



wwPDB EM Validation Summary Report ⓘ

Mar 20, 2026 – 10:28 AM UTC

PDB ID : 8H6J / pdb_00008h6j
EMDB ID : EMD-34505
Title : Cryo-EM structure of human exon-defined spliceosome in the mature pre-B state.
Authors : Zhang, W.; Zhan, X.; Zhang, X.; Lei, J.; Yan, C.; Shi, Y.
Deposited on : 2022-10-18
Resolution : 3.25 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:

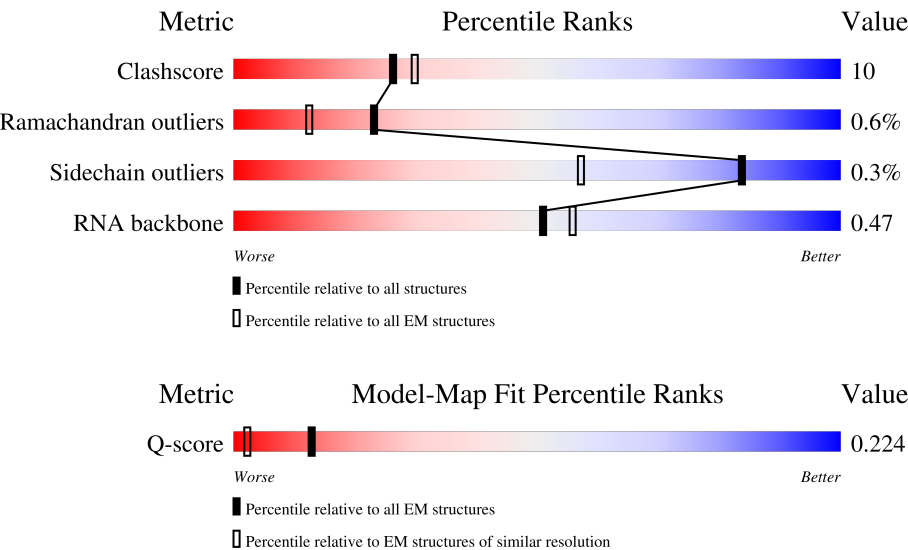
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.25 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14599 (2.75 - 3.75)

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	144	29% 8% 15% 71%
2	6A	107	21% 32% 10% 7% 50%
3	6a	95	94% 87% 5% 6%

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Mol	Chain	Length	Quality of chain
4	6b	102	
5	6c	139	
6	6d	91	
7	6e	80	
8	6f	103	
9	6g	96	
10	5A	117	
11	5B	2335	
12	5C	972	
13	5D	2136	
14	5E	357	
15	2a	231	
15	4a	231	
15	5a	231	
16	2b	119	
16	4b	119	
16	5b	119	
17	2c	118	
17	4c	118	
17	5c	118	
18	2d	86	
18	4d	86	
18	5d	86	
19	2e	92	
19	4e	92	

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Mol	Chain	Length	Quality of chain
19	5e	92	
20	2f	76	
20	4f	76	
20	5f	76	
21	2g	126	
21	4g	126	
21	5g	126	
22	4A	144	
23	4B	683	
24	4C	522	
25	4D	499	
26	4E	128	
27	4F	142	
28	4G	941	
29	4R	480	
30	4S	800	
31	4T	565	
32	4U	820	
33	4X	155	
34	4Y	1007	
35	2A	188	
36	2B	255	
37	2C	225	
38	2D	793	
39	2E	464	

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Mol	Chain	Length	Quality of chain
40	2F	501	84% 5% 16%
41	2G	1304	80% 50% 28% 20%
42	2H	895	20% 18% 80%
43	2I	1217	96% 83% 13%
44	2J	424	18% 17% 82%
45	2K	125	86% 74% 12% 14%
46	2L	110	81% 73% 8% 19%
47	2M	86	77% 52% 23% 23%

2 Entry composition

There are 51 unique types of molecules in this entry. The entry contains 96473 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	A	42	Total	C	N	O	P	0	0
			864	387	124	311	42		

- Molecule 2 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	6A	54	Total	C	N	O	P	0	0
			1142	509	206	373	54		

- Molecule 3 is a protein called U6 snRNA-associated Sm-like protein LSm2.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	6a	89	Total	C	N	O	0	0
			356	178	89	89		

- Molecule 4 is a protein called U6 snRNA-associated Sm-like protein LSm3.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	6b	74	Total	C	N	O	0	0
			296	148	74	74		

- Molecule 5 is a protein called U6 snRNA-associated Sm-like protein LSm4.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	6c	74	Total	C	N	O	0	0
			296	148	74	74		

- Molecule 6 is a protein called U6 snRNA-associated Sm-like protein LSm5.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	6d	72	Total	C	N	O	0	0
			288	144	72	72		

- Molecule 7 is a protein called U6 snRNA-associated Sm-like protein LSm6.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	6e	70	Total	C	N	O	0	0
			280	140	70	70		

- Molecule 8 is a protein called U6 snRNA-associated Sm-like protein LSm7.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	6f	65	Total	C	N	O	0	0
			260	130	65	65		

- Molecule 9 is a protein called U6 snRNA-associated Sm-like protein LSm8.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	6g	61	Total	C	N	O	0	0
			244	122	61	61		

- Molecule 10 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	5A	114	Total	C	N	O	P	0	0
			2398	1074	398	812	114		

- Molecule 11 is a protein called Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	5B	2209	Total	C	N	O	S	0	0
			18244	11760	3170	3235	79		

- Molecule 12 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	5C	852	Total	C	N	O	S	0	0
			6727	4300	1127	1266	34		

- Molecule 13 is a protein called U5 small nuclear ribonucleoprotein 200 kDa helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	5D	2001	Total	C	N	O	S	0	0
			16077	10235	2767	2991	84		

- Molecule 14 is a protein called U5 small nuclear ribonucleoprotein 40 kDa protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	5E	301	Total	C	N	O	0	0
			1481	879	301	301		

- Molecule 15 is a protein called Isoform SM-B of Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	5a	86	Total	C	N	O	0	0
			344	172	86	86		
15	4a	82	Total	C	N	O	0	0
			405	241	82	82		
15	2a	85	Total	C	N	O	0	0
			340	170	85	85		

- Molecule 16 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	5b	82	Total	C	N	O	0	0
			328	164	82	82		
16	4b	81	Total	C	N	O	0	0
			401	239	81	81		
16	2b	82	Total	C	N	O	0	0
			328	164	82	82		

- Molecule 17 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	5c	97	Total	C	N	O	0	0
			388	194	97	97		
17	4c	92	Total	C	N	O	0	0
			455	271	92	92		
17	2c	85	Total	C	N	O	0	0
			340	170	85	85		

- Molecule 18 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	5d	73	Total	C	N	O	0	0
			292	146	73	73		
18	4d	72	Total	C	N	O	0	0
			351	207	72	72		
18	2d	74	Total	C	N	O	0	0
			296	148	74	74		

- Molecule 19 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	5e	79	Total	C	N	O	0	0
			316	158	79	79		
19	4e	76	Total	C	N	O	0	0
			376	224	76	76		
19	2e	79	Total	C	N	O	0	0
			316	158	79	79		

- Molecule 20 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	5f	74	Total	C	N	O	0	0
			296	148	74	74		
20	4f	74	Total	C	N	O	0	0
			363	215	74	74		
20	2f	66	Total	C	N	O	0	0
			264	132	66	66		

- Molecule 21 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	5g	77	Total	C	N	O	0	0
			308	154	77	77		
21	4g	83	Total	C	N	O	0	0
			409	243	83	83		
21	2g	80	Total	C	N	O	0	0
			320	160	80	80		

- Molecule 22 is a RNA chain called U4 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	4A	125	Total	C	N	O	P	0	0
			2656	1188	468	876	124		

- Molecule 23 is a protein called U4/U6 small nuclear ribonucleoprotein Prp3.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	4B	193	Total	C	N	O	0	0
			953	567	193	193		

- Molecule 24 is a protein called U4/U6 small nuclear ribonucleoprotein Prp4.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	4C	359	Total	C	N	O	0	0
			1765	1047	359	359		

- Molecule 25 is a protein called U4/U6 small nuclear ribonucleoprotein Prp31.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	4D	270	Total	C	N	O	0	0
			1340	800	270	270		

- Molecule 26 is a protein called NHP2-like protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	4E	124	Total	C	N	O	0	0
			615	367	124	124		

- Molecule 27 is a protein called Thioredoxin-like protein 4A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	4F	141	Total	C	N	O	S	0	0
			1169	751	194	214	10		

- Molecule 28 is a protein called Pre-mRNA-processing factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	4G	784	Total	C	N	O	S	0	0
			4539	2745	884	901	9		

- Molecule 29 is a protein called RNA-binding protein 42.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	4R	106	Total	C	N	O	S	0	0
			874	553	160	157	4		

- Molecule 30 is a protein called U4/U6.U5 tri-snRNP-associated protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	4S	61	Total	C	N	O	S	0	0
			505	317	94	91	3		

- Molecule 31 is a protein called U4/U6.U5 tri-snRNP-associated protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	4T	456	Total	C	N	O	S	0	0
			3749	2427	635	673	14		

- Molecule 32 is a protein called Probable ATP-dependent RNA helicase DDX23.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	4U	578	Total	C	N	O	S	1	0
			3414	2063	682	667	2		

- Molecule 33 is a protein called U4/U6.U5 small nuclear ribonucleoprotein 27 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	4X	21	Total	C	N	O	S	0	0
			184	115	40	28	1		

- Molecule 34 is a protein called Serine/threonine-protein kinase PRP4 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	4Y	322	Total	C	N	O		0	0
			1595	951	322	322			

- Molecule 35 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	2A	109	Total	C	N	O	P	0	0
			2311	1032	396	774	109		

- Molecule 36 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	2B	162	Total	C	N	O		0	0
			648	324	162	162			

- Molecule 37 is a protein called U2 small nuclear ribonucleoprotein B'.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	2C	94	Total	C	N	O		0	0
			376	188	94	94			

- Molecule 38 is a protein called Splicing factor 3A subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	2D	124	Total	C	N	O	0	0
			496	248	124	124		

- Molecule 39 is a protein called Splicing factor 3A subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	2E	94	Total	C	N	O	0	0
			376	188	94	94		

- Molecule 40 is a protein called Splicing factor 3A subunit 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	2F	423	Total	C	N	O	0	0
			1693	847	423	423		

- Molecule 41 is a protein called Splicing factor 3B subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	2G	1048	Total	C	N	O	0	0
			4192	2096	1048	1048		

- Molecule 42 is a protein called Splicing factor 3B subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	2H	182	Total	C	N	O	0	0
			728	364	182	182		

- Molecule 43 is a protein called Splicing factor 3B subunit 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	2I	1168	Total	C	N	O	0	0
			4672	2336	1168	1168		

- Molecule 44 is a protein called Splicing factor 3B subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	2J	78	Total	C	N	O	0	0
			312	156	78	78		

- Molecule 45 is a protein called Splicing factor 3B subunit 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	2K	108	Total	C	N	O	0	0
			432	216	108	108		

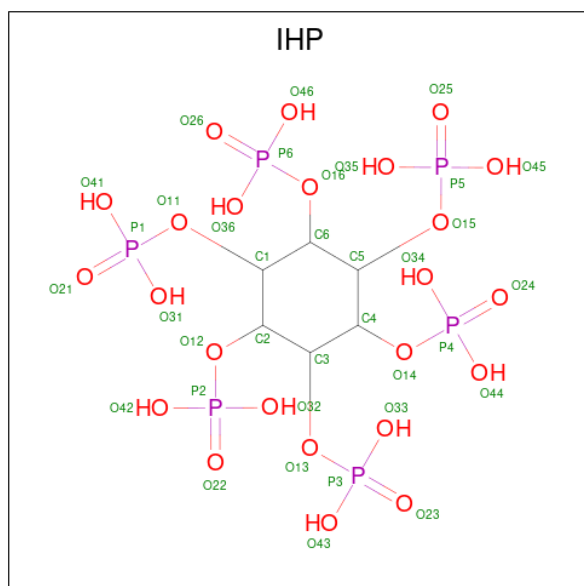
- Molecule 46 is a protein called PHD finger-like domain-containing protein 5A.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	2L	89	Total	C	N	O	0	0
			356	178	89	89		

- Molecule 47 is a protein called Splicing factor 3B subunit 5.

Mol	Chain	Residues	Atoms				AltConf	Trace
47	2M	66	Total	C	N	O	0	0
			264	132	66	66		

- Molecule 48 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: $C_6H_{18}O_{24}P_6$).

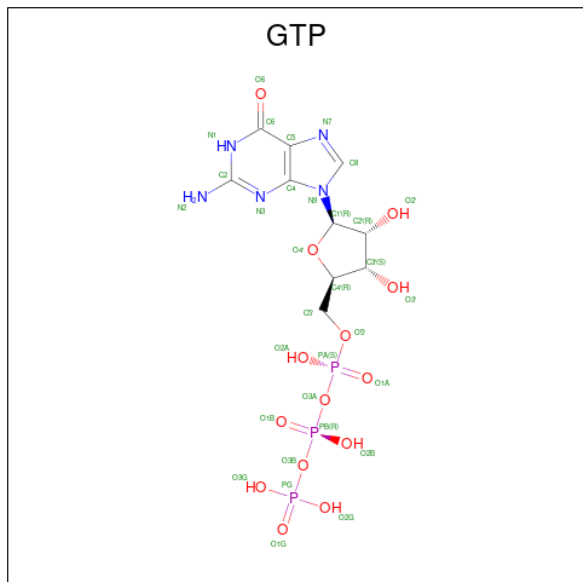


Mol	Chain	Residues	Atoms				AltConf
48	5B	1	Total	C	O	P	0
			36	6	24	6	

- Molecule 49 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
49	5C	1	Total	Mg	0
			1	1	

- Molecule 50 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
50	5C	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 51 is ZINC ION (CCD ID: ZN) (formula: Zn).

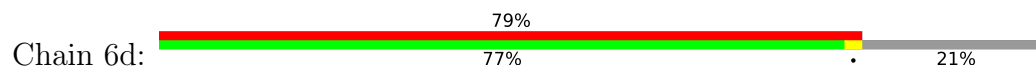
Mol	Chain	Residues	Atoms		AltConf
51	4T	1	Total	Zn	0
			1	1	



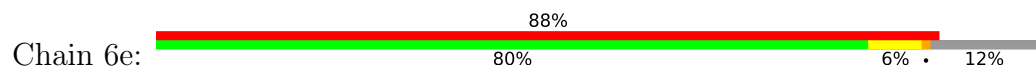
• Molecule 5: U6 snRNA-associated Sm-like protein LSm4



• Molecule 6: U6 snRNA-associated Sm-like protein LSm5

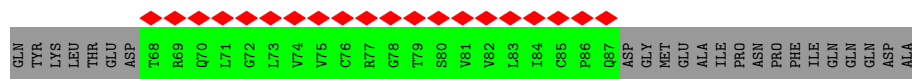


• Molecule 7: U6 snRNA-associated Sm-like protein LSm6

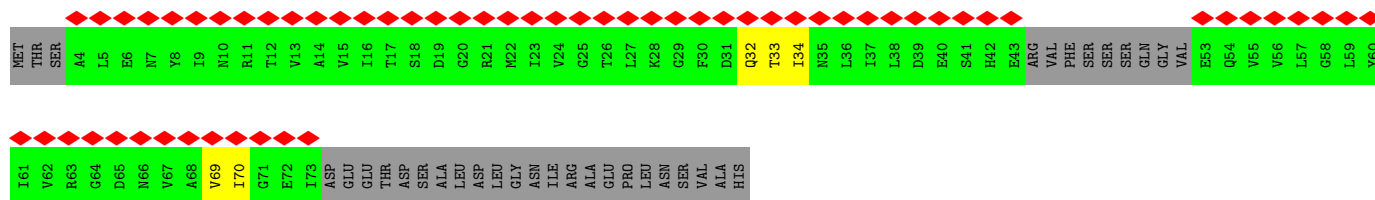


• Molecule 8: U6 snRNA-associated Sm-like protein LSm7

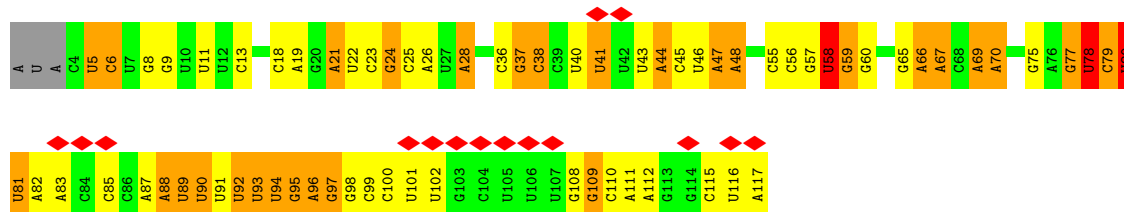




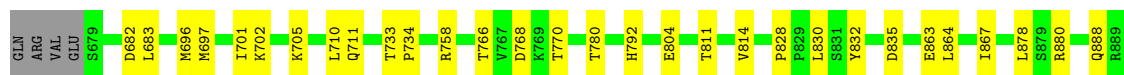
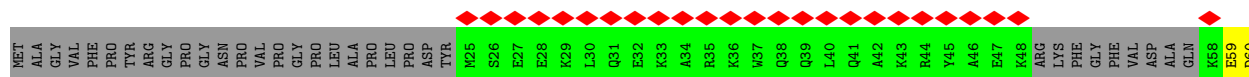
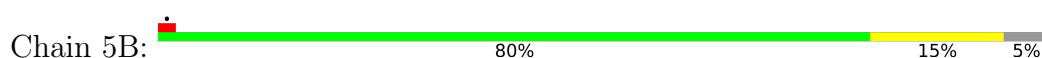
• Molecule 9: U6 snRNA-associated Sm-like protein LSm8

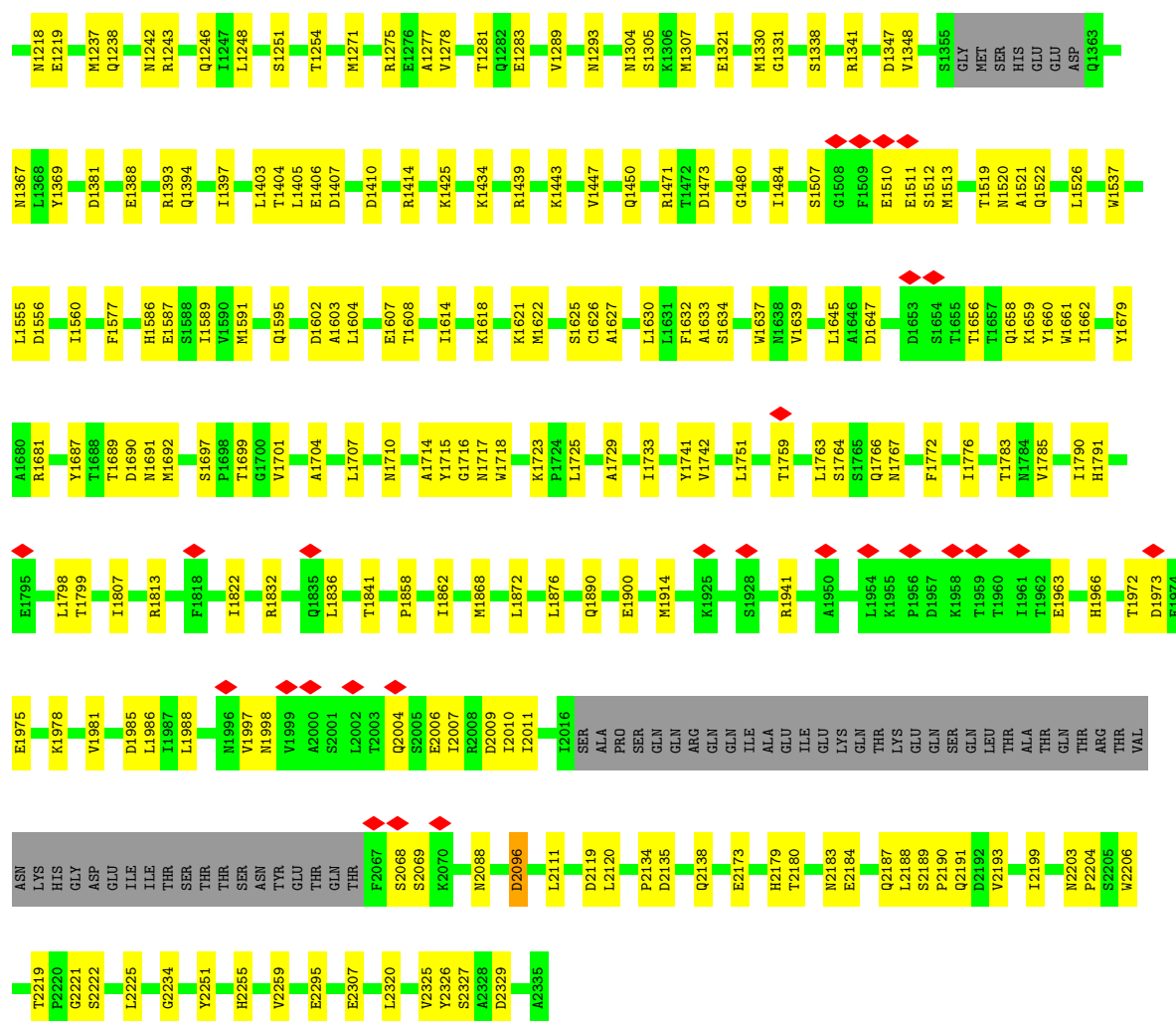


• Molecule 10: U5 snRNA

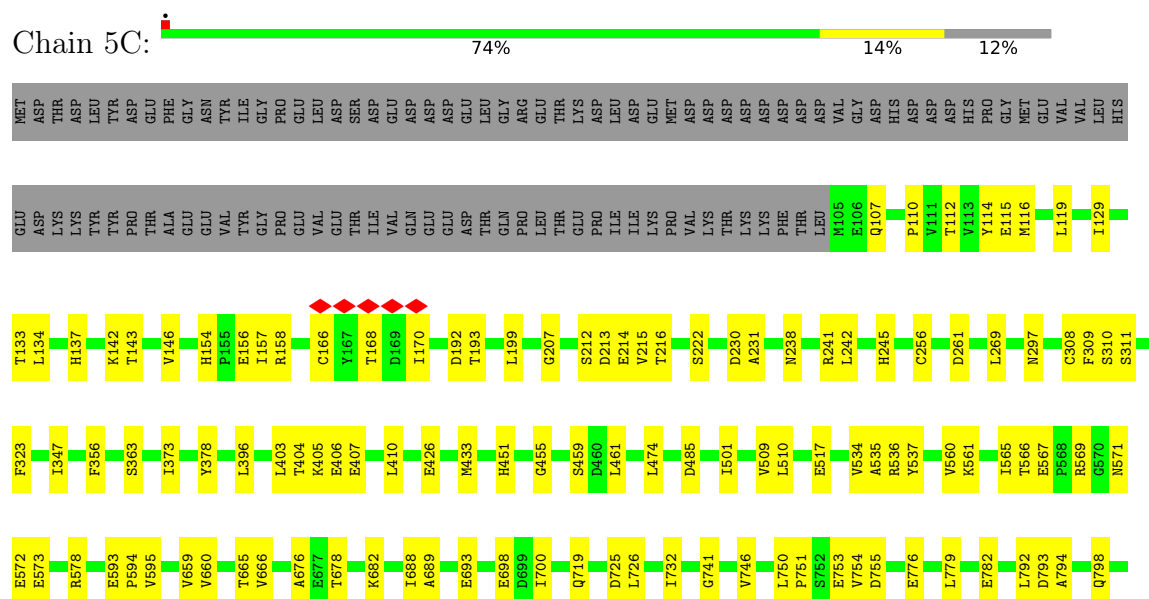


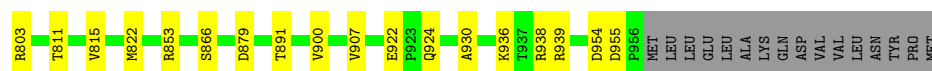
• Molecule 11: Pre-mRNA-processing-splicing factor 8



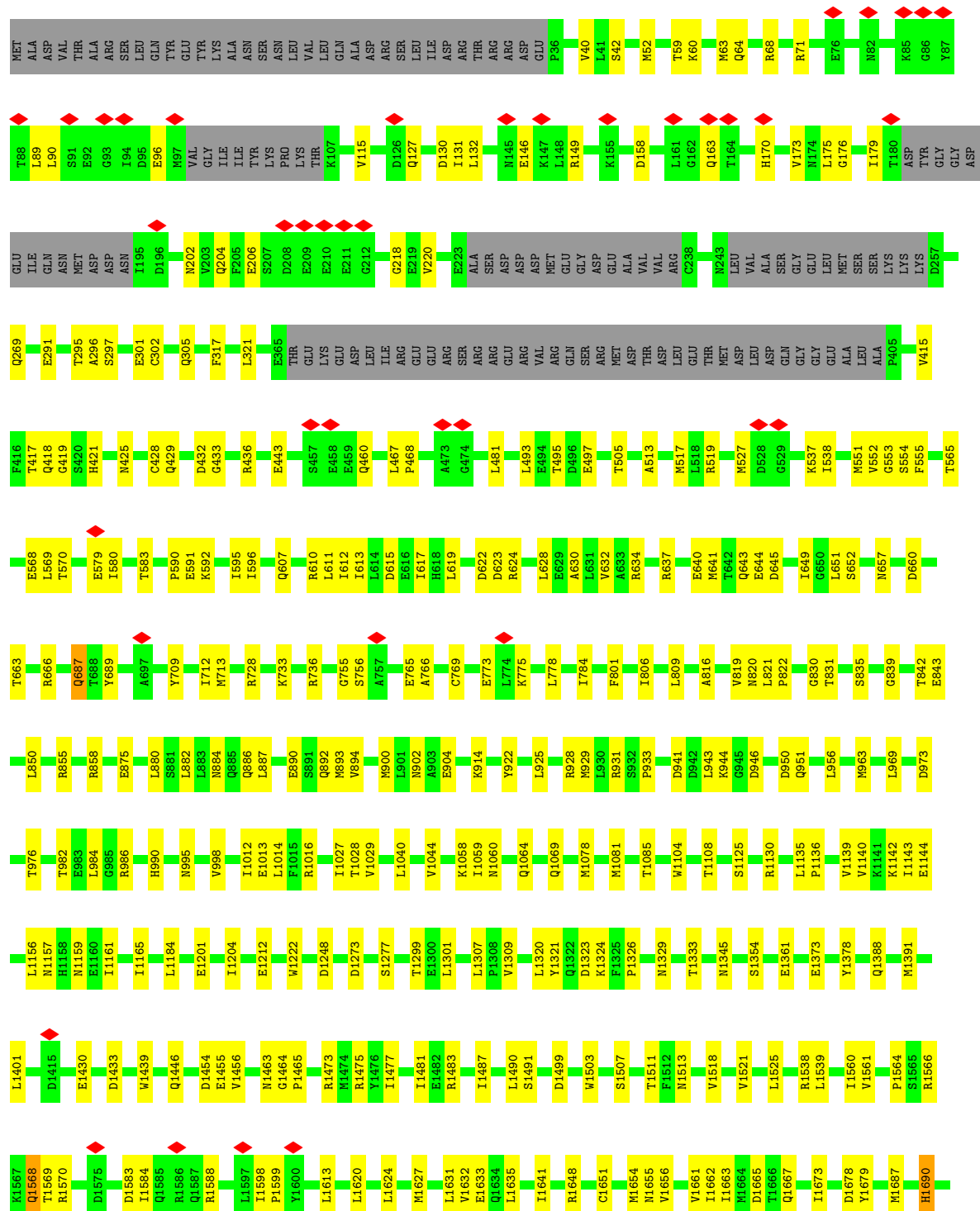
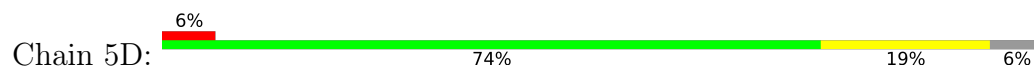


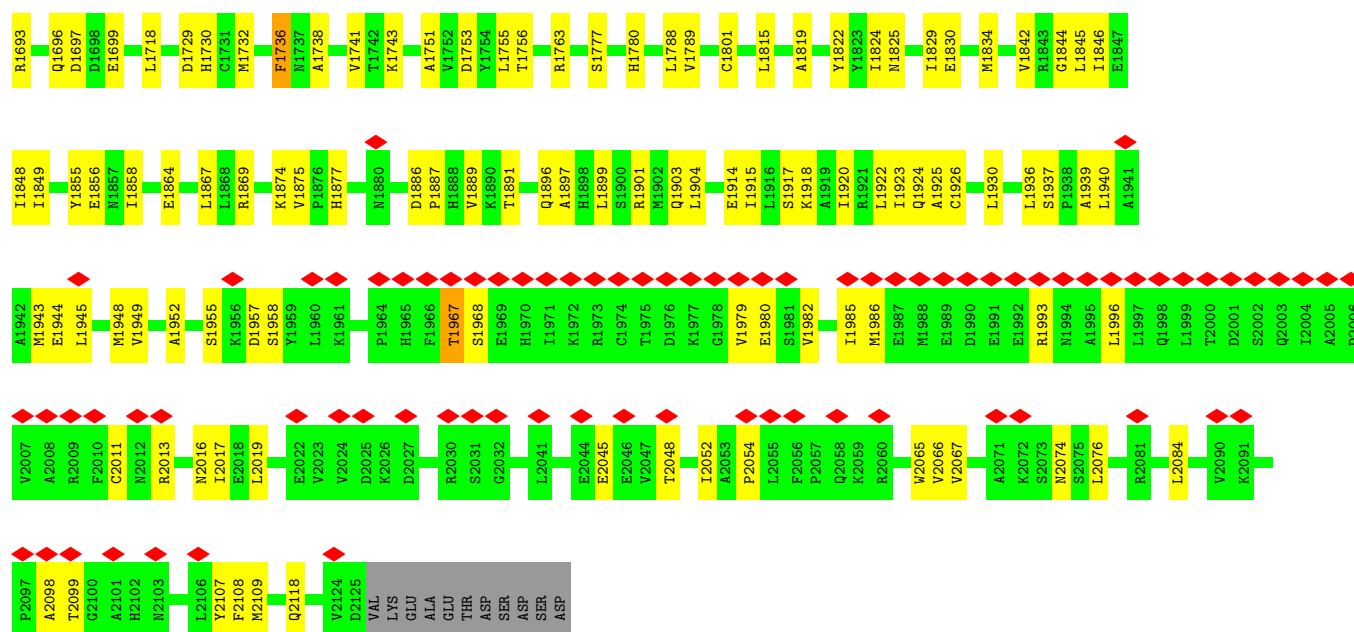
- Molecule 12: 116 kDa U5 small nuclear ribonucleoprotein component



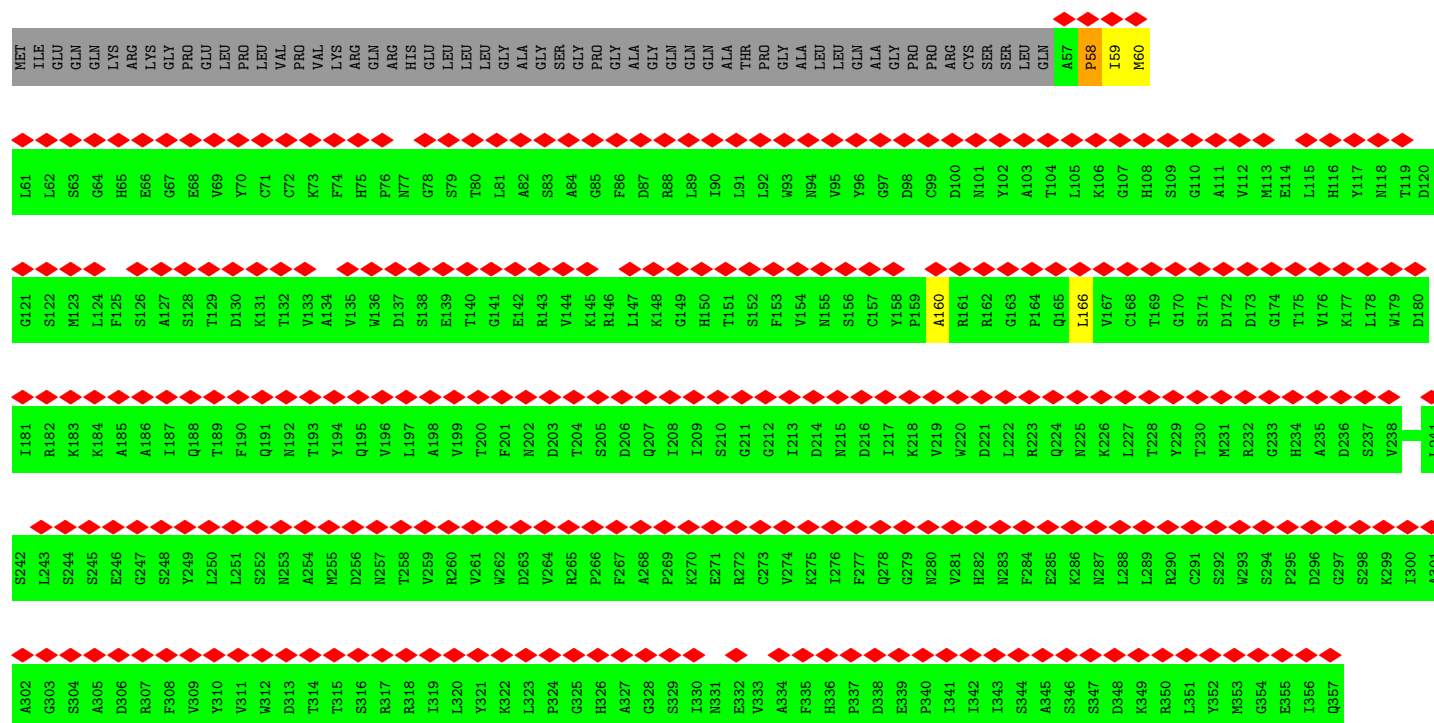
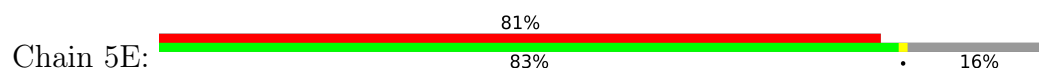


- Molecule 13: U5 small nuclear ribonucleoprotein 200 kDa helicase



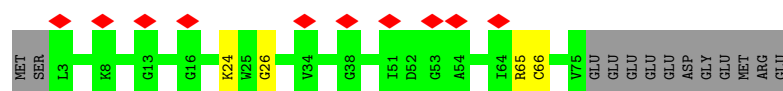
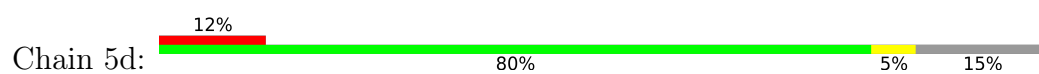


- Molecule 14: U5 small nuclear ribonucleoprotein 40 kDa protein

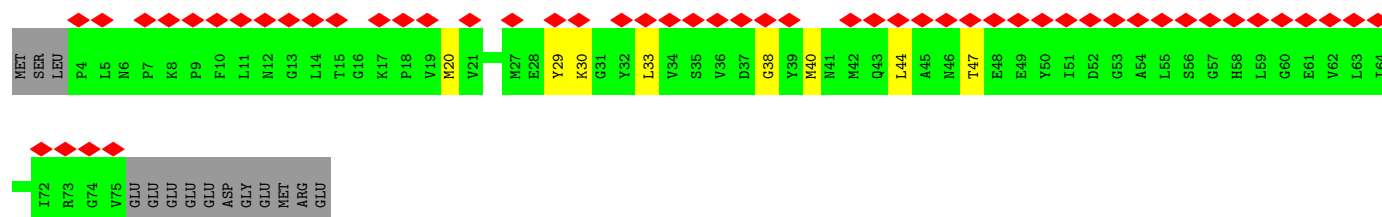
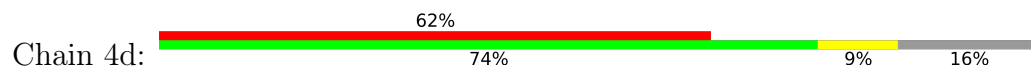


- Molecule 15: Isoform SM-B of Small nuclear ribonucleoprotein-associated proteins B and B'

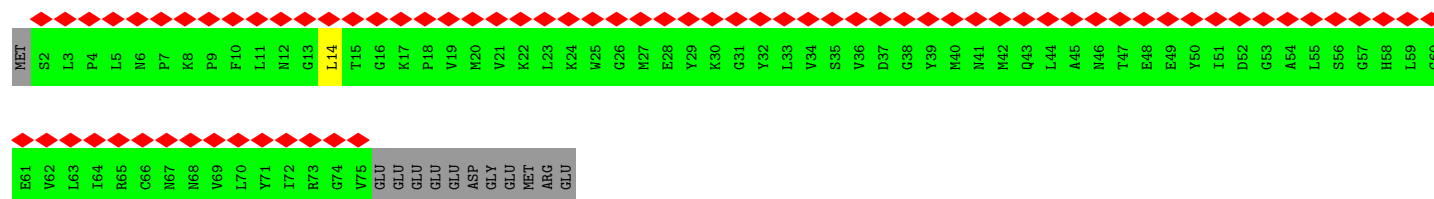
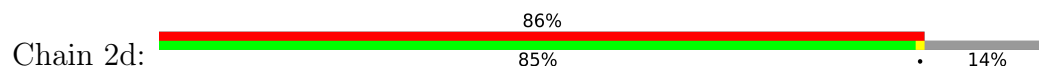




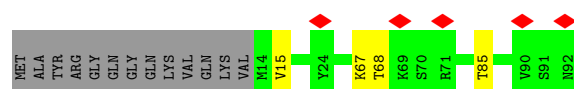
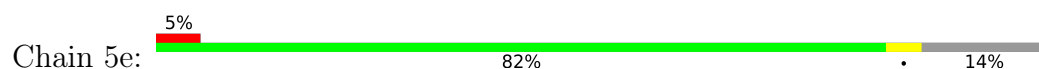
- Molecule 18: Small nuclear ribonucleoprotein F



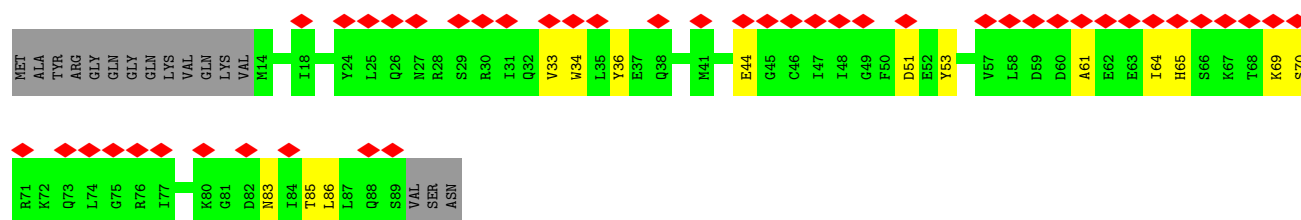
- Molecule 18: Small nuclear ribonucleoprotein F



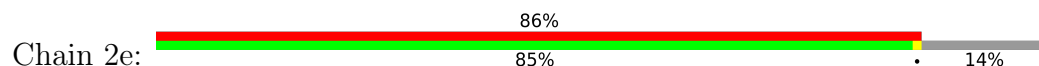
- Molecule 19: Small nuclear ribonucleoprotein E

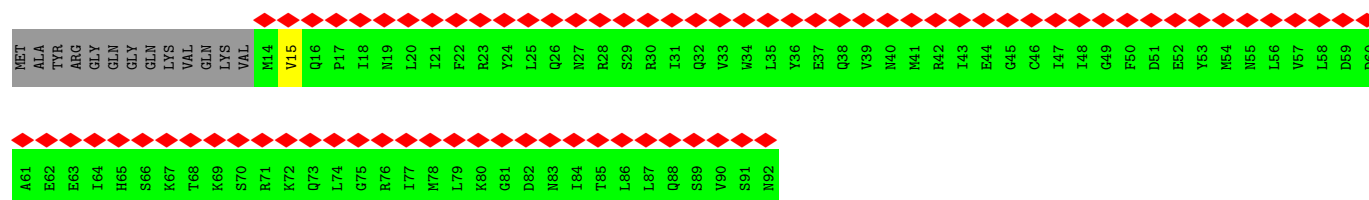


- Molecule 19: Small nuclear ribonucleoprotein E

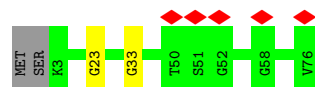


- Molecule 19: Small nuclear ribonucleoprotein E

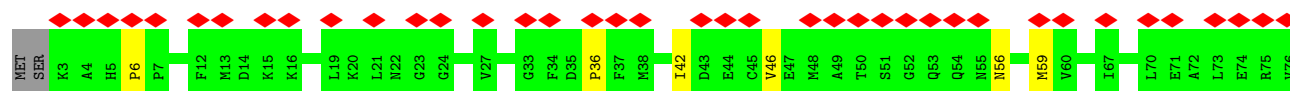
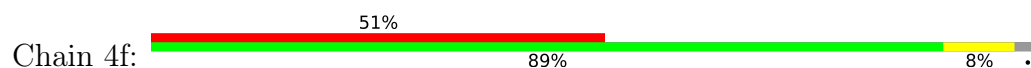




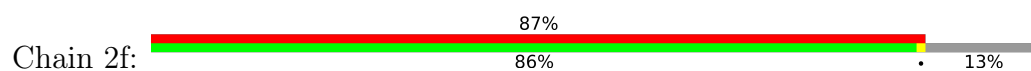
• Molecule 20: Small nuclear ribonucleoprotein G



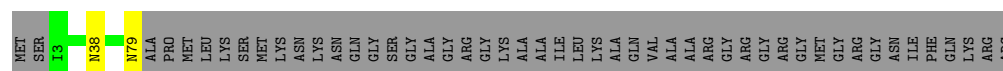
• Molecule 20: Small nuclear ribonucleoprotein G



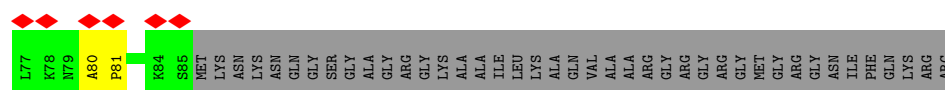
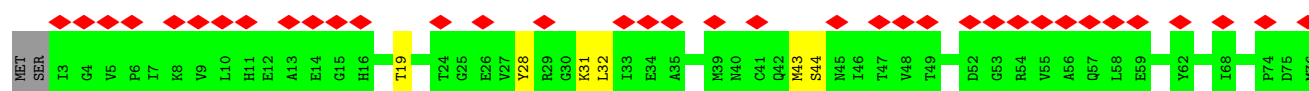
• Molecule 20: Small nuclear ribonucleoprotein G



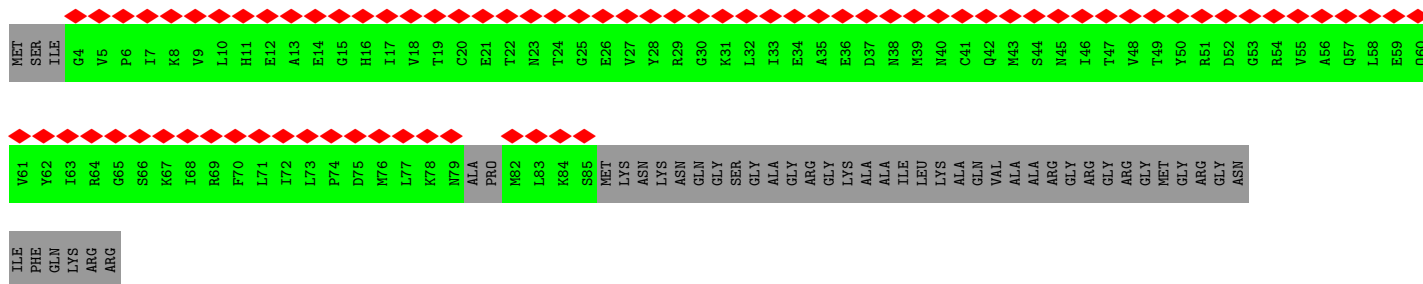
• Molecule 21: Small nuclear ribonucleoprotein Sm D3



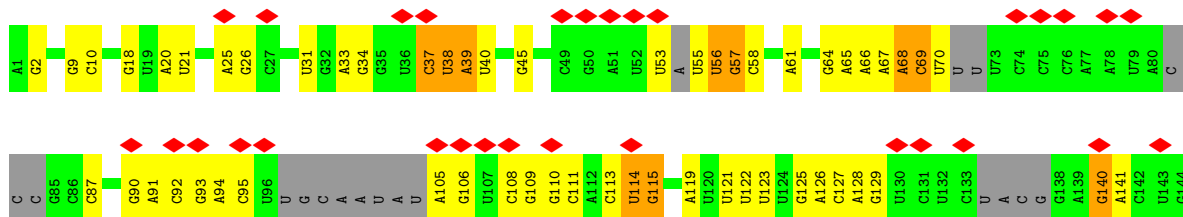
• Molecule 21: Small nuclear ribonucleoprotein Sm D3



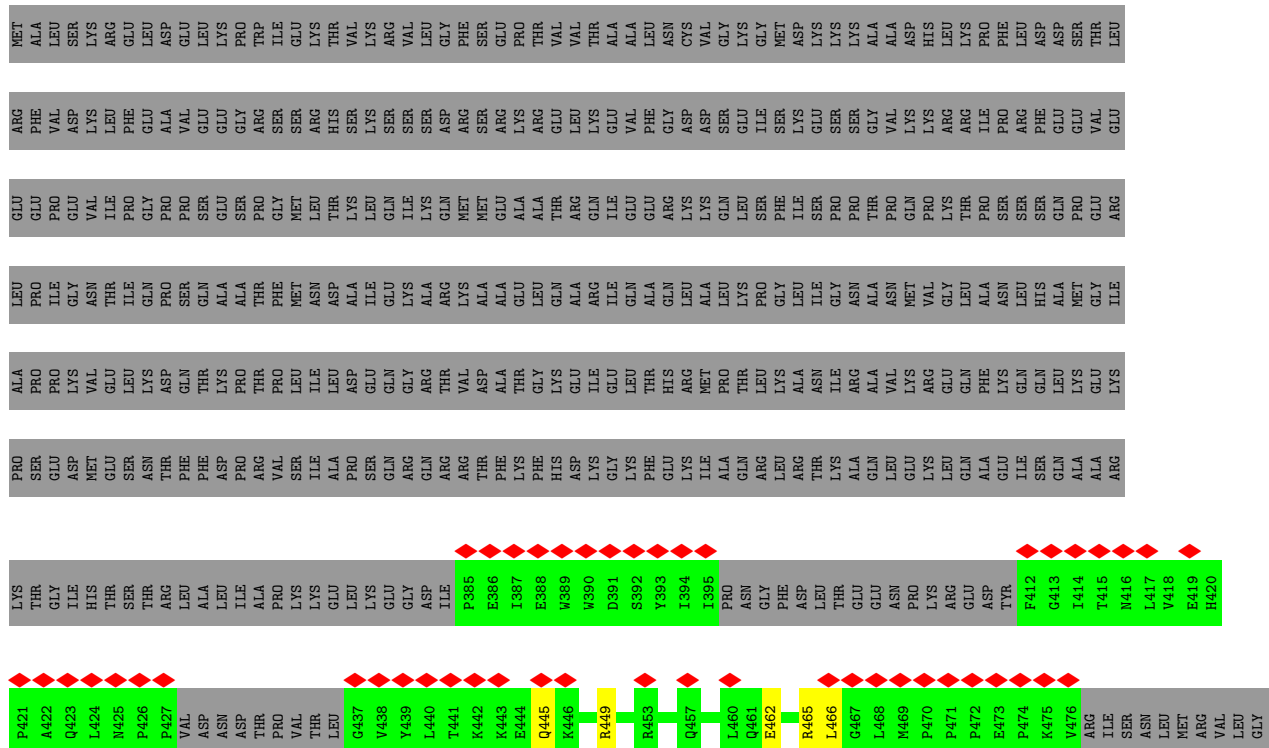
Chain 2g:

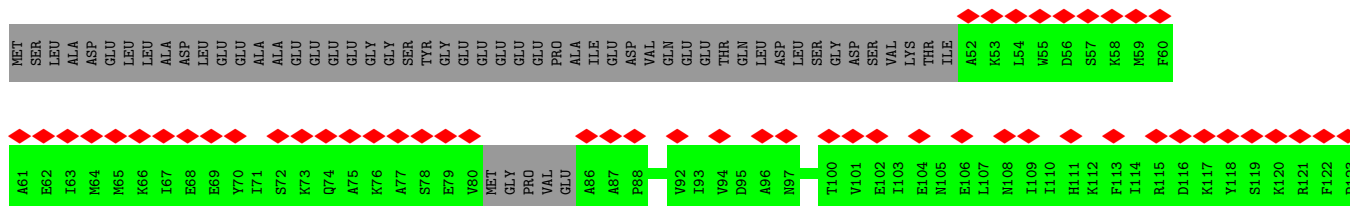


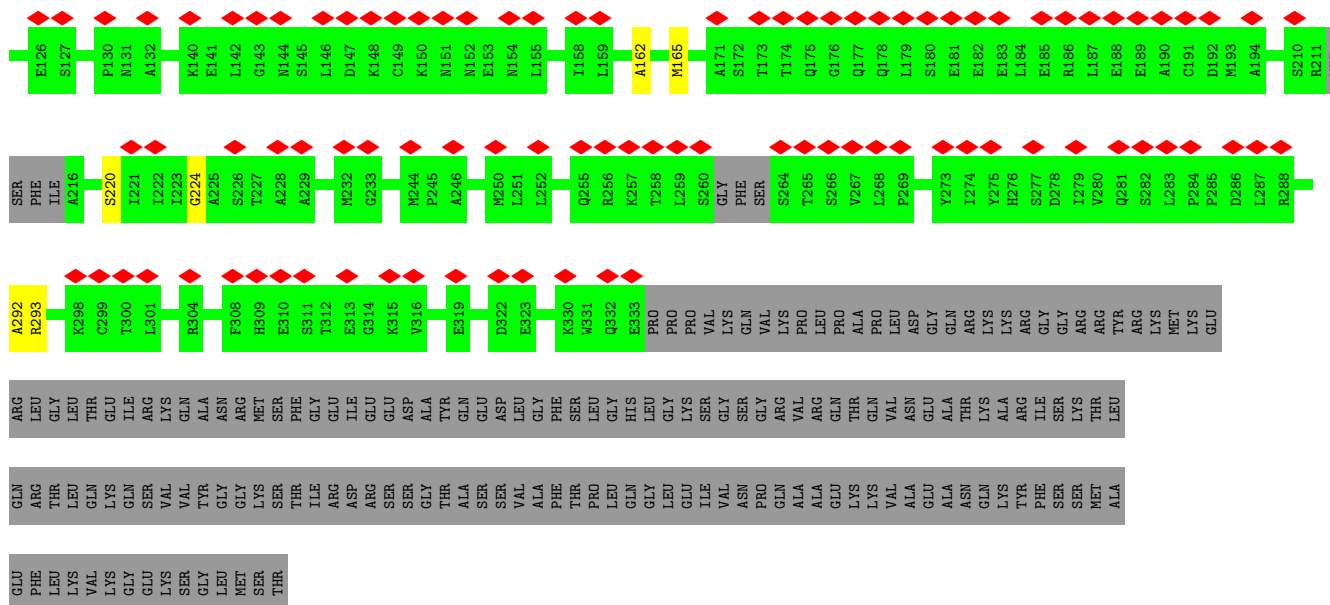
Chain 4A:



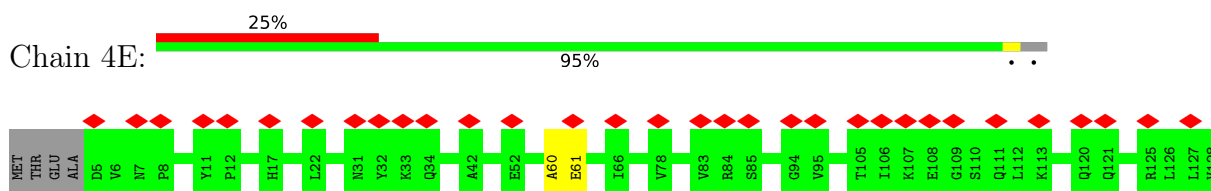
Chain 4B:



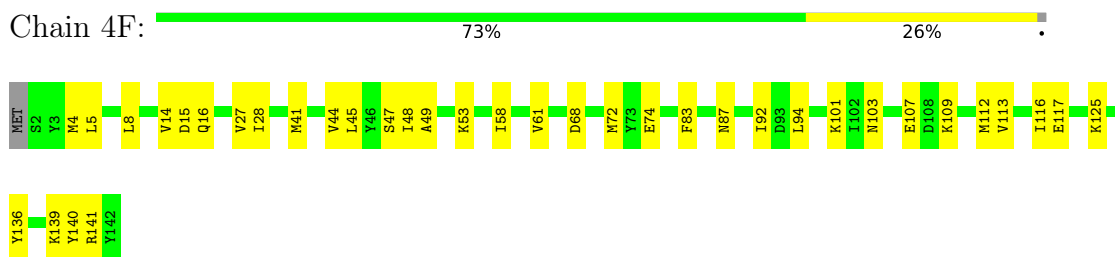




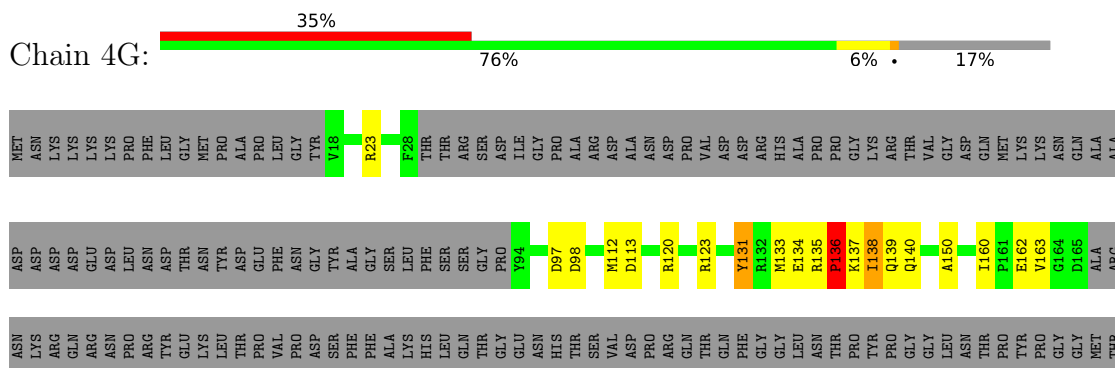
- Molecule 26: NHP2-like protein 1



- Molecule 27: Thioredoxin-like protein 4A



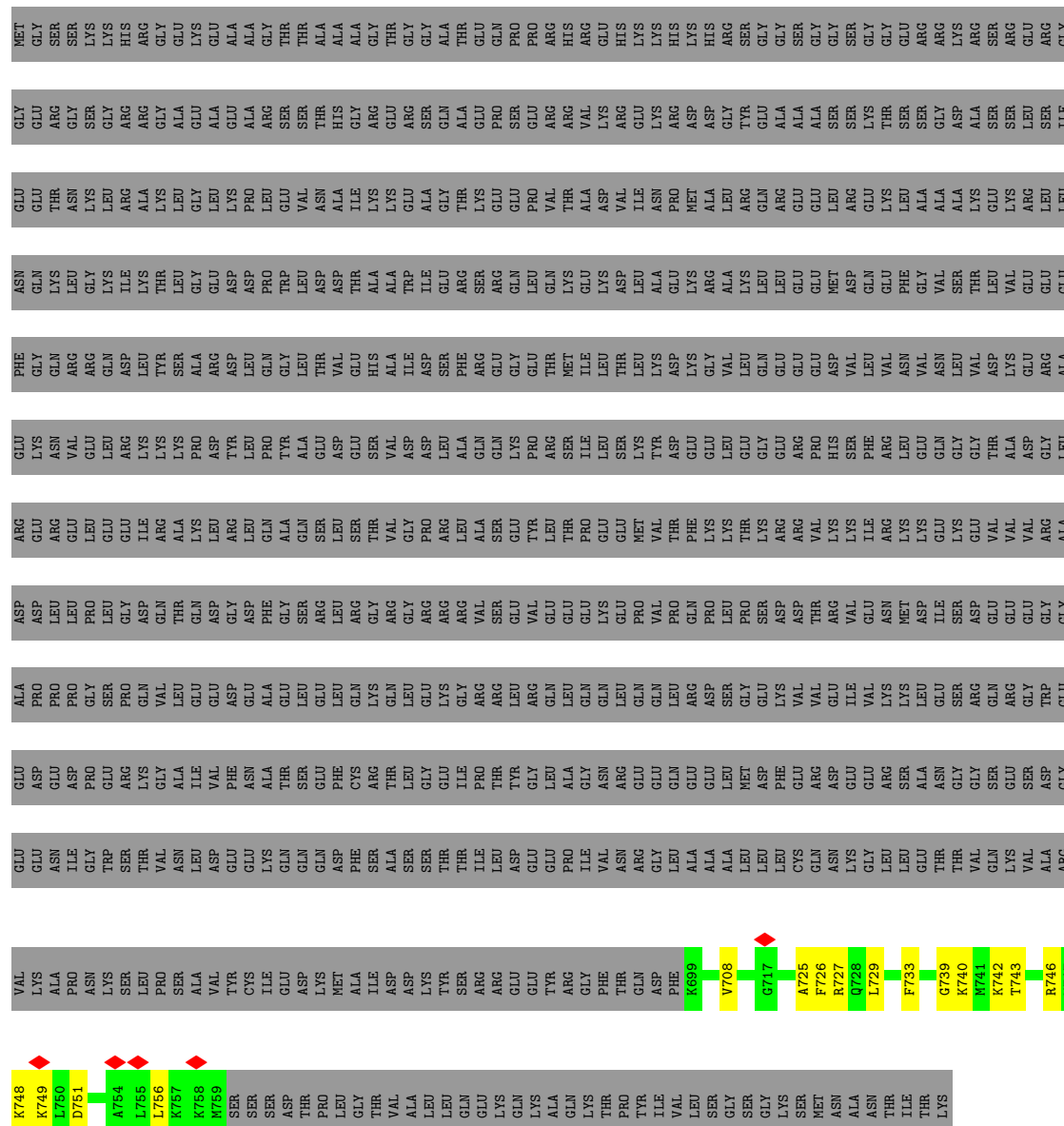
- Molecule 28: Pre-mRNA-processing factor 6



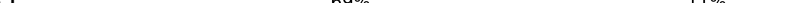


- Molecule 30: U4/U6.U5 tri-snRNP-associated protein 1

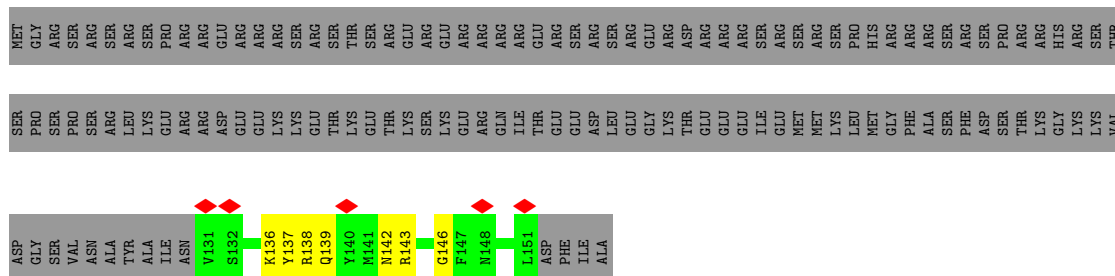
Chain 4S: 6% 92%

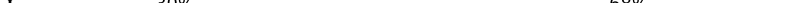


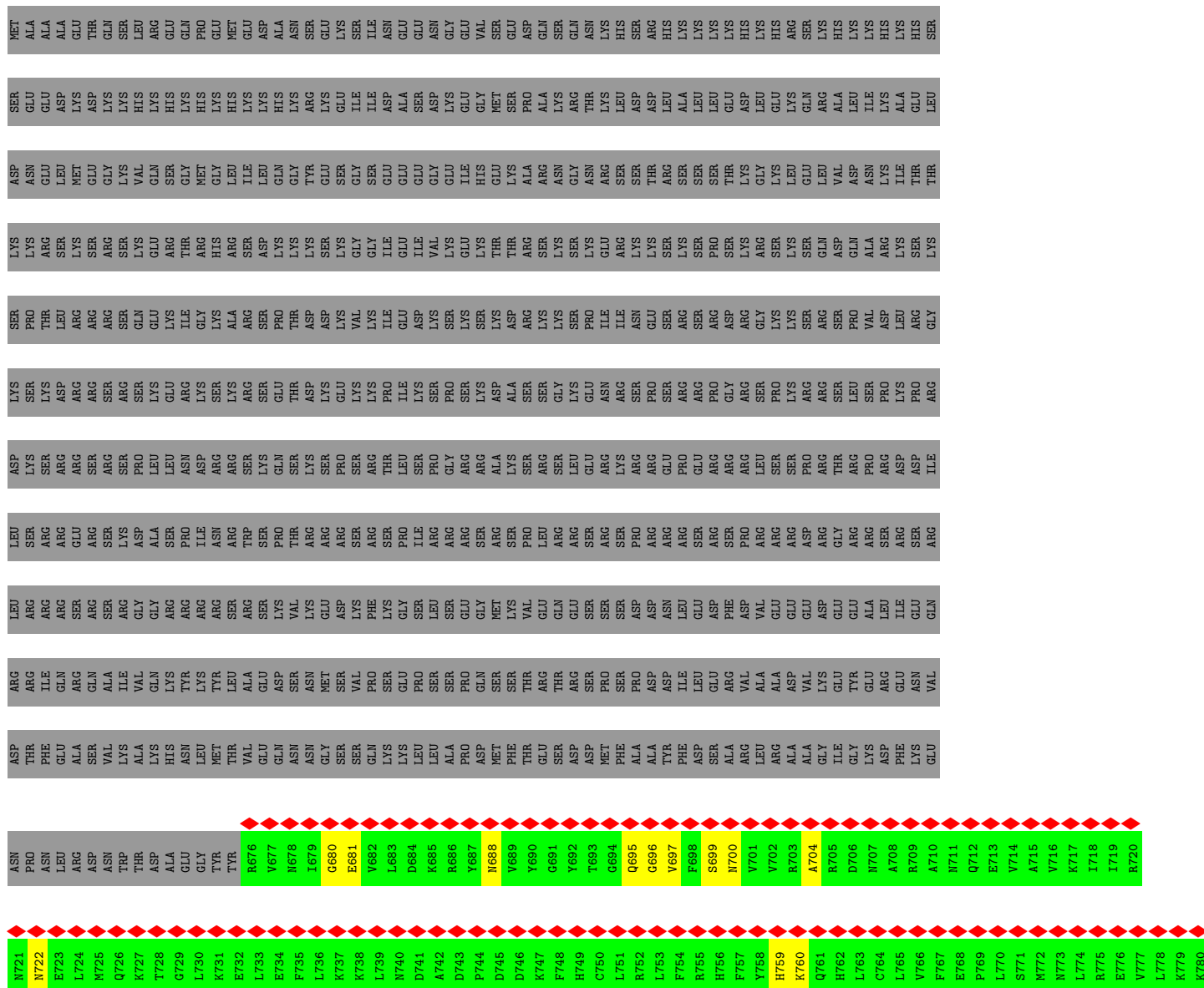
- Molecule 31: U4/U6.U5 tri-snRNP-associated protein 2

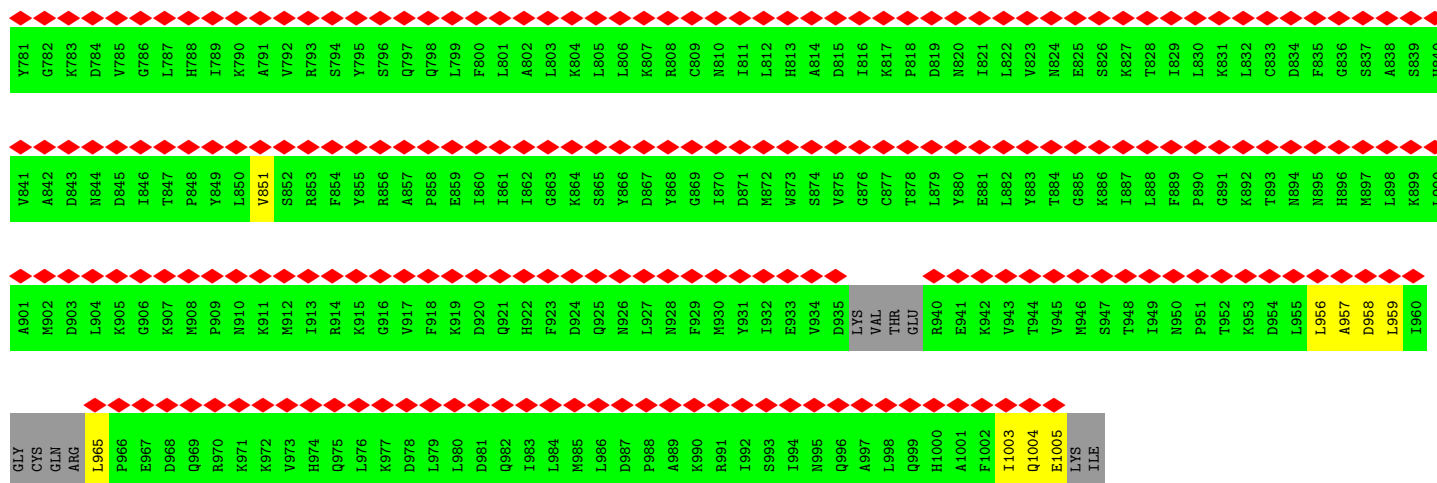
Chain 4T:  69% 11% 19%

- Chain 4X: 9% 5% 86%

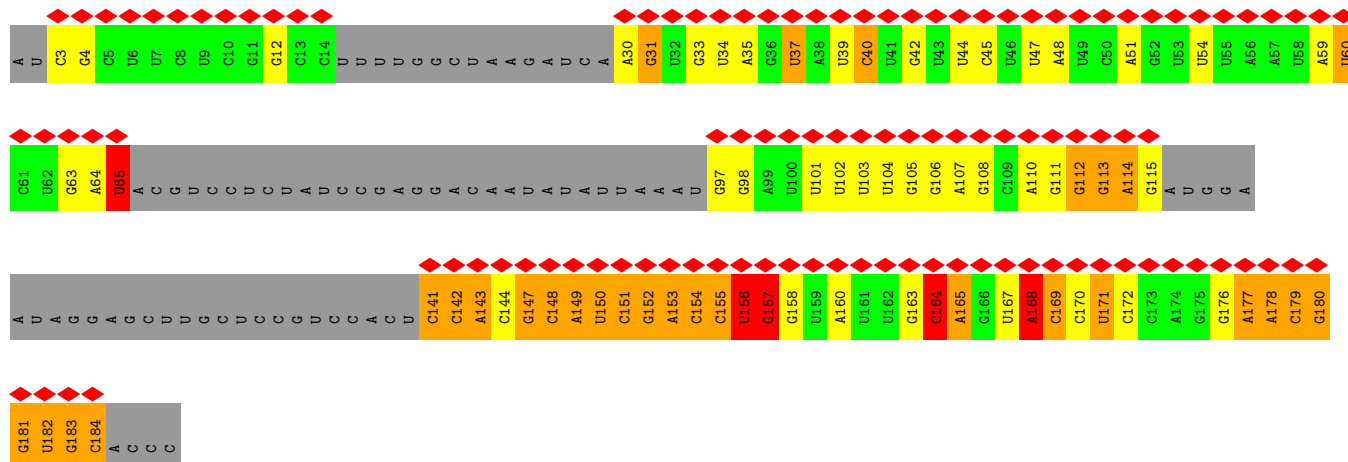


- Chain 4Y: 

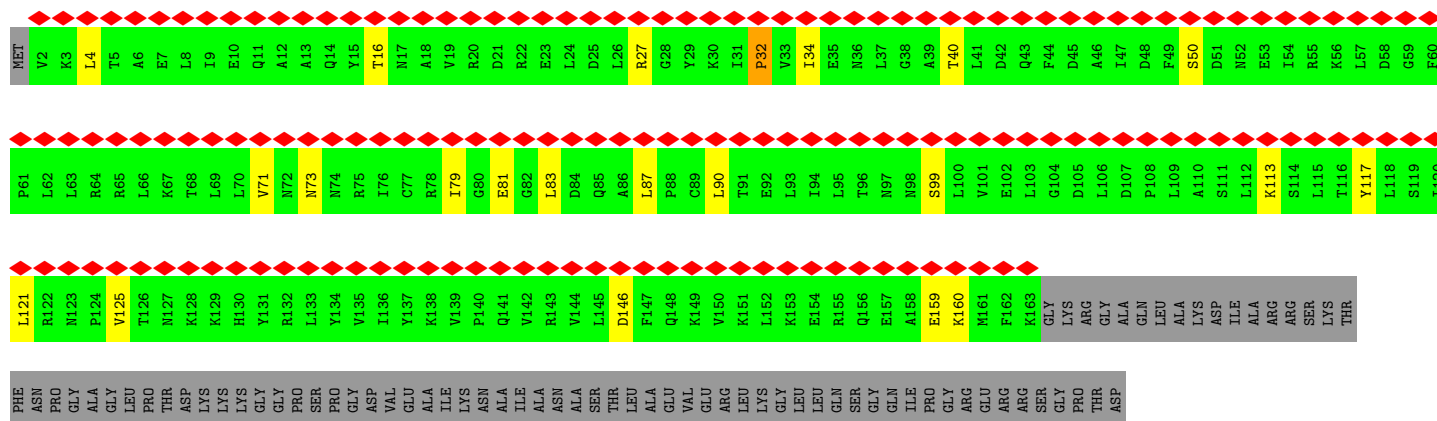




• Molecule 35: U2 snRNA



• Molecule 36: U2 small nuclear ribonucleoprotein A'



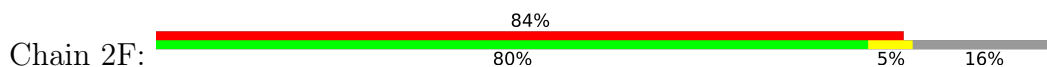


[illegible]

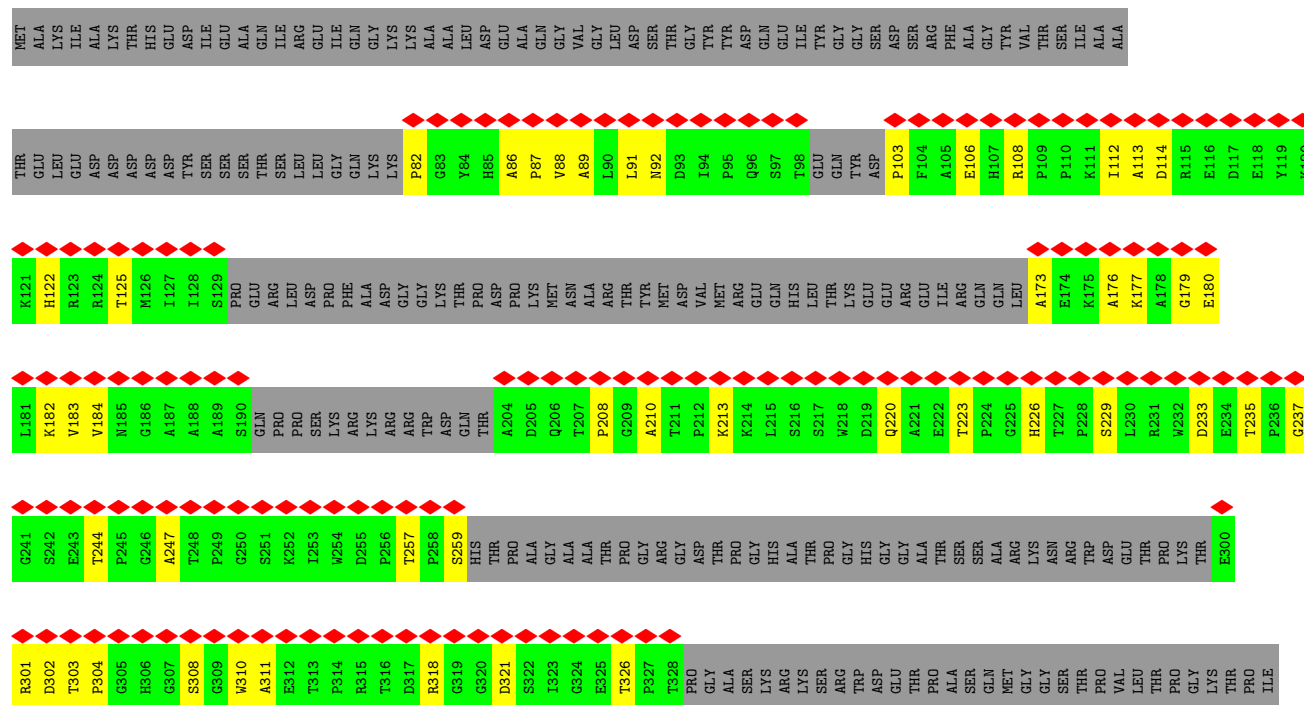
- Molecule 39: Splicing factor 3A subunit 2

[illegible]

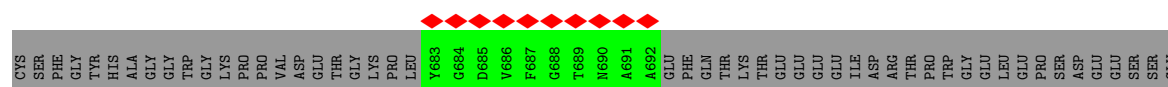
- Molecule 40: Splicing factor 3A subunit 3



M1	E2	T3	T4	L5	E6	Q7	Q8	R9	R10	Y11	H12	E13	E14	K15	E16	R17	L18	M19	D20	V21	W22	A23	K24	E25	W26	L27	T28	K29	X30	S31	T32	L33	R34	D35	Q36	R37	I38	S39	ASN	D40	H41	K42	T43	R44	S45	V46	Q47	D48	R49	V50	M51	E52	V53	S54	E55	N56	L57	E58	D59
Y61	D62	D63	K64	D65	G66	L67	R68	K69	E70	E71	L72	T73	A74	I75	S76	G77	P78	N79	E80	F81	A82	E83	F84	Y85	N86	R87	L88	K89	Q90	I91	K92	E93	F94	H95	R96	H98	PRO	ASN	GLU	ILE	CYS	VAL	PRO	MET	SER	VAL	GLU	F110	E111	E112	L113	L114	K115	A116	R117	E118	N119	P120	

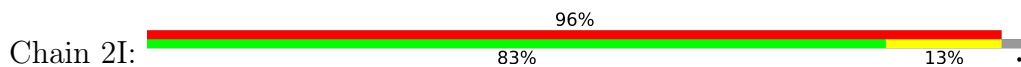


F1081	T1021	V961	Q901	A841	D781	I721	R661	A601	S541	D481	Y421	GLY
G1082	P1022	M962	E902	N842	E782	E722	H662	K602	P542	V482	V422	THR
Y1083	I1023	K963	Q903	K843	E783	S723	T663	A603	T543	D483	P423	PRO
I1084	L1024	T964	T904	V844	M784	F724	G664	A604	L544	E484	I424	ALA
A1085	K1025	C965	T905	G845	K785	D725	I665	G605	E545	S485	R425	ASN
K1086	N1026	Q966	E906	A846	K786	S726	K666	L606	D546	THR	R426	MET
A1087	R1027	E967	D907	A847	I787	V727	I667	A607	Q547	LEU	T427	ALA
I1088	H1028	E968	S908	E848	V788	L728	V668	T608	E548	PRO	P427	THR
G1089	E1029	K969	V909	T849	L789	K729	Q669	M609	R549	THR	A428	PRO
P1090	K1030	L970	M910	T850	K790	P730	Q670	I610	H550	GLY	K430	PRO
H1091	V1031	M971	L911	S851	V791	L731	I671	S611	L551	GLY	R439	HIS
D1092	Q1032	G972	N912	R852	V792	V732	A672	T612	L552	ILE	K431	ILE
L1094	H1034	L974	F914	V854	Q794	K734	L674	M614	V553	SER	T432	MET
A1095	C1035	G975	G915	D855	C795	I735	M675	P615	K554	THR	A433	THR
T1096	I1036	V976	T916	D856	C796	R736	G676	D616	V555	PRO	P435	PRO
L1097	D1037	V977	V917	L857	G797	Q737	C677	I617	I556	GLU	T436	GLU
L1098	L1038	L978	V918	K858	T798	H738	A678	D618	D557	GLN	P437	GLN
M1099	V1039	Y979	N919	D859	D799	R739	I679	N619	R558	LEU	L438	LEU
N1100	G1040	E980	A920	E860	G800	G740	L680	M620	I559	GLN	G439	GLN
L1101	R1041	Y981	L921	A861	V801	K741	P681	D621	L560	ALA	G440	ALA
K1102	I1042	L982	G922	E862	E802	G742	H682	E622	Y561	TRP	M441	TRP
V1103	A1043	G983	K923	Q863	A903	L743	L683	Y623	K562	ARG	T442	ARG
I1104	D1044	E984	R924	Y864	N804	A744	G684	V624	L563	GLU	G443	GLU
E1105	R1045	E985	V925	R865	T805	A745	S685	R625	D564	GLU	F444	GLU
L1106	G1046	Y986	K926	K866	I806	F746	L686	N626	D565	ILE	H445	ILE
Q1107	A1047	P987	P927	K867	K807	L747	V687	T627	L566	ASP	M446	ASP
N1108	E1048	E988	Y928	V868	T808	K748	G688	T628	V567	THR	Q447	THR
L1109	Y1049	V989	L929	H869	E809	A749	I689	A629	R568	GLU	THR	GLU
V1110	Y1050	G991	P930	E870	I810	I750	I690	R630	P569	N396	ASP	N396
C1111	S1051	G992	Q931	T871	L811	G751	E691	A631	P510	R397	ASP	R397
T1112	A1052	S992	I932	T872	P812	V752	H692	R632	M511	P398	THR	P398
T1113	R1053	L993	C933	E873	P813	L753	G693	F632	R512	L399	THR	L399
V1114	E1054	G994	G934	K874	F814	I754	L694	V634	K513	S400	MET	S400
A1115	W1055	G995	T935	L875	F815	P755	V695	V635	A514	D401	S455	D401
I1116	M1056	A996	V936	H876	K816	L756	D696	A636	A515	E402	V456	E402
A1117	R1057	L997	L937	G877	H817	M757	E697	S637	L516	E403	N457	E403
I1118	I1058	K998	V938	N878	F818	D758	Q698	A638	R517	D405	D458	D405
V1119	C1059	A999	R939	L879	M819	A759	Q699	L639	I518	M407	Q459	M407
A1120	F1060	I1000	L940	G880	Q820	E760	K700	G640	I519	A406	P460	A406
E1121	E1061	V1001	N941	A881	H821	V761	V701	I641	T520	F408	S461	F408
T1122	L1062	N1002	N942	A882	R822	A762	R702	P642	D521	P409	M462	P409
C1123	L1063	V1003	K943	D883	M823	M763	T703	S643	A523	E410	L464	E410
S1124	E1064	I1004	S944	T884	A824	V764	I704	L644	R524	G411	P465	G411
P1125	L1065	G1005	A945	D885	L825	V765	S705	L645	E525	Y412	F466	Y412
F1126	M1066	K946	K946	H886	D826	T766	A706	P646	F526	K413	L467	K413
T1127	K1067	V947	V947	K887	R827	R767	L707	F647	D527	V414	K468	V414
V1128	M1068	K948	R948	L888	R828	E768	A708	L648	A528	L415	P469	L415
L1129	M1069	K949	Q949	E889	N829	V769	I709	K649	G529	P416	D470	P416
P1130	K1070	N1010	Q950	E890	Y830	M770	A710	A650	P530	P417	D471	P417
A1131	P1011	A951	A951	Q891	R831	L771	A711	V651	L531	P418	I472	P418
L1132	M1012	A952	A952	L892	Q832	I772	L712	C652	F532	A419	Q473	A419
M1133	I1013	D953	D953	T893	L833	L773	A713	K653	N533	G420	Y474	G420
N1134	K1014	L954	L954	D894	V834	I774	E714	S654	Q534		Y475	
E1135	D1015	G955	G955	K895	D835	R775	A715	K655	I535		F476	
Y1136	L1016	L896	L896	T896	T836	E776	A716	K656	L536		D477	
R1137	L1017	L897	L897	T897	T837	F777	A717	S657	P537		K478	
V1138	T1077	L957	T957	L898	V837	Q778	T717	K658	L538		L479	
P1139	V1078	T958	T958	L899	V838	F779	T718	S659	L539		V480	
E1140	M1079	R1019	A959	A899	E839	S779	Y719	Q659	N599			
	T1080	L1020	V960	F900	L840	P780	G720	A660	L600			



THR	GLN	LYS	TYR	GLU	GLU	HIS	VAL	ARG	GLU	GLN	GLN	ALA	ALA	GLN	VAL	GLU	LYS	GLU	ASP	PHE	SER	ASP	MET	VAL	ALA	ALA	HIS	ALA	ALA	LYS	GLN	LYS	LYS	LYS	LYS	LYS	ALA	ALA	ARG	ASP	GLN	GLN	TYR	LYS	LYS	GLY	ARG	ASP	GLN	GLN	GLU	PHE	LYS	THR	THR
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- Molecule 43: Splicing factor 3B subunit 3



R601	K541	A481	P421	I361	F301	G241	M181	L121	V61	M1
S602	K542	T482	Q422	A362	L302	S242	F182	A122	I62	F2
R603	T543	L483	L483	H363	A303	D243	A183	D243	R63	L3
F604	I544	V484	Y424	L364	Q304	G244	C184	D124	S64	Y4
L605	V545	L485	V425	G365	T305	S245	L185	P125	L65	N5
A606	K546	S486	A426	D366	E306	S246	E186	K126	H66	L6
G607	C547	I487	A426	D366	G307	G247	D187	G127	A67	T7
V608	A548	C488	Q428	D368	G308	V248	D188	K128	F68	L8
L609	V549	E489	R429	E369	D309	L249	Y189	A129	R69	Q9
V610	N550	T490	G430	E370	I310	I250	E190	V130	L70	R10
D611	Q551	V491	P431	P371	F311	C251	E191	M131	T71	A11
N612	R552	E492	R432	E372	K312	S252	A192	I132	G72	T12
T613	Q553	E493	S433	F373	I313	E253	D193	S133	G73	G13
V614	V554	V494	S434	S374	T314	N254	N194	A134	T74	I14
R615	V555	T495	L435	S375	L315	V255	D195	I135	K75	S15
I616	I556	D496	R436	A376	E316	I256	P196	E136	D76	F16
S617	A557	L497	V437	M377	T317	T257	T197	K137	Y77	A17
L618	L558	G498	L438	PR0	D318	V258	G198	Q138	I78	I18
V619	T559	F499	R439	GLU	E319	K259	E199	K139	V79	H19
D620	G560	L500	HIS	GLU	D320	N260	A200	L140	V80	G20
P621	G561	G501	G441	GLY	M321	F261	A201	V141	G81	N21
S622	E562	T502	L442	ASP	V322	G262	A202	Y142	S82	F22
G623	L563	T503	E443	T384	T323	D263	N203	D143	D83	S23
C624	V564	P504	V444	F385	E324	Q264	T204	L144	S84	G24
L625	Y565	T505	S445	F386	I325	P265	Q205	N145	G85	T25
Q626	F566	L506	E446	F387	R326	D266	Q206	R146	R86	K26
P627	E567	S507	M447	Q388	L327	I267	T207	D147	I87	Q27
L628	M568	C508	R448	P389	K328	R268	L208	A148	V88	Q28
S629	D569	S509	V449	R390	Y329	C269	T209	A149	I89	E29
M630	P570	L510	S450	P391	F330	P270	F210	A150	L90	I30
G631	S571	G511	E451	L392	D331	I271	Y211	R151	E91	V31
A632	G572	G512	L452	K393	T332	P272	E212	L152	Y92	V32
L633	Q573	D513	P453	N394	V333	R273	L213	T153	Q93	S33
P634	L574	D514	G454	L395	P334	R274	D214	I154	P94	R34
A635	N575	A515	M455	V396	V335	R275	L215	S155	S95	G35
Q636	E576	L516	P456	L397	A336	N276	G216	S156	X96	X36
P637	Y577	V517	M457	V398	A337	D277	L217	P157	X97	I37
E638	T578	Q518	A458	D399	A338	L278	N218	L158	X98	L38
S639	E579	V519	V459	E400	M339	D279	H219	E159	F99	E39
L640	R580	Y520	V460	L401	C340	D280	V220	A160	E100	L40
C641	K581	P521	T461	D402	V341	P281	V221	H161	K101	L41
I642	E582	D522	V462	S403	L342	E282	R222	K162	I102	R42
V643	M583	G523	L463	L404	K343	R283	K223	A163	H103	P43
E644	S584	I524	R464	S405	T344	G284	Y224	N164	Q104	D44
M645	A585	R525	H465	P406	G345	M285	S225	T165	E105	P45
GLY	D586	H526	I466	I407	F346	I286	E226	L166	T106	M46
GLY	V587	I527	E467	L408	L347	F287	P227	V167	F107	T47
THR	V588	R528	D468	F409	F348	V288	L228	V168	G108	G48
LYS	C589	A529	E469	C410	V349	C289	E229	H169	K109	R49
GLN	M590	D530	F470	Q411	A350	S290	E230	V170	S110	V50
ASP	S591	L471	D471	I412	S351	A291	H231	V171	G111	H51
GLU	L592	R332	A472	A413	E352	T292	G232	G172	C112	T52
LEU	L593	G533	Y473	D414	F353	H293	N233	V173	R113	L53
GLY	A594	V534	I474	L415	G354	K294	F234	D174	R114	L54
GLU	ARC	NS34	I475	A416	N355	T295	L235	V175	I115	T55
GLY	V595	E535	I476	M417	N356	K296	T236	G176	V116	V56
SER	P596	W536	V476	M418	H356	S297	T237	F177	P117	E57
ILE	P597	K537	S477	E418	V357	T297	V238	E178	G118	V58
	G598	T538	F478	D419	L358	M298	V239	E179	G119	F59
	P599	P539	V479	T420	V359	F299	P239	N179	Q119	T60
	P600	C540	N480		C600	T300	C240	D180	T120	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	116801	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.326	Depositor
Minimum map value	-0.959	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.062	Depositor
Recommended contour level	0.25	Depositor
Map size ($\text{\AA}$)	563.2, 563.2, 563.2	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.1, 1.1, 1.1	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.69	6/956 (0.6%)	0.75	2/1481 (0.1%)
2	6A	0.30	0/1274	0.48	2/1976 (0.1%)
3	6a	0.70	0/355	1.27	0/442
4	6b	0.75	0/294	1.37	3/364 (0.8%)
5	6c	0.59	0/294	1.32	3/364 (0.8%)
6	6d	0.71	0/286	1.28	2/354 (0.6%)
7	6e	0.71	0/279	1.40	2/347 (0.6%)
8	6f	0.60	0/258	1.14	0/319
9	6g	0.68	0/242	1.21	1/299 (0.3%)
10	5A	0.22	0/2673	0.55	8/4156 (0.2%)
11	5B	0.13	0/18748	0.31	0/25452
12	5C	0.13	0/6879	0.32	0/9344
13	5D	0.12	0/16393	0.31	0/22174
14	5E	0.26	0/1480	0.67	0/2056
15	2a	0.86	0/339	1.19	2/422 (0.5%)
15	4a	0.30	0/404	0.71	0/561
15	5a	0.87	0/343	1.20	3/427 (0.7%)
16	2b	0.89	0/327	1.10	0/407
16	4b	0.32	0/400	0.78	0/556
16	5b	0.89	0/327	1.11	0/407
17	2c	1.18	0/338	1.20	1/419 (0.2%)
17	4c	0.34	0/454	0.78	0/631
17	5c	1.14	1/387 (0.3%)	1.22	1/482 (0.2%)
18	2d	1.24	1/295 (0.3%)	1.26	0/367
18	4d	0.39	0/350	0.78	0/483
18	5d	1.23	0/291	1.26	0/362
19	2e	1.02	0/315	1.26	0/392
19	4e	0.33	0/375	0.91	2/521 (0.4%)
19	5e	1.03	0/315	1.27	1/392 (0.3%)
20	2f	0.85	0/262	1.04	0/324
20	4f	0.34	0/362	0.81	0/501
20	5f	0.86	0/295	1.05	0/367

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
21	2g	0.81	0/318	1.01	0/394
21	4g	0.30	0/408	0.71	0/566
21	5g	0.78	0/307	1.01	0/382
22	4A	0.35	1/2963 (0.0%)	0.49	5/4603 (0.1%)
23	4B	0.17	0/948	0.40	0/1312
24	4C	0.13	0/1764	0.36	0/2450
25	4D	0.16	0/1336	0.33	0/1858
26	4E	0.11	0/614	0.29	0/855
27	4F	0.12	0/1198	0.31	0/1620
28	4G	0.29	4/4561 (0.1%)	0.51	11/6271 (0.2%)
29	4R	0.12	0/891	0.34	0/1188
30	4S	0.13	0/512	0.33	0/673
31	4T	0.12	0/3845	0.34	0/5208
32	4U	0.61	0/3422	0.89	5/4659 (0.1%)
33	4X	0.12	0/187	0.34	0/245
34	4Y	0.49	0/1592	0.99	2/2215 (0.1%)
35	2A	0.71	12/2576 (0.5%)	1.11	27/4003 (0.7%)
36	2B	0.99	0/647	2.34	33/807 (4.1%)
37	2C	0.96	0/375	1.97	7/467 (1.5%)
38	2D	0.37	0/493	0.98	2/611 (0.3%)
39	2E	0.38	0/373	1.77	4/461 (0.9%)
40	2F	0.39	0/1688	0.92	2/2102 (0.1%)
41	2G	1.72	36/4184 (0.9%)	1.43	29/5216 (0.6%)
42	2H	1.17	0/722	1.25	3/892 (0.3%)
43	2I	1.39	24/4664 (0.5%)	1.20	10/5816 (0.2%)
44	2J	1.02	0/311	0.99	0/387
45	2K	1.27	2/431 (0.5%)	1.27	1/537 (0.2%)
46	2L	1.15	0/355	1.10	0/442
47	2M	1.59	1/263 (0.4%)	1.24	0/327
All	All	0.61	88/98538 (0.1%)	0.73	174/133716 (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
15	4a	0	1
17	2c	0	1
17	5c	0	1
18	4d	0	1
19	4e	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
22	4A	0	1
24	4C	0	1
28	4G	0	2
40	2F	0	1
41	2G	0	11
42	2H	0	3
43	2I	0	11
45	2K	0	1
47	2M	0	1
All	All	0	37

The worst 5 of 88 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	2G	407	MET	N-CA	22.59	1.71	1.46
41	2G	406	ALA	C-N	14.97	1.52	1.33
41	2G	1243	PRO	N-CA	-9.49	1.35	1.47
22	4A	87	C	O3'-P	9.19	1.75	1.61
41	2G	944	SER	N-CA	-8.47	1.34	1.46

The worst 5 of 174 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	2E	146	MET	CA-C-N	21.08	146.19	119.84
39	2E	146	MET	C-N-CA	21.08	146.19	119.84
41	2G	406	ALA	CA-C-N	17.64	147.35	120.89
41	2G	406	ALA	C-N-CA	17.64	147.35	120.89
41	2G	406	ALA	CA-C-O	-13.03	105.77	120.24

There are no chirality outliers.

5 of 37 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
22	4A	90	G	Sidechain
24	4C	459	PRO	Peptide
28	4G	569	VAL	Mainchain
28	4G	572	SER	Mainchain
17	5c	112	ASN	Peptide

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	A	864	0	443	142	0
2	6A	1142	0	575	39	0
3	6a	356	0	94	2	0
4	6b	296	0	76	5	0
5	6c	296	0	77	0	0
6	6d	288	0	78	0	0
7	6e	280	0	81	8	0
8	6f	260	0	75	0	0
9	6g	244	0	71	3	0
10	5A	2398	0	1215	98	0
11	5B	18244	0	18075	266	0
12	5C	6727	0	6735	93	0
13	5D	16077	0	16192	305	0
14	5E	1481	0	675	2	0
15	2a	340	0	90	4	0
15	4a	405	0	170	4	0
15	5a	344	0	93	0	0
16	2b	328	0	89	0	0
16	4b	401	0	165	1	0
16	5b	328	0	89	5	0
17	2c	340	0	87	1	0
17	4c	455	0	187	3	0
17	5c	388	0	102	6	0
18	2d	296	0	87	0	0
18	4d	351	0	155	4	0
18	5d	292	0	86	9	0
19	2e	316	0	85	1	0
19	4e	376	0	157	6	0
19	5e	316	0	85	4	0
20	2f	264	0	73	1	0
20	4f	363	0	160	3	0
20	5f	296	0	84	4	0
21	2g	320	0	88	0	0
21	4g	409	0	180	4	0
21	5g	308	0	86	5	0
22	4A	2656	0	1349	50	0
23	4B	953	0	411	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	4C	1765	0	801	7	0
25	4D	1340	0	616	5	0
26	4E	615	0	279	4	0
27	4F	1169	0	1141	42	0
28	4G	4539	0	3081	49	0
29	4R	874	0	883	23	0
30	4S	505	0	530	16	0
31	4T	3749	0	3767	46	0
32	4U	3414	0	2245	16	0
33	4X	184	0	192	8	0
34	4Y	1595	0	694	11	0
35	2A	2311	0	1170	143	0
36	2B	648	0	167	0	0
37	2C	376	0	102	0	0
38	2D	496	0	118	2	0
39	2E	376	0	85	0	0
40	2F	1693	0	454	22	0
41	2G	4192	0	1110	233	0
42	2H	728	0	183	9	0
43	2I	4672	0	1260	71	0
44	2J	312	0	87	3	0
45	2K	432	0	114	6	0
46	2L	356	0	105	5	0
47	2M	264	0	70	12	0
48	5B	36	0	6	2	0
49	5C	1	0	0	0	0
50	5C	32	0	12	0	0
51	4T	1	0	0	0	0
All	All	96473	0	67892	1662	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 10.

The worst 5 of 1662 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)
23:4B:466:LEU:CA	29:4R:432:PRO:HG3	1.12	1.54
41:2G:407:MET:N	41:2G:407:MET:CA	1.71	1.51
2:6A:76:A:N1	23:4B:562:ALA:HB1	1.21	1.45
1:A:30:C:C2'	1:A:31:C:H5''	1.54	1.38
23:4B:466:LEU:CA	29:4R:432:PRO:CG	2.08	1.28

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	6a	87/95 (92%)	76 (87%)	7 (8%)	4 (5%)	2	11
4	6b	70/102 (69%)	64 (91%)	3 (4%)	3 (4%)	2	13
5	6c	70/139 (50%)	64 (91%)	5 (7%)	1 (1%)	9	33
6	6d	68/91 (75%)	63 (93%)	4 (6%)	1 (2%)	8	32
7	6e	68/80 (85%)	64 (94%)	2 (3%)	2 (3%)	3	20
8	6f	61/103 (59%)	56 (92%)	5 (8%)	0	100	100
9	6g	57/96 (59%)	52 (91%)	4 (7%)	1 (2%)	6	29
11	5B	2195/2335 (94%)	2099 (96%)	96 (4%)	0	100	100
12	5C	850/972 (87%)	823 (97%)	27 (3%)	0	100	100
13	5D	1989/2136 (93%)	1912 (96%)	77 (4%)	0	100	100
14	5E	299/357 (84%)	280 (94%)	17 (6%)	2 (1%)	18	48
15	2a	83/231 (36%)	81 (98%)	2 (2%)	0	100	100
15	4a	80/231 (35%)	71 (89%)	9 (11%)	0	100	100
15	5a	84/231 (36%)	82 (98%)	2 (2%)	0	100	100
16	2b	80/119 (67%)	77 (96%)	3 (4%)	0	100	100
16	4b	79/119 (66%)	75 (95%)	4 (5%)	0	100	100
16	5b	80/119 (67%)	77 (96%)	3 (4%)	0	100	100
17	2c	81/118 (69%)	78 (96%)	3 (4%)	0	100	100
17	4c	90/118 (76%)	84 (93%)	6 (7%)	0	100	100
17	5c	95/118 (80%)	91 (96%)	4 (4%)	0	100	100
18	2d	72/86 (84%)	68 (94%)	4 (6%)	0	100	100
18	4d	70/86 (81%)	69 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	5d	71/86 (83%)	68 (96%)	3 (4%)	0	100	100
19	2e	77/92 (84%)	76 (99%)	1 (1%)	0	100	100
19	4e	74/92 (80%)	71 (96%)	3 (4%)	0	100	100
19	5e	77/92 (84%)	76 (99%)	1 (1%)	0	100	100
20	2f	62/76 (82%)	60 (97%)	2 (3%)	0	100	100
20	4f	72/76 (95%)	66 (92%)	6 (8%)	0	100	100
20	5f	72/76 (95%)	70 (97%)	2 (3%)	0	100	100
21	2g	76/126 (60%)	74 (97%)	2 (3%)	0	100	100
21	4g	81/126 (64%)	76 (94%)	5 (6%)	0	100	100
21	5g	75/126 (60%)	73 (97%)	2 (3%)	0	100	100
23	4B	183/683 (27%)	177 (97%)	6 (3%)	0	100	100
24	4C	357/522 (68%)	333 (93%)	24 (7%)	0	100	100
25	4D	262/499 (52%)	252 (96%)	10 (4%)	0	100	100
26	4E	122/128 (95%)	114 (93%)	8 (7%)	0	100	100
27	4F	139/142 (98%)	136 (98%)	3 (2%)	0	100	100
28	4G	776/941 (82%)	739 (95%)	33 (4%)	4 (0%)	24	55
29	4R	104/480 (22%)	93 (89%)	11 (11%)	0	100	100
30	4S	59/800 (7%)	57 (97%)	2 (3%)	0	100	100
31	4T	454/565 (80%)	425 (94%)	29 (6%)	0	100	100
32	4U	559/820 (68%)	541 (97%)	17 (3%)	1 (0%)	43	70
33	4X	19/155 (12%)	19 (100%)	0	0	100	100
34	4Y	316/1007 (31%)	294 (93%)	18 (6%)	4 (1%)	9	34
36	2B	160/255 (63%)	146 (91%)	12 (8%)	2 (1%)	9	34
37	2C	92/225 (41%)	90 (98%)	2 (2%)	0	100	100
38	2D	118/793 (15%)	106 (90%)	6 (5%)	6 (5%)	1	10
39	2E	88/464 (19%)	63 (72%)	16 (18%)	9 (10%)	0	2
40	2F	413/501 (82%)	367 (89%)	41 (10%)	5 (1%)	10	36
41	2G	1032/1304 (79%)	845 (82%)	165 (16%)	22 (2%)	5	25
42	2H	170/895 (19%)	151 (89%)	15 (9%)	4 (2%)	4	23
43	2I	1152/1217 (95%)	1053 (91%)	89 (8%)	10 (1%)	14	42
44	2J	76/424 (18%)	75 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	2K	106/125 (85%)	85 (80%)	18 (17%)	3 (3%)	4	20
46	2L	87/110 (79%)	75 (86%)	12 (14%)	0	100	100
47	2M	64/86 (74%)	55 (86%)	8 (12%)	1 (2%)	7	30
All	All	14353/22191 (65%)	13407 (93%)	861 (6%)	85 (1%)	23	51

5 of 85 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	6a	55	LEU
4	6b	84	MET
6	6d	70	ASP
7	6e	52	VAL
7	6e	55	GLN

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	
11	5B	1978/2108 (94%)	1975 (100%)	3 (0%)	87	87
12	5C	754/866 (87%)	754 (100%)	0	100	100
13	5D	1779/1908 (93%)	1773 (100%)	6 (0%)	86	86
27	4F	129/130 (99%)	129 (100%)	0	100	100
28	4G	185/792 (23%)	179 (97%)	6 (3%)	34	58
29	4R	94/369 (26%)	94 (100%)	0	100	100
30	4S	54/681 (8%)	54 (100%)	0	100	100
31	4T	418/511 (82%)	418 (100%)	0	100	100
32	4U	133/721 (18%)	133 (100%)	0	100	100
33	4X	19/144 (13%)	19 (100%)	0	100	100
All	All	5543/8230 (67%)	5528 (100%)	15 (0%)	84	86

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	5D	1874	LYS
28	4G	138	ILE
13	5D	1967	THR
28	4G	242	LYS
28	4G	135	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 53 such sidechains are listed below:

Mol	Chain	Res	Type
13	5D	726	HIS
13	5D	1341	ASN
31	4T	293	HIS
13	5D	785	HIS
13	5D	1101	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	41/144 (28%)	27 (65%)	9 (21%)
10	5A	113/117 (96%)	39 (34%)	6 (5%)
2	6A	50/107 (46%)	8 (16%)	3 (6%)
22	4A	119/144 (82%)	21 (17%)	2 (1%)
35	2A	105/188 (55%)	22 (20%)	3 (2%)
All	All	428/700 (61%)	117 (27%)	23 (5%)

5 of 117 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	8	U
1	A	9	U
1	A	10	C
1	A	11	C
1	A	12	U

5 of 23 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
10	5A	78	U
10	5A	96	A
10	5A	94	U
22	4A	68	A

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Mol	Chain	Res	Type
1	A	38	C

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 4 ligands modelled in this entry, 2 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	$\# Z > 2$
48	IHP	5B	2401	-	36,36,36	0.74	0	60,60,60	1.22	3 (5%)
50	GTP	5C	1002	49	33,34,34	0.94	1 (3%)	50,54,54	1.54	8 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	IHP	5B	2401	-	-	2/30/54/54	0/1/1/1
50	GTP	5C	1002	49	-	4/22/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	5C	1002	GTP	C2-N3	2.07	1.38	1.33

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	5C	1002	GTP	C5-C4-N3	-4.91	120.58	128.39
50	5C	1002	GTP	C2-N3-C4	4.67	120.35	112.30
48	5B	2401	IHP	C5-C4-C3	3.34	117.76	110.43
50	5C	1002	GTP	N9-C4-N3	3.14	132.22	125.95
50	5C	1002	GTP	C2-N1-C6	-3.02	119.64	125.11

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
50	5C	1002	GTP	C5'-O5'-PA-O3A
50	5C	1002	GTP	C5'-O5'-PA-O2A
50	5C	1002	GTP	O4'-C4'-C5'-O5'
50	5C	1002	GTP	C3'-C4'-C5'-O5'
48	5B	2401	IHP	C1-O11-P1-O41

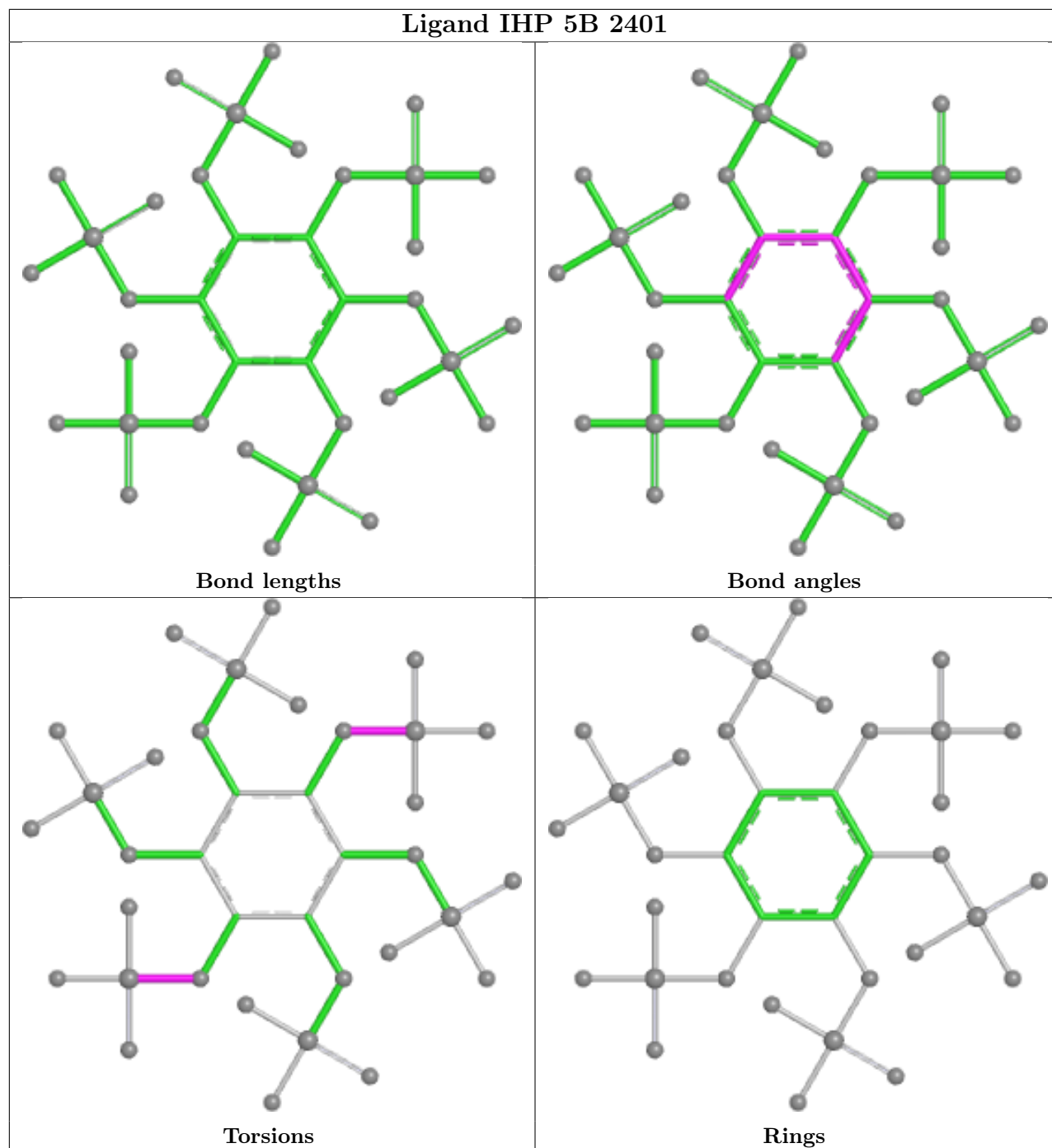
There are no ring outliers.

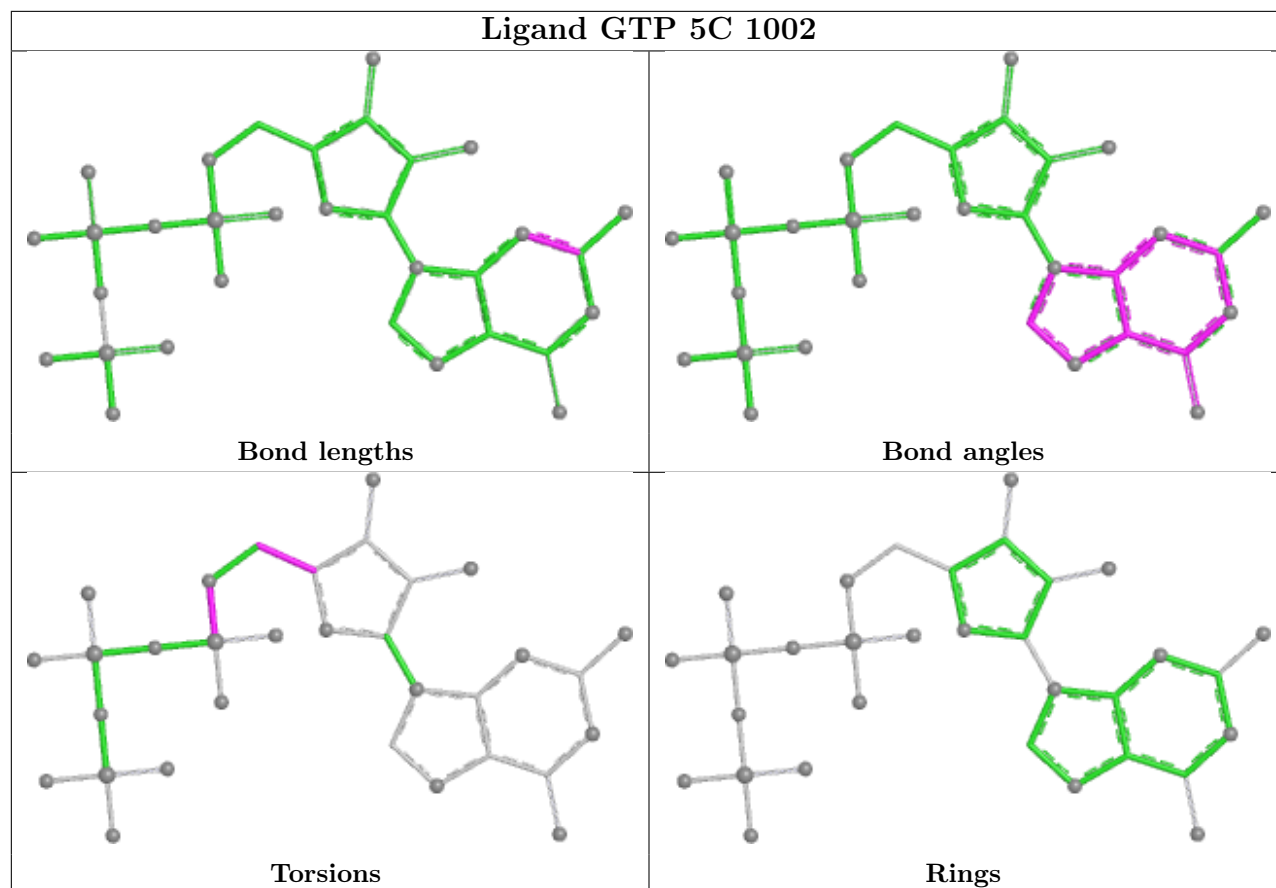
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
48	5B	2401	IHP	2	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.

Ligand IHP 5B 2401





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.

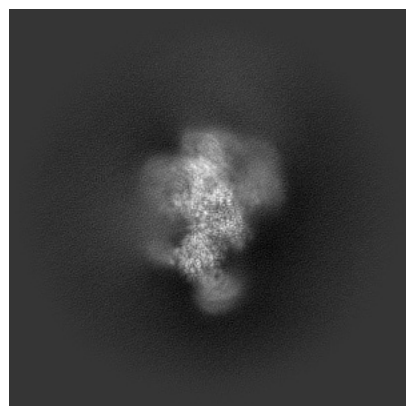
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34505. These allow visual inspection of the internal detail of the map and identification of artifacts.

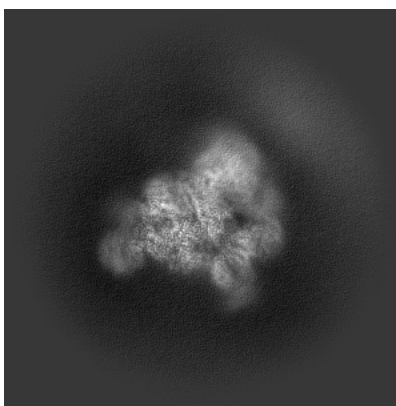
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

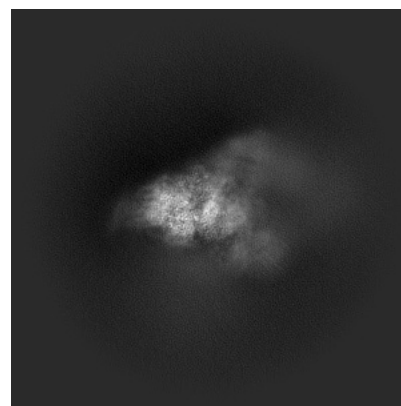
6.1.1 Primary map



X

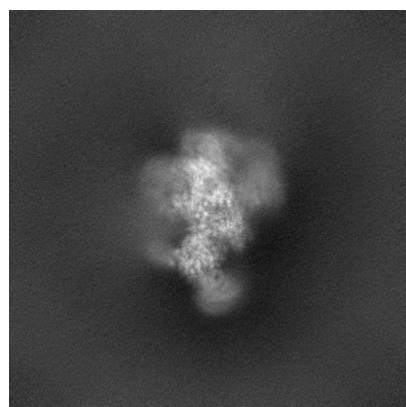


Y

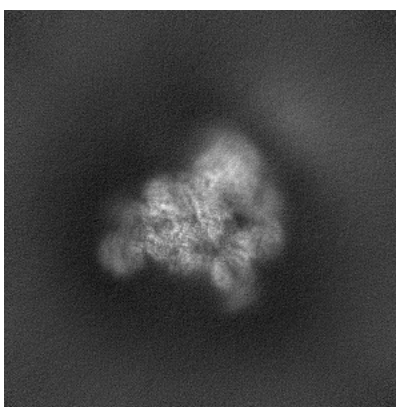


Z

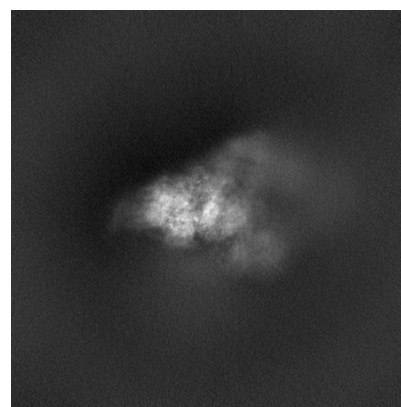
6.1.2 Raw map



X



Y

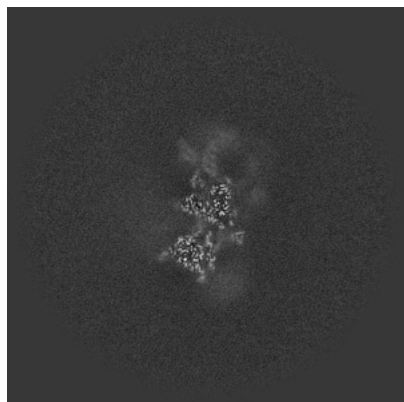


Z

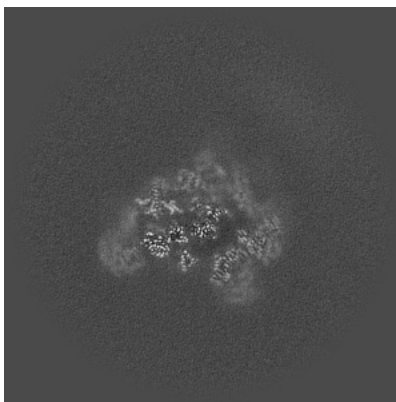
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

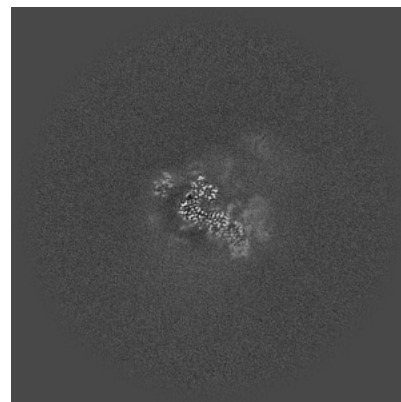
6.2.1 Primary map



X Index: 256

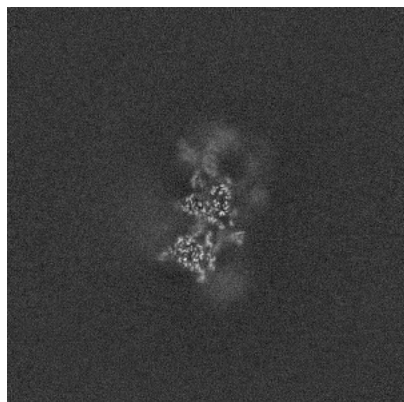


Y Index: 256

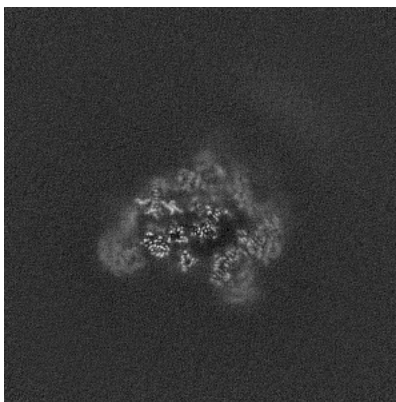


Z Index: 256

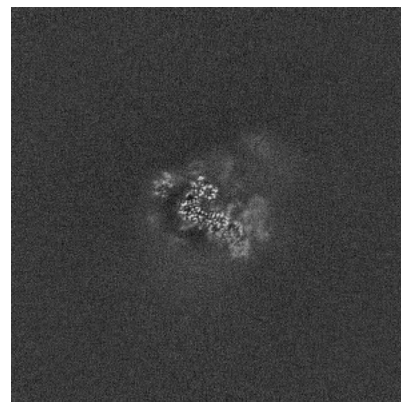
6.2.2 Raw map



X Index: 256



Y Index: 256

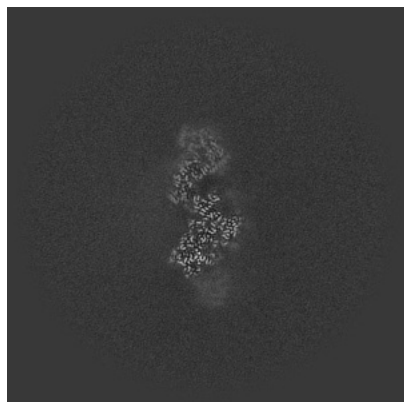


Z Index: 256

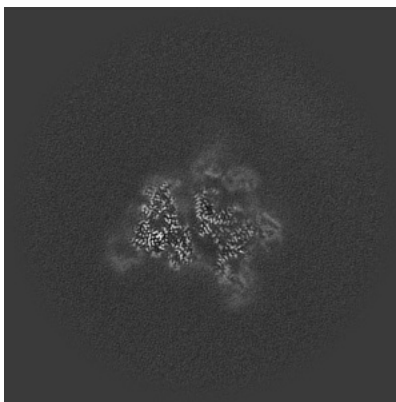
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

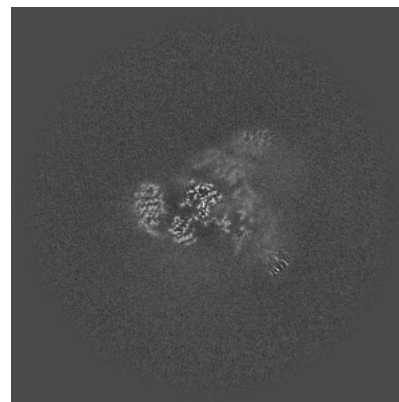
6.3.1 Primary map



X Index: 222

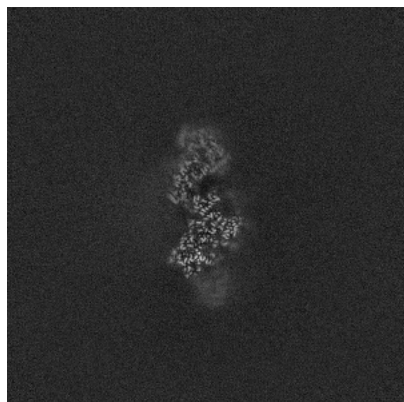


Y Index: 242

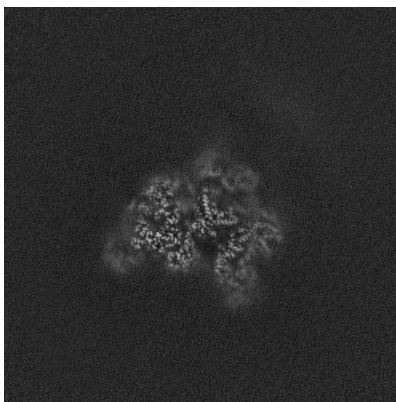


Z Index: 272

6.3.2 Raw map



X Index: 222



Y Index: 245

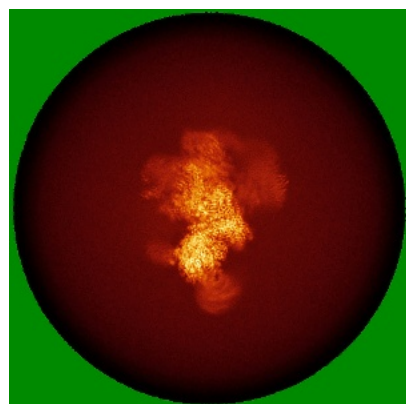


Z Index: 272

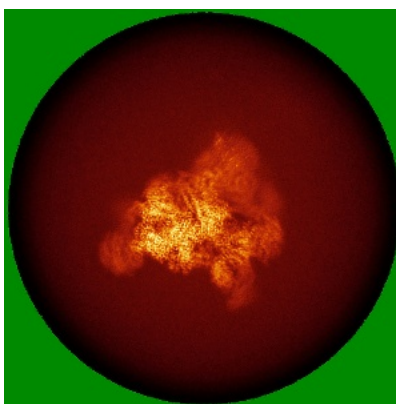
The images above show the largest variance slices of the map in three orthogonal directions.

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

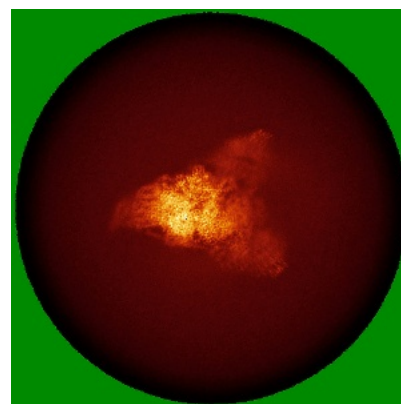
6.4.1 Primary map



X

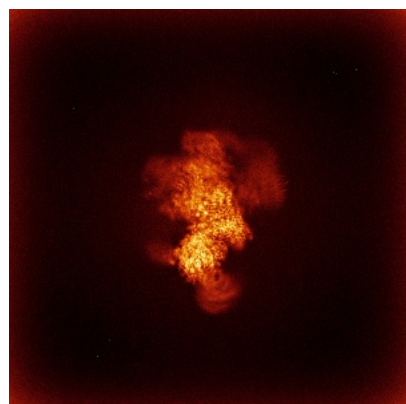


Y

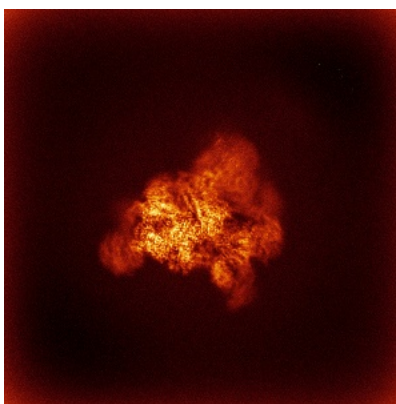


Z

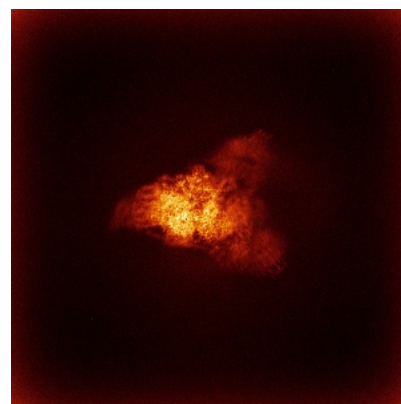
6.4.2 Raw map



X



Y

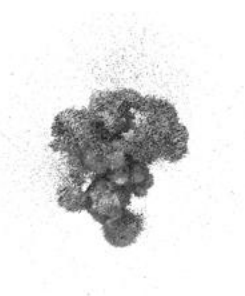


Z

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



X



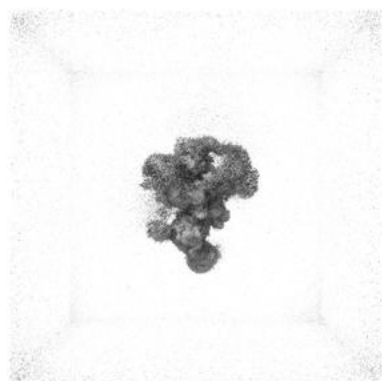
Y



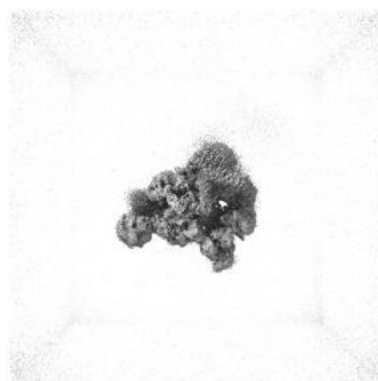
Z

The images above show the 3D surface view of the map at the recommended contour level 0.25. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

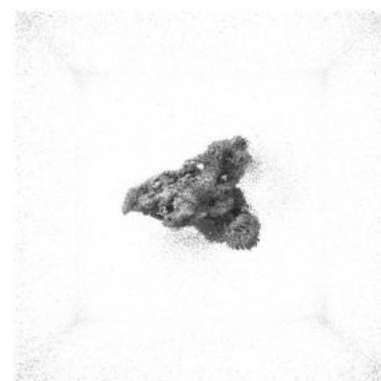
6.5.2 Raw map



X



Y



Z

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.

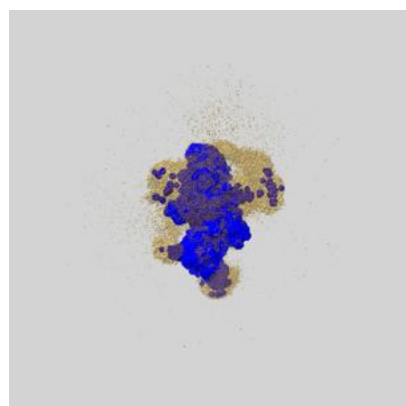
6.6 Mask visualisation [i](#)

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

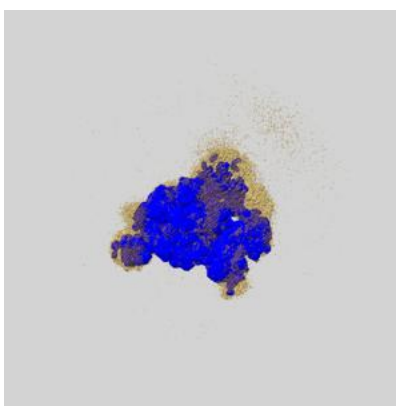
A mask typically either:

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

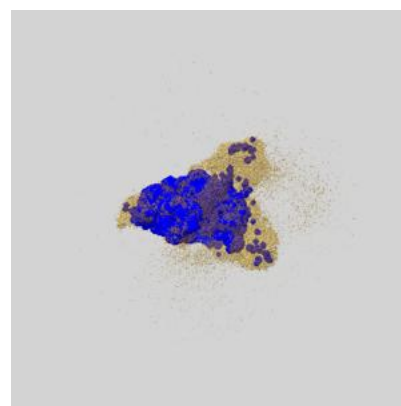
6.6.1 emd_34505_msk_1.map [i](#)



X



Y

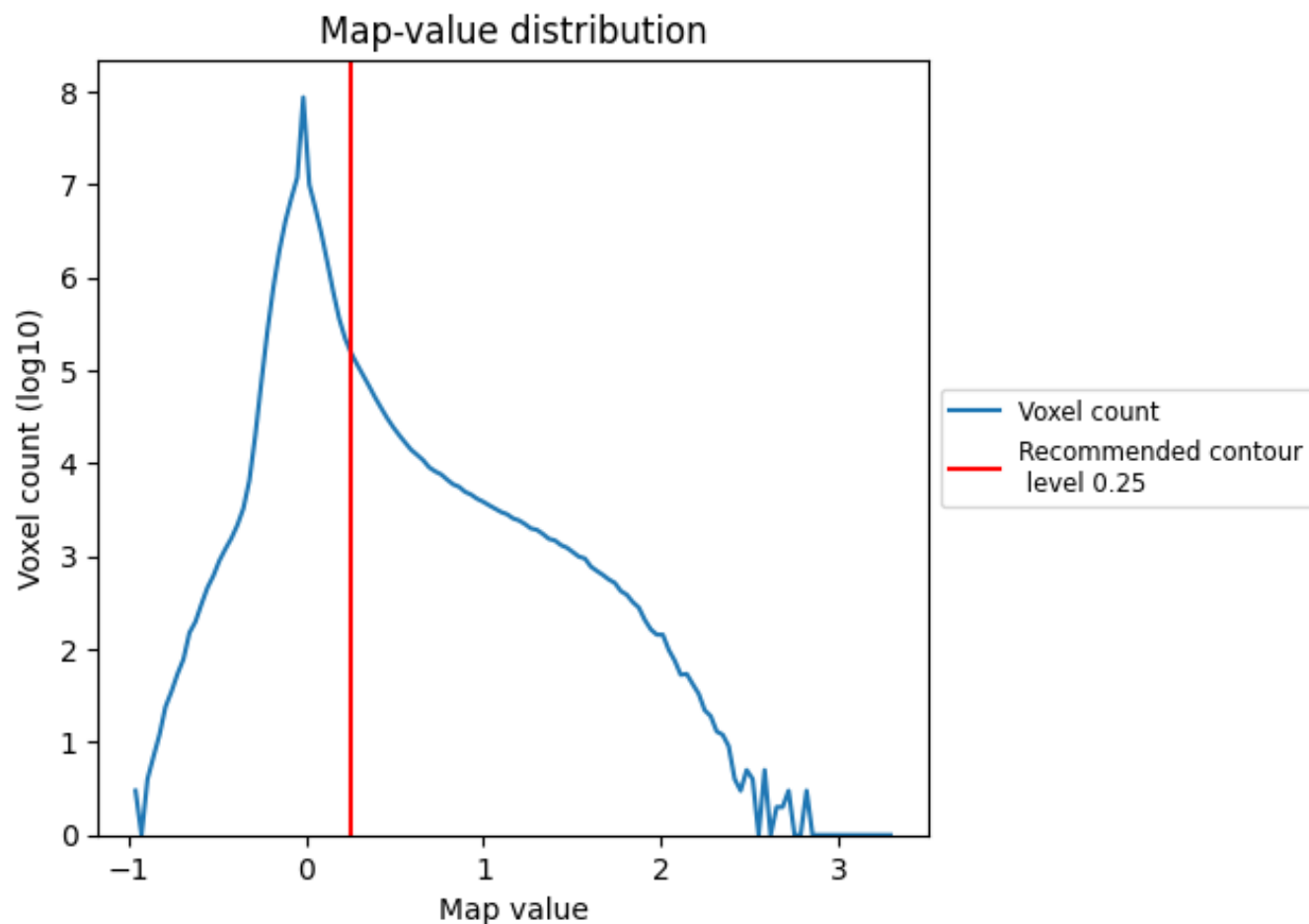


Z

7 Map analysis [i](#)

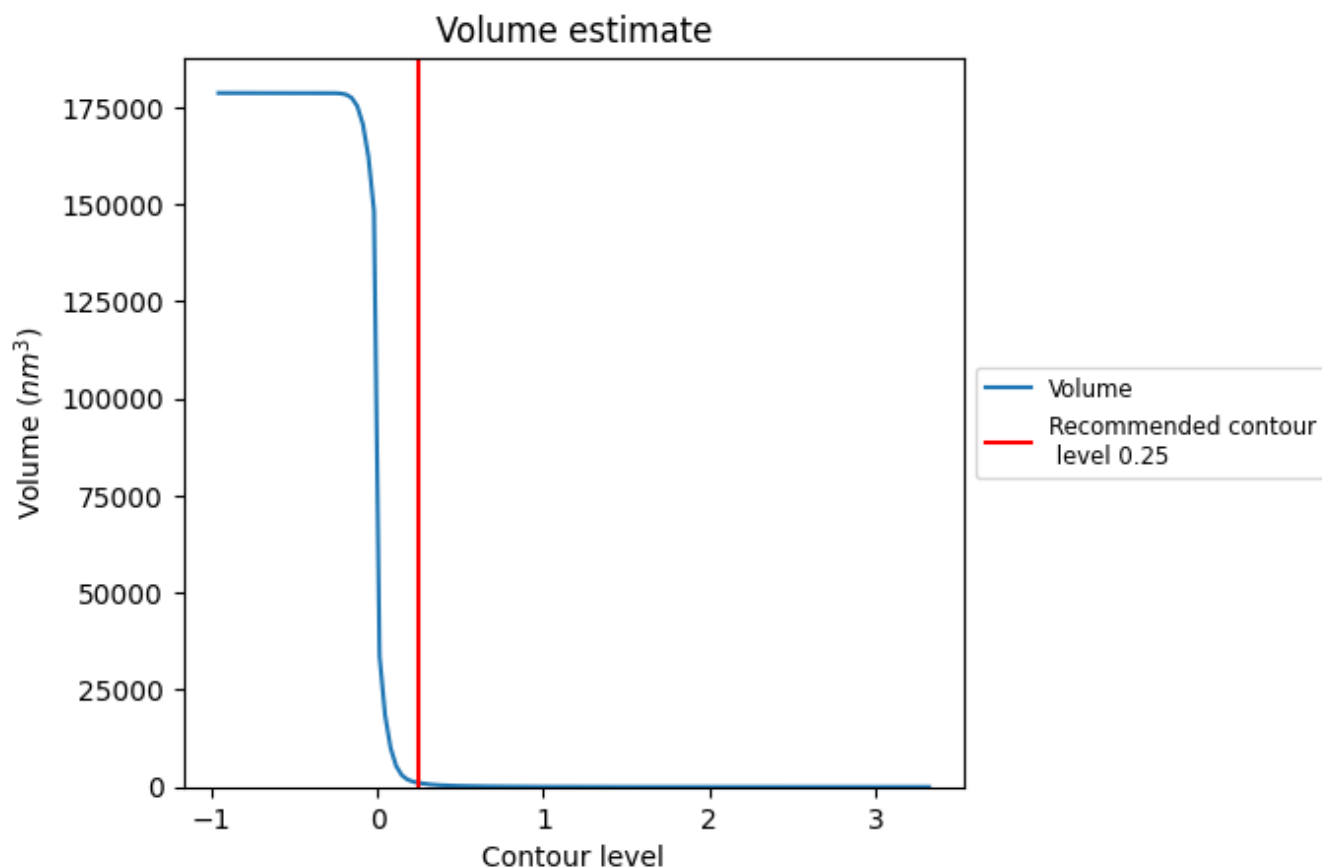
This section contains the results of statistical analysis of the map.

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.

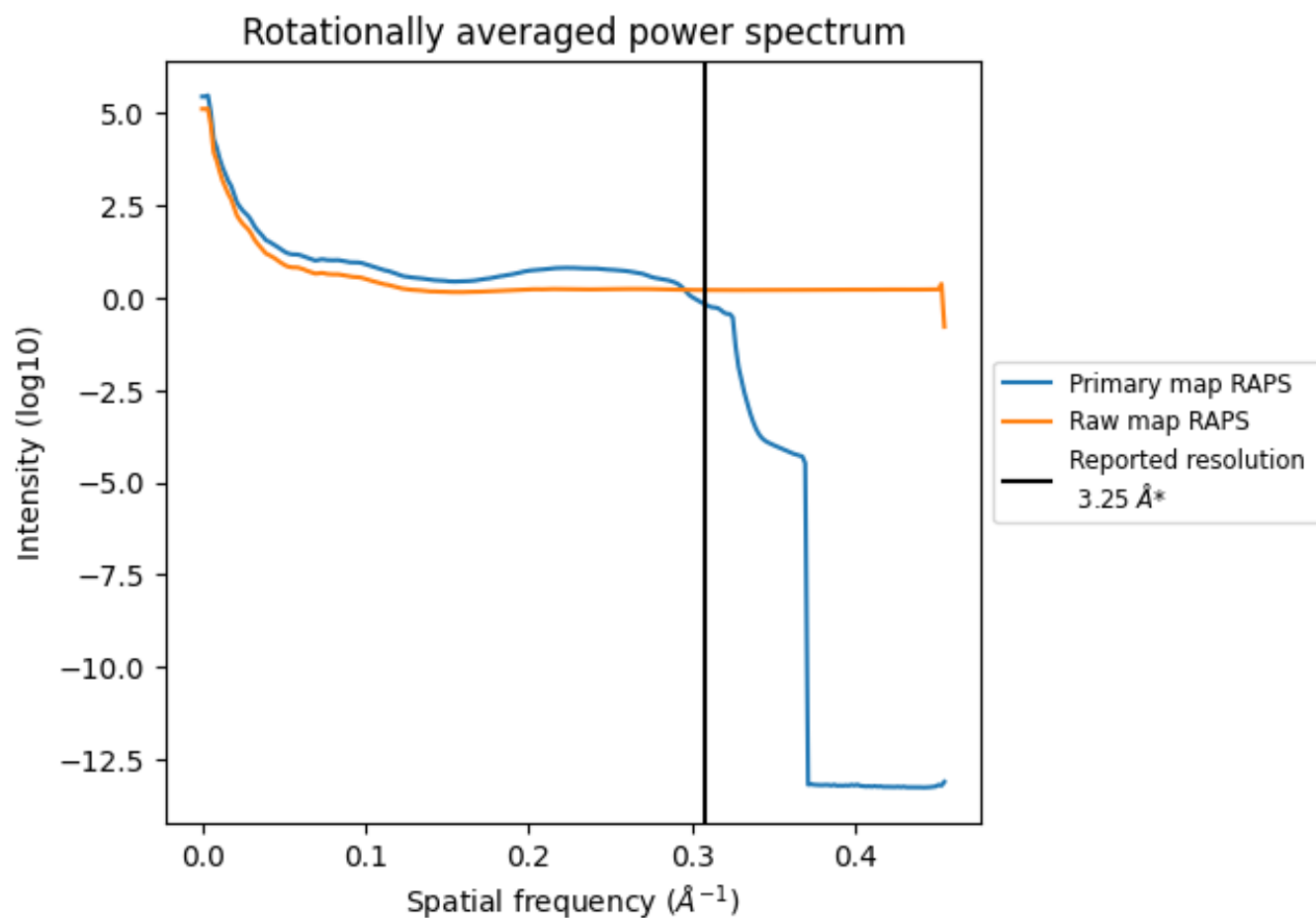
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1031 nm^3 ; this corresponds to an approximate mass of 932 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 ⓘ

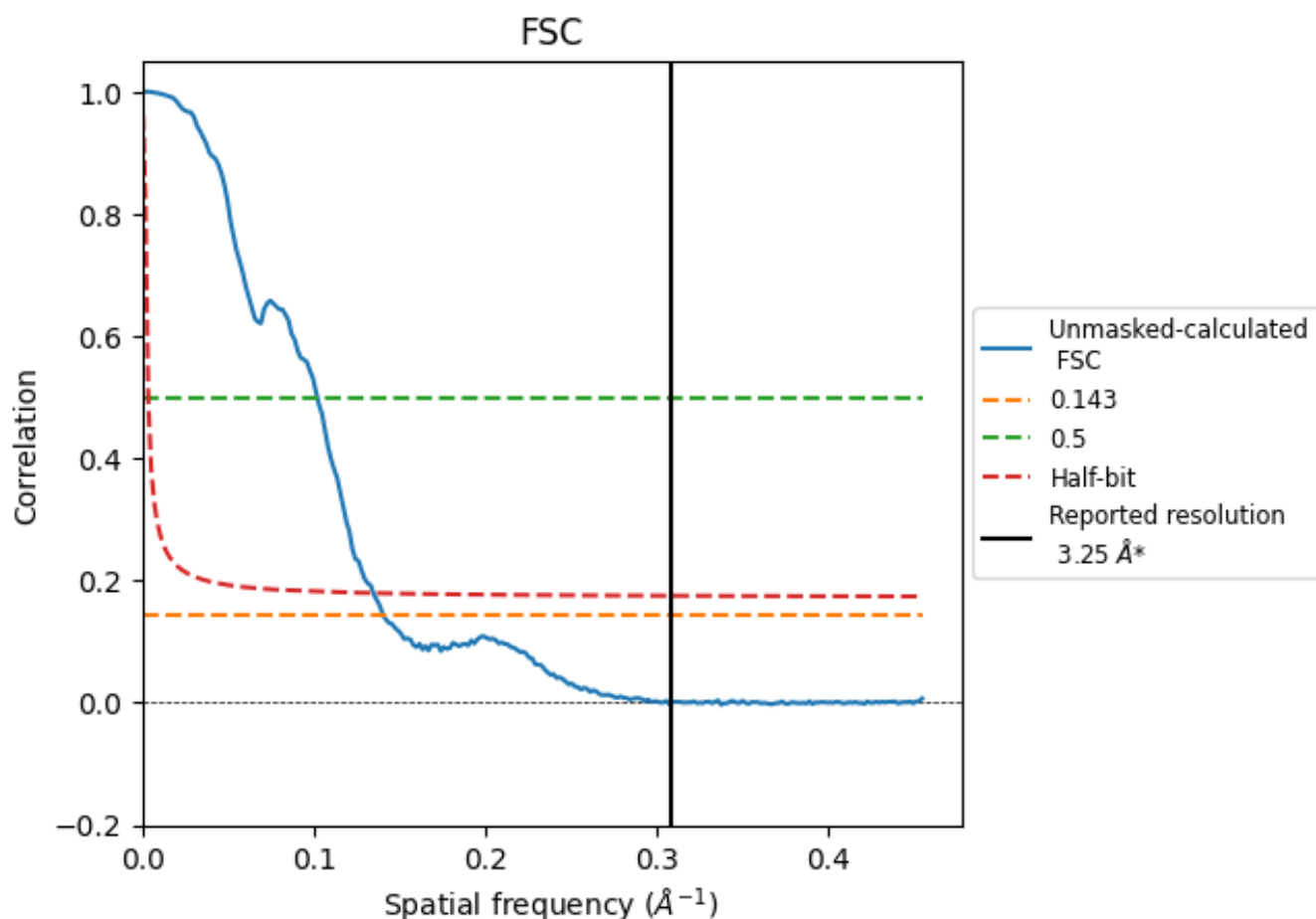


*Reported resolution corresponds to spatial frequency of 0.308 Å⁻¹

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 0.308 Å⁻¹

8.2 Resolution estimates [i](#)

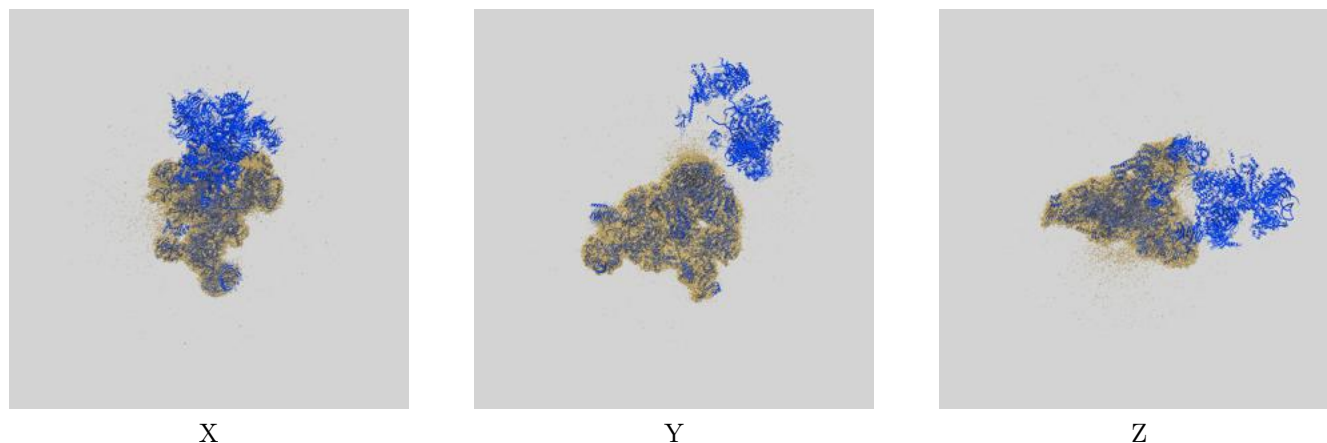
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.25	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.13	9.80	7.42

*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 7.13 differs from the reported value 3.25 by more than 10 %

9 Map-model fit [i](#)

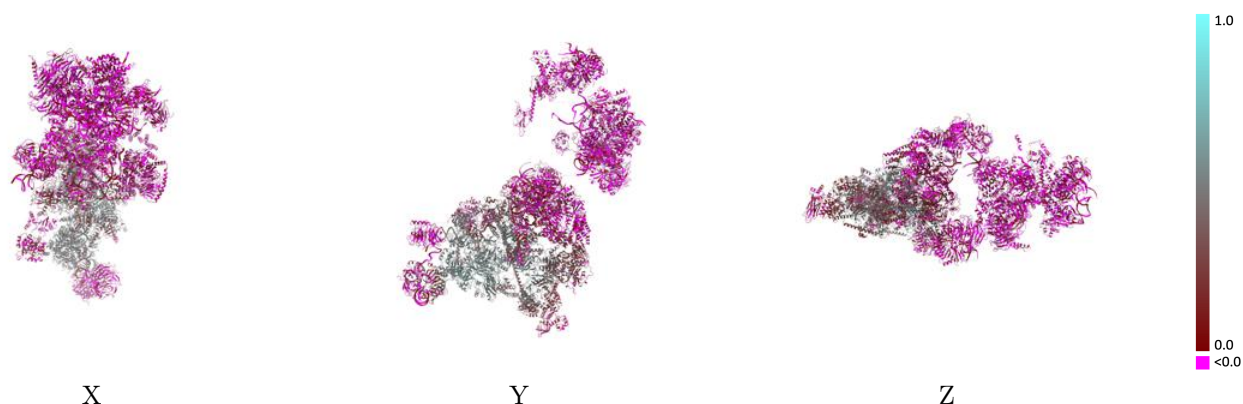
This section contains information regarding the fit between EMDB map EMD-34505 and PDB model 8H6J. Per-residue inclusion information can be found in [section 3](#) on [page 15](#).

9.1 Map-model overlay [i](#)



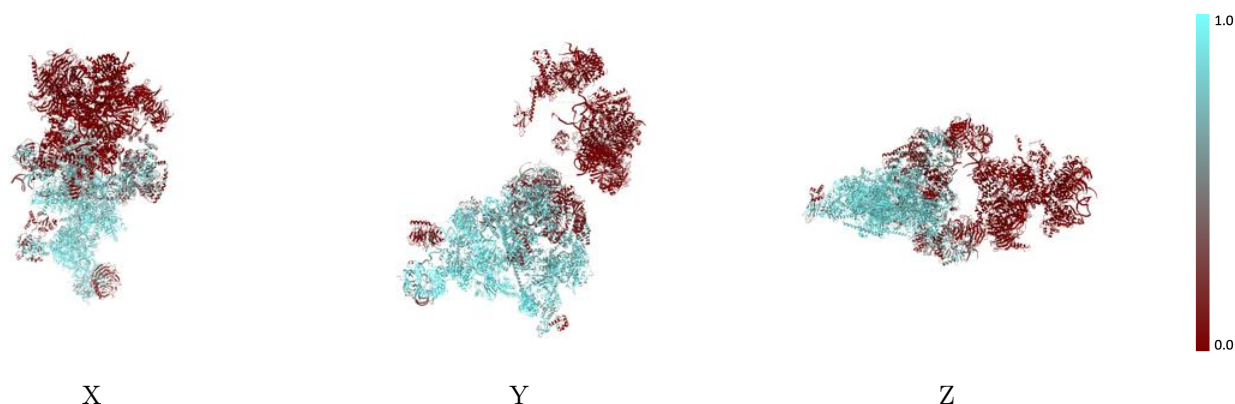
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



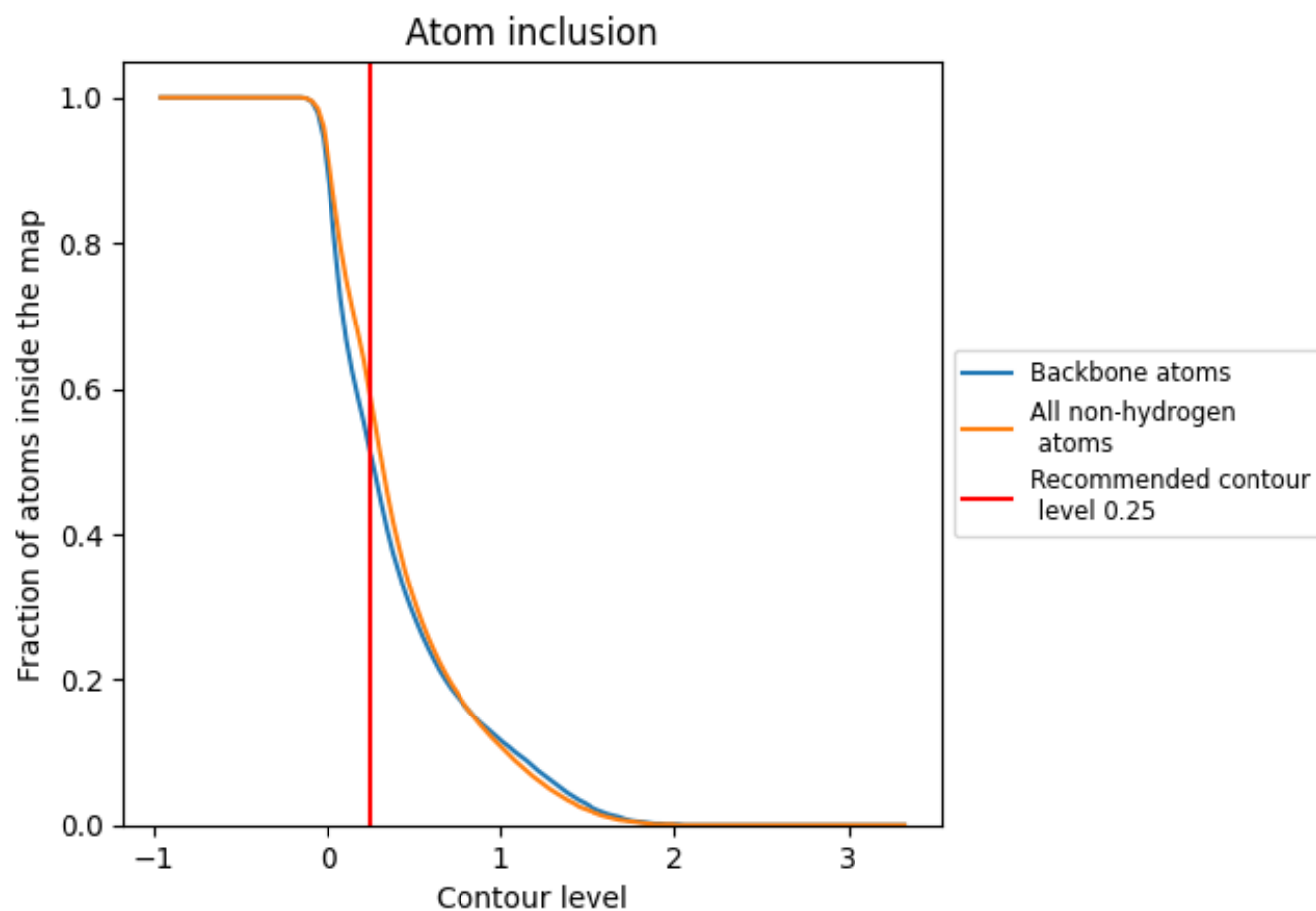
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.25).

9.4 Atom inclusion [i](#)



At the recommended contour level, 51% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5890	 0.2240
2A	 0.0010	 -0.0090
2B	 0.0000	 0.0020
2C	 0.0000	 -0.0250
2D	 0.0000	 -0.0050
2E	 0.0000	 -0.0070
2F	 0.0000	 -0.0040
2G	 0.0000	 -0.0130
2H	 0.0000	 -0.0150
2I	 0.0000	 -0.0050
2J	 0.0000	 0.0460
2K	 0.0000	 0.0320
2L	 0.0030	 0.0220
2M	 0.0040	 0.0130
2a	 0.0000	 -0.0400
2b	 0.0000	 0.0190
2c	 0.0000	 0.0430
2d	 0.0000	 -0.0030
2e	 0.0000	 0.0050
2f	 0.0040	 0.0320
2g	 0.0000	 -0.0340
4A	 0.6140	 0.0630
4B	 0.3690	 0.0180
4C	 0.4930	 0.0170
4D	 0.4580	 0.1080
4E	 0.6550	 0.1050
4F	 0.9280	 0.3440
4G	 0.6020	 0.1260
4R	 0.6290	 0.1390
4S	 0.7320	 0.2420
4T	 0.9740	 0.4940
4U	 0.5510	 0.1870
4X	 0.6610	 0.0650
4Y	 0.0040	 0.0250
4a	 0.5210	 0.0460



Continued on next page...

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Chain	Atom inclusion	Q-score
4b	 0.5810	 0.0520
4c	 0.3080	 0.0180
4d	 0.3190	 0.0190
4e	 0.4070	 0.0180
4f	 0.4790	 0.0320
4g	 0.4910	 0.0270
5A	 0.8090	 0.2300
5B	 0.9200	 0.4330
5C	 0.9680	 0.5180
5D	 0.8510	 0.3060
5E	 0.0920	 -0.0080
5a	 0.7880	 0.1740
5b	 0.8840	 0.1430
5c	 0.7550	 0.0820
5d	 0.7940	 0.0890
5e	 0.8700	 0.1520
5f	 0.8580	 0.2450
5g	 0.9770	 0.3590
6A	 0.5270	 0.0800
6a	 0.0000	 -0.0160
6b	 0.0000	 0.0040
6c	 0.0000	 0.0300
6d	 0.0000	 0.0130
6e	 0.0000	 0.0170
6f	 0.0000	 0.0310
6g	 0.0000	 0.0220
A	 0.0000	 -0.0130