wwPDB EM Validation Summary Report ⓘ

Nov 9, 2022 – 03:22 AM JST

PDB ID	:	6AHD
EMDB ID	:	EMD-9624
Title	:	The Cryo-EM Structure of Human Pre-catalytic Spliceosome (B complex) at 3.8 angstrom resolution
Authors	:	Zhan, X.; Yan, C.; Zhang, X.; Shi, Y.
Deposited on	:	2018-08-17
Resolution	:	3.80 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:

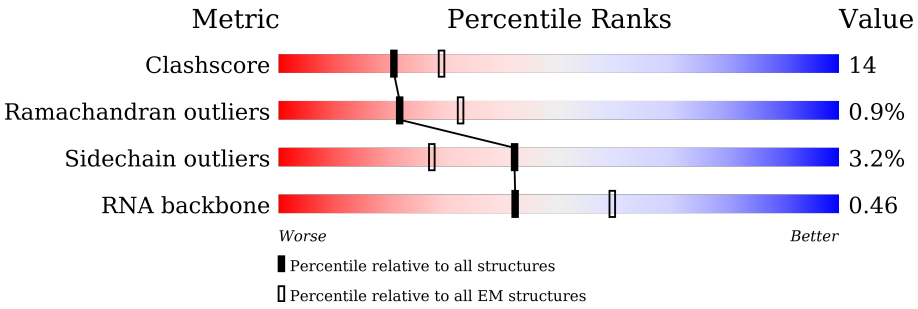
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.80 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	2335	77% 17% • 5%
2	I	144	47% 35% 39% 20% 6%
3	B	117	34% 32% 41% 24% • •
4	F	107	45% 40% 31% 15% • 12%
5	G	274	19% 5% 8% 15% 72%
6	O	142	80% 18% • •
7	C	972	65% 18% 16%

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Mol	Chain	Length	Quality of chain
8	N	941	16% 71% 10% 17%
9	M	128	84% 12%
10	L	499	63% 12% 25%
11	9	800	11% 6% 79%
12	J	683	29% 5% 67%
13	U	231	26% 26% 72%
13	a	231	32% 37% 63%
13	i	231	37% 37% 63%
14	V	119	66% 68% 31%
14	b	119	58% 69% 31%
14	j	119	69% 69% 31%
15	P	118	62% 60% 37%
15	c	118	81% 81% 18%
15	k	118	72% 71% 28%
16	Q	86	81% 79% 17%
16	d	86	86% 86% 14%
16	l	86	86% 86% 14%
17	R	92	83% 84% 15%
17	e	92	83% 86% 14%
17	m	92	86% 86% 14%
18	S	76	92% 91% 5%
18	f	76	95% 97%
18	n	76	89% 89% 11%
19	T	126	52% 56% 44%
19	g	126	52% 64% 36%

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Mol	Chain	Length	Quality of chain
19	h	126	63% 63% 37%
20	E	357	80% 81% 16%
21	X	376	11% 19% 80%
22	W	177	19% 90% 6% 5%
23	A0	73	5% 71% 21% 8%
24	0	439	6% 9% 90%
25	Z	312	15% 54% 44%
26	8	199	8% 26% 72%
27	Y	513	88% 83% 5% 12%
28	H	188	58% 19% 20% 16% 42%
29	o	255	64% 63% 36%
30	p	225	42% 42% 58%
31	u	793	16% 15% 84%
32	v	464	20% 18% 80%
33	w	501	84% 83% 16%
34	q	95	95% 91% 5%
35	r	102	73% 70% 27%
36	s	139	53% 53% 47%
37	t	91	79% 78% 21%
38	x	80	88% 85% 12%
39	y	103	63% 63% 37%
40	z	96	64% 63% 36%
41	K	522	71% 7% 21%
42	1	1304	79% 57% 22% 20%
43	3	1217	96% 86% 10%

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Mol	Chain	Length	Quality of chain
44	5	125	86% 75% 11% 14%
45	6	110	78% 72% 9% 19%
46	7	86	74% 58% 19% 23%
47	2	895	20% 18% 80%
48	4	424	18% 17% 82%
49	D	2136	52% 76% 20%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
50	IHP	A	3000	-	-	X	-

2 Entry composition (i)

There are 52 unique types of molecules in this entry. The entry contains 85302 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 protein called Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	2209	17290	10998	3094	3128	70	0	0

- Molecule 2 is a RNA chain called U4snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	I	136	2881	1288	498	959	136	0	0

- Molecule 3 is a RNA chain called U5snRNA.

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

- Molecule 4 is a RNA chain called U6snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	F	94	1995	891	362	648	94	0	0

- Molecule 5 is a RNA chain called pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	G	77	1612	722	261	552	77	0	0

- Molecule 6 is a protein called Thioredoxin-like protein 4A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	O	141	1152	739	194	209	10	0	0

- Molecule 7 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	818	Total	C	N	O	S	0	0
			6440	4117	1086	1205	32		

- Molecule 8 is a protein called Pre-mRNA-processing factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	N	781	Total	C	N	O	S	0	0
			4518	2759	876	878	5		

- Molecule 9 is a protein called NHP2-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	M	124	Total	C	N	O	S	0	0
			962	608	171	178	5		

- Molecule 10 is a protein called U4/U6 small nuclear ribonucleoprotein Prp31.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	376	Total	C	N	O	S	0	0
			2874	1788	524	550	12		

- Molecule 11 is a protein called U4/U6.U5 tri-snRNP-associated protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	9	165	Total	C	N	O	S	0	0
			1087	669	205	212	1		

- Molecule 12 is a protein called U4/U6 small nuclear ribonucleoprotein Prp3.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	J	227	Total	C	N	O	S	0	0
			1273	724	283	263	3		

- Molecule 13 is a protein called SmB.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	a	86	Total	C	N	O	0	0
			344	172	86	86		
13	i	86	Total	C	N	O	0	0
			344	172	86	86		

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Mol	Chain	Residues	Atoms				AltConf	Trace
13	U	64	Total 256	C 128	N 64	O 64	0	0

- Molecule 14 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	b	82	Total 328	C 164	N 82	O 82	0	0
14	j	82	Total 328	C 164	N 82	O 82	0	0
14	V	82	Total 334	C 170	N 82	O 82	0	0

- Molecule 15 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	c	97	Total 388	C 194	N 97	O 97	0	0
15	k	85	Total 340	C 170	N 85	O 85	0	0
15	P	74	Total 300	C 152	N 74	O 74	0	0

- Molecule 16 is a protein called SmE.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	d	74	Total 296	C 148	N 74	O 74	0	0
16	l	74	Total 296	C 148	N 74	O 74	0	0
16	Q	71	Total 292	C 150	N 71	O 71	0	0

- Molecule 17 is a protein called SmF.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	e	79	Total 316	C 158	N 79	O 79	0	0
17	m	79	Total 316	C 158	N 79	O 79	0	0
17	R	78	Total 314	C 158	N 78	O 78	0	0

- Molecule 18 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	f	74	Total	C	N	O	0	0
			296	148	74	74		
18	n	68	Total	C	N	O	0	0
			272	136	68	68		
18	S	73	Total	C	N	O	0	0
			298	152	73	73		

- Molecule 19 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	g	81	Total	C	N	O	0	0
			324	162	81	81		
19	h	80	Total	C	N	O	0	0
			320	160	80	80		
19	T	71	Total	C	N	O	0	0
			288	146	71	71		

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

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

- Molecule 21 is a protein called WW domain-binding protein 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	X	75	Total	C	N	O	0	0
			378	228	75	75		

- Molecule 22 is a protein called Peptidyl-prolyl cis-trans isomerase H.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	W	169	Total	C	N	O	0	0
			844	506	169	169		

- Molecule 23 is a protein called Ubiquitin-like protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	A0	73	Total	C	N	O	S	0	0
			581	375	93	109	4		

- Molecule 24 is a protein called Microfibrillar-associated protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	0	45	Total	C	N	O	0	0
			225	135	45	45		

- Molecule 25 is a protein called Pre-mRNA-splicing factor 38A.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	Z	176	Total	C	N	O	0	0
			883	531	176	176		

- Molecule 26 is a protein called Zinc finger matrin-type protein 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	8	56	Total	C	N	O	0	0
			277	165	56	56		

- Molecule 27 is a protein called WD40 repeat-containing protein SMU1.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	Y	453	Total	C	N	O	0	0
			2258	1352	453	453		

- Molecule 28 is a RNA chain called U2snRNA.

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

- Molecule 29 is a protein called U2 small nuclear ribonucleoprotein A'.

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

- Molecule 30 is a protein called U2 small nuclear ribonucleoprotein B".

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

- Molecule 31 is a protein called Splicing factor 3A subunit 1.

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

- Molecule 32 is a protein called Splicing factor 3A subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	v	94	Total 376	C 188	N 94	O 94	0	0

- Molecule 33 is a protein called Splicing factor 3A subunit 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	w	423	Total 1693	C 847	N 423	O 423	0	0

- Molecule 34 is a protein called U6 snRNA-associated Sm-like protein LSm2.

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

- Molecule 35 is a protein called U6 snRNA-associated Sm-like protein LSm3.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	r	74	Total 296	C 148	N 74	O 74	0	0

- Molecule 36 is a protein called U6 snRNA-associated Sm-like protein LSm4.

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

- Molecule 37 is a protein called U6 snRNA-associated Sm-like protein LSm5.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	t	72	Total 288	C 144	N 72	O 72	0	0

- Molecule 38 is a protein called U6 snRNA-associated Sm-like protein LSm6.

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

- Molecule 39 is a protein called U6 snRNA-associated Sm-like protein LSm7.

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

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

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

- Molecule 41 is a protein called U4/U6 small nuclear ribonucleoprotein Prp4.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	K	414	Total 1821	C 969	N 423	O 428	S 1	0	0

- Molecule 42 is a protein called Splicing factor 3B subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	1	1048	Total 4192	C 2096	N 1048	O 1048	0	0

- Molecule 43 is a protein called Splicing factor 3B subunit 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	3	1168	Total 4672	C 2336	N 1168	O 1168	0	0

- Molecule 44 is a protein called SF3b14a, Splicing factor 3B subunit 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	5	108	Total 432	C 216	N 108	O 108	0	0

- Molecule 45 is a protein called PHD finger-like domain-containing protein 5A.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	6	89	Total 356	C 178	N 89	O 89	0	0

- Molecule 46 is a protein called SF3b5, Splicing factor 3B subunit 5.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	7	66	Total 264	C 132	N 66	O 66	0	0

- Molecule 47 is a protein called SF3b145, Splicing factor 3B subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
47	2	182	Total 728	C 364	N 182	O 182	0	0

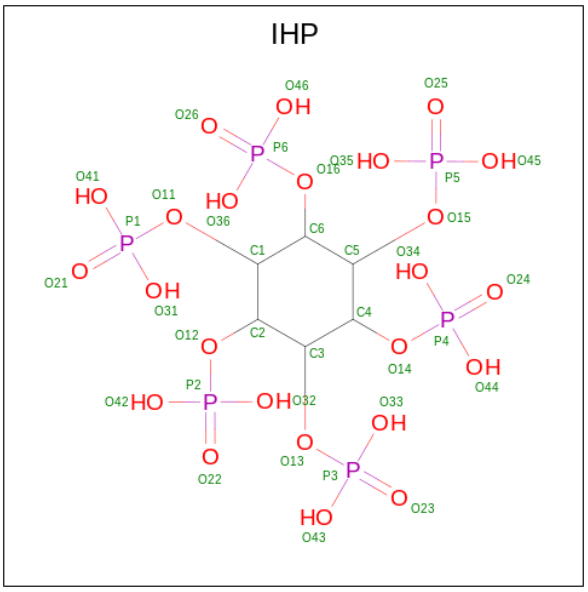
- Molecule 48 is a protein called SF3b49, Splicing factor 3B subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	4	78	Total 312	C 156	N 78	O 78	0	0

- Molecule 49 is a protein called Brr2, U5 small nuclear ribonucleoprotein 200 kDa helicase.

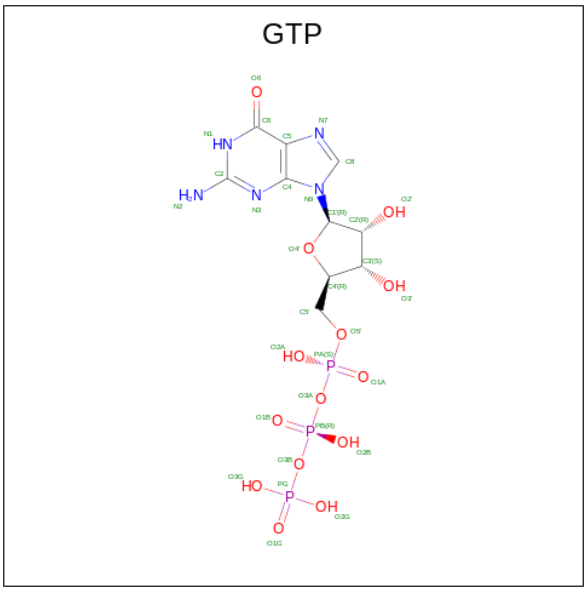
Mol	Chain	Residues	Atoms				AltConf	Trace
49	D	1699	Total 6796	C 3398	N 1699	O 1699	0	0

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



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

- Molecule 51 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	
51	C	1	32	10	5	14	3	0

- Molecule 52 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

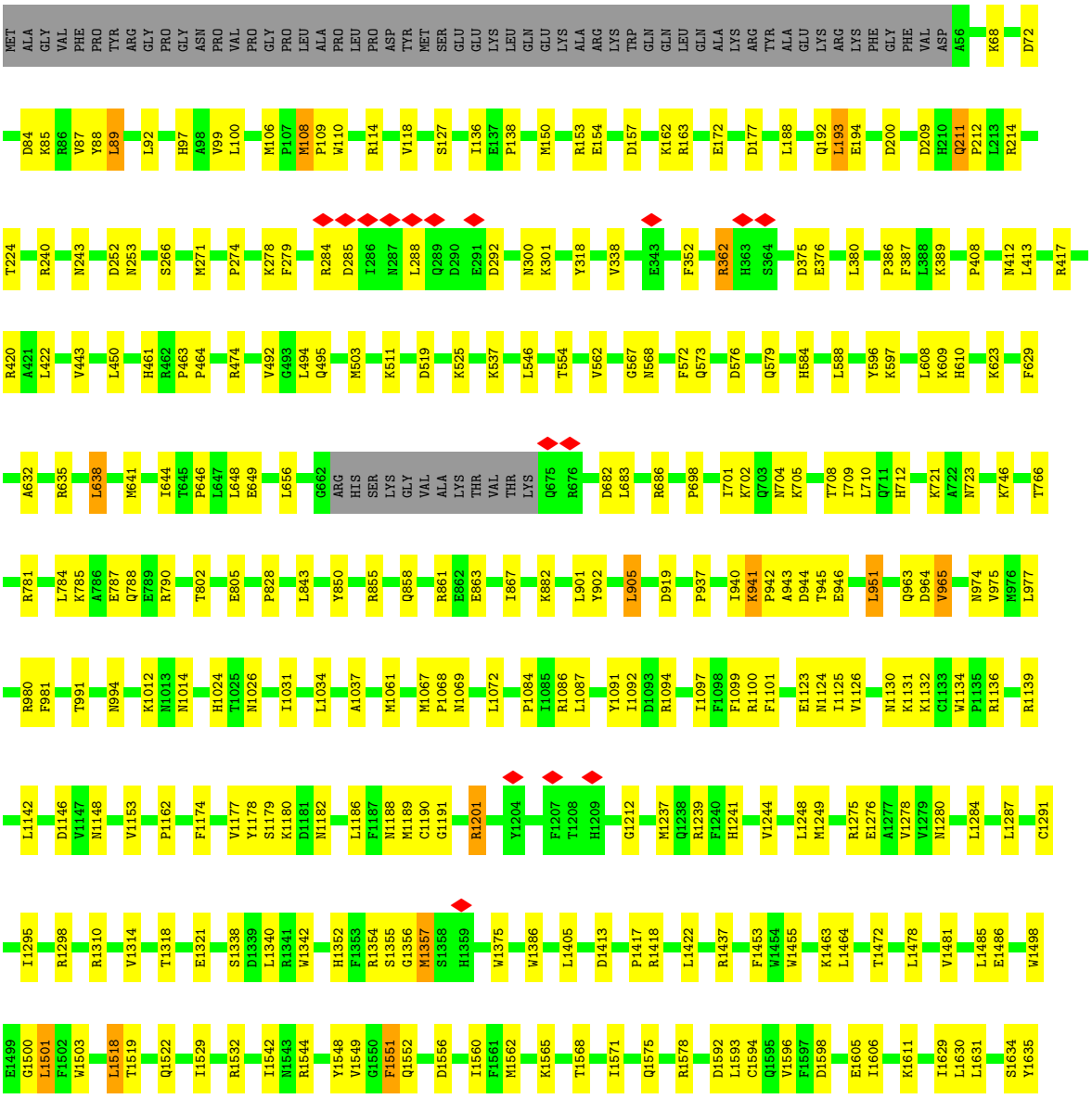
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
52	C	1	1	1	0

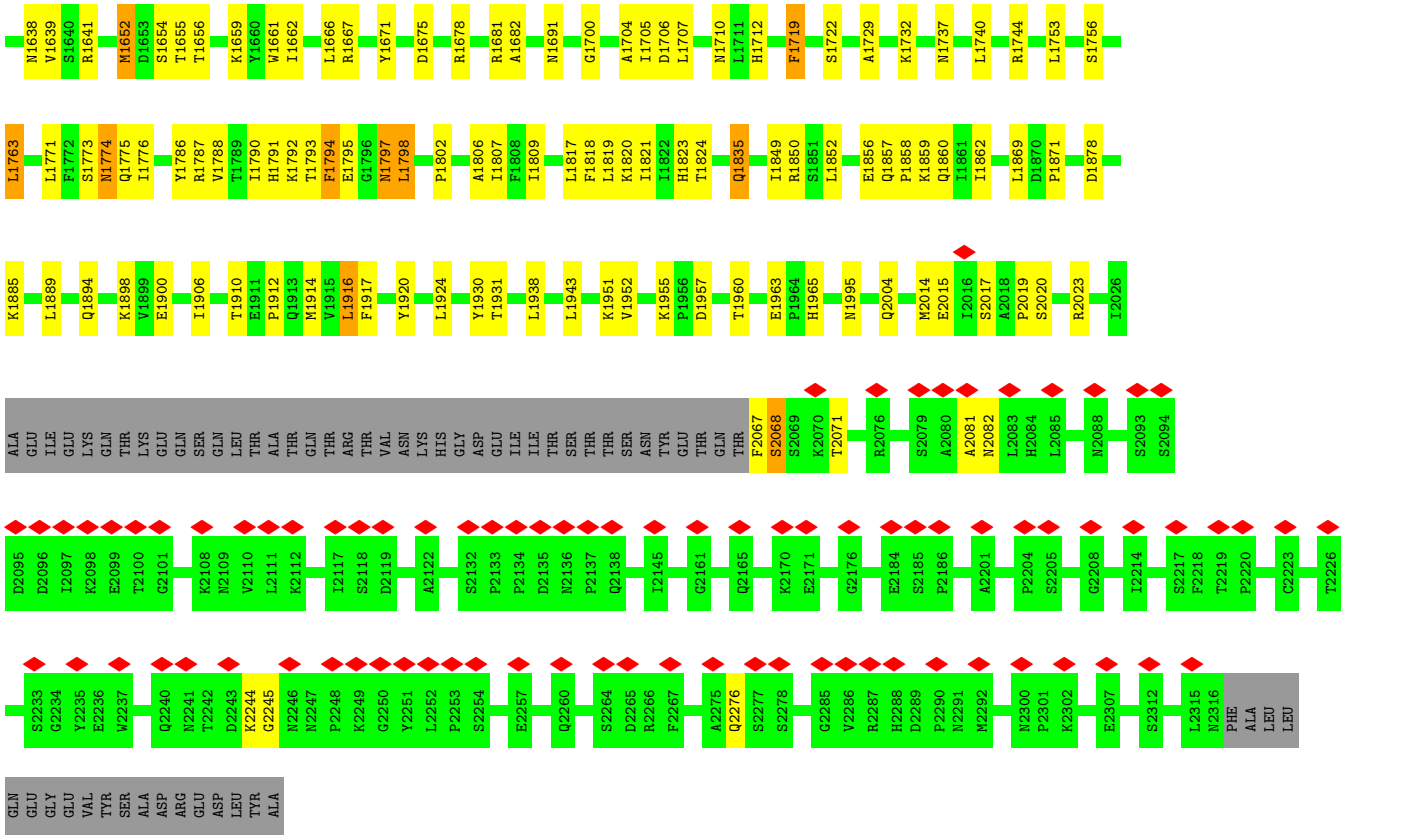
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Pre-mRNA-processing-splicing factor 8

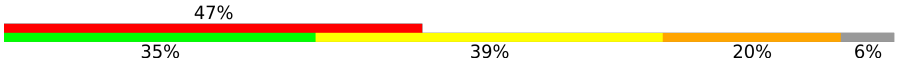
Chain A:

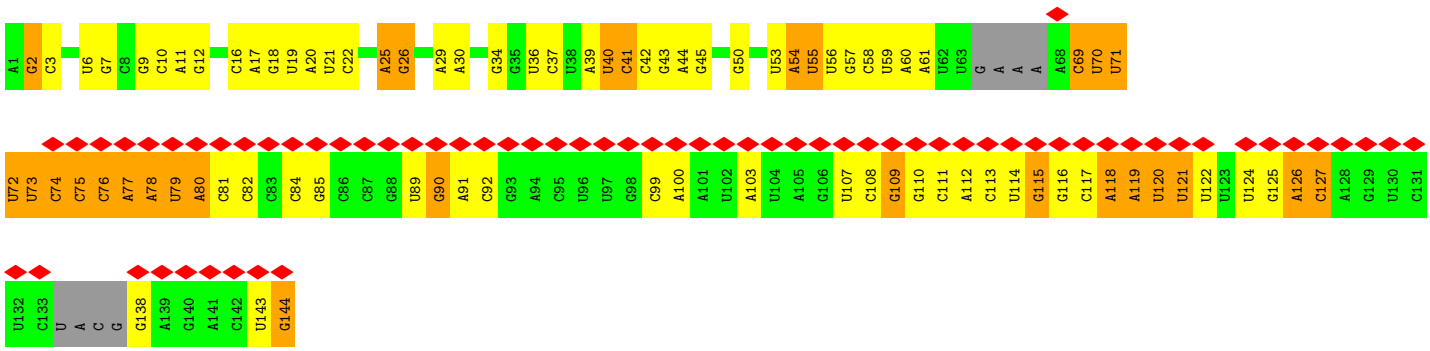




• Molecule 2: U4snRNA

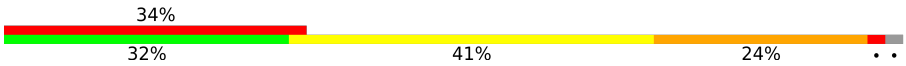
Chain I:

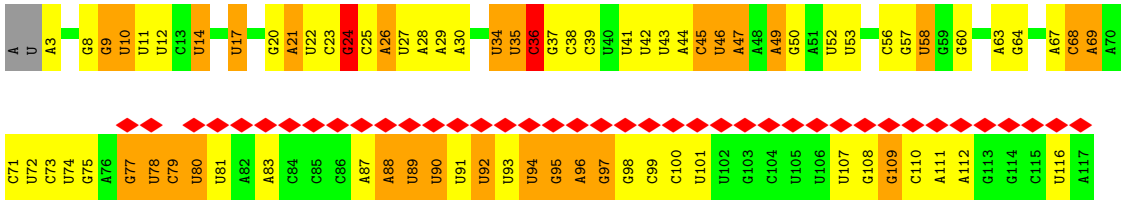




• Molecule 3: U5snRNA

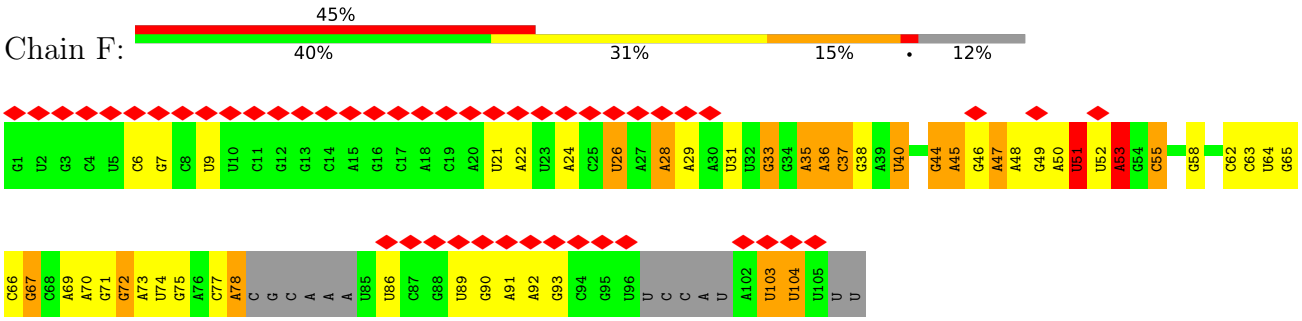
Chain B:





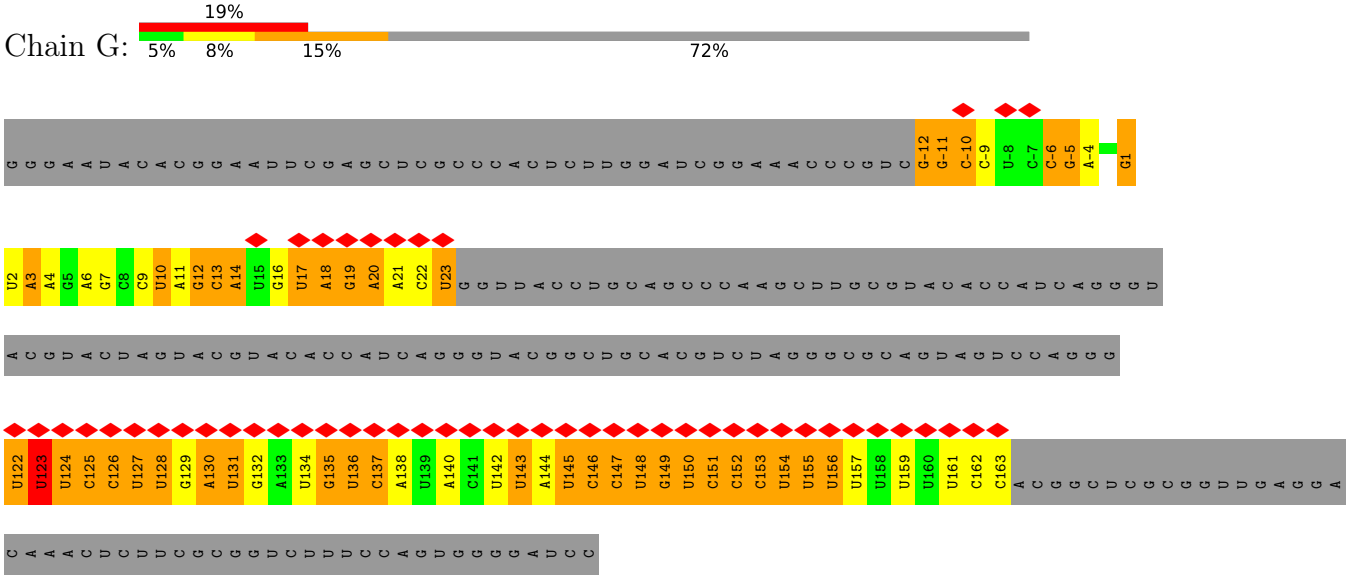
• Molecule 4: U6snRNA

Chain F:



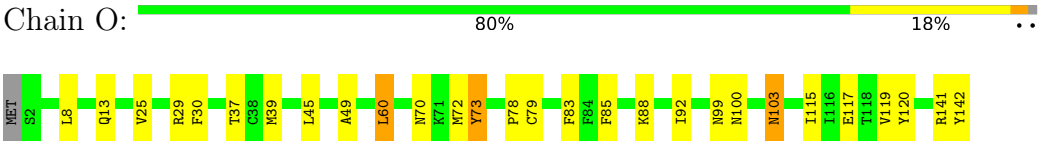
• Molecule 5: pre-mRNA

Chain G:



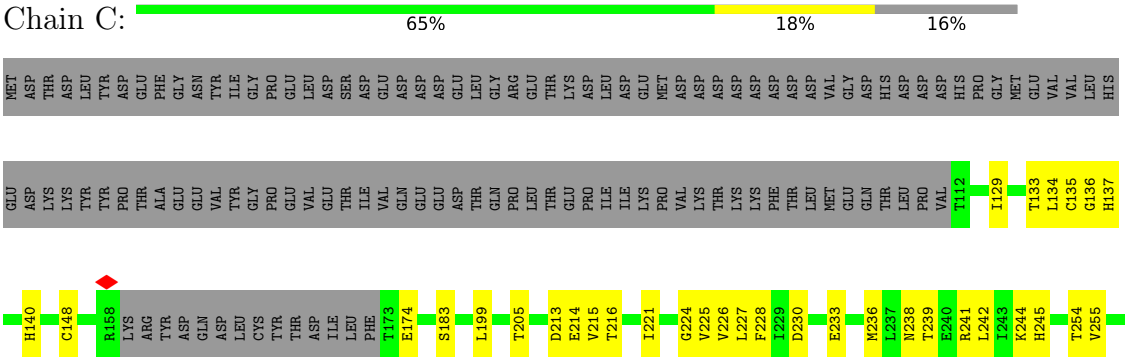
• Molecule 6: Thioredoxin-like protein 4A

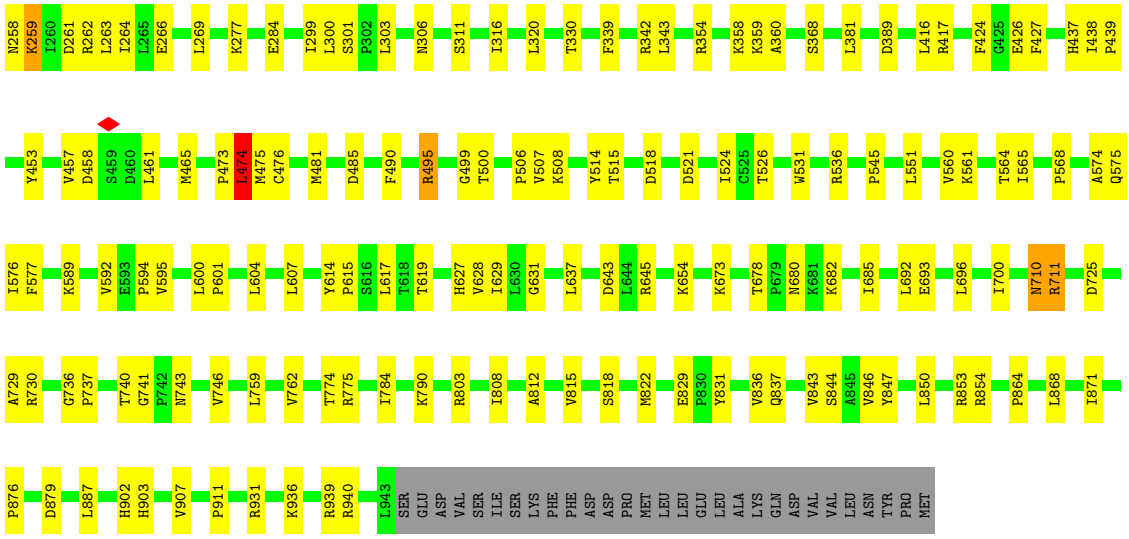
Chain O:



• Molecule 7: 116 kDa U5 small nuclear ribonucleoprotein component

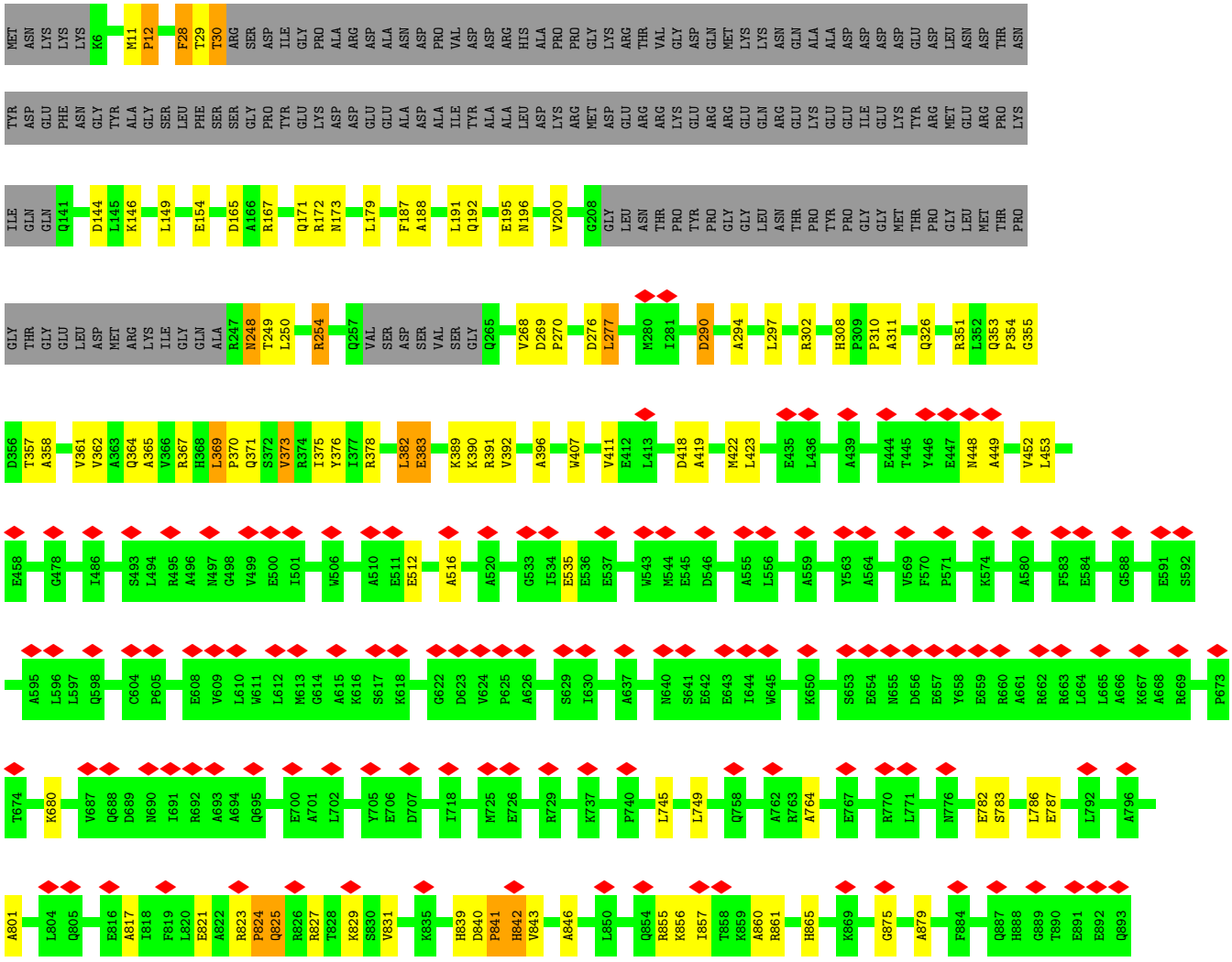
Chain C:

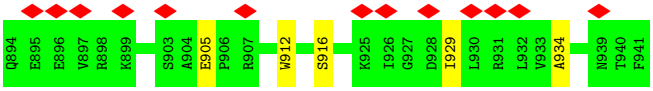




• Molecule 8: Pre-mRNA-processing factor 6

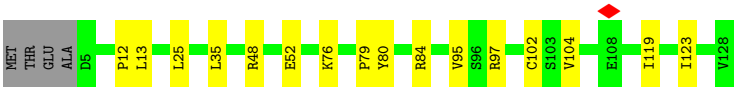
Chain N:





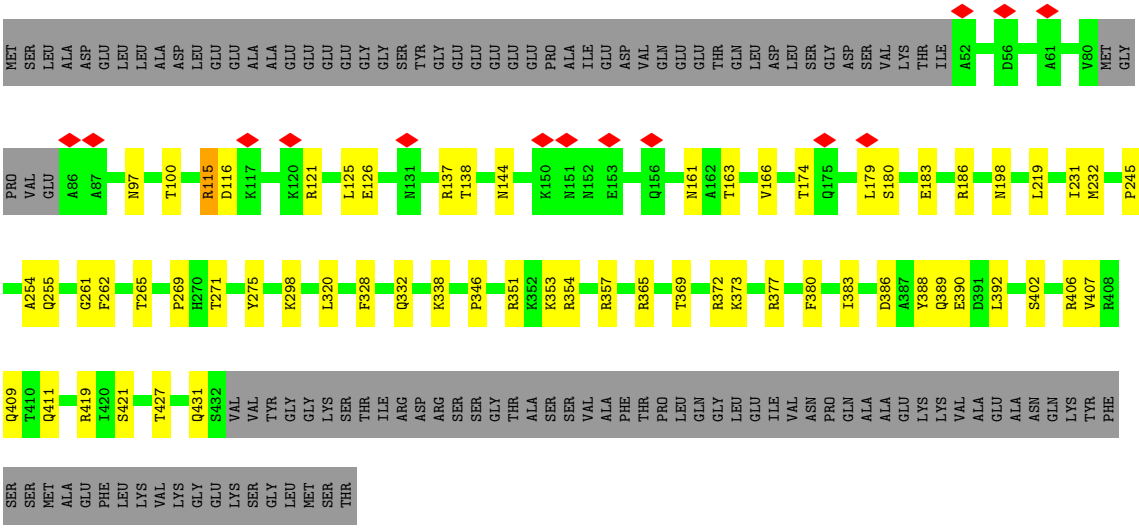
• Molecule 9: NHP2-like protein 1

Chain M:



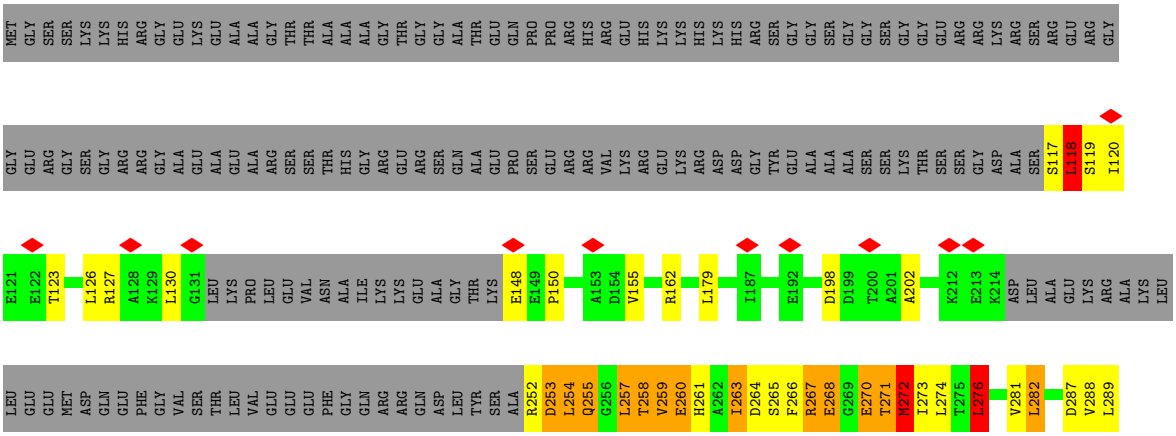
• Molecule 10: U4/U6 small nuclear ribonucleoprotein Prp31

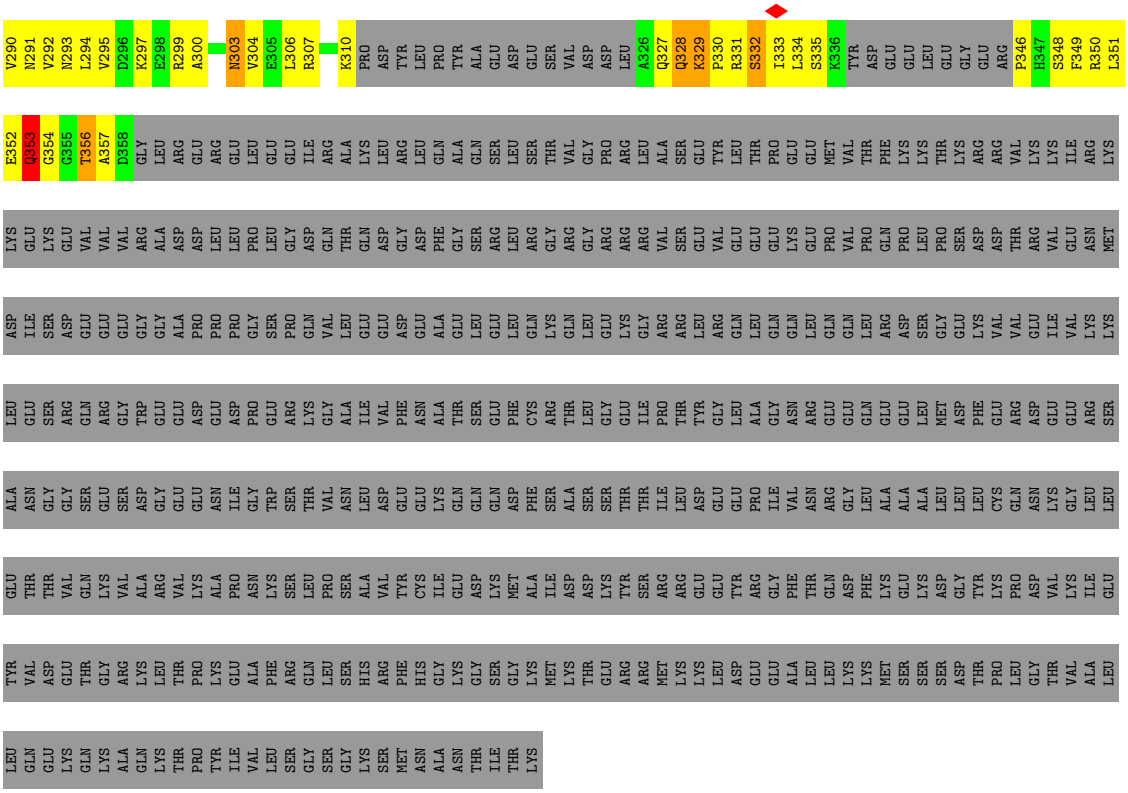
Chain L:



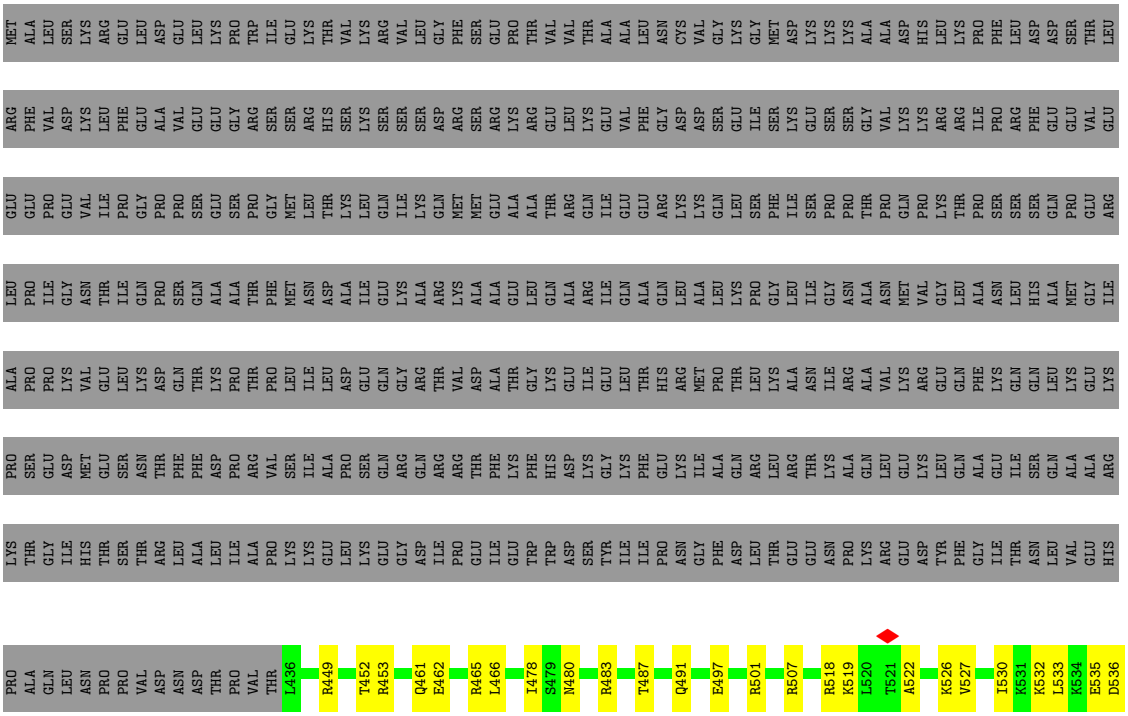
• Molecule 11: U4/U6.U5 tri-snRNP-associated protein 1

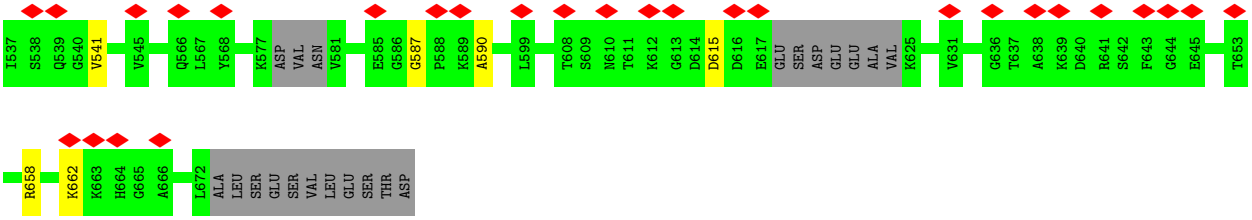
Chain 9:





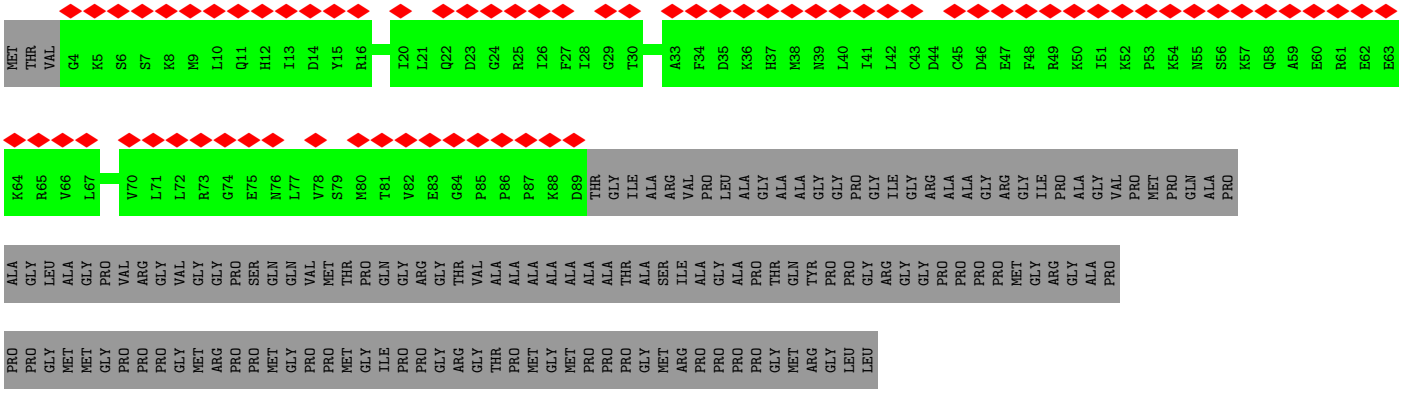
• Molecule 12: U4/U6 small nuclear ribonucleoprotein Prp3





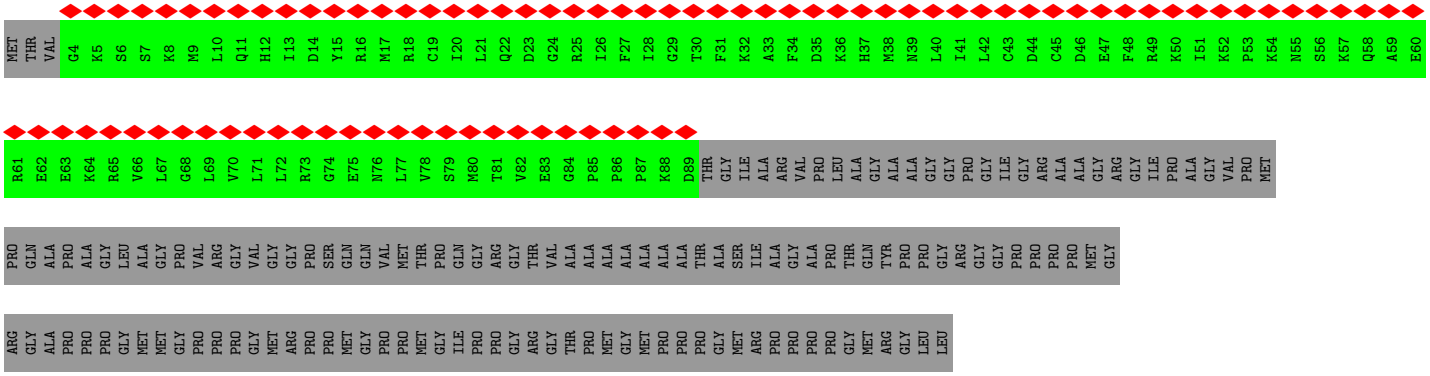
• Molecule 13: SmB

Chain a:



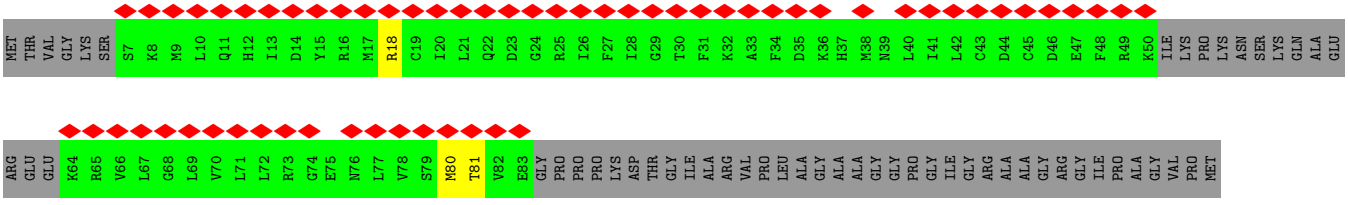
• Molecule 13: SmB

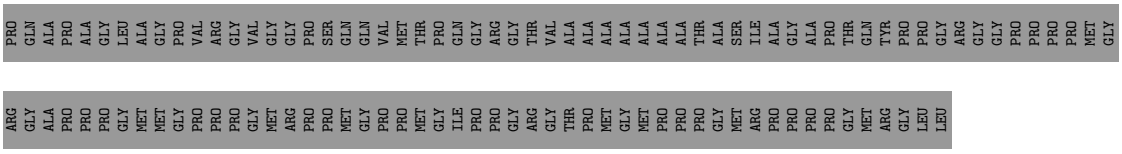
Chain i:



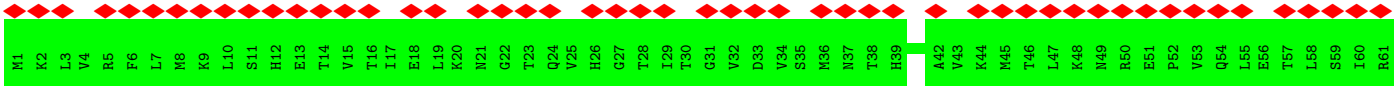
• Molecule 13: SmB

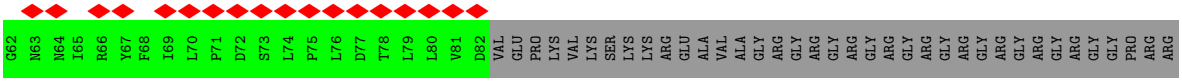
Chain U:



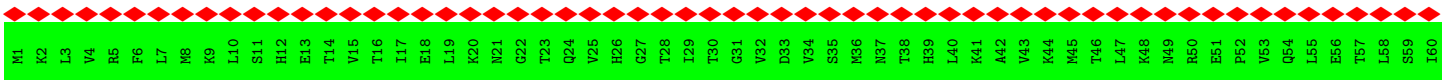


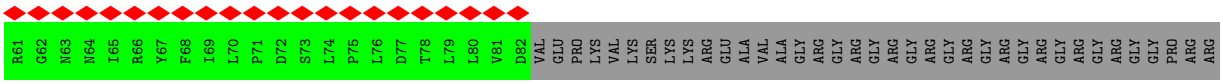
• Molecule 14: Small nuclear ribonucleoprotein Sm D1



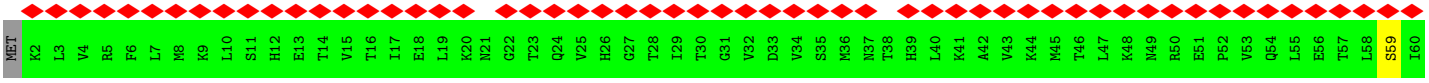


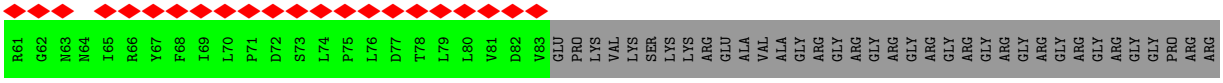
• Molecule 14: Small nuclear ribonucleoprotein Sm D1



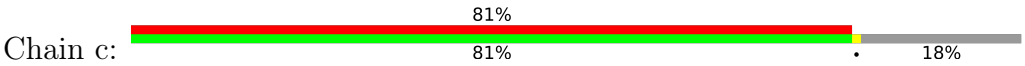


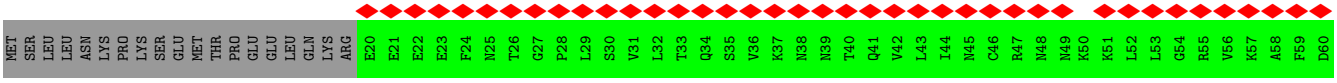
• Molecule 14: Small nuclear ribonucleoprotein Sm D1

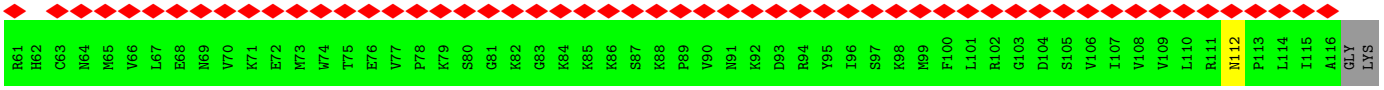




• Molecule 15: Small nuclear ribonucleoprotein Sm D2

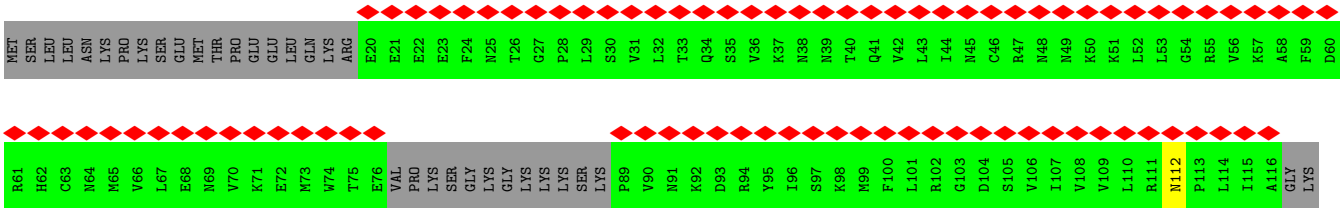






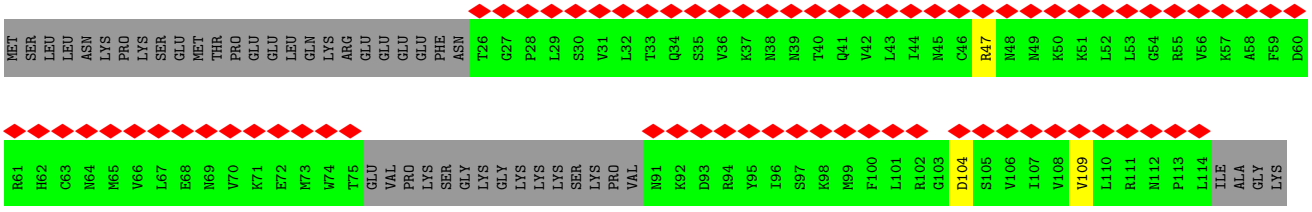
• Molecule 15: Small nuclear ribonucleoprotein Sm D2

Chain k:



• Molecule 15: Small nuclear ribonucleoprotein Sm D2

Chain P:



• Molecule 16: SmE

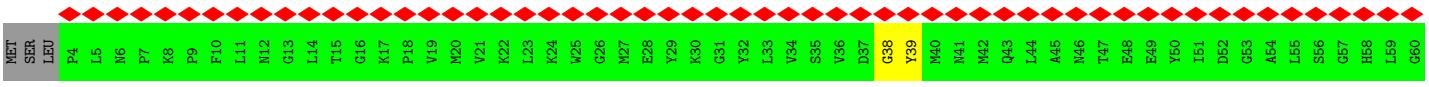
Chain d:

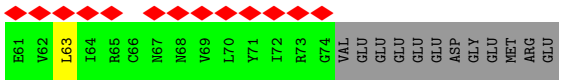
• Molecule 16: SmE

Chain l:

• Molecule 16: SmE

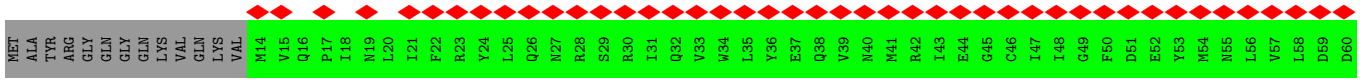
Chain Q:

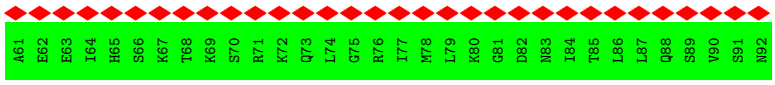




• Molecule 17: SmF

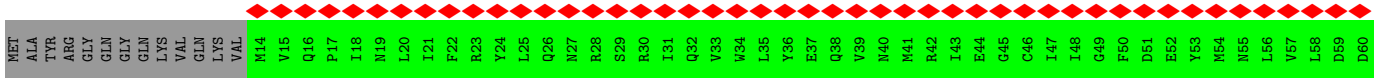
Chain e:

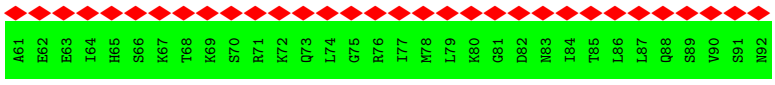




• Molecule 17: SmF

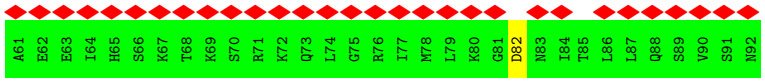
Chain m:





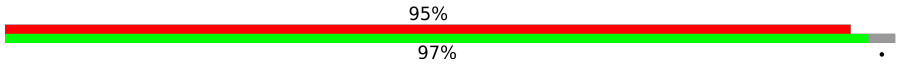
• Molecule 17: SmF

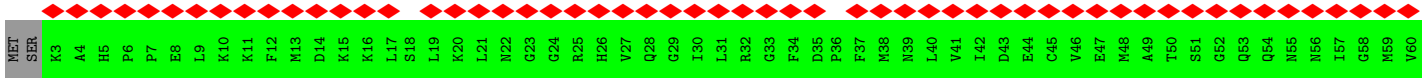
Chain R:

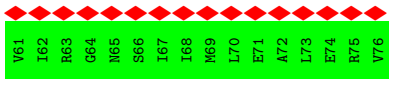


• Molecule 18: Small nuclear ribonucleoprotein G

Chain f:

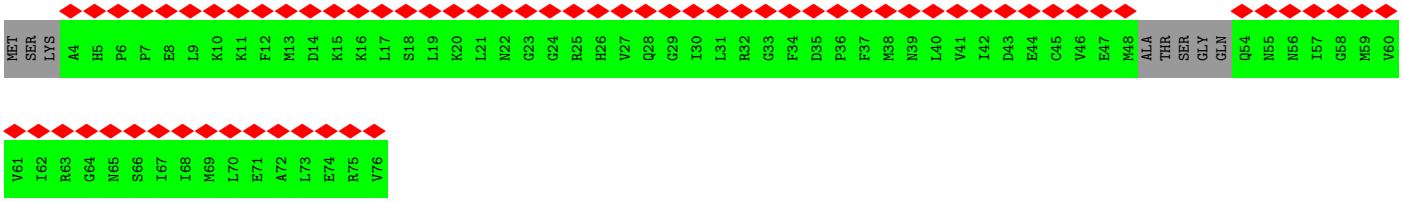




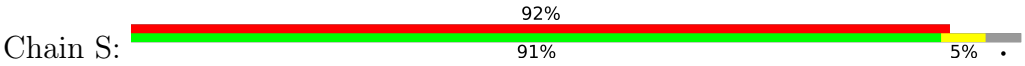


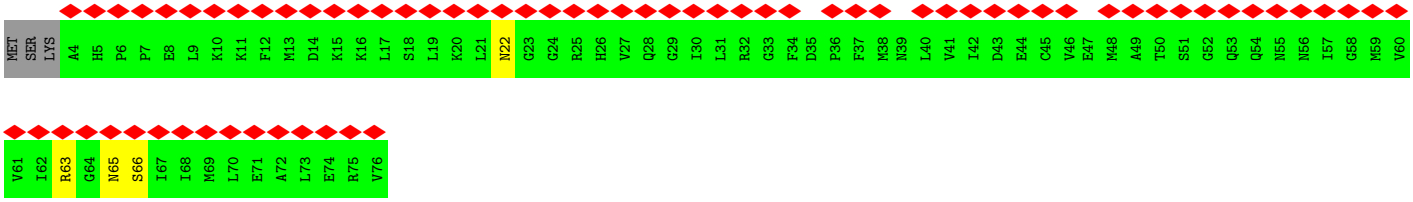
• Molecule 18: Small nuclear ribonucleoprotein G

Chain n:

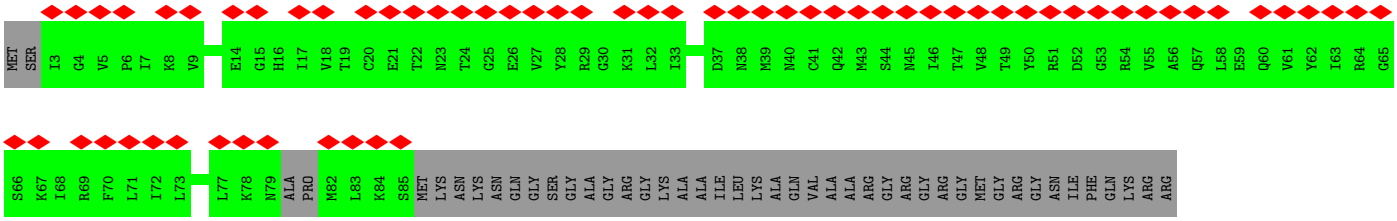


• Molecule 18: Small nuclear ribonucleoprotein G

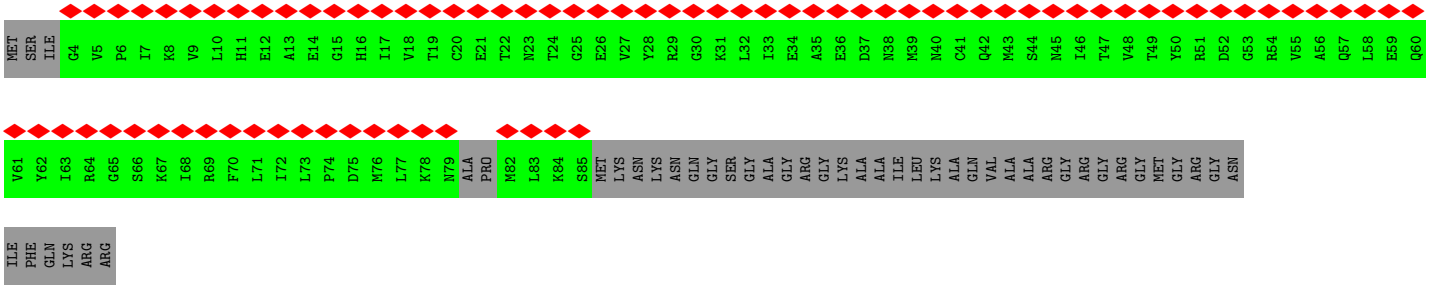




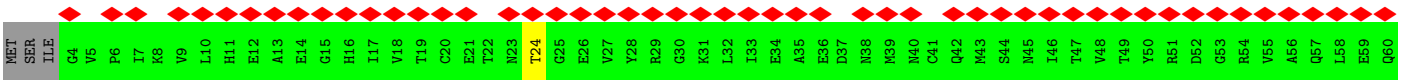
• Molecule 19: Small nuclear ribonucleoprotein Sm D3

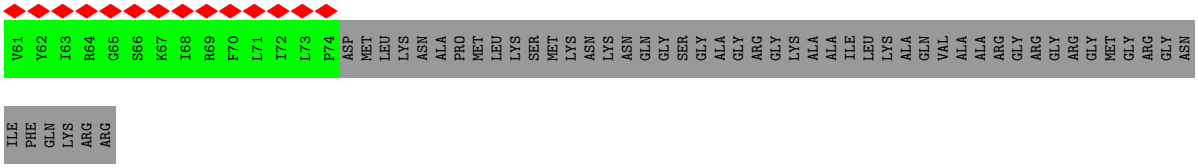


• Molecule 19: Small nuclear ribonucleoprotein Sm D3



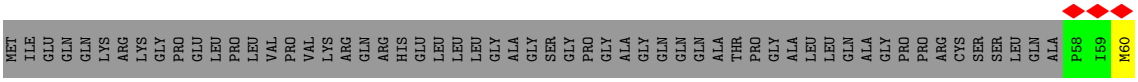
• Molecule 19: Small nuclear ribonucleoprotein Sm D3

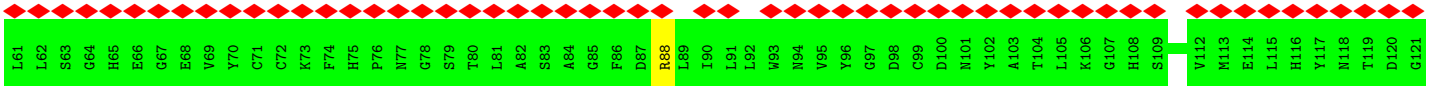


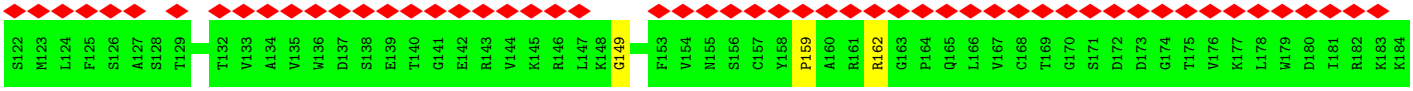


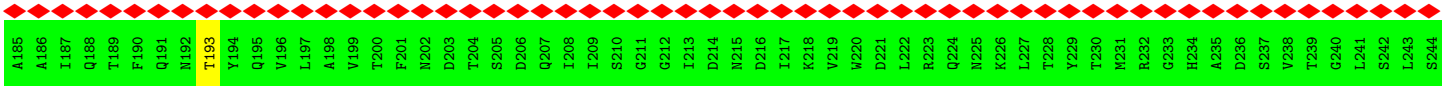
• Molecule 20: U5 small nuclear ribonucleoprotein 40 kDa protein

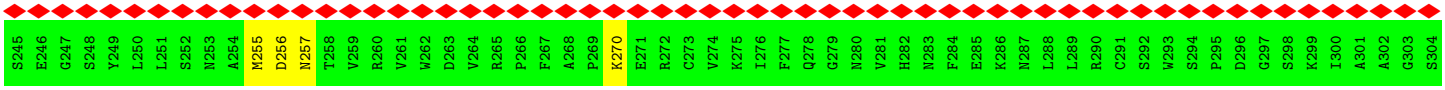
Chain E:

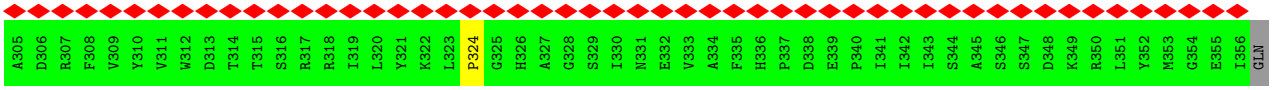






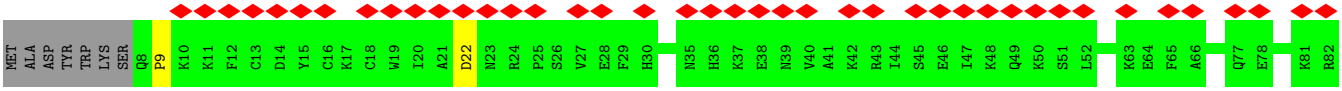


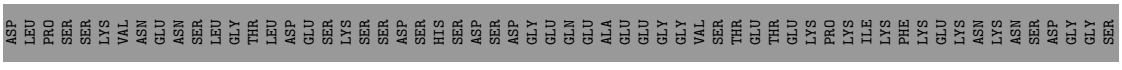




• Molecule 21: WW domain-binding protein 4

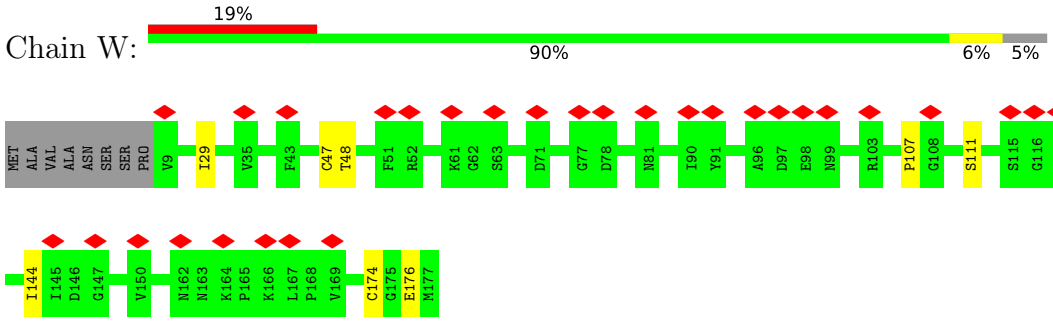
Chain X:





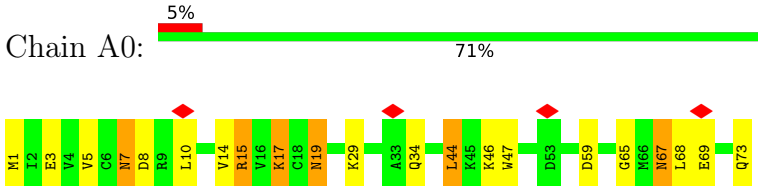
• Molecule 22: Peptidyl-prolyl cis-trans isomerase H

Chain W:



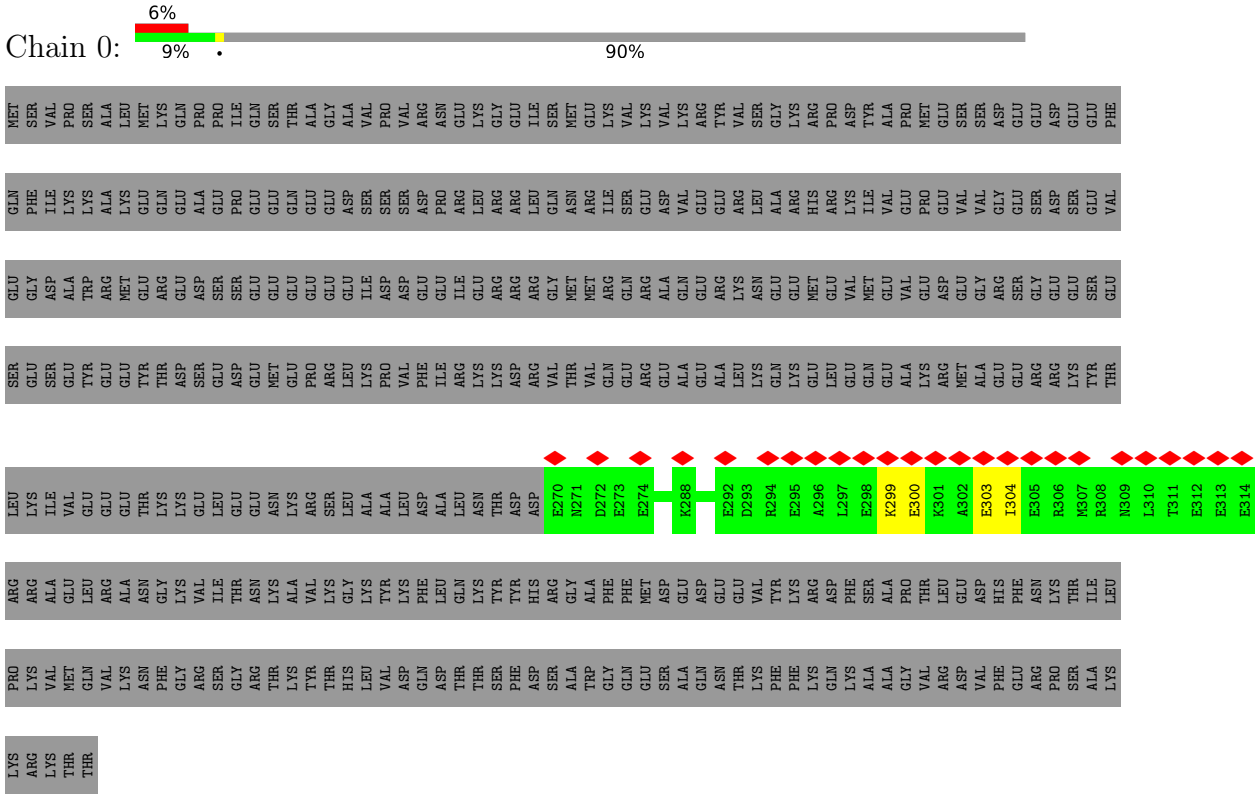
• Molecule 23: Ubiquitin-like protein 5

Chain A0:



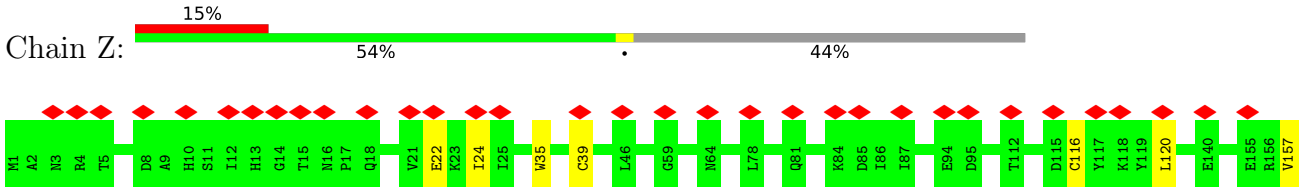
• Molecule 24: Microfibrillar-associated protein 1

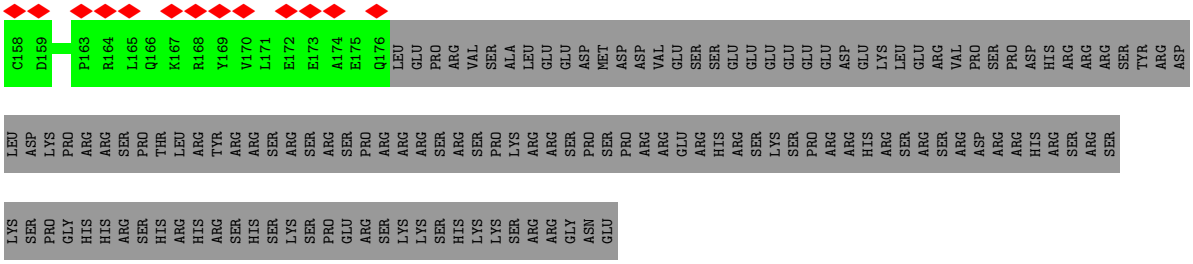
Chain 0:



• Molecule 25: Pre-mRNA-splicing factor 38A

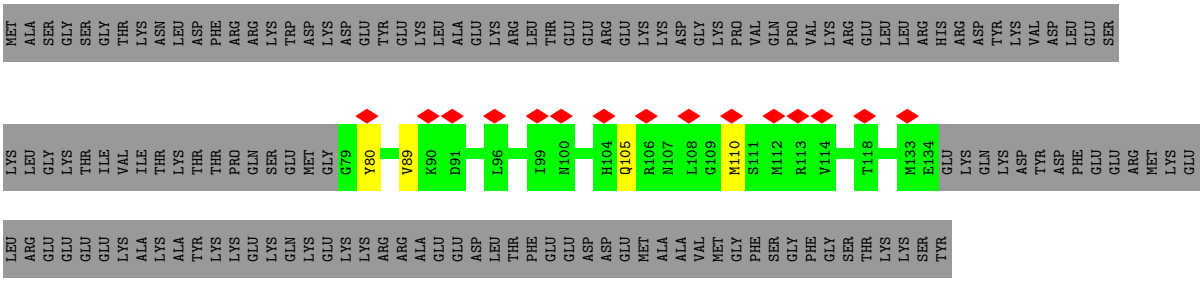
Chain Z:





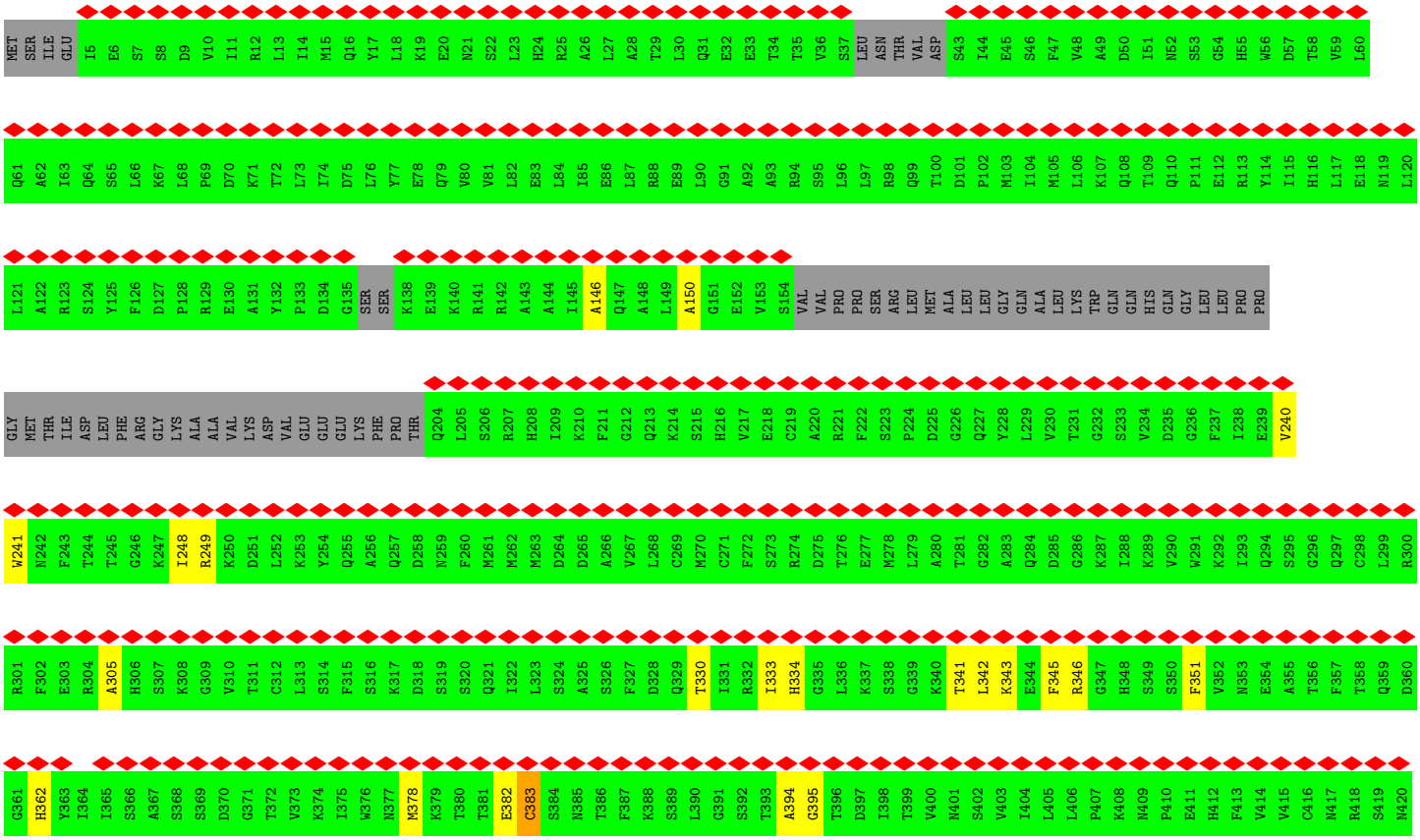
• Molecule 26: Zinc finger matrin-type protein 2

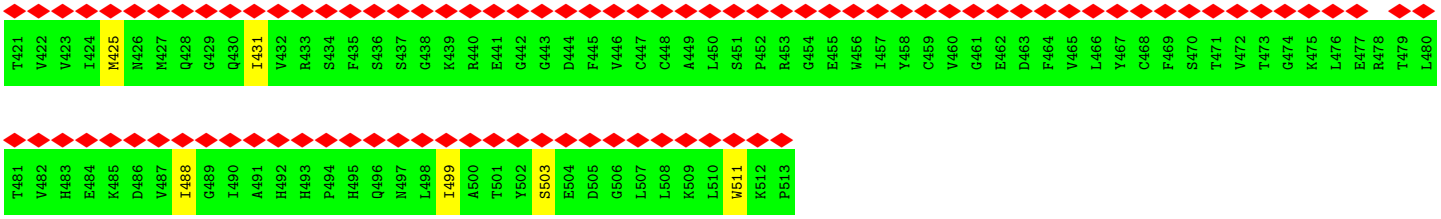
Chain 8:



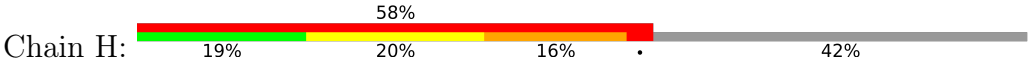
• Molecule 27: WD40 repeat-containing protein SMU1

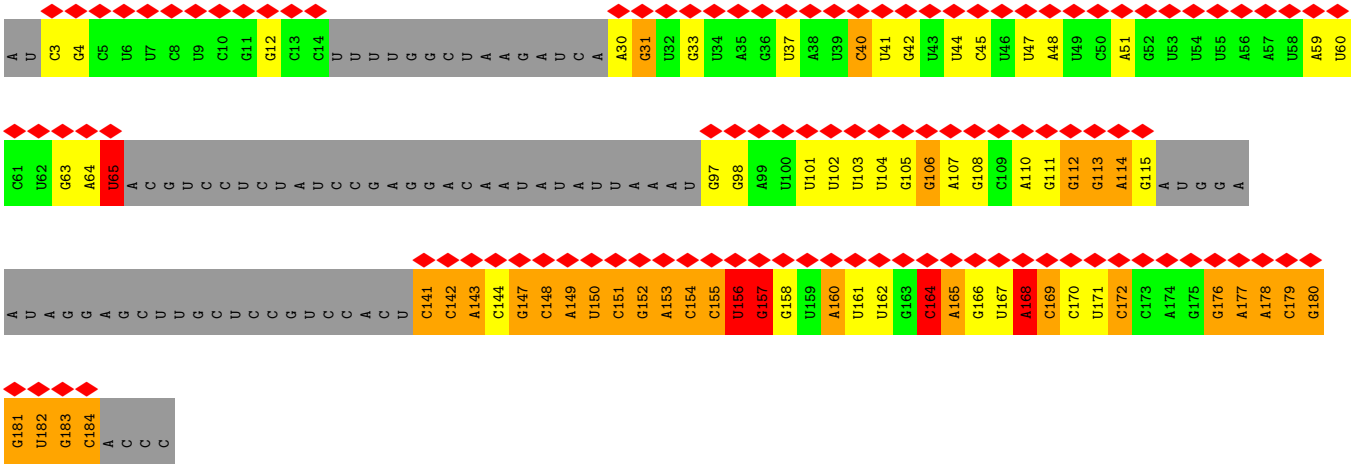
Chain Y:



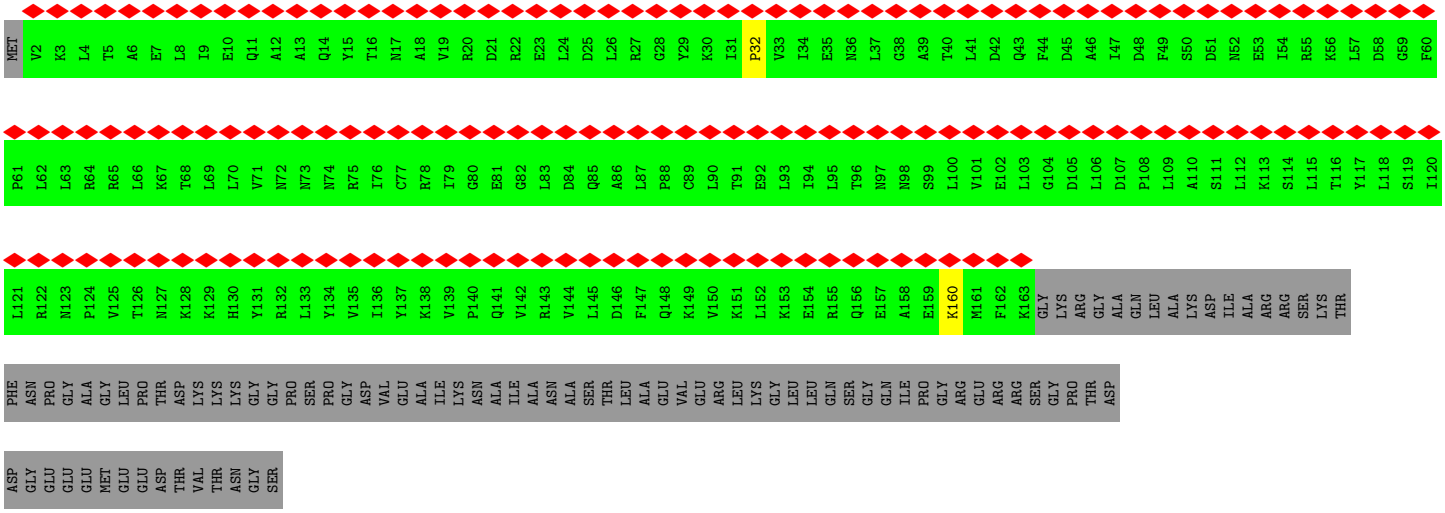


• Molecule 28: U2snRNA

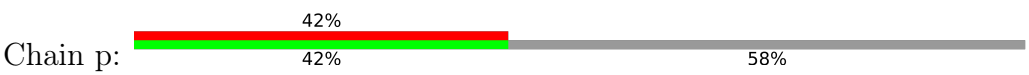


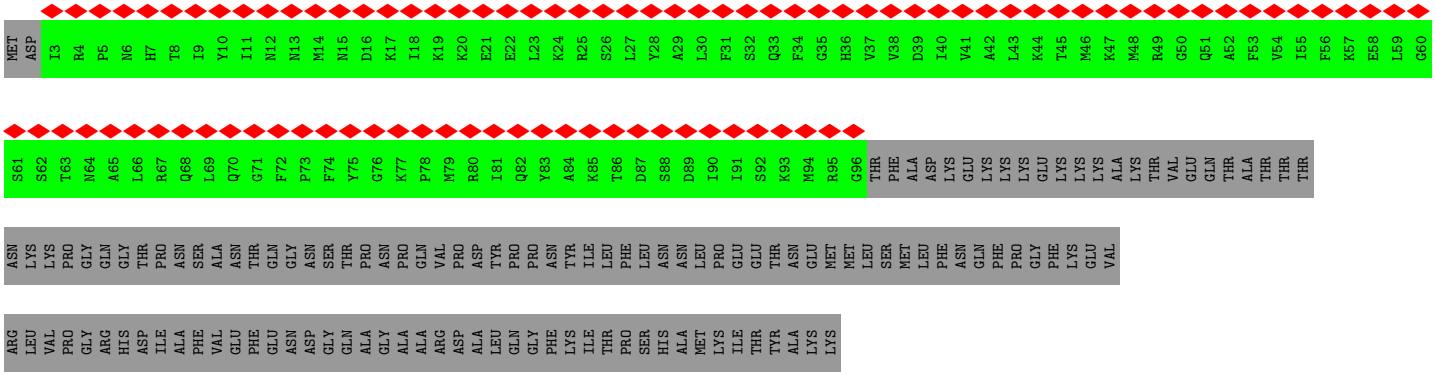


• Molecule 29: U2 small nuclear ribonucleoprotein A'



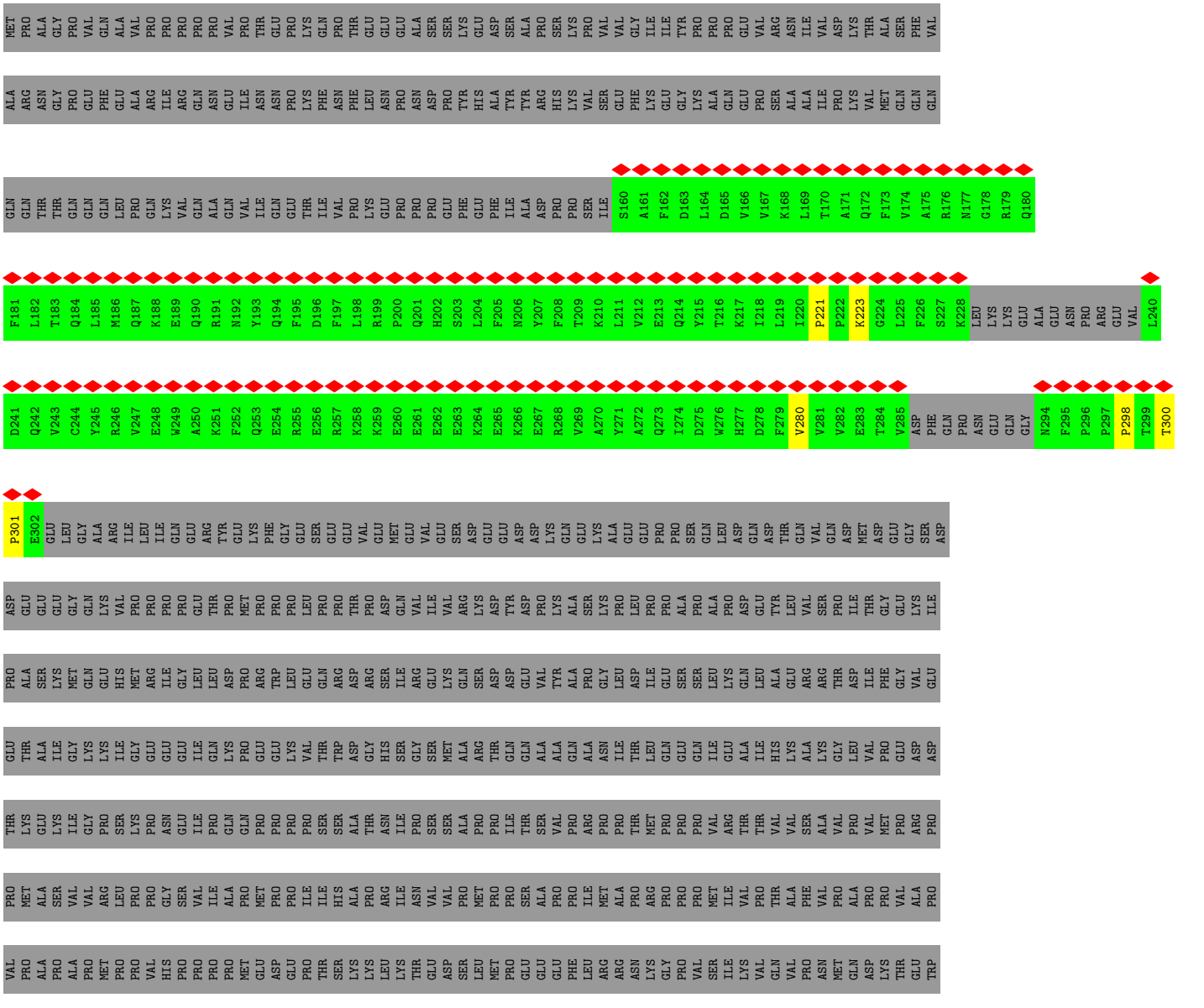
• Molecule 30: U2 small nuclear ribonucleoprotein B"

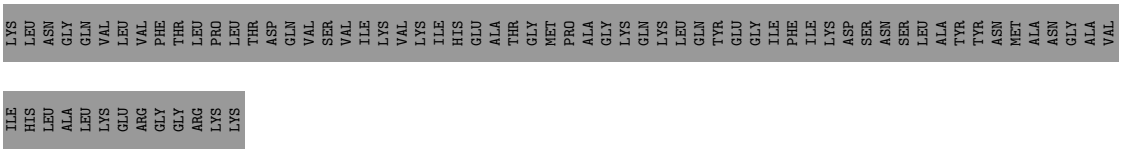




• Molecule 31: Splicing factor 3A subunit 1

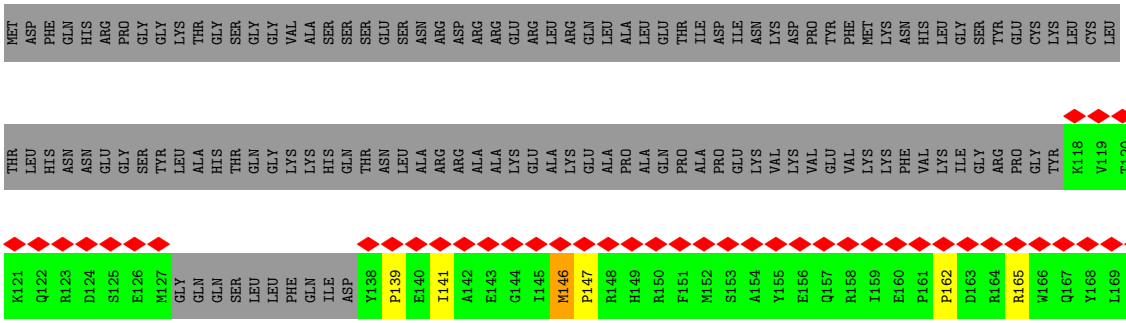
Chain u:





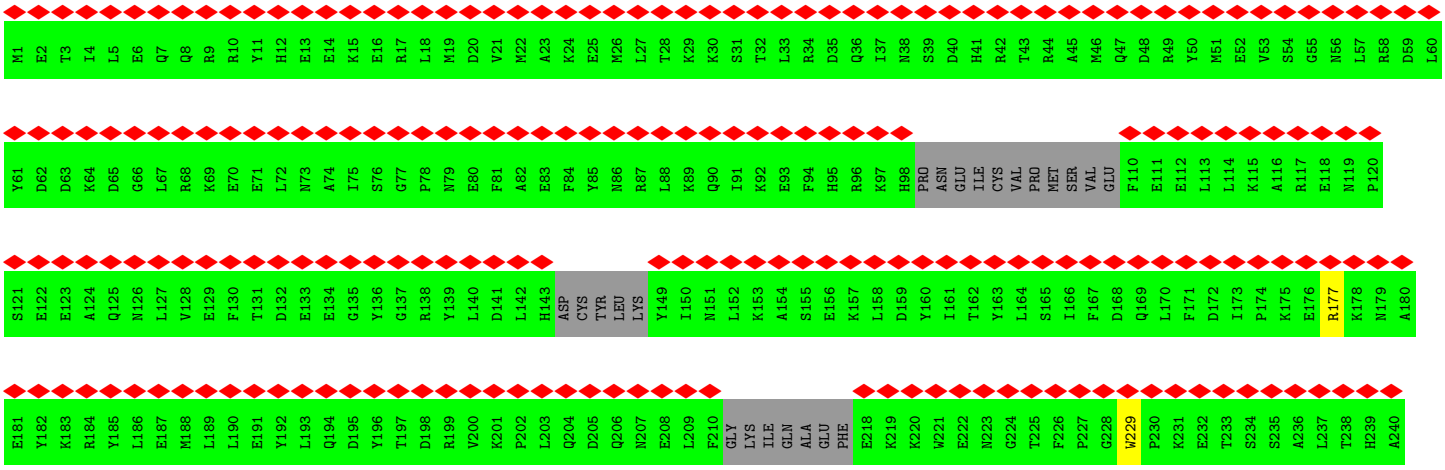
• Molecule 32: Splicing factor 3A subunit 2

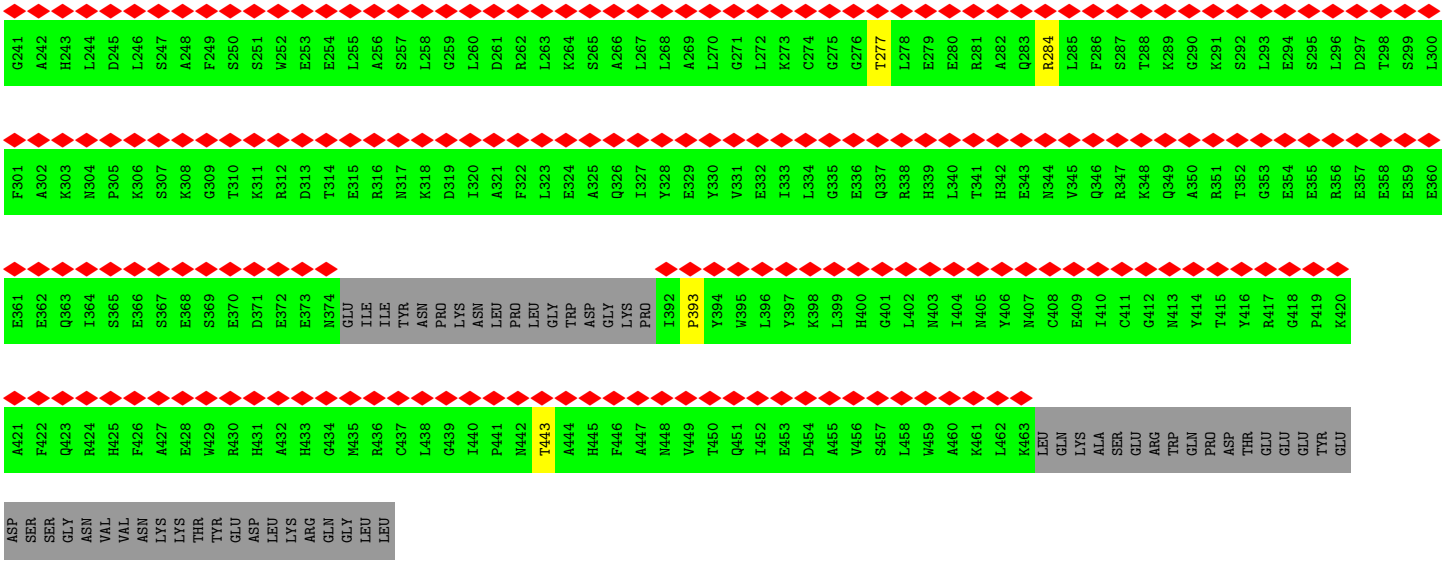
Chain v:



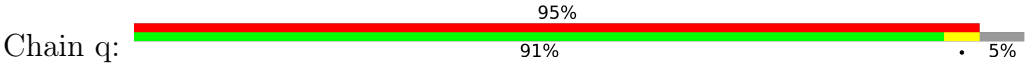
• Molecule 33: Splicing factor 3A subunit 3

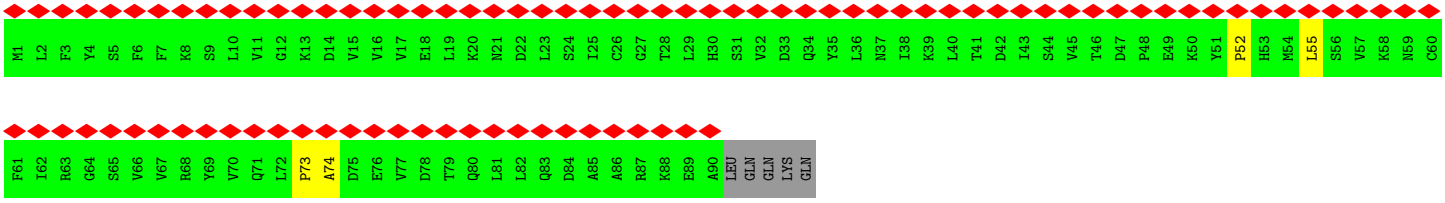
Chain w:





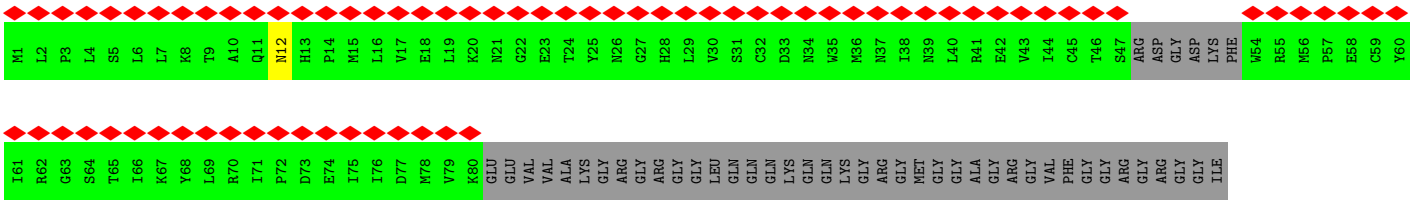
- Molecule 34: U6 snRNA-associated Sm-like protein LSm2



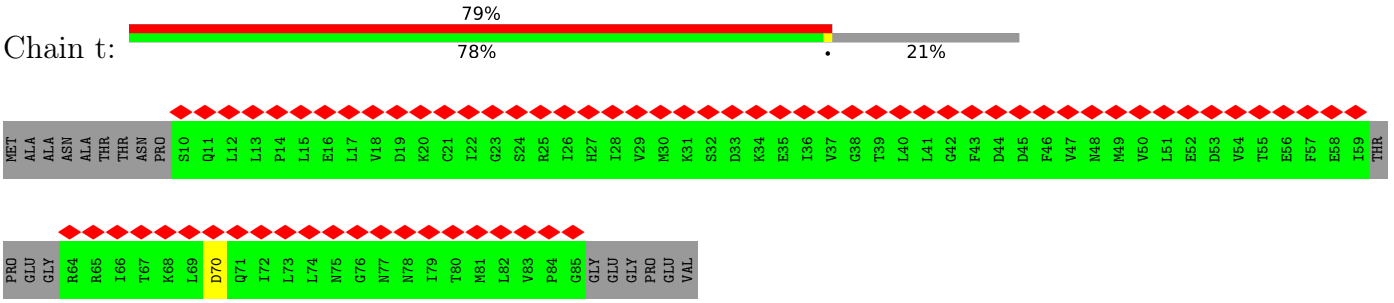


- Molecule 35: U6 snRNA-associated Sm-like protein LSm3

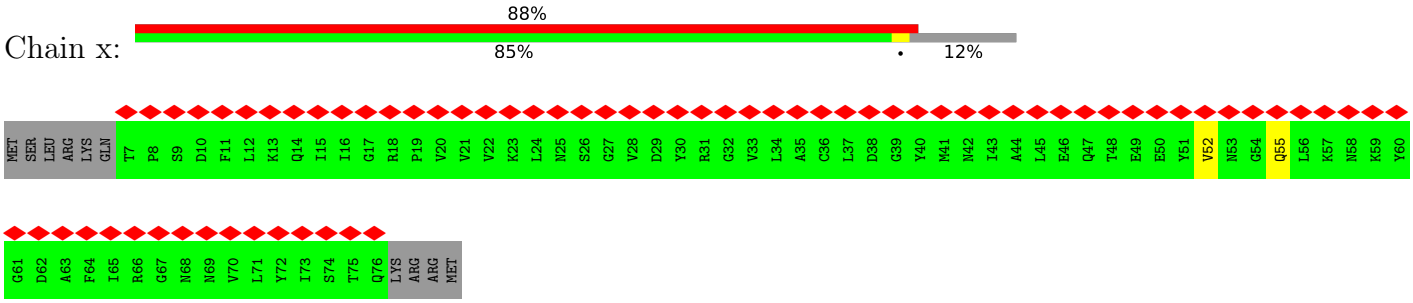
- Molecule 36: U6 snRNA-associated Sm-like protein LSm4



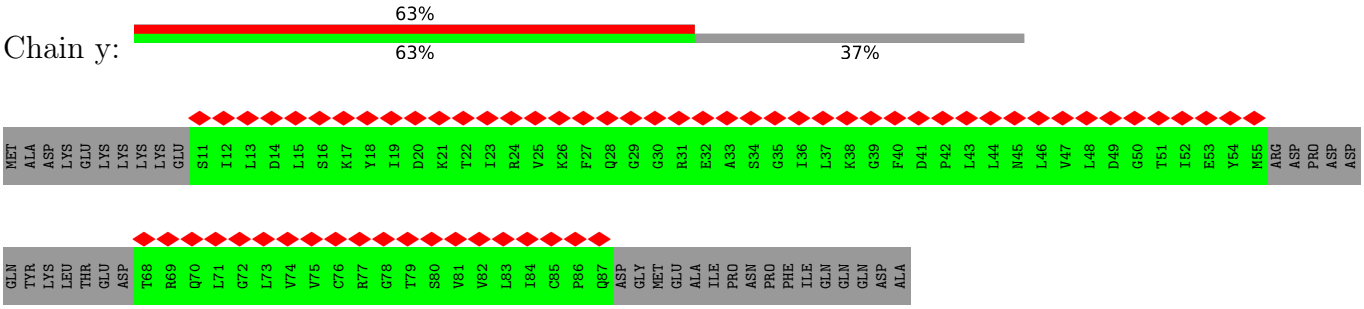
• Molecule 37: U6 snRNA-associated Sm-like protein LSm5



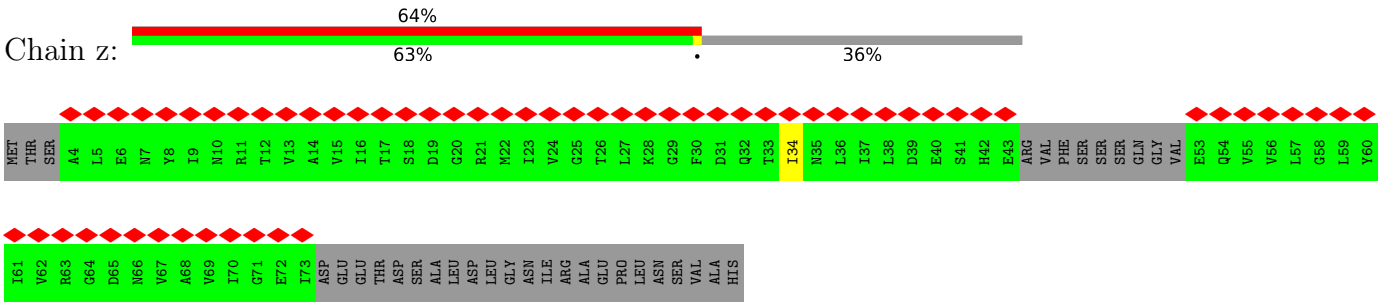
• Molecule 38: U6 snRNA-associated Sm-like protein LSm6



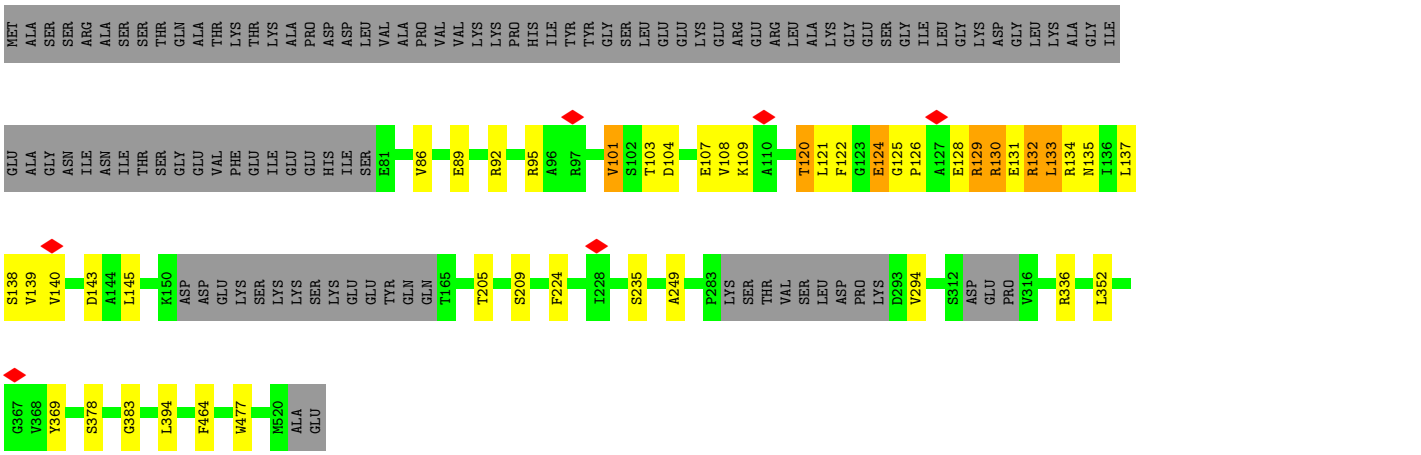
• Molecule 39: U6 snRNA-associated Sm-like protein LSm7



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

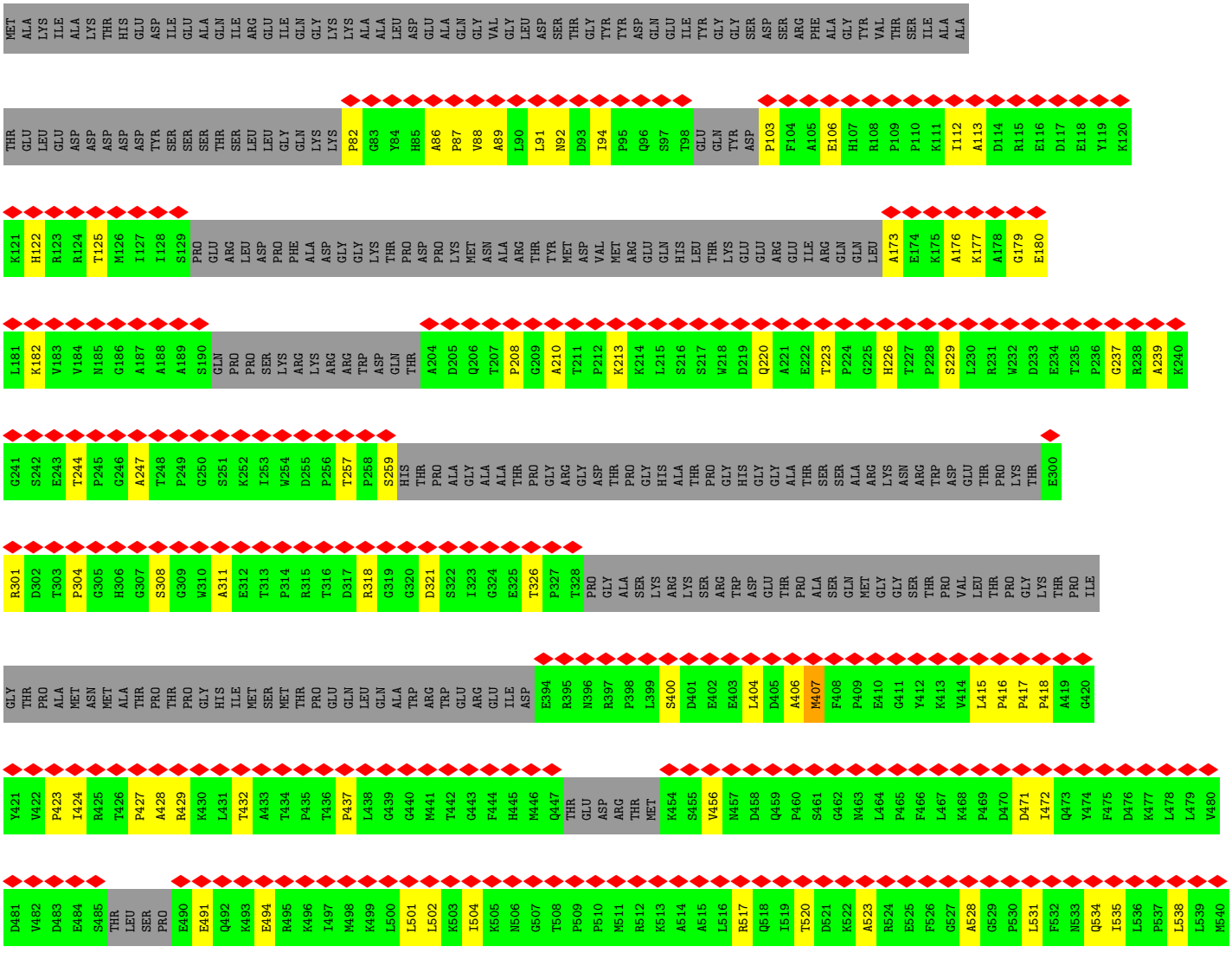


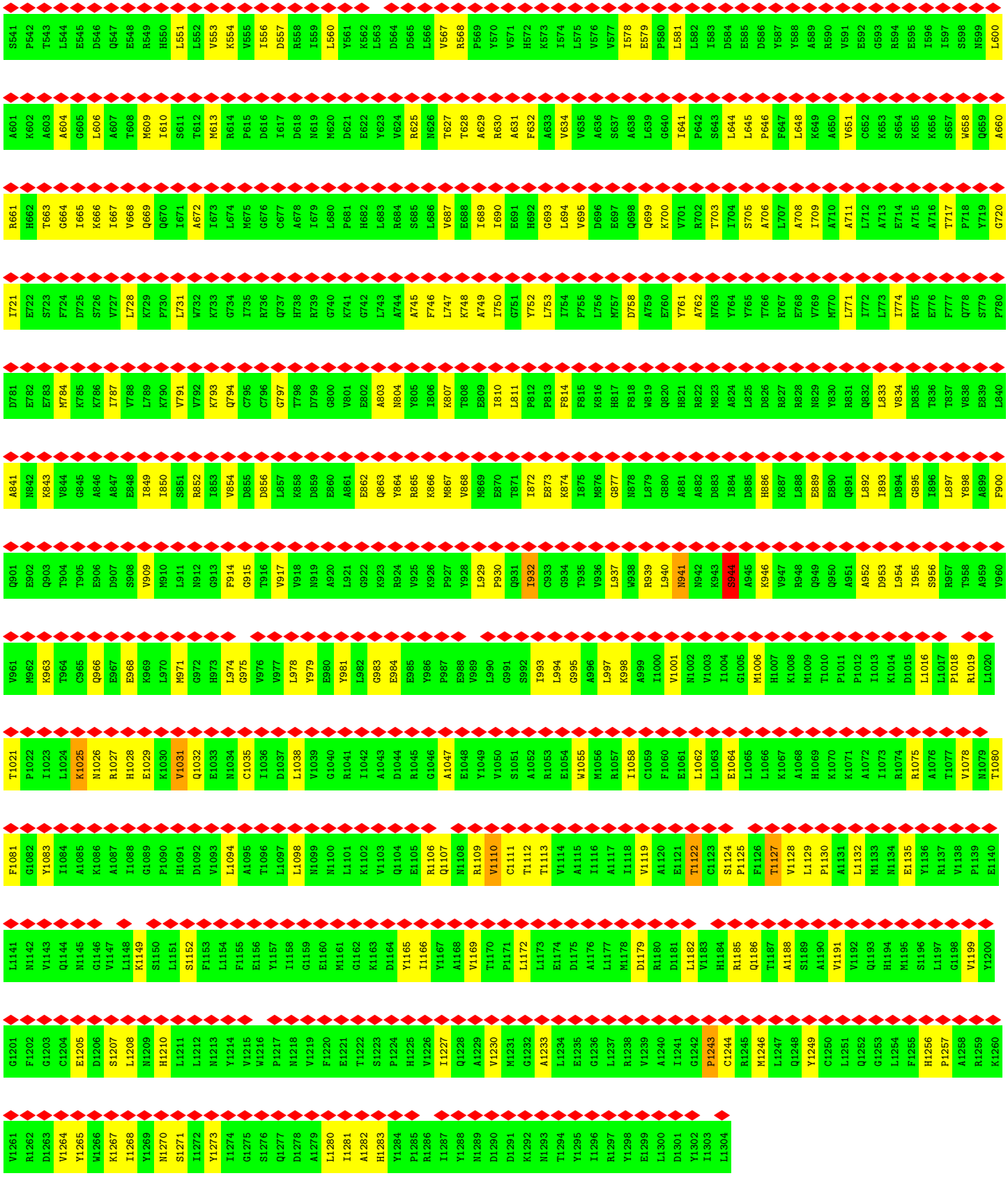
• Molecule 41: U4/U6 small nuclear ribonucleoprotein Prp4



• Molecule 42: Splicing factor 3B subunit 1

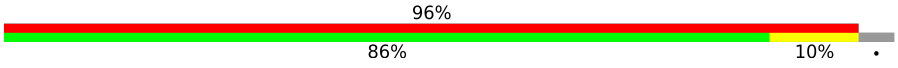
Chain 1:

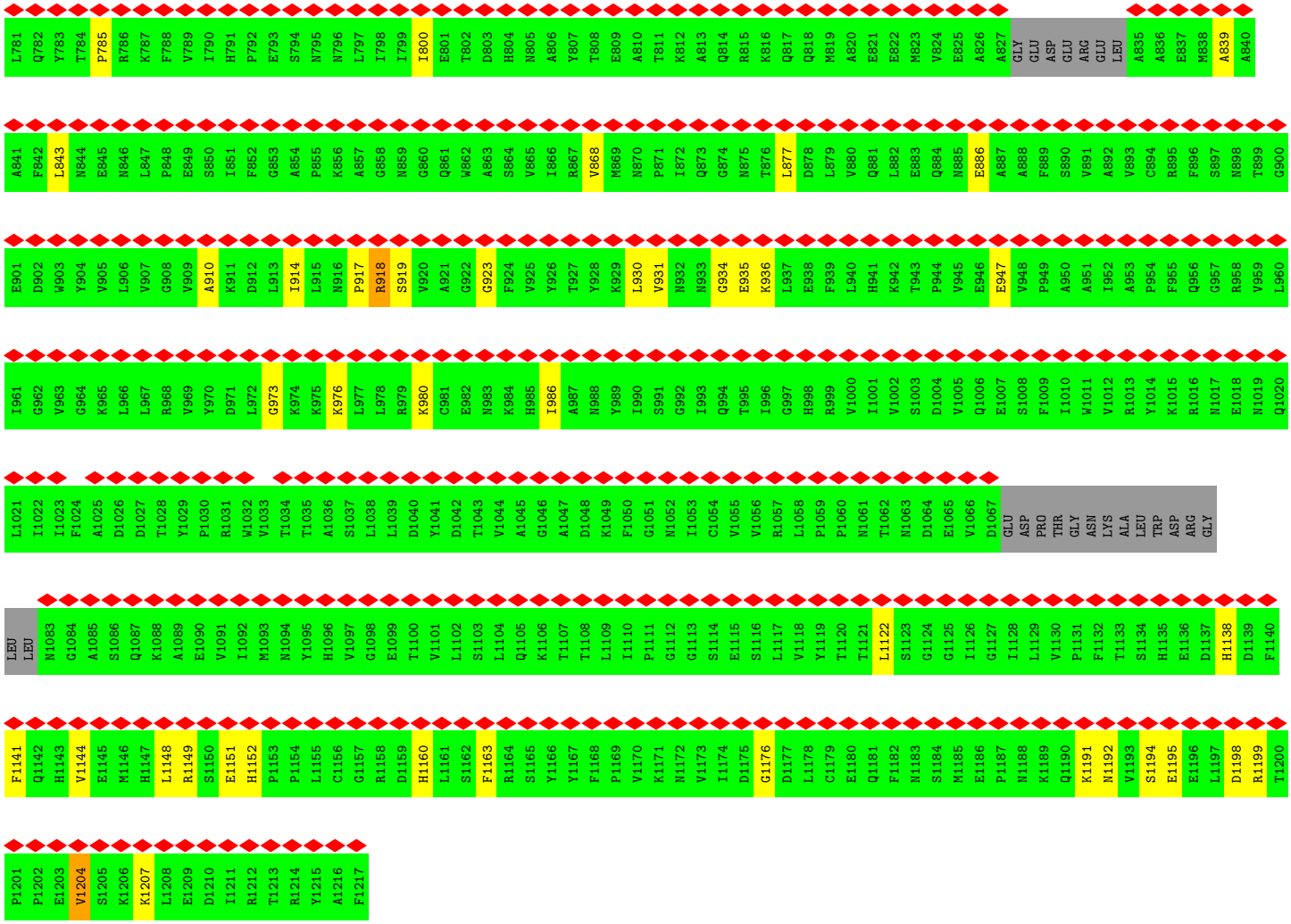




- Molecule 43: Splicing factor 3B subunit 3

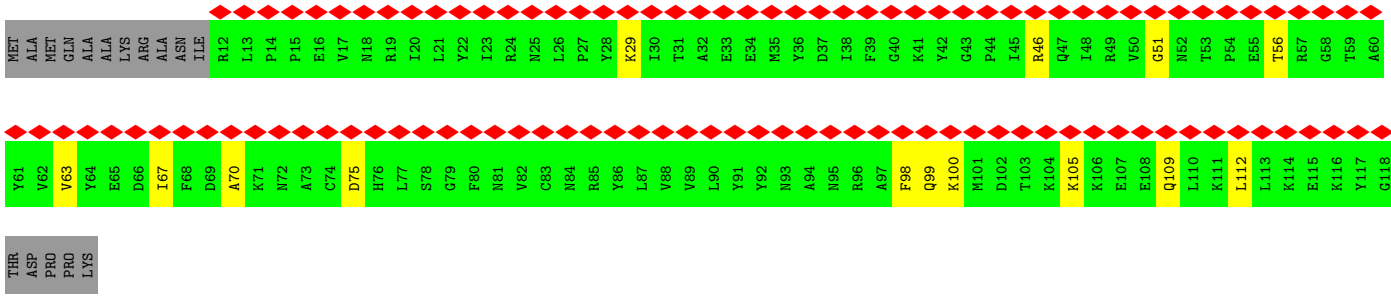
Chain 3:





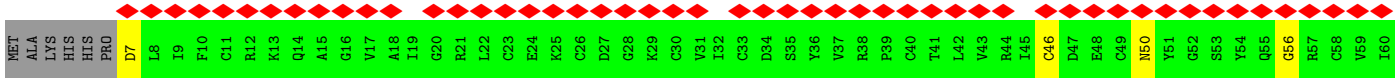
• Molecule 44: SF3b14a, Splicing factor 3B subunit 6

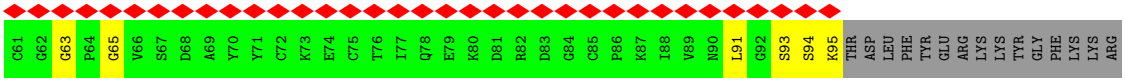
Chain 5:



• Molecule 45: PHD finger-like domain-containing protein 5A

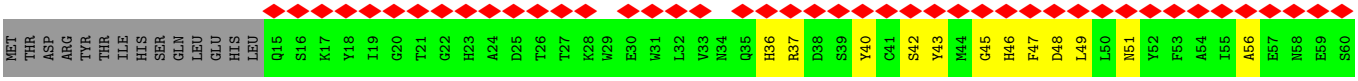
Chain 6:

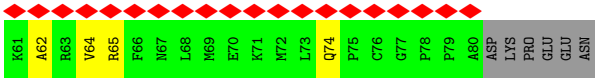




• Molecule 46: SF3b5, Splicing factor 3B subunit 5

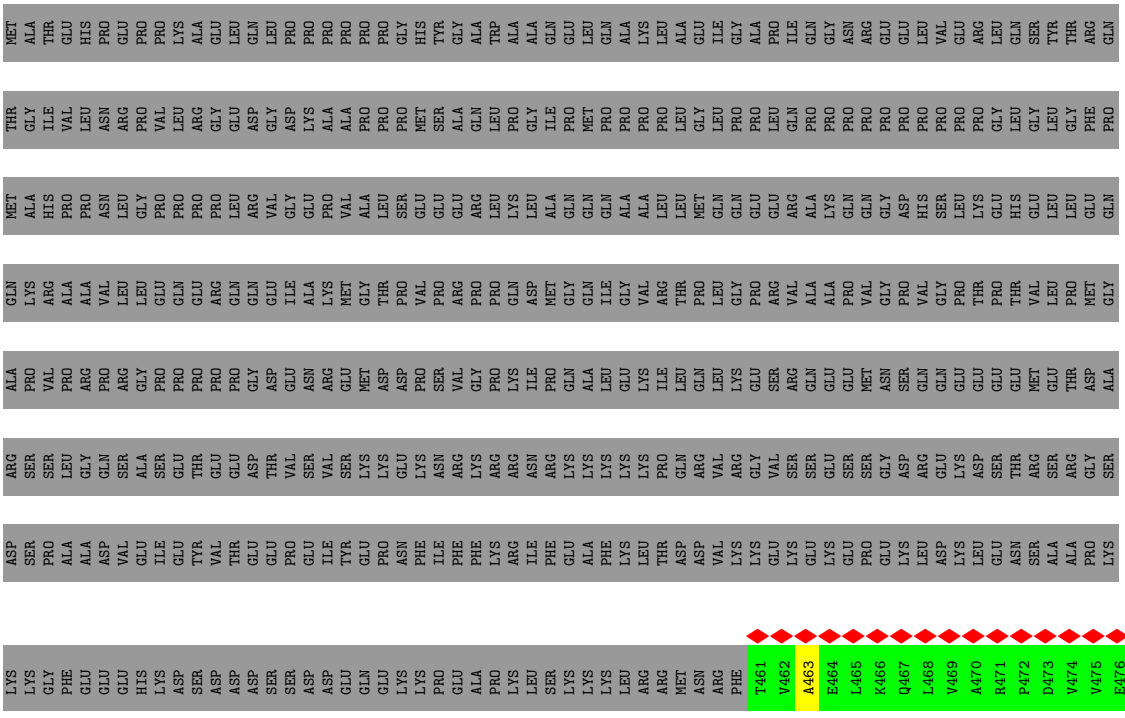
Chain 7:

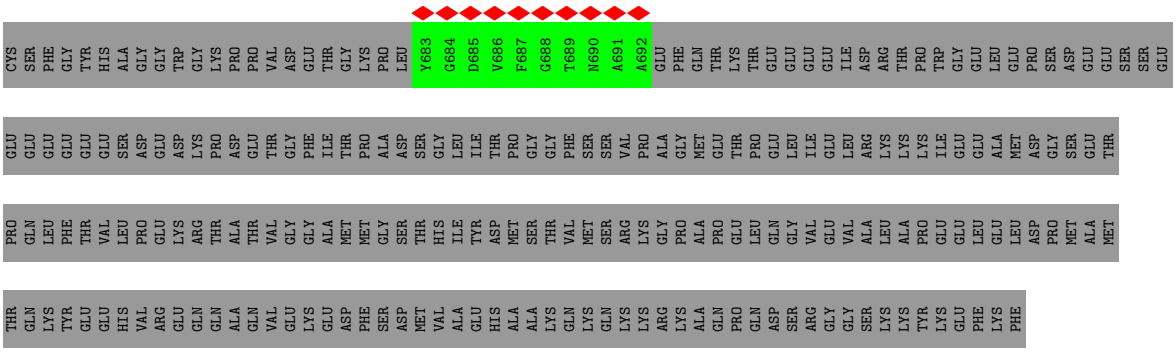




• Molecule 47: SF3b145, Splicing factor 3B subunit 2

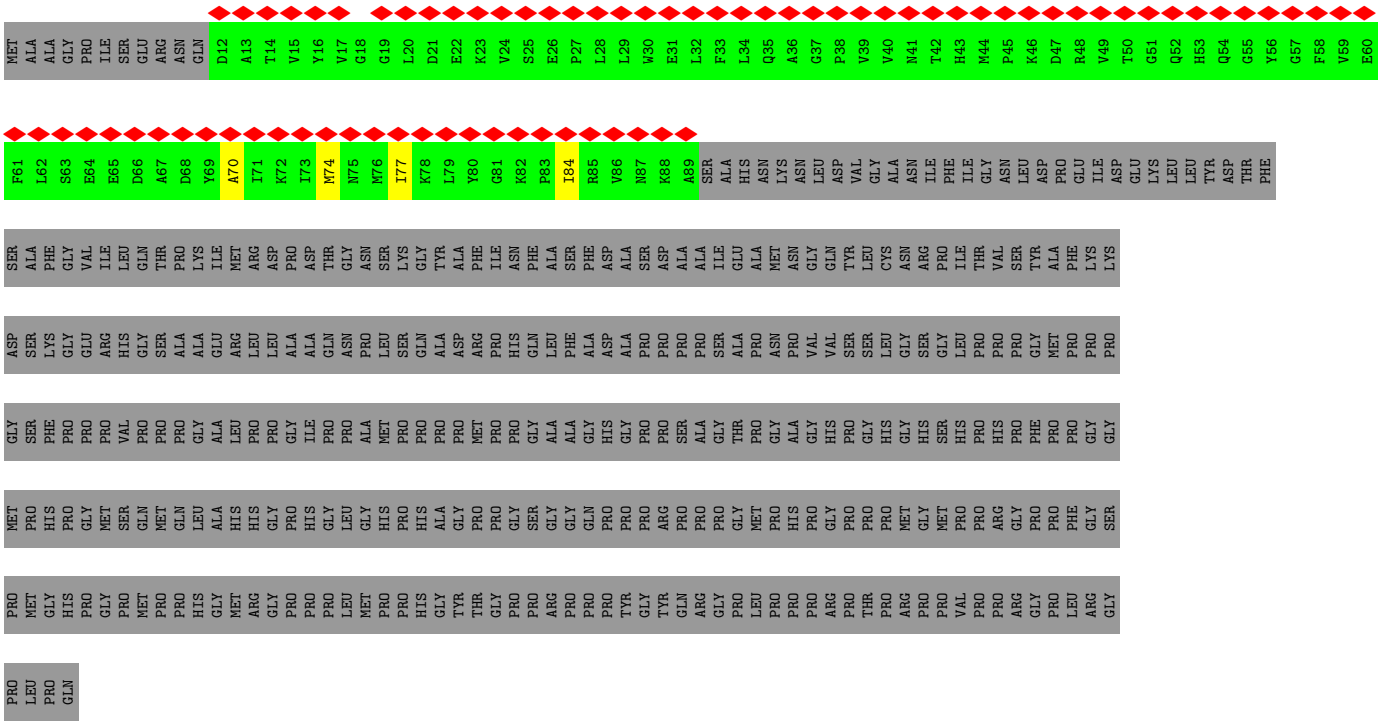
Chain 2:





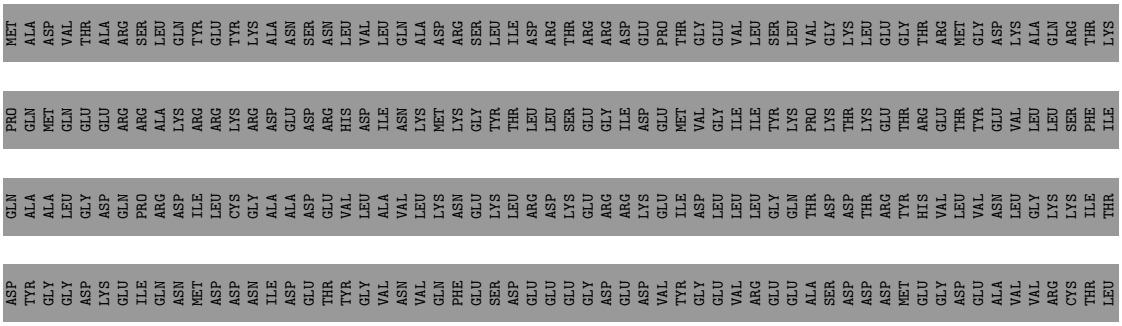
• Molecule 48: SF3b49, Splicing factor 3B subunit 4

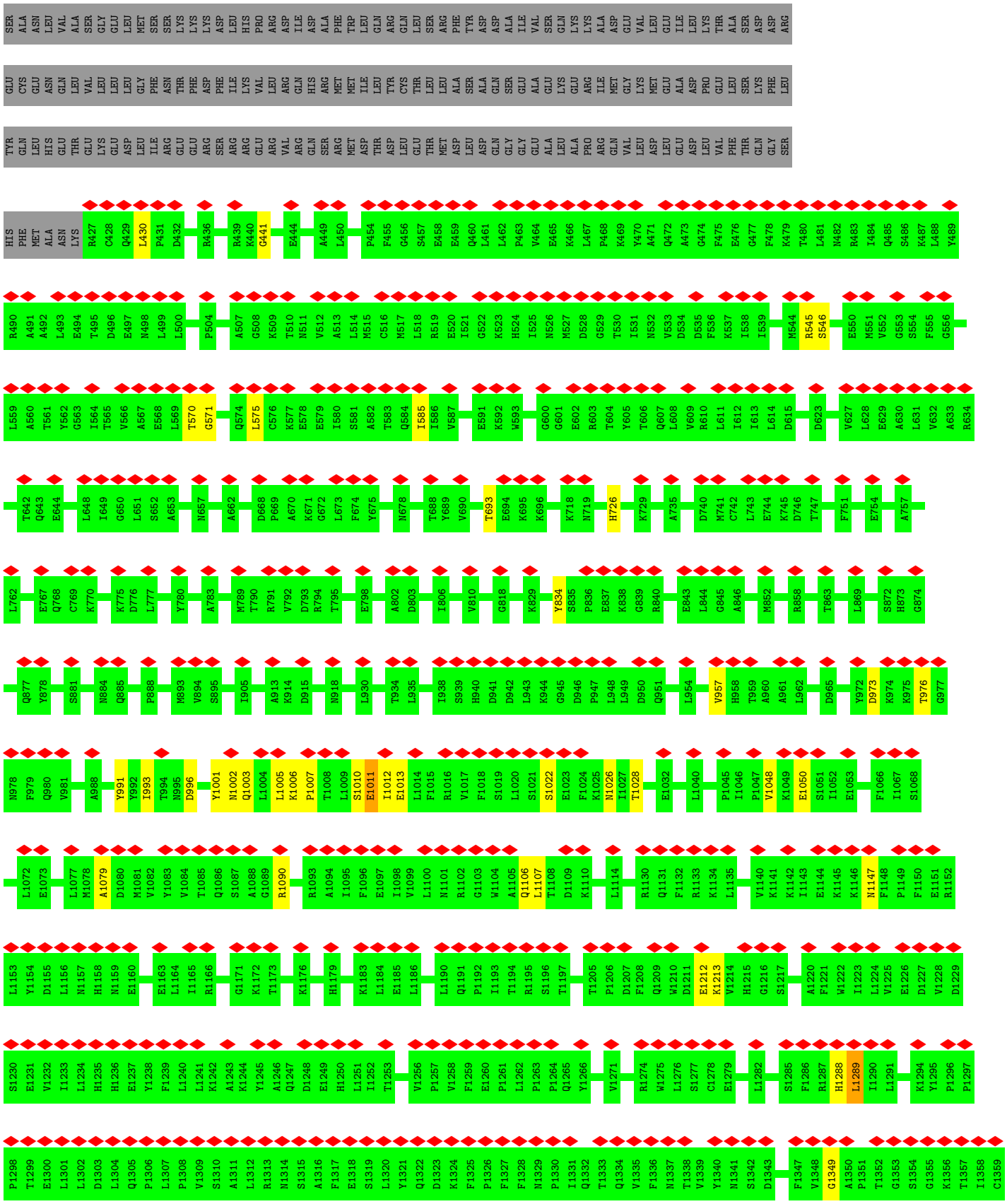
Chain 4:

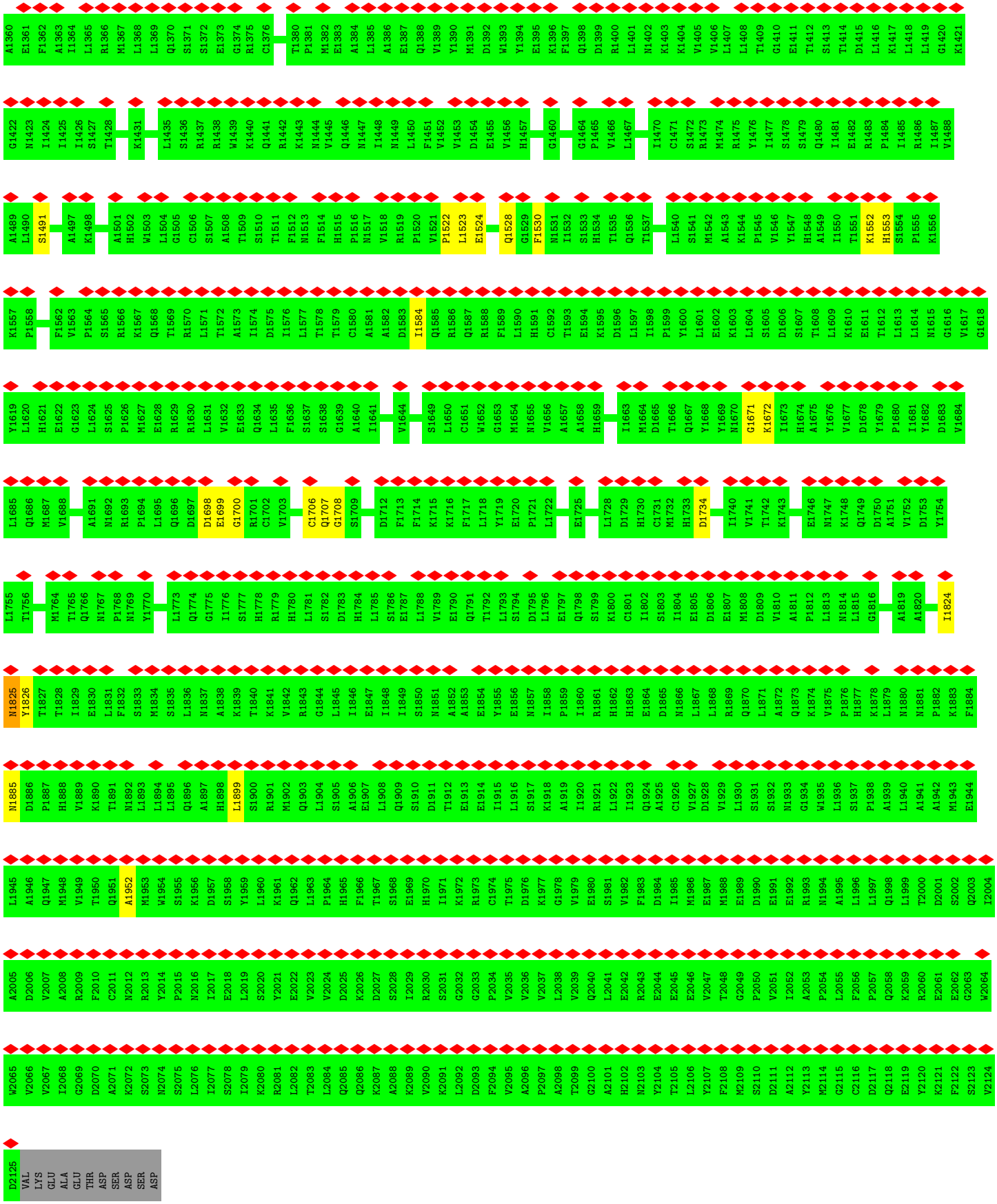


• Molecule 49: Brr2, U5 small nuclear ribonucleoprotein 200 kDa helicase

Chain D:




SER ALA ASN LEU VAL ALA SER GLY GLU LEU MET SER SER LYS LYS LYS LYS ASP LEU HIS PRO ARG ASP ASP ILE ASP ALA PHE TRP LEU GLN ARG GLN LEU GLU ILE ASP ASP ALA ILE VAL SER GLN LYS LYS ALA ASP GLU VAL LEU LEU GLU ILE LEU LYS THR ALA SER ASP ASP ARG
GLU CYS GLU ASN GLN LEU VAL LEU LEU LEU GLY PHE ASN THR PHE ASP PHE ILE LYS VAL LEU ARG GLN HIS ARG MET MET ILE LEU TYR CYS THR LEU LEU ALA SER ALA GLN SER GLU ALA GLU LYS GLU ARG ILE MET GLY LYS MET GLU ALA ASP PRO GLU LEU SER LYS PHE LEU
TYR GLN LEU HIS GLU THR GLU LYS GLU ASP LEU ILE ARG GLU GLU ARG SER ARG ARG GLU ARG VAL ARG GLN SER ARG MET ASP THR ASP LEU GLU THR GLN VAL LEU ASP LEU ASP GLN GLY GLY GLU ALA LEU ALA PRO ARG GLN VAL LEU ASP LEU VAL PHE THR GLN GLY SER
HIS PHE MET ALA ASN LYS R427 C428 Q429 L430 P431 D432 R436 R439 K440 G441 E444 A449 L450 P454 F455 G456 S457 E458 E459 Q460 L461 L462 P463 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 P504 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 M544 R545 S546 E550 M551 V552 G553 S554 F555 G556
L559 A560 T561 Y562 G563 I564 T565 V566 A567 E568 L569 T570 G571 Q574 L575 C576 K577 E578 E579 I580 S581 A582 T583 Q584 I585 I586 V587 E591 K592 W593 G600 G601 E602 R603 T604 Y605 T606 Q607 L608 V609 R610 L611 I612 I613 L614 D615 D623 V627 L628 E629 A630 L631 V632 A633 R634
T642 Q643 E644 L648 I649 G650 L651 S652 A653 N657 A662 D668 P669 A670 K671 G672 L673 F674 Y675 N678 T688 Y689 V690 T693 E694 K695 K696 K718 N719 H726 K729 A735 D740 M741 C742 L743 E744 K745 D746 T747 F751 E754 A757
L762 E767 Q768 C769 K770 K775 D776 L777 Y780 A783 M789 T790 R791 V792 D793 R794 T795 E798 A802 D803 I806 V810 G818 K829 Y834 S835 P836 E837 K838 G839 R840 E843 L844 G845 A846 M852 R858 T863 L869 S872 H873 G874
Q877 Y878 S881 N884 Q885 P888 M893 V894 S895 I905 A913 K914 D915 N918 L930 T934 L935 I938 S939 H940 D941 D942 L943 K944 G945 D946 P947 L948 L949 D950 Q951 L954 V957 H958 T959 A960 A961 L962 D965 Y972 D973 K974 K975 T976 G977
N978 P979 Q980 V981 A988 Y991 Y992 I993 T994 N995 D996 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 E1032 L1040 P1045 I1046 P1047 V1048 K1049 E1050 S1051 I1052 E1053 F1066 I1067 S1068
L1072 E1073 L1077 M1078 A1079 D1080 M1081 V1082 Y1083 V1084 T1085 Q1086 S1087 A1088 G1089 R1090 R1093 A1094 I1095 F1096 E1097 I1098 V1099 L1100 N1101 R1102 G1103 W1104 A1105 Q1106 L1107 T1108 D1109 K1110 L1114 R1130 Q1131 F1132 R1133 K1134 L1135 V1140 K1141 K1142 I1143 E1144 K1145 K1146 F1148 P1149 F1150 E1151 R1152
L1153 Y1154 D1155 L1156 N1157 H1158 N1159 E1160 E1163 L1164 I1165 R1166 G1171 K1172 T1173 K1176 H1179 K1183 L1184 E1185 L1186 L1190 Q1191 P1192 I1193 T1194 R1195 S1196 T1197 T1205 P1206 D1207 F1208 Q1209 W1210 D1211 E1212 K1213 V1214 H1215 G1216 S1217 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 V1256 P1257 V1258 F1259 E1260 P1261 L1262 P1263 P1264 Q1265 Y1266 V1271 R1274 W1275 L1276 S1277 C1278 E1279 L1282 S1285 F1286 R1287 H1288 L1289 I1290 L1291 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 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
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
K1431
L1435 S1436 R1437 R1438 W1439 K1440 Q1441 R1442 K1443 N1444 V1445 Q1446 N1447 I1448 N1449 L1450 F1451 V1452 V1453 D1454 E1455 V1456 H1457
G1460
G1464 P1465 V1466 L1467
I1470 C1471 S1472 R1473 M1474 R1475 Y1476 I1477 S1478 S1479 Q1480 I1481 E1482 R1483 P1484 I1485 R1486 I1487 V1488
A1489 L1490 S1491
A1497 K1498
A1501 H1502 W1503 L1504 G1505 C1506 S1507 A1508 T1509 S1510 T1511 F1512 N1513 F1514 H1515 P1516 N1517 V1518 R1519 P1520 V1521
P1522 L1523 E1524
Q1528 G1529 F1530
N1531 I1532 S1533 H1534 T1535 Q1536 T1537
L1540 S1541 M1542 A1543 K1544 P1545 V1546 Y1547 H1548 A1549 I1550 T1551
K1552 H1553 S1554 P1555 K1556
K1557 P1558
F1562 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 T1608 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
V1644
S1649 L1650 C1651 W1652 G1653 M1654 N1655 V1656 A1657 A1658 H1659
T1663 M1664 D1665 T1666 Q1667 Y1668 Y1669 N1670
G1671 K1672
I1673 H1674 A1675 Y1676 V1677 D1678 Y1679 P1680 I1681 Y1682 D1683 V1684
L1685 Q1686 M1687 V1688
A1691 N1692 R1693 P1694 L1695 Q1696 D1697
D1698 E1699 G1700 R1701 C1702 V1703
C1706 Q1707 G1708
S1709
D1712 F1713 F1714 K1715 K1716 F1717 L1718 Y1719 E1720 P1721 L1722
E1725
L1728 D1729 H1730 C1731 M1732 H1733
D1734
I1740 V1741 T1742 K1743
E1746 N1747 K1748 Q1749 D1750 A1751 V1752 D1753 Y1754
L1755 T1756
M1764 T1765 Q1766 N1767 P1768 N1769 Y1770
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
A1819 A1820
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 G1934 K1874 V1875 P1876 H1877 K1878 L1879 N1880 N1881 P1882 K1883 F1884
N1885 D1886 P1887 H1888 M1889 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 P2010 C2011 N2012 R2013 Y2014 P2015 N2016 I2017 E2018 L2019 S2020 Y2021 E2022 V2023 V2024 D2025 K2026 D2027 S2028 I2029 R2030 S2031 G2032 G2033 P2034 V2035 V2036 V2037 L2038 V2039 Q2040 L2041 E2042 R2043 E2044 E2045 E2046 V2047 T2048 G2049 P2050 V2051 I2052 A2053 P2054 L2055 F2056 P2057 Q2058 K2059 R2060 E2061 E2062 G2063 W2064
W2065 V2066 V2067 I2068 G2069 D2070 A2071 K2072 S2073 N2074 S2075 L2076 I2077 S2078 I2079 K2080 R2081 L2082 T2083 L2084 Q2085 Q2086 K2087 A2088 K2089 V2090 K2091 L2092 D2093 P2094 V2095 A2096 P2097 A2098 T2099 G2100 A2101 H2102 N2103 Y2104 T2105 L2106 Y2107 F2108 M2109 S2110 D2111 A2112 Y2113 M2114 G2115 C2116 D2117 Q2118 E2119 Y2120 K2121 F2122 S2123 V2124
D2125
VAL LYS GLU ALA GLU THR ASP SER ASP SER ASP

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	137853	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	45	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.251	Depositor
Minimum map value	-0.129	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	535.2, 535.2, 535.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.338, 1.338, 1.338	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, GTP, 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	A	0.47	0/17735	0.64	10/23951 (0.0%)
2	I	0.52	0/3214	0.97	7/4998 (0.1%)
3	B	0.47	0/2698	1.05	25/4195 (0.6%)
4	F	0.50	1/2230 (0.0%)	1.02	9/3468 (0.3%)
5	G	0.65	6/1793 (0.3%)	0.93	2/2783 (0.1%)
6	O	0.50	0/1180	0.65	1/1594 (0.1%)
7	C	0.38	0/6584	0.63	1/8942 (0.0%)
8	N	0.44	0/4568	0.60	2/6320 (0.0%)
9	M	0.36	0/974	0.60	0/1316
10	L	0.36	0/2912	0.60	0/3924
11	9	0.77	0/1091	0.91	3/1478 (0.2%)
12	J	0.50	0/1278	0.61	0/1657
13	U	0.22	0/254	0.48	0/314
13	a	0.50	0/343	0.69	0/427
13	i	0.50	0/343	0.69	0/427
14	V	0.22	0/333	0.47	0/416
14	b	0.57	0/327	0.67	0/407
14	j	0.56	0/327	0.68	0/407
15	P	0.23	0/298	0.48	0/370
15	c	0.69	0/387	0.72	0/482
15	k	0.70	0/338	0.73	0/419
16	Q	0.24	0/291	0.49	0/363
16	d	0.77	0/295	0.76	0/367
16	l	0.78	0/295	0.76	0/367
17	R	0.22	0/313	0.49	0/390
17	e	0.65	0/315	0.75	0/392
17	m	0.64	0/315	0.75	0/392
18	S	0.24	0/297	0.51	0/371
18	f	0.54	0/295	0.61	0/367
18	n	0.55	0/270	0.63	0/334
19	T	0.23	0/287	0.49	0/358
19	g	0.47	0/322	0.55	0/399

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
19	h	0.47	0/318	0.56	0/394
20	E	0.67	0/1195	0.71	0/1492
21	X	0.24	0/379	0.35	0/530
22	W	0.25	0/853	0.47	0/1188
23	A0	0.38	0/591	0.84	2/799 (0.3%)
24	0	0.22	0/224	0.29	0/312
25	Z	0.23	0/888	0.40	0/1241
26	8	0.22	0/276	0.43	0/383
27	Y	0.24	0/2265	0.45	0/3156
28	H	0.85	11/2576 (0.4%)	1.43	55/4003 (1.4%)
29	o	0.63	0/647	1.42	0/807
30	p	0.61	0/375	1.20	0/467
31	u	0.22	0/493	0.42	0/611
32	v	0.21	0/373	0.58	1/461 (0.2%)
33	w	0.25	0/1688	0.47	0/2102
34	q	0.42	0/359	0.67	0/447
35	r	0.47	0/294	0.75	0/364
36	s	0.34	0/294	0.61	0/364
37	t	0.43	0/286	0.59	0/354
38	x	0.43	0/279	0.72	0/347
39	y	0.38	0/258	0.61	0/319
40	z	0.41	0/242	0.64	0/299
41	K	0.27	0/1818	0.63	0/2308
42	1	1.04	4/4184 (0.1%)	0.83	2/5216 (0.0%)
43	3	0.85	0/4664	0.76	0/5816
44	5	0.79	0/431	0.79	0/537
45	6	0.73	0/355	0.68	0/442
46	7	1.01	0/263	0.77	0/327
47	2	0.74	0/722	0.72	0/892
48	4	0.62	0/311	0.64	0/387
49	D	0.30	0/6795	0.58	0/8492
All	All	0.54	22/87198 (0.0%)	0.75	120/117252 (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
1	A	0	12
7	C	0	6
8	N	0	8

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Mol	Chain	#Chirality outliers	#Planarity outliers
15	c	0	1
15	k	0	1
23	A0	0	2
33	w	0	1
42	1	0	11
43	3	0	11
44	5	0	1
46	7	0	1
47	2	0	3
49	D	0	1
All	All	0	59

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	1	407	MET	N-CA	12.36	1.71	1.46
42	1	406	ALA	C-N	7.99	1.52	1.34
28	H	142	C	C1'-N1	7.29	1.59	1.48
42	1	1243	PRO	N-CA	-7.11	1.35	1.47
28	H	182	U	C1'-N1	6.93	1.59	1.48

The worst 5 of 120 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	H	167	U	C5-C4-O4	11.72	132.93	125.90
23	A0	8	ASP	CB-CG-OD1	10.83	128.05	118.30
42	1	406	ALA	C-N-CA	10.26	147.36	121.70
28	H	164	C	N1-C2-O2	-10.13	112.82	118.90
8	N	277	LEU	CA-CB-CG	9.42	136.96	115.30

There are no chirality outliers.

5 of 59 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	108	MET	Peptide
1	A	211	GLN	Peptide
1	A	408	PRO	Peptide
1	A	463	PRO	Peptide
1	A	802	THR	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	17290	0	16495	383	0
2	I	2881	0	1461	123	0
3	B	2420	0	1226	94	0
4	F	1995	0	1006	61	0
5	G	1612	0	821	192	0
6	O	1152	0	1123	21	0
7	C	6440	0	6465	127	0
8	N	4518	0	3121	96	0
9	M	962	0	1012	12	0
10	L	2874	0	2856	46	0
11	9	1087	0	921	252	0
12	J	1273	0	903	32	0
13	U	256	0	70	2	0
13	a	344	0	93	0	0
13	i	344	0	93	0	0
14	V	334	0	92	1	0
14	b	328	0	89	0	0
14	j	328	0	89	0	0
15	P	300	0	80	4	0
15	c	388	0	102	0	0
15	k	340	0	87	0	0
16	Q	292	0	93	6	0
16	d	296	0	87	0	0
16	l	296	0	87	0	0
17	R	314	0	86	3	0
17	e	316	0	85	0	0
17	m	316	0	85	0	0
18	S	298	0	89	5	0
18	f	296	0	84	0	0
18	n	272	0	75	0	0
19	T	288	0	84	1	0
19	g	324	0	89	0	0
19	h	320	0	88	0	0
20	E	1196	0	337	2	0
21	X	378	0	190	1	0
22	W	844	0	426	16	0
23	A0	581	0	567	45	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	0	225	0	98	2	0
25	Z	883	0	414	6	0
26	8	277	0	114	2	0
27	Y	2258	0	1064	38	0
28	H	2311	0	1170	141	0
29	o	648	0	167	0	0
30	p	376	0	102	0	0
31	u	496	0	118	0	0
32	v	376	0	85	0	0
33	w	1693	0	454	0	0
34	q	360	0	95	0	0
35	r	296	0	76	0	0
36	s	296	0	77	0	0
37	t	288	0	78	0	0
38	x	280	0	81	0	0
39	y	260	0	75	0	0
40	z	244	0	71	0	0
41	K	1821	0	759	50	0
42	1	4192	0	1110	173	0
43	3	4672	0	1260	62	0
44	5	432	0	114	6	0
45	6	356	0	105	7	0
46	7	264	0	70	8	0
47	2	728	0	183	8	0
48	4	312	0	87	3	0
49	D	6796	0	1778	106	0
50	A	36	0	6	9	0
51	C	32	0	12	0	0
52	C	1	0	0	0	0
All	All	85302	0	50580	1753	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

The worst 5 of 1753 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1790:ILE:HD13	11:9:266:PHE:CE2	1.27	1.66
11:9:352:GLU:HG3	11:9:357:ALA:CB	1.28	1.59
1:A:1790:ILE:HD13	11:9:266:PHE:CD2	1.40	1.54
42:1:407:MET:N	42:1:407:MET:CA	1.71	1.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1790:ILE:CD1	11:9:266:PHE:CE2	1.92	1.46

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	2203/2335 (94%)	2043 (93%)	150 (7%)	10 (0%)	29	66
6	O	139/142 (98%)	125 (90%)	13 (9%)	1 (1%)	22	60
7	C	814/972 (84%)	756 (93%)	54 (7%)	4 (0%)	29	66
8	N	773/941 (82%)	685 (89%)	78 (10%)	10 (1%)	12	48
9	M	122/128 (95%)	118 (97%)	4 (3%)	0	100	100
10	L	372/499 (74%)	351 (94%)	21 (6%)	0	100	100
11	9	155/800 (19%)	141 (91%)	13 (8%)	1 (1%)	25	62
12	J	221/683 (32%)	207 (94%)	12 (5%)	2 (1%)	17	54
13	U	60/231 (26%)	57 (95%)	3 (5%)	0	100	100
13	a	84/231 (36%)	82 (98%)	2 (2%)	0	100	100
13	i	84/231 (36%)	82 (98%)	2 (2%)	0	100	100
14	V	80/119 (67%)	76 (95%)	4 (5%)	0	100	100
14	b	80/119 (67%)	77 (96%)	3 (4%)	0	100	100
14	j	80/119 (67%)	77 (96%)	3 (4%)	0	100	100
15	P	70/118 (59%)	68 (97%)	2 (3%)	0	100	100
15	c	95/118 (80%)	91 (96%)	4 (4%)	0	100	100
15	k	81/118 (69%)	78 (96%)	3 (4%)	0	100	100
16	Q	69/86 (80%)	67 (97%)	2 (3%)	0	100	100
16	d	72/86 (84%)	69 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	l	72/86 (84%)	68 (94%)	4 (6%)	0	100	100
17	R	76/92 (83%)	70 (92%)	6 (8%)	0	100	100
17	e	77/92 (84%)	76 (99%)	1 (1%)	0	100	100
17	m	77/92 (84%)	76 (99%)	1 (1%)	0	100	100
18	S	71/76 (93%)	67 (94%)	4 (6%)	0	100	100
18	f	72/76 (95%)	70 (97%)	2 (3%)	0	100	100
18	n	64/76 (84%)	62 (97%)	2 (3%)	0	100	100
19	T	69/126 (55%)	69 (100%)	0	0	100	100
19	g	77/126 (61%)	75 (97%)	2 (3%)	0	100	100
19	h	76/126 (60%)	75 (99%)	1 (1%)	0	100	100
20	E	297/357 (83%)	272 (92%)	16 (5%)	9 (3%)	4	33
21	X	73/376 (19%)	70 (96%)	3 (4%)	0	100	100
22	W	167/177 (94%)	158 (95%)	9 (5%)	0	100	100
23	A0	71/73 (97%)	68 (96%)	3 (4%)	0	100	100
24	0	43/439 (10%)	42 (98%)	1 (2%)	0	100	100
25	Z	174/312 (56%)	158 (91%)	15 (9%)	1 (1%)	25	62
26	8	54/199 (27%)	47 (87%)	7 (13%)	0	100	100
27	Y	445/513 (87%)	432 (97%)	12 (3%)	1 (0%)	47	79
29	o	160/255 (63%)	146 (91%)	12 (8%)	2 (1%)	12	48
30	p	92/225 (41%)	90 (98%)	2 (2%)	0	100	100
31	u	118/793 (15%)	106 (90%)	6 (5%)	6 (5%)	2	23
32	v	88/464 (19%)	63 (72%)	16 (18%)	9 (10%)	0	9
33	w	413/501 (82%)	367 (89%)	41 (10%)	5 (1%)	13	50
34	q	88/95 (93%)	77 (88%)	7 (8%)	4 (4%)	2	25
35	r	70/102 (69%)	64 (91%)	3 (4%)	3 (4%)	2	26
36	s	70/139 (50%)	63 (90%)	6 (9%)	1 (1%)	11	46
37	t	68/91 (75%)	63 (93%)	4 (6%)	1 (2%)	10	46
38	x	68/80 (85%)	64 (94%)	2 (3%)	2 (3%)	4	34
39	y	61/103 (59%)	56 (92%)	5 (8%)	0	100	100
40	z	57/96 (59%)	52 (91%)	4 (7%)	1 (2%)	8	42
41	K	406/522 (78%)	343 (84%)	62 (15%)	1 (0%)	47	79

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
42	1	1032/1304 (79%)	844 (82%)	166 (16%)	22 (2%)	7 40
43	3	1152/1217 (95%)	1053 (91%)	89 (8%)	10 (1%)	17 54
44	5	106/125 (85%)	84 (79%)	19 (18%)	3 (3%)	5 35
45	6	87/110 (79%)	76 (87%)	10 (12%)	1 (1%)	14 51
46	7	64/86 (74%)	55 (86%)	7 (11%)	2 (3%)	4 33
47	2	170/895 (19%)	151 (89%)	15 (9%)	4 (2%)	6 37
48	4	76/424 (18%)	75 (99%)	1 (1%)	0	100 100
49	D	1697/2136 (79%)	1604 (94%)	82 (5%)	11 (1%)	25 62
All	All	13852/21253 (65%)	12701 (92%)	1024 (7%)	127 (1%)	21 54

5 of 127 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	C	474	LEU
8	N	842	HIS
12	J	541	VAL
20	E	193	THR
27	Y	383	CYS

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
1	A	1775/2108 (84%)	1742 (98%)	33 (2%)	57 76
6	O	126/130 (97%)	123 (98%)	3 (2%)	49 71
7	C	719/866 (83%)	710 (99%)	9 (1%)	69 82
8	N	196/792 (25%)	185 (94%)	11 (6%)	21 52
9	M	108/111 (97%)	108 (100%)	0	100 100
10	L	299/424 (70%)	292 (98%)	7 (2%)	50 72
11	9	81/681 (12%)	54 (67%)	27 (33%)	0 1
12	J	72/599 (12%)	67 (93%)	5 (7%)	15 46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
21	X	2/333 (1%)	2 (100%)	0	100 100
22	W	10/148 (7%)	10 (100%)	0	100 100
23	A0	60/66 (91%)	56 (93%)	4 (7%)	16 47
25	Z	6/293 (2%)	6 (100%)	0	100 100
27	Y	11/450 (2%)	11 (100%)	0	100 100
41	K	29/442 (7%)	17 (59%)	12 (41%)	0 0
All	All	3494/7443 (47%)	3383 (97%)	111 (3%)	42 65

5 of 111 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	L	161	ASN
41	K	139	VAL
11	9	260	GLU
41	K	138	SER
41	K	86	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 55 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1894	GLN
7	C	837	GLN
23	A0	67	ASN
11	9	291	ASN
6	O	70	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	I	133/144 (92%)	54 (40%)	5 (3%)
28	H	105/188 (55%)	22 (20%)	3 (2%)
3	B	114/117 (97%)	43 (37%)	6 (5%)
4	F	90/107 (84%)	32 (35%)	5 (5%)
5	G	76/274 (27%)	44 (57%)	15 (19%)
All	All	518/830 (62%)	195 (37%)	34 (6%)

5 of 195 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	I	2	G
2	I	9	G
2	I	11	A
2	I	12	G
2	I	18	G

5 of 34 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	G	153	C
5	G	155	U
28	H	164	C
4	F	35	A
4	F	28	A

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
51	GTP	C	1500	52	26,34,34	1.40	3 (11%)	32,54,54	1.79	8 (25%)
50	IHP	A	3000	-	36,36,36	0.82	0	54,60,60	1.20	2 (3%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
51	GTP	C	1500	52	-	6/18/38/38	0/3/3/3
50	IHP	A	3000	-	-	6/30/54/54	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	C	1500	GTP	C5-C6	-5.03	1.37	1.47
51	C	1500	GTP	C2-N3	2.38	1.38	1.33
51	C	1500	GTP	O4'-C4'	-2.00	1.40	1.45

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	C	1500	GTP	PB-O3B-PG	-5.03	115.58	132.83
51	C	1500	GTP	PA-O3A-PB	-4.55	117.22	132.83
50	A	3000	IHP	C6-C5-C4	3.80	118.73	110.41
51	C	1500	GTP	C3'-C2'-C1'	3.17	105.76	100.98
51	C	1500	GTP	C5-C6-N1	2.94	119.14	113.95

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
50	A	3000	IHP	C2-O12-P2-O42
50	A	3000	IHP	C3-O13-P3-O23
51	C	1500	GTP	C3'-C4'-C5'-O5'
51	C	1500	GTP	C4'-C5'-O5'-PA
51	C	1500	GTP	O4'-C4'-C5'-O5'

There are no ring outliers.

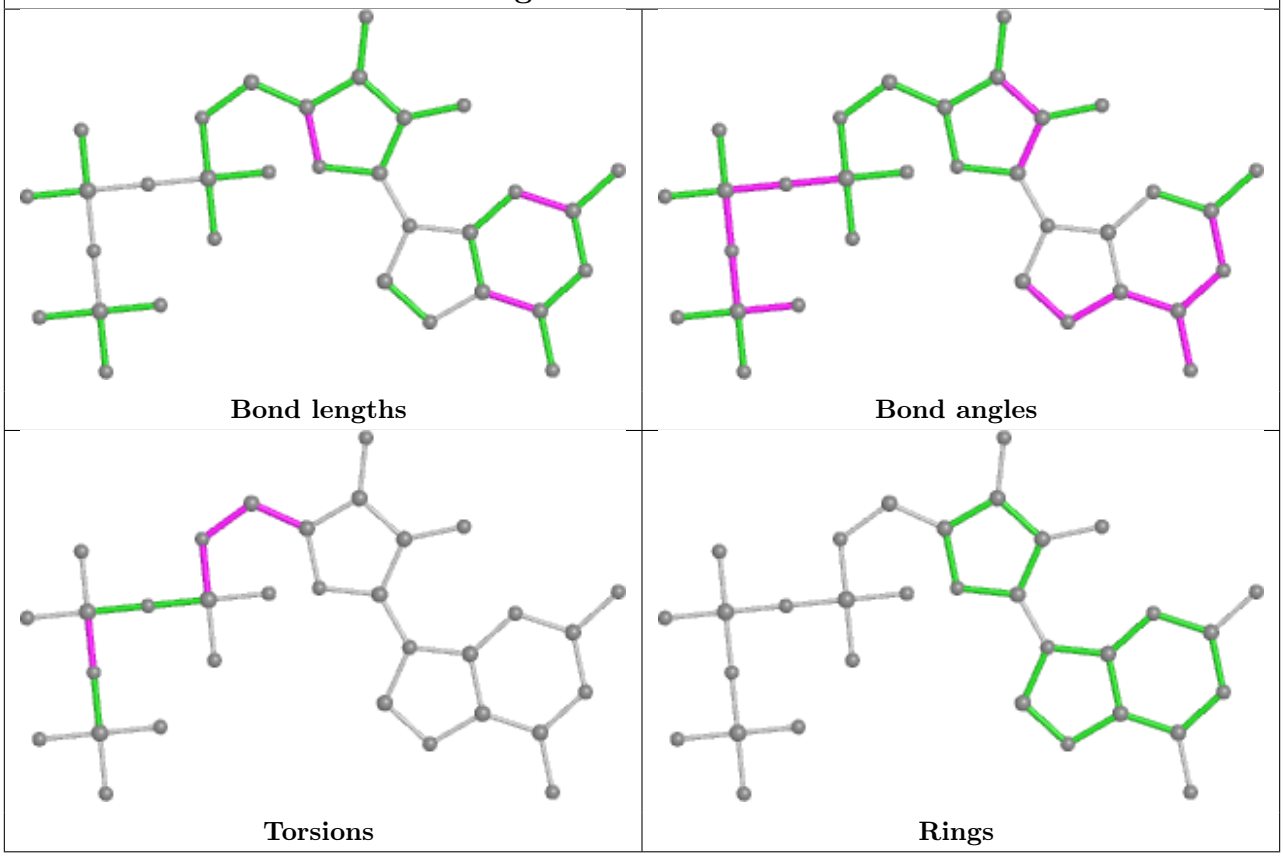
1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
50	A	3000	IHP	9	0

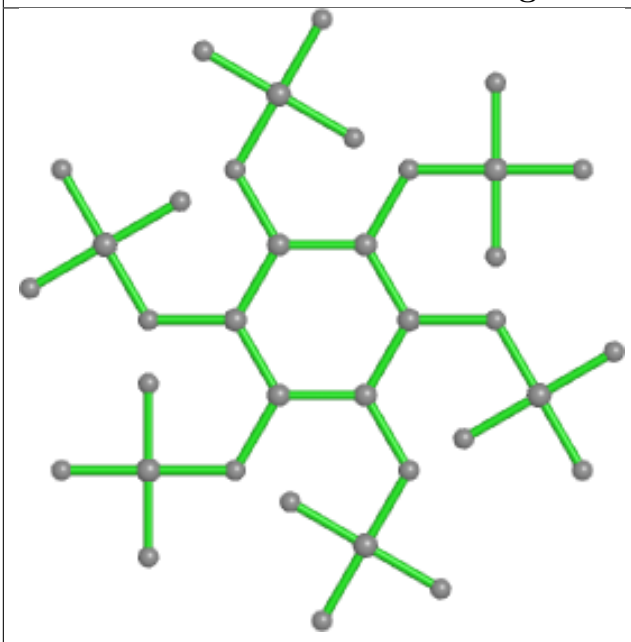
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

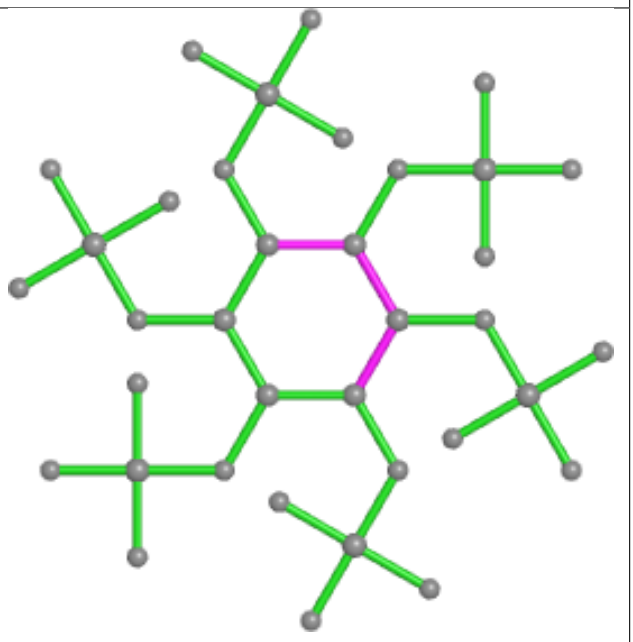
Ligand GTP C 1500



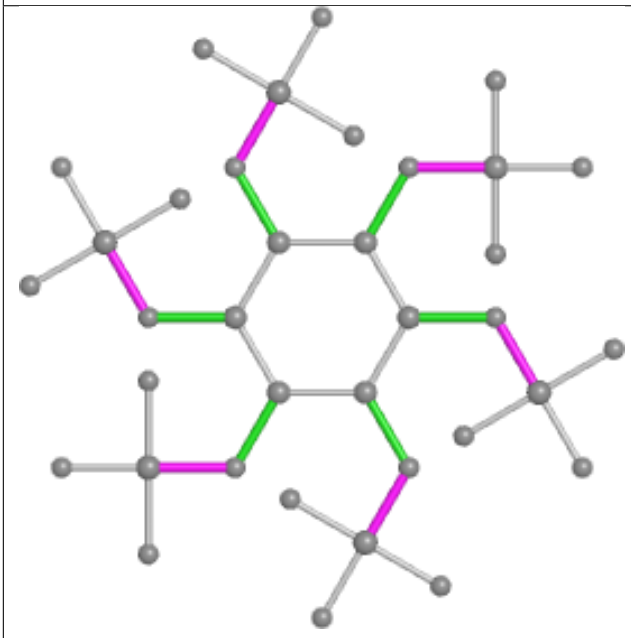
Ligand IHP A 3000



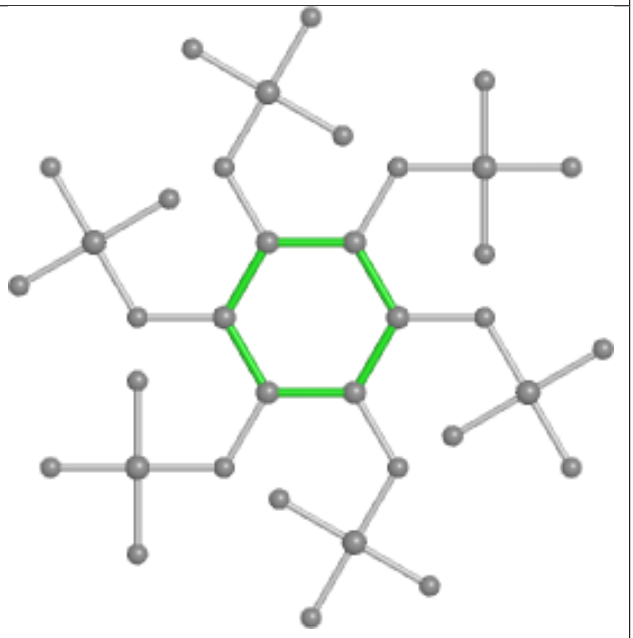
Bond lengths



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.

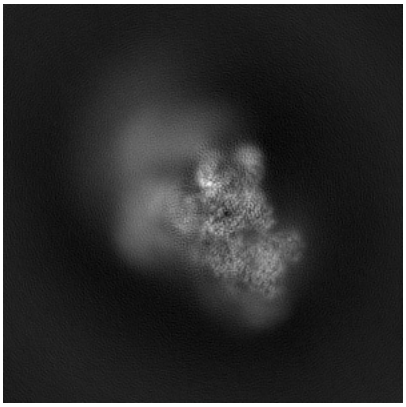
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-9624. These allow visual inspection of the internal detail of the map and identification of artifacts.

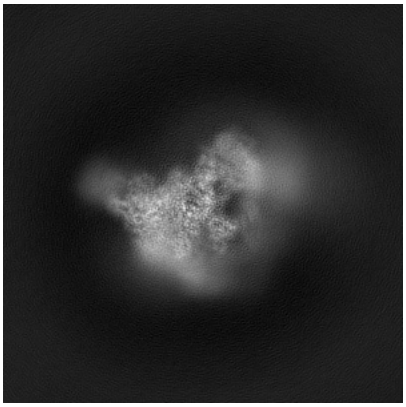
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

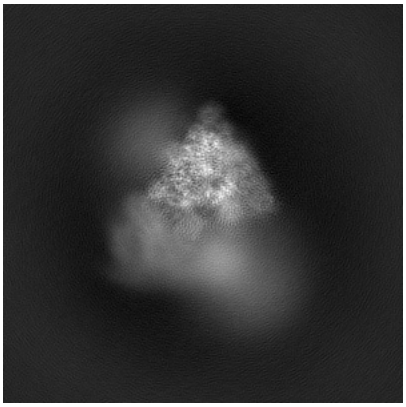
6.1.1 Primary map



X



Y

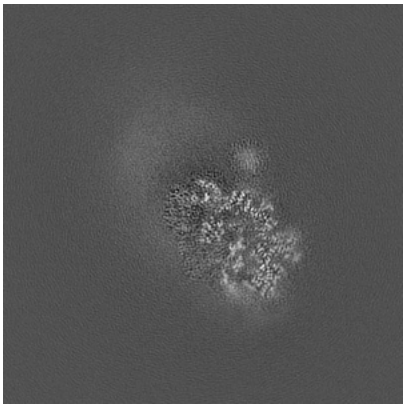


Z

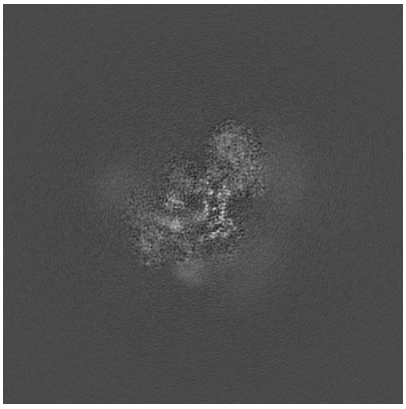
The images above show the map projected in three orthogonal directions.

6.2 Central slices

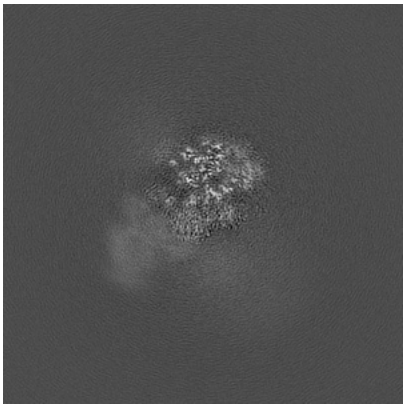
6.2.1 Primary map



X Index: 200



Y Index: 200

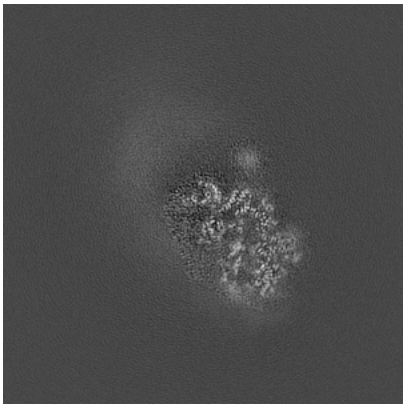


Z Index: 200

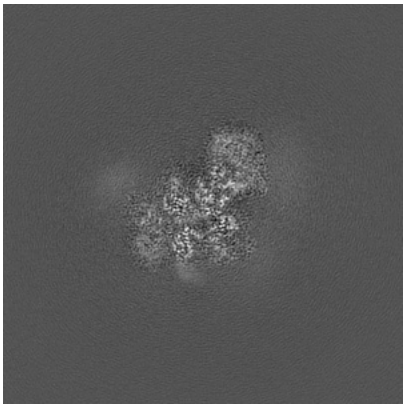
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

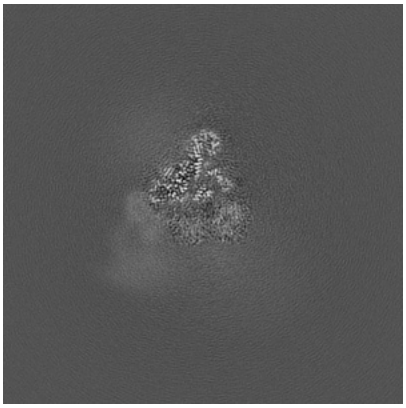
6.3.1 Primary map



X Index: 201



Y Index: 207



Z Index: 181

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

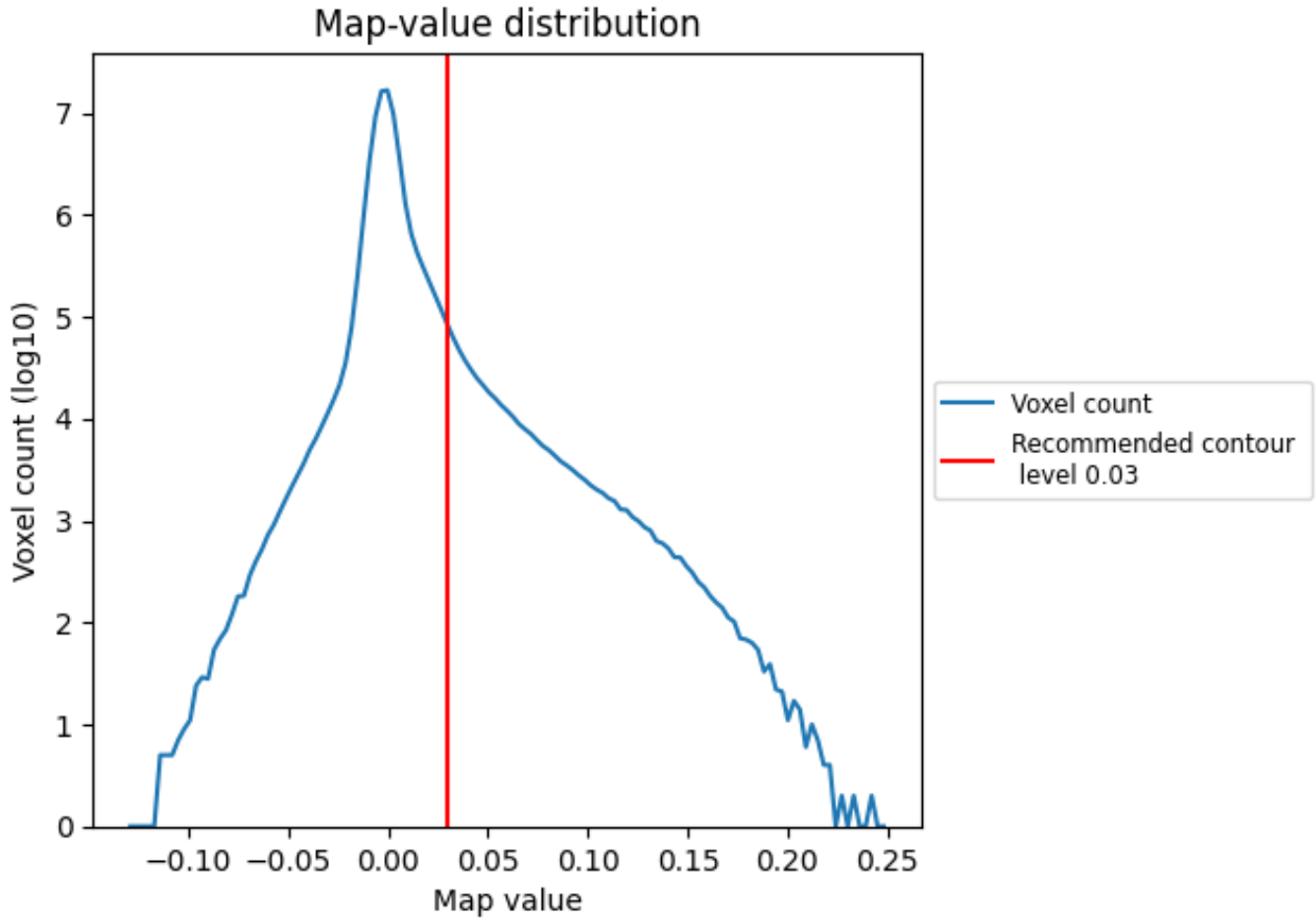
6.5 Mask visualisation (i)

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

7 Map analysis

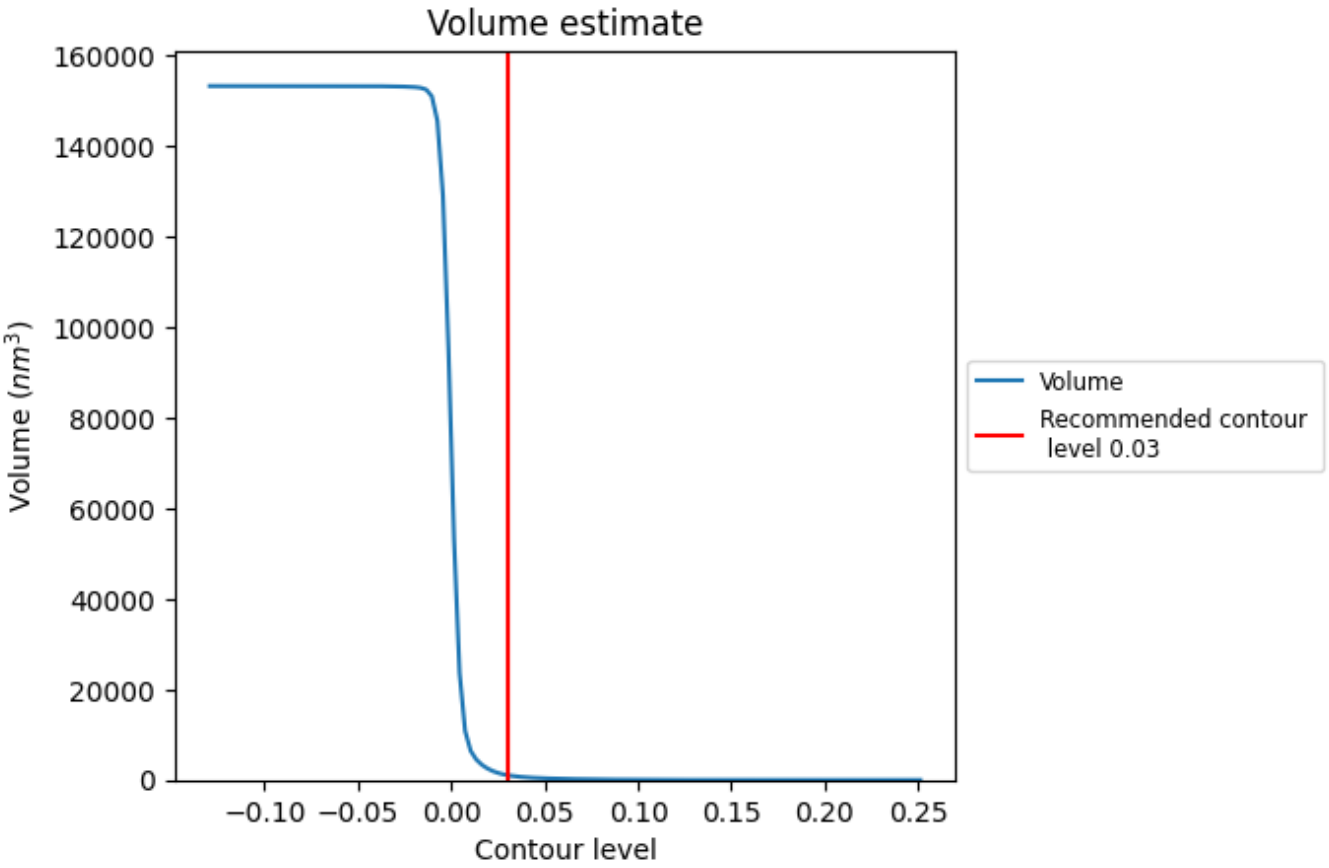
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

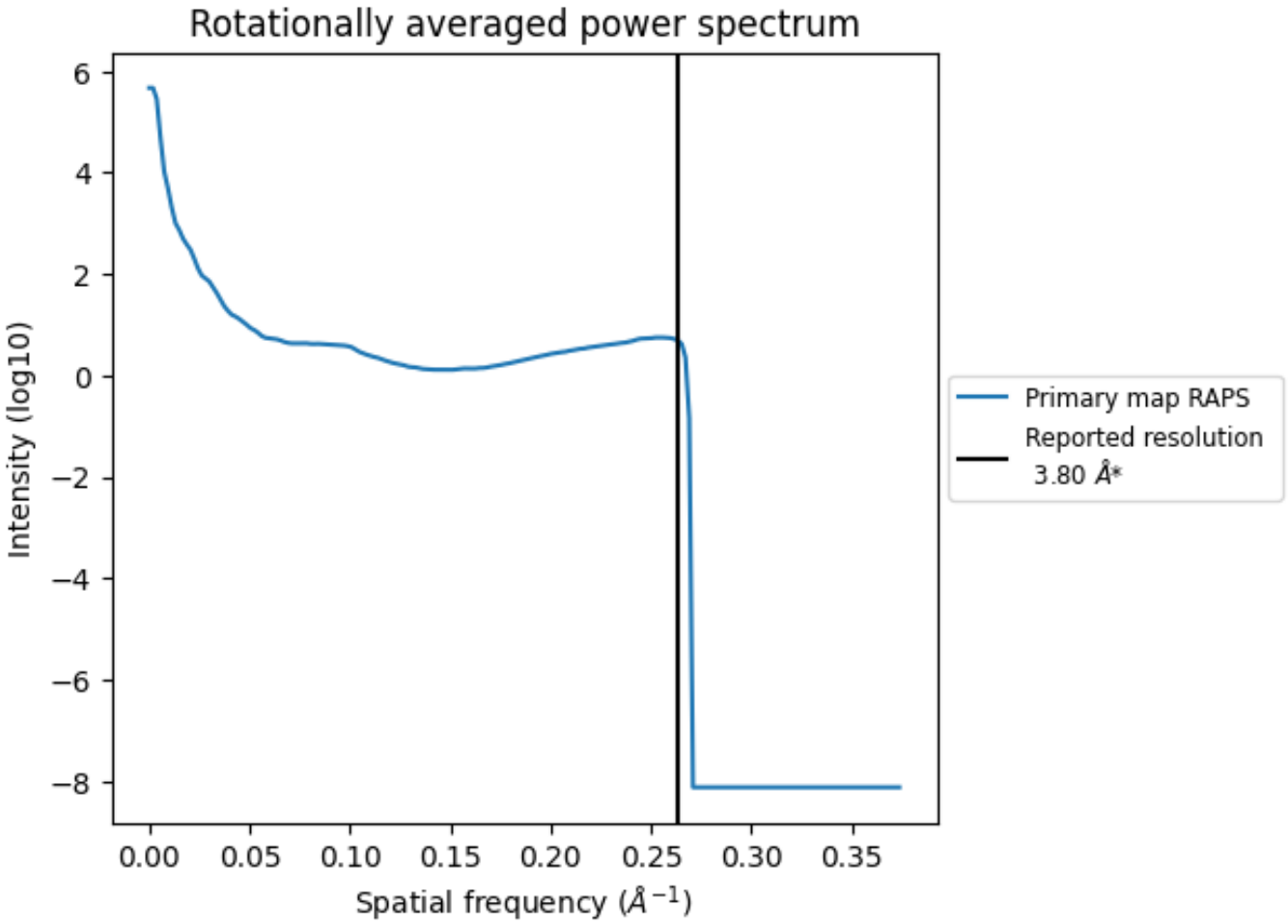
7.2 Volume estimate (i)



The volume at the recommended contour level is 1073 nm^3; this corresponds to an approximate mass of 969 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 0.263 Å^{-1}

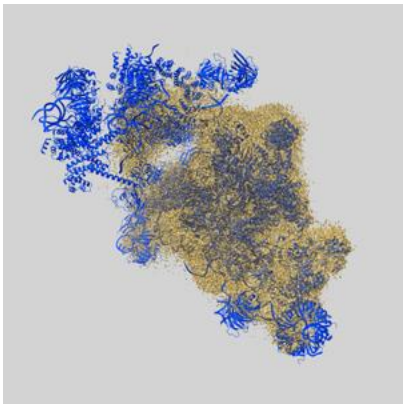
8 Fourier-Shell correlation (i)

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

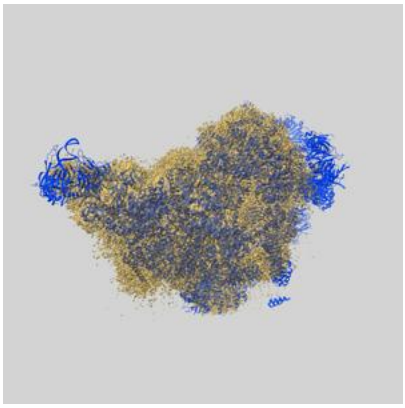
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-9624 and PDB model 6AHD. Per-residue inclusion information can be found in section 3 on page 16.

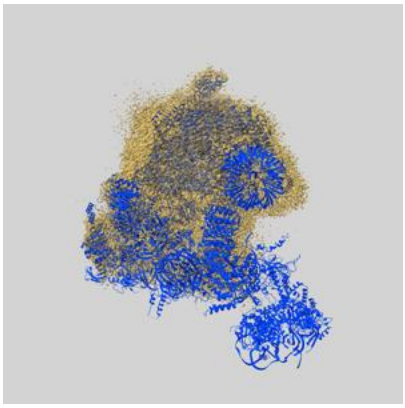
9.1 Map-model overlay



X



Y



Z

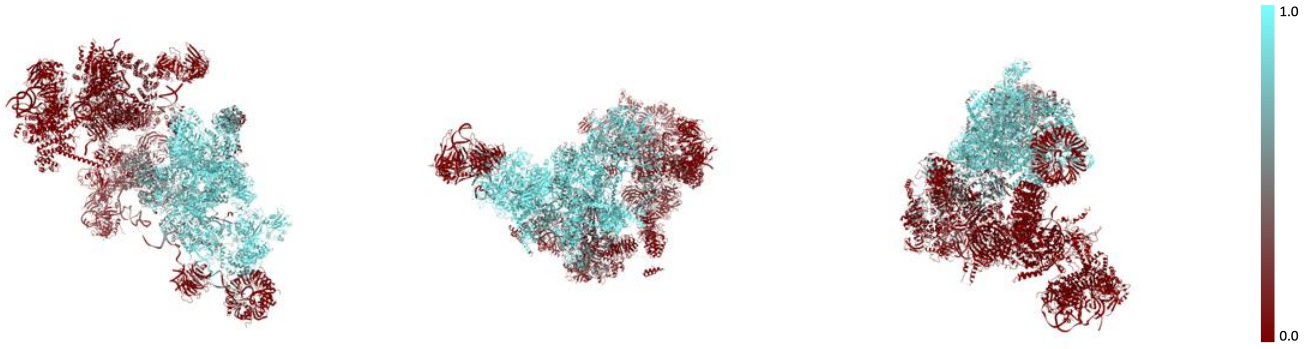
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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.

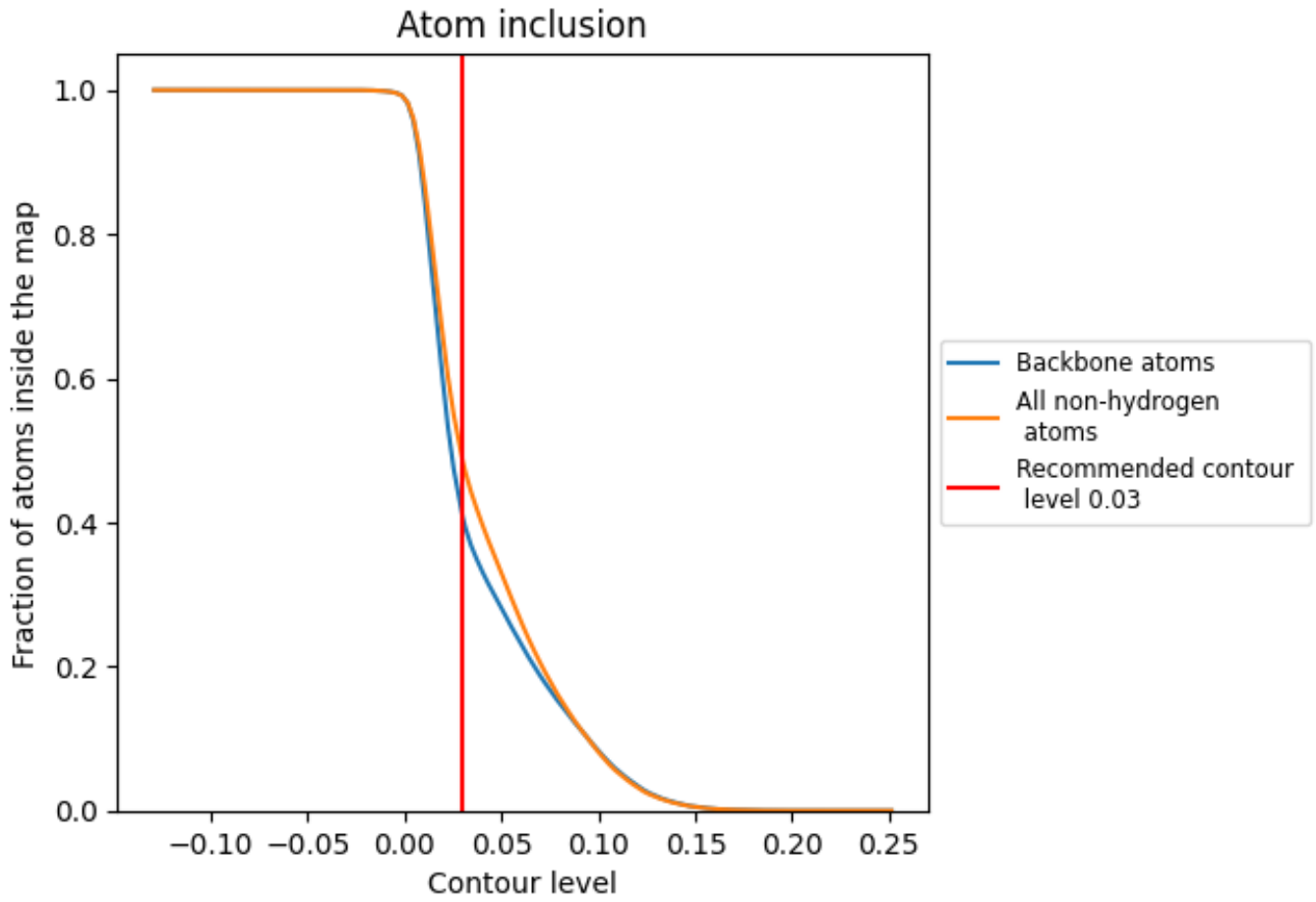
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.03).

9.4 Atom inclusion (i)



At the recommended contour level, 41% of all backbone atoms, 48% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4849	0.1890
0	0.4622	0.0350
1	0.0198	-0.0020
2	0.0508	0.0150
3	0.0101	-0.0120
4	0.0449	0.0080
5	0.0000	-0.0120
6	0.0449	0.0060
7	0.0492	-0.0460
8	0.6245	0.1170
9	0.8108	0.3010
A	0.8924	0.4270
A0	0.7330	0.3980
B	0.6269	0.2100
C	0.9038	0.3920
D	0.2706	0.0170
E	0.0426	0.0270
F	0.4842	0.1360
G	0.3251	0.0910
H	0.0286	0.0170
I	0.5259	0.1780
J	0.7912	0.2650
K	0.8964	0.2760
L	0.8375	0.3490
M	0.8955	0.4130
N	0.7584	0.2080
O	0.9210	0.4500
P	0.0267	-0.0080
Q	0.0171	-0.0430
R	0.0382	0.0530
S	0.0570	0.0570
T	0.0521	0.0070
U	0.0508	0.0040
V	0.0359	0.0450
W	0.6682	0.0810

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Chain	Atom inclusion	Q-score
X	0.4709	0.0330
Y	0.0257	0.0100
Z	0.6693	0.1560
a	0.1279	-0.0110
b	0.1250	0.0190
c	0.0412	0.0080
d	0.0101	-0.0090
e	0.0222	0.0010
f	0.0338	-0.0570
g	0.1852	0.0140
h	0.0000	-0.0180
i	0.0000	0.0150
j	0.0000	-0.0030
k	0.0000	-0.0090
l	0.0000	-0.0360
m	0.0000	0.0330
n	0.0000	-0.0400
o	0.0000	0.0220
p	0.0000	-0.0370
q	0.0000	0.0190
r	0.0000	0.0090
s	0.0000	-0.0050
t	0.0000	0.0350
u	0.0000	0.0260
v	0.0000	0.0080
w	0.0006	0.0110
x	0.0071	0.0140
y	0.0000	-0.0360
z	0.0000	-0.0230