wwPDB EM Validation Summary Report

Mar 19, 2024 – 05:50 PM JST

PDB ID	:	6AH0
EMDB ID	:	EMD-9621
Title	:	The Cryo-EM Structure of the Precusor of Human Pre-catalytic Spliceosome (pre-B complex)
Authors	:	Zhan, X.; Yan, C.; Zhang, X.; Shi, Y.
Deposited on	:	2018-08-15
Resolution	:	5.70 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:

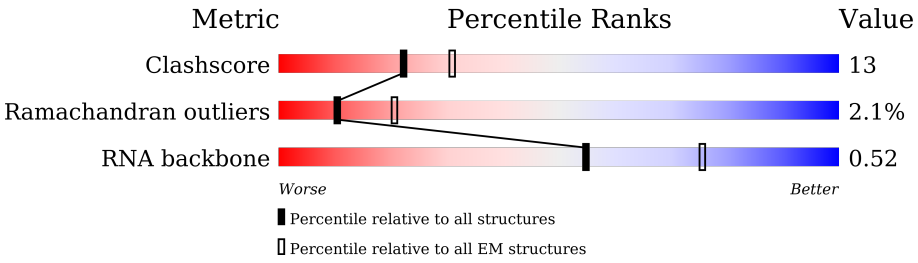
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 5.70 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
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	B	117	38% 44% 16%
2	D	2136	86% 12%
3	E	357	18% 81% 16%
4	P	118	61% 37%
4	a	118	66% 34%
4	k	118	72% 71% 28%
5	Q	86	6% 81% 17%
5	b	86	10% 85% 15%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	m	86	86% 86% 14%
6	R	92	7% 85% 15%
6	c	92	5% 85% 15%
6	l	92	86% 86% 14%
7	S	76	7% 93%
7	d	76	9% 91% 9%
7	n	76	89% 89% 11%
8	T	126	5% 56% 44%
8	e	126	62% 38%
8	h	126	63% 63% 37%
9	U	231	26% 72%
9	f	231	28% 72%
9	i	231	32% 32% 68%
10	V	119	64% 5% 31%
10	g	119	5% 78% 22%
10	j	119	69% 69% 31%
11	F	107	12% 39% 21% 36%
12	q	95	95% 91% 5%
13	r	102	74% 72% 26%
14	s	139	53% 53% 47%
15	t	91	82% 79% 18%
16	x	80	88% 86% 12%
17	y	103	63% 63% 37%
18	z	96	64% 63% 36%
19	G	274	15% 5% 8% 85%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
20	H	188	54% 20% 21% 15% 42%
21	o	255	64% 63% 36%
22	p	225	42% 42% 58%
23	u	793	16% 15% 84%
24	v	464	21% 19% 79%
25	w	501	88% 87% 12%
26	1	1304	77% 56% 22% 21%
27	2	895	20% 19% 79%
28	3	1217	96% 87% 10%
29	4	424	18% 17% 82%
30	5	125	86% 75% 11% 14%
31	6	110	81% 72% 8% 19%
32	7	86	77% 59% 16% 23%
33	J	683	23% 76%
34	K	522	58% 7% 34%
35	N	941	53% 9% 38%
36	L	499	45% 55%
37	M	128	93% 5%
38	O	142	95%
39	W	565	5% 61% 17% 18%
40	I	144	38% 31% 13% 19%
41	X	820	50% 50%
42	A	2335	86% 9% 5%
43	C	972	77% 7% 16%

2 Entry composition (i)

There are 46 unique types of molecules in this entry. The entry contains 63369 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 U5snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	B	115	2419	1084	402	818	115	0	0

- Molecule 2 is a protein called U5 small nuclear ribonucleoprotein 200 kDa helicase.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	D	1874	7496	3748	1874	1874	0	0

- Molecule 3 is a protein called U5 small nuclear ribonucleoprotein 40 kDa protein.

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

- Molecule 4 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	a	78	318	162	78	78	0	0
4	k	85	340	170	85	85	0	0
4	P	74	300	152	74	74	0	0

- Molecule 5 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	b	73	300	154	73	73	0	0
5	m	74	296	148	74	74	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
5	Q	71	Total 292	C 150	N 71	O 71	0	0

- Molecule 6 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	c	78	Total 314	C 158	N 78	O 78	0	0
6	l	79	Total 316	C 158	N 79	O 79	0	0
6	R	78	Total 314	C 158	N 78	O 78	0	0

- Molecule 7 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	d	69	Total 282	C 144	N 69	O 69	0	0
7	n	68	Total 272	C 136	N 68	O 68	0	0
7	S	73	Total 298	C 152	N 73	O 73	0	0

- Molecule 8 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	e	78	Total 318	C 162	N 78	O 78	0	0
8	h	80	Total 320	C 160	N 80	O 80	0	0
8	T	71	Total 288	C 146	N 71	O 71	0	0

- Molecule 9 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	f	64	Total 260	C 132	N 64	O 64	0	0
9	i	73	Total 292	C 146	N 73	O 73	0	0
9	U	64	Total 256	C 128	N 64	O 64	0	0

- Molecule 10 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	g	93	Total 380	C 194	N 93	O 93	0	0
10	j	82	Total 328	C 164	N 82	O 82	0	0
10	V	82	Total 334	C 170	N 82	O 82	0	0

- Molecule 11 is a RNA chain called U6snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	F	69	Total 1470	C 656	N 259	O 486	P 69	0	0

- Molecule 12 is a protein called U6 snRNA-associated Sm-like protein LSm2.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	q	90	Total 360	C 180	N 90	O 90	0	0

- Molecule 13 is a protein called U6 snRNA-associated Sm-like protein LSm3.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	r	75	Total 300	C 150	N 75	O 75	0	0

- Molecule 14 is a protein called U6 snRNA-associated Sm-like protein LSm4.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	s	74	Total 296	C 148	N 74	O 74	0	0

- Molecule 15 is a protein called U6 snRNA-associated Sm-like protein LSm5.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	t	75	Total 300	C 150	N 75	O 75	0	0

- Molecule 16 is a protein called U6 snRNA-associated Sm-like protein LSm6.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	x	70	Total 280	C 140	N 70	O 70	0	0

- Molecule 17 is a protein called U6 snRNA-associated Sm-like protein LSm7.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	y	65	Total 260	C 130	N 65	O 65	0	0

- Molecule 18 is a protein called U6 snRNA-associated Sm-like protein LSm8.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	z	61	Total 244	C 122	N 61	O 61	0	0

- Molecule 19 is a RNA chain called pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	G	42	Total 862	C 387	N 122	O 311	P 42	0	0

- Molecule 20 is a RNA chain called U2snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	H	109	Total 2311	C 1032	N 396	O 774	P 109	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
21	o	162	Total 648	C 324	N 162	O 162	0	0

- Molecule 22 is a protein called U2 small nuclear ribonucleoprotein B".

Mol	Chain	Residues	Atoms				AltConf	Trace
22	p	94	Total 376	C 188	N 94	O 94	0	0

- Molecule 23 is a protein called Splicing factor 3A subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	u	124	Total 496	C 248	N 124	O 124	0	0

- Molecule 24 is a protein called Splicing factor 3A subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	v	99	Total 396	C 198	N 99	O 99	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
25	w	443	Total 1773	C 887	N 443	O 443	0	0

- Molecule 26 is a protein called Splicing factor 3B subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	1	1030	Total 4120	C 2060	N 1030	O 1030	0	0

- Molecule 27 is a protein called Splicing factor 3B subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	2	186	Total 744	C 372	N 186	O 186	0	0

- Molecule 28 is a protein called Splicing factor 3B subunit 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	3	1174	Total 4696	C 2348	N 1174	O 1174	0	0

- Molecule 29 is a protein called Splicing factor 3B subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	4	78	Total 312	C 156	N 78	O 78	0	0

- Molecule 30 is a protein called Splicing factor 3B subunit 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	5	108	Total 432	C 216	N 108	O 108	0	0

- Molecule 31 is a protein called PHD finger-like domain-containing protein 5A.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	6	89	Total 356	C 178	N 89	O 89	0	0

- Molecule 32 is a protein called Splicing factor 3B subunit 5.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	7	66	Total 264	C 132	N 66	O 66	0	0

- Molecule 33 is a protein called U4/U6 small nuclear ribonucleoprotein Prp3.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	J	167	Total 668	C 334	N 167	O 167	0	0

- Molecule 34 is a protein called U4/U6 small nuclear ribonucleoprotein Prp4.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	K	343	Total 1371	C 686	N 343	O 342	0	0

- Molecule 35 is a protein called Pre-mRNA-processing factor 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	N	579	Total 2316	C 1158	N 579	O 579	0	0

- Molecule 36 is a protein called U4/U6 small nuclear ribonucleoprotein Prp31.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	L	226	Total 904	C 452	N 226	O 226	0	0

- Molecule 37 is a protein called NHP2-like protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	M	125	Total	C	N	O	0	0
			500	250	125	125		

- Molecule 38 is a protein called Thioredoxin-like protein 4A.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	O	139	Total	C	N	O	0	0
			556	278	139	139		

- Molecule 39 is a protein called U4/U6.U5 tri-snRNP-associated protein 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	W	463	Total	C	N	O	0	0
			1852	926	463	463		

- Molecule 40 is a RNA chain called U4snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	I	117	Total	C	N	O	P	0	0
			2491	1112	439	823	117		

- Molecule 41 is a protein called Probable ATP-dependent RNA helicase DDX23.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	X	414	Total	C	N	O	0	0
			1661	833	414	414		

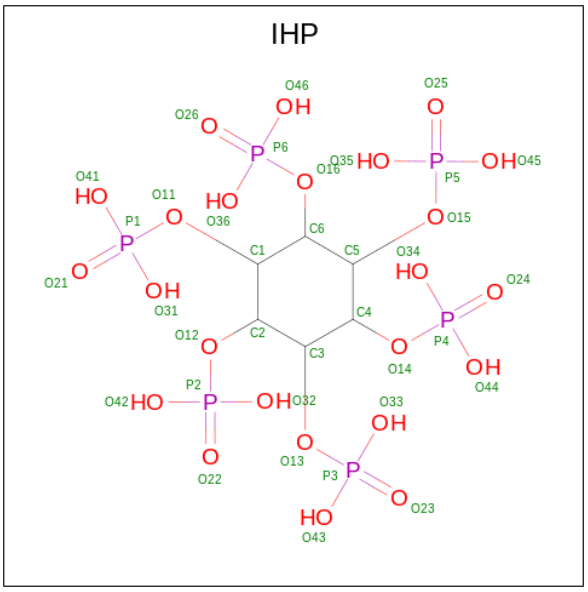
- Molecule 42 is a protein called Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	A	2221	Total	C	N	O	0	0
			8884	4442	2221	2221		

- Molecule 43 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

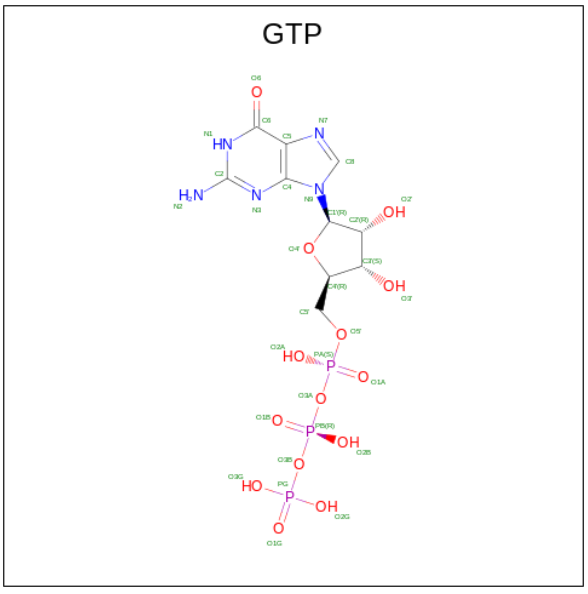
Mol	Chain	Residues	Atoms				AltConf	Trace
43	C	818	Total	C	N	O	0	0
			3272	1636	818	818		

- Molecule 44 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
44	A	1	36	6	24	6	0

- Molecule 45 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

- Molecule 46 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

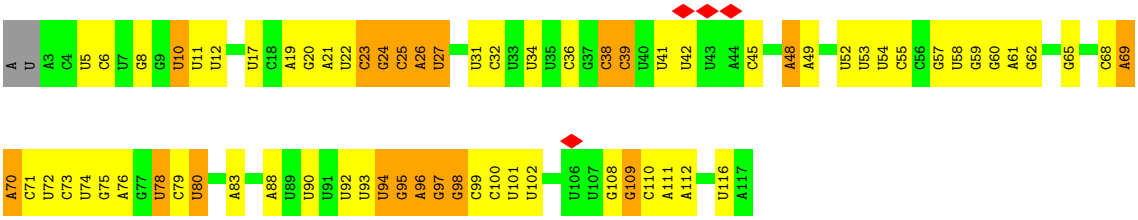
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
46	C	1	1	1	0

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.

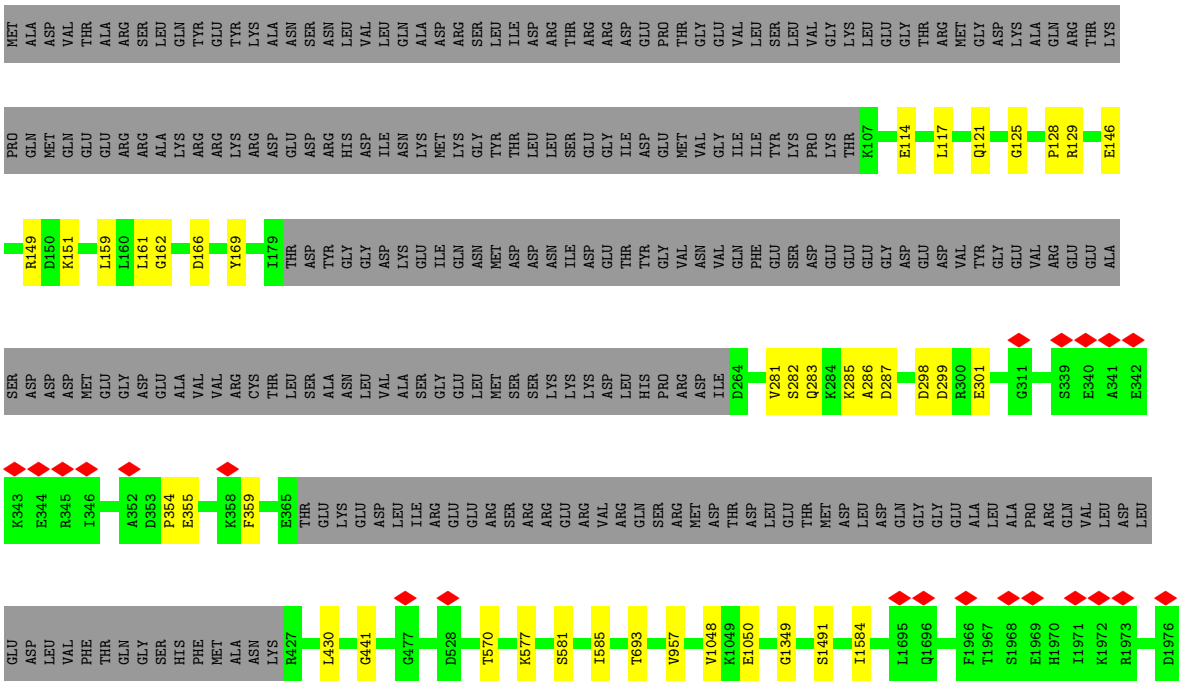
• Molecule 1: U5snRNA

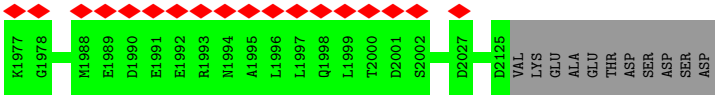
Chain B:



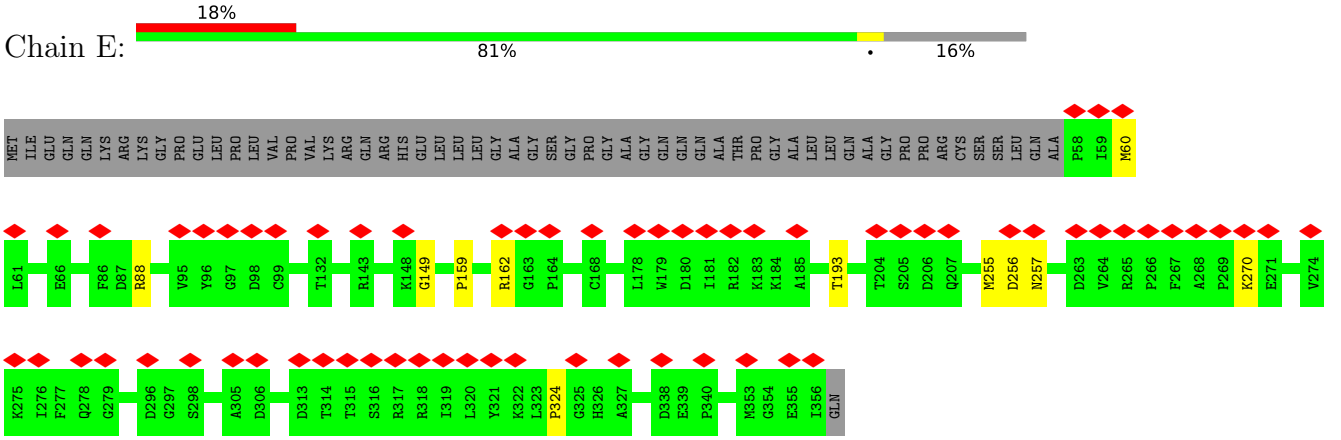
• Molecule 2: U5 small nuclear ribonucleoprotein 200 kDa helicase

Chain D:

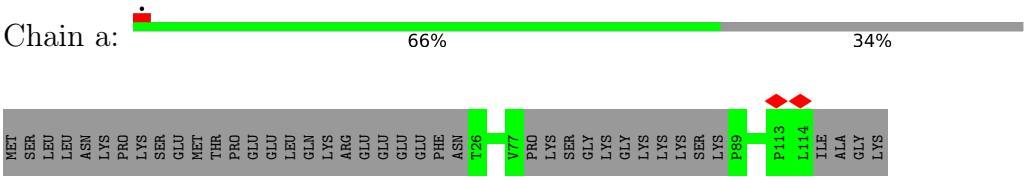




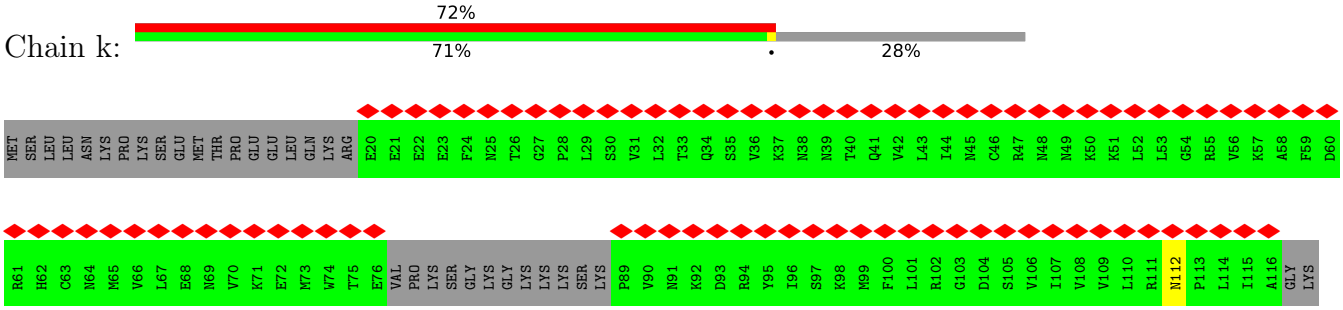
• Molecule 3: U5 small nuclear ribonucleoprotein 40 kDa protein



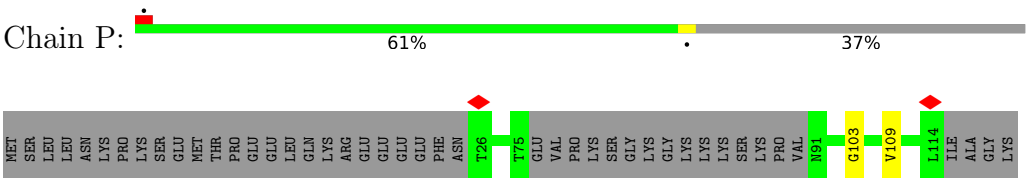
• Molecule 4: Small nuclear ribonucleoprotein Sm D2



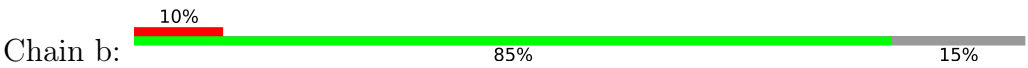
• Molecule 4: Small nuclear ribonucleoprotein Sm D2

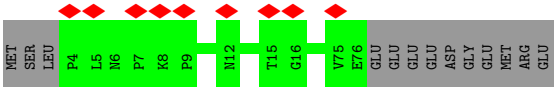


• Molecule 4: Small nuclear ribonucleoprotein Sm D2

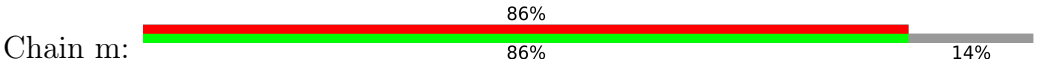


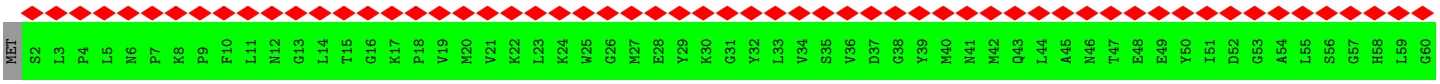
• Molecule 5: Small nuclear ribonucleoprotein F

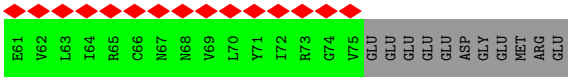




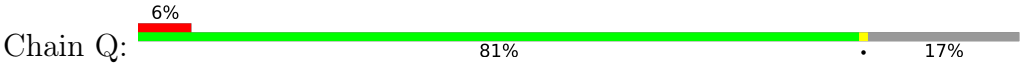
• Molecule 5: Small nuclear ribonucleoprotein F

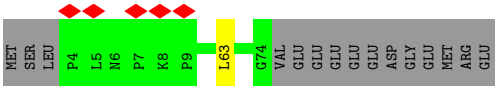




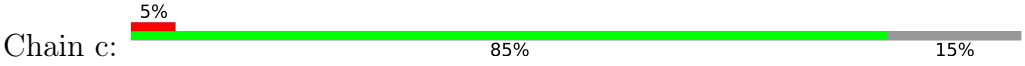


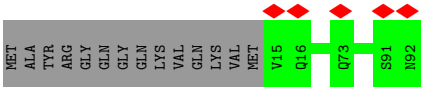
• Molecule 5: Small nuclear ribonucleoprotein F



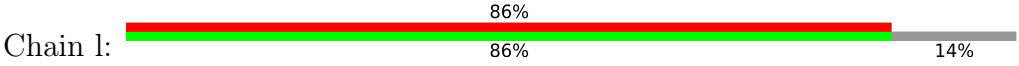


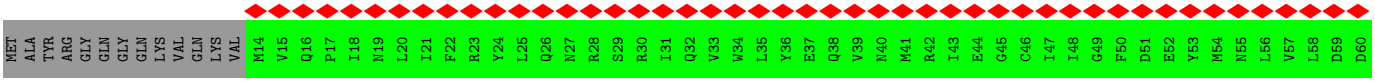
• Molecule 6: Small nuclear ribonucleoprotein E

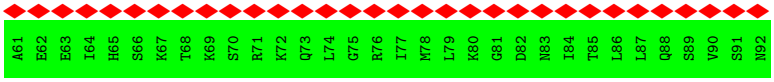




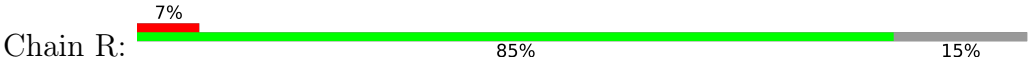
• Molecule 6: Small nuclear ribonucleoprotein E

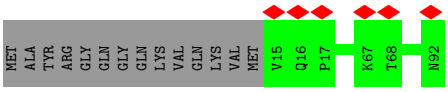






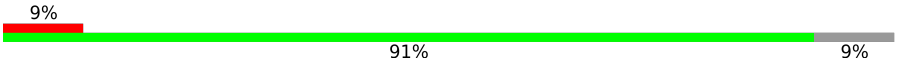
• Molecule 6: Small nuclear ribonucleoprotein E

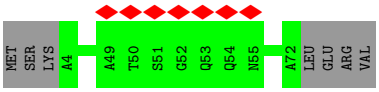




• Molecule 7: Small nuclear ribonucleoprotein G

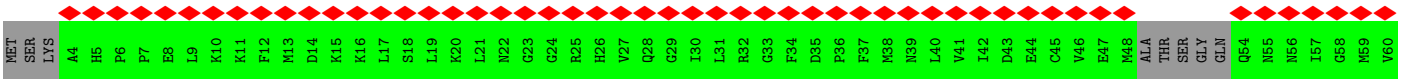
Chain d:

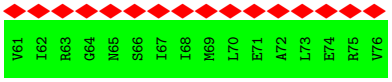




• Molecule 7: Small nuclear ribonucleoprotein G

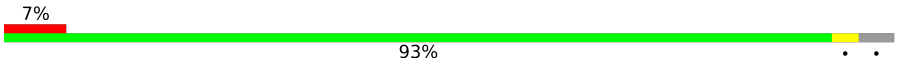
Chain n:

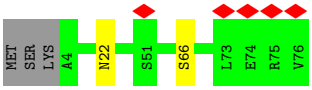




• Molecule 7: Small nuclear ribonucleoprotein G

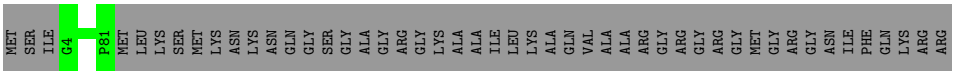
Chain S:





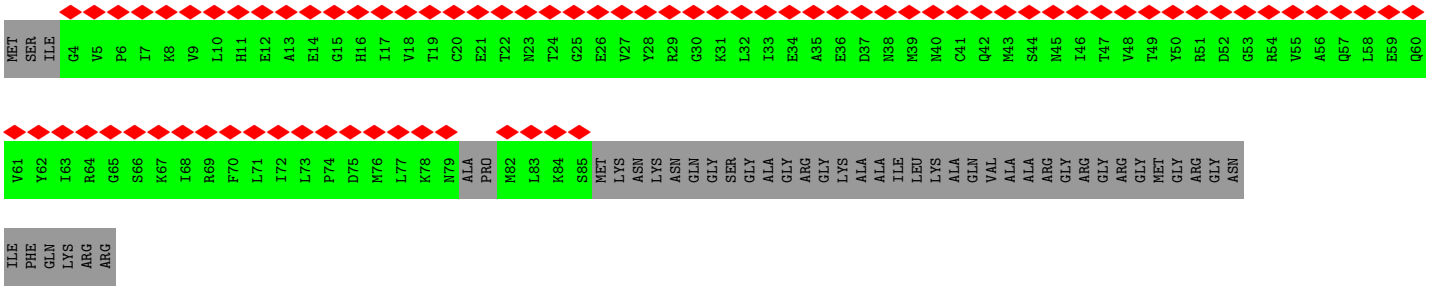
• Molecule 8: Small nuclear ribonucleoprotein Sm D3

Chain e:



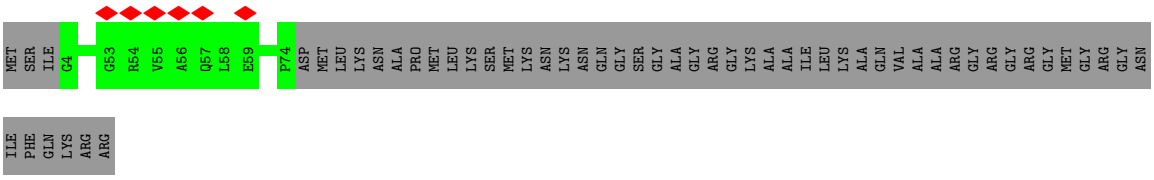
• Molecule 8: Small nuclear ribonucleoprotein Sm D3

Chain h:



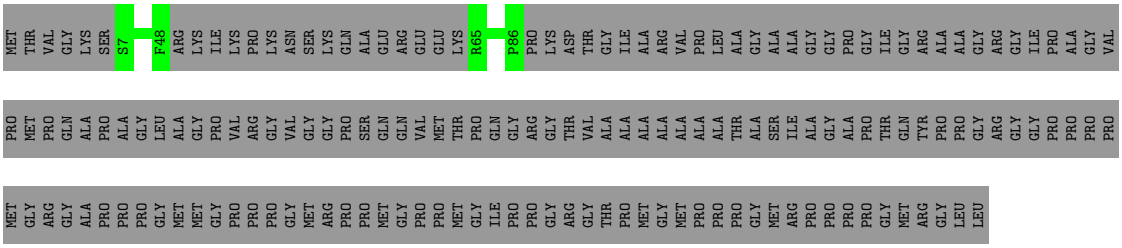
• Molecule 8: Small nuclear ribonucleoprotein Sm D3

Chain T:



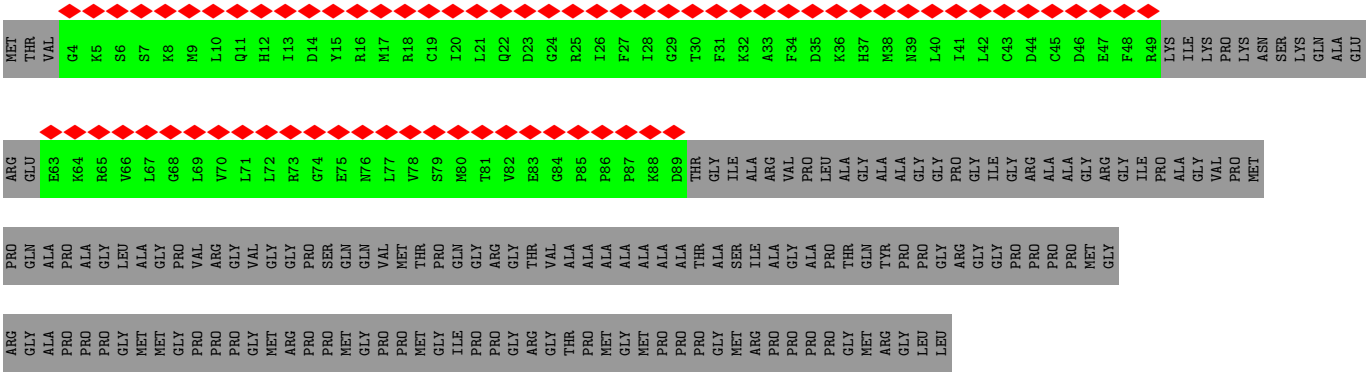
• Molecule 9: Small nuclear ribonucleoprotein-associated proteins B and B'

Chain f:



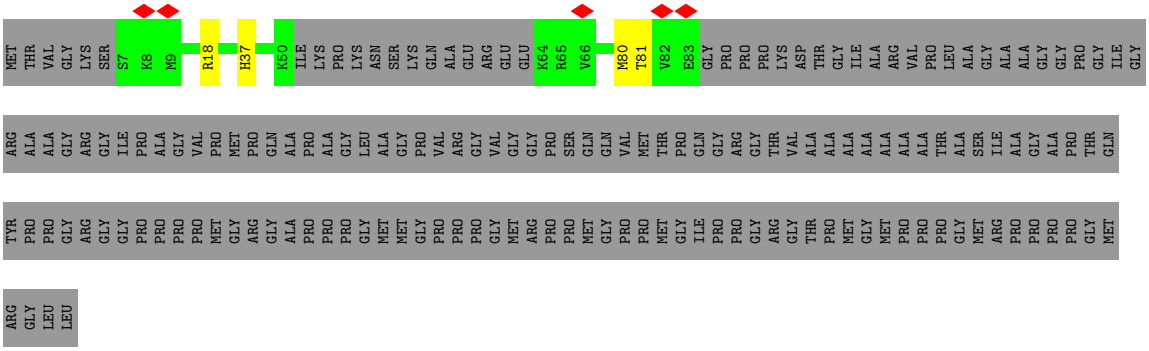
• Molecule 9: Small nuclear ribonucleoprotein-associated proteins B and B'

Chain i:



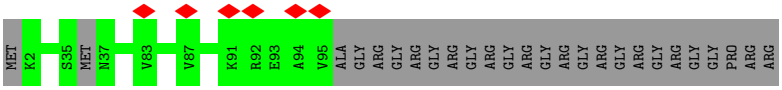
• Molecule 9: Small nuclear ribonucleoprotein-associated proteins B and B'

Chain U:



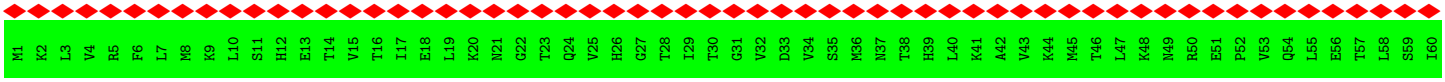
• Molecule 10: Small nuclear ribonucleoprotein Sm D1

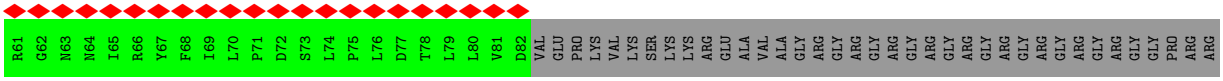
Chain g:



• Molecule 10: Small nuclear ribonucleoprotein Sm D1

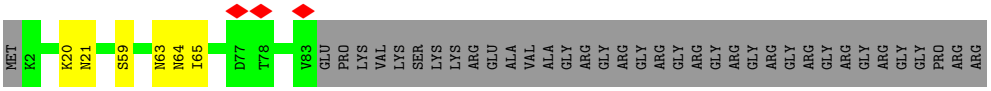
Chain j:





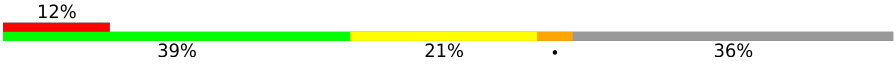
• Molecule 10: Small nuclear ribonucleoprotein Sm D1

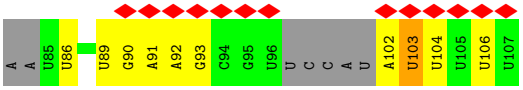
Chain V:



• Molecule 11: U6snRNA

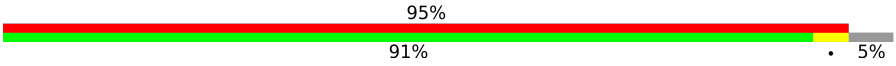
Chain F:

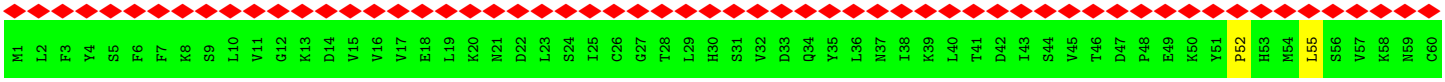


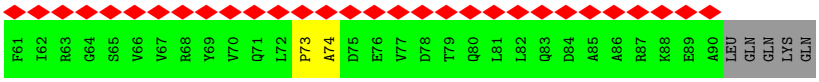


• Molecule 12: U6 snRNA-associated Sm-like protein LSm2

Chain q:





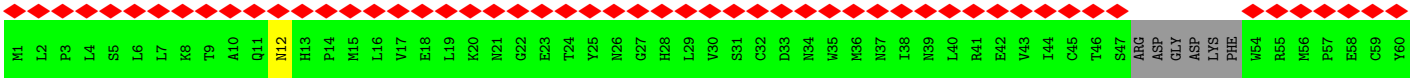


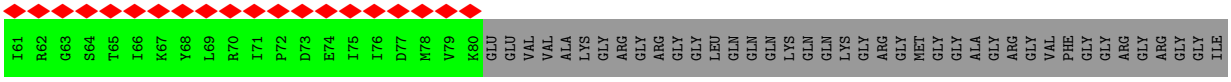
• Molecule 13: U6 snRNA-associated Sm-like protein LSm3

Chain r:

• Molecule 14: U6 snRNA-associated Sm-like protein LSm4

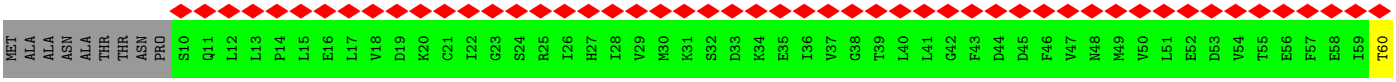
Chain s:

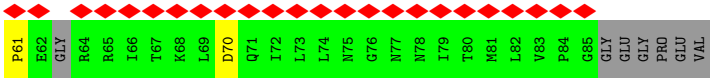




• Molecule 15: U6 snRNA-associated Sm-like protein LSm5

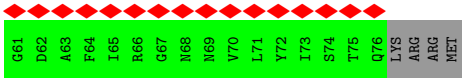
Chain t:





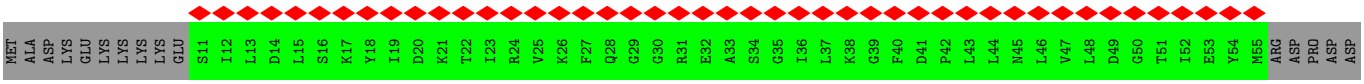
• Molecule 16: U6 snRNA-associated Sm-like protein LSm6

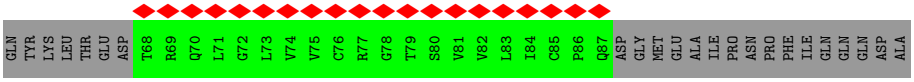
Chain x:



• Molecule 17: U6 snRNA-associated Sm-like protein LSm7

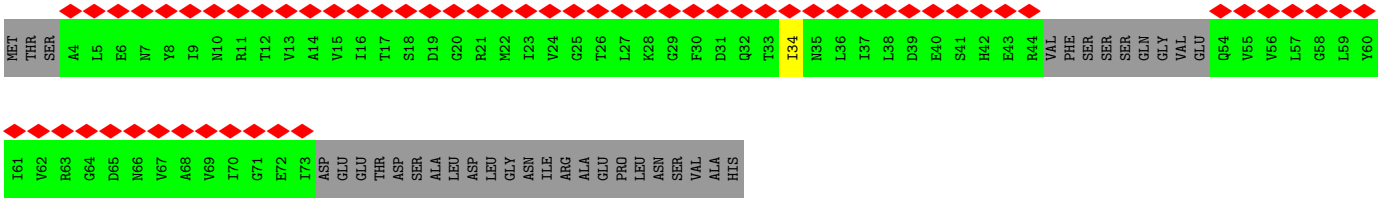
Chain y:





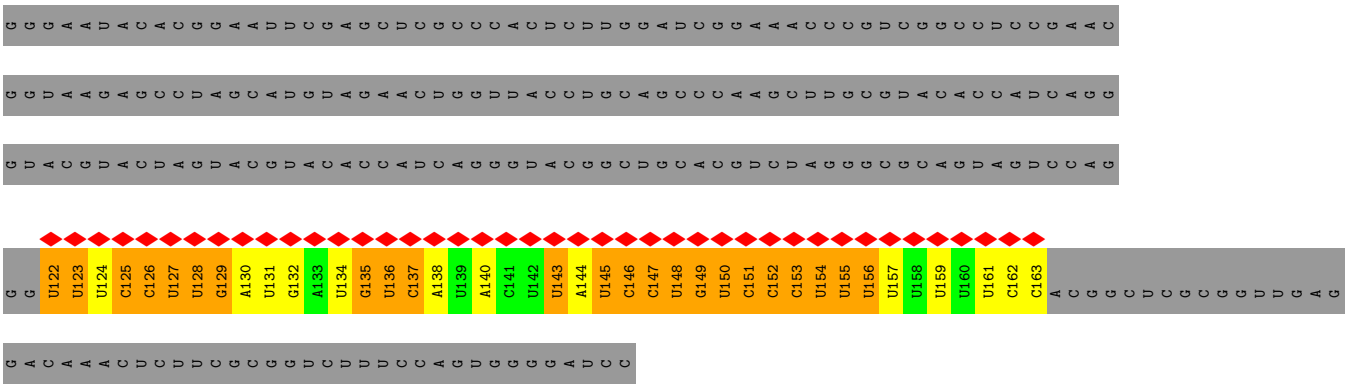
• Molecule 18: U6 snRNA-associated Sm-like protein LSm8

Chain z:



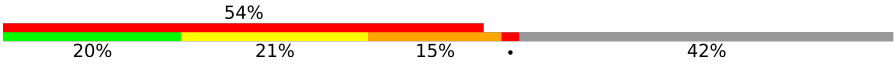
• Molecule 19: pre-mRNA

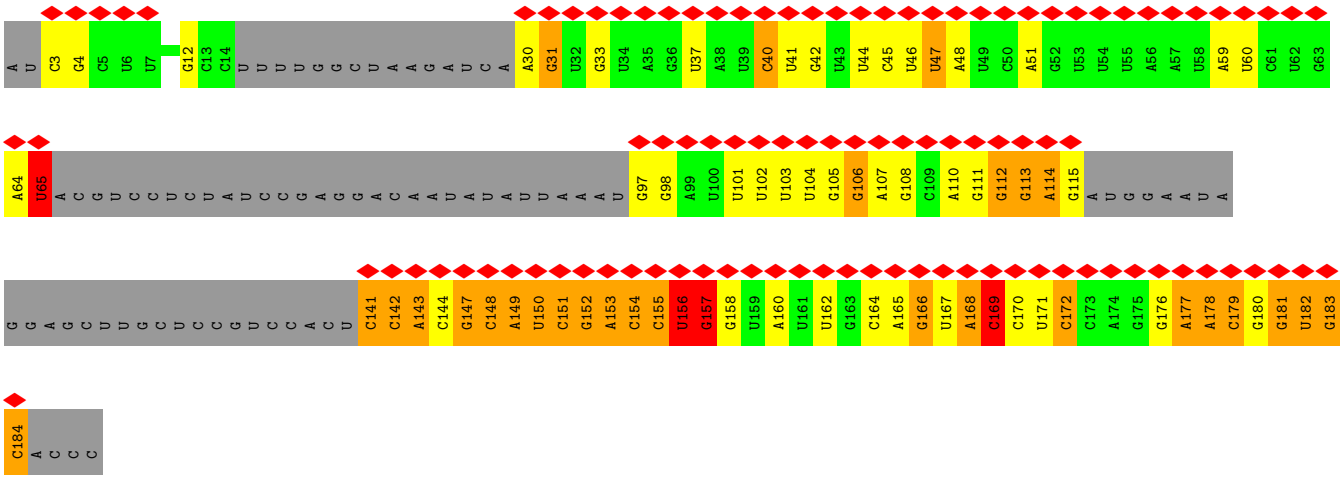
Chain G:



• Molecule 20: U2snRNA

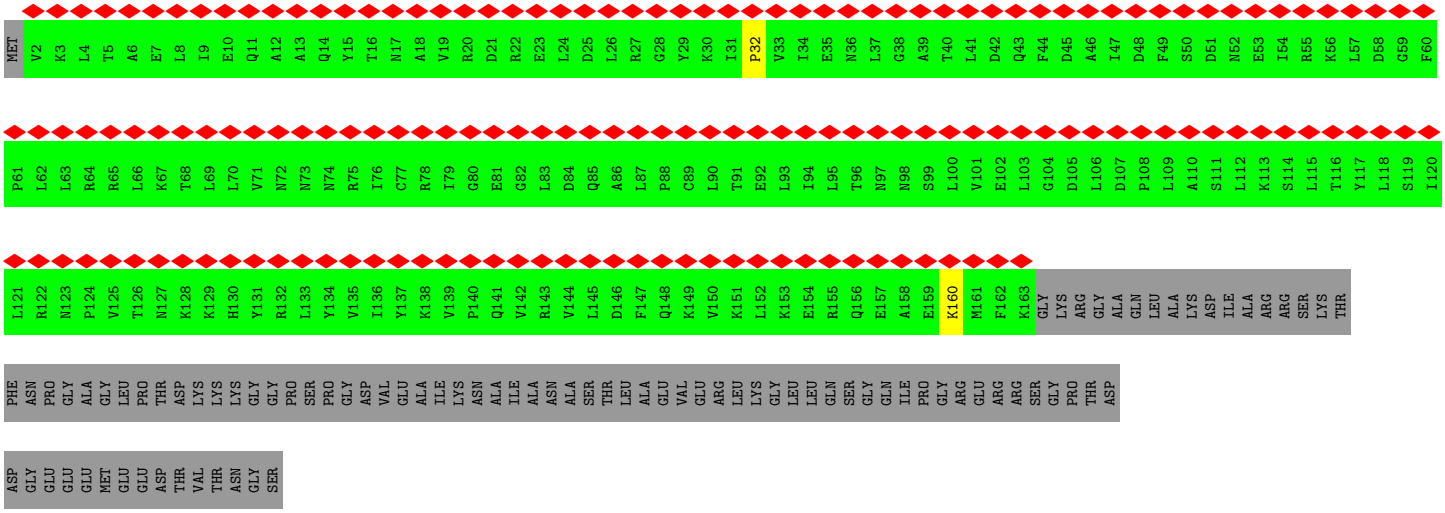
Chain H:





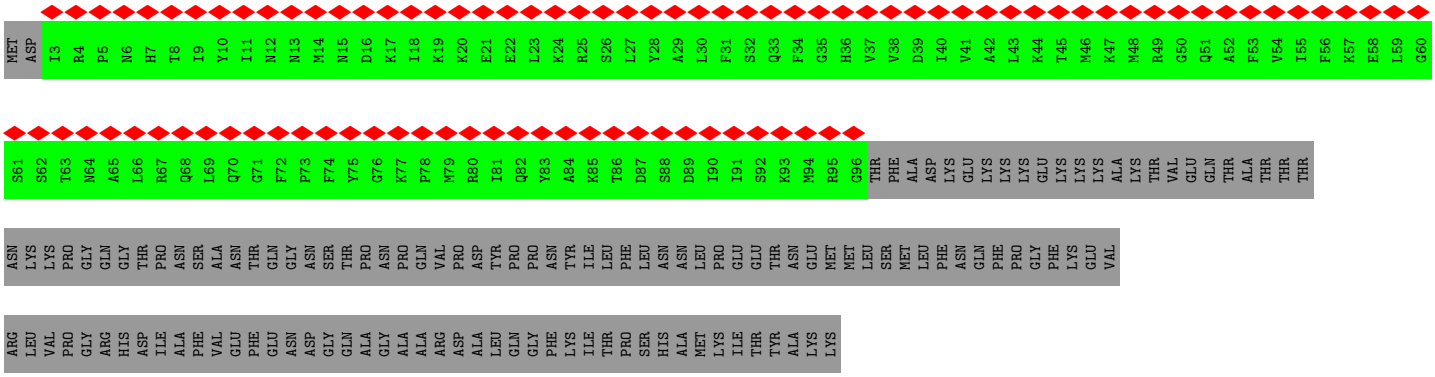
• Molecule 21: U2 small nuclear ribonucleoprotein A'

Chain o:



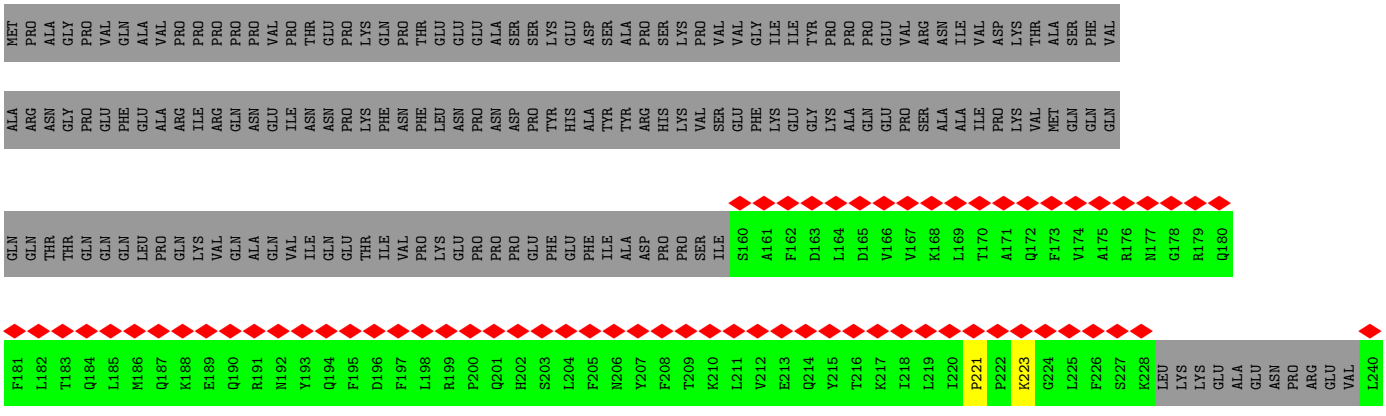
• Molecule 22: U2 small nuclear ribonucleoprotein B”

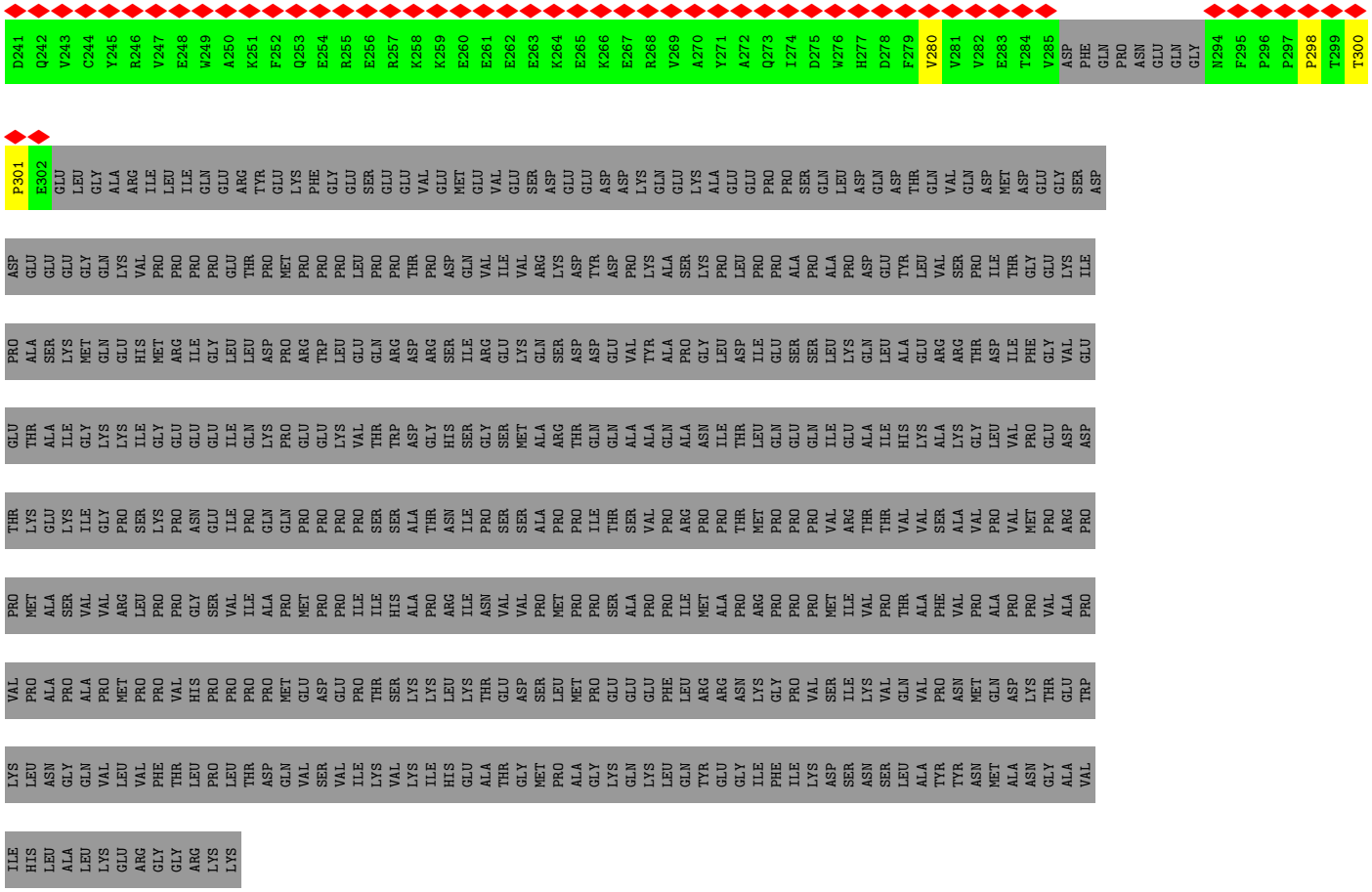
Chain p:



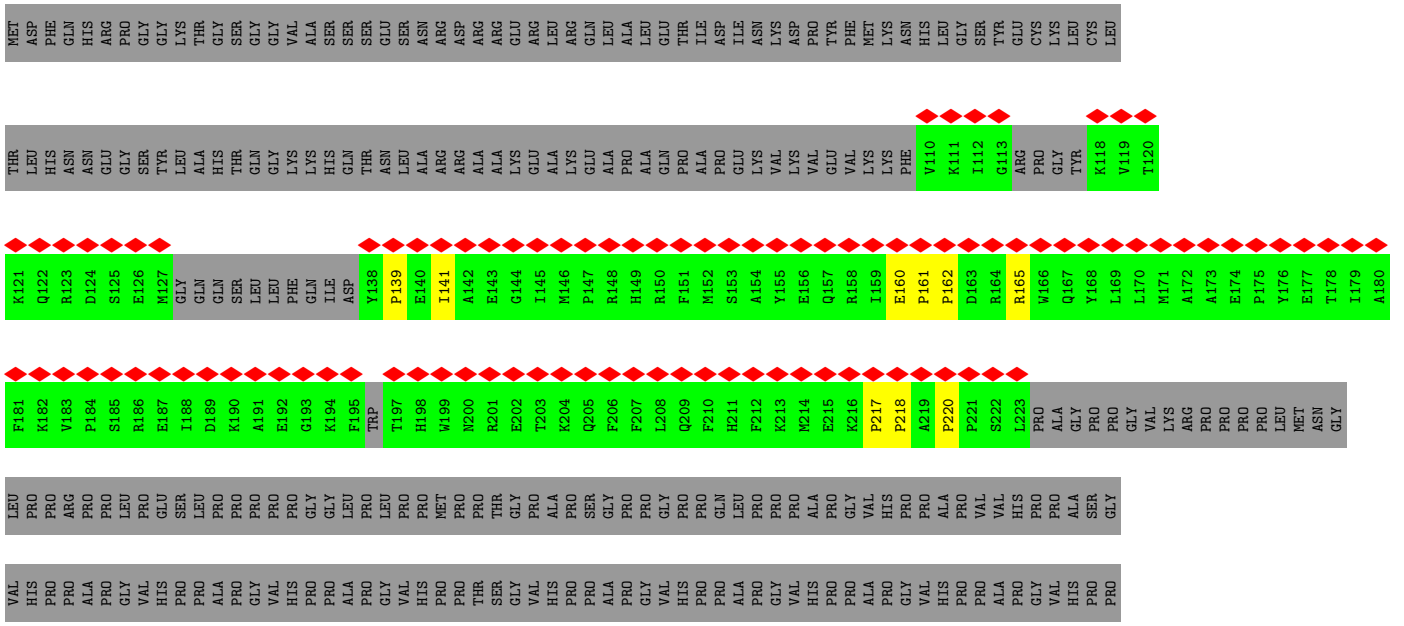
• Molecule 23: Splicing factor 3A subunit 1

Chain u:





• Molecule 24: Splicing factor 3A subunit 2



ALA PRO GLY VAL HIS PRO PRO PRO SER ALA GLY VAL HIS PRO GLN ALA PRO GLY VAL HIS PRO PRO PRO GLY VAL HIS PRO GLN ALA PRO GLY VAL HIS PRO PRO ALA PRO GLY MET HIS PRO GLN ALA PRO GLY VAL HIS PRO GLN PRO PRO GLY VAL HIS PRO SER ALA PRO GLY

VAL HIS PRO GLN PRO PRO GLY VAL HIS PRO SER ASN PRO GLY VAL HIS PRO PRO PRO THR PRO MET PRO PRO PRO MET LEU ARG PRO PRO LEU PRO SER GLU GLY GLY PRO GLY ASN ILE PRO PRO PRO PRO PRO THR ASN

• Molecule 25: Splicing factor 3A subunit 3

Chain w:

M1 E2 T3 I4 L5 E6 Q7 Q8 R9 R10 Y11 H12 E13 E14 K15 E16 R17 L18 M19 D20 V21 M22 A23 K24 E25 M26 L27 T28 K29 K30 S31 T32 L33 R34 D35 Q36 I37 N38 S39 D40 H41 R42 T43 R44 A45 M46 Q47 D48 R49 Y50 M51 E52 V53 S54 G55 N56 L57 R58 D59 L60

Y61 D62 D63 K64 D65 G66 L67 R68 K69 E70 E71 L72 N73 A74 I75 S76 G77 P78 N79 E80 F81 A82 E83 F84 Y85 N86 R87 L88 K89 Q90 I91 K92 E93 F94 H95 R96 K97 H98 PRO ASN GLU ILE CYS VAL PRO MET SER VAL GLU F110 E111 E112 L113 L114 K115 A116 R117 E118 N119 P120

S121 E122 E123 A124 Q125 N126 L127 V128 E129 F130 T131 D132 E133 E134 G135 Y136 G137 R138 Y139 L140 D141 L142 H143 ASP CYS TYR LEU LYS Y149 I150 N151 L152 K153 A154 S155 E156 K157 L158 D159 Y160 I161 T162 Y163 L164 S165 I166 F167 D168 Q169 L170 F171 D172 I173 P174 K175 E176 R177 K178 N179 A180

E181 Y182 K183 R184 Y185 L186 E187 M188 L189 L190 E191 Y192 L193 Q194 D195 Y196 T197 D198 R199 V200 K201 P202 L203 Q204 D205 Q206 N207 E208 L209 F210 GLY LYS ILE GLN ALA GLU PHE E218 K219 K220 W221 E222 N223 G224 T225 F226 P227 G228 W229 P230 K231 E232 T233 S234 S235 A236 L237 T238 H239 A240

G241 A242 H243 L244 D245 L246 S247 A248 F249 S250 S251 W252 E253 E254 L255 A256 S257 L258 G259 L260 D261 R262 L263 K264 S265 A266 L267 L268 A269 L270 G271 L272 K273 C274 G275 G276 T277 L278 E279 E280 R281 A282 Q283 R284 L285 F286 S287 T288 K289 G290 K291 S292 L293 E294 S295 L296 D297 T298 S299 L300

F301 A302 K303 N304 P305 K306 S307 K308 G309 T310 K311 R312 D313 T314 E315 R316 N317 K318 D319 I320 A321 F322 L323 E324 A325 Q326 I327 Y328 E329 Y330 V331 E332 I333 L334 G335 E336 Q337 R338 H339 L340 T341 H342 E343 N344 V345 Q346 R347 K348 Q349 A350 R351 T352 G353 E354 E355 R356 E357 E358 E359 E360

E361 E362 Q363 I364 S365 E366 S367 E368 S369 E370 D371 E372 E373 N374 GLU ILE ILE TYR ASN PRO LYS ASN LEU PRO LEU GLY TRP ASP GLY LYS PRO I392 P393 Y394 W395 L396 Y397 K398 L399 H400 G401 L402 N403 I404 N405 Y406 N407 C408 E409 I410 C411 G412 N413 Y414 T415 Y416 R417 G418 P419 K420

A421 F422 Q423 R424 H425 F426 A427 E428 W429 R430 H431 A432 H433 G434 M435 R436 C437 L438 G439 I440 P441 N442 T443 A444 H445 F446 A447 N448 V449 T450 Q451 I452 E453 D454 A455 V456 S457 L458 W459 A460 K461 L462 K463 LEU GLN LYS ALA SER GLU ARG TRP GLN PRO ASP THR GLU GLU GLU TYR E480

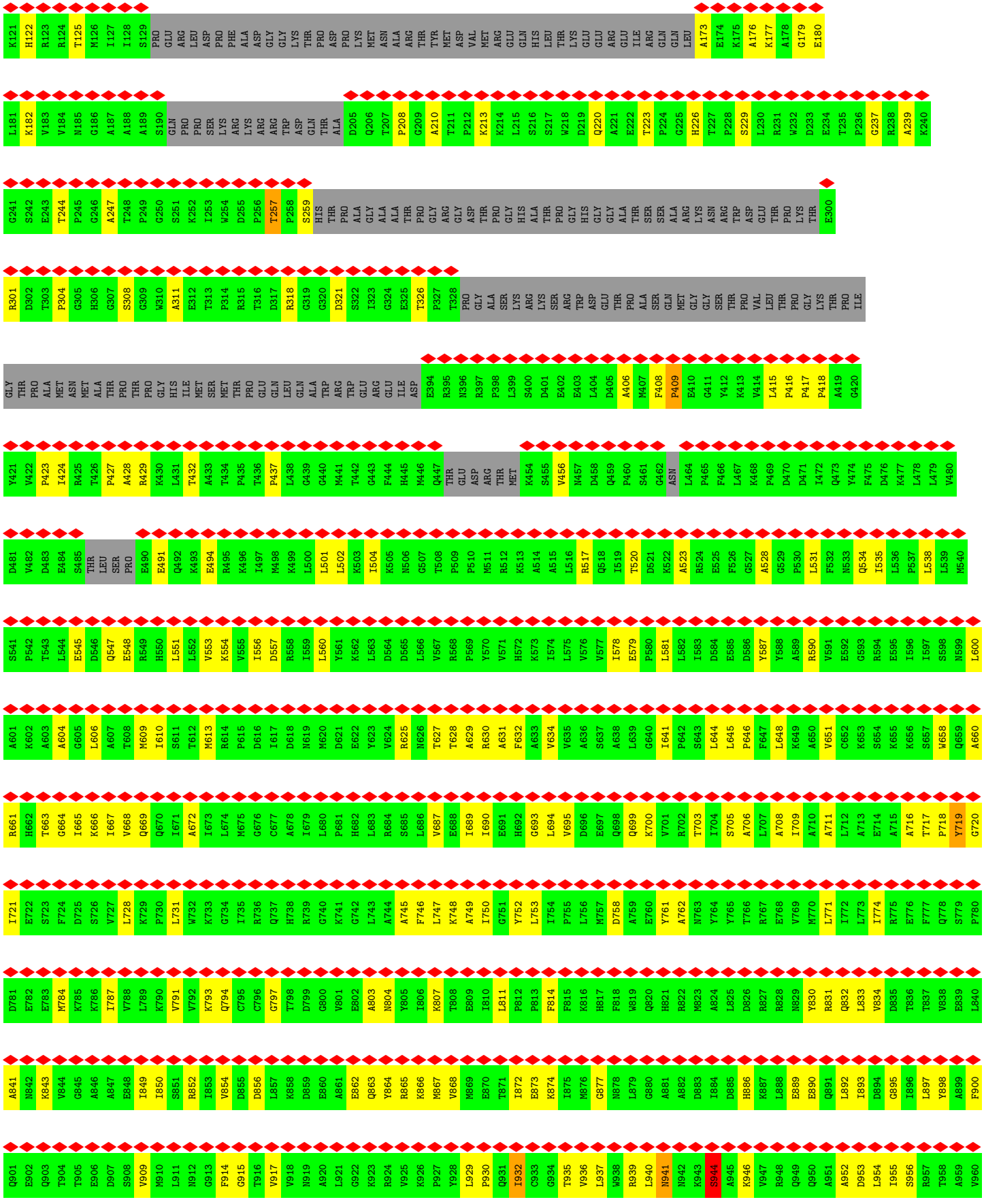
D481 S482 S483 G484 N485 V486 V487 N488 K489 K490 T491 Y492 E493 D494 L495 K496 R497 Q498 G499 LEU LEU

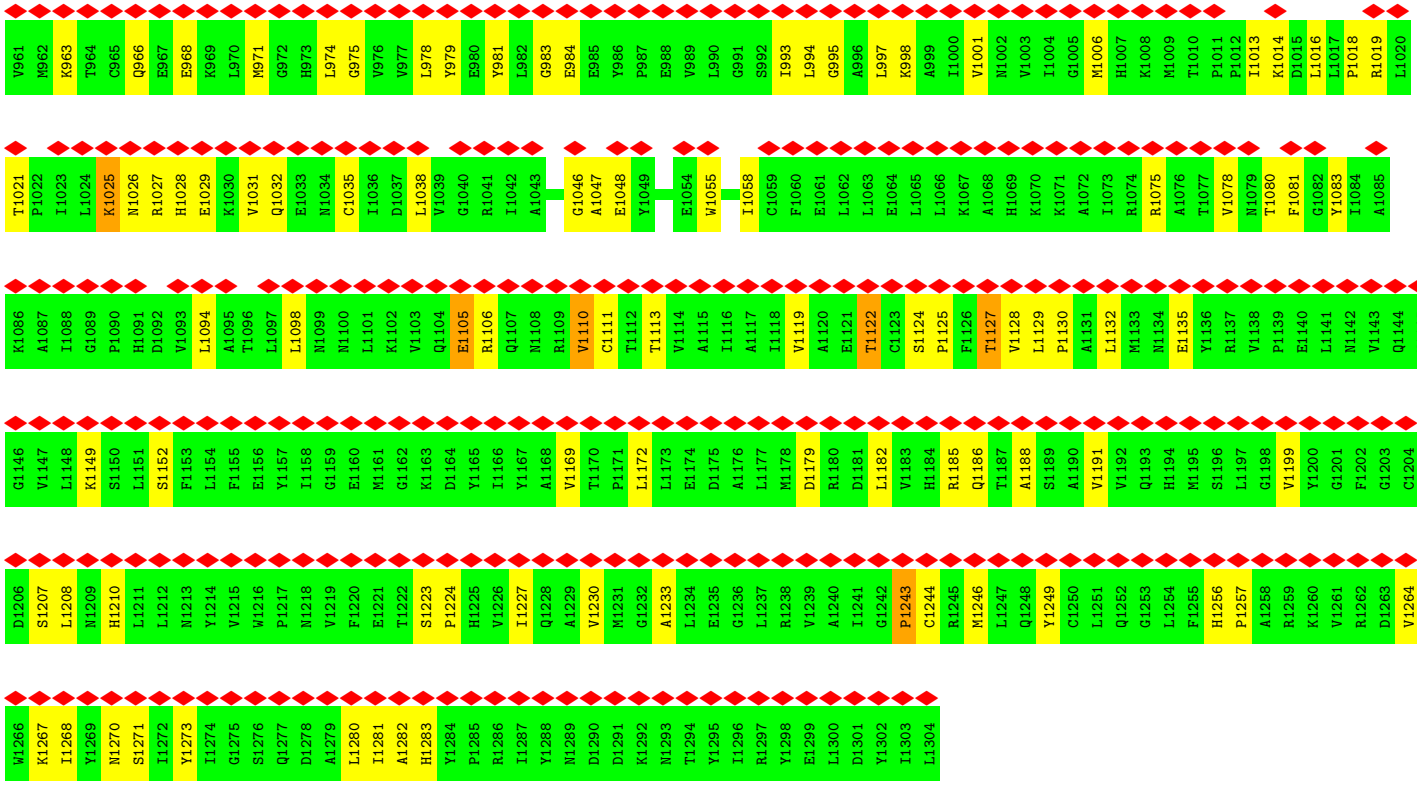
• Molecule 26: Splicing factor 3B subunit 1

Chain 1:

MET ALA LYS ILE ALA LYS THR HIS GLU ASP ILE GLU ALA GLN ILE ARG GLU ILE GLN GLY LYS LYS ALA ALA LEU ASP GLU ALA GLN GLY VAL GLY LEU ASP SER THR GLY TYR TYR ASP GLN GLU ILE TYR GLY GLY SER ASP SER ARG PHE ALA GLY TYR VAL THR SER ILE ALA ALA

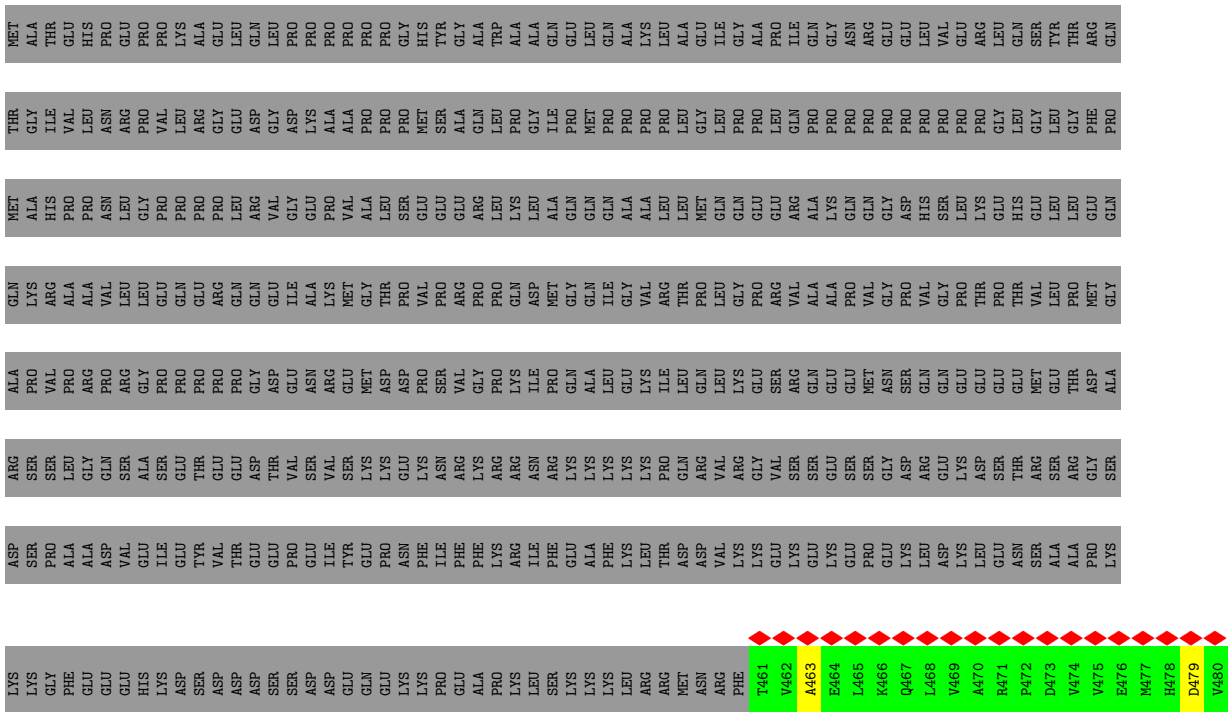
THR GLU LEU GLU ASP ASP ASP ASP TYR SER SER SER THR SER LEU LEU GLY GLN LYS LYS PRO GLY TYR HIS ALA PRO VAL ALA LEU LEU ASN ASP ILE PRO GLN SER THR GLU GLN TYR D102 P103 F104 A105 E106 H107 R108 P109 P110 K111 I112 A113 D114 R115 E116 D117 E118 Y119 K120

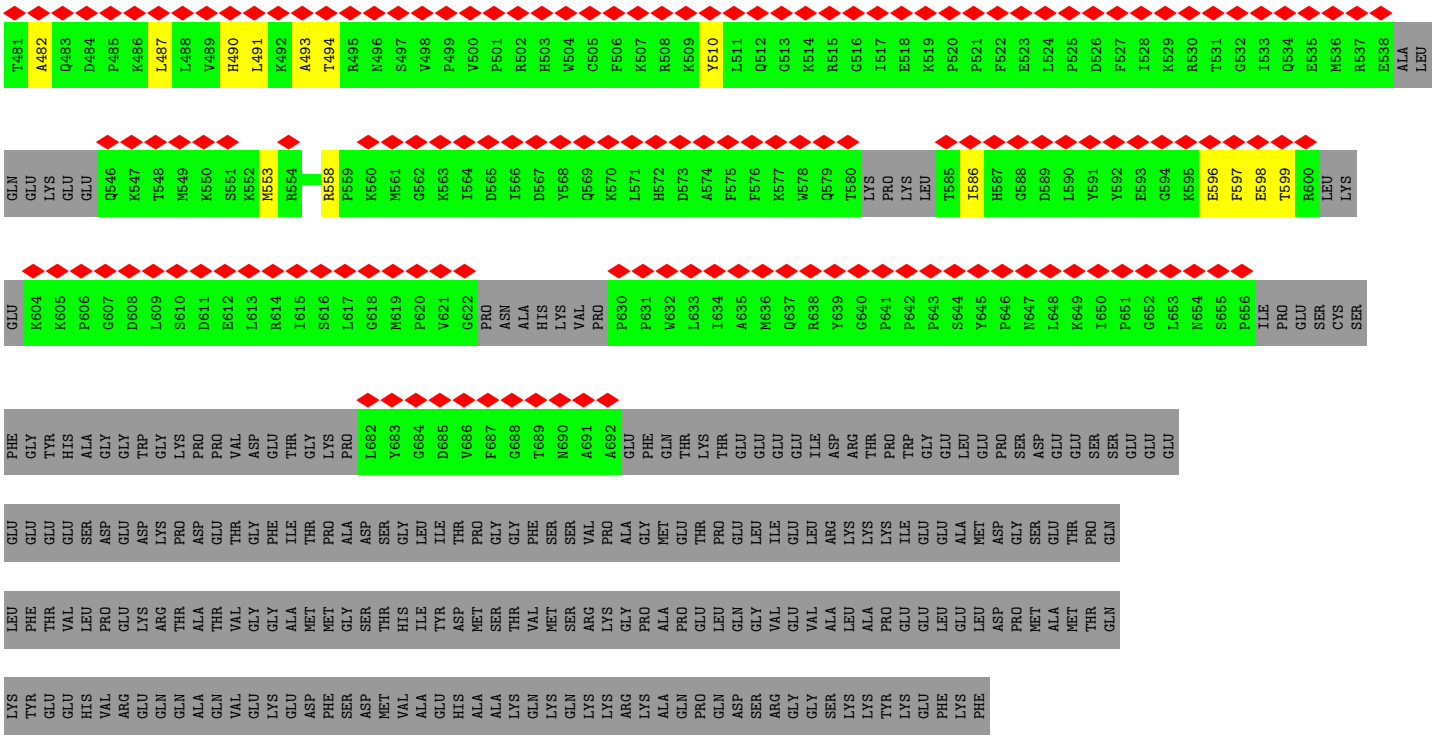

K121 H122 R123 R124 T125 M126 I127 I128 S129 PRO GLU ARG LEU ASP PRO PHE ALA ASP GLY GLY LYS THR PRO ASP PRO LYS MET ASN ALA ARG THR TYR MET ASP VAL MET ARG GLU GLN HIS LEU THR LYS GLU GLU ARG GLU ILE ARG GLN GLN LEU A173 E174 K175 A176 K177 A178 G179 E180
L181 K182 V183 V184 N185 G186 A187 A188 A189 S190 GLN PRO PRO SER LYS ARG LYS ARG ARG TRP ASP GLN THR ALA D205 Q206 T207 P208 G209 A210 T211 P212 K213 K214 L215 S216 S217 W218 D219 Q220 A221 E222 T223 P224 G225 H226 T227 P228 S229 L230 R231 W232 D233 E234 T235 P236 G237 R238 A239 K240
G241 S242 E243 T244 P245 G246 A247 T248 P249 G250 S251 K252 I253 W254 D255 P256 T257 P258 S259 HIS THR PRO ALA GLY ALA ALA THR PRO GLY ARG GLY ASP THR PRO GLY HIS ALA THR PRO GLY HIS GLY GLY ALA THR SER SER ALA ARG LYS ASN ARG TRP ASP GLU THR PRO LYS THR E300
R301 D302 T303 P304 G305 H306 G307 S308 G309 W310 A311 E312 T313 P314 R315 T316 D317 R318 G319 G320 D321 S322 I323 G324 E325 T326 P327 T328 PRO GLY ALA SER LYS ARG LYS SER ARG TRP ASP GLU THR PRO ALA SER GLN MET GLY GLY SER THR PRO VAL LEU THR PRO GLY LYS THR PRO ILE
GLY THR PRO ALA MET ASN MET ALA THR PRO THR PRO GLY HIS ILE MET SER MET THR PRO GLU GLN LEU GLN ALA TRP ARG TRP GLU ARG GLU ILE ASP E394 R395 N396 R397 P398 L399 S400 D401 E402 E403 L404 D405 A406 M407 F408 P409 E410 G411 Y412 K413 V414 L415 P416 P417 P418 A419 G420
Y421 V422 P423 I424 R425 T426 P427 A428 R429 K430 L431 T432 A433 T434 P435 T436 P437 L438 G439 G440 M441 T442 G443 F444 H445 M446 Q447 THR GLU ASP ARG THR MET K454 S455 V456 N457 D458 Q459 P460 S461 G462 ASN L464 P465 F466 L467 K468 P469 D470 D471 I472 Q473 Y474 F475 D476 K477 L478 L479 V480
D481 V482 D483 E484 S485 THR LEU SER PRO E490 E491 Q492 K493 E494 R495 K496 I497 M498 K499 L500 L501 L502 K503 I504 K505 N506 G507 T508 P509 P510 M511 R512 K513 A514 A515 L516 R517 Q518 I519 T520 D521 K522 A523 R524 E525 F526 G527 A528 G529 P530 L531 F532 N533 Q534 I535 L536 P537 L538 L539 N540
S541 P542 T543 L544 E545 D546 Q547 E548 R549 H550 L551 L552 V553 K554 V555 I556 D557 R558 I559 L560 Y561 K562 L563 D564 D565 L566 V567 R568 P569 Y570 V571 H572 K573 I574 L575 V576 V577 I578 E579 P580 L581 L582 I583 D584 E585 D586 Y587 Y588 A589 R590 V591 E592 G593 R594 E595 I596 L597 S598 N599 L600
A601 K602 A603 A604 G605 L606 A607 T608 M609 I610 S611 T612 M613 R614 P615 D616 I617 D618 N619 M620 D621 E622 Y623 V624 R625 N626 T627 T628 A629 R630 A631 F632 A633 V634 V635 A636 S637 A638 L639 G640 I641 P642 S643 L644 L645 P646 F647 L648 K649 A650 V651 C652 K653 S654 K655 K656 S657 W658 Q659 A660
R661 H662 T663 G664 I665 K666 I667 V668 Q669 Q670 I671 A672 I673 L674 M675 G676 C677 A678 I679 L680 P681 H682 L683 R684 S685 L686 V687 E688 I689 I690 E691 H692 G693 L694 V695 D696 E697 Q698 Q699 K700 V701 R702 T703 I704 S705 A706 L707 A708 I709 A710 A711 L712 A713 E714 A715 A716 T717 P718 Y719 G720
I721 E722 S723 F724 D725 S726 V727 L728 K729 P730 L731 W732 K733 G734 I735 R736 Q737 H738 R739 G740 K741 G742 L743 A744 A745 F746 L747 K748 A749 I750 G751 Y752 L753 I754 P755 L756 M757 D758 A759 E760 Y761 A762 N763 Y764 Y765 T766 R767 E768 V769 M770 L771 I772 L773 I774 R775 E776 F777 Q778 S779 P780
D781 E782 E783 M784 K785 K786 I787 V788 L789 K790 V791 V792 K793 Q794 C795 C796 G797 T798 D799 G800 V801 E802 A803 N804 Y805 I806 K807 T808 E809 I810 L811 P812 P813 F814 F815 K816 H817 F818 W819 Q820 H821 R822 M823 A824 L825 D826 R827 R828 N829 Y830 R831 Q832 L833 V834 D835 T836 T837 V838 E839 L840
A841 N842 K843 V844 G845 A846 A847 E848 I849 I850 S851 R852 I853 V854 D855 D856 L857 K858 D859 E860 A861 E862 Q863 Y864 R865 K866 M867 V868 M869 E870 T871 I872 E873 K874 I875 M876 G877 N878 L879 G880 A881 A882 D883 I884 D885 H886 K887 L888 E889 E890 Q891 L892 I893 D894 G895 I896 L897 Y898 A899 F900
Q901 E902 Q903 T904 T905 E906 D907 S908 V909 M910 L911 N912 G913 F914 G915 T916 V917 V918 N919 A920 L921 G922 K923 R924 V925 K926 P927 Y928 L929 P930 Q931 I932 C933 G934 T935 V936 L937 W938 R939 L940 N941 N942 K943 S944 A945 K946 V947 R948 Q949 Q950 A951 A952 D953 L954 I955 S956 R957 T958 A959 V960



- Molecule 27: Splicing factor 3B subunit 2

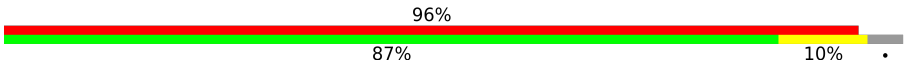
Chain 2: 20% 19% 79%

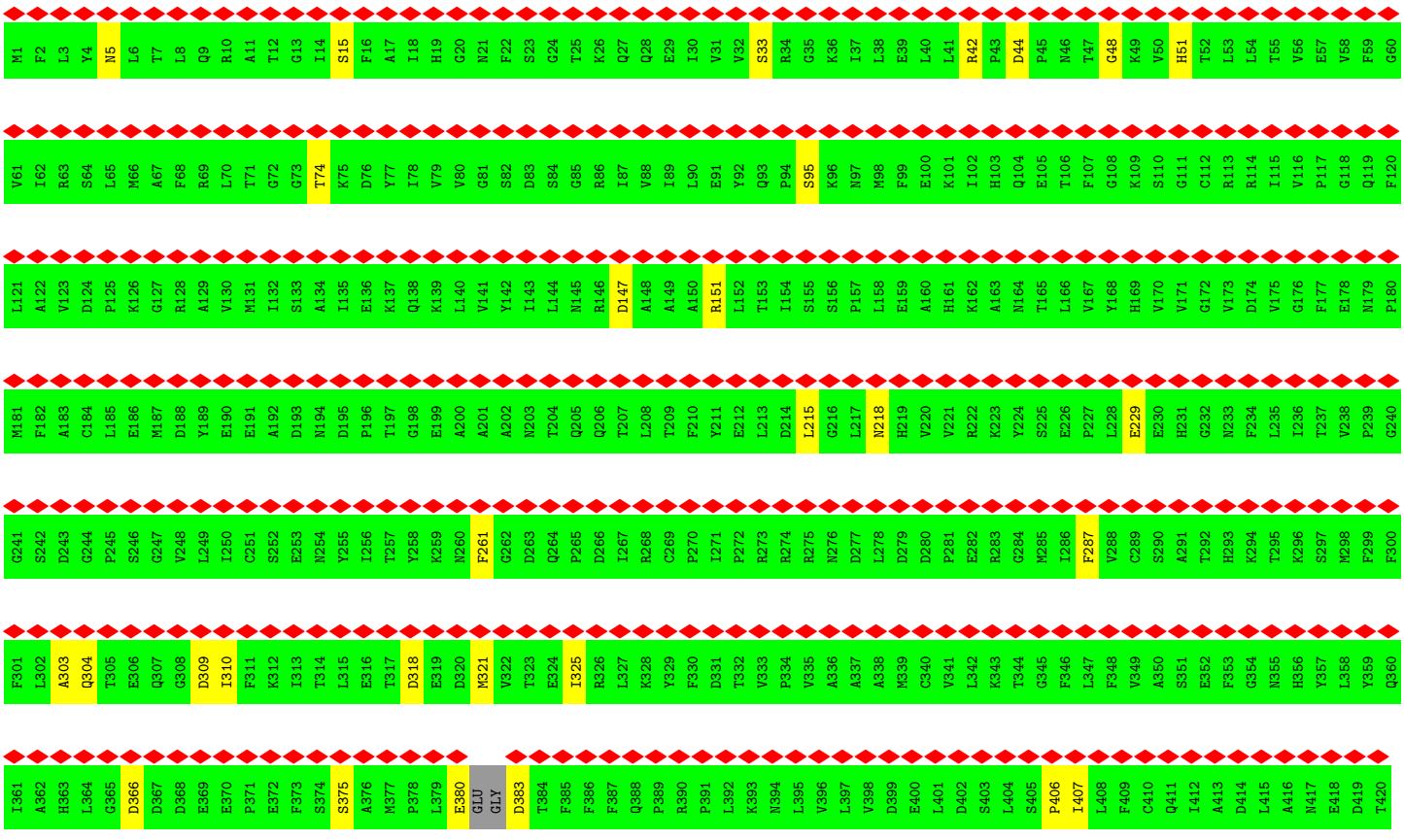


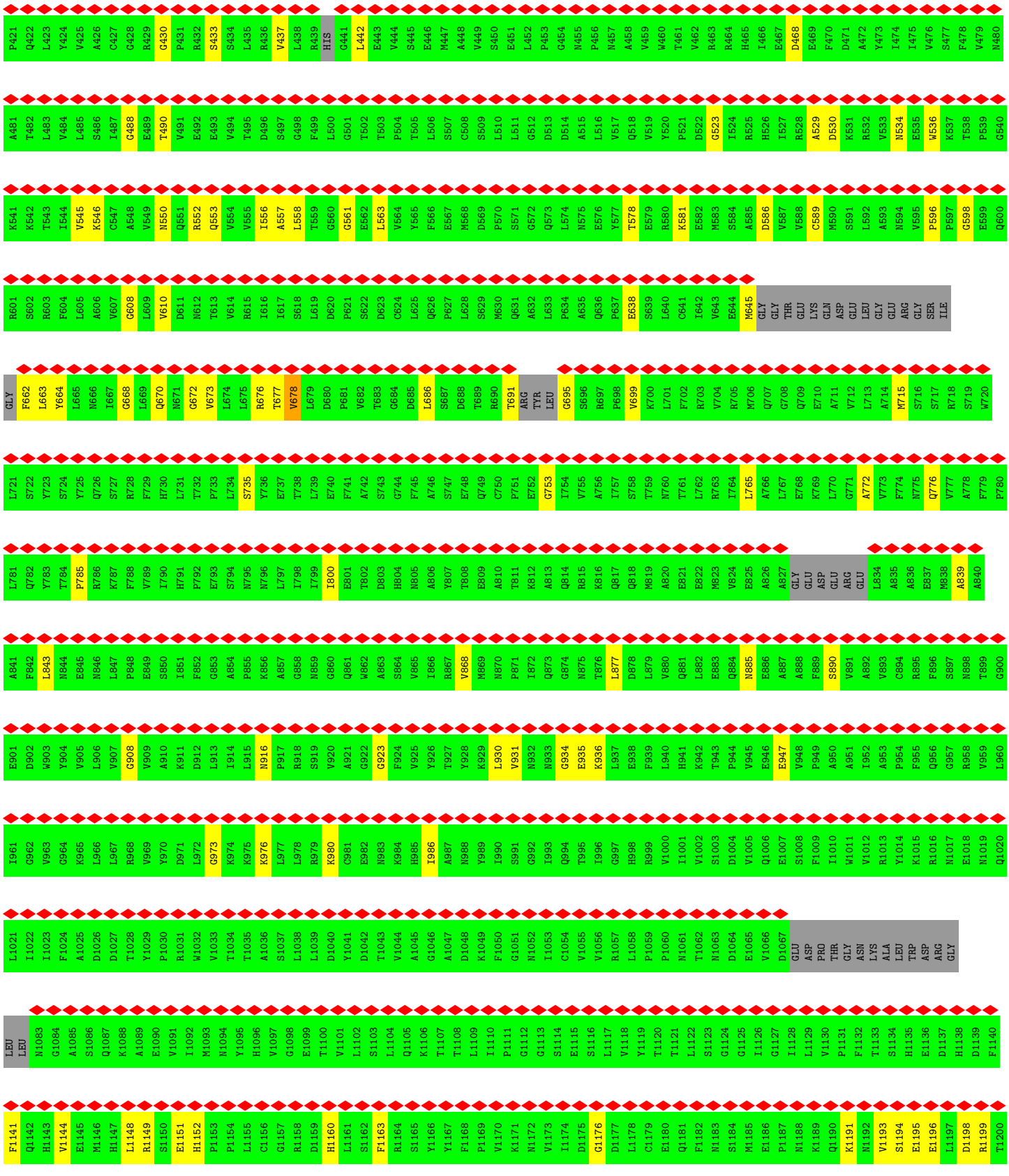


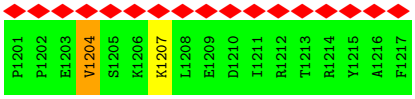
• Molecule 28: Splicing factor 3B subunit 3

Chain 3:



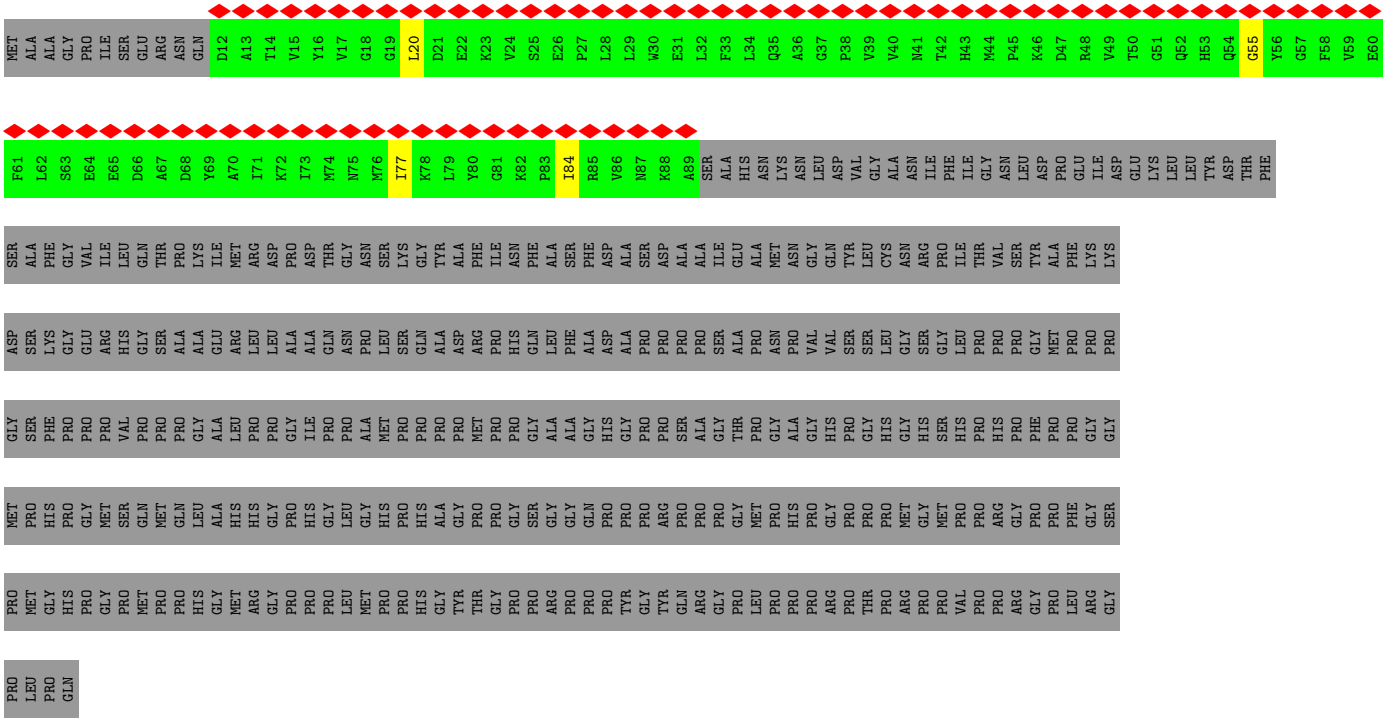



P421 Q422 L423 Y424 V425 A426 C427 G428 R429 G430 P431 R432 S433 S434 L435 R436 V437 L438 R439 HIS G441 L442 E443 V444 S445 E446 M447 A448 V449 S450 E451 L452 P453 G454 N455 P456 N457 A458 V459 W460 T461 V462 R463 R464 H465 I466 E467 D468 E469 F470 D471 A472 Y473 I474 I475 V476 S477 F478 V479 N480
A481 T482 L483 V484 L485 S486 I487 G488 E489 T490 V491 E492 E493 V494 T495 D496 S497 G498 F499 L500 G501 T502 T503 P504 T505 L506 S507 C508 S509 L510 L511 G512 D513 D514 A515 L516 V517 Q518 V519 Y520 P521 D522 G523 I524 R525 H526 I527 R528 A529 D530 K531 R532 V533 N534 E535 W536 K537 T538 P539 G540
K541 K542 T543 I544 V545 K546 C547 A548 V549 N550 Q551 R552 Q553 V554 V555 I556 A557 L558 T559 G560 G561 E562 L563 V564 Y565 F566 E567 M568 D569 P570 S571 G572 Q573 L574 N575 E576 Y577 T578 E579 R580 K581 E582 M583 S584 A585 D586 V587 V588 C589 M590 S591 L592 A593 N594 V595 P596 P597 G598 E599 Q600
R601 S602 R603 F604 L605 A606 V607 G608 L609 V610 D611 N612 T613 V614 R615 I616 I617 S618 L619 D620 P621 S622 D623 G624 L625 Q626 P627 L628 S629 M630 Q631 A632 L633 P634 A635 Q636 P637 E638 S639 L640 C641 I642 V643 E644 M645 GLY GLY THR GLU LYS GLN ASP GLU LEU GLY GLU ARG GLY SER ILE
GLY F662 L663 Y664 L665 N666 I667 G668 L669 Q670 N671 G672 V673 L674 L675 R676 T677 V678 L679 D680 P681 V682 T683 G684 D685 L686 S687 D688 T689 R690 T691 ARG TYR LEU G695 S696 R697 P698 V699 K700 L701 F702 R703 V704 R705 M706 Q707 G708 Q709 E710 A711 V712 L713 A714 M715 S716 S717 R718 S719 W720
L721 S722 Y723 S724 Y725 Q726 S727 R728 F729 H730 L731 T732 P733 L734 S735 Y736 E737 T738 L739 E740 F741 A742 S743 G744 F745 A746 S747 E748 Q749 C750 P751 E752 G753 I764 V755 A756 I757 S758 T759 N760 T761 L762 R763 I764 L765 A766 L767 E768 K769 L770 G771 A772 V773 F774 N775 Q776 V777 A778 F779 P780
L781 Q782 Y783 T784 P785 R786 K787 F788 V789 I790 H791 P792 E793 S794 N795 N796 L797 T798 I799 I800 E801 T802 D803 H804 N805 A806 Y807 T808 E809 A810 T811 K812 A813 Q814 R815 K816 Q817 Q818 M819 A820 E821 E822 M823 V824 E825 A826 A827 GLY GLU ASP GLU ARG GLU L834 A835 A836 E837 M838 A839 A840
A841 F842 L843 N844 E845 N846 L847 P848 E849 S850 I851 F852 G853 A854 P855 K856 A857 G858 N859 G860 Q861 W862 A863 S864 V865 I866 R867 V868 M869 N870 P871 I872 Q873 G874 N875 T876 L877 D878 L879 V880 Q881 L882 E883 Q884 N885 E886 A887 A888 F889 S890 V891 A892 V893 C894 R895 F896 S897 N898 T899 G900
E901 D902 W903 Y904 V905 L906 V907 G908 V909 A910 K911 D912 L913 I914 L915 N916 P917 R918 S919 V920 A921 G922 G923 F924 V925 Y926 T927 Y928 K929 L930 V931 N932 N933 G934 E935 K936 L937 E938 F939 L940 H941 K942 T943 P944 V945 E946 E947 V948 P949 A950 A951 I952 A953 P954 F955 Q956 G957 R958 V959 L960
I961 G962 V963 G964 K965 L966 L967 R968 V969 Y970 D971 L972 G973 K974 K975 K976 L977 L978 R979 K980 C981 E982 N983 K984 H985 I986 A987 N988 Y989 I990 S991 G992 I993 Q994 T995 I996 G997 H998 R999 V1000 I1001 H1002 S1003 D1004 V1005 Q1006 E1007 S1008 F1009 I1010 W1011 V1012 R1013 Y1014 K1015 R1016 N1017 E1018 N1019 Q1020
L1021 I1022 I1023 F1024 A1025 D1026 D1027 T1028 Y1029 P1030 R1031 W1032 V1033 T1034 T1035 A1036 S1037 L1038 L1039 D1040 Y1041 D1042 T1043 V1044 A1045 G1046 A1047 D1048 K1049 F1050 G1051 N1052 I1053 C1054 V1055 V1056 R1057 L1058 P1059 P1060 N1061 T1062 N1063 D1064 E1065 V1066 D1067 GLU ASP PRO THR GLY ASN LYS ALA LEU TRP ASP ARG GLY
LEU LEU N1083 G1084 A1085 S1086 Q1087 K1088 A1089 E1090 V1091 I1092 M1093 N1094 Y1095 H1096 V1097 G1098 E1099 T1100 V1101 L1102 S1103 L1104 Q1105 K1106 T1107 T1108 L1109 I1110 P1111 G1112 G1113 S1114 E1115 S1116 L1117 V1118 Y1119 T1120 T1121 L1122 S1123 G1124 G1125 I1126 G1127 I1128 L1129 V1130 P1131 F1132 T1133 S1134 H1135 E1136 D1137 H1138 D1139 F1140
F1141 Q1142 H1143 V1144 E1145 M1146 H1147 L1148 R1149 S1150 E1151 H1152 P1153 P1154 L1155 C1156 G1157 R1158 D1159 H1160 L1161 S1162 F1163 R1164 S1165 Y1166 Y1167 F1168 P1169 V1170 K1171 N1172 V1173 I1174 D1175 G1176 D1177 L1178 C1179 E1180 Q1181 F1182 N1183 S1184 M1185 E1186 P1187 N1188 K1189 Q1190 K1191 N1192 V1193 S1194 E1195 E1196 L1197 D1198 R1199 T1200



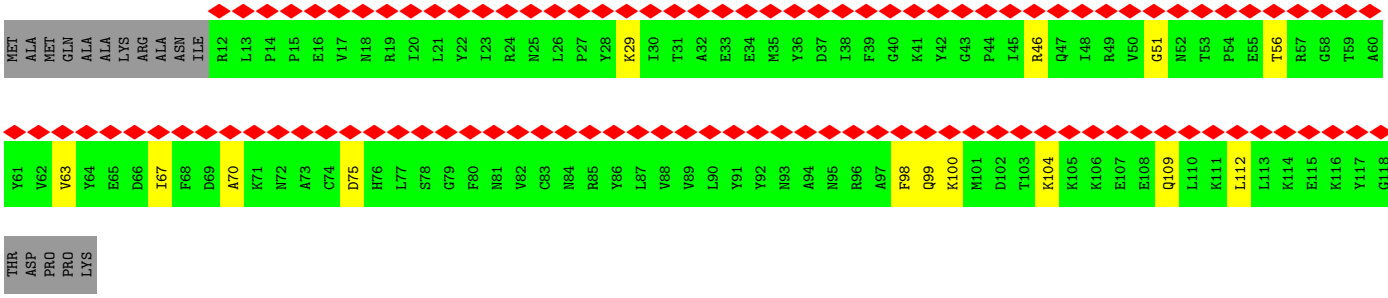
• Molecule 29: Splicing factor 3B subunit 4

Chain 4:



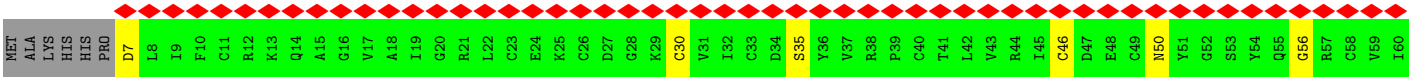
• Molecule 30: Splicing factor 3B subunit 6

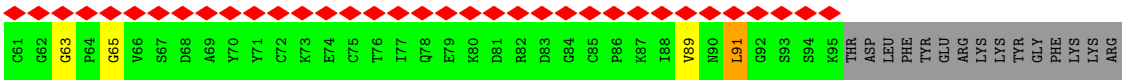
Chain 5:



• Molecule 31: PHD finger-like domain-containing protein 5A

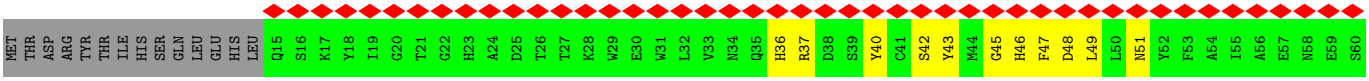
Chain 6:

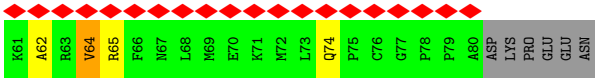




• Molecule 32: Splicing factor 3B subunit 5

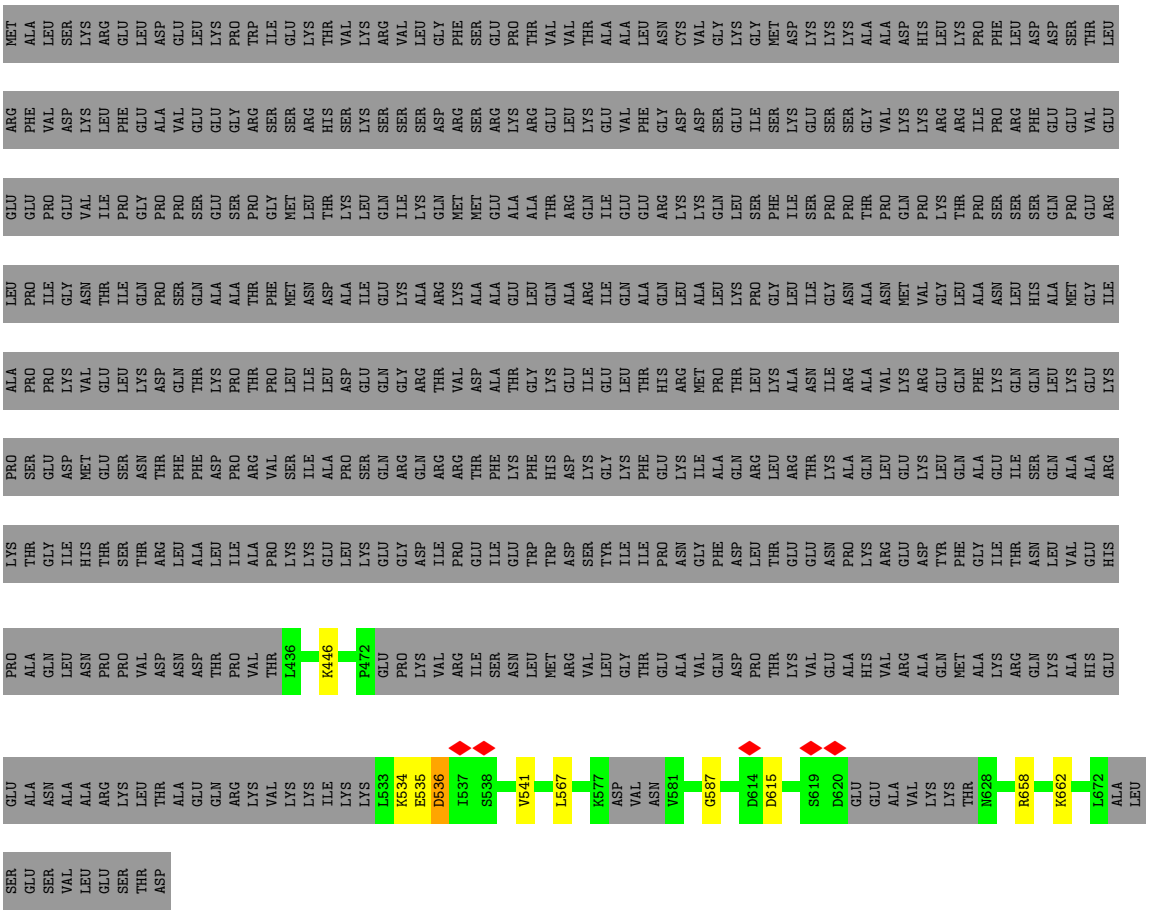
Chain 7:





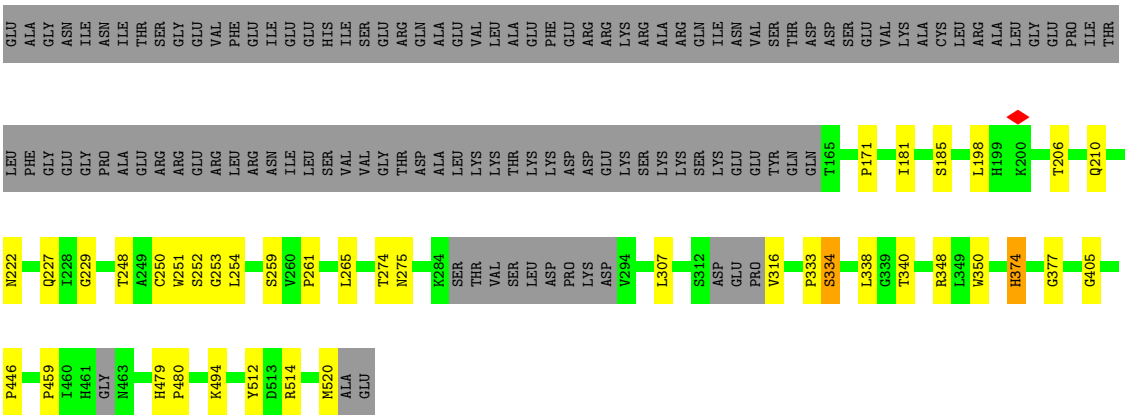
• Molecule 33: U4/U6 small nuclear ribonucleoprotein Prp3

Chain J:

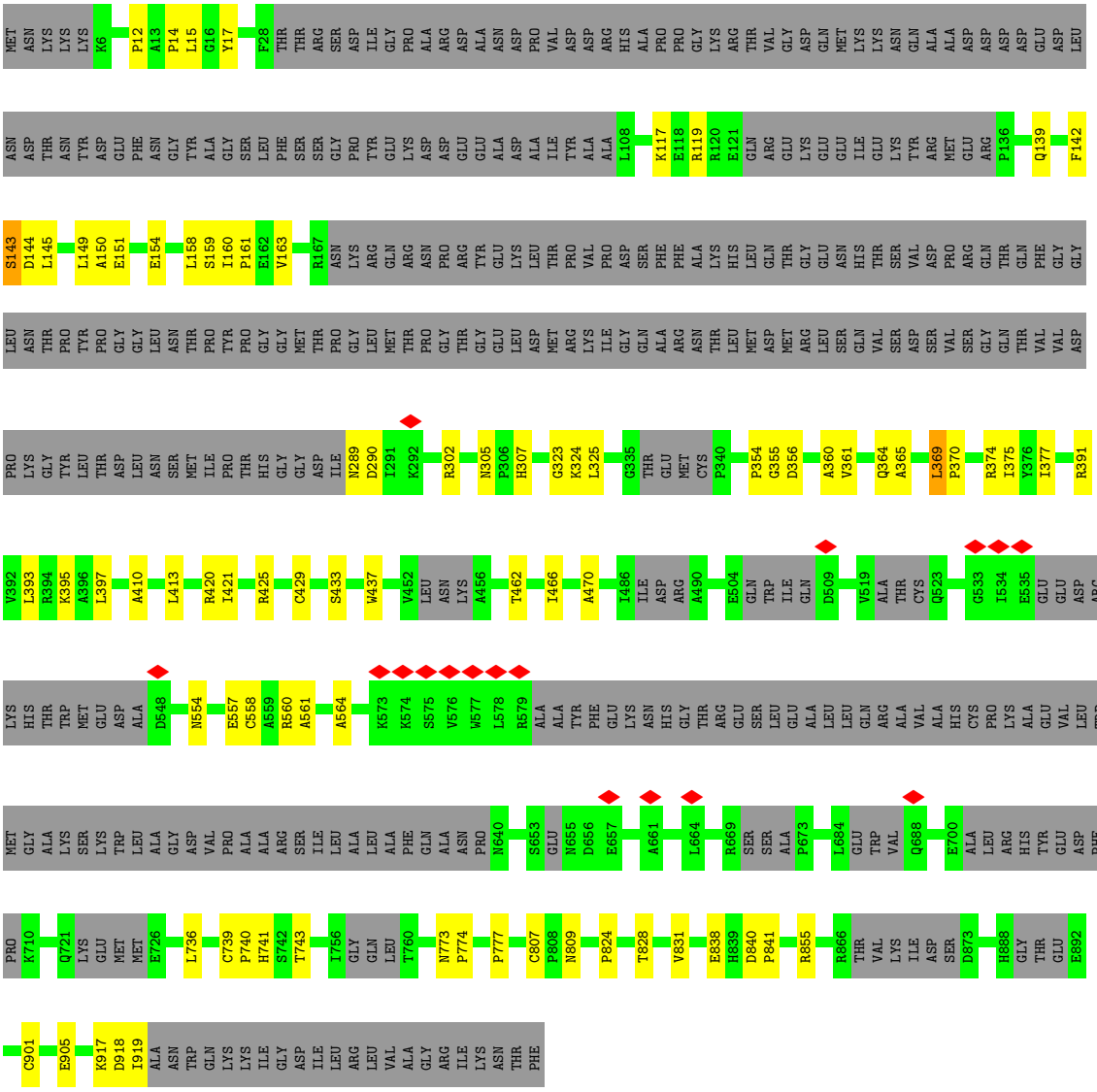


• Molecule 34: U4/U6 small nuclear ribonucleoprotein Prp4

Chain K:

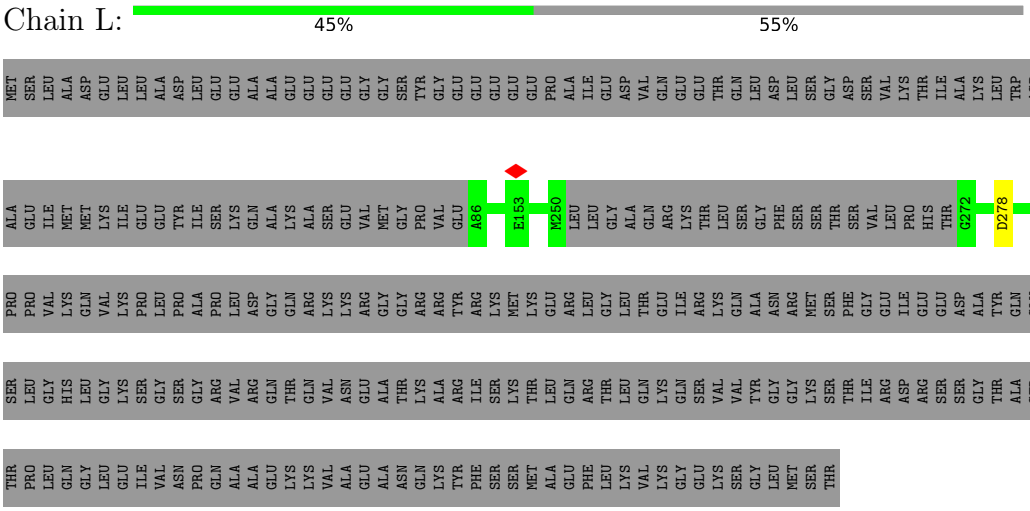


• Molecule 35: Pre-mRNA-processing factor 6



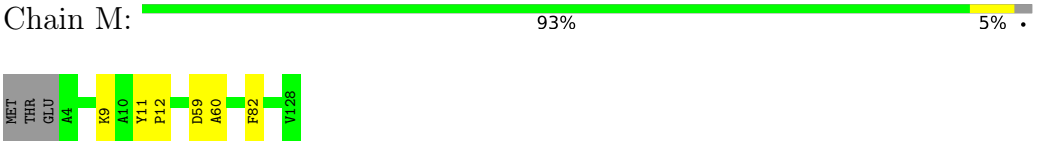
• Molecule 36: U4/U6 small nuclear ribonucleoprotein Prp31

Chain L:



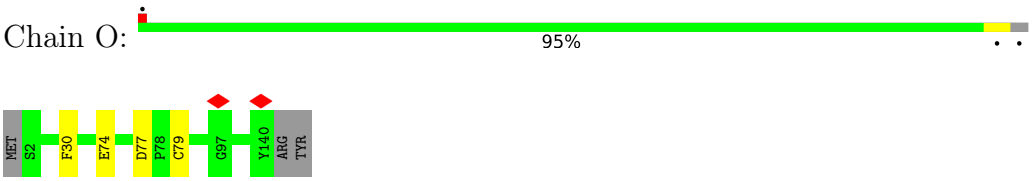
• Molecule 37: NHP2-like protein 1

Chain M:



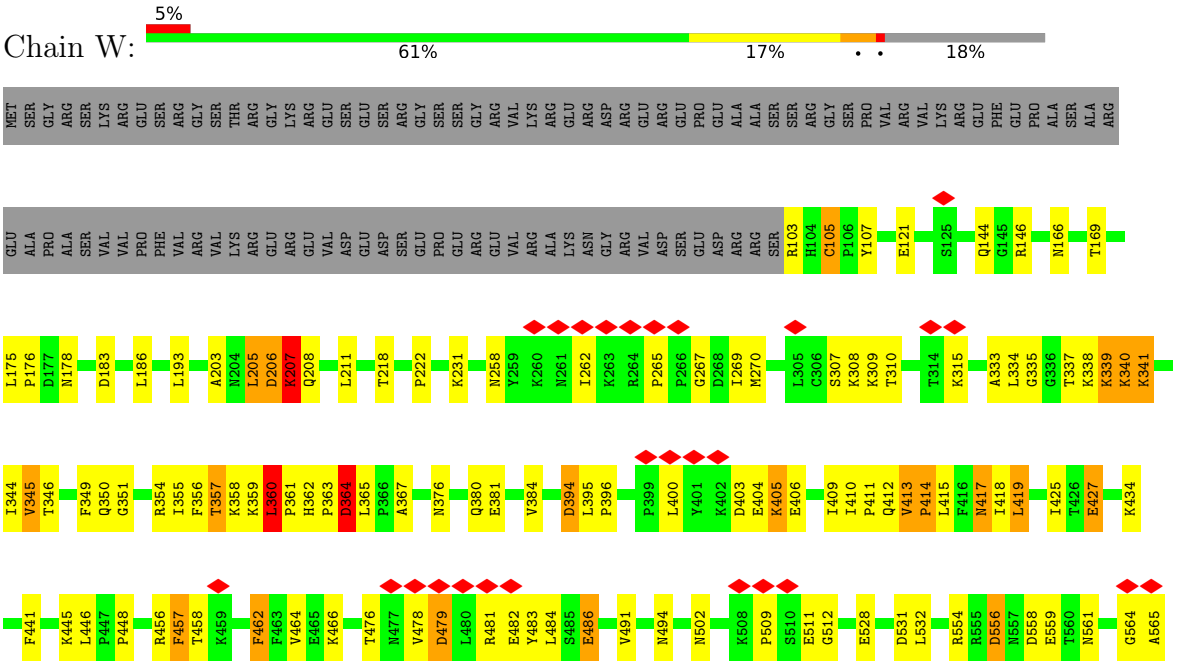
• Molecule 38: Thioredoxin-like protein 4A

Chain O:



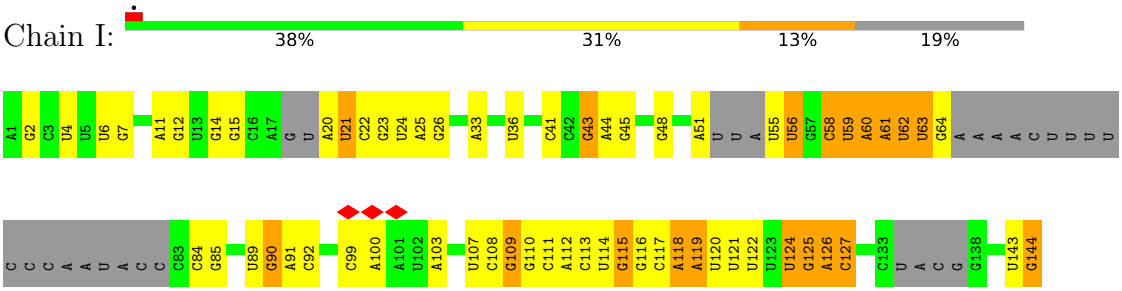
• Molecule 39: U4/U6.U5 tri-snRNP-associated protein 2

Chain W:



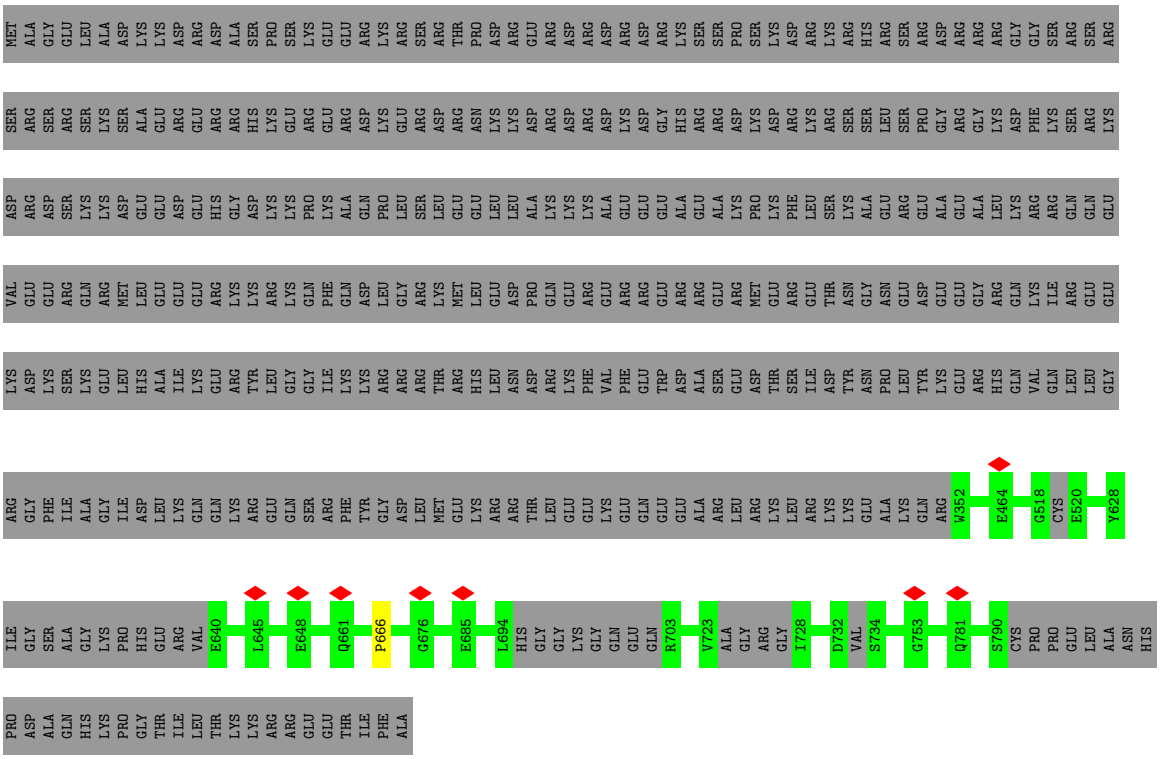
• Molecule 40: U4snRNA

Chain I:



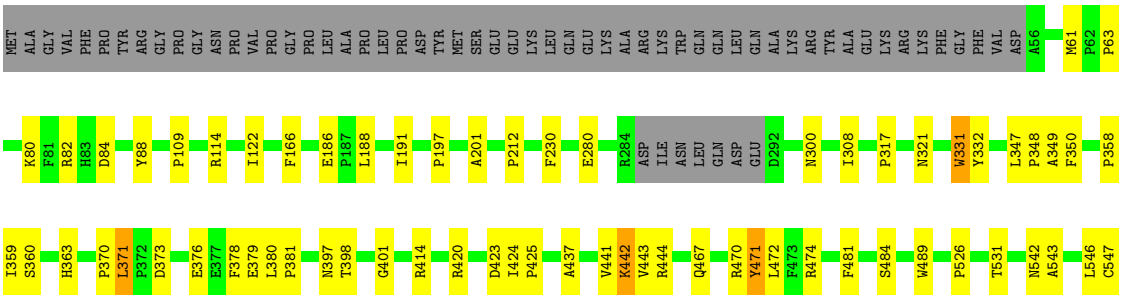
• Molecule 41: Probable ATP-dependent RNA helicase DDX23

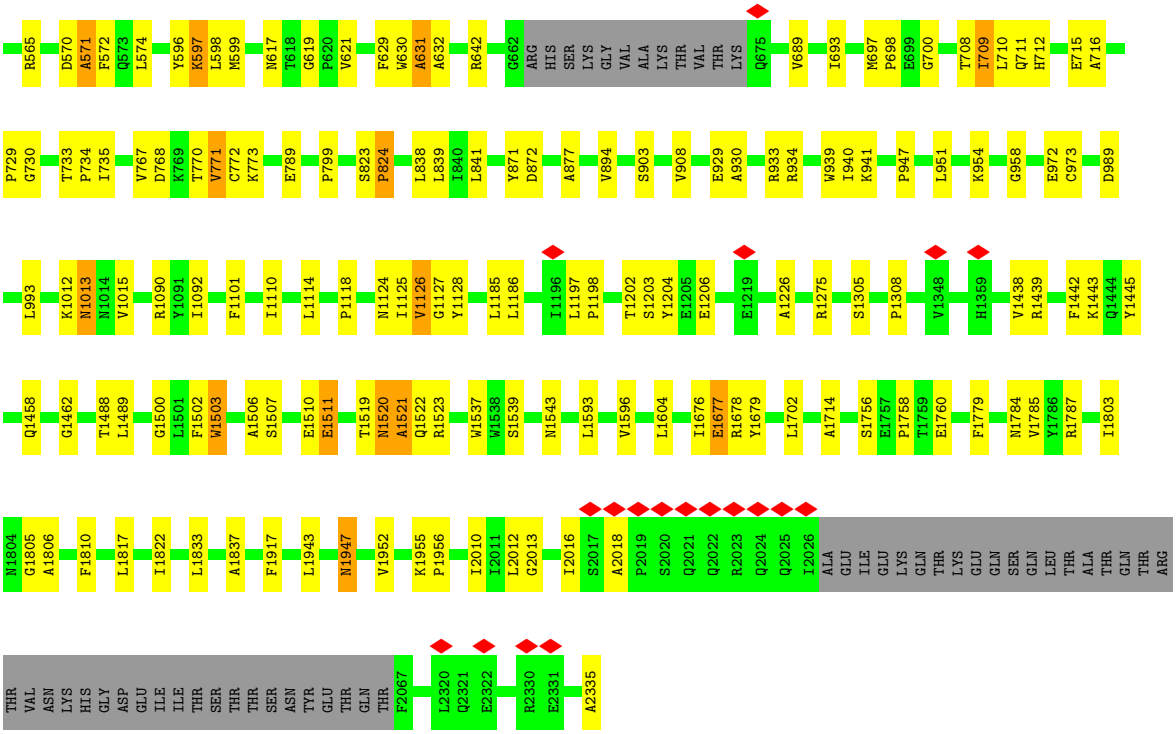
Chain X:



• Molecule 42: Pre-mRNA-processing-splicing factor 8

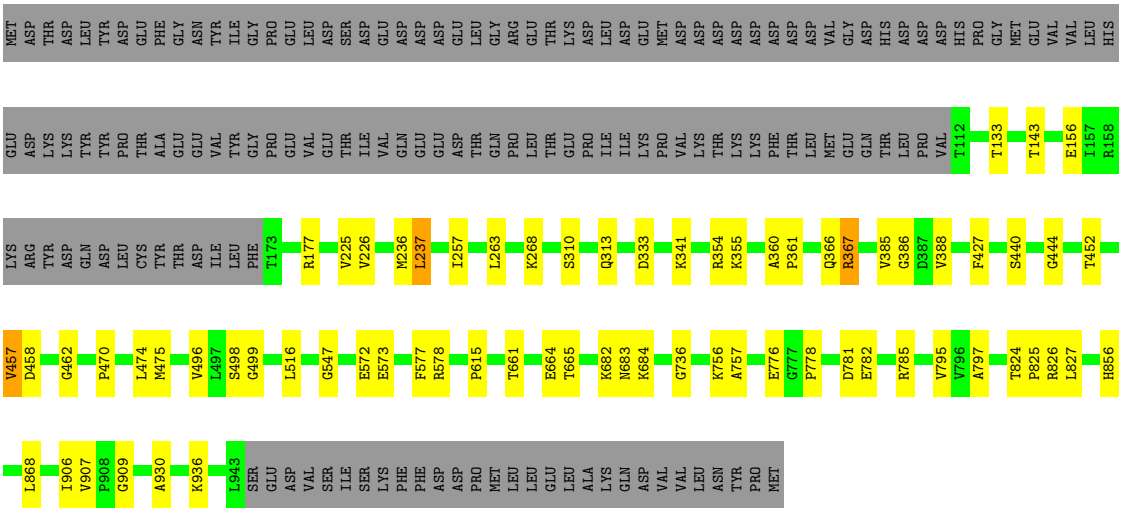
Chain A:





• Molecule 43: 116 kDa U5 small nuclear ribonucleoprotein component

Chain C:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	186162	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	45	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.116	Depositor
Minimum map value	-0.035	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	535.2, 535.2, 535.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.338, 1.338, 1.338	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	B	0.18	0/2697	0.76	0/4193
2	D	0.32	0/7493	0.57	0/9361
3	E	0.67	0/1195	0.71	0/1492
4	P	0.23	0/298	0.48	0/370
4	a	0.23	0/316	0.48	0/392
4	k	0.70	0/338	0.73	0/419
5	Q	0.24	0/291	0.49	0/363
5	b	0.24	0/299	0.49	0/373
5	m	0.78	0/295	0.76	0/367
6	R	0.22	0/313	0.49	0/390
6	c	0.22	0/313	0.49	0/390
6	l	0.63	0/315	0.75	0/392
7	S	0.24	0/297	0.51	0/371
7	d	0.24	0/281	0.52	0/351
7	n	0.55	0/270	0.63	0/334
8	T	0.23	0/287	0.49	0/358
8	e	0.23	0/317	0.52	0/396
8	h	0.47	0/318	0.56	0/394
9	U	0.22	0/254	0.48	0/314
9	f	0.23	0/258	0.48	0/320
9	i	0.47	0/290	0.65	0/359
10	V	0.22	0/333	0.47	0/416
10	g	0.22	0/378	0.46	0/471
10	j	0.56	0/327	0.68	0/407
11	F	0.26	0/1639	0.72	0/2545
12	q	0.42	0/359	0.67	0/447
13	r	0.46	0/298	0.77	0/369
14	s	0.34	0/294	0.61	0/364
15	t	0.42	0/298	0.57	0/369
16	x	0.43	0/279	0.66	0/347
17	y	0.38	0/258	0.61	0/319
18	z	0.42	0/242	0.65	0/299

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
19	G	0.62	2/954 (0.2%)	0.87	0/1477
20	H	0.77	11/2576 (0.4%)	1.24	32/4003 (0.8%)
21	o	0.63	0/647	1.42	0/807
22	p	0.62	0/375	1.20	0/467
23	u	0.22	0/493	0.42	0/611
24	v	0.23	0/392	0.55	0/483
25	w	0.24	0/1767	0.46	0/2199
26	1	1.03	4/4112 (0.1%)	0.81	0/5126
27	2	0.72	0/738	0.72	0/912
28	3	0.85	0/4689	0.76	0/5849
29	4	0.66	0/311	0.70	0/387
30	5	0.77	0/431	0.77	0/537
31	6	0.75	0/355	0.70	0/442
32	7	1.01	0/263	0.77	0/327
33	J	0.68	0/664	0.66	0/823
34	K	0.73	0/1367	0.79	0/1702
35	N	0.55	0/2297	0.68	1/2838 (0.0%)
36	L	0.34	0/902	0.51	0/1124
37	M	0.38	0/499	0.62	0/622
38	O	0.74	0/555	0.73	0/692
39	W	0.50	0/1851	1.16	7/2312 (0.3%)
40	I	0.23	1/2779 (0.0%)	0.70	0/4319
41	X	0.43	0/1655	0.56	0/2062
42	A	0.62	2/8880 (0.0%)	0.72	2/11093 (0.0%)
43	C	0.65	1/3270 (0.0%)	0.73	0/4084
All	All	0.59	21/64262 (0.0%)	0.75	42/83350 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	0	1
4	k	0	1
16	x	0	1
25	w	0	1
26	1	0	15
27	2	0	2
28	3	0	13
30	5	0	1
31	6	0	2

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
32	7	0	1
34	K	0	1
35	N	0	6
39	W	0	62
43	C	0	1
All	All	0	108

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	A	597	LYS	C-N	10.75	1.58	1.34
20	H	142	C	C1'-N1	7.31	1.59	1.48
26	1	1243	PRO	N-CA	-7.12	1.35	1.47
42	A	877	ALA	C-N	7.10	1.50	1.34
20	H	182	U	C1'-N1	6.93	1.59	1.48

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	H	162	U	N3-C2-O2	-9.04	115.88	122.20
20	H	169	C	P-O3'-C3'	8.24	129.58	119.70
35	N	369	LEU	C-N-CA	-8.00	88.41	122.00
42	A	877	ALA	O-C-N	7.84	135.24	122.70
20	H	114	A	OP2-P-O3'	7.27	121.19	105.20

There are no chirality outliers.

5 of 108 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	1	110	PRO	Peptide
2	D	430	LEU	Peptide
4	k	112	ASN	Peptide
25	w	443	THR	Peptide
16	x	51	TYR	Peptide

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	B	2419	0	1224	60	0
2	D	7496	0	1961	18	0
3	E	1196	0	337	2	0
4	P	300	0	80	9	0
4	a	318	0	86	0	0
4	k	340	0	87	0	0
5	Q	292	0	93	1	0
5	b	300	0	95	0	0
5	m	296	0	87	0	0
6	R	314	0	86	0	0
6	c	314	0	86	0	0
6	l	316	0	85	0	0
7	S	298	0	89	1	0
7	d	282	0	85	0	0
7	n	272	0	75	0	0
8	T	288	0	84	0	0
8	e	318	0	92	0	0
8	h	320	0	88	0	0
9	U	256	0	70	3	0
9	f	260	0	74	0	0
9	i	292	0	80	0	0
10	V	334	0	92	16	0
10	g	380	0	103	0	0
10	j	328	0	89	0	0
11	F	1470	0	745	49	0
12	q	360	0	95	0	0
13	r	300	0	77	0	0
14	s	296	0	77	0	0
15	t	300	0	80	0	0
16	x	280	0	81	0	0
17	y	260	0	75	0	0
18	z	244	0	71	0	0
19	G	862	0	441	136	0
20	H	2311	0	1170	139	0
21	o	648	0	167	0	0
22	p	376	0	102	0	0
23	u	496	0	118	0	0
24	v	396	0	91	0	0
25	w	1773	0	477	0	0
26	1	4120	0	1091	171	0
27	2	744	0	189	5	0
28	3	4696	0	1266	59	0
29	4	312	0	87	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	5	432	0	114	7	0
31	6	356	0	105	5	0
32	7	264	0	70	9	0
33	J	668	0	179	8	0
34	K	1371	0	384	17	0
35	N	2316	0	581	45	0
36	L	904	0	235	1	0
37	M	500	0	128	4	0
38	O	556	0	147	1	0
39	W	1852	0	477	30	0
40	I	2491	0	1262	118	0
41	X	1661	0	440	0	0
42	A	8884	0	2283	148	0
43	C	3272	0	874	50	0
44	A	36	0	6	0	0
45	C	32	0	12	4	0
46	C	1	0	0	0	0
All	All	63369	0	19125	1003	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 13.

The worst 5 of 1003 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)
19:G:145:U:C2'	19:G:146:C:H5"	1.54	1.37
33:J:536:ASP:CA	33:J:587:GLY:CA	2.11	1.28
43:C:470:PRO:CA	43:C:499:GLY:HA2	1.64	1.27
40:I:63:U:H2'	40:I:64:G:C8	1.69	1.26
33:J:536:ASP:CA	33:J:587:GLY:HA3	1.64	1.25

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	D	1868/2136 (88%)	1770 (95%)	93 (5%)	5 (0%)	41 76
3	E	297/357 (83%)	272 (92%)	16 (5%)	9 (3%)	4 28
4	P	70/118 (59%)	68 (97%)	2 (3%)	0	100 100
4	a	74/118 (63%)	71 (96%)	3 (4%)	0	100 100
4	k	81/118 (69%)	78 (96%)	3 (4%)	0	100 100
5	Q	69/86 (80%)	67 (97%)	2 (3%)	0	100 100
5	b	71/86 (83%)	70 (99%)	1 (1%)	0	100 100
5	m	72/86 (84%)	68 (94%)	4 (6%)	0	100 100
6	R	76/92 (83%)	70 (92%)	6 (8%)	0	100 100
6	c	76/92 (83%)	70 (92%)	6 (8%)	0	100 100
6	l	77/92 (84%)	76 (99%)	1 (1%)	0	100 100
7	S	71/76 (93%)	67 (94%)	4 (6%)	0	100 100
7	d	67/76 (88%)	63 (94%)	4 (6%)	0	100 100
7	n	64/76 (84%)	62 (97%)	2 (3%)	0	100 100
8	T	69/126 (55%)	69 (100%)	0	0	100 100
8	e	76/126 (60%)	73 (96%)	3 (4%)	0	100 100
8	h	76/126 (60%)	75 (99%)	1 (1%)	0	100 100
9	U	60/231 (26%)	57 (95%)	3 (5%)	0	100 100
9	f	60/231 (26%)	57 (95%)	3 (5%)	0	100 100
9	i	69/231 (30%)	68 (99%)	1 (1%)	0	100 100
10	V	80/119 (67%)	76 (95%)	4 (5%)	0	100 100
10	g	89/119 (75%)	84 (94%)	5 (6%)	0	100 100
10	j	80/119 (67%)	77 (96%)	3 (4%)	0	100 100
12	q	88/95 (93%)	77 (88%)	7 (8%)	4 (4%)	2 22
13	r	71/102 (70%)	66 (93%)	3 (4%)	2 (3%)	5 30
14	s	70/139 (50%)	64 (91%)	5 (7%)	1 (1%)	11 46
15	t	71/91 (78%)	64 (90%)	4 (6%)	3 (4%)	3 22
16	x	68/80 (85%)	66 (97%)	2 (3%)	0	100 100
17	y	61/103 (59%)	56 (92%)	5 (8%)	0	100 100
18	z	57/96 (59%)	52 (91%)	4 (7%)	1 (2%)	8 40

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
21	o	160/255 (63%)	146 (91%)	12 (8%)	2 (1%)	12 48
22	p	92/225 (41%)	90 (98%)	2 (2%)	0	100 100
23	u	118/793 (15%)	106 (90%)	6 (5%)	6 (5%)	2 19
24	v	91/464 (20%)	66 (72%)	16 (18%)	9 (10%)	0 9
25	w	431/501 (86%)	385 (89%)	41 (10%)	5 (1%)	13 49
26	1	1014/1304 (78%)	821 (81%)	171 (17%)	22 (2%)	6 35
27	2	174/895 (19%)	155 (89%)	14 (8%)	5 (3%)	4 29
28	3	1160/1217 (95%)	1062 (92%)	90 (8%)	8 (1%)	22 62
29	4	76/424 (18%)	74 (97%)	2 (3%)	0	100 100
30	5	106/125 (85%)	83 (78%)	20 (19%)	3 (3%)	5 30
31	6	87/110 (79%)	76 (87%)	11 (13%)	0	100 100
32	7	64/86 (74%)	55 (86%)	8 (12%)	1 (2%)	9 43
33	J	159/683 (23%)	148 (93%)	7 (4%)	4 (2%)	5 32
34	K	335/522 (64%)	295 (88%)	26 (8%)	14 (4%)	3 22
35	N	541/941 (58%)	475 (88%)	41 (8%)	25 (5%)	2 21
36	L	222/499 (44%)	214 (96%)	8 (4%)	0	100 100
37	M	123/128 (96%)	117 (95%)	6 (5%)	0	100 100
38	O	137/142 (96%)	126 (92%)	9 (7%)	2 (2%)	10 45
39	W	461/565 (82%)	327 (71%)	77 (17%)	57 (12%)	0 5
41	X	402/820 (49%)	393 (98%)	8 (2%)	1 (0%)	47 81
42	A	2213/2335 (95%)	2046 (92%)	100 (4%)	67 (3%)	4 28
43	C	814/972 (84%)	751 (92%)	40 (5%)	23 (3%)	5 30
All	All	13158/19749 (67%)	11964 (91%)	915 (7%)	279 (2%)	10 36

5 of 279 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	354	PRO
2	D	957	VAL
2	D	1584	ILE
3	E	193	THR
12	q	55	LEU

5.3.2 Protein sidechains (i)

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

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	B	114/117 (97%)	38 (33%)	2 (1%)
11	F	65/107 (60%)	10 (15%)	2 (3%)
19	G	41/274 (14%)	28 (68%)	9 (21%)
20	H	105/188 (55%)	25 (23%)	2 (1%)
40	I	112/144 (77%)	31 (27%)	4 (3%)
All	All	437/830 (52%)	132 (30%)	19 (4%)

5 of 132 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	B	8	G
1	B	10	U
1	B	20	G
1	B	21	A
1	B	22	U

5 of 19 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
20	H	168	A
40	I	99	C
40	I	114	U
40	I	58	C
19	G	150	U

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
45	GTP	C	1500	46	26,34,34	1.27	1 (3%)	32,54,54	1.62	3 (9%)
44	IHP	A	3000	-	36,36,36	0.82	0	54,60,60	1.20	2 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	GTP	C	1500	46	-	3/18/38/38	0/3/3/3
44	IHP	A	3000	-	-	6/30/54/54	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	C	1500	GTP	C6-N1	-3.66	1.32	1.37

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	C	1500	GTP	PB-O3B-PG	-5.86	112.72	132.83
44	A	3000	IHP	C6-C5-C4	3.80	118.73	110.41
45	C	1500	GTP	PA-O3A-PB	-3.76	119.91	132.83
44	A	3000	IHP	C5-C4-C3	2.46	115.80	110.41
45	C	1500	GTP	C5-C6-N1	2.40	118.19	113.95

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
44	A	3000	IHP	C2-O12-P2-O42
44	A	3000	IHP	C3-O13-P3-O23
45	C	1500	GTP	C5'-O5'-PA-O3A
44	A	3000	IHP	C6-O16-P6-O46
44	A	3000	IHP	C5-O15-P5-O25

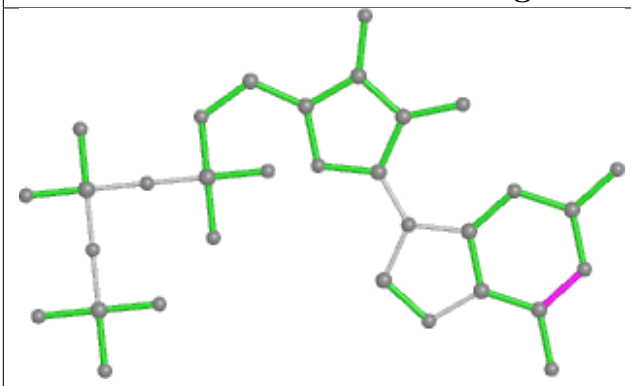
There are no ring outliers.

1 monomer is involved in 4 short contacts:

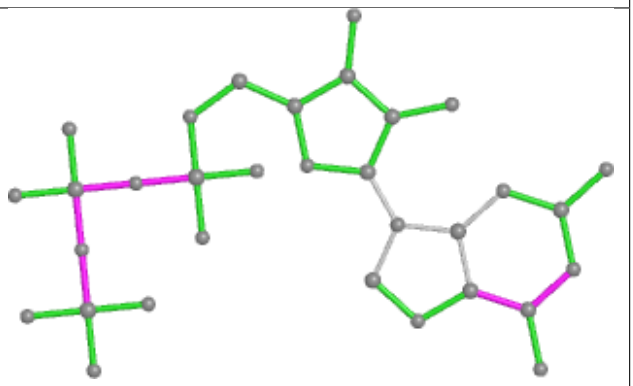
Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	C	1500	GTP	4	0

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

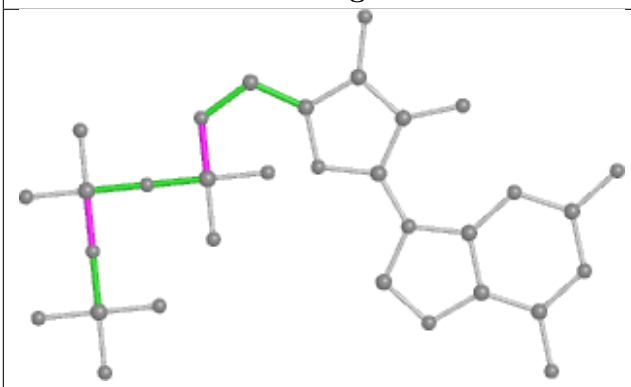
Ligand GTP C 1500



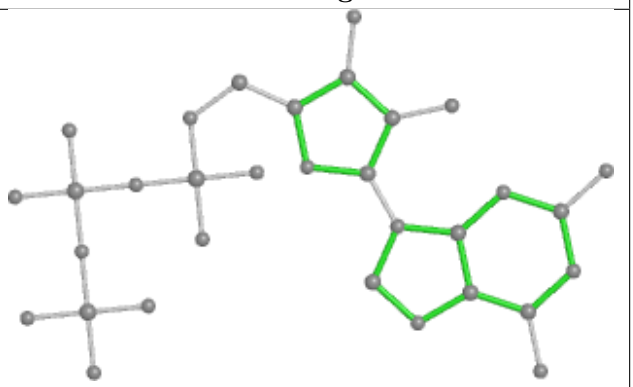
Bond lengths



Bond angles

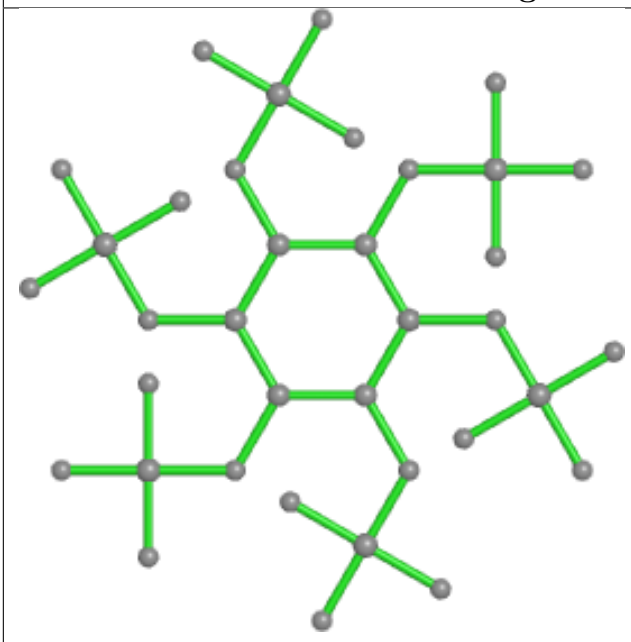


Torsions

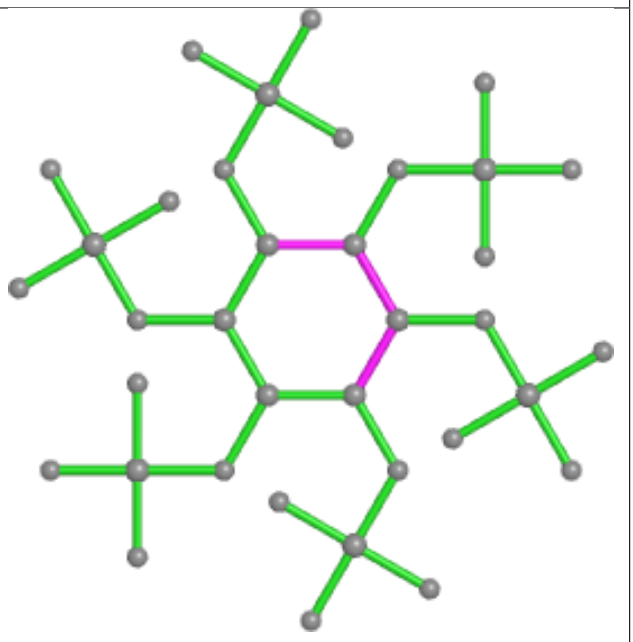


Rings

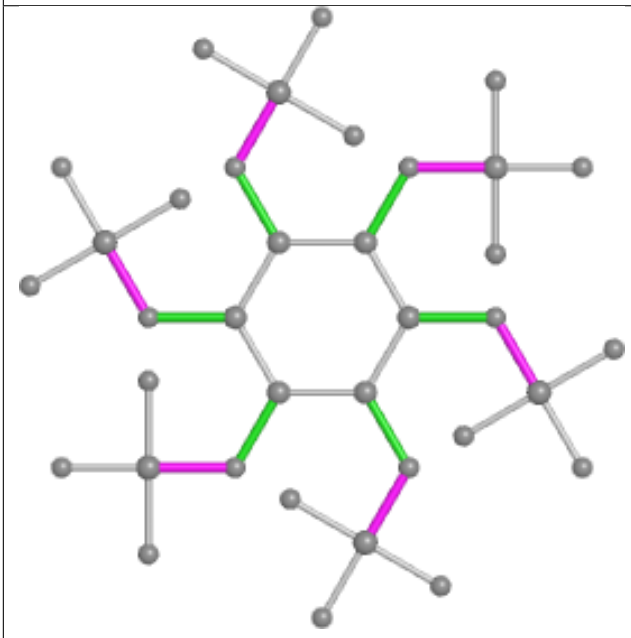
Ligand IHP A 3000



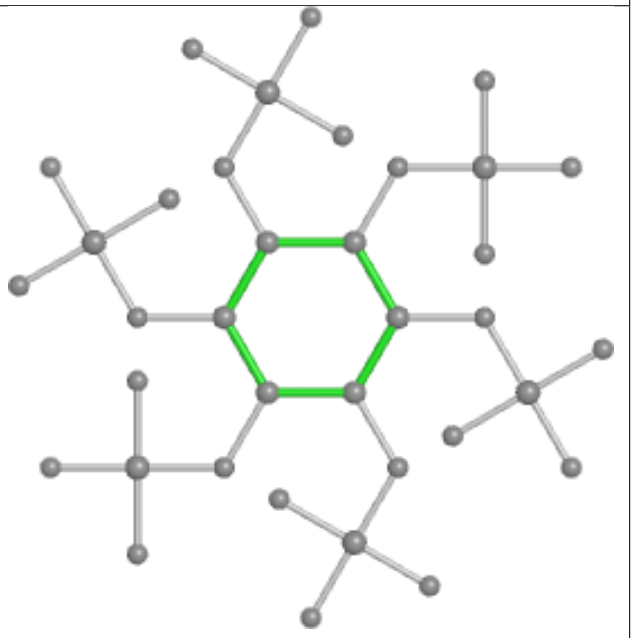
Bond lengths



Bond angles



Torsions



Rings

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.

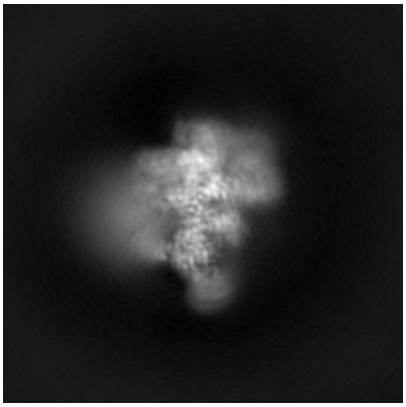
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-9621. These allow visual inspection of the internal detail of the map and identification of artifacts.

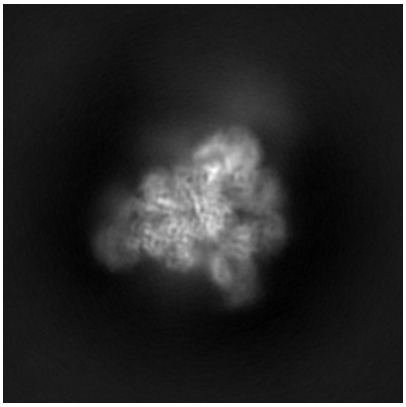
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

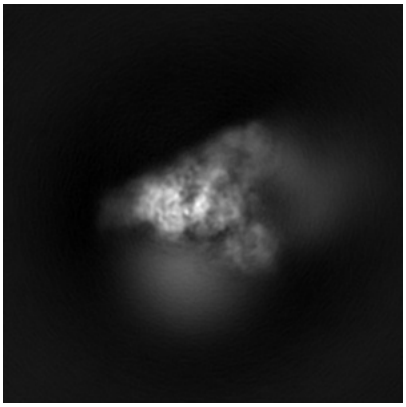
6.1.1 Primary map



X



Y

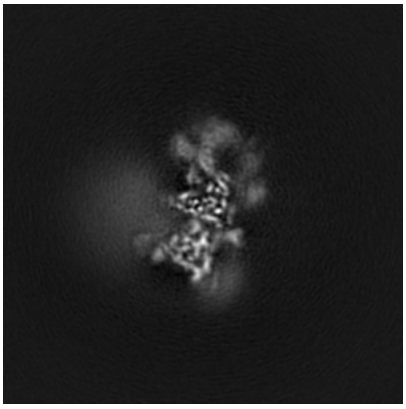


Z

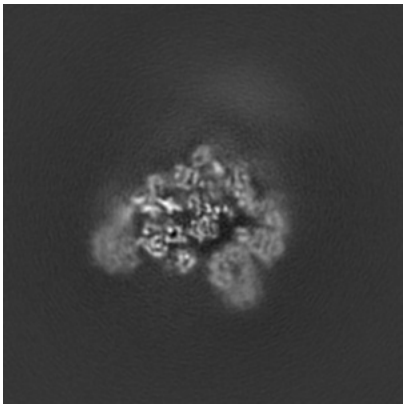
The images above show the map projected in three orthogonal directions.

6.2 Central slices

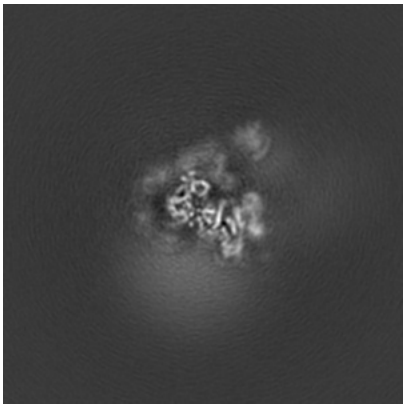
6.2.1 Primary map



X Index: 200



Y Index: 200

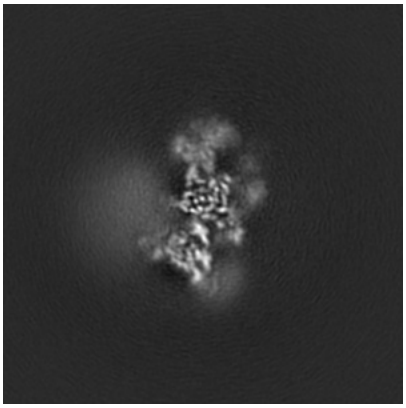


Z Index: 200

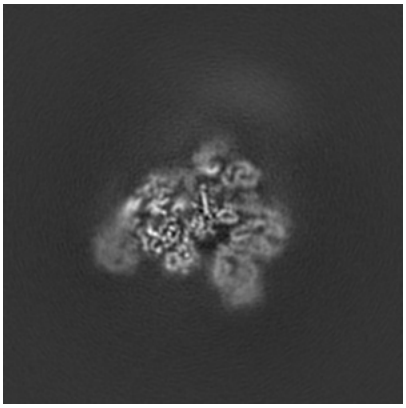
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

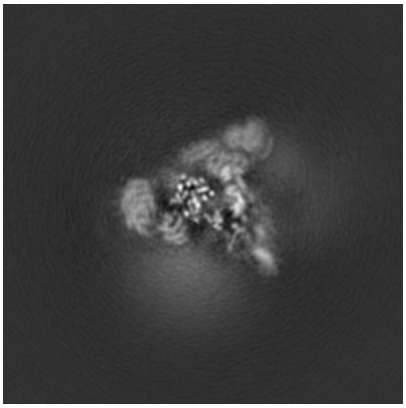
6.3.1 Primary map



X Index: 197



Y Index: 193

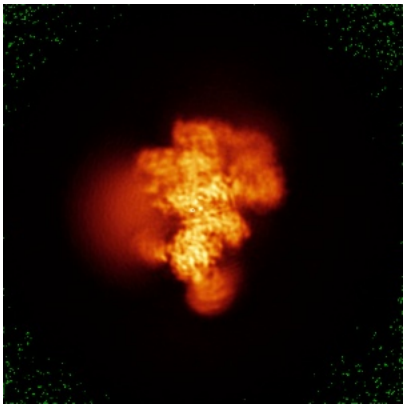


Z Index: 213

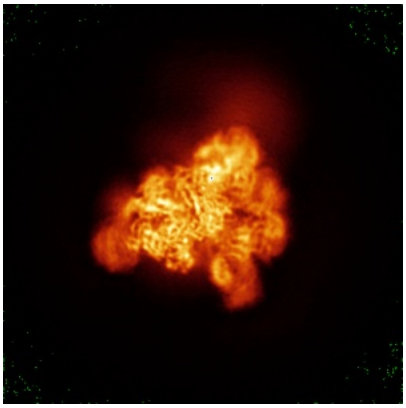
The images above show the largest variance slices of the map in three orthogonal directions.

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

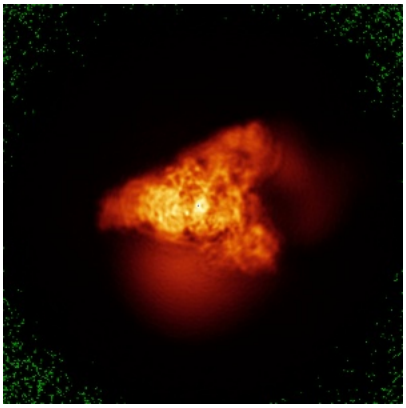
6.4.1 Primary map



X



Y



Z

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 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

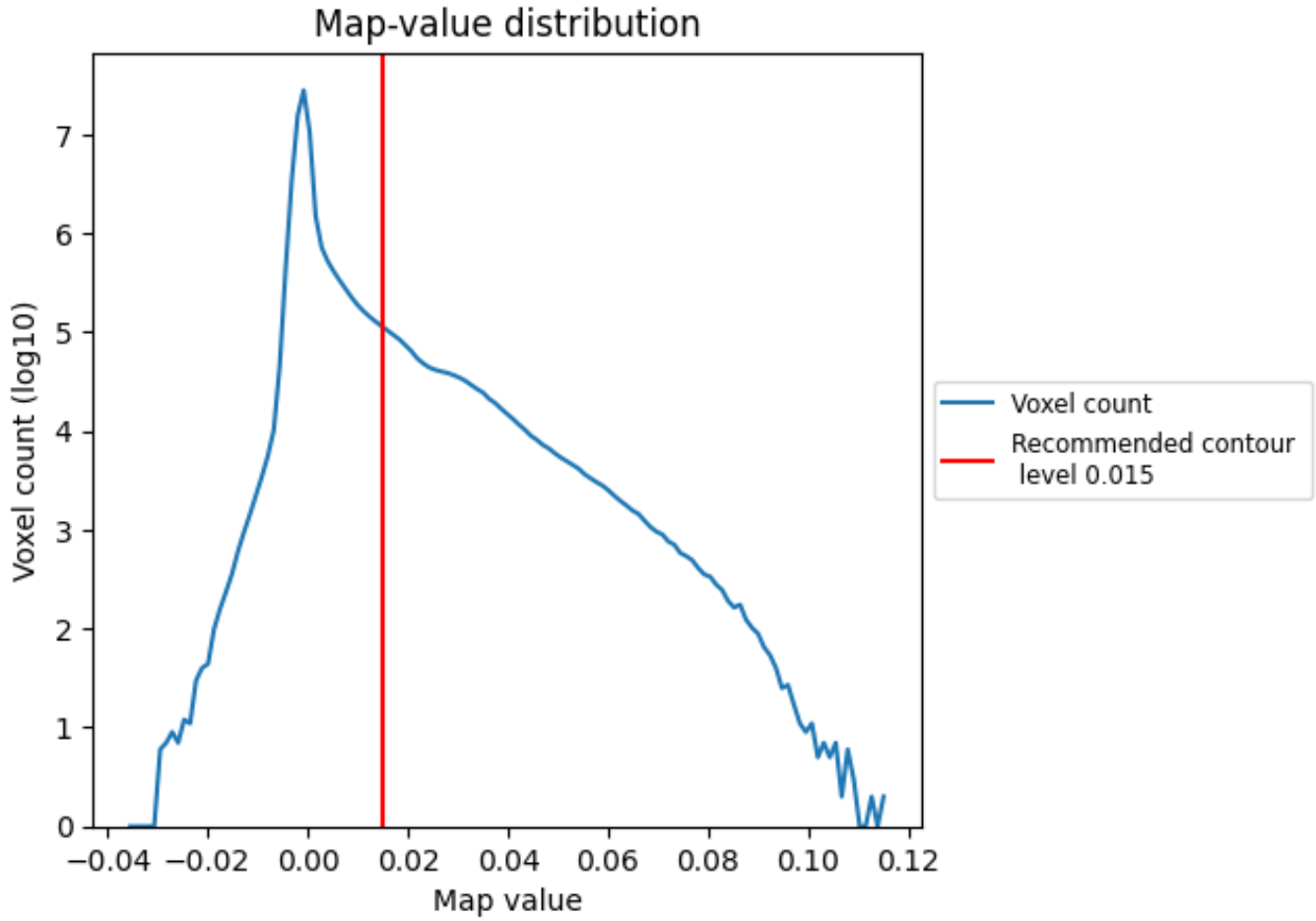
6.6 Mask visualisation (i)

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

7 Map analysis

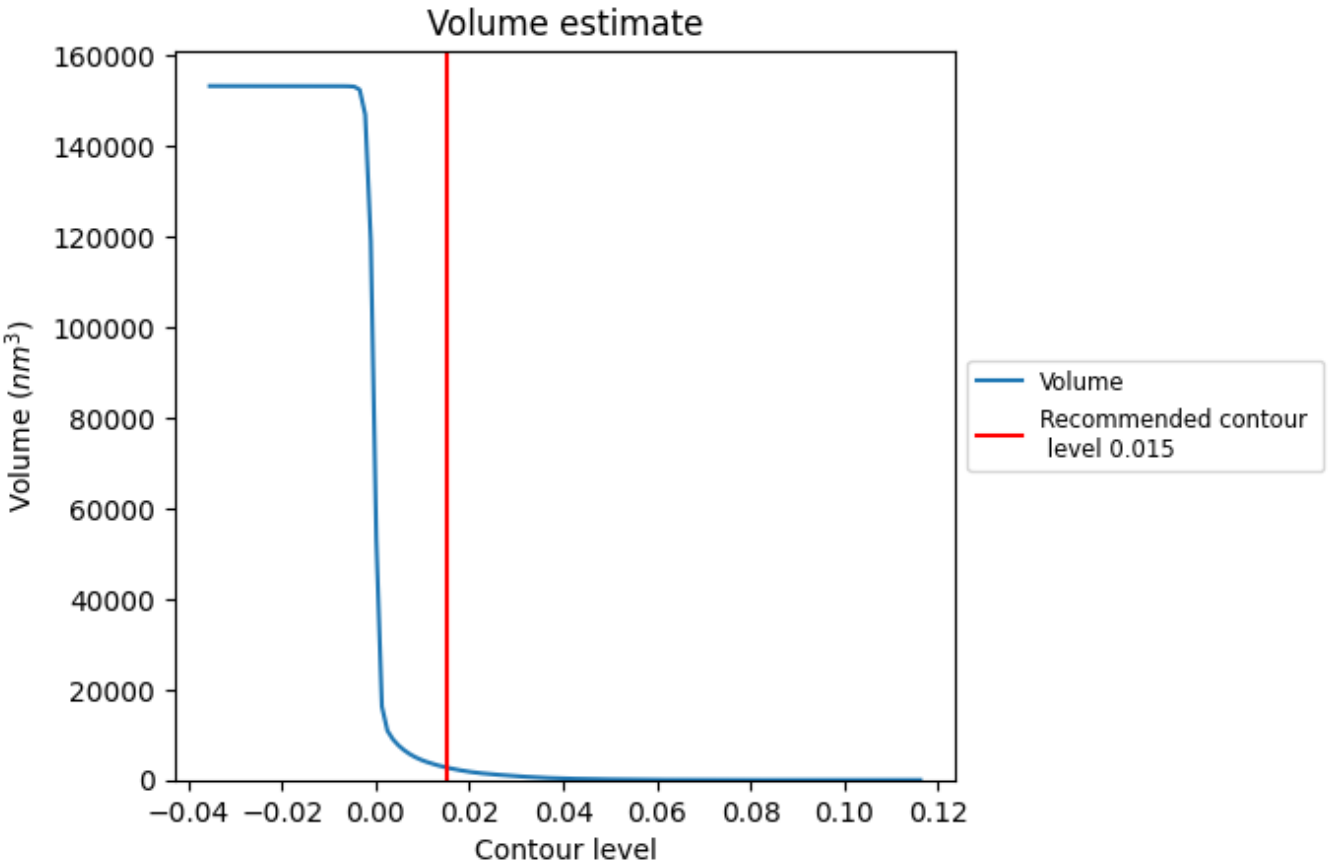
This section contains the results of statistical analysis of the map.

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.

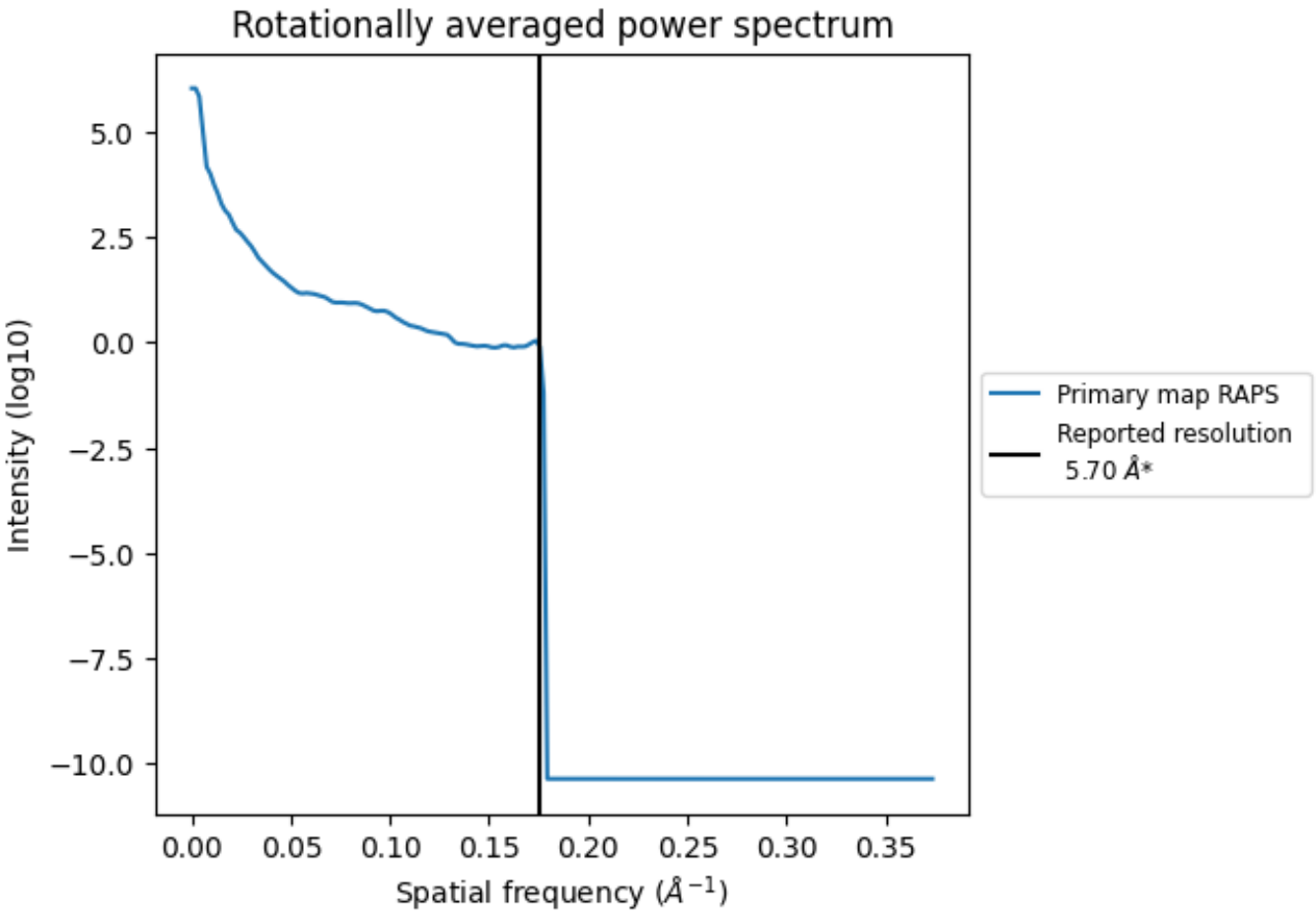
7.2 Volume estimate (i)



The volume at the recommended contour level is 2784 nm^3; this corresponds to an approximate mass of 2515 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 0.175 $Å^{-1}$

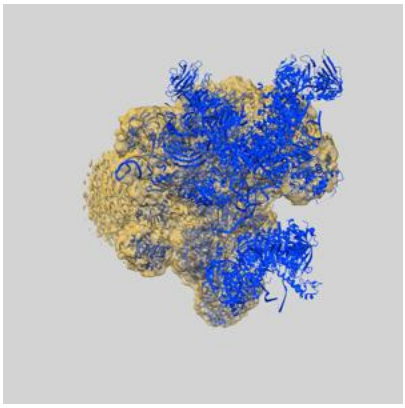
8 Fourier-Shell correlation

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

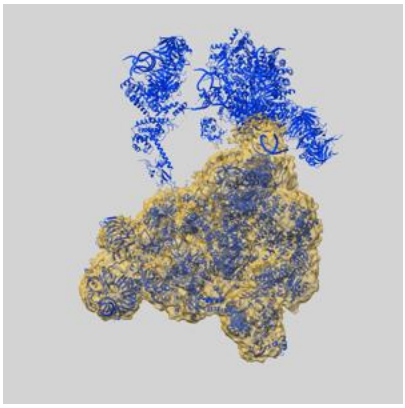
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-9621 and PDB model 6AH0. Per-residue inclusion information can be found in section 3 on page 14.

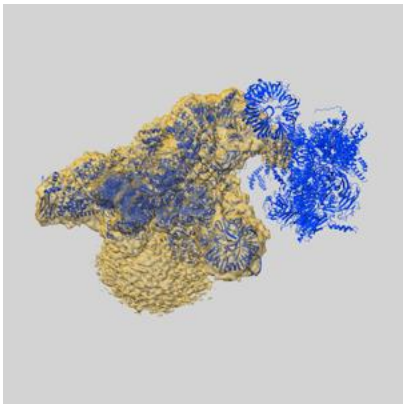
9.1 Map-model overlay



X



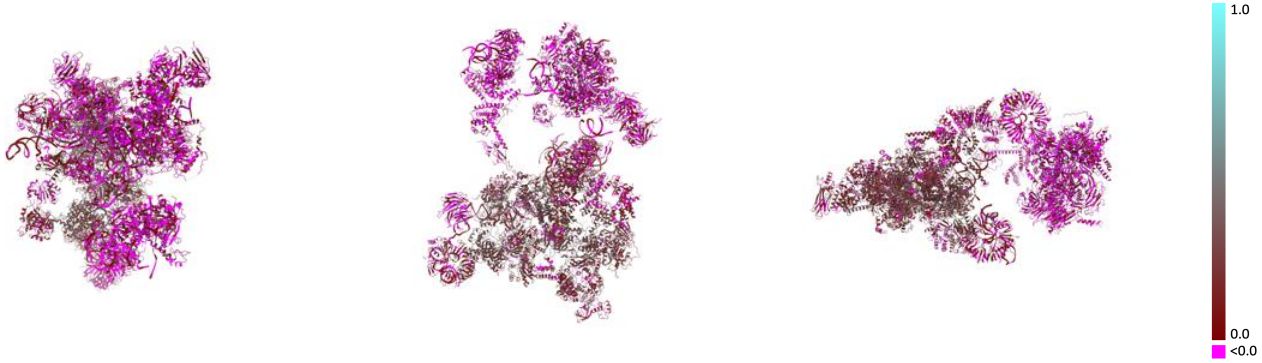
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.015 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.

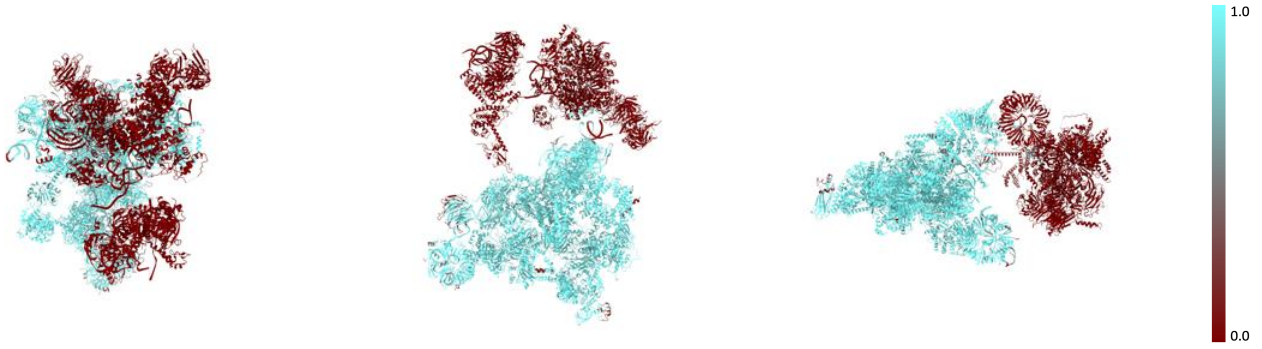
9.2 Q-score mapped to coordinate model



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.

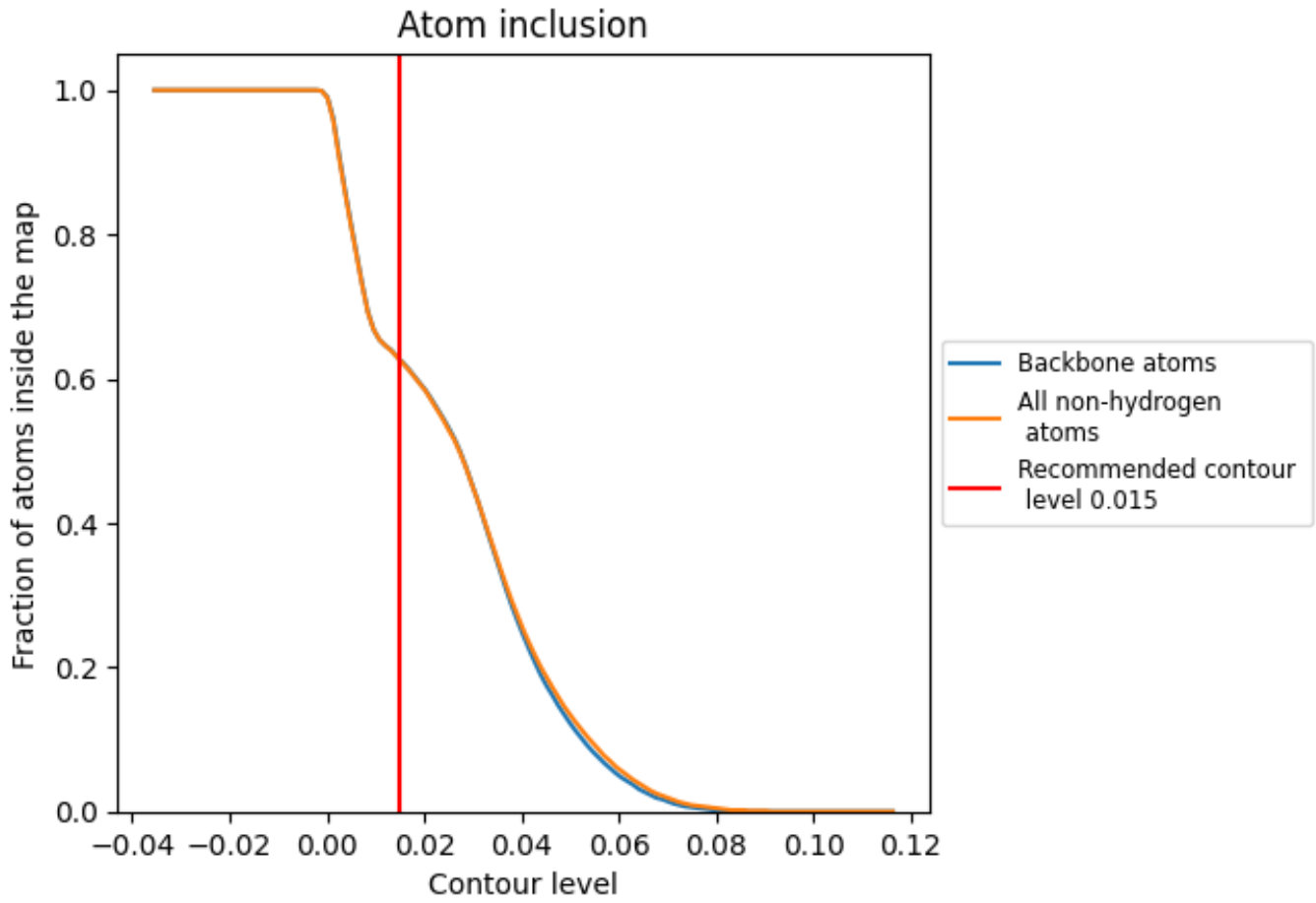
9.3 Atom inclusion mapped to coordinate model



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 (0.015).

9.4 Atom inclusion (i)



At the recommended contour level, 63% of all backbone atoms, 63% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6260	0.1190
1	0.0190	0.0020
2	0.0360	0.0050
3	0.0000	-0.0030
4	0.0000	-0.0090
5	0.0000	-0.0110
6	0.0000	-0.0050
7	0.0000	0.0920
A	0.9900	0.2830
B	0.9360	0.1220
C	1.0000	0.2810
D	0.9740	0.1980
E	0.7270	-0.0190
F	0.7860	0.1010
G	0.0000	0.0150
H	0.0530	-0.0000
I	0.9330	0.1200
J	0.9580	0.0740
K	0.9940	0.0920
L	0.9870	0.1530
M	0.9900	0.2130
N	0.9580	0.1260
O	0.9750	0.2170
P	0.9570	0.1190
Q	0.9210	0.0870
R	0.8920	0.0800
S	0.9230	0.1050
T	0.9060	0.0760
U	0.9100	0.0820
V	0.9550	0.1500
W	0.9250	0.1840
X	0.9610	0.1200
a	0.9650	0.1010
b	0.8400	0.0480
c	0.9040	0.0990

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
d	0.8760	0.1480
e	1.0000	0.2090
f	1.0000	0.1490
g	0.9290	0.1560
h	0.0000	0.0120
i	0.0000	-0.0140
j	0.0000	-0.0180
k	0.0000	0.0390
l	0.0000	0.0120
m	0.0000	0.0380
n	0.0000	0.0170
o	0.0000	-0.0050
p	0.0000	0.0060
q	0.0000	0.0370
r	0.0000	0.0420
s	0.0000	-0.0520
t	0.0000	-0.0050
u	0.0000	0.0100
v	0.0000	0.0170
w	0.0000	-0.0140
x	0.0000	0.0050
y	0.0000	0.0190
z	0.0000	-0.0140