wwPDB EM Validation Summary Report ⓘ

Nov 19, 2022 – 11:36 pm GMT

PDB ID	:	6G90
EMDB ID	:	EMD-4364
Title	:	Prespliceosome structure provides insight into spliceosome assembly and regulation (map A2)
Authors	:	Plaschka, C.; Lin, P.-C.; Charenton, C.; Nagai, K.
Deposited on	:	2018-04-10
Resolution	:	4.00 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:

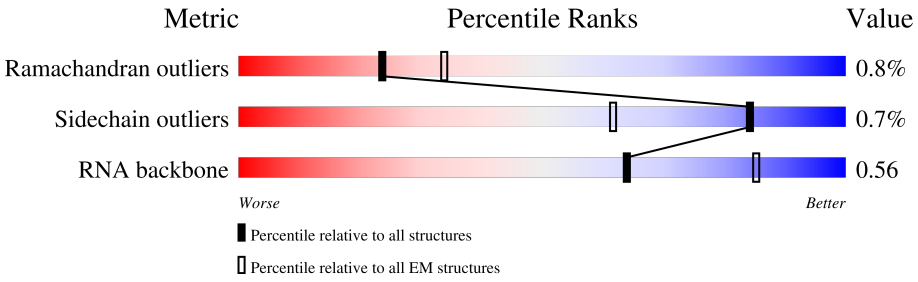
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.00 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	1	407	17% 59% 16% 5% 20%
2	2	143	100% 36% 52% 10% •
3	A	298	• 33% 67%
4	B	300	38% 62% • 36%
5	C	231	9% 73% • 23%
6	D	629	13% 79% • 19%
7	E	544	6% 91% 8% ••
8	F	523	• 30% • 67%

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Mol	Chain	Length	Quality of chain
9	G	492	43% 56%
10	H	261	18% 60% 39%
11	I	38	74% 76% 24%
12	J	620	7% 93%
13	O	971	86% 86% 14%
14	P	1361	87% 86% 13%
15	Q	435	51% 50% 49%
16	R	213	81% 81% 19%
17	S	107	96% 96%
18	T	530	87% 86% 13%
19	U	266	74% 73% 26%
20	V	280	45% 45% 55%
21	W	238	71% 62% 8% 29%
22	X	51	31% 100%
23	Y	111	76% 74% 24%
24	Z	85	98% 96%
25	b	196	8% 59% 38%
25	s	196	33% 33% 67%
26	d	101	89% 8%
26	v	101	81% 79% 19%
27	e	94	9% 79% 18%
27	w	94	82% 81% 18%
28	f	86	14% 83% 15%
28	x	86	85% 85% 15%
29	g	77	6% 91% 6%

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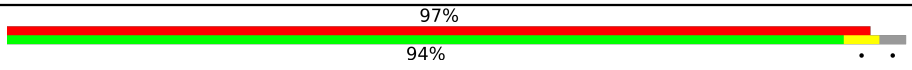
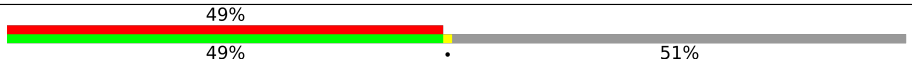
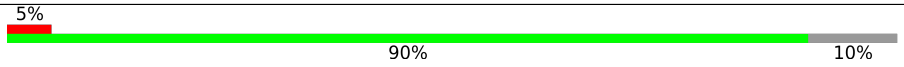
Mol	Chain	Length	Quality of chain
29	y	77	
30	h	146	
30	t	146	
31	i	110	
31	u	110	

2 Entry composition (i)

There are 32 unique types of molecules in this entry. The entry contains 65050 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 U1 snRNA,U1 snRNA,U1 snRNA,U1 snRNA,U1 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	1	327	6625	2951	1072	2275	327	0	0

- Molecule 2 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	2	143	3025	1352	513	1017	143	0	0

- Molecule 3 is a protein called U1 small nuclear ribonucleoprotein A,U1 small nuclear ribonucleoprotein A,U1 small nuclear ribonucleoprotein A,U1 small nuclear ribonucleoprotein A,U1 small nuclear ribonucleoprotein A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	A	99	492	294	99	99	0	0

- Molecule 4 is a protein called U1 small nuclear ribonucleoprotein 70 kDa homolog,U1 small nuclear ribonucleoprotein 70 kDa homolog,U1 small nuclear ribonucleoprotein 70 kDa homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	B	193	1450	929	261	258	2	0	0

- Molecule 5 is a protein called U1 small nuclear ribonucleoprotein C.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	C	177	1323	832	246	240	5	0	0

- Molecule 6 is a protein called Pre-mRNA-processing factor 39.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	509	Total	C	N	O	S	0	0
			3462	2188	608	659	7		

- Molecule 7 is a protein called U1 small nuclear ribonucleoprotein component PRP42.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	E	541	Total	C	N	O	S	0	0
			4574	2996	723	836	19		

- Molecule 8 is a protein called Protein NAM8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	F	175	Total	C	N	O	S	0	0
			1337	840	232	255	10		

- Molecule 9 is a protein called 56 kDa U1 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	G	216	Total	C	N	O	S	0	0
			1684	1098	274	301	11		

- Molecule 10 is a protein called Protein LUC7,Protein LUC7,Protein LUC7.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	H	158	Total	C	N	O	S	0	0
			1083	675	198	201	9		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	83	VAL	GLU	conflict	UNP Q07508
H	84	GLU	VAL	conflict	UNP Q07508

- Molecule 11 is a RNA chain called Yeast UBC4 pre-mRNA (mutant).

Mol	Chain	Residues	Atoms					AltConf	Trace
11	I	38	Total	C	N	O	P	0	0
			789	355	132	264	38		

- Molecule 12 is a protein called U1 small nuclear ribonucleoprotein component SNU71.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	J	42	Total	C	N	O	0	0
			324	210	55	59		

- Molecule 13 is a protein called U2 snRNP component HSH155.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	O	833	Total	C	N	O	S	0	0
			6612	4258	1121	1192	41		

- Molecule 14 is a protein called Pre-mRNA-splicing factor RSE1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	P	1186	Total	C	N	O	S	0	0
			9437	6034	1589	1763	51		

- Molecule 15 is a protein called Cold sensitive U2 snRNA suppressor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Q	220	Total	C	N	O	S	0	0
			1786	1157	307	313	9		

- Molecule 16 is a protein called Protein HSH49.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	R	173	Total	C	N	O	S	0	0
			1429	930	239	258	2		

- Molecule 17 is a protein called Pre-mRNA-splicing factor RDS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	103	Total	C	N	O	S	0	0
			814	503	154	143	14		

- Molecule 18 is a protein called Pre-mRNA-splicing factor PRP9.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	462	Total	C	N	O	S	0	0
			3915	2487	677	735	16		

- Molecule 19 is a protein called Pre-mRNA-splicing factor PRP11,Pre-mRNA-splicing factor PRP11,Pre-mRNA-splicing factor PRP11.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	196	Total	C	N	O	S	0	0
			1489	934	258	291	6		

- Molecule 20 is a protein called Pre-mRNA-splicing factor PRP21.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	127	Total	C	N	O	S	0	0
			1084	689	193	196	6		

- Molecule 21 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	170	Total	C	N	O	S	0	0
			1383	866	253	257	7		

- Molecule 22 is a protein called Unknown.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	X	51	Total	C	N	O	0	0
			255	153	51	51		

- Molecule 23 is a protein called U2 small nuclear ribonucleoprotein B".

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Y	84	Total	C	N	O	S	0	0
			683	439	119	122	3		

- Molecule 24 is a protein called RDS3 complex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Z	83	Total	C	N	O	S	0	0
			685	424	129	131	1		

- Molecule 25 is a protein called Small nuclear ribonucleoprotein-associated protein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	b	121	Total	C	N	O	S	0	0
			972	613	183	173	3		
25	s	65	Total	C	N	O	S	0	0
			518	331	91	93	3		

- Molecule 26 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	d	93	Total	C	N	O	S	0	0
			714	453	125	133	3		
26	v	82	Total	C	N	O	S	0	0
			632	402	109	119	2		

- Molecule 27 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	e	77	Total	C	N	O	S	0	0
			600	395	96	106	3		
27	w	77	Total	C	N	O	S	0	0
			602	396	95	108	3		

- Molecule 28 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	f	73	Total	C	N	O	S	0	0
			585	376	102	106	1		
28	x	73	Total	C	N	O	S	0	0
			585	376	102	106	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	g	72	Total	C	N	O	S	0	0
			556	352	97	105	2		
29	y	75	Total	C	N	O	S	0	0
			577	363	100	112	2		

- Molecule 30 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	h	107	Total	C	N	O	S	0	0
			834	525	149	157	3		
30	t	72	Total	C	N	O	S	0	0
			569	364	99	104	2		

- Molecule 31 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	i	99	Total	C	N	O	S	0	0
			805	514	148	139	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
31	u	92	Total	C	N	O	S	0	0
			752	481	136	131	4		

- Molecule 32 is ZINC ION (three-letter code: ZN) (formula: Zn).

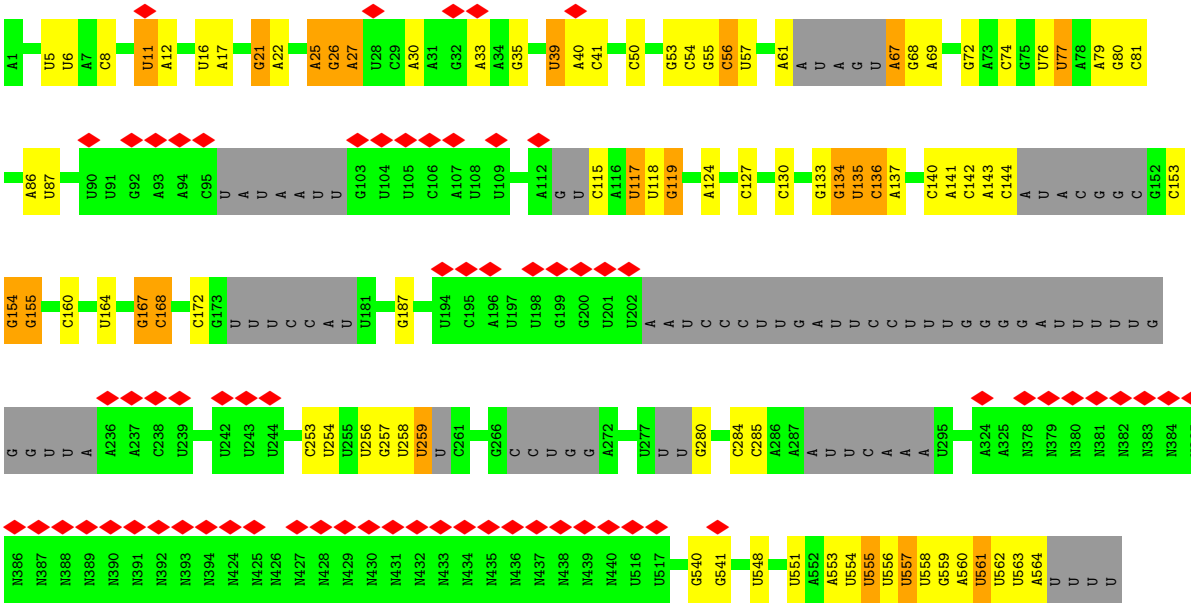
Mol	Chain	Residues	Atoms		AltConf
32	C	1	Total	Zn	0
			1	1	
32	H	2	Total	Zn	0
			2	2	
32	S	3	Total	Zn	0
			3	3	
32	T	2	Total	Zn	0
			2	2	
32	U	1	Total	Zn	0
			1	1	

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.

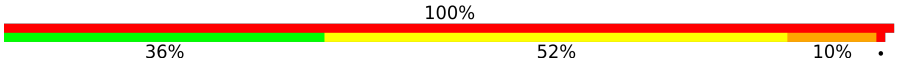
• Molecule 1: U1 snRNA,U1 snRNA,U1 snRNA,U1 snRNA,U1 snRNA

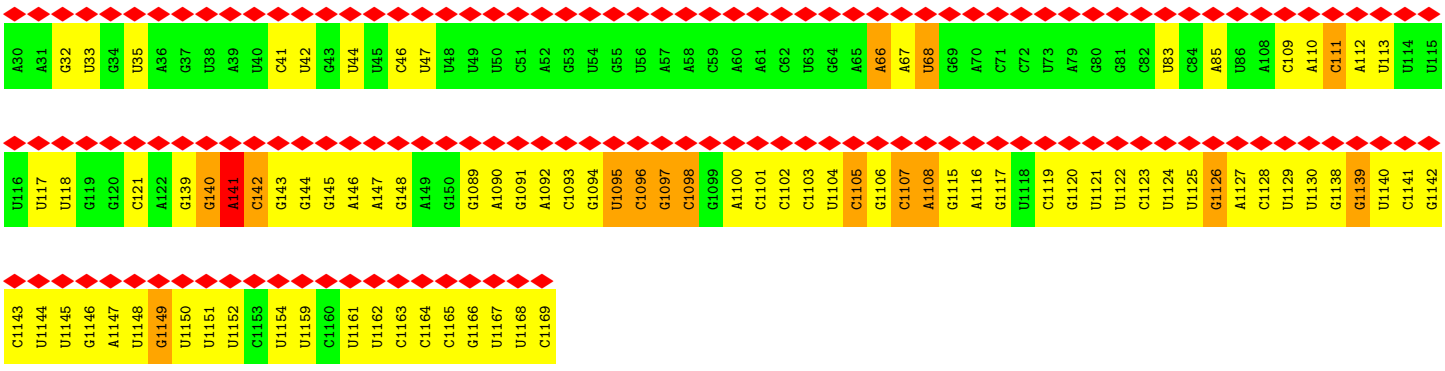
Chain 1:



• Molecule 2: U2 snRNA

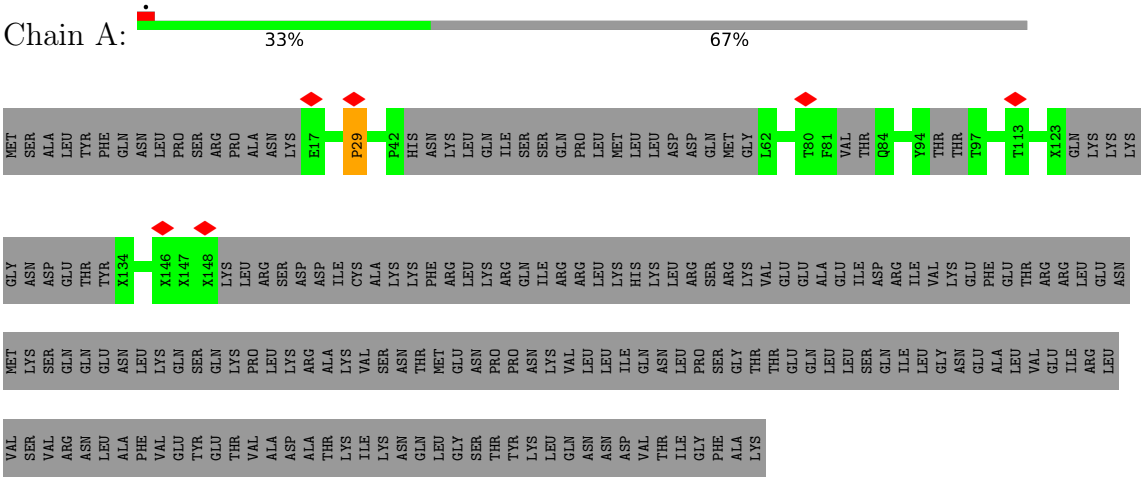
Chain 2:





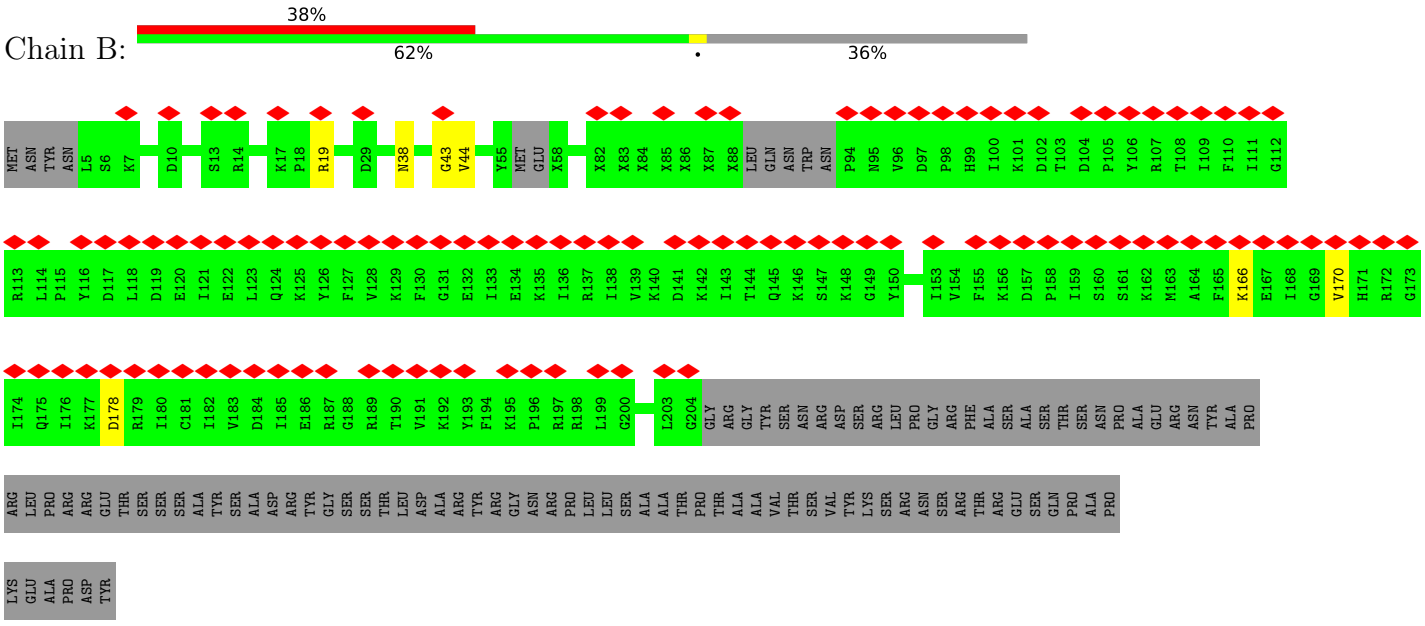
• Molecule 3: U1 small nuclear ribonucleoprotein A,U1 small nuclear ribonucleoprotein A,U1 small nuclear ribonucleoprotein A,U1 small nuclear ribonucleoprotein A,U1 small nuclear ribonucleoprotein A

Chain A:



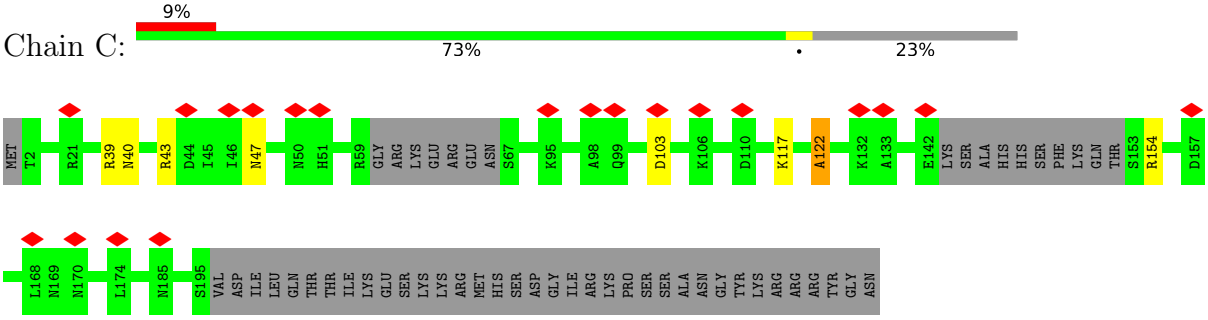
• Molecule 4: U1 small nuclear ribonucleoprotein 70 kDa homolog,U1 small nuclear ribonucleoprotein 70 kDa homolog,U1 small nuclear ribonucleoprotein 70 kDa homolog

Chain B:



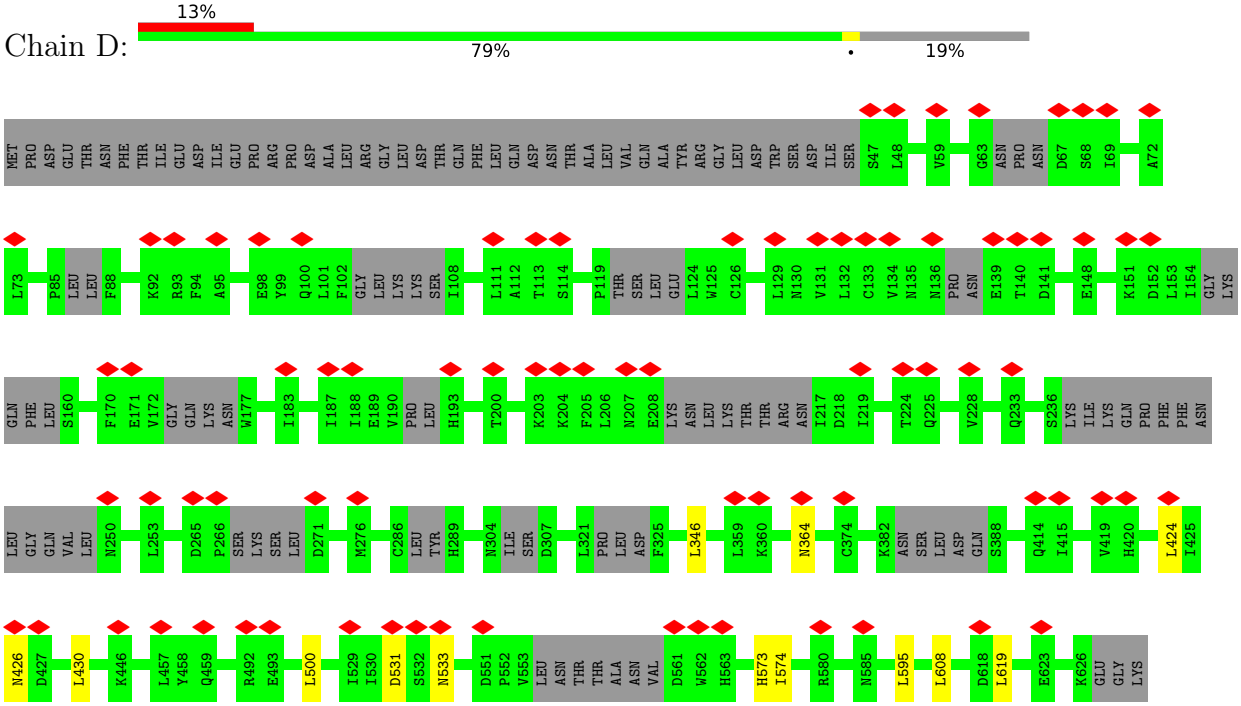
• Molecule 5: U1 small nuclear ribonucleoprotein C

Chain C:



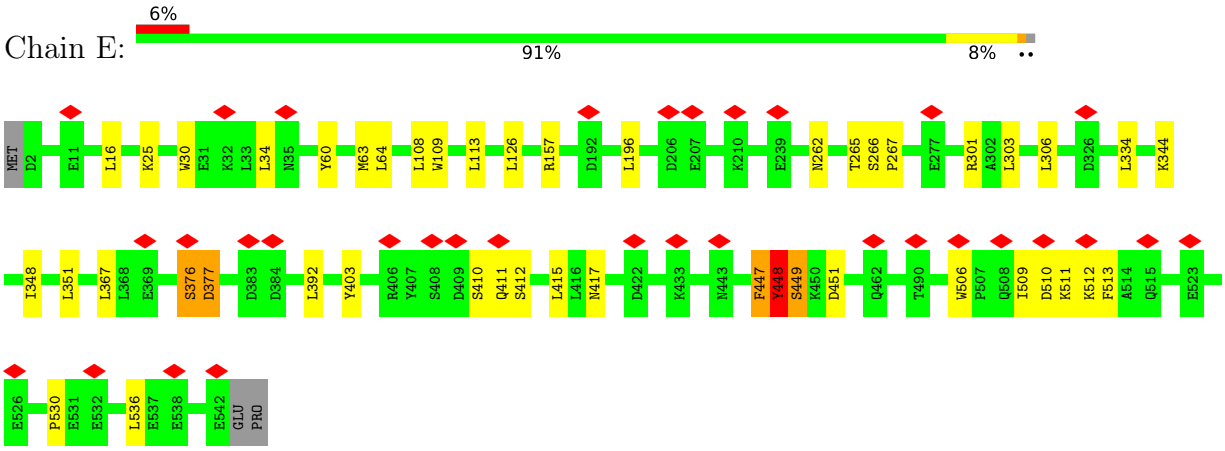
• Molecule 6: Pre-mRNA-processing factor 39

Chain D:



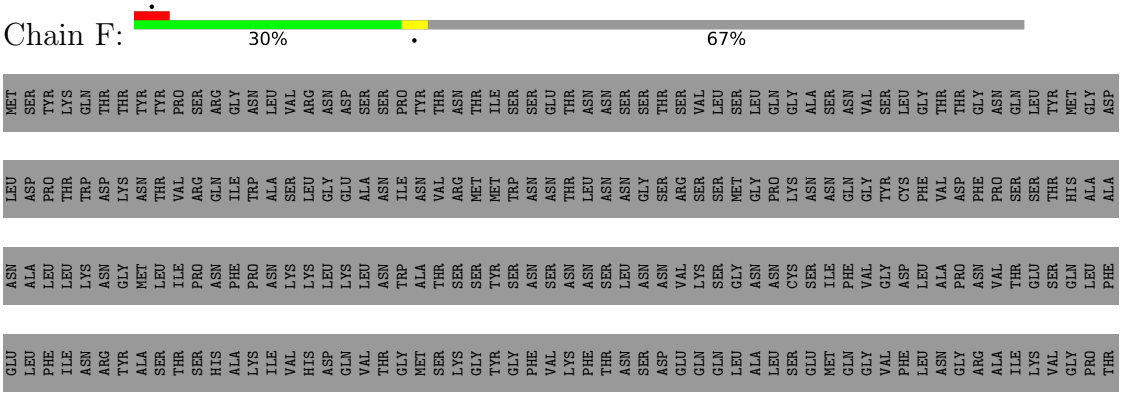
• Molecule 7: U1 small nuclear ribonucleoprotein component PRP42

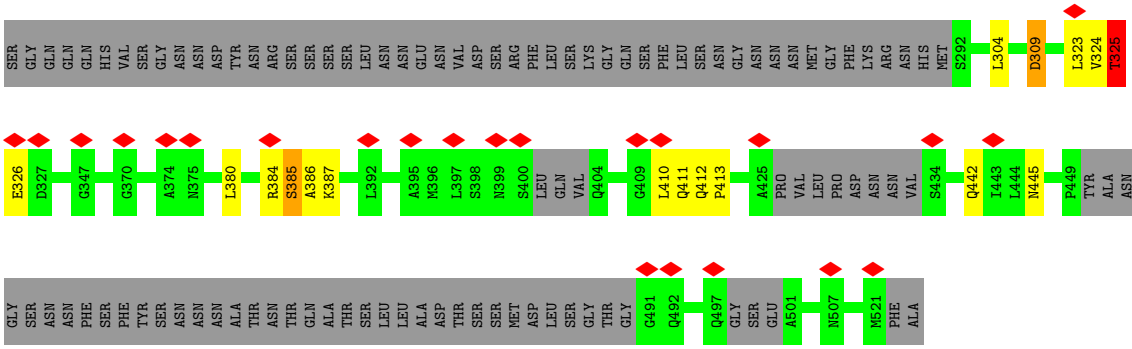
Chain E:



• Molecule 8: Protein NAM8

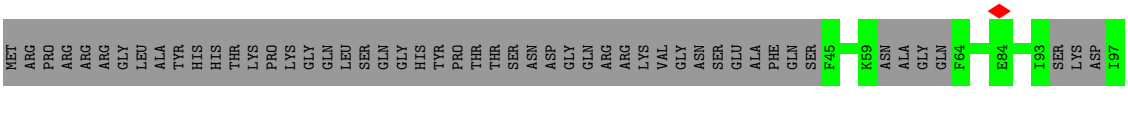
Chain F:

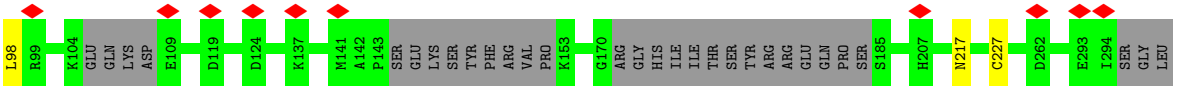


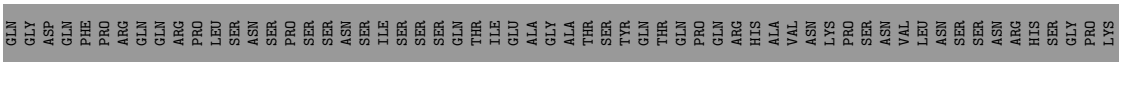


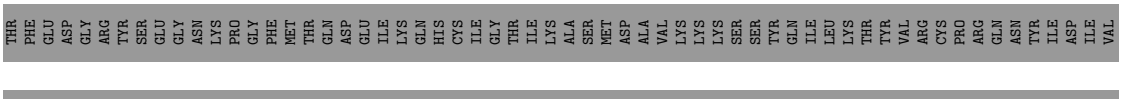
• Molecule 9: 56 kDa U1 small nuclear ribonucleoprotein component

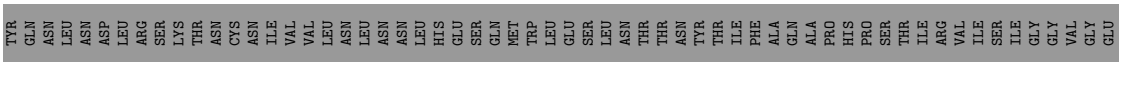
Chain G:





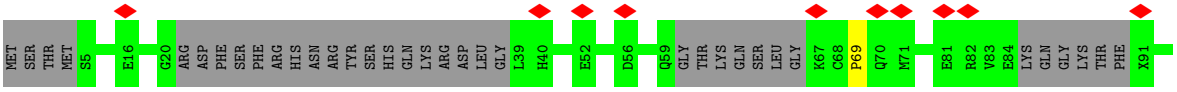


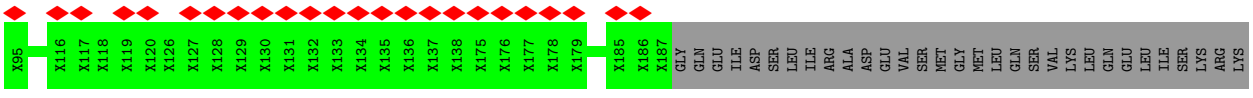


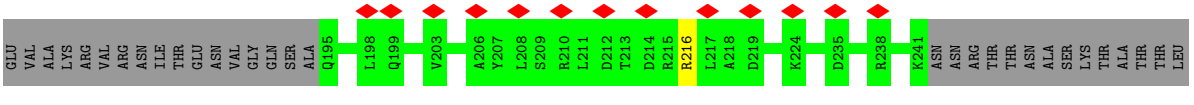


• Molecule 10: Protein LUC7,Protein LUC7,Protein LUC7

Chain H:

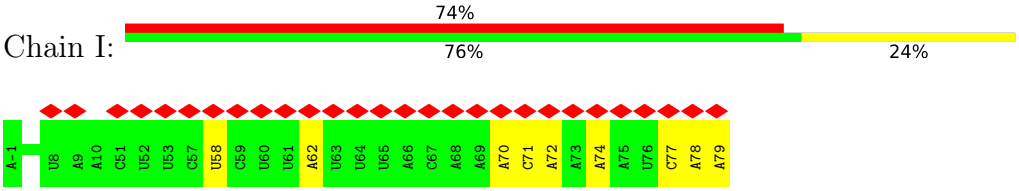






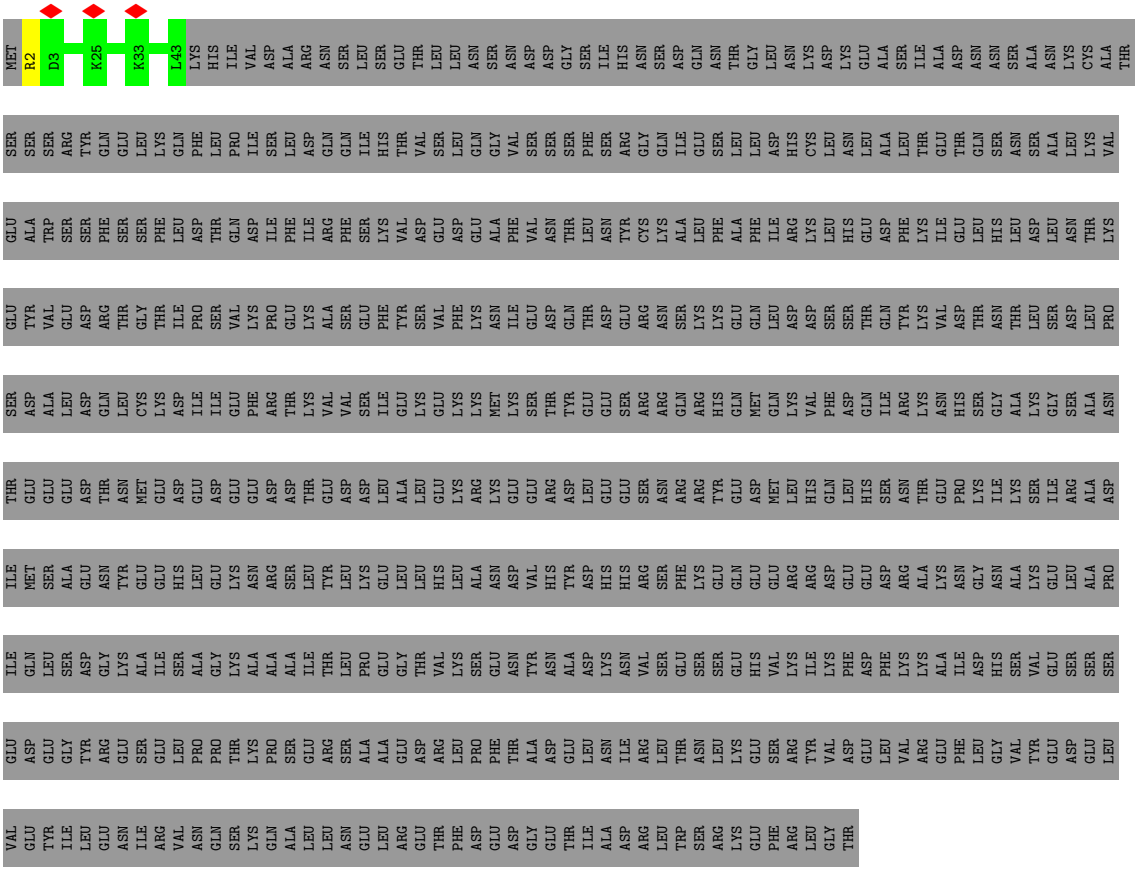
• Molecule 11: Yeast UBC4 pre-mRNA (mutant)

Chain I:



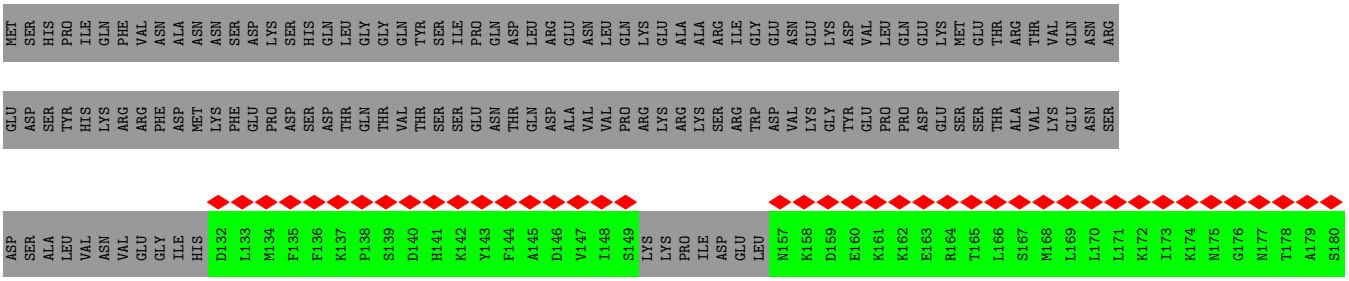
• Molecule 12: U1 small nuclear ribonucleoprotein component SNU71

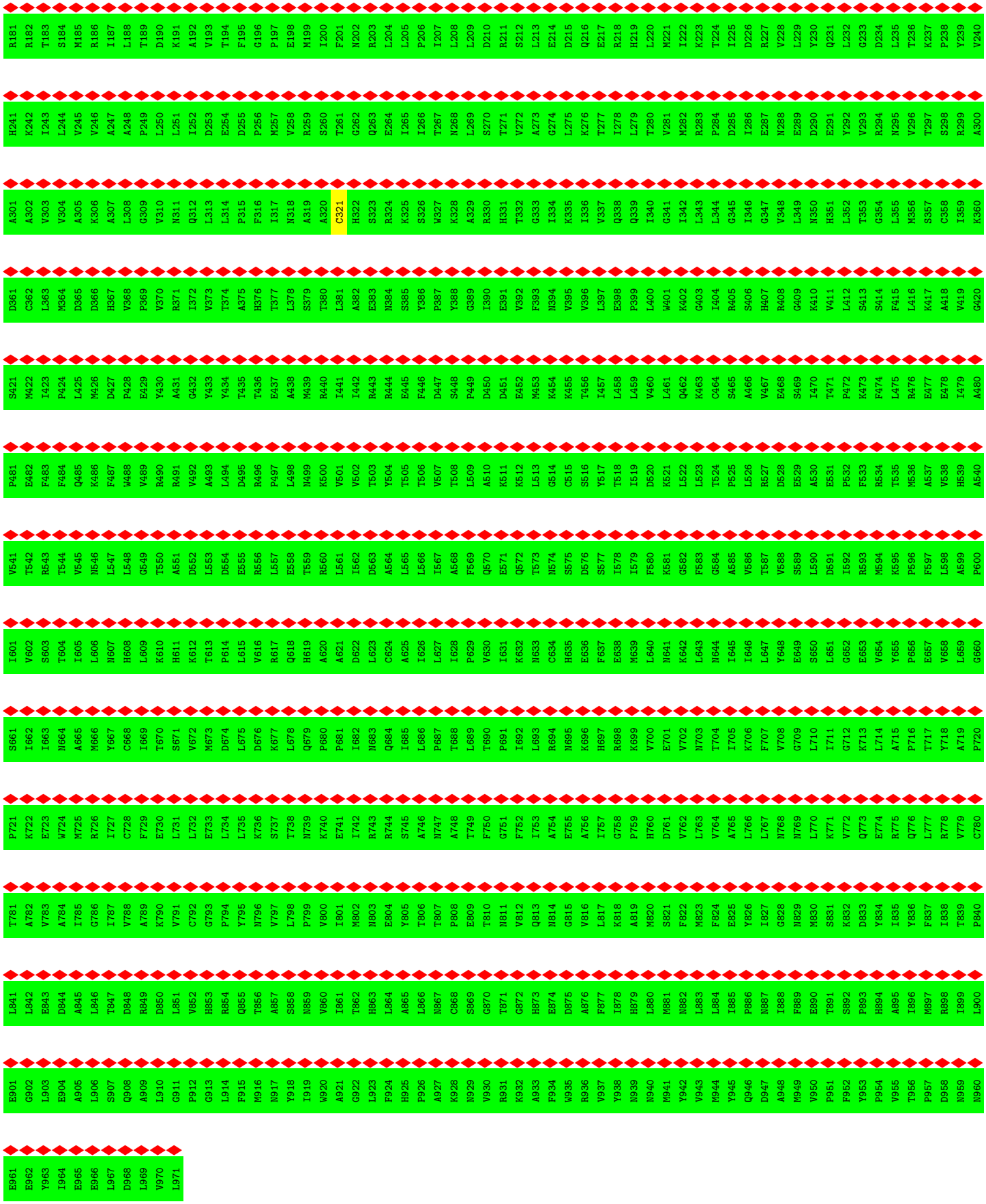
Chain J:



• Molecule 13: U2 snRNP component HSH155

Chain O:

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H241 K242 I243 L244 V245 V246 A247 A248 P249 L250 L251 I252 D253 E254 D255 P256 M257 V258 R259 S260 T261 G262 Q263 E264 I265 I266 T267 N268 L269 S270 T271 V272 A273 G274 L275 K276 T277 I278 L279 T280 V281 M282 R283 P284 D285 I286 E287 N288 E289 D290 E291 Y292 V293 R294 N295 V296 T297 S298 R299 A300
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D361 C362 L363 M364 D365 D366 H367 V368 P369 V370 R371 I372 V373 T374 A375 H376 T377 L378 S379 T380 L381 A382 E383 N384 S385 Y386 P387 Y388 G389 I390 E391 V392 P393 N394 V395 V396 L397 E398 P399 L400 W401 K402 G403 I404 R405 S406 H407 R408 G409 K410 V411 L412 S413 S414 F415 L416 K417 A418 V419 G420
S421 M422 I423 P424 L425 M426 D427 P428 E429 Y430 A431 G432 Y433 Y434 T435 T436 E437 A438 M439 R440 I441 I442 R443 R444 E445 F446 D447 S448 P449 D450 D451 E452 M453 K454 K455 T456 I457 L458 L459 V460 L461 Q462 K463 C464 S465 A466 V467 E468 S469 I470 T471 P472 K473 F474 L475 R476 E477 E478 I479 A480
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I601 V602 S603 T604 I605 L606 N607 H608 L609 K610 H611 K612 T613 P614 L615 V616 R617 Q618 H619 A620 A621 D622 L623 C624 A625 I626 L627 I628 P629 V630 I631 K632 N633 C634 H635 E636 F637 E638 M639 L640 N641 K642 L643 N644 I645 I646 L647 Y648 E649 S650 L651 G652 E653 V654 Y655 P656 E657 V658 L659 G660
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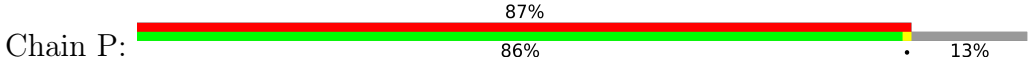
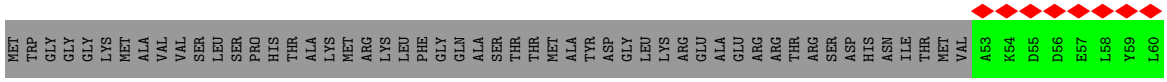
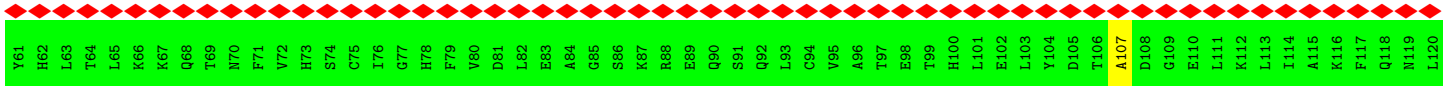
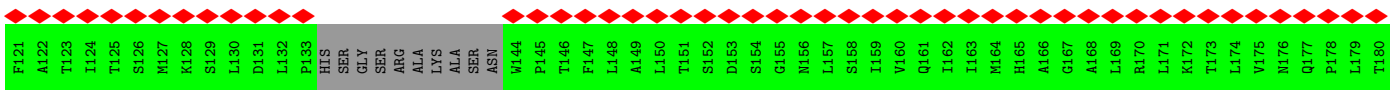
• Molecule 14: Pre-mRNA-splicing factor RSE1

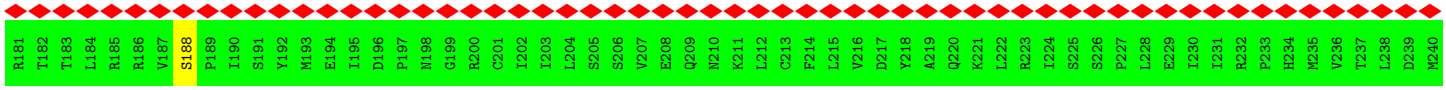
Chain P:

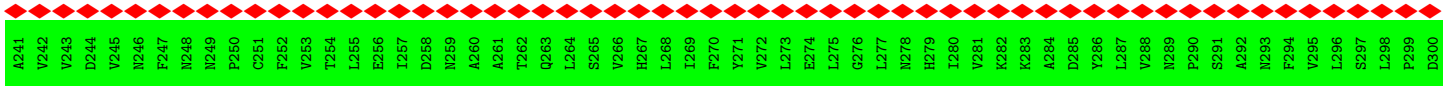


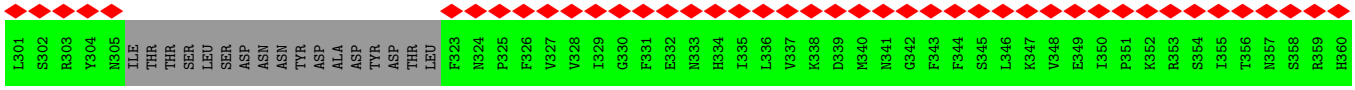


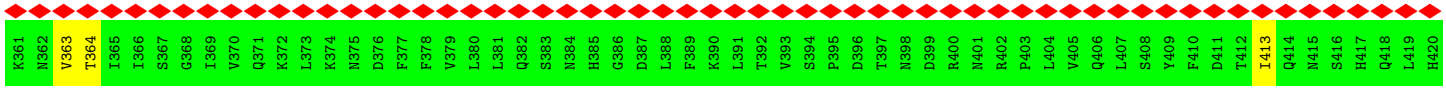


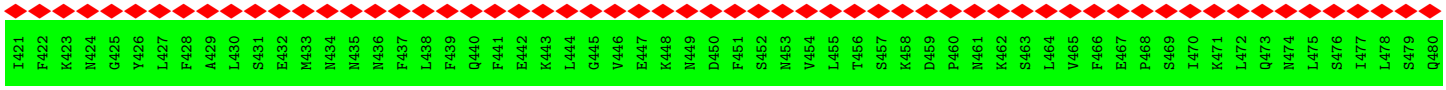


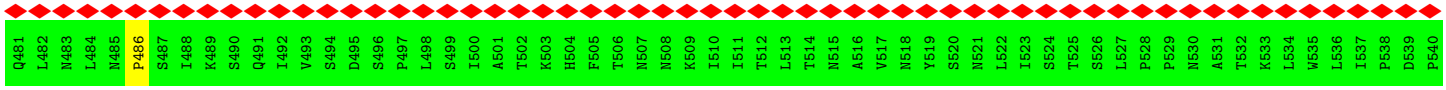


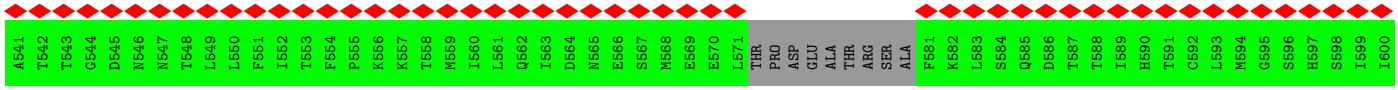


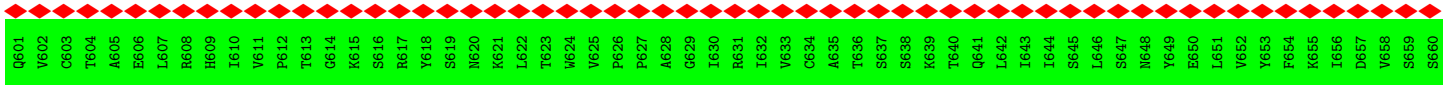


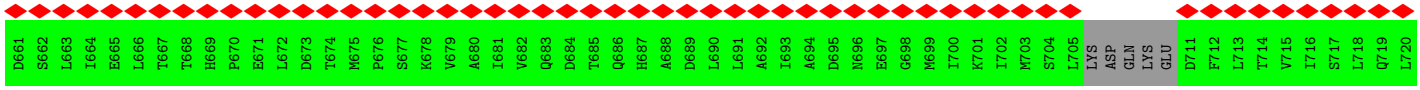


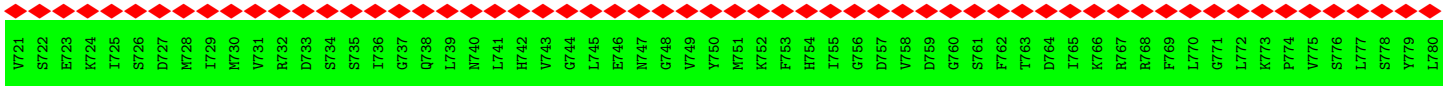


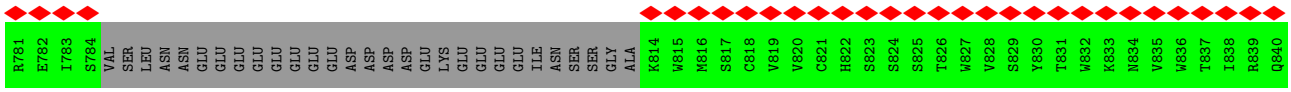


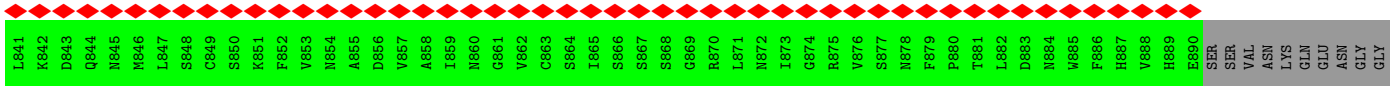


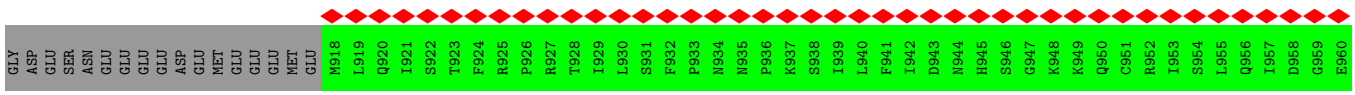


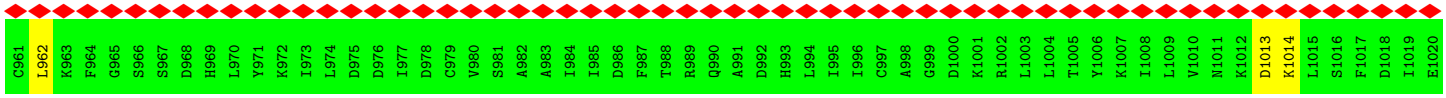


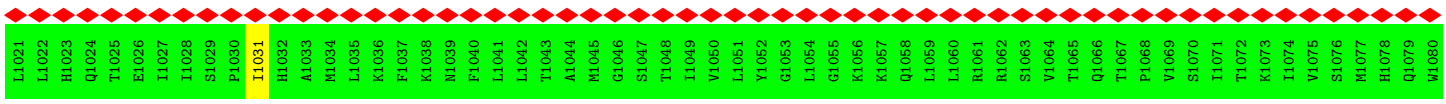


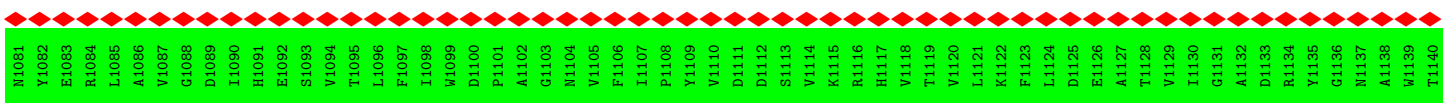


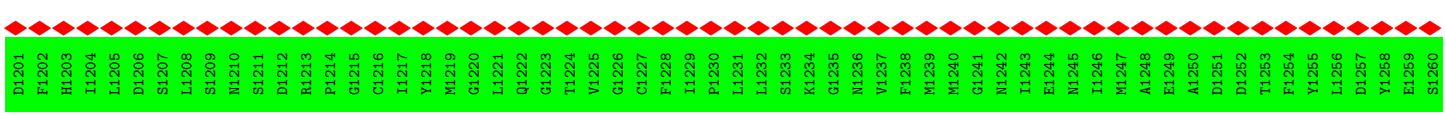


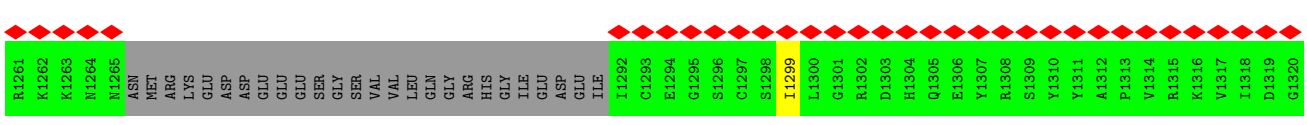


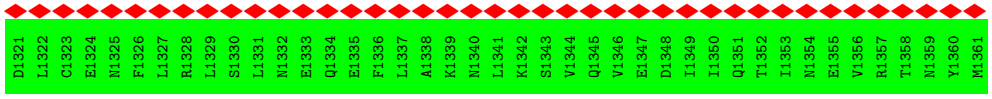






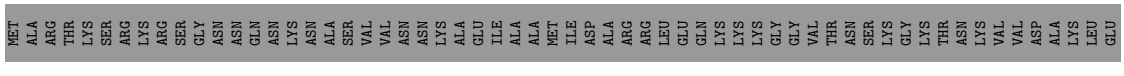


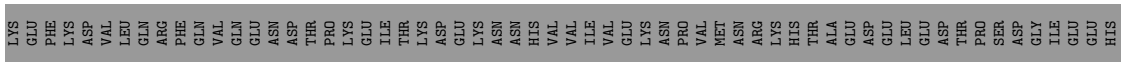


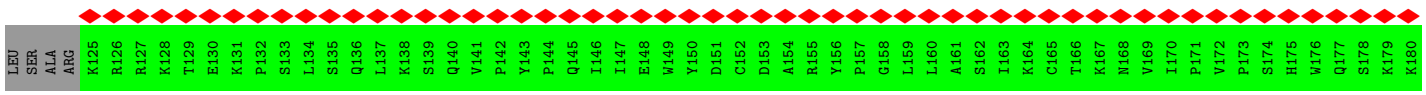


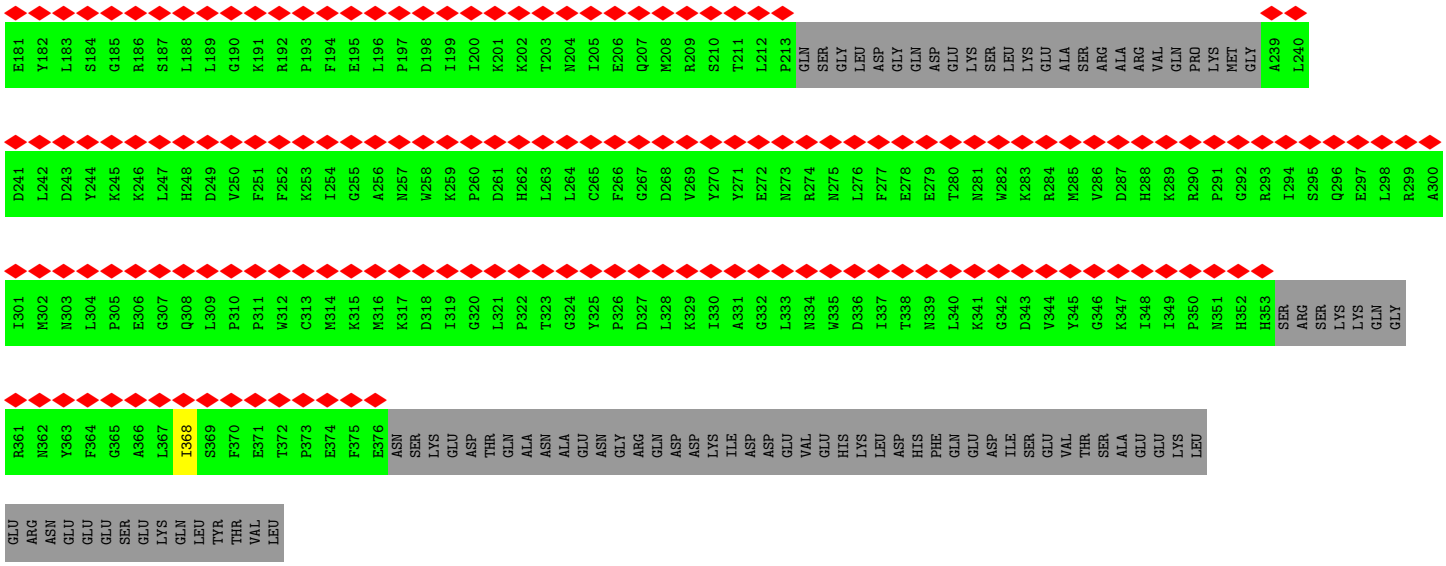
• Molecule 15: Cold sensitive U2 snRNA suppressor 1

Chain Q:

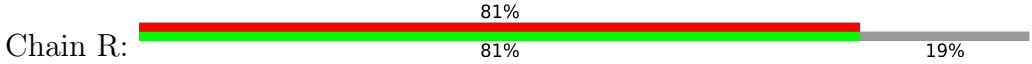


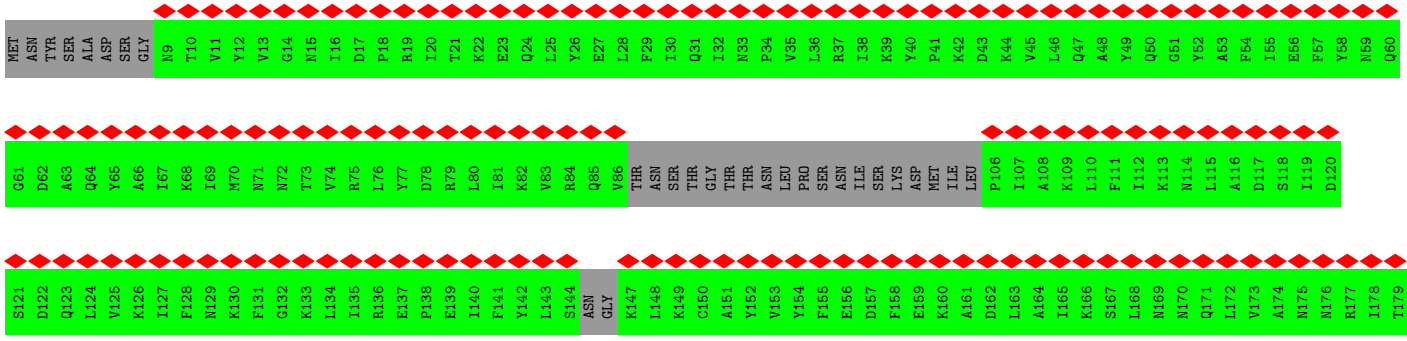






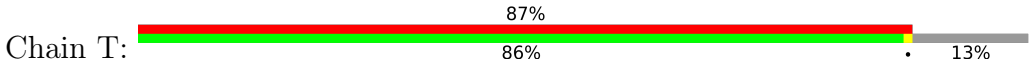
• Molecule 16: Protein HSH49

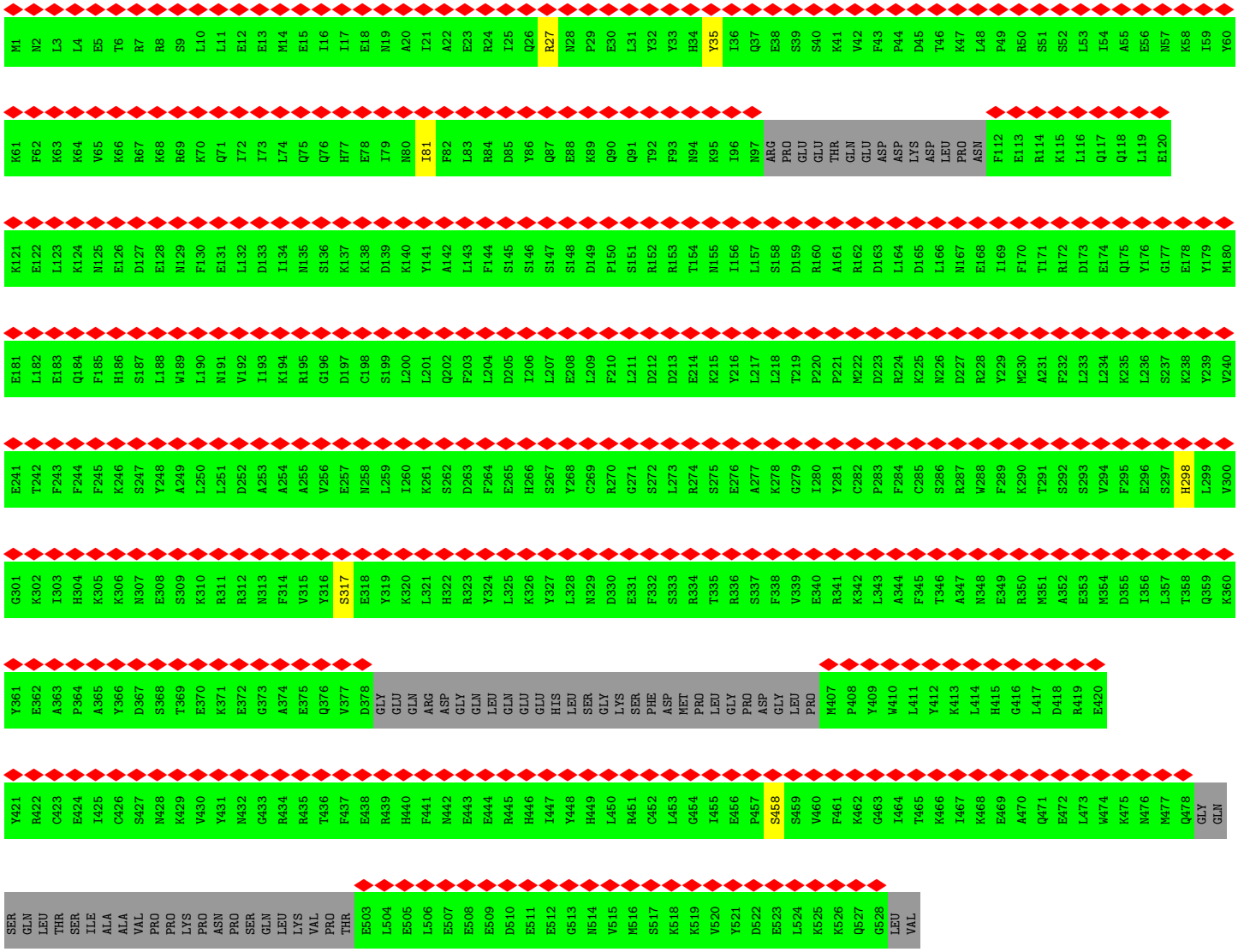




• Molecule 17: Pre-mRNA-splicing factor RDS3

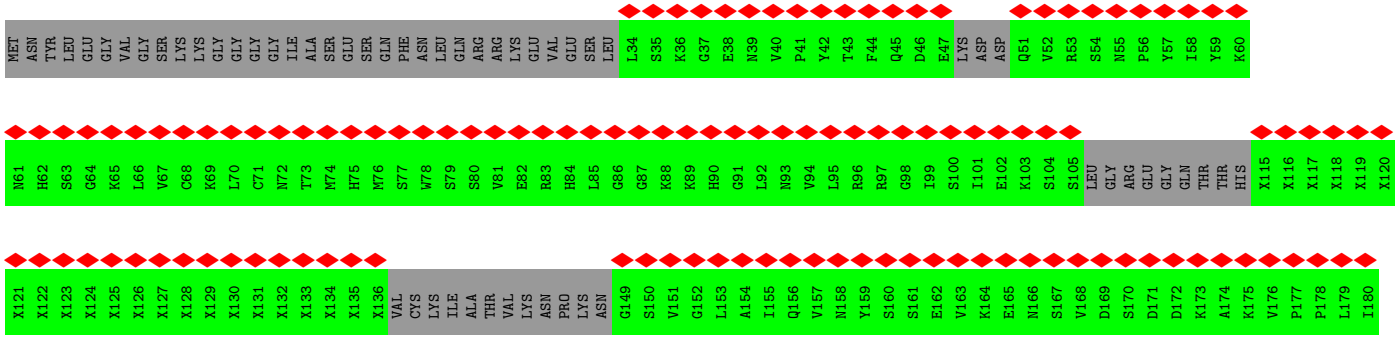
• Molecule 18: Pre-mRNA-splicing factor PRP9



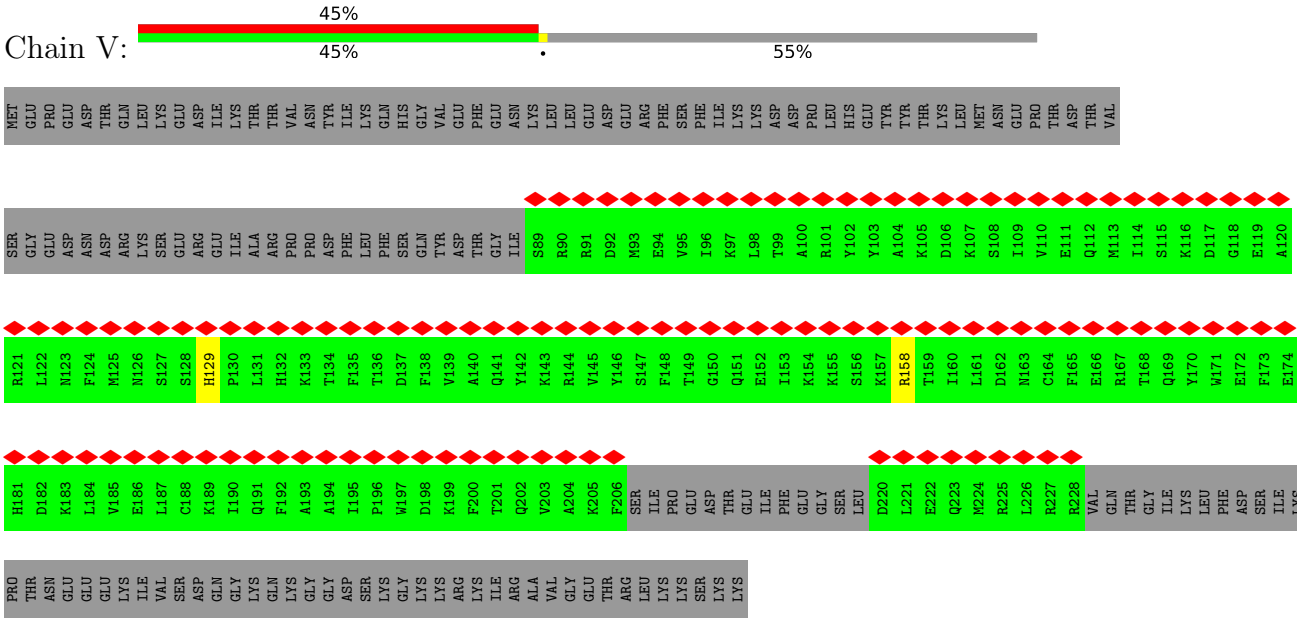


• Molecule 19: Pre-mRNA-splicing factor PRP11,Pre-mRNA-splicing factor PRP11,Pre-mRNA-splicing factor PRP11

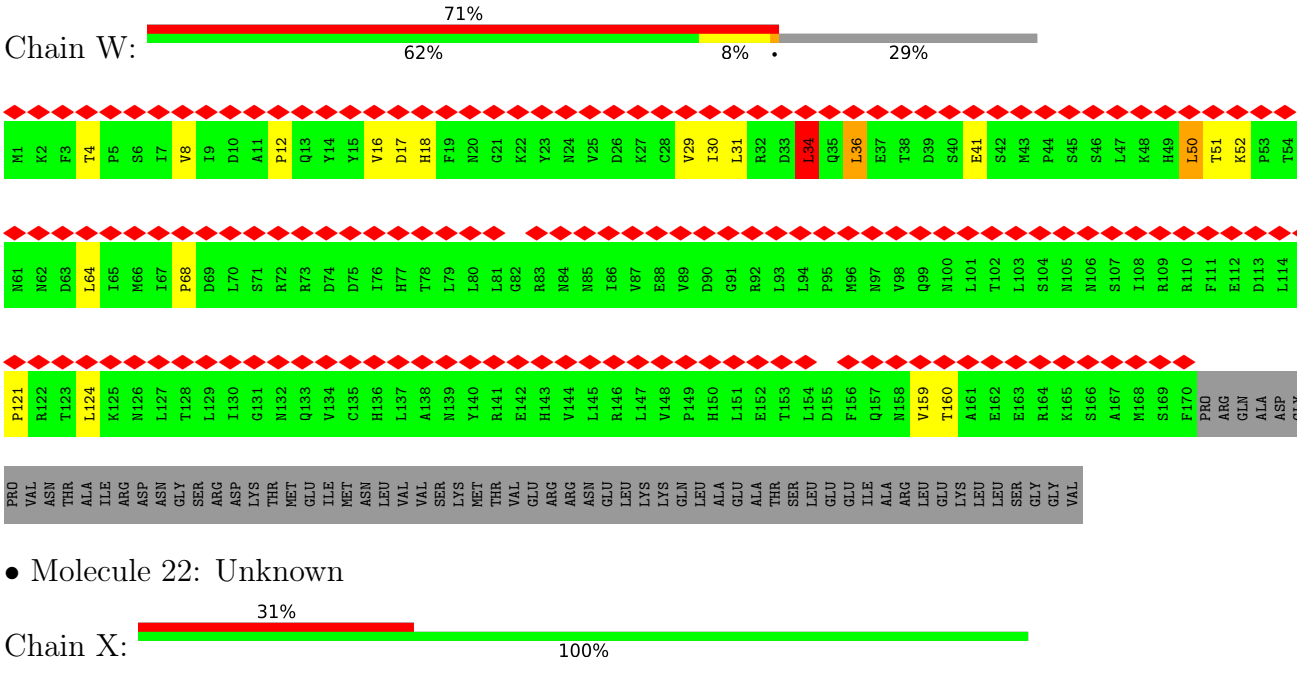
Chain U:



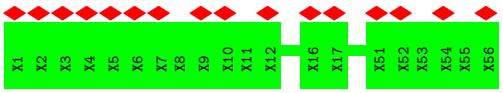
• Molecule 20: Pre-mRNA-splicing factor PRP21



• Molecule 21: U2 small nuclear ribonucleoprotein A'

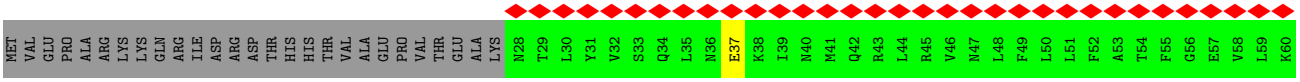


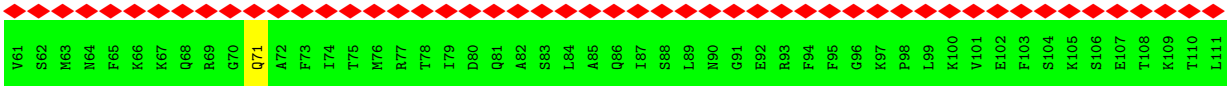
• Molecule 22: Unknown



• Molecule 23: U2 small nuclear ribonucleoprotein B"

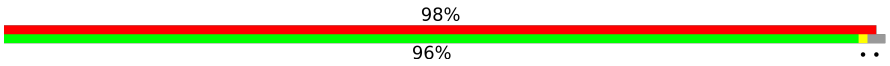
Chain Y:

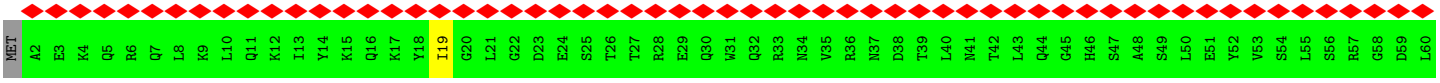


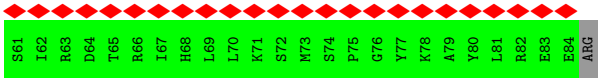


• Molecule 24: RDS3 complex subunit 10

Chain Z:

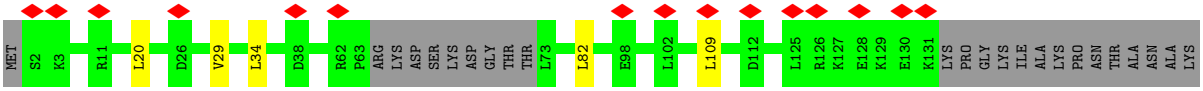






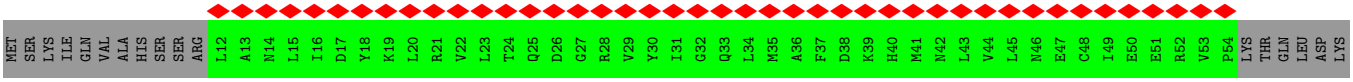
• Molecule 25: Small nuclear ribonucleoprotein-associated protein B

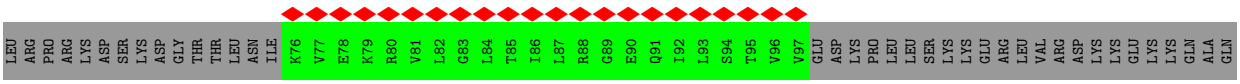
Chain b:



• Molecule 25: Small nuclear ribonucleoprotein-associated protein B

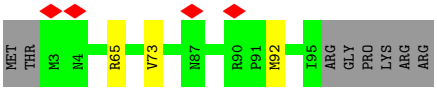
Chain s:





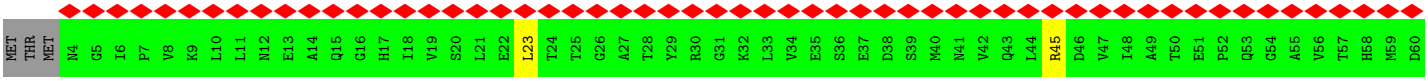
• Molecule 26: Small nuclear ribonucleoprotein Sm D3

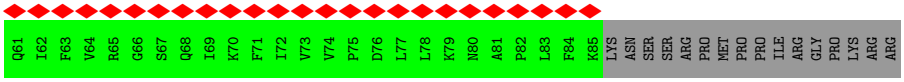
Chain d:



• Molecule 26: Small nuclear ribonucleoprotein Sm D3

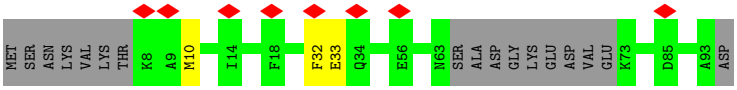
Chain v:





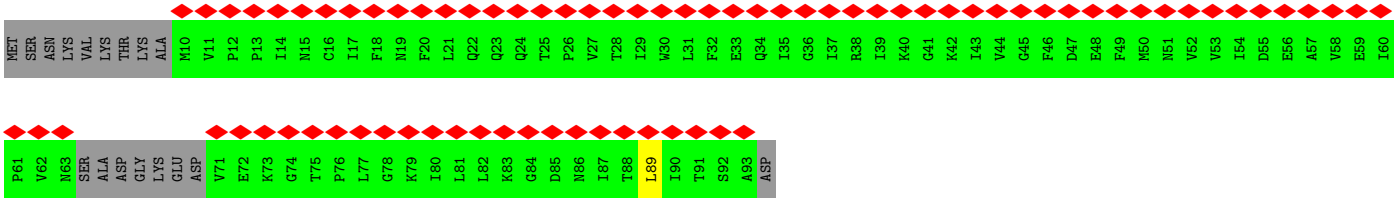
• Molecule 27: Small nuclear ribonucleoprotein E

Chain e:



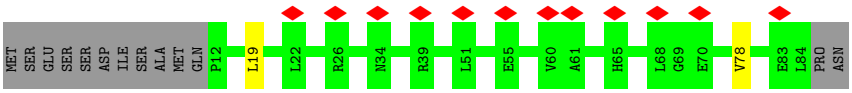
• Molecule 27: Small nuclear ribonucleoprotein E

Chain w:



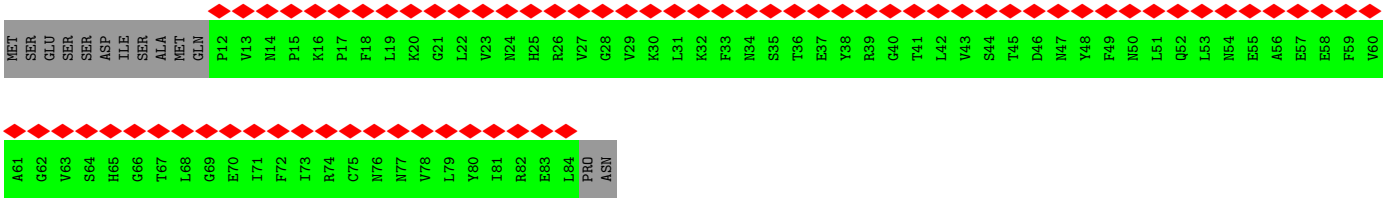
• Molecule 28: Small nuclear ribonucleoprotein F

Chain f:

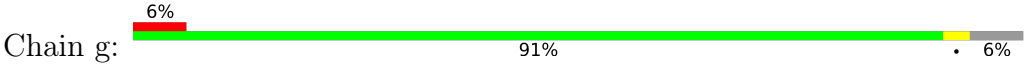


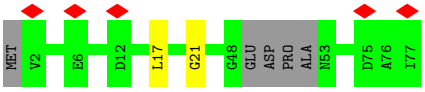
• Molecule 28: Small nuclear ribonucleoprotein F

Chain x:

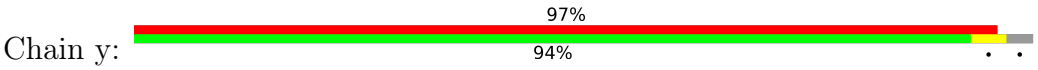


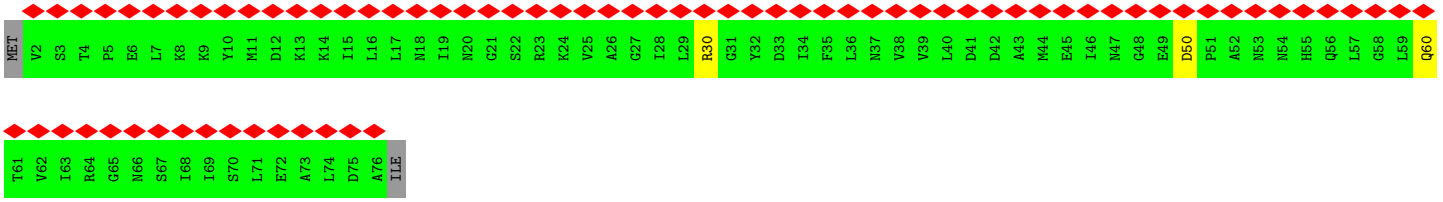
• Molecule 29: Small nuclear ribonucleoprotein G



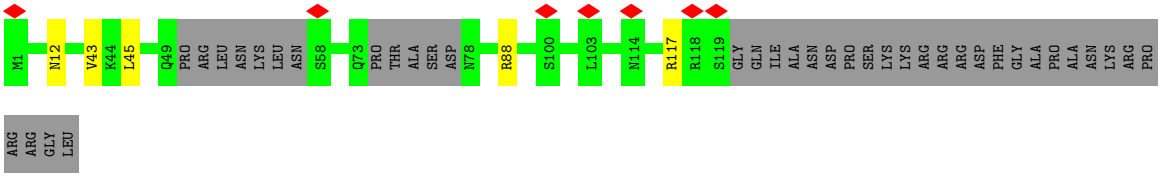


• Molecule 29: Small nuclear ribonucleoprotein G

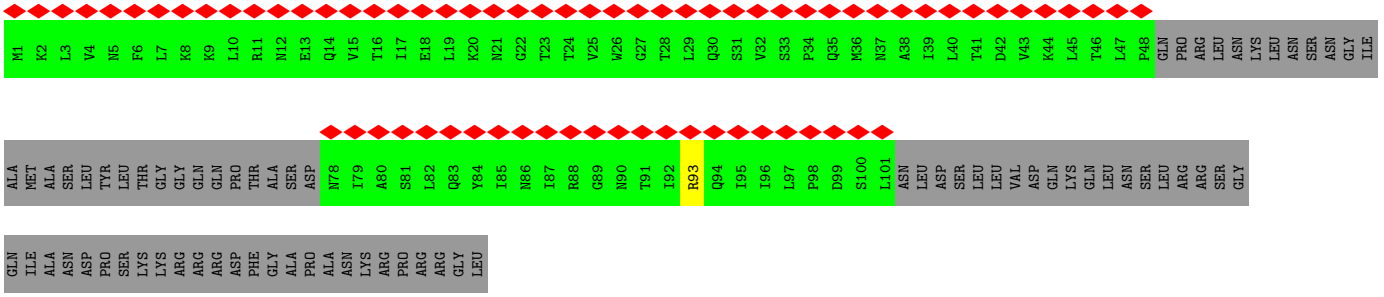




• Molecule 30: Small nuclear ribonucleoprotein Sm D1

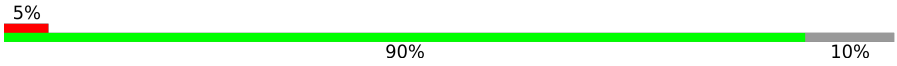


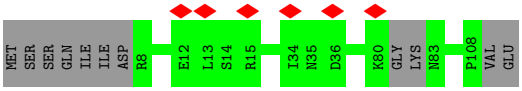
• Molecule 30: Small nuclear ribonucleoprotein Sm D1



• Molecule 31: Small nuclear ribonucleoprotein Sm D2

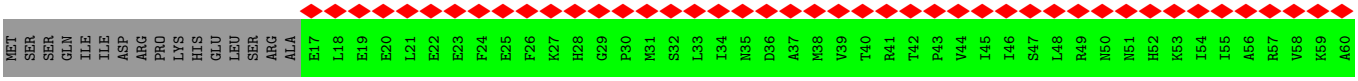
Chain i:

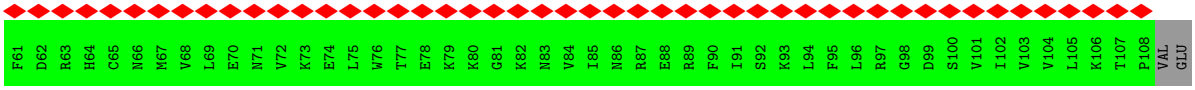




• Molecule 31: Small nuclear ribonucleoprotein Sm D2

Chain u:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	153556	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 ($e^-/Å^2$)	43	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	105000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.152	Depositor
Minimum map value	-0.083	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0369	Depositor
Map size (Å)	632.8, 632.8, 632.8	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.13, 1.13, 1.13	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	1	0.76	0/6890	1.31	72/10700 (0.7%)
2	2	1.40	52/3302 (1.6%)	1.72	120/5123 (2.3%)
3	A	0.28	0/388	0.60	1/535 (0.2%)
4	B	0.45	0/1325	0.79	2/1784 (0.1%)
5	C	0.57	0/1348	0.76	2/1825 (0.1%)
6	D	0.51	0/3499	0.71	7/4772 (0.1%)
7	E	0.77	4/4688 (0.1%)	0.94	26/6331 (0.4%)
8	F	0.65	0/1361	0.89	3/1843 (0.2%)
9	G	0.58	0/1716	0.74	1/2314 (0.0%)
10	H	0.49	0/816	0.69	0/1094
11	I	0.48	0/878	0.93	0/1357
12	J	0.50	0/331	0.78	0/448
13	O	0.28	0/6745	0.45	0/9157
14	P	0.30	1/9623 (0.0%)	0.53	1/13041 (0.0%)
15	Q	0.27	0/1835	0.46	0/2480
16	R	0.26	0/1453	0.42	0/1954
17	S	0.29	0/827	0.46	0/1105
18	T	0.27	0/3992	0.41	0/5346
19	U	0.24	0/1403	0.40	0/1889
20	V	0.24	0/1105	0.36	0/1475
21	W	0.41	0/1406	0.69	4/1905 (0.2%)
23	Y	0.30	0/692	0.54	0/923
24	Z	0.28	0/694	0.47	0/929
25	b	0.65	1/978 (0.1%)	0.93	4/1306 (0.3%)
25	s	0.39	0/521	0.62	0/701
26	d	0.68	1/726 (0.1%)	0.83	1/984 (0.1%)
26	v	0.43	0/641	0.65	2/868 (0.2%)
27	e	0.58	0/610	0.79	0/826
27	w	0.40	0/612	0.61	1/830 (0.1%)
28	f	0.63	1/597 (0.2%)	0.89	2/807 (0.2%)
28	x	0.42	0/597	0.63	0/807
29	g	0.63	0/559	0.83	0/751

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
29	y	0.26	0/582	0.49	0/785
30	h	0.52	0/839	0.77	2/1132 (0.2%)
30	t	0.42	0/574	0.68	1/777 (0.1%)
31	i	0.57	0/818	0.75	0/1099
31	u	0.40	0/764	0.57	0/1026
All	All	0.57	60/65735 (0.1%)	0.84	252/91029 (0.3%)

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
2	2	0	1
4	B	0	3
5	C	0	3
6	D	0	5
7	E	0	12
8	F	0	8
9	G	0	1
10	H	0	1
14	P	0	2
18	T	0	1
21	W	0	1
27	e	0	1
29	g	0	1
30	h	0	1
All	All	0	41

The worst 5 of 60 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1149	G	O3'-P	24.38	1.90	1.61
2	2	143	G	O3'-P	18.83	1.83	1.61
2	2	1161	U	O3'-P	-15.58	1.42	1.61
2	2	143	G	C3'-O3'	15.30	1.63	1.42
2	2	1092	A	O3'-P	-14.80	1.43	1.61

The worst 5 of 252 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	144	G	C4'-C3'-O3'	-16.52	74.71	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	1162	U	C5'-C4'-O4'	14.81	126.87	109.10
2	2	1093	C	P-O5'-C5'	14.80	144.59	120.90
2	2	1147	A	C5'-C4'-C3'	-14.18	93.31	116.00
2	2	1092	A	C2'-C3'-O3'	14.12	140.56	109.50

There are no chirality outliers.

5 of 41 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	2	141	A	Sidechain
4	B	166	LYS	Peptide
4	B	170	VAL	Peptide
4	B	43	GLY	Peptide
5	C	103	ASP	Peptide

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	A	72/298 (24%)	59 (82%)	12 (17%)	1 (1%)	11 46
4	B	158/300 (53%)	135 (85%)	22 (14%)	1 (1%)	25 63
5	C	171/231 (74%)	152 (89%)	18 (10%)	1 (1%)	25 63
6	D	475/629 (76%)	435 (92%)	37 (8%)	3 (1%)	25 63
7	E	539/544 (99%)	482 (89%)	44 (8%)	13 (2%)	6 36
8	F	165/523 (32%)	142 (86%)	17 (10%)	6 (4%)	3 28
9	G	204/492 (42%)	186 (91%)	18 (9%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	H	94/261 (36%)	89 (95%)	5 (5%)	0	100	100
12	J	40/620 (6%)	34 (85%)	6 (15%)	0	100	100
13	O	829/971 (85%)	788 (95%)	41 (5%)	0	100	100
14	P	1170/1361 (86%)	1059 (90%)	104 (9%)	7 (1%)	25	63
15	Q	214/435 (49%)	202 (94%)	11 (5%)	1 (0%)	29	67
16	R	165/213 (78%)	162 (98%)	3 (2%)	0	100	100
17	S	101/107 (94%)	88 (87%)	13 (13%)	0	100	100
18	T	454/530 (86%)	416 (92%)	38 (8%)	0	100	100
19	U	168/266 (63%)	143 (85%)	24 (14%)	1 (1%)	25	63
20	V	123/280 (44%)	112 (91%)	11 (9%)	0	100	100
21	W	168/238 (71%)	129 (77%)	28 (17%)	11 (6%)	1	18
23	Y	82/111 (74%)	76 (93%)	5 (6%)	1 (1%)	13	49
24	Z	81/85 (95%)	76 (94%)	4 (5%)	1 (1%)	13	49
25	b	117/196 (60%)	108 (92%)	9 (8%)	0	100	100
25	s	61/196 (31%)	58 (95%)	3 (5%)	0	100	100
26	d	91/101 (90%)	87 (96%)	4 (4%)	0	100	100
26	v	80/101 (79%)	77 (96%)	3 (4%)	0	100	100
27	e	73/94 (78%)	68 (93%)	4 (6%)	1 (1%)	11	46
27	w	73/94 (78%)	72 (99%)	1 (1%)	0	100	100
28	f	71/86 (83%)	66 (93%)	5 (7%)	0	100	100
28	x	71/86 (83%)	69 (97%)	2 (3%)	0	100	100
29	g	68/77 (88%)	61 (90%)	6 (9%)	1 (2%)	10	45
29	y	73/77 (95%)	64 (88%)	6 (8%)	3 (4%)	3	25
30	h	101/146 (69%)	97 (96%)	4 (4%)	0	100	100
30	t	68/146 (47%)	67 (98%)	1 (2%)	0	100	100
31	i	95/110 (86%)	90 (95%)	5 (5%)	0	100	100
31	u	90/110 (82%)	89 (99%)	1 (1%)	0	100	100
All	All	6605/10115 (65%)	6038 (91%)	515 (8%)	52 (1%)	24	58

5 of 52 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	D	426	ASN

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Mol	Chain	Res	Type
6	D	608	LEU
7	E	448	TYR
8	F	325	THR
8	F	385	SER

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
4	B	136/236 (58%)	135 (99%)	1 (1%)	84 90
5	C	127/214 (59%)	124 (98%)	3 (2%)	49 69
6	D	266/603 (44%)	266 (100%)	0	100 100
7	E	515/519 (99%)	512 (99%)	3 (1%)	86 92
8	F	148/451 (33%)	144 (97%)	4 (3%)	44 66
9	G	175/448 (39%)	174 (99%)	1 (1%)	86 92
10	H	84/183 (46%)	83 (99%)	1 (1%)	71 84
12	J	34/568 (6%)	33 (97%)	1 (3%)	42 65
13	O	739/867 (85%)	738 (100%)	1 (0%)	93 97
14	P	1093/1244 (88%)	1093 (100%)	0	100 100
15	Q	192/391 (49%)	192 (100%)	0	100 100
16	R	154/189 (82%)	154 (100%)	0	100 100
17	S	93/97 (96%)	93 (100%)	0	100 100
18	T	429/492 (87%)	424 (99%)	5 (1%)	71 84
19	U	158/216 (73%)	157 (99%)	1 (1%)	86 92
20	V	118/259 (46%)	116 (98%)	2 (2%)	60 78
21	W	161/219 (74%)	151 (94%)	10 (6%)	18 46
23	Y	76/100 (76%)	75 (99%)	1 (1%)	69 82
24	Z	75/77 (97%)	75 (100%)	0	100 100
25	b	108/176 (61%)	108 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
25	s	58/176 (33%)	58 (100%)	0	100 100
26	d	81/89 (91%)	80 (99%)	1 (1%)	71 84
26	v	71/89 (80%)	71 (100%)	0	100 100
27	e	68/83 (82%)	67 (98%)	1 (2%)	65 80
27	w	69/83 (83%)	69 (100%)	0	100 100
28	f	65/77 (84%)	65 (100%)	0	100 100
28	x	65/77 (84%)	65 (100%)	0	100 100
29	g	62/66 (94%)	62 (100%)	0	100 100
29	y	64/66 (97%)	64 (100%)	0	100 100
30	h	96/129 (74%)	94 (98%)	2 (2%)	53 72
30	t	67/129 (52%)	67 (100%)	0	100 100
31	i	90/103 (87%)	90 (100%)	0	100 100
31	u	85/103 (82%)	85 (100%)	0	100 100
All	All	5822/8819 (66%)	5784 (99%)	38 (1%)	84 90

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
21	W	36	LEU
27	e	10	MET
21	W	41	GLU
21	W	160	THR
30	h	117	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 99 such sidechains are listed below:

Mol	Chain	Res	Type
14	P	1117	HIS
18	T	415	HIS
14	P	1203	HIS
16	R	50	GLN
21	W	99	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	281/407 (69%)	66 (23%)	12 (4%)
11	I	35/38 (92%)	8 (22%)	2 (5%)
2	2	136/143 (95%)	46 (33%)	25 (18%)
All	All	452/588 (76%)	120 (26%)	39 (8%)

5 of 120 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	8	C
1	1	11	U
1	1	12	A
1	1	17	A
1	1	21	G

5 of 39 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	2	1122	U
2	2	1144	U
2	2	1123	C
2	2	1138	G
11	I	77	C

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

5 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#\|Z\| > 2$
2	PSU	2	42	2,11	18,21,22	1.09	1 (5%)	22,30,33	1.72	4 (18%)
2	PSU	2	44	2,11	18,21,22	1.03	1 (5%)	22,30,33	1.66	4 (18%)
1	PSU	1	5	1	18,21,22	1.47	2 (11%)	22,30,33	1.25	2 (9%)
1	PSU	1	6	1,11	18,21,22	1.35	1 (5%)	22,30,33	1.21	2 (9%)
2	PSU	2	35	2,11	18,21,22	1.06	1 (5%)	22,30,33	1.72	5 (22%)

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
2	PSU	2	42	2,11	-	0/7/25/26	0/2/2/2
2	PSU	2	44	2,11	-	0/7/25/26	0/2/2/2
1	PSU	1	5	1	-	0/7/25/26	0/2/2/2
1	PSU	1	6	1,11	-	0/7/25/26	0/2/2/2
2	PSU	2	35	2,11	-	0/7/25/26	0/2/2/2

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	5	PSU	C2-N1	4.33	1.42	1.36
1	1	6	PSU	C2-N1	3.91	1.42	1.36
2	2	42	PSU	C6-C5	3.50	1.39	1.35
2	2	35	PSU	C6-C5	3.33	1.39	1.35
2	2	44	PSU	C6-C5	3.25	1.39	1.35

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	42	PSU	C4-N3-C2	-4.58	119.74	126.34
2	2	35	PSU	C4-N3-C2	-4.47	119.90	126.34
2	2	42	PSU	N1-C2-N3	4.38	120.09	115.13
2	2	35	PSU	N1-C2-N3	4.36	120.07	115.13
2	2	44	PSU	N1-C2-N3	4.32	120.02	115.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	2	10
1	1	4
11	I	2
10	H	2
22	X	1

The worst 5 of 19 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	10:A	O3'	51:C	P	64.91
1	1	440:N	O3'	516:U	P	49.12
1	1	325:A	O3'	378:N	P	48.87
1	2	122:A	O3'	139:G	P	46.36
1	1	532:U	O3'	538:C	P	25.27

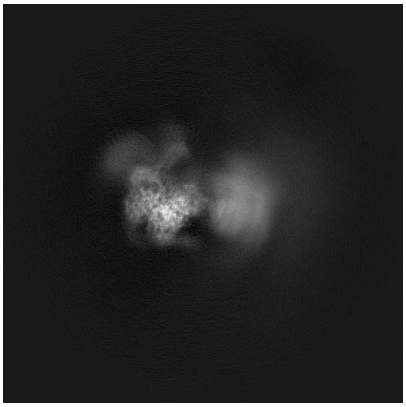
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4364. These allow visual inspection of the internal detail of the map and identification of artifacts.

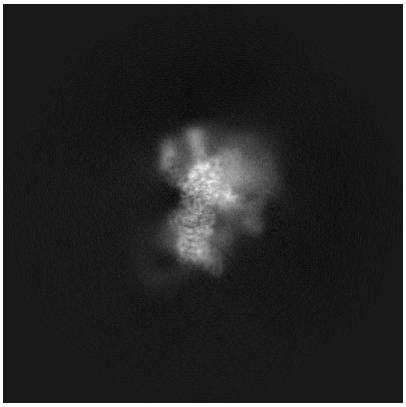
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

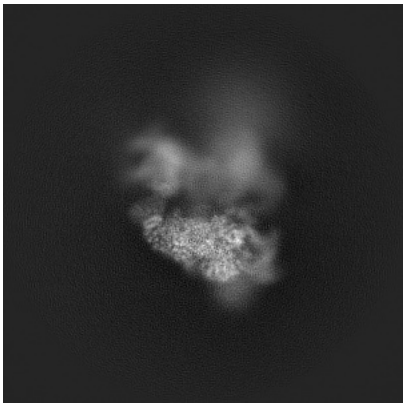
6.1.1 Primary map



X



Y

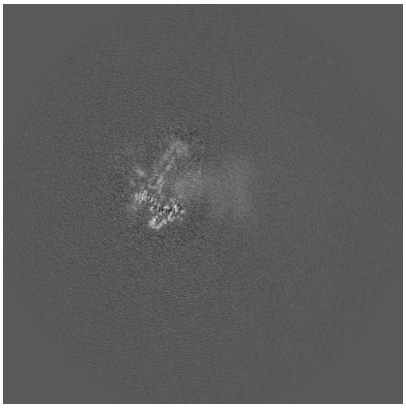


Z

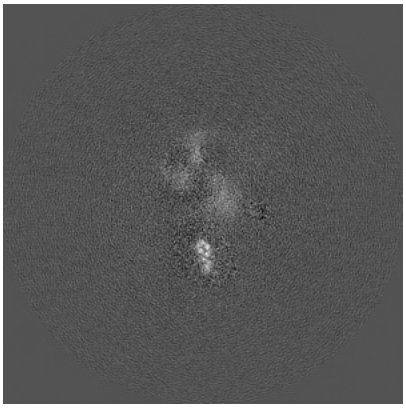
The images above show the map projected in three orthogonal directions.

6.2 Central slices

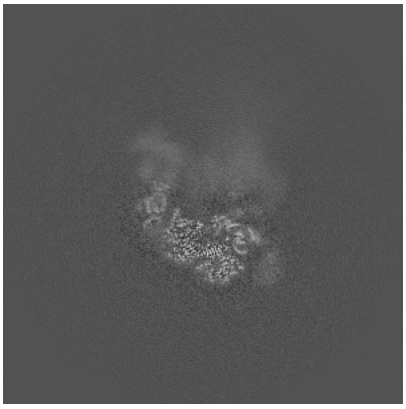
6.2.1 Primary map



X Index: 280



Y Index: 280

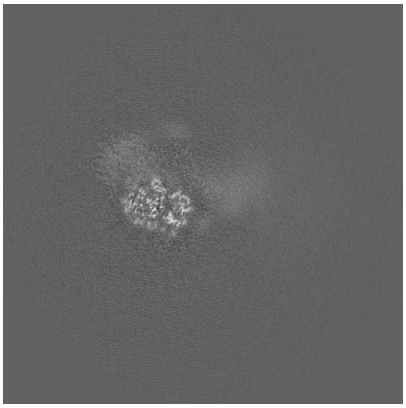


Z Index: 280

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

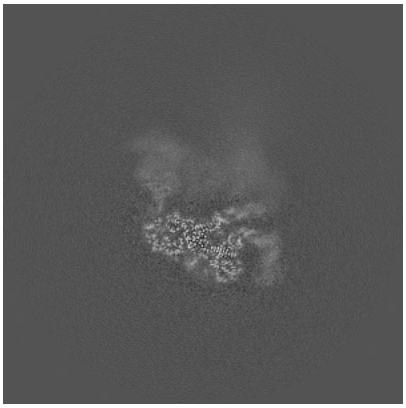
6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 303

Y Index: 225



Z Index: 271

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.0369. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

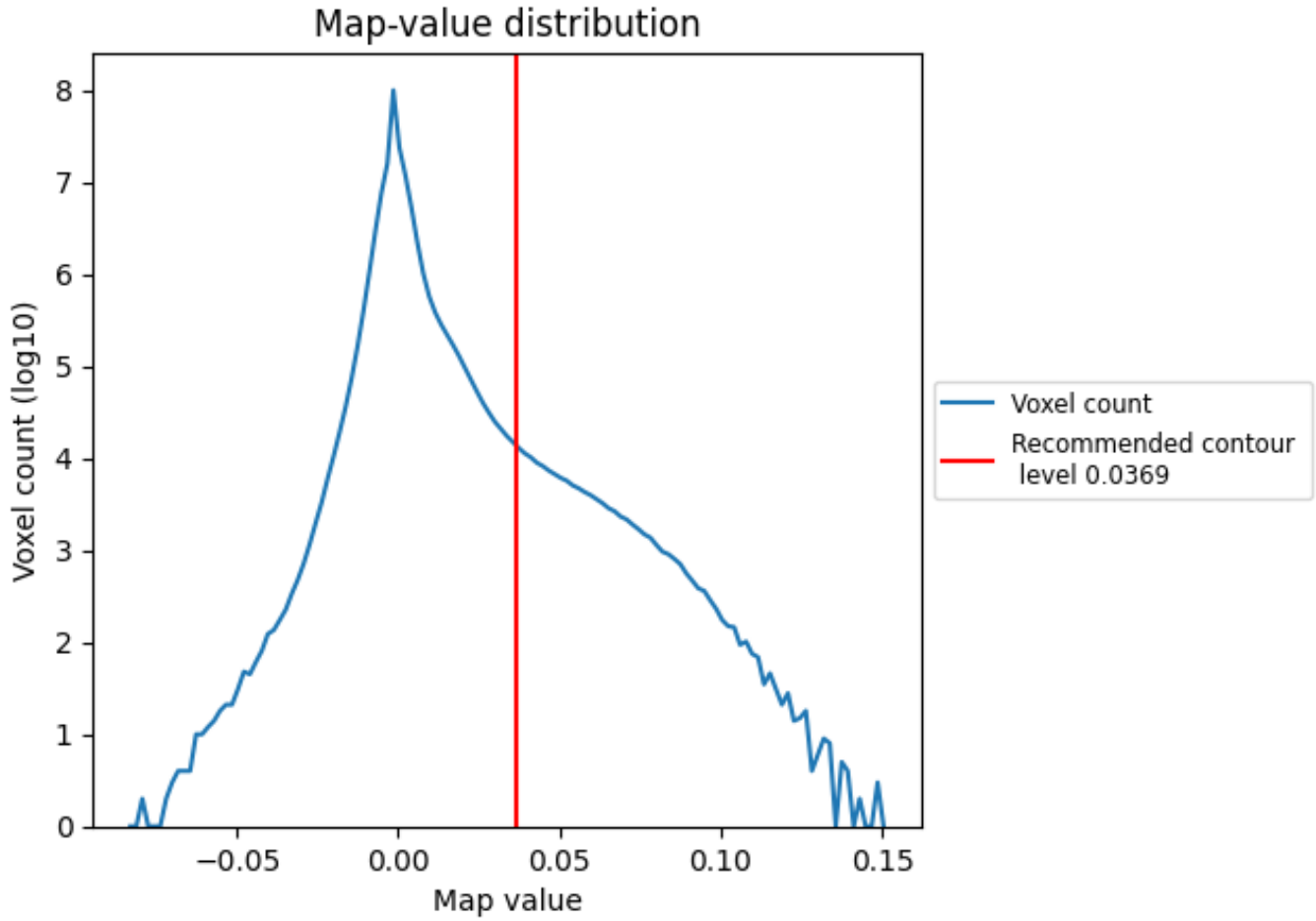
6.5 Mask visualisation (i)

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

7 Map analysis

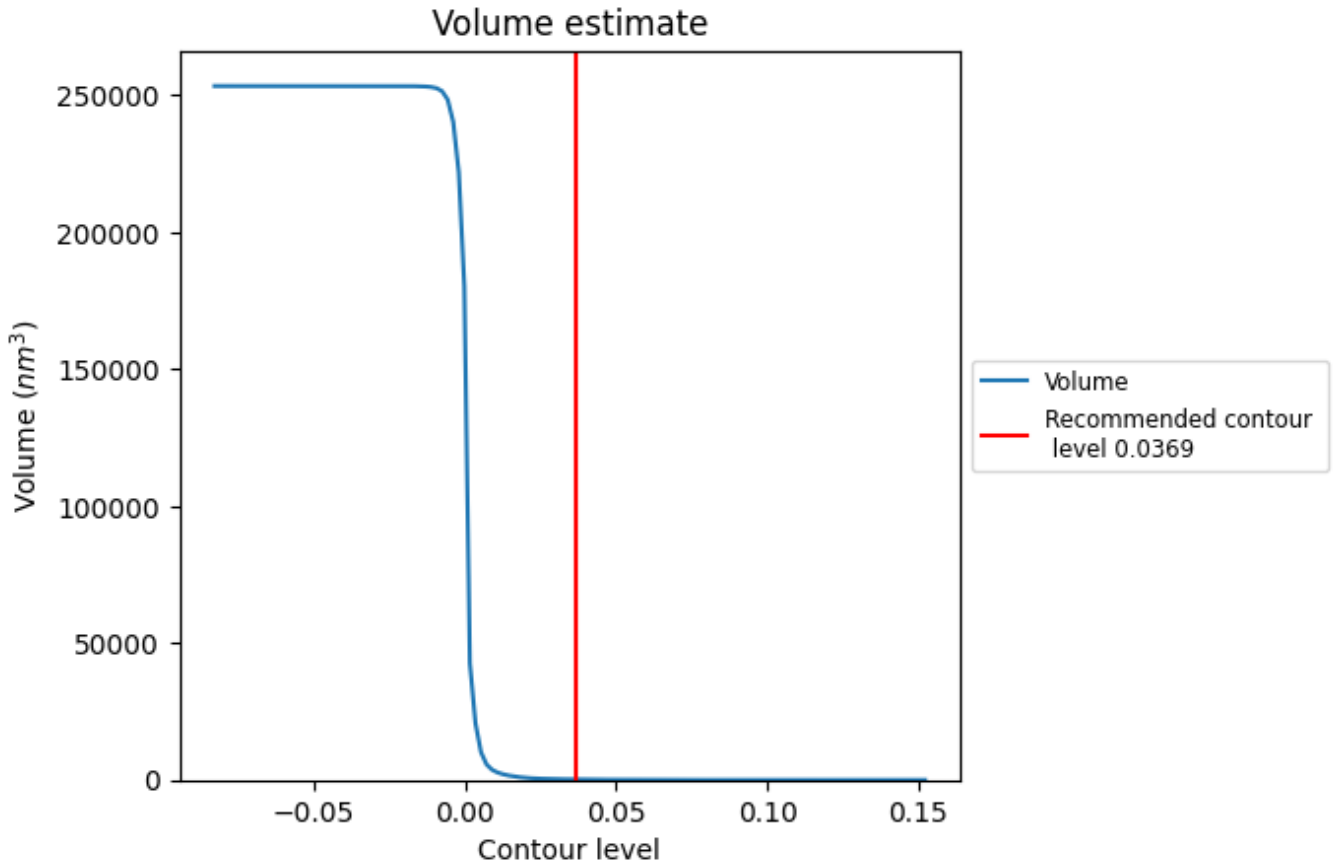
This section contains the results of statistical analysis of the map.

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.

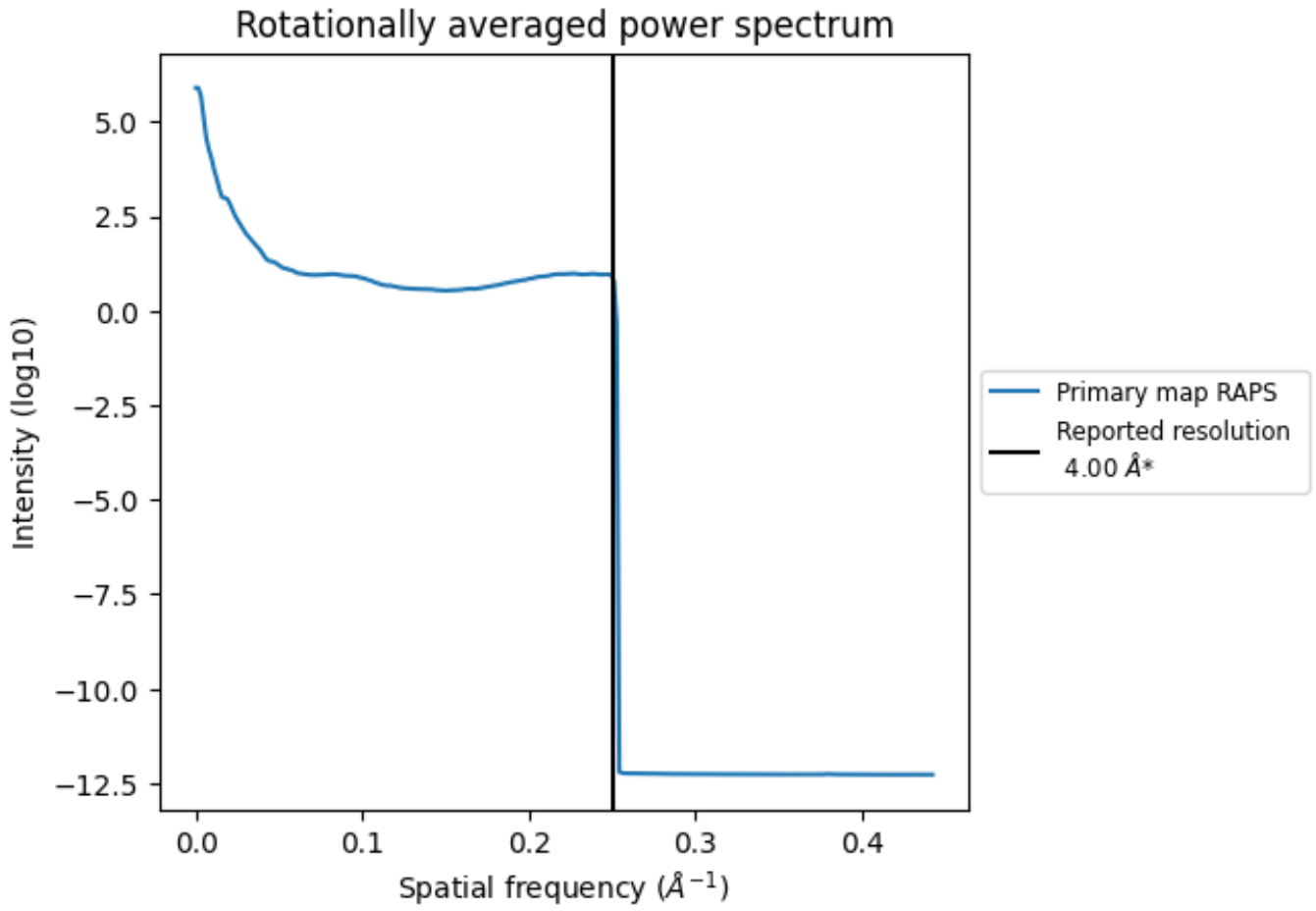
7.2 Volume estimate (i)



The volume at the recommended contour level is 189 nm^3; this corresponds to an approximate mass of 171 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 0.250 $Å^{-1}$

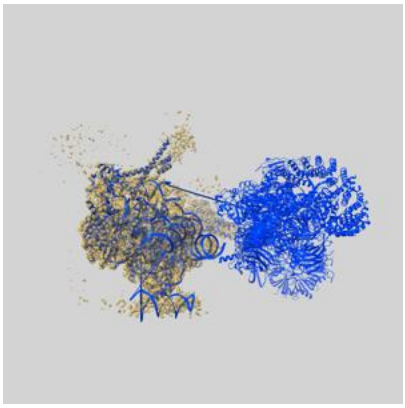
8 Fourier-Shell correlation (i)

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

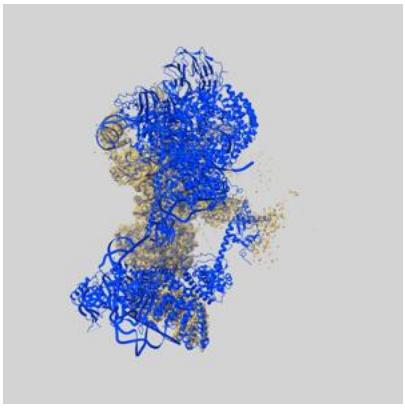
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4364 and PDB model 6G90. Per-residue inclusion information can be found in section 3 on page 11.

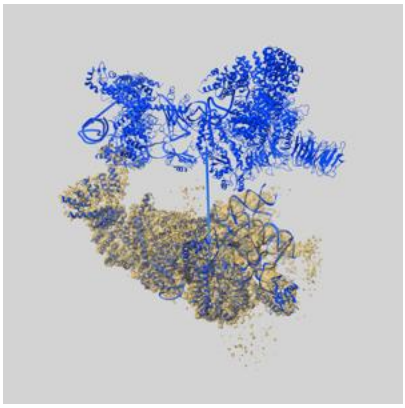
9.1 Map-model overlay



X



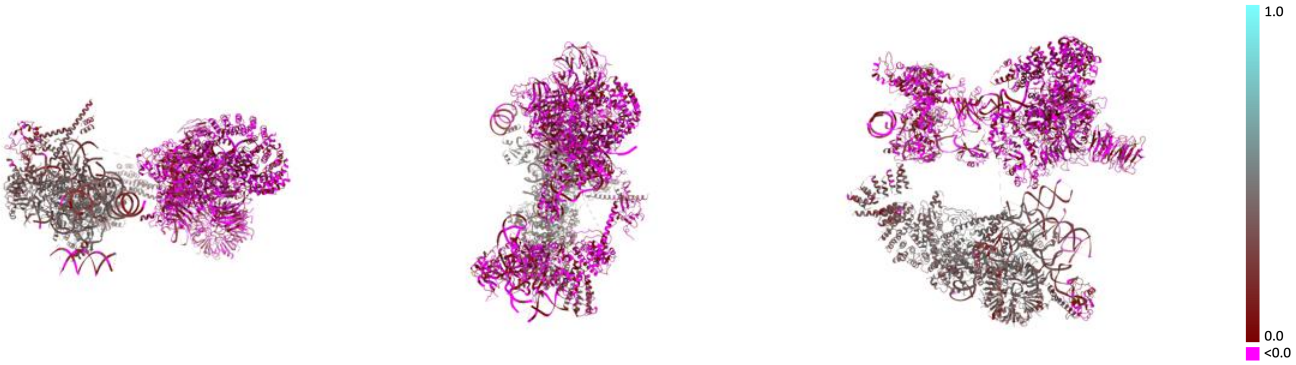
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0369 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.

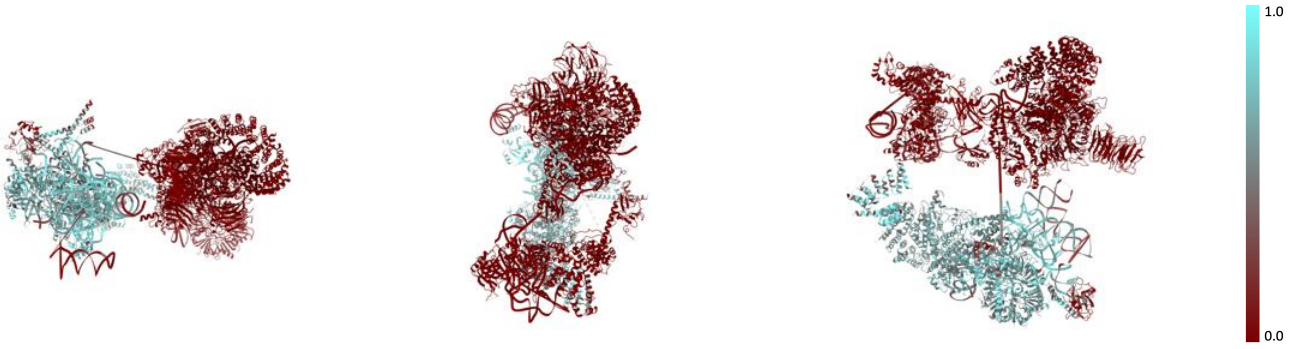
9.2 Q-score mapped to coordinate model (i)



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.

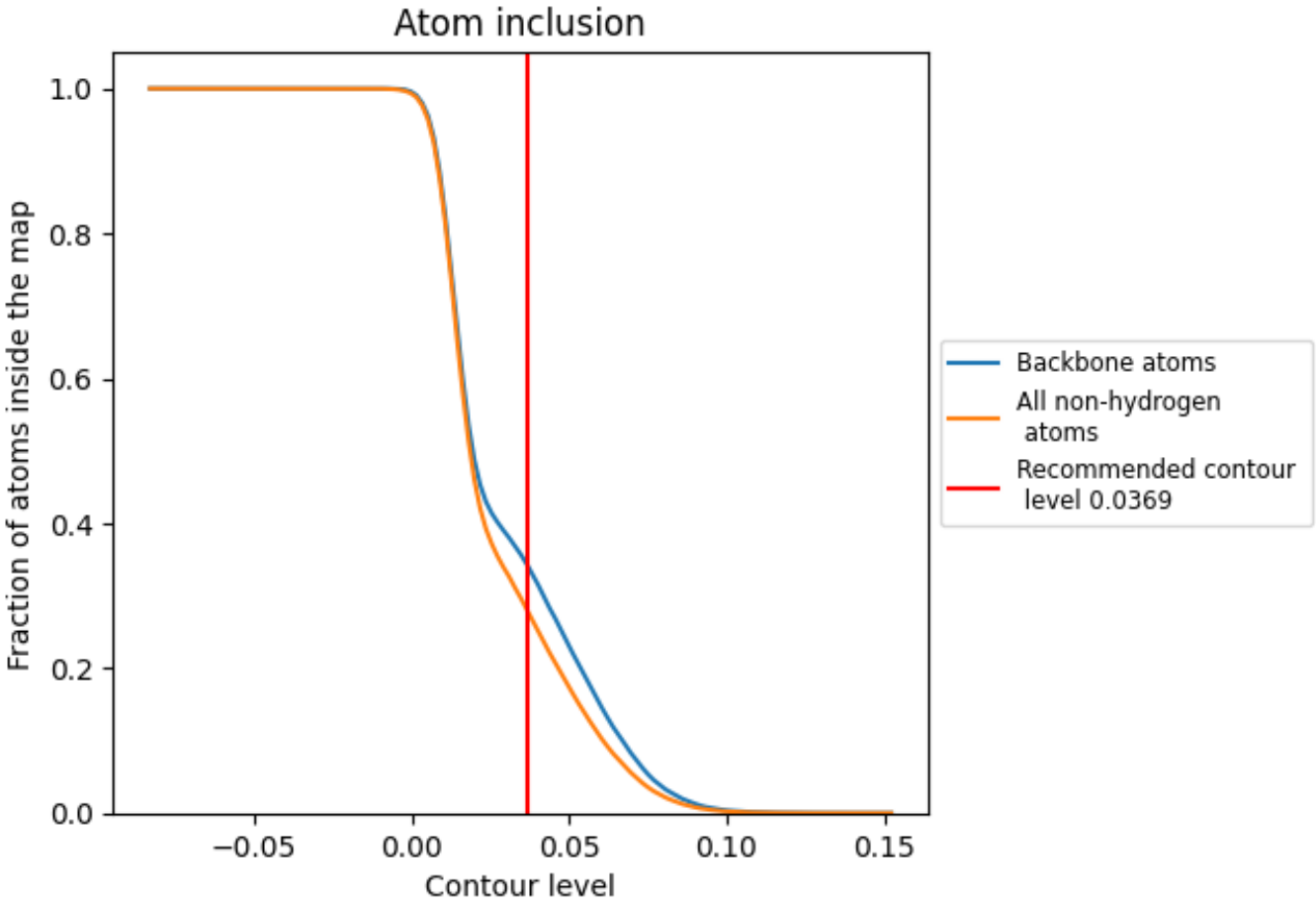
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0369).

9.4 Atom inclusion (i)



At the recommended contour level, 34% of all backbone atoms, 28% 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 (0.0369) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.2785	0.1520
1	0.6777	0.2970
2	0.0000	0.0010
A	0.7988	0.3950
B	0.3392	0.1890
C	0.6654	0.4050
D	0.6578	0.3440
E	0.6803	0.3970
F	0.6371	0.3920
G	0.6574	0.3800
H	0.5708	0.3040
I	0.2193	0.0990
J	0.7044	0.4150
O	0.0000	-0.0020
P	0.0000	0.0010
Q	0.0000	-0.0020
R	0.0000	0.0120
S	0.0000	0.0090
T	0.0000	0.0070
U	0.0000	0.0040
V	0.0000	-0.0060
W	0.0311	0.0250
X	0.6118	0.3000
Y	0.0208	0.0230
Z	0.0000	0.0080
b	0.6263	0.4070
d	0.6766	0.4380
e	0.6248	0.3770
f	0.6289	0.3320
g	0.6442	0.4250
h	0.6395	0.3970
i	0.6244	0.3460
s	0.0000	-0.0080
t	0.0000	-0.0400
u	0.0000	0.0300

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Chain	Atom inclusion	Q-score
v	0.0000	0.0160
w	0.0000	-0.0150
x	0.0000	0.0370
y	0.0000	0.0090