Full wwPDB EM Validation Report

May 25, 2024 – 11:15 am BST

PDB ID	:	8R0A
EMDB ID	:	EMD-18788
Title	:	Cryo-EM structure of the cross-exon pre-B+5'ss complex
Authors	:	Zhang, Z.; Kumar, V.; Dybkov, O.; Will, C.L.; Zhong, J.; Ludwig, S.; Urlaub, H.; Kastner, B.; Stark, H.; Luehrmann, R.
Deposited on	:	2023-10-31
Resolution	:	5.80 Å(reported)

This is a Full wwPDB EM Validation 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 (i) 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 (i)) were used in the production of this report:

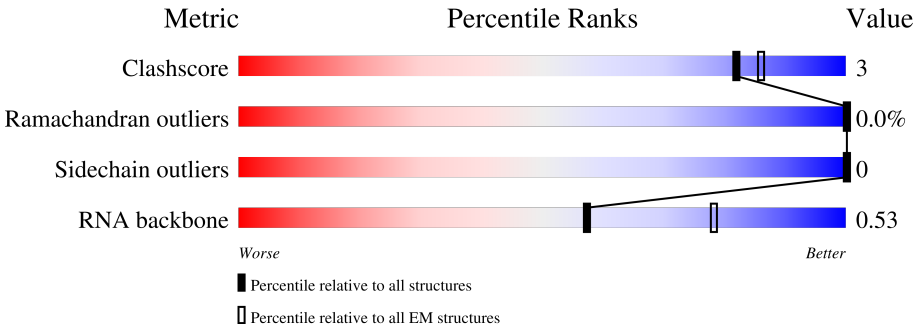
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance

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

The reported resolution of this entry is 5.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	5	117	46% 35% 15%
2	C	972	83% 14%
3	D	142	99%
4	E	357	83% 14%
5	F	522	65% 31%
6	M	128	91% 5%
7	R	480	21% 78%

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Mol	Chain	Length	Quality of chain
8	U	565	74% 7% 19%
9	X	155	14% 86%
10	Z	347	96%
11	z	11	55% 45%
12	A	2335	93% 5%
13	B	2136	92% 7%
14	2	188	17% 35% 13% 48%
15	4	144	45% 29% 8% 14%
16	6	106	42% 10% 44%
17	7	793	14% 20% 80%
18	8	464	18% 30% 69%
19	B4	424	18% 82%
20	9	501	62% 76% 24%
21	B2	895	23% 77%
22	B5	86	78% 20%
23	B3	1217	19% 95%
24	BP	110	91% 9%
25	B1	1304	67% 33%
26	B6	125	67% 5% 28%
27	22	118	81% 81% 19%
27	42	118	13% 77% 22%
27	52	118	82% 18%
28	2B	225	32% 40% 59%
29	2f	86	84% 84% 16%
29	4f	86	10% 84% 16%

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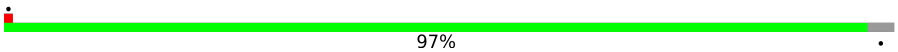
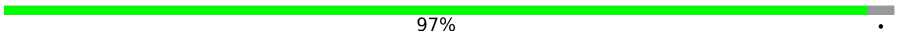
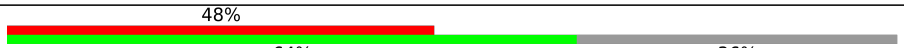
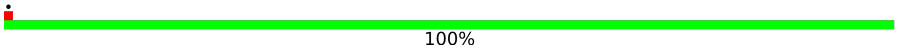
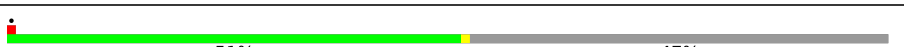
Mol	Chain	Length	Quality of chain
29	5f	86	
30	2b	240	
30	4b	240	
30	5b	240	
31	23	126	
31	43	126	
31	53	126	
32	2g	76	
32	4g	76	
32	5g	76	
33	2e	92	
33	4e	92	
33	5e	92	
34	21	119	
34	41	119	
34	51	119	
35	2A	255	
36	66	80	
37	67	103	
38	62	95	
39	63	102	
40	68	96	
41	64	139	
42	65	91	
43	J	683	

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Mol	Chain	Length	Quality of chain
44	K	1007	
45	G	820	
46	L	499	
47	S	800	
48	N	941	

2 Entry composition

There are 48 unique types of molecules in this entry. The entry contains 80982 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 U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	5	115	2420	1084	403	818	115	0	0

- Molecule 2 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	C	836	4223	2551	836	836	0	0

- Molecule 3 is a protein called Thioredoxin-like protein 4A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	D	141	708	426	141	141	0	0

- Molecule 4 is a protein called U5 small nuclear ribonucleoprotein 40 kDa protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	E	307	1531	917	307	307	0	0

- Molecule 5 is a protein called U4/U6 small nuclear ribonucleoprotein Prp4.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	F	359	1795	1077	359	359	0	0

- Molecule 6 is a protein called NHP2-like protein 1, N-terminally processed.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	M	123	622	376	123	123	0	0

- Molecule 7 is a protein called RNA-binding protein 42.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	R	106	Total	C	N	O	0	0
			531	319	106	106		

- Molecule 8 is a protein called Ubiquitin carboxyl-terminal hydrolase 39.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	U	456	Total	C	N	O	0	0
			2308	1396	456	456		

- Molecule 9 is a protein called U4/U6.U5 small nuclear ribonucleoprotein 27 kDa protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	X	22	Total	C	N	O	0	0
			110	66	22	22		

- Molecule 10 is a RNA chain called pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Z	15	Total	C	N	O	P	0	0
			314	141	51	107	15		

- Molecule 11 is a RNA chain called 5'ss oligo.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	z	11	Total	C	N	O	P	0	0
			239	107	46	75	11		

- Molecule 12 is a protein called Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	A	2210	Total	C	N	O	0	0
			11208	6788	2210	2210		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
13	B	1981	Total	C	N	O	0	0
			9980	6018	1981	1981		

- Molecule 14 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	2	97	Total	C	N	O	P	0	0
			2052	917	346	692	97		

- Molecule 15 is a RNA chain called U4 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	4	124	Total	C	N	O	P	0	0
			2636	1179	466	868	123		

- Molecule 16 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	6	59	Total	C	N	O	P	0	0
			1265	565	230	411	59		

- Molecule 17 is a protein called Splicing factor 3A subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	7	159	Total	C	N	O	0	0
			799	481	159	159		

- Molecule 18 is a protein called Splicing factor 3A subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	8	144	Total	C	N	O	0	0
			729	441	144	144		

- Molecule 19 is a protein called Splicing factor 3B subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	B4	78	Total	C	N	O	0	0
			391	235	78	78		

- Molecule 20 is a protein called Splicing factor 3A subunit 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	9	383	Total	C	N	O	0	0
			1920	1154	383	383		

- Molecule 21 is a protein called Splicing factor 3B subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	B2	208	Total 1072	C 656	N 208	O 208	0	0

- Molecule 22 is a protein called Splicing factor 3B subunit 5.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	B5	69	Total 347	C 209	N 69	O 69	0	0

- Molecule 23 is a protein called Splicing factor 3B subunit 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	B3	1186	Total 5969	C 3597	N 1186	O 1186	0	0

- Molecule 24 is a protein called PHD finger-like domain-containing protein 5A.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	BP	100	Total 498	C 298	N 100	O 100	0	0

- Molecule 25 is a protein called Splicing factor 3B subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	B1	870	Total 4383	C 2643	N 870	O 870	0	0

- Molecule 26 is a protein called Splicing factor 3B subunit 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	B6	90	Total 455	C 275	N 90	O 90	0	0

- Molecule 27 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	22	95	Total 482	C 292	N 95	O 95	0	0
27	52	97	Total 388	C 194	N 97	O 97	0	0
27	42	92	Total 463	C 279	N 92	O 92	0	0

- Molecule 28 is a protein called U2 small nuclear ribonucleoprotein B".

Mol	Chain	Residues	Atoms				AltConf	Trace
28	2B	92	Total	C	N	O	0	0
			461	277	92	92		

- Molecule 29 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	2f	72	Total	C	N	O	0	0
			359	215	72	72		
29	5f	74	Total	C	N	O	0	0
			296	148	74	74		
29	4f	72	Total	C	N	O	0	0
			359	215	72	72		

- Molecule 30 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	2b	82	Total	C	N	O	0	0
			413	249	82	82		
30	5b	86	Total	C	N	O	0	0
			344	172	86	86		
30	4b	82	Total	C	N	O	0	0
			413	249	82	82		

- Molecule 31 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	23	83	Total	C	N	O	0	0
			415	249	83	83		
31	53	77	Total	C	N	O	0	0
			308	154	77	77		
31	43	83	Total	C	N	O	0	0
			415	249	83	83		

- Molecule 32 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	2g	73	Total	C	N	O	0	0
			364	218	73	73		
32	5g	74	Total	C	N	O	0	0
			296	148	74	74		

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Mol	Chain	Residues	Atoms				AltConf	Trace
32	4g	74	Total 369	C 221	N 74	O 74	0	0

- Molecule 33 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	2e	81	Total 403	C 241	N 81	O 81	0	0
33	5e	79	Total 316	C 158	N 79	O 79	0	0
33	4e	76	Total 378	C 226	N 76	O 76	0	0

- Molecule 34 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	21	80	Total 402	C 242	N 80	O 80	0	0
34	51	82	Total 328	C 164	N 82	O 82	0	0
34	41	81	Total 407	C 245	N 81	O 81	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
35	2A	162	Total 816	C 492	N 162	O 162	0	0

- Molecule 36 is a protein called U6 snRNA-associated Sm-like protein LSm6.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	66	72	Total 357	C 213	N 72	O 72	0	0

- Molecule 37 is a protein called U6 snRNA-associated Sm-like protein LSm7.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	67	77	Total 384	C 230	N 77	O 77	0	0

- Molecule 38 is a protein called U6 snRNA-associated Sm-like protein LSm2.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	62	95	Total	C	N	O	0	0
			478	288	95	95		

- Molecule 39 is a protein called U6 snRNA-associated Sm-like protein LSm3.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	63	85	Total	C	N	O	0	0
			429	259	85	85		

- Molecule 40 is a protein called U6 snRNA-associated Sm-like protein LSm8.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	68	95	Total	C	N	O	0	0
			469	279	95	95		

- Molecule 41 is a protein called U6 snRNA-associated Sm-like protein LSm4.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	64	73	Total	C	N	O	0	0
			369	223	73	73		

- Molecule 42 is a protein called U6 snRNA-associated Sm-like protein LSm5.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	65	76	Total	C	N	O	0	0
			378	226	76	76		

- Molecule 43 is a protein called U4/U6 small nuclear ribonucleoprotein Prp3.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	J	159	Total	C	N	O	0	0
			792	474	159	159		

- Molecule 44 is a protein called Serine/threonine-protein kinase PRP4 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	K	322	Total	C	N	O	0	0
			1615	971	322	322		

- Molecule 45 is a protein called Probable ATP-dependent RNA helicase DDX23.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	G	415	Total 2128	C 1286	N 421	O 421	6	0

- Molecule 46 is a protein called U4/U6 small nuclear ribonucleoprotein Prp31.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	L	292	Total 1464	C 880	N 292	O 292	0	0

- Molecule 47 is a protein called U4/U6.U5 tri-snRNP-associated protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
47	S	86	Total 428	C 256	N 86	O 86	0	0

- Molecule 48 is a protein called Pre-mRNA-processing factor 6.

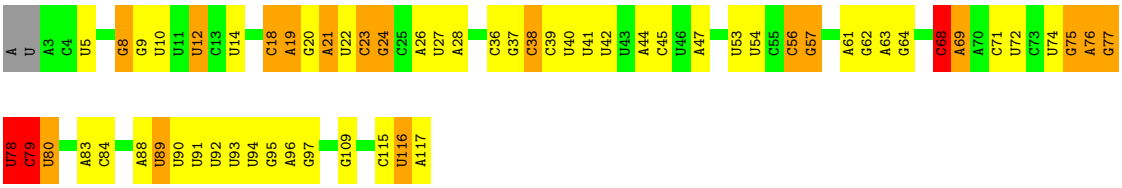
Mol	Chain	Residues	Atoms				AltConf	Trace
48	N	792	Total 3991	C 2407	N 792	O 792	0	0

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.

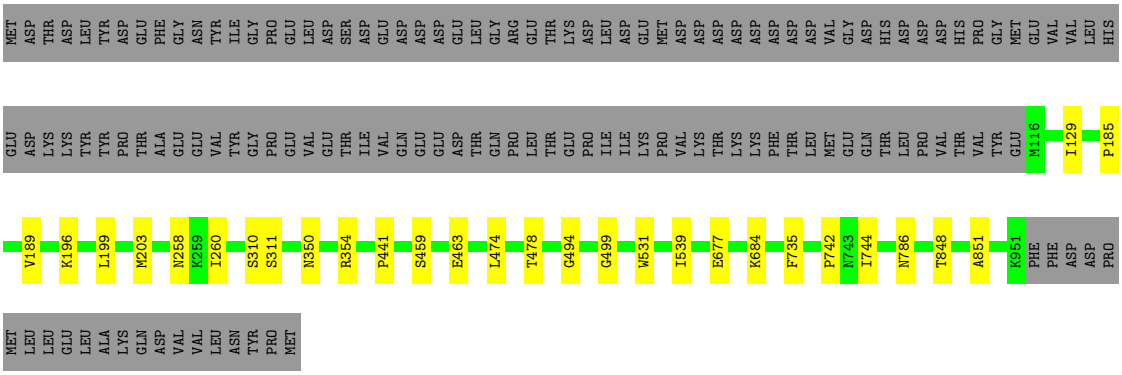
• Molecule 1: U5 snRNA

Chain 5:



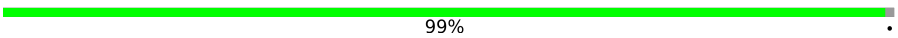
• Molecule 2: 116 kDa U5 small nuclear ribonucleoprotein component

Chain C:



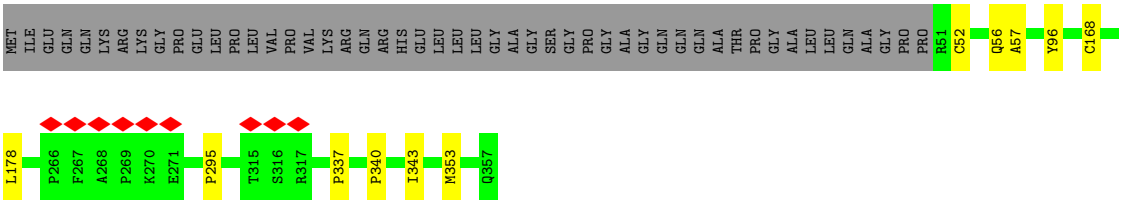
• Molecule 3: Thioredoxin-like protein 4A

Chain D:



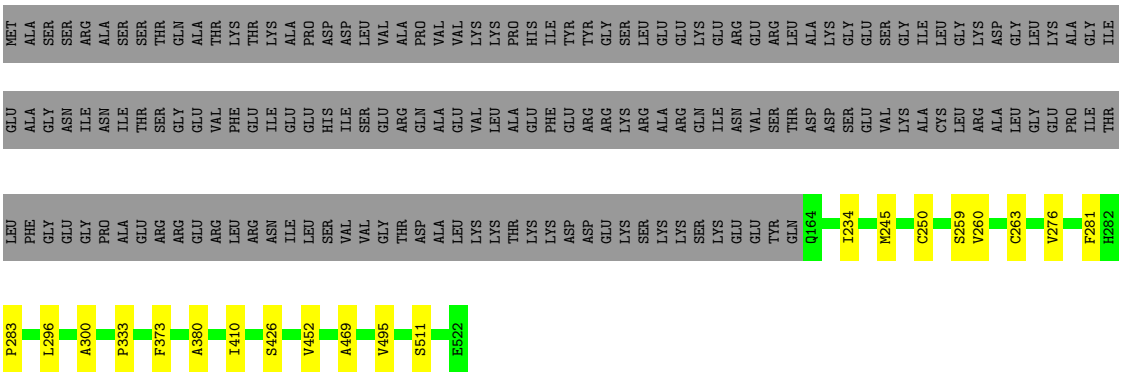
• Molecule 4: U5 small nuclear ribonucleoprotein 40 kDa protein

Chain E:



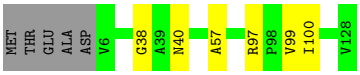
• Molecule 5: U4/U6 small nuclear ribonucleoprotein Prp4

Chain F:



• Molecule 6: NHP2-like protein 1, N-terminally processed

Chain M:

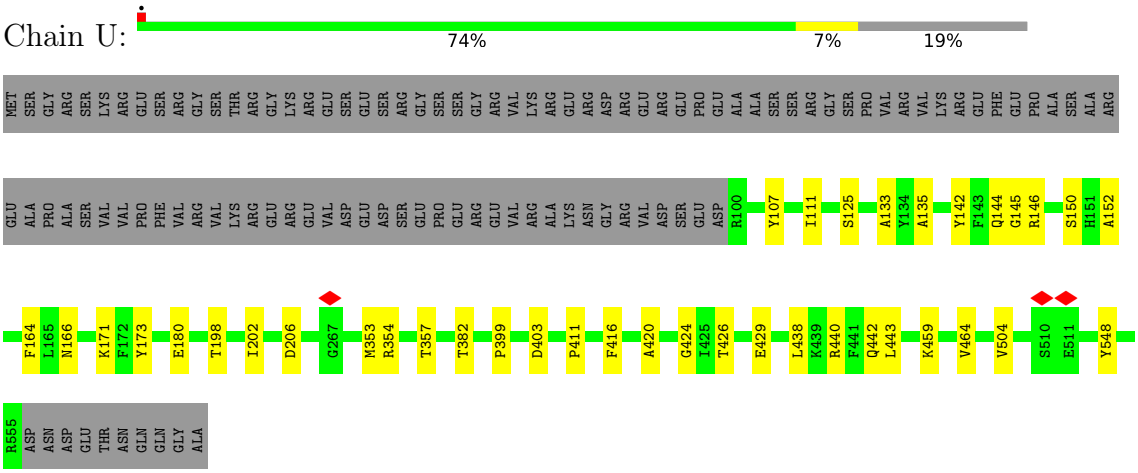


• Molecule 7: RNA-binding protein 42

Chain R:

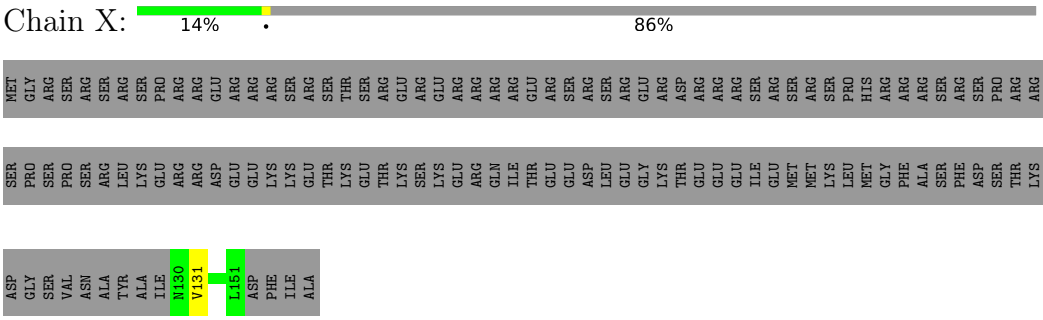
• Molecule 8: Ubiquitin carboxyl-terminal hydrolase 39

Chain U:



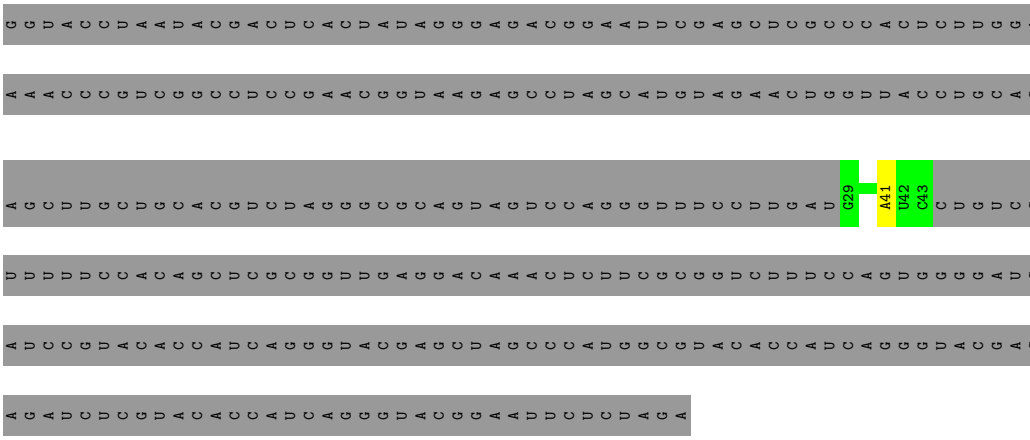
• Molecule 9: U4/U6.U5 small nuclear ribonucleoprotein 27 kDa protein

Chain X:



• Molecule 10: pre-mRNA

Chain Z:

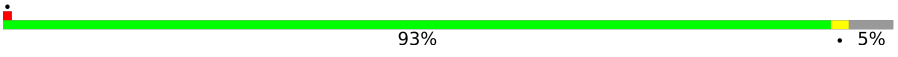


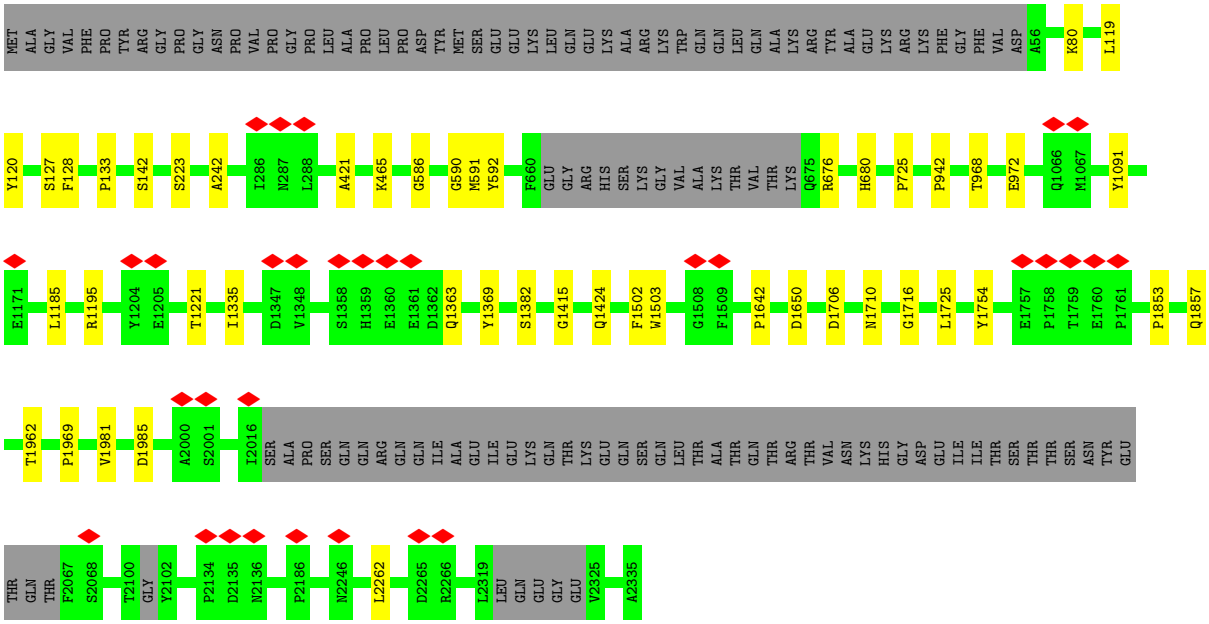
• Molecule 11: 5'ss oligo

Chain z:

• Molecule 12: Pre-mRNA-processing-splicing factor 8

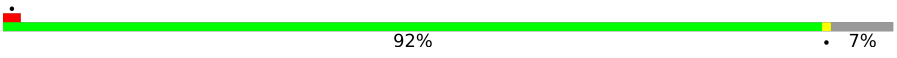
Chain A:

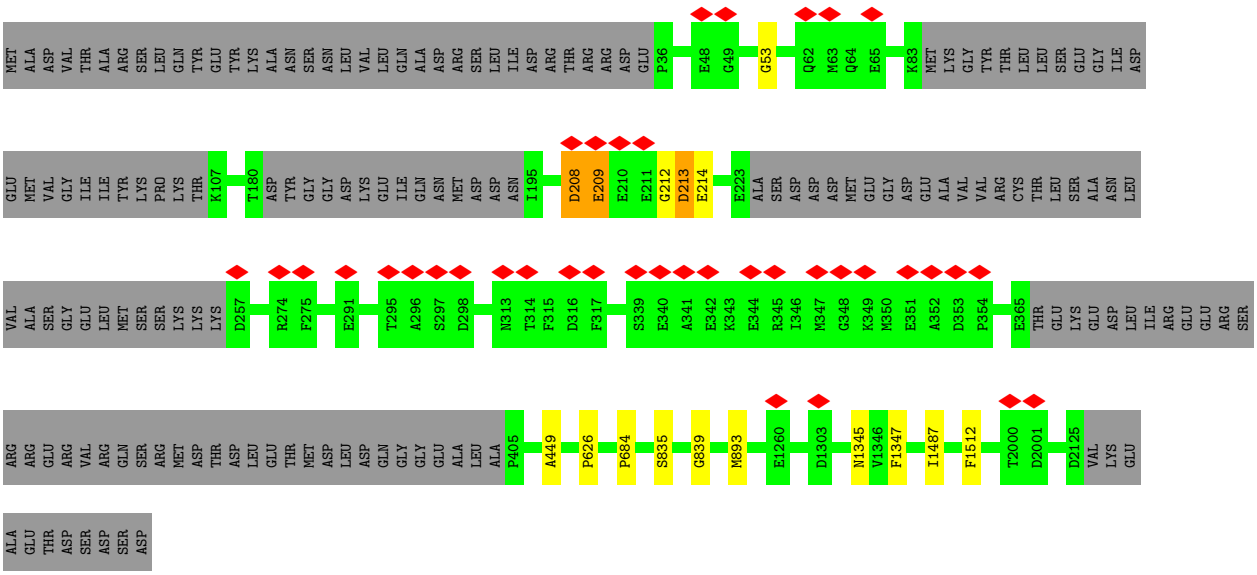




• Molecule 13: U5 small nuclear ribonucleoprotein 200 kDa helicase

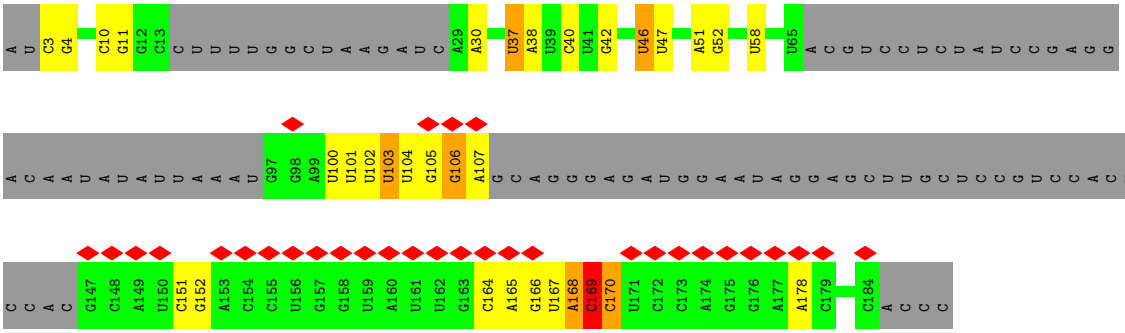
Chain B:





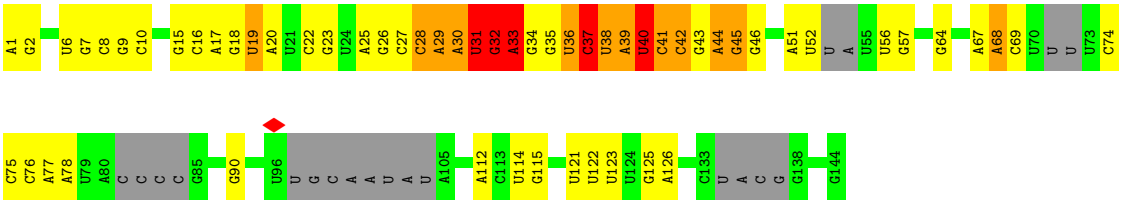
• Molecule 14: U2 snRNA

Chain 2:



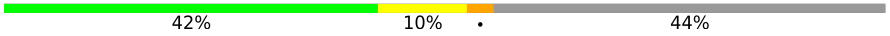
• Molecule 15: U4 snRNA

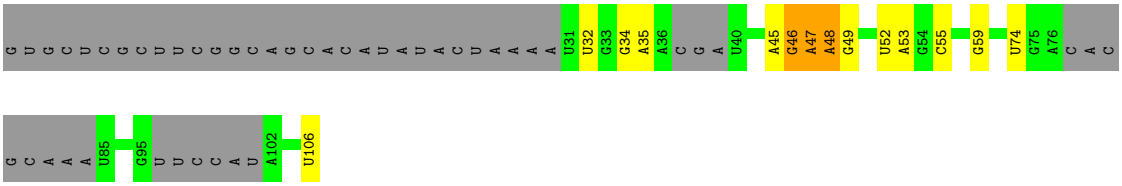
Chain 4:



• Molecule 16: U6 snRNA

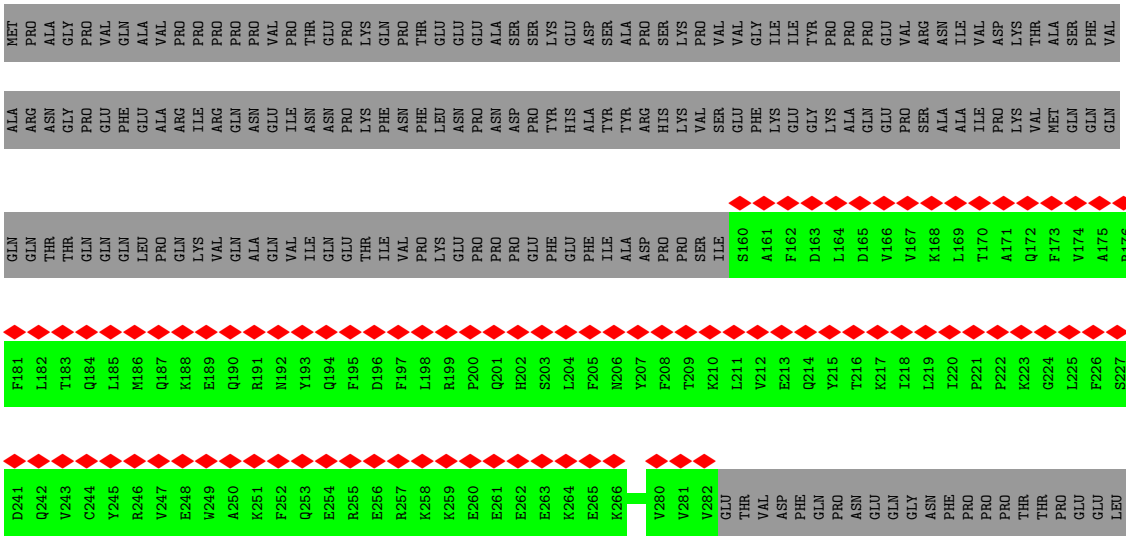
Chain 6:

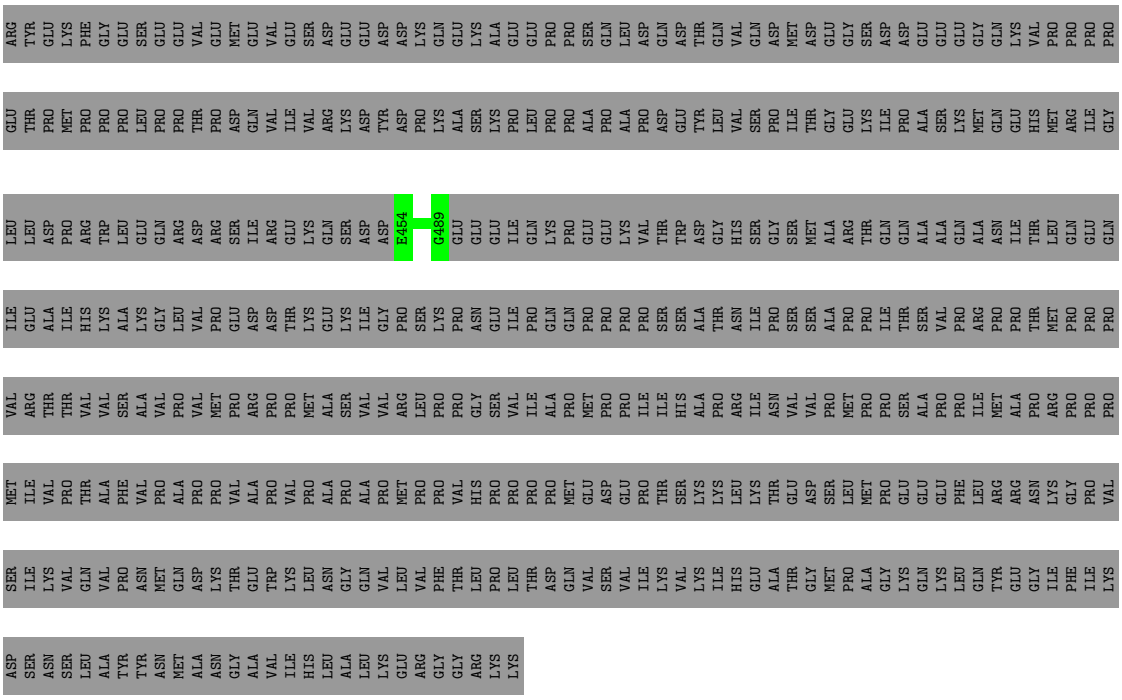




• Molecule 17: Splicing factor 3A subunit 1

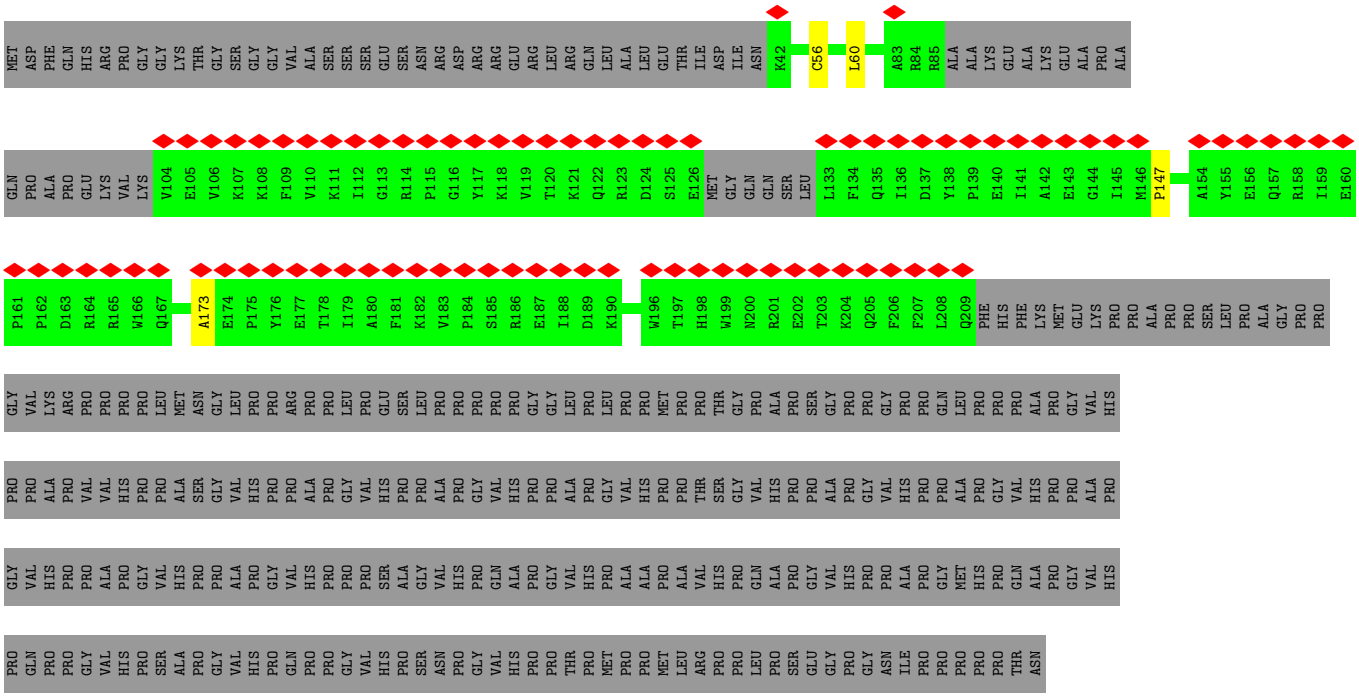
Chain 7:





• Molecule 18: Splicing factor 3A subunit 2

Chain 8:

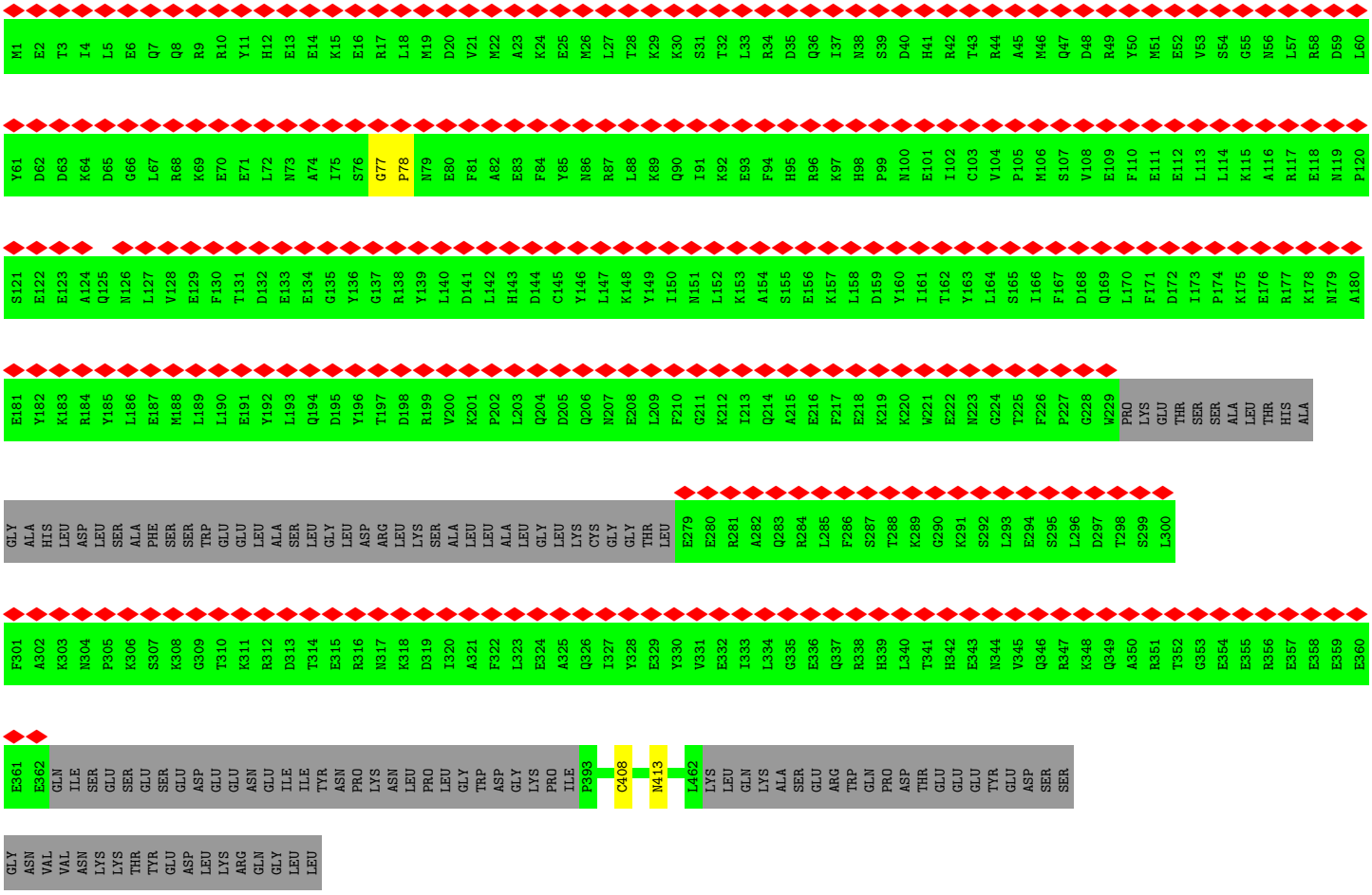


• Molecule 19: Splicing factor 3B subunit 4

Chain B4:

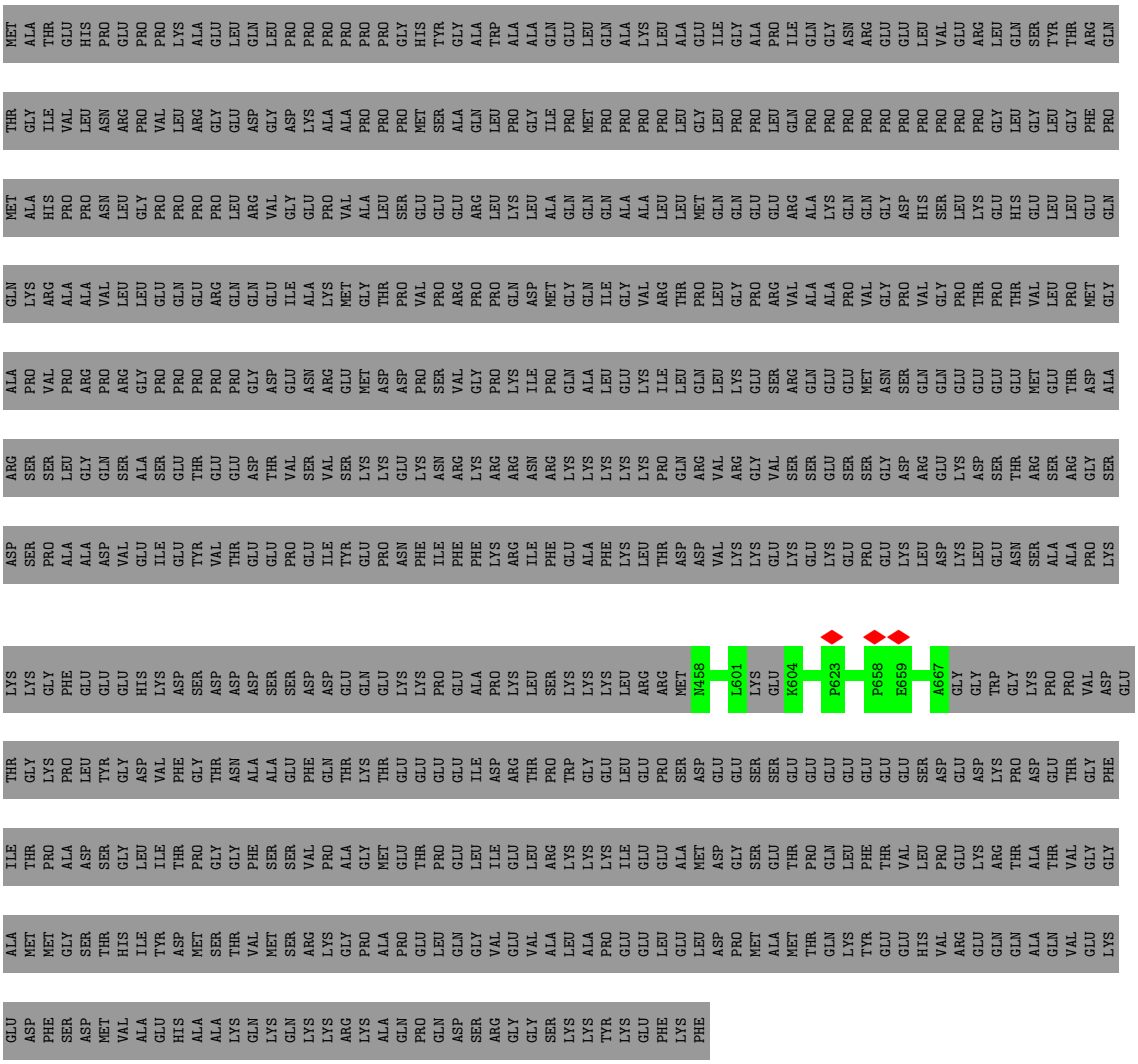
• Molecule 20: Splicing factor 3A subunit 3

Chain 9:



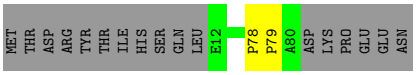
• Molecule 21: Splicing factor 3B subunit 2

Chain B2:



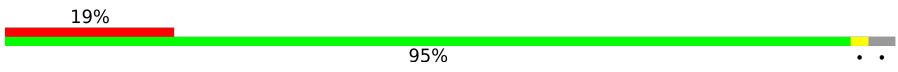
• Molecule 22: Splicing factor 3B subunit 5

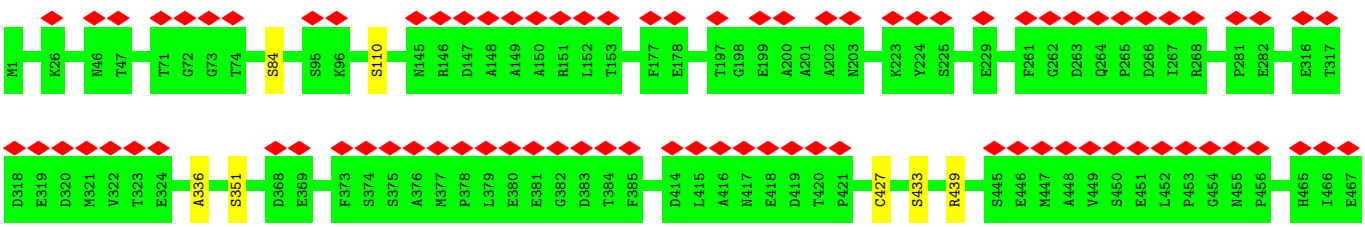
Chain B5:

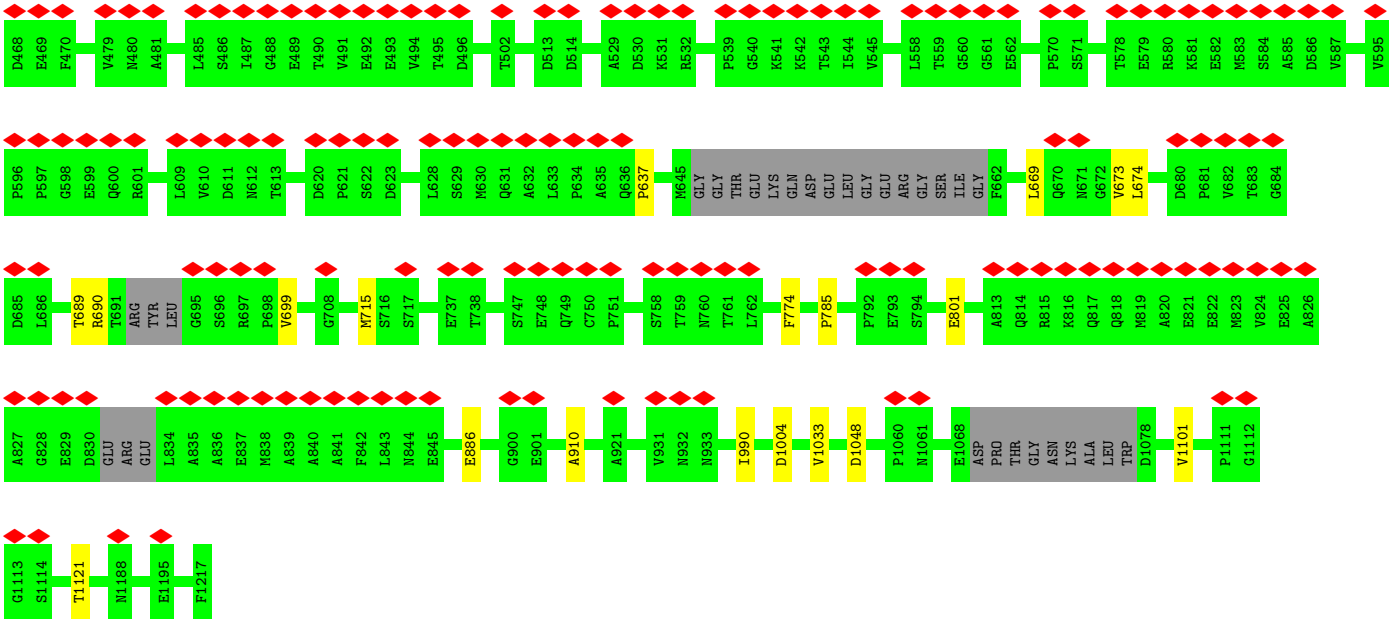


• Molecule 23: Splicing factor 3B subunit 3

Chain B3:

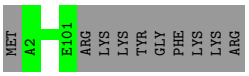






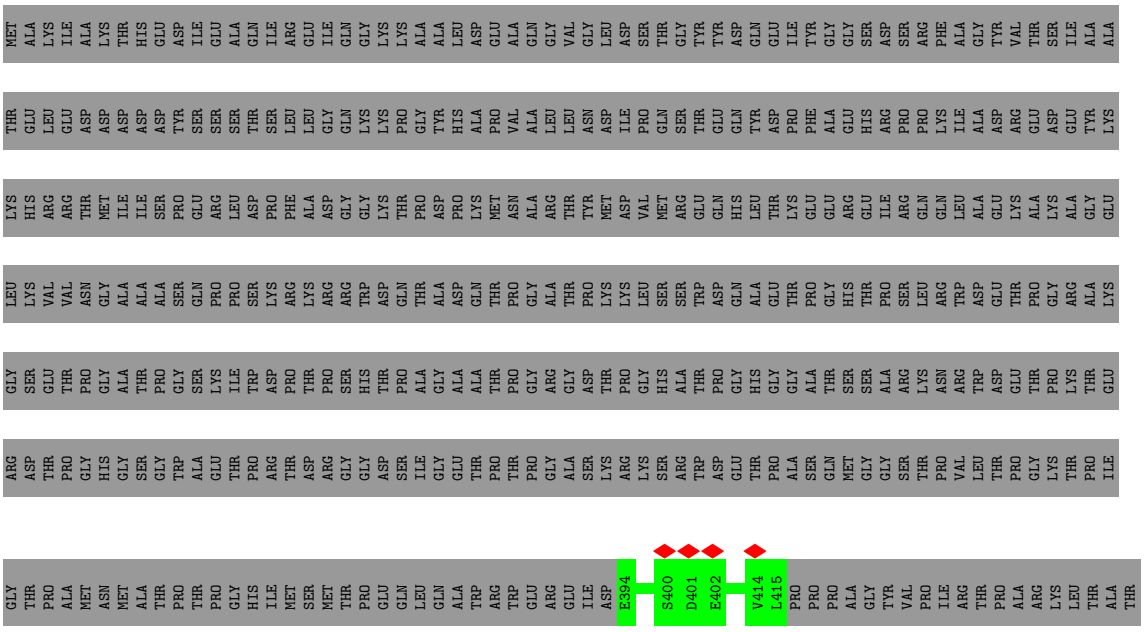
• Molecule 24: PHD finger-like domain-containing protein 5A

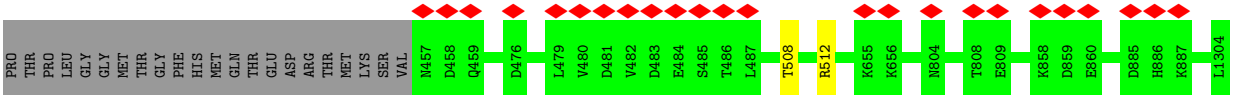
Chain BP:



• Molecule 25: Splicing factor 3B subunit 1

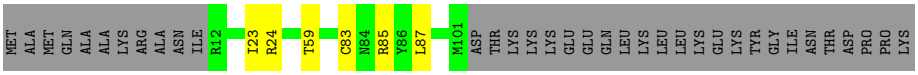
Chain B1:





• Molecule 26: Splicing factor 3B subunit 6

Chain B6:

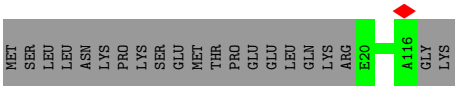


• Molecule 27: Small nuclear ribonucleoprotein Sm D2

Chain 22:

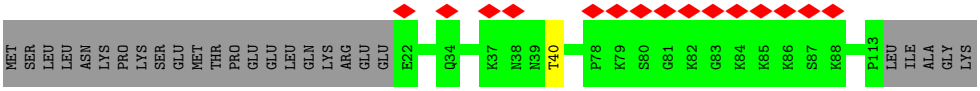
• Molecule 27: Small nuclear ribonucleoprotein Sm D2

Chain 52:



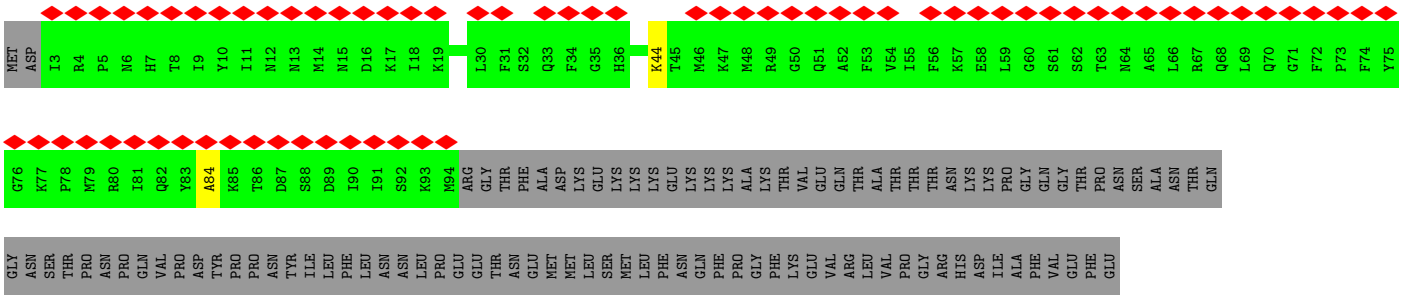
• Molecule 27: Small nuclear ribonucleoprotein Sm D2

Chain 42:



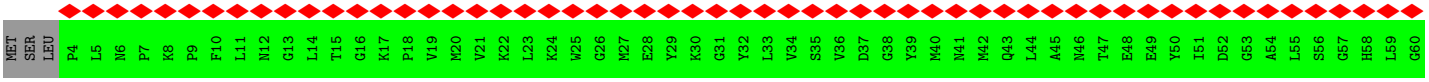
• Molecule 28: U2 small nuclear ribonucleoprotein B"

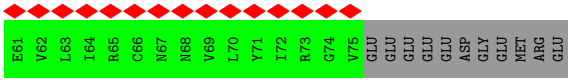
Chain 2B:



• Molecule 29: Small nuclear ribonucleoprotein F

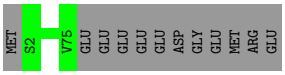
Chain 2f:





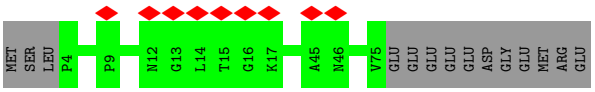
• Molecule 29: Small nuclear ribonucleoprotein F

Chain 5f:



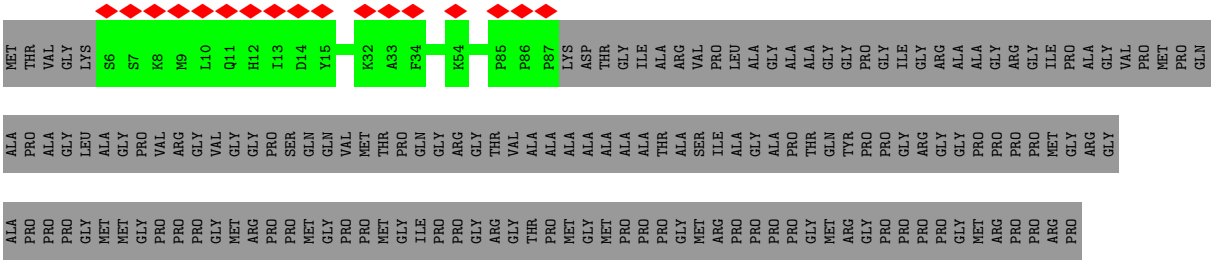
• Molecule 29: Small nuclear ribonucleoprotein F

Chain 4f:



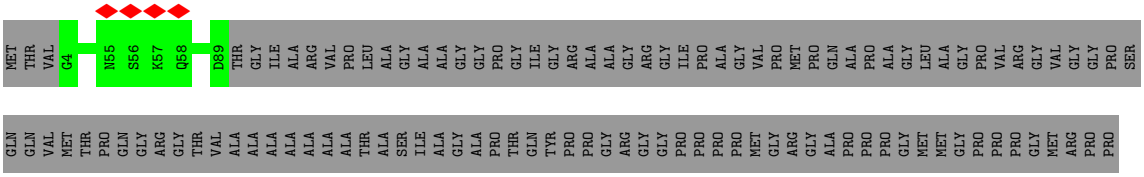
• Molecule 30: Small nuclear ribonucleoprotein-associated proteins B and B'

Chain 2b:



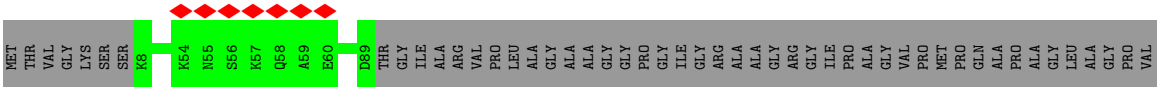
• Molecule 30: Small nuclear ribonucleoprotein-associated proteins B and B'

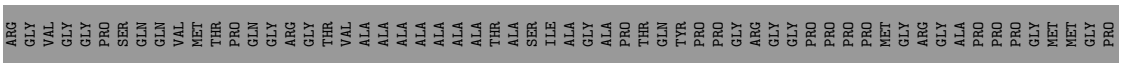
Chain 5b:



• Molecule 30: Small nuclear ribonucleoprotein-associated proteins B and B'

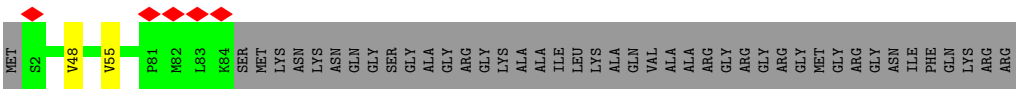
Chain 4b:





• Molecule 31: Small nuclear ribonucleoprotein Sm D3

Chain 23:



• Molecule 31: Small nuclear ribonucleoprotein Sm D3

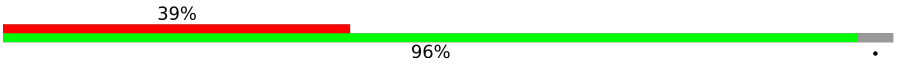
Chain 53:

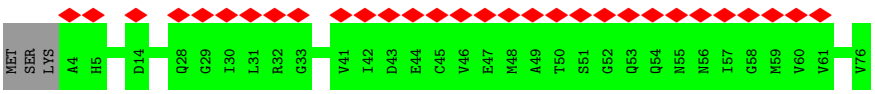
• Molecule 31: Small nuclear ribonucleoprotein Sm D3

Chain 43:

• Molecule 32: Small nuclear ribonucleoprotein G

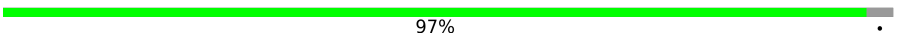
Chain 2g:

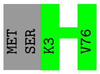




• Molecule 32: Small nuclear ribonucleoprotein G

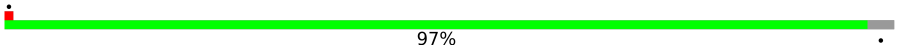
Chain 5g:

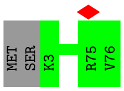




• Molecule 32: Small nuclear ribonucleoprotein G

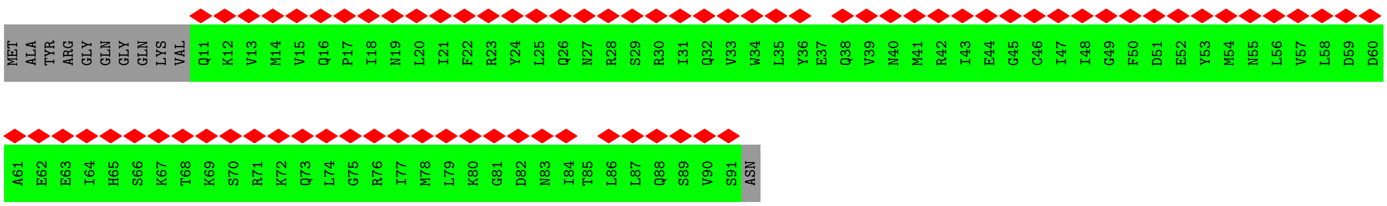
Chain 4g:





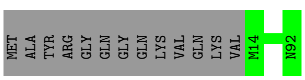
• Molecule 33: Small nuclear ribonucleoprotein E

Chain 2e:



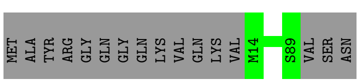
• Molecule 33: Small nuclear ribonucleoprotein E

Chain 5e:



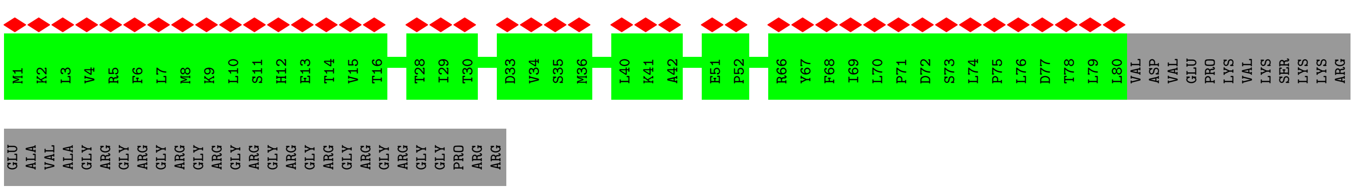
• Molecule 33: Small nuclear ribonucleoprotein E

Chain 4e:



• Molecule 34: Small nuclear ribonucleoprotein Sm D1

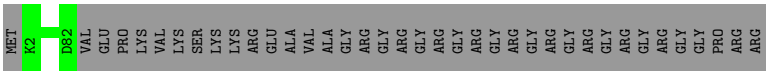
Chain 21:



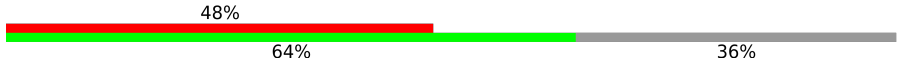
• Molecule 34: Small nuclear ribonucleoprotein Sm D1

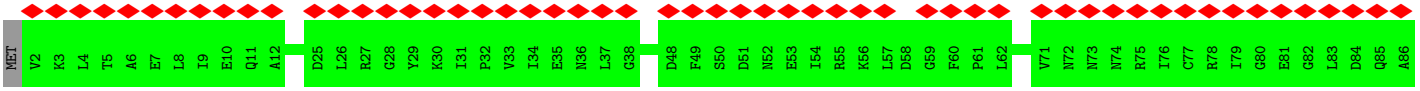
Chain 51:

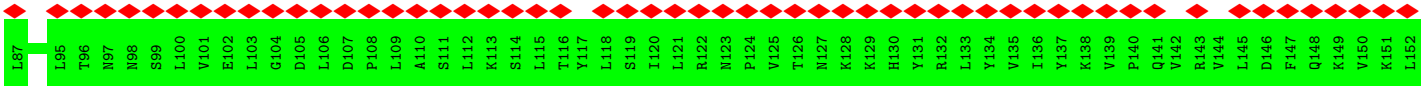
• Molecule 34: Small nuclear ribonucleoprotein Sm D1

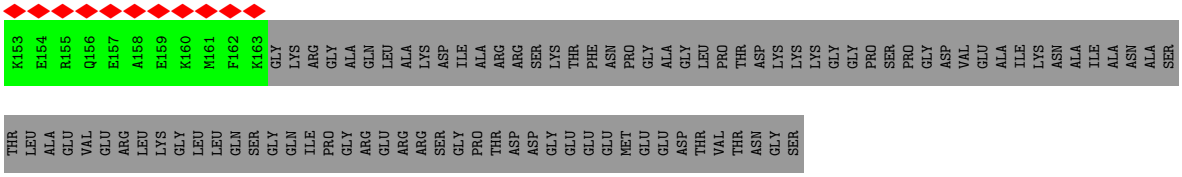


• Molecule 35: U2 small nuclear ribonucleoprotein A'

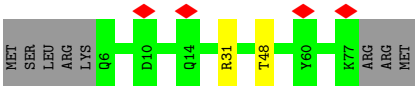




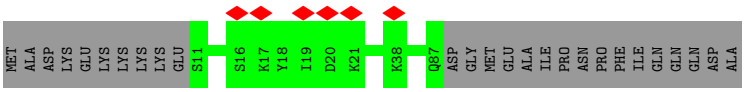




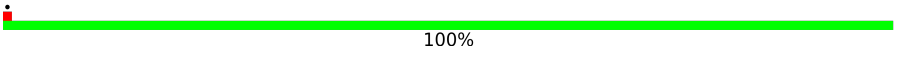
• Molecule 36: U6 snRNA-associated Sm-like protein LSm6

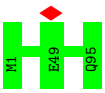


• Molecule 37: U6 snRNA-associated Sm-like protein LSm7



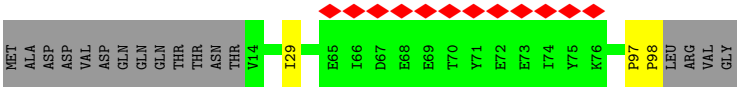
• Molecule 38: U6 snRNA-associated Sm-like protein LSm2





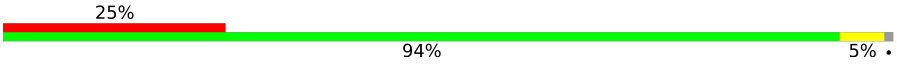
• Molecule 39: U6 snRNA-associated Sm-like protein LSm3

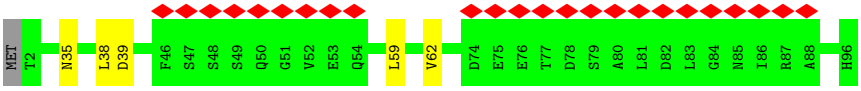
Chain 63:



• Molecule 40: U6 snRNA-associated Sm-like protein LSm8

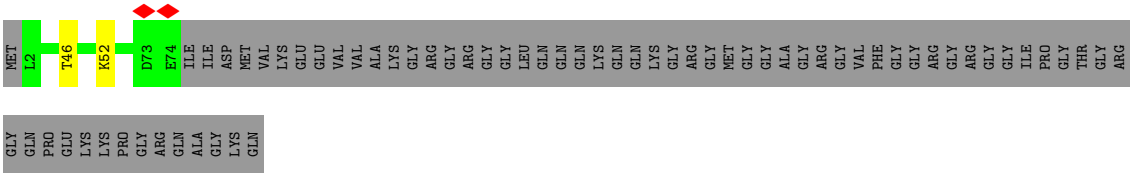
Chain 68:





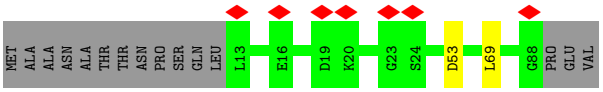
• Molecule 41: U6 snRNA-associated Sm-like protein LSm4

Chain 64:



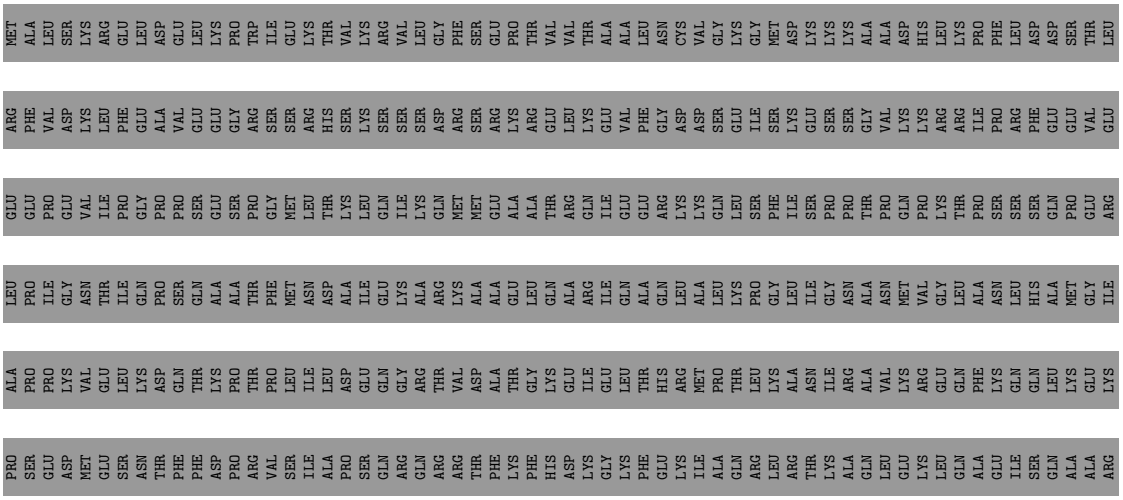
• Molecule 42: U6 snRNA-associated Sm-like protein LSm5

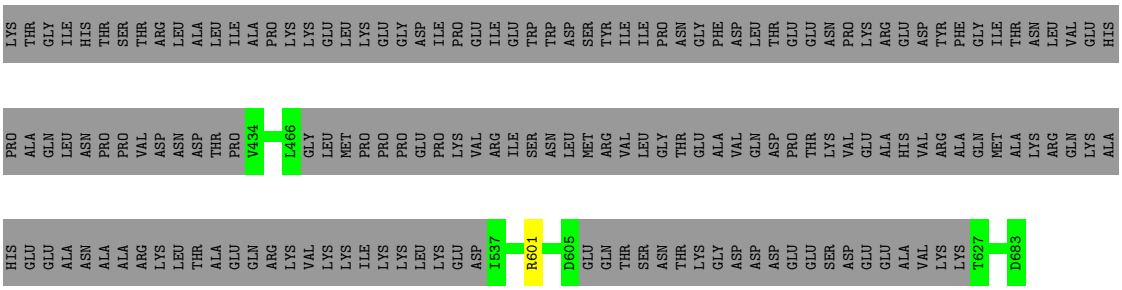
Chain 65:



• Molecule 43: U4/U6 small nuclear ribonucleoprotein Prp3

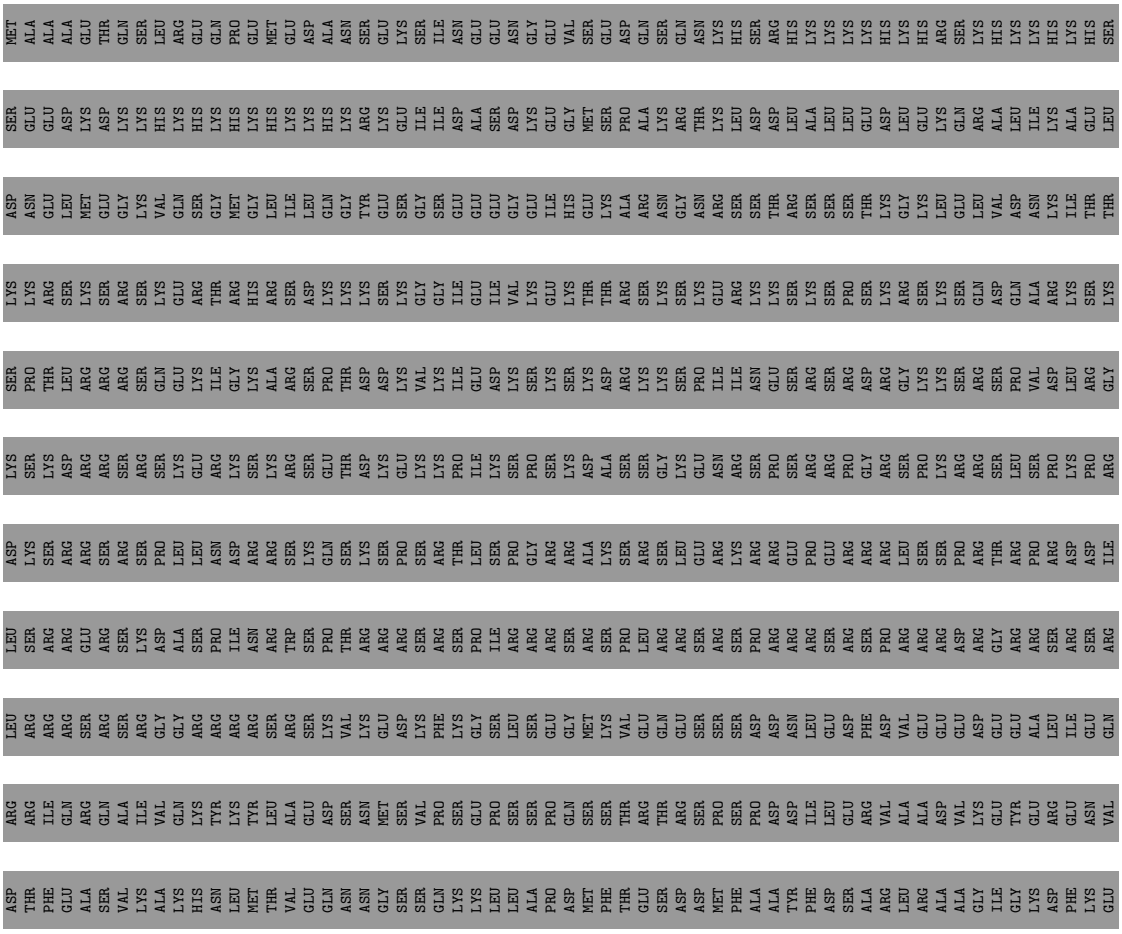
Chain J:

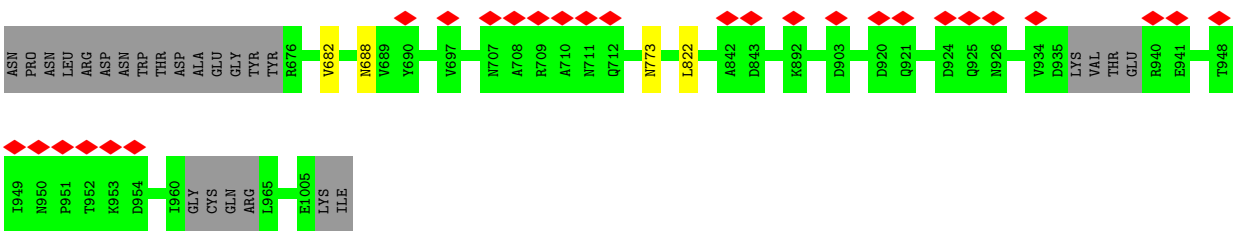




• Molecule 44: Serine/threonine-protein kinase PRP4 homolog

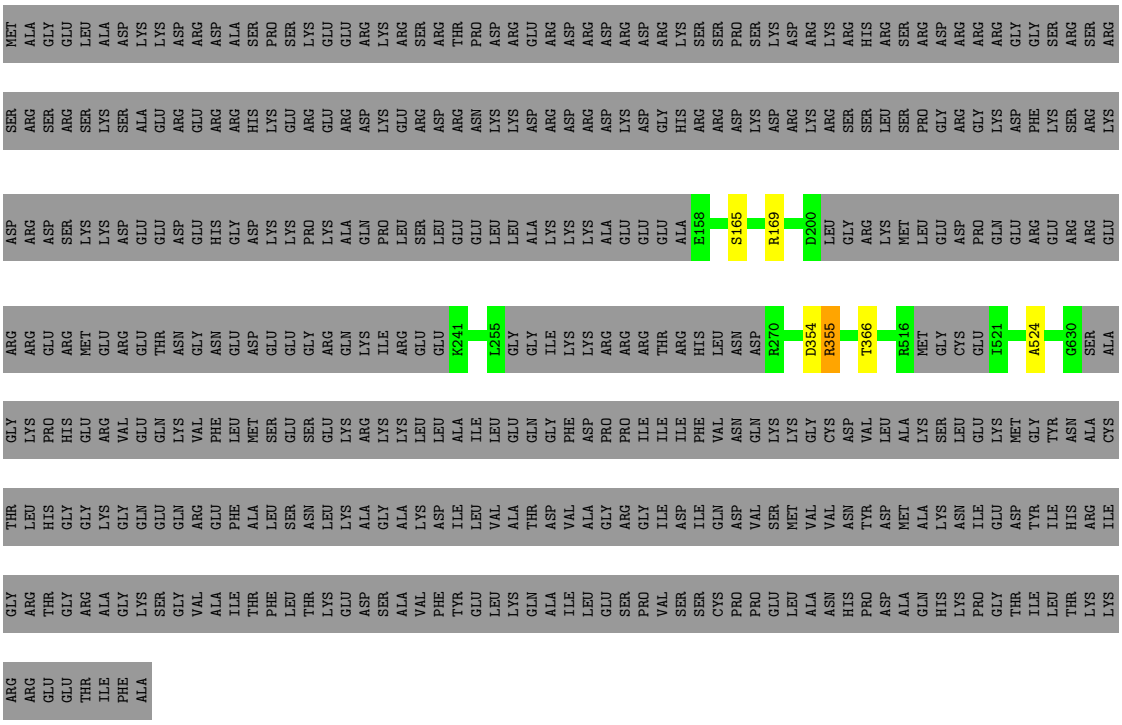
Chain K:





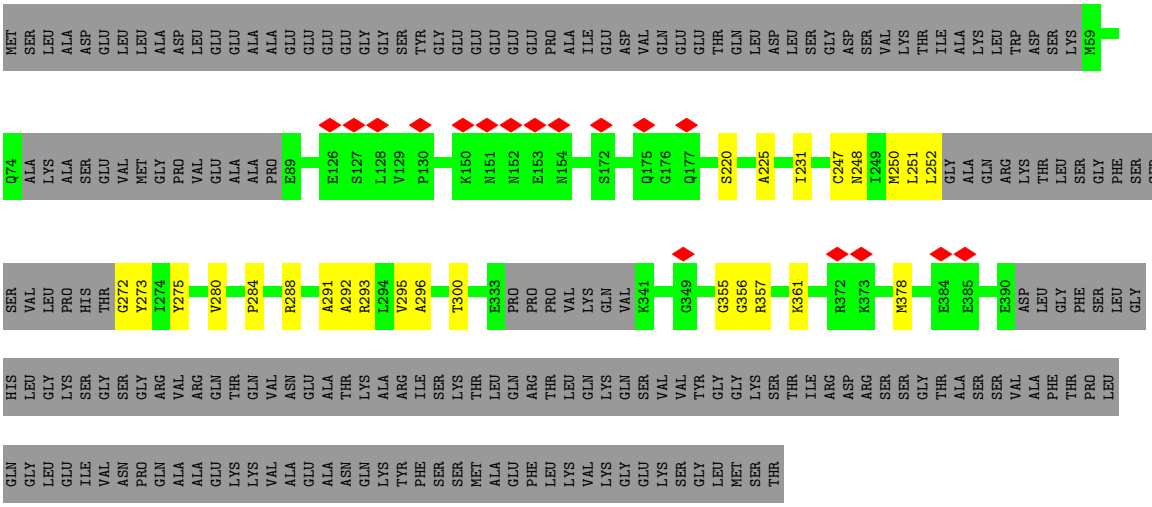
• Molecule 45: Probable ATP-dependent RNA helicase DDX23

Chain G:



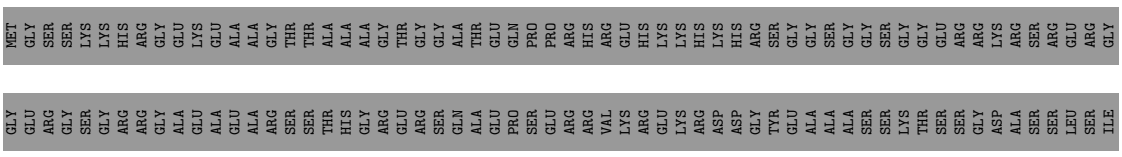
• Molecule 46: U4/U6 small nuclear ribonucleoprotein Prp31

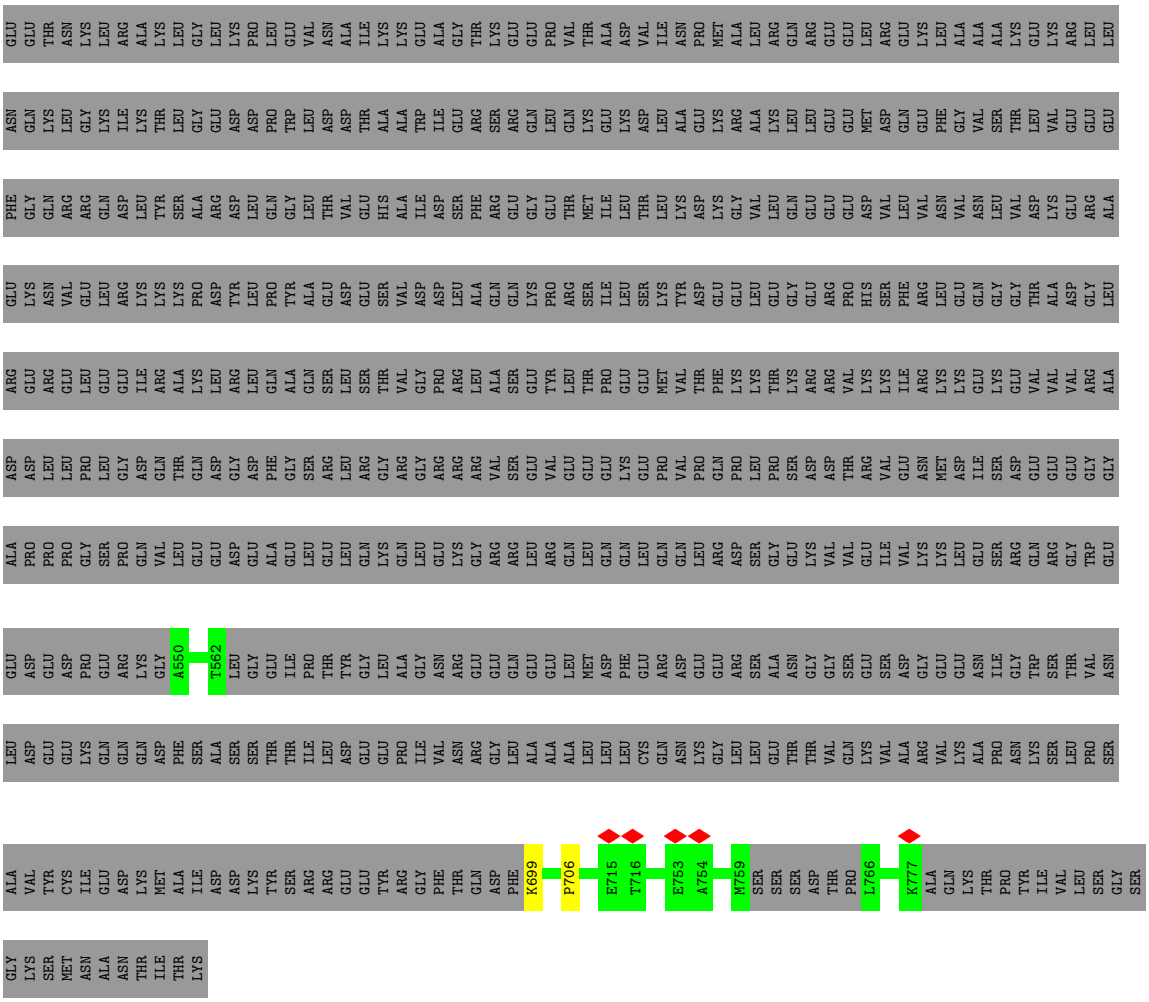
Chain L:



• Molecule 47: U4/U6.U5 tri-snRNP-associated protein 1

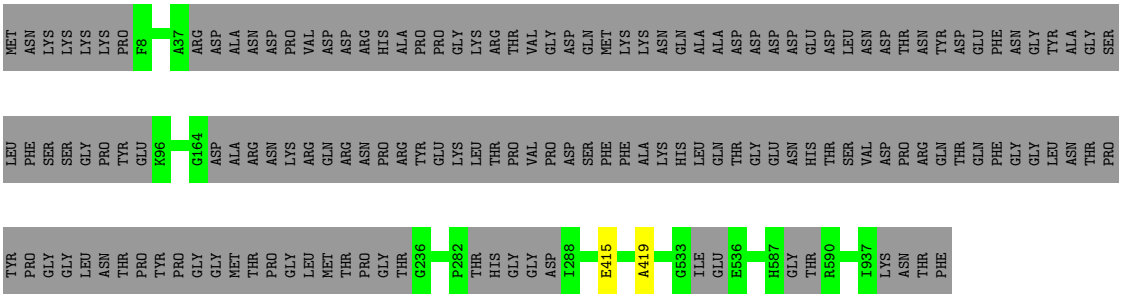
Chain S:





• Molecule 48: Pre-mRNA-processing factor 6

Chain N:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	176879	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	45	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.034	Depositor
Minimum map value	-0.010	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.007	Depositor
Map size (Å)	580.0, 580.0, 580.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.16, 1.16, 1.16	Depositor

5 Model quality

5.1 Standard geometry

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	5	0.26	0/2698	0.89	12/4195 (0.3%)
2	C	0.24	0/4270	0.42	0/5983
3	D	0.23	0/712	0.42	0/995
4	E	0.28	0/1540	0.49	0/2148
5	F	0.24	0/1809	0.46	0/2525
6	M	0.34	0/627	0.44	0/878
7	R	0.24	0/534	0.41	0/745
8	U	0.23	0/2330	0.41	0/3268
9	X	0.41	0/110	0.48	0/152
10	Z	0.23	0/349	0.94	0/540
11	z	0.17	0/268	0.73	0/416
12	A	0.24	0/11329	0.41	0/15897
13	B	0.25	0/10059	0.41	0/14084
14	2	0.32	0/2286	1.00	12/3550 (0.3%)
15	4	0.29	0/2941	0.88	12/4569 (0.3%)
16	6	0.16	0/1413	0.71	0/2194
17	7	0.24	0/802	0.38	0/1120
18	8	0.24	0/734	0.46	0/1025
19	B4	0.26	0/394	0.44	0/549
20	9	0.24	0/1928	0.39	0/2692
21	B2	0.25	0/1092	0.42	0/1536
22	B5	0.24	0/349	0.36	0/487
23	B3	0.25	0/6024	0.47	0/8425
24	BP	0.24	0/501	0.44	0/697
25	B1	0.26	0/4421	0.41	0/6190
26	B6	0.23	0/459	0.41	0/642
27	22	0.24	0/485	0.43	0/677
27	42	0.33	0/466	0.51	0/651
27	52	0.23	0/387	0.50	0/482
28	2B	0.23	0/463	0.41	0/646
29	2f	0.26	0/362	0.49	0/502
29	4f	0.25	0/362	0.49	0/502
29	5f	0.24	0/295	0.50	0/367
30	2b	0.24	0/416	0.46	0/581

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
30	4b	0.25	0/416	0.47	0/581
30	5b	0.24	0/343	0.51	0/427
31	23	0.26	0/417	0.48	0/581
31	43	0.25	0/417	0.49	0/581
31	53	0.25	0/307	0.50	0/382
32	2g	0.25	0/366	0.48	0/509
32	4g	0.23	0/371	0.46	0/516
32	5g	0.24	0/295	0.51	0/367
33	2e	0.24	0/403	0.44	0/561
33	4e	0.24	0/378	0.46	0/526
33	5e	0.23	0/315	0.50	0/392
34	21	0.23	0/404	0.47	0/564
34	41	0.23	0/409	0.48	0/571
34	51	0.23	0/327	0.50	0/407
35	2A	0.24	0/821	0.45	0/1149
36	66	0.25	0/358	0.46	0/497
37	67	0.23	0/386	0.47	0/537
38	62	0.24	0/480	0.44	0/671
39	63	0.24	0/432	0.47	0/604
40	68	0.24	0/469	0.49	0/651
41	64	0.25	0/372	0.47	0/520
42	65	0.24	0/380	0.48	0/528
43	J	0.25	0/792	0.39	0/1101
44	K	0.24	0/1622	0.42	0/2265
45	G	0.27	0/2146	0.43	1/3003 (0.0%)
46	L	0.31	0/1469	0.39	0/2049
47	S	0.24	0/427	0.38	0/591
48	N	0.25	0/4017	0.39	0/5620
All	All	0.25	0/82554	0.51	37/116661 (0.0%)

There are no bond length outliers.

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	4	37	C	P-O3'-C3'	-9.75	108.00	119.70
15	4	32	G	P-O3'-C3'	-9.60	108.19	119.70
15	4	41	C	P-O3'-C3'	-9.51	108.29	119.70
15	4	30	A	P-O3'-C3'	-9.48	108.32	119.70
1	5	76	A	P-O3'-C3'	-9.40	108.42	119.70
15	4	40	U	P-O3'-C3'	-9.24	108.61	119.70
14	2	168	A	P-O3'-C3'	-8.93	108.99	119.70
1	5	77	G	P-O3'-C3'	-8.83	109.10	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	4	39	A	P-O3'-C3'	-8.82	109.12	119.70
14	2	167	U	P-O3'-C3'	-8.66	109.31	119.70
15	4	33	A	P-O3'-C3'	-8.42	109.59	119.70
15	4	38	U	P-O3'-C3'	-8.30	109.74	119.70
1	5	79	C	P-O3'-C3'	-8.13	109.94	119.70
15	4	31	U	P-O3'-C3'	-8.08	110.01	119.70
1	5	68	C	N1-C2-O2	8.05	123.73	118.90
14	2	169	C	P-O3'-C3'	-7.94	110.17	119.70
1	5	68	C	C2-N1-C1'	7.72	127.29	118.80
1	5	78	U	P-O3'-C3'	-7.17	111.10	119.70
14	2	106	G	P-O3'-C3'	7.05	128.16	119.70
14	2	103	U	OP2-P-O3'	7.00	120.59	105.20
15	4	29	A	P-O3'-C3'	-6.80	111.55	119.70
14	2	103	U	P-O3'-C3'	6.79	127.84	119.70
14	2	46	U	P-O3'-C3'	6.68	127.72	119.70
15	4	28	C	P-O3'-C3'	-6.68	111.69	119.70
15	4	42	C	P-O3'-C3'	-6.62	111.75	119.70
1	5	80	U	P-O3'-C3'	-6.53	111.86	119.70
1	5	68	C	N3-C2-O2	-6.44	117.39	121.90
14	2	170	C	P-O3'-C3'	-6.37	112.06	119.70
1	5	75	G	P-O3'-C3'	-6.04	112.45	119.70
45	G	524	ALA	C-N-CA	5.63	135.78	121.70
14	2	58	U	N1-C2-O2	5.30	126.51	122.80
1	5	68	C	C6-N1-C1'	-5.29	114.45	120.80
14	2	166	G	P-O3'-C3'	-5.26	113.39	119.70
1	5	115	C	C6-N1-C2	-5.26	118.19	120.30
1	5	68	C	C6-N1-C2	-5.19	118.22	120.30
14	2	58	U	N3-C2-O2	-5.11	118.62	122.20
14	2	37	U	P-O3'-C3'	5.10	125.82	119.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	5	2420	0	1226	29	0
2	C	4223	0	2099	17	0
3	D	708	0	328	0	0
4	E	1531	0	747	8	0
5	F	1795	0	891	10	0
6	M	622	0	313	8	0
7	R	531	0	253	3	0
8	U	2308	0	1104	23	0
9	X	110	0	50	1	0
10	Z	314	0	160	0	0
11	z	239	0	119	0	0
12	A	11208	0	5481	28	0
13	B	9980	0	4817	9	0
14	2	2052	0	1038	11	0
15	4	2636	0	1339	65	0
16	6	1265	0	638	17	0
17	7	799	0	377	0	0
18	8	729	0	356	2	0
19	B4	391	0	197	0	0
20	9	1920	0	902	2	0
21	B2	1072	0	563	0	0
22	B5	347	0	171	1	0
23	B3	5969	0	2985	13	0
24	BP	498	0	241	0	0
25	B1	4383	0	2195	1	0
26	B6	455	0	227	3	0
27	22	482	0	220	0	0
27	42	463	0	211	1	0
27	52	388	0	102	0	0
28	2B	461	0	218	2	0
29	2f	359	0	179	0	0
29	4f	359	0	179	0	0
29	5f	296	0	87	0	0
30	2b	413	0	194	0	0
30	4b	413	0	194	0	0
30	5b	344	0	93	0	0
31	23	415	0	198	1	0
31	43	415	0	198	1	0
31	53	308	0	86	2	0
32	2g	364	0	176	0	0
32	4g	369	0	178	0	0
32	5g	296	0	84	0	0
33	2e	403	0	173	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	4e	378	0	163	0	0
33	5e	316	0	85	0	0
34	21	402	0	184	0	0
34	41	407	0	183	0	0
34	51	328	0	89	0	0
35	2A	816	0	386	0	0
36	66	357	0	169	1	0
37	67	384	0	178	0	0
38	62	478	0	222	0	0
39	63	429	0	199	2	0
40	68	469	0	220	3	0
41	64	369	0	172	1	0
42	65	378	0	174	1	0
43	J	792	0	366	4	0
44	K	1615	0	754	2	0
45	G	2128	0	1038	2	0
46	L	1464	0	708	25	0
47	S	428	0	200	2	0
48	N	3991	0	2047	1	0
All	All	80982	0	39124	262	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 3.

All (262) 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)
46:L:251:LEU:HA	46:L:272:GLY:HA3	1.27	1.08
46:L:251:LEU:HA	46:L:272:GLY:CA	1.85	1.04
31:23:48:VAL:O	31:23:55:VAL:HA	1.74	0.87
4:E:56:GLN:H	4:E:96:TYR:HA	1.39	0.87
23:B3:886:GLU:HA	23:B3:910:ALA:O	1.76	0.83
16:6:74:U:OP1	43:J:601:ARG:CB	2.27	0.83
15:4:8:C:H2'	15:4:9:G:C8	2.14	0.82
8:U:164:PHE:H	8:U:173:TYR:H	1.28	0.80
1:5:75:G:H2'	1:5:76:A:C8	2.18	0.79
23:B3:699:VAL:HA	23:B3:715:MET:O	1.85	0.76
15:4:33:A:H4'	15:4:45:G:H21	1.50	0.76
1:5:78:U:H4'	1:5:79:C:C5	2.23	0.73
15:4:29:A:O4'	15:4:33:A:H5'	1.88	0.73
2:C:196:LYS:CB	31:53:12:GLU:CA	2.68	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:38:GLY:HA3	15:4:32:G:C6	2.24	0.71
15:4:41:C:N4	46:L:296:ALA:HB2	2.04	0.71
7:R:387:ASP:H	15:4:68:A:H61	1.38	0.71
15:4:7:G:H2'	15:4:8:C:H6	1.56	0.70
2:C:478:THR:HA	2:C:494:GLY:HA3	1.73	0.70
15:4:7:G:H2'	15:4:8:C:C6	2.27	0.70
46:L:250:MET:H	46:L:273:TYR:CB	2.06	0.69
12:A:1706:ASP:O	12:A:1710:ASN:N	2.26	0.68
2:C:350:ASN:O	2:C:354:ARG:N	2.27	0.68
1:5:19:A:N3	1:5:21:A:N6	2.42	0.67
46:L:251:LEU:HA	46:L:272:GLY:HA2	1.76	0.67
1:5:75:G:H2'	1:5:76:A:H8	1.59	0.67
6:M:38:GLY:HA2	15:4:30:A:O3'	1.96	0.64
1:5:23:C:O2'	1:5:57:G:N2	2.27	0.64
15:4:33:A:C4'	15:4:45:G:H21	2.10	0.63
13:B:1345:ASN:HA	13:B:1487:ILE:O	1.98	0.62
46:L:220:SER:CB	46:L:225:ALA:HA	2.30	0.62
8:U:504:VAL:HA	8:U:548:TYR:H	1.64	0.62
46:L:247:CYS:CB	46:L:300:THR:HA	2.31	0.61
8:U:173:TYR:HA	8:U:180:GLU:HA	1.82	0.60
46:L:251:LEU:CA	46:L:272:GLY:CA	2.73	0.60
1:5:78:U:H2'	1:5:78:U:O2	2.01	0.60
15:4:9:G:H2'	15:4:10:C:C6	2.36	0.60
1:5:78:U:H4'	1:5:79:C:C6	2.36	0.60
20:9:408:CYS:O	20:9:413:ASN:HA	2.02	0.60
23:B3:427:CYS:O	23:B3:433:SER:HA	2.01	0.60
15:4:30:A:O4'	15:4:44:A:N6	2.35	0.59
1:5:18:C:HO2'	1:5:19:A:H8	1.49	0.59
15:4:35:G:H2'	15:4:37:C:OP2	2.02	0.58
1:5:21:A:H2'	1:5:23:C:H5"	1.85	0.58
15:4:40:U:C5	46:L:250:MET:HA	2.38	0.58
14:2:165:A:H61	28:2B:84:ALA:HB1	1.68	0.57
23:B3:990:ILE:HA	23:B3:1004:ASP:HA	1.85	0.57
6:M:99:VAL:HA	15:4:30:A:H3'	1.85	0.57
15:4:31:U:OP1	15:4:31:U:H6	1.87	0.57
26:B6:23:ILE:O	26:B6:59:THR:HA	2.05	0.57
6:M:40:ASN:N	15:4:32:G:O6	2.37	0.56
1:5:97:G:H1	1:5:116:U:H3	1.52	0.56
40:68:38:LEU:O	40:68:59:LEU:HA	2.05	0.56
15:4:39:A:H2	46:L:293:ARG:CB	2.17	0.56
1:5:36:C:H2'	1:5:37:G:H8	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:1382:SER:HA	12:A:1415:GLY:HA2	1.88	0.56
2:C:185:PRO:HA	2:C:203:MET:HA	1.86	0.56
13:B:208:ASP:O	13:B:209:GLU:C	2.44	0.55
13:B:212:GLY:C	13:B:214:GLU:H	2.09	0.55
15:4:64:G:H22	15:4:67:A:H5'	1.71	0.55
1:5:74:U:H2'	1:5:75:G:C8	2.41	0.55
15:4:74:C:N4	16:6:34:G:O6	2.39	0.55
15:4:78:A:N6	16:6:32:U:O4	2.38	0.55
12:A:1725:LEU:HA	47:S:706:PRO:HG3	1.89	0.55
15:4:36:U:O5'	15:4:39:A:N6	2.40	0.55
1:5:78:U:O3'	1:5:79:C:H2'	2.06	0.54
15:4:33:A:H4'	15:4:45:G:N2	2.21	0.54
1:5:5:U:C4	1:5:77:G:C2	2.94	0.54
2:C:677:GLU:HA	2:C:684:LYS:HA	1.90	0.54
5:F:245:MET:HA	5:F:260:VAL:H	1.72	0.54
46:L:231:ILE:HA	46:L:250:MET:CB	2.37	0.54
4:E:56:GLN:N	4:E:96:TYR:HA	2.17	0.54
8:U:198:THR:O	8:U:202:ILE:N	2.39	0.54
12:A:942:PRO:HD3	12:A:1091:TYR:HA	1.89	0.54
8:U:403:ASP:HA	12:A:725:PRO:HB3	1.90	0.54
15:4:29:A:O3'	15:4:32:G:H4'	2.07	0.54
15:4:34:G:O5'	15:4:34:G:H8	1.90	0.54
12:A:1221:THR:O	12:A:2262:LEU:CB	2.56	0.54
14:2:170:C:H2'	28:2B:44:LYS:O	2.07	0.54
8:U:125:SER:N	8:U:142:TYR:O	2.41	0.53
26:B6:24:ARG:O	26:B6:87:LEU:HA	2.08	0.53
15:4:30:A:C4	15:4:44:A:C6	2.97	0.53
16:6:55:C:N4	46:L:355:GLY:O	2.34	0.53
36:66:31:ARG:O	36:66:48:THR:HA	2.09	0.53
15:4:35:G:C6	15:4:42:C:C2	2.97	0.53
4:E:52:CYS:O	4:E:340:PRO:HD2	2.09	0.53
15:4:8:C:H2'	15:4:9:G:H8	1.66	0.52
46:L:284:PRO:O	46:L:288:ARG:N	2.36	0.52
6:M:97:ARG:CB	15:4:29:A:H2'	2.38	0.52
12:A:1502:PHE:O	12:A:1754:TYR:N	2.43	0.52
16:6:74:U:OP1	43:J:601:ARG:CA	2.57	0.52
15:4:22:C:H2'	15:4:23:G:H8	1.75	0.52
15:4:33:A:H2'	15:4:34:G:O4'	2.10	0.51
8:U:429:GLU:HA	8:U:438:LEU:HA	1.93	0.51
15:4:19:U:H4'	15:4:20:A:C8	2.45	0.51
2:C:735:PHE:HA	2:C:744:ILE:HA	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:410:ILE:HA	5:F:426:SER:HA	1.94	0.50
12:A:119:LEU:O	12:A:128:PHE:N	2.38	0.50
14:2:168:A:H3'	14:2:169:C:C6	2.46	0.50
15:4:29:A:O2'	15:4:30:A:H5"	2.10	0.50
8:U:357:THR:N	8:U:382:THR:O	2.44	0.50
15:4:34:G:H4'	15:4:46:G:O2'	2.11	0.50
23:B3:673:VAL:HA	23:B3:690:ARG:CB	2.42	0.50
6:M:38:GLY:N	15:4:30:A:O2'	2.45	0.49
8:U:133:ALA:HA	8:U:144:GLN:HA	1.94	0.49
1:5:12:U:OP1	12:A:223:SER:N	2.45	0.49
14:2:168:A:H2'	14:2:168:A:N3	2.27	0.49
23:B3:1033:VAL:HA	23:B3:1048:ASP:HA	1.94	0.49
40:68:39:ASP:HA	40:68:59:LEU:H	1.78	0.49
2:C:350:ASN:O	2:C:354:ARG:CA	2.61	0.49
2:C:474:LEU:HA	2:C:499:GLY:HA3	1.95	0.49
15:4:6:U:H2'	15:4:7:G:C8	2.48	0.49
44:K:682:VAL:HA	44:K:688:ASN:HA	1.94	0.49
39:63:29:ILE:HA	39:63:98:PRO:HD3	1.95	0.48
14:2:168:A:H5"	14:2:169:C:H5	1.78	0.48
8:U:135:ALA:HA	8:U:142:TYR:HA	1.94	0.48
12:A:1335:ILE:N	12:A:1363:GLN:O	2.45	0.48
15:4:32:G:O2'	15:4:43:G:N2	2.32	0.48
15:4:38:U:H3	15:4:42:C:H4'	1.78	0.48
7:R:414:ARG:HA	7:R:421:THR:HA	1.96	0.48
8:U:353:MET:HA	8:U:443:LEU:HA	1.96	0.48
15:4:17:A:N3	16:6:59:G:N2	2.62	0.48
15:4:28:C:O2'	15:4:33:A:H5"	2.14	0.48
5:F:452:VAL:HA	5:F:469:ALA:HA	1.94	0.48
5:F:276:VAL:HA	5:F:300:ALA:HA	1.96	0.48
23:B3:336:ALA:HA	23:B3:351:SER:HA	1.96	0.48
4:E:168:CYS:HA	4:E:178:LEU:HA	1.96	0.47
4:E:295:PRO:HG2	4:E:337:PRO:HA	1.94	0.47
15:4:33:A:H1'	15:4:45:G:O2'	2.13	0.47
1:5:8:G:H21	1:5:71:C:H5	1.61	0.47
15:4:43:G:H4'	15:4:44:A:H5'	1.96	0.47
42:65:53:ASP:HA	42:65:69:LEU:HA	1.95	0.47
2:C:189:VAL:HA	2:C:199:LEU:HA	1.97	0.47
7:R:387:ASP:N	15:4:68:A:H61	2.07	0.47
5:F:283:PRO:HG2	5:F:333:PRO:HA	1.97	0.47
1:5:23:C:H42	12:A:465:LYS:C	2.17	0.47
12:A:1642:PRO:HB3	12:A:1716:GLY:HA2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:4:33:A:N6	15:4:43:G:H1'	2.30	0.47
16:6:34:G:H2'	16:6:35:A:C8	2.49	0.47
44:K:773:ASN:HA	44:K:822:LEU:HA	1.95	0.47
1:5:24:G:O6	1:5:56:C:N4	2.46	0.47
1:5:71:C:H2'	1:5:72:U:H4'	1.97	0.47
15:4:67:A:H61	16:6:46:G:H1	1.63	0.47
16:6:74:U:OP1	43:J:601:ARG:HA	2.15	0.47
15:4:76:C:H2'	15:4:77:A:C8	2.50	0.46
15:4:33:A:H3'	15:4:34:G:C8	2.51	0.46
4:E:56:GLN:O	4:E:57:ALA:C	2.54	0.46
16:6:47:A:H4'	16:6:48:A:H3'	1.97	0.46
5:F:281:PHE:HA	5:F:296:LEU:HA	1.97	0.46
2:C:531:TRP:HA	2:C:539:ILE:HA	1.98	0.46
8:U:399:PRO:HD3	8:U:411:PRO:HG3	1.98	0.46
15:4:28:C:H2'	15:4:33:A:H4'	1.98	0.46
15:4:39:A:C2	46:L:293:ARG:CB	2.98	0.46
13:B:835:SER:O	13:B:839:GLY:N	2.49	0.46
15:4:57:G:H1	16:6:55:C:H42	1.63	0.46
45:G:165:SER:O	45:G:169:ARG:N	2.48	0.45
15:4:56:U:H2'	15:4:57:G:C8	2.51	0.45
15:4:27:C:N3	15:4:28:C:N4	2.65	0.45
15:4:33:A:H2'	15:4:34:G:C8	2.52	0.45
16:6:74:U:P	43:J:601:ARG:CB	3.04	0.45
15:4:67:A:N1	16:6:46:G:N2	2.58	0.45
12:A:1650:ASP:O	47:S:699:LYS:N	2.49	0.45
23:B3:785:PRO:HA	23:B3:801:GLU:HA	1.97	0.45
1:5:37:G:H2'	1:5:38:C:H4'	1.99	0.45
8:U:399:PRO:HG3	8:U:411:PRO:HD3	1.99	0.45
48:N:415:GLU:O	48:N:419:ALA:N	2.48	0.45
18:8:147:PRO:HB3	18:8:173:ALA:HB2	1.99	0.45
1:5:77:G:C8	1:5:79:C:N4	2.85	0.44
8:U:166:ASN:H	8:U:171:LYS:N	2.15	0.44
1:5:89:U:N3	31:53:38:ASN:O	2.43	0.44
8:U:354:ARG:N	8:U:442:GLN:O	2.50	0.44
12:A:968:THR:O	12:A:972:GLU:N	2.49	0.44
2:C:459:SER:O	2:C:463:GLU:N	2.41	0.44
23:B3:439:ARG:O	23:B3:774:PHE:HA	2.18	0.44
14:2:168:A:H3'	14:2:169:C:C5	2.53	0.44
1:5:26:A:H2'	1:5:27:U:O4'	2.18	0.44
8:U:416:PHE:O	8:U:420:ALA:N	2.50	0.44
8:U:426:THR:HA	8:U:440:ARG:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:459:LYS:HA	8:U:464:VAL:HA	1.99	0.44
23:B3:674:LEU:O	23:B3:689:THR:N	2.51	0.44
23:B3:637:PRO:HA	23:B3:669:LEU:HA	2.00	0.44
46:L:280:VAL:HA	46:L:291:ALA:HB1	2.00	0.44
9:X:131:VAL:H	27:42:40:THR:HA	1.83	0.43
46:L:275:TYR:HA	46:L:292:ALA:HB2	1.99	0.43
1:5:68:C:H2'	1:5:69:A:C4	2.52	0.43
31:43:45:ASN:HA	31:43:58:LEU:O	2.19	0.43
46:L:251:LEU:CA	46:L:272:GLY:HA2	2.43	0.43
13:B:626:PRO:HG3	13:B:893:MET:HA	1.99	0.43
46:L:231:ILE:CB	46:L:248:ASN:HA	2.48	0.43
5:F:373:PHE:HA	5:F:380:ALA:HA	2.00	0.43
15:4:51:A:H2'	15:4:52:U:C6	2.53	0.43
25:B1:508:THR:O	25:B1:512:ARG:N	2.46	0.43
13:B:449:ALA:HB1	13:B:684:PRO:HB2	2.00	0.43
46:L:291:ALA:O	46:L:295:VAL:N	2.52	0.43
12:A:676:ARG:O	12:A:680:HIS:N	2.39	0.43
6:M:38:GLY:HA3	15:4:32:G:N1	2.34	0.43
14:2:3:C:H2'	14:2:4:G:H8	1.84	0.43
46:L:357:ARG:O	46:L:361:LYS:N	2.47	0.43
2:C:258:ASN:HA	2:C:310:SER:O	2.19	0.43
14:2:151:C:H2'	14:2:152:G:H8	1.83	0.42
14:2:10:C:H2'	14:2:11:G:H8	1.84	0.42
2:C:350:ASN:O	2:C:354:ARG:HA	2.19	0.42
5:F:259:SER:O	5:F:263:CYS:N	2.51	0.42
1:5:78:U:O2	1:5:78:U:C2'	2.68	0.42
8:U:146:ARG:H	8:U:150:SER:CB	2.33	0.42
1:5:53:U:H2'	1:5:54:U:C6	2.54	0.42
1:5:61:A:H2'	1:5:62:G:C8	2.54	0.42
2:C:260:ILE:H	2:C:311:SER:HA	1.85	0.42
5:F:234:ILE:HA	5:F:250:CYS:HA	2.01	0.42
15:4:57:G:N2	16:6:55:C:N3	2.59	0.42
22:B5:78:PRO:HA	22:B5:79:PRO:HD3	1.94	0.42
2:C:848:THR:O	2:C:851:ALA:HB3	2.20	0.42
15:4:32:G:N3	15:4:43:G:C2	2.87	0.42
16:6:55:C:H41	46:L:356:GLY:HA2	1.85	0.42
40:68:35:ASN:HA	40:68:62:VAL:O	2.20	0.42
1:5:63:A:H2'	1:5:64:G:C8	2.54	0.42
41:64:46:THR:HA	41:64:52:LYS:HA	2.02	0.42
46:L:251:LEU:N	46:L:273:TYR:H	2.17	0.42
12:A:1185:LEU:O	12:A:1195:ARG:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:1706:ASP:O	12:A:1710:ASN:CA	2.68	0.42
8:U:420:ALA:O	8:U:424:GLY:N	2.51	0.41
12:A:591:MET:O	12:A:592:TYR:C	2.58	0.41
15:4:9:G:H2'	15:4:10:C:H6	1.82	0.41
18:8:56:CYS:O	18:8:60:LEU:HA	2.20	0.41
39:63:97:PRO:HA	39:63:98:PRO:HD3	1.93	0.41
46:L:252:LEU:H	46:L:273:TYR:N	2.18	0.41
12:A:142:SER:HA	12:A:242:ALA:HB2	2.02	0.41
23:B3:1101:VAL:HA	23:B3:1121:THR:HA	2.03	0.41
8:U:202:ILE:O	8:U:206:ASP:N	2.44	0.41
12:A:133:PRO:HB2	12:A:421:ALA:HB3	2.02	0.41
15:4:44:A:O3'	15:4:45:G:H4'	2.20	0.41
2:C:129:ILE:O	2:C:441:PRO:HD3	2.19	0.41
15:4:31:U:H3'	15:4:32:G:C5'	2.50	0.41
12:A:120:TYR:HA	12:A:127:SER:HA	2.01	0.41
12:A:1369:TYR:O	13:B:53:GLY:N	2.39	0.41
8:U:145:GLY:HA3	8:U:152:ALA:H	1.85	0.41
20:9:77:GLY:HA3	20:9:78:PRO:HD3	1.84	0.41
2:C:742:PRO:HB2	2:C:786:ASN:H	1.85	0.41
14:2:51:A:H2'	14:2:52:G:H8	1.85	0.41
4:E:343:ILE:HA	4:E:353:MET:HA	2.03	0.41
4:E:56:GLN:H	4:E:96:TYR:CA	2.21	0.41
6:M:57:ALA:HB3	6:M:100:ILE:HA	2.01	0.41
12:A:586:GLY:O	12:A:590:GLY:HA2	2.21	0.41
12:A:1503:TRP:O	46:L:378:MET:N	2.51	0.41
13:B:1347:PHE:O	13:B:1512:PHE:N	2.52	0.41
15:4:15:G:H2'	15:4:16:C:C6	2.56	0.41
15:4:90:G:O6	15:4:112:A:N6	2.54	0.41
23:B3:84:SER:HA	23:B3:110:SER:HA	2.03	0.41
15:4:16:C:H2'	15:4:17:A:O4'	2.21	0.41
26:B6:83:CYS:O	26:B6:85:ARG:N	2.52	0.41
45:G:354:ASP:O	45:G:355:ARG:CB	2.68	0.41
46:L:280:VAL:HA	46:L:291:ALA:CB	2.50	0.41
8:U:107:TYR:O	8:U:111:ILE:N	2.55	0.40
15:4:75:C:H1'	16:6:35:A:N1	2.37	0.40
5:F:495:VAL:HA	5:F:511:SER:HA	2.03	0.40
12:A:1424:GLN:HA	13:B:213:ASP:O	2.21	0.40
12:A:1853:PRO:O	12:A:1857:GLN:N	2.52	0.40
12:A:1981:VAL:O	12:A:1985:ASP:N	2.45	0.40
14:2:151:C:H2'	14:2:152:G:C8	2.56	0.40
16:6:52:U:H2'	16:6:53:A:H8	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:77:G:C5	1:5:79:C:C5	3.09	0.40
12:A:1962:THR:HA	12:A:1969:PRO:HA	2.03	0.40

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	
2	C	834/972 (86%)	813 (98%)	21 (2%)	0	100	100
3	D	139/142 (98%)	136 (98%)	3 (2%)	0	100	100
4	E	305/357 (85%)	301 (99%)	4 (1%)	0	100	100
5	F	357/522 (68%)	348 (98%)	9 (2%)	0	100	100
6	M	121/128 (94%)	121 (100%)	0	0	100	100
7	R	104/480 (22%)	101 (97%)	3 (3%)	0	100	100
8	U	454/565 (80%)	441 (97%)	13 (3%)	0	100	100
9	X	20/155 (13%)	20 (100%)	0	0	100	100
12	A	2200/2335 (94%)	2116 (96%)	83 (4%)	1 (0%)	100	100
13	B	1971/2136 (92%)	1940 (98%)	28 (1%)	3 (0%)	47	81
17	7	155/793 (20%)	155 (100%)	0	0	100	100
18	8	138/464 (30%)	135 (98%)	3 (2%)	0	100	100
19	B4	76/424 (18%)	76 (100%)	0	0	100	100
20	9	377/501 (75%)	372 (99%)	5 (1%)	0	100	100
21	B2	204/895 (23%)	200 (98%)	4 (2%)	0	100	100
22	B5	67/86 (78%)	66 (98%)	1 (2%)	0	100	100
23	B3	1176/1217 (97%)	1144 (97%)	32 (3%)	0	100	100
24	BP	98/110 (89%)	96 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	B1	866/1304 (66%)	847 (98%)	19 (2%)	0	100	100
26	B6	88/125 (70%)	84 (96%)	4 (4%)	0	100	100
27	22	91/118 (77%)	91 (100%)	0	0	100	100
27	42	90/118 (76%)	89 (99%)	1 (1%)	0	100	100
27	52	95/118 (80%)	88 (93%)	7 (7%)	0	100	100
28	2B	90/225 (40%)	90 (100%)	0	0	100	100
29	2f	70/86 (81%)	68 (97%)	2 (3%)	0	100	100
29	4f	70/86 (81%)	69 (99%)	1 (1%)	0	100	100
29	5f	72/86 (84%)	72 (100%)	0	0	100	100
30	2b	80/240 (33%)	80 (100%)	0	0	100	100
30	4b	80/240 (33%)	79 (99%)	1 (1%)	0	100	100
30	5b	84/240 (35%)	78 (93%)	6 (7%)	0	100	100
31	23	81/126 (64%)	78 (96%)	3 (4%)	0	100	100
31	43	81/126 (64%)	81 (100%)	0	0	100	100
31	53	75/126 (60%)	72 (96%)	3 (4%)	0	100	100
32	2g	71/76 (93%)	71 (100%)	0	0	100	100
32	4g	72/76 (95%)	70 (97%)	2 (3%)	0	100	100
32	5g	72/76 (95%)	69 (96%)	3 (4%)	0	100	100
33	2e	79/92 (86%)	79 (100%)	0	0	100	100
33	4e	74/92 (80%)	74 (100%)	0	0	100	100
33	5e	77/92 (84%)	77 (100%)	0	0	100	100
34	21	78/119 (66%)	75 (96%)	3 (4%)	0	100	100
34	41	79/119 (66%)	78 (99%)	1 (1%)	0	100	100
34	51	80/119 (67%)	76 (95%)	4 (5%)	0	100	100
35	2A	160/255 (63%)	158 (99%)	2 (1%)	0	100	100
36	66	70/80 (88%)	69 (99%)	1 (1%)	0	100	100
37	67	75/103 (73%)	74 (99%)	1 (1%)	0	100	100
38	62	93/95 (98%)	89 (96%)	4 (4%)	0	100	100
39	63	83/102 (81%)	82 (99%)	1 (1%)	0	100	100
40	68	93/96 (97%)	91 (98%)	2 (2%)	0	100	100
41	64	71/139 (51%)	70 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	65	74/91 (81%)	71 (96%)	3 (4%)	0	100	100
43	J	153/683 (22%)	151 (99%)	2 (1%)	0	100	100
44	K	316/1007 (31%)	307 (97%)	9 (3%)	0	100	100
45	G	413/820 (50%)	405 (98%)	6 (2%)	2 (0%)	29	69
46	L	284/499 (57%)	280 (99%)	4 (1%)	0	100	100
47	S	80/800 (10%)	79 (99%)	1 (1%)	0	100	100
48	N	780/941 (83%)	769 (99%)	11 (1%)	0	100	100
All	All	14236/22218 (64%)	13911 (98%)	319 (2%)	6 (0%)	100	100

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
45	G	355	ARG
12	A	80	LYS
13	B	208	ASP
13	B	213	ASP
45	G	366	THR
13	B	209	GLU

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	48/866 (6%)	48 (100%)	0	100	100
3	D	5/130 (4%)	5 (100%)	0	100	100
4	E	10/300 (3%)	10 (100%)	0	100	100
5	F	15/442 (3%)	15 (100%)	0	100	100
6	M	6/111 (5%)	6 (100%)	0	100	100
7	R	4/369 (1%)	4 (100%)	0	100	100
8	U	23/511 (4%)	23 (100%)	0	100	100
9	X	1/144 (1%)	1 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	A	126/2108 (6%)	126 (100%)	0	100	100
13	B	84/1908 (4%)	84 (100%)	0	100	100
17	7	5/709 (1%)	5 (100%)	0	100	100
18	8	8/382 (2%)	8 (100%)	0	100	100
19	B4	4/336 (1%)	4 (100%)	0	100	100
20	9	11/446 (2%)	11 (100%)	0	100	100
21	B2	22/776 (3%)	22 (100%)	0	100	100
22	B5	3/77 (4%)	3 (100%)	0	100	100
23	B3	60/1051 (6%)	60 (100%)	0	100	100
24	BP	4/95 (4%)	4 (100%)	0	100	100
25	B1	40/1104 (4%)	40 (100%)	0	100	100
26	B6	5/109 (5%)	5 (100%)	0	100	100
27	22	5/110 (4%)	5 (100%)	0	100	100
27	42	4/110 (4%)	4 (100%)	0	100	100
28	2B	3/195 (2%)	3 (100%)	0	100	100
29	2f	4/74 (5%)	4 (100%)	0	100	100
29	4f	4/74 (5%)	4 (100%)	0	100	100
30	2b	4/177 (2%)	4 (100%)	0	100	100
30	4b	4/177 (2%)	4 (100%)	0	100	100
31	23	3/101 (3%)	3 (100%)	0	100	100
31	43	3/101 (3%)	3 (100%)	0	100	100
32	2g	3/66 (4%)	3 (100%)	0	100	100
32	4g	3/66 (4%)	3 (100%)	0	100	100
33	2e	1/84 (1%)	1 (100%)	0	100	100
33	4e	1/84 (1%)	1 (100%)	0	100	100
34	21	3/101 (3%)	3 (100%)	0	100	100
34	41	3/101 (3%)	3 (100%)	0	100	100
35	2A	6/218 (3%)	6 (100%)	0	100	100
36	66	2/70 (3%)	2 (100%)	0	100	100
37	67	3/91 (3%)	3 (100%)	0	100	100
38	62	3/88 (3%)	3 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	63	4/94 (4%)	4 (100%)	0	100	100
40	68	1/82 (1%)	1 (100%)	0	100	100
41	64	4/111 (4%)	4 (100%)	0	100	100
42	65	3/80 (4%)	3 (100%)	0	100	100
43	J	3/599 (0%)	3 (100%)	0	100	100
44	K	10/919 (1%)	10 (100%)	0	100	100
45	G	22/721 (3%)	22 (100%)	0	100	100
46	L	9/424 (2%)	9 (100%)	0	100	100
47	S	2/681 (0%)	2 (100%)	0	100	100
48	N	32/792 (4%)	32 (100%)	0	100	100
All	All	636/18565 (3%)	636 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	5	114/117 (97%)	42 (36%)	1 (0%)
10	Z	14/347 (4%)	1 (7%)	0
11	z	10/11 (90%)	5 (50%)	0
14	2	93/188 (49%)	16 (17%)	4 (4%)
15	4	119/144 (82%)	21 (17%)	3 (2%)
16	6	55/106 (51%)	6 (10%)	0
All	All	405/913 (44%)	91 (22%)	8 (1%)

All (91) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	5	8	G
1	5	9	G
1	5	10	U
1	5	12	U
1	5	14	U
1	5	18	C
1	5	19	A

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Mol	Chain	Res	Type
1	5	20	G
1	5	21	A
1	5	22	U
1	5	23	C
1	5	24	G
1	5	28	A
1	5	38	C
1	5	39	C
1	5	40	U
1	5	41	U
1	5	42	U
1	5	44	A
1	5	45	C
1	5	47	A
1	5	56	C
1	5	57	G
1	5	68	C
1	5	69	A
1	5	78	U
1	5	79	C
1	5	80	U
1	5	83	A
1	5	84	C
1	5	88	A
1	5	89	U
1	5	90	U
1	5	91	U
1	5	92	U
1	5	93	U
1	5	94	U
1	5	95	G
1	5	96	A
1	5	109	G
1	5	116	U
1	5	117	A
10	Z	41	A
11	z	-2	A
11	z	1	G
11	z	2	U
11	z	3	A
11	z	7	A
14	2	30	A

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Mol	Chain	Res	Type
14	2	38	A
14	2	40	C
14	2	42	G
14	2	47	U
14	2	100	U
14	2	101	U
14	2	102	U
14	2	103	U
14	2	104	U
14	2	105	G
14	2	106	G
14	2	107	A
14	2	164	C
14	2	169	C
14	2	178	A
15	4	2	G
15	4	18	G
15	4	19	U
15	4	25	A
15	4	26	G
15	4	31	U
15	4	32	G
15	4	33	A
15	4	36	U
15	4	37	C
15	4	40	U
15	4	44	A
15	4	45	G
15	4	68	A
15	4	69	C
15	4	115	G
15	4	121	U
15	4	122	U
15	4	123	U
15	4	125	G
15	4	126	A
16	6	45	A
16	6	46	G
16	6	47	A
16	6	48	A
16	6	49	G
16	6	106	U

All (8) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	5	19	A
14	2	37	U
14	2	46	U
14	2	103	U
14	2	106	G
15	4	1	A
15	4	68	A
15	4	114	U

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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.

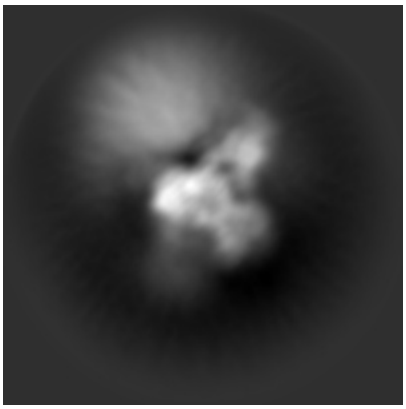
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-18788. These allow visual inspection of the internal detail of the map and identification of artifacts.

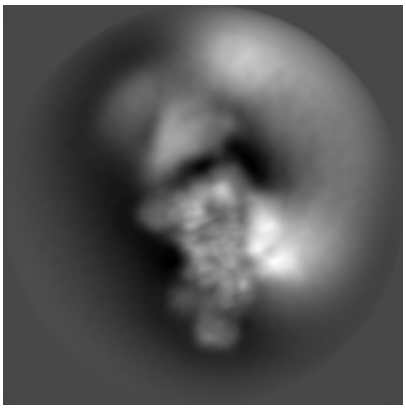
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

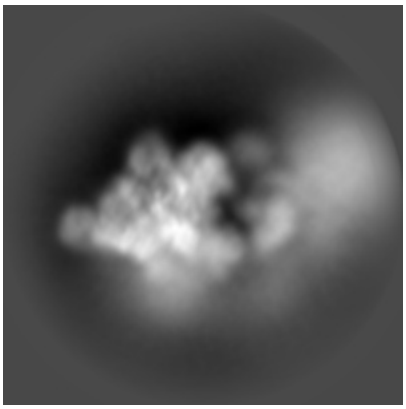
6.1.1 Primary map



X

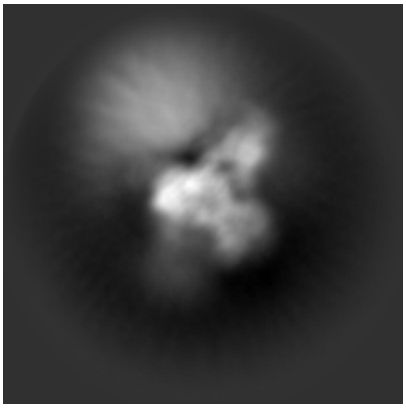


Y

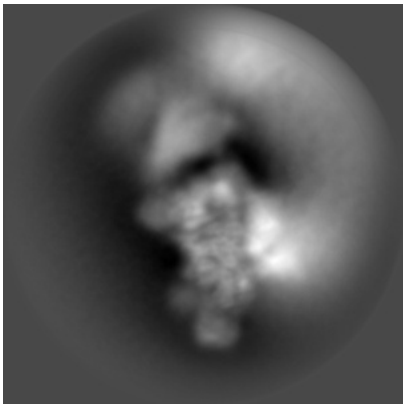


Z

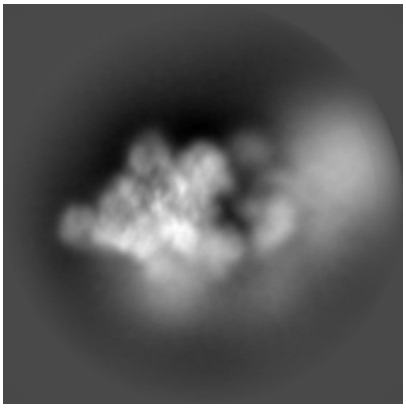
6.1.2 Raw map



X



Y

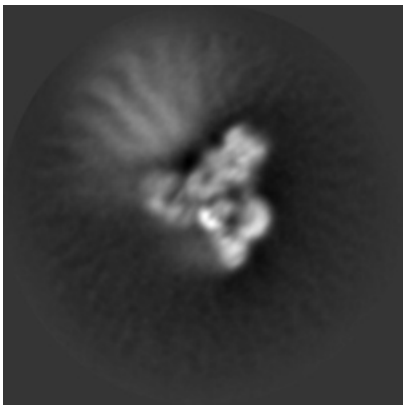


Z

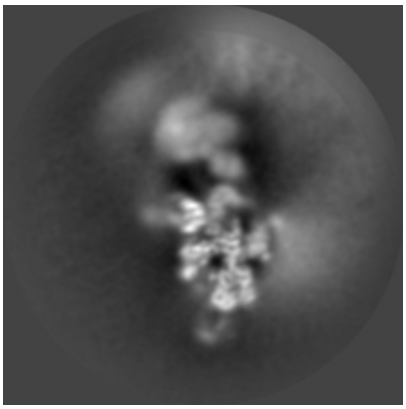
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

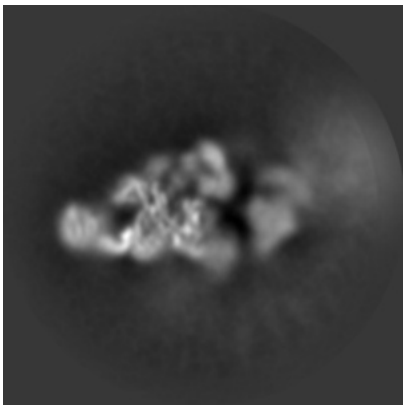
6.2.1 Primary map



X Index: 250

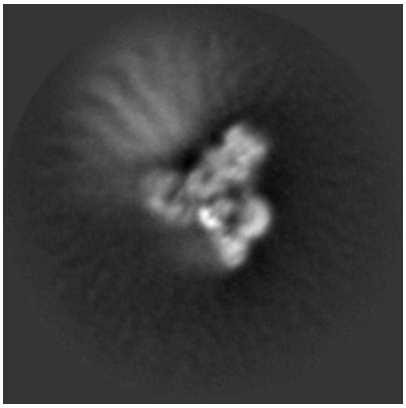


Y Index: 250

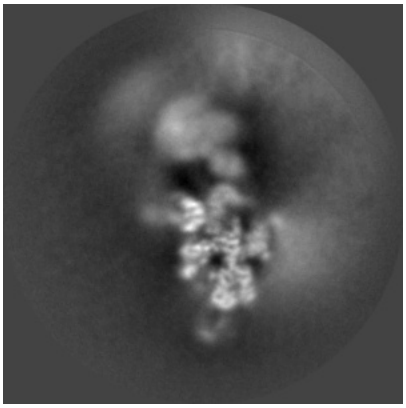


Z Index: 250

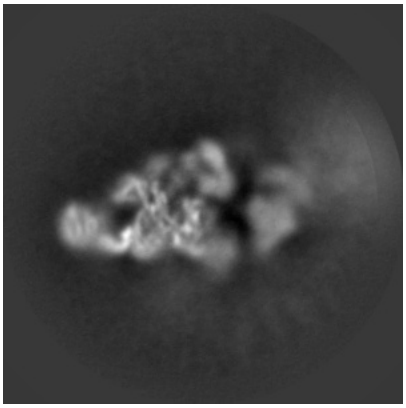
6.2.2 Raw map



X Index: 250



Y Index: 250

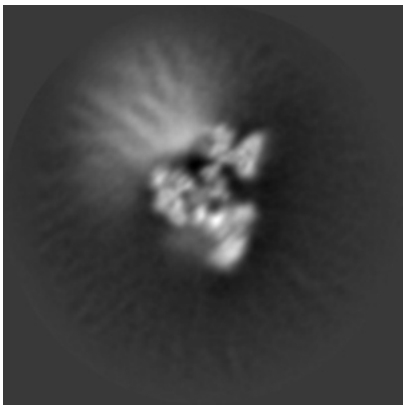


Z Index: 250

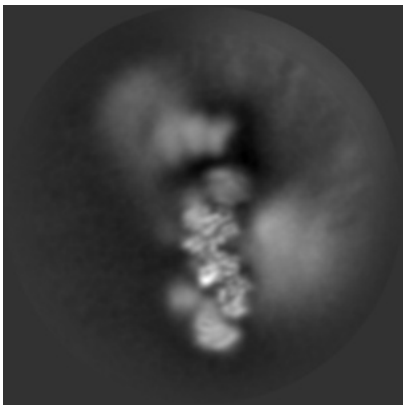
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

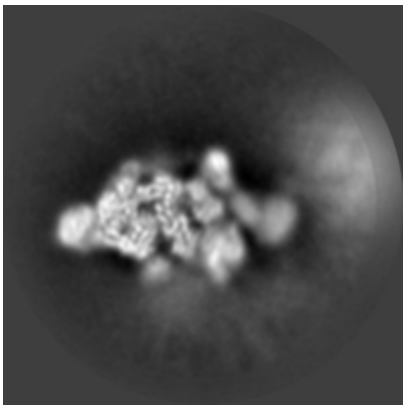
6.3.1 Primary map



X Index: 225

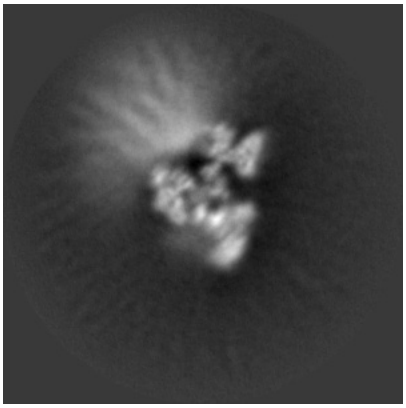


Y Index: 214

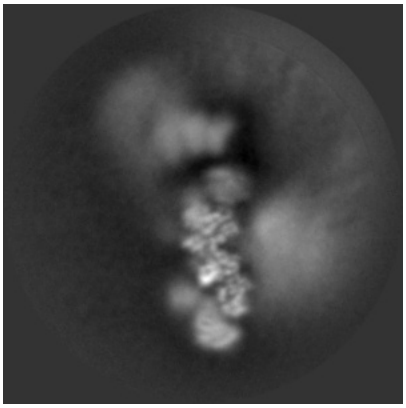


Z Index: 275

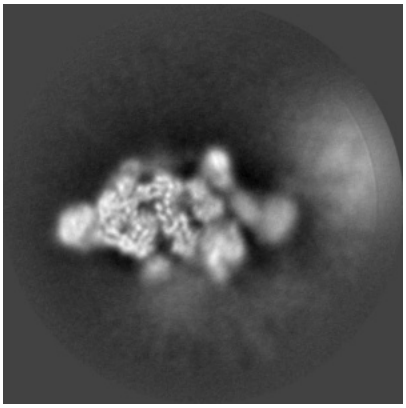
6.3.2 Raw map



X Index: 225



Y Index: 214

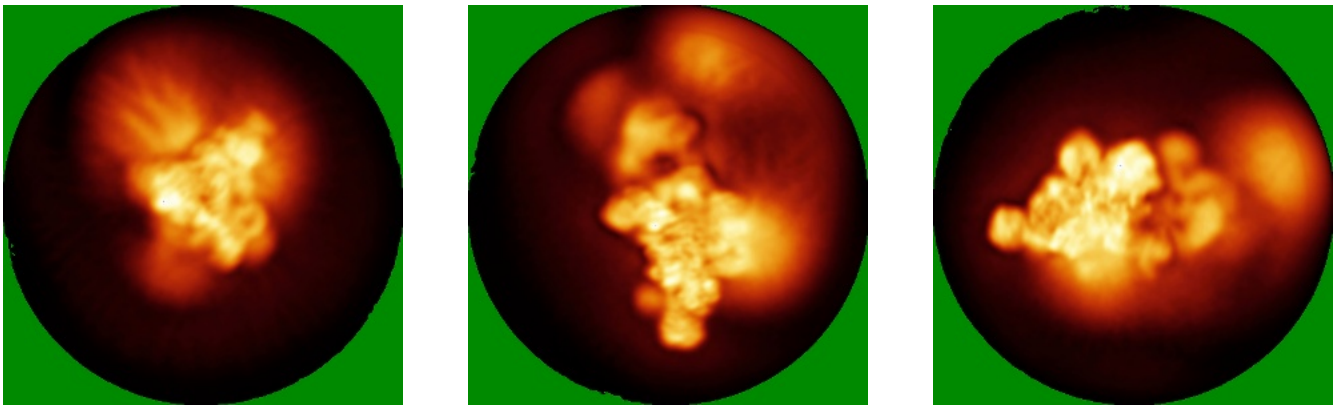


Z Index: 275

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

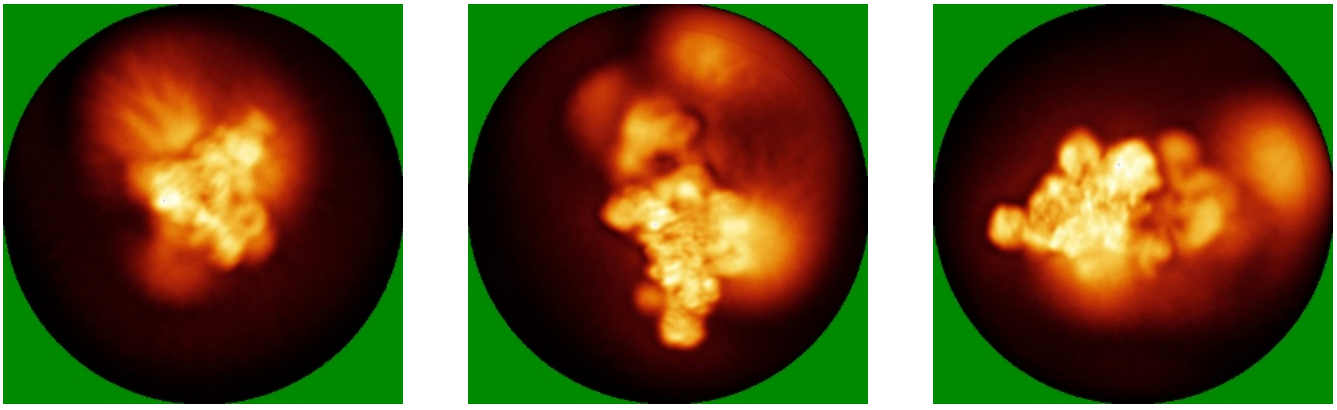
6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map



X Y Z

6.4.2 Raw map

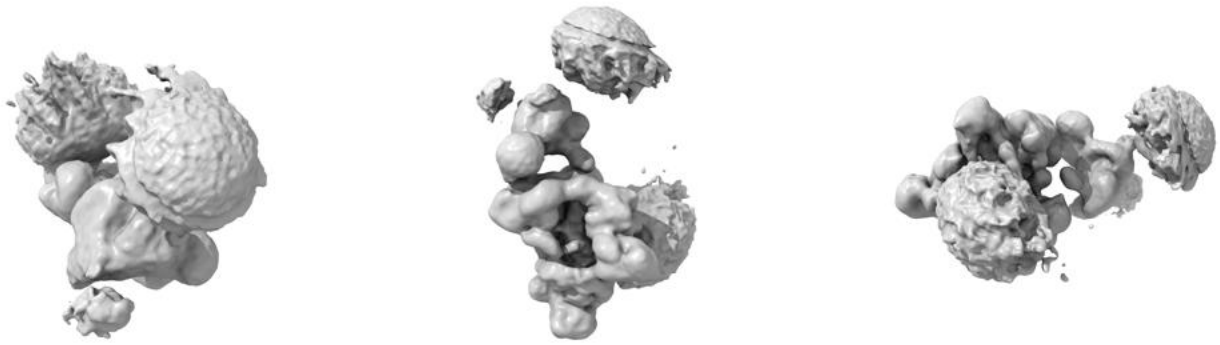


X Y Z

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 0.007. 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.

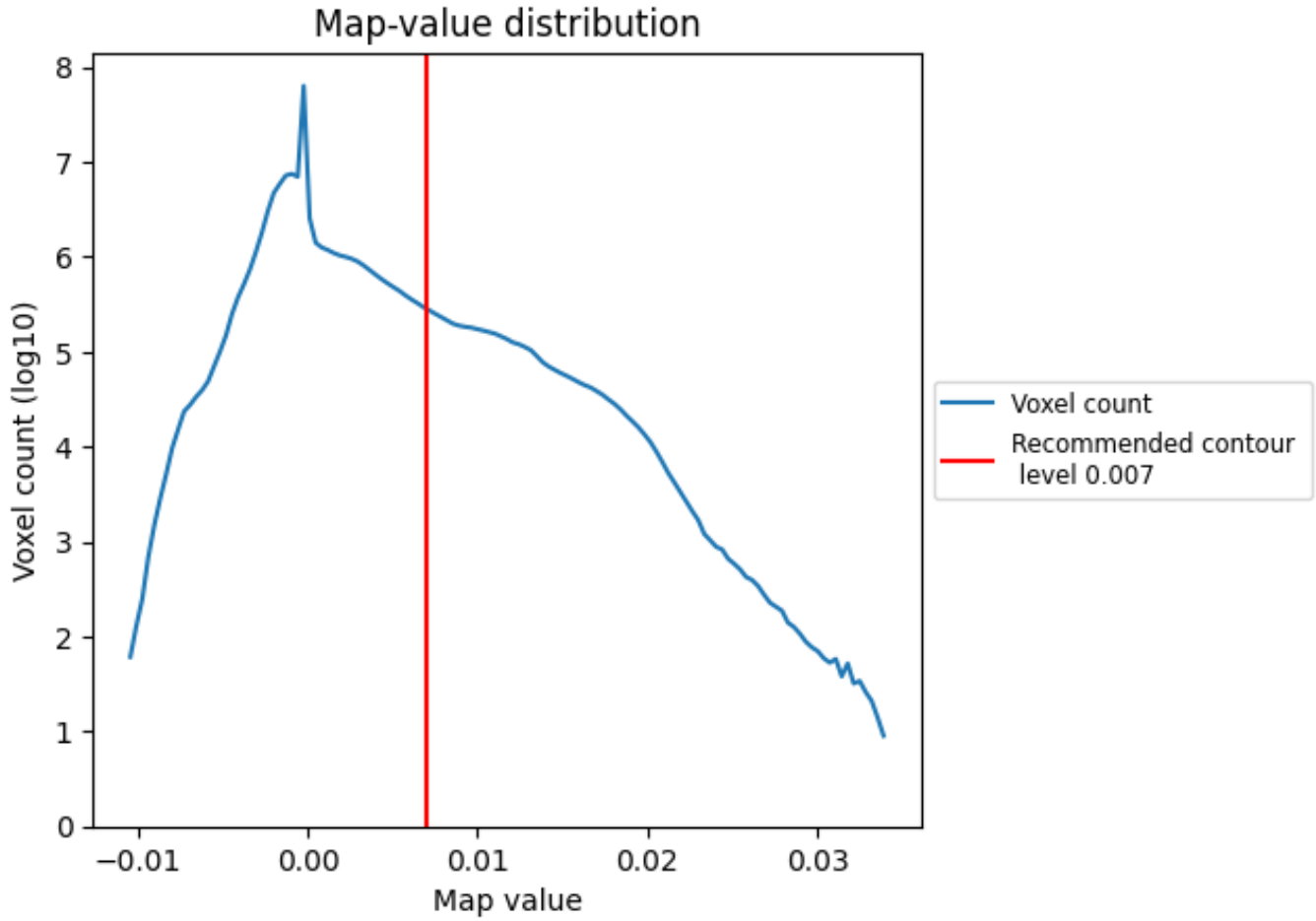
6.6 Mask visualisation (i)

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

7 Map analysis

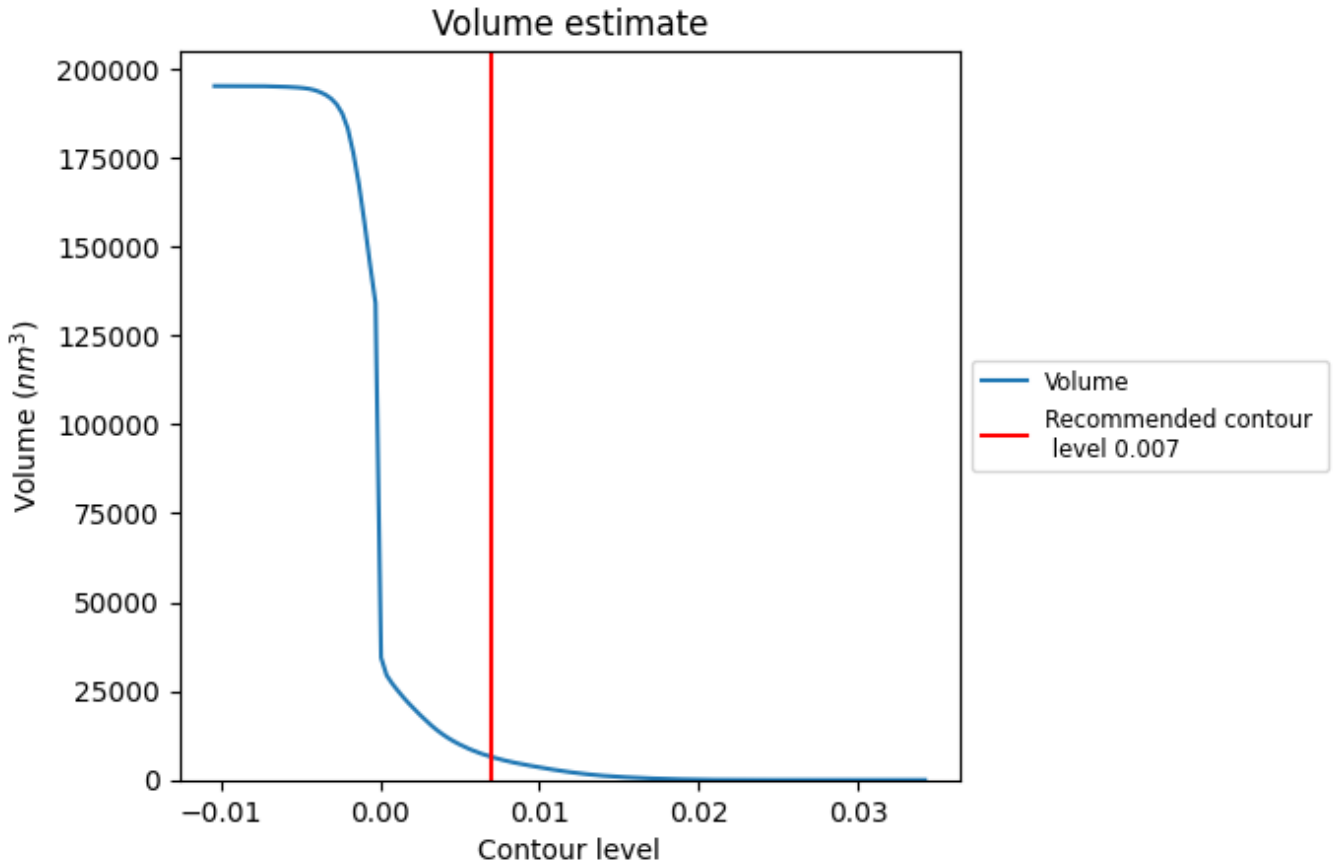
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

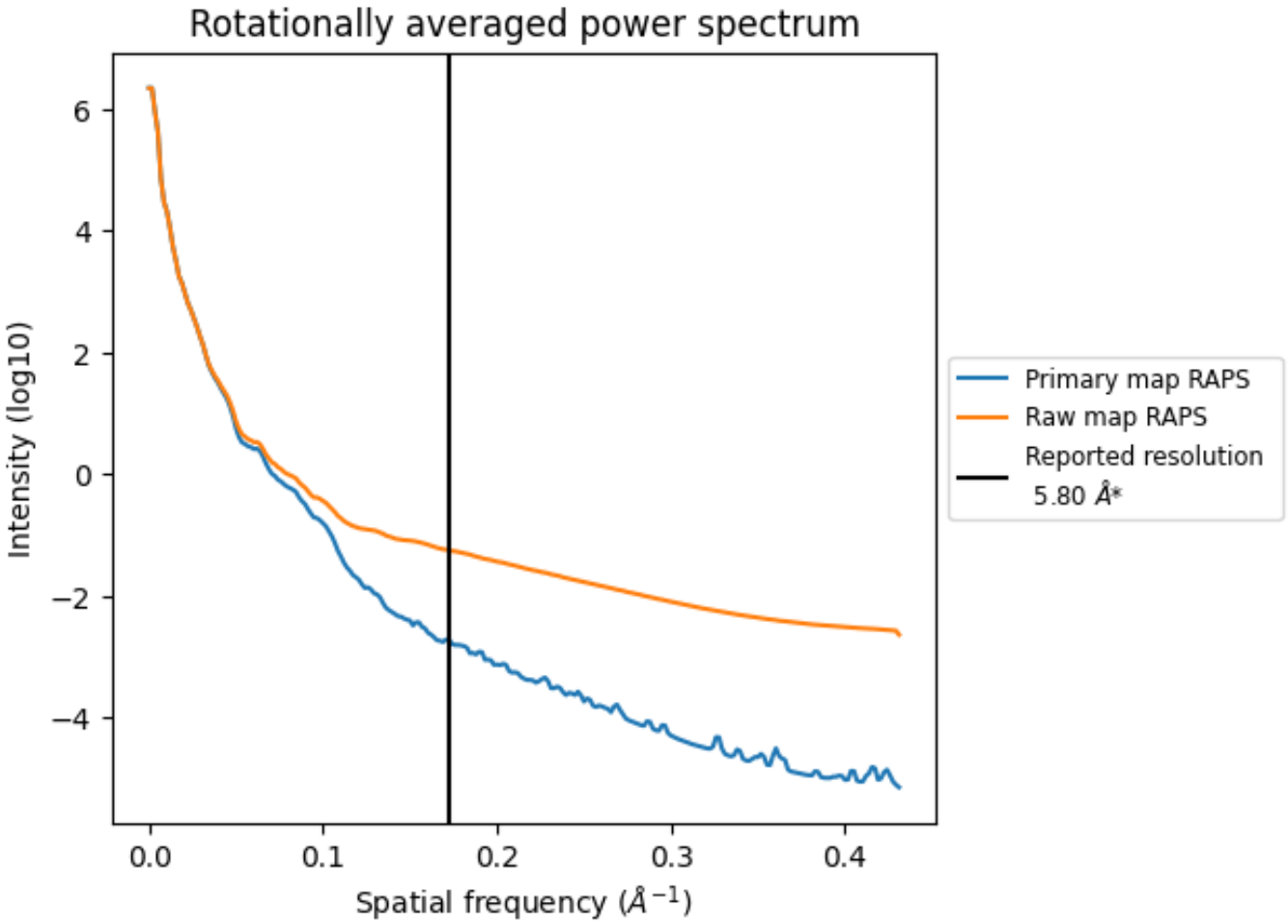
7.2 Volume estimate



The volume at the recommended contour level is 6461 nm^3; this corresponds to an approximate mass of 5837 kDa.

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

7.3 Rotationally averaged power spectrum (i)

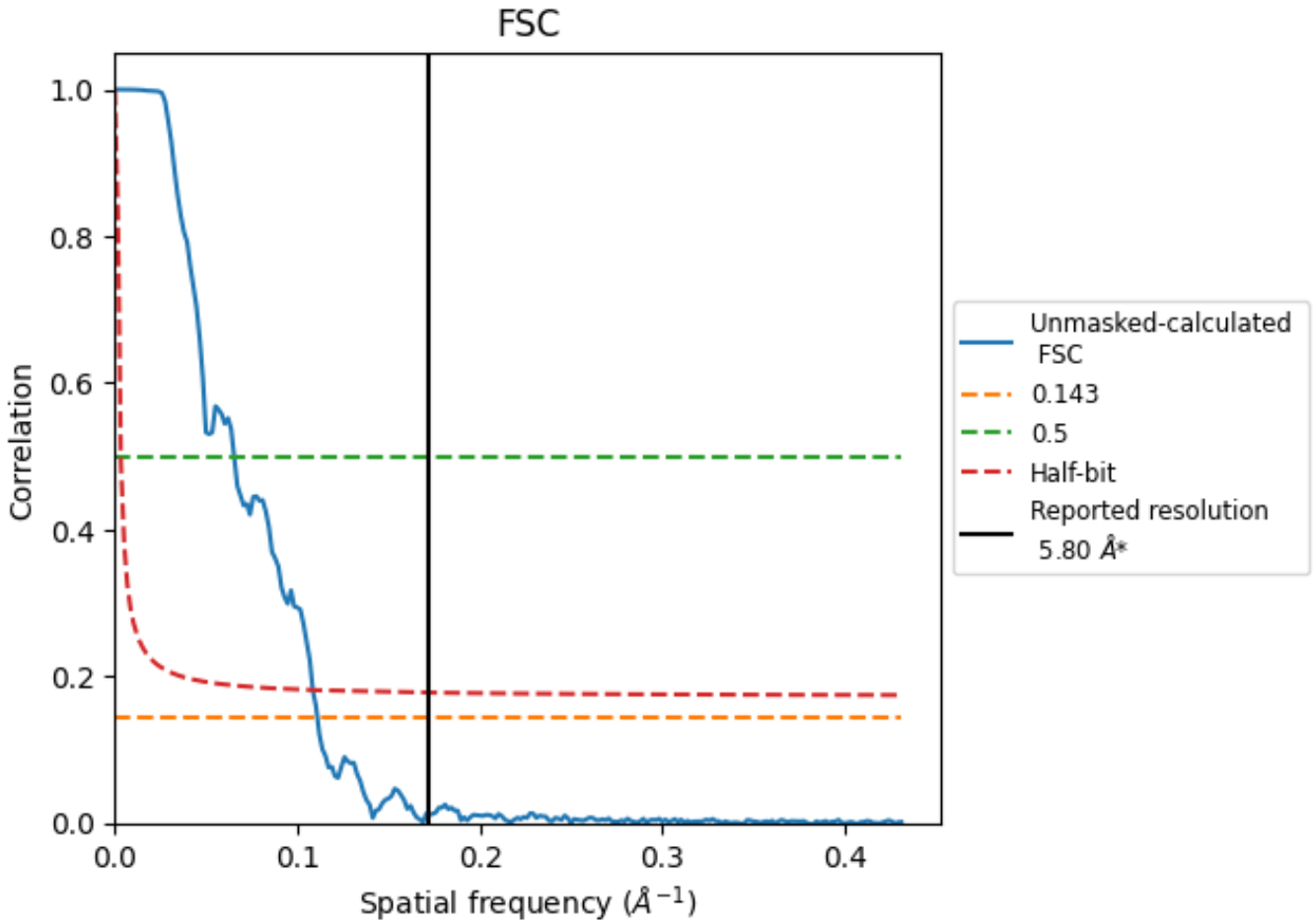


*Reported resolution corresponds to spatial frequency of 0.172 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.172 Å^{-1}

8.2 Resolution estimates (i)

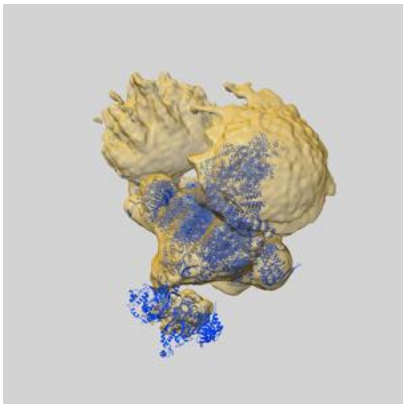
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	9.00	15.29	9.21

*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 9.00 differs from the reported value 5.8 by more than 10 %

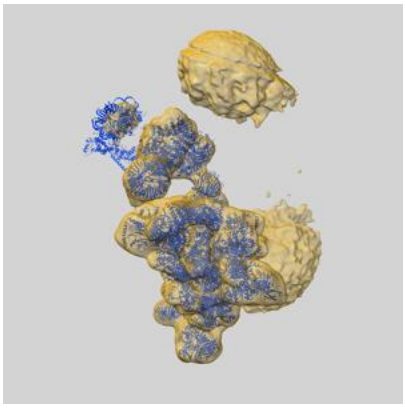
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-18788 and PDB model 8R0A. Per-residue inclusion information can be found in section 3 on page 14.

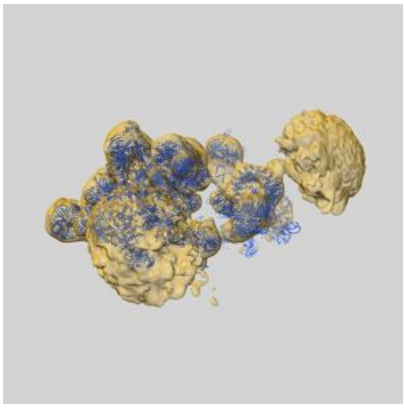
9.1 Map-model overlay



X



Y



Z

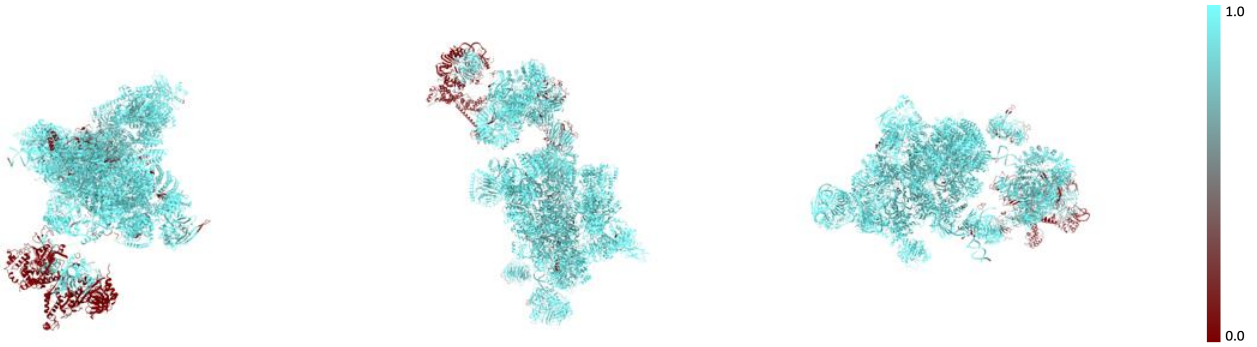
The images above show the 3D surface view of the map at the recommended contour level 0.007 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)

X Y Z

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.

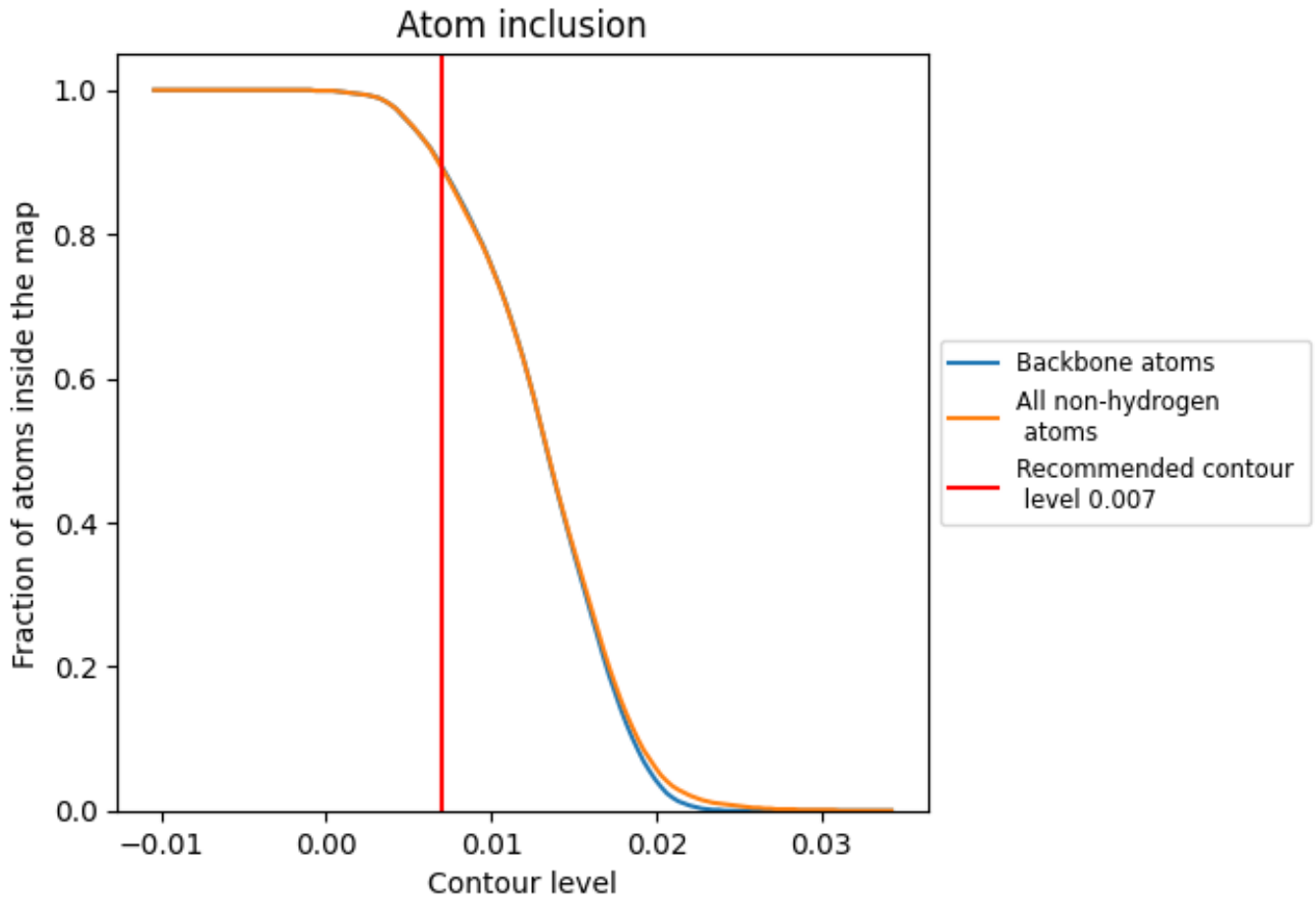
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.007).

9.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 89% 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 (0.007) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8920	0.1020
2	0.6380	0.0370
21	0.4280	0.0200
22	0.0000	0.0180
23	0.9320	0.0480
2A	0.2590	0.0420
2B	0.2360	0.0590
2b	0.7840	0.0540
2e	0.0420	0.0060
2f	0.0000	0.0250
2g	0.5520	0.0420
4	0.9890	0.1110
41	0.9980	0.0310
42	0.8380	0.0320
43	1.0000	0.0640
4b	0.9150	0.0410
4e	0.9970	0.0560
4f	0.8610	0.0550
4g	0.9760	0.0550
5	0.9990	0.1350
51	1.0000	0.1270
52	0.9850	0.1190
53	1.0000	0.1820
5b	0.9420	0.1270
5e	1.0000	0.1160
5f	1.0000	0.0940
5g	1.0000	0.1230
6	0.9950	0.1250
62	0.9750	0.0290
63	0.8580	0.0350
64	0.9840	0.0430
65	0.9130	0.0530
66	0.9470	0.0610
67	0.8960	0.0520
68	0.7570	0.0270

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Chain	Atom inclusion	Q-score
7	0.2980	0.0330
8	0.4110	0.0230
9	0.1850	0.0270
A	0.9810	0.1670
B	0.9780	0.1280
B1	0.9650	0.0470
B2	0.9830	0.0530
B3	0.7940	0.0540
B4	1.0000	0.0620
B5	1.0000	0.0440
B6	0.9960	0.0690
BP	1.0000	0.0400
C	0.9980	0.1670
D	1.0000	0.1670
E	0.9650	0.0430
F	0.9990	0.0850
G	0.9950	0.1320
J	1.0000	0.1420
K	0.9110	0.0690
L	0.9300	0.1040
M	1.0000	0.1130
N	0.9980	0.1300
R	0.9980	0.1140
S	0.9210	0.1450
U	0.9920	0.1450
X	1.0000	0.0610
Z	1.0000	0.0800
z	1.0000	0.1530