



wwPDB EM Validation Summary Report ⓘ

May 19, 2025 – 02:21 pm BST

PDB ID : 9ESH / pdb_00009esh
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

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.dev118
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
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) : 2.43.1

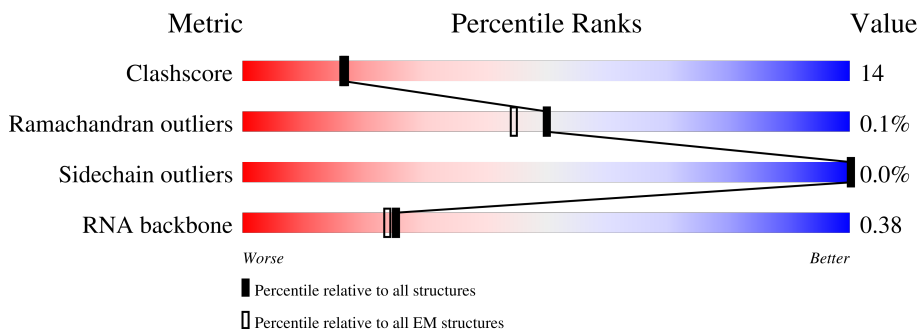
1 Overall quality at a glance

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 ≥ 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	<div> <div>62%</div> <div>28% 48% 24%</div> </div>
2	2	186	<div> <div>8%</div> <div>5% 6% 87%</div> </div>
3	5	120	<div> <div>54%</div> <div>23% 8% 15%</div> </div>
4	6	99	<div> <div>37%</div> <div>25% 42% 25% 7%</div> </div>
5	A	2363	<div> <div>54%</div> <div>19% 26%</div> </div>
6	B	984	<div> <div>67%</div> <div>26% 7%</div> </div>
7	C	340	<div> <div>9%</div> <div>56% 32% 11%</div> </div>

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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	

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Mol	Chain	Length	Quality of chain
30	c	887	
31	d	155	
32	f	22	
33	m	797	
34	r	346	
35	y	534	
36	z	647	

2 Entry composition

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
1	1	29	Total	C	N	O	P	0	0
			605	272	91	213	29		

- Molecule 2 is a RNA chain called U2snRNA.

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

- Molecule 3 is a RNA chain called U5snRNA.

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

- Molecule 4 is a RNA chain called U6snRNA.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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
21	Q	90	Total	C	N	O	S	0	0
			752	467	146	138	1		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 32 is a protein called UNK1.

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

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

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

- 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		

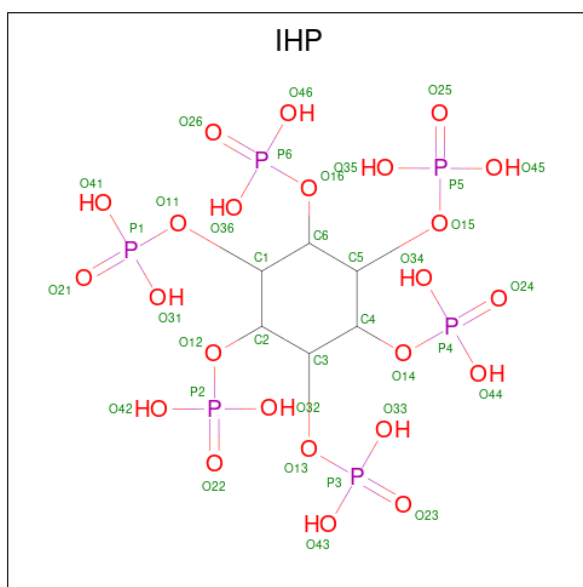
- Molecule 37 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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 (CCD ID: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

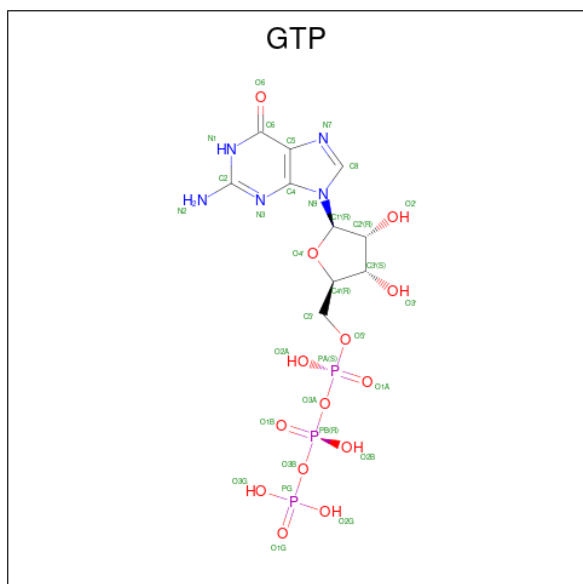
Mol	Chain	Residues	Atoms		AltConf
38	6	1	Total	K	0
			1	1	

- Molecule 39 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: C₆H₁₈O₂₄P₆) (labeled as "Ligand of Interest" by depositor).



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

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

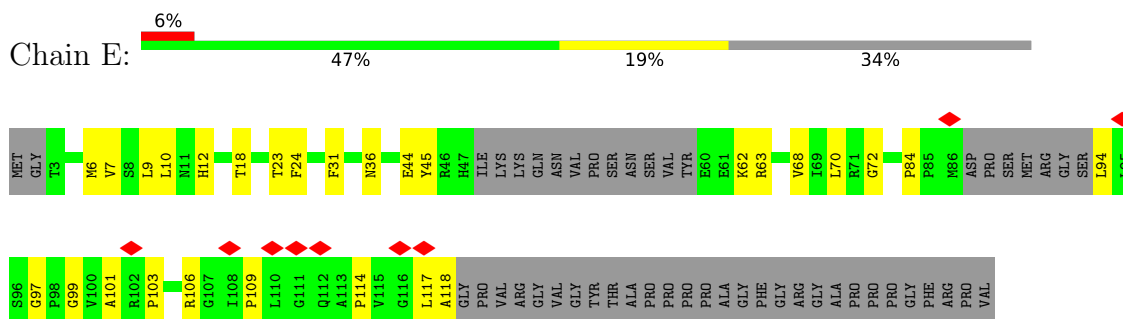


Mol	Chain	Residues	Atoms					AltConf
40	B	1	Total	C	N	O	P	0
			32	10	5	14	3	

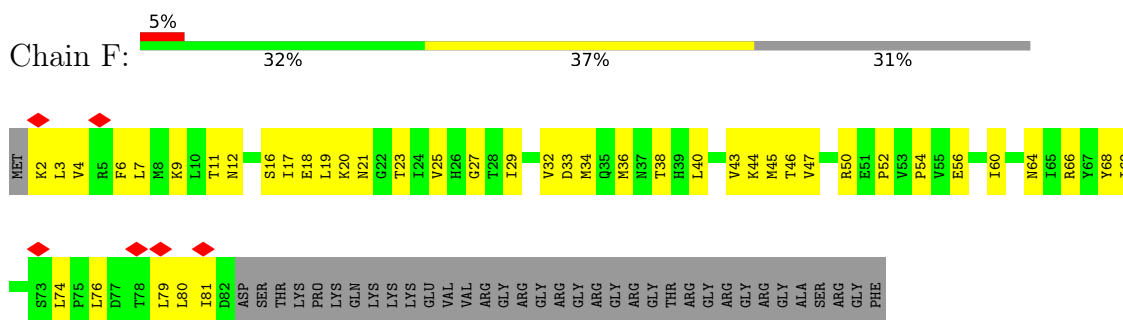
- Molecule 41 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
41	M	2	Total 2	Zn 2	0
41	O	3	Total 3	Zn 3	0
41	P	1	Total 1	Zn 1	0

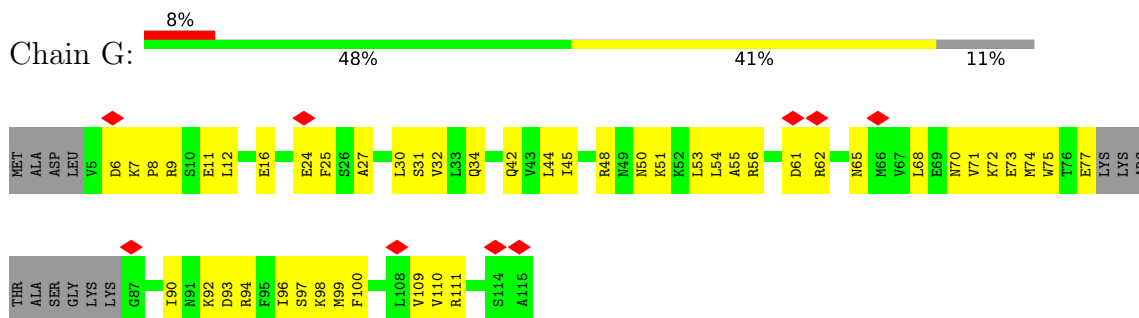
- Molecule 9: Small nuclear ribonucleoprotein-associated protein B



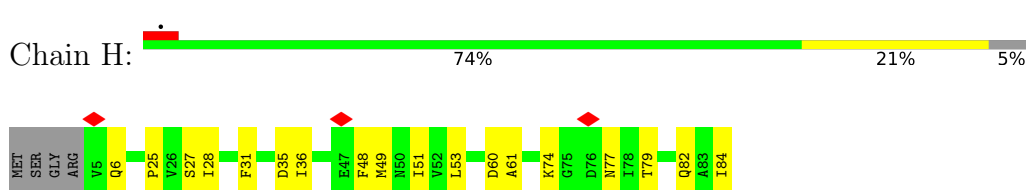
- Molecule 10: Small nuclear ribonucleoprotein Sm D1



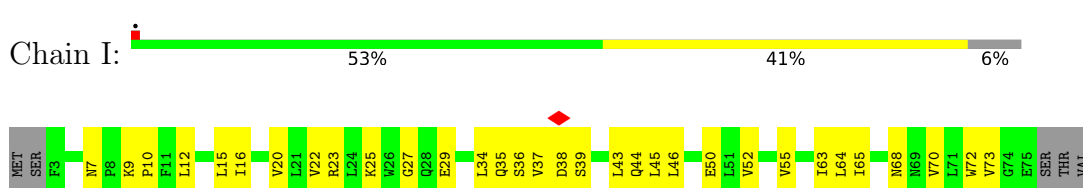
- Molecule 11: Small nuclear ribonucleoprotein Sm D2



- Molecule 12: Small nuclear ribonucleoprotein E



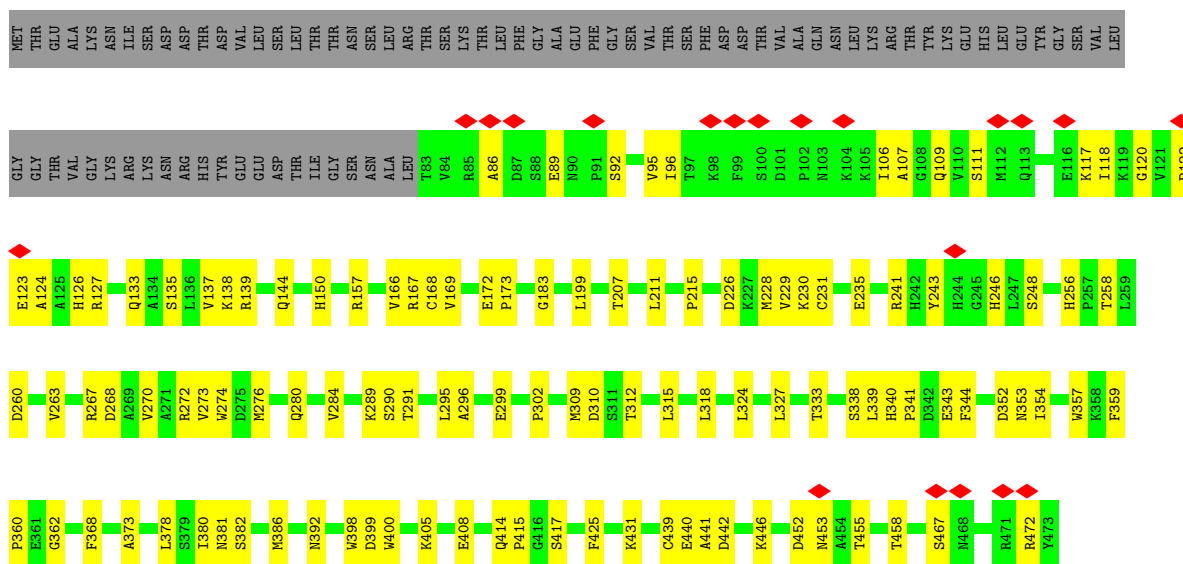
- Molecule 13: Small nuclear ribonucleoprotein F

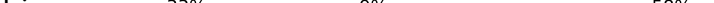


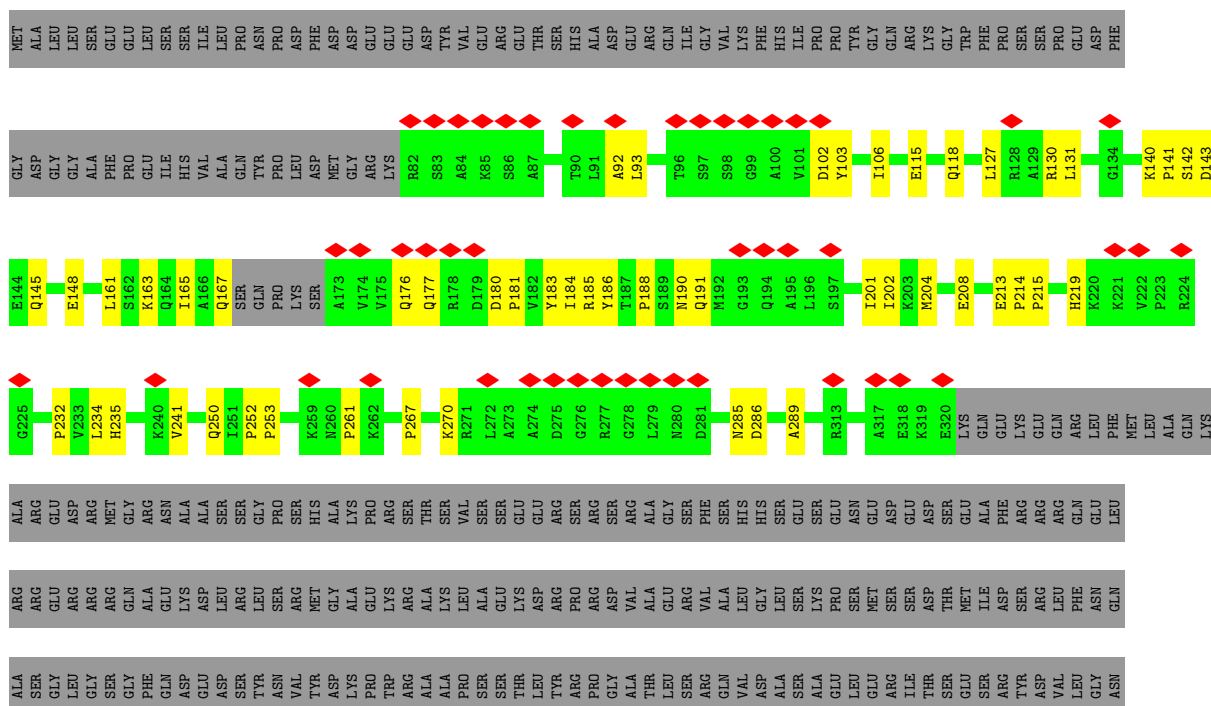
- Molecule 14: Small nuclear ribonucleoprotein G

ME1	S8	F18	L21	N22	R25	K26	V27	Y28	R32	G33	N39	E43	E48	D51	G52	E53	K54	R63	T68	M69	I70	E71	T72	L73	D74	K75	ME1	THR
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Chain K:  58% 25% 17%




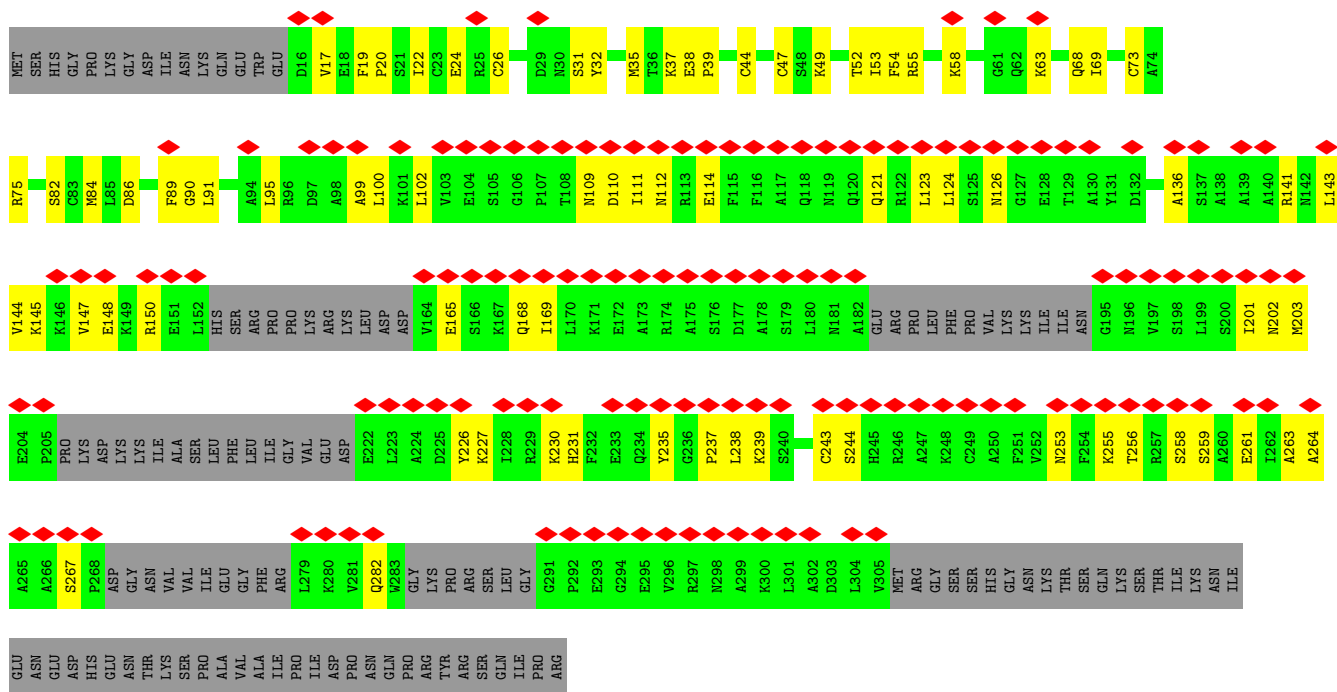
Chain L: 



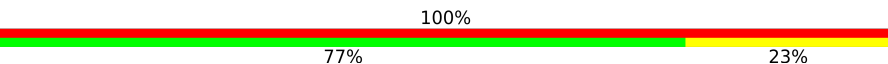
ALA
HIS
LYS
LYS
PHE
PRO
LYS
GLY
SER
ASP
ASP
GLU
VAL
VAL
GLU
SER
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ARG
ALA
GLY
PRO
VAL
THR
PHE
GLU
LYS
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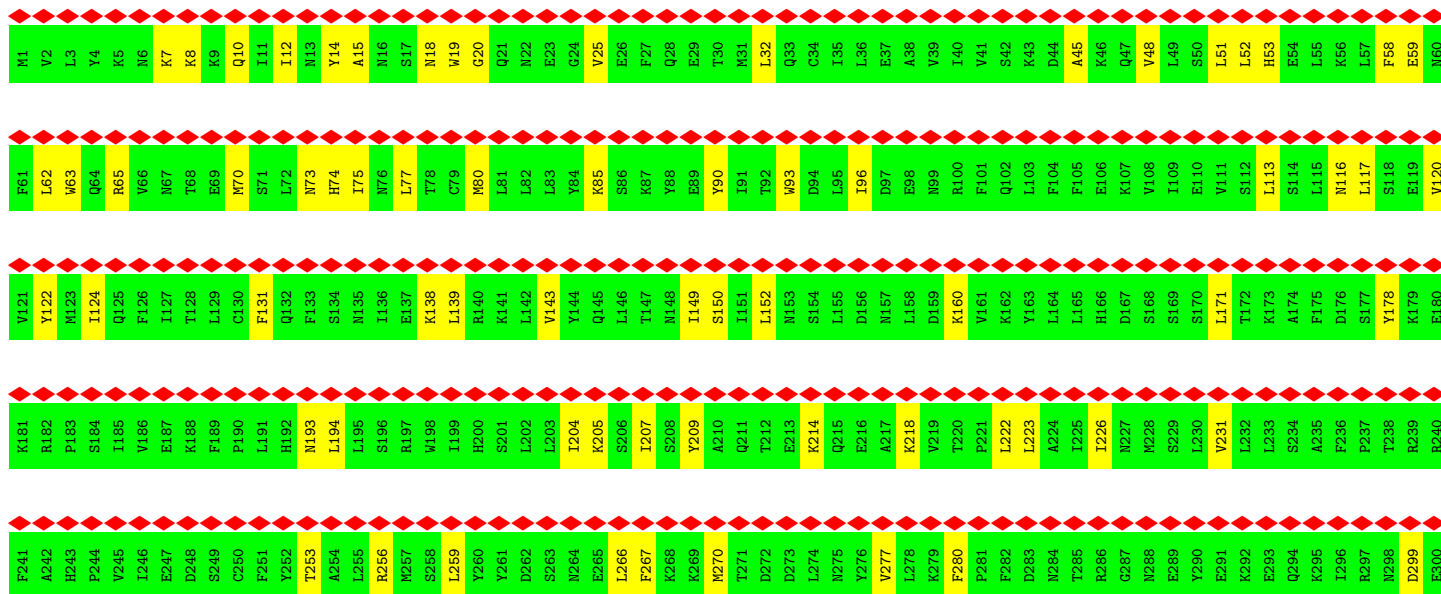
• Molecule 17: Pre-mRNA-splicing factor cwf5

Chain M: 



• Molecule 18: Pre-mRNA-splicing factor cwf11

Chain N: 

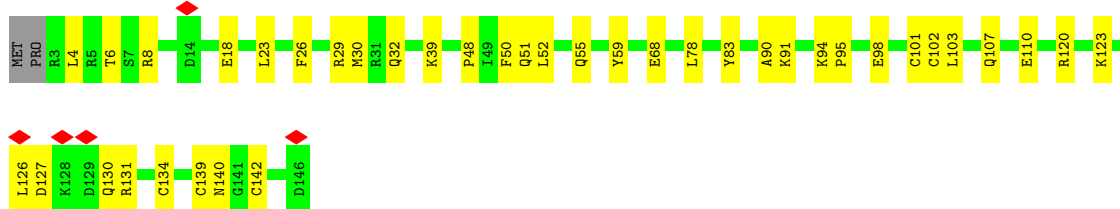


M1021	T961	T901	I841	M781	S721	G661	Y601	K541	M481	Q421	P361	L301
M1022	R962	Y902	Q842	F782	N722	L662	R602	L542	M482	N422	E362	V302
T1023	L963	R903	A843	S783	R723	R663	P603	L543	F483	T423	K363	Y303
S1024	G964	K904	P844	M784	L724	S664	K604	H544	K484	A424	Y364	Y304
M1025	T965	D905	G845	M785	Y725	I665	Q605	G545	T486	I425	A365	H305
G1026	L966	R906	S846	T786	T726	Y666	L406	N546	T486	Q426	I366	L306
S1027	K967	F907	H847	L787	Y727	A667	K607	A547	S487	Y427	K367	Q307
L1028	E968	F908	D848	F788	N728	R668	F608	L548	V488	L428	V368	L308
F1029	K969	D909	A849	T789	D729	R669	R609	D549	A489	S429	V369	T309
K1030	G970	Y910	S850	L790	K730	L670	F610	P550	P490	I430	F370	L310
R1031	F971	A911	P851	L791	Q731	F671	A611	L551	P491	S431	E371	F311
L1032	C972	T912	D852	E792	L732	N672	L612	E552	Q492	F432	F372	S312
R1033	F973	K913	T853	K793	E733	T673	V613	G553	I493	F433	L373	D313
Y1034	N974	L914	A854	A794	S734	V674	L614	V554	G494	M434	K374	F314
L1035	N975	Y915	L855	R795	I735	E675	S615	T555	Q495	R435	N375	Q315
K1036	L976	G916	Y856	C796	L736	Q676	P616	D556	V496	Q436	V376	K316
S1037	I977	E917	F857	F797	L737	L677	E617	F557	P497	S437	I377	L317
L1038	R978	L918	R858	H798	G738	Q678	A618	T558	P498	S438	I378	L318
I1039	M979	E919	D859	Q799	S739	S679	R619	I559	Q499	K439	N379	G319
I1040	N980	Y920	A860	G800	Q740	V680	K620	A560	F500	A440	T380	D320
D1041	S981	R921	Y861	H801	P741	L681	Y621	T561	V501	Y441	Y381	L321
L1042	Q982	F922	T862	L802	G742	P682	N622	I562	K502	K442	D382	V322
M1043	N983	Q923	K863	L803	L743	R683	L623	C563	C503	K443	R383	F323
T1044	I984	Q924	R864	Y804	T744	C684	D624	N564	Q504	L444	T384	C324
Q1045	S985	L925	L865	L805	N745	H685	L625	D565	M505	L445	R385	T325
Y1046	E986	E926	R866	S806	V746	V686	N626	D566	G506	L446	L386	Q326
M1047	S987	E927	E867	D807	N747	P687	I627	V567	L507	R447	V387	T327
V1048	S988	R928	K868	E808	G748	S688	L628	G568	S508	S448	N388	S328
R1049	I989	R929	Y869	G809	P749	R689	V629	M569	R509	L449	D389	L329
E1050	T990	P930	L870	K810	T750	L690	S630	F570	P510	Y450	Y390	Q330
S1051	S991	F931	R871	D811	R751	S691	L631	Q771	G511	A451	D391	Q331
I1052	I992	G932	T872	E812	C752	T692	L632	S572	P512	E452	E392	R332
S1053	L993	L933	H873	T813	G753	E693	N633	D573	F513	L453	I393	Q333
L1054	R994	L934	D874	L814	K754	S694	R634	N574	H514	L454	I394	K334
L1055	S995	R935	D875	E815	H755	L695	A635	Q775	S515	N455	N395	L335
C1056	N996	Y936	K876	R816	V756	L696	K636	S576	A516	F456	F396	E336
S1057	C997	Y937	D877	Y817	L757	I697	E637	D577	L517	S457	T397	E337
S1058	E998	E938	R878	G818	V758	K698	F638	S578	R518	E458	I338	I338
I1059	P999	D939	Y879	T819	C759	F699	P639	D579	D519	Q459	K399	T339
Y1060	T1000	Q940	D880	L820	K760	Y700	K640	N580	L520	Y460	D400	S340
P1061	G1001	E941	A881	S821	L761	T701	W641	K581	K521	R461	V401	F341
L1062	F1002	L942	Y882	S822	L762	N702	F642	S582	N522	R462	L402	L342
D1063	D1003	Y943	R883	W823	E763	Q703	E643	I583	S523	L463	G403	S343
I1064	R1004	A944	R884	T824	V764	N704	D644	N584	I524	S464	E404	F344
L1065	L1005	L945	F885	S825	L765	K705	L645	V585	K525	L465	R405	N345
T1066	V1006	C946	P886	K826	Q766	I706	F646	V586	S526	K466	S406	S346
V1067	L1007	Q947	F887	L827	D767	S707	L647	L587	P527	N467	V407	L347
D1068	L1008	Q948	H888	P828	T768	A708	G648	S588	F528	A468	M408	K348
S1069	G1009	S949	S889	G829	S769	D709	F649	P589	L529	T469	D409	S349
N1010	N1010	R950	Y890	L830	P770	W710	G650	F590	C530	K470	Q410	L350
Q1011	Q1011	P951	F891	L831	N771	T711	T651	Y591	L531	N471	E411	C351
N1012	N1012	I952	G892	R832	D772	A712	P652	Y592	I532	L472	N412	S352
K1013	K1013	G953	D893	E833	R773	S713	D653	H593	Y533	T473	S413	K353
R1014	T1014	C954	K894	T834	T774	D714	I654	S594	I534	K474	L414	C354
L1015	S1015	T955	S895	G835	V775	R715	C655	L595	S535	D475	T415	Y355
D1016	G1016	Y956	K896	R836	V776	H716	A656	A596	K536	N476	N416	L356
Y1017	N1017	T957	R897	L837	L777	F717	F657	G597	D537	F477	Y417	R357
G1018	Q1018	S958	P898	L838	S778	L718	P658	L598	M538	F478	F418	T358
N1019	D1019	L959	T899	A839	D779	L719	N659	G599	E539	S479	L419	S359
S1080	I1020	S960	E900	S840	S780	P720	A660	E600	Y540	L480	L420	F360



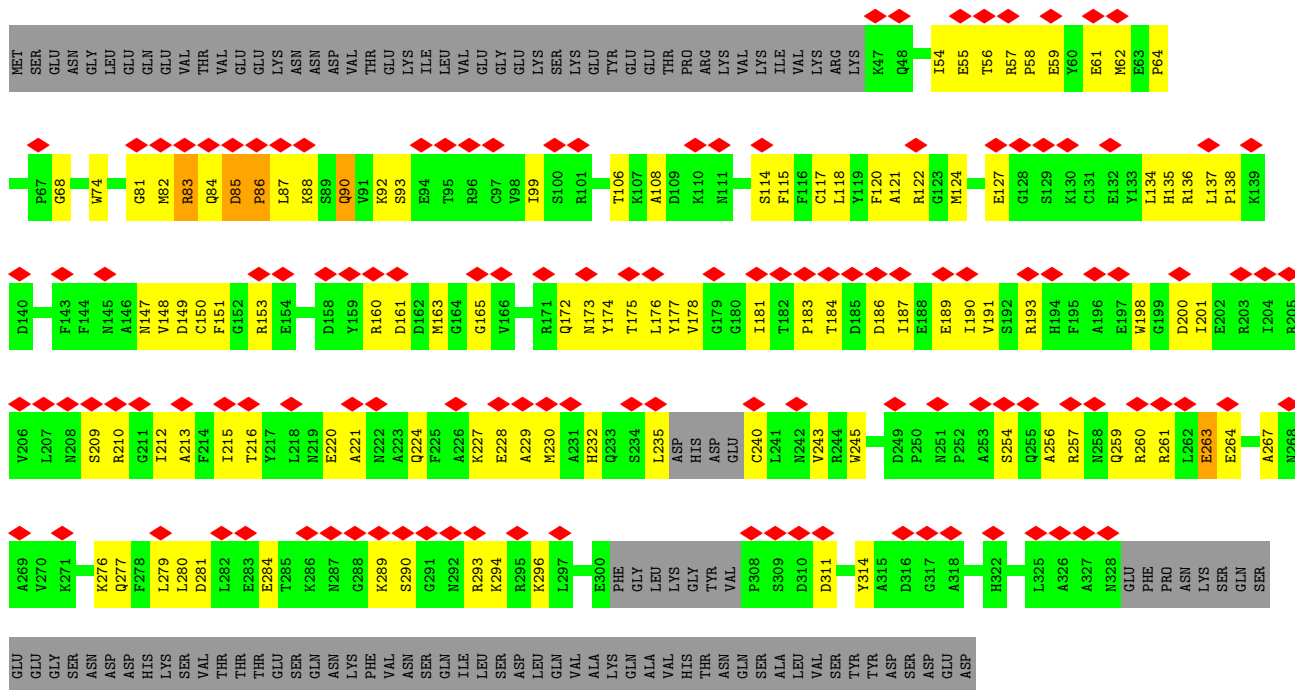
• Molecule 19: Pre-mRNA-splicing factor cwf14

Chain O: 72% 27%

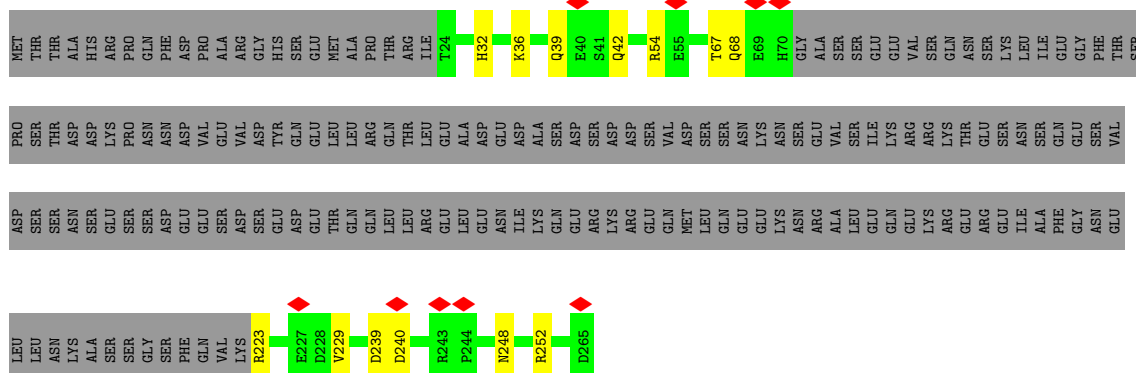


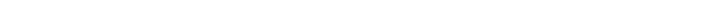
• Molecule 20: Pre-mRNA-splicing factor cwf2

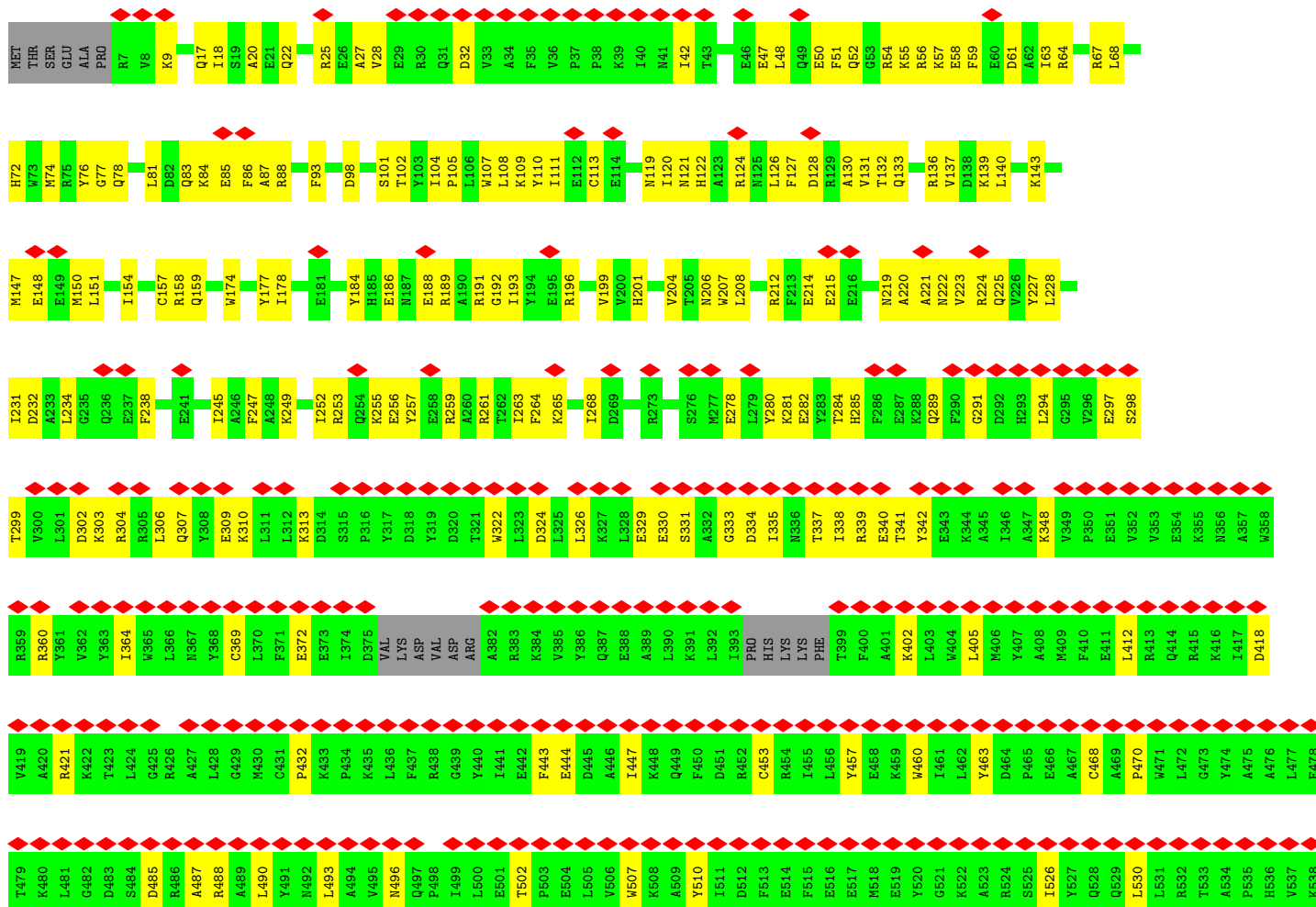
Chain P: 33% 42% 27% 30%

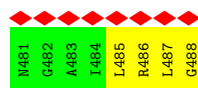


Chain Q: 29% 5% 66%

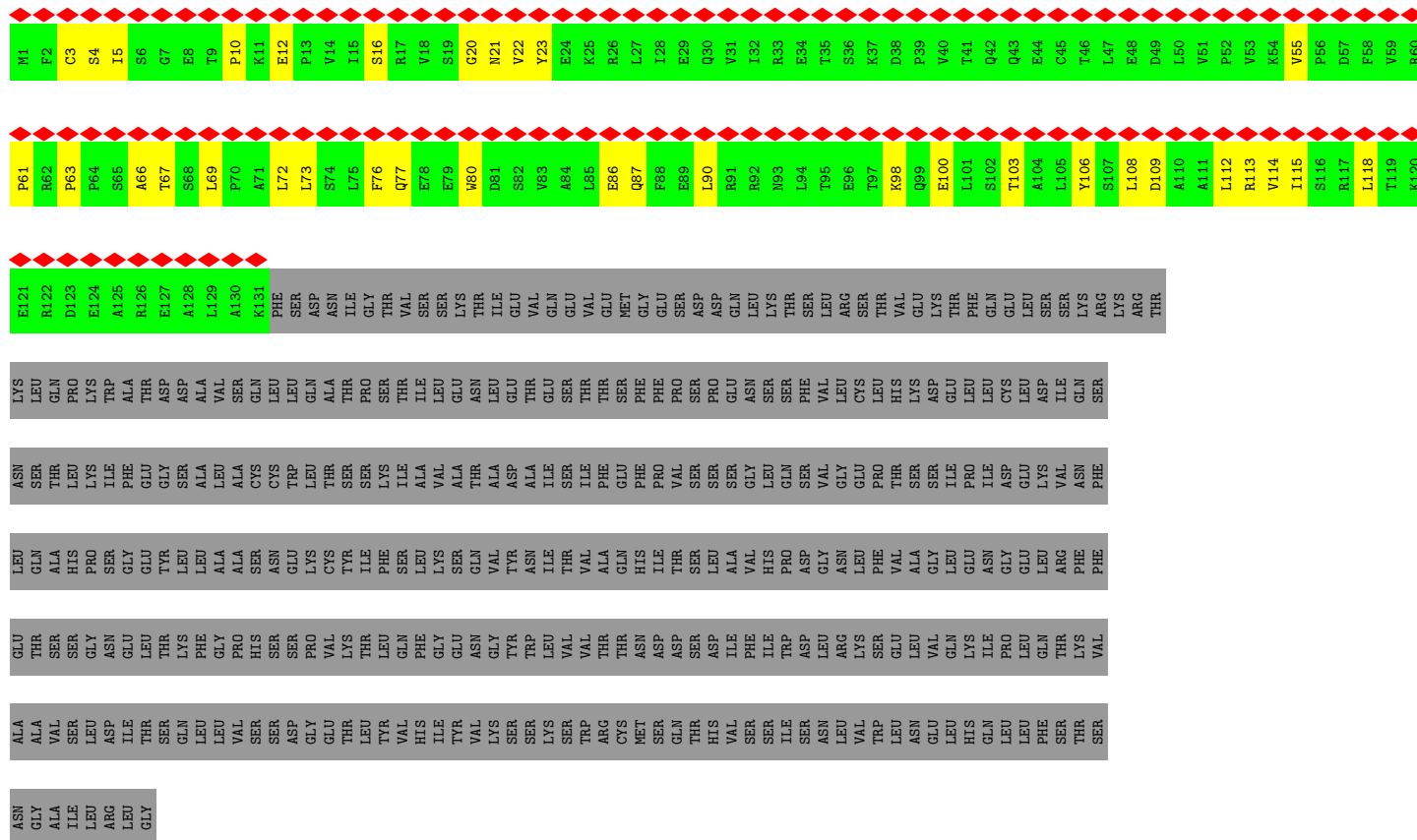


Chain R: 

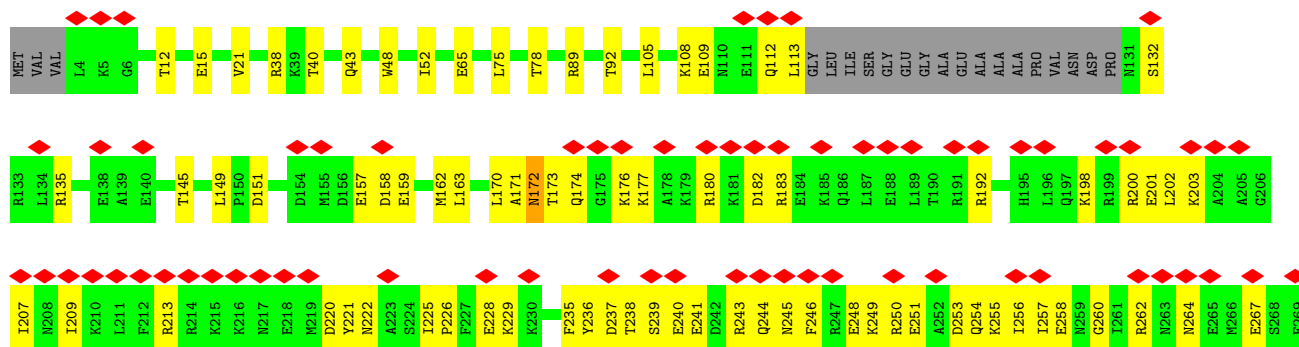
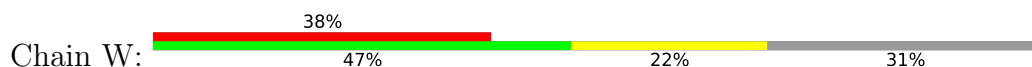


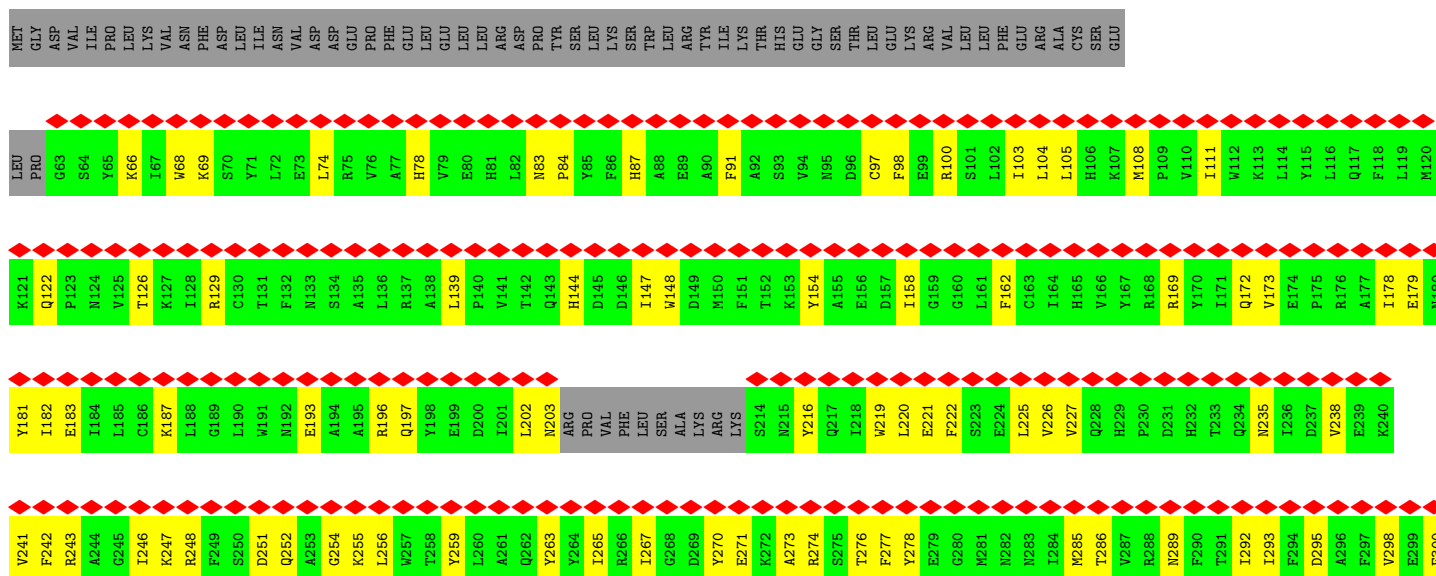


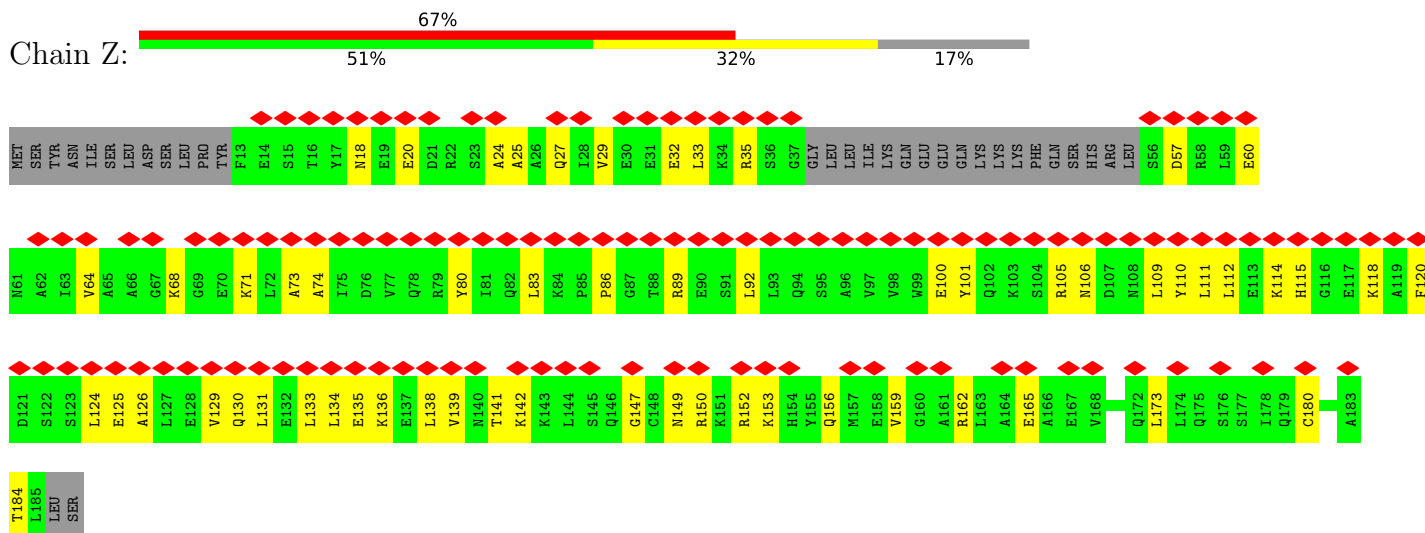
• Molecule 23: Pre-mRNA-processing factor 19



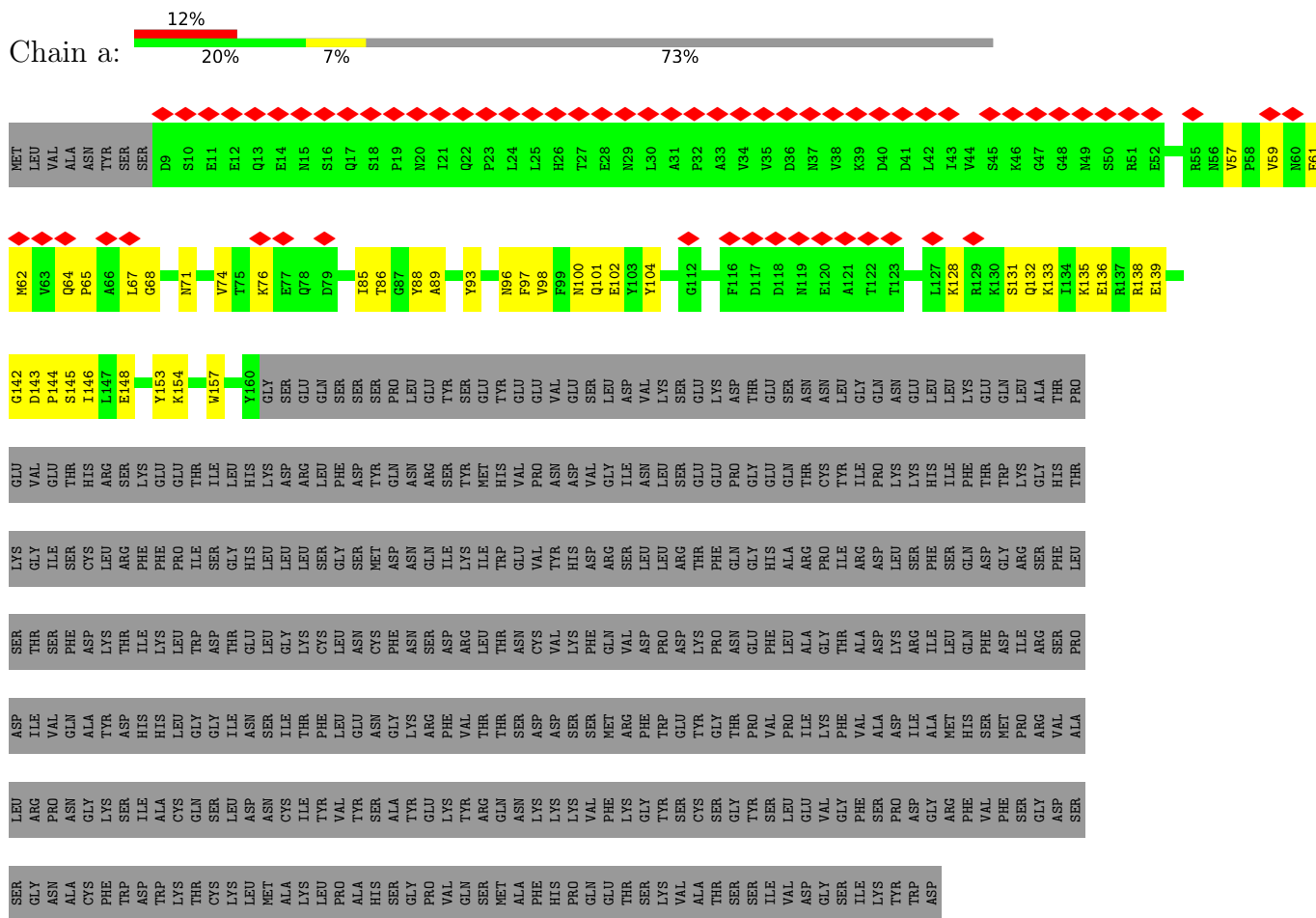
• Molecule 24: Pre-mRNA-splicing factor cdc5







- Molecule 28: Pre-mRNA-processing factor 17

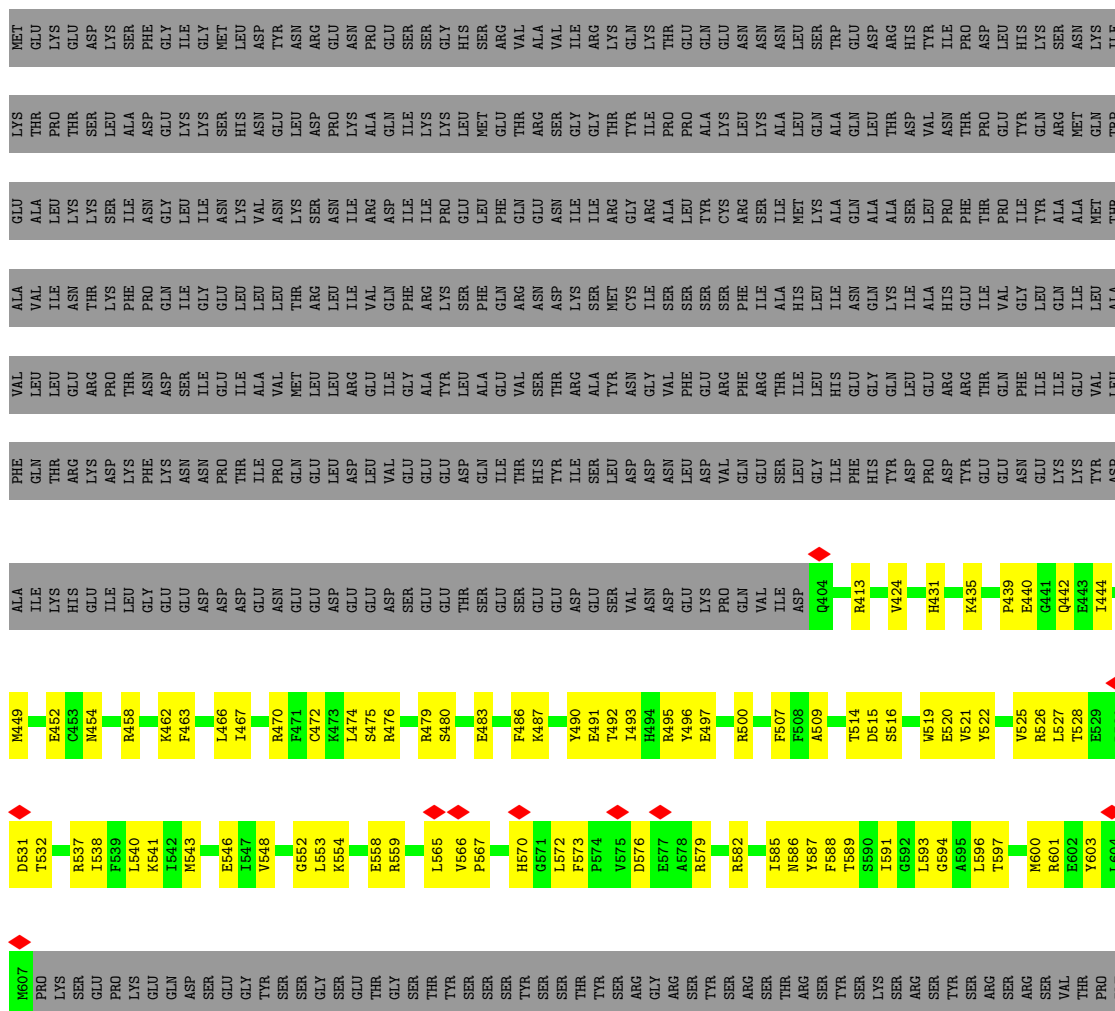


- Molecule 29: Pre-mRNA-splicing factor cwf21



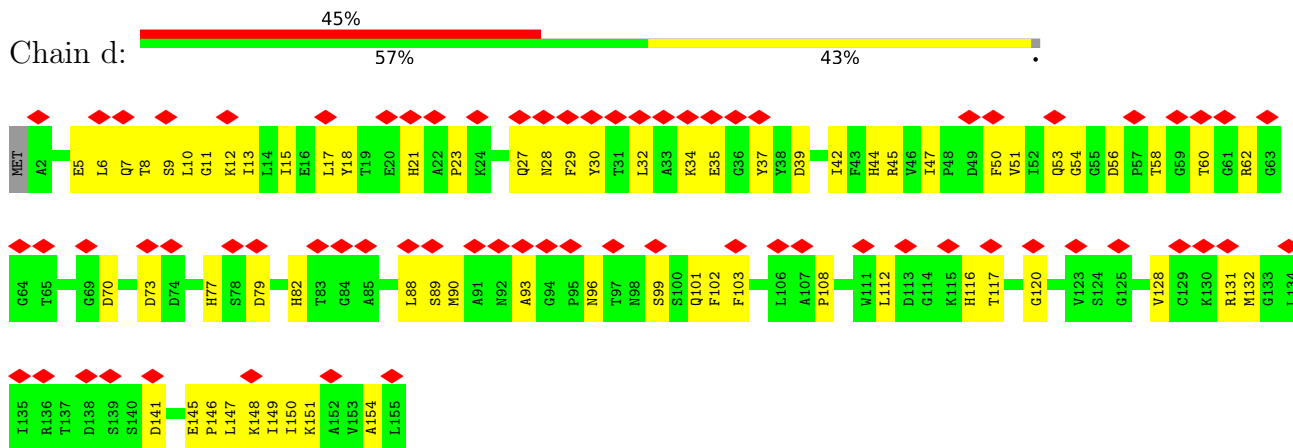
- Molecule 30: Pre-mRNA-splicing factor cwf22

Chain c:  14% 9% 77%

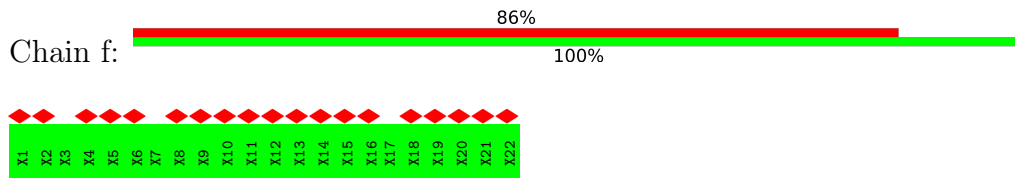


[illegible]

- Molecule 31: Peptidyl-prolyl cis-trans isomerase *ppi1*



- Molecule 32: UNK1



- Molecule 33: G-patch domain-containing protein C1486.03

[illegible]



T307	A370	D430	D491	K552	Y616
S308	Y371	E431	A492	F553	S617
I309	S372	S432	F493	S554	S618
T310	L373	G433	V494	I555	A619
I311	M374	M434	A495	F556	V620
D312	K375	L435		T557	E621
G313	E376	T436	S498	A558	S622
I314	E377	D437	F499	Q559	E623
V315	F378	F438	F500	R560	T624
Y316	E379	L439	A501	L561	Q625
V317	A380	G440	N502	P562	T626
V318	D381	I441	E503	S563	F627
D319	I382	Q442	G504	S564	V628
S320	L383	I443	D505	D565	K629
G321	N384	S444	I506	C566	N630
F322	C385	M445	I507	S567	I631
N323	D386	S446	T508	K568	S632
K324	M387	F447	A509	I569	K633
Q325	S388	L448	L510	L570	
R326	P389	D449	N511	K571	F637
I327	L390	A450	V512	C572	W638
F328	V391	M451	F513	L573	L639
N329	L392	I452	E514	L574	D640
P330	F393	S453	S515	D575	K641
T331	L394	K454	F516	G576	Y642
T332	K395	A455	V517	F577	Y643
R333	G396	L456	G518	V578	K644
T334	L397	L457	N519	R579	R645
S335	G398	T458	K520	N580	GLU
K336	L399	S459	K521	V581	LYS
L337	M400	M460	D522	A582	
	N401	Q461	L523	Q585	
I342	I402	F462	Q524	N586	
S343	L403	G463	N525	D587	
K344	Q404	C464	C526		
S345	F405	E467	R527	K591	
S346	Q406	I468	K528	T592	
A347	F407	L469	N529	I593	
I348	F408	S470	Y530	G594	
Q349	V409	I471	L531	G595	
R350	R410	A472	N532	K596	
S351	P411	S473	Y533		
G352	P412	I474	Q534	W599	
R353	T413	L475	T535	L600	
A354	V414	T476	L536	D601	
G355	H415	A477	R537	S602	
R356	L416	G478	Q538	S603	
M358	M417	E479	A539	S604	
R359	A418	V480	L540	V605	
R359	A419	F481	D541	L606	
G360	L420	Y482	I542	H607	
K361	E421	M483	R543	E608	
V362	D422	P484	T544	K609	
F363	L423	T485	H545	R610	
R364	Y424	S486	L546	T611	
L365	L425	S487	V547	P612	
T366	Q426	K489	N548	W613	
T367	V428	M490	L550	I614	
E368	L429			N615	
K369					

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 ⓘ

5.1 Standard geometry ⓘ

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

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	0.17	0/673	0.40	0/1043
2	2	0.12	0/554	0.24	0/856
3	5	0.18	0/2397	0.25	0/3727
4	6	0.14	0/2207	0.35	0/3438
5	A	0.24	0/14793	0.43	5/20040 (0.0%)
6	B	0.22	0/7459	0.43	0/10117
7	C	0.18	0/2376	0.48	0/3216
8	D	0.21	0/772	0.43	0/1038
9	E	0.17	0/737	0.43	0/993
10	F	0.22	0/646	0.57	0/875
11	G	0.23	0/829	0.66	0/1111
12	H	0.16	0/662	0.44	0/894
13	I	0.16	0/585	0.48	0/794
14	J	0.19	0/578	0.48	0/774
15	K	0.23	0/3130	0.47	0/4251
16	L	0.19	0/1885	0.43	0/2545
17	M	0.19	0/1841	0.47	0/2468
18	N	0.12	0/10690	0.33	0/14463
19	O	0.24	0/1199	0.49	0/1609
20	P	0.28	0/2222	0.58	3/2991 (0.1%)
21	Q	0.16	0/767	0.35	0/1028
22	R	0.19	0/5235	0.48	1/7067 (0.0%)
23	S	0.21	0/1072	0.47	0/1453
23	T	0.23	0/1086	0.61	0/1472
23	U	0.14	0/2897	0.42	1/3914 (0.0%)
23	V	0.19	0/1060	0.48	0/1437
24	W	0.20	0/4407	0.50	3/5907 (0.1%)
25	X	0.16	0/5599	0.40	0/7566
26	Y	0.17	0/1065	0.50	0/1413
27	Z	0.17	0/1244	0.43	0/1667
28	a	0.18	0/1055	0.45	0/1443
29	b	0.17	0/829	0.38	0/1111

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
30	c	0.20	0/1711	0.46	0/2312
31	d	0.20	0/1206	0.50	0/1636
33	m	0.14	0/663	0.38	0/895
35	y	0.18	0/1511	0.52	0/2032
36	z	0.16	0/5079	0.41	0/6875
All	All	0.19	0/92721	0.44	13/126471 (0.0%)

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	531	ILE	N-CA-C	-6.22	105.65	112.80
24	W	626	THR	CA-C-N	-5.86	112.92	120.65
24	W	626	THR	C-N-CA	-5.86	112.92	120.65
5	A	533	ARG	N-CA-C	-5.85	106.38	112.93
23	U	118	LEU	CA-CB-CG	5.68	136.19	116.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	605	0	302	12	0
2	2	500	0	257	14	0
3	5	2149	0	1085	23	0
4	6	1970	0	994	53	0
5	A	14402	0	14306	361	0
6	B	7298	0	7336	189	0
7	C	2328	0	2276	89	0
8	D	760	0	776	28	0
9	E	726	0	750	24	0
10	F	638	0	682	37	0
11	G	819	0	845	49	0
12	H	652	0	680	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	I	574	0	591	28	0
14	J	573	0	602	14	0
15	K	3053	0	3011	92	0
16	L	1849	0	1879	55	0
17	M	1818	0	1822	74	0
18	N	10461	0	10412	198	0
19	O	1176	0	1167	37	0
20	P	2178	0	2101	108	0
21	Q	752	0	729	15	0
22	R	5108	0	5024	185	0
23	S	1055	0	1075	61	0
23	T	1069	0	1084	74	0
23	U	2870	0	2403	85	0
23	V	1044	0	1066	47	0
24	W	4346	0	4375	184	0
25	X	5467	0	5372	163	0
26	Y	1049	0	1052	54	0
27	Z	1232	0	1242	59	0
28	a	1035	0	837	40	0
29	b	822	0	820	28	0
30	c	1678	0	1659	63	0
31	d	1179	0	1169	60	0
32	f	110	0	29	0	0
33	m	649	0	641	16	0
34	r	335	0	77	8	0
35	y	1480	0	1379	62	0
36	z	4980	0	5047	153	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	2460	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 14.

The worst 5 of 2460 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

5.3.1 Protein backbone

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

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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 ⓘ

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%)	1569 (100%)	1 (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%)	532 (100%)	0	100	100
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%)	469 (100%)	0	100	100
25	X	586/707 (83%)	586 (100%)	0	100	100
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	z	564/585 (96%)	564 (100%)	0	100	100
All	All	9245/14625 (63%)	9244 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	A	1209	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 100 such sidechains are listed below:

Mol	Chain	Res	Type
20	P	324	GLN
24	W	387	ASN
36	z	384	ASN
22	R	119	ASN
23	T	42	GLN

5.3.3 RNA ⓘ

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
39	IHP	A	2401	-	36,36,36	1.39	13 (36%)	54,60,60	1.47	9 (16%)
40	GTP	B	1001	37	26,34,34	1.22	2 (7%)	32,54,54	1.69	7 (21%)

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

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

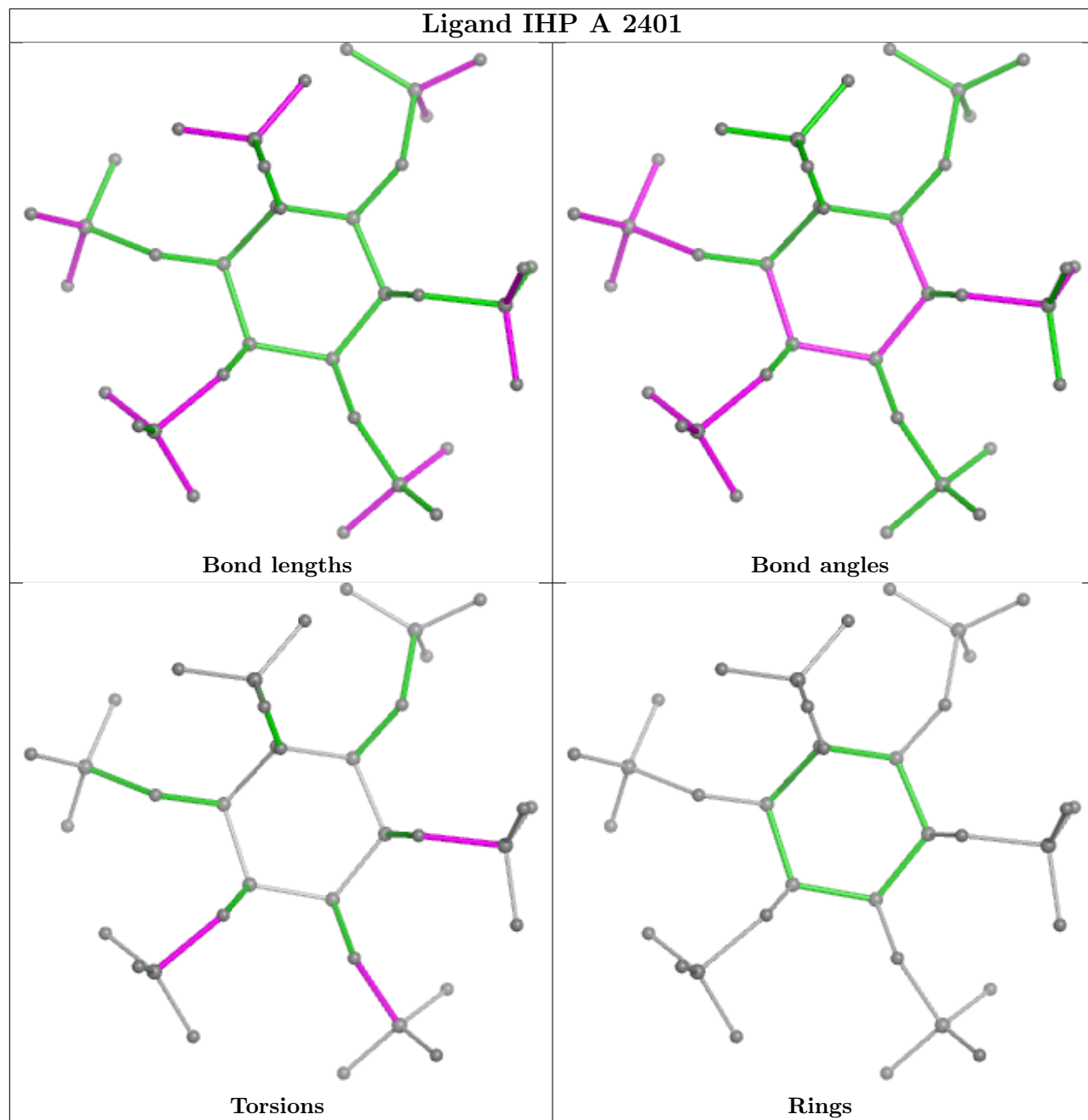
There are no ring outliers.

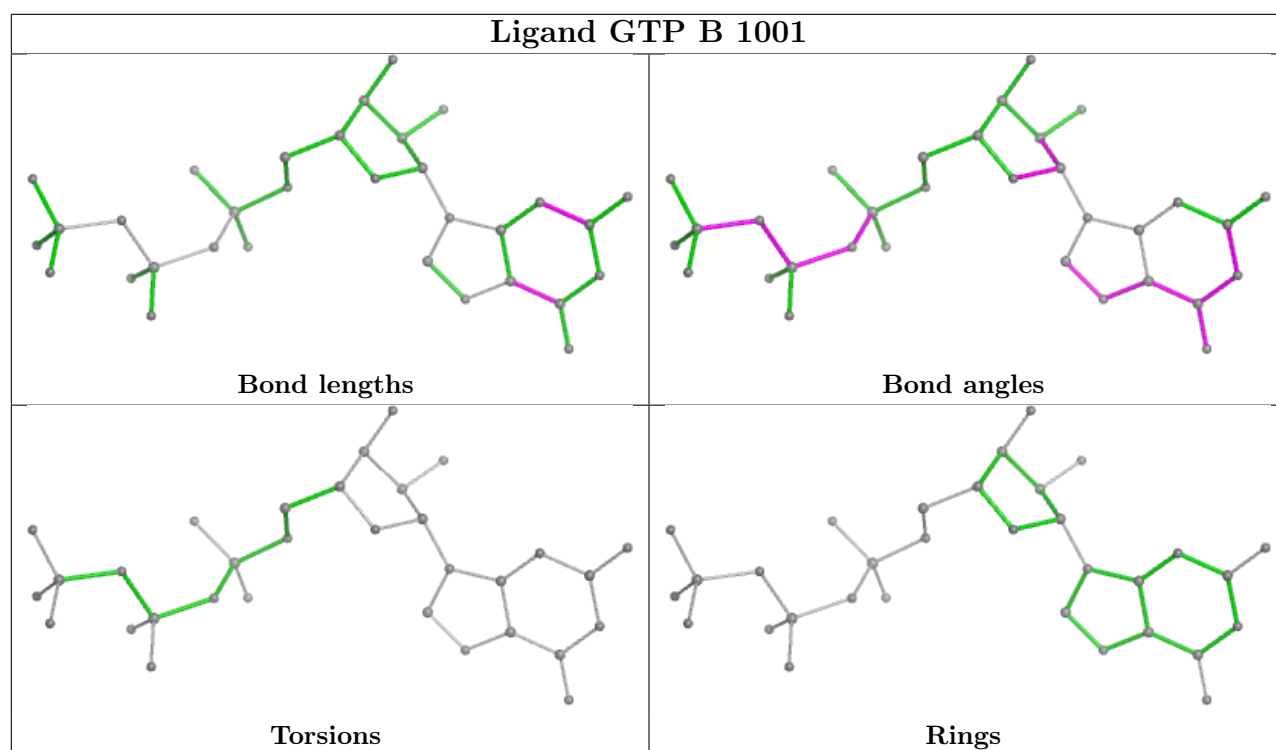
1 monomer is involved in 3 short contacts:

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.

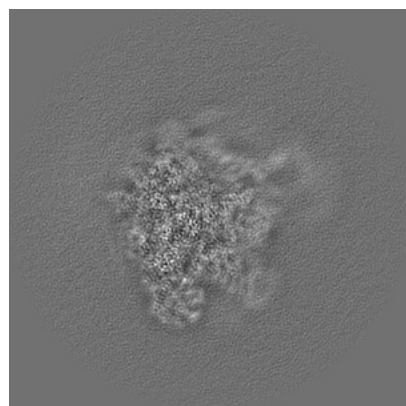
6 Map visualisation [i](#)

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.

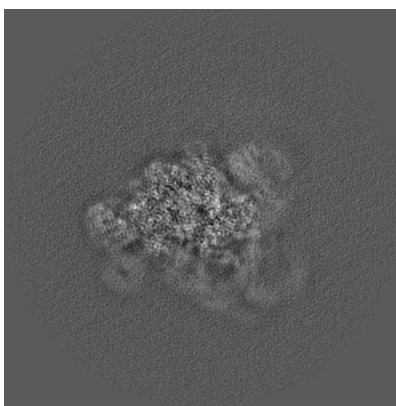
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

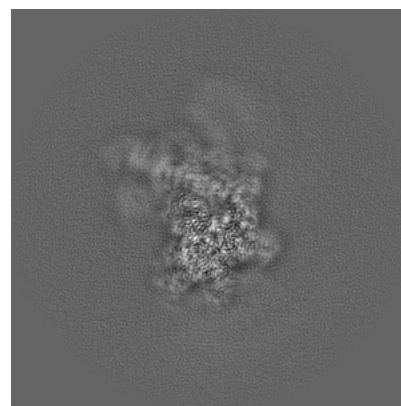
6.1.1 Primary map



X

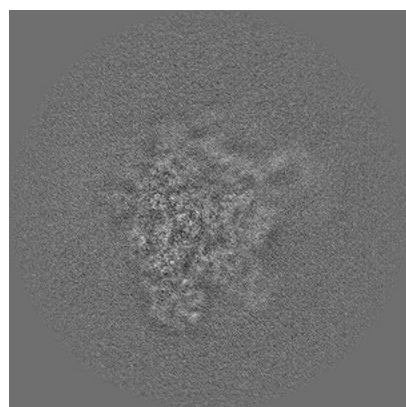


Y

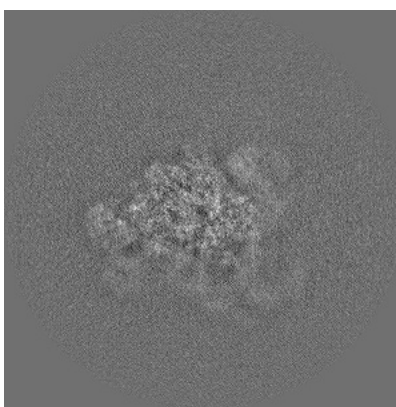


Z

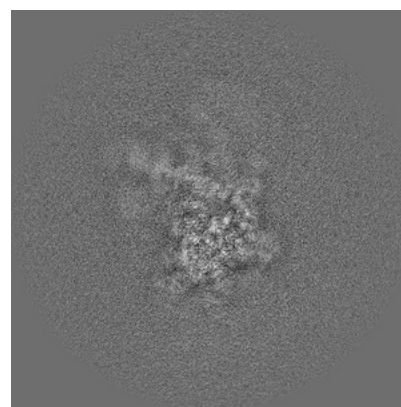
6.1.2 Raw map



X



Y

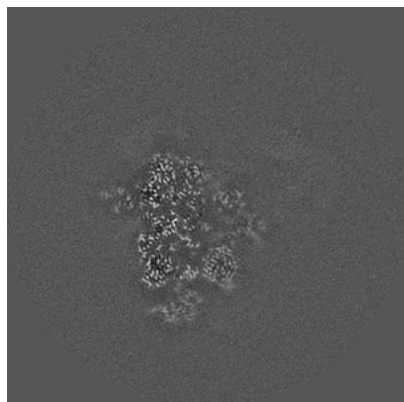


Z

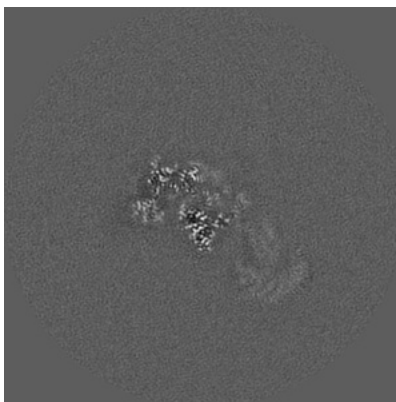
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

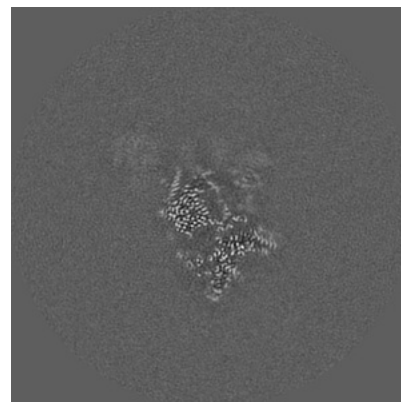
6.2.1 Primary map



X Index: 280

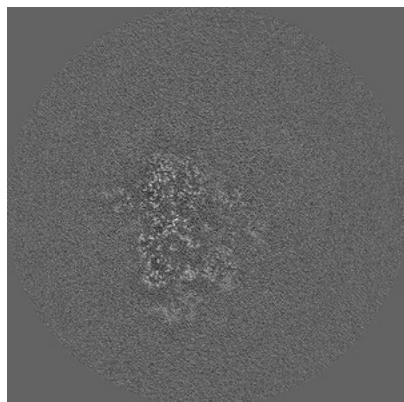


Y Index: 280

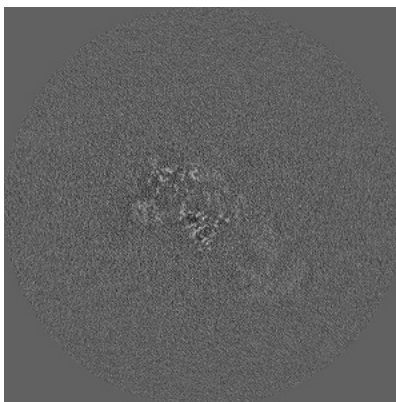


Z Index: 280

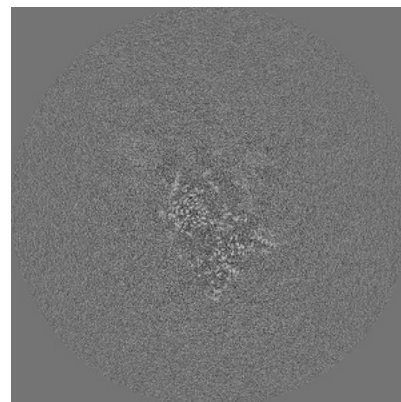
6.2.2 Raw map



X Index: 280



Y Index: 280

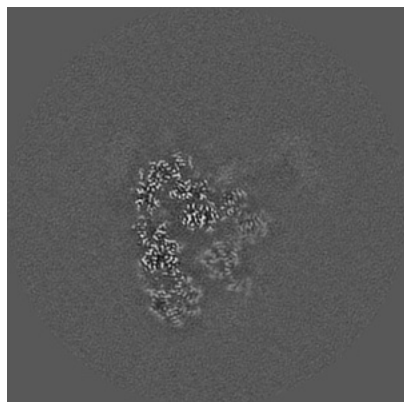


Z Index: 280

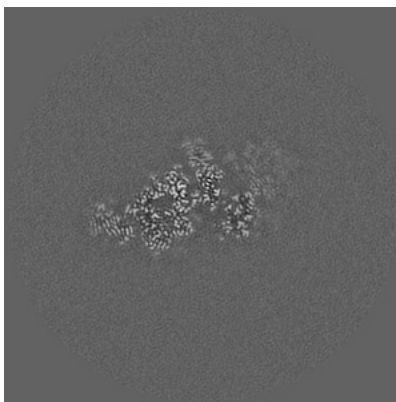
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

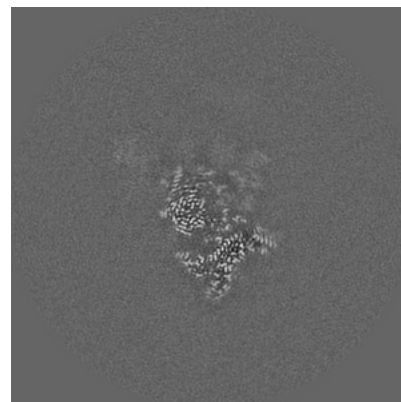
6.3.1 Primary map



X Index: 263

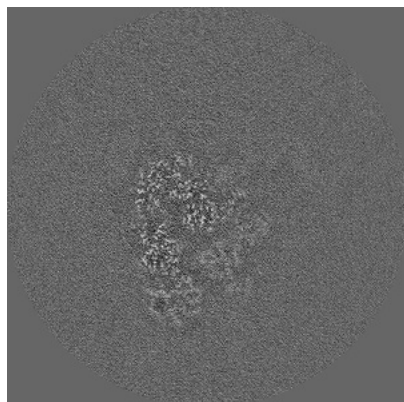


Y Index: 220

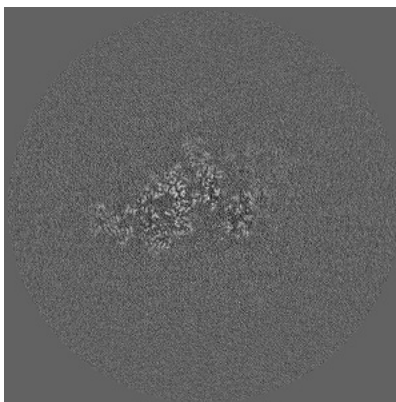


Z Index: 282

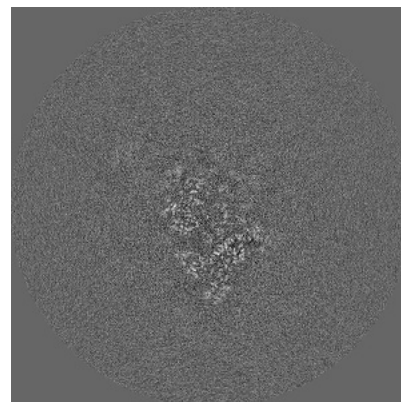
6.3.2 Raw map



X Index: 263



Y Index: 220

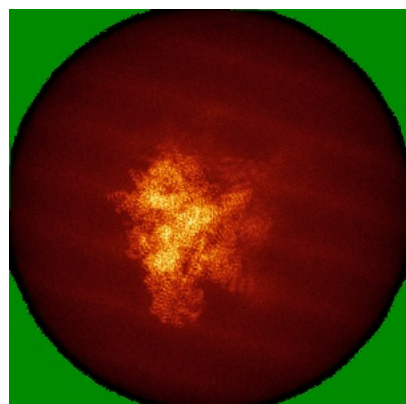


Z Index: 284

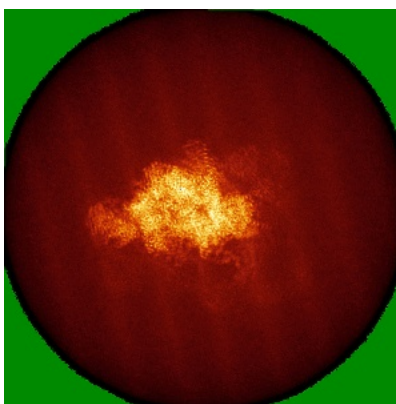
The images above show the largest variance slices of the map in three orthogonal directions.

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

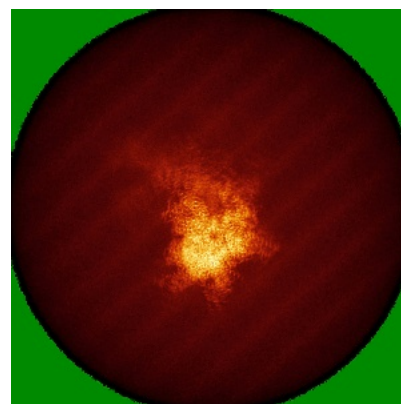
6.4.1 Primary map



X

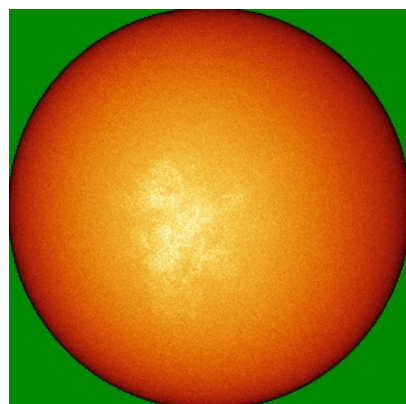


Y

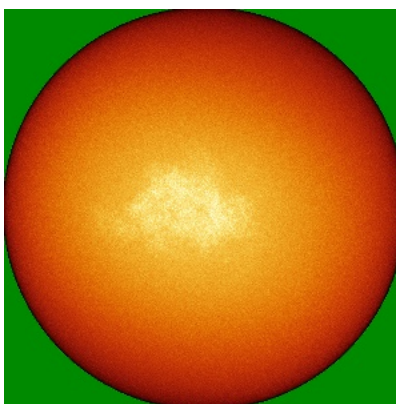


Z

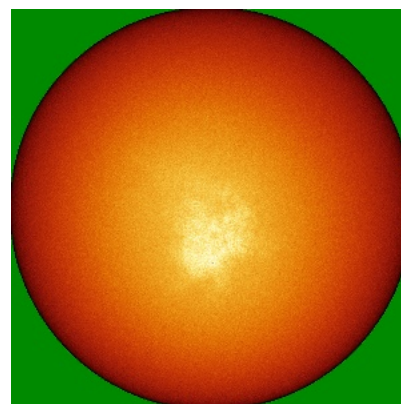
6.4.2 Raw map



X



Y

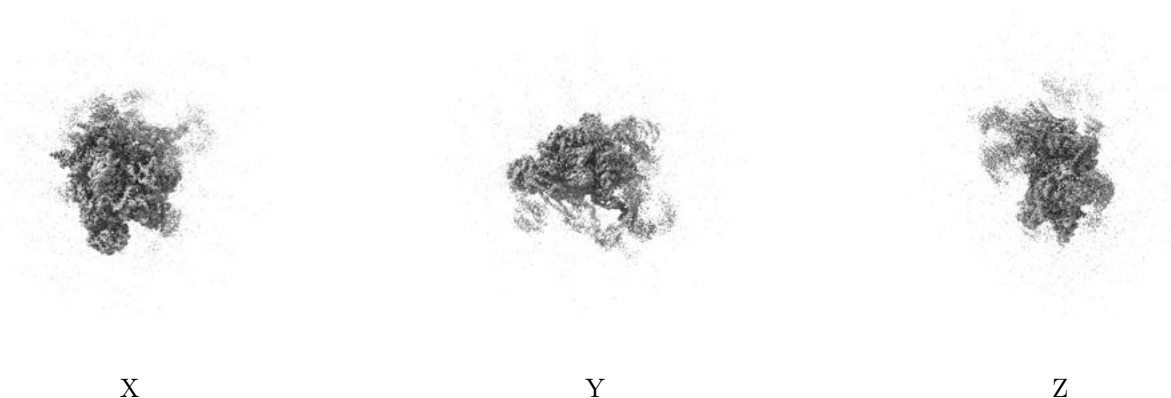


Z

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.

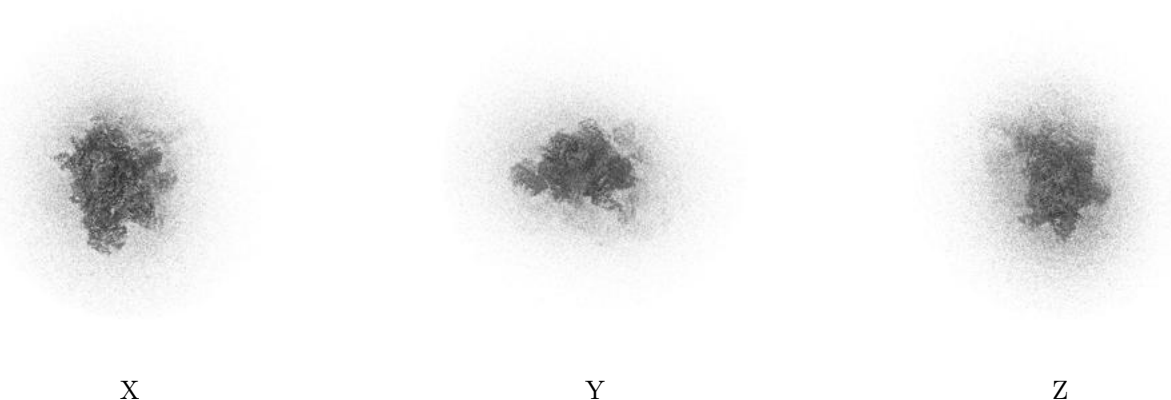
6.5 Orthogonal surface views [i](#)

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.

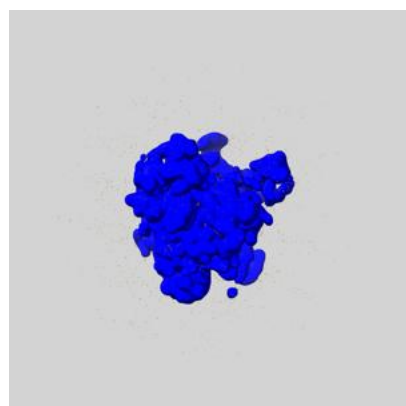
6.6 Mask visualisation [i](#)

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

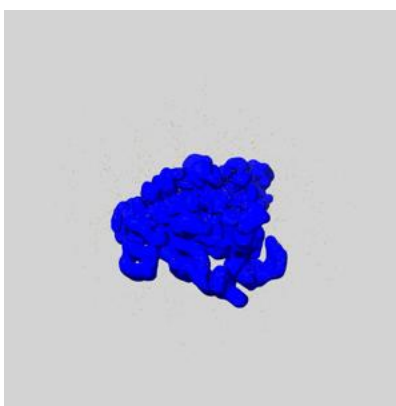
A mask typically either:

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

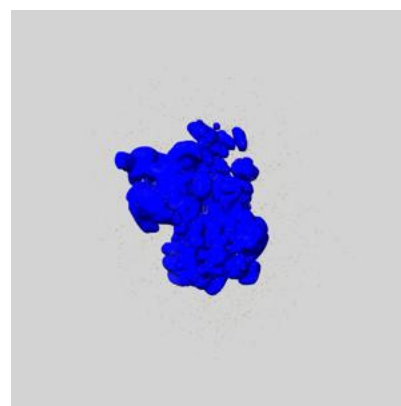
6.6.1 emd_19941_msk_1.map [i](#)



X



Y

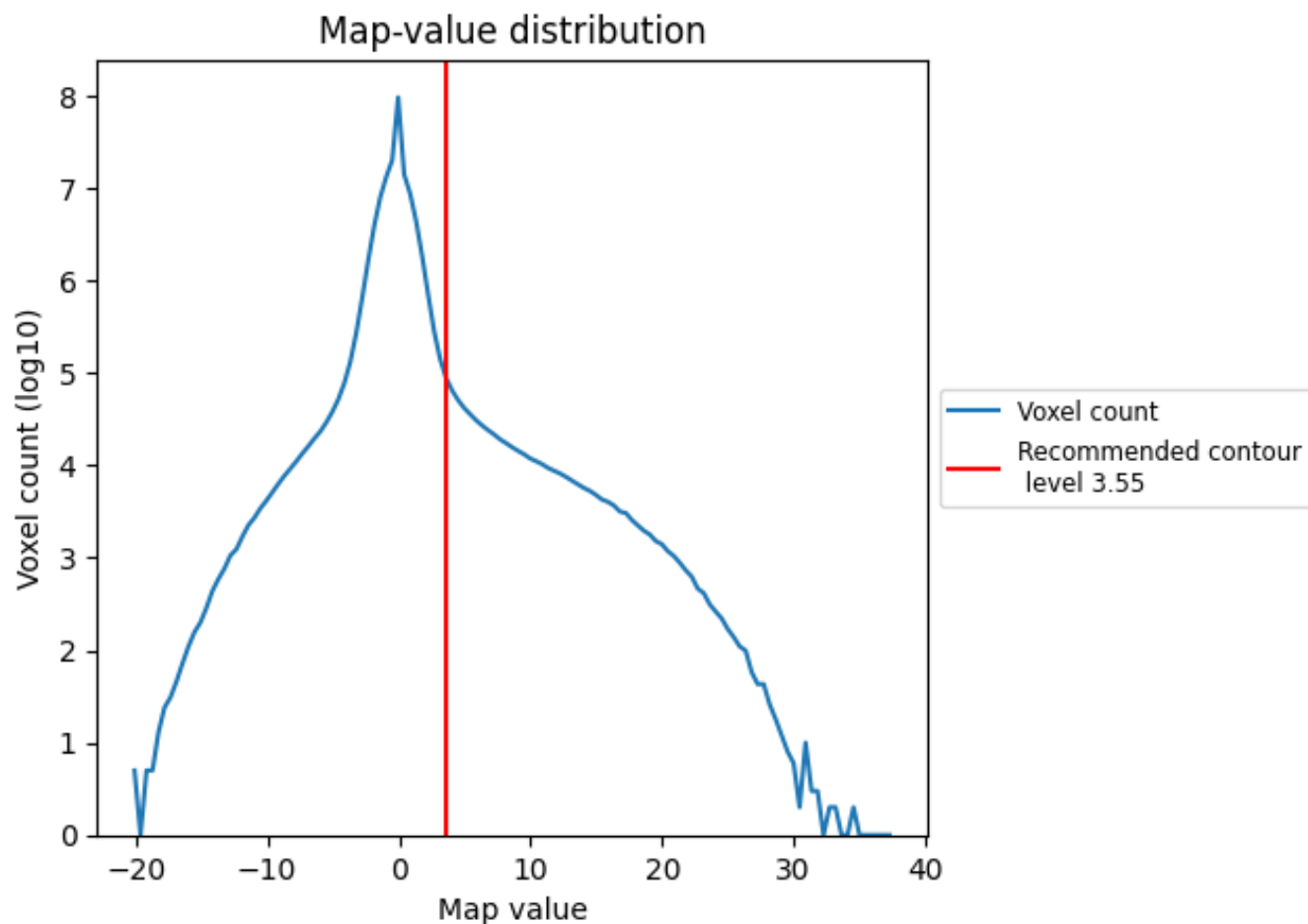


Z

7 Map analysis [i](#)

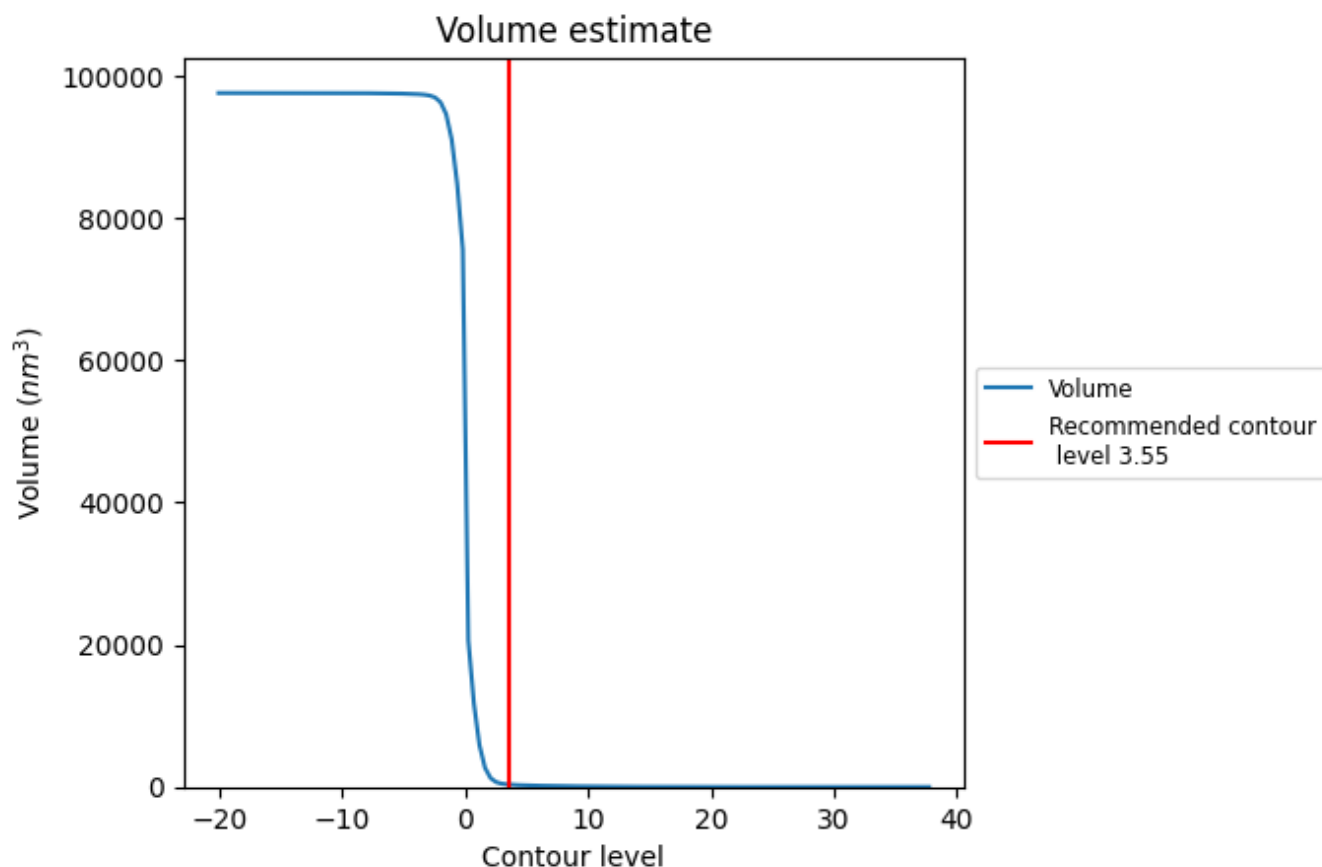
This section contains the results of statistical analysis of the map.

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.

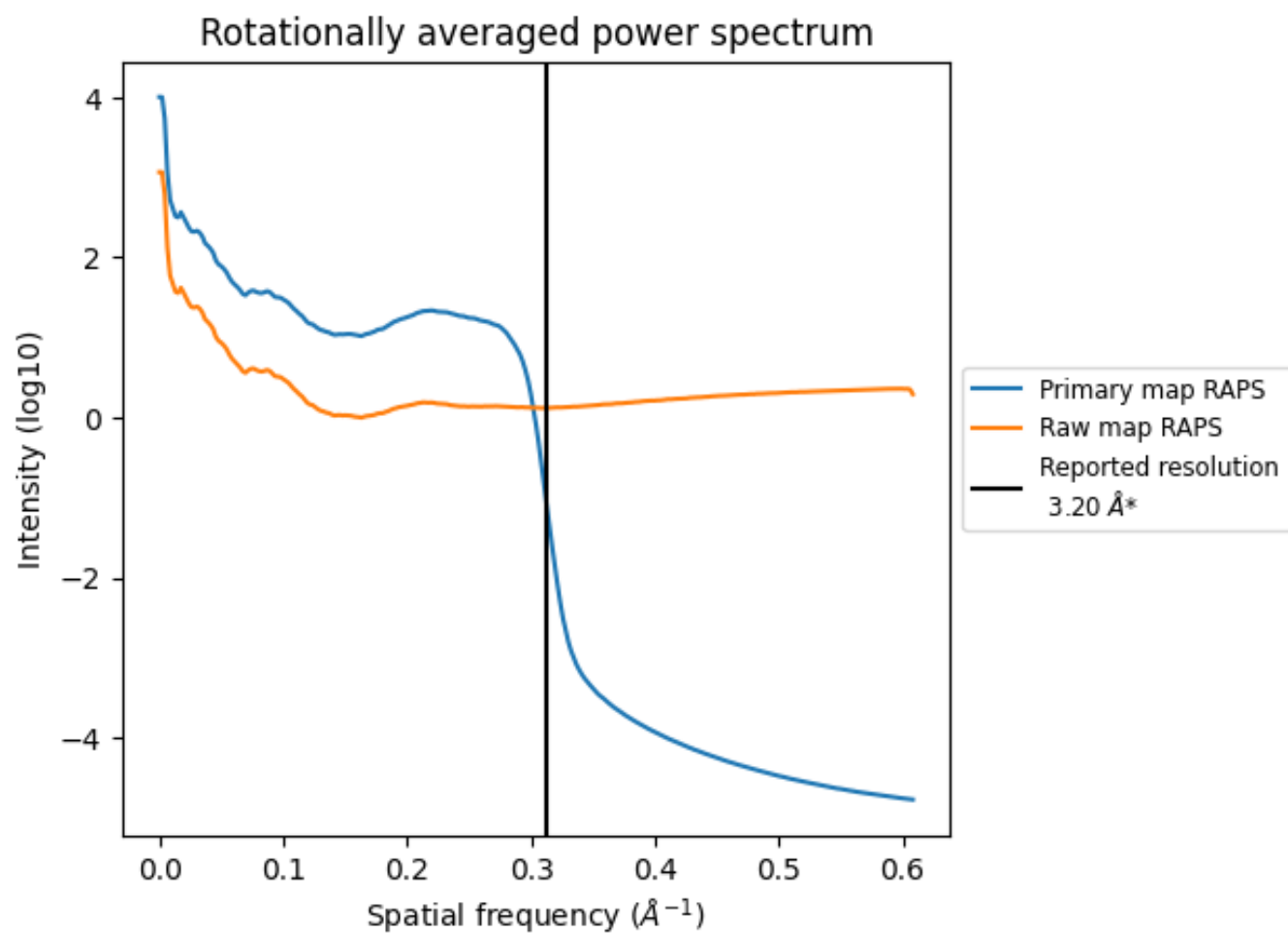
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 341 nm^3 ; 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 ⓘ

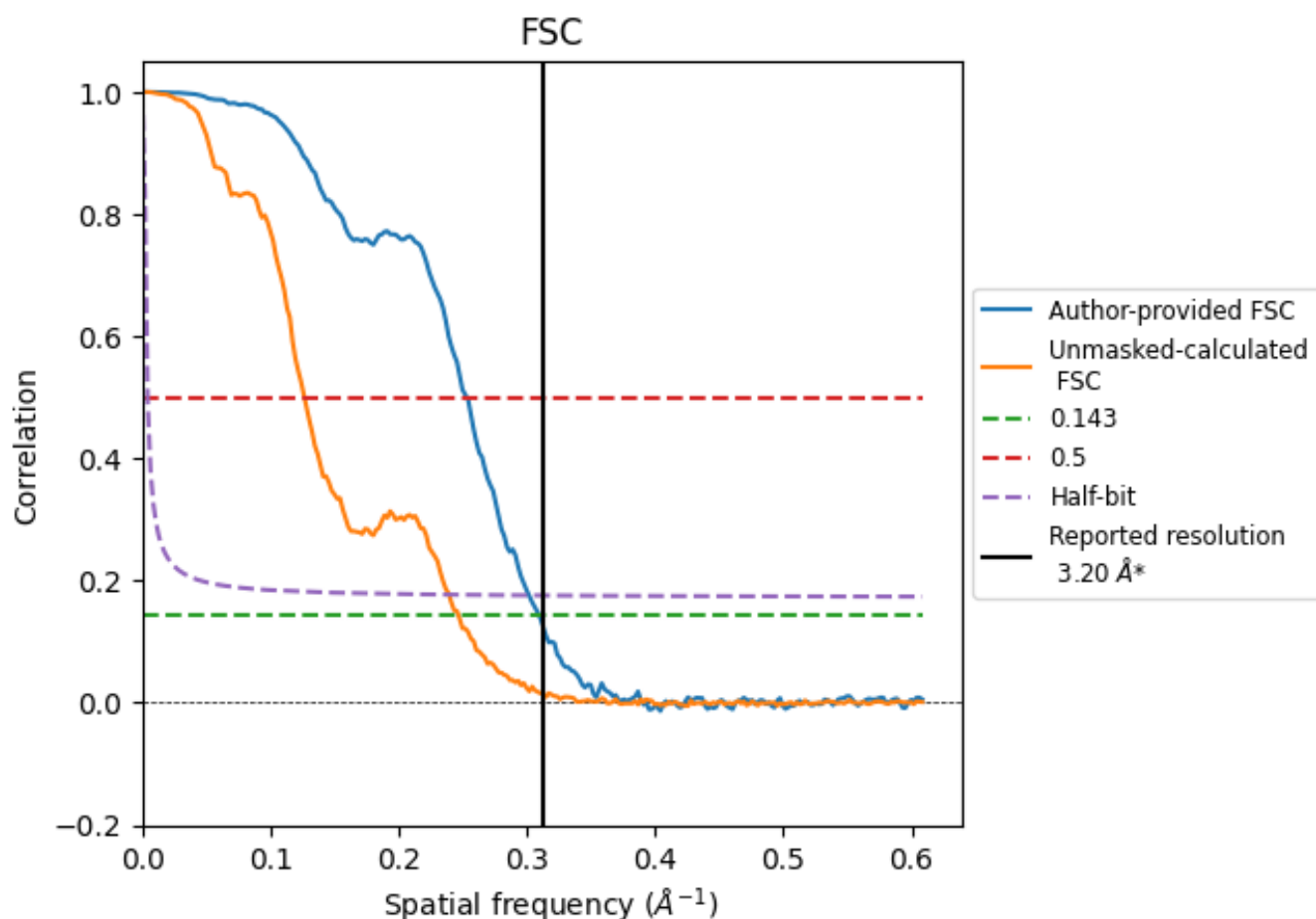


*Reported resolution corresponds to spatial frequency of 0.312 \AA^{-1}

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⁻¹

8.2 Resolution estimates [i](#)

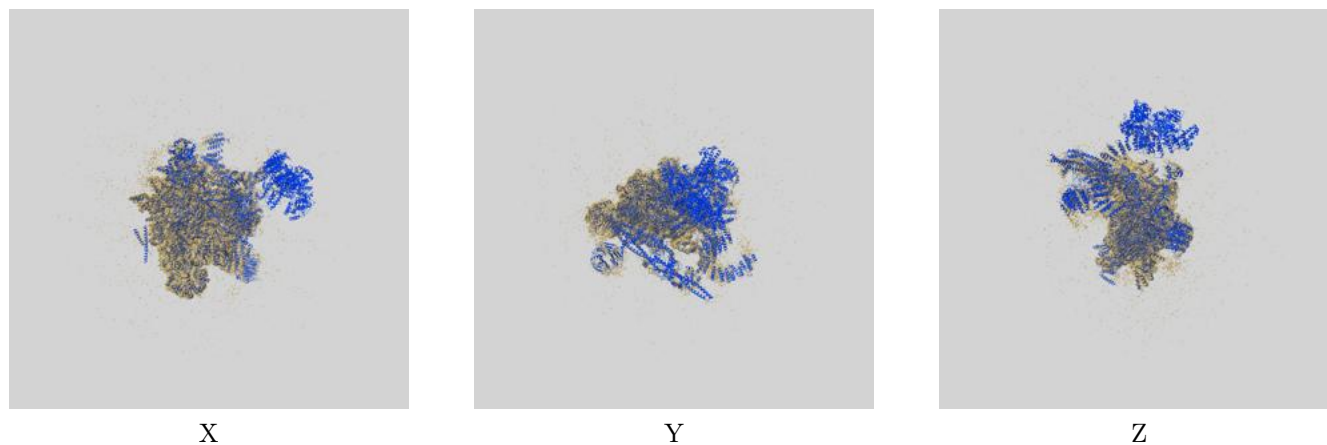
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.23	3.95	3.31
Unmasked-calculated*	4.06	7.91	4.18

*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](#)

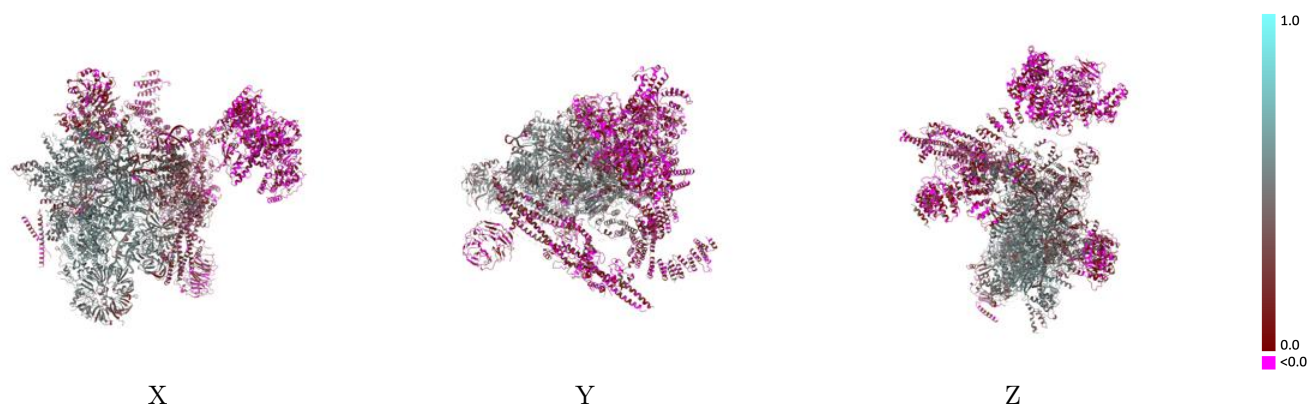
This section contains information regarding the fit between EMDB map EMD-19941 and PDB model 9ESH. Per-residue inclusion information can be found in [section 3](#) on [page 13](#).

9.1 Map-model overlay [i](#)



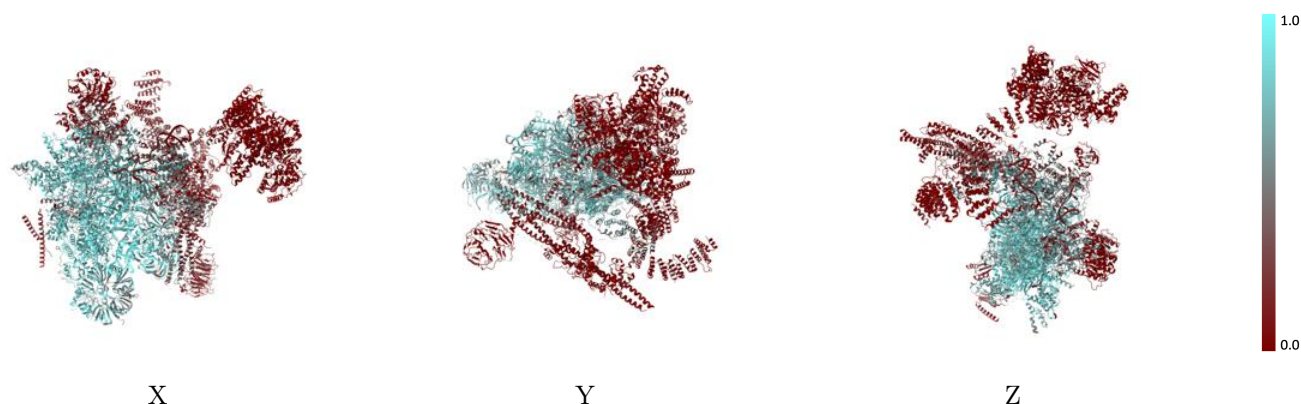
The images above show the 3D surface view of the map at the recommended contour level 3.55 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



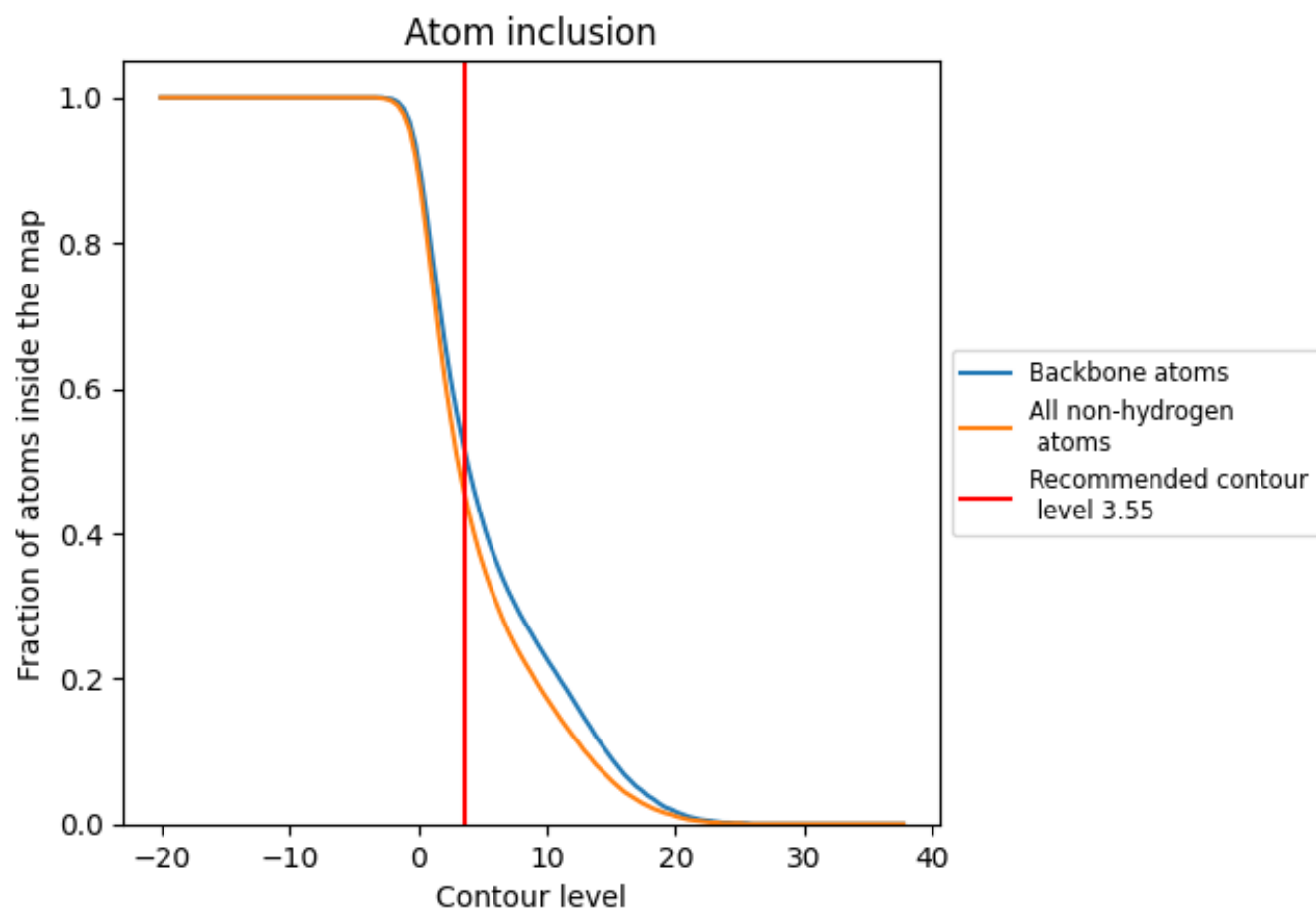
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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...

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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