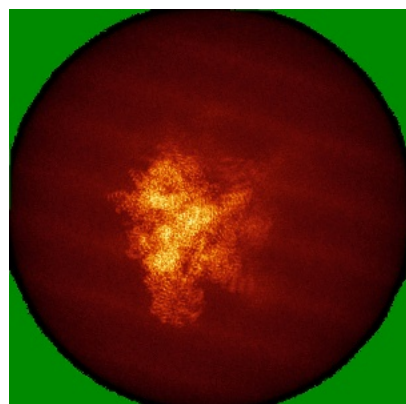


Z Index: 284

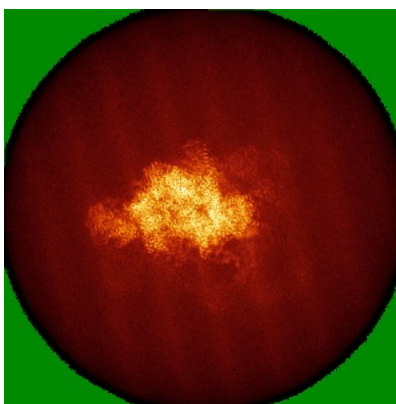
The images above show the largest variance slices of the map in three orthogonal directions.

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

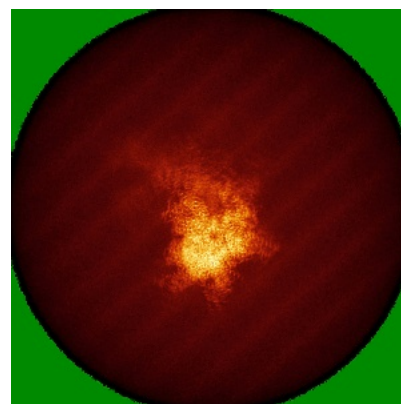
### 6.4.1 Primary map



X

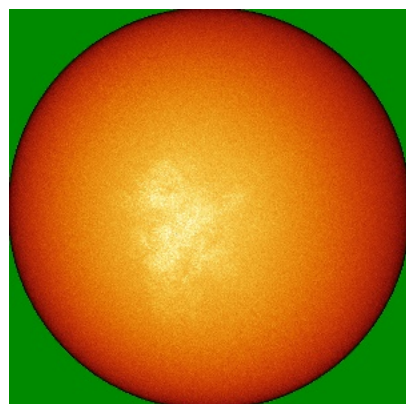


Y

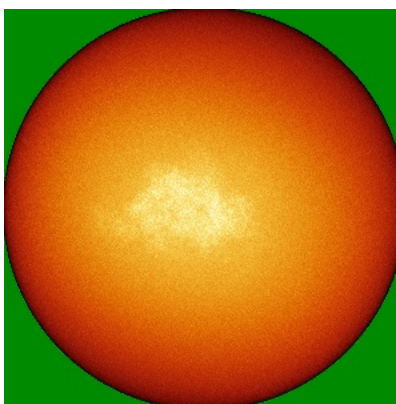


Z

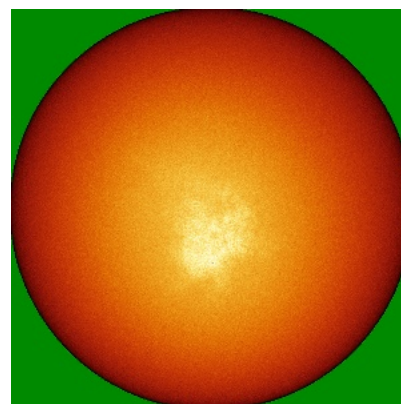
### 6.4.2 Raw map



X



Y



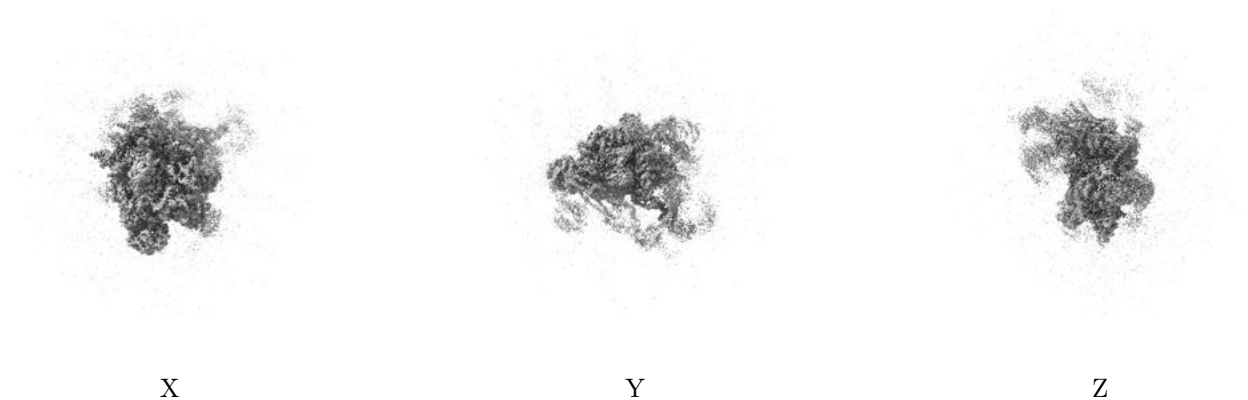
Z

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



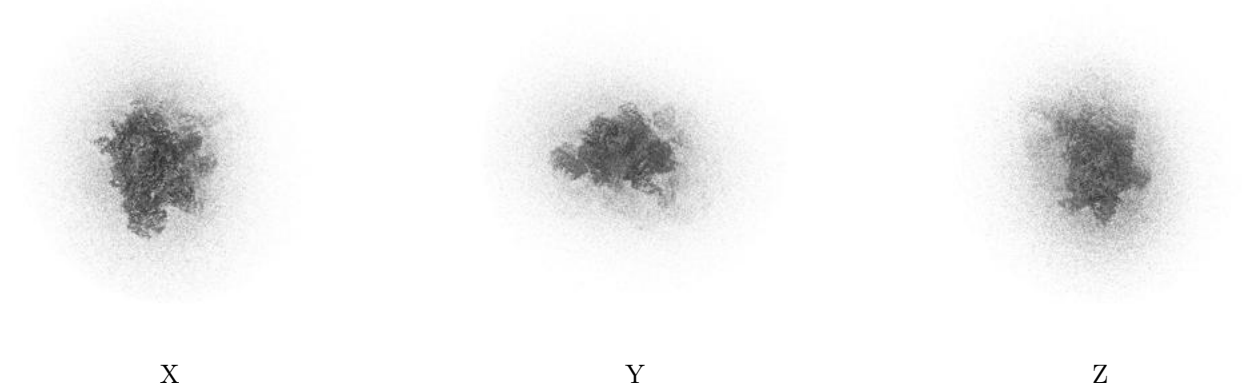
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.55. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

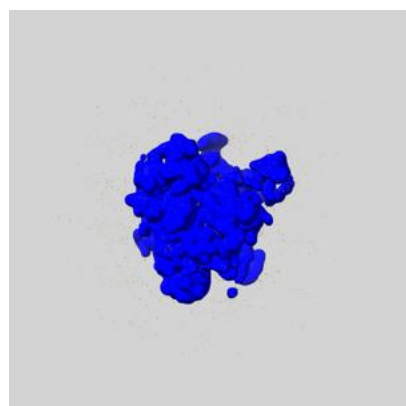
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

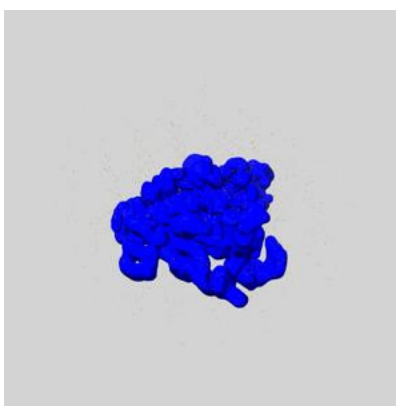
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

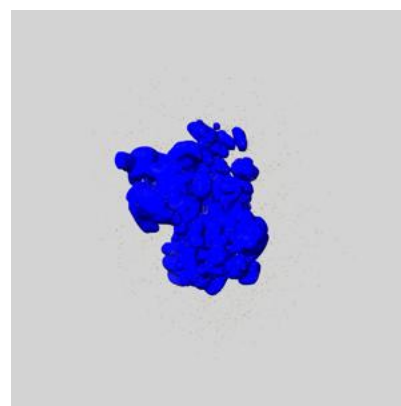
### 6.6.1 emd\_19941\_msk\_1.map [i](#)



X



Y

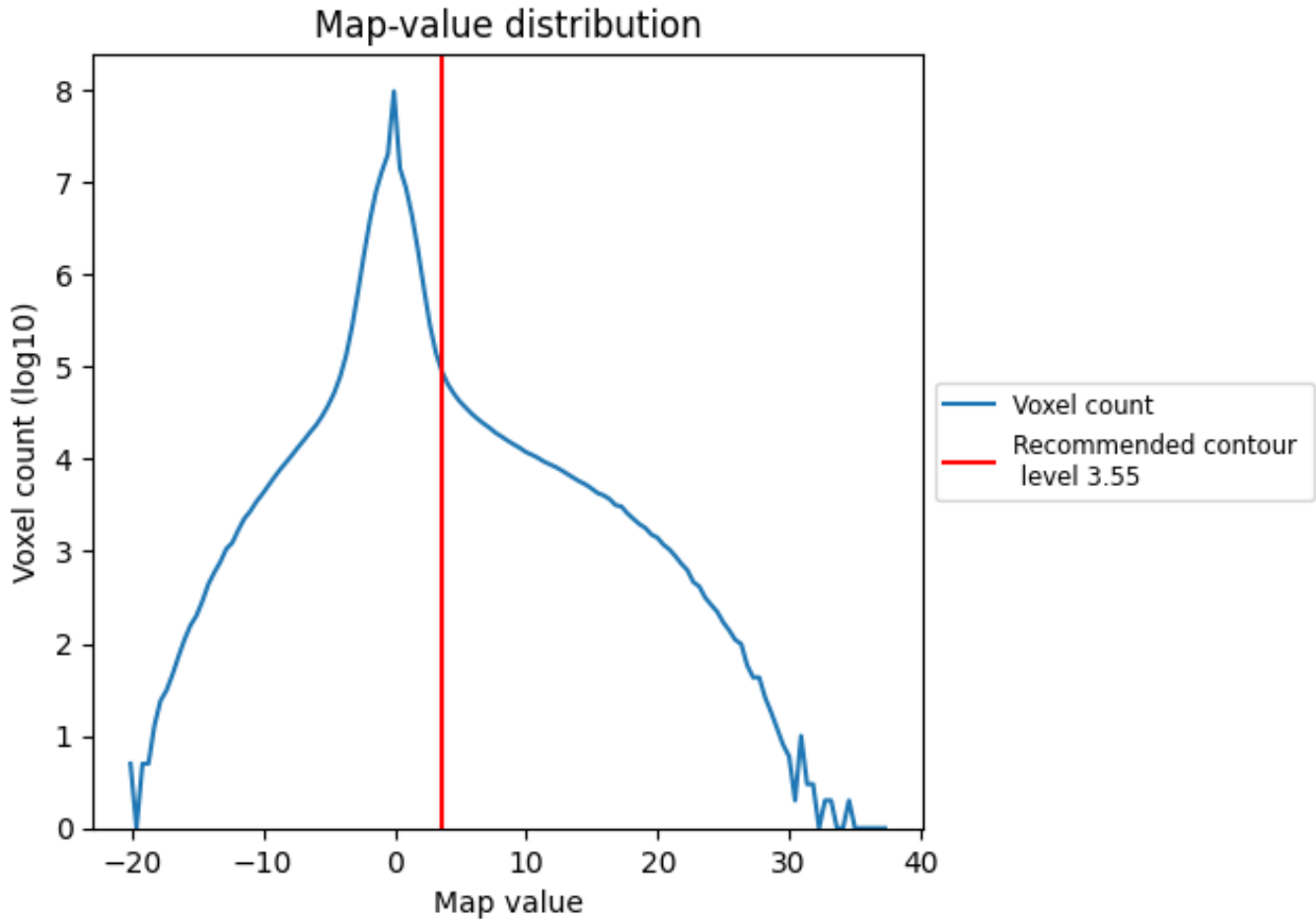


Z

## 7 Map analysis [i](#)

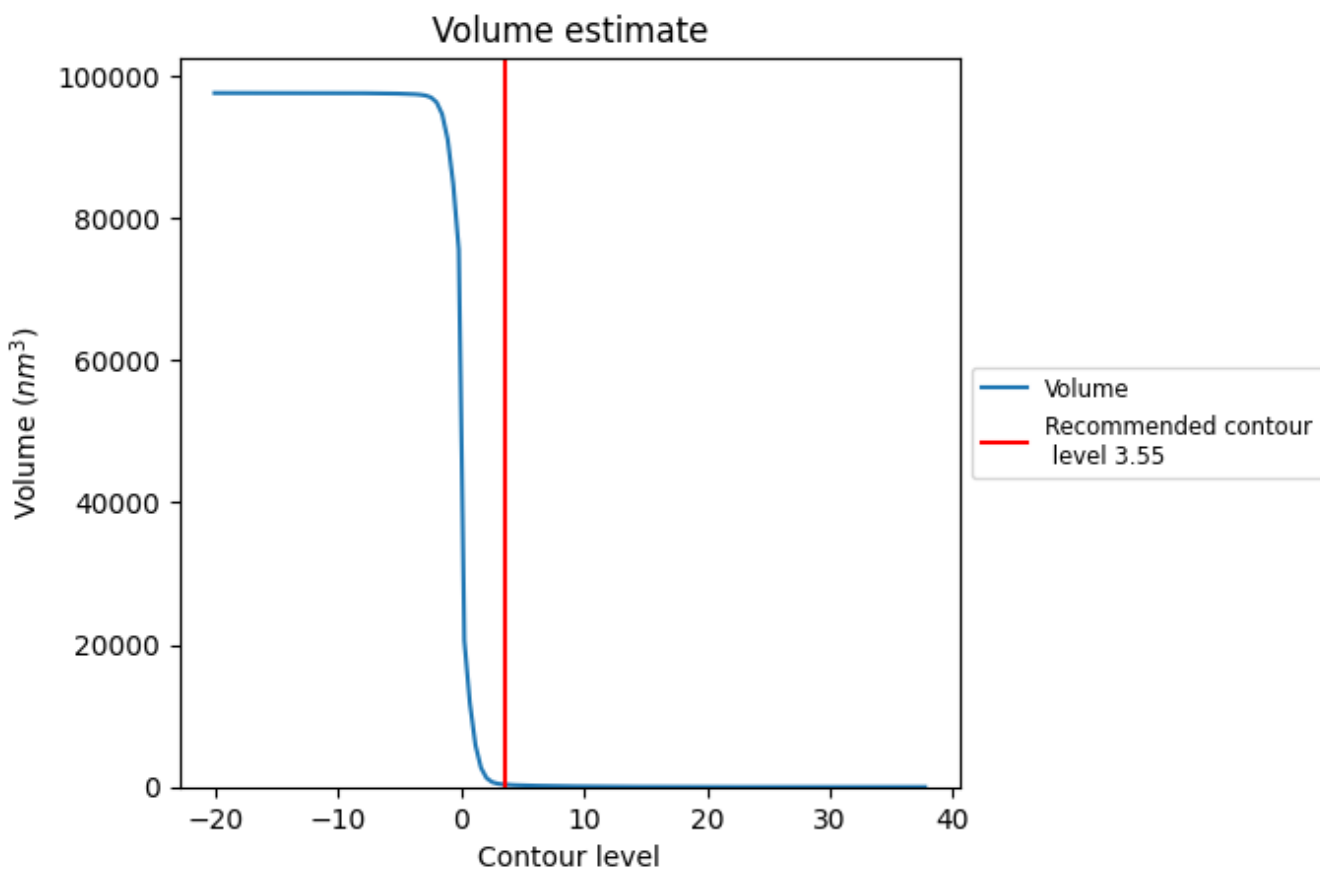
This section contains the results of statistical analysis of the map.

### 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.

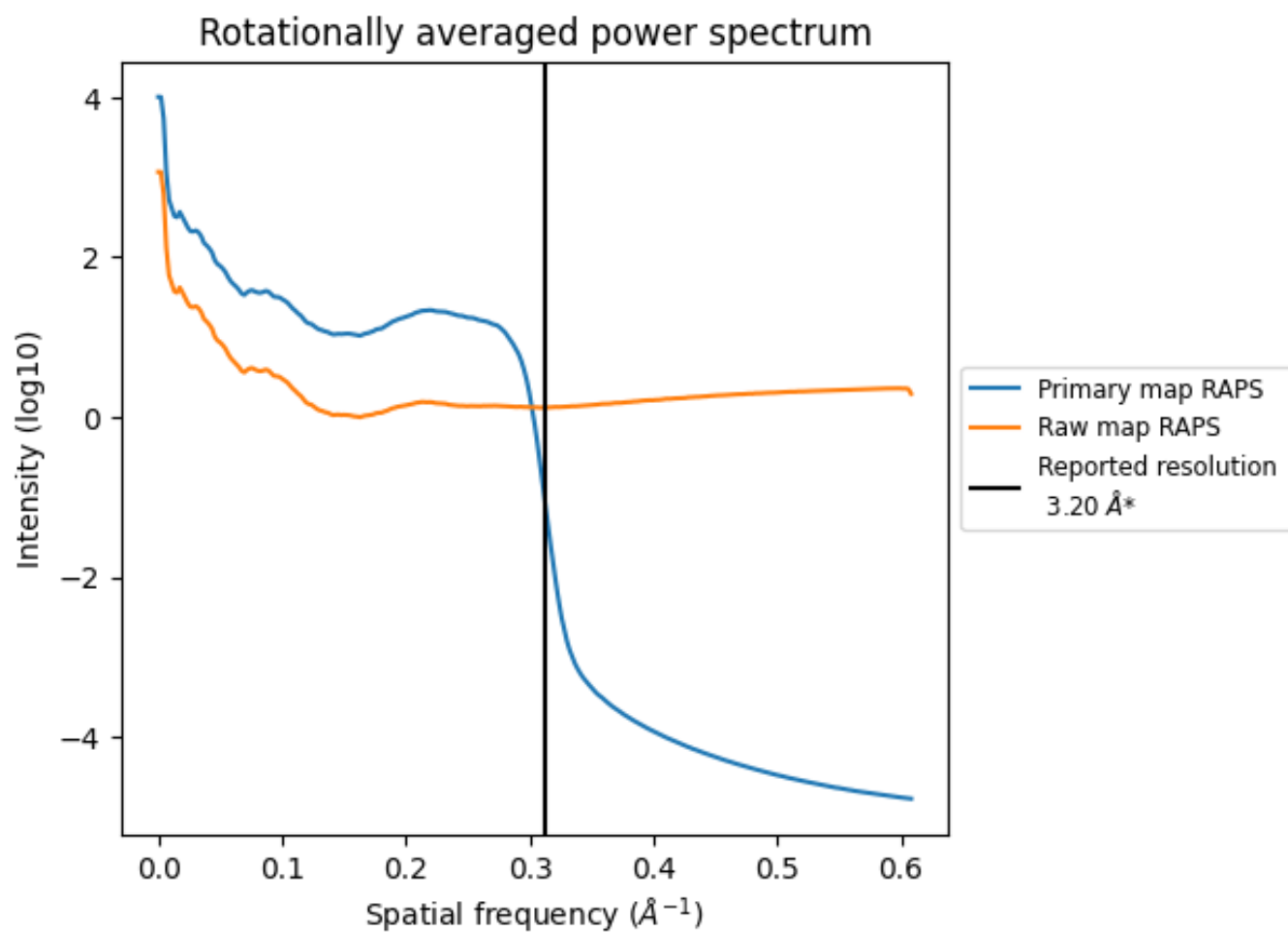
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 341 nm<sup>3</sup>; this corresponds to an approximate mass of 308 kDa.

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

### 7.3 Rotationally averaged power spectrum [i](#)

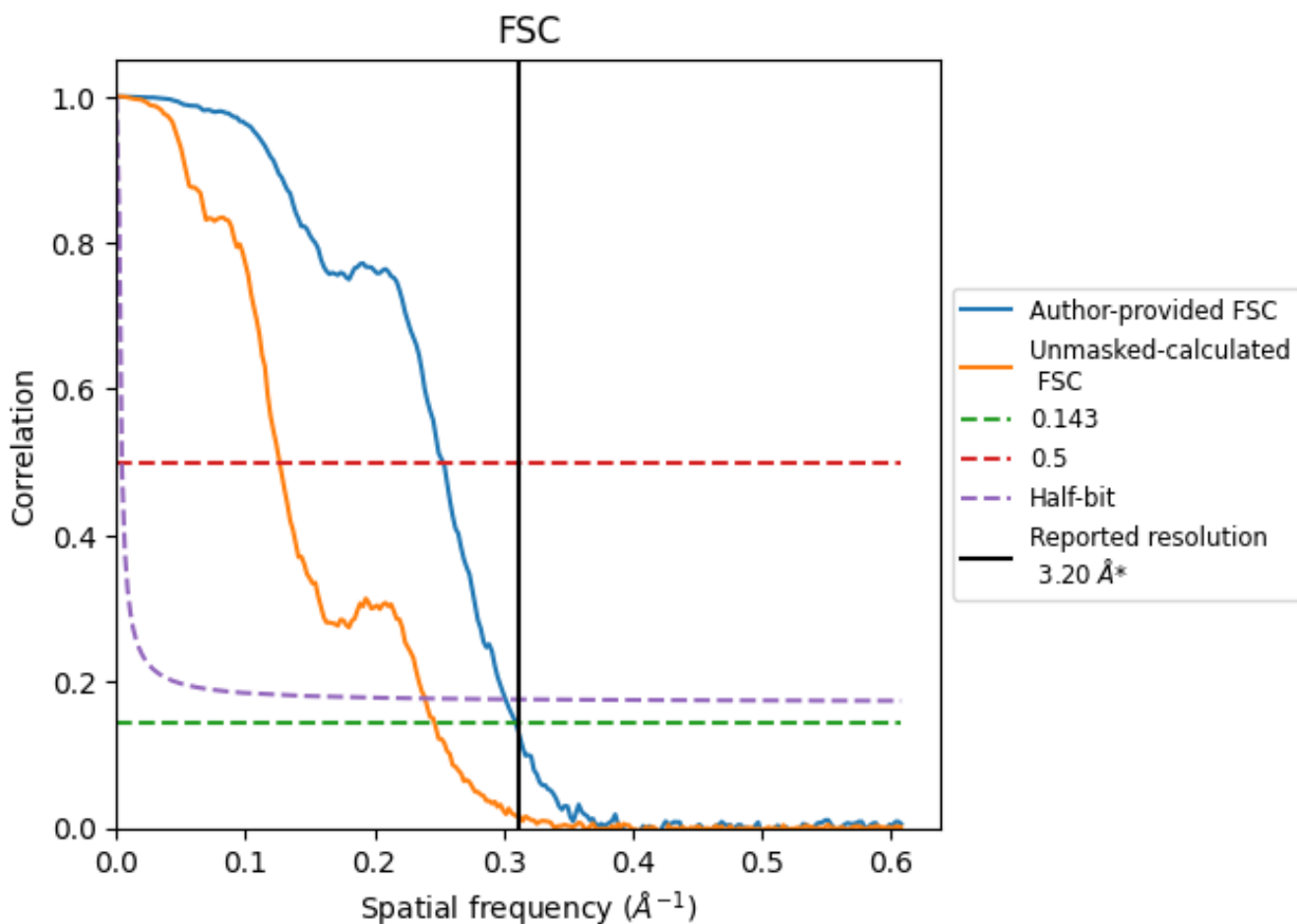


\*Reported resolution corresponds to spatial frequency of 0.312 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.312 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

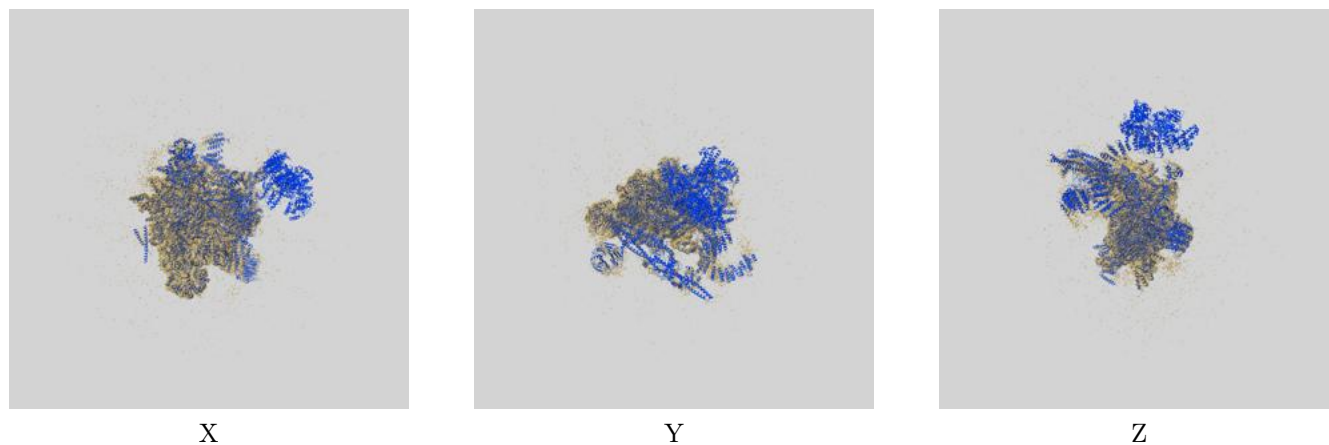
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.23	3.95	3.31
Unmasked-calculated*	4.06	7.91	4.18

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.06 differs from the reported value 3.2 by more than 10 %

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

This section contains information regarding the fit between EMDB map EMD-19941 and PDB model 9ESH. Per-residue inclusion information can be found in section 3 on page 13.

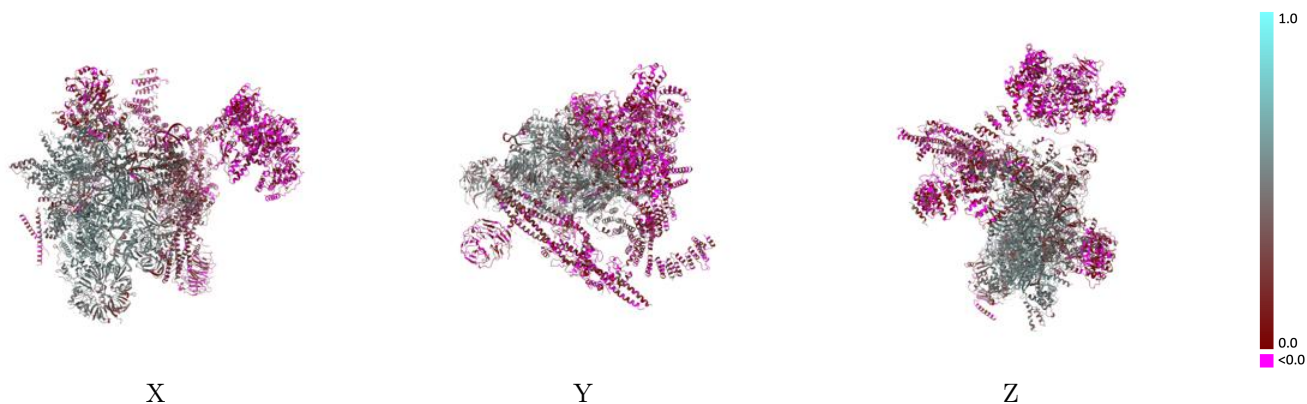
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 3.55 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.

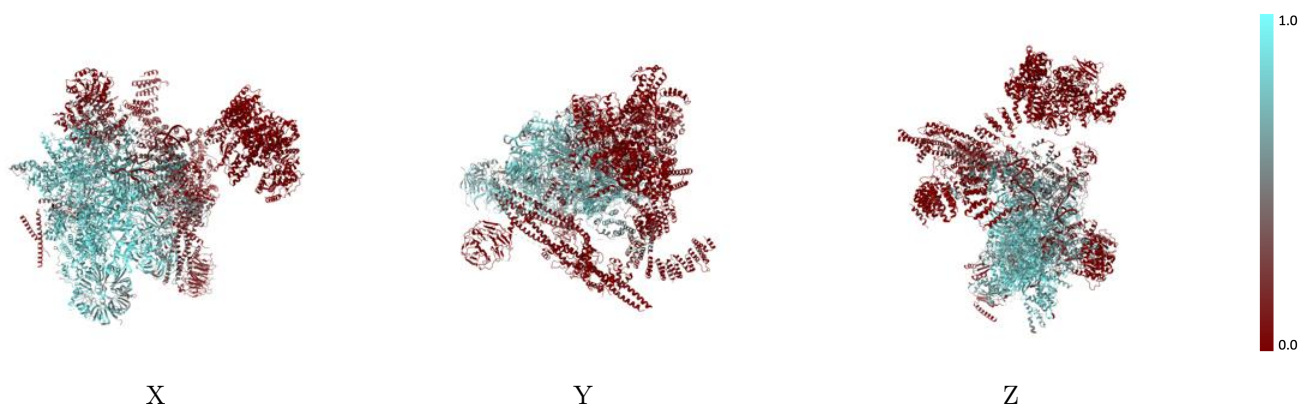


## 9.2 Q-score mapped to coordinate model [i](#)



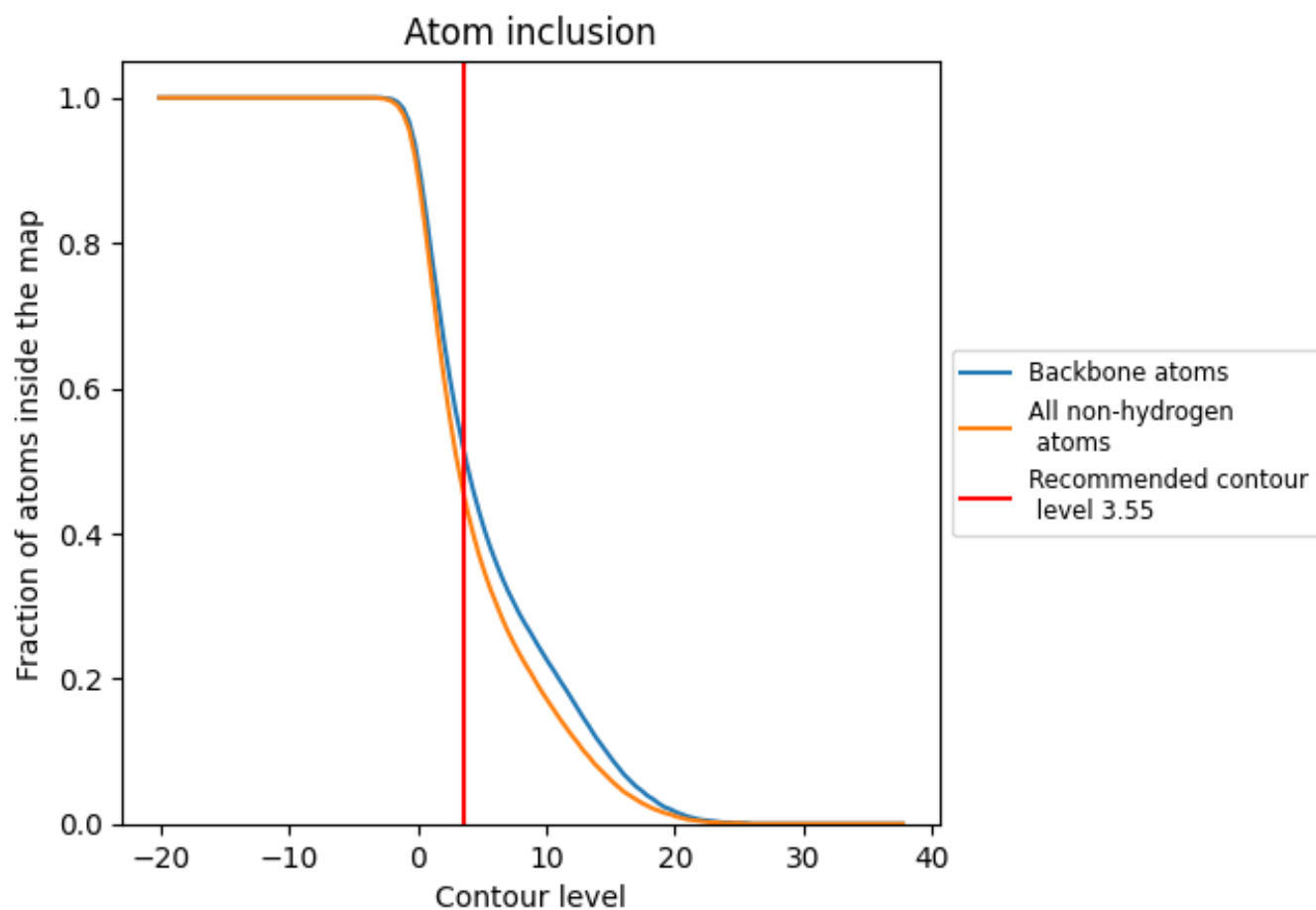
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3.55).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 52% of all backbone atoms, 46% 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 (3.55) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4560	 0.3240
1	 0.4260	 0.3460
2	 0.4240	 0.3160
5	 0.8960	 0.5180
6	 0.5250	 0.3510
A	 0.8180	 0.5270
B	 0.8010	 0.5140
C	 0.6820	 0.4410
D	 0.8140	 0.5290
E	 0.7040	 0.4790
F	 0.6540	 0.4320
G	 0.6130	 0.3800
H	 0.7050	 0.4650
I	 0.7230	 0.4510
J	 0.7460	 0.5120
K	 0.8210	 0.5120
L	 0.6500	 0.4400
M	 0.3530	 0.3180
N	 0.0010	 0.0390
O	 0.7960	 0.5120
P	 0.4460	 0.3400
Q	 0.7420	 0.5080
R	 0.3340	 0.2400
S	 0.0210	 0.0950
T	 0.0830	 0.1130
U	 0.0550	 0.1060
V	 0.0350	 0.0900
W	 0.3780	 0.2880
X	 0.0550	 0.0880
Y	 0.2010	 0.2840
Z	 0.1880	 0.1880
a	 0.5000	 0.3400
b	 0.2540	 0.2530
c	 0.7340	 0.4730
d	 0.4530	 0.3460



*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion	Q-score
f	 0.2270	 0.2320
m	 0.1690	 0.3020
r	 0.1580	 0.1660
y	 0.3800	 0.2950
z	 0.1960	 0.1910