



wwPDB EM Validation Summary Report ⓘ

Dec 12, 2022 – 06:30 PM EST

PDB ID : 3JB9
EMDB ID : EMD-6413
Title : Cryo-EM structure of the yeast spliceosome at 3.6 angstrom resolution
Authors : Yan, C.; Hang, J.; Wan, R.; Huang, M.; Wong, C.; Shi, Y.
Deposited on : 2015-08-09
Resolution : 3.60 Å (reported)
Based on initial models : 2YTC, 1GV2, 4WZJ, 2XL2, 4I43, 3J7P, 3LRV, 2BAY, 3U1L, 4YVD

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:

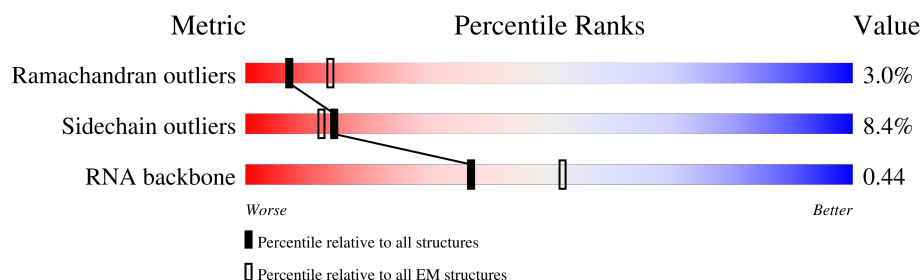
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

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 3.60 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	A	2363	<div> <div>7%</div> <div>71%</div> <div>11%</div> <div>17%</div> </div>
2	B	984	<div> <div>85%</div> <div>7%</div> <div>8%</div> </div>
3	C	120	<div> <div>42%</div> <div>45%</div> <div>12%</div> </div>
4	D	97	<div> <div>85%</div> <div>14%</div> </div>
4	Z	97	<div> <div>82%</div> <div>73%</div> <div>9%</div> <div>18%</div> </div>
5	E	147	<div> <div>62%</div> <div>5%</div> <div>33%</div> </div>
5	b	147	<div> <div>50%</div> <div>46%</div> <div>50%</div> </div>
6	F	117	<div> <div>63%</div> <div>6%</div> <div>30%</div> </div>




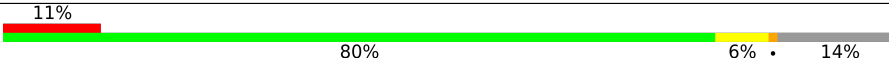
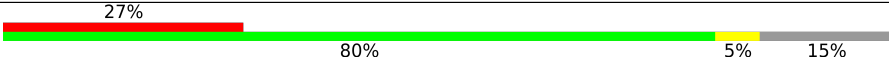

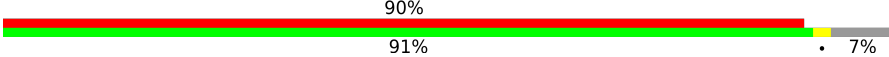



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Mol	Chain	Length	Quality of chain
6	f	117	
7	G	115	
7	l	115	
8	H	84	
8	m	84	
9	I	78	
9	n	78	
10	J	77	
10	o	77	
11	K	473	
12	L	340	
13	M	557	
14	N	99	
15	O	8	
16	Q	13	
17	P	186	
18	S	488	
18	T	488	
18	U	488	
18	V	488	
19	W	757	
20	Y	388	
21	a	354	
22	c	639	
23	d	155	

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Mol	Chain	Length	Quality of chain
24	e	146	
25	g	558	
26	h	265	
27	i	187	
28	R	674	
29	r	790	
30	X	1284	
31	j	239	
32	k	111	
33	x	412	

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 86551 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Pre-mRNA-splicing factor spp42.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1964	Total	C	N	O	S	0	0
			16230	10413	2859	2893	65		

- Molecule 2 is a protein called Pre-mRNA-splicing factor cwf10.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	904	Total	C	N	O	S	0	0
			7196	4586	1235	1340	35		

- Molecule 3 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	105	Total	C	N	O	P	0	0
			2209	990	364	750	105		

- Molecule 4 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	96	Total	C	N	O	S	0	0
			760	470	147	136	7		
4	Z	80	Total	C	N	O	S	0	0
			639	396	118	118	7		

- Molecule 5 is a protein called Small nuclear ribonucleoprotein-associated protein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	98	Total	C	N	O	S	0	0
			730	464	130	131	5		
5	b	74	Total	C	N	O	S	0	0
			576	365	99	107	5		

- Molecule 6 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	82	Total	C	N	O	S	0	0
			646	412	110	119	5		
6	f	82	Total	C	N	O	S	0	0
			646	412	110	119	5		

- Molecule 7 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	95	Total	C	N	O	S	0	0
			751	472	141	134	4		
7	l	87	Total	C	N	O	S	0	0
			696	440	128	124	4		

- Molecule 8 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	76	Total	C	N	O	S	0	0
			620	401	107	110	2		
8	m	76	Total	C	N	O	S	0	0
			620	401	107	110	2		

- Molecule 9 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	73	Total	C	N	O	S	0	0
			570	369	95	104	2		
9	n	73	Total	C	N	O	S	0	0
			570	369	95	104	2		

- Molecule 10 is a protein called Small nuclear ribonucleoprotein G.

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

- Molecule 11 is a protein called Pre-mRNA-splicing factor prp5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	373	Total	C	N	O	S	0	0
			2730	1720	492	505	13		

- Molecule 12 is a protein called Pre-mRNA-splicing factor cwf17.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	293	Total	C	N	O	S	0	0
			2273	1425	407	430	11		

- Molecule 13 is a protein called Pre-mRNA-processing protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	207	Total	C	N	O	S	0	0
			1661	1044	309	304	4		

- Molecule 14 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	90	Total	C	N	O	P	0	0
			1928	863	357	618	90		

- Molecule 15 is a RNA chain called RNA (5'-R(P*GP*UP*AP*UP*GP*UP*AP*U)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	8	Total	C	N	O	P	0	0
			170	76	28	58	8		

- Molecule 16 is a RNA chain called RNA (5'-R(P*UP*UP*UP*AP*UP*AP*CP*UP*AP*A P*CP*AP*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	13	Total	C	N	O	P	0	0
			270	122	44	91	13		

- Molecule 17 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	111	Total	C	N	O	P	0	0
			2323	1039	365	808	111		

- Molecule 18 is a protein called Pre-mRNA-processing factor 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	132	Total	C	N	O	S	0	0
			1052	663	181	205	3		
18	T	134	Total	C	N	O	S	0	0
			1069	671	183	212	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
18	U	430	Total	C	N	O	S	0	0
			2864	1801	492	562	9		
18	V	131	Total	C	N	O	S	0	0
			1037	652	177	205	3		

- Molecule 19 is a protein called Pre-mRNA-splicing factor cdc5.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	W	426	Total	C	N	O	S	0	0
			3024	1881	562	574	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Y	261	Total	C	N	O	S	0	0
			2008	1252	365	381	10		

- Molecule 21 is a protein called Pre-mRNA-splicing factor cwf5.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	a	255	Total	C	N	O	S	0	0
			1751	1088	324	325	14		

- Molecule 22 is a protein called Pre-mRNA-splicing factor cwf19.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	c	300	Total	C	N	O	S	0	0
			2425	1541	422	447	15		

- Molecule 23 is a protein called Peptidyl-prolyl cis-trans isomerase ppl1.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	d	155	Total	C	N	O	S	0	0
			1187	755	203	224	5		

- Molecule 24 is a protein called Pre-mRNA-splicing factor cwf14.

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

- Molecule 25 is a protein called Pre-mRNA-processing factor 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	g	148	Total	C	N	O	S	0	0
			1013	631	181	200	1		

- Molecule 26 is a protein called Pre-mRNA-splicing factor cwf15.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	i	161	Total	C	N	O	S	0	0
			1218	758	219	238	3		

- Molecule 28 is a protein called Pre-mRNA-splicing factor cwf4.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	R	575	Total	C	N	O	S	0	0
			3800	2363	718	706	13		

- Molecule 29 is a protein called Pre-mRNA-splicing factor cwf3.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	r	573	Total	C	N	O	S	0	0
			3299	2039	619	640	1		

- Molecule 30 is a protein called Pre-mRNA-splicing factor cwf11.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	X	1195	Total	C	N	O	S	0	0
			9764	6282	1619	1820	43		

- Molecule 31 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	j	160	Total	C	N	O	S	0	0
			1108	707	187	211	3		

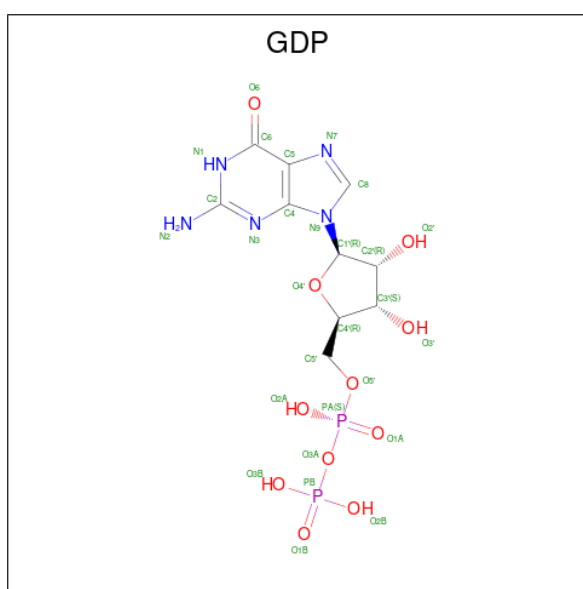
- Molecule 32 is a protein called Probable U2 small nuclear ribonucleoprotein B''.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	k	89	Total	C	N	O	S	0	0
			618	405	102	109	2		

- Molecule 33 is a protein called unknown chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	x	272	Total	C	N	O		0	0
			1360	816	272	272			

- Molecule 34 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					AltConf
34	B	1	Total	C	N	O	P	0
			28	10	5	11	2	

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

Mol	Chain	Residues	Atoms		AltConf
35	N	4	Total	Mg	0
			4	4	

- Molecule 36 is ZINC ION (three-letter code: ZN) (formula: Zn).

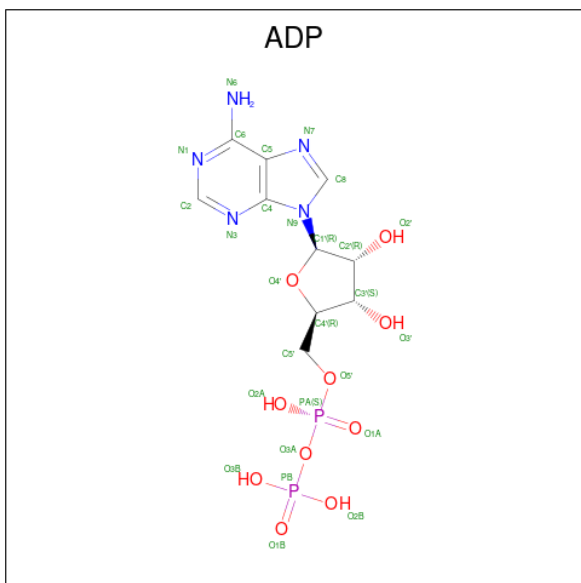
Mol	Chain	Residues	Atoms		AltConf
36	Y	1	Total	Zn	0
			1	1	

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Mol	Chain	Residues	Atoms	AltConf
36	a	2	Total Zn 2 2	0
36	c	1	Total Zn 1 1	0
36	e	3	Total Zn 3 3	0

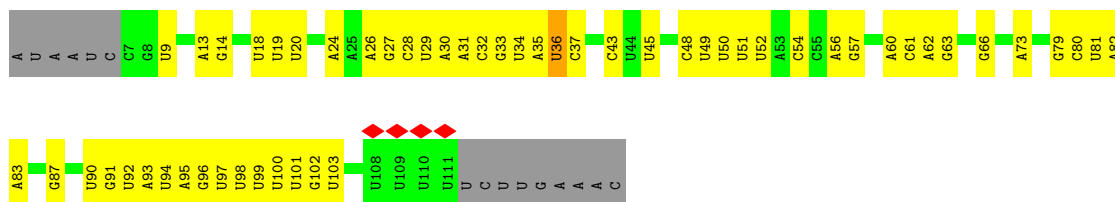
- Molecule 37 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$).



Mol	Chain	Residues	Atoms					AltConf
37	X	1	Total 27	C 10	N 5	O 10	P 2	0

- Molecule 2: Pre-mRNA-splicing factor cwf10

Chain C:  42% 45% 12%

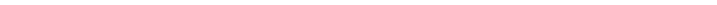


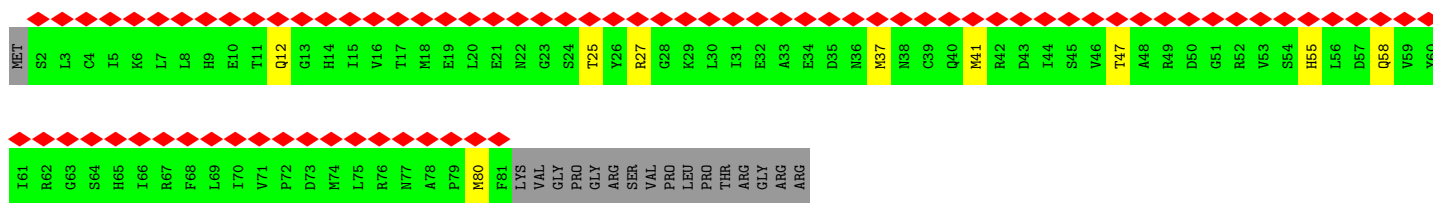
- Molecule 4: Small nuclear ribonucleoprotein Sm D3

Chain D: 85% 14%



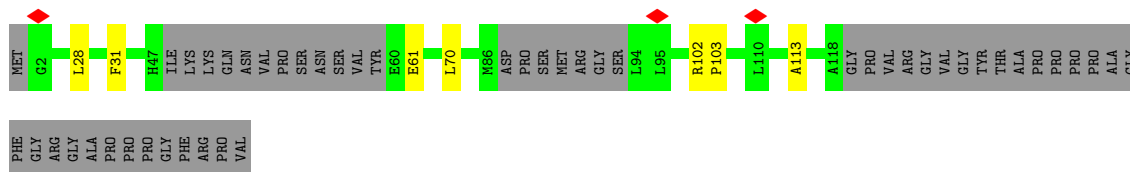
- Molecule 4: Small nuclear ribonucleoprotein Sm D3

Chain Z: 



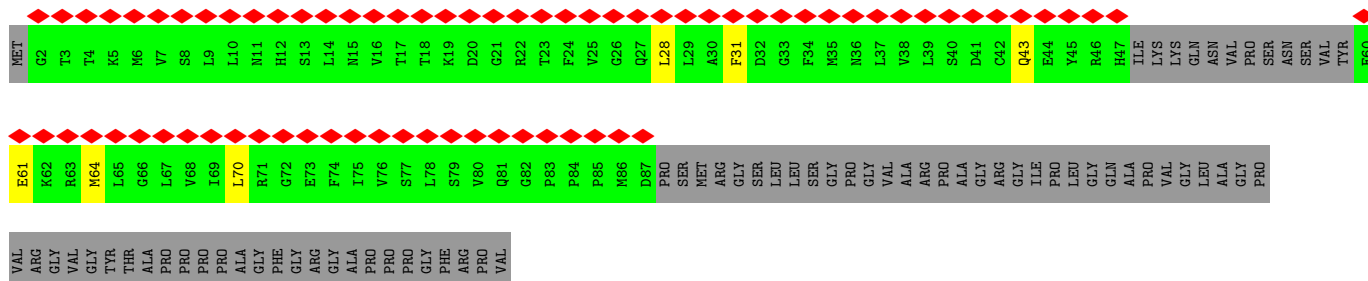
- Molecule 5: Small nuclear ribonucleoprotein-associated protein B

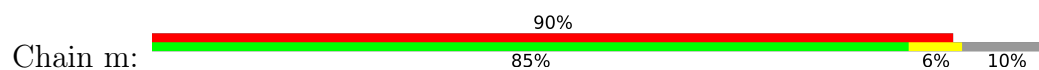
Chain E:  62% 5% 33%



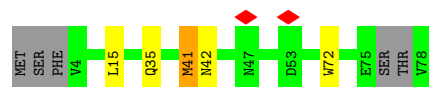
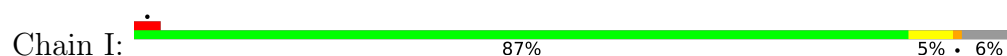
- Molecule 5: Small nuclear ribonucleoprotein-associated protein B

Chain b: 50% 46% 50%

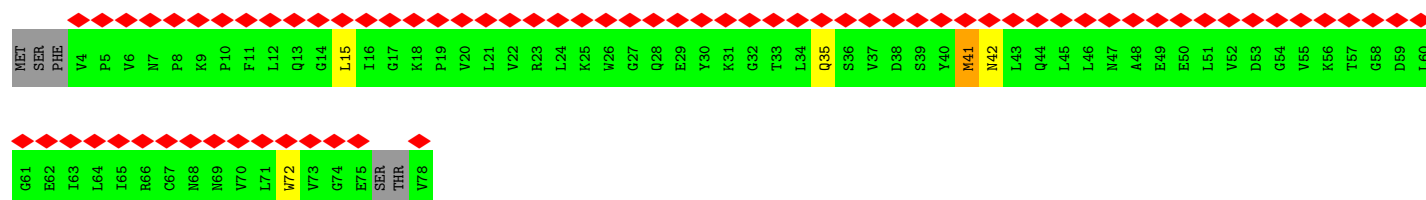
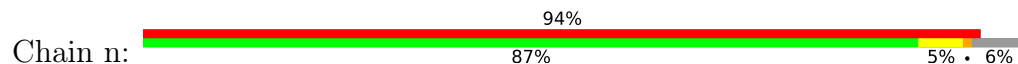




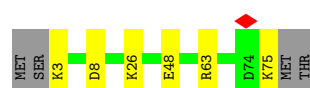
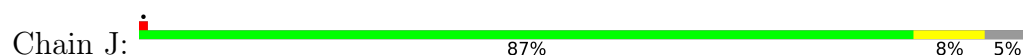
- Molecule 9: Small nuclear ribonucleoprotein F



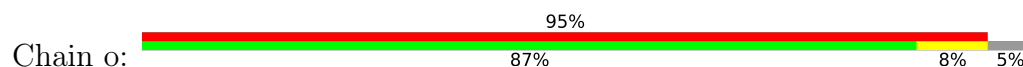
- Molecule 9: Small nuclear ribonucleoprotein F



- Molecule 10: Small nuclear ribonucleoprotein G

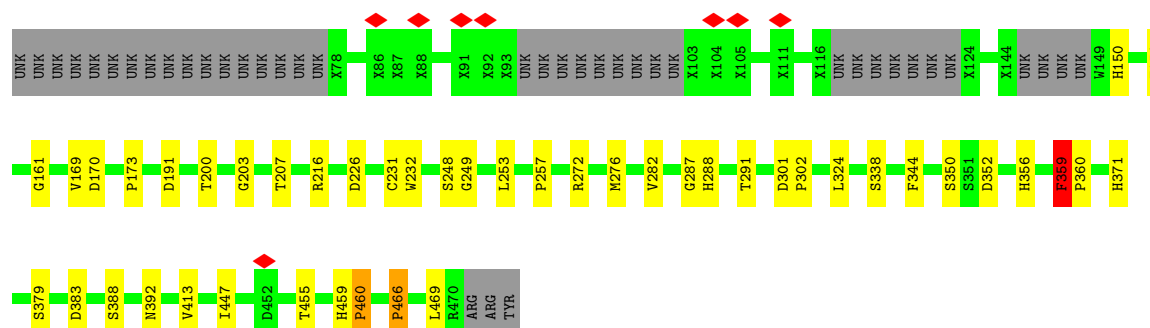


- Molecule 10: Small nuclear ribonucleoprotein G

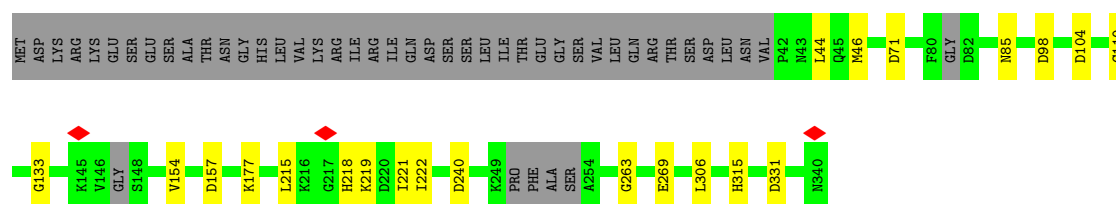
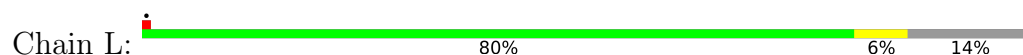


- Molecule 11: Pre-mRNA-splicing factor prp5

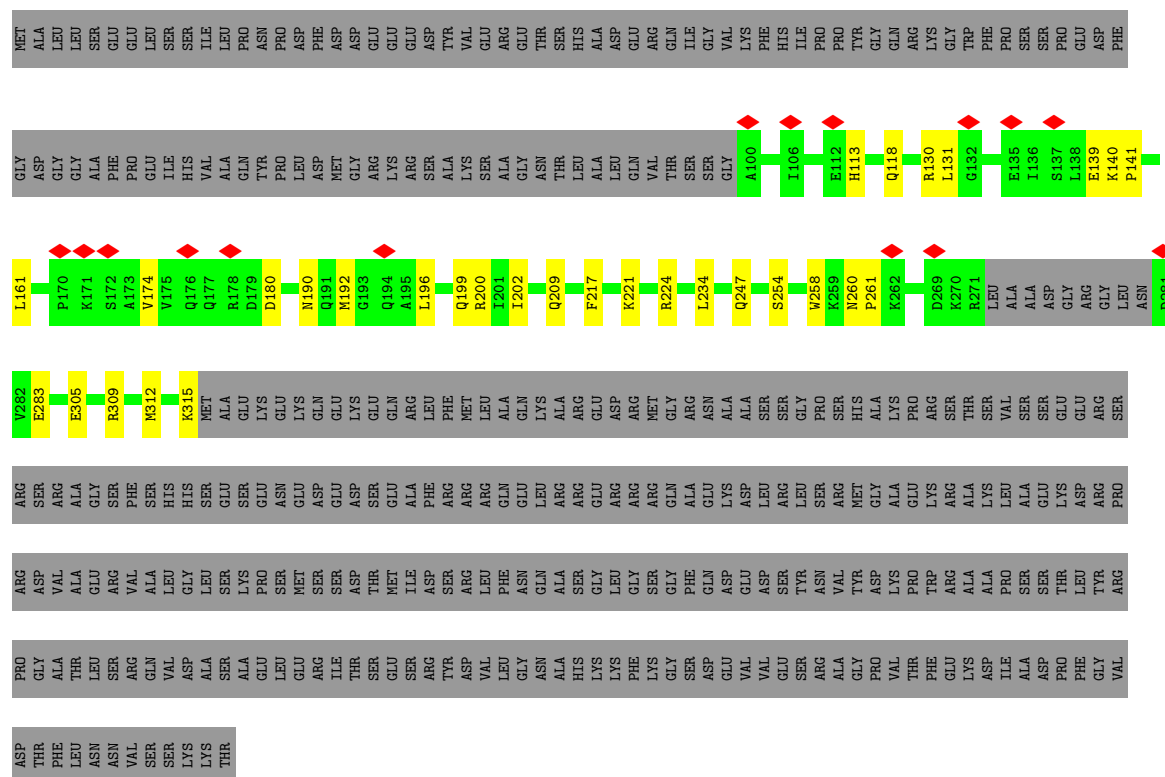




- Molecule 12: Pre-mRNA-splicing factor cwf17



- Molecule 13: Pre-mRNA-processing protein 45



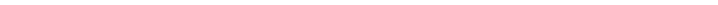
- Molecule 14: U6 snRNA

- Chain O:

Diagram illustrating a sequence of nodes: G100, U101, A102, U103, G104, and U107. U103 and G104 are highlighted in yellow, and U107 is highlighted in green. A red diamond is positioned above U107.

- Chain Q: 

U492	U493	U494	A495	U496	A497	C498	U499	A500	A501	C502	A503	C504
------	------	------	------	------	------	------	------	------	------	------	------	------

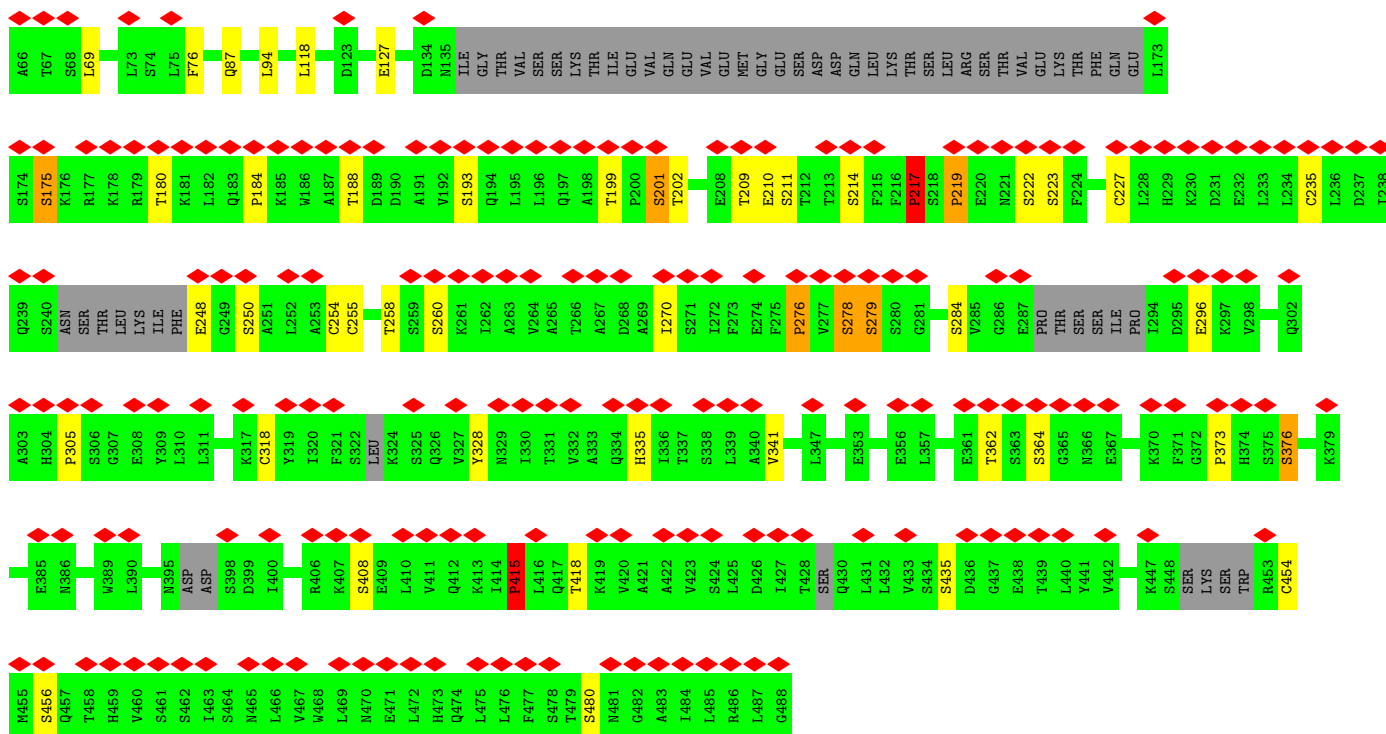
- Chain P:  47% 29% 27% 40%

[illegible]

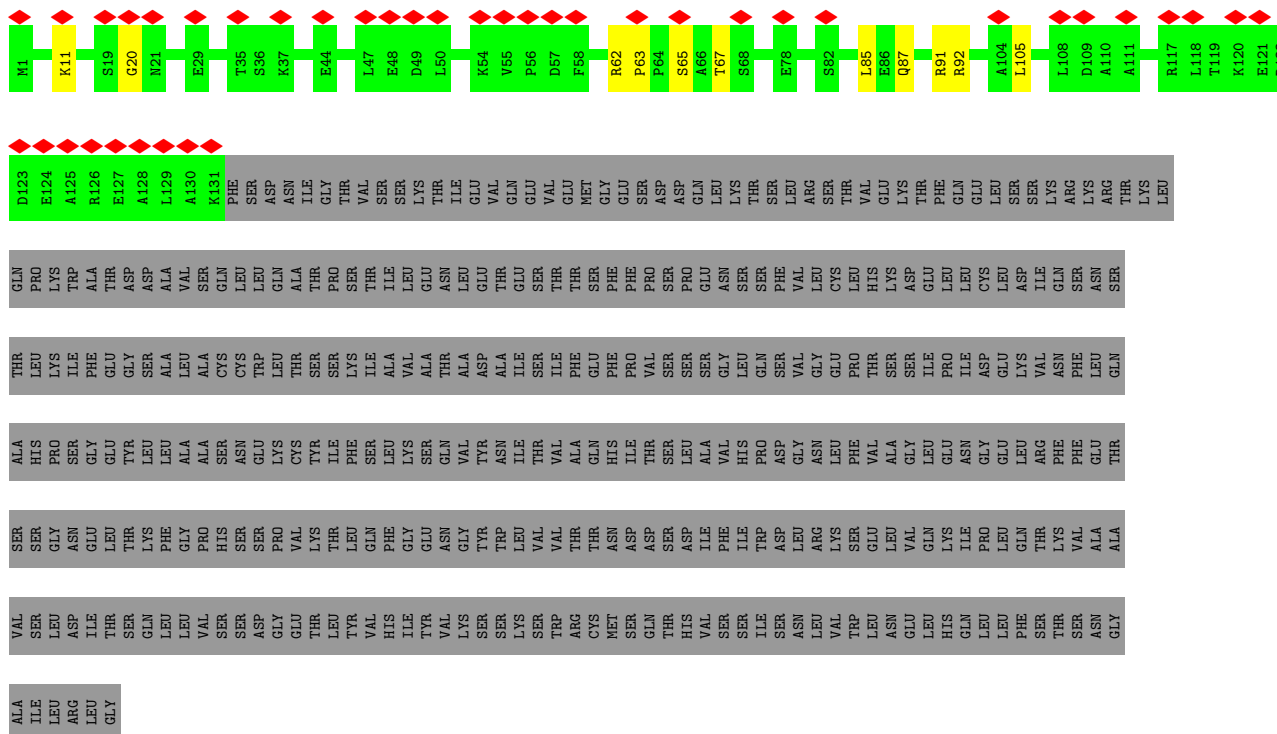
- Chain S: 

1000 samples

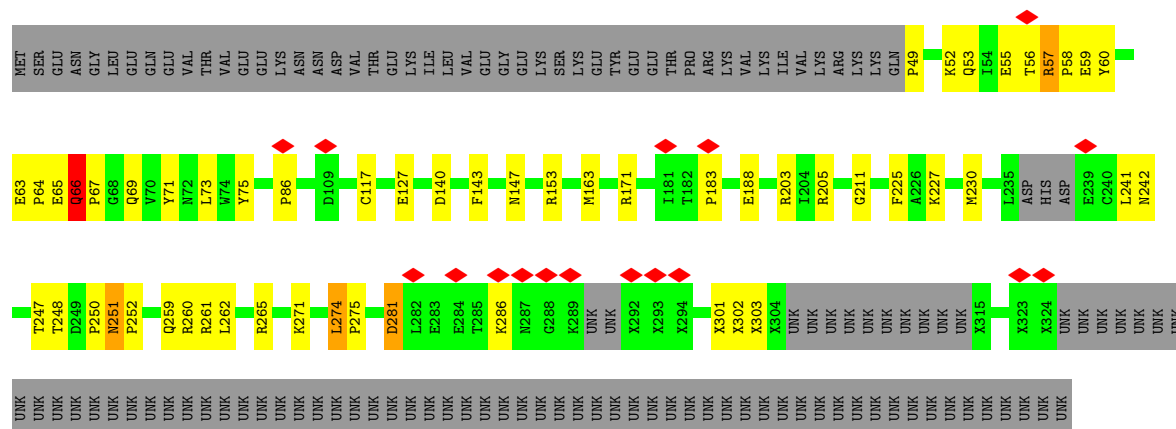
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G7	10
E8	10
T9	10
P10	10
K11	10
I15	10
V18	10
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V22	10
R26	10
L27	10
V31	10
I32	10
R33	10
R33	10
R33	10
T35	10
S36	10
K37	10
V40	10
T41	10
Q42	10
Q42	10
Q43	10
E44	10
E44	10
T46	10
L47	10
E48	10
V53	10
K54	10
D57	10
F58	10
V59	10
R60	10
P61	10
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S102	10
T103	10
A104	10
L105	10
T106	10



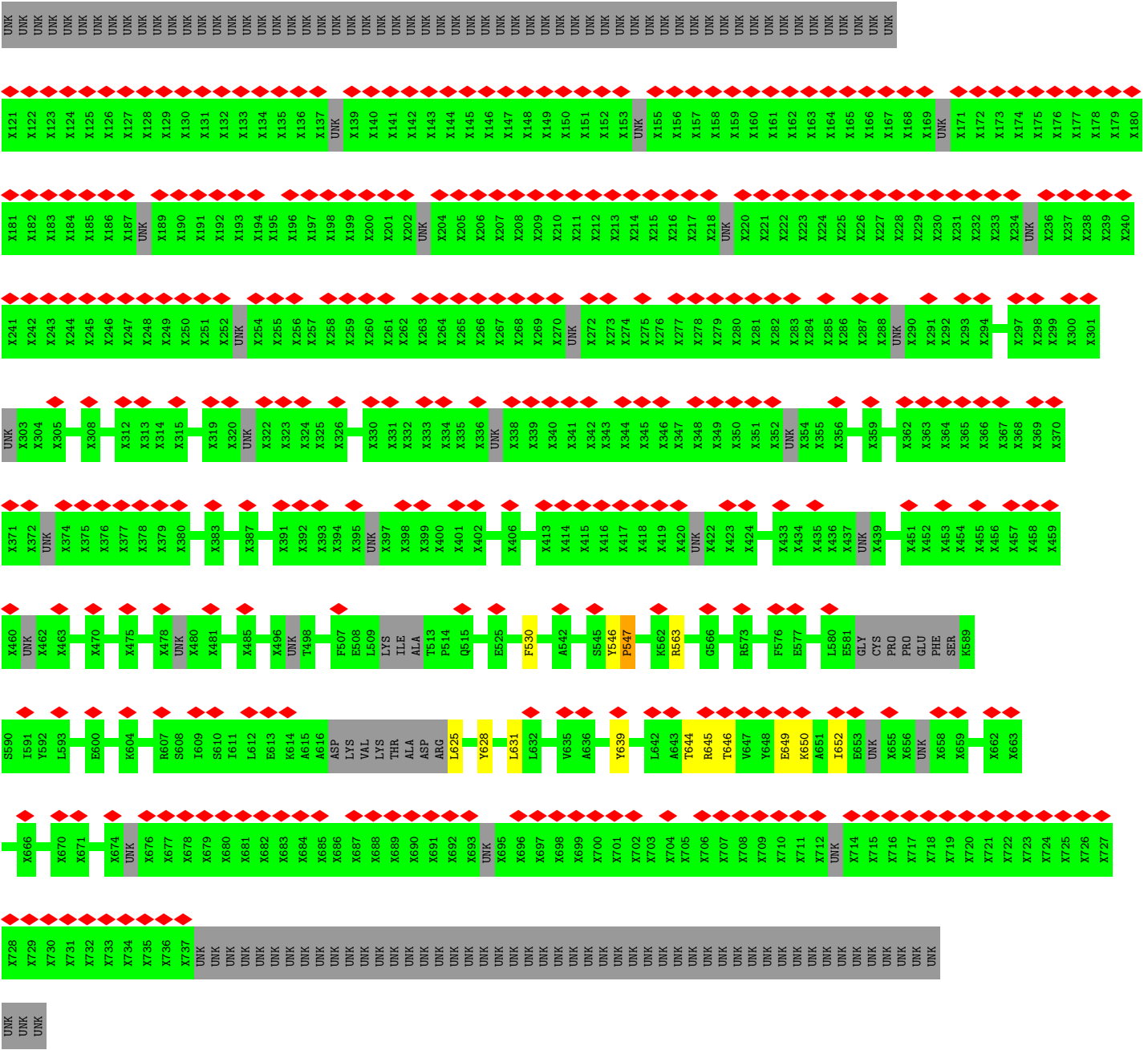
• Molecule 18: Pre-mRNA-processing factor 19



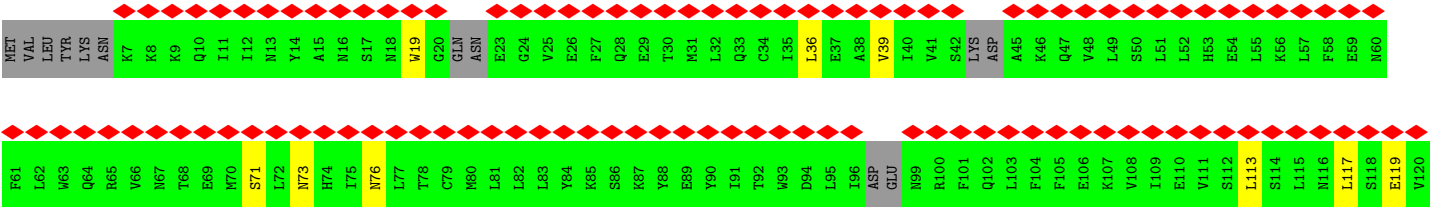
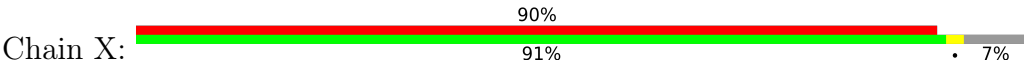
• Molecule 19: Pre-mRNA-splicing factor cdc5

[illegible]

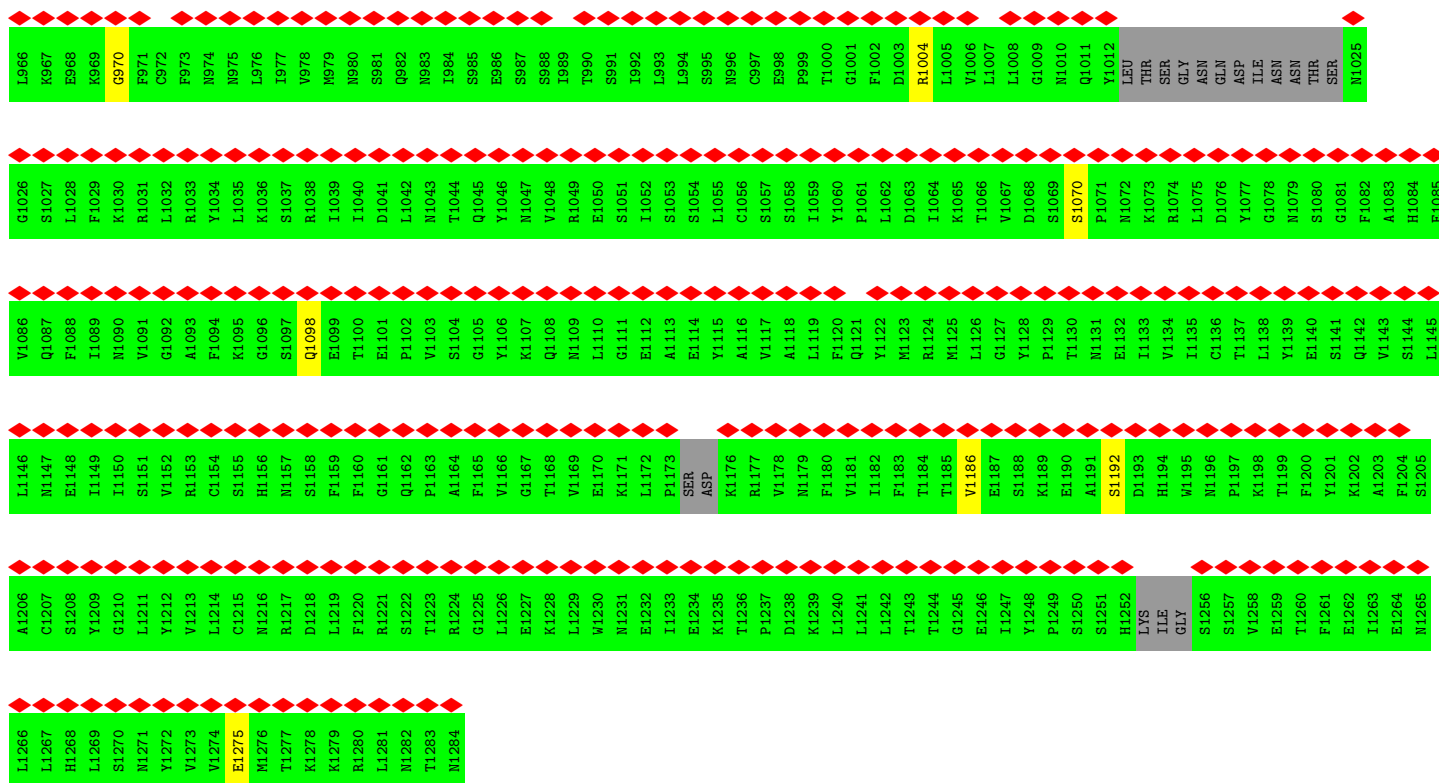




● Molecule 30: Pre-mRNA-splicing factor cwf11

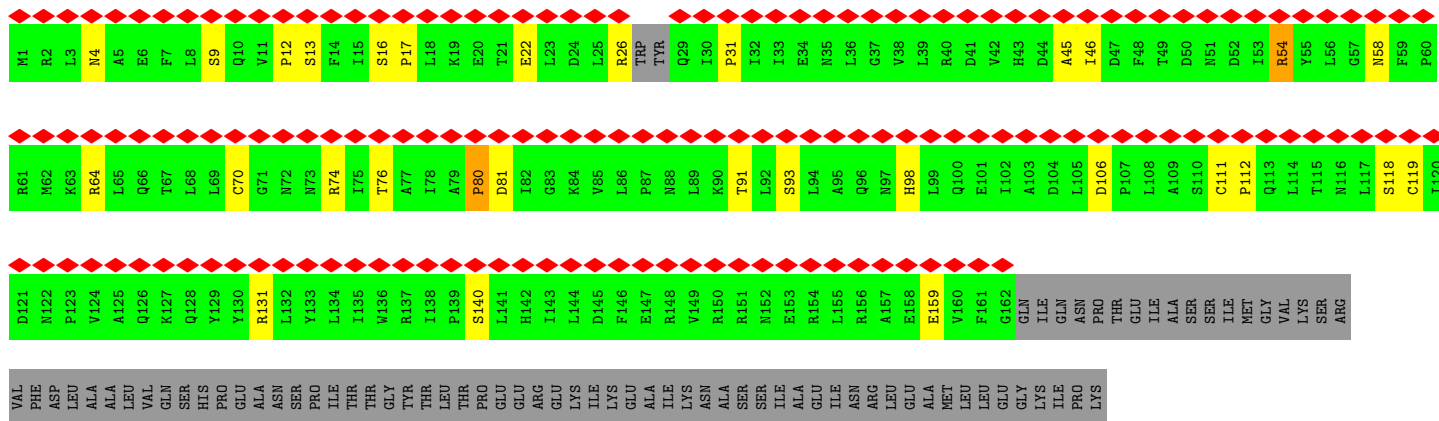


V121	K181	F241	L301	Y364	Q426	T486	N546	L606	V666	T786	S846	N906
Y122	R182	A242	V302	A365	Y427	S487	A547	K607	A667	L787	H847	F907
M123	P183	H243	Q307	I366	L428	V488	L548	F608	R668	F788	D848	F908
I124	SER	P244	I308	K367	S429	A489	D549	N609	N669	T789	A849	D909
Q125	I1E	P245	L308	V368	I430	P490	P650	F610	L670	L790	S850	Y910
T126	V186	I246	L309	D369	S431	GLN	L551	A611	N671	L791	P851	A911
I127	E187	E247	L310	F370	F432	I1E	E552	L612	N672	E792	D852	T912
T128	K188	D248	F311	E371	F433	GLY	V554	V613	T673	K793	T853	K913
L129	F189	S249	S312	F372	M434	GLN	T555	L614	V674	A794	A854	L914
C130	P190	C250	D313	L373	R435	VAL	D556	S615	E675	R795	L855	Y915
F131	L191	F251	F314	K374	Q436	L497	F557	PRO	Q676	C796	Y856	G916
Q132	H192	Y252	Q315	F377	Q437	P498	T558	GLU	L677	F797	F857	E917
F133	N193	T253	LYS	F377	S438	Q499	F558	ALA	Q678	H798	R858	L918
S134	L194	A254	GLU	I378	K439	F500	L559	GLN	N679	S799	D859	E919
N135	L195	L255	LEU	N379	A440	V501	A560	K620	S679	Q739	T860	Y920
I136	S196	R256	ASP	D382	Y441	K502	T561	Y621	V680	Q740	A860	Y920
E137	R197	S257	VAL	R383	K442	C503	L562	N622	L681	P741	Y861	M921
K138	W198	S258	PHE	THR	K443	Q504	C563	L623	P682	G742	T862	F922
L139	I199	L259	CYS	R385	K444	M505	N564	D624	N683	L743	K863	Q923
R140	H200	Y260	THR	L445	L445	G506	L564	L625	C684	T744	R864	Q924
K141	S201	Y261	THR	L446	L446	L507	D565	N626	H685	M745	L865	L925
L142	L202	Y262	SER	V387	R447	S508	D566	L627	V686	W746	Y866	E926
V143	L203	S263	L329	N388	S448	R509	G568	L628	P687	N747	D807	E927
Y144	I204	N264	Q330	D389	L449	P510	M569	V629	S688	G748	E808	I928
Q145	K205	E265	Q331	Y390	Y450	PRO	F570	S630	N689	P749	C809	R929
L146	S206	L266	R332	D391	A451	GLN	ASP	L631	L690	T750	L870	P930
T147	I207	F267	Q333	E392	E452	SER	ASP	L632	S691	R751	N871	F931
N148	S208	K268	K334	I393	L453	HTS	N574	N633	T692	C752	T872	G932
I149	Y209	K269	L335	I394	L454	A516	Q575	R634	E693	G753	L873	L933
A210	A210	K270	E336	N395	N455	L517	S576	A635	S694	K754	E874	L934
Q211	Q211	M270	E337	F396	F456	R518	S577	K636	L696	V756	ASP	R935
THR	THR	T271	I338	T397	S457	D519	D577	E637	L697	L757	K876	Y936
GLU	GLU	D272	I339	L398	E458	L520	S578	F638	T697	L758	D877	Y937
K214	Q215	D273	S340	K399	Q459	K521	D579	P639	K698	T759	S878	E938
Q215	E216	L274	F341	D400	Y460	N522	N580	K640	F699	C759	V879	D939
E216	E217	N275	L342	V401	R461	S523	K581	N641	Y700	K760	D880	Q940
ASP	A217	Y276	L343	L402	R462	I1E	S582	F642	T701	L761	S822	E941
K218	K218	V277	S343	G403	R463	LYS	S583	E643	M702	L762	W823	L942
V219	V219	L278	F344	E404	L463	S526	N584	D644	Q703	E763	T824	Y943
T220	T220	K279	N345	R405	S464	S527	V585	L645	M704	V764	S825	A944
P221	P221	F280	S346	R406	I465	F528	V586	L646	K705	L765	K826	L945
L222	L222	P281	S347	S406	K466	L529	L587	F646	I1E	Q766	L827	C946
F282	F282	V281	L347	V407	N467	C530	S588	L647	S707	D767	P828	Q947
D283	D283	K282	K348	M408	A468	L531	P589	G648	A708	E767	G829	Q948
N284	N284	N285	L350	D409	T469	I532	F590	F649	D709	T768	L830	S949
T285	T285	R286	C351	E411	K470	V533	V591	G650	V710	P770	L831	Y950
R286	R286	G287	S352	M412	N471	I534	V592	T651	N711	T771	R832	F951
G287	G287	K288	S353	S413	L472	S535	H593	P652	A712	D772	E833	I952
M228	M228	N288	C354	S413	THR	K536	S594	D653	S713	R773	T834	Q953
S229	S229	E289	Y355	T415	ASP	D537	L595	T654	D714	T774	G835	C954
L230	L230	Y290	L356	M416	N476	M538	A596	A656	R715	V775	R836	T955
V231	V231	E291	L356	THR	F477	E539	G597	F657	H716	V776	L837	W956
L232	L232	K292	T358	PHE	F478	Y540	L598	P658	L777	L777	A838	R957
L233	L233	E293	S359	LEU	S479	K541	G599	N659	LEU	S778	P898	S958
S234	S234	Q294	F360	LEU	L480	L542	E600	A660	LEU	D779	S840	L959
A235	A235	K295	P361	GLN	N481	L543	N601	Q660	PRO	D779	T841	Y960
F236	F236	I296	E362	THR	N482	H544	R602	S664	S721	S780	Q842	T961
P237	P237	R297	K363	A424	F483	G545	P603	L665	N722	F782	A843	R962
T238	T238	N298	Y485	I425	K484		K604		R723	S783	P844	L963
R239	R239	D299			V485		Q605		L724	M784	G845	Q964
K179	K179	E300							Y726	N785		T965



• Molecule 31: U2 small nuclear ribonucleoprotein A'

Chain j:

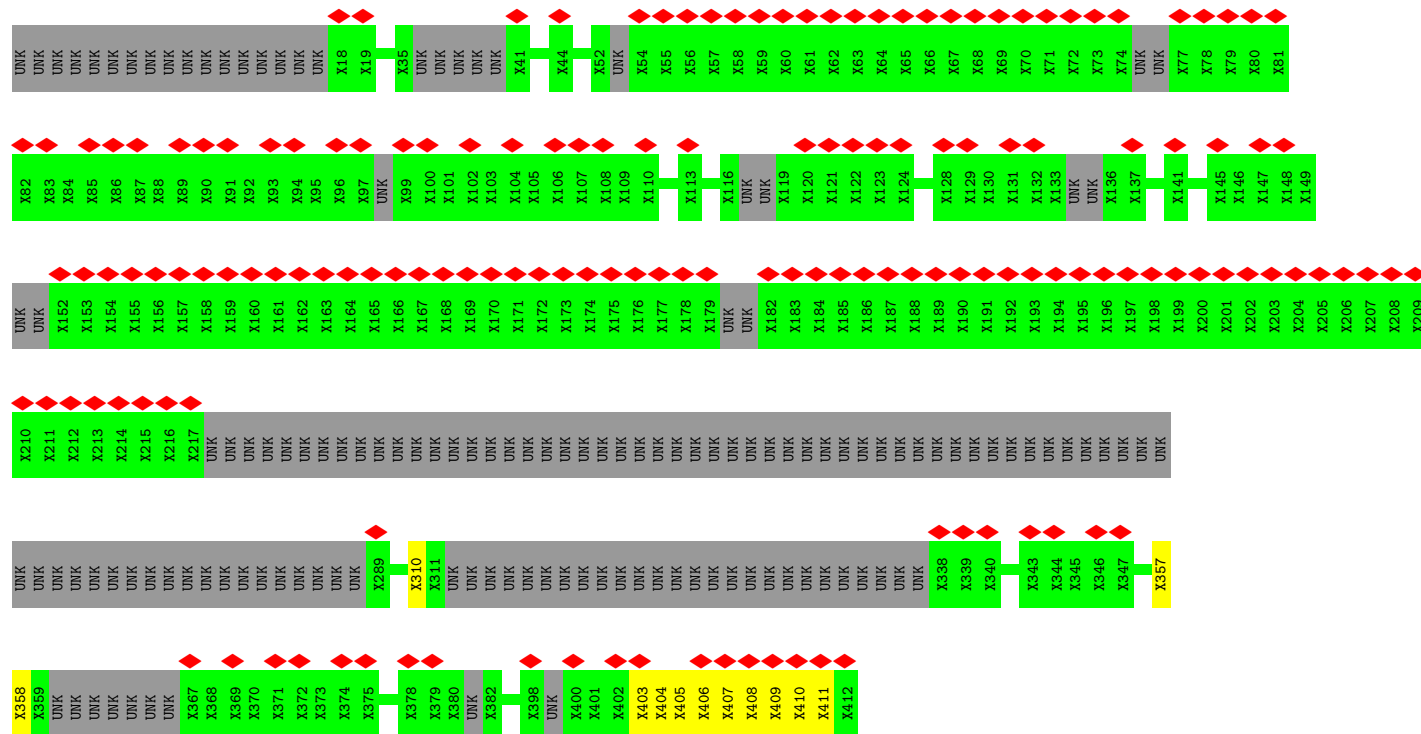
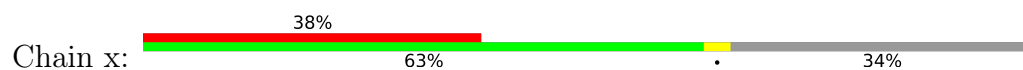


• Molecule 32: Probable U2 small nuclear ribonucleoprotein B''

Chain k:



● Molecule 33: unknown chain



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	112795	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	
Minimum defocus (nm)	3.0	Depositor
Maximum defocus (nm)	1.5	Depositor
Magnification	Not provided	
Image detector	GATAN K2 (4k x 4k)	Depositor
Maximum map value	0.189	Depositor
Minimum map value	-0.087	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0203	Depositor
Map size (\AA)	475.2, 475.2, 475.2	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.32, 1.32, 1.32	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ADP, GDP, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.35	0/16654	0.57	0/22571
2	B	0.33	0/7357	0.57	0/9980
3	C	0.32	0/2463	0.72	1/3829 (0.0%)
4	D	0.29	0/772	0.56	0/1038
4	Z	0.29	0/648	0.54	0/871
5	E	0.30	0/741	0.54	0/998
5	b	0.32	0/584	0.55	0/785
6	F	0.27	0/654	0.50	0/885
6	f	0.27	0/654	0.50	0/885
7	G	0.27	0/760	0.46	0/1016
7	l	0.27	0/705	0.47	0/945
8	H	0.28	0/630	0.47	0/851
8	m	0.28	0/630	0.47	0/851
9	I	0.28	0/579	0.50	0/785
9	n	0.28	0/579	0.50	0/785
10	J	0.27	0/578	0.51	0/774
10	o	0.27	0/578	0.51	0/774
11	K	0.39	0/2539	0.67	2/3453 (0.1%)
12	L	0.30	0/2317	0.56	0/3130
13	M	0.33	0/1698	0.54	0/2295
14	N	0.22	0/2160	0.68	0/3365
15	O	0.19	0/189	0.65	0/292
16	Q	0.18	0/300	0.63	0/463
17	P	0.92	22/2580 (0.9%)	1.48	66/4000 (1.6%)
18	S	0.30	0/1069	0.48	0/1449
18	T	0.29	0/1086	0.51	0/1472
18	U	1.33	36/2888 (1.2%)	0.78	4/3898 (0.1%)
18	V	0.30	0/1053	0.48	0/1429
19	W	0.30	0/2300	0.50	1/3087 (0.0%)
20	Y	0.44	5/1934 (0.3%)	0.69	7/2609 (0.3%)
21	a	0.57	5/1479 (0.3%)	0.60	2/1980 (0.1%)
22	c	0.31	0/2486	0.52	1/3360 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
23	d	0.30	0/1214	0.47	0/1646
24	e	0.33	0/1199	0.60	0/1609
25	g	0.47	2/1033 (0.2%)	0.65	6/1412 (0.4%)
26	h	0.33	0/767	0.55	0/1028
27	i	0.30	0/1231	0.44	0/1657
28	R	0.31	0/2243	0.52	0/3016
29	r	0.42	0/1161	0.57	1/1565 (0.1%)
30	X	0.32	0/9957	0.53	0/13430
31	j	1.67	12/1118 (1.1%)	1.71	18/1513 (1.2%)
32	k	0.81	2/624 (0.3%)	1.36	5/838 (0.6%)
All	All	0.48	84/82191 (0.1%)	0.67	114/112619 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
11	K	0	2
20	Y	0	3
33	x	0	12
All	All	0	22

The worst 5 of 84 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	j	118	SER	CB-OG	31.06	1.82	1.42
18	U	318	CYS	CB-SG	-19.87	1.48	1.82
18	U	227	CYS	CB-SG	-19.43	1.49	1.82
31	j	70	CYS	CB-SG	-17.93	1.51	1.82
31	j	111	CYS	CB-SG	-17.52	1.52	1.82

The worst 5 of 114 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	Y	57	ARG	C-N-CD	-16.30	84.75	120.60
31	j	54	ARG	NE-CZ-NH1	14.95	127.77	120.30
31	j	54	ARG	CD-NE-CZ	13.77	142.87	123.60
17	P	167	U	C5-C4-O4	11.99	133.10	125.90
31	j	54	ARG	NE-CZ-NH2	-11.81	114.40	120.30

There are no chirality outliers.

5 of 22 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1191	THR	Peptide
1	A	1440	ILE	Peptide
1	A	187	PHE	Peptide
1	A	457	HIS	Peptide
1	A	964	LYS	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1956/2363 (83%)	1657 (85%)	220 (11%)	79 (4%)	3	26
2	B	902/984 (92%)	783 (87%)	97 (11%)	22 (2%)	6	37
4	D	94/97 (97%)	80 (85%)	8 (8%)	6 (6%)	1	17
4	Z	78/97 (80%)	71 (91%)	6 (8%)	1 (1%)	12	50
5	E	92/147 (63%)	81 (88%)	9 (10%)	2 (2%)	6	39
5	b	70/147 (48%)	67 (96%)	3 (4%)	0	100	100
6	F	80/117 (68%)	72 (90%)	6 (8%)	2 (2%)	5	36
6	f	80/117 (68%)	72 (90%)	6 (8%)	2 (2%)	5	36
7	G	91/115 (79%)	88 (97%)	3 (3%)	0	100	100
7	l	83/115 (72%)	81 (98%)	2 (2%)	0	100	100
8	H	74/84 (88%)	69 (93%)	5 (7%)	0	100	100
8	m	74/84 (88%)	69 (93%)	5 (7%)	0	100	100
9	I	70/78 (90%)	64 (91%)	4 (6%)	2 (3%)	4	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	n	70/78 (90%)	65 (93%)	3 (4%)	2 (3%)	4	33
10	J	71/77 (92%)	66 (93%)	5 (7%)	0	100	100
10	o	71/77 (92%)	66 (93%)	5 (7%)	0	100	100
11	K	320/473 (68%)	246 (77%)	50 (16%)	24 (8%)	1	12
12	L	285/340 (84%)	239 (84%)	41 (14%)	5 (2%)	8	43
13	M	203/557 (36%)	172 (85%)	22 (11%)	9 (4%)	2	23
18	S	130/488 (27%)	122 (94%)	7 (5%)	1 (1%)	19	59
18	T	132/488 (27%)	123 (93%)	8 (6%)	1 (1%)	19	59
18	U	414/488 (85%)	383 (92%)	20 (5%)	11 (3%)	5	35
18	V	129/488 (26%)	121 (94%)	4 (3%)	4 (3%)	4	32
19	W	266/757 (35%)	244 (92%)	13 (5%)	9 (3%)	3	31
20	Y	234/388 (60%)	200 (86%)	24 (10%)	10 (4%)	2	24
21	a	189/354 (53%)	167 (88%)	18 (10%)	4 (2%)	7	40
22	c	298/639 (47%)	254 (85%)	31 (10%)	13 (4%)	2	23
23	d	153/155 (99%)	137 (90%)	13 (8%)	3 (2%)	7	41
24	e	142/146 (97%)	120 (84%)	17 (12%)	5 (4%)	3	30
25	g	146/558 (26%)	123 (84%)	15 (10%)	8 (6%)	2	19
26	h	86/265 (32%)	75 (87%)	7 (8%)	4 (5%)	2	22
27	i	157/187 (84%)	144 (92%)	10 (6%)	3 (2%)	8	42
28	R	248/674 (37%)	219 (88%)	20 (8%)	9 (4%)	3	29
29	r	130/790 (16%)	120 (92%)	6 (5%)	4 (3%)	4	32
30	X	1143/1284 (89%)	1032 (90%)	87 (8%)	24 (2%)	7	40
31	j	156/239 (65%)	140 (90%)	14 (9%)	2 (1%)	12	50
32	k	87/111 (78%)	85 (98%)	2 (2%)	0	100	100
All	All	9004/14646 (62%)	7917 (88%)	816 (9%)	271 (3%)	7	33

5 of 271 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	67	GLY
1	A	68	VAL
1	A	155	ARG
1	A	188	PRO
1	A	232	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1775/2138 (83%)	1565 (88%)	210 (12%)	5	28
2	B	809/881 (92%)	758 (94%)	51 (6%)	18	53
4	D	85/86 (99%)	77 (91%)	8 (9%)	8	38
4	Z	72/86 (84%)	64 (89%)	8 (11%)	6	31
5	E	80/118 (68%)	75 (94%)	5 (6%)	18	53
5	b	66/118 (56%)	60 (91%)	6 (9%)	9	39
6	F	77/102 (76%)	70 (91%)	7 (9%)	9	39
6	f	77/102 (76%)	70 (91%)	7 (9%)	9	39
7	G	81/101 (80%)	79 (98%)	2 (2%)	47	75
7	l	76/101 (75%)	75 (99%)	1 (1%)	69	86
8	H	69/76 (91%)	64 (93%)	5 (7%)	14	47
8	m	69/76 (91%)	64 (93%)	5 (7%)	14	47
9	I	64/69 (93%)	60 (94%)	4 (6%)	18	53
9	n	64/69 (93%)	60 (94%)	4 (6%)	18	53
10	J	63/67 (94%)	57 (90%)	6 (10%)	8	37
10	o	63/67 (94%)	57 (90%)	6 (10%)	8	37
11	K	261/278 (94%)	239 (92%)	22 (8%)	11	42
12	L	251/292 (86%)	234 (93%)	17 (7%)	16	50
13	M	182/477 (38%)	160 (88%)	22 (12%)	5	26
18	S	120/443 (27%)	110 (92%)	10 (8%)	11	42
18	T	123/443 (28%)	112 (91%)	11 (9%)	9	40
18	U	223/443 (50%)	206 (92%)	17 (8%)	13	45
18	V	118/443 (27%)	111 (94%)	7 (6%)	19	55
19	W	234/294 (80%)	213 (91%)	21 (9%)	9	39
20	Y	194/253 (77%)	158 (81%)	36 (19%)	1	10
21	a	142/222 (64%)	123 (87%)	19 (13%)	4	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	c	259/579 (45%)	224 (86%)	35 (14%)	4	23
23	d	129/129 (100%)	125 (97%)	4 (3%)	40	71
24	e	130/132 (98%)	123 (95%)	7 (5%)	22	57
25	g	78/496 (16%)	62 (80%)	16 (20%)	1	7
26	h	79/240 (33%)	70 (89%)	9 (11%)	5	29
27	i	118/163 (72%)	108 (92%)	10 (8%)	10	41
28	R	224/224 (100%)	192 (86%)	32 (14%)	3	21
29	r	117/136 (86%)	107 (92%)	10 (8%)	10	41
30	X	1106/1188 (93%)	1100 (100%)	6 (0%)	88	95
31	j	87/214 (41%)	83 (95%)	4 (5%)	27	61
32	k	49/96 (51%)	46 (94%)	3 (6%)	18	53
All	All	7814/11442 (68%)	7161 (92%)	653 (8%)	14	42

5 of 653 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
21	a	38	GLU
28	R	136	ARG
21	a	237	PRO
21	a	27	LEU
24	e	17	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 137 such sidechains are listed below:

Mol	Chain	Res	Type
30	X	605	GLN
30	X	983	ASN
7	l	34	GLN
5	E	36	ASN
4	D	65	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	N	89/99 (89%)	53 (59%)	12 (13%)
15	O	8/8 (100%)	3 (37%)	1 (12%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
16	Q	12/13 (92%)	4 (33%)	2 (16%)
17	P	106/186 (56%)	28 (26%)	8 (7%)
3	C	104/120 (86%)	54 (51%)	13 (12%)
All	All	319/426 (74%)	142 (44%)	36 (11%)

5 of 142 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	C	9	U
3	C	14	G
3	C	18	U
3	C	19	U
3	C	20	U

5 of 36 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
17	P	14	C
17	P	168	A
17	P	17	U
17	P	104	G
3	C	100	U

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	$\# Z > 2$
34	GDP	B	1000	-	24,30,30	1.02	1 (4%)	30,47,47	1.12	3 (10%)
37	ADP	X	1500	-	24,29,29	0.96	1 (4%)	29,45,45	1.50	4 (13%)

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
34	GDP	B	1000	-	-	5/12/32/32	0/3/3/3
37	ADP	X	1500	-	-	6/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	X	1500	ADP	C5-C4	2.51	1.47	1.40
34	B	1000	GDP	C6-N1	-2.49	1.34	1.37

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	X	1500	ADP	PA-O3A-PB	-3.59	120.52	132.83
37	X	1500	ADP	C3'-C2'-C1'	3.50	106.25	100.98
37	X	1500	ADP	N3-C2-N1	-3.14	123.77	128.68
37	X	1500	ADP	C4-C5-N7	-2.70	106.59	109.40
34	B	1000	GDP	O6-C6-C5	-2.36	119.77	124.37

There are no chirality outliers.

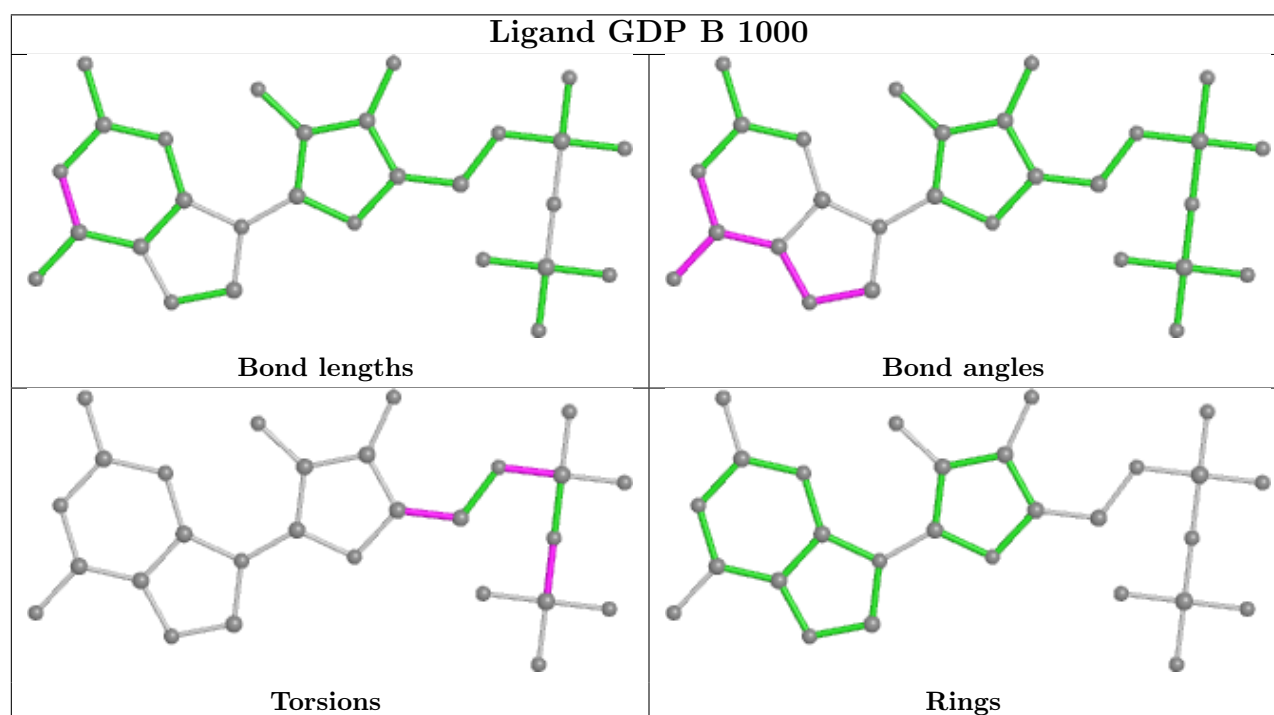
5 of 11 torsion outliers are listed below:

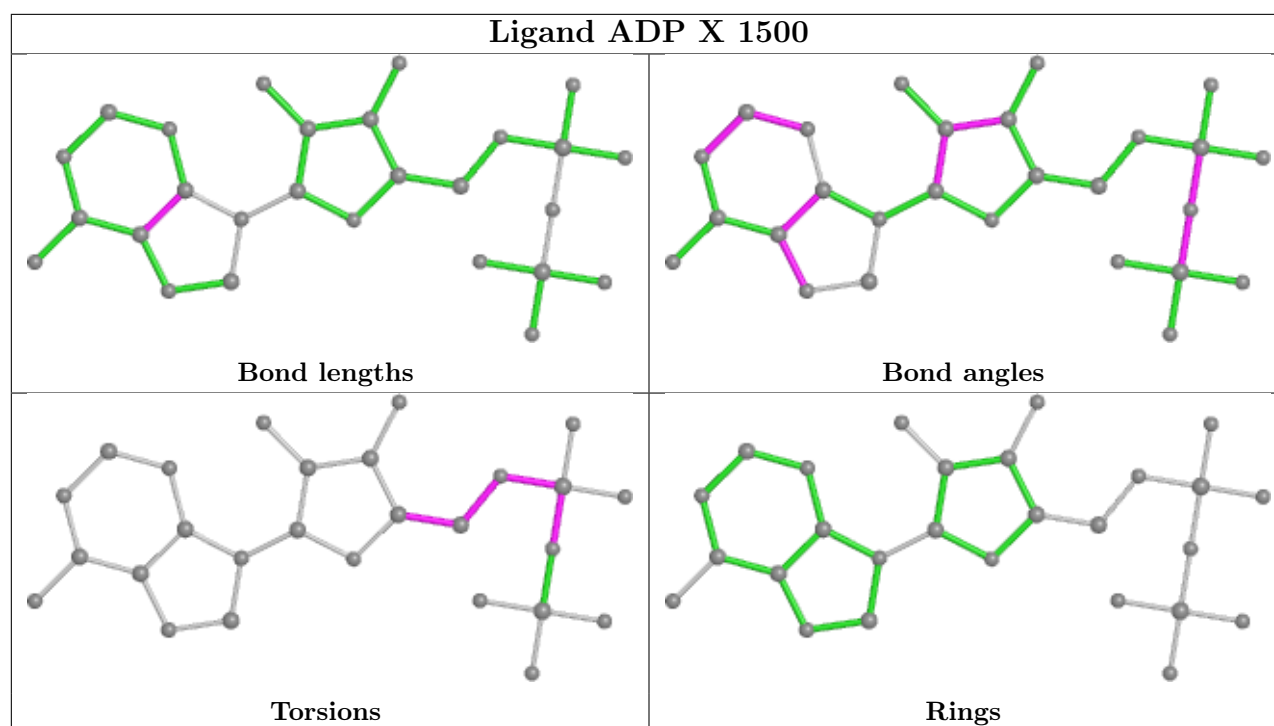
Mol	Chain	Res	Type	Atoms
34	B	1000	GDP	C5'-O5'-PA-O3A
34	B	1000	GDP	C3'-C4'-C5'-O5'
37	X	1500	ADP	C5'-O5'-PA-O3A
37	X	1500	ADP	C4'-C5'-O5'-PA
34	B	1000	GDP	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

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.

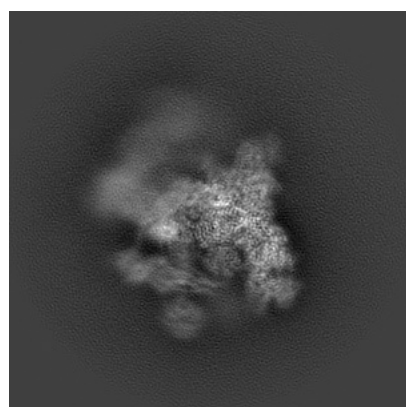
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6413. These allow visual inspection of the internal detail of the map and identification of artifacts.

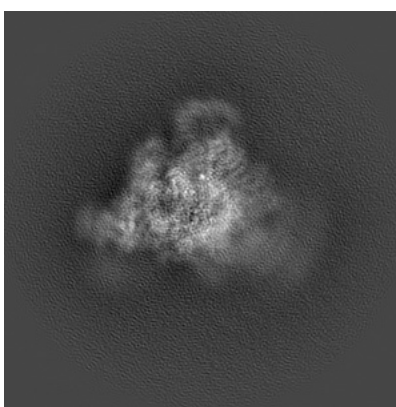
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

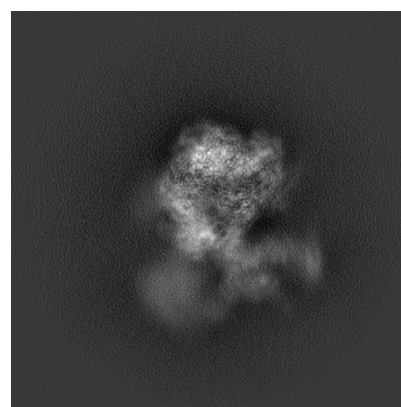
6.1.1 Primary map



X



Y

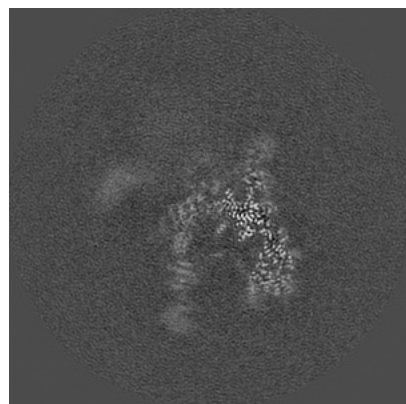


Z

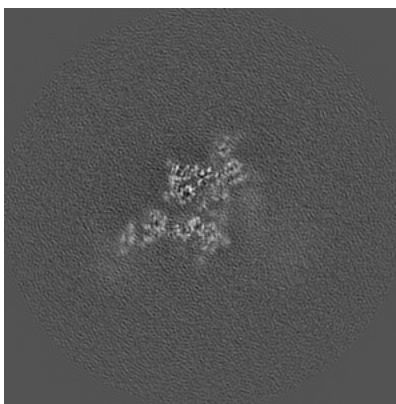
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

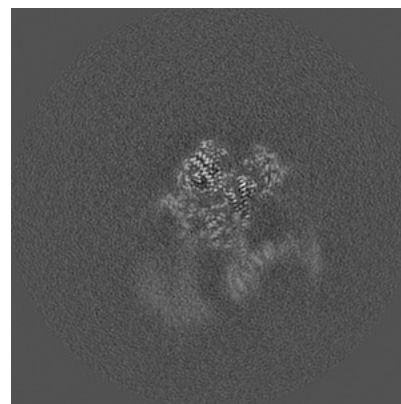
6.2.1 Primary map



X Index: 180



Y Index: 180

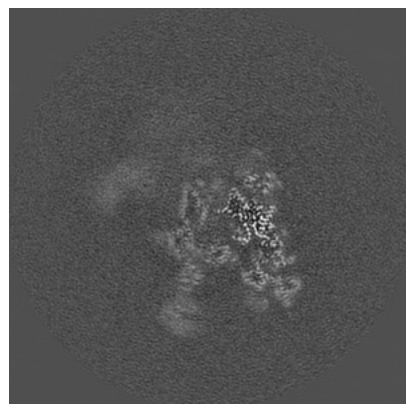


Z Index: 180

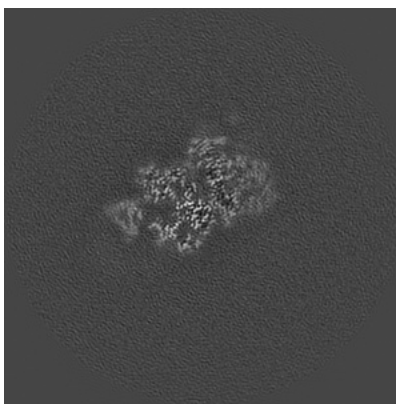
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

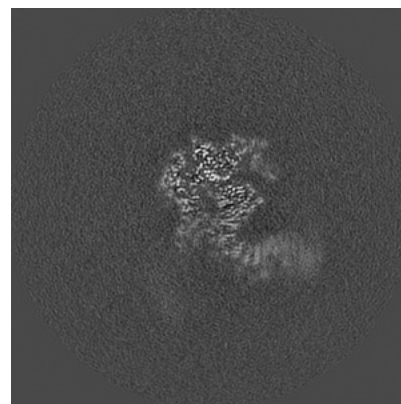
6.3.1 Primary map



X Index: 174



Y Index: 217

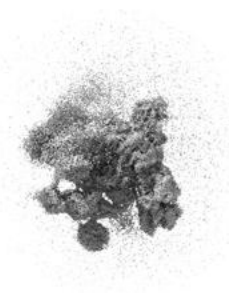


Z Index: 165

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0203. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

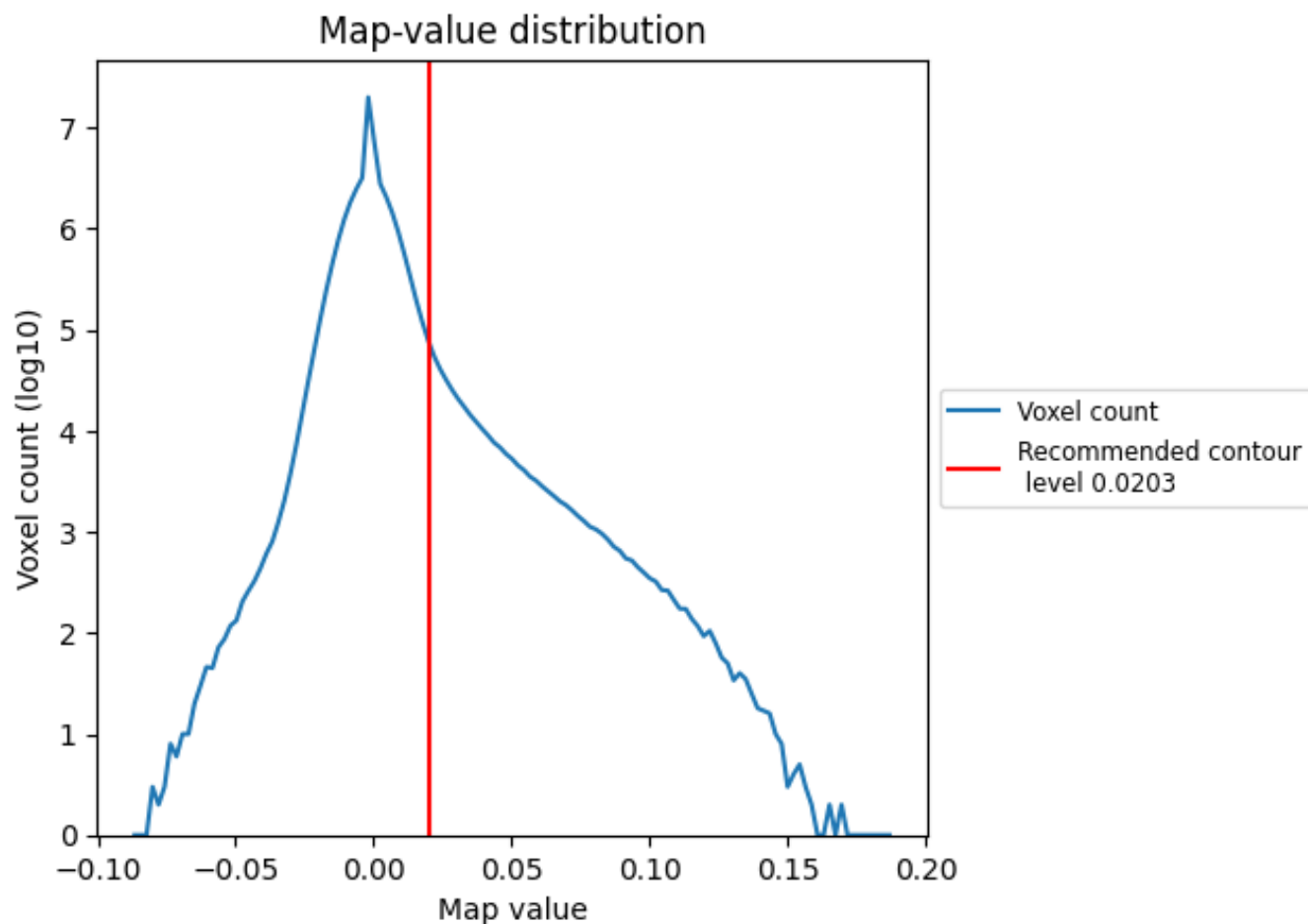
6.5 Mask visualisation

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

7 Map analysis [i](#)

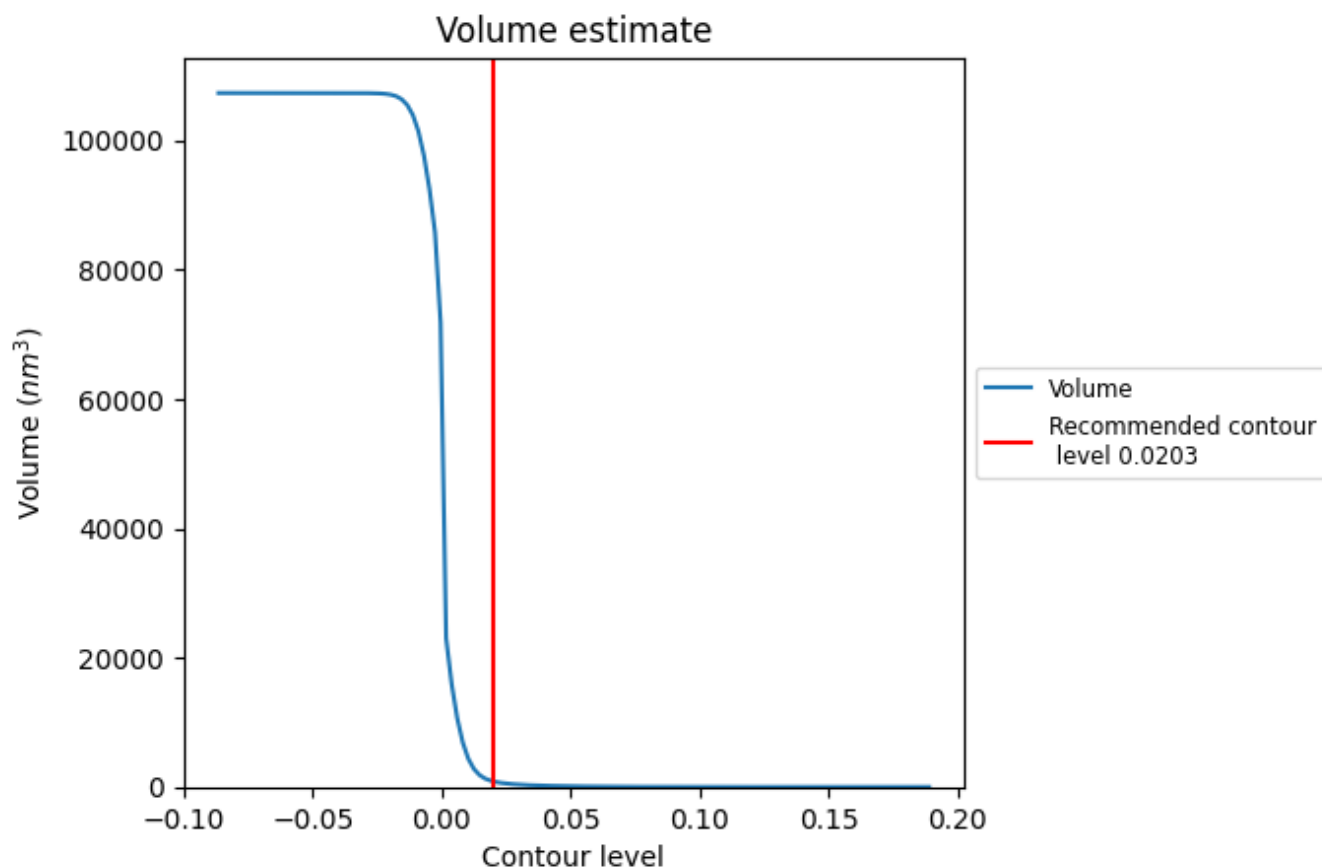
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

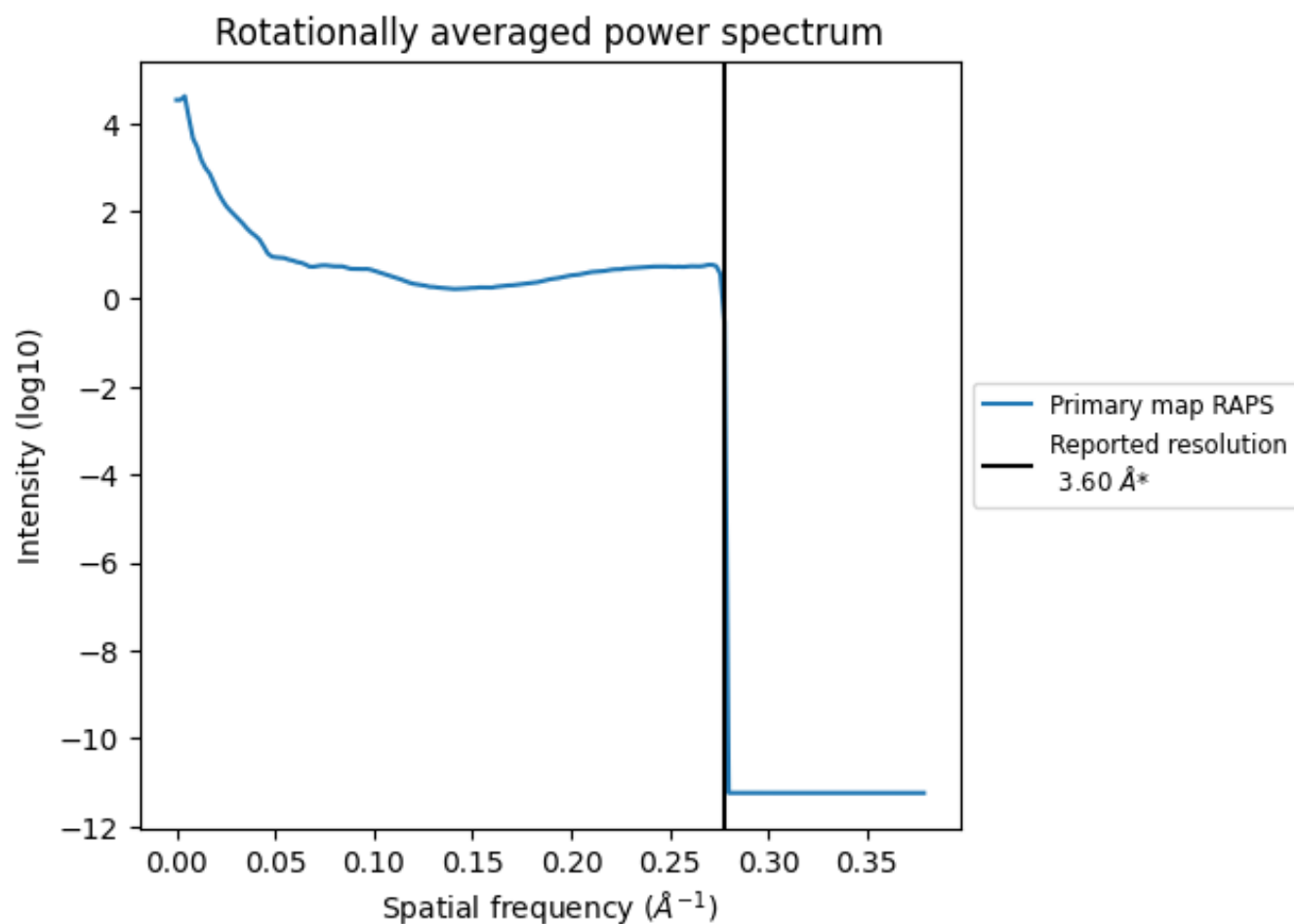
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 836 nm^3 ; this corresponds to an approximate mass of 755 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 0.278 \AA^{-1}

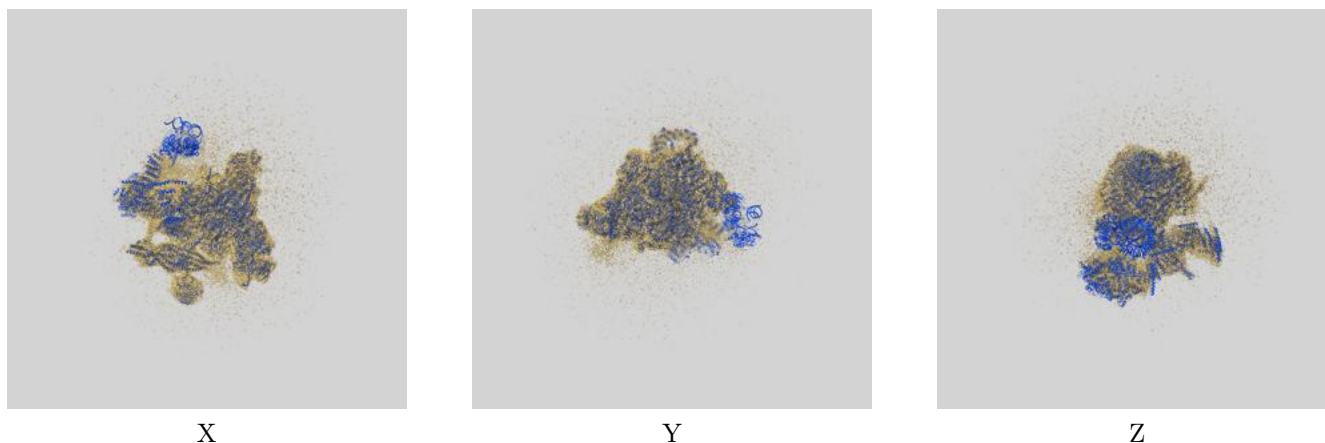
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

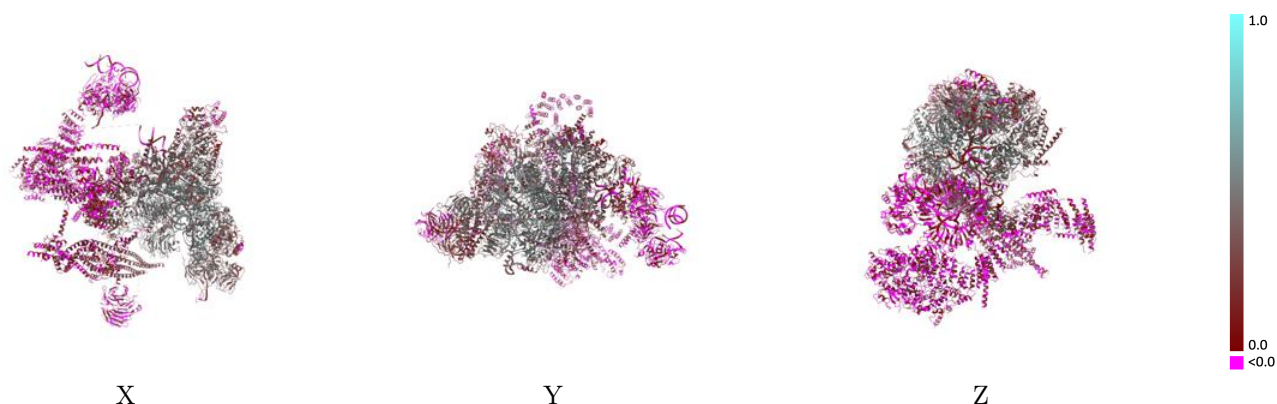
This section contains information regarding the fit between EMDB map EMD-6413 and PDB model 3JB9. Per-residue inclusion information can be found in [section 3](#) on [page 12](#).

9.1 Map-model overlay [i](#)



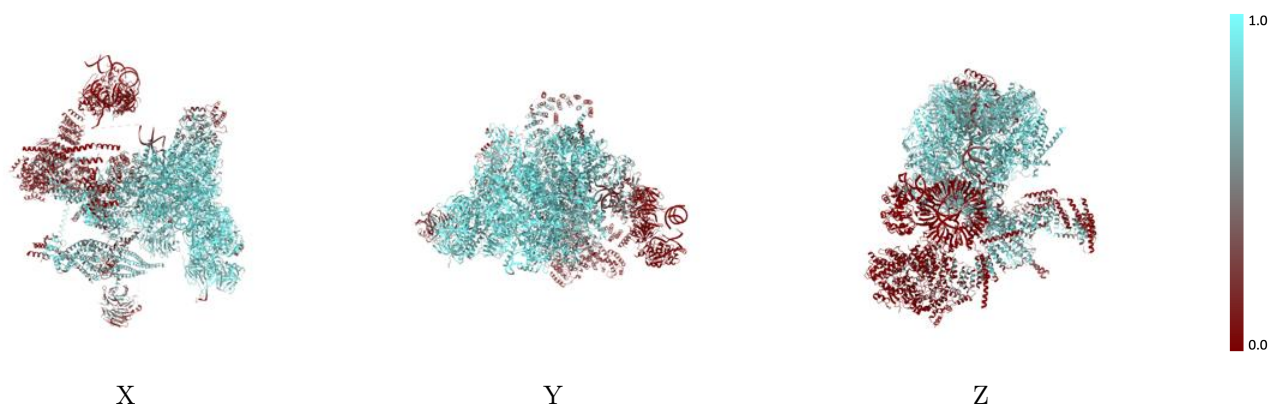
The images above show the 3D surface view of the map at the recommended contour level 0.0203 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



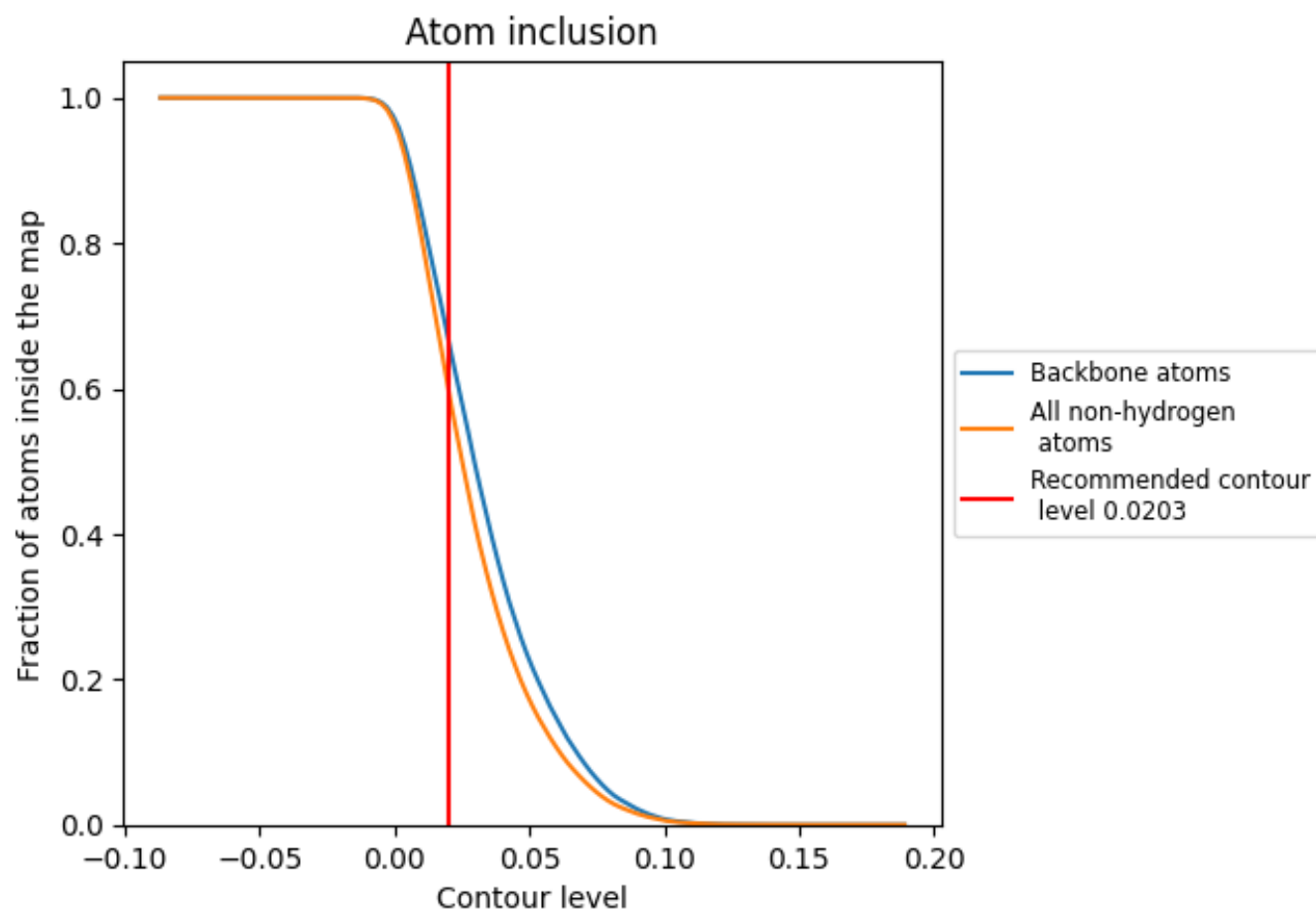
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0203).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 59% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ



















The table lists the average atom inclusion at the recommended contour level (0.0203) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5928	 0.2520
A	 0.8041	 0.4010
B	 0.8677	 0.4180
C	 0.9294	 0.4420
D	 0.8886	 0.4500
E	 0.8480	 0.3960
F	 0.7736	 0.3100
G	 0.7333	 0.2220
H	 0.8069	 0.3130
I	 0.7740	 0.2540
J	 0.8221	 0.3800
K	 0.8765	 0.4390
L	 0.8577	 0.4210
M	 0.7384	 0.3490
N	 0.8106	 0.3390
O	 0.7118	 0.2310
P	 0.1830	 0.0590
Q	 0.2222	 0.0640
R	 0.6467	 0.2420
S	 0.5141	 0.1110
T	 0.6351	 0.1600
U	 0.3927	 0.0610
V	 0.5483	 0.1070
W	 0.6940	 0.2420
X	 0.0763	 0.0030
Y	 0.7698	 0.2860
Z	 0.0080	 0.0210
a	 0.6502	 0.2880
b	 0.0053	 0.0380
c	 0.6499	 0.3140
d	 0.7451	 0.3010
e	 0.8977	 0.4560
f	 0.0031	 0.0210
g	 0.7292	 0.3180
h	 0.7500	 0.4070



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Chain	Atom inclusion	Q-score
i	 0.6583	 0.1600
j	 0.0037	 -0.0160
k	 0.0049	 0.0040
l	 0.0029	 -0.0040
m	 0.0000	 -0.0030
n	 0.0018	 -0.0110
o	 0.0036	 -0.0400
r	 0.4199	 0.0610
x	 0.4110	 0.0850