wwPDB EM Validation Summary Report ⓘ

Nov 20, 2022 – 02:49 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 ⓘ symbol.

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

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

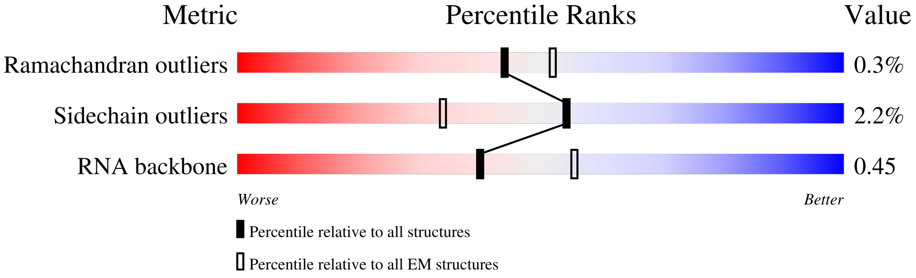
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance ⓘ

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

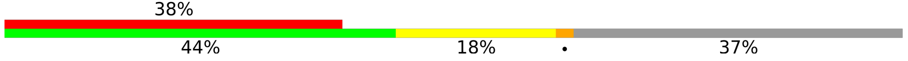
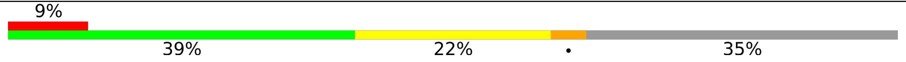
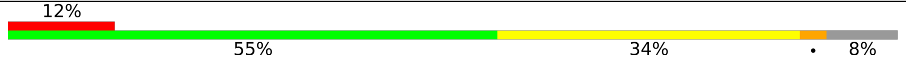
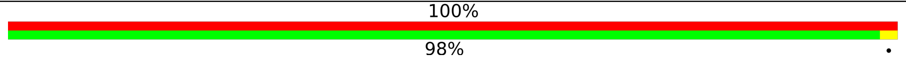
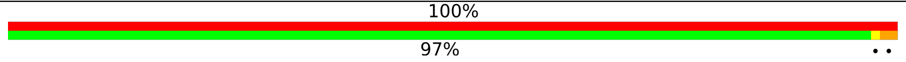
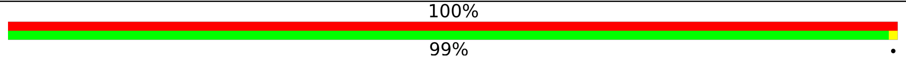
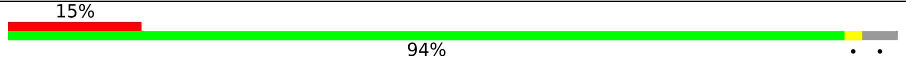
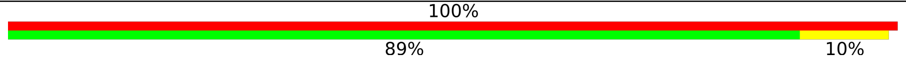
The reported resolution of this entry is 3.30 Å.

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	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	2	189	
2	5	116	
3	6	106	
4	7	390	
5	8	91	
6	9	144	
7	A	2335	
8	B	1722	

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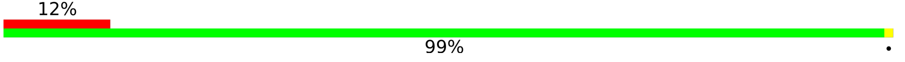
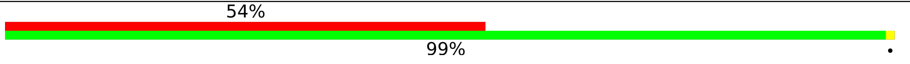
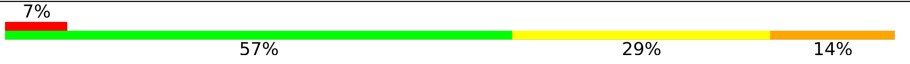
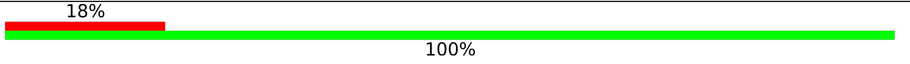
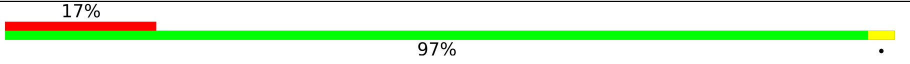
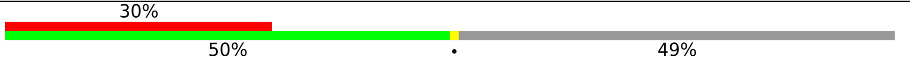
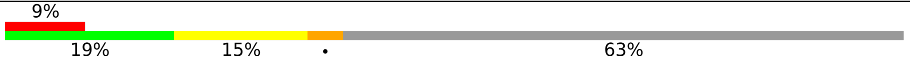
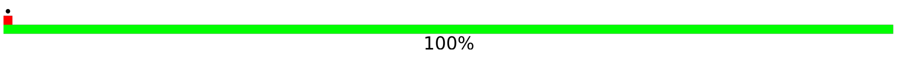
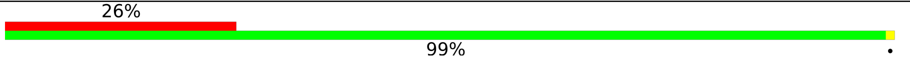
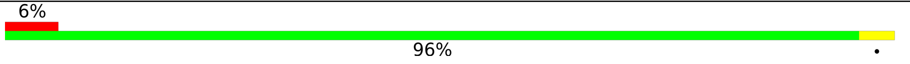
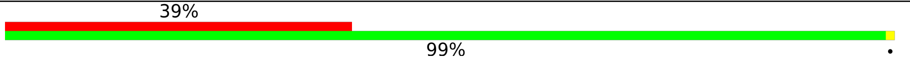
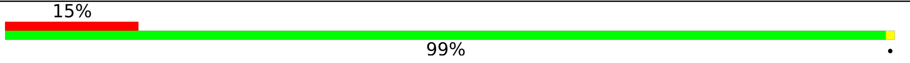
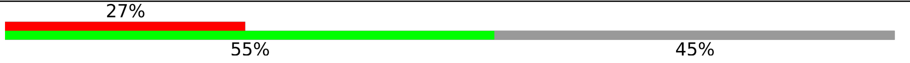
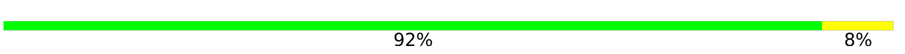
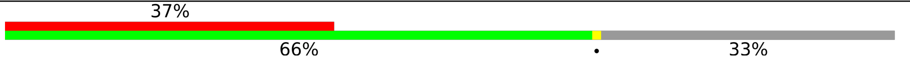
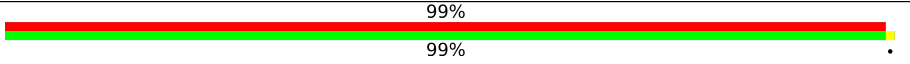
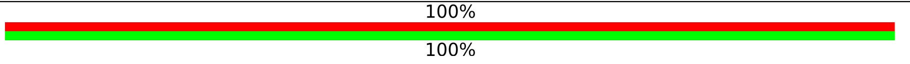
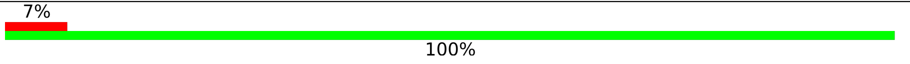
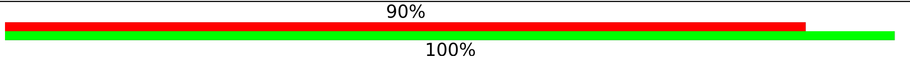
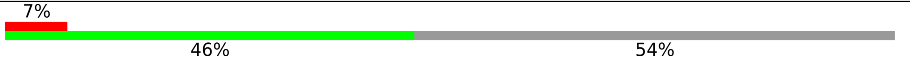
Mol	Chain	Length	Quality of chain
9	C	899	
10	D	123	
11	E	14	
12	F	122	
13	G	60	
14	H	908	
15	I	113	
16	J	320	
17	K	295	
18	L	144	
19	M	289	
20	N	306	
21	O	802	
22	P	229	
23	R	26	
24	S	848	
25	T	855	
26	U	1485	
27	V	1220	
28	W	162	
29	Y	92	
30	Z	30	
31	b	82	
31	k	82	
32	c	586	

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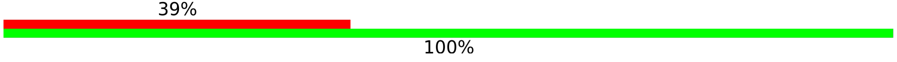
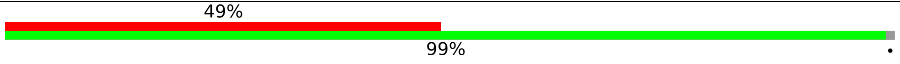
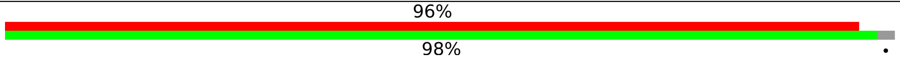
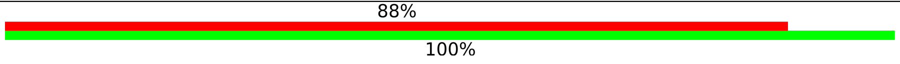
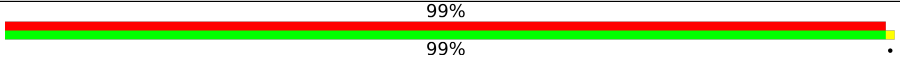
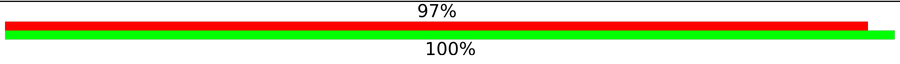
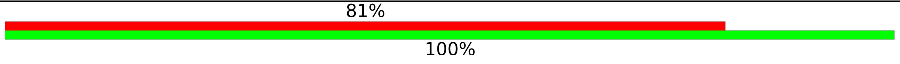
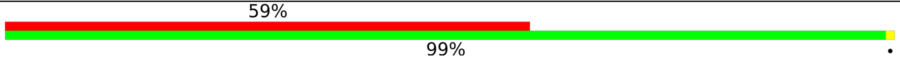
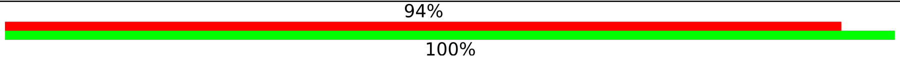
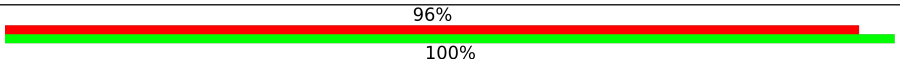
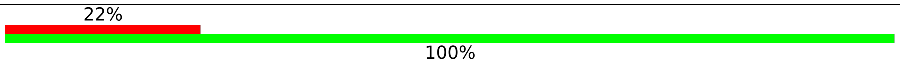
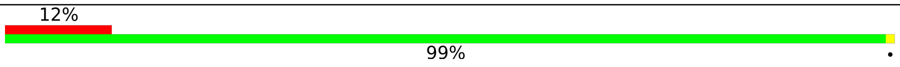
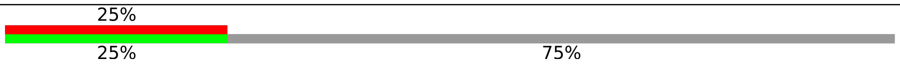
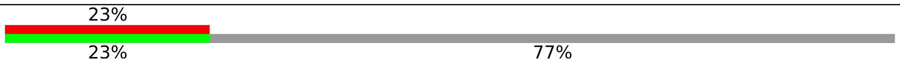
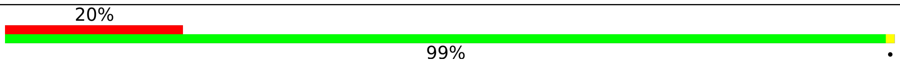
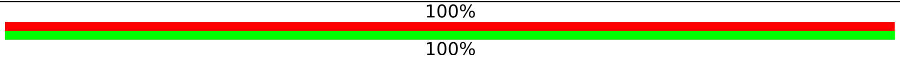
Mol	Chain	Length	Quality of chain
33	d	84	
33	n	84	
34	e	81	
34	p	81	
35	f	72	
35	q	72	
36	g	73	
36	r	73	
37	h	80	
37	l	80	
38	i	164	
39	j	118	
39	m	118	
40	o	513	
41	s	225	
42	t	504	
42	u	504	
42	v	504	
42	w	504	
43	y	144	
44	z	34	

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.

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

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
7	?	-	GLU	deletion	UNP P38919
7	405	MET	-	expression tag	UNP P38919
7	406	ASN	-	expression tag	UNP P38919
7	407	VAL	-	expression tag	UNP P38919
7	408	ALA	-	expression tag	UNP P38919
7	409	ASP	-	expression tag	UNP P38919
7	410	LEU	-	expression tag	UNP P38919
7	411	ILE	-	expression tag	UNP P38919

- 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

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
8	151	VAL	-	expression tag	UNP Q9Y5S9
8	152	ARG	-	expression tag	UNP Q9Y5S9
8	153	GLY	-	expression tag	UNP Q9Y5S9
8	154	PRO	-	expression tag	UNP Q9Y5S9

- 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

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
9	146	LYS	-	expression tag	UNP Q96A72
9	147	PRO	-	expression tag	UNP Q96A72
9	148	ILE	-	expression tag	UNP Q96A72

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

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

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

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

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

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

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
			Total	C	N	O	S		
10	D	123	1013	635	193	180	5	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	140	LEU	-	expression tag	UNP Q9H875
D	141	ALA	-	expression tag	UNP Q9H875
D	142	LYS	-	expression tag	UNP Q9H875

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

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

- Molecule 12 is a protein called Cactin.

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

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 504	C 314	N 96	O 92	S 2	0	0

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

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

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

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

- Molecule 16 is a protein called Pleiotropic regulator 1.

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

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

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

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	?	-	GLU	deletion	UNP Q13573
K	330	LYS	-	expression tag	UNP Q13573
K	331	ALA	-	expression tag	UNP Q13573
K	332	ARG	-	expression tag	UNP Q13573
K	333	GLU	-	expression tag	UNP Q13573
K	334	ARG	-	expression tag	UNP Q13573
K	335	ARG	-	expression tag	UNP Q13573

- Molecule 18 is a protein called Protein BUD31 homolog.

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

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

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

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
			Total	C	N	O	S		
20	N	306	2394	1501	422	457	14	0	0

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
			Total	C	N	O	S		
21	O	441	3416	2116	648	639	13	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	163	LYS	-	expression tag	UNP P09661

- 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 745 480 130 130 5	0	0

- 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 230 140 43 45 2	0	0

- 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 545 347 95 96 7	0	0
31	k	82	Total C N O S 664 419 121 117 7	0	0

- 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 2215 1392 397 418 8	0	0

- 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 658 412 116 124 6	0	0
33	n	83	Total C N O S 652 409 115 122 6	0	0

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

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

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

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

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

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
h	79	LEU	-	expression tag	UNP P62314
h	80	LEU	-	expression tag	UNP P62314
l	79	LEU	-	expression tag	UNP P62314
l	80	LEU	-	expression tag	UNP P62314

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

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
i	165	SER	-	expression tag	UNP Q9Y3C6
i	166	GLY	-	expression tag	UNP Q9Y3C6

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

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

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

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

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

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

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

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
y	240	GLY	-	expression tag	UNP O95926
y	241	THR	-	expression tag	UNP O95926
y	242	ALA	-	expression tag	UNP O95926
y	243	VAL	-	expression tag	UNP O95926

- 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 280 166 59 53 2	0	0

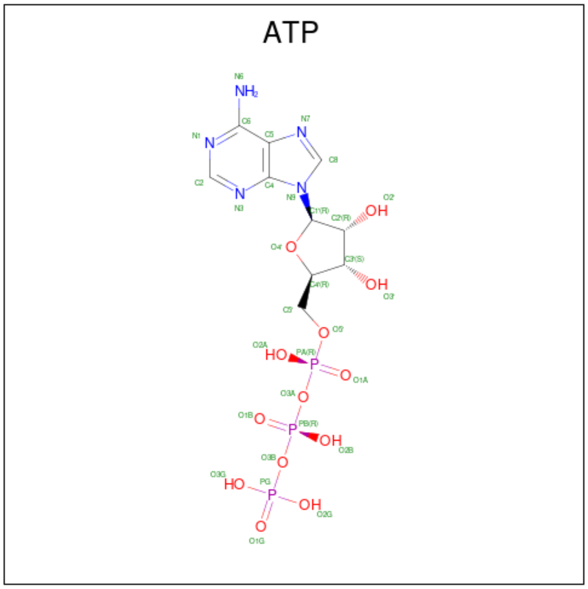
- Molecule 45 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

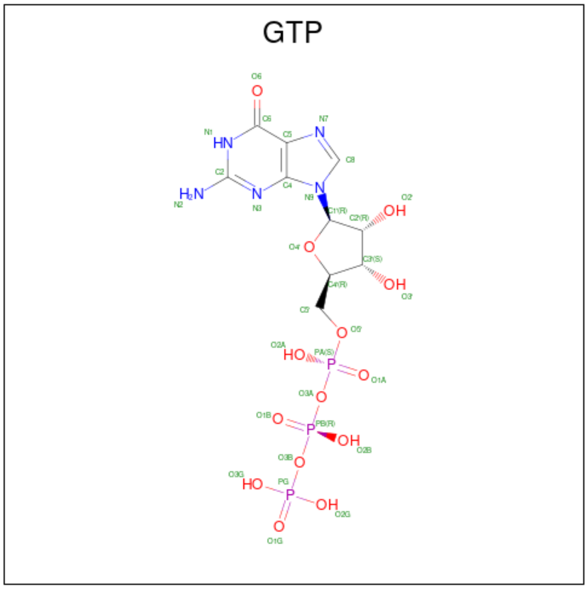
Mol	Chain	Residues	Atoms	AltConf
46	6	1	Total K 1 1	0

- 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 31 10 5 13 3	0

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

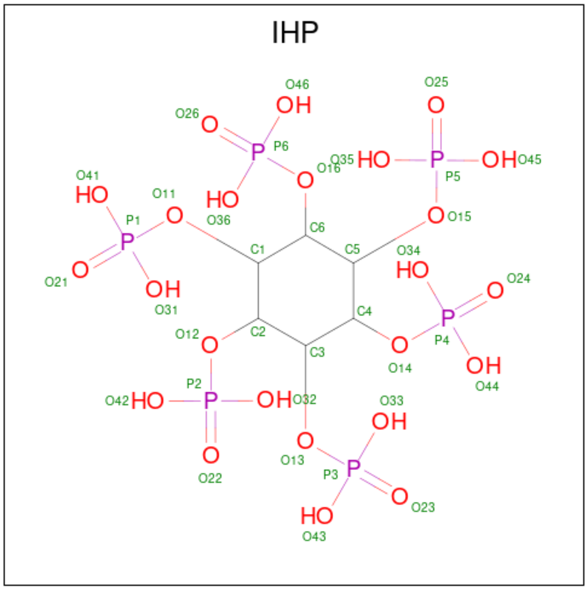


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
48	C	1	32	10	5	14	3	0

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

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

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



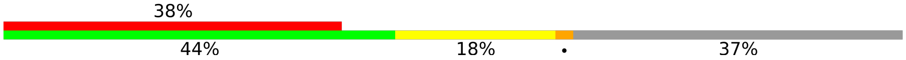
Mol	Chain	Residues	Atoms	AltConf
50	c	1	Total C O P 36 6 24 6	0

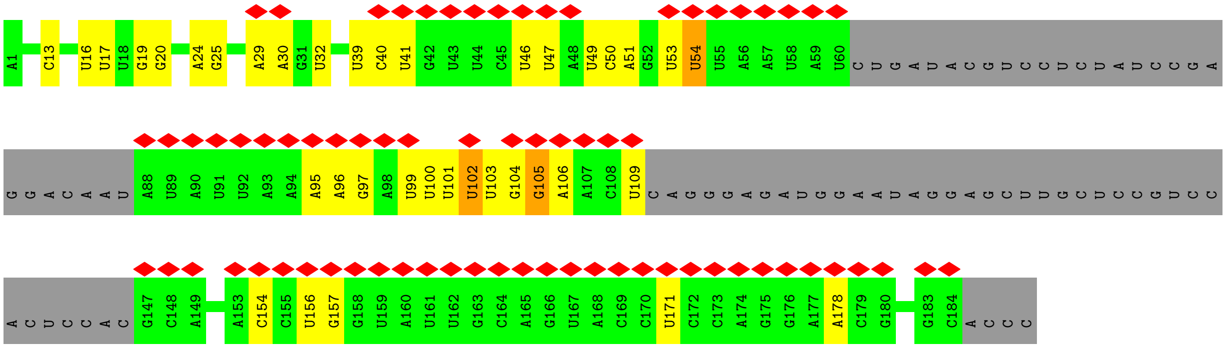
3 Residue-property plots ⓘ

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

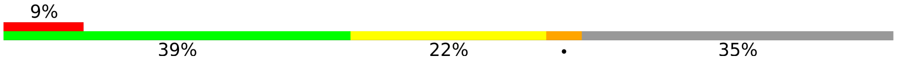
Chain 2:

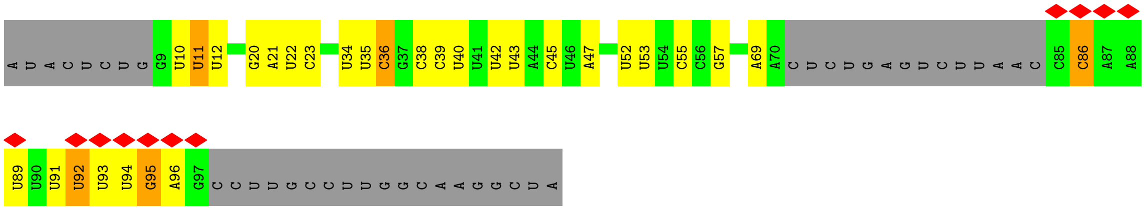




- Molecule 2: U5 snRNA

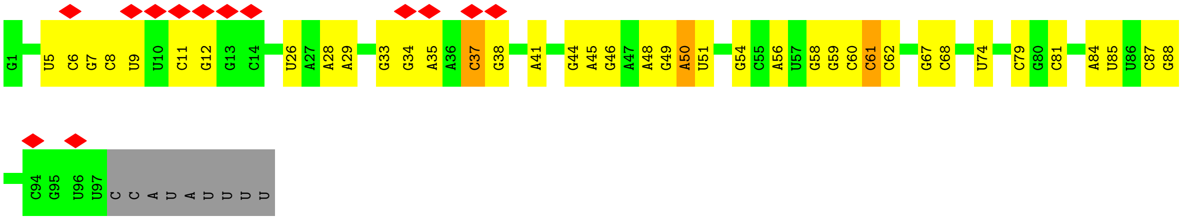
Chain 5:



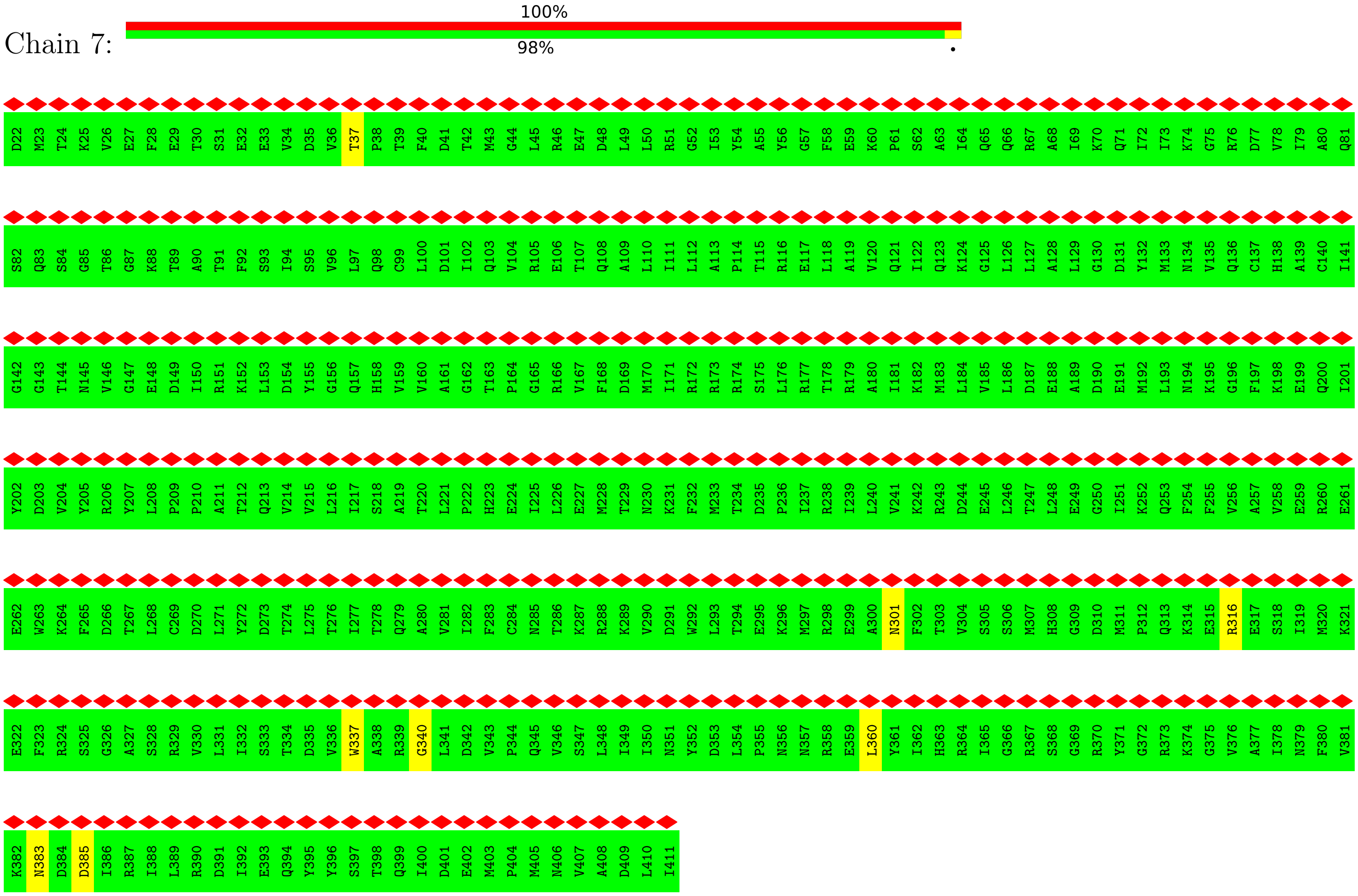


- Molecule 3: U6 snRNA

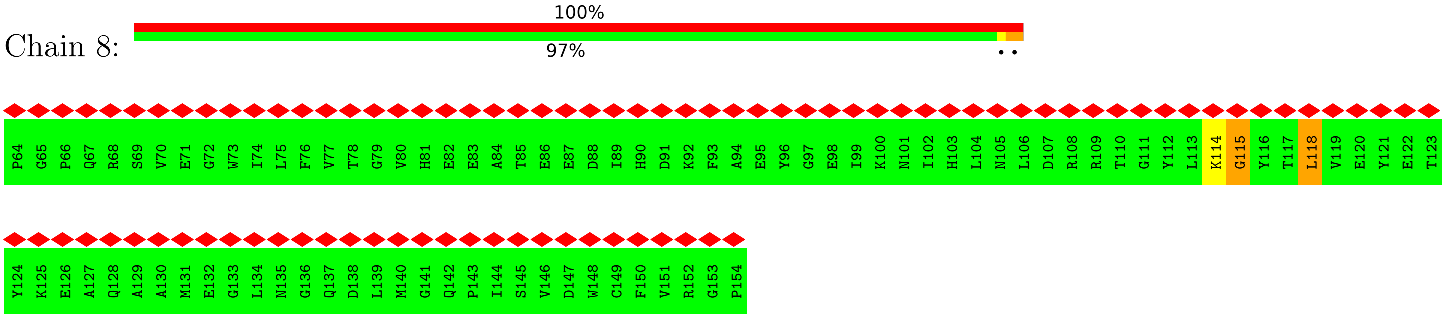
Chain 6:



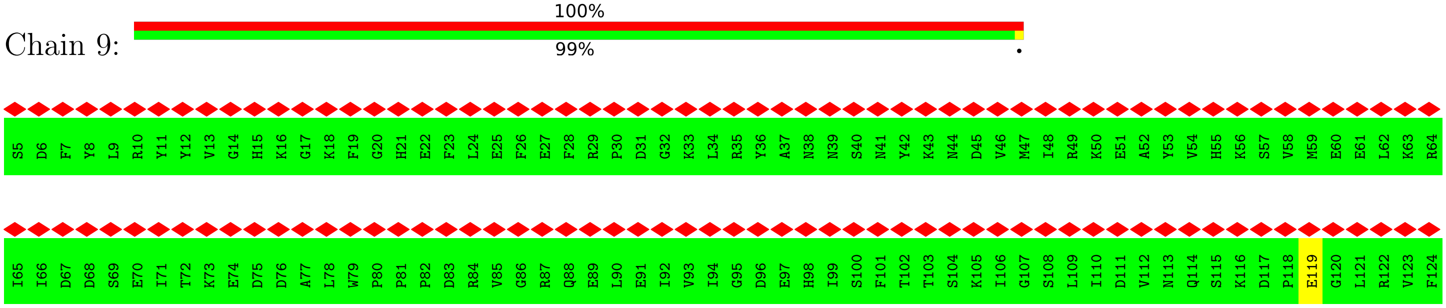
- Molecule 4: Eukaryotic initiation factor 4A-III

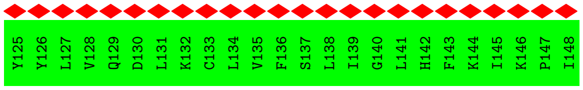


- Molecule 5: RNA-binding protein 8A



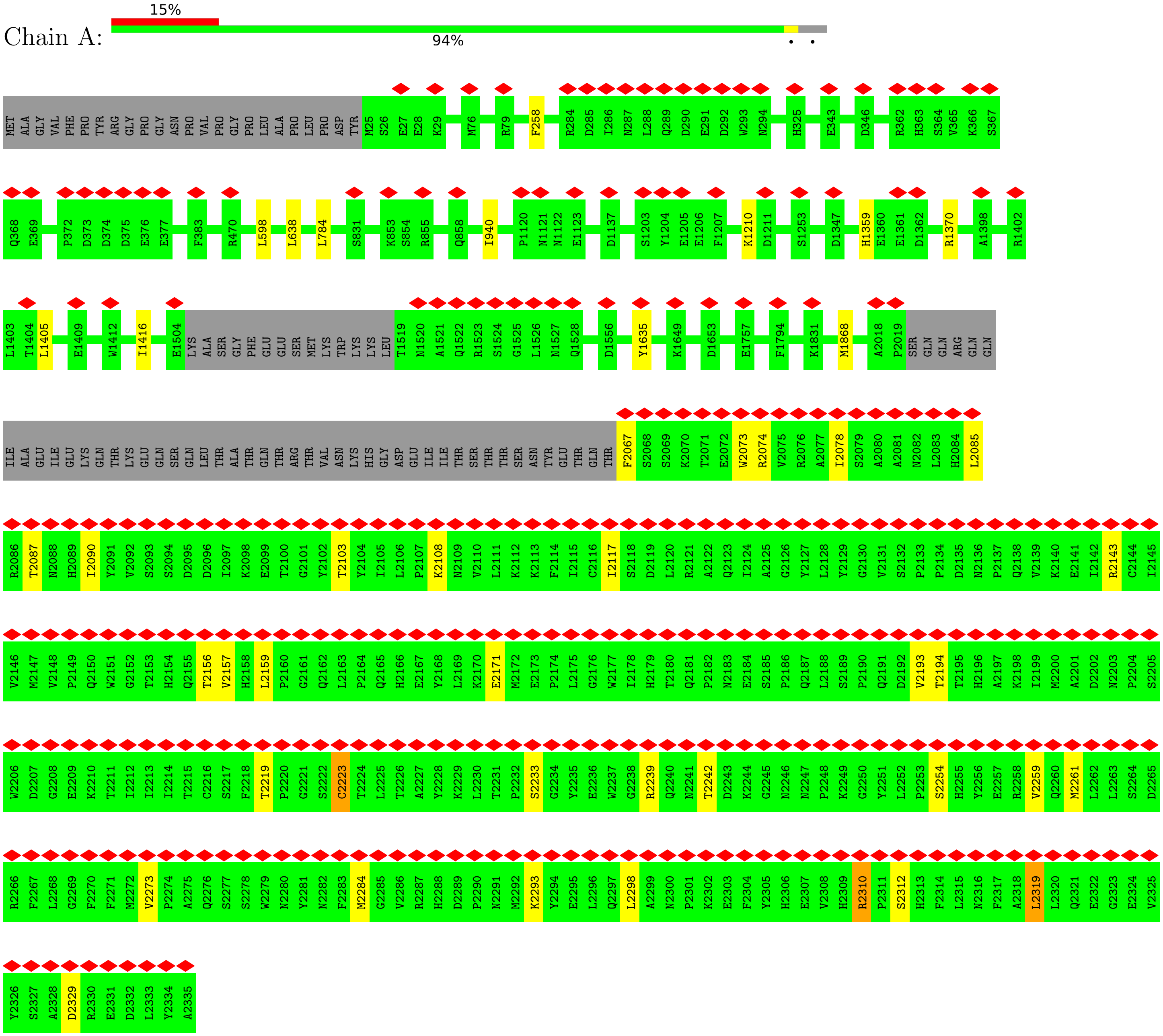
- Molecule 6: Protein mago nashi homolog 2





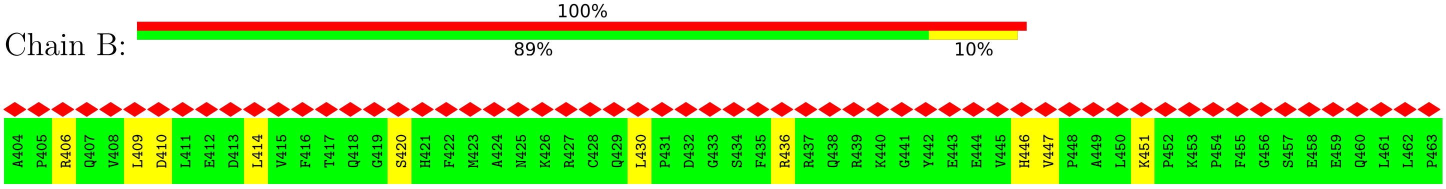
- Molecule 7: Pre-mRNA-processing-splicing factor 8

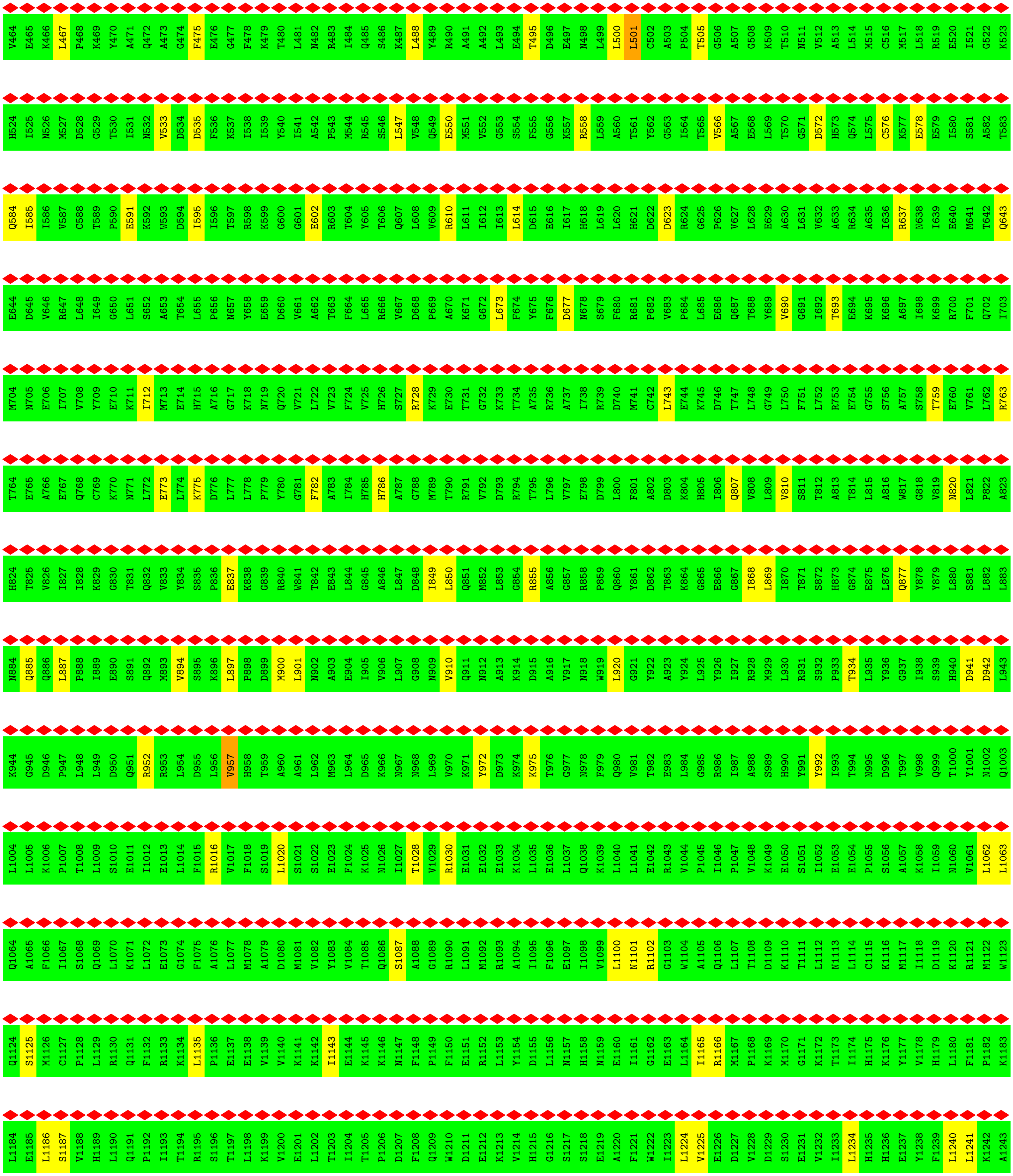
Chain A:



- Molecule 8: U5 small nuclear ribonucleoprotein 200 kDa helicase

Chain B:





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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

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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

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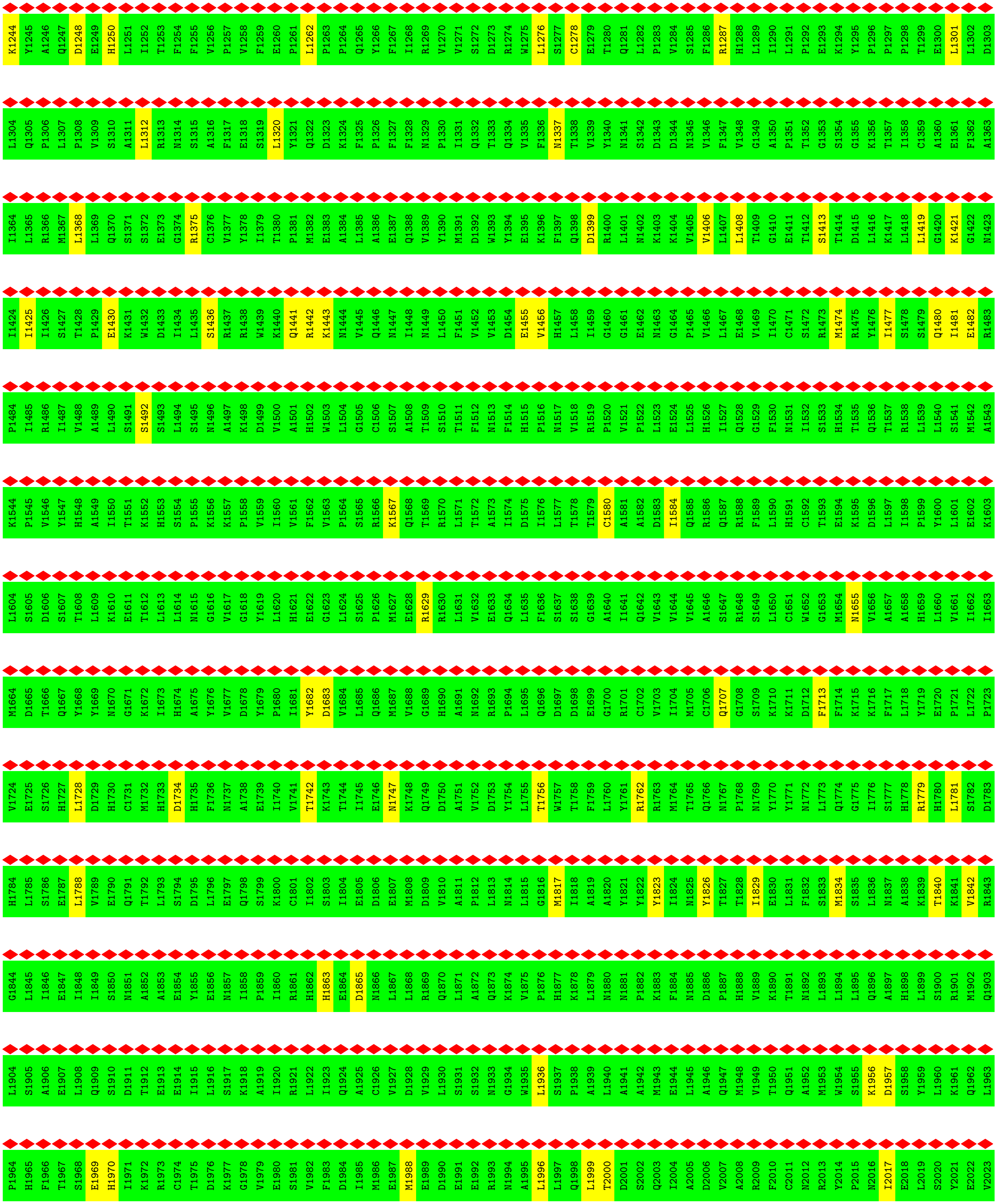
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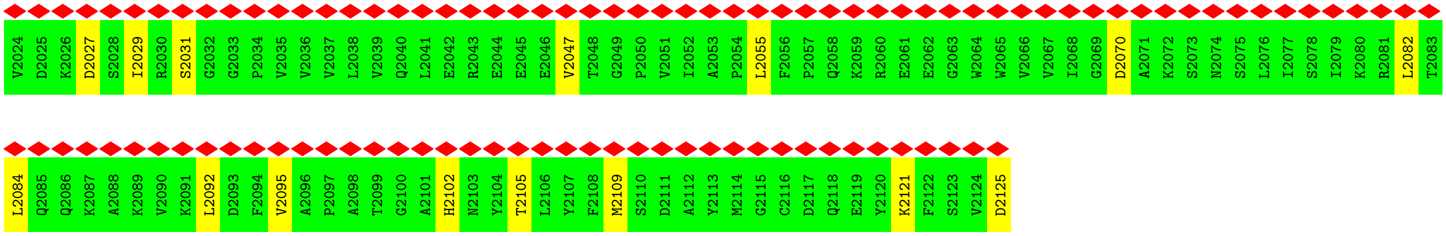
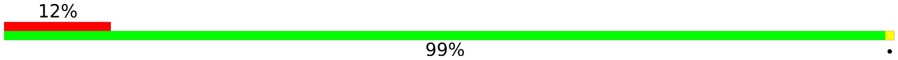
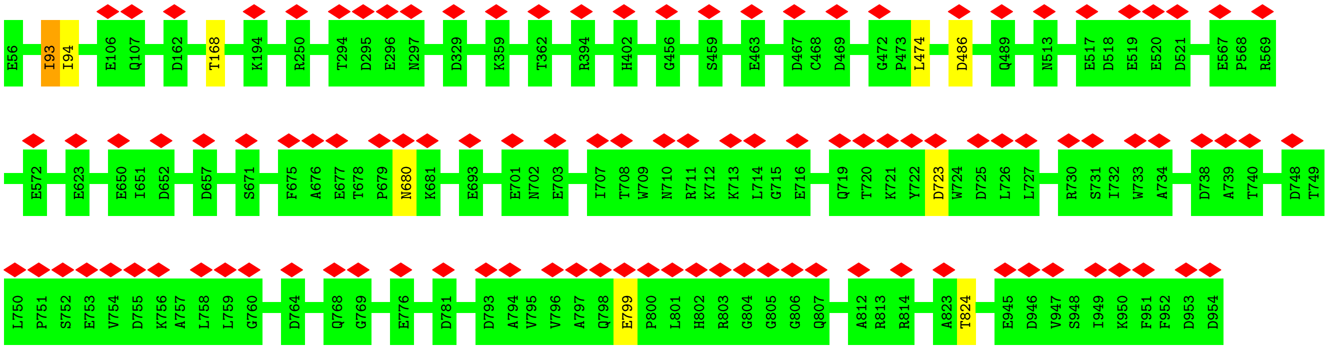


- Molecule 9: 116 kDa U5 small nuclear ribonucleoprotein component

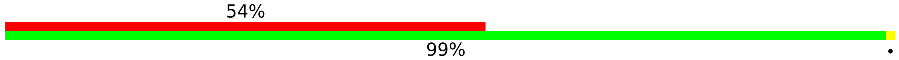
Chain C:





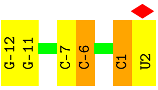
- Molecule 10: PRKR-interacting protein 1

Chain D:



- Molecule 11: Ligated exons: MINX mRNA

Chain E:



- Molecule 12: Cactin

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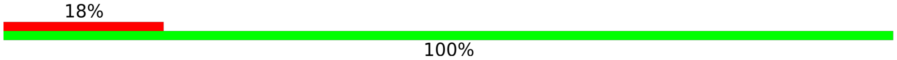
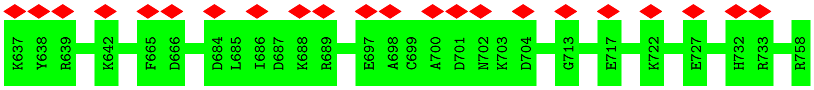
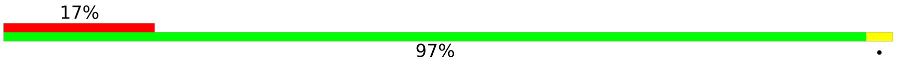
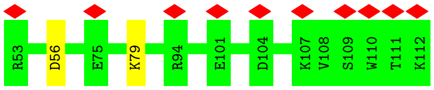




- Molecule 13: Protein FAM32A

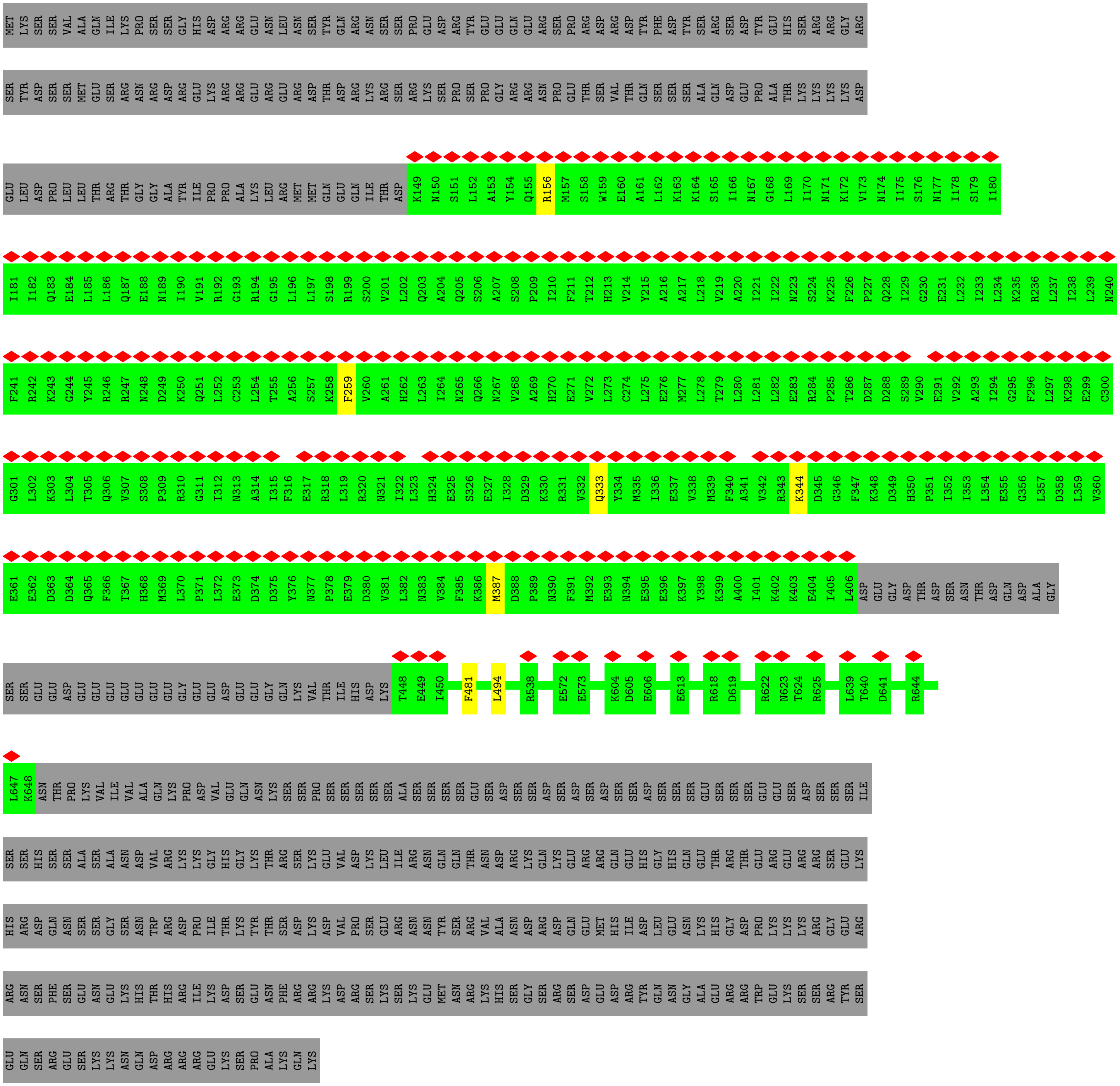
Chain G:



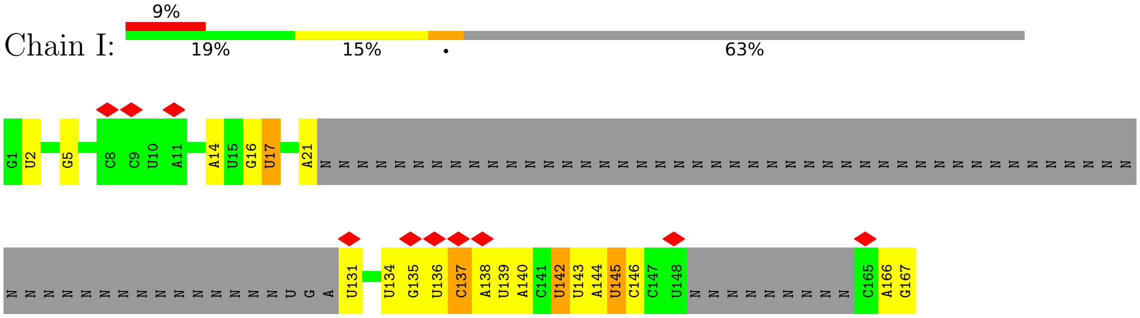


- Molecule 14: Pre-mRNA-splicing factor CWC22 homolog

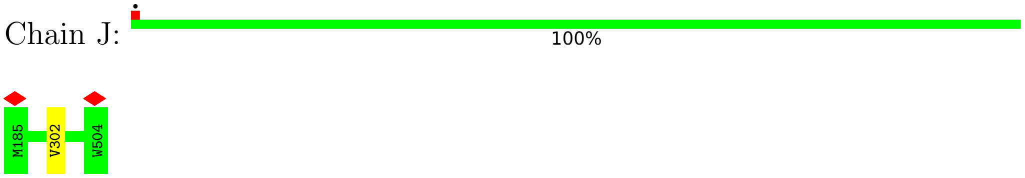
Chain H:



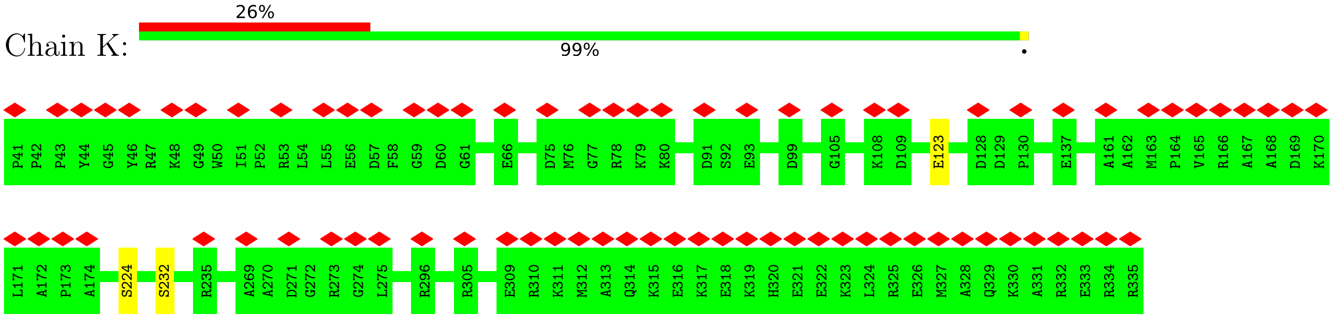
- Molecule 15: Intron lariat: MINX RNA



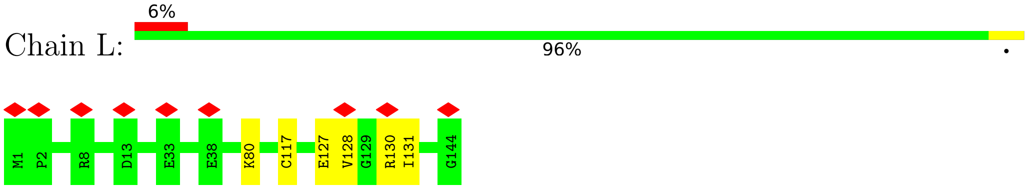
- Molecule 16: Pleiotropic regulator 1



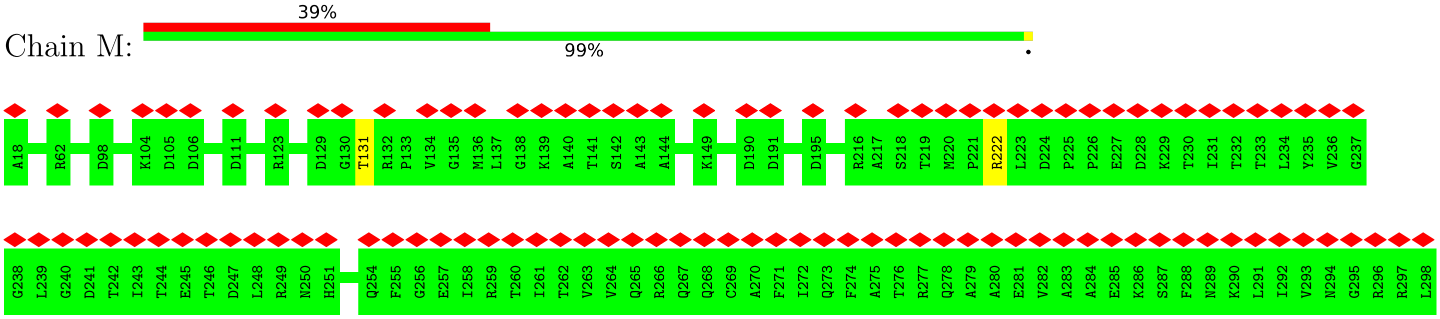
- Molecule 17: SNW domain-containing protein 1

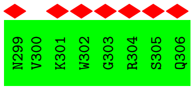


- Molecule 18: Protein BUD31 homolog



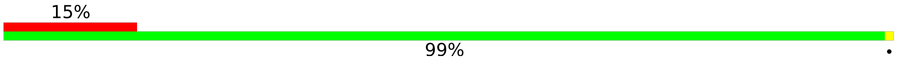
- Molecule 19: Pre-mRNA-splicing factor RBM22

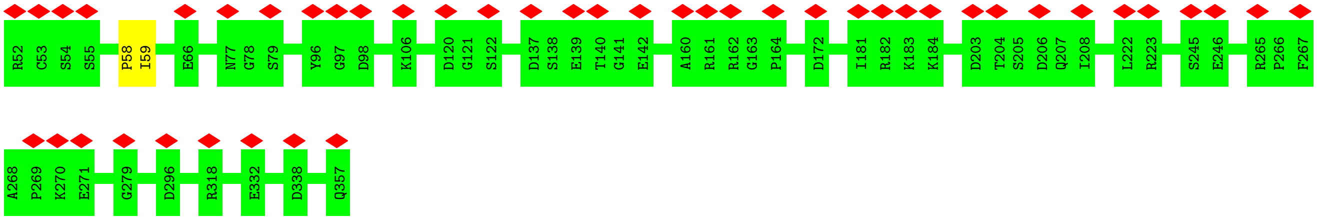




- Molecule 20: U5 small nuclear ribonucleoprotein 40 kDa protein

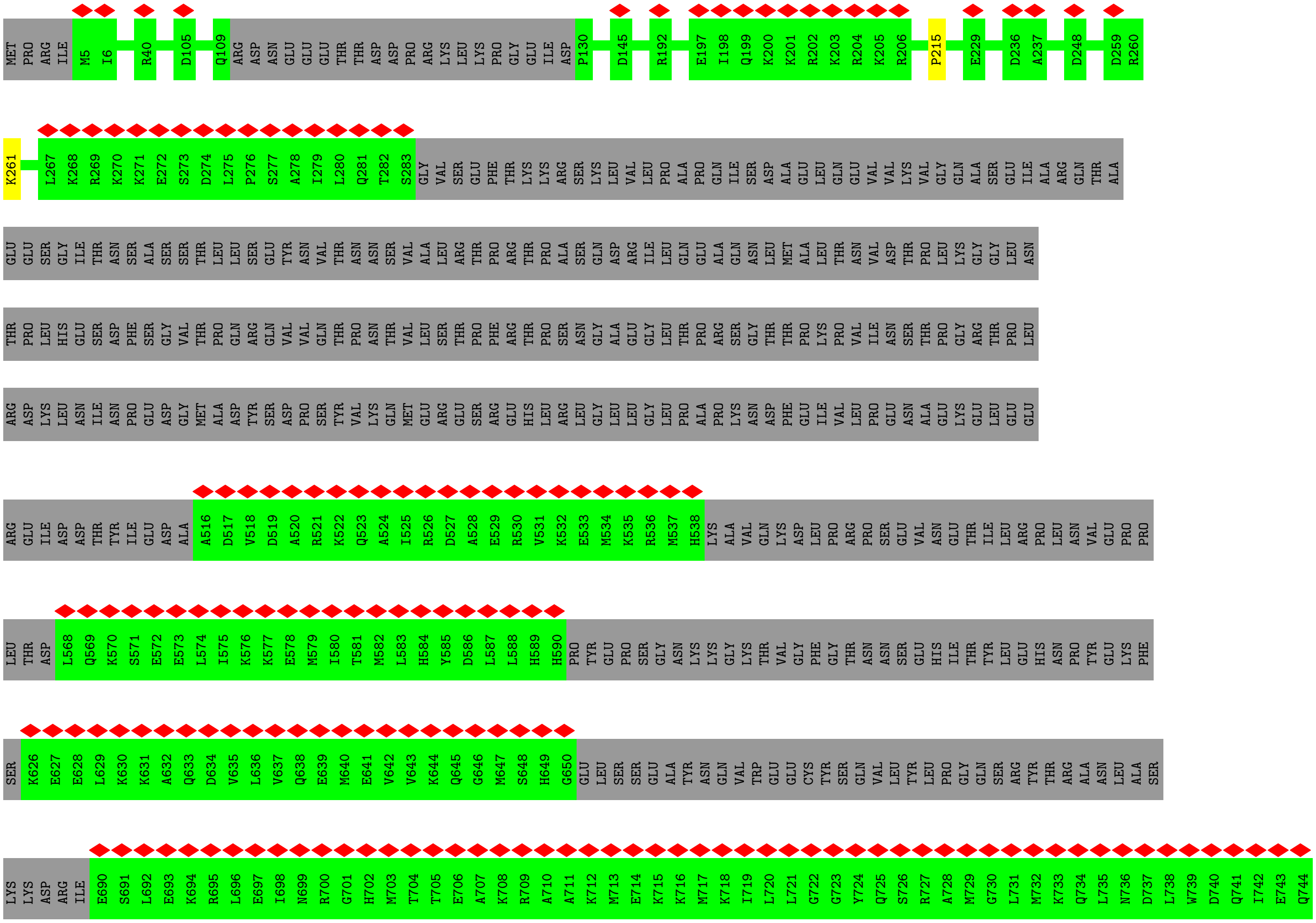
Chain N:

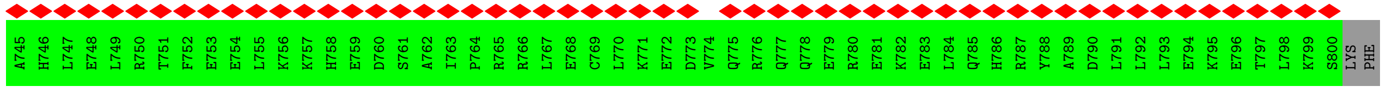




- Molecule 21: Cell division cycle 5-like protein

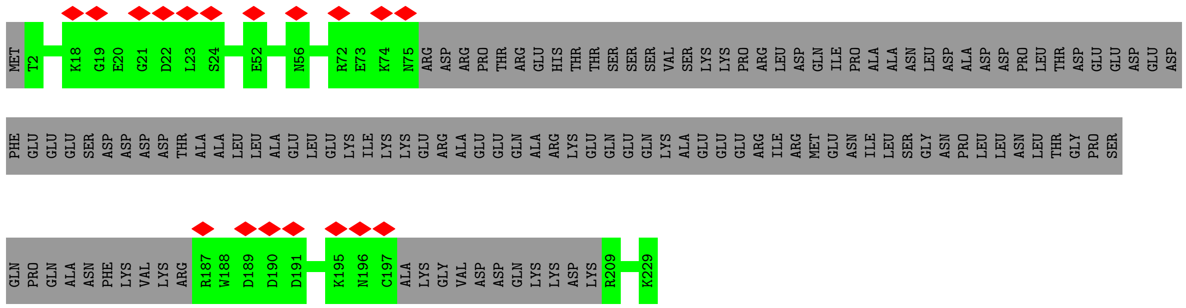
Chain O:





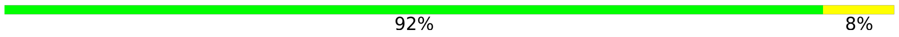
- Molecule 22: Spliceosome-associated protein CWC15 homolog

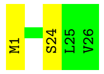
Chain P:



- Molecule 23: Serine/arginine repetitive matrix protein 2

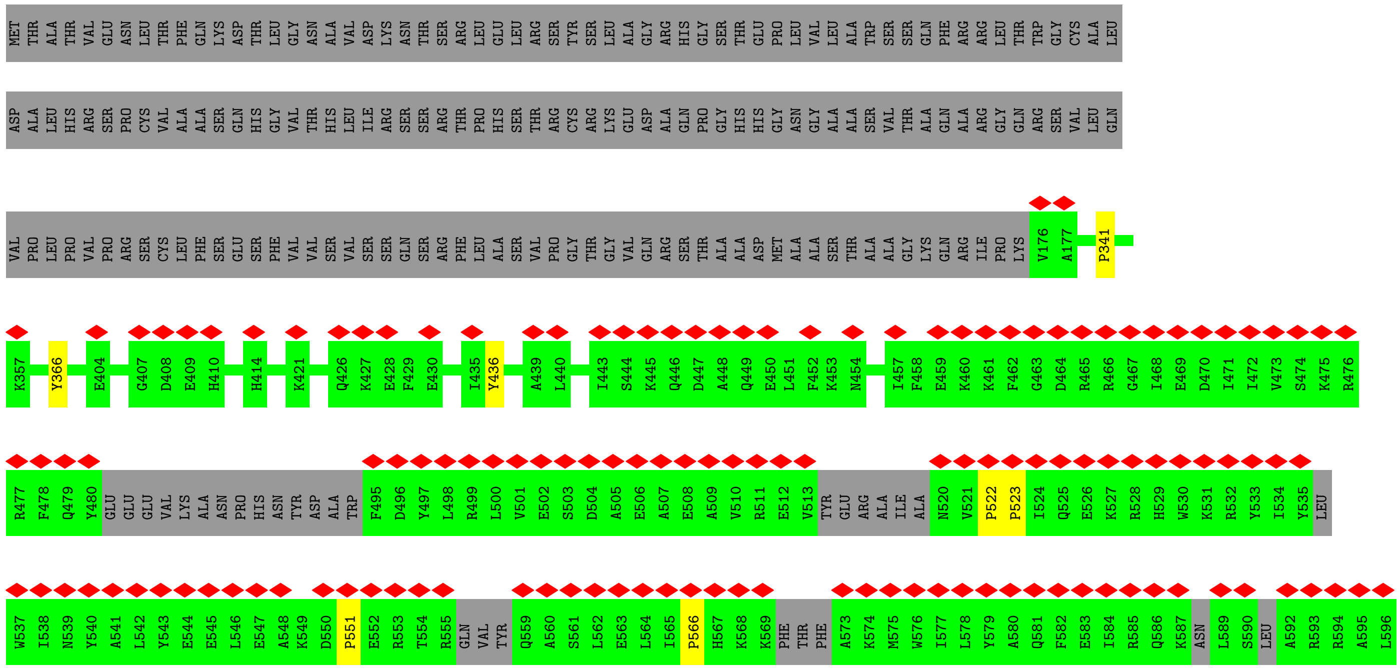
Chain R:

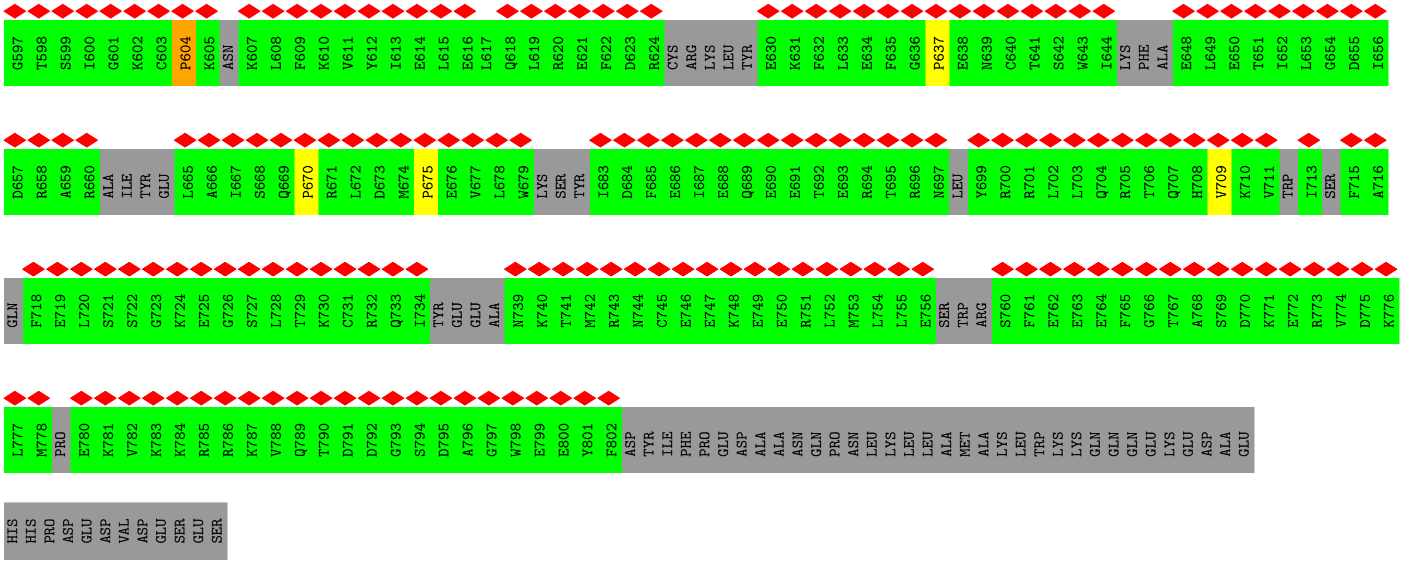




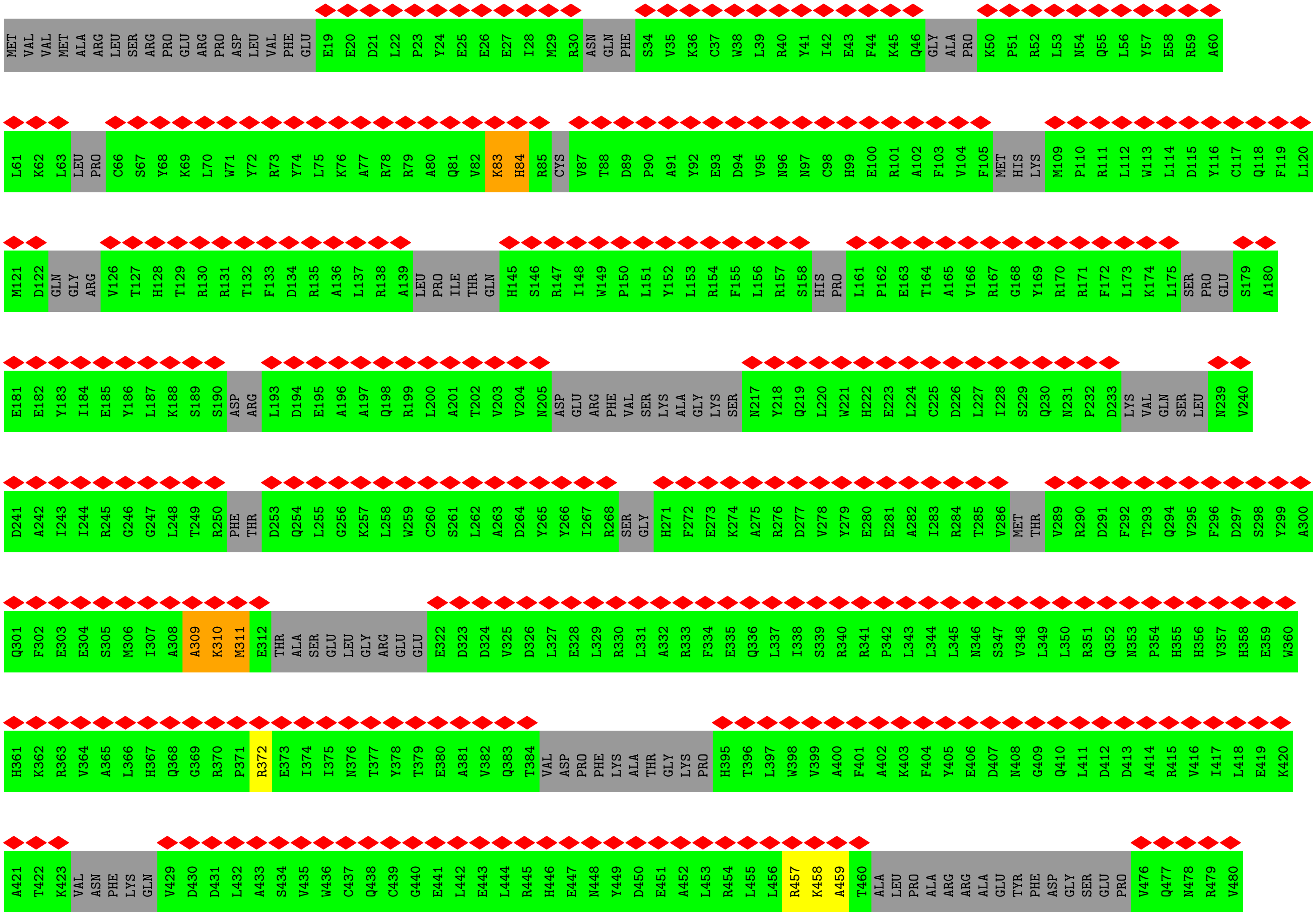
- Molecule 24: Crooked neck-like protein 1

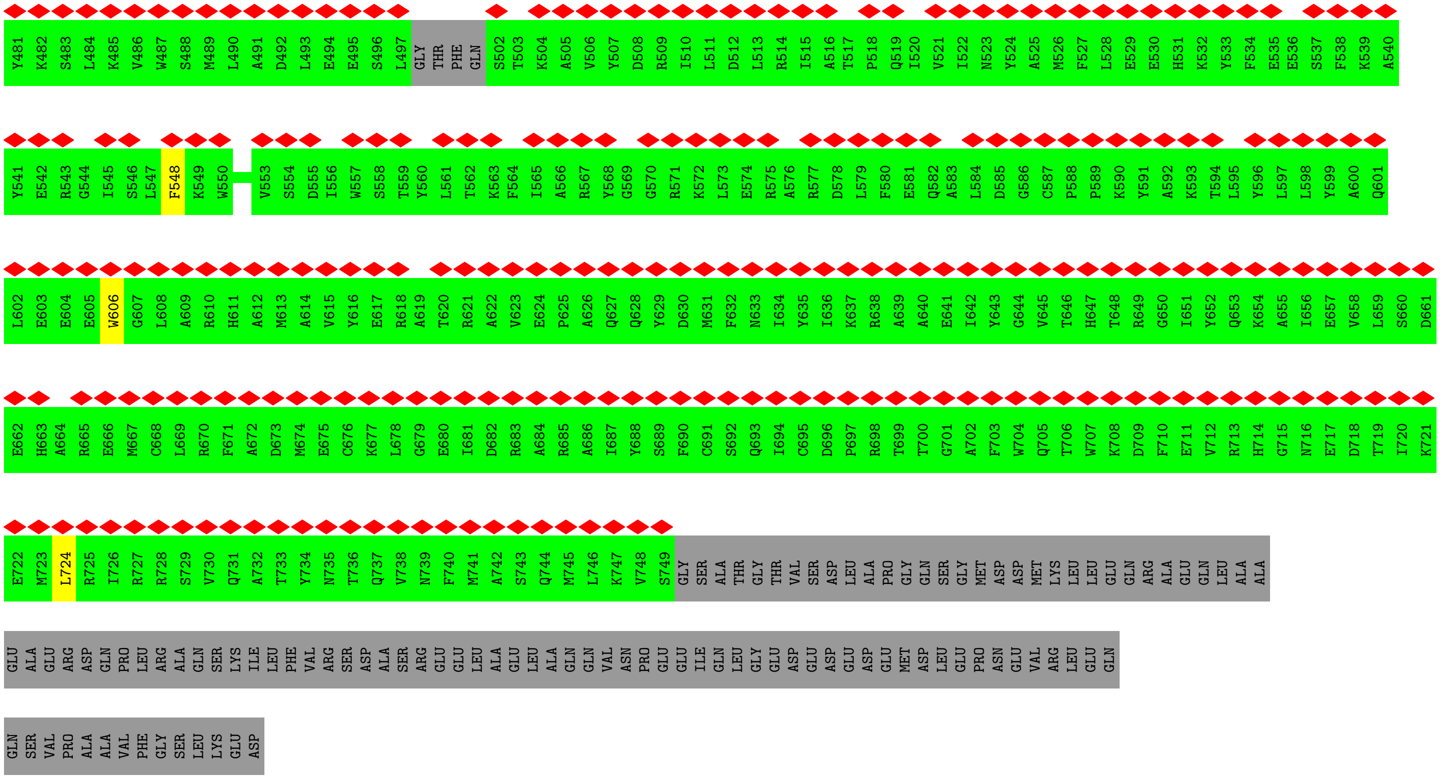
Chain S:





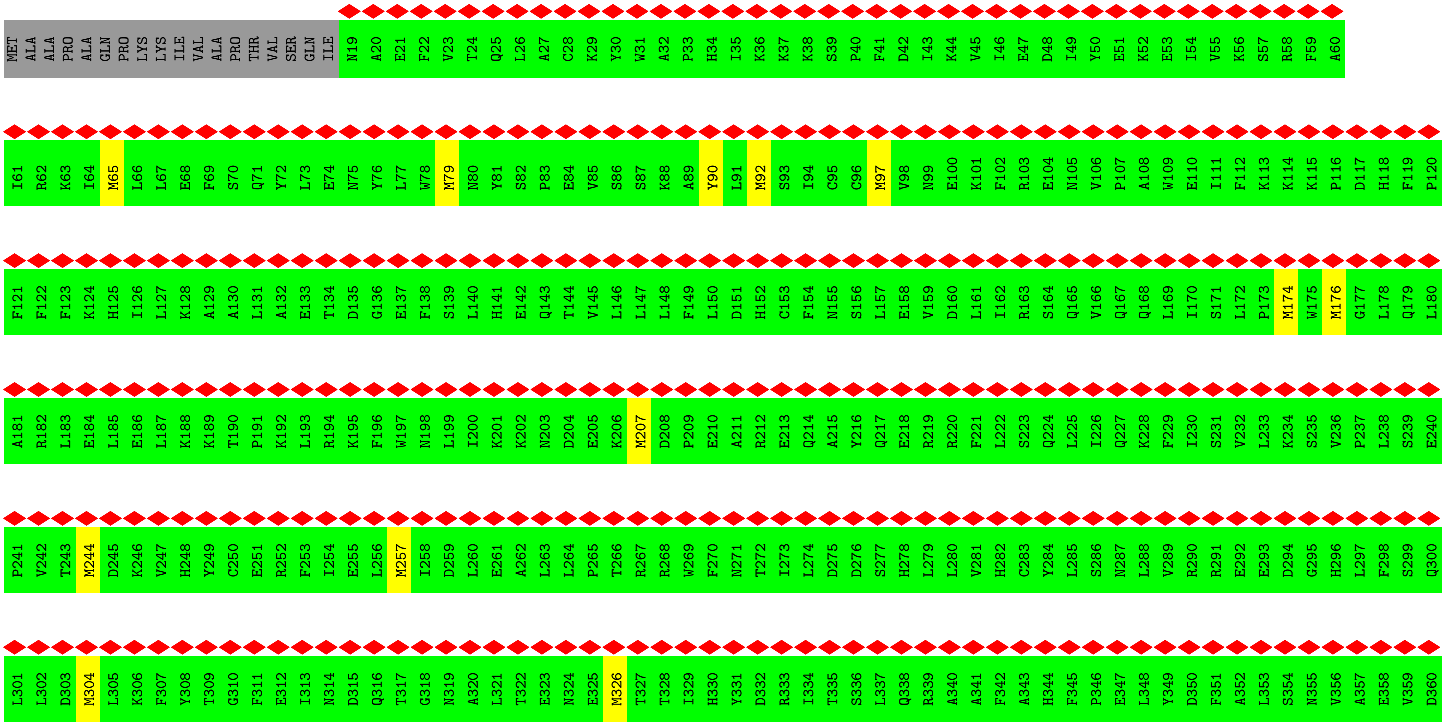
- Molecule 25: Pre-mRNA-splicing factor SYF1

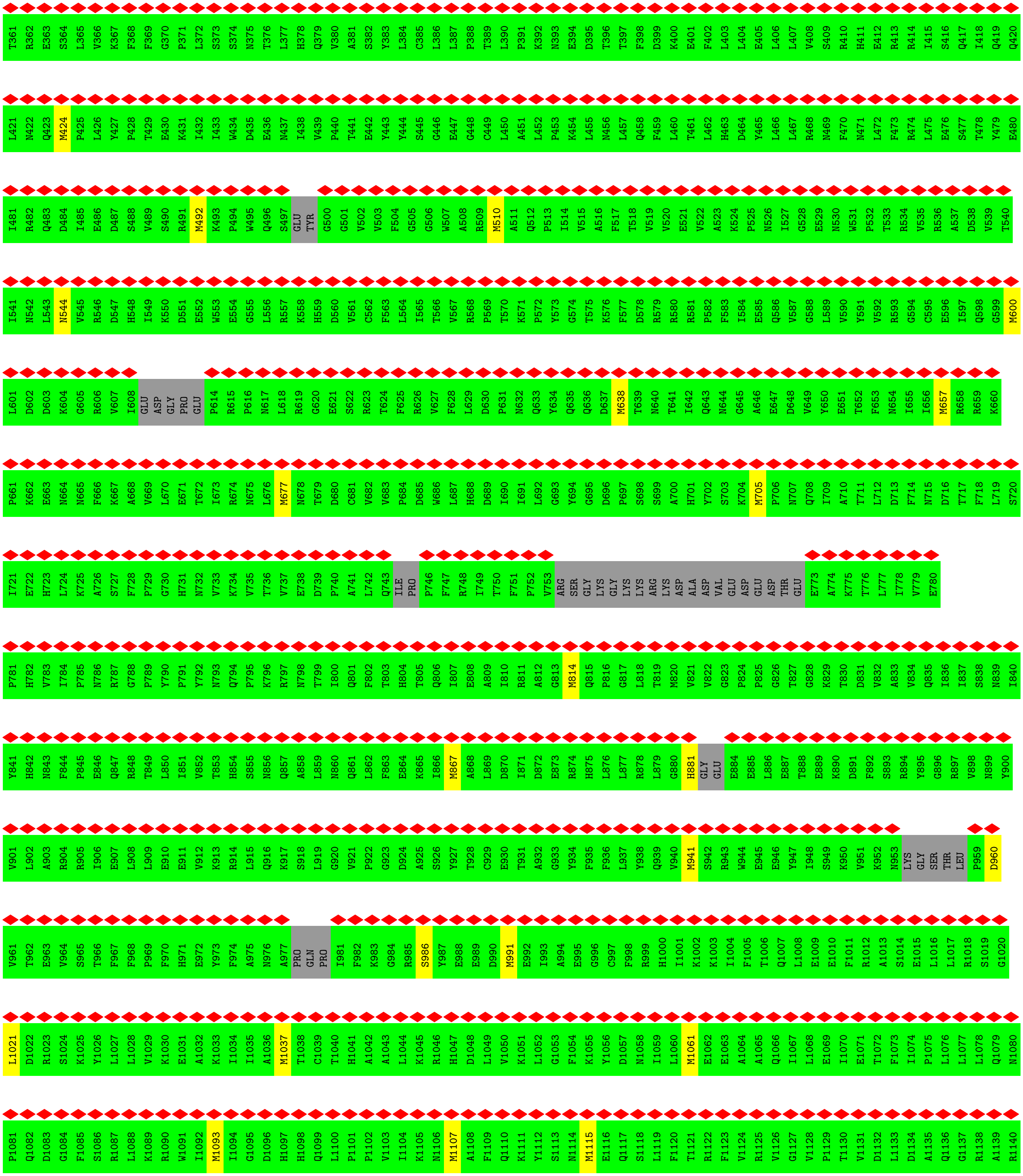




- Molecule 26: Intron-binding protein aquarius

Chain U:





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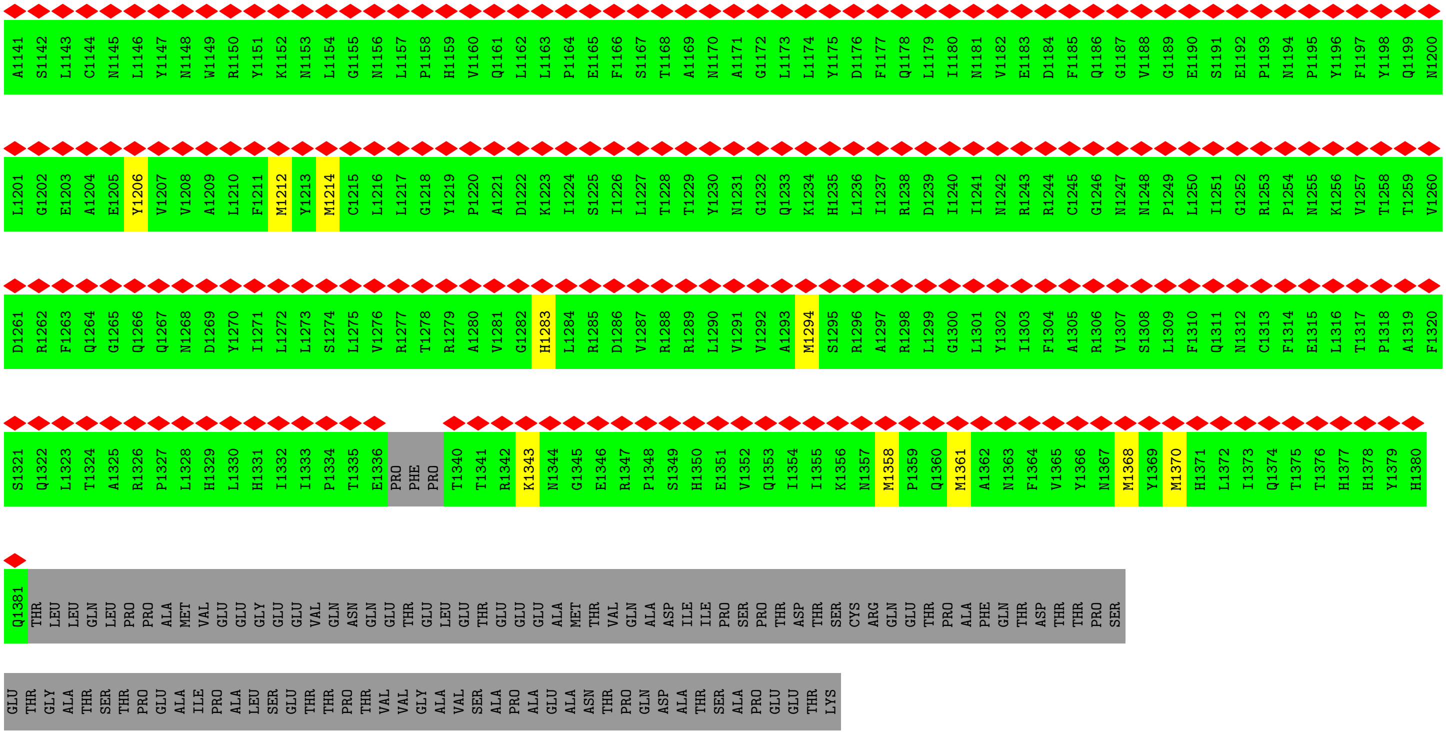
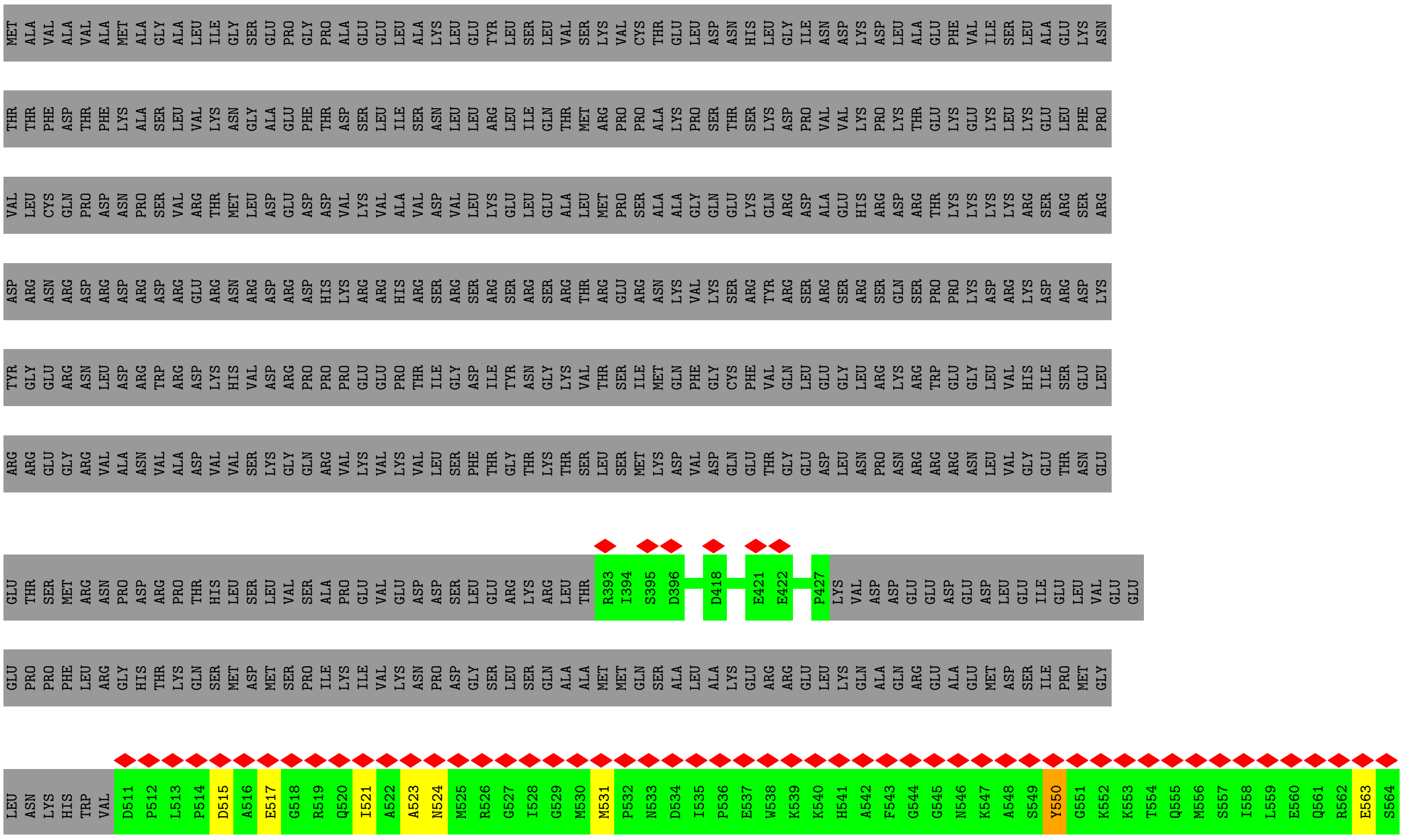
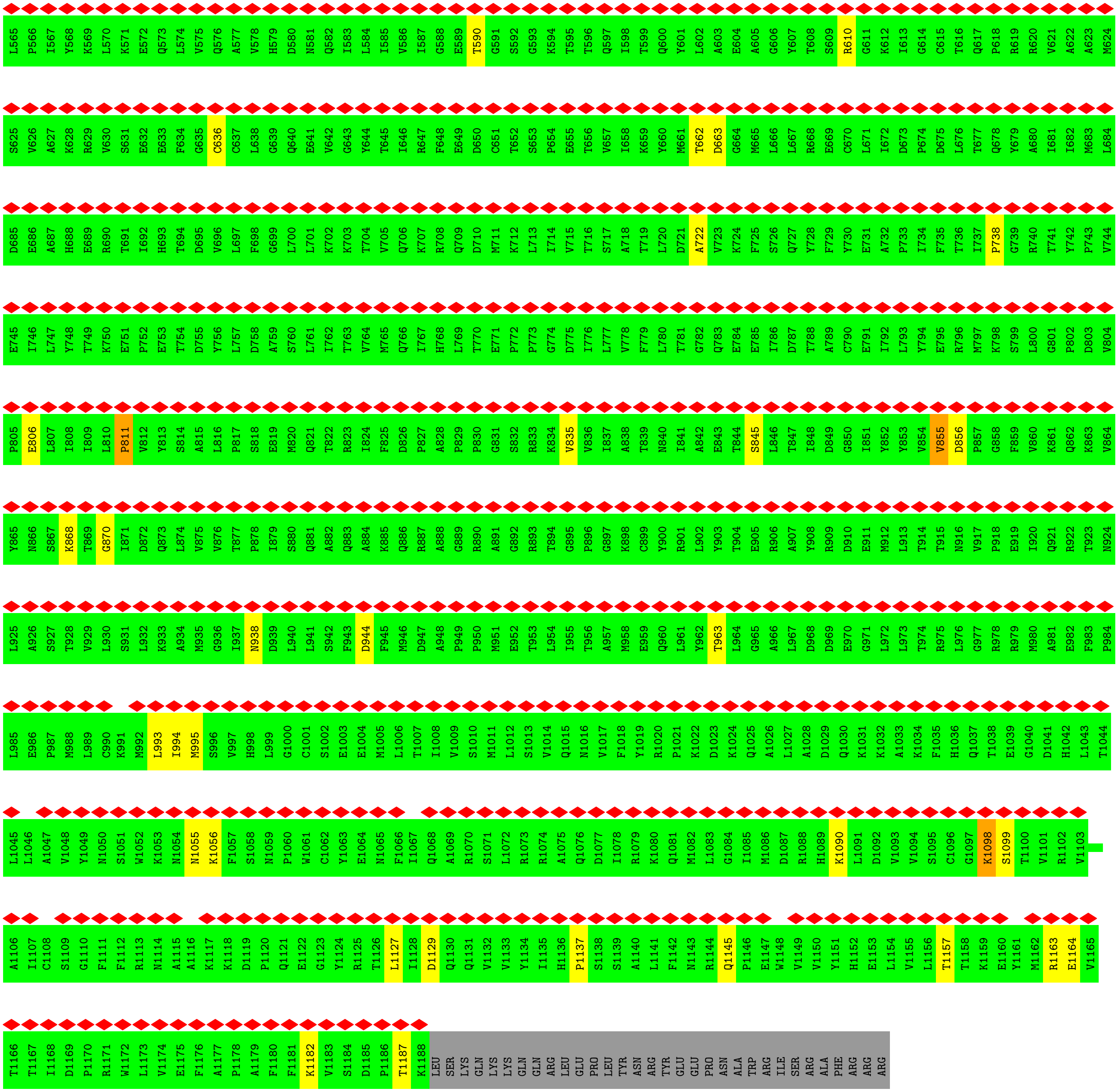


- Molecule 27: ATP-dependent RNA helicase DHX8

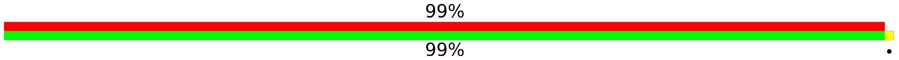
Chain V:

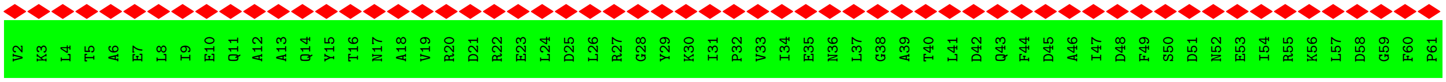


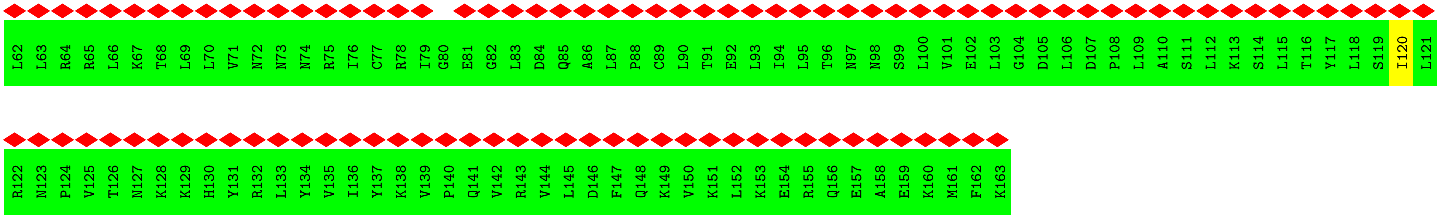


- Molecule 28: U2 small nuclear ribonucleoprotein A’

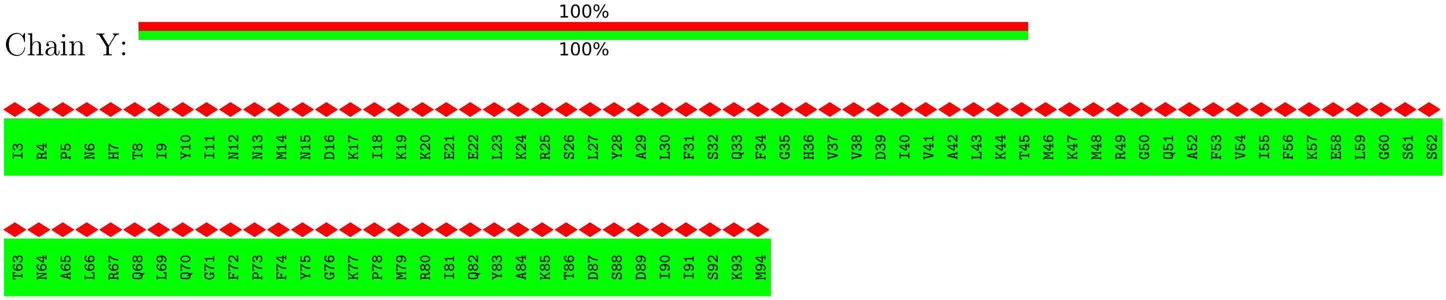
Chain W:



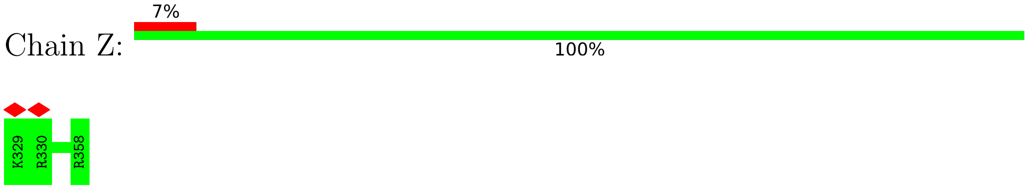




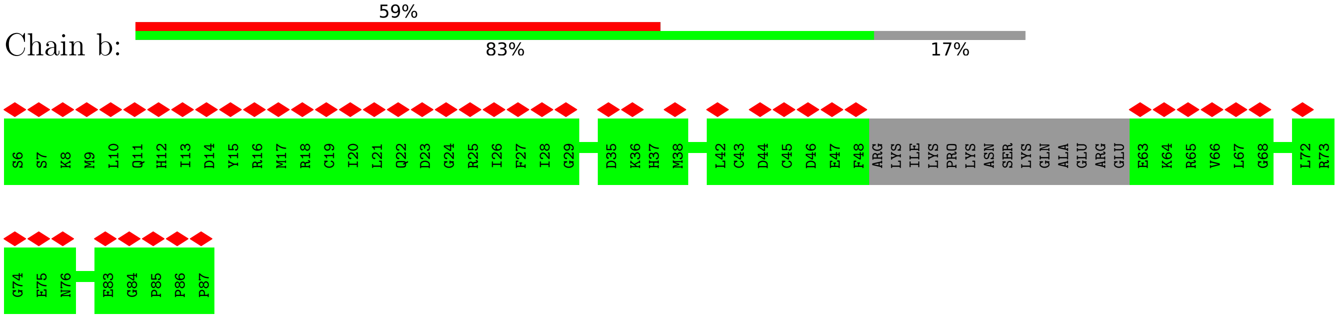
- Molecule 29: U2 small nuclear ribonucleoprotein B"



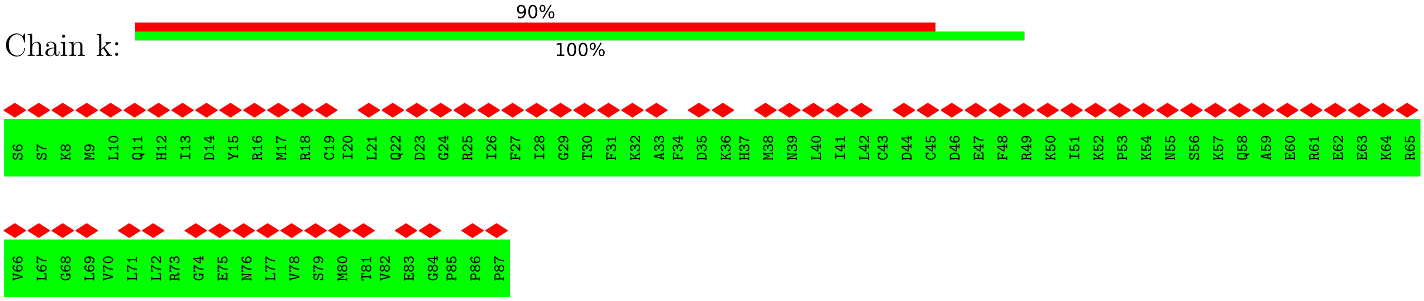
- Molecule 30: NF-kappa-B-activating protein



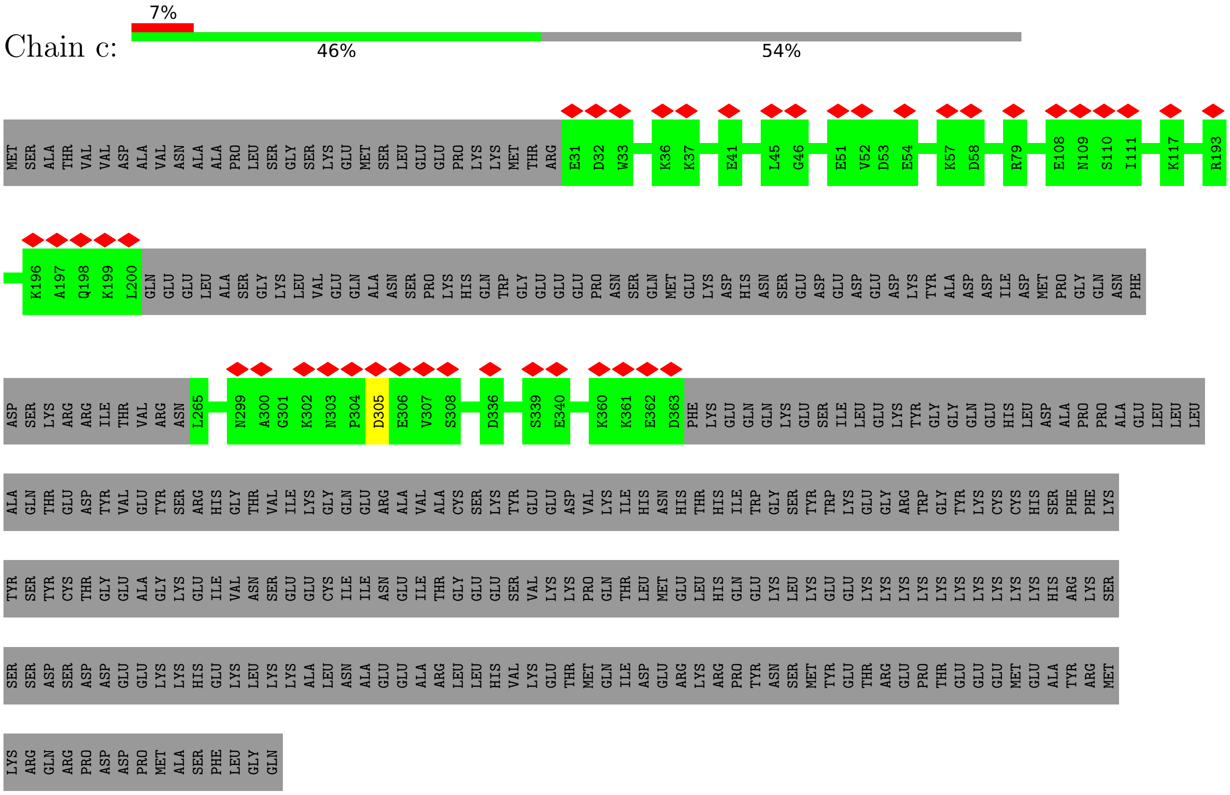
- Molecule 31: Small nuclear ribonucleoprotein-associated proteins B and B'



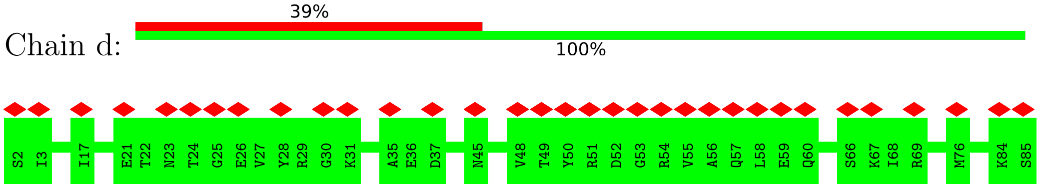
- Molecule 31: Small nuclear ribonucleoprotein-associated proteins B and B'



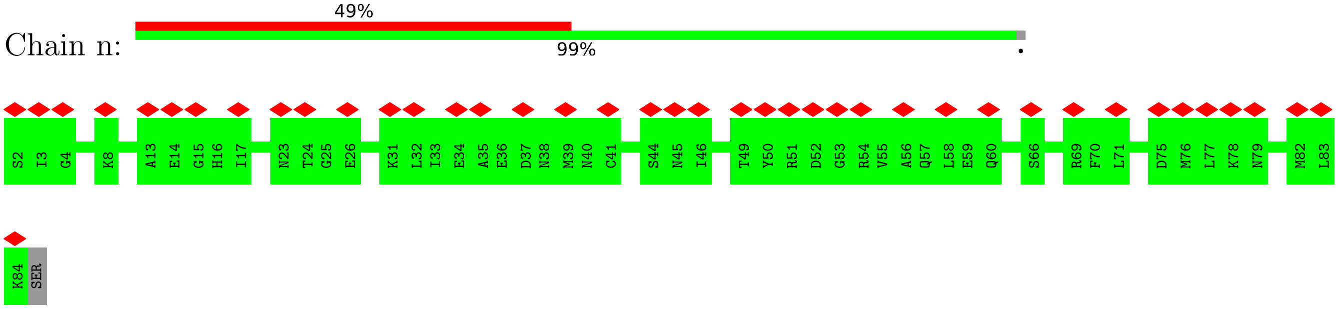
- Molecule 32: Pre-mRNA-splicing factor SLU7


Chain c:

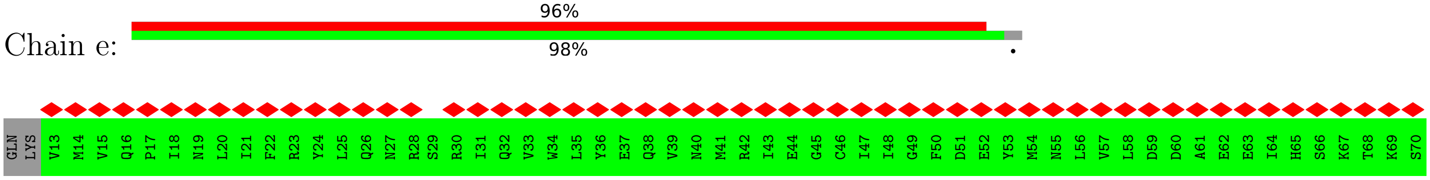
- Molecule 33: Small nuclear ribonucleoprotein Sm D3

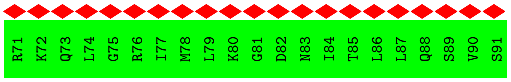

Chain d:

- Molecule 33: Small nuclear ribonucleoprotein Sm D3

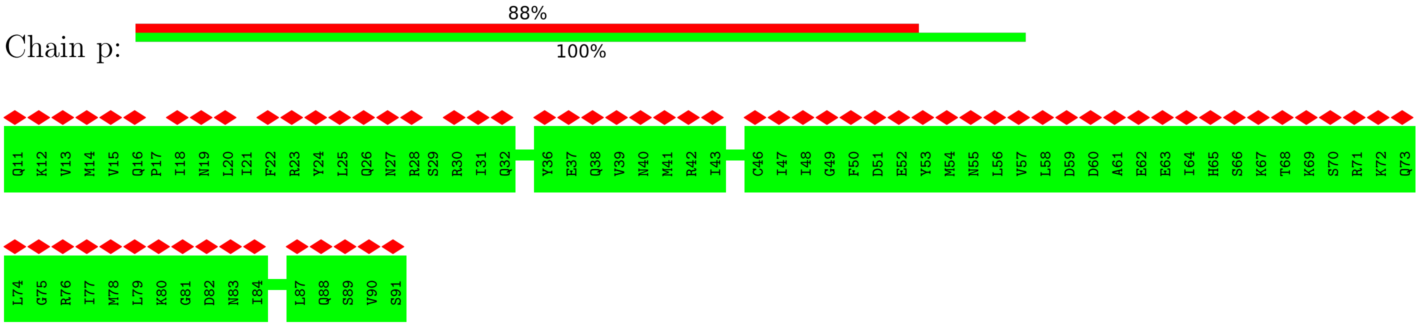

Chain n:

- Molecule 34: Small nuclear ribonucleoprotein E

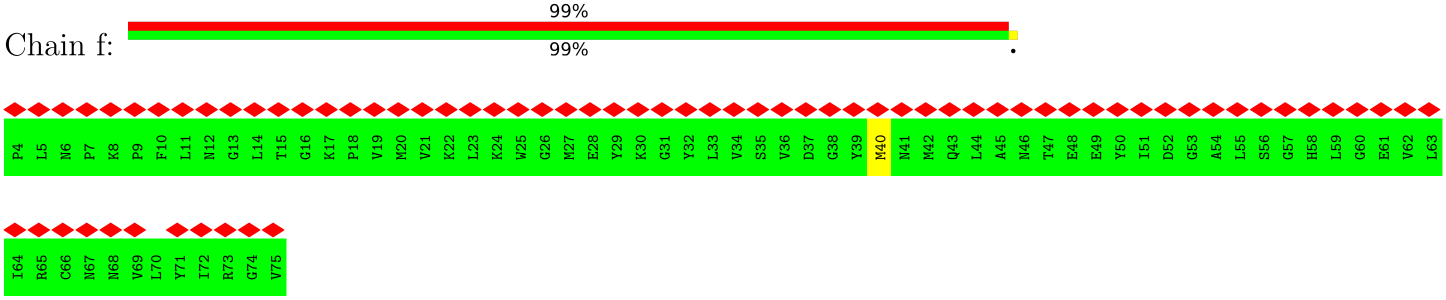

Chain e:



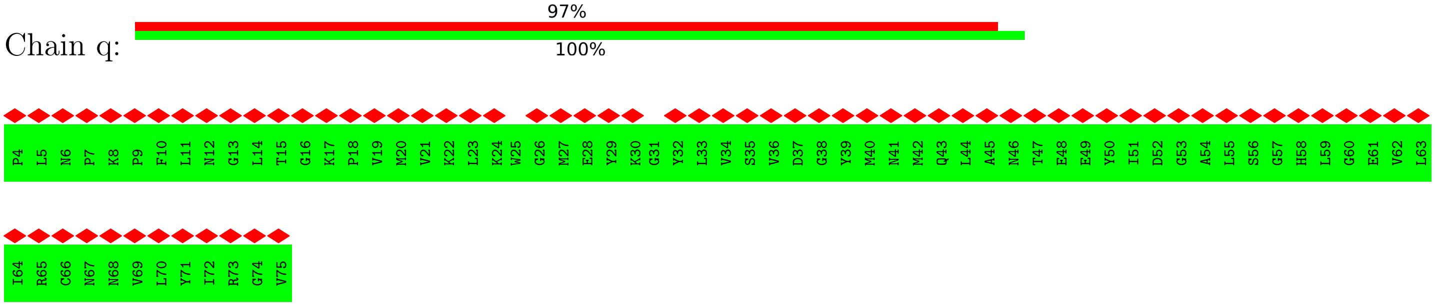
- Molecule 34: Small nuclear ribonucleoprotein E



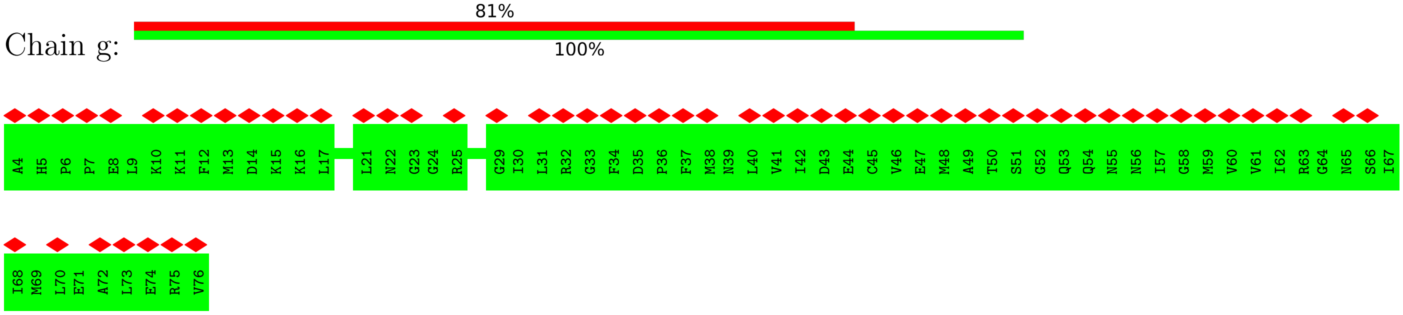
- Molecule 35: Small nuclear ribonucleoprotein F



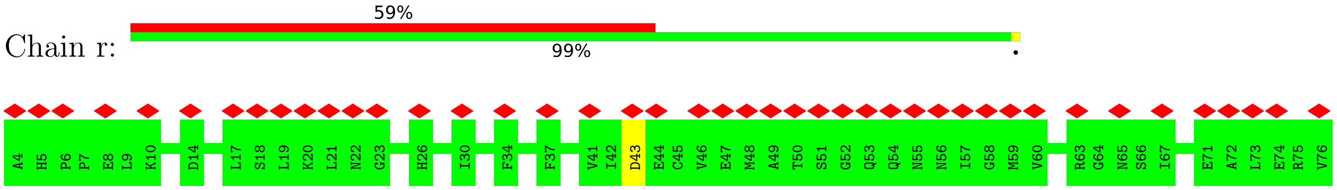
- Molecule 35: Small nuclear ribonucleoprotein F



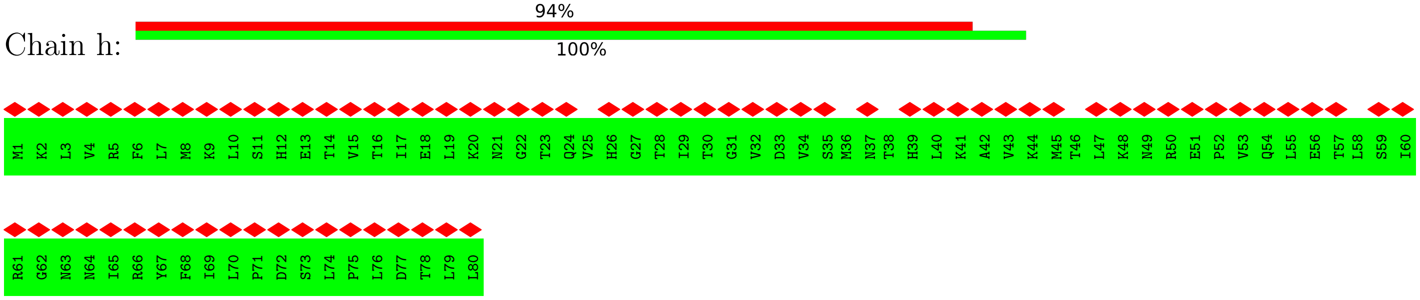
- Molecule 36: Small nuclear ribonucleoprotein G



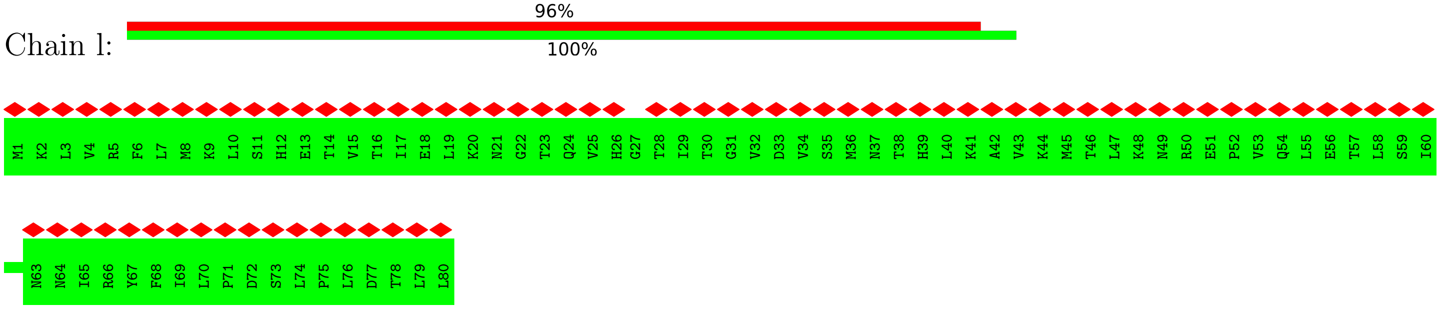
- Molecule 36: Small nuclear ribonucleoprotein G



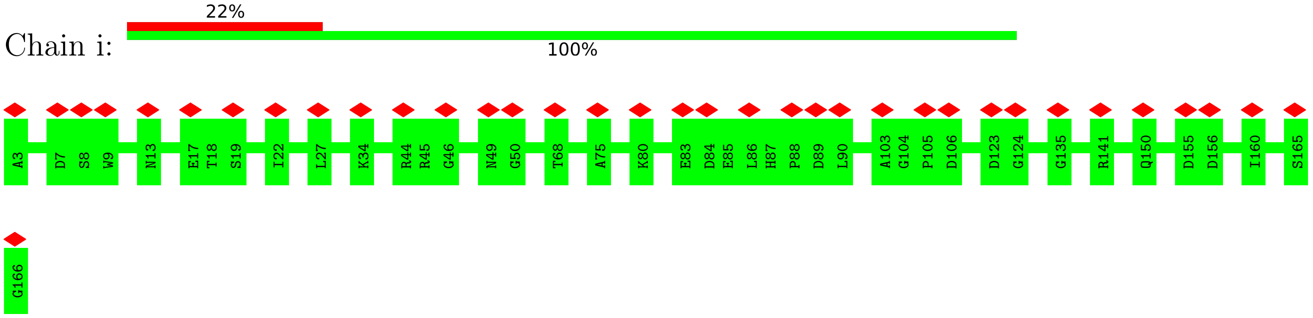
- Molecule 37: Small nuclear ribonucleoprotein Sm D1



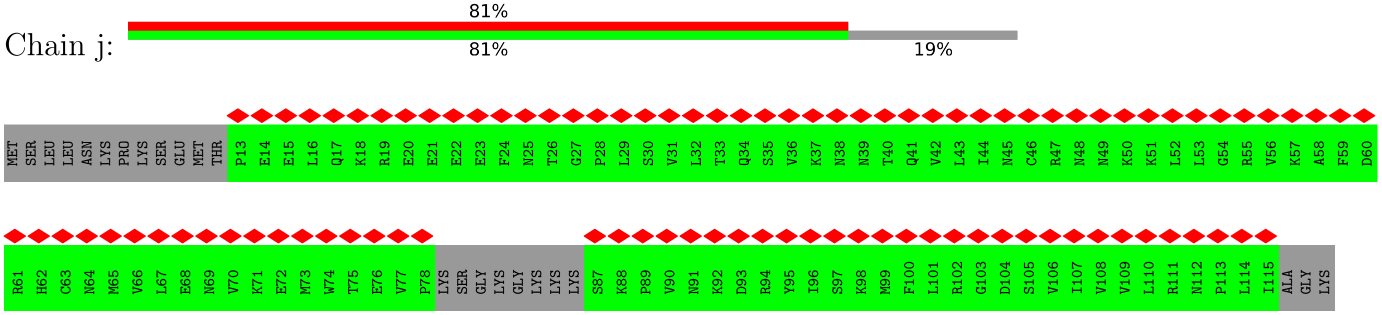
- Molecule 37: Small nuclear ribonucleoprotein Sm D1



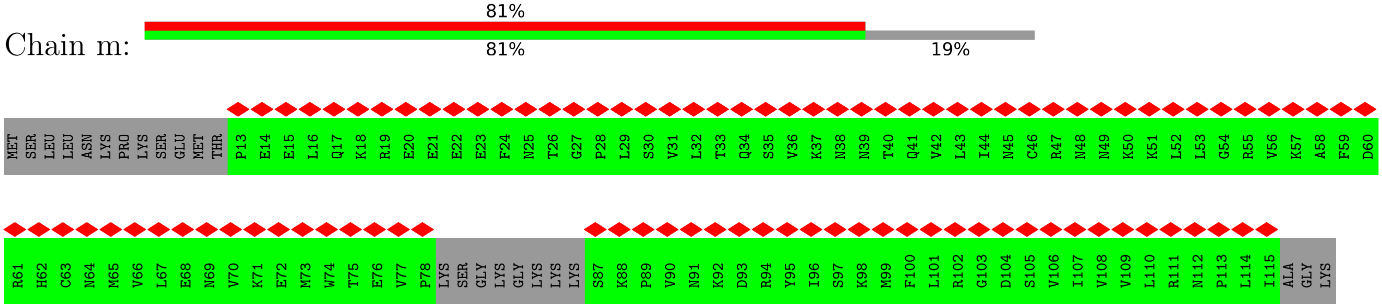
- Molecule 38: Peptidyl-prolyl cis-trans isomerase-like 1



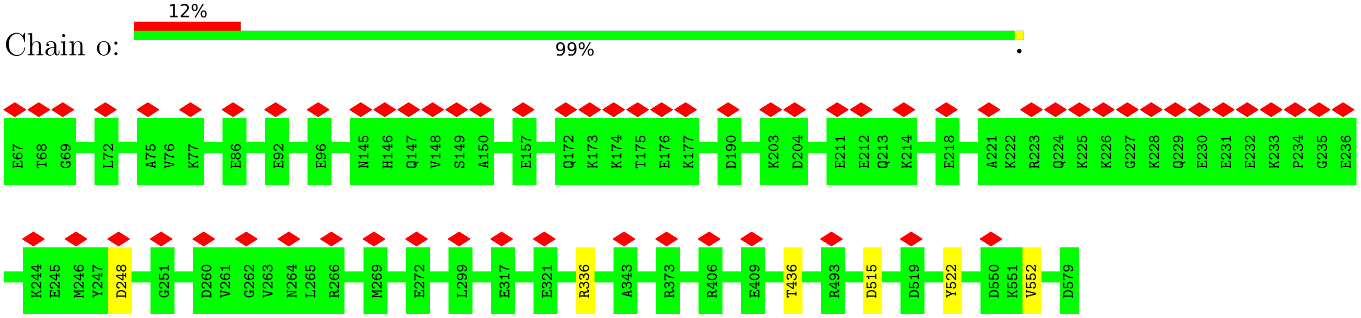
- Molecule 39: Small nuclear ribonucleoprotein Sm D2



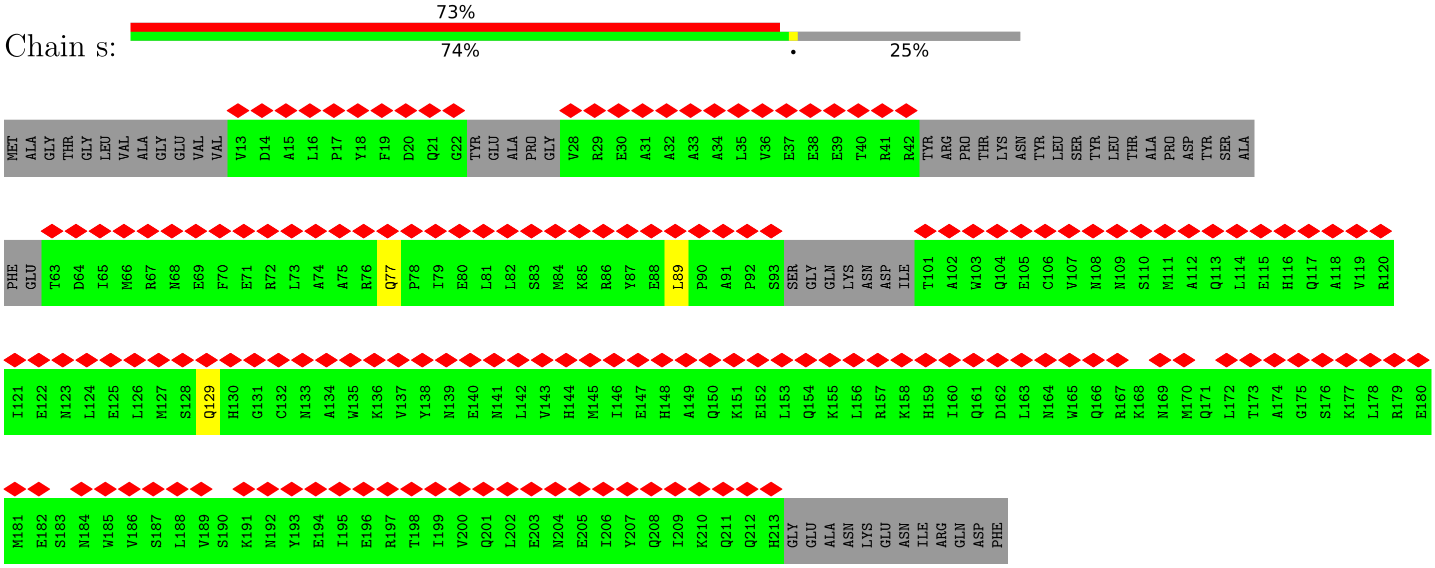
- Molecule 39: Small nuclear ribonucleoprotein Sm D2



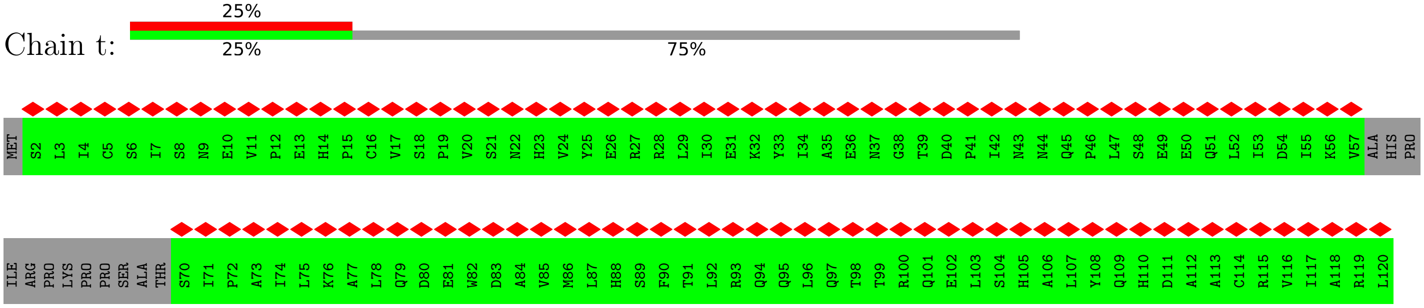
- Molecule 40: Pre-mRNA-processing factor 17

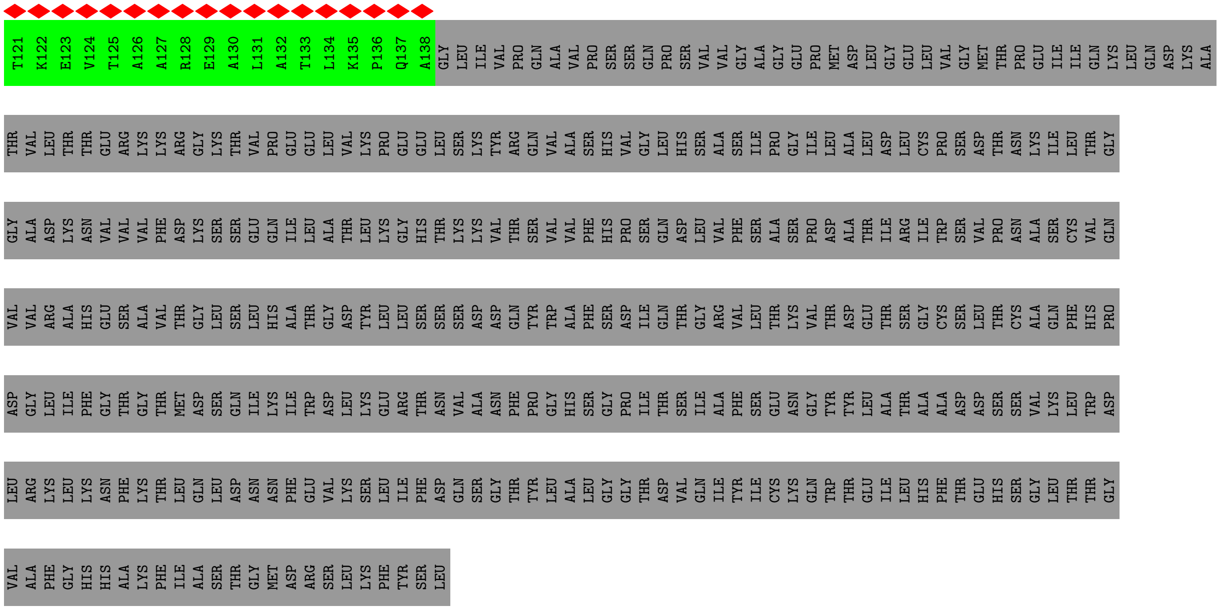


- Molecule 41: Pre-mRNA-splicing factor SPF27



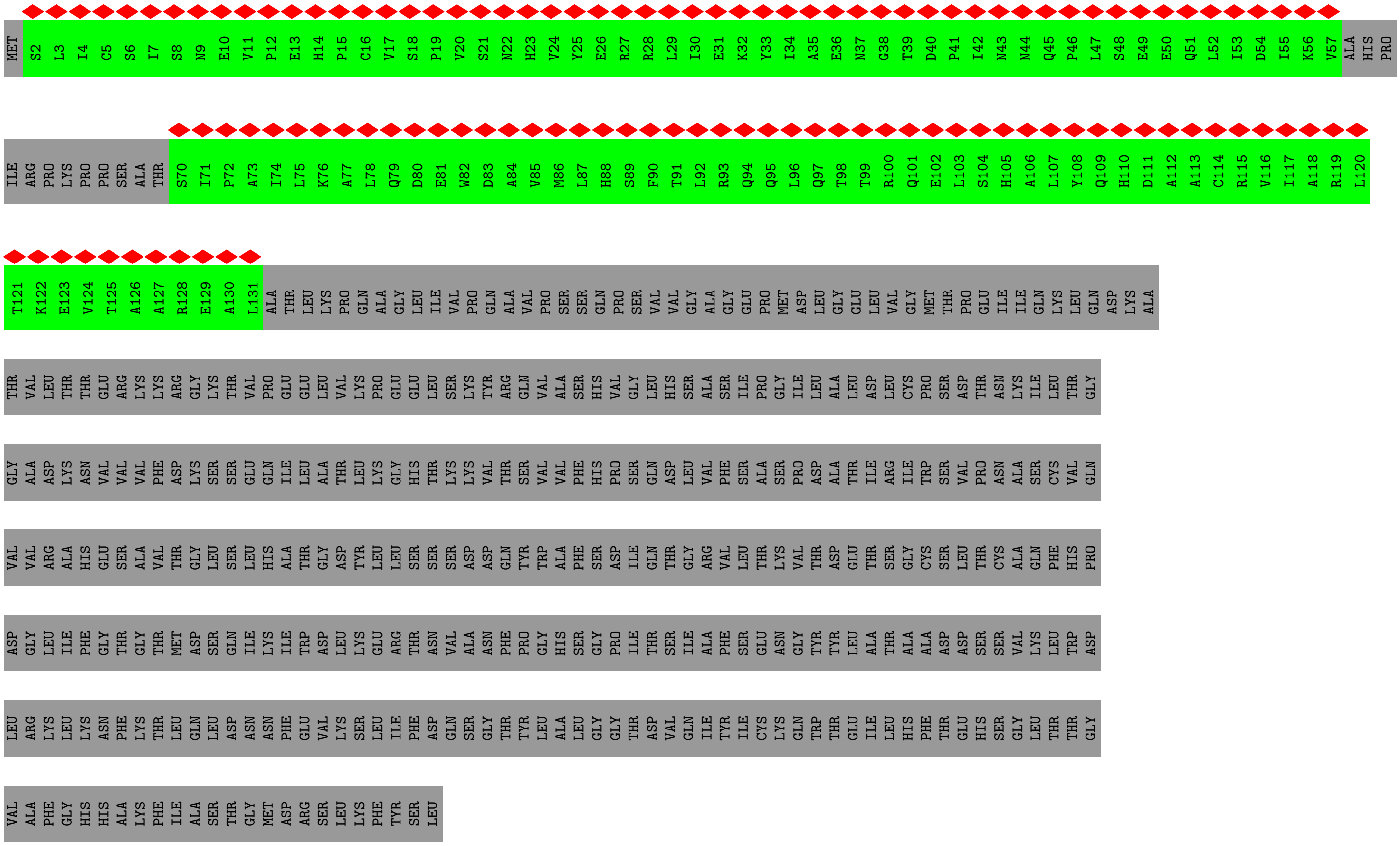
- Molecule 42: Pre-mRNA-processing factor 19





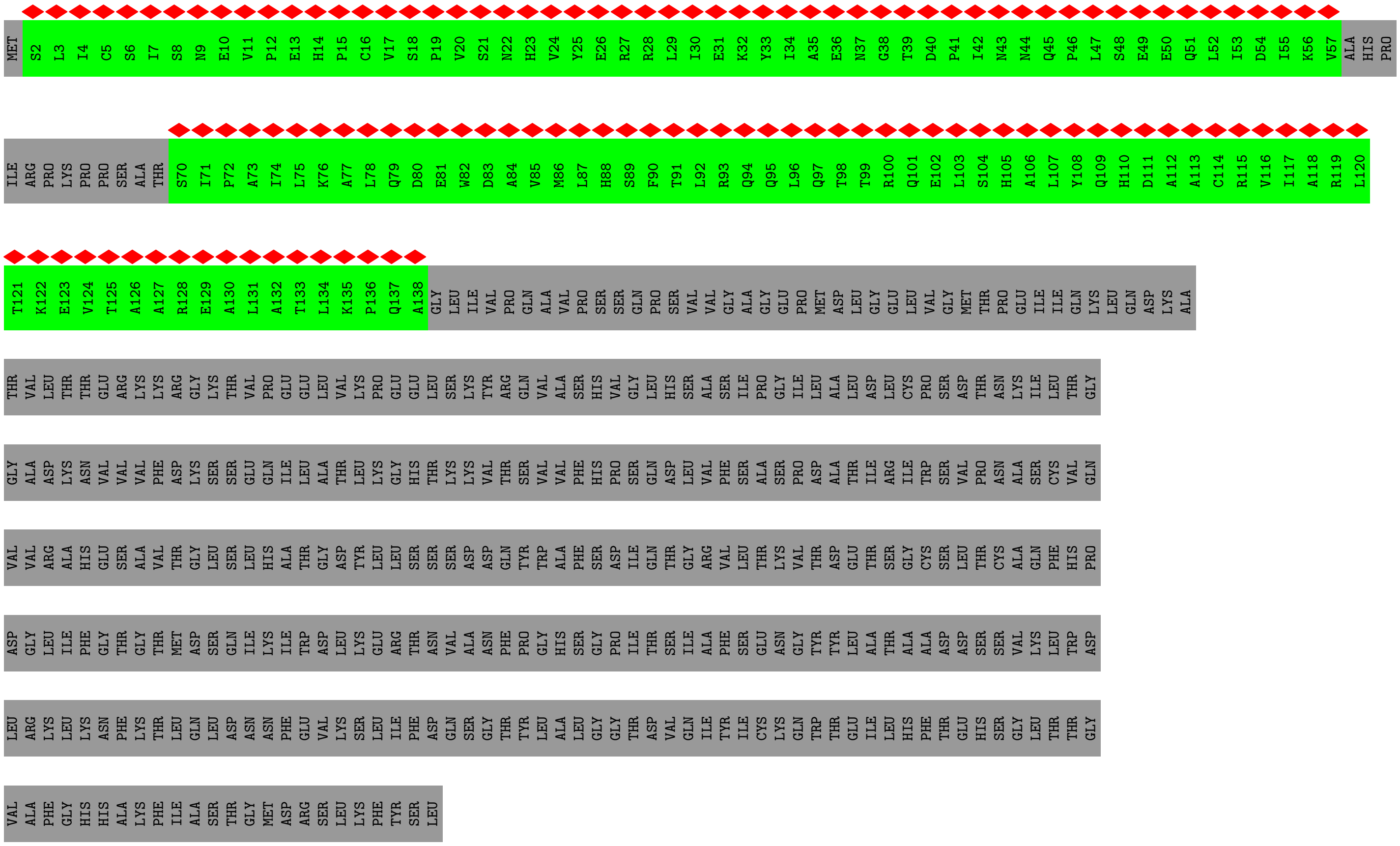
- Molecule 42: Pre-mRNA-processing factor 19

Chain u:



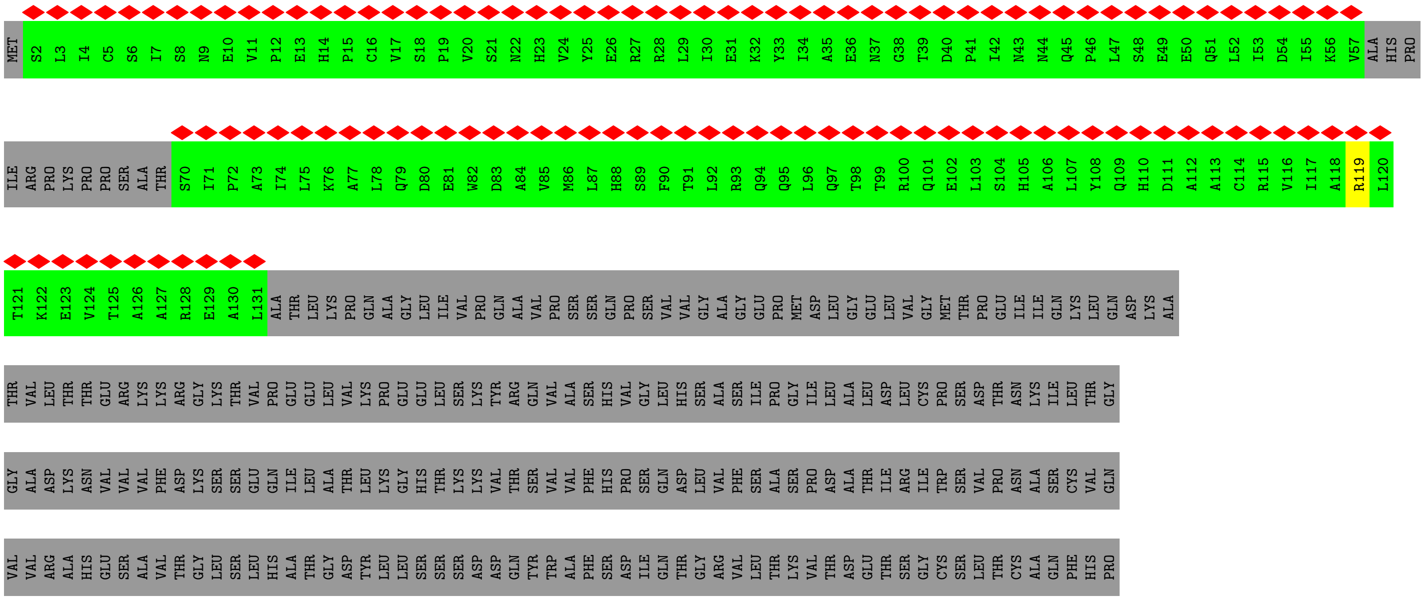
- Molecule 42: Pre-mRNA-processing factor 19

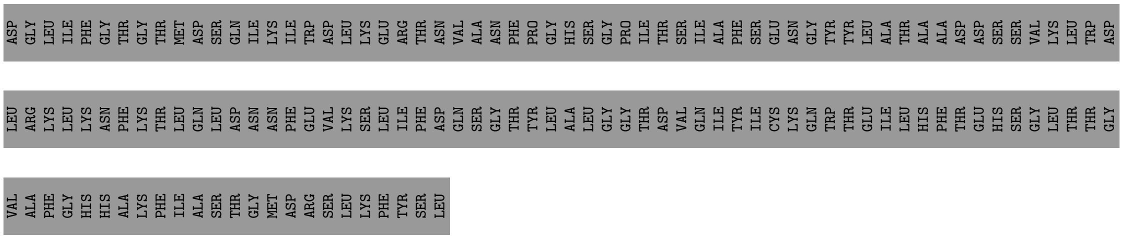
Chain v:



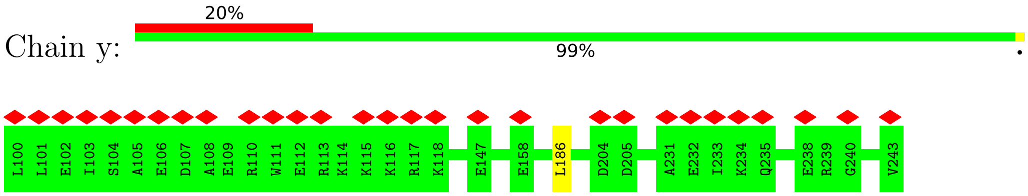
- Molecule 42: Pre-mRNA-processing factor 19

Chain w:

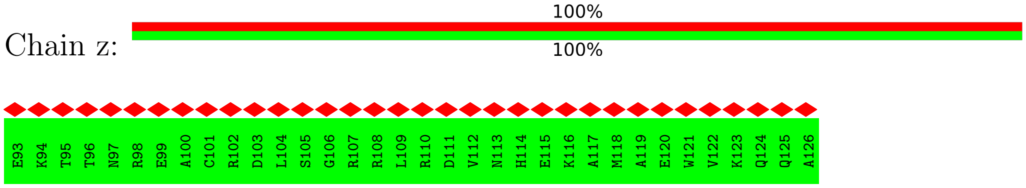




- Molecule 43: Pre-mRNA-splicing factor SYF2



- Molecule 44: Replication stress response regulator SDE2



4 Experimental information ⓘ

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 ($e^-/\text{Å}^2$)	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: K, GTP, ATP, SEP, IHP, ZN, 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	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 ⓘ

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	7	388/390 (100%)	376 (97%)	9 (2%)	3 (1%)	19	51
5	8	89/91 (98%)	87 (98%)	1 (1%)	1 (1%)	14	45
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%)	47	77
9	C	897/899 (100%)	828 (92%)	67 (8%)	2 (0%)	47	77
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%)	22	54
21	O	429/802 (54%)	416 (97%)	12 (3%)	1 (0%)	47	77
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%)	25	57
25	T	597/855 (70%)	584 (98%)	12 (2%)	1 (0%)	47	77
26	U	1308/1485 (88%)	1283 (98%)	25 (2%)	0	100	100
27	V	709/1220 (58%)	617 (87%)	60 (8%)	32 (4%)	2	15
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

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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%)	47	77
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%)	44	71

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 ⓘ

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%)	67	82
5	8	76/76 (100%)	75 (99%)	1 (1%)	69	82
6	9	132/132 (100%)	131 (99%)	1 (1%)	81	89
7	A	2033/2108 (96%)	1996 (98%)	37 (2%)	59	78
8	B	1541/1541 (100%)	1363 (88%)	178 (12%)	5	22
9	C	799/799 (100%)	797 (100%)	2 (0%)	92	96
10	D	106/106 (100%)	105 (99%)	1 (1%)	78	87
12	F	110/110 (100%)	110 (100%)	0	100	100
13	G	54/55 (98%)	53 (98%)	1 (2%)	57	77
14	H	410/838 (49%)	403 (98%)	7 (2%)	60	78
16	J	276/276 (100%)	275 (100%)	1 (0%)	91	95
17	K	246/247 (100%)	246 (100%)	0	100	100
18	L	130/130 (100%)	127 (98%)	3 (2%)	50	73
19	M	254/254 (100%)	253 (100%)	1 (0%)	91	95
20	N	263/263 (100%)	263 (100%)	0	100	100
21	O	322/709 (45%)	321 (100%)	1 (0%)	92	96
22	P	94/203 (46%)	94 (100%)	0	100	100
23	R	21/21 (100%)	20 (95%)	1 (5%)	25	56
24	S	275/751 (37%)	273 (99%)	2 (1%)	84	90
25	T	213/749 (28%)	210 (99%)	3 (1%)	67	82
26	U	1202/1336 (90%)	1193 (99%)	9 (1%)	84	90
27	V	31/1085 (3%)	31 (100%)	0	100	100
28	W	139/147 (95%)	138 (99%)	1 (1%)	84	90
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%)	91	95
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

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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%)	62	79
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%)	73	85
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%)	78	87
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%)	54	74

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

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Mol	Chain	Res	Type
34	p	88	GLN

5.3.3 RNA ⓘ

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	137	C
3	6	33	G
15	I	142	U
3	6	58	G

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

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	-	8,9,10	1.57	1 (12%)	8,12,14	1.47	2 (25%)
17	SEP	K	224	-	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	-	-	3/5/8/10	-
17	SEP	K	224	-	-	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\#\|Z\| > 2$
47	ATP	7	702	45	26,33,33	0.92	1 (3%)	31,52,52	1.55	5 (16%)
48	GTP	C	1500	45	26,34,34	1.24	1 (3%)	32,54,54	1.70	7 (21%)
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
47	ATP	7	702	45	-	0/18/38/38	0/3/3/3
48	GTP	C	1500	45	-	5/18/38/38	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:

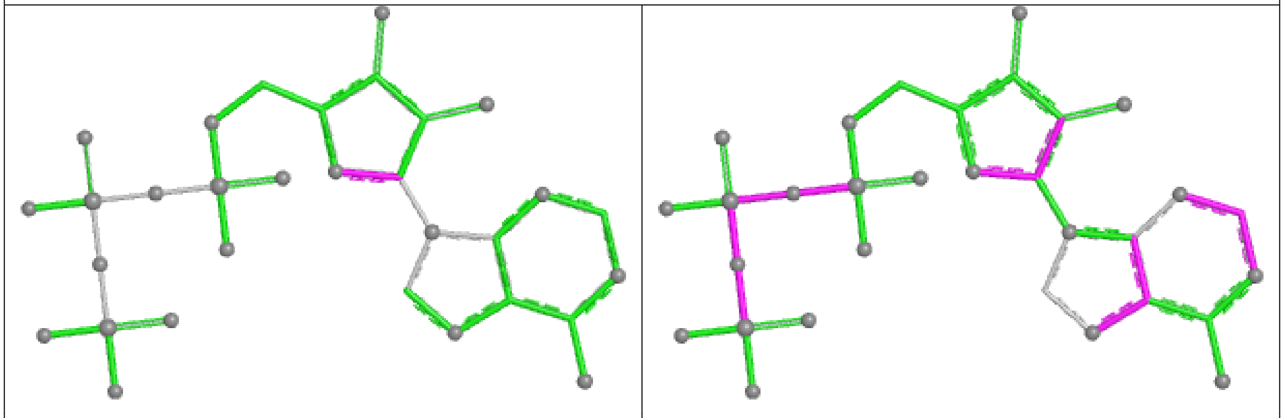
Mol	Chain	Res	Type	Atoms
48	C	1500	GTP	C5'-O5'-PA-O3A
48	C	1500	GTP	C5'-O5'-PA-O1A
48	C	1500	GTP	C5'-O5'-PA-O2A
50	c	601	IHP	C2-O12-P2-O42
50	c	601	IHP	C5-O15-P5-O25

There are no ring outliers.

No monomer is involved in short contacts.

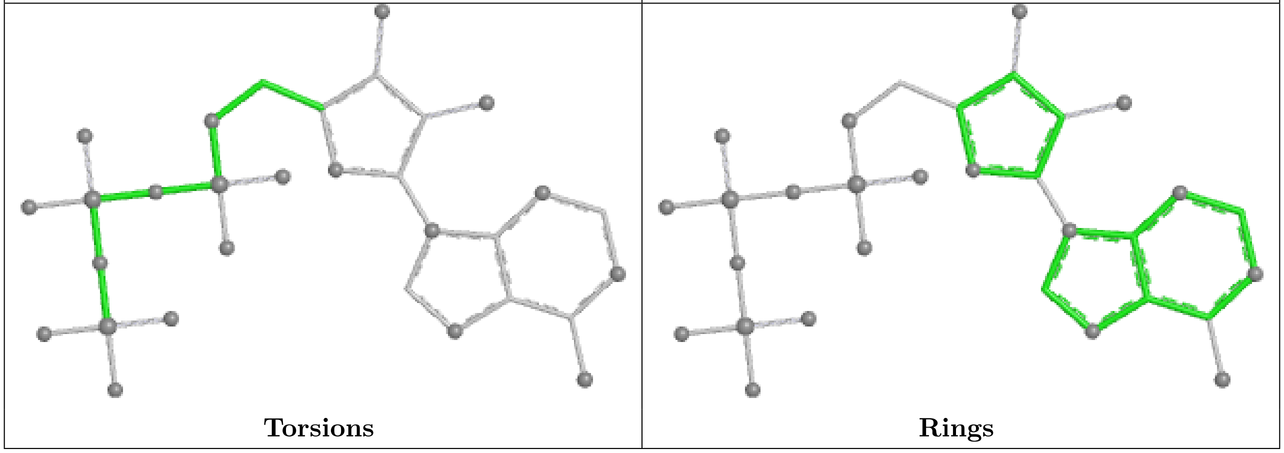
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

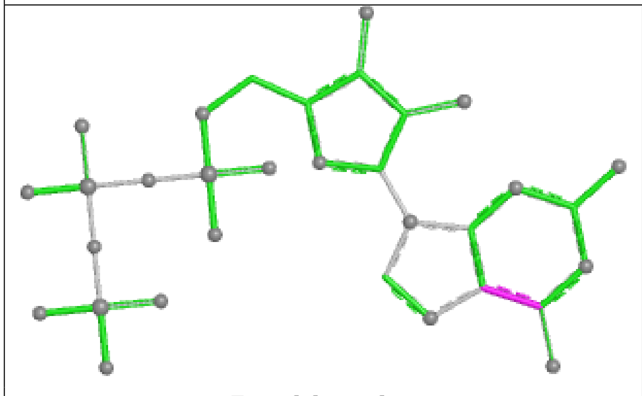
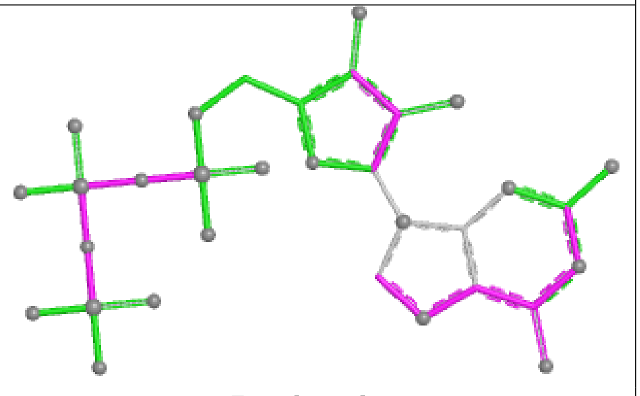
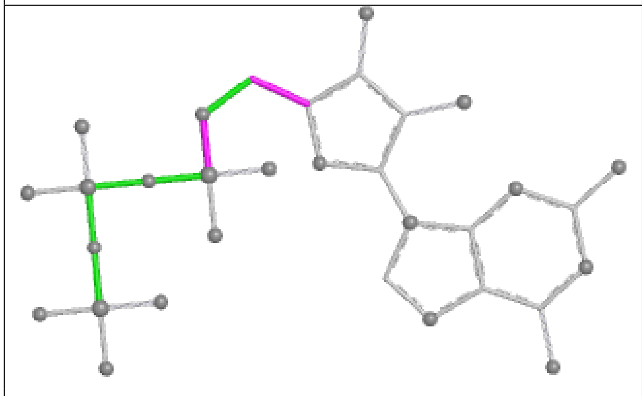
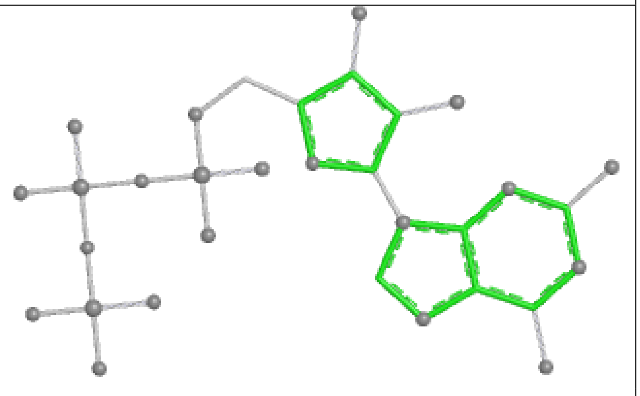
Bond angles



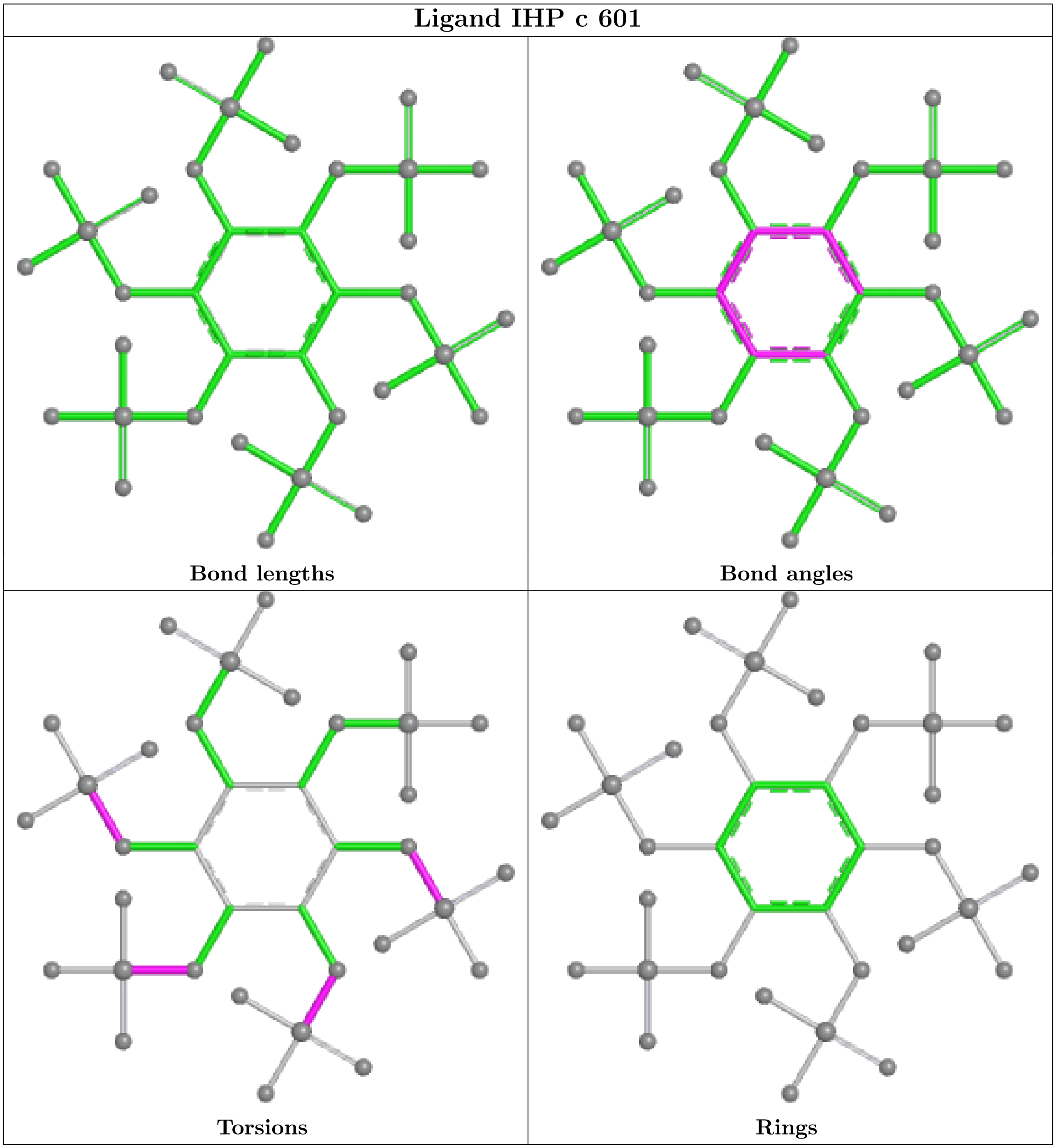
Torsions

Rings

Ligand GTP C 1500

 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Ligand IHP c 601



Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

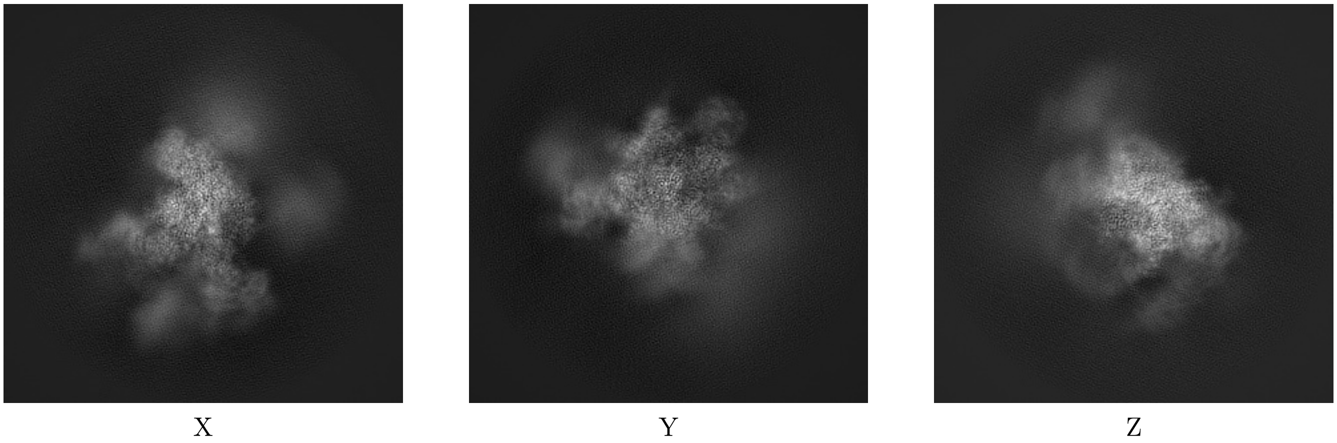
6 Map visualisation ⓘ

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 ⓘ

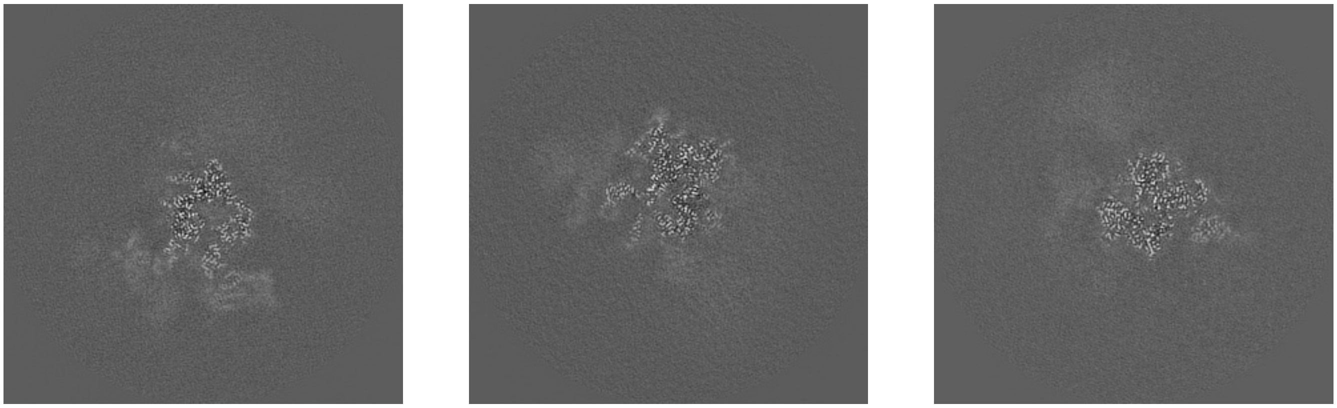
6.1.1 Primary map



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

6.2 Central slices ⓘ

6.2.1 Primary map

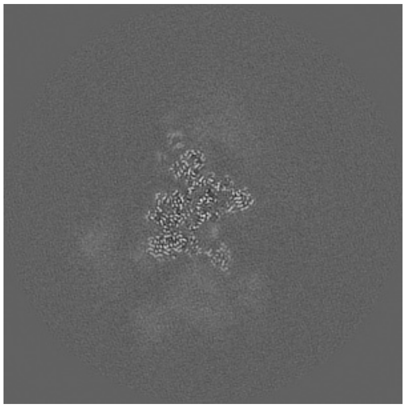


X Index: 205 Y Index: 205 Z Index: 205

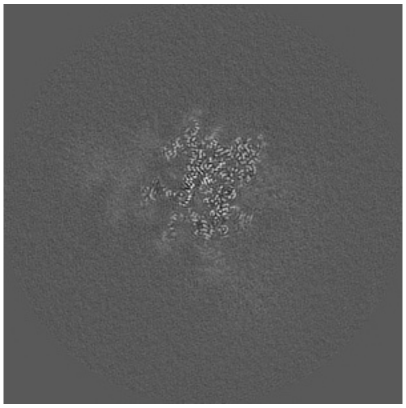
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices

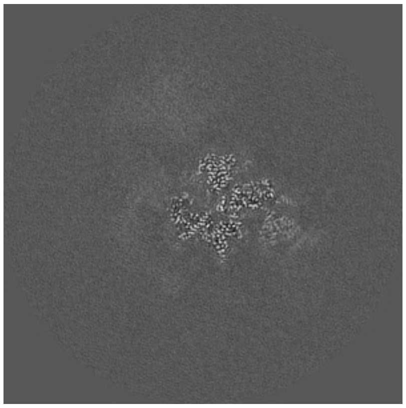
6.3.1 Primary map



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 surface views

6.4.1 Primary map

X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.024. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

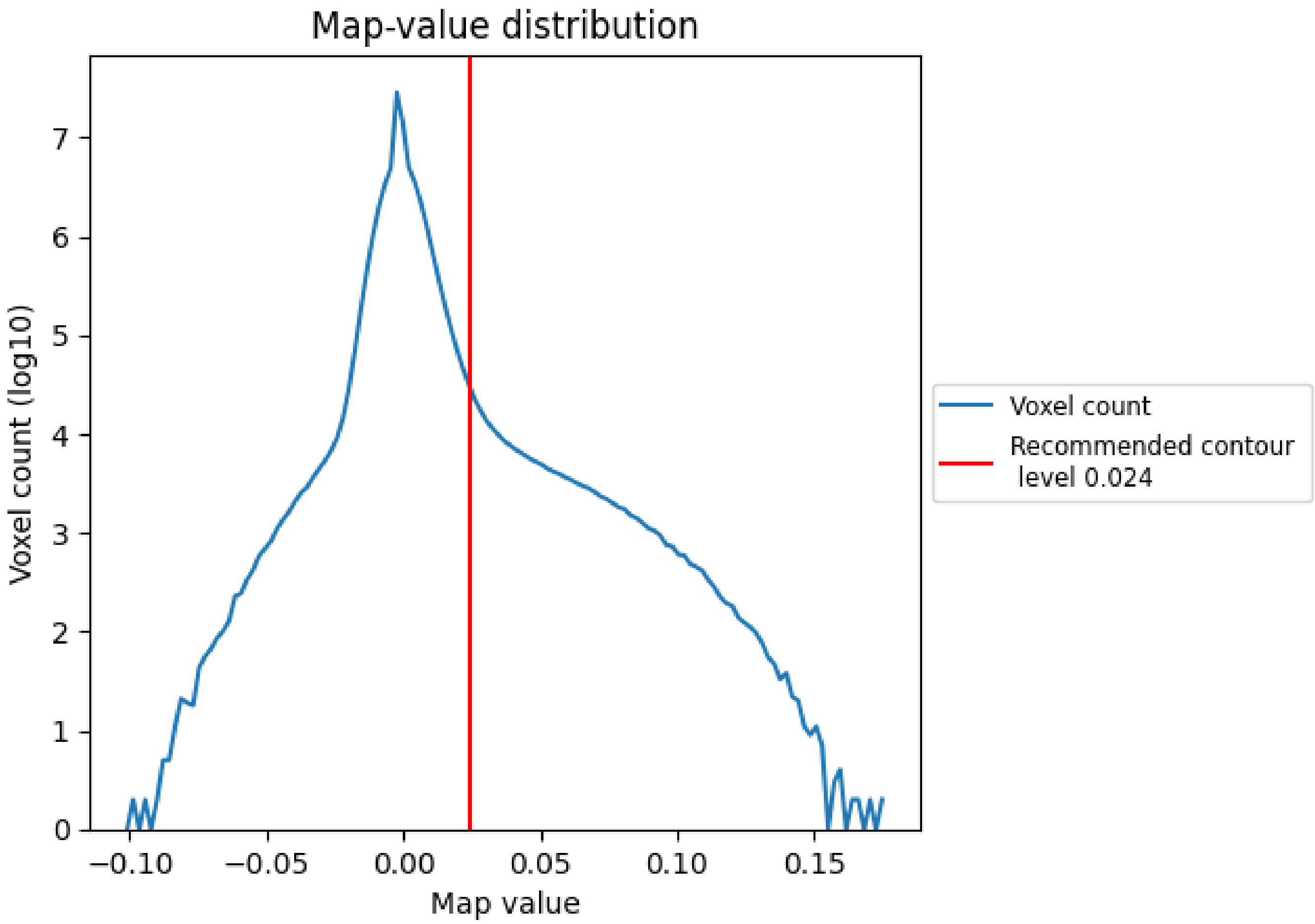
6.5 Mask visualisation ⓘ

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

7 Map analysis (i)

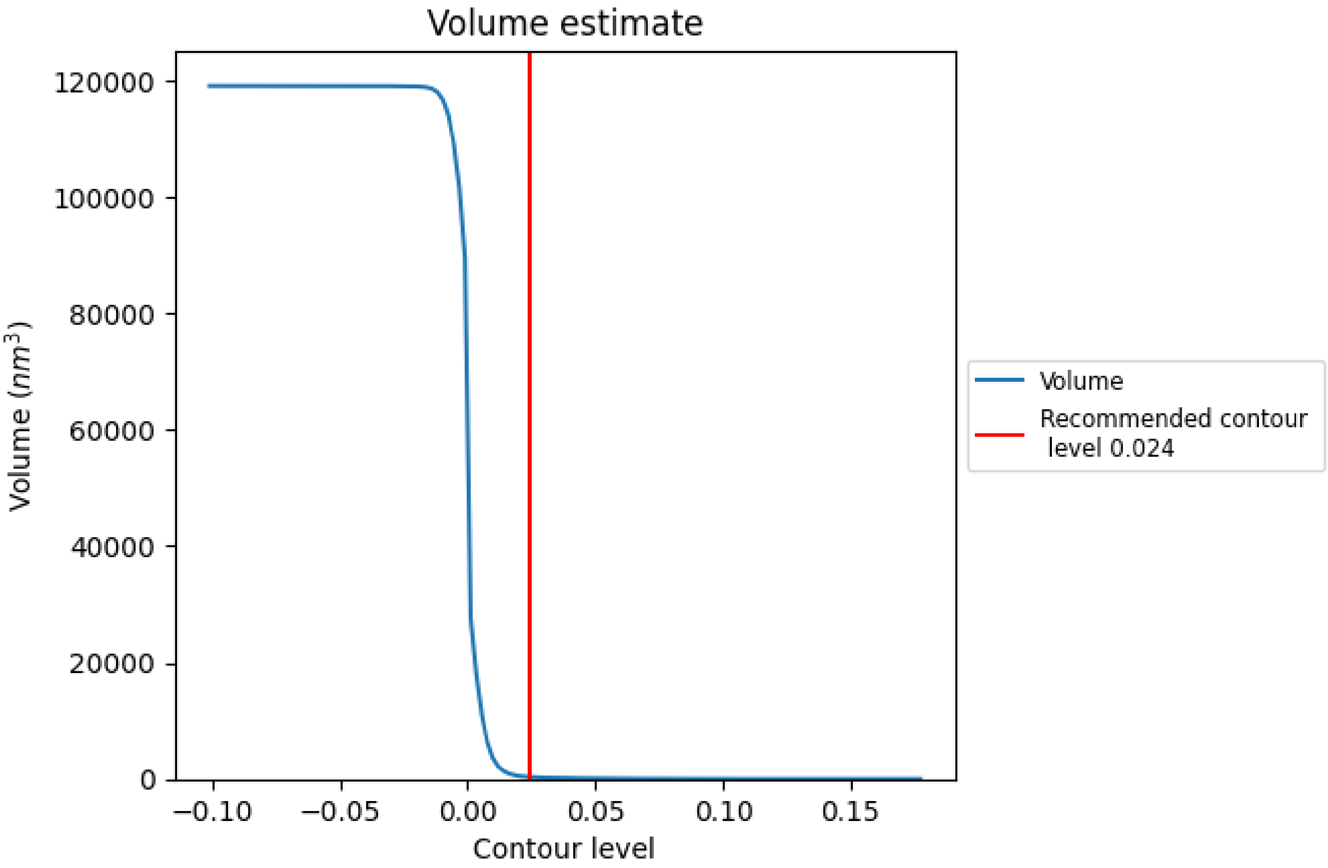
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

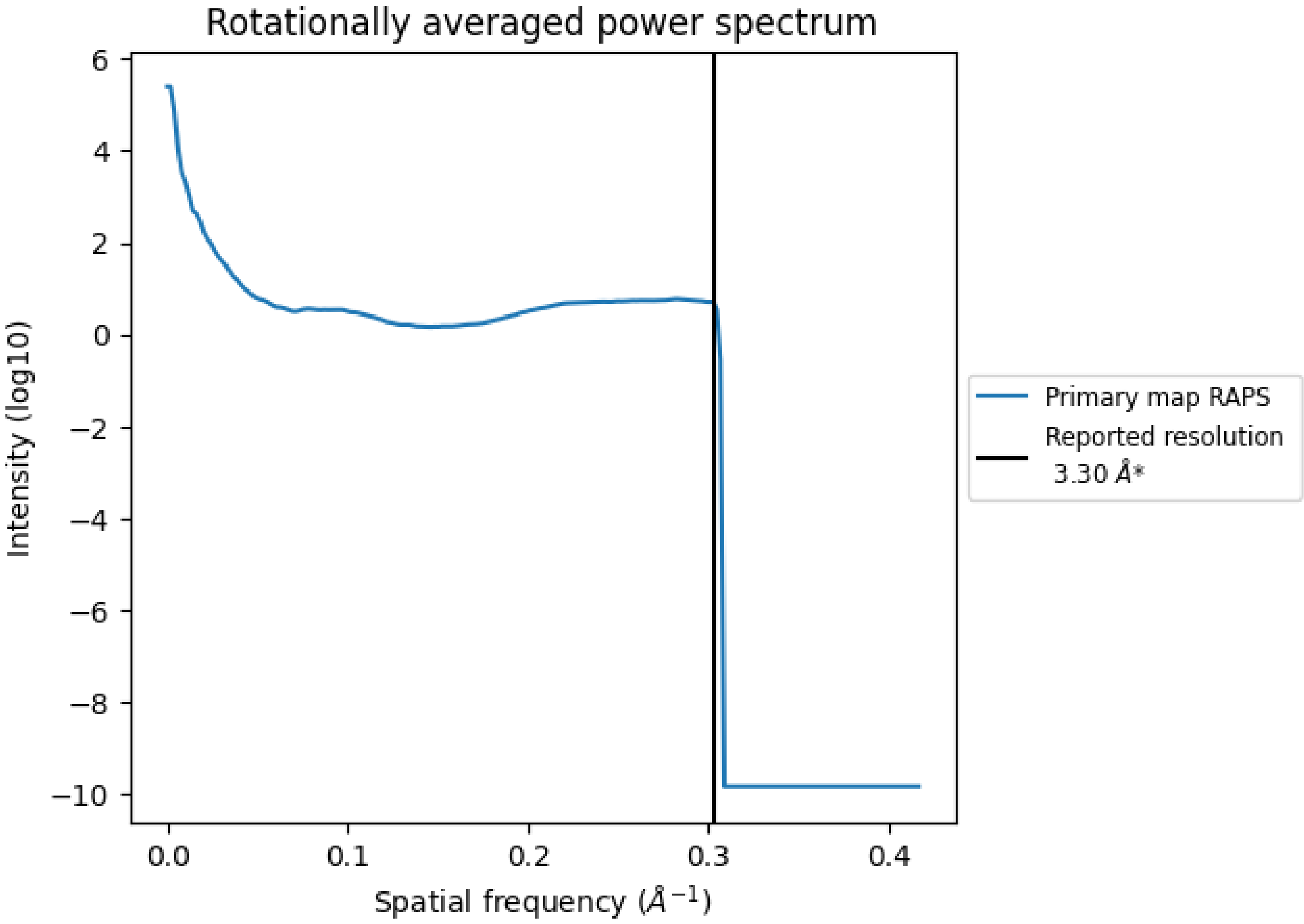
7.2 Volume estimate ⓘ



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 ⓘ

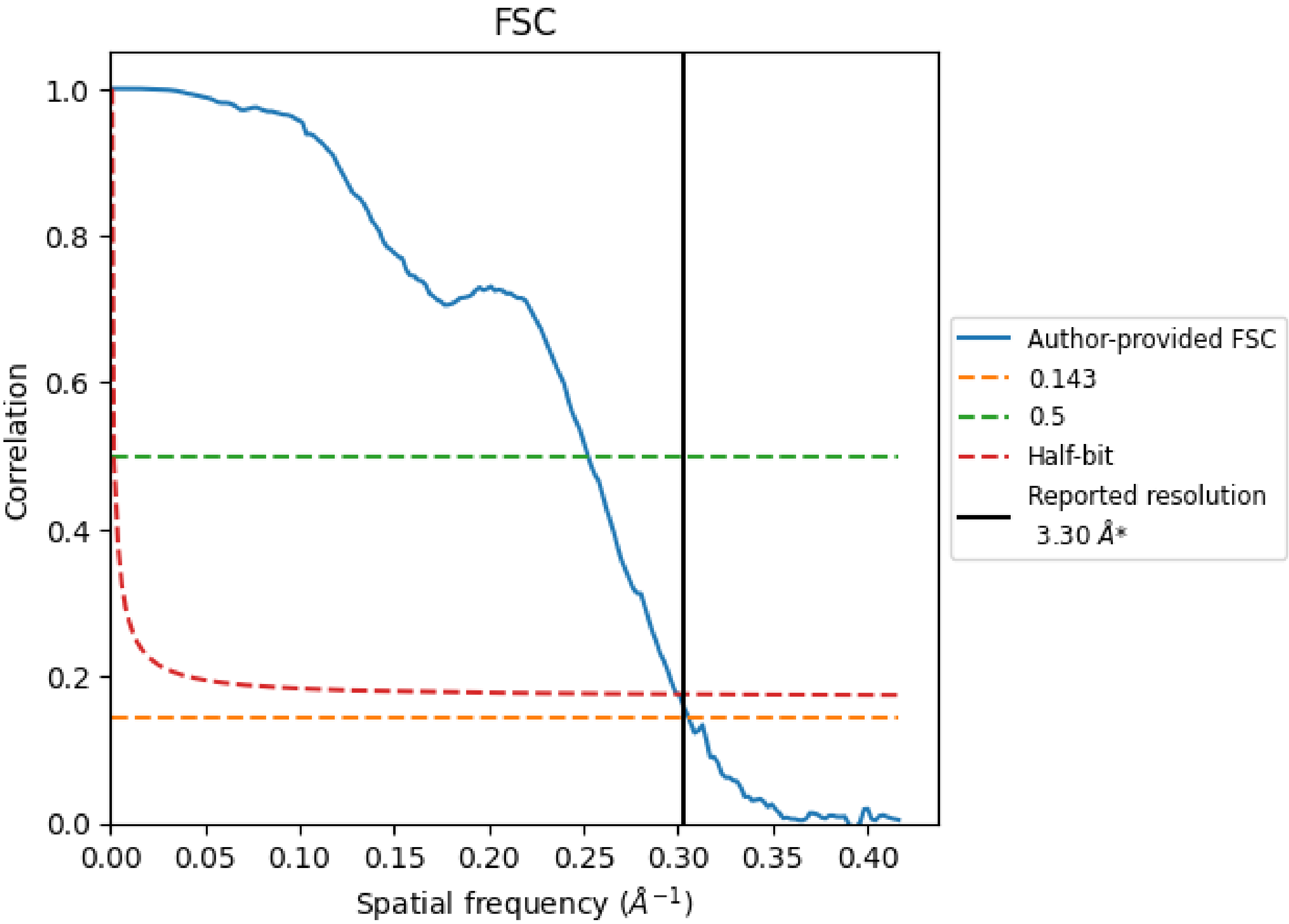


*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



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

8.2 Resolution estimates ⓘ

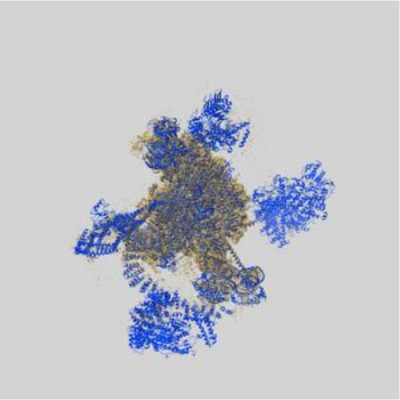
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.27	3.96	3.33
Unmasked-calculated*	-	-	-

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

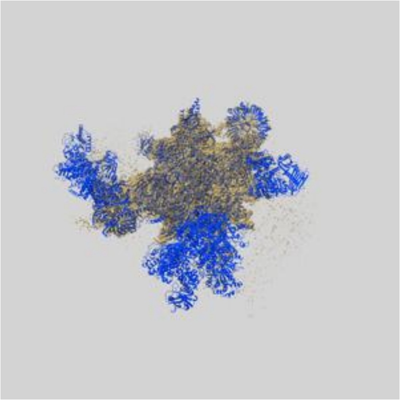
9 Map-model fit ⓘ

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 17.

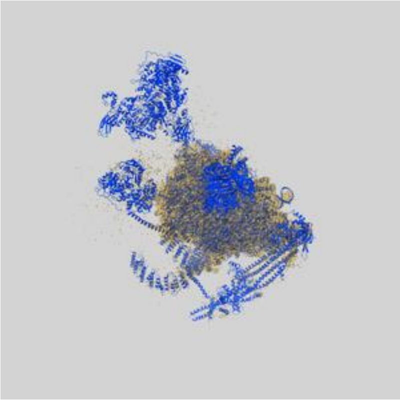
9.1 Map-model overlay ⓘ



X



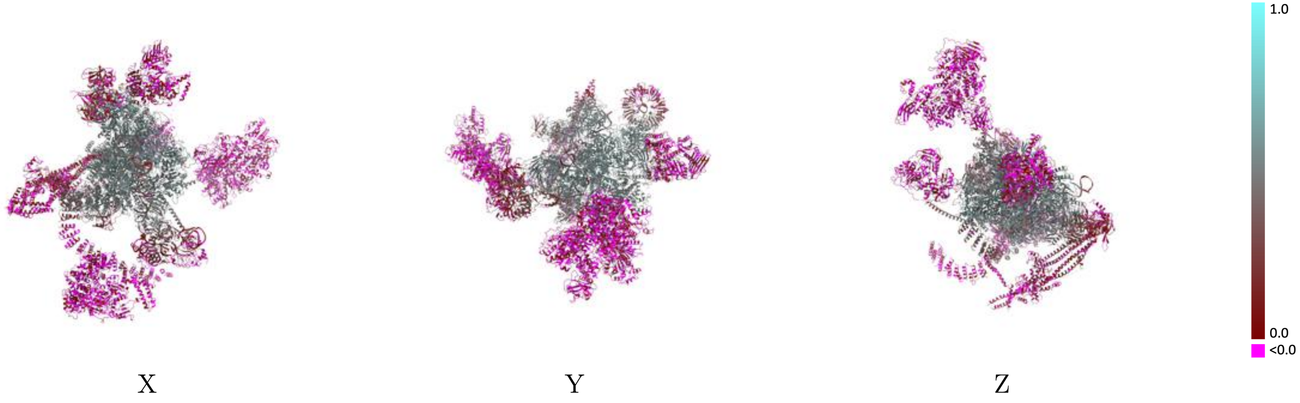
Y



Z

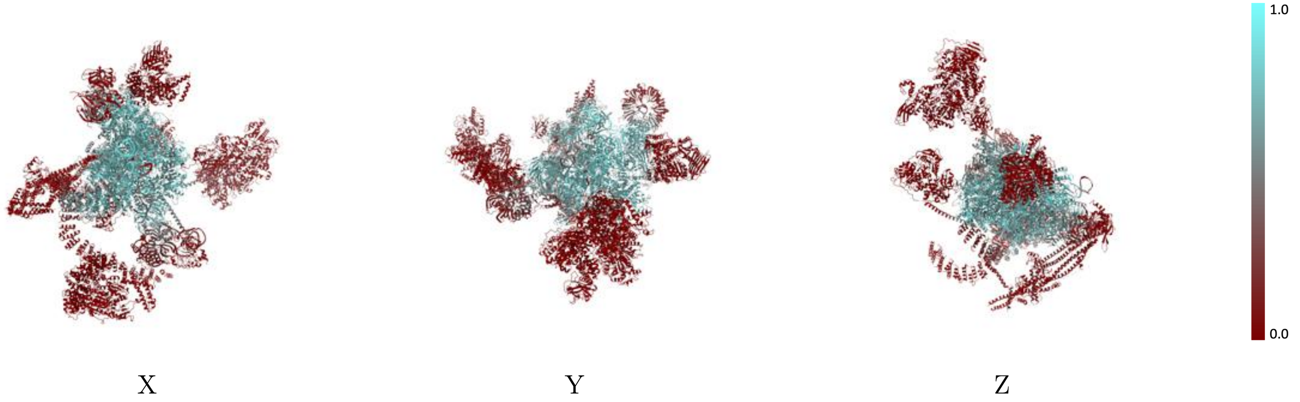
The images above show the 3D surface view of the map at the recommended contour level 0.024 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model ⓘ



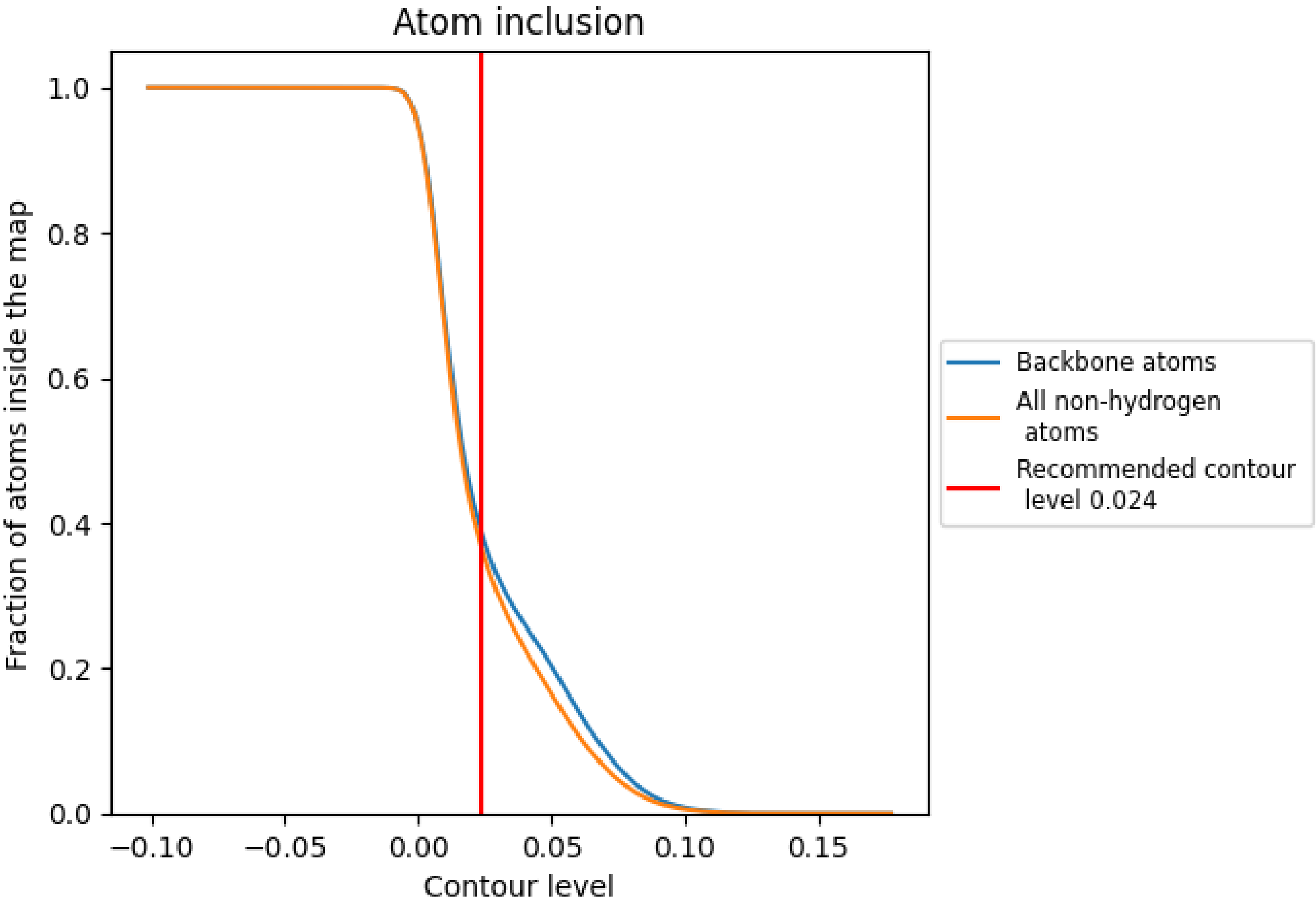
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 ⓘ



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	0.3639	0.2780
2	0.4154	0.2640
5	0.7511	0.4540
6	0.7381	0.4570
7	0.0049	0.0600
8	0.0000	-0.0230
9	0.0000	0.0230
A	0.6844	0.4780
B	0.0007	0.0020
C	0.6848	0.5010
D	0.4081	0.3490
E	0.8412	0.5300
F	0.6278	0.4670
G	0.5772	0.5060
H	0.3249	0.2530
I	0.6044	0.3950
J	0.8354	0.5600
K	0.5775	0.4700
L	0.7396	0.5240
M	0.5155	0.4410
N	0.6243	0.4720
O	0.4296	0.3550
P	0.6534	0.5150
R	0.8342	0.5500
S	0.4421	0.3340
T	0.0662	0.1560
U	0.0014	-0.0010
V	0.0732	0.0630
W	0.0215	0.0440
Y	0.0479	0.0930
Z	0.6516	0.5040
b	0.2809	0.2660
c	0.6516	0.4960
d	0.4341	0.3790
e	0.0740	0.1380

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Chain	Atom inclusion	Q-score
f	0.0417	0.1010
g	0.2161	0.2880
h	0.1072	0.1720
i	0.5726	0.4500
j	0.0501	0.0950
k	0.2065	0.2370
l	0.1232	0.1500
m	0.0607	0.0830
n	0.3693	0.3190
o	0.6617	0.4960
p	0.2236	0.2290
q	0.1141	0.1190
r	0.3482	0.3330
s	0.0730	0.1200
t	0.0258	0.0690
u	0.0163	0.0240
v	0.0237	0.1160
w	0.0098	0.0760
y	0.6404	0.4890
z	0.0112	0.1960