



wwPDB EM Validation Summary Report ⓘ

Mar 25, 2026 – 06:00 AM UTC

PDB ID : 8H6L / pdb_00008h6l
EMDB ID : EMD-34508
Title : Cryo-EM structure of human exon-defined spliceosome in the early B state.
Authors : Zhang, W.; Zhan, X.; Zhang, X.; Bai, R.; Lei, J.; Yan, C.; Shi, Y.
Deposited on : 2022-10-18
Resolution : 2.60 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:

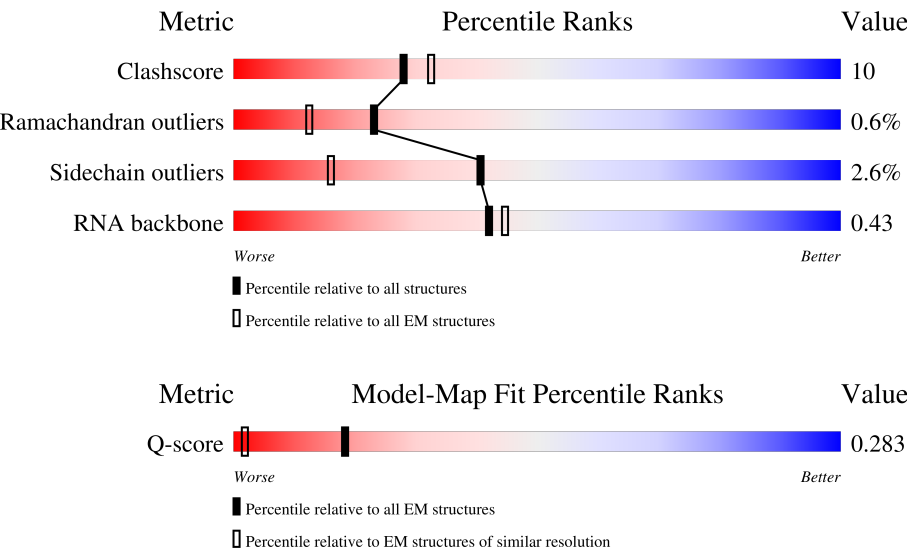
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.60 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.



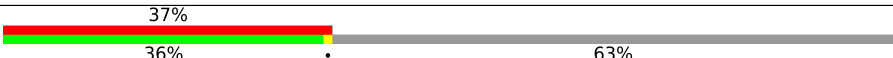
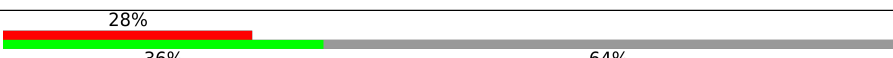
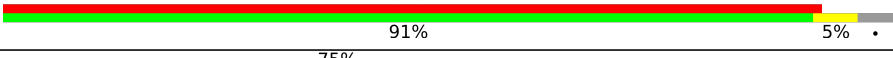
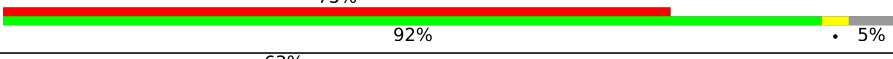
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	8728 (2.10 - 3.10)

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	
2	5A	117	
3	5B	2335	

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Mol	Chain	Length	Quality of chain
4	5C	972	
5	5D	2136	
6	5E	357	
7	2a	231	
7	4a	231	
7	5a	231	
8	2b	119	
8	4b	119	
8	5b	119	
9	2c	118	
9	4c	118	
9	5c	118	
10	2d	86	
10	4d	86	
10	5d	86	
11	2e	92	
11	4e	92	
11	5e	92	
12	2f	76	
12	4f	76	
12	5f	76	
13	2g	126	
13	4g	126	
13	5g	126	
14	6A	107	

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Mol	Chain	Length	Quality of chain
15	6a	95	
16	6b	102	
17	6c	139	
18	6d	91	
19	6e	80	
20	6f	103	
21	6g	96	
22	4A	145	
23	4B	683	
24	4C	522	
25	4D	499	
26	4E	128	
27	4F	142	
28	4G	941	
29	4H	177	
30	4I	376	
31	4J	800	
32	4Z	513	
33	2A	188	
34	2B	255	
35	2C	225	
36	2D	793	
37	2E	464	
38	2F	501	
39	2G	1304	

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Mol	Chain	Length	Quality of chain
40	2H	895	
41	2I	1217	
42	2J	424	
43	2K	125	
44	2L	110	
45	2M	86	

2 Entry composition

There are 49 unique types of molecules in this entry. The entry contains 94667 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	57	Total	C	N	O	P	0	0
			1187	531	183	416	57		

- Molecule 2 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	5A	115	Total	C	N	O	P	0	0
			2420	1084	403	818	115		

- Molecule 3 is a protein called Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	5B	2253	Total	C	N	O	S	0	0
			18642	11992	3250	3319	81		

- Molecule 4 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	5C	818	Total	C	N	O	S	0	0
			6436	4114	1085	1205	32		

- Molecule 5 is a protein called U5 small nuclear ribonucleoprotein 200 kDa helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5D	1696	Total	C	N	O	S	0	0
			13633	8715	2329	2519	70		

- Molecule 6 is a protein called U5 small nuclear ribonucleoprotein 40 kDa protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	5E	299	Total	C	N	O	0	0
			1196	598	299	299		

- Molecule 7 is a protein called Isoform SM-B of Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	5a	84	Total	C	N	O	0	0
			336	168	84	84		
7	4a	64	Total	C	N	O	0	0
			256	128	64	64		
7	2a	86	Total	C	N	O	0	0
			344	172	86	86		

- Molecule 8 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	5b	82	Total	C	N	O	0	0
			328	164	82	82		
8	4b	82	Total	C	N	O	0	0
			334	170	82	82		
8	2b	82	Total	C	N	O	0	0
			328	164	82	82		

- Molecule 9 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	5c	97	Total	C	N	O	0	0
			388	194	97	97		
9	4c	74	Total	C	N	O	0	0
			300	152	74	74		
9	2c	85	Total	C	N	O	0	0
			340	170	85	85		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
10	5d	74	Total	C	N	O	0	0
			296	148	74	74		
10	4d	71	Total	C	N	O	0	0
			292	150	71	71		
10	2d	74	Total	C	N	O	0	0
			296	148	74	74		

- Molecule 11 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	5e	79	Total	C	N	O	0	0
			316	158	79	79		
11	4e	78	Total	C	N	O	0	0
			314	158	78	78		
11	2e	79	Total	C	N	O	0	0
			316	158	79	79		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
12	5f	72	Total	C	N	O	0	0
			288	144	72	72		
12	4f	73	Total	C	N	O	0	0
			298	152	73	73		
12	2f	68	Total	C	N	O	0	0
			272	136	68	68		

- Molecule 13 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	5g	76	Total	C	N	O	0	0
			304	152	76	76		
13	4g	71	Total	C	N	O	0	0
			288	146	71	71		
13	2g	80	Total	C	N	O	0	0
			320	160	80	80		

- Molecule 14 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	6A	59	Total	C	N	O	P	0	0
			1251	558	230	404	59		

- Molecule 15 is a protein called U6 snRNA-associated Sm-like protein LSm2.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	6a	90	Total	C	N	O	0	0
			360	180	90	90		

- Molecule 16 is a protein called U6 snRNA-associated Sm-like protein LSm3.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	6b	74	Total	C	N	O	0	0
			296	148	74	74		

- Molecule 17 is a protein called U6 snRNA-associated Sm-like protein LSm4.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	6c	74	Total	C	N	O	0	0
			296	148	74	74		

- Molecule 18 is a protein called U6 snRNA-associated Sm-like protein LSm5.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	6d	72	Total	C	N	O	0	0
			288	144	72	72		

- Molecule 19 is a protein called U6 snRNA-associated Sm-like protein LSm6.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	6e	70	Total	C	N	O	0	0
			280	140	70	70		

- Molecule 20 is a protein called U6 snRNA-associated Sm-like protein LSm7.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	6f	65	Total	C	N	O	0	0
			260	130	65	65		

- Molecule 21 is a protein called U6 snRNA-associated Sm-like protein LSm8.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	6g	61	Total	C	N	O	0	0
			244	122	61	61		

- Molecule 22 is a RNA chain called U4 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	4A	129	Total	C	N	O	P	0	0
			2744	1225	472	917	130		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	4B	256	Total	C	N	O	S	0	0
			2076	1316	385	367	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	4C	426	Total	C	N	O	S	0	0
			3370	2118	612	620	20		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	4D	376	Total	C	N	O	S	0	0
			2874	1788	524	550	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	4E	124	Total	C	N	O	S	0	0
			962	608	171	178	5		

- 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	801	Total	C	N	O	S	0	0
			5504	3419	1043	1026	16		

- Molecule 29 is a protein called Peptidyl-prolyl cis-trans isomerase H.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	4H	169	Total	C	N	O	0	0
			844	506	169	169		

- Molecule 30 is a protein called WW domain-binding protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	4I	75	Total	C	N	O	S	0	0
			494	304	96	91	3		

- Molecule 31 is a protein called U4/U6.U5 tri-snRNP-associated protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	4J	153	Total	C	N	O	S	0	0
			1153	715	206	230	2		

- Molecule 32 is a protein called WD40 repeat-containing protein SMU1.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	4Z	420	Total	C	N	O	0	0
			2093	1253	420	420		

- Molecule 33 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	2A	109	Total	C	N	O	P	0	0
			2311	1032	396	774	109		

- Molecule 34 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	2B	162	Total	C	N	O	0	0
			648	324	162	162		

- Molecule 35 is a protein called U2 small nuclear ribonucleoprotein B'.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	2C	94	Total	C	N	O	0	0
			376	188	94	94		

- Molecule 36 is a protein called Splicing factor 3A subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	2D	236	Total	C	N	O	S	0	0
			1380	793	285	299	3		

- Molecule 37 is a protein called Splicing factor 3A subunit 2.

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
38	2F	423	Total	C	N	O	0	0
			1693	847	423	423		

- Molecule 39 is a protein called Splicing factor 3B subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	2G	1048	Total	C	N	O	0	0
			4192	2096	1048	1048		

- Molecule 40 is a protein called Splicing factor 3B subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	2H	213	Total	C	N	O	S	0	0
			959	510	220	226	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
41	2I	1168	Total	C	N	O	0	0
			4672	2336	1168	1168		

- Molecule 42 is a protein called Splicing factor 3B subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	2J	78	Total	C	N	O	0	0
			312	156	78	78		

- Molecule 43 is a protein called Splicing factor 3B subunit 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	2K	108	Total	C	N	O	0	0
			432	216	108	108		

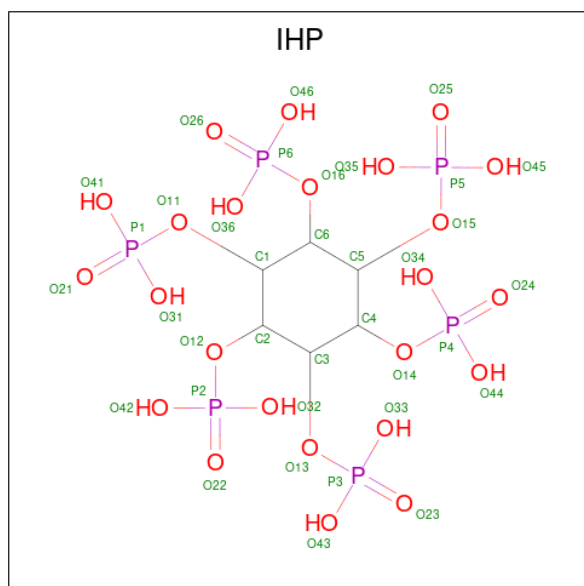
- Molecule 44 is a protein called PHD finger-like domain-containing protein 5A.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	2L	89	Total	C	N	O	0	0
			356	178	89	89		

- Molecule 45 is a protein called Splicing factor 3B subunit 5.

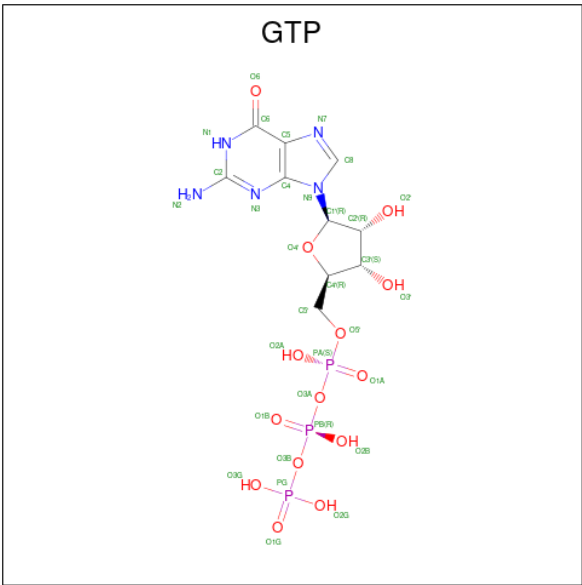
Mol	Chain	Residues	Atoms				AltConf	Trace
45	2M	66	Total	C	N	O	0	0
			264	132	66	66		

- Molecule 46 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: $C_6H_{18}O_{24}P_6$).



Mol	Chain	Residues	Atoms				AltConf
46	5B	1	Total	C	O	P	0
			36	6	24	6	

- Molecule 47 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
47	5C	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 48 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
48	5C	1	Total	Mg	0
			1	1	

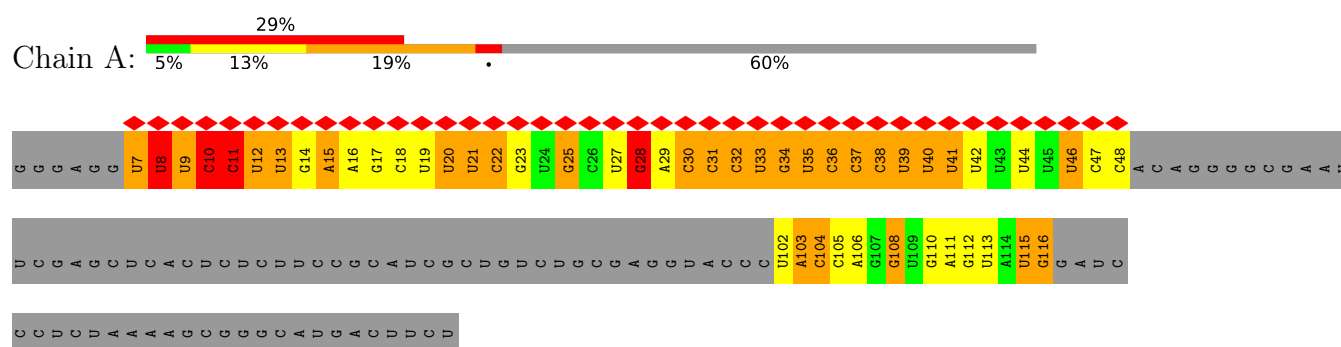
- Molecule 49 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
49	4I	1	Total	Zn	0
			1	1	

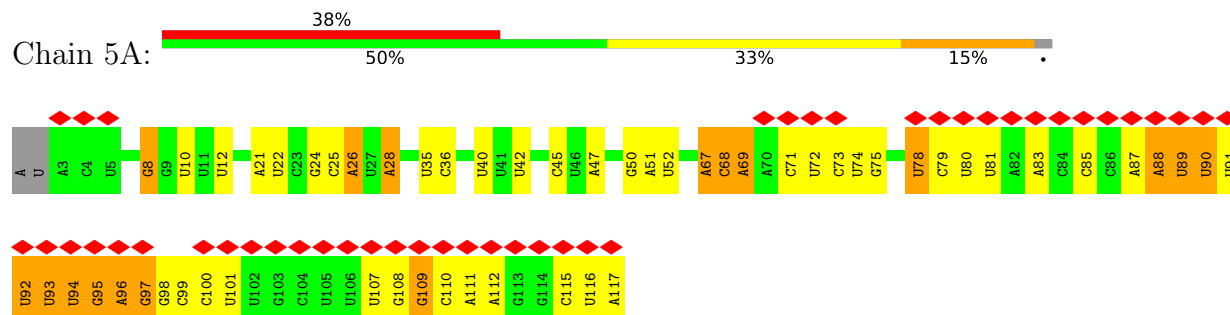
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

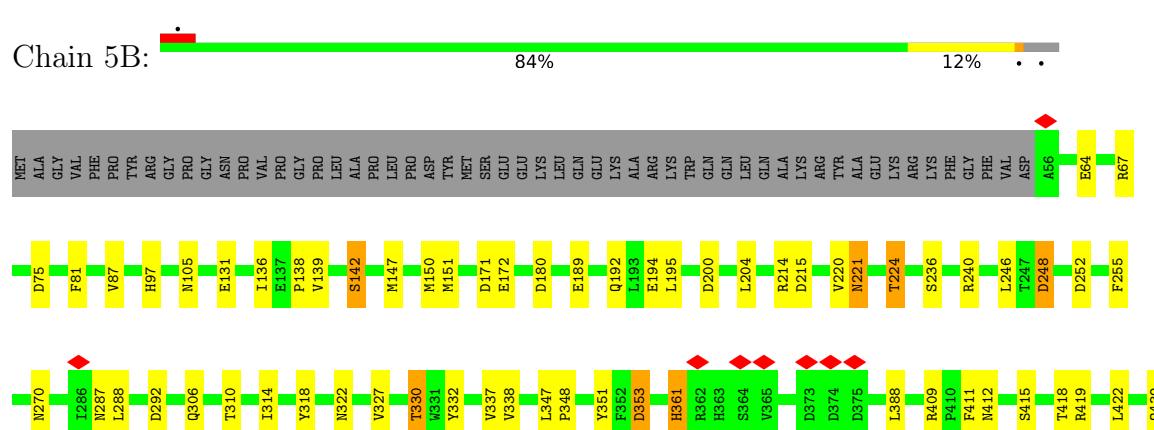
• Molecule 1: pre-mRNA



• Molecule 2: U5 snRNA



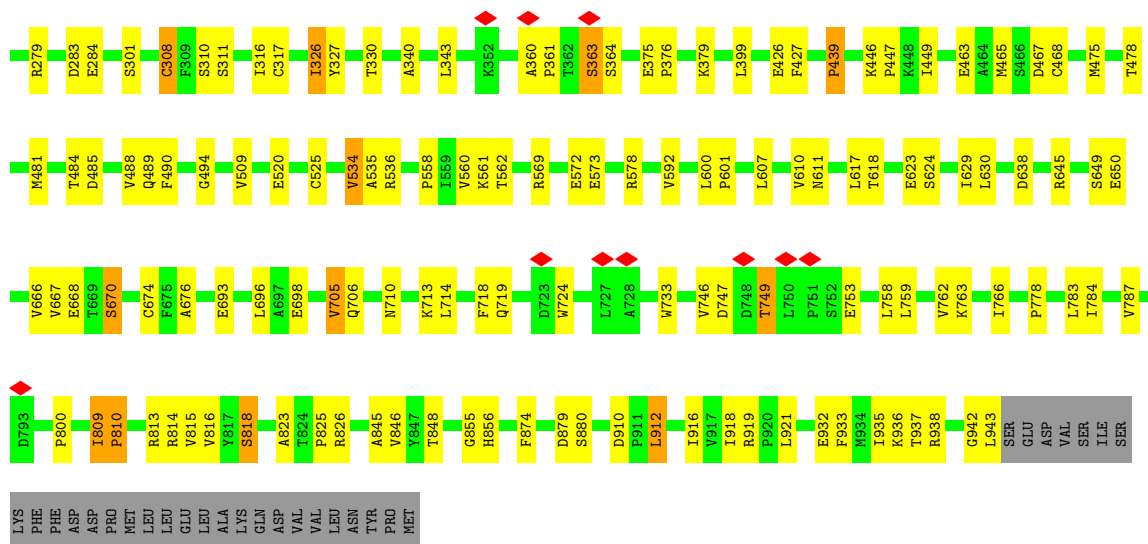
• Molecule 3: Pre-mRNA-processing-splicing factor 8



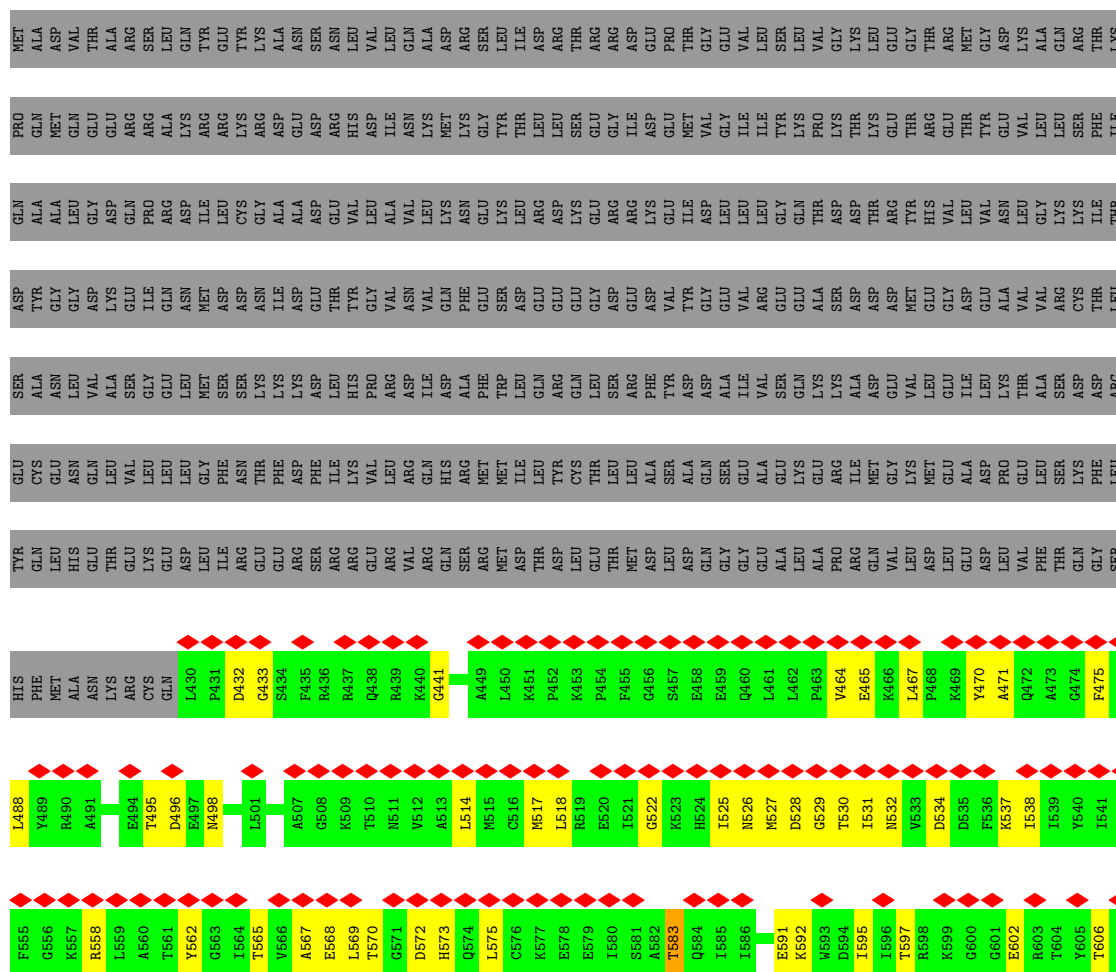


- Molecule 4: 116 kDa U5 small nuclear ribonucleoprotein component



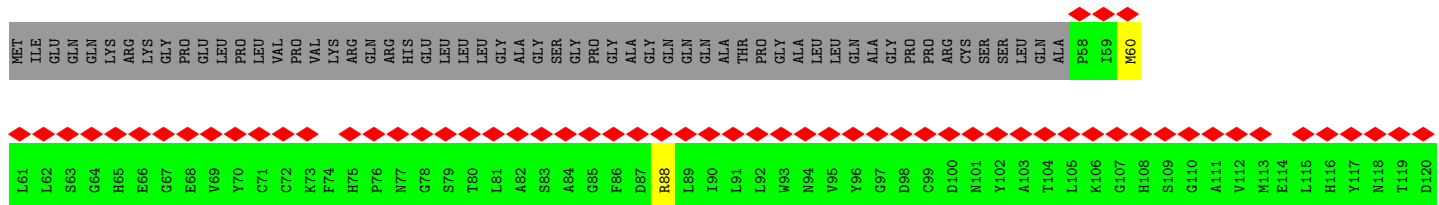
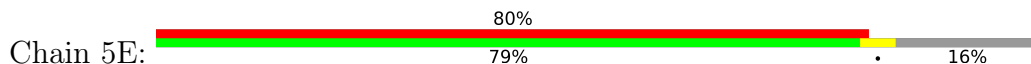


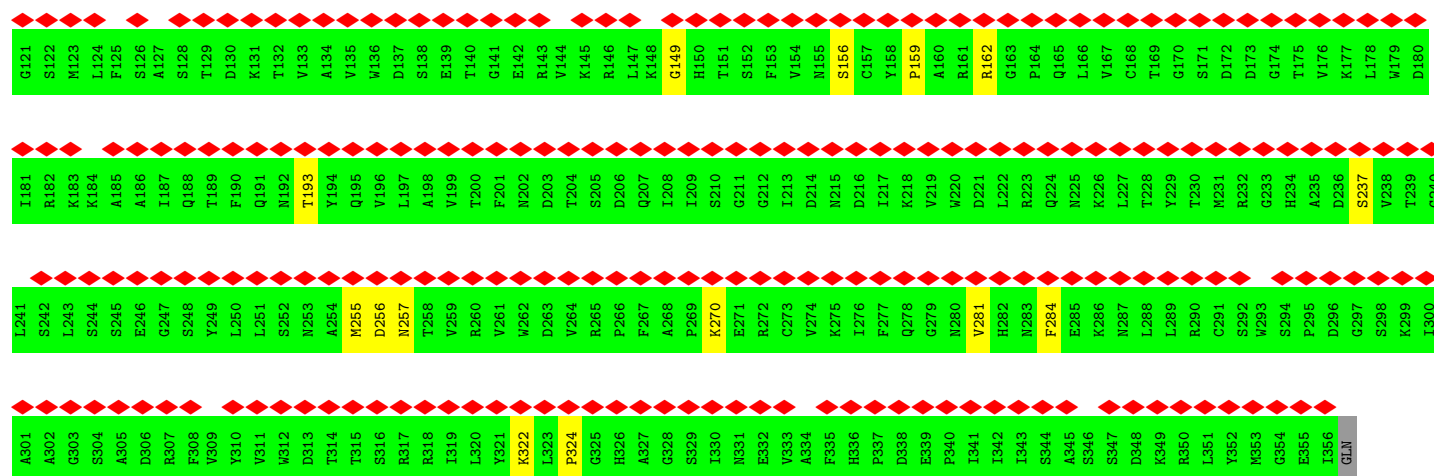
● Molecule 5: U5 small nuclear ribonucleoprotein 200 kDa helicase



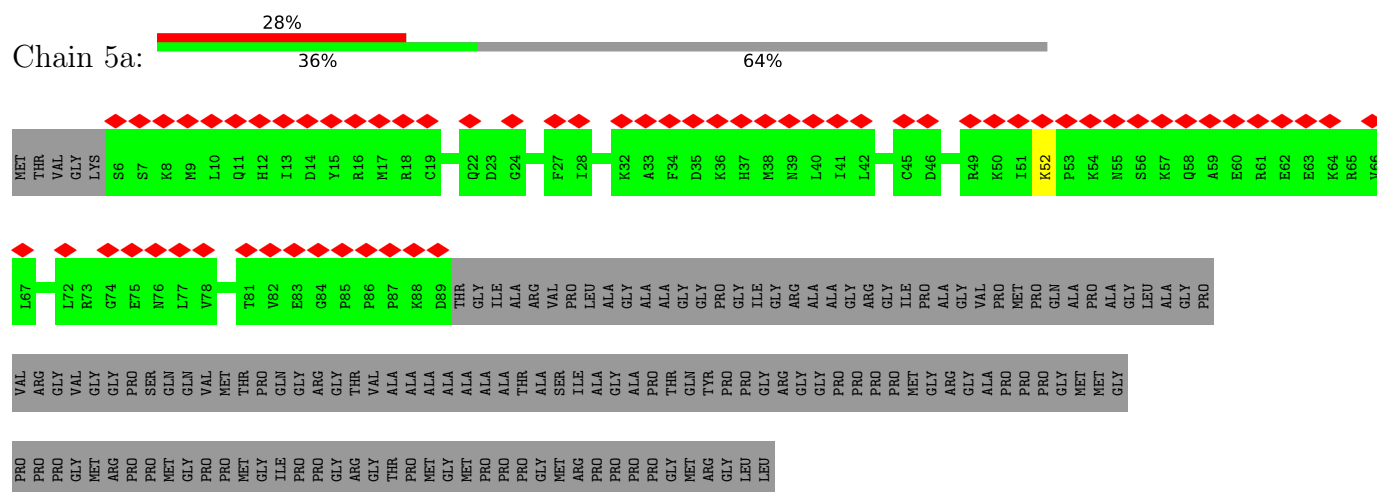


- Molecule 6: U5 small nuclear ribonucleoprotein 40 kDa protein

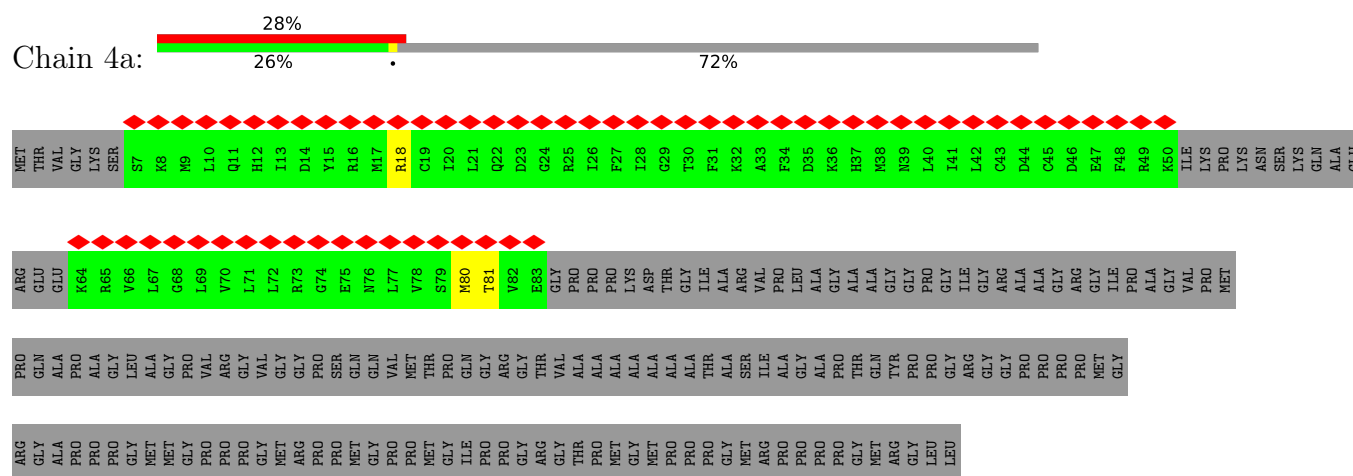




- Molecule 7: Isoform SM-B of Small nuclear ribonucleoprotein-associated proteins B and B'

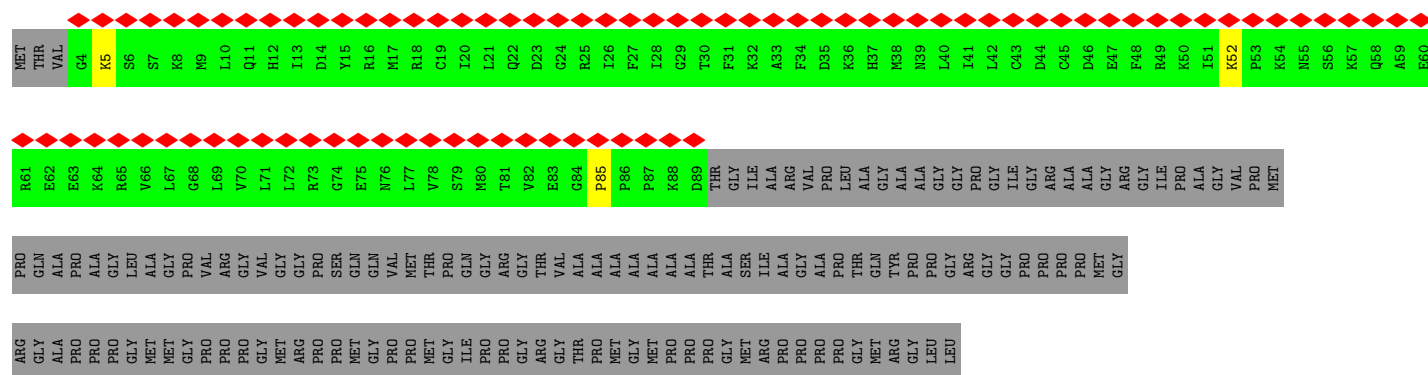


- Molecule 7: Isoform SM-B of Small nuclear ribonucleoprotein-associated proteins B and B'

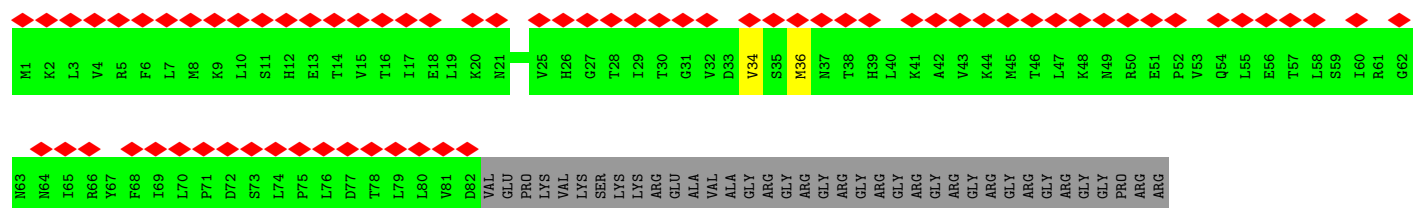


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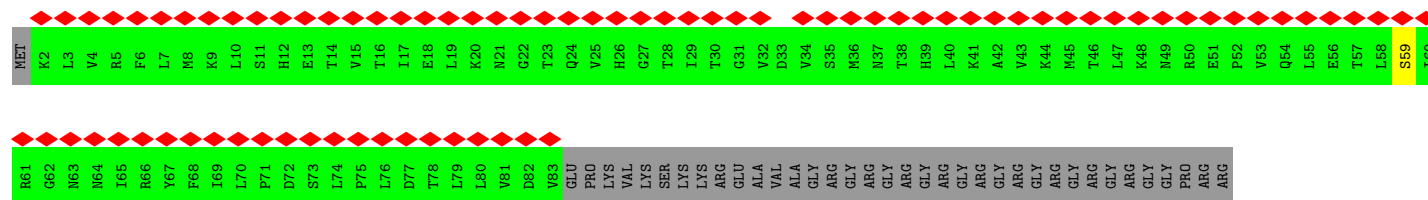




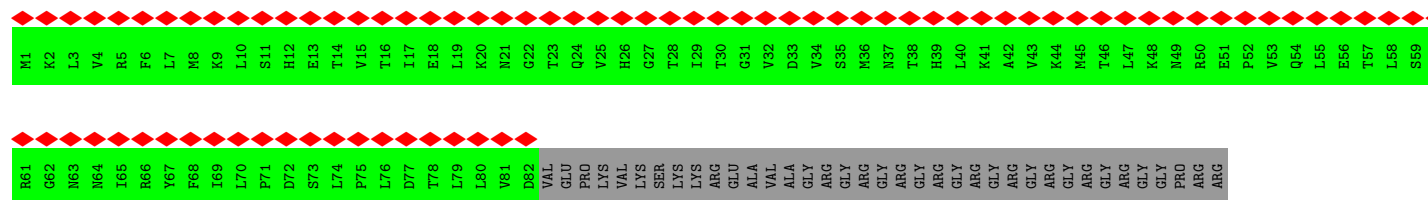
• Molecule 8: Small nuclear ribonucleoprotein Sm D1



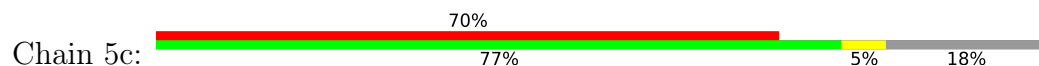
• Molecule 8: Small nuclear ribonucleoprotein Sm D1



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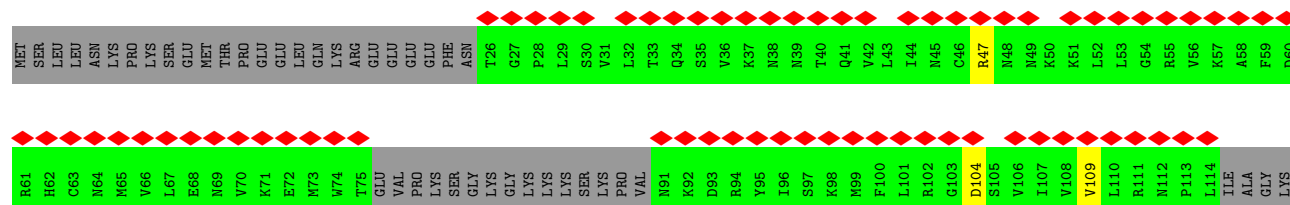


• Molecule 9: Small nuclear ribonucleoprotein Sm D2





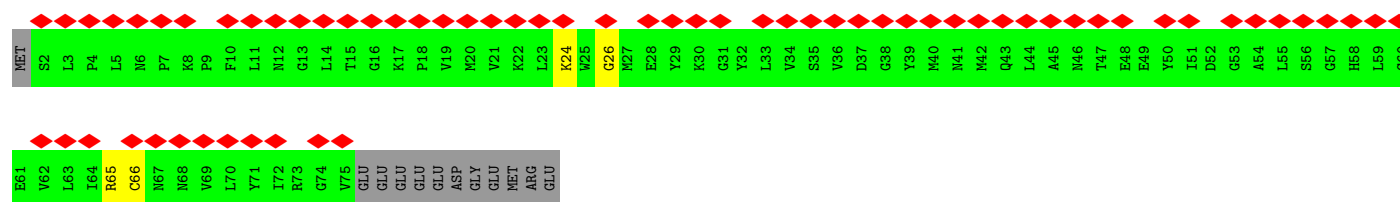
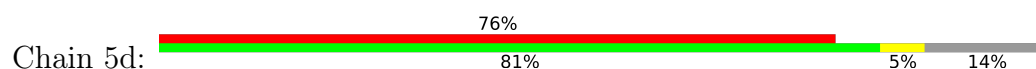
• Molecule 9: Small nuclear ribonucleoprotein Sm D2



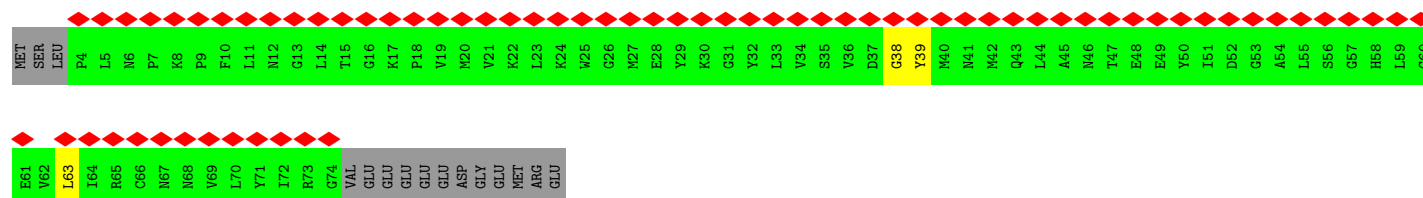
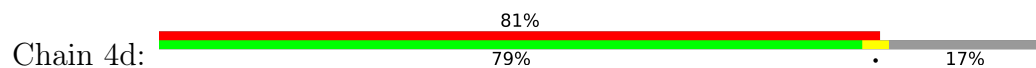
• Molecule 9: Small nuclear ribonucleoprotein Sm D2



• Molecule 10: Small nuclear ribonucleoprotein F

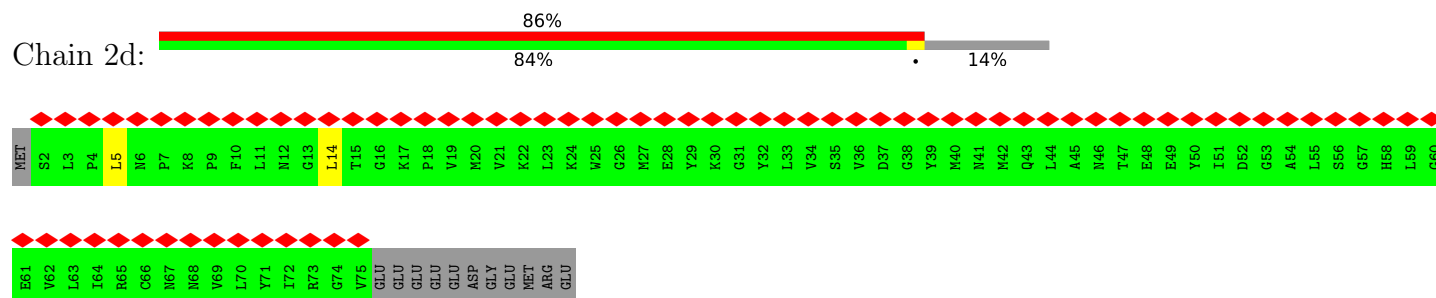


• Molecule 10: Small nuclear ribonucleoprotein F



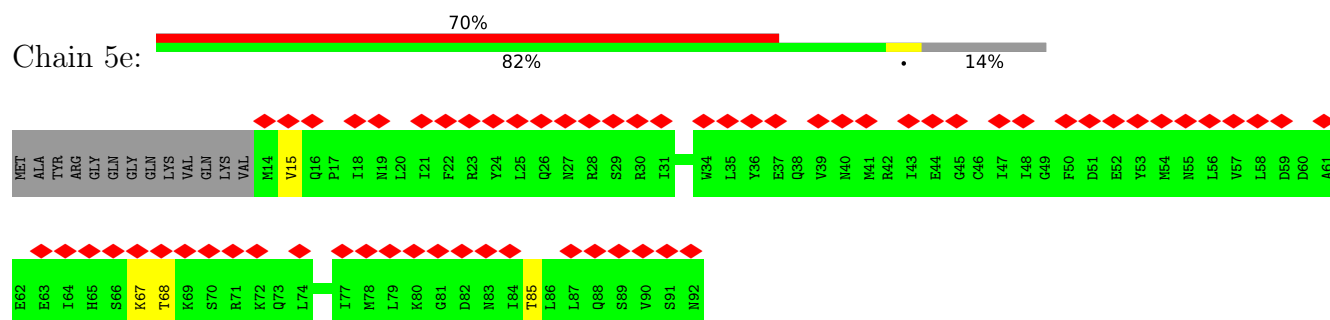
• Molecule 10: Small nuclear ribonucleoprotein F

Chain 2d:



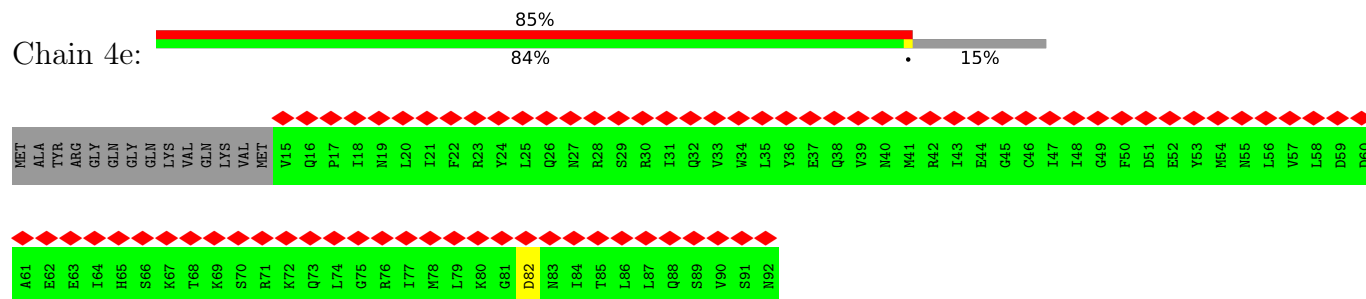
• Molecule 11: Small nuclear ribonucleoprotein E

Chain 5e:



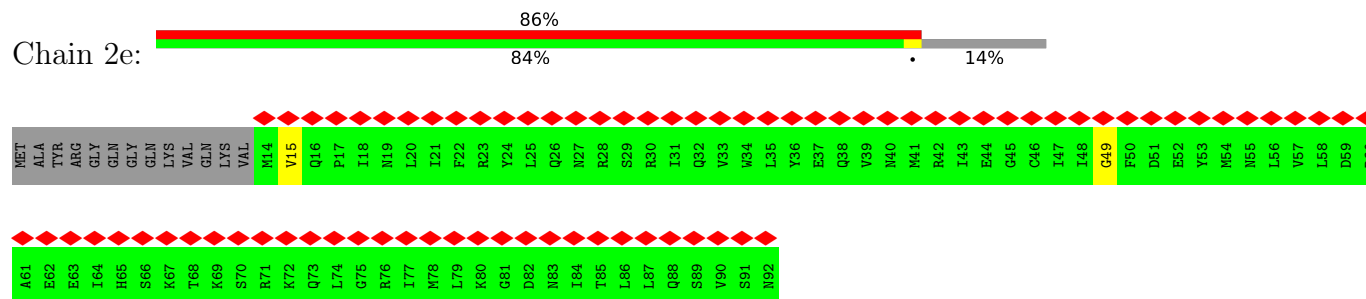
• Molecule 11: Small nuclear ribonucleoprotein E

Chain 4e:



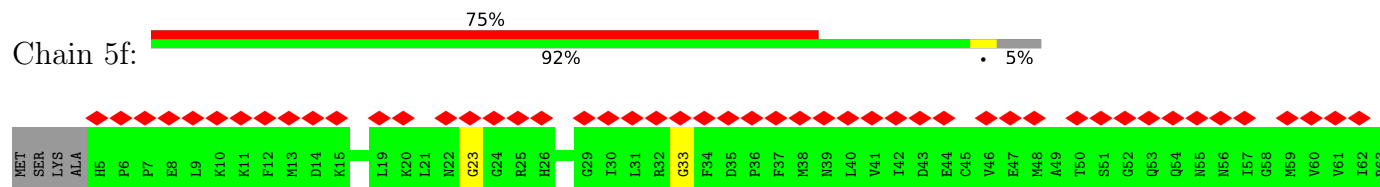
• Molecule 11: Small nuclear ribonucleoprotein E

Chain 2e:

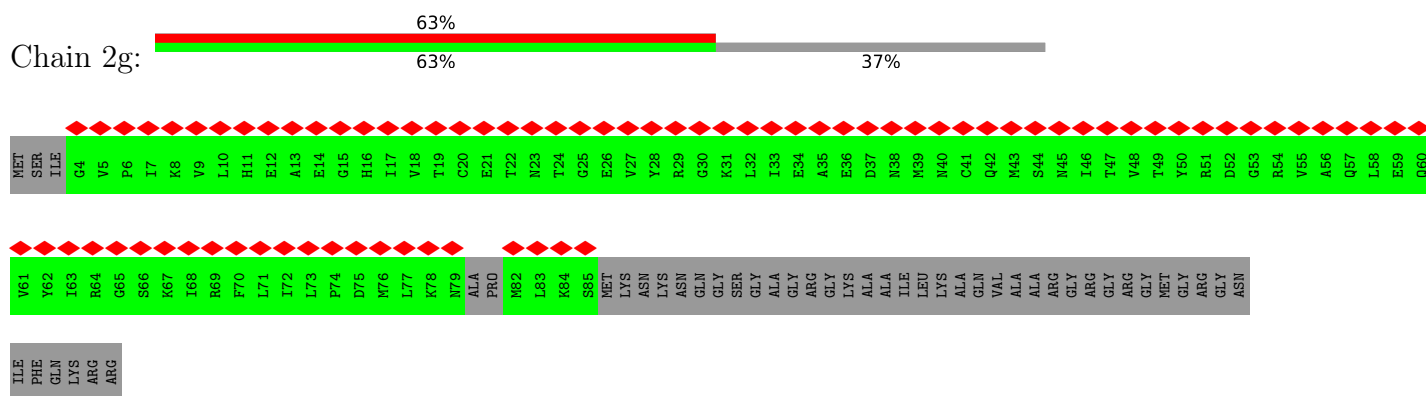


• Molecule 12: Small nuclear ribonucleoprotein G

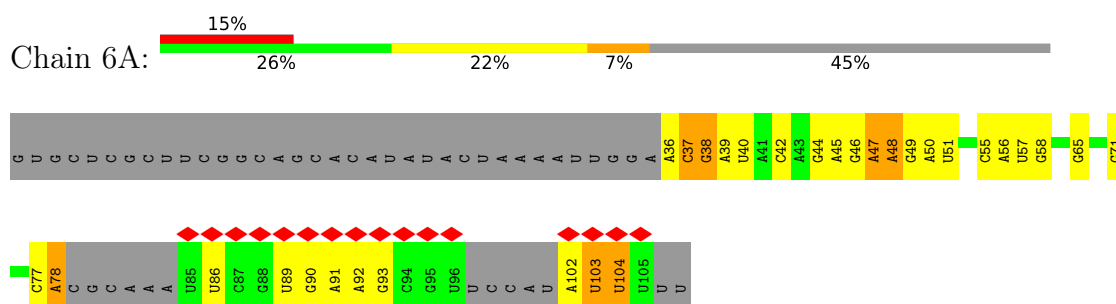
Chain 5f:



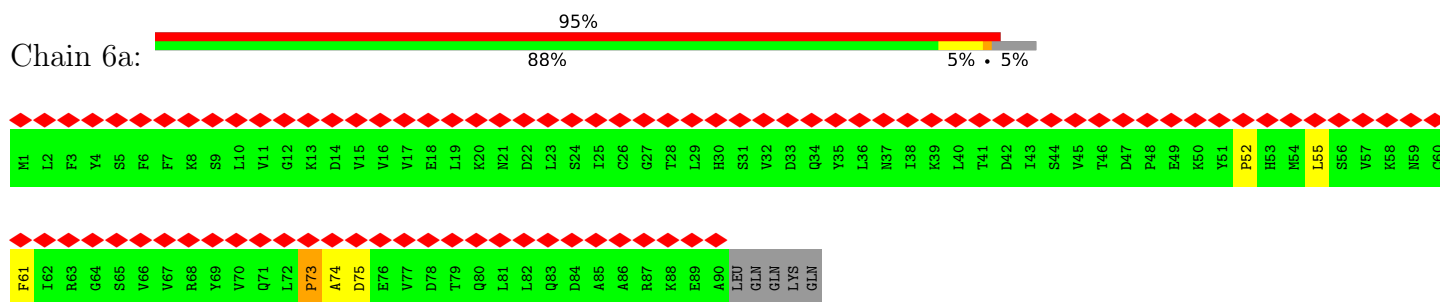
- Molecule 13: Small nuclear ribonucleoprotein Sm D3



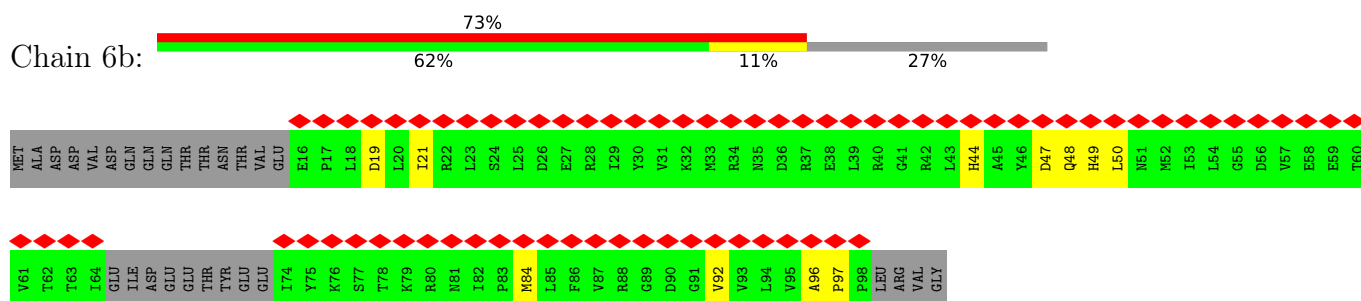
- Molecule 14: U6 snRNA



- Molecule 15: U6 snRNA-associated Sm-like protein LSm2

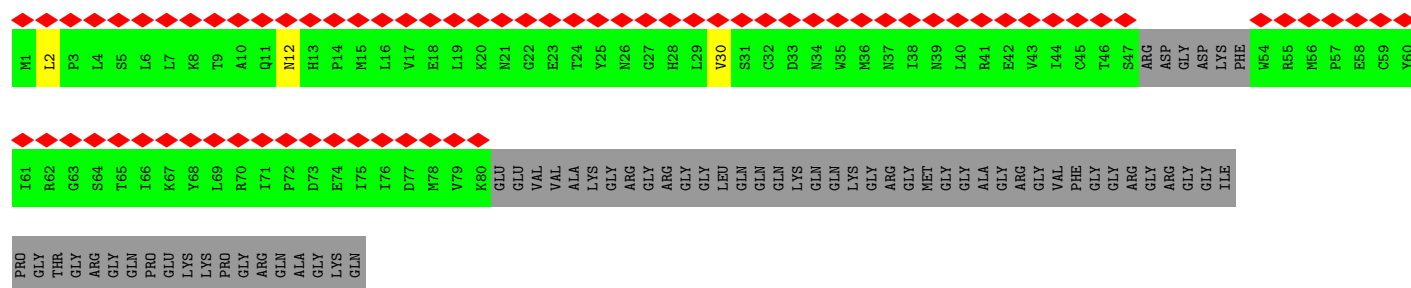


- Molecule 16: U6 snRNA-associated Sm-like protein LSm3

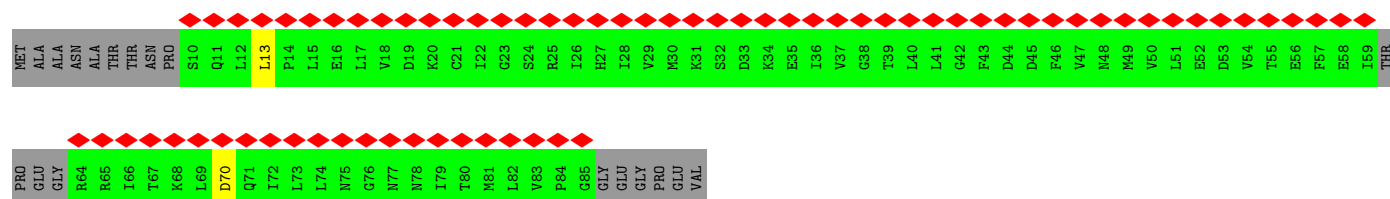
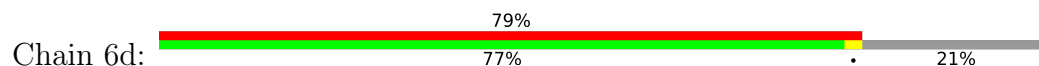


- Molecule 17: U6 snRNA-associated Sm-like protein LSm4

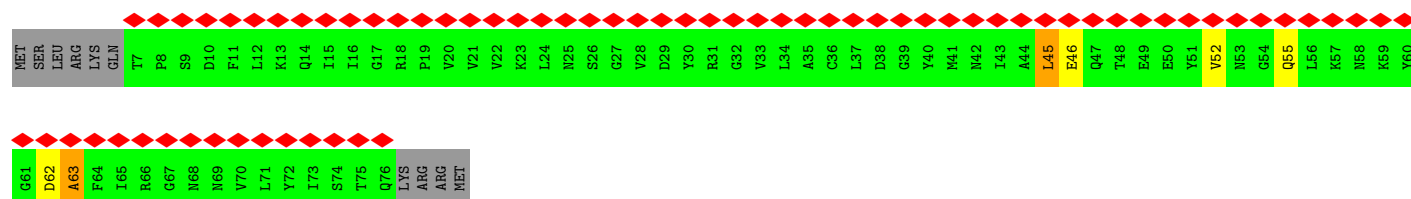
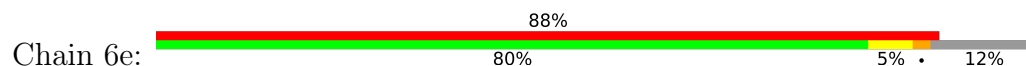




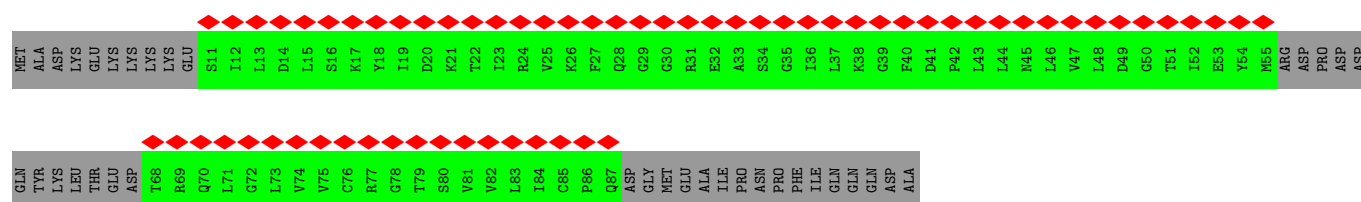
- Molecule 18: U6 snRNA-associated Sm-like protein LSm5



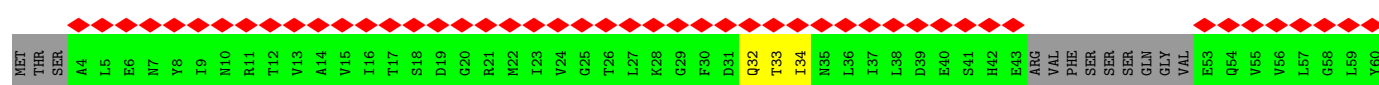
- Molecule 19: U6 snRNA-associated Sm-like protein LSm6



- Molecule 20: U6 snRNA-associated Sm-like protein LSm7

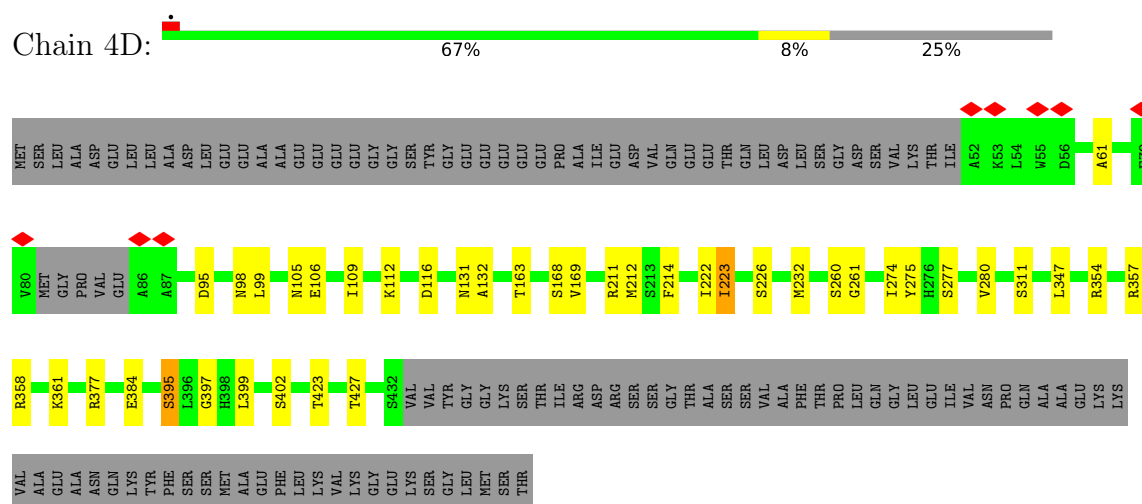


- Molecule 21: U6 snRNA-associated Sm-like protein LSm8

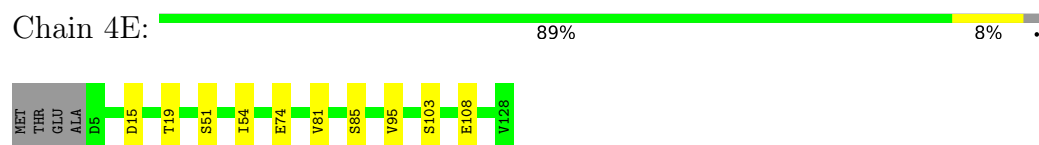




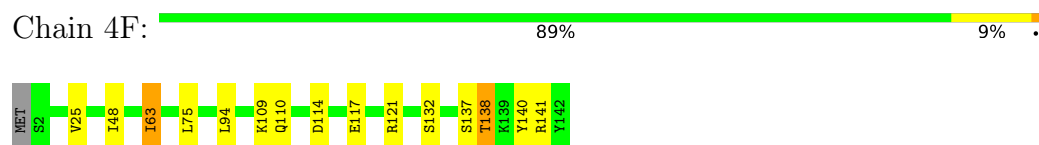
- Molecule 25: U4/U6 small nuclear ribonucleoprotein Prp31



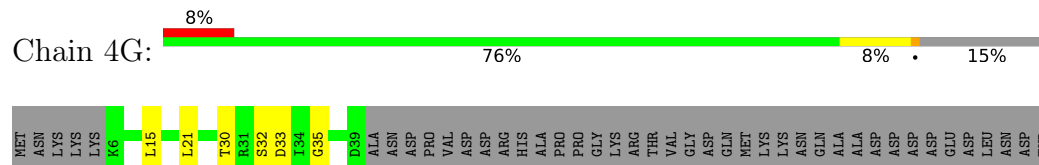
- Molecule 26: NHP2-like protein 1

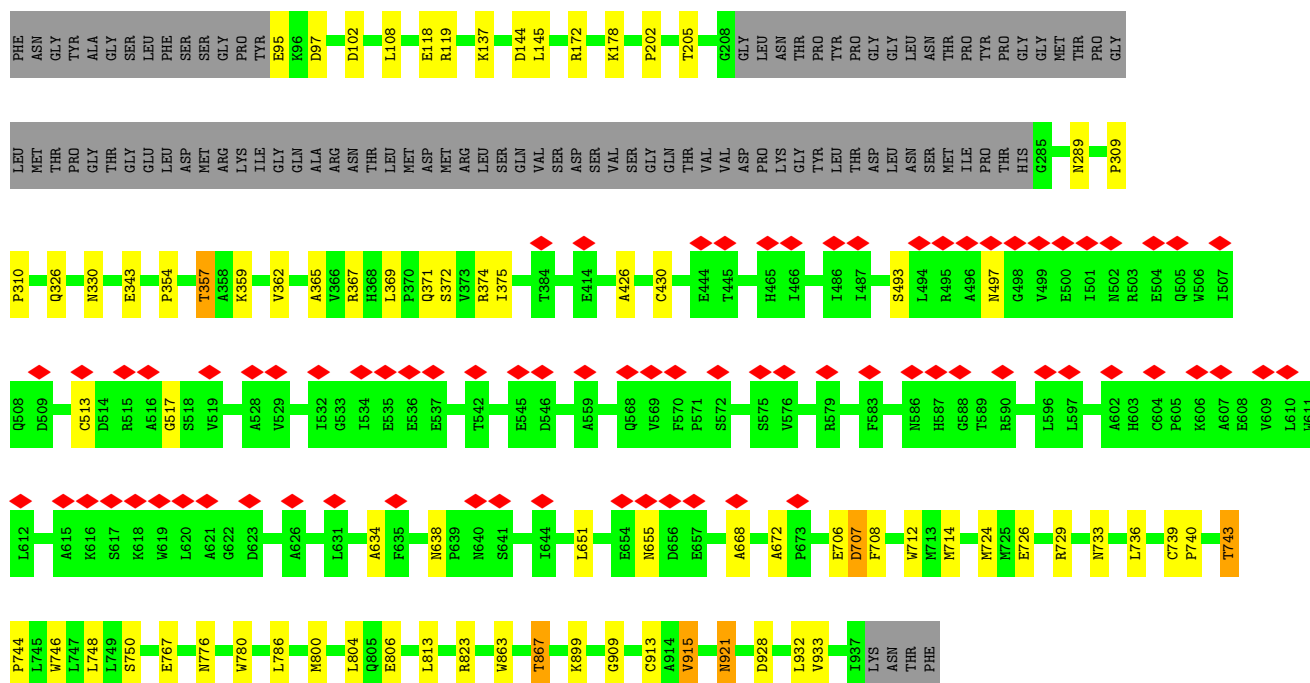


- Molecule 27: Thioredoxin-like protein 4A



- Molecule 28: Pre-mRNA-processing factor 6

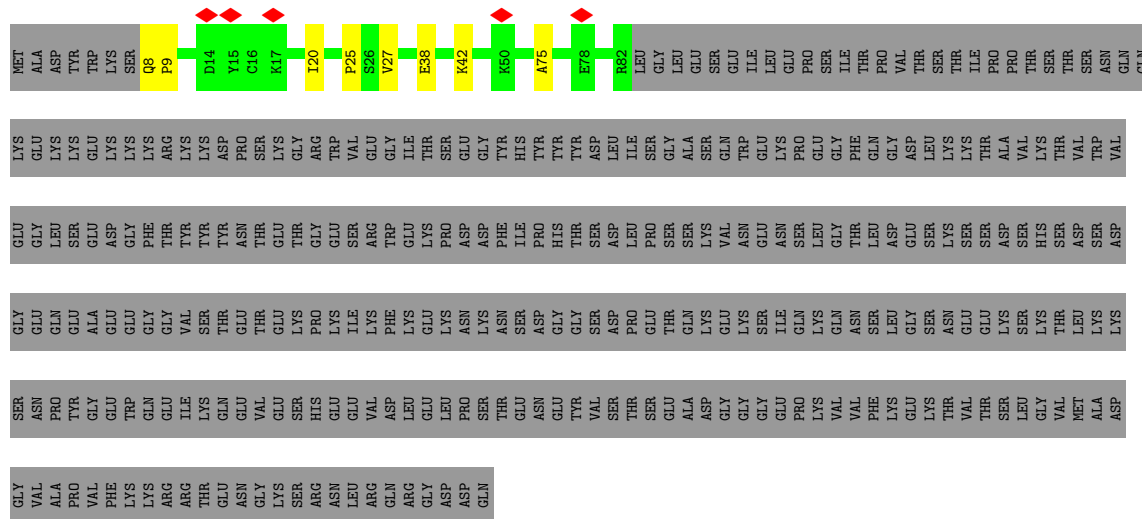




- Molecule 29: Peptidyl-prolyl cis-trans isomerase H



- Molecule 30: WW domain-binding protein 4

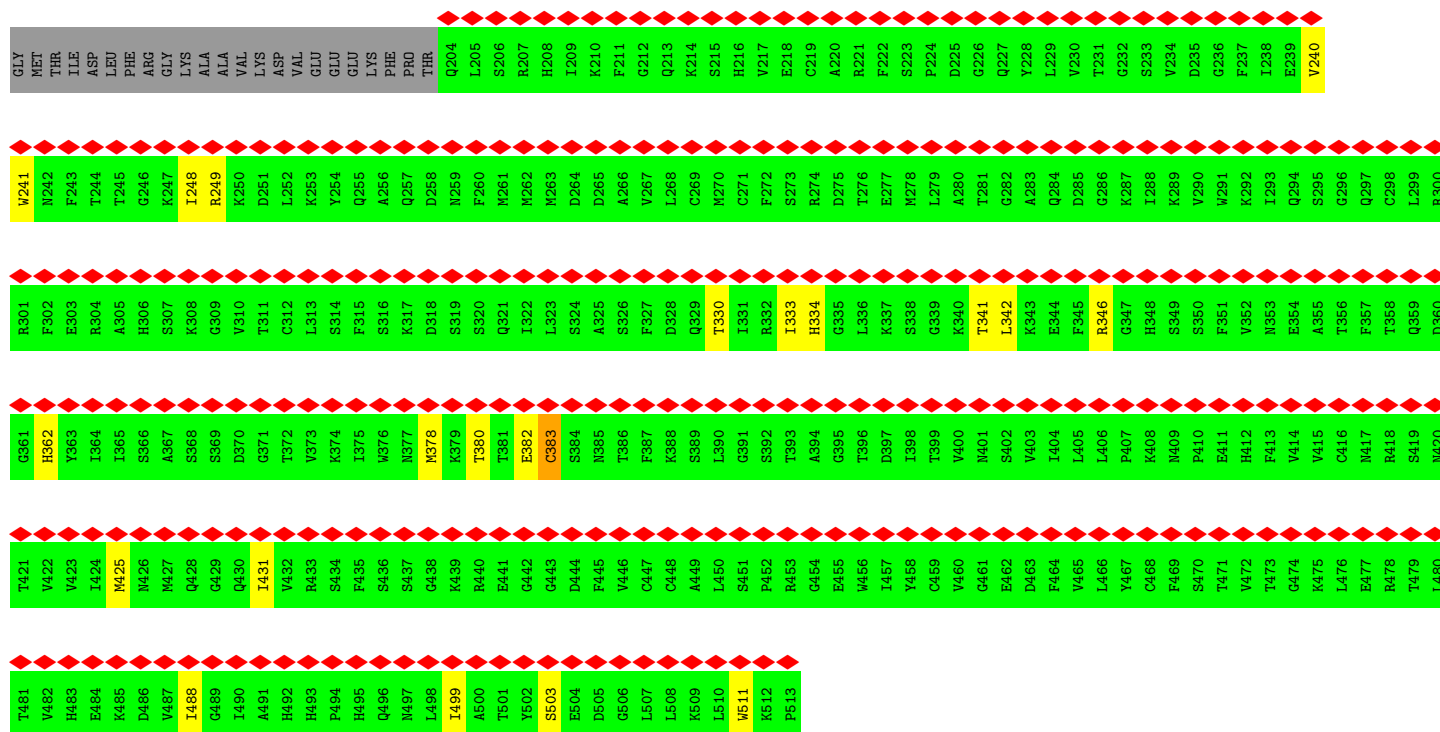


- Molecule 31: U4/U6.U5 tri-snRNP-associated protein 1

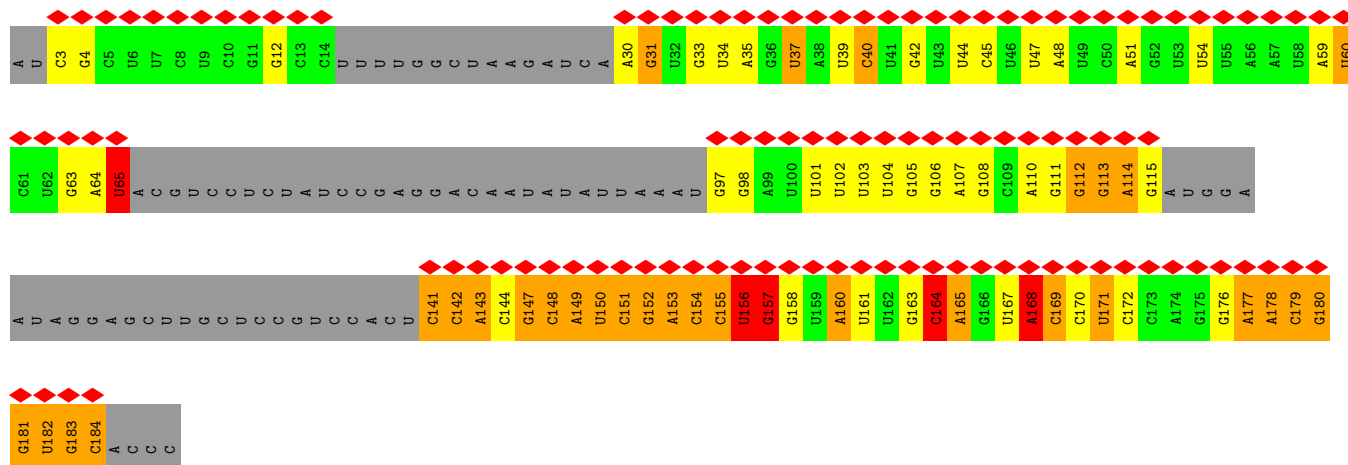
[illegible]

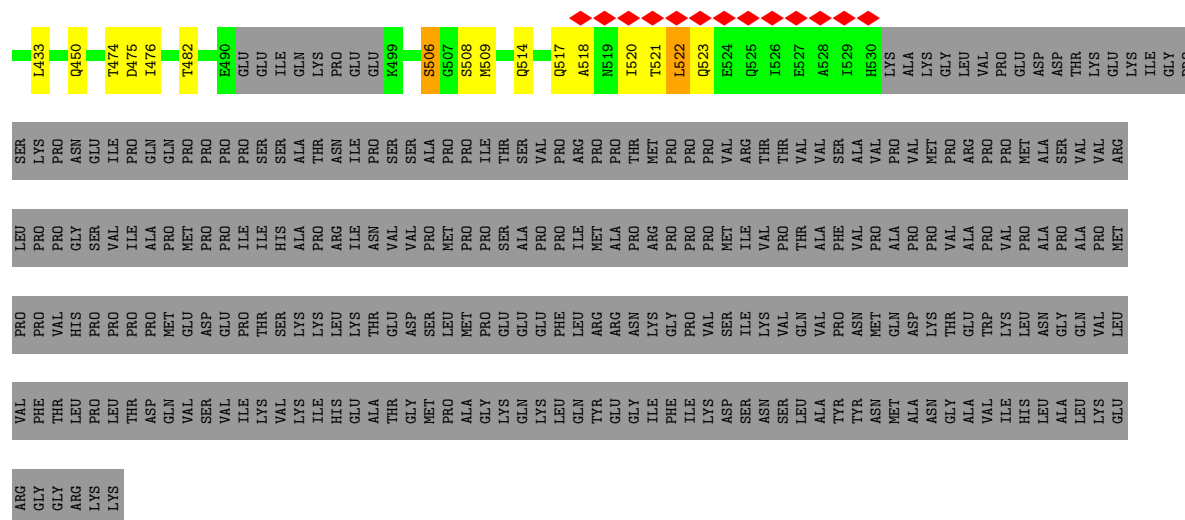
Chain 4Z: 82% 77% 1% 18%

Met	Ser	Ile	Glu	Ile	Glu	Ser	Ser	Asp	Val	Ile	Arg	Leu	Ile	Met	Gln	Tyr	Leu	Lys	Glu	Asn	Ser	Ser	Leu	His	Arg	Ala	Leu	Ala	Thr	Leu	Gln	Glu	Thr	Thr	Val	Ser	Leu	Asn	Thr	Val	Asp	S43	I44	E45	S46	F47	V48	A49	D50	I51	N52	S53	G54	H55	W56	D57	T58	V59	L60
Q61	A62	I63	Q64	S65	L66	K67	L68	P69	D70	K71	T72	L73	I74	D75	L76	Y77	E78	Q79	V80	V81	L82	E83	L84	I85	E86	L87	R88	E89	L90	G91	A92	A93	R94	S95	L96	L97	R98	Q99	T100	D101	P102	M103	I104	M105	L106	K107	Q108	T109	Q110	P111	E112	R113	Y114	I115	H116	L117	E118	N119	L120
L121	A122	R123	S124	Y125	F126	D127	P128	R129	E130	A131	Y132	P133	D134	G135	Ser	K138	E139	K140	R141	R142	A143	A144	I145	A146	Q147	A148	L149	A150	G151	E152	V153	S154	Val	Val	Pro	Pro	Ser	Arg	Leu	Met	Leu	Gly	Gln	Ala	Leu	Lys	Trp	Gln	Gln	His	Gln	Leu	Pro	Pro					

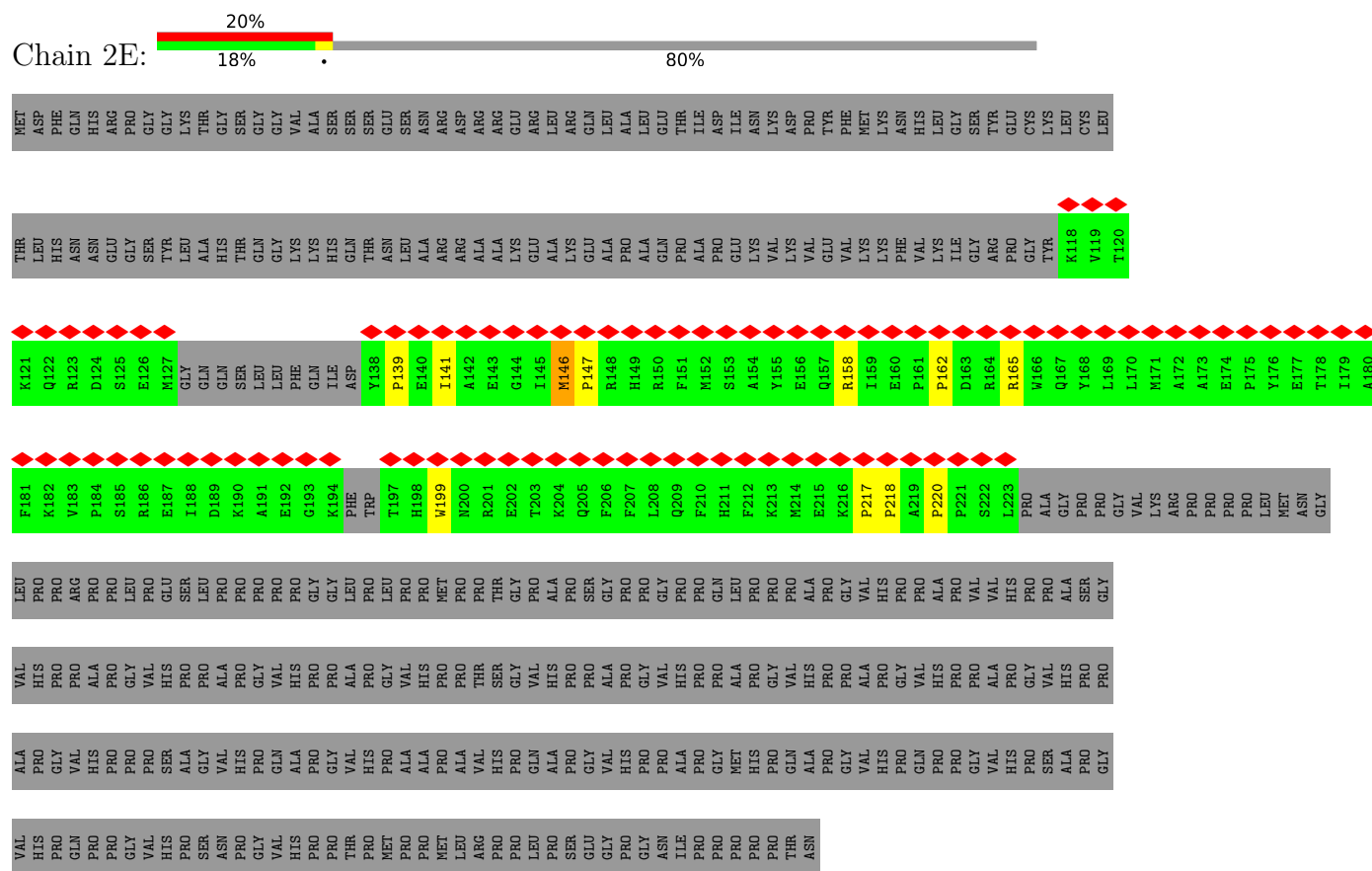


• Molecule 33: U2 snRNA

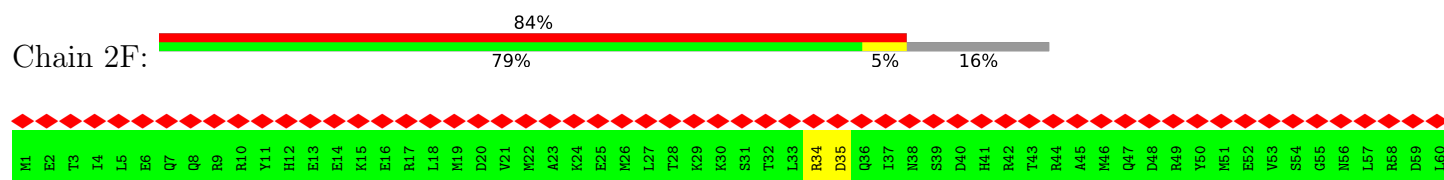




• Molecule 37: Splicing factor 3A subunit 2



• Molecule 38: Splicing factor 3A subunit 3



T1021	V961	Q901	A841	R661	A601	S541	D481	Y421	R301
P1022	M962	E902	B842	H662	K602	P542	V482	V422	D302
I1023	K963	E903	R843	T663	A603	T543	D483	P423	T303
L1024	T964	T904	V844	G664	A604	L544	E484	I424	P304
K1025	C965	T905	B845	I665	G605	E545	S485	R425	G305
N1026	Q966	E906	G846	K666	L606	D546	T486	L426	H306
R1027	E967	D907	A847	I667	A607	Q547	S487	P427	G307
H1028	E968	S908	E848	V668	T608	E548	P488	A428	S308
E1029	K969	V909	T849	Q669	M609	R549	E489	R429	G309
K1030	L970	M910	T850	Q670	I610	H550	E491	K430	W310
V1031	M971	L911	S851	I671	S611	L551	Q492	L431	A311
Q1032	G972	H912	R852	A672	T612	L552	K493	T432	E312
E1033	H973	G913	T853	I673	M613	V553	E494	A433	T313
N1034	L974	F914	B854	L674	R614	K554	R495	T434	P314
C1035	G975	G915	D855	M675	P615	V555	K496	P435	R315
I1036	V976	T916	D856	Q676	D616	I556	I497	T436	T316
D1037	V977	V917	L857	C677	I617	D557	M498	L437	D317
L1038	L978	V918	K858	H738	D618	R558	K499	L438	R318
V1039	Y979	H919	D859	I679	M620	I559	L500	G439	G319
G1040	E980	A920	E860	L680	M620	L560	L501	G440	G320
R1041	Y881	L921	A861	P681	D621	Y561	L502	M441	D321
I1042	L982	E922	K862	H682	Y623	K562	K503	T442	S322
A1043	G983	A803	L683	L683	Y623	L563	I504	G443	I323
D1044	E984	N804	B684	B684	V624	D564	K505	F444	G324
N1045	E985	Y805	S685	S685	R625	D565	N506	H445	E325
G1046	Y986	T806	L686	L686	N626	L566	G507	M446	T326
A1047	P987	K807	L747	V687	T627	V567	T508	Q447	T327
E1048	E988	T808	K748	E688	T628	R568	P509	T488	P328
Y1049	V989	E809	A749	I689	A629	P569	P510	GLY	PRO
F1050	G991	T810	I750	I690	R630	Y570	M511	ASP	GLY
S1051	S992	P812	G751	E691	A631	V571	R512	ALA	ALA
A1052	E993	E873	L753	H692	F632	H572	K313	SER	SER
E1053	L994	K874	L754	G693	A633	K573	A514	LYS	LYS
W1055	G995	F815	P755	V695	V635	L575	L516	ARG	ARG
M1056	A996	K816	L756	D696	A636	V576	R517	LYS	LYS
R1057	L997	H817	M757	E697	S637	V577	Q518	SER	SER
I1058	K998	F818	D758	Q698	A638	V578	I519	TRP	TRP
C1059	A999	H819	A759	Q699	L639	E579	T520	ASP	ASP
F1060	I1000	Q820	E760	Q700	L640	P580	D521	GLU	GLU
E1061	V1001	H821	V761	V701	T641	L581	K522	THR	THR
L1062	N1002	R822	A762	R702	P642	L582	A523	A406	ALA
L1063	V1003	M823	N763	T703	S643	I583	R524	M407	ALA
E1064	I1004	A824	Y764	I704	L644	D584	E525	F408	SER
L1065	G1005	L825	V765	S705	L645	E585	F526	P409	GLN
L1066	M1006	D826	T766	A706	P646	D586	G527	E410	GLY
K1067	H1007	R827	R767	L707	F647	Y587	A528	L464	GLY
A1068	K1008	R828	E768	A708	L648	Y588	G529	P465	THR
H1069	M1009	H829	V769	I709	K649	A589	P469	D470	THR
K1070	P1010	Y830	M770	A710	A650	A589	P530	P416	PRO
P1071	P1011	R831	L771	A711	V651	R591	L531	D471	GLY
A1072	E1012	K832	I772	L712	G652	E592	F532	I472	THR
I1073	I1013	L833	L773	A713	K653	G593	Q534	Q473	PRO
R1074	K1014	B834	E774	E714	S654	R594	I535	Y474	ILE
R1075	D1015	D835	R775	A715	K655	E595	L536	F475	
A1076	L1016	T836	E776	A716	K656	I596	L537	D476	
T1077	L1017	T837	F777	T717	S657	I597	L538	K477	
V1078	Y898	B838	Q778	T718	S658	I598	L539	L478	
N1079	R1019	E839	S779	Y719	Q659	N599	M540	L479	
T1080	L1020	V960	P780	G720	A660	L600		V480	





K61	A62	R63	V64	R65	F66	N67	L68	M69	E70	K71	M72	L73	Q74	P75	C76	G77	P78	P79	A80	ASP	LYS	PRO	GLU	GLU	ASN
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	716083	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	0.163	Depositor
Minimum map value	-0.121	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.008	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: M7M, IHP, ZN, 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	0.60	6/1317 (0.5%)	0.68	2/2042 (0.1%)
2	5A	0.20	0/2698	0.39	0/4195
3	5B	0.16	0/19157	0.32	2/26004 (0.0%)
4	5C	0.15	1/6580 (0.0%)	0.41	5/8938 (0.1%)
5	5D	0.15	0/13923	0.32	2/18868 (0.0%)
6	5E	1.08	0/1195	1.21	5/1492 (0.3%)
7	2a	0.86	0/343	1.21	3/427 (0.7%)
7	4a	0.13	0/254	0.39	0/314
7	5a	0.85	0/335	1.18	2/417 (0.5%)
8	2b	0.89	0/327	1.11	0/407
8	4b	0.15	0/333	0.46	0/416
8	5b	0.89	0/327	1.11	0/407
9	2c	1.18	0/338	1.20	1/419 (0.2%)
9	4c	0.16	0/298	0.49	0/370
9	5c	1.14	0/387	1.21	1/482 (0.2%)
10	2d	1.24	1/295 (0.3%)	1.26	0/367
10	4d	0.21	0/291	0.47	0/363
10	5d	1.23	0/295	1.26	0/367
11	2e	1.02	0/315	1.26	0/392
11	4e	0.17	0/313	0.47	0/390
11	5e	1.03	0/315	1.27	1/392 (0.3%)
12	2f	0.86	0/270	1.05	0/334
12	4f	0.24	0/297	0.59	0/371
12	5f	0.85	0/287	1.03	0/357
13	2g	0.81	0/318	1.01	0/394
13	4g	0.14	0/287	0.35	0/358
13	5g	0.78	0/302	1.02	0/374
14	6A	0.17	0/1398	0.34	0/2172
15	6a	0.69	0/359	1.28	0/447
16	6b	0.75	0/294	1.37	3/364 (0.8%)
17	6c	0.58	0/294	1.32	3/364 (0.8%)
18	6d	0.71	0/286	1.28	2/354 (0.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
19	6e	0.71	0/279	1.40	2/347 (0.6%)
20	6f	0.60	0/258	1.14	0/319
21	6g	0.67	0/242	1.21	1/299 (0.3%)
22	4A	0.22	0/3025	0.37	0/4702
23	4B	0.12	0/2114	0.29	0/2836
24	4C	0.14	0/3452	0.33	0/4675
25	4D	0.15	0/2912	0.31	0/3924
26	4E	0.14	0/974	0.27	0/1316
27	4F	0.16	0/1198	0.32	0/1620
28	4G	0.11	0/5592	0.31	2/7615 (0.0%)
29	4H	0.09	0/853	0.26	0/1188
30	4I	0.19	0/502	0.55	2/683 (0.3%)
31	4J	0.12	0/1158	0.31	0/1553
32	4Z	0.17	0/2101	0.48	1/2928 (0.0%)
33	2A	0.71	12/2576 (0.5%)	1.11	27/4003 (0.7%)
34	2B	0.99	0/647	2.34	33/807 (4.1%)
35	2C	0.97	0/375	1.97	7/467 (1.5%)
36	2D	0.24	0/1388	0.62	2/1813 (0.1%)
37	2E	0.38	0/373	1.77	4/461 (0.9%)
38	2F	0.38	0/1688	0.92	3/2102 (0.1%)
39	2G	1.72	38/4184 (0.9%)	1.43	27/5216 (0.5%)
40	2H	1.02	0/957	1.09	2/1209 (0.2%)
41	2I	1.39	25/4664 (0.5%)	1.20	9/5816 (0.2%)
42	2J	1.02	0/311	0.99	0/387
43	2K	1.27	2/431 (0.5%)	1.27	1/537 (0.2%)
44	2L	1.16	0/355	1.12	0/442
45	2M	1.59	1/263 (0.4%)	1.23	0/327
All	All	0.61	86/96900 (0.1%)	0.70	155/130950 (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
3	5B	0	1
9	2c	0	1
9	5c	0	1
25	4D	0	1
38	2F	0	1
39	2G	0	11
40	2H	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
41	2I	0	11
43	2K	0	1
45	2M	0	1
All	All	0	32

The worst 5 of 86 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	2G	407	MET	N-CA	22.52	1.71	1.46
39	2G	406	ALA	C-N	14.95	1.52	1.33
39	2G	1243	PRO	N-CA	-9.49	1.35	1.47
39	2G	944	SER	N-CA	-8.41	1.34	1.46
41	2I	84	SER	CA-C	-7.80	1.42	1.53

The worst 5 of 155 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	2E	146	MET	CA-C-N	21.07	146.17	119.84
37	2E	146	MET	C-N-CA	21.07	146.17	119.84
39	2G	406	ALA	CA-C-N	17.67	147.39	120.89
39	2G	406	ALA	C-N-CA	17.67	147.39	120.89
4	5C	810	PRO	CA-N-CD	-14.59	91.58	112.00

There are no chirality outliers.

5 of 32 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
38	2F	443	THR	Peptide
39	2G	220	GLN	Peptide
25	4D	358	ARG	Sidechain
3	5B	941	LYS	Peptide
9	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	1187	0	605	151	0
2	5A	2420	0	1226	77	0
3	5B	18642	0	18499	189	0
4	5C	6436	0	6453	105	0
5	5D	13633	0	13769	313	0
6	5E	1196	0	337	2	0
7	2a	344	0	93	4	0
7	4a	256	0	70	2	0
7	5a	336	0	89	0	0
8	2b	328	0	89	0	0
8	4b	334	0	92	1	0
8	5b	328	0	89	5	0
9	2c	340	0	87	1	0
9	4c	300	0	80	5	0
9	5c	388	0	102	7	0
10	2d	296	0	87	1	0
10	4d	292	0	93	7	0
10	5d	296	0	87	10	0
11	2e	316	0	85	2	0
11	4e	314	0	86	3	0
11	5e	316	0	85	4	0
12	2f	272	0	75	1	0
12	4f	298	0	89	5	0
12	5f	288	0	82	5	0
13	2g	320	0	88	0	0
13	4g	288	0	84	1	0
13	5g	304	0	82	6	0
14	6A	1251	0	630	25	0
15	6a	360	0	95	2	0
16	6b	296	0	76	5	0
17	6c	296	0	77	0	0
18	6d	288	0	78	0	0
19	6e	280	0	81	8	0
20	6f	260	0	75	0	0
21	6g	244	0	71	3	0
22	4A	2744	0	1395	67	0
23	4B	2076	0	2148	18	0
24	4C	3370	0	3300	49	0
25	4D	2874	0	2856	24	0
26	4E	962	0	1012	5	0
27	4F	1169	0	1139	6	0
28	4G	5504	0	4772	57	0
29	4H	844	0	426	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	4I	494	0	384	6	0
31	4J	1153	0	1107	13	0
32	4Z	2093	0	993	15	0
33	2A	2311	0	1170	144	0
34	2B	648	0	167	1	0
35	2C	376	0	102	0	0
36	2D	1380	0	999	20	0
37	2E	376	0	85	0	0
38	2F	1693	0	454	22	0
39	2G	4192	0	1110	234	0
40	2H	959	0	417	11	0
41	2I	4672	0	1260	71	0
42	2J	312	0	87	3	0
43	2K	432	0	114	6	0
44	2L	356	0	105	5	0
45	2M	264	0	70	11	0
46	5B	36	0	6	1	0
47	5C	32	0	12	0	0
48	5C	1	0	0	0	0
49	4I	1	0	0	0	0
All	All	94667	0	69576	1572	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 1572 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)
39:2G:407:MET:N	39:2G:407:MET:CA	1.71	1.53
1:A:30:C:C2'	1:A:31:C:H5''	1.54	1.35
1:A:30:C:N4	1:A:31:C:C4	2.10	1.18
1:A:38:C:H4'	1:A:39:U:OP1	1.42	1.18
3:5B:2036:GLN:O	5:5D:1035:LEU:HD13	1.40	1.17

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	5B	2249/2335 (96%)	2145 (95%)	104 (5%)	0	100	100
4	5C	814/972 (84%)	745 (92%)	68 (8%)	1 (0%)	48	70
5	5D	1694/2136 (79%)	1618 (96%)	75 (4%)	1 (0%)	48	70
6	5E	297/357 (83%)	272 (92%)	16 (5%)	9 (3%)	3	6
7	2a	84/231 (36%)	82 (98%)	2 (2%)	0	100	100
7	4a	60/231 (26%)	57 (95%)	3 (5%)	0	100	100
7	5a	82/231 (36%)	80 (98%)	2 (2%)	0	100	100
8	2b	80/119 (67%)	77 (96%)	3 (4%)	0	100	100
8	4b	80/119 (67%)	76 (95%)	4 (5%)	0	100	100
8	5b	80/119 (67%)	77 (96%)	3 (4%)	0	100	100
9	2c	81/118 (69%)	78 (96%)	3 (4%)	0	100	100
9	4c	70/118 (59%)	68 (97%)	2 (3%)	0	100	100
9	5c	95/118 (80%)	91 (96%)	4 (4%)	0	100	100
10	2d	72/86 (84%)	68 (94%)	4 (6%)	0	100	100
10	4d	69/86 (80%)	67 (97%)	2 (3%)	0	100	100
10	5d	72/86 (84%)	69 (96%)	3 (4%)	0	100	100
11	2e	77/92 (84%)	76 (99%)	1 (1%)	0	100	100
11	4e	76/92 (83%)	70 (92%)	6 (8%)	0	100	100
11	5e	77/92 (84%)	76 (99%)	1 (1%)	0	100	100
12	2f	64/76 (84%)	62 (97%)	2 (3%)	0	100	100
12	4f	71/76 (93%)	67 (94%)	4 (6%)	0	100	100
12	5f	70/76 (92%)	68 (97%)	2 (3%)	0	100	100
13	2g	76/126 (60%)	75 (99%)	1 (1%)	0	100	100
13	4g	69/126 (55%)	69 (100%)	0	0	100	100
13	5g	72/126 (57%)	70 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	6a	88/95 (93%)	77 (88%)	7 (8%)	4 (4%)	2	2
16	6b	70/102 (69%)	64 (91%)	3 (4%)	3 (4%)	2	2
17	6c	70/139 (50%)	63 (90%)	6 (9%)	1 (1%)	9	19
18	6d	68/91 (75%)	63 (93%)	4 (6%)	1 (2%)	8	18
19	6e	68/80 (85%)	64 (94%)	2 (3%)	2 (3%)	3	6
20	6f	61/103 (59%)	56 (92%)	5 (8%)	0	100	100
21	6g	57/96 (59%)	52 (91%)	4 (7%)	1 (2%)	6	14
23	4B	248/683 (36%)	229 (92%)	19 (8%)	0	100	100
24	4C	422/522 (81%)	388 (92%)	33 (8%)	1 (0%)	43	66
25	4D	372/499 (74%)	354 (95%)	18 (5%)	0	100	100
26	4E	122/128 (95%)	112 (92%)	10 (8%)	0	100	100
27	4F	139/142 (98%)	134 (96%)	5 (4%)	0	100	100
28	4G	795/941 (84%)	745 (94%)	50 (6%)	0	100	100
29	4H	167/177 (94%)	156 (93%)	11 (7%)	0	100	100
30	4I	73/376 (19%)	71 (97%)	2 (3%)	0	100	100
31	4J	143/800 (18%)	136 (95%)	7 (5%)	0	100	100
32	4Z	414/513 (81%)	401 (97%)	12 (3%)	1 (0%)	43	66
34	2B	160/255 (63%)	146 (91%)	12 (8%)	2 (1%)	9	21
35	2C	92/225 (41%)	90 (98%)	2 (2%)	0	100	100
36	2D	226/793 (28%)	208 (92%)	12 (5%)	6 (3%)	4	7
37	2E	88/464 (19%)	63 (72%)	16 (18%)	9 (10%)	0	0
38	2F	413/501 (82%)	367 (89%)	41 (10%)	5 (1%)	10	23
39	2G	1032/1304 (79%)	844 (82%)	166 (16%)	22 (2%)	5	11
40	2H	199/895 (22%)	179 (90%)	16 (8%)	4 (2%)	6	12
41	2I	1152/1217 (95%)	1053 (91%)	89 (8%)	10 (1%)	14	30
42	2J	76/424 (18%)	75 (99%)	1 (1%)	0	100	100
43	2K	106/125 (85%)	85 (80%)	18 (17%)	3 (3%)	4	6
44	2L	87/110 (79%)	74 (85%)	13 (15%)	0	100	100
45	2M	64/86 (74%)	55 (86%)	7 (11%)	2 (3%)	3	5
All	All	13703/20230 (68%)	12707 (93%)	908 (7%)	88 (1%)	23	42

5 of 88 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	5D	1086	GLN
6	5E	193	THR
15	6a	55	LEU
16	6b	84	MET
18	6d	70	ASP

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	
3	5B	2034/2108 (96%)	1974 (97%)	60 (3%)	37	65
4	5C	718/866 (83%)	693 (96%)	25 (4%)	32	59
5	5D	1517/1908 (80%)	1514 (100%)	3 (0%)	87	95
23	4B	225/599 (38%)	216 (96%)	9 (4%)	28	55
24	4C	362/442 (82%)	345 (95%)	17 (5%)	23	48
25	4D	299/424 (70%)	289 (97%)	10 (3%)	33	61
26	4E	108/111 (97%)	104 (96%)	4 (4%)	30	57
27	4F	129/130 (99%)	122 (95%)	7 (5%)	20	42
28	4G	417/792 (53%)	405 (97%)	12 (3%)	37	65
29	4H	10/148 (7%)	10 (100%)	0	100	100
30	4I	32/333 (10%)	31 (97%)	1 (3%)	35	63
31	4J	113/681 (17%)	107 (95%)	6 (5%)	20	43
32	4Z	11/450 (2%)	11 (100%)	0	100	100
36	2D	95/709 (13%)	89 (94%)	6 (6%)	16	36
40	2H	26/776 (3%)	26 (100%)	0	100	100
All	All	6096/10477 (58%)	5936 (97%)	160 (3%)	41	68

5 of 160 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
25	4D	168	SER
28	4G	750	SER

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Mol	Chain	Res	Type
25	4D	226	SER
27	4F	94	LEU
31	4J	288	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 69 such sidechains are listed below:

Mol	Chain	Res	Type
26	4E	77	ASN
28	4G	173	ASN
31	4J	261	HIS
4	5C	280	HIS
3	5B	2288	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	55/144 (38%)	35 (63%)	10 (18%)
14	6A	55/107 (51%)	14 (25%)	2 (3%)
2	5A	114/117 (97%)	30 (26%)	5 (4%)
22	4A	124/145 (85%)	35 (28%)	4 (3%)
33	2A	105/188 (55%)	22 (20%)	3 (2%)
All	All	453/701 (64%)	136 (30%)	24 (5%)

5 of 136 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 24 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	5A	96	A
22	4A	18	G
14	6A	77	C
22	4A	38	U
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	$\# Z > 2$
47	GTP	5C	1500	48	33,34,34	0.92	1 (3%)	50,54,54	1.56	8 (16%)
46	IHP	5B	3000	-	36,36,36	0.73	0	60,60,60	1.12	2 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	GTP	5C	1500	48	-	6/22/38/38	0/3/3/3
46	IHP	5B	3000	-	-	3/30/54/54	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	5C	1500	GTP	C2-N3	2.08	1.38	1.33

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	5C	1500	GTP	C5-C4-N3	-4.92	120.56	128.39
47	5C	1500	GTP	C2-N3-C4	4.64	120.30	112.30
47	5C	1500	GTP	N9-C4-N3	3.04	132.04	125.95
47	5C	1500	GTP	C2-N1-C6	-2.93	119.80	125.11
47	5C	1500	GTP	N9-C8-N7	-2.67	108.45	113.40

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

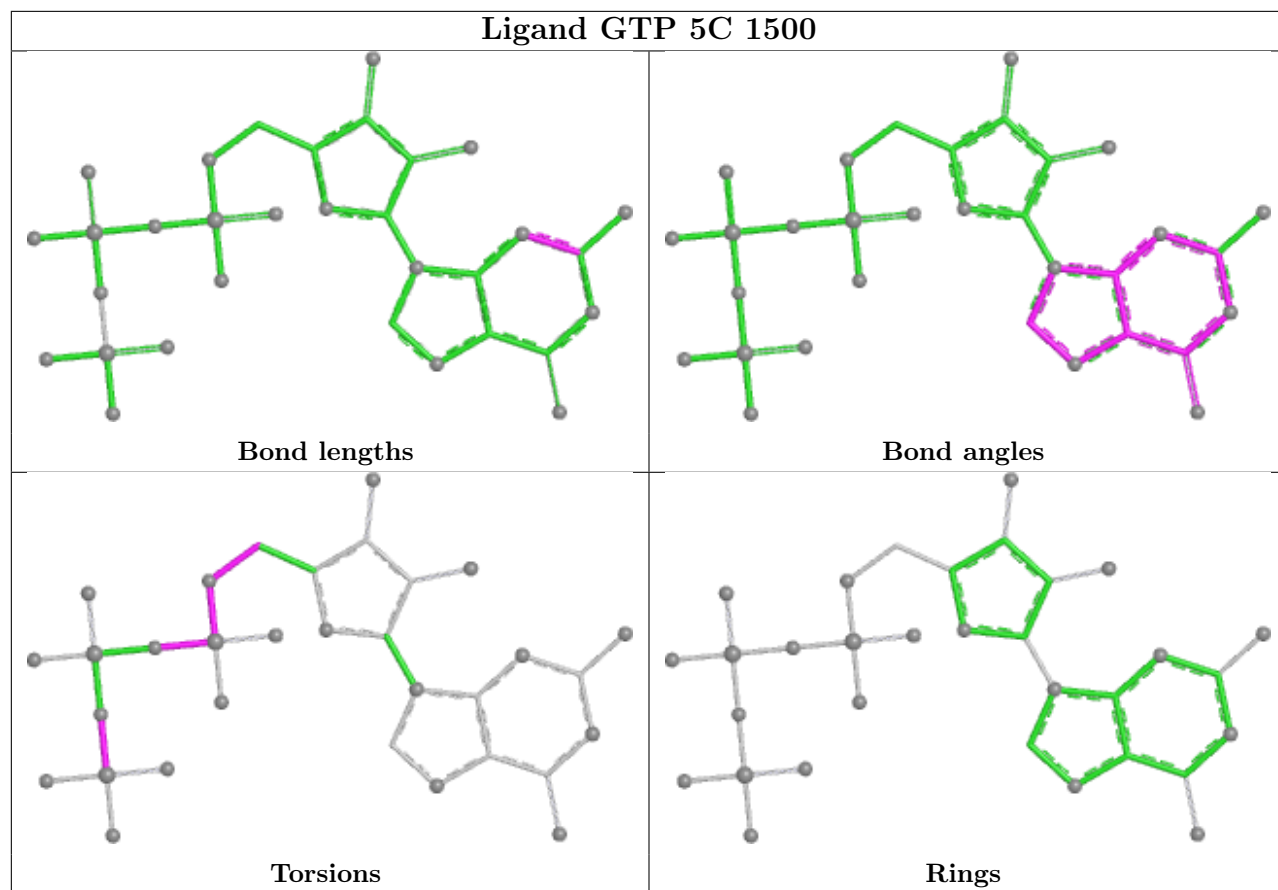
Mol	Chain	Res	Type	Atoms
47	5C	1500	GTP	PB-O3B-PG-O3G
47	5C	1500	GTP	C5'-O5'-PA-O3A
47	5C	1500	GTP	C5'-O5'-PA-O1A
47	5C	1500	GTP	PB-O3A-PA-O5'
47	5C	1500	GTP	C5'-O5'-PA-O2A

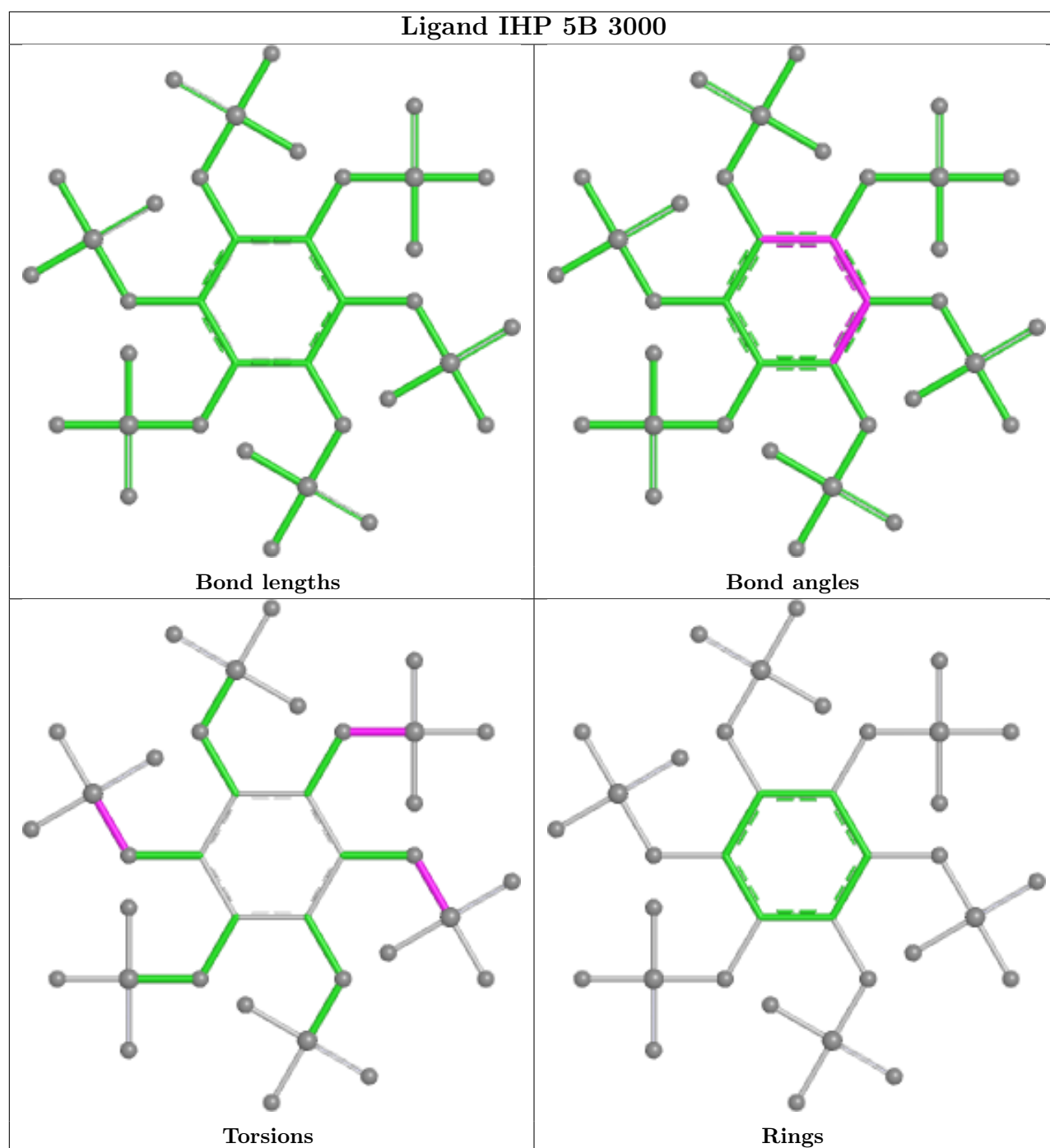
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
46	5B	3000	IHP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

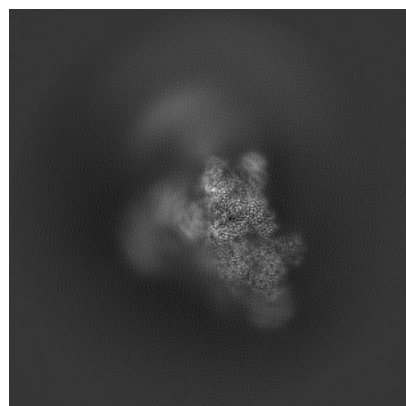
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34508. These allow visual inspection of the internal detail of the map and identification of artifacts.

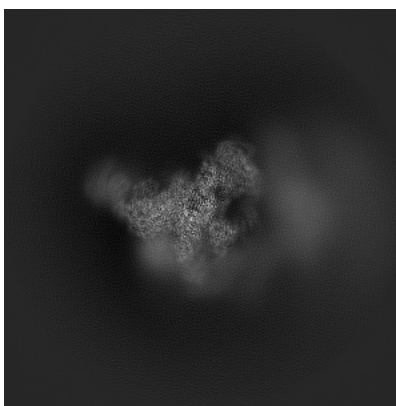
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

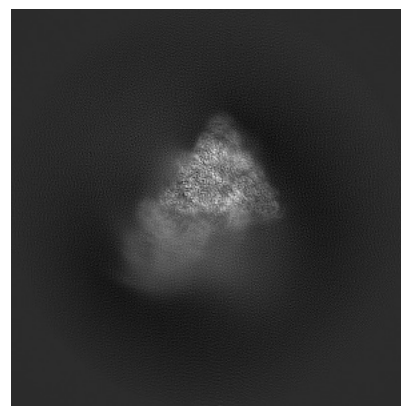
6.1.1 Primary map



X

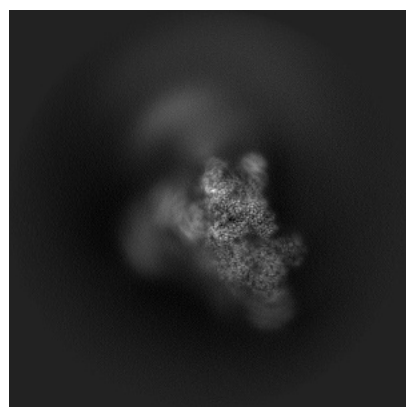


Y

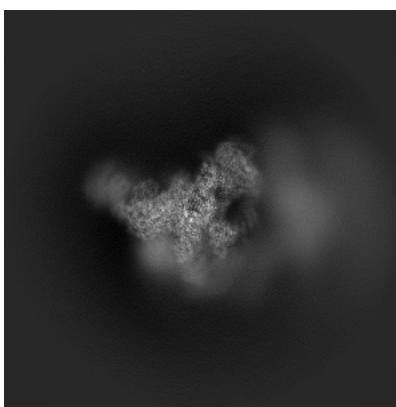


Z

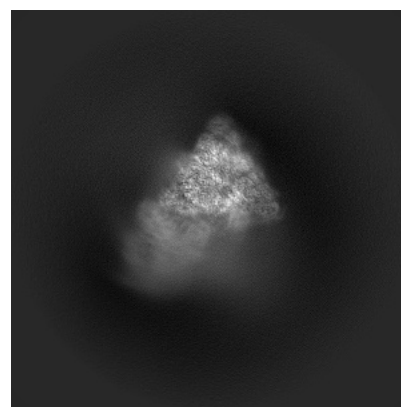
6.1.2 Raw map



X



Y

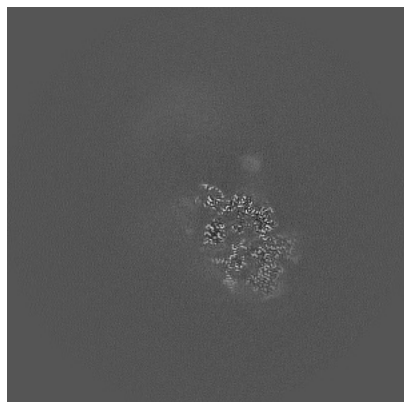


Z

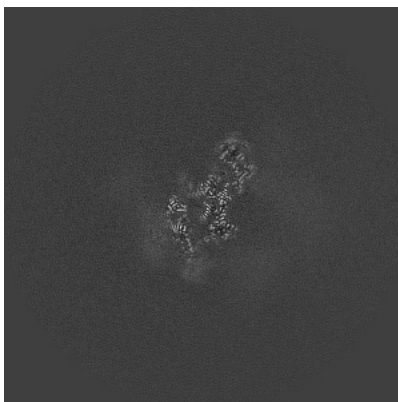
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

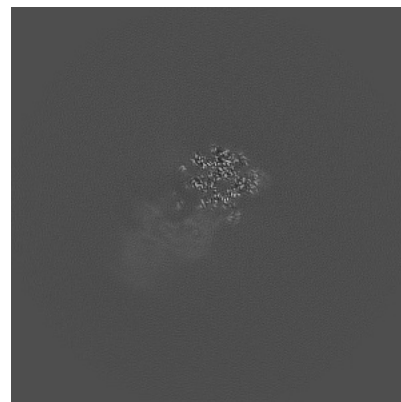
6.2.1 Primary map



X Index: 256

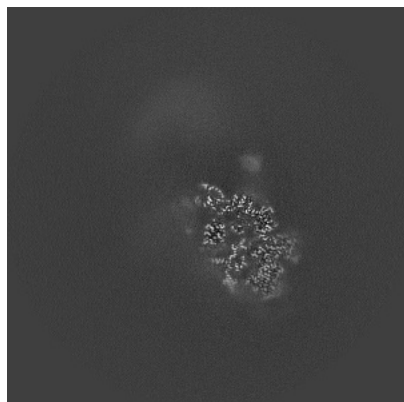


Y Index: 256

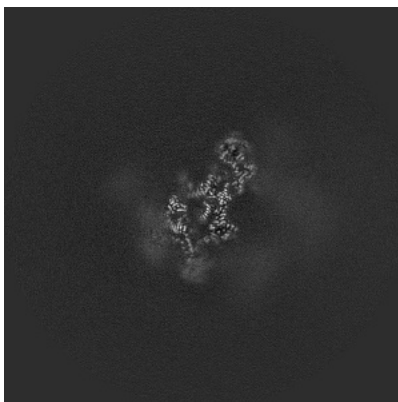


Z Index: 256

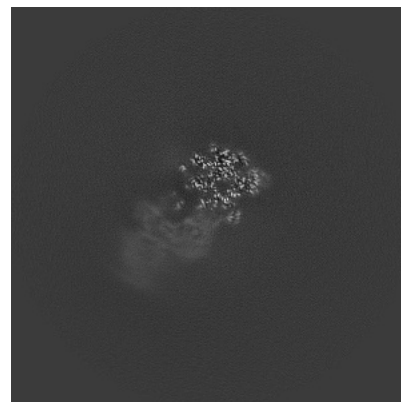
6.2.2 Raw map



X Index: 256



Y Index: 256

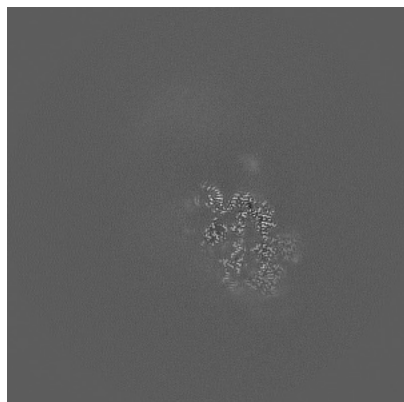


Z Index: 256

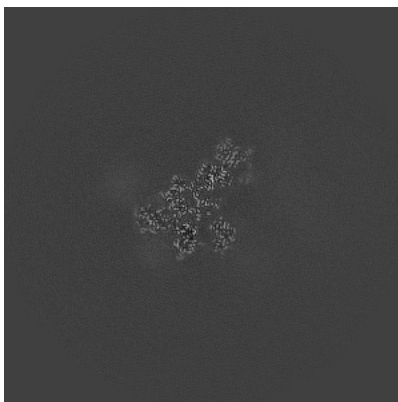
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

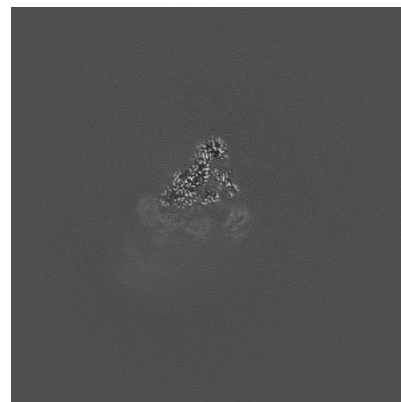
6.3.1 Primary map



X Index: 259

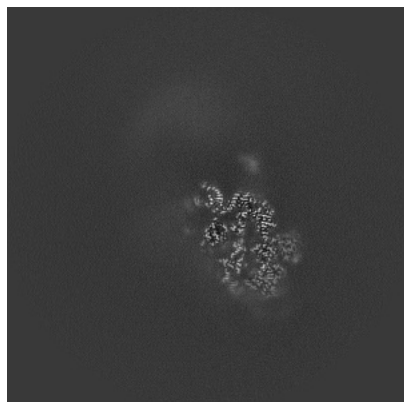


Y Index: 274

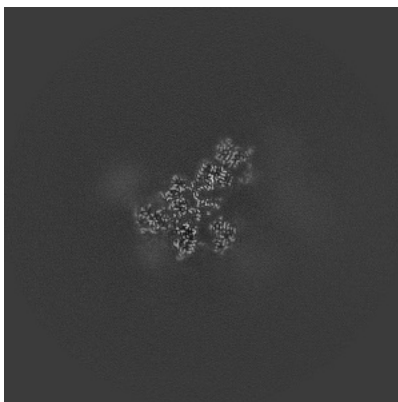


Z Index: 234

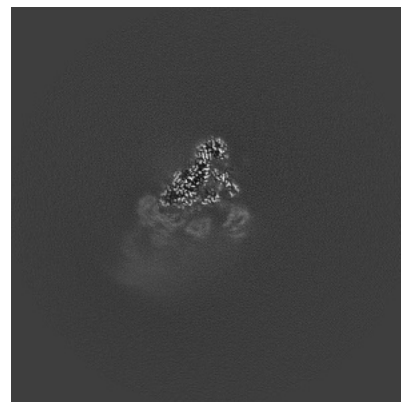
6.3.2 Raw map



X Index: 259



Y Index: 274

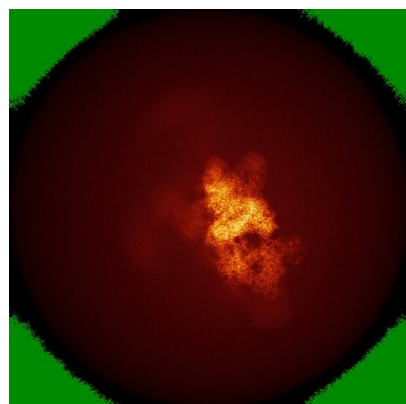


Z Index: 234

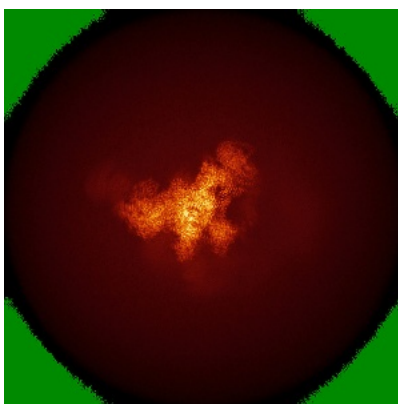
The images above show the largest variance slices of the map in three orthogonal directions.

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

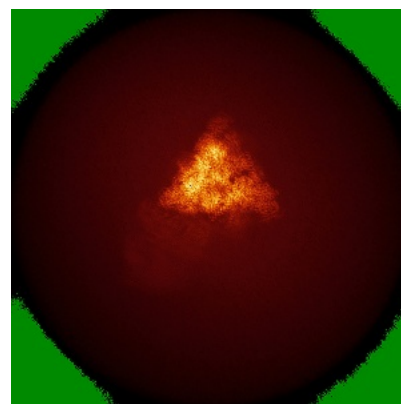
6.4.1 Primary map



X

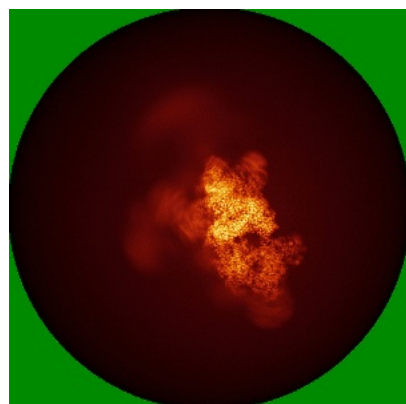


Y

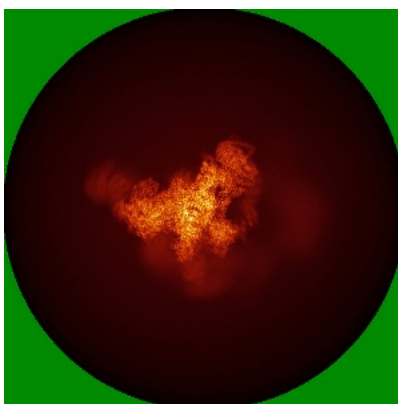


Z

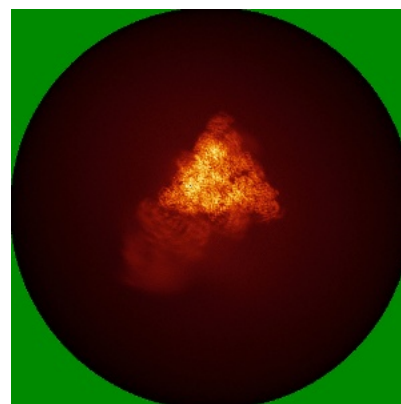
6.4.2 Raw map



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



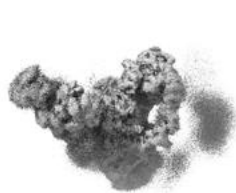
Z

The images above show the 3D surface view of the map at the recommended contour level 0.008. 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.

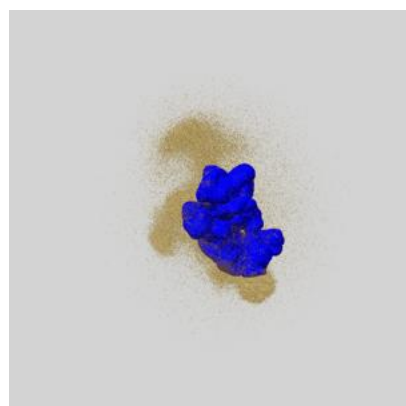
6.6 Mask visualisation [i](#)

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

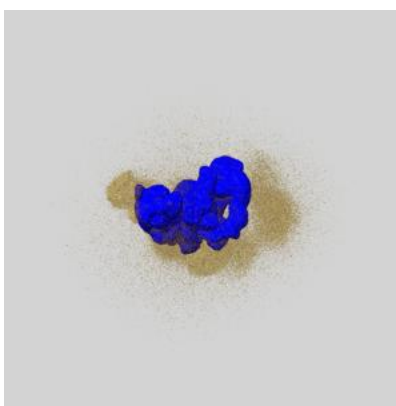
A mask typically either:

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

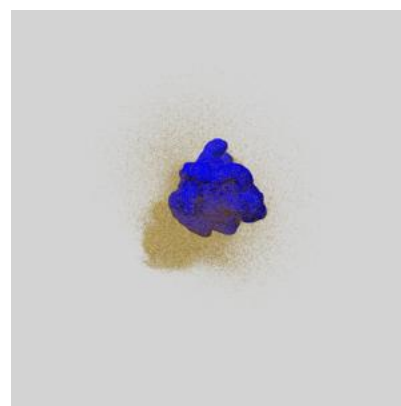
6.6.1 emd_34508_msk_1.map [i](#)



X



Y

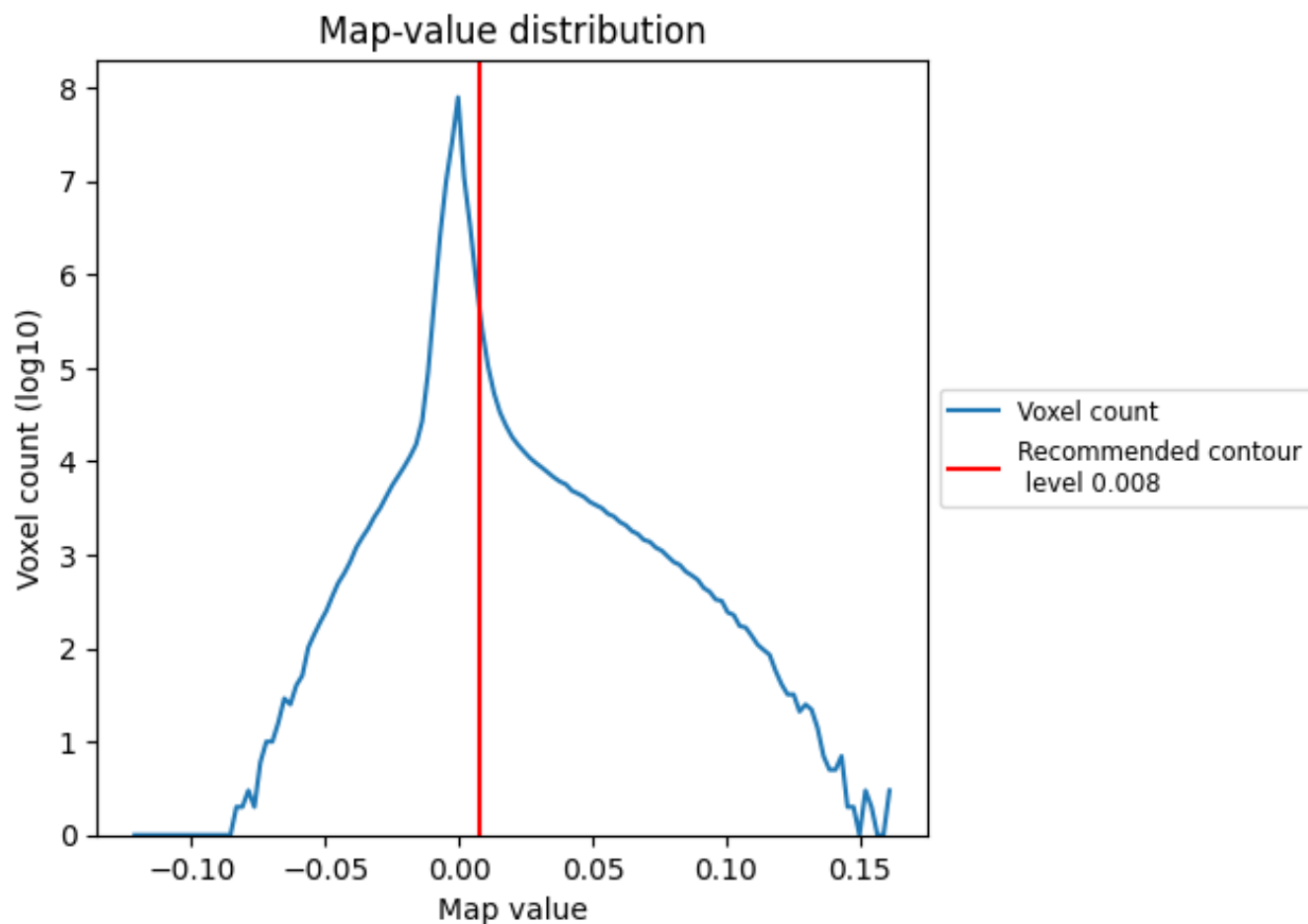


Z

7 Map analysis [i](#)

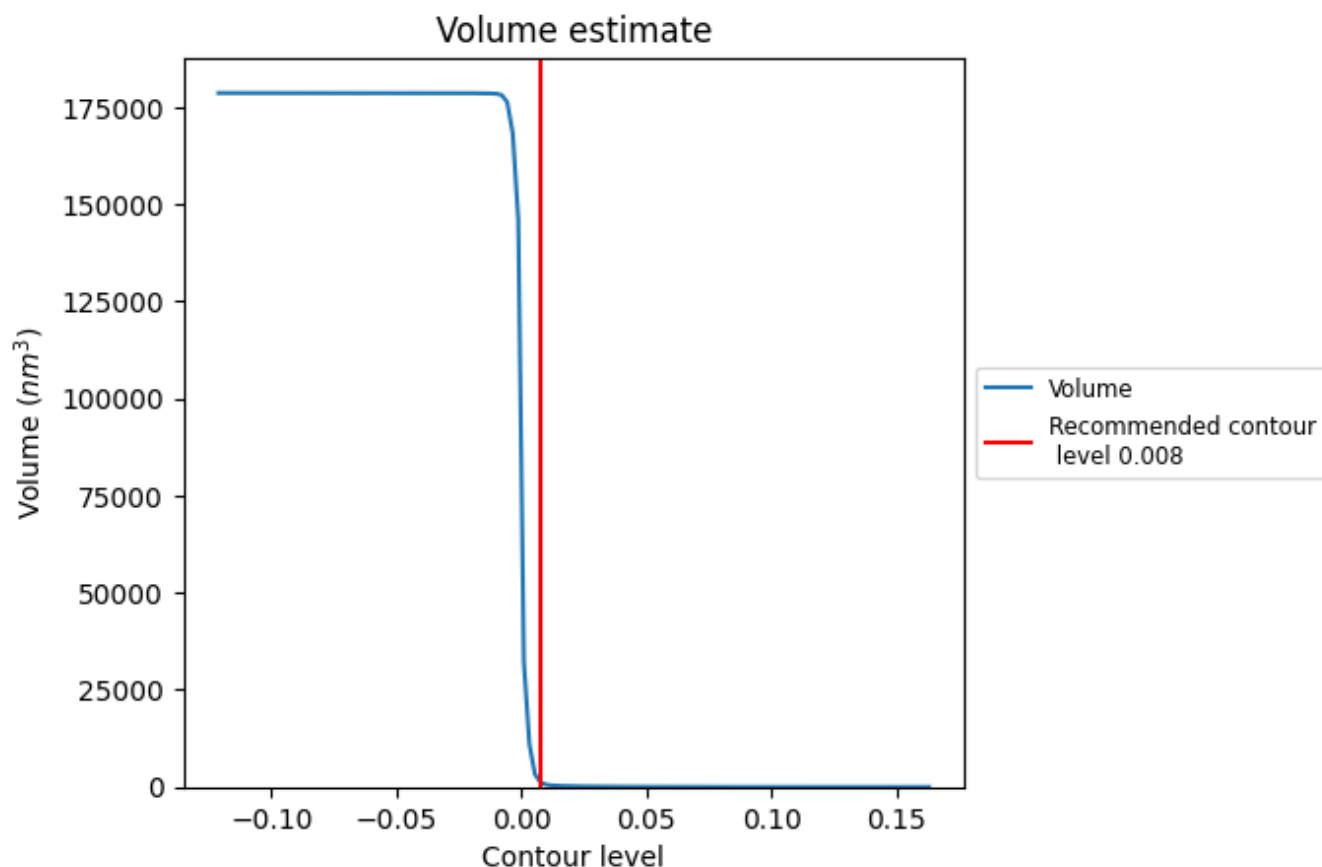
This section contains the results of statistical analysis of the map.

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.

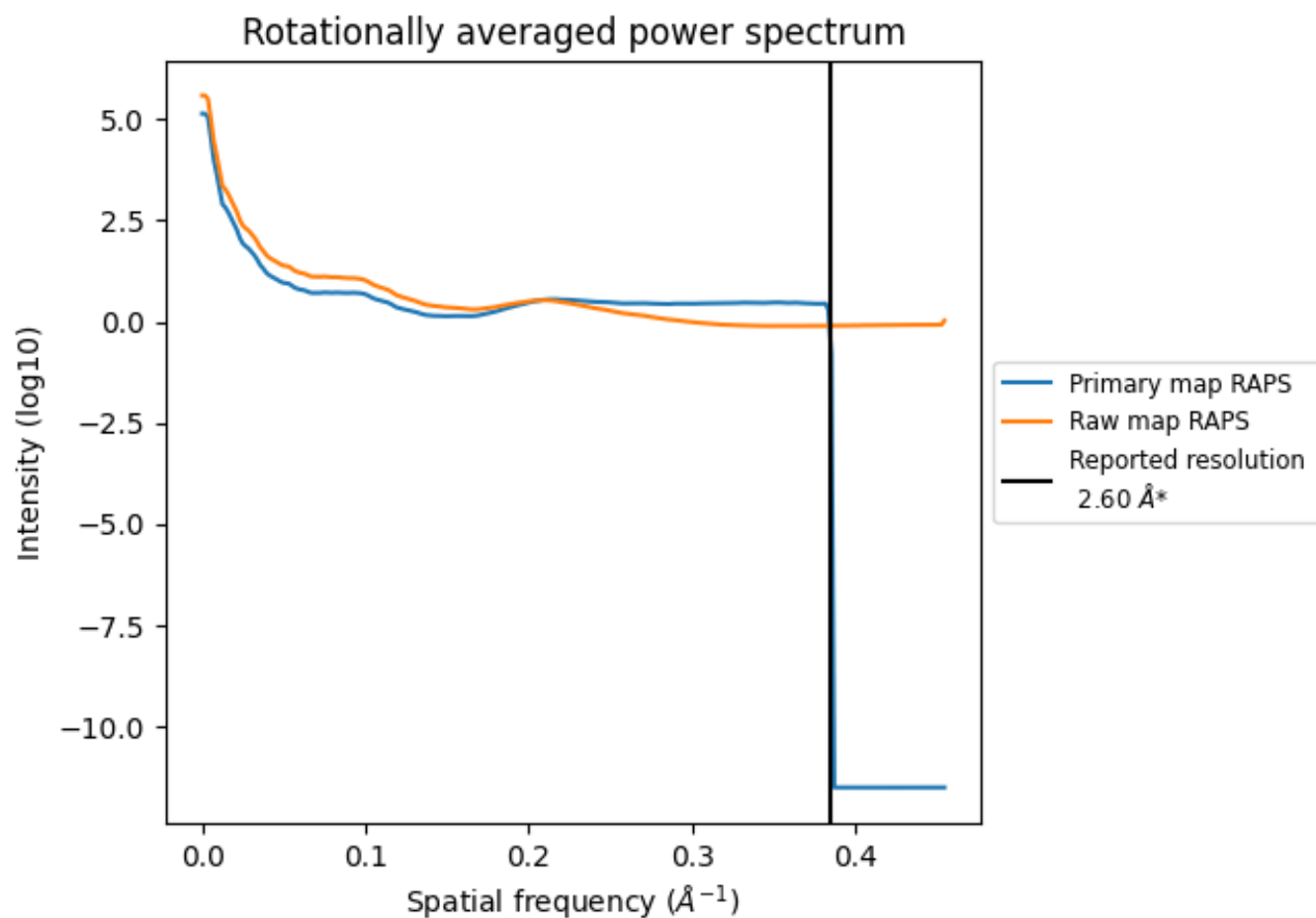
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1104 nm³; this corresponds to an approximate mass of 997 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 ⓘ

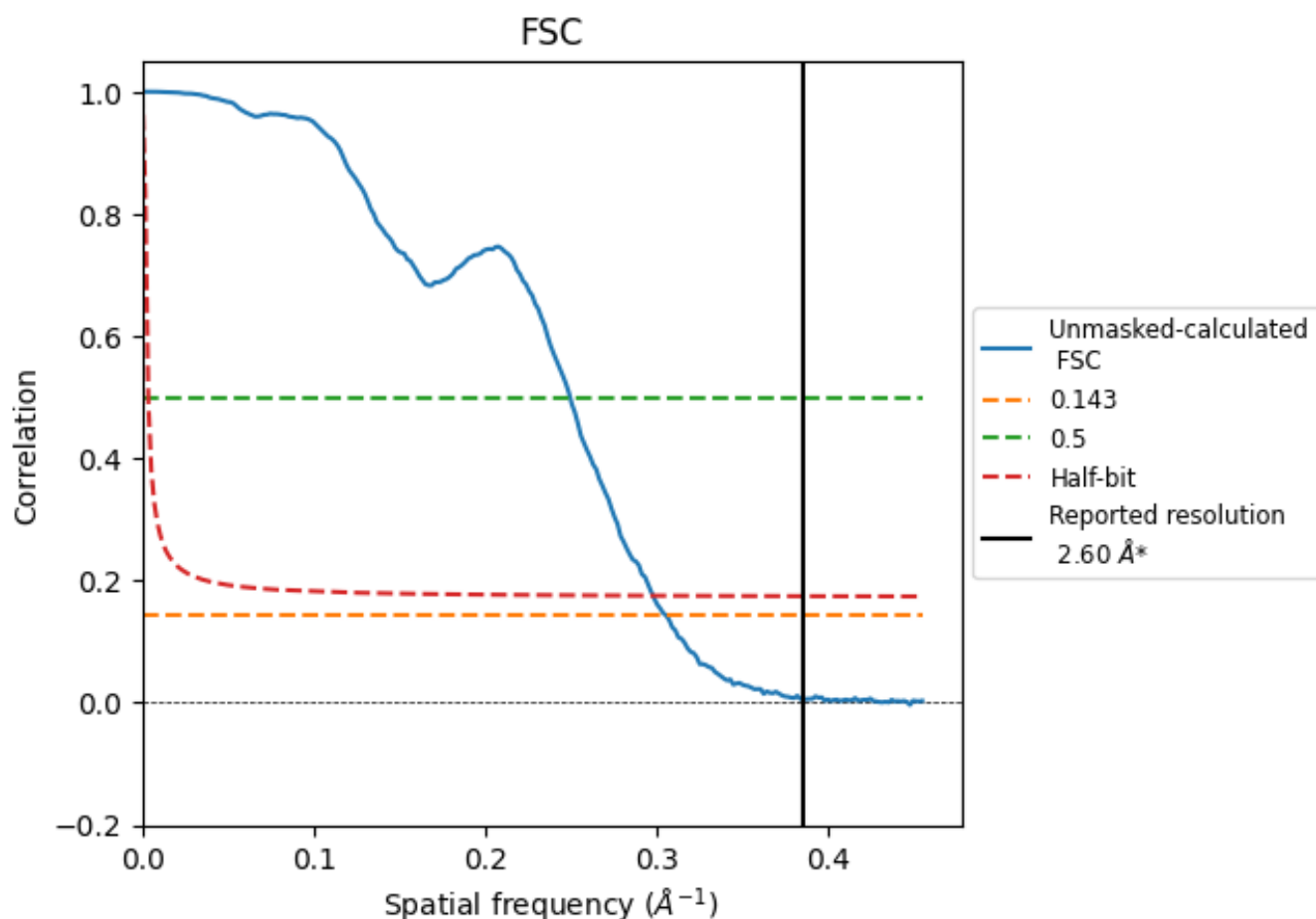


*Reported resolution corresponds to spatial frequency of 0.385 Å⁻¹

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 0.385 Å⁻¹

8.2 Resolution estimates [i](#)

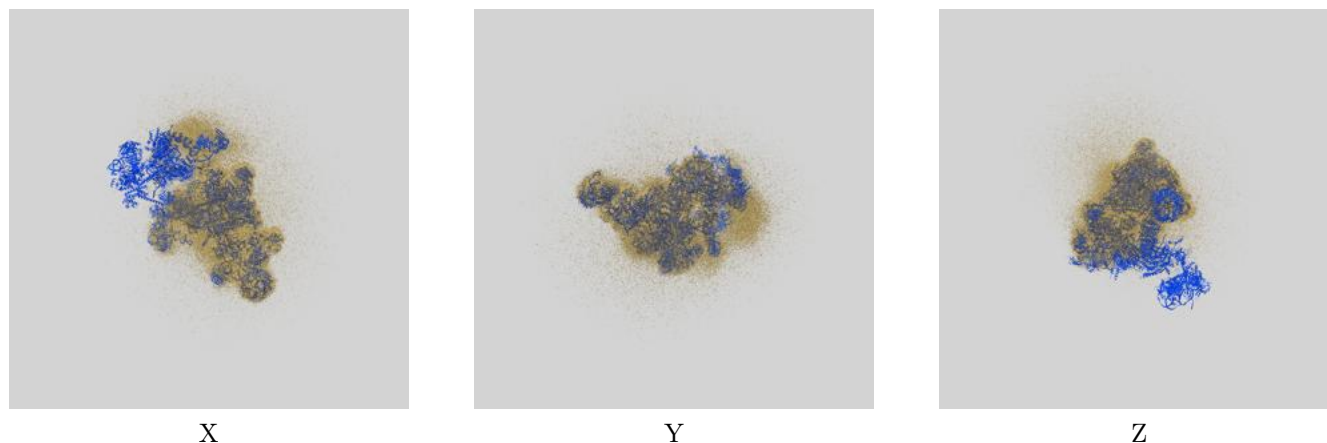
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.28	4.01	3.36

*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 3.28 differs from the reported value 2.6 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-34508 and PDB model 8H6L. Per-residue inclusion information can be found in [section 3](#) on [page 15](#).

9.1 Map-model overlay [i](#)



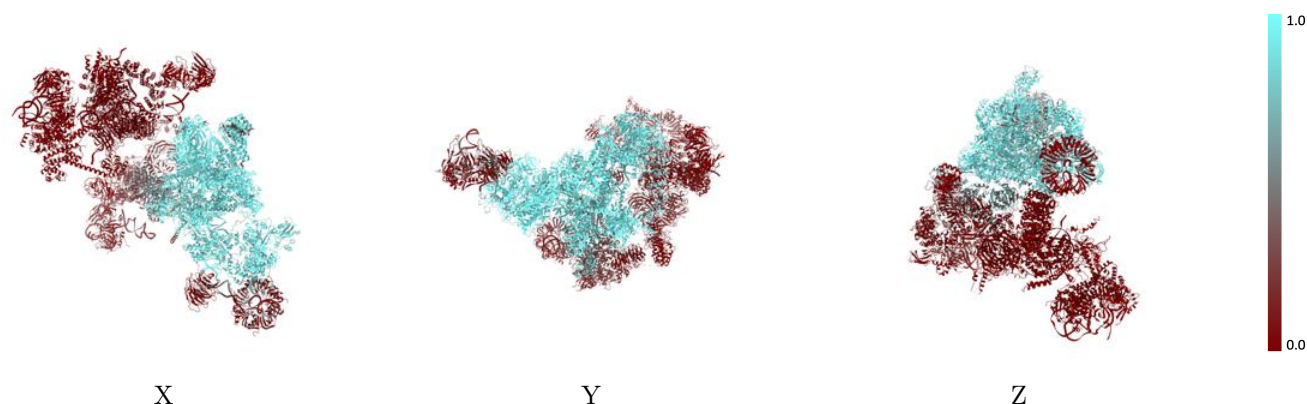
The images above show the 3D surface view of the map at the recommended contour level 0.008 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



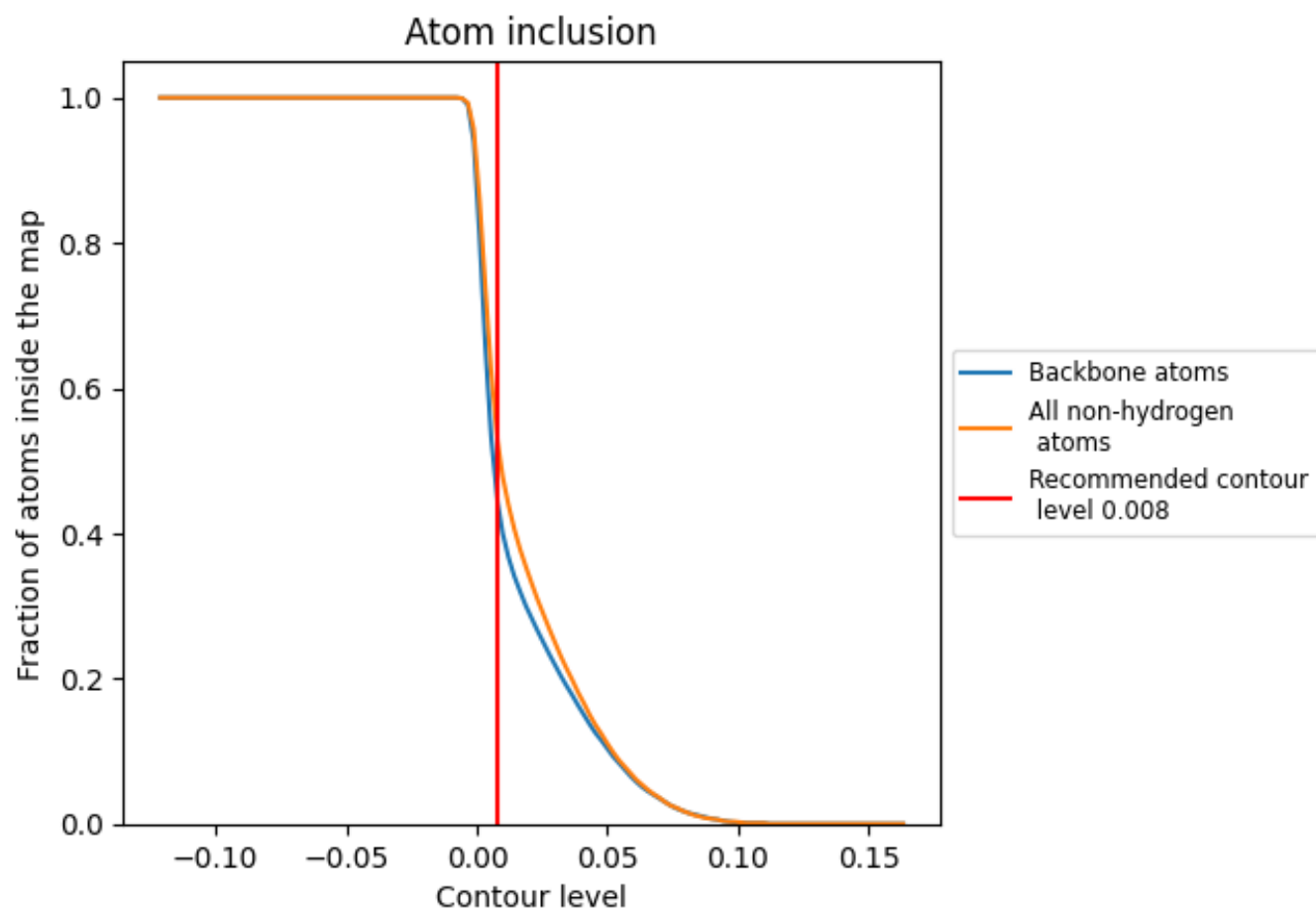
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.008).

9.4 Atom inclusion [i](#)



At the recommended contour level, 44% of all backbone atoms, 53% 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 (0.008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5260	 0.2830
2A	 0.0030	 0.0080
2B	 0.0000	 0.0230
2C	 0.0000	 0.0180
2D	 0.5430	 0.3300
2E	 0.0000	 0.0370
2F	 0.0000	 0.0030
2G	 0.0050	 0.0040
2H	 0.2340	 0.1520
2I	 0.0010	 0.0030
2J	 0.0030	 -0.0330
2K	 0.0000	 0.0130
2L	 0.0000	 -0.0350
2M	 0.0110	 0.0050
2a	 0.0000	 0.0390
2b	 0.0000	 -0.0010
2c	 0.0000	 -0.0030
2d	 0.0000	 0.0150
2e	 0.0000	 -0.0110
2f	 0.0000	 0.0220
2g	 0.0000	 -0.0050
4A	 0.5380	 0.3160
4B	 0.9470	 0.5370
4C	 0.9600	 0.5400
4D	 0.9580	 0.5830
4E	 0.9860	 0.6400
4F	 0.9950	 0.6570
4G	 0.8880	 0.4510
4H	 0.9260	 0.3380
4I	 0.7670	 0.3290
4J	 0.9200	 0.5340
4Z	 0.0570	 -0.0000
4a	 0.0190	 -0.0450
4b	 0.0240	 -0.0130
4c	 0.0730	 -0.0240



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Chain	Atom inclusion	Q-score
4d	 0.0580	 -0.0190
4e	 0.0450	 -0.0350
4f	 0.0600	 0.0000
4g	 0.0620	 0.0350
5A	 0.6410	 0.3220
5B	 0.9230	 0.5570
5C	 0.9400	 0.5080
5D	 0.2680	 0.0360
5E	 0.0720	 0.0020
5a	 0.2230	 -0.0220
5b	 0.1550	 -0.0160
5c	 0.1470	 0.0070
5d	 0.1350	 0.0090
5e	 0.1610	 -0.0140
5f	 0.1980	 -0.0280
5g	 0.2570	 -0.0050
6A	 0.7150	 0.4220
6a	 0.0060	 0.0080
6b	 0.0030	 -0.0140
6c	 0.0030	 0.0150
6d	 0.0070	 0.0160
6e	 0.0210	 0.0620
6f	 0.0040	 0.0110
6g	 0.0080	 -0.0300
A	 0.2650	 0.1630