wwPDB EM Validation Summary Report (i)

Nov 2, 2024 – 09:39 pm GMT

PDB ID	:	6QDV
EMDB ID	:	EMD-4525
Title	:	Human post-catalytic P complex spliceosome
Authors	:	Fica, S.M.; Oubridge, C.; Wilkinson, M.E.; Newman, A.J.; Nagai, K.
Deposited on	:	2019-01-03
Resolution	:	3.30 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

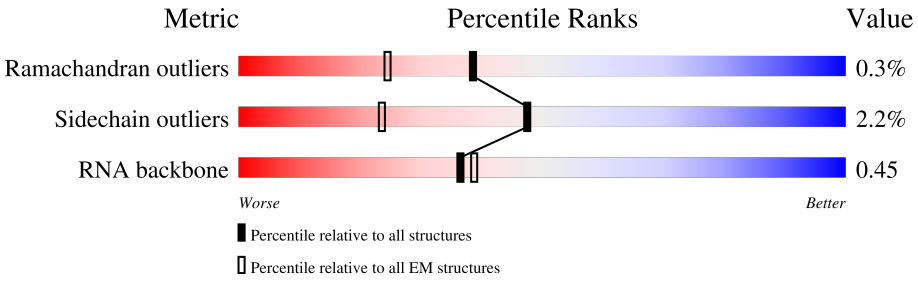
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.30 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	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	2	189	38% 44% 18% · 37%
2	5	116	9% 39% 22% · 35%
3	6	106	12% 55% 34% · 8%
4	7	390	100% 98% ·
5	8	91	100% 97% · ·
6	9	144	100% 99% ·
7	A	2335	15% 94% · ·
8	B	1722	100% 89% 10%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	C	899	12% 99%
10	D	123	54% 99%
11	E	14	7% 57% 29% 14%
12	F	122	18% 100%
13	G	60	17% 97%
14	H	908	30% 50% 49%
15	I	113	9% 19% 15% 63%
16	J	320	100%
17	K	295	26% 99%
18	L	144	6% 96%
19	M	289	39% 99%
20	N	306	15% 99%
21	O	802	27% 55% 45%
22	P	229	8% 46% 54%
23	R	26	92% 8%
24	S	848	37% 66% 33%
25	T	855	73% 73% 25%
26	U	1485	89% 86% 11%
27	V	1220	55% 55% 42%
28	W	162	99% 99%
29	Y	92	100% 100%
30	Z	30	7% 100%
31	b	82	59% 83% 17%
31	k	82	90% 100%
32	c	586	7% 46% 54%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
33	d	84	39% 100%
33	n	84	49% 99%
34	e	81	96% 98%
34	p	81	88% 100%
35	f	72	99% 99%
35	q	72	97% 100%
36	g	73	81% 100%
36	r	73	59% 99%
37	h	80	94% 100%
37	l	80	96% 100%
38	i	164	22% 100%
39	j	118	81% 81% 19%
39	m	118	81% 81% 19%
40	o	513	12% 99%
41	s	225	73% 74% 25%
42	t	504	25% 25% 75%
42	u	504	23% 23% 77%
42	v	504	25% 25% 75%
42	w	504	23% 23% 77%
43	y	144	20% 99%
44	z	34	100% 100%

2 Entry composition (i)

There are 50 unique types of molecules in this entry. The entry contains 121152 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 U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	2	120	2535	1135	428	852	120	0	0

- Molecule 2 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	5	75	1579	708	264	532	75	0	0

- Molecule 3 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	6	97	2075	928	381	669	97	0	0

- Molecule 4 is a protein called Eukaryotic initiation factor 4A-III, N-terminally processed.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	7	390	3130	1976	546	589	19	0	0

- Molecule 5 is a protein called RNA-binding protein 8A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	8	91	730	463	122	142	3	0	0

- Molecule 6 is a protein called Protein mago nashi homolog 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	9	144	1196	772	200	221	3	0	0

- Molecule 7 is a protein called Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	2250	Total	C	N	O	S	0	0
			18655	12009	3256	3309	81		

- Molecule 8 is a protein called U5 small nuclear ribonucleoprotein 200 kDa helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	1722	Total	C	N	O	S	0	0
			13846	8848	2369	2557	72		

- Molecule 9 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	899	Total	C	N	O	S	0	0
			7116	4553	1184	1345	34		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	SER	deletion	UNP Q15029

- Molecule 10 is a protein called PRKR-interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D	123	Total	C	N	O	S	0	0
			1013	635	193	180	5		

- Molecule 11 is a RNA chain called Ligated exons: MINX mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	E	14	Total	C	N	O	P	0	0
			296	132	52	98	14		

- Molecule 12 is a protein called Cactin.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F	122	Total	C	N	O	S	0	0
			1084	712	197	173	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	654	ALA	GLU	conflict	UNP Q8WUQ7

- Molecule 13 is a protein called Protein FAM32A.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G	60	Total	C	N	O	S	0	0
			504	314	96	92	2		

- Molecule 14 is a protein called Pre-mRNA-splicing factor CWC22 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	H	459	Total	C	N	O	S	0	0
			3713	2380	634	678	21		

- Molecule 15 is a RNA chain called Intron lariat: MINX RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	I	42	Total	C	N	O	P	0	0
			872	390	148	292	42		

- Molecule 16 is a protein called Pleiotropic regulator 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	J	320	Total	C	N	O	S	0	0
			2523	1594	457	464	8		

- Molecule 17 is a protein called SNW domain-containing protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	K	295	Total	C	N	O	P	S	0	0
			2360	1479	431	435	2	13		

- Molecule 18 is a protein called Protein BUD31 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	L	144	Total	C	N	O	S	0	0
			1188	748	218	210	12		

- Molecule 19 is a protein called Pre-mRNA-splicing factor RBM22.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	M	289	Total	C	N	O	S	0	0
			2318	1455	416	428	19		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	143	ALA	THR	conflict	UNP Q9NW64
M	144	ALA	SER	conflict	UNP Q9NW64
M	145	ALA	ASP	conflict	UNP Q9NW64
M	146	ALA	MET	conflict	UNP Q9NW64

- Molecule 20 is a protein called U5 small nuclear ribonucleoprotein 40 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	N	306	Total	C	N	O	S	0	0
			2394	1501	422	457	14		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	?	-	ALA	deletion	UNP Q96DI7

- Molecule 21 is a protein called Cell division cycle 5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	O	441	Total	C	N	O	S	0	0
			3416	2116	648	639	13		

- Molecule 22 is a protein called Spliceosome-associated protein CWC15 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	P	106	Total	C	N	O	S	0	0
			888	544	174	168	2		

- Molecule 23 is a protein called Serine/arginine repetitive matrix protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	R	26	Total	C	N	O	S	0	0
			193	120	36	36	1		

- Molecule 24 is a protein called Crooked neck-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	S	570	Total	C	N	O	S	0	0
			3965	2482	740	737	6		

- Molecule 25 is a protein called Pre-mRNA-splicing factor SYF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	T	639	Total	C	N	O	S	0	0
			4003	2479	748	763	13		

- Molecule 26 is a protein called Intron-binding protein aquarius.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	U	1322	Total	C	N	O	S	4	0
			10885	6989	1879	1963	54		

- Molecule 27 is a protein called ATP-dependent RNA helicase DHX8.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	V	713	Total	C	N	O	S	0	0
			2995	1538	722	734	1		

- Molecule 28 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	W	162	Total	C	N	O	S	0	0
			1282	820	219	240	3		

- Molecule 29 is a protein called U2 small nuclear ribonucleoprotein B".

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Y	92	Total	C	N	O	S	0	0
			745	480	130	130	5		

- Molecule 30 is a protein called NF-kappa-B-activating protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Z	30	Total	C	N	O	S	0	0
			230	140	43	45	2		

- Molecule 31 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	b	68	Total	C	N	O	S	0	0
			545	347	95	96	7		
31	k	82	Total	C	N	O	S	0	0
			664	419	121	117	7		

- Molecule 32 is a protein called Pre-mRNA-splicing factor SLU7.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	c	269	Total	C	N	O	S	0	0
			2215	1392	397	418	8		

- Molecule 33 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	d	84	Total	C	N	O	S	0	0
			658	412	116	124	6		
33	n	83	Total	C	N	O	S	0	0
			652	409	115	122	6		

- Molecule 34 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	e	79	Total	C	N	O	S	0	0
			651	413	115	118	5		
34	p	81	Total	C	N	O	S	0	0
			669	424	119	121	5		

- Molecule 35 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	f	72	Total	C	N	O	S	0	0
			562	364	93	100	5		
35	q	72	Total	C	N	O	S	0	0
			562	364	93	100	5		

- Molecule 36 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	g	73	Total	C	N	O	S	0	0
			568	358	102	102	6		
36	r	73	Total	C	N	O	S	0	0
			568	358	102	102	6		

- Molecule 37 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	h	80	Total	C	N	O	S	0	0
			634	404	111	115	4		
37	l	80	Total	C	N	O	S	0	0
			634	404	111	115	4		

- Molecule 38 is a protein called Peptidyl-prolyl cis-trans isomerase-like 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	i	164	Total	C	N	O	S	0	0
			1270	810	220	233	7		

- Molecule 39 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	j	95	Total	C	N	O	S	0	0
			774	486	141	142	5		
39	m	95	Total	C	N	O	S	0	0
			774	486	141	142	5		

- Molecule 40 is a protein called Pre-mRNA-processing factor 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	o	513	Total	C	N	O	S	0	0
			4157	2643	719	771	24		

- Molecule 41 is a protein called Pre-mRNA-splicing factor SPF27.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	s	169	Total	C	N	O	S	0	0
			1402	872	257	264	9		

- Molecule 42 is a protein called Pre-mRNA-processing factor 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	t	125	Total	C	N	O	S	0	0
			988	618	176	190	4		
42	u	118	Total	C	N	O	S	0	0
			938	586	167	181	4		
42	v	125	Total	C	N	O	S	0	0
			988	618	176	190	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
42	w	118	Total	C	N	O	S	0	0
			938	586	167	181	4		

- Molecule 43 is a protein called Pre-mRNA-splicing factor SYF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	y	144	Total	C	N	O	S	0	0
			1218	758	225	233	2		

- Molecule 44 is a protein called Replication stress response regulator SDE2.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	z	34	Total	C	N	O	S	0	0
			280	166	59	53	2		

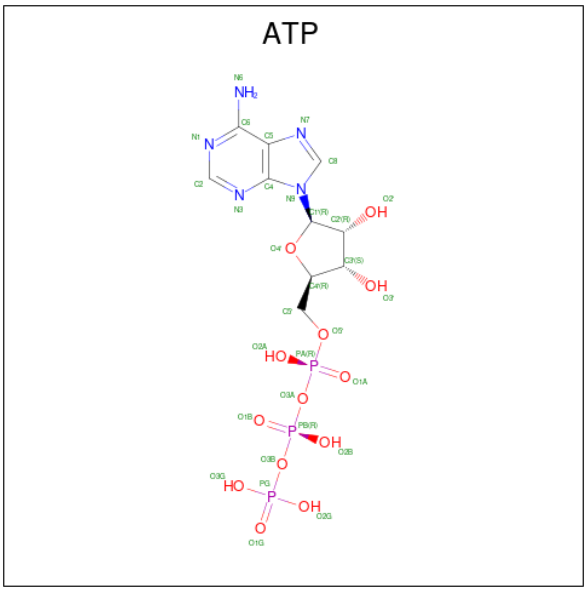
- Molecule 45 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
45	6	5	Total	Mg	0
			5	5	
45	7	1	Total	Mg	0
			1	1	
45	C	1	Total	Mg	0
			1	1	

- Molecule 46 is POTASSIUM ION (three-letter code: K) (formula: K).

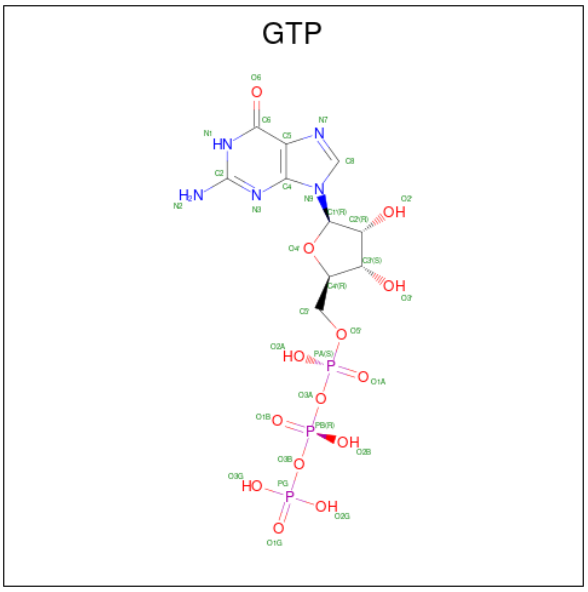
Mol	Chain	Residues	Atoms		AltConf
46	6	1	Total	K	0
			1	1	

- Molecule 47 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
47	7	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 48 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

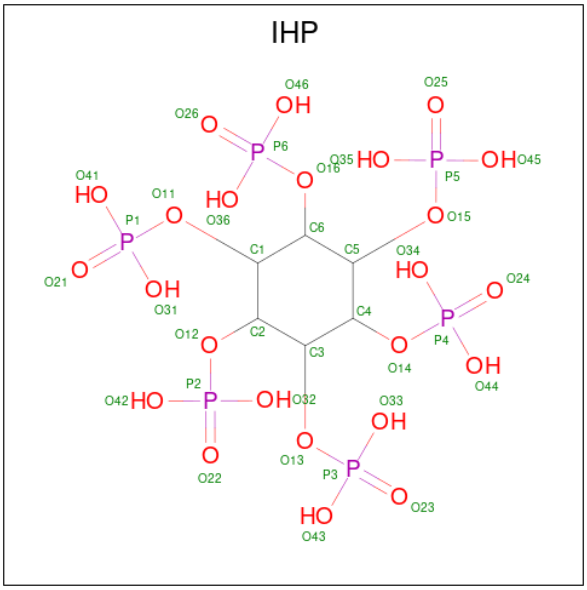


Mol	Chain	Residues	Atoms					AltConf
48	C	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 49 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
49	L	3	Total Zn 3 3	0
49	M	3	Total Zn 3 3	0
49	c	1	Total Zn 1 1	0

- Molecule 50 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$).



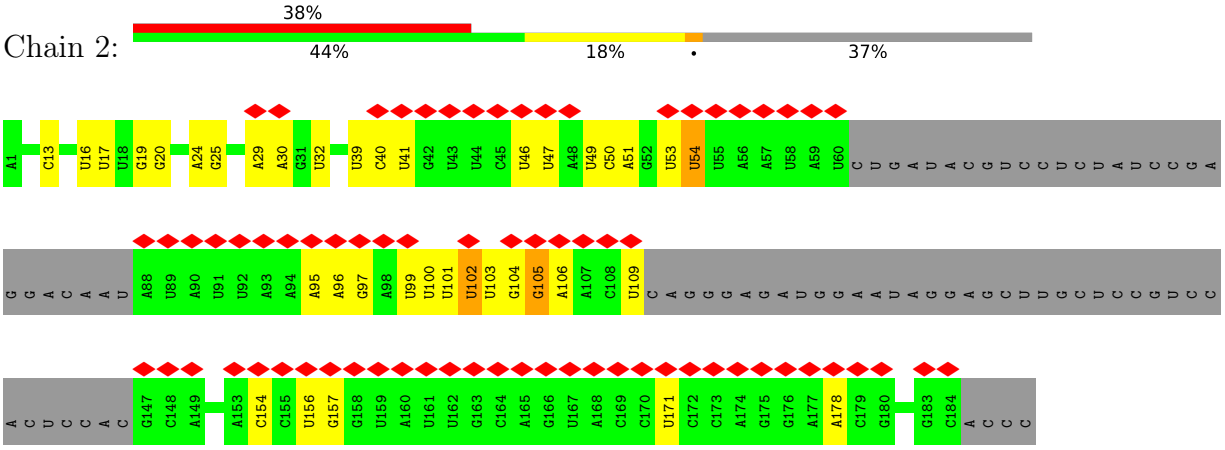
Mol	Chain	Residues	Atoms	AltConf
50	c	1	Total C O P 36 6 24 6	0

3 Residue-property plots

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.

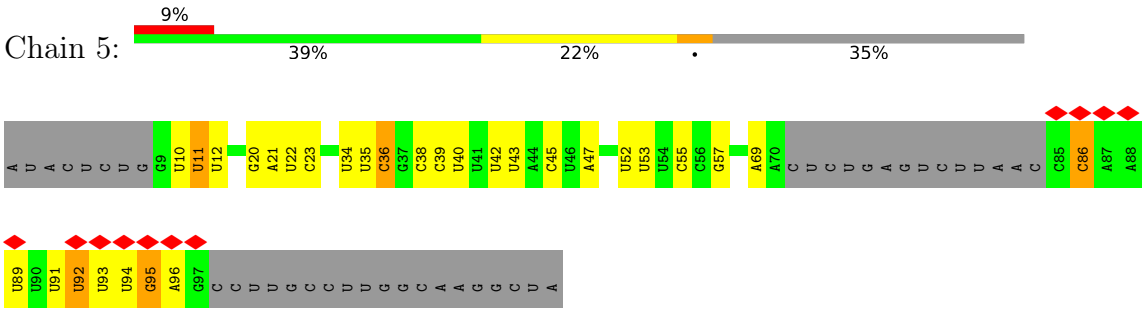
- Molecule 1: U2 snRNA

Chain 2:



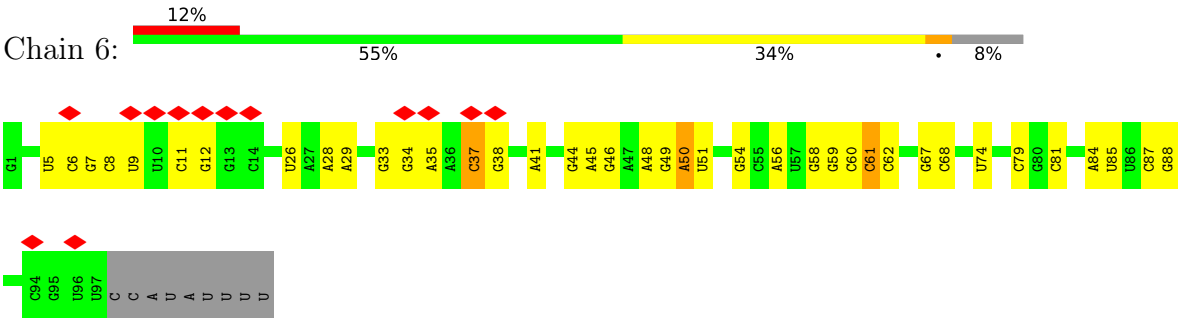
- Molecule 2: U5 snRNA

Chain 5:



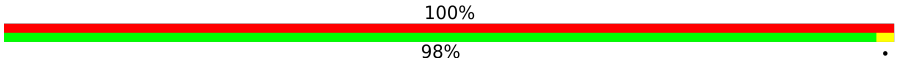
- Molecule 3: U6 snRNA

Chain 6:



- Molecule 4: Eukaryotic initiation factor 4A-III, N-terminally processed

Chain 7:



D22 M23 T24 K25 V26 E27 F28 E29 T30 S31 E32 E33 V34 D35 V36 T37 P38 T39 F40 D41 T42 M43 G44 L45 R46 E47 D48 L49 L50 R51 G52 I53 Y54 A55 Y56 G57 F58 E59 K60 P61 S62 A63 I64 Q65 Q66 R67 A68 I69 K70 Q71 I72 I73 K74 G75 R76 D77 V78 I79 A80 Q81
S82 Q83 S84 G85 T86 G87 K88 T89 A90 T91 F92 S93 I94 S95 V96 L97 Q98 C99 L100 D101 I102 Q103 V104 R105 E106 T107 Q108 A109 L110 I111 L112 A113 P114 T115 R116 E117 L118 A119 V120 Q121 I122 Q123 K124 G125 L126 L127 A128 L129 G130 D131 Y132 M133 N134 V135 Q136 C137 H138 A139 C140 I141
G142 G143 T144 N145 V146 G147 E148 D149 I150 R151 K152 L153 D154 Y155 G156 Q157 H158 V159 V160 A161 G162 T163 P164 G165 R166 V167 F168 D169 M170 I171 R172 R173 R174 S175 L176 R177 T178 R179 A180 I181 K182 M183 L184 V185 L186 D187 E188 A189 D190 E191 M192 L193 N194 K195 G196 F197 K198 E199 Q200 I201
Y202 D203 V204 Y205 R206 Y207 L208 P209 P210 A211 T212 Q213 V214 V215 L216 I217 S218 A219 T220 L221 P222 H223 E224 I225 L226 E227 M228 T229 N230 K231 F232 M233 T234 D235 P236 I237 R238 I239 L240 V241 K242 R243 D244 E245 L246 T247 L248 E249 G250 I251 K252 Q253 F254 P255 V256 A257 V258 E259 R260 E261
E262 W263 K264 F265 D266 T267 L268 C269 D270 L271 Y272 D273 T274 L275 T276 I277 T278 Q279 A280 V281 I282 F283 C284 N285 T286 K287 R288 K289 V290 D291 W292 L293 T294 E295 K296 M297 R298 E299 A300 N301 F302 T303 V304 S305 S306 M307 H308 G309 D310 M311 P312 Q313 K314 E315 R316 E317 S318 I319 M320 K321
E322 F323 R324 S325 G326 A327 S328 R329 V330 L331 I332 S333 T334 D335 V336 W337 A338 R339 G340 L341 D342 V343 P344 Q345 V346 S347 L348 I349 I350 N351 Y352 D353 L354 P355 N356 N357 R358 E359 L360 Y361 I362 H363 R364 I365 G366 R367 S368 G369 R370 Y371 G372 R373 K374 G375 V376 A377 I378 N379 F380 V381
K382 N383 D384 D385 I386 R387 I388 L389 R390 D391 I392 E393 Q394 Y395 Y396 S397 T398 Q399 I400 D401 E402 M403 P404 M405 N406 V407 A408 D409 L410 I411

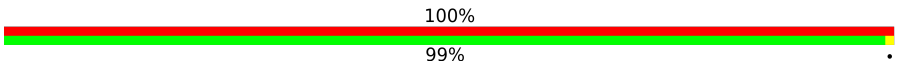
• Molecule 5: RNA-binding protein 8A

Chain 8:

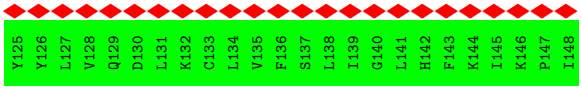
P64 G65 P66 Q67 R68 S69 V70 E71 G72 W73 I74 L75 F76 V77 T78 G79 V80 H81 E82 E83 A84 T85 E86 E87 D88 I89 H90 D91 K92 F93 A94 E95 Y96 G97 E98 I99 K100 N101 I102 H103 L104 N105 L106 D107 R108 R109 T110 G111 Y112 L113 K114 G115 Y116 T117 L118 V119 E120 Y121 E122 T123
Y124 K125 E126 A127 Q128 A129 A130 M131 E132 G133 L134 N135 G136 Q137 D138 L139 M140 G141 Q142 P143 I144 S145 V146 D147 W148 C149 F150 V151 R152 G153 P154

• Molecule 6: Protein mago nashi homolog 2

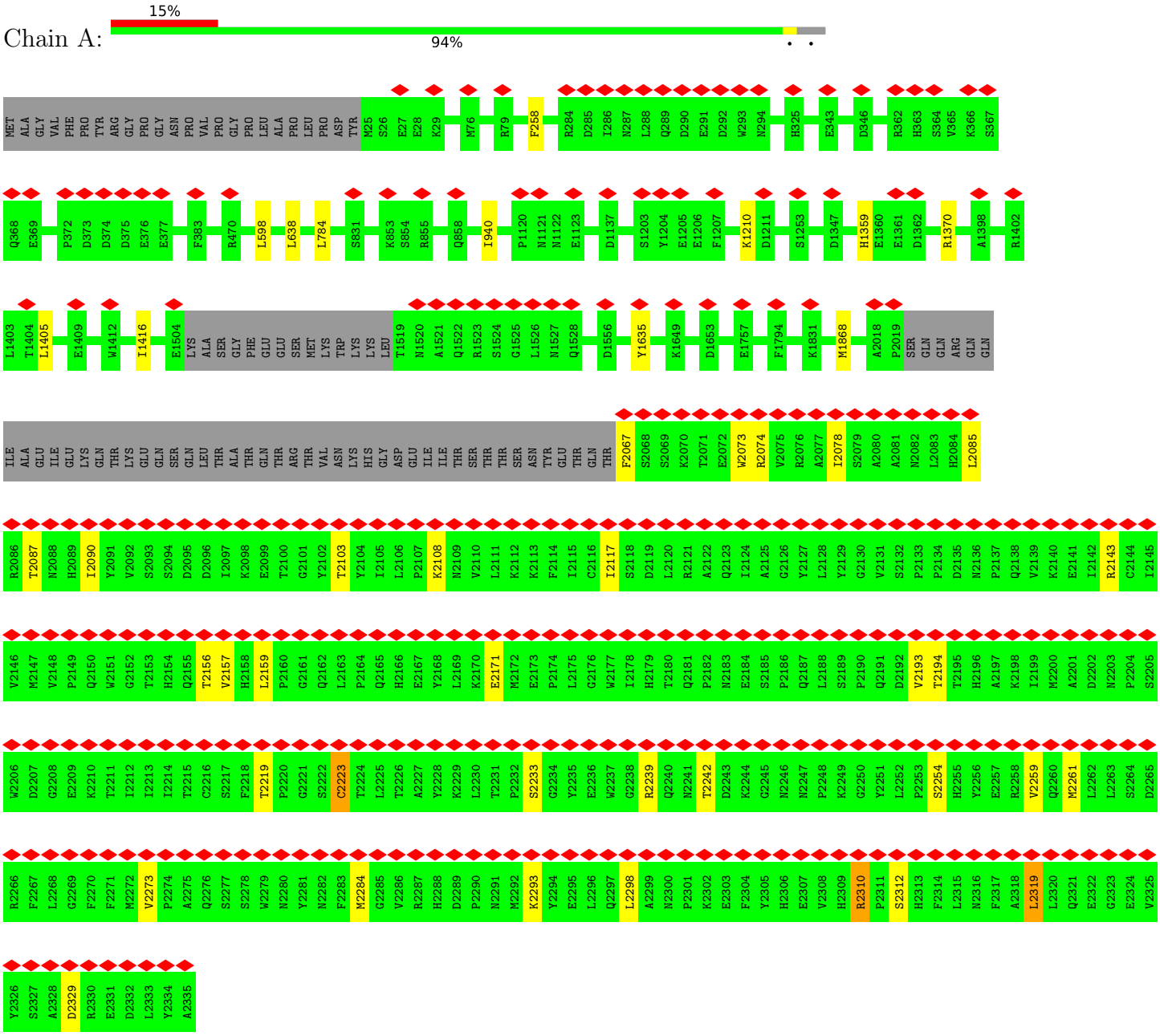
Chain 9:



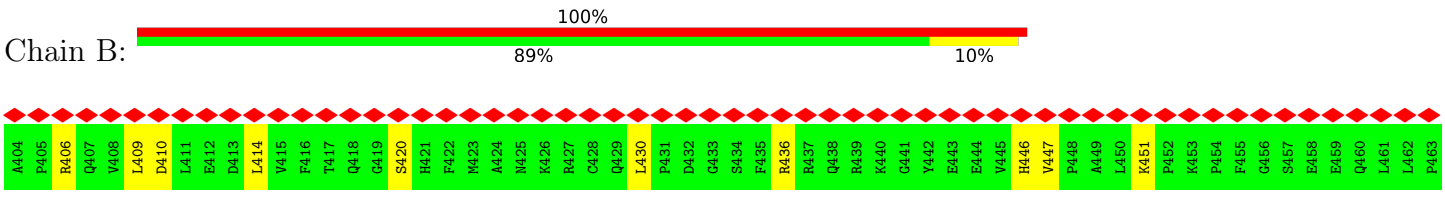
S5 D6 F7 Y8 L9 R10 Y11 Y12 V13 G14 H15 K16 G17 K18 F19 G20 H21 E22 F23 L24 E25 F26 E27 F28 R29 P30 D31 G32 K33 L34 R35 Y36 A37 N38 N39 S40 N41 Y42 K43 N44 D45 V46 M47 I48 R49 K50 E51 A52 Y53 V54 H55 K56 S57 V58 M59 E60 E61 L62 K63 R64
I65 I66 D67 D68 S69 E70 I71 T72 K73 E74 D75 D76 A77 L78 W79 P80 P81 P82 D83 R84 V85 G86 R87 Q88 E89 L90 E91 I92 V93 I94 G95 D96 E97 H98 I99 S100 F101 T102 T103 S104 K105 I106 G107 S108 L109 I110 D111 V112 N113 Q114 S115 K116 D117 P118 E119 G120 L121 R122 V123 F124

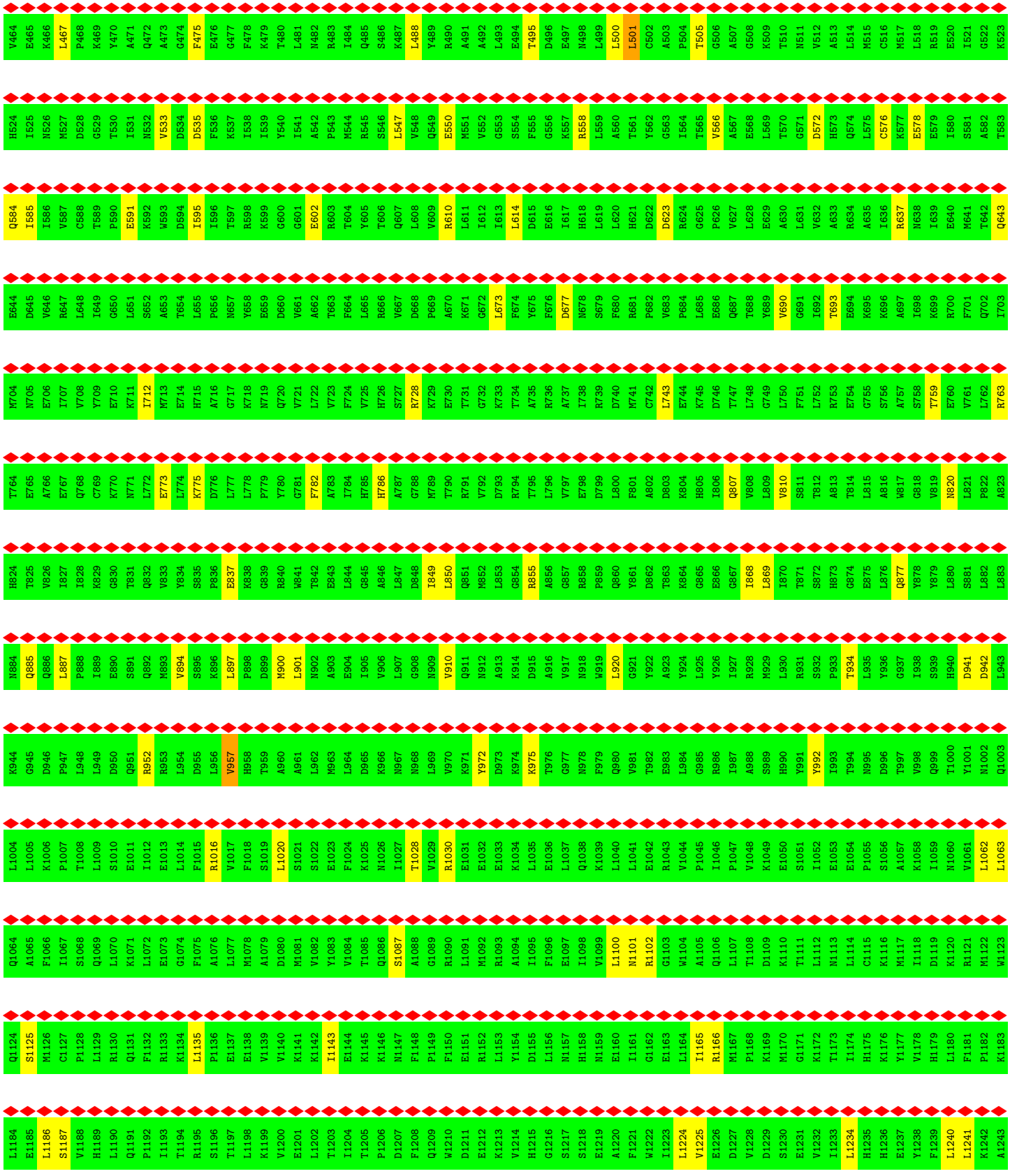


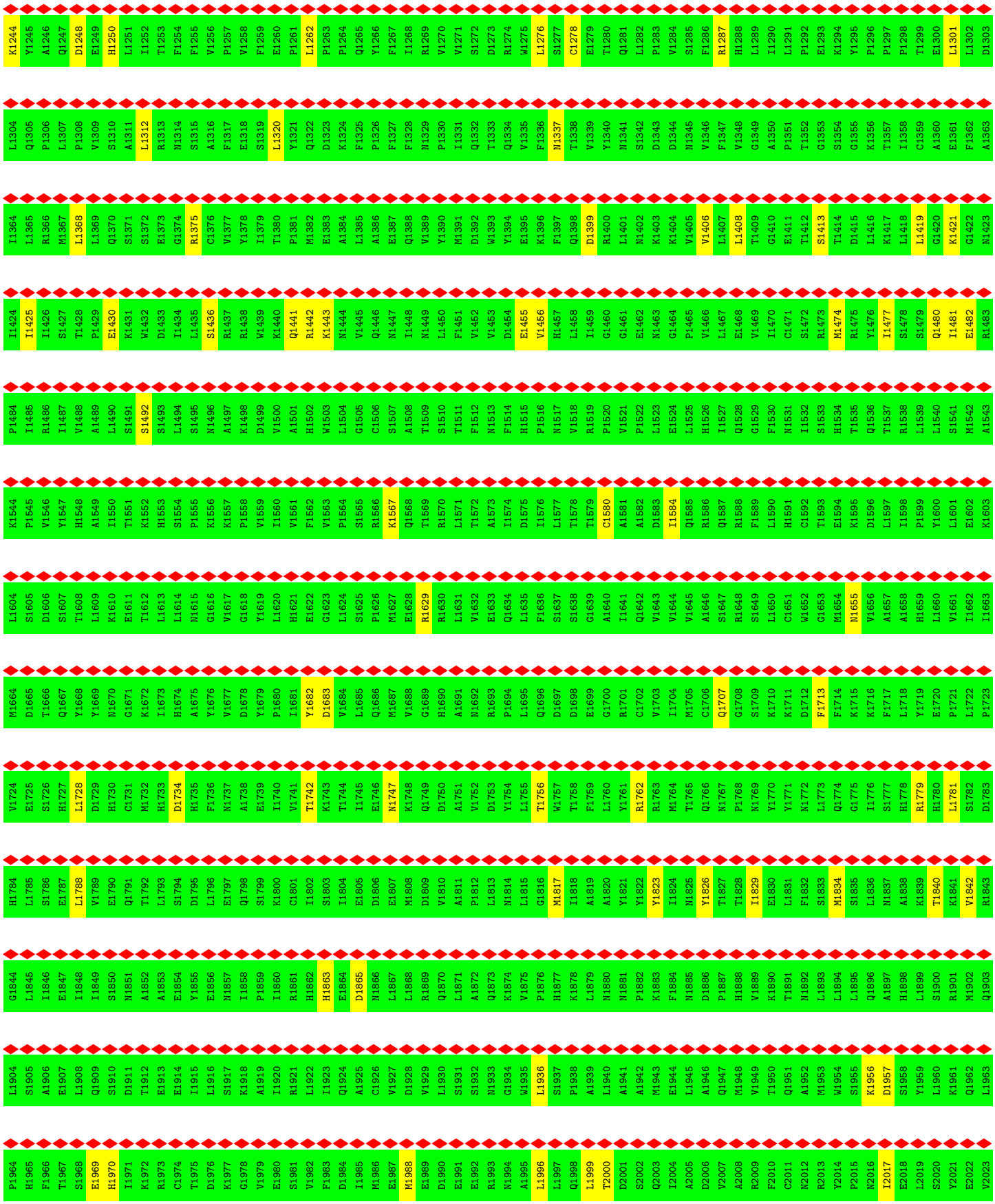
• Molecule 7: Pre-mRNA-processing-splicing factor 8

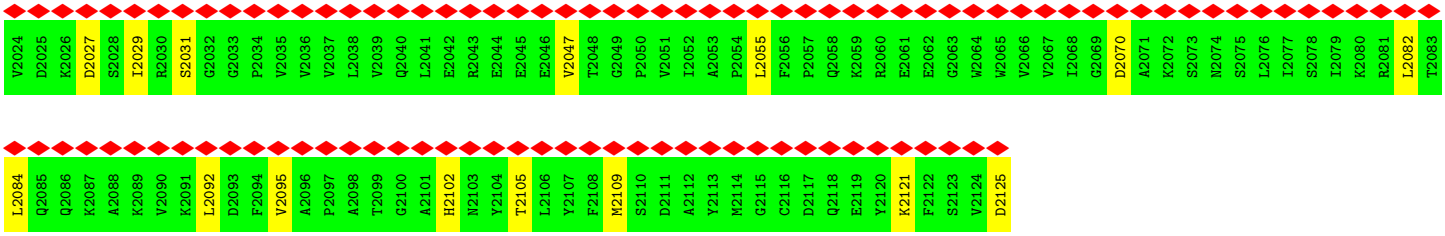


• Molecule 8: U5 small nuclear ribonucleoprotein 200 kDa helicase

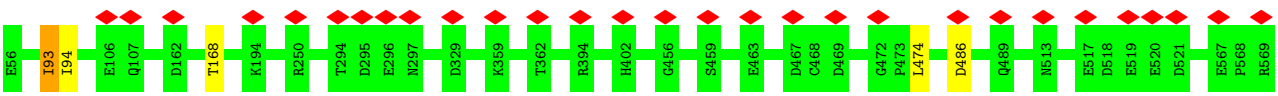



V464 E465 K466 L467 P468 K469 Y470 A471 Q472 A473 G474 F475 E476 G477 F478 K479 T480 L481 N482 R483 I484 Q485 S486 K487 L488 Y489 R490 A491 A492 L493 E494 T495 D496 E497 N498 L499 L500 L501 C502 A503 P504 T505 G506 A507 G508 K509 T510 N511 V512 A513 L514 M515 C516 M517 L518 R519 E520 I521 G522 K523
H524 I525 N526 M527 D528 G529 T530 I531 N532 V533 D534 D535 F536 K537 I538 I539 Y540 I541 A542 P543 M544 R545 S546 L547 V548 Q549 E550 M551 V552 G553 S554 F555 G556 K557 R558 L559 A560 T561 Y562 G563 I564 T565 V566 A567 E568 L569 T570 G571 D572 H573 Q574 L575 C576 K577 E578 E579 I580 S581 A582 T583
Q584 I585 I586 V587 C588 T589 P590 E591 K592 W593 D594 I595 I596 T597 R598 K599 G600 G601 E602 R603 T604 Y605 T606 Q607 L608 V609 R610 L611 I612 I613 L614 D615 E616 I617 H618 L619 L620 H621 D622 D623 R624 G625 P626 V627 L628 E629 A630 L631 V632 A633 R634 A635 I636 R637 N638 I639 E640 M641 T642 Q643
E644 D645 V646 R647 L648 I649 G650 L651 S652 A653 T654 L655 P656 N657 Y658 E659 D660 V661 A662 T663 F664 L665 R666 V667 D668 P669 A670 K671 G672 L673 F674 Y675 F676 D677 N678 S679 F680 R681 P682 V683 P684 L685 E686 Q687 T688 Y689 V690 G691 I692 T693 E694 K695 K696 A697 I698 K699 R700 F701 Q702 I703
M704 N705 E706 I707 V708 Y709 E710 K711 I712 M713 E714 H715 A716 G717 K718 N719 Q720 V721 L722 V723 F724 V725 H726 S727 R728 K729 E730 T731 G732 K733 T734 A735 R736 A737 I738 R739 D740 M741 C742 L743 E744 K745 D746 T747 L748 G749 L750 F751 L752 R753 E754 G755 S756 A757 S758 T759 E760 V761 L762 R763
T764 E765 A766 E767 Q768 C769 K770 N771 L772 E773 L774 K775 D776 L777 L778 P779 Y780 G781 F782 A783 I784 H785 H786 A787 G788 M789 T790 R791 V792 D793 R794 T795 L796 V797 E798 D799 L800 F801 A802 D803 K804 H805 I806 Q807 V808 L809 V810 S811 T812 A813 T814 L815 A816 W817 G818 V819 N820 L821 P822 A823
H824 T825 V826 I827 I828 K829 G830 T831 Q832 V833 Y834 S835 P836 E837 K838 G839 R840 W841 T842 E843 L844 G845 A846 L847 D848 I849 L850 Q851 M852 L853 G854 R855 A856 G857 R858 P859 Q860 Y861 D862 D863 K864 G865 E866 G867 I868 L869 I870 T871 S872 H873 G874 E875 L876 Q877 Y878 Y879 L880 S881 L882 L883
N884 Q885 Q886 L887 P888 I889 E890 S891 Q892 M893 V894 S895 K896 L897 P898 D899 M900 L901 N902 A903 E904 I905 V906 L907 G908 N909 V910 Q911 N912 A913 K914 D915 A916 V917 N918 W919 L920 G921 Y922 A923 Y924 L925 Y926 I927 R928 M929 L930 R931 S932 P933 T934 L935 Y936 G937 I938 S939 H940 D941 D942 L943
K944 G945 D946 P947 L948 L949 D950 Q951 R952 R953 L954 D955 L956 V957 H958 T959 A960 A961 L962 M963 L964 D965 K966 N967 N968 L969 V970 K971 Y972 D973 K974 K975 T976 G977 N978 F979 Q980 V981 T982 E983 L984 G985 R986 I987 A988 S989 H990 Y991 Y992 I993 T994 N995 D996 T997 V998 Q999 T1000 Y1001 N1002 Q1003
L1004 L1005 K1006 P1007 T1008 L1009 S1010 E1011 I1012 E1013 L1014 F1015 R1016 V1017 F1018 S1019 L1020 S1021 S1022 E1023 F1024 K1025 N1026 I1027 T1028 V1029 R1030 E1031 E1032 E1033 K1034 L1035 E1036 L1037 Q1038 K1039 L1040 L1041 E1042 R1043 V1044 P1045 I1046 P1047 V1048 K1049 E1050 S1051 I1052 E1053 E1054 P1055 S1056 A1057 K1058 I1059 N1060 V1061 L1062 L1063
Q1064 A1065 F1066 I1067 S1068 Q1069 L1070 K1071 L1072 E1073 G1074 F1075 A1076 L1077 M1078 A1079 D1080 M1081 V1082 Y1083 V1084 T1085 Q1086 S1087 A1088 G1089 R1090 L1091 M1092 R1093 A1094 I1095 F1096 E1097 I1098 V1099 L1100 N1101 R1102 G1103 W1104 A1105 Q1106 L1107 T1108 D1109 K1110 T1111 L1112 N1113 L1114 C1115 K1116 M1117 I1118 D1119 K1120 R1121 M1122 W1123
Q1124 S1125 M1126 C1127 P1128 L1129 R1130 Q1131 F1132 R1133 K1134 L1135 P1136 E1137 E1138 V1139 V1140 K1141 K1142 I1143 E1144 K1145 K1146 N1147 F1148 P1149 F1150 E1151 R1152 L1153 Y1154 D1155 L1156 N1157 H1158 N1159 E1160 I1161 G1162 E1163 L1164 I1165 R1166 M1167 P1168 K1169 M1170 G1171 K1172 T1173 I1174 H1175 K1176 Y1177 V1178 H1179 L1180 F1181 P1182 K1183
L1184 E1185 L1186 S1187 V1188 H1189 L1190 Q1191 P1192 I1193 T1194 R1195 S1196 T1197 L1198 K1199 V1200 E1201 L1202 T1203 I1204 T1205 P1206 D1207 F1208 Q1209 W1210 D1211 E1212 K1213 V1214 H1215 G1216 S1217 S1218 E1219 A1220 F1221 W1222 I1223 L1224 V1225 E1226 D1227 V1228 D1229 S1230 E1231 V1232 I1233 L1234 H1235 H1236 E1237 Y1238 F1239 L1240 L1241 K1242 A1243

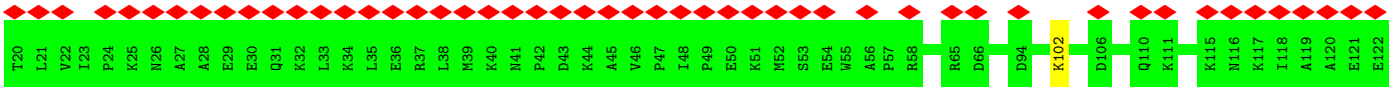

K1244 Y1245 A1246 Q1247 D1248 E1249 H1250 L1251 I1252 T1253 F1254 F1255 V1256 P1257 V1258 F1259 E1260 P1261 L1262 P1263 P1264 Q1265 Y1266 F1267 I1268 R1269 V1270 V1271 S1272 D1273 R1274 W1275 L1276 S1277 C1278 E1279 T1280 Q1281 L1282 P1283 V1284 S1285 F1286 R1287 H1288 L1289 I1290 L1291 P1292 E1293 K1294 Y1295 P1296 P1297 P1298 T1299 E1300 L1301 L1302 D1303
L1304 Q1305 P1306 L1307 P1308 V1309 S1310 A1311 L1312 R1313 N1314 S1315 A1316 F1317 E1318 S1319 L1320 Y1321 Q1322 D1323 K1324 F1325 P1326 F1327 F1328 N1329 P1330 I1331 Q1332 T1333 Q1334 V1335 F1336 N1337 T1338 V1339 Y1340 N1341 S1342 D1343 D1344 N1345 V1346 F1347 V1348 G1349 A1350 P1351 T1352 G1353 S1354 G1355 K1356 T1357 I1358 C1359 A1360 E1361 F1362 A1363
I1364 L1365 R1366 M1367 L1368 L1369 Q1370 S1371 S1372 E1373 G1374 R1375 C1376 V1377 Y1378 I1379 T1380 P1381 M1382 E1383 A1384 L1385 A1386 E1387 Q1388 V1389 Y1390 M1391 D1392 W1393 Y1394 E1395 K1396 F1397 Q1398 D1399 R1400 L1401 N1402 K1403 K1404 V1405 V1406 L1407 L1408 T1409 G1410 E1411 T1412 S1413 T1414 D1415 L1416 K1417 L1418 L1419 G1420 K1421 G1422 N1423
I1424 I1425 I1426 S1427 T1428 P1429 E1430 K1431 W1432 D1433 I1434 L1435 S1436 R1437 R1438 W1439 K1440 Q1441 R1442 K1443 N1444 V1445 Q1446 N1447 I1448 N1449 L1450 F1451 V1452 V1453 D1454 E1455 V1456 H1457 L1458 I1459 G1460 G1461 E1462 N1463 G1464 P1465 V1466 L1467 E1468 V1469 I1470 C1471 S1472 R1473 M1474 R1475 Y1476 I1477 S1478 S1479 Q1480 I1481 E1482 R1483
P1484 I1485 R1486 I1487 V1488 A1489 L1490 S1491 S1492 S1493 L1494 S1495 N1496 A1497 K1498 D1499 V1500 A1501 H1502 W1503 L1504 G1505 C1506 S1507 A1508 T1509 S1510 T1511 F1512 N1513 F1514 H1515 P1516 N1517 V1518 R1519 P1520 V1521 P1522 L1523 E1524 L1525 H1526 I1527 Q1528 G1529 F1530 N1531 I1532 S1533 H1534 T1535 Q1536 L1537 R1538 L1539 L1540 S1541 M1542 A1543
K1544 P1545 V1546 Y1547 H1548 A1549 I1550 T1551 K1552 H1553 S1554 P1555 K1556 K1557 P1558 V1559 I1560 V1561 P1562 V1563 P1564 S1565 R1566 K1567 Q1568 T1569 R1570 L1571 T1572 A1573 I1574 D1575 I1576 L1577 T1578 T1579 C1580 A1581 A1582 D1583 I1584 Q1585 R1586 Q1587 R1588 F1589 L1590 H1591 C1592 T1593 E1594 K1595 D1596 L1597 I1598 P1599 Y1600 L1601 E1602 K1603
L1604 S1605 D1606 S1607 Y1608 L1609 K1610 E1611 T1612 L1613 L1614 N1615 G1616 V1617 G1618 Y1619 L1620 H1621 E1622 G1623 L1624 S1625 P1626 M1627 E1628 R1629 R1630 L1631 V1632 E1633 Q1634 L1635 F1636 S1637 S1638 G1639 A1640 I1641 Q1642 V1643 V1644 V1645 A1646 S1647 R1648 S1649 L1650 C1651 W1652 G1653 M1654 N1655 V1656 A1657 A1658 H1659 L1660 V1661 I1662 I1663
M1664 D1665 T1666 Q1667 H1668 Y1669 N1670 G1671 K1672 I1673 H1674 A1675 Y1676 V1677 D1678 Y1679 P1680 I1681 Y1682 D1683 Y1684 L1685 Q1686 M1687 V1688 G1689 H1690 A1691 N1692 R1693 P1694 L1695 Q1696 D1697 D1698 E1699 G1700 R1701 C1702 V1703 I1704 M1705 C1706 Q1707 G1708 S1709 K1710 K1711 D1712 F1713 F1714 K1715 K1716 F1717 L1718 Y1719 E1720 P1721 L1722 P1723
V1724 E1725 S1726 H1727 L1728 D1729 H1730 C1731 M1732 H1733 D1734 H1735 F1736 N1737 A1738 E1739 I1740 V1741 T1742 K1743 T1744 I1745 E1746 N1747 K1748 Q1749 D1750 A1751 V1752 D1753 Y1754 L1755 T1756 W1757 T1758 F1759 L1760 Y1761 R1762 R1763 M1764 T1765 Q1766 N1767 P1768 N1769 Y1770 Y1771 N1772 L1773 Q1774 G1775 I1776 S1777 H1778 R1779 H1780 L1781 S1782 D1783
H1784 L1785 S1786 E1787 L1788 V1789 E1790 Q1791 T1792 L1793 S1794 D1795 L1796 E1797 Q1798 S1799 K1800 C1801 I1802 S1803 I1804 E1805 D1806 E1807 M1808 D1809 V1810 A1811 P1812 L1813 N1814 L1815 G1816 M1817 I1818 A1819 A1820 Y1821 Y1822 Y1823 I1824 N1825 Y1826 T1827 T1828 I1829 E1830 L1831 F1832 S1833 M1834 S1835 L1836 N1837 A1838 K1839 T1840 K1841 V1842 R1843
G1844 L1845 I1846 E1847 I1848 I1849 S1850 N1851 A1852 A1853 E1854 Y1855 E1856 N1857 I1858 P1859 I1860 R1861 H1862 H1863 E1864 D1865 N1866 L1867 L1868 R1869 Q1870 L1871 A1872 Q1873 K1874 V1875 P1876 H1877 K1878 L1879 N1880 N1881 P1882 K1883 F1884 N1885 D1886 P1887 H1888 V1889 K1890 T1891 N1892 L1893 L1894 L1895 Q1896 A1897 H1898 L1899 S1900 R1901 M1902 Q1903
L1904 S1905 A1906 E1907 L1908 Q1909 S1910 D1911 T1912 E1913 E1914 I1915 L1916 S1917 K1918 A1919 I1920 R1921 L1922 I1923 Q1924 A1925 C1926 V1927 D1928 V1929 L1930 S1931 S1932 N1933 G1934 W1935 L1936 S1937 P1938 A1939 L1940 A1941 A1942 M1943 E1944 L1945 A1946 Q1947 M1948 V1949 T1950 Q1951 A1952 M1953 W1954 S1955 K1956 D1957 S1958 Y1959 L1960 K1961 Q1962 L1963
P1964 H1965 F1966 T1967 S1968 E1969 H1970 I1971 K1972 R1973 C1974 T1975 D1976 K1977 G1978 V1979 E1980 S1981 V1982 F1983 D1984 I1985 M1986 E1987 M1988 E1989 D1990 E1991 E1992 R1993 N1994 A1995 L1996 L1997 Q1998 L1999 T2000 D2001 S2002 Q2003 I2004 A2005 D2006 V2007 A2008 R2009 F2010 C2011 N2012 R2013 Y2014 P2015 N2016 I2017 E2018 L2019 S2020 Y2021 E2022 V2023



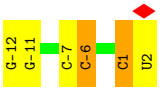
• Molecule 9: 116 kDa U5 small nuclear ribonucleoprotein component



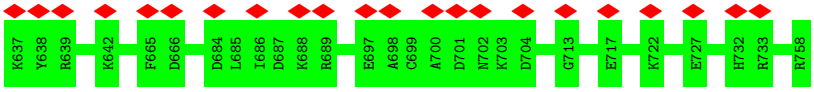
• Molecule 10: PRKR-interacting protein 1



• Molecule 11: Ligated exons: MINX mRNA

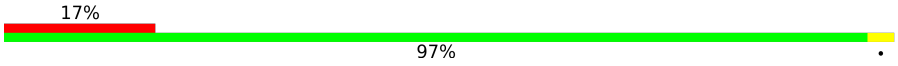


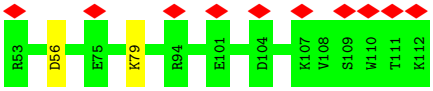
• Molecule 12: Cactin



• Molecule 13: Protein FAM32A

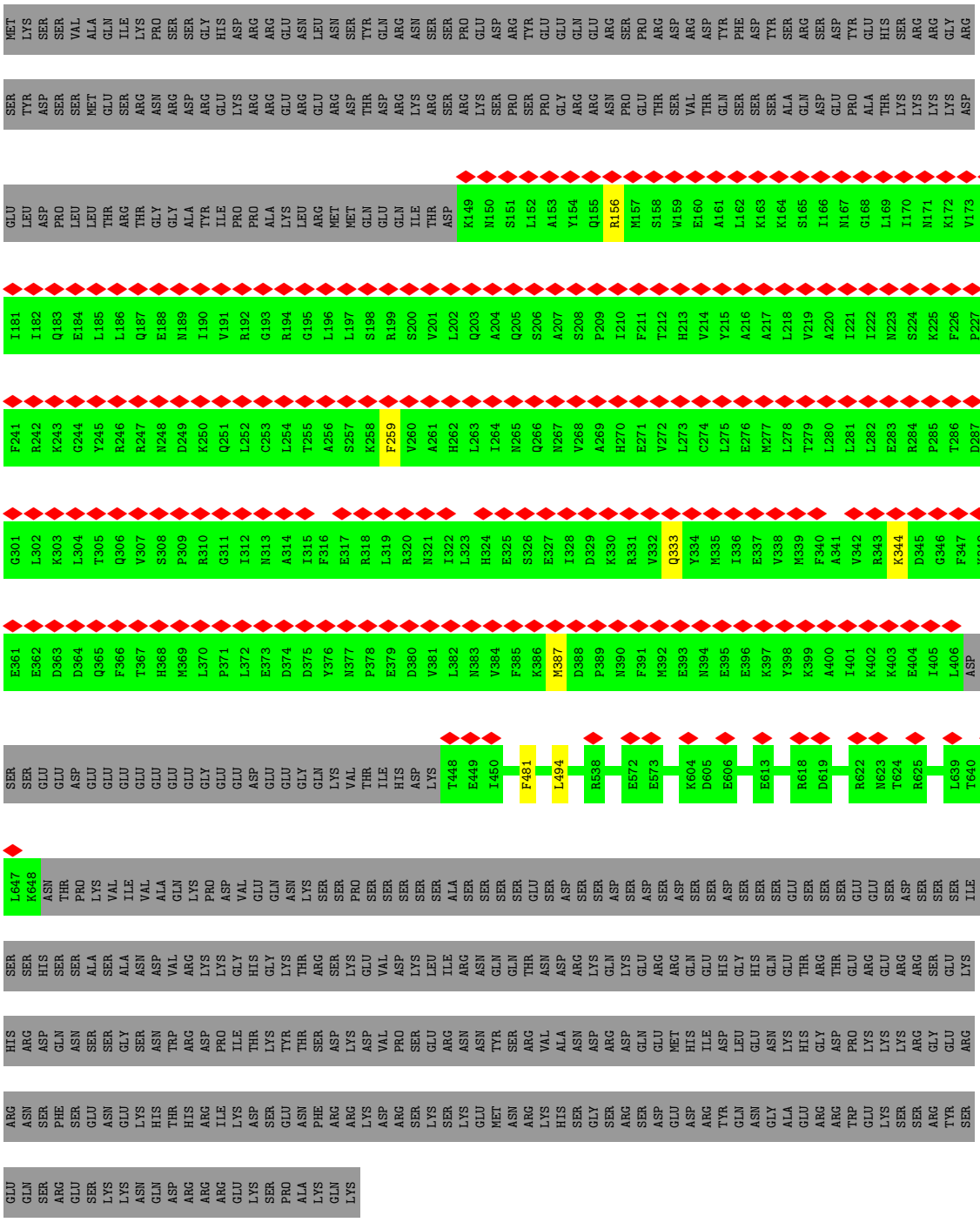
Chain G:





• Molecule 14: Pre-mRNA-splicing factor CWC22 homolog

Chain H:



• Molecule 15: Intron lariat: MINX RNA

Chain I:

• Molecule 16: Pleiotropic regulator 1

Chain J:

• Molecule 17: SNW domain-containing protein 1

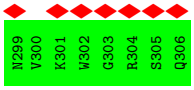
Chain K:

• Molecule 18: Protein BUD31 homolog

Chain L:

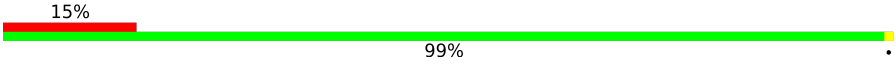
• Molecule 19: Pre-mRNA-splicing factor RBM22

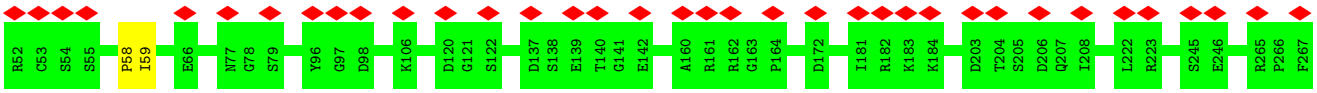
Chain M:

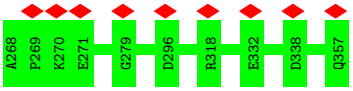


• Molecule 20: U5 small nuclear ribonucleoprotein 40 kDa protein

Chain N:

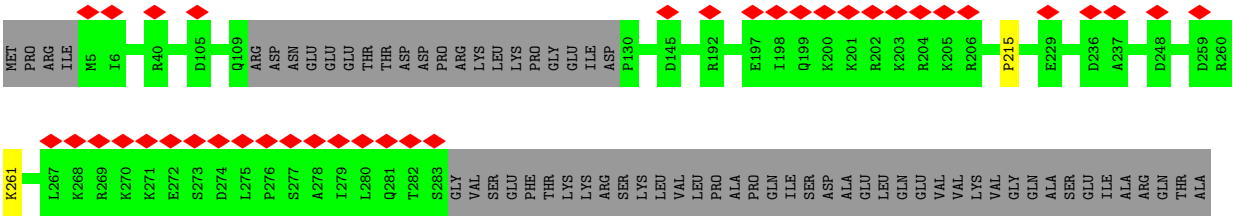


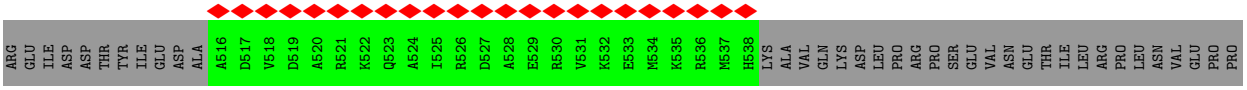


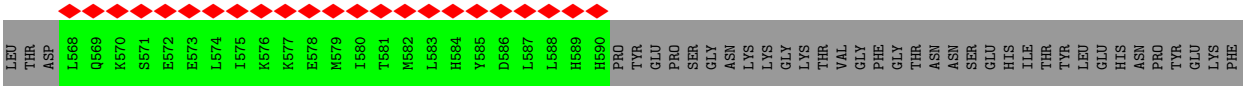


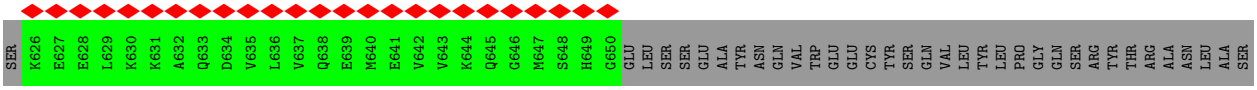
• Molecule 21: Cell division cycle 5-like protein

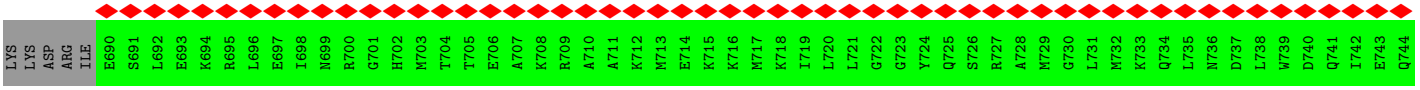
Chain O:

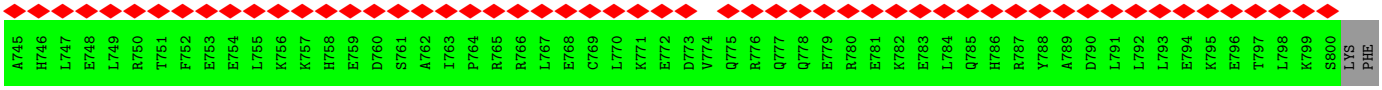






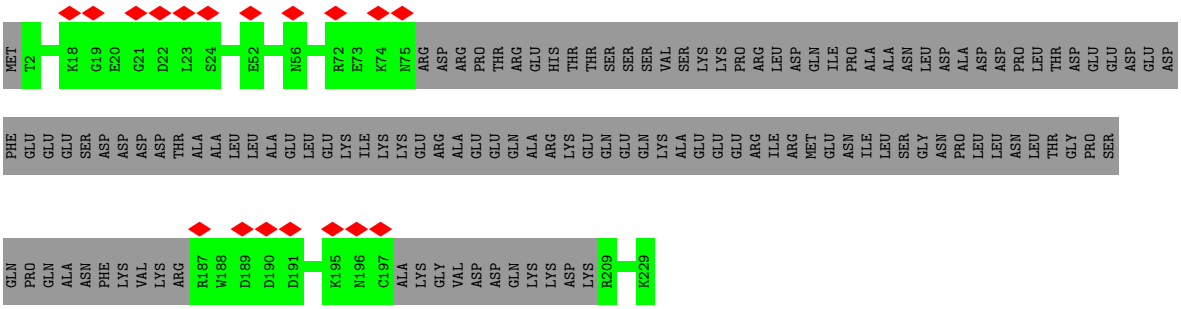






• Molecule 22: Spliceosome-associated protein CWC15 homolog

Chain P:

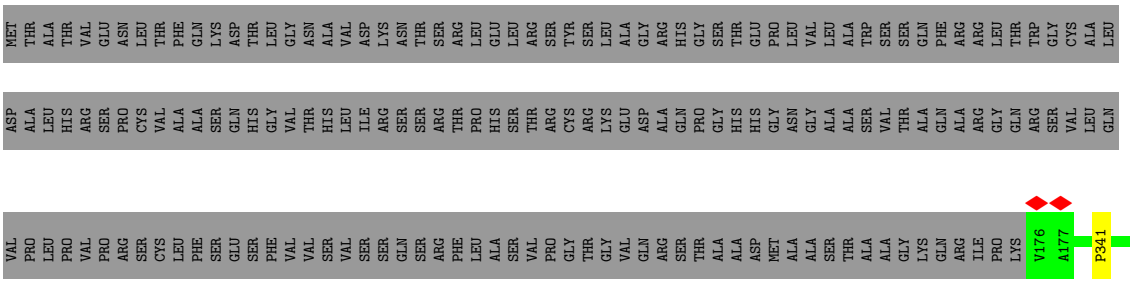


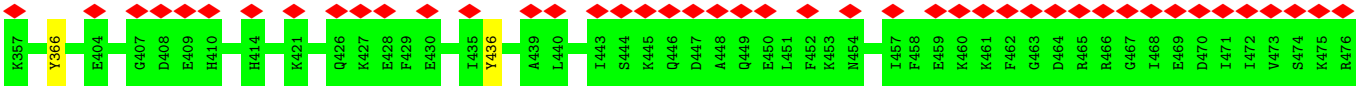
• Molecule 23: Serine/arginine repetitive matrix protein 2

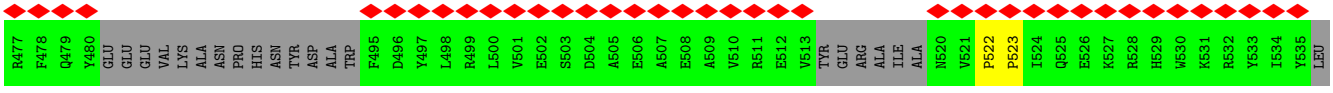
Chain R:

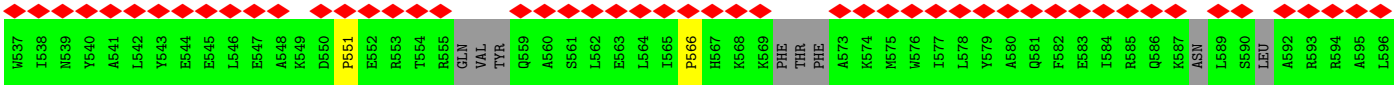
• Molecule 24: Crooked neck-like protein 1

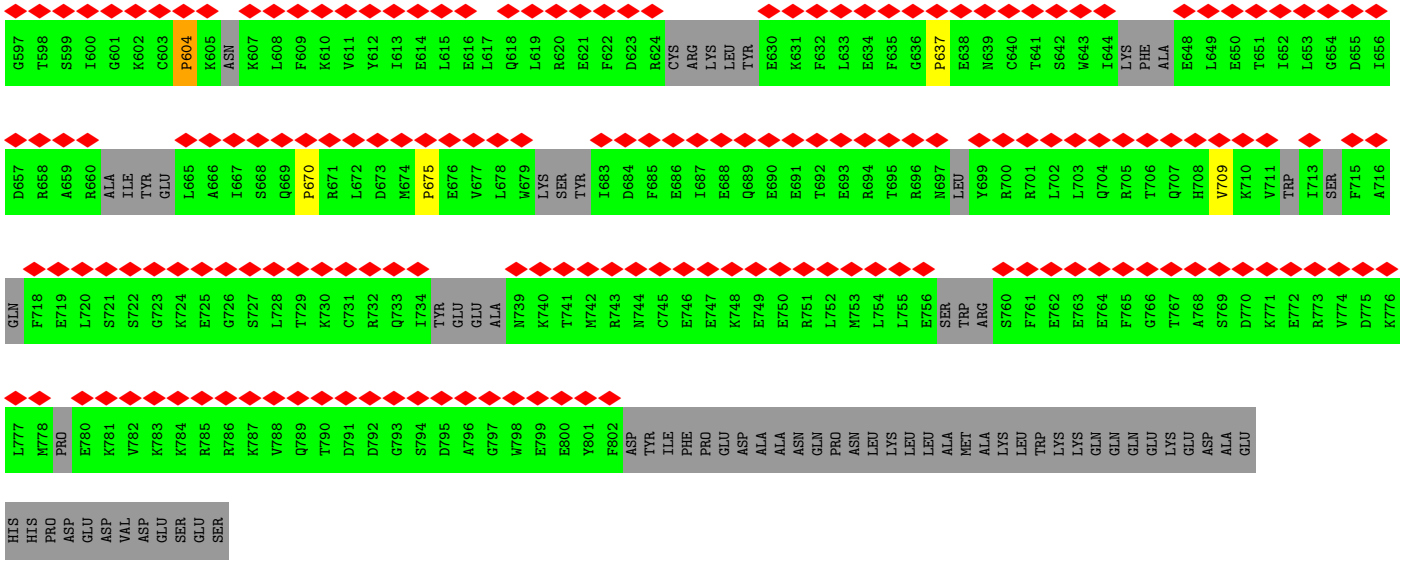
Chain S:





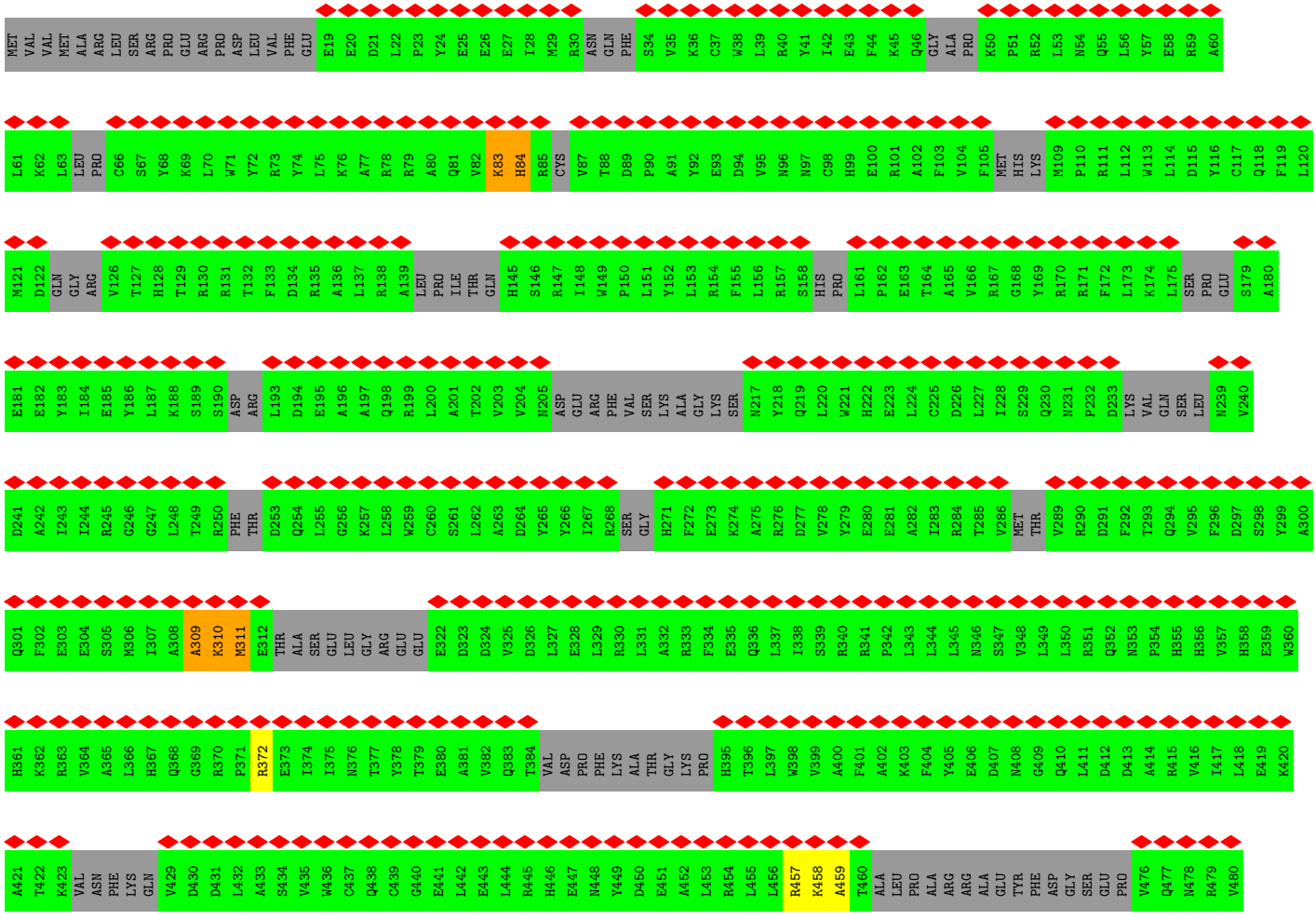


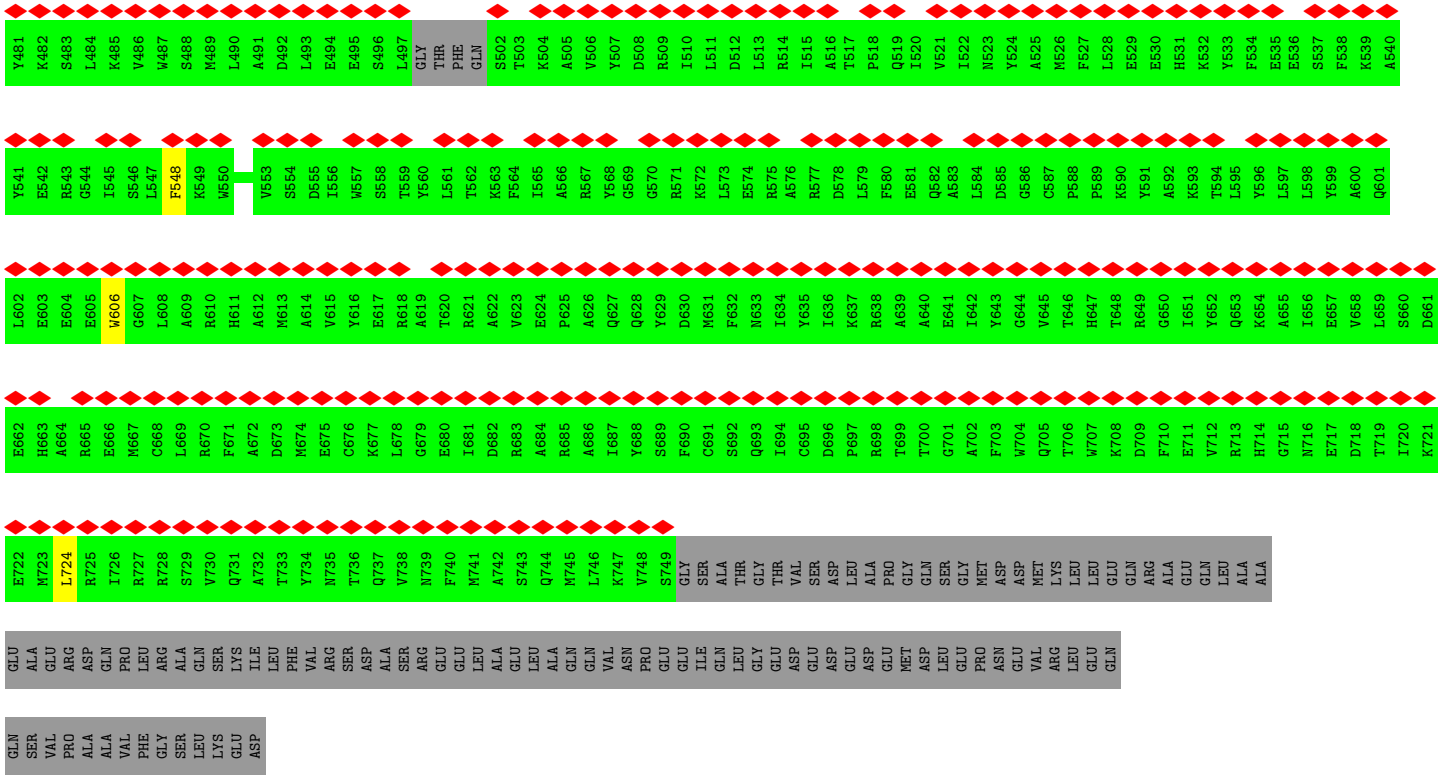




• Molecule 25: Pre-mRNA-splicing factor SYF1

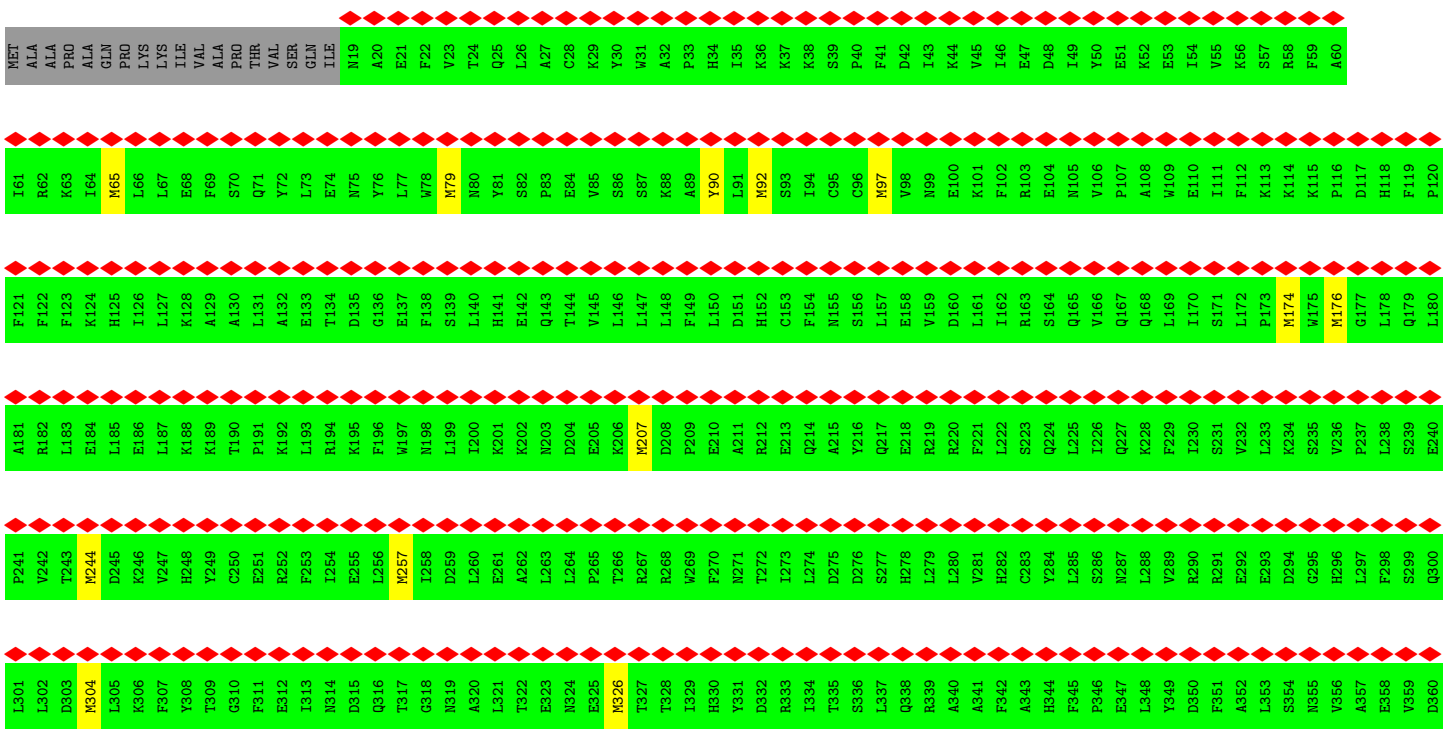
Chain T:

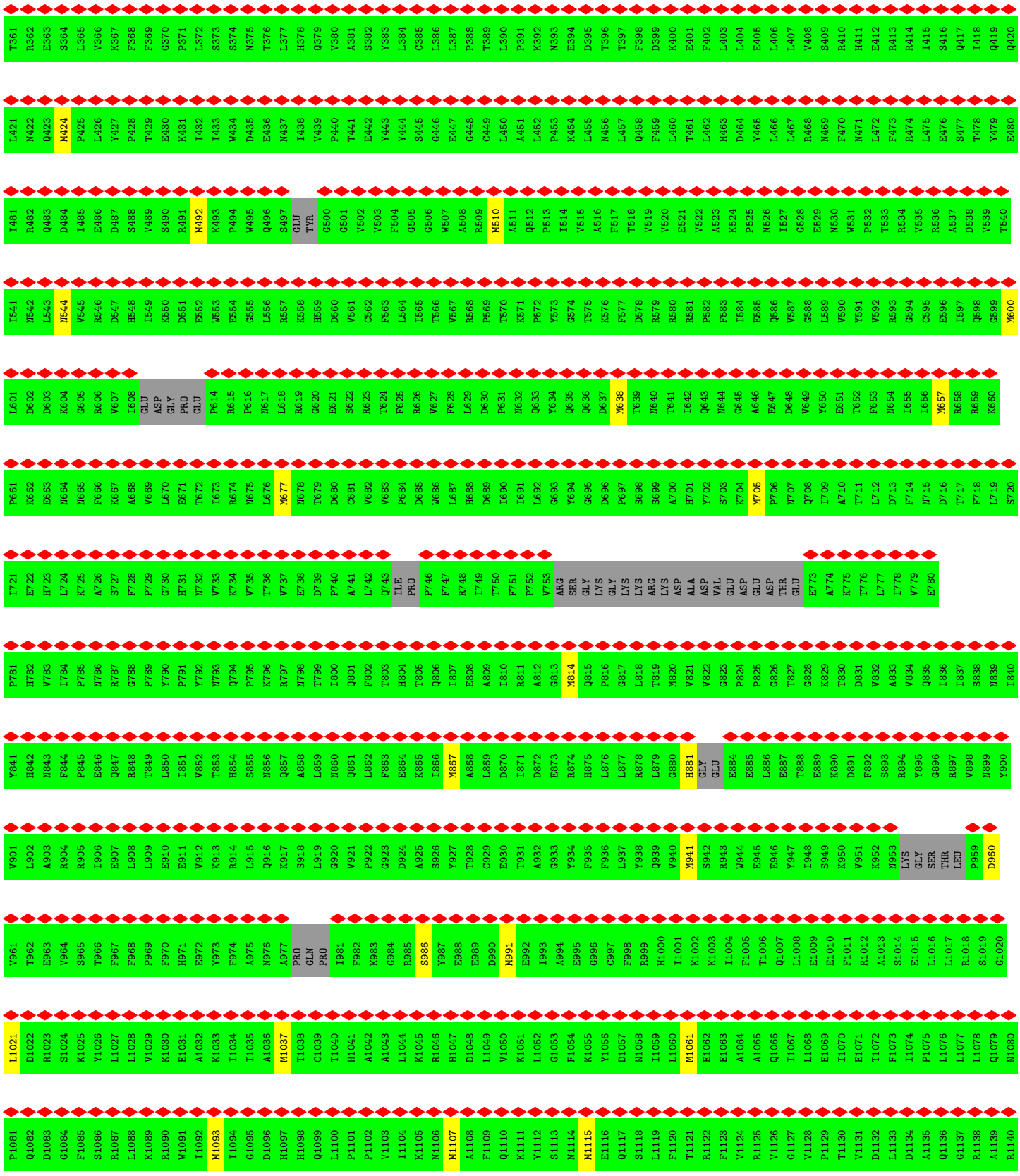


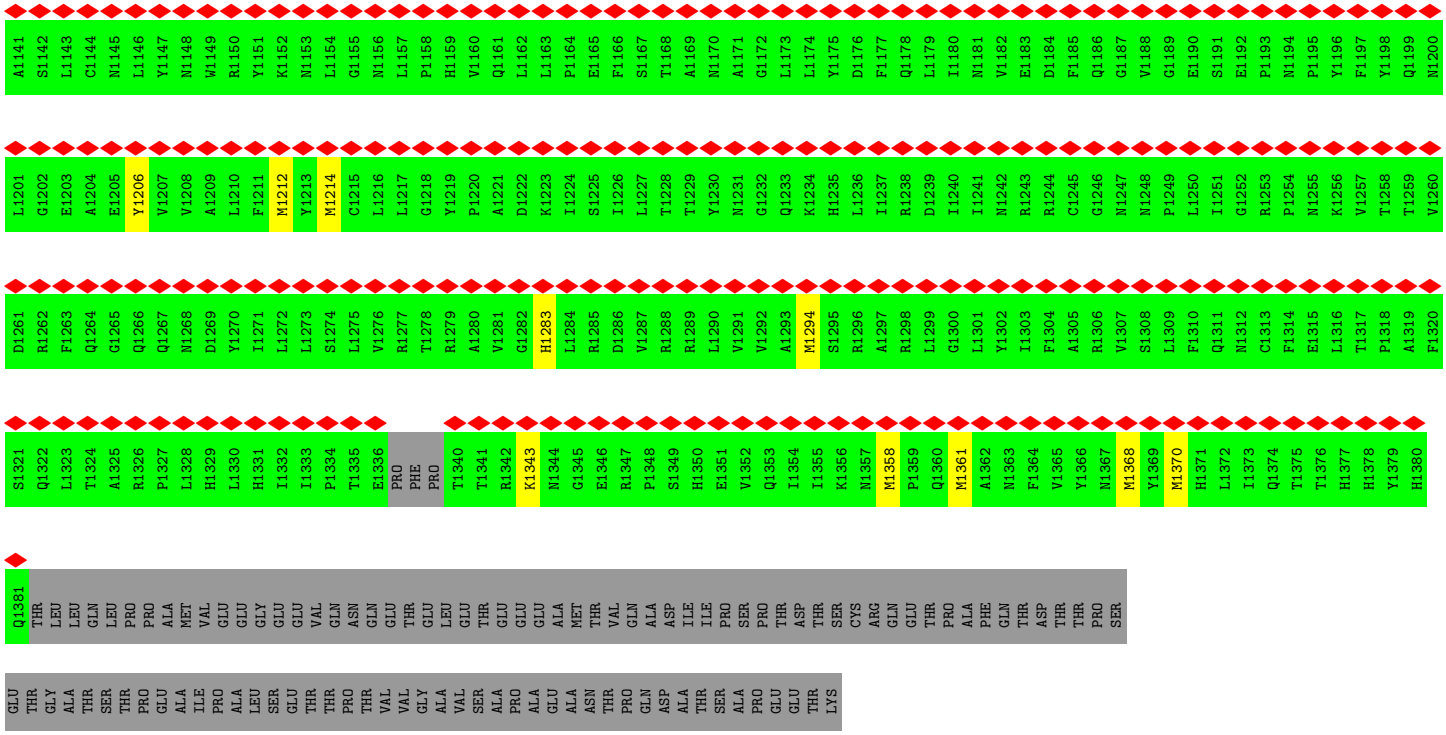


- Molecule 26: Intron-binding protein aquarius

Chain U:

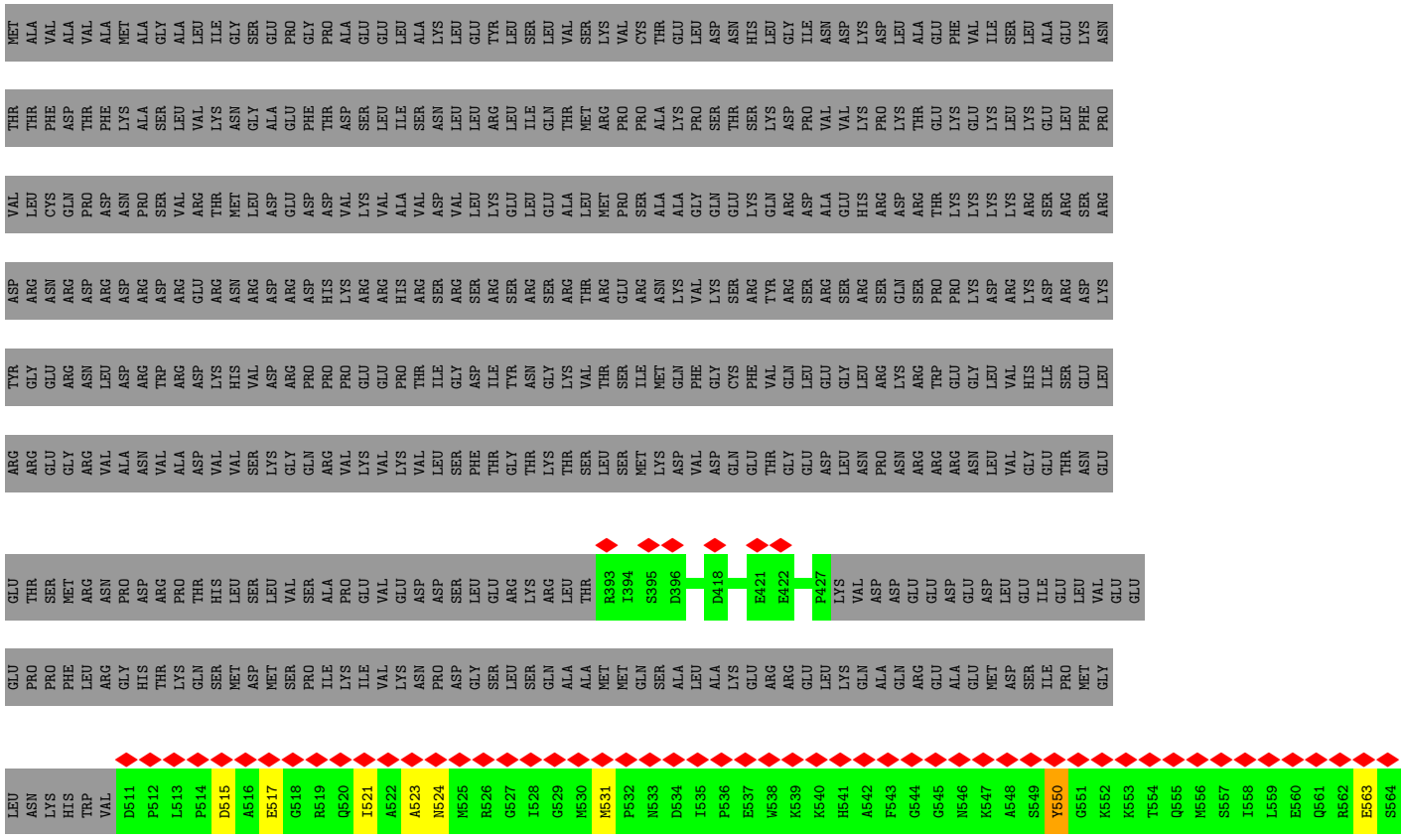


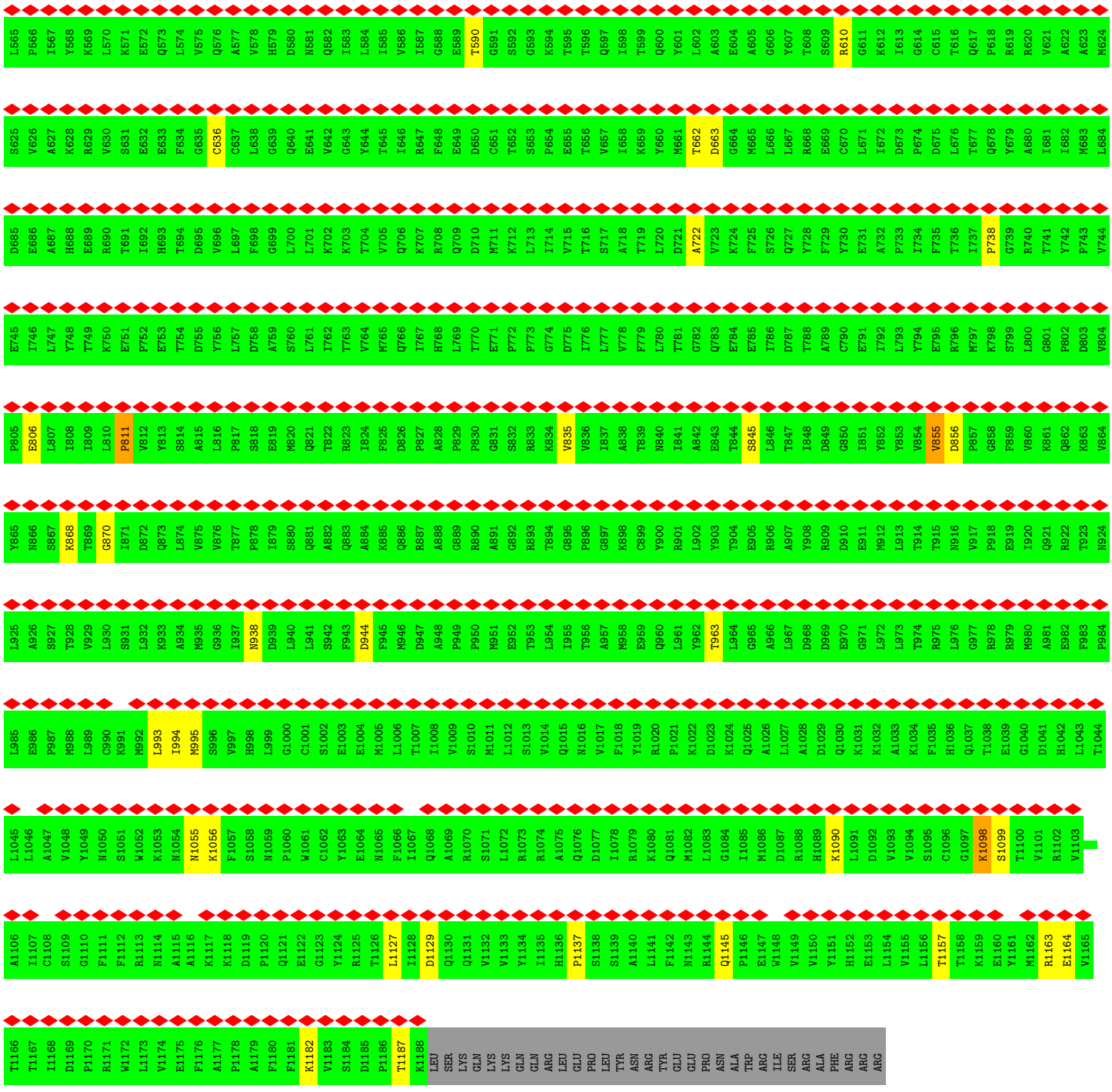

T361 R362 E363 S364 L365 V366 K367 F368 F369 G370 P371 L372 S373 S374 N375 T376 L377 H378 Q379 V380 A381 S382 Y383 L384 C385 L386 L387 P388 T389 L390 P391 K392 N393 E394 D395 T396 T397 F398 D399 K400 E401 F402 L403 L404 E405 L406 L407 V408 S409 R410 H411 E412 R413 R414 I415 S416 Q417 I418 Q419 Q420
L421 N422 Q423 M424 P425 L426 Y427 P428 T429 E430 K431 I432 I433 W434 D435 E436 N437 I438 V439 P440 T441 E442 Y443 Y444 S445 G446 E447 G448 C449 L450 A451 L452 P453 K454 L455 N456 L457 Q458 F459 L460 T461 L462 H463 D464 Y465 L466 L467 R468 N469 F470 N471 L472 F473 R474 L475 E476 S477 T478 Y479 E480
I481 R482 Q483 D484 I485 E486 D487 S488 V489 S490 R491 M492 K493 P494 W495 Q496 S497 GLU TYR G500 G501 V502 V503 F504 G505 G506 W507 A508 R509 M510 A511 Q512 P513 I514 V515 A516 F517 T518 V519 V520 E521 V522 A523 K524 P525 N526 I527 G528 E529 N530 W531 P532 T533 R534 V535 R536 A537 D538 V539 T540
I541 N542 L543 N544 V545 R546 D547 H548 I549 K550 D551 E552 W553 E554 G555 L556 R557 K558 H559 D560 V561 C562 F563 L564 I565 T566 V567 R568 P569 T570 K571 P572 Y573 G574 T575 K576 F577 D578 R579 R580 R581 P582 F583 I584 E585 Q586 V587 G588 L589 V590 Y591 V592 R593 G594 C595 E596 I597 Q598 G599 M600
L601 D602 D603 K604 G605 R606 V607 I608 GLU ASP GLY PRO GLU P614 R615 P616 N617 L618 R619 G620 E621 S622 R623 T624 F625 R626 V627 F628 L629 D630 P631 N632 Q633 Y634 Q635 Q636 D637 M638 T639 N640 T641 I642 Q643 N644 G645 A646 E647 D648 V649 Y650 E651 T652 F653 N654 I655 I656 M657 R658 R659 K660
P661 K662 E663 N664 N665 F666 K667 A668 V669 L670 E671 T672 I673 R674 N675 L676 M677 N678 T679 D680 C681 V682 V683 P684 D685 W686 L687 H688 D689 I690 I691 L692 G693 Y694 G695 D696 P697 S698 S699 A700 H701 Y702 S703 K704 M705 P706 N707 Q708 I709 A710 T711 L712 D713 F714 N715 D716 T717 F718 L719 S720
I721 E722 H723 L724 K725 A726 S727 F728 P729 G730 H731 N732 V733 K734 V735 T736 V737 E738 D739 P740 A741 L742 Q743 ILE PRO P746 F747 R748 I749 T750 F751 P752 V753 ARG SER GLY LYS GLY LYS LYS ARG LYS ASP ALA ASP VAL GLU ASP GLU ASP THR GLU E773 A774 K775 T776 L777 I778 V779 E780
P781 H782 V783 I784 P785 N786 R787 G788 P789 Y790 P791 Y792 N793 Q794 P795 K796 R797 N798 T799 I800 Q801 F802 T803 H804 T805 Q806 I807 E808 A809 I810 R811 A812 G813 M814 Q815 P816 G817 L818 T819 M820 V821 V822 G823 P824 P825 G826 T827 G828 K829 T830 D831 V832 A833 V834 Q835 I836 I837 S838 N839 I840
Y841 H842 N843 F844 P845 E846 Q847 R848 T849 L850 I851 V852 T853 H854 S855 N856 Q857 A858 L859 N860 Q861 L862 F863 E864 K865 I866 M867 A868 L869 D870 I871 D872 E873 R874 H875 L876 L877 R878 L879 G880 H881 GLY GLU E884 E885 L886 E887 T888 E889 K890 D891 F892 S893 R894 Y895 G896 R897 V898 N899 Y900
V901 L902 A903 R904 R905 I906 E907 L908 L909 E910 E911 V912 K913 R914 L915 Q916 K917 S918 L919 G920 V921 P922 G923 D924 A925 S926 Y927 T928 C929 E930 T931 A932 G933 Y934 F935 F936 L937 Y938 Q939 V940 M941 S942 R943 W944 E945 E946 Y947 I948 S949 K950 V951 K952 N953 LYS GLY SER THR LEU P959 D960
V961 T962 E963 V964 S965 T966 F967 F968 P969 F970 H971 E972 Y973 F974 A975 N976 A977 PRO GLN PRO I981 P982 K983 G984 R985 S986 Y987 E988 E989 D990 M991 E992 I993 A994 E995 G996 C997 F998 R999 H1000 I1001 K1002 K1003 I1004 F1005 T1006 Q1007 L1008 E1009 E1010 F1011 R1012 A1013 S1014 E1015 L1016 L1017 R1018 S1019 G1020
L1021 D1022 R1023 S1024 K1025 Y1026 L1027 L1028 V1029 K1030 E1031 A1032 K1033 I1034 I1035 A1036 M1037 T1038 C1039 T1040 H1041 A1042 A1043 L1044 K1045 R1046 H1047 D1048 L1049 V1050 K1051 L1052 G1053 F1054 K1055 Y1056 D1057 N1058 I1059 L1060 M1061 E1062 E1063 A1064 A1065 Q1066 I1067 L1068 E1069 I1070 E1071 T1072 F1073 I1074 P1075 L1076 L1077 L1078 Q1079 N1080
P1081 Q1082 D1083 G1084 F1085 S1086 R1087 L1088 K1089 R1090 W1091 I1092 M1093 I1094 G1095 D1096 H1097 H1098 Q1099 L1100 P1101 P1102 V1103 I1104 K1105 N1106 M1107 A1108 F1109 Q1110 K1111 Y1112 S1113 N1114 M1115 E1116 Q1117 S1118 L1119 F1120 T1121 R1122 F1123 V1124 R1125 V1126 G1127 V1128 P1129 T1130 V1131 D1132 L1133 D1134 A1135 Q1136 G1137 R1138 A1139 R1140



- Molecule 27: ATP-dependent RNA helicase DHX8

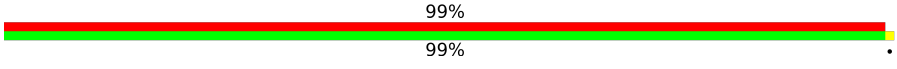
Chain V:

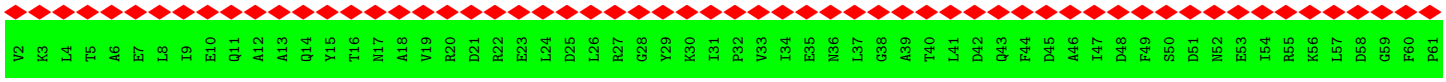


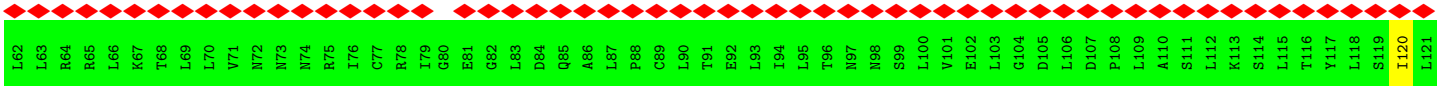


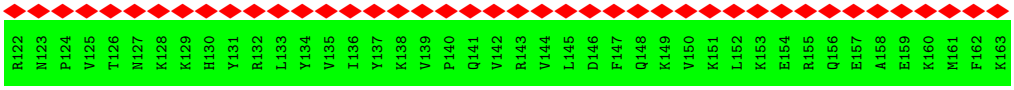
• Molecule 28: U2 small nuclear ribonucleoprotein A'

Chain W:



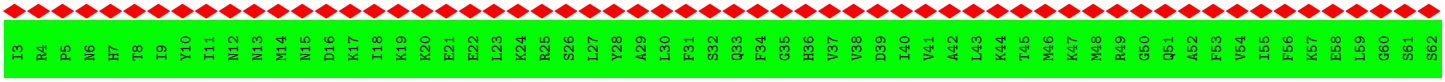


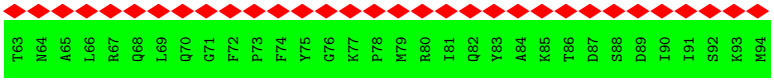




• Molecule 29: U2 small nuclear ribonucleoprotein B"

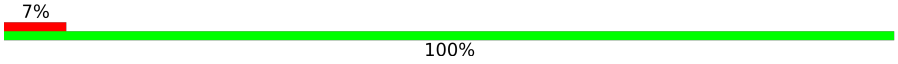
Chain Y:





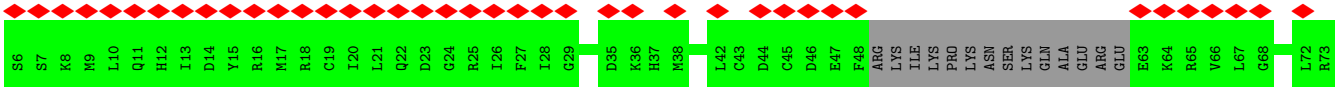
• Molecule 30: NF-kappa-B-activating protein

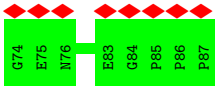
Chain Z:



• Molecule 31: Small nuclear ribonucleoprotein-associated proteins B and B'

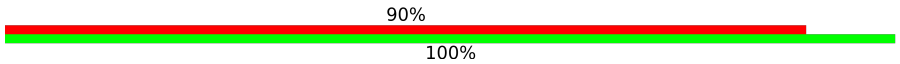
Chain b:

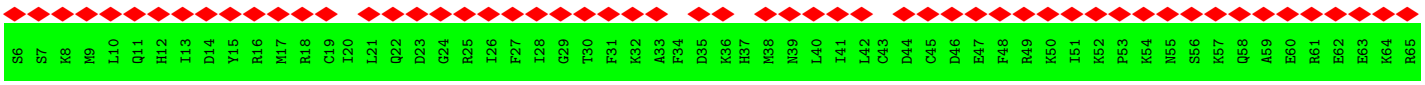


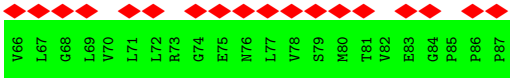


• Molecule 31: Small nuclear ribonucleoprotein-associated proteins B and B'

Chain k:

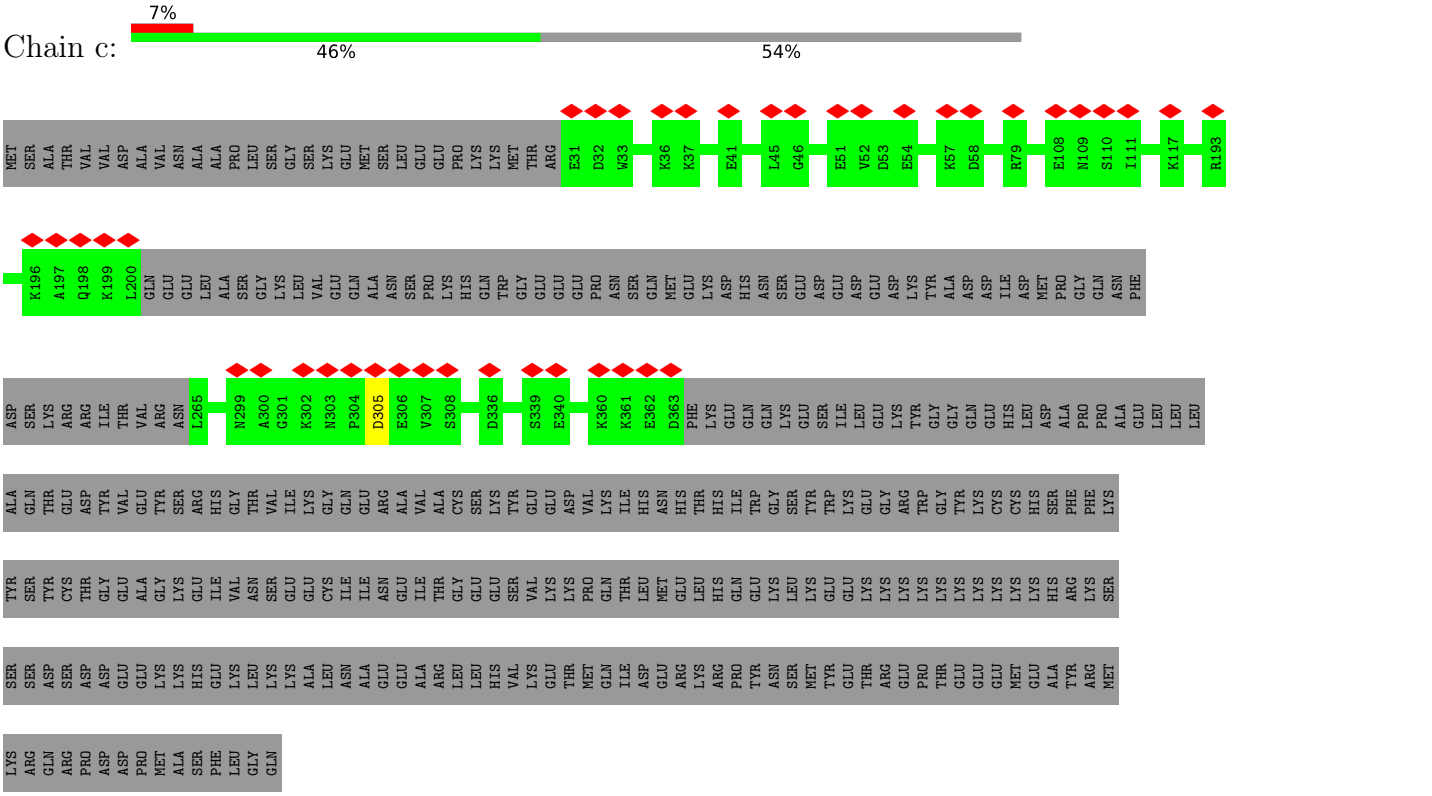






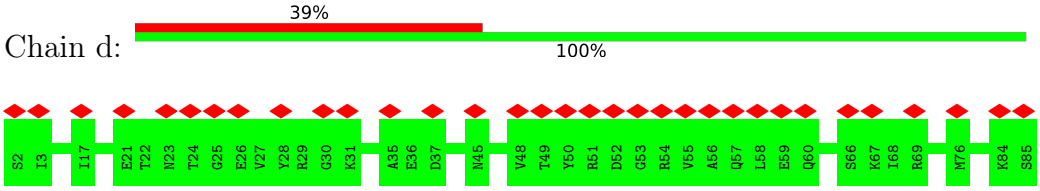
• Molecule 32: Pre-mRNA-splicing factor SLU7

Chain c:



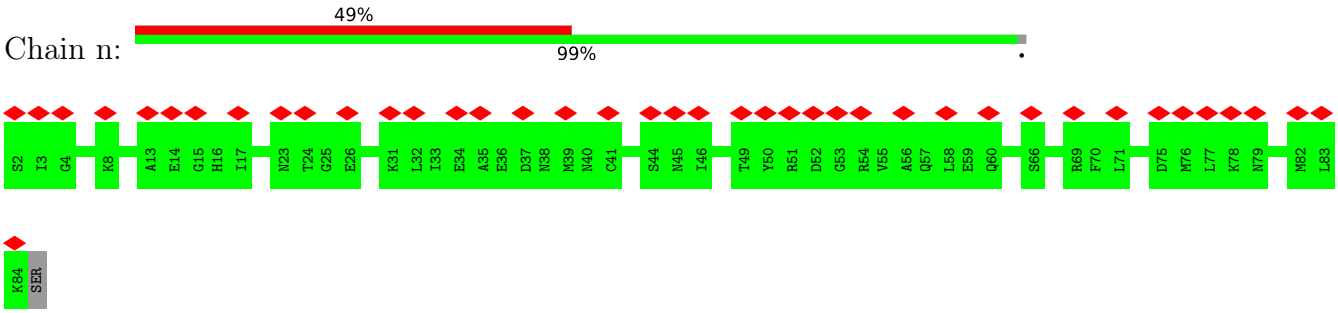
• Molecule 33: Small nuclear ribonucleoprotein Sm D3

Chain d:



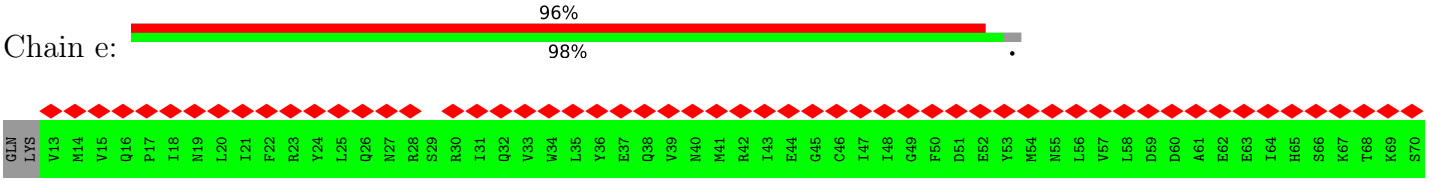
• Molecule 33: Small nuclear ribonucleoprotein Sm D3

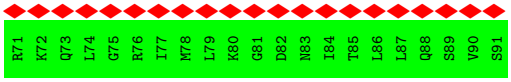
Chain n:



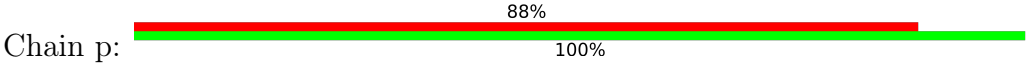
• Molecule 34: Small nuclear ribonucleoprotein E

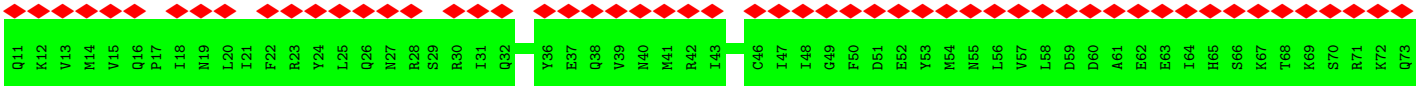
Chain e:

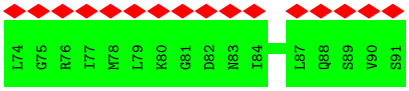




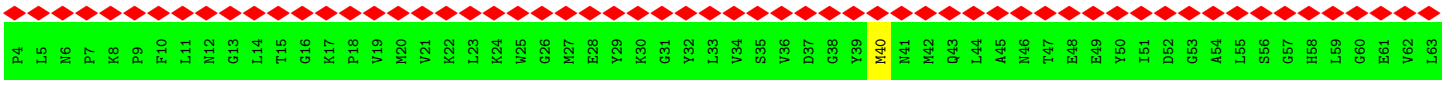
• Molecule 34: Small nuclear ribonucleoprotein E

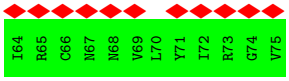




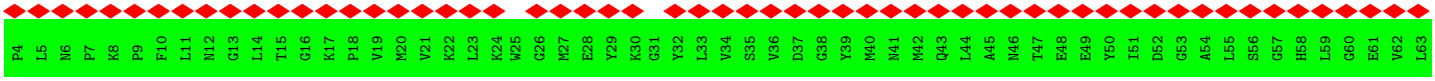


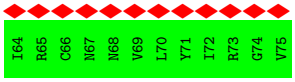
• Molecule 35: Small nuclear ribonucleoprotein F



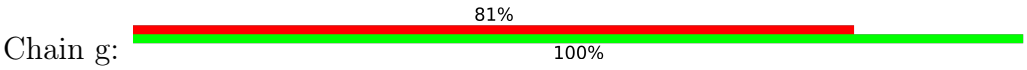


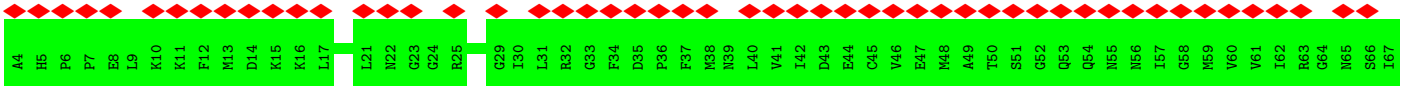
• Molecule 35: Small nuclear ribonucleoprotein F

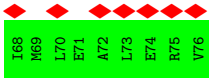




• Molecule 36: Small nuclear ribonucleoprotein G

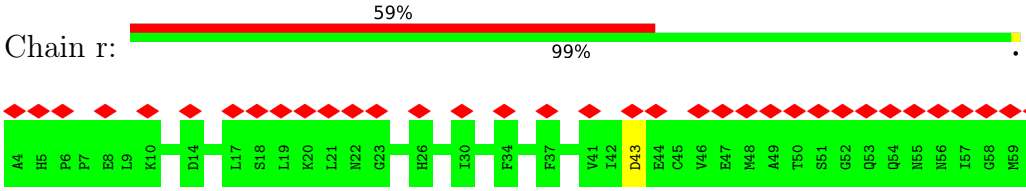






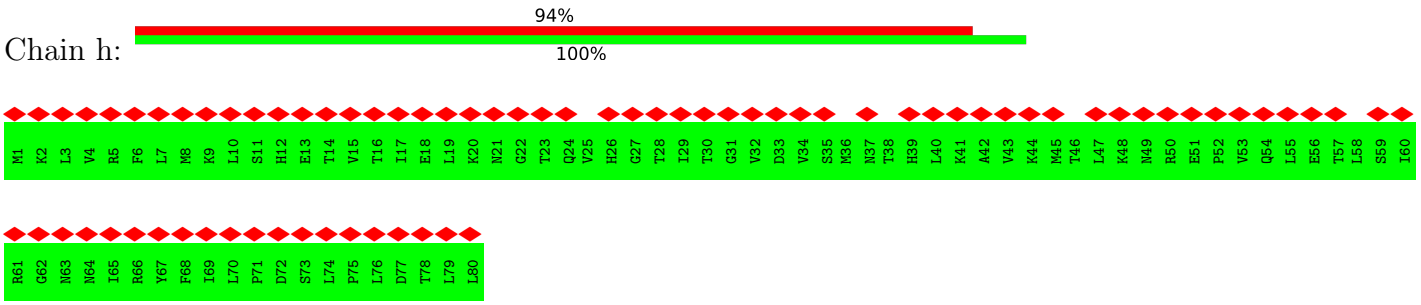
• Molecule 36: Small nuclear ribonucleoprotein G

Chain r:



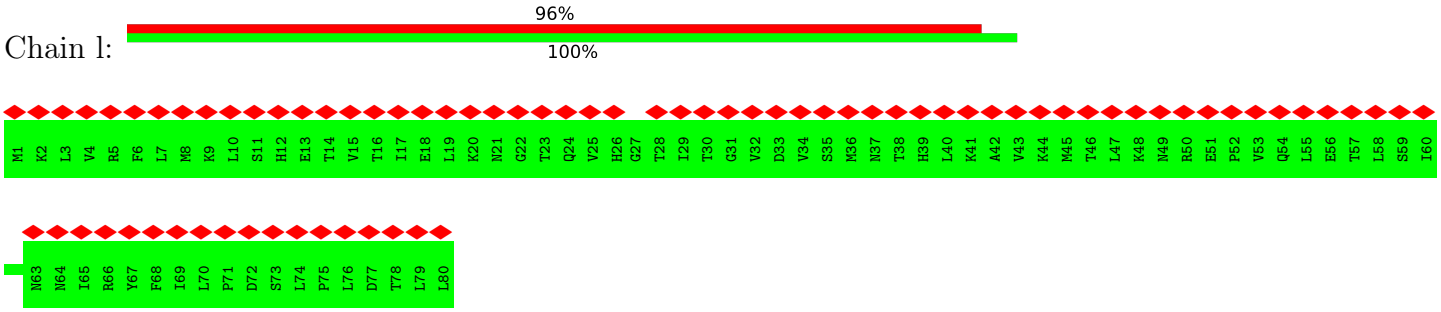
• Molecule 37: Small nuclear ribonucleoprotein Sm D1

Chain h:



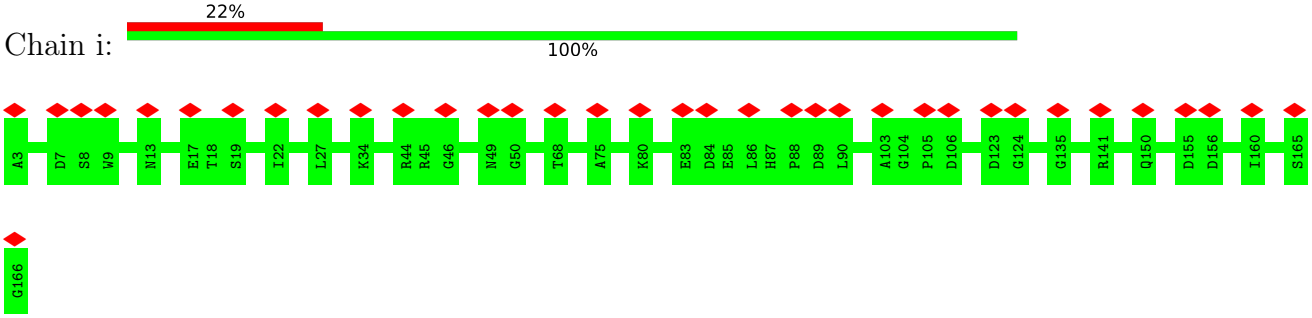
• Molecule 37: Small nuclear ribonucleoprotein Sm D1

Chain l:



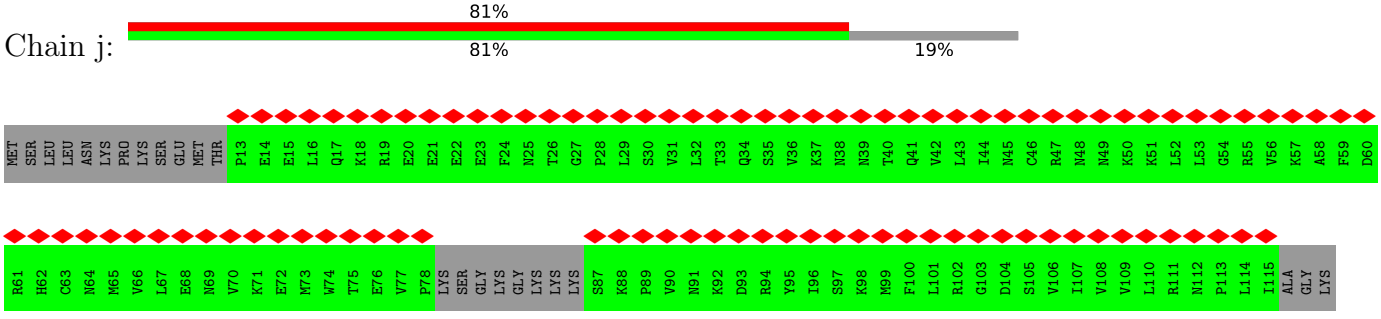
• Molecule 38: Peptidyl-prolyl cis-trans isomerase-like 1

Chain i:



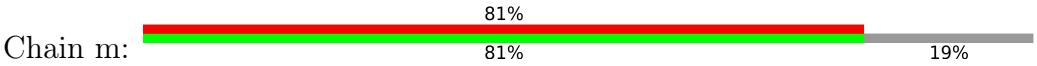
• Molecule 39: Small nuclear ribonucleoprotein Sm D2

Chain j:



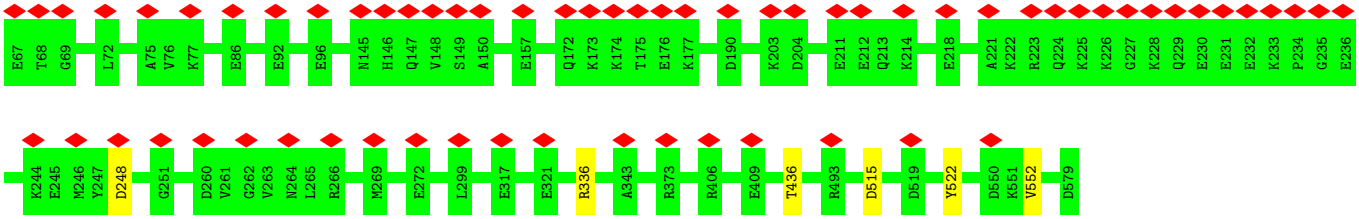
• Molecule 39: Small nuclear ribonucleoprotein Sm D2

Chain m:



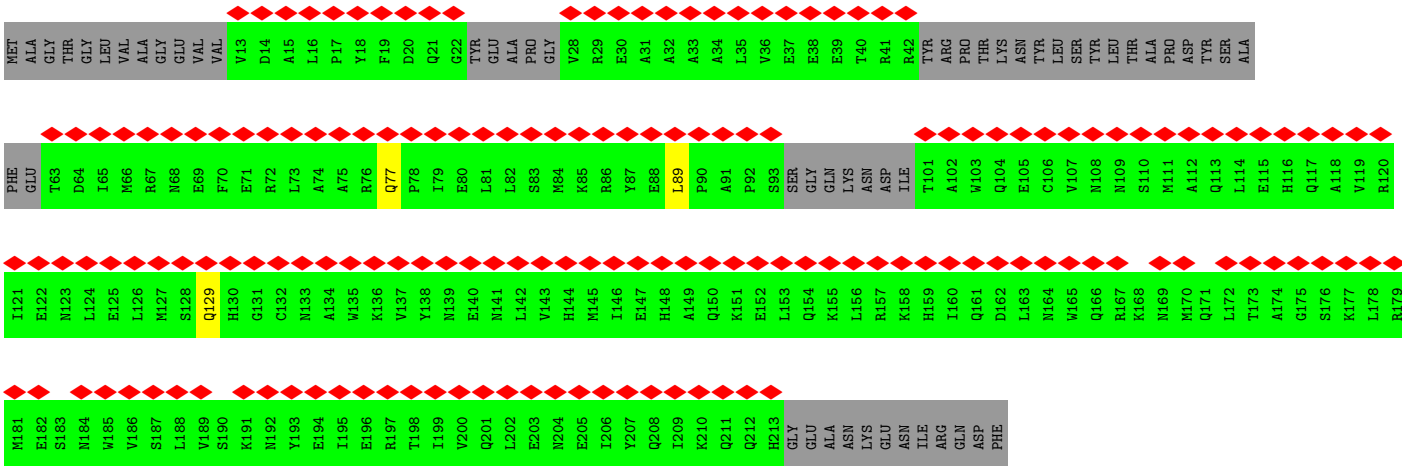
• Molecule 40: Pre-mRNA-processing factor 17

Chain o:



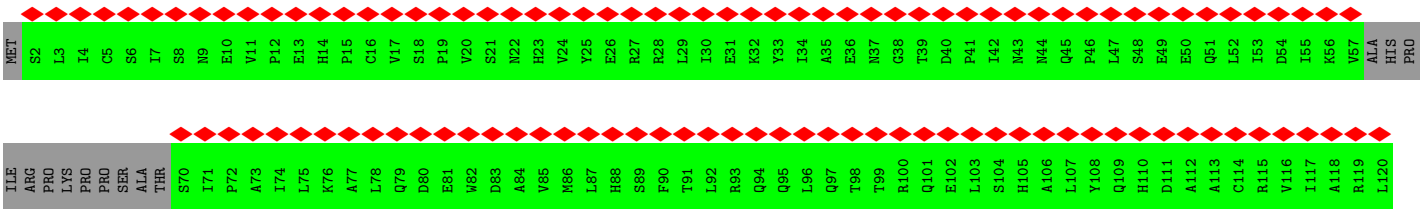
• Molecule 41: Pre-mRNA-splicing factor SPF27

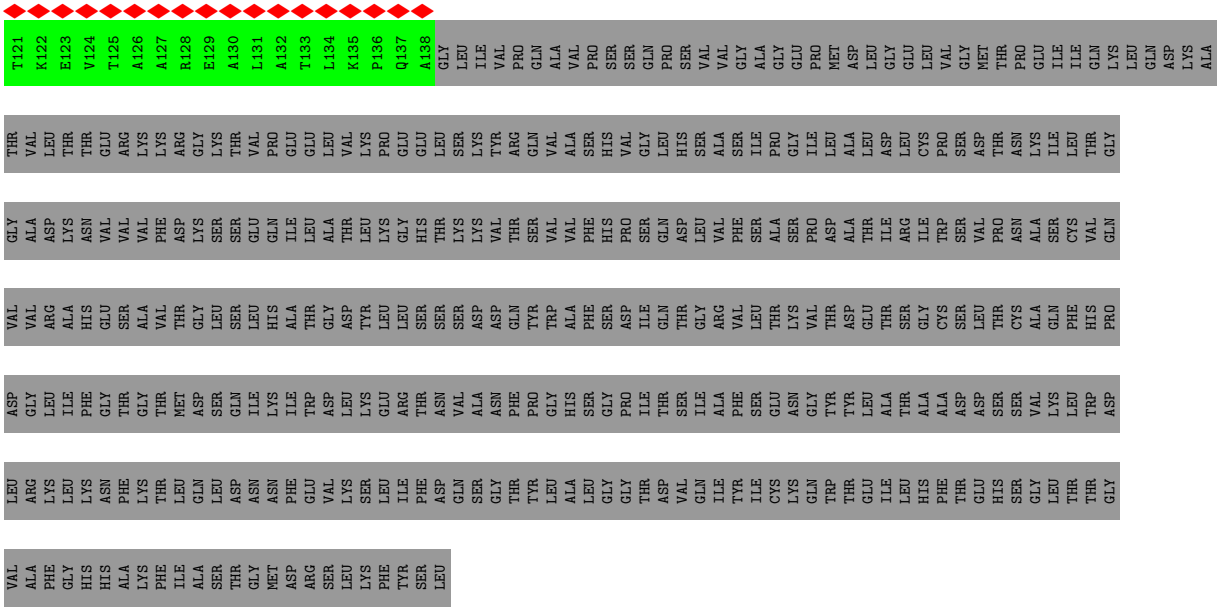
Chain s:



• Molecule 42: Pre-mRNA-processing factor 19

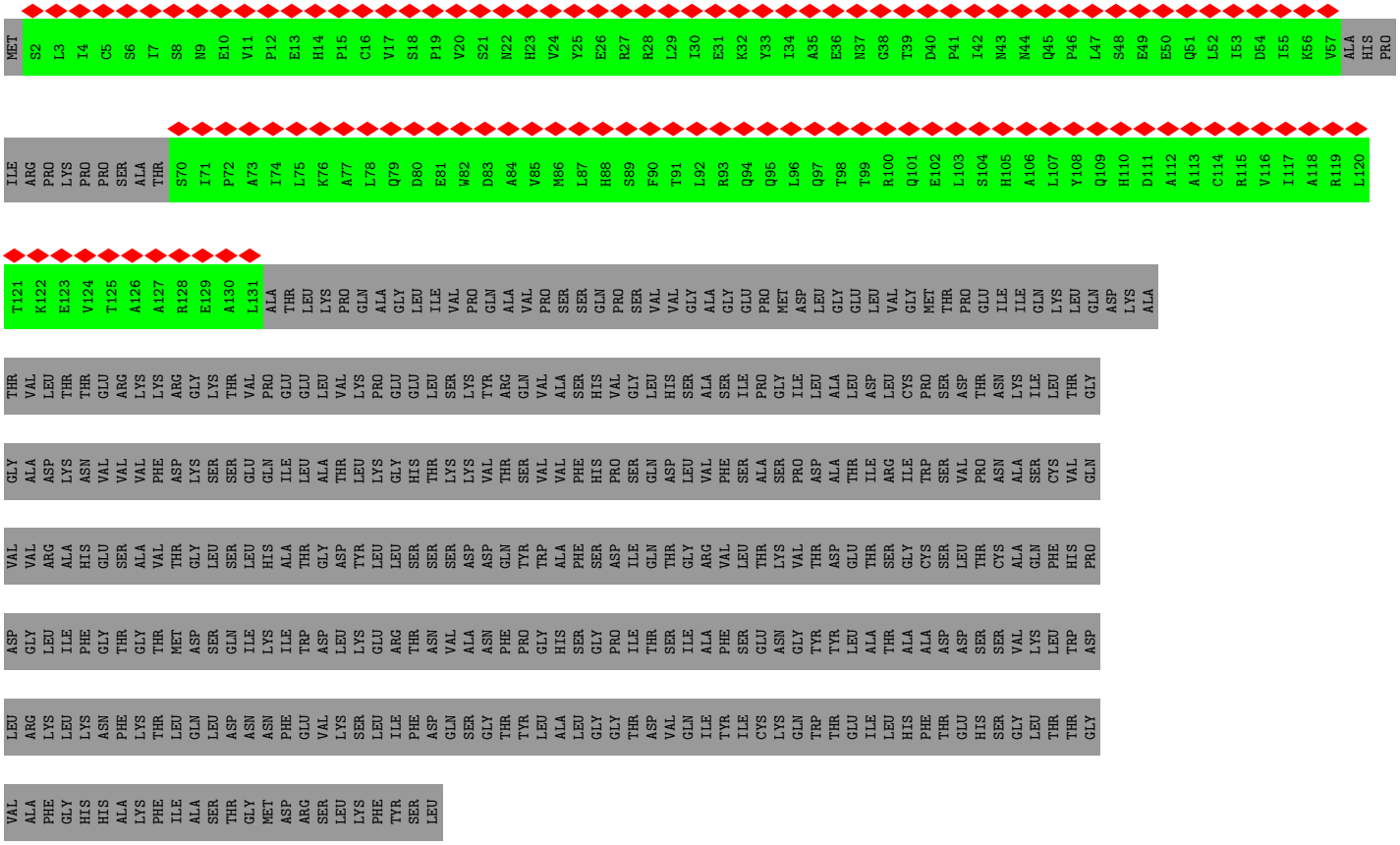
Chain t:





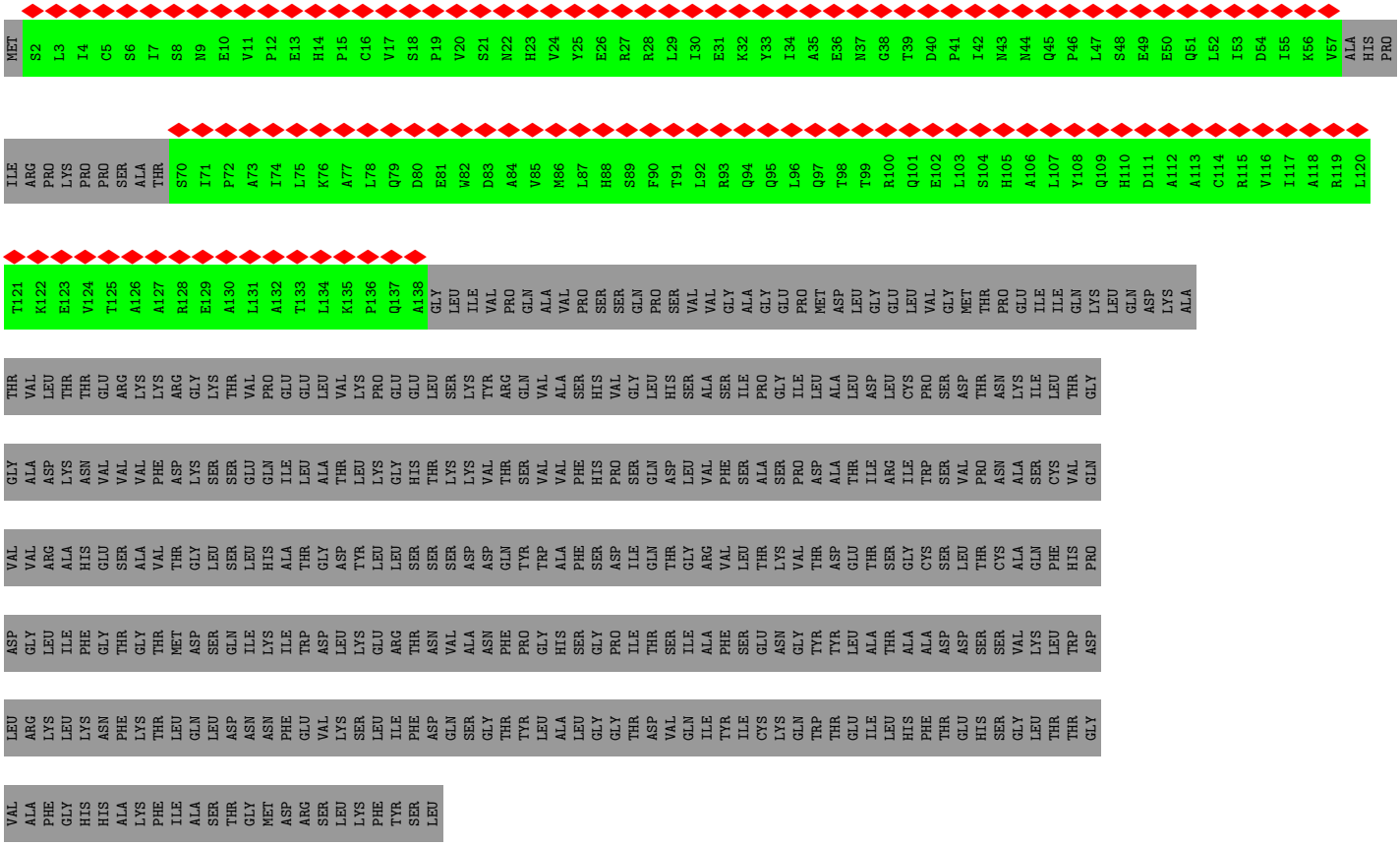
• Molecule 42: Pre-mRNA-processing factor 19

Chain u:



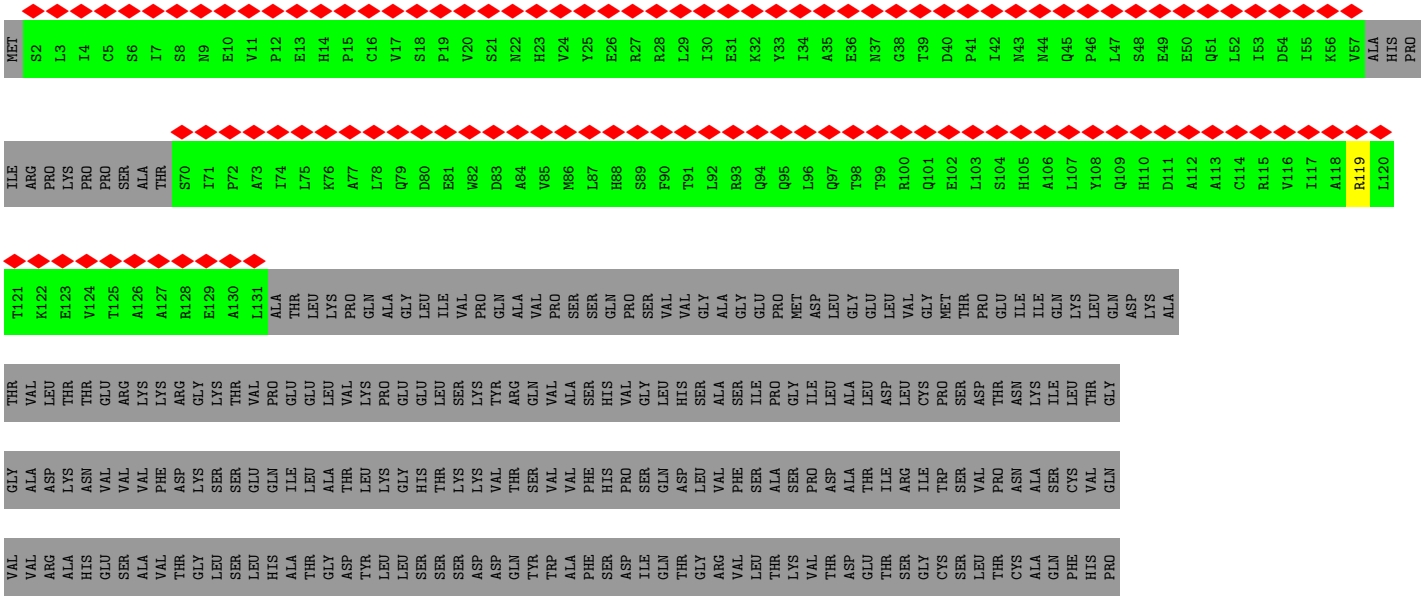
• Molecule 42: Pre-mRNA-processing factor 19

Chain v:



• Molecule 42: Pre-mRNA-processing factor 19

Chain w:



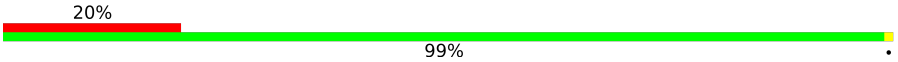
ASP GLY LEU ILE PHE GLY THR GLY THR MET ASP SER GLN ILE LYS ILE TRP ASP LEU LYS GLU ARG THR ASN VAL ALA ASN PHE PRO GLY HIS SER GLY PRO ILE THR SER ILE ALA PHE SER GLU ASN GLY TYR TYR LEU ALA THR ALA ALA ASP ASP SER SER VAL LYS LEU TRP ASP

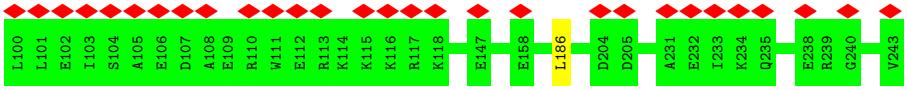
LEU ARG LYS LEU LYS ASN PHE LYS THR LEU GLN LEU ASP ASN ASN PHE GLU VAL LYS SER LEU ILE PHE ASP GLN SER GLY THR TYR LEU ALA LEU GLY GLY THR ASP VAL GLN ILE TYR ILE CYS LYS GLN TRP THR GLU ILE LEU HIS PHE THR GLU HIS SER GLY LEU THR THR GLY

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

- Molecule 43: Pre-mRNA-splicing factor SYF2

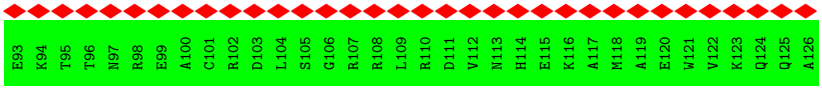
Chain y:





- Molecule 44: Replication stress response regulator SDE2

Chain z:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	103860	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 ($e^-/Å^2$)	53	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	135000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.177	Depositor
Minimum map value	-0.101	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.024	Depositor
Map size (Å)	492.00003, 492.00003, 492.00003	wwPDB
Map dimensions	410, 410, 410	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2, 1.2, 1.2	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: MG, ATP, SEP, GTP, ZN, K, IHP

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	2	0.56	0/2827	1.12	16/4393 (0.4%)
2	5	0.58	0/1760	1.27	25/2733 (0.9%)
3	6	0.53	0/2323	0.98	3/3619 (0.1%)
4	7	0.38	0/3179	0.65	0/4291
5	8	0.36	0/748	0.71	3/1012 (0.3%)
6	9	0.38	0/1225	0.60	0/1648
7	A	0.43	1/19172 (0.0%)	0.58	7/26014 (0.0%)
8	B	0.37	0/14140	0.58	2/19159 (0.0%)
9	C	0.39	0/7277	0.62	4/9887 (0.0%)
10	D	0.34	0/1030	0.59	0/1371
11	E	0.60	0/329	1.18	4/510 (0.8%)
12	F	0.32	0/1129	0.53	0/1525
13	G	0.27	0/513	0.55	1/683 (0.1%)
14	H	0.33	0/3779	0.50	0/5087
15	I	0.41	0/971	1.20	10/1504 (0.7%)
16	J	0.46	0/2592	0.63	0/3535
17	K	0.35	0/2387	0.57	0/3205
18	L	0.45	1/1214 (0.1%)	0.58	0/1627
19	M	0.36	0/2366	0.57	1/3193 (0.0%)
20	N	0.31	0/2448	0.58	0/3316
21	O	0.32	0/3457	0.50	0/4627
22	P	0.34	0/902	0.54	0/1201
23	R	0.58	1/196 (0.5%)	0.53	0/265
24	S	0.38	0/4013	0.55	8/5432 (0.1%)
25	T	0.41	0/4031	0.81	8/5500 (0.1%)
26	U	0.43	35/11155 (0.3%)	0.41	0/15095
27	V	0.47	0/3000	0.93	0/3777
28	W	0.31	0/1299	0.62	0/1761
29	Y	0.38	0/759	0.50	0/1016
30	Z	0.32	0/232	0.48	0/307
31	b	0.33	0/553	0.53	0/739
31	k	0.45	0/674	0.55	0/899

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	c	0.36	0/2268	0.53	0/3052
33	d	0.39	0/666	0.55	0/897
33	n	0.47	0/660	0.61	0/889
34	e	0.29	0/659	0.54	0/885
34	p	0.47	0/677	0.60	0/908
35	f	0.30	0/574	0.55	0/775
35	q	0.49	0/574	0.59	0/775
36	g	0.34	0/575	0.59	0/768
36	r	0.47	0/575	0.62	0/768
37	h	0.28	0/642	0.53	0/867
37	l	0.41	0/642	0.55	0/867
38	i	0.31	0/1304	0.57	0/1767
39	j	0.28	0/784	0.51	0/1053
39	m	0.42	0/784	0.56	0/1053
40	o	0.37	0/4265	0.60	0/5761
41	s	0.35	0/1423	0.51	0/1914
42	t	0.32	0/1004	0.50	0/1365
42	u	0.34	0/953	0.49	0/1295
42	v	0.34	0/1004	0.51	0/1365
42	w	0.31	0/953	0.49	0/1295
43	y	0.33	0/1241	0.56	1/1662 (0.1%)
44	z	0.44	0/282	0.50	0/375
All	All	0.40	38/124189 (0.0%)	0.64	93/169287 (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
7	A	0	4
8	B	0	1
9	C	0	2
17	K	0	1
18	L	0	2
25	T	0	5
27	V	0	15
35	f	0	1
41	s	0	3
All	All	0	34

The worst 5 of 38 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	2223	CYS	CB-SG	-6.69	1.70	1.82
18	L	117	CYS	CB-SG	-6.56	1.71	1.82
23	R	24	SER	CA-CB	-5.95	1.44	1.52
26	U	1107	MET	CG-SD	5.78	1.96	1.81
26	U	244	MET	CG-SD	5.75	1.96	1.81

The worst 5 of 93 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	5	86	C	N1-C2-O2	14.03	127.32	118.90
2	5	86	C	C2-N1-C1'	11.76	131.73	118.80
2	5	86	C	N3-C2-O2	-11.61	113.78	121.90
1	2	50	C	N1-C2-O2	10.30	125.08	118.90
1	2	50	C	C2-N1-C1'	9.37	129.10	118.80

There are no chirality outliers.

5 of 34 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	A	1210	LYS	Peptide
7	A	1416	ILE	Peptide
7	A	1635	TYR	Peptide
7	A	940	ILE	Peptide
8	B	430	LEU	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
4	7	388/390 (100%)	376 (97%)	9 (2%)	3 (1%)	16 46
5	8	89/91 (98%)	87 (98%)	1 (1%)	1 (1%)	12 40
6	9	142/144 (99%)	138 (97%)	4 (3%)	0	100 100
7	A	2244/2335 (96%)	2105 (94%)	139 (6%)	0	100 100
8	B	1720/1722 (100%)	1633 (95%)	84 (5%)	3 (0%)	44 71
9	C	897/899 (100%)	828 (92%)	67 (8%)	2 (0%)	44 71
10	D	121/123 (98%)	116 (96%)	5 (4%)	0	100 100
12	F	120/122 (98%)	107 (89%)	13 (11%)	0	100 100
13	G	58/60 (97%)	56 (97%)	2 (3%)	0	100 100
14	H	455/908 (50%)	440 (97%)	15 (3%)	0	100 100
16	J	318/320 (99%)	303 (95%)	15 (5%)	0	100 100
17	K	291/295 (99%)	271 (93%)	20 (7%)	0	100 100
18	L	142/144 (99%)	134 (94%)	8 (6%)	0	100 100
19	M	287/289 (99%)	271 (94%)	16 (6%)	0	100 100
20	N	304/306 (99%)	283 (93%)	19 (6%)	2 (1%)	19 50
21	O	429/802 (54%)	416 (97%)	12 (3%)	1 (0%)	44 71
22	P	100/229 (44%)	97 (97%)	3 (3%)	0	100 100
23	R	24/26 (92%)	17 (71%)	7 (29%)	0	100 100
24	S	531/848 (63%)	500 (94%)	28 (5%)	3 (1%)	22 53
25	T	597/855 (70%)	584 (98%)	12 (2%)	1 (0%)	44 71
26	U	1308/1485 (88%)	1283 (98%)	25 (2%)	0	100 100
27	V	709/1220 (58%)	617 (87%)	60 (8%)	32 (4%)	2 13
28	W	160/162 (99%)	147 (92%)	13 (8%)	0	100 100
29	Y	90/92 (98%)	88 (98%)	2 (2%)	0	100 100
30	Z	28/30 (93%)	27 (96%)	1 (4%)	0	100 100
31	b	64/82 (78%)	62 (97%)	2 (3%)	0	100 100
31	k	80/82 (98%)	74 (92%)	6 (8%)	0	100 100
32	c	265/586 (45%)	248 (94%)	17 (6%)	0	100 100
33	d	82/84 (98%)	77 (94%)	5 (6%)	0	100 100
33	n	81/84 (96%)	76 (94%)	5 (6%)	0	100 100
34	e	77/81 (95%)	75 (97%)	2 (3%)	0	100 100
34	p	79/81 (98%)	77 (98%)	2 (2%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	f	70/72 (97%)	69 (99%)	1 (1%)	0	100	100
35	q	70/72 (97%)	69 (99%)	1 (1%)	0	100	100
36	g	71/73 (97%)	68 (96%)	3 (4%)	0	100	100
36	r	71/73 (97%)	69 (97%)	2 (3%)	0	100	100
37	h	78/80 (98%)	76 (97%)	2 (3%)	0	100	100
37	l	78/80 (98%)	75 (96%)	3 (4%)	0	100	100
38	i	162/164 (99%)	149 (92%)	13 (8%)	0	100	100
39	j	91/118 (77%)	87 (96%)	4 (4%)	0	100	100
39	m	91/118 (77%)	86 (94%)	5 (6%)	0	100	100
40	o	511/513 (100%)	465 (91%)	45 (9%)	1 (0%)	44	71
41	s	161/225 (72%)	148 (92%)	13 (8%)	0	100	100
42	t	121/504 (24%)	118 (98%)	3 (2%)	0	100	100
42	u	114/504 (23%)	113 (99%)	1 (1%)	0	100	100
42	v	121/504 (24%)	119 (98%)	2 (2%)	0	100	100
42	w	114/504 (23%)	113 (99%)	1 (1%)	0	100	100
43	y	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
44	z	32/34 (94%)	30 (94%)	2 (6%)	0	100	100
All	All	14378/18759 (77%)	13605 (95%)	724 (5%)	49 (0%)	38	66

5 of 49 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	7	383	ASN
8	B	957	VAL
8	B	1584	ILE
20	N	59	ILE
27	V	531	MET

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	7	345/345 (100%)	340 (99%)	5 (1%)	62 78
5	8	76/76 (100%)	75 (99%)	1 (1%)	65 79
6	9	132/132 (100%)	131 (99%)	1 (1%)	79 87
7	A	2033/2108 (96%)	1996 (98%)	37 (2%)	54 74
8	B	1541/1541 (100%)	1363 (88%)	178 (12%)	4 18
9	C	799/799 (100%)	797 (100%)	2 (0%)	91 94
10	D	106/106 (100%)	105 (99%)	1 (1%)	75 85
12	F	110/110 (100%)	110 (100%)	0	100 100
13	G	54/55 (98%)	53 (98%)	1 (2%)	52 72
14	H	410/838 (49%)	403 (98%)	7 (2%)	56 74
16	J	276/276 (100%)	275 (100%)	1 (0%)	89 93
17	K	246/247 (100%)	246 (100%)	0	100 100
18	L	130/130 (100%)	127 (98%)	3 (2%)	45 68
19	M	254/254 (100%)	253 (100%)	1 (0%)	89 93
20	N	263/263 (100%)	263 (100%)	0	100 100
21	O	322/709 (45%)	321 (100%)	1 (0%)	91 94
22	P	94/203 (46%)	94 (100%)	0	100 100
23	R	21/21 (100%)	20 (95%)	1 (5%)	21 50
24	S	275/751 (37%)	273 (99%)	2 (1%)	81 88
25	T	213/749 (28%)	210 (99%)	3 (1%)	62 78
26	U	1202/1336 (90%)	1193 (99%)	9 (1%)	81 88
27	V	31/1085 (3%)	31 (100%)	0	100 100
28	W	139/147 (95%)	138 (99%)	1 (1%)	81 88
29	Y	81/82 (99%)	81 (100%)	0	100 100
30	Z	25/25 (100%)	25 (100%)	0	100 100
31	b	62/75 (83%)	62 (100%)	0	100 100
31	k	75/75 (100%)	75 (100%)	0	100 100
32	c	236/520 (45%)	235 (100%)	1 (0%)	89 93
33	d	74/74 (100%)	74 (100%)	0	100 100
33	n	73/74 (99%)	73 (100%)	0	100 100
34	e	74/76 (97%)	74 (100%)	0	100 100
34	p	76/76 (100%)	76 (100%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	f	61/61 (100%)	61 (100%)	0	100	100
35	q	61/61 (100%)	61 (100%)	0	100	100
36	g	63/63 (100%)	63 (100%)	0	100	100
36	r	63/63 (100%)	62 (98%)	1 (2%)	58	76
37	h	75/75 (100%)	75 (100%)	0	100	100
37	l	75/75 (100%)	75 (100%)	0	100	100
38	i	133/133 (100%)	133 (100%)	0	100	100
39	j	91/110 (83%)	91 (100%)	0	100	100
39	m	91/110 (83%)	91 (100%)	0	100	100
40	o	451/451 (100%)	446 (99%)	5 (1%)	70	82
41	s	152/196 (78%)	152 (100%)	0	100	100
42	t	111/435 (26%)	111 (100%)	0	100	100
42	u	106/435 (24%)	106 (100%)	0	100	100
42	v	111/435 (26%)	111 (100%)	0	100	100
42	w	106/435 (24%)	105 (99%)	1 (1%)	75	85
43	y	129/129 (100%)	129 (100%)	0	100	100
44	z	29/29 (100%)	29 (100%)	0	100	100
All	All	11756/16654 (71%)	11493 (98%)	263 (2%)	47	69

5 of 263 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	H	481	PHE
21	O	261	LYS
40	o	552	VAL
8	B	855	ARG
8	B	837	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 117 such sidechains are listed below:

Mol	Chain	Res	Type
20	N	101	ASN
42	v	79	GLN
28	W	72	ASN
42	v	43	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	p	88	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	117/189 (61%)	30 (25%)	5 (4%)
11	E	14/14 (100%)	5 (35%)	1 (7%)
15	I	39/113 (34%)	19 (48%)	2 (5%)
2	5	73/116 (62%)	24 (32%)	2 (2%)
3	6	96/106 (90%)	37 (38%)	5 (5%)
All	All	339/538 (63%)	115 (33%)	15 (4%)

5 of 115 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	16	U
1	2	17	U
1	2	19	G
1	2	20	G
1	2	24	A

5 of 15 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	6	5	U
15	I	90	C
3	6	33	G
15	I	95	U
3	6	58	G

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

2 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	$\#\|Z\|>2$
17	SEP	K	232	17	8,9,10	1.57	1 (12%)	8,12,14	1.47	2 (25%)
17	SEP	K	224	17	8,9,10	1.54	1 (12%)	8,12,14	1.58	1 (12%)

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
17	SEP	K	232	17	-	3/5/8/10	-
17	SEP	K	224	17	-	0/5/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	K	232	SEP	P-O1P	3.39	1.61	1.50
17	K	224	SEP	P-O1P	3.34	1.61	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	K	224	SEP	P-OG-CB	-3.83	107.75	118.30
17	K	232	SEP	P-OG-CB	-2.85	110.45	118.30
17	K	232	SEP	OG-CB-CA	2.46	110.54	108.14

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	K	232	SEP	CB-OG-P-O2P
17	K	232	SEP	CB-OG-P-O3P
17	K	232	SEP	CB-OG-P-O1P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 15 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
48	GTP	C	1500	45	26,34,34	1.24	1 (3%)	32,54,54	1.70	7 (21%)
47	ATP	7	702	45	26,33,33	0.92	1 (3%)	31,52,52	1.55	5 (16%)
50	IHP	c	601	-	36,36,36	0.74	0	54,60,60	0.91	3 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	GTP	C	1500	45	-	5/18/38/38	0/3/3/3
47	ATP	7	702	45	-	0/18/38/38	0/3/3/3
50	IHP	c	601	-	-	6/30/54/54	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	C	1500	GTP	C5-C6	-4.41	1.38	1.47
47	7	702	ATP	O4'-C1'	2.08	1.44	1.41

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	C	1500	GTP	PA-O3A-PB	-4.43	117.62	132.83
47	7	702	ATP	PB-O3B-PG	-4.34	117.95	132.83
47	7	702	ATP	N3-C2-N1	-4.09	122.29	128.68
48	C	1500	GTP	PB-O3B-PG	-3.51	120.78	132.83
48	C	1500	GTP	C5-C6-N1	3.47	120.07	113.95

There are no chirality outliers.

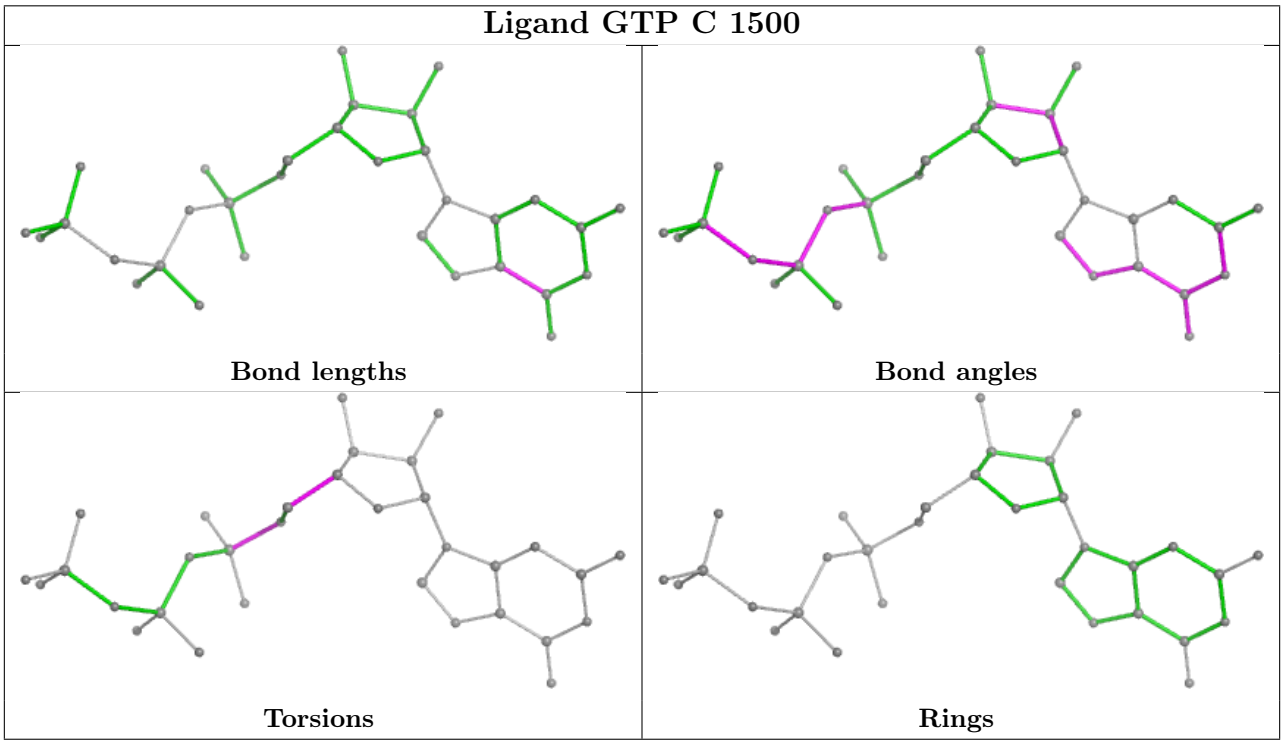
5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
48	C	1500	GTP	C5'-O5'-PA-O3A
48	C	1500	GTP	C5'-O5'-PA-O1A
48	C	1500	GTP	C5'-O5'-PA-O2A
50	c	601	IHP	C2-O12-P2-O42
50	c	601	IHP	C5-O15-P5-O25

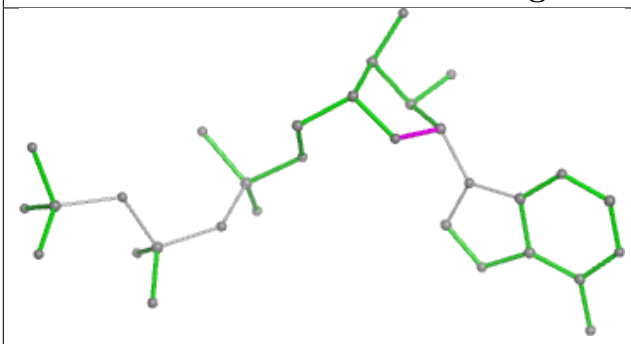
There are no ring outliers.

No monomer is involved in short contacts.

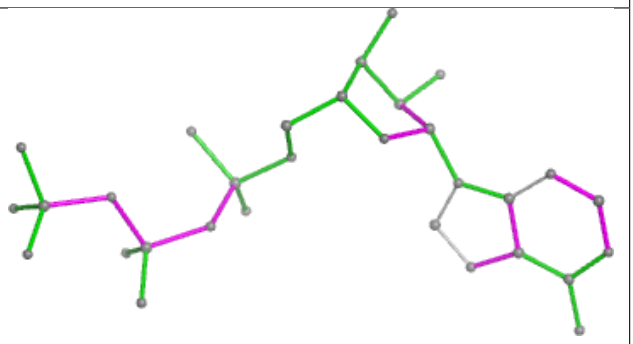
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



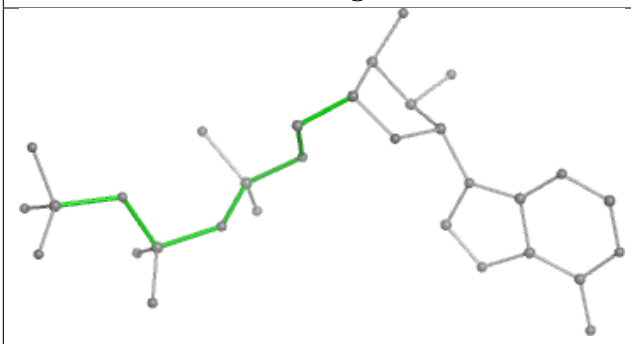
Ligand ATP 7 702



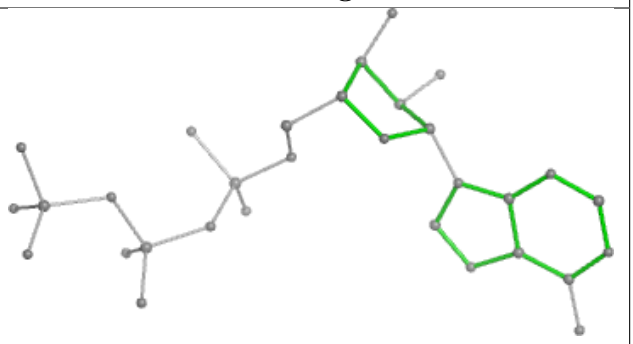
Bond lengths



Bond angles

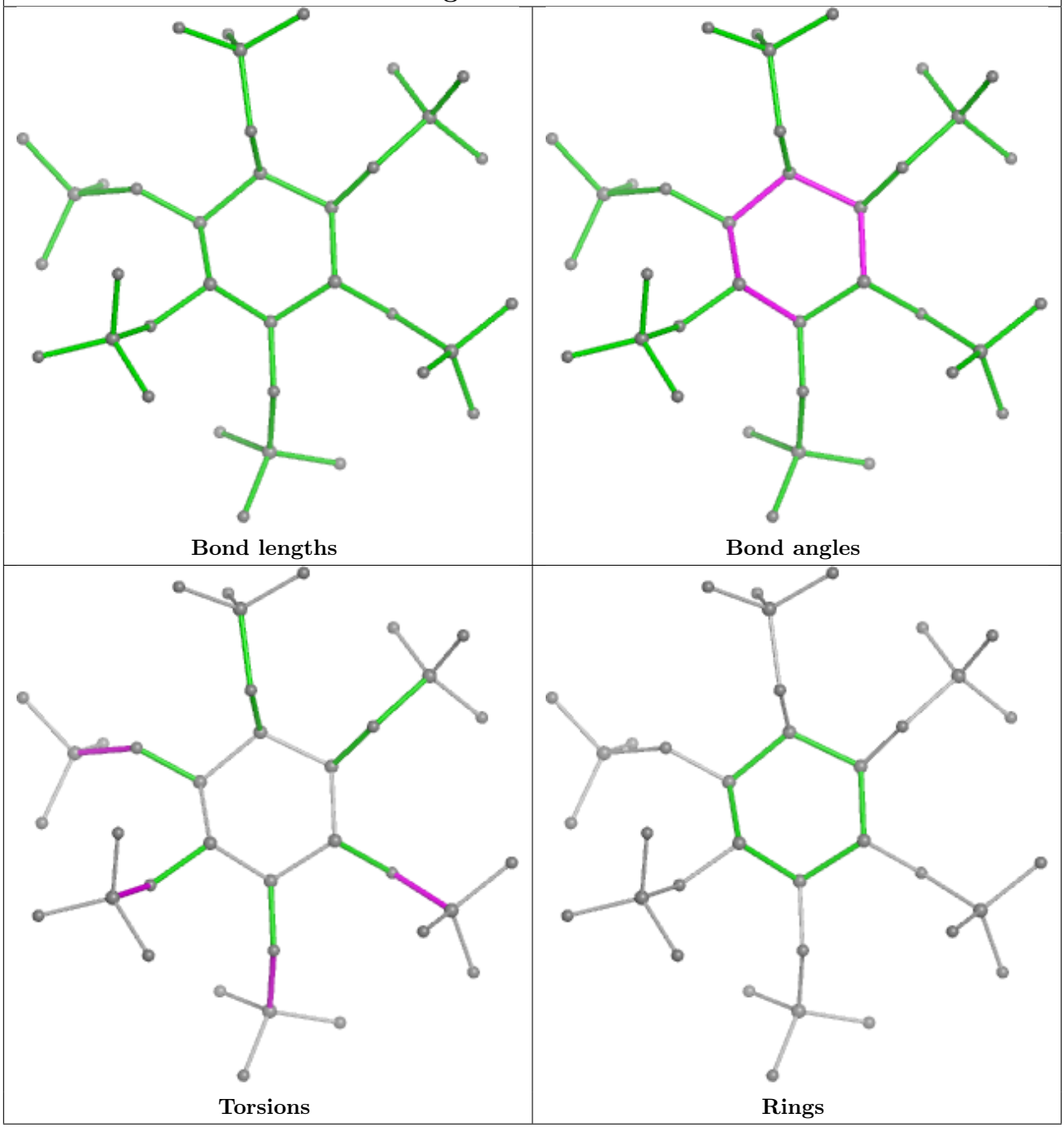


Torsions



Rings

Ligand IHP c 601



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
15	I	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	83:A	O3'	84:U	P	83.48

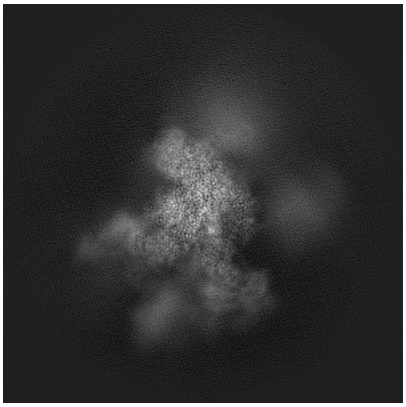
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4525. These allow visual inspection of the internal detail of the map and identification of artifacts.

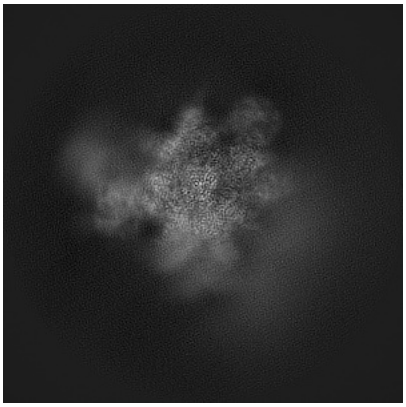
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

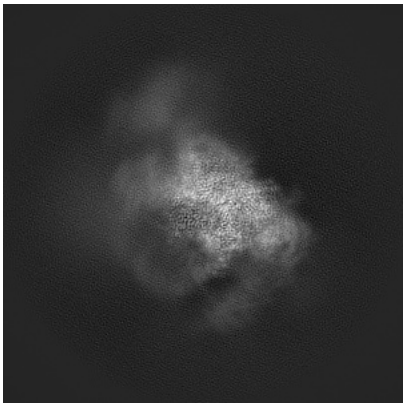
6.1.1 Primary map



X



Y

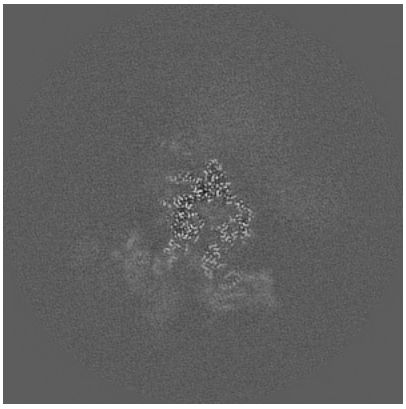


Z

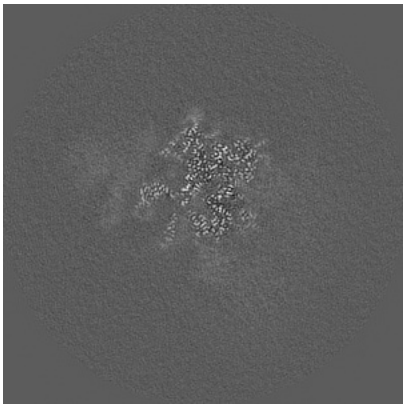
The images above show the map projected in three orthogonal directions.

6.2 Central slices

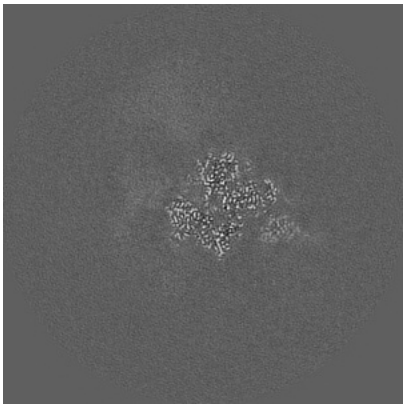
6.2.1 Primary map



X Index: 205



Y Index: 205

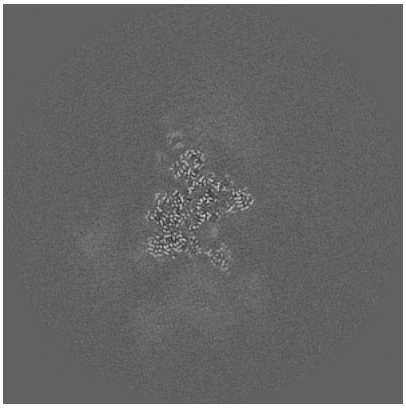


Z Index: 205

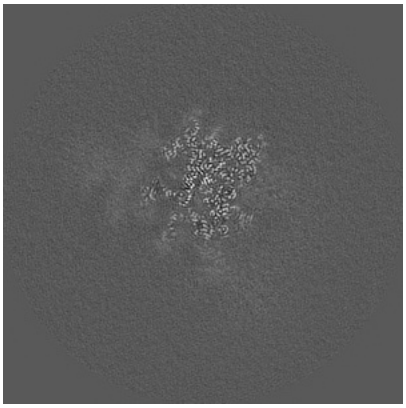
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

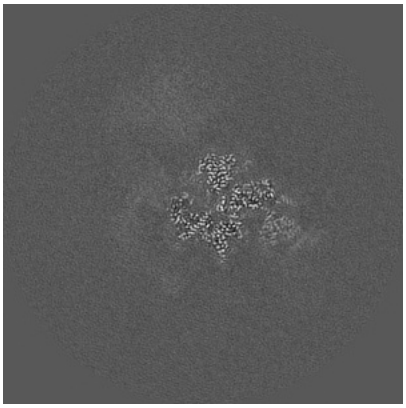
6.3.1 Primary map



X Index: 231



Y Index: 203

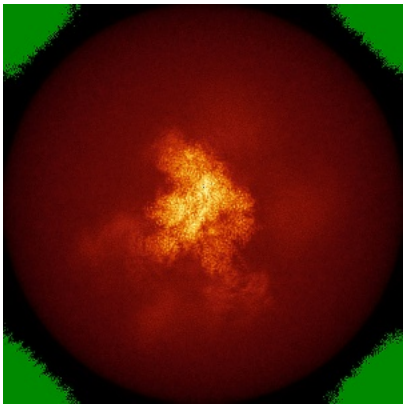


Z Index: 202

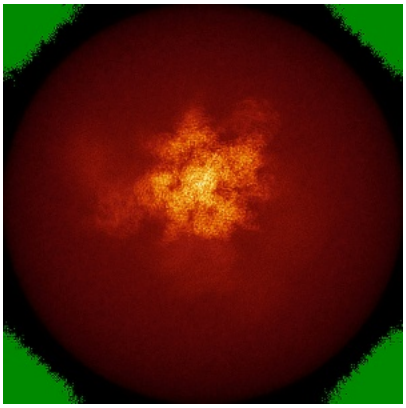
The images above show the largest variance slices of the map in three orthogonal directions.

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

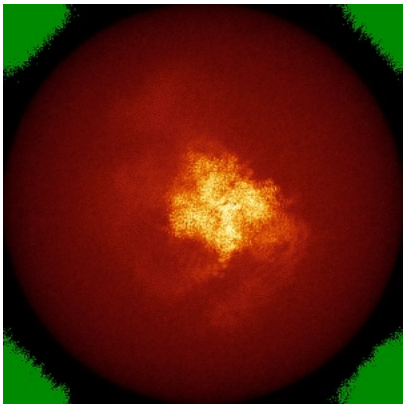
6.4.1 Primary map



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

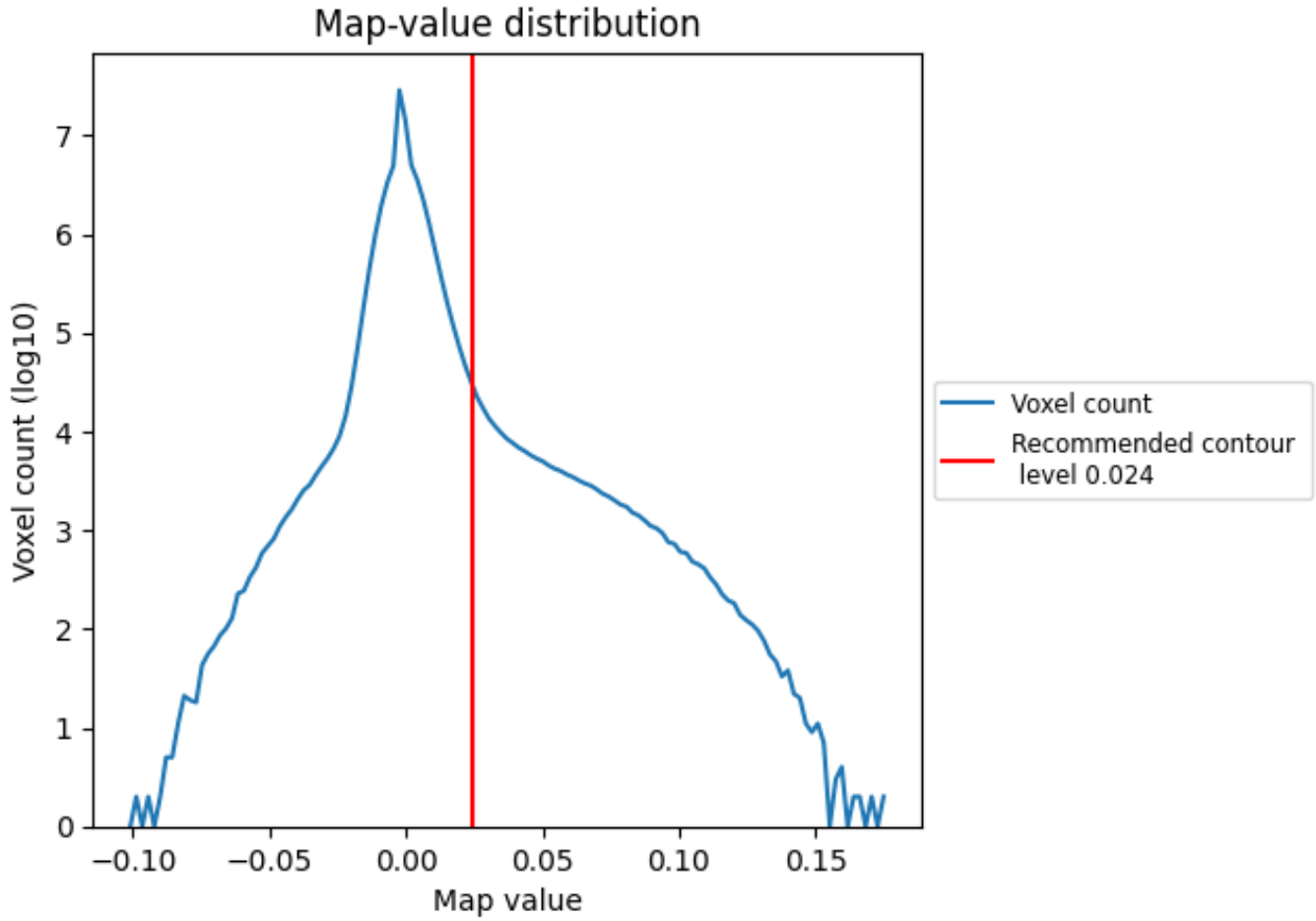
6.6 Mask visualisation (i)

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

7 Map analysis

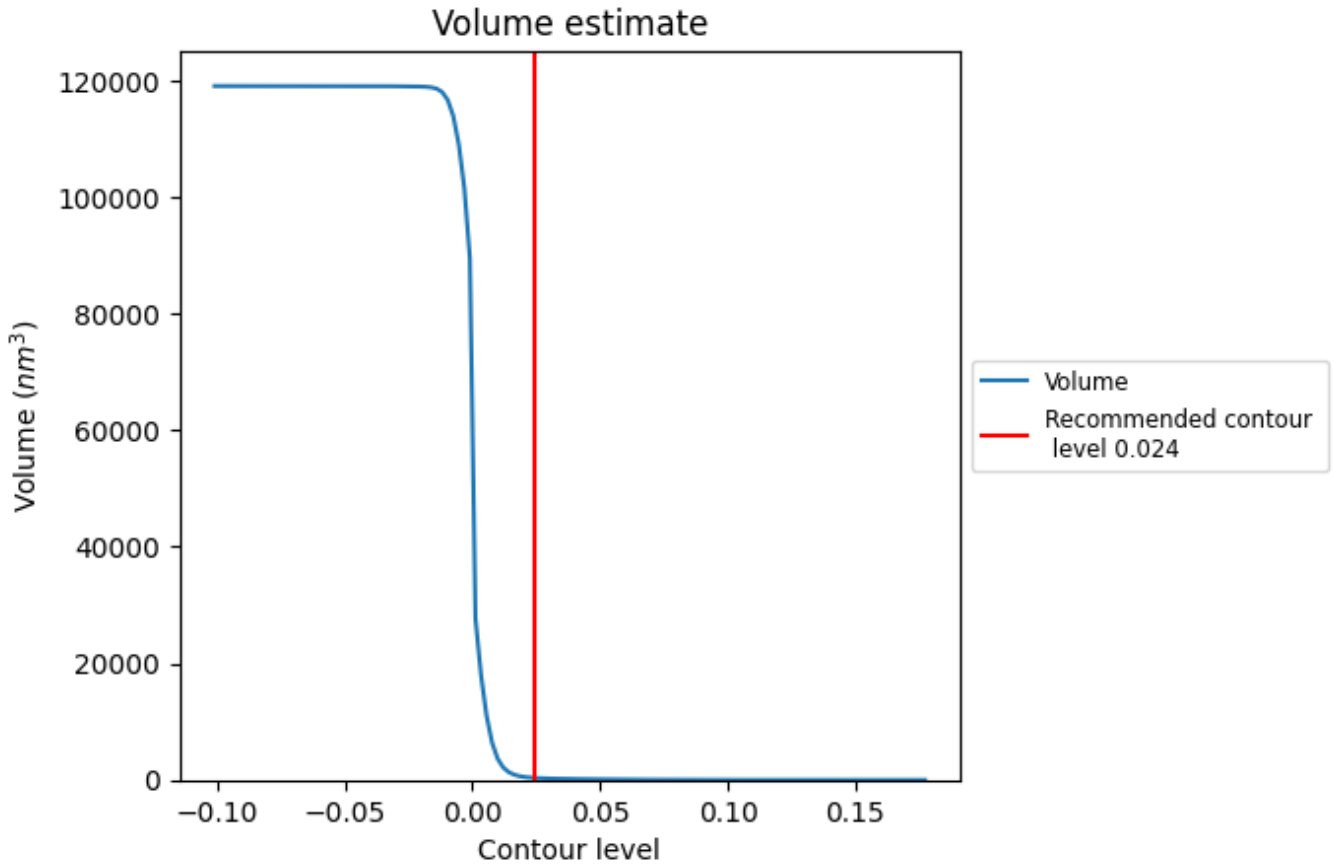
This section contains the results of statistical analysis of the map.

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.

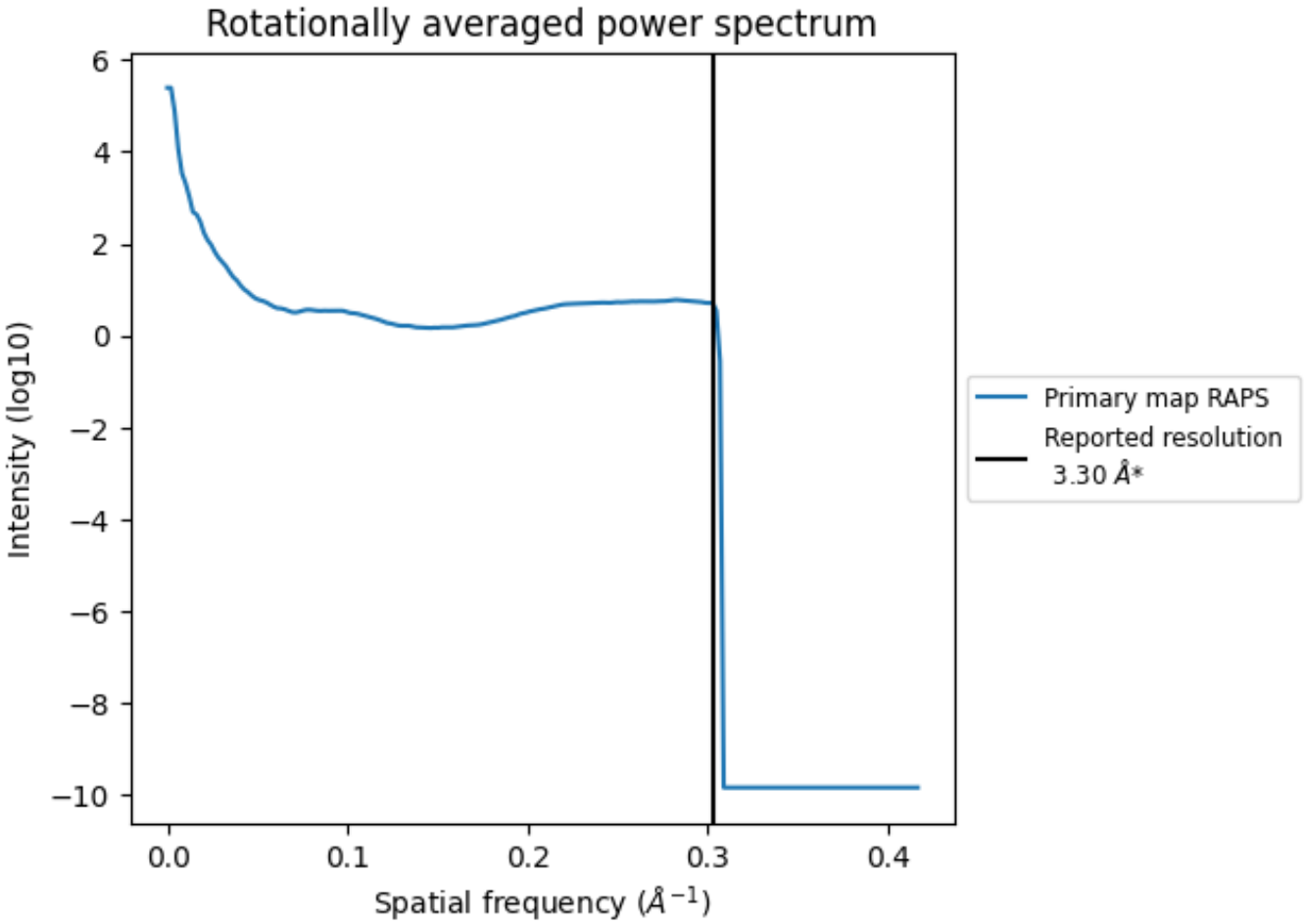
7.2 Volume estimate (i)



The volume at the recommended contour level is 356 nm^3; this corresponds to an approximate mass of 321 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)

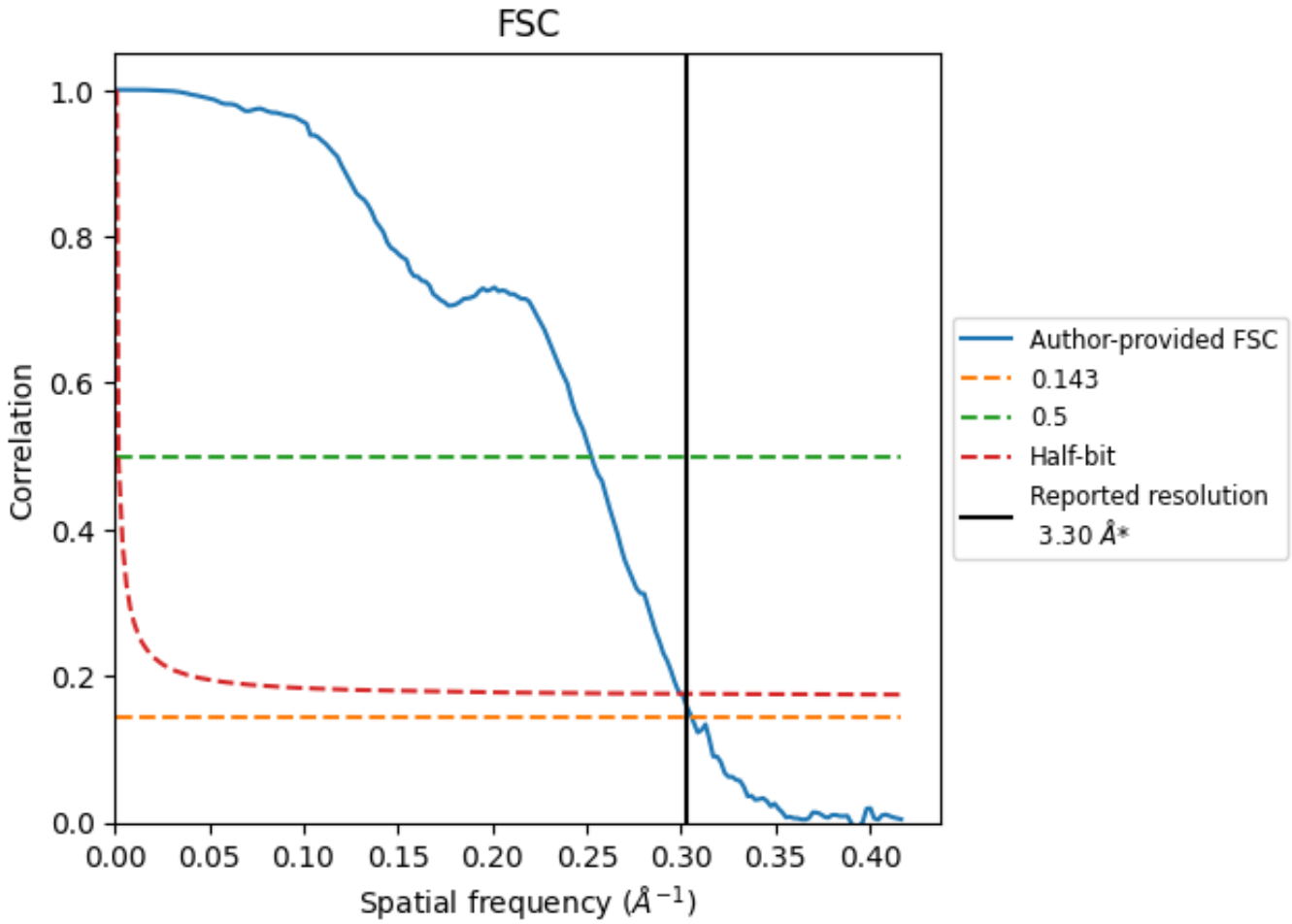


*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

8.2 Resolution estimates (i)

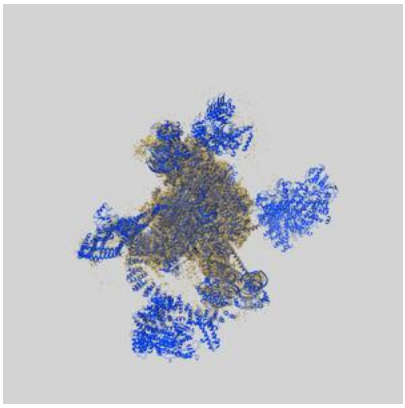
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.27	3.96	3.33
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

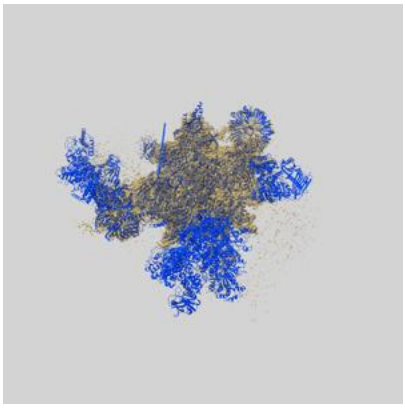
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4525 and PDB model 6QDV. Per-residue inclusion information can be found in section 3 on page 15.

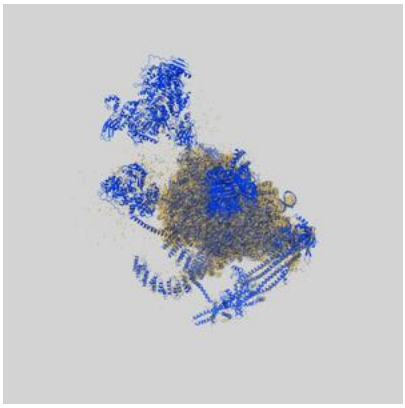
9.1 Map-model overlay



X



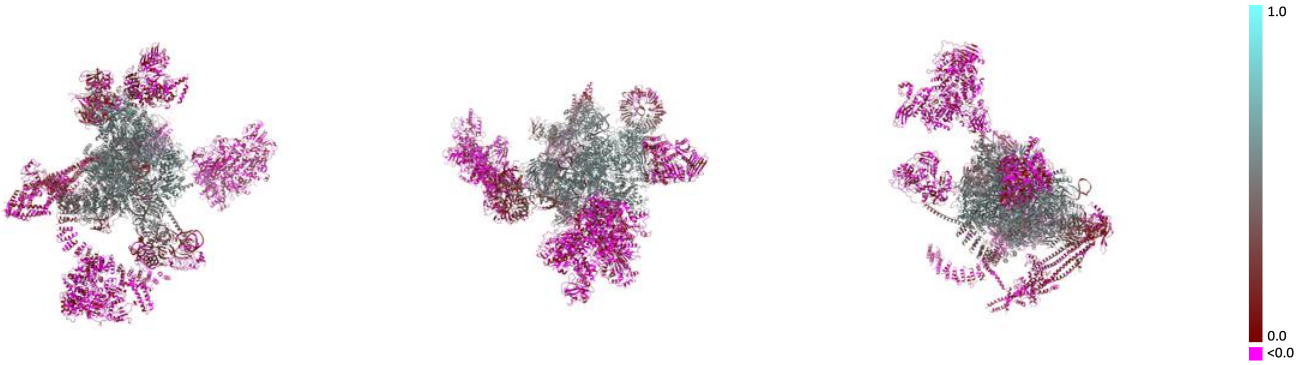
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.024 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.

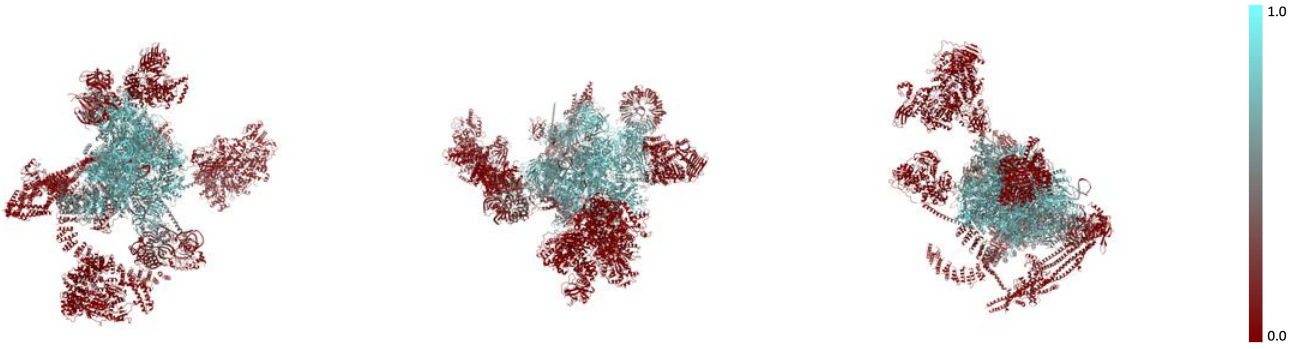
9.2 Q-score mapped to coordinate model (i)



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.

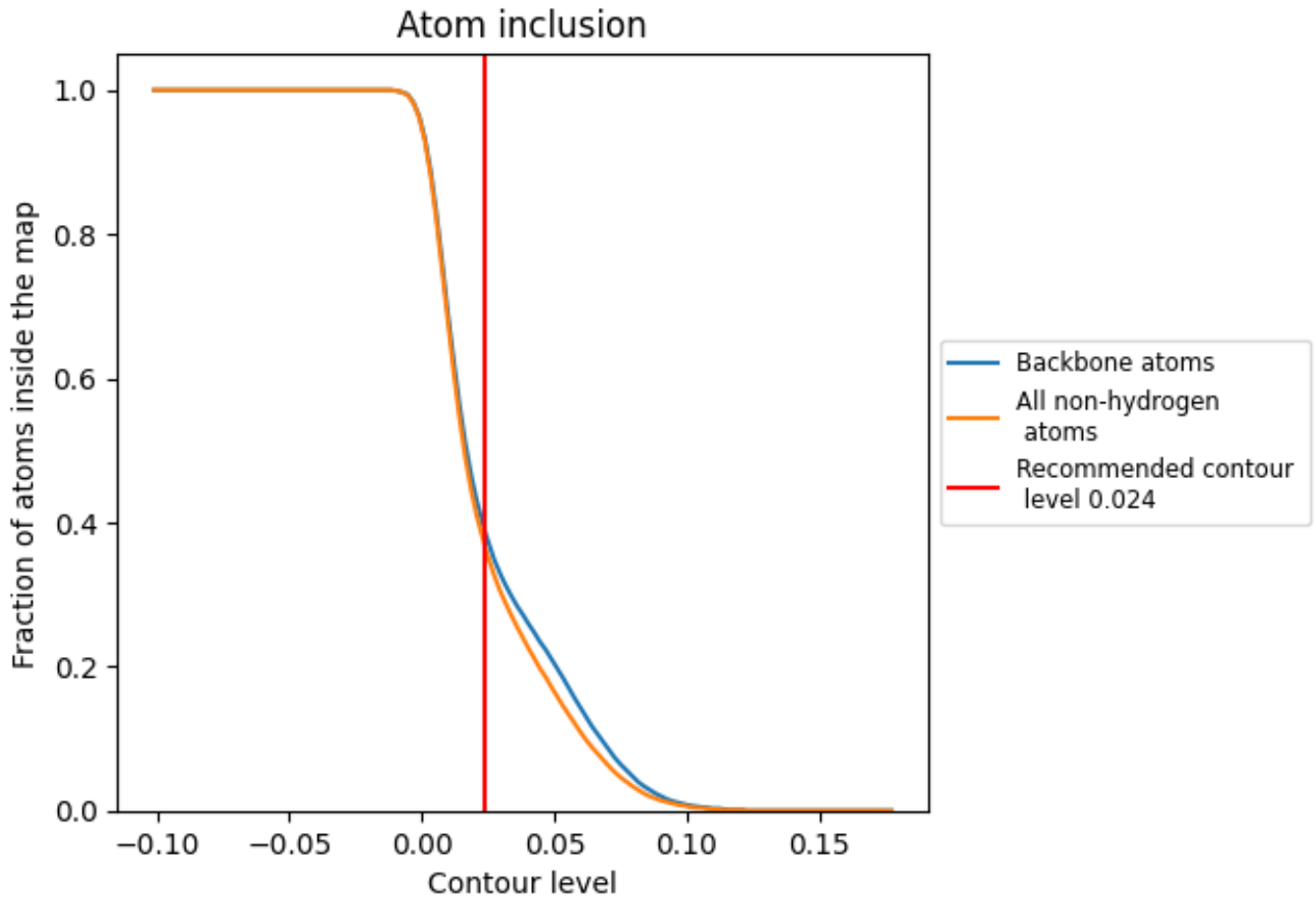
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.024).

9.4 Atom inclusion (i)



At the recommended contour level, 38% of all backbone atoms, 36% 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 (0.024) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3640	0.2780
2	0.4150	0.2640
5	0.7510	0.4540
6	0.7380	0.4570
7	0.0050	0.0600
8	0.0000	-0.0230
9	0.0000	0.0230
A	0.6840	0.4780
B	0.0010	0.0020
C	0.6850	0.5010
D	0.4080	0.3490
E	0.8410	0.5300
F	0.6280	0.4670
G	0.5770	0.5060
H	0.3250	0.2530
I	0.6040	0.3950
J	0.8350	0.5600
K	0.5780	0.4700
L	0.7400	0.5240
M	0.5150	0.4410
N	0.6240	0.4720
O	0.4300	0.3550
P	0.6530	0.5150
R	0.8340	0.5500
S	0.4420	0.3340
T	0.0660	0.1560
U	0.0010	-0.0010
V	0.0730	0.0630
W	0.0210	0.0440
Y	0.0480	0.0930
Z	0.6520	0.5040
b	0.2810	0.2660
c	0.6520	0.4960
d	0.4340	0.3790
e	0.0740	0.1380

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
f	0.0420	0.1010
g	0.2160	0.2880
h	0.1070	0.1720
i	0.5730	0.4500
j	0.0500	0.0950
k	0.2060	0.2370
l	0.1230	0.1500
m	0.0610	0.0830
n	0.3690	0.3190
o	0.6620	0.4960
p	0.2240	0.2290
q	0.1140	0.1190
r	0.3480	0.3330
s	0.0730	0.1200
t	0.0260	0.0690
u	0.0160	0.0240
v	0.0240	0.1160
w	0.0100	0.0760
y	0.6400	0.4900
z	0.0110	0.1960