wwPDB EM Validation Summary Report ⓘ

Nov 22, 2022 – 01:33 AM JST

PDB ID : 7DVQ
EMDB ID : EMD-30875
Title : Cryo-EM Structure of the Activated Human Minor Spliceosome (minor Bact Complex)
Authors : Bai, R.; Wan, R.; Wang, L.; Xu, K.; Zhang, Q.; Lei, J.; Shi, Y.
Deposited on : 2021-01-14
Resolution : 2.89 Å(reported)

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

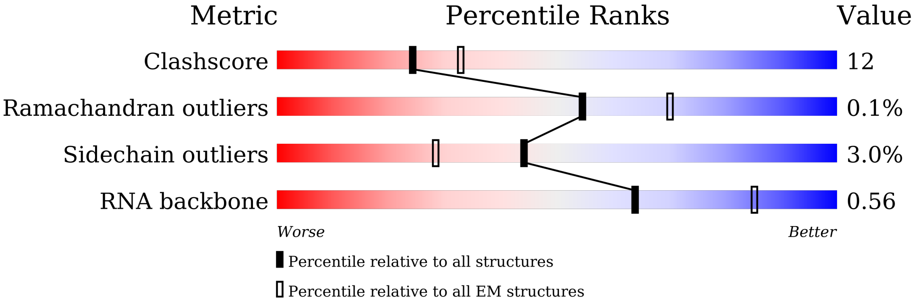
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance ⓘ

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

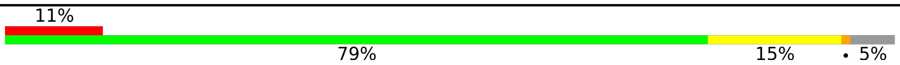
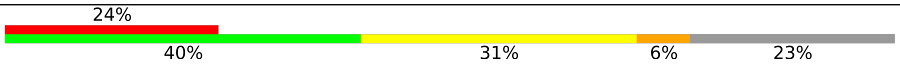
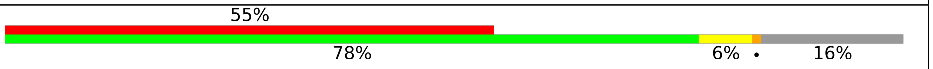
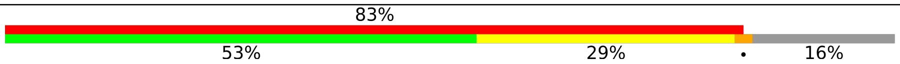
The reported resolution of this entry is 2.89 Å.

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	
2	B	117	
3	C	972	
4	D	2136	
5	E	357	
6	a	126	
6	h	126	

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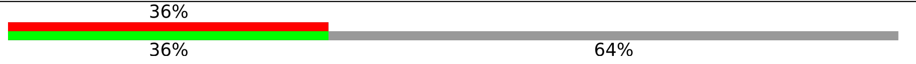
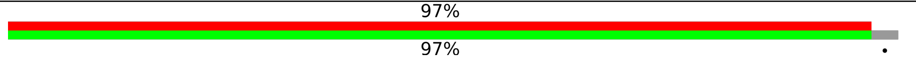
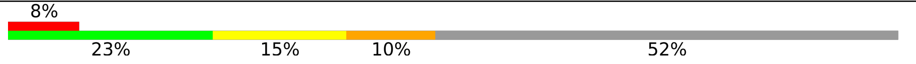
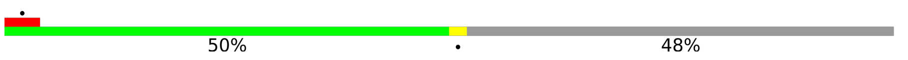
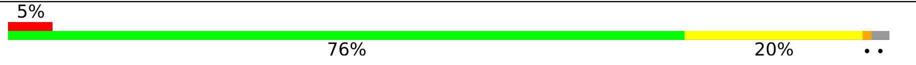
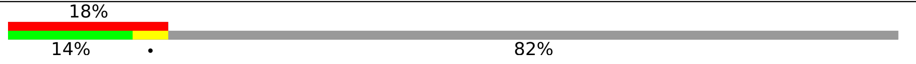
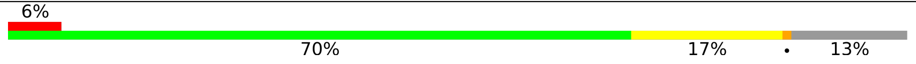
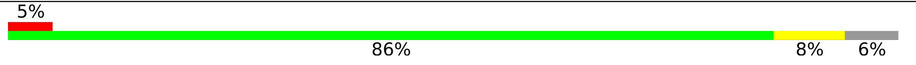
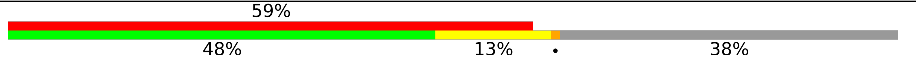
Mol	Chain	Length	Quality of chain
7	b	240	
7	i	240	
8	c	119	
8	j	119	
9	d	118	
9	k	118	
10	f	86	
10	m	86	
11	e	92	
11	l	92	
12	g	76	
12	n	76	
13	F	124	
14	G	142	
15	H	150	
16	v	230	
17	1	1304	
18	2	895	
19	3	1217	
20	4	424	
21	5	125	
22	6	110	
23	7	86	
24	L	802	
25	J	848	

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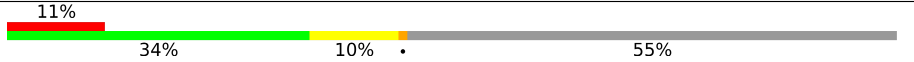
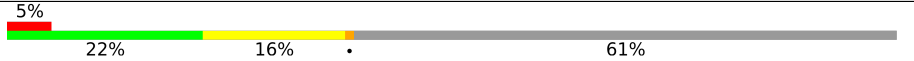
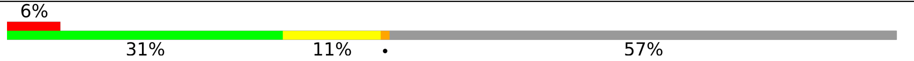
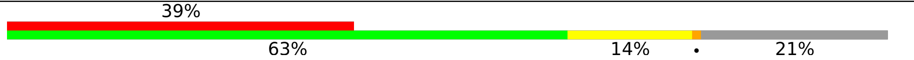
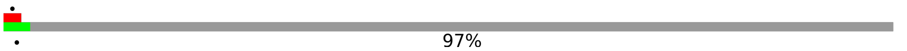
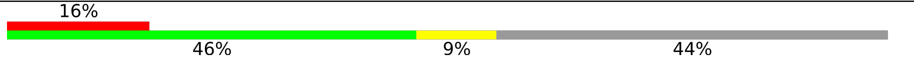
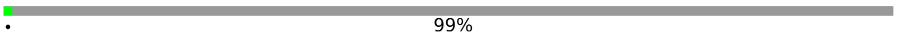
Mol	Chain	Length	Quality of chain
26	P	229	
27	R	536	
28	T	514	
29	X	396	
30	Y	322	
31	Z	619	
32	9	520	
33	z	472	
34	x	1041	
35	y	476	
36	M	343	
37	U	2752	
38	V	908	
39	8	904	
40	0	101	
41	I	367	
42	K	198	

2 Entry composition ⓘ

There are 49 unique types of molecules in this entry. The entry contains 99906 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	2223	18354	11832	3206	3236	80	0	0

- Molecule 2 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	90	1898	850	320	638	90	0	0

- Molecule 3 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	902	7125	4560	1185	1345	35	0	0

- Molecule 4 is a protein called U5 small nuclear ribonucleoprotein 200 kDa helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	1803	9215	5522	1841	1851	1	0	0

- Molecule 5 is a protein called U5 small nuclear ribonucleoprotein 40 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	299	2337	1470	409	445	13	0	0

- Molecule 6 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	a	81	399	237	81	81	0	0

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Mol	Chain	Residues	Atoms	AltConf	Trace
6	h	80	Total C N O 392 233 79 80	0	0

- Molecule 7 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues	Atoms	AltConf	Trace
7	b	82	Total C N O 405 241 82 82	0	0
7	i	86	Total C N O 422 250 86 86	0	0

- Molecule 8 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms	AltConf	Trace
8	c	82	Total C N O 406 242 82 82	0	0
8	j	82	Total C N O 406 242 82 82	0	0

- Molecule 9 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms	AltConf	Trace
9	d	97	Total C N O 480 286 97 97	0	0
9	k	85	Total C N O 422 252 85 85	0	0

- Molecule 10 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms	AltConf	Trace
10	f	74	Total C N O 361 213 74 74	0	0
10	m	74	Total C N O 361 213 74 74	0	0

- Molecule 11 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms	AltConf	Trace
11	e	79	Total C N O 391 233 79 79	0	0
11	l	79	Total C N O 391 233 79 79	0	0

- Molecule 12 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
12	g	74	363	215	74	74	0	0
12	n	68	334	198	68	68	0	0

- Molecule 13 is a RNA chain called U6atac snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
13	F	60	1294	577	242	415	60	0	0

- Molecule 14 is a RNA chain called pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
14	G	63	1303	585	197	458	63	0	0

- Molecule 15 is a RNA chain called U12 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
15	H	63	1350	604	247	436	63	0	0

- Molecule 16 is a protein called Sodium channel modifier 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	v	119	963	601	179	178	5	0	0

- Molecule 17 is a protein called Splicing factor 3B subunit 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
17	1	986	7879	5035	1361	1435	1	47	0	0

- Molecule 18 is a protein called Splicing factor 3B subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	2	216	1674	1067	296	305	6	0	0

- Molecule 19 is a protein called Splicing factor 3B subunit 3.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
19	3	1193	9352	5932	1590	1784	1	45	0	0

- Molecule 20 is a protein called Splicing factor 3B subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
20	4	78	383	227	78	78	0	0

- Molecule 21 is a protein called Splicing factor 3B subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	5	109	906	582	157	163	4	0	0

- Molecule 22 is a protein called PHD finger-like domain-containing protein 5A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	6	105	811	502	145	151	13	0	0

- Molecule 23 is a protein called Splicing factor 3B subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	7	81	669	422	117	124	6	0	0

- Molecule 24 is a protein called Cell division cycle 5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	L	101	843	540	152	147	4	0	0

- Molecule 25 is a protein called Crooked neck-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	J	522	3457	2153	654	645	5	0	0

- Molecule 26 is a protein called Spliceosome-associated protein CWC15 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	P	44	384	243	71	68	2	0	0

- Molecule 27 is a protein called SNW domain-containing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	R	241	1923	1191	347	374	11	0	0

- Molecule 28 is a protein called Pleiotropic regulator 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	T	320	2507	1582	456	462	7	0	0

- Molecule 29 is a protein called Smad nuclear-interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	X	156	1271	815	227	227	2	0	0

- Molecule 30 is a protein called RNA-binding motif protein, X-linked 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	Y	140	1095	692	192	206	5	0	0

- Molecule 31 is a protein called BUD13 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	Z	140	1129	703	214	207	5	0	0

- Molecule 32 is a protein called RING-type E3 ubiquitin-protein ligase PPIL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	9	409	2691	1672	487	525	7	0	0

- Molecule 33 is a protein called Peptidyl-prolyl cis-trans isomerase CWC27 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	z	177	Total 1400	C 883	N 245	O 267	S 5	0	0

- Molecule 34 is a protein called Pre-mRNA-splicing factor ATP-dependent RNA helicase DHX16.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	x	599	Total 3007	C 1794	N 607	O 605	S 1	0	0

- Molecule 35 is a protein called G-patch domain and KOW motifs-containing protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	y	13	Total 105	C 66	N 22	O 17	0	0

- Molecule 36 is a protein called RING finger protein 113A.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	M	191	Total 1572	C 983	N 282	O 295	S 12	0	0

- Molecule 37 is a protein called Serine/arginine repetitive matrix protein 2.

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

- Molecule 38 is a protein called Pre-mRNA-splicing factor CWC22 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	V	468	Total 3008	C 1873	N 548	O 574	S 13	0	0

- Molecule 39 is a protein called Serine/arginine repetitive matrix protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	8	126	Total 1011	C 652	N 168	O 185	S 6	0	0

- Molecule 40 is a protein called Cysteine-rich PDZ-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	0	100	770	475	142	144	9	0	0

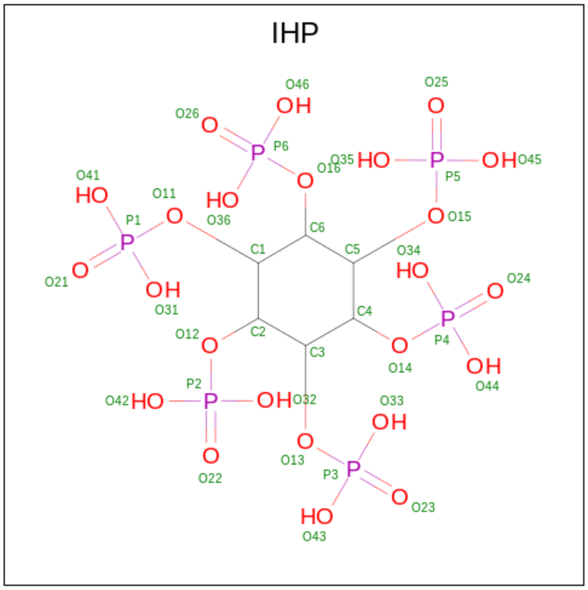
- Molecule 41 is a protein called RNA-binding protein 48.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	I	128	1062	683	184	190	5	0	0

- Molecule 42 is a protein called Armadillo repeat-containing protein 7.

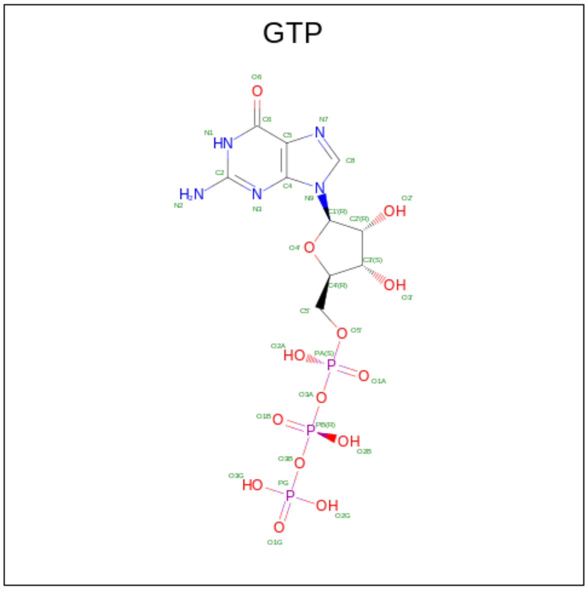
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	K	188	1314	824	229	256	5	0	0

- Molecule 43 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 44 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



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

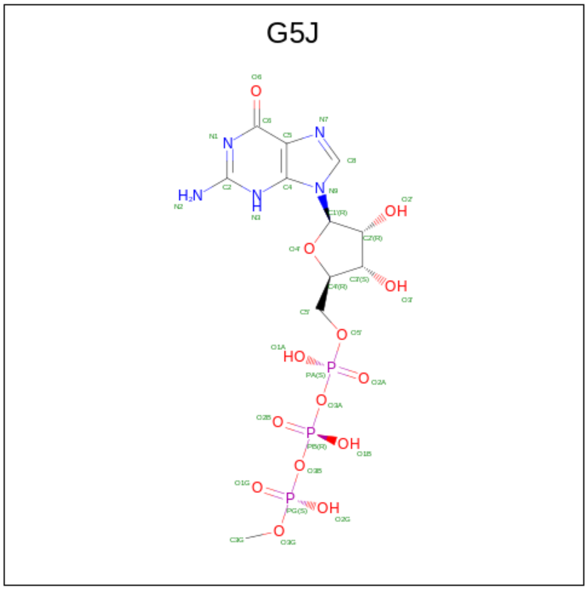
- Molecule 45 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
45	C	1	Total 1	Mg 1	0
45	F	4	Total 4	Mg 4	0

- Molecule 46 is POTASSIUM ION (three-letter code: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
46	F	2	Total 2	K 2	0

- Molecule 47 is 5'-O-[(S)-hydroxy{[(R)-hydroxy{[(S)-hydroxy(methoxy)phosphoryl]oxy} phosphoryl]oxy}phosphoryl]guanosine (three-letter code: G5J) (formula: $C_{11}H_{18}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
47	F	1	33	11	5	14	3	0

- Molecule 48 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
48	v	1	Total 1	Zn 1	0
48	6	3	Total 3	Zn 3	0
48	M	1	Total 1	Zn 1	0
48	0	2	Total 2	Zn 2	0

- Molecule 49 is water.

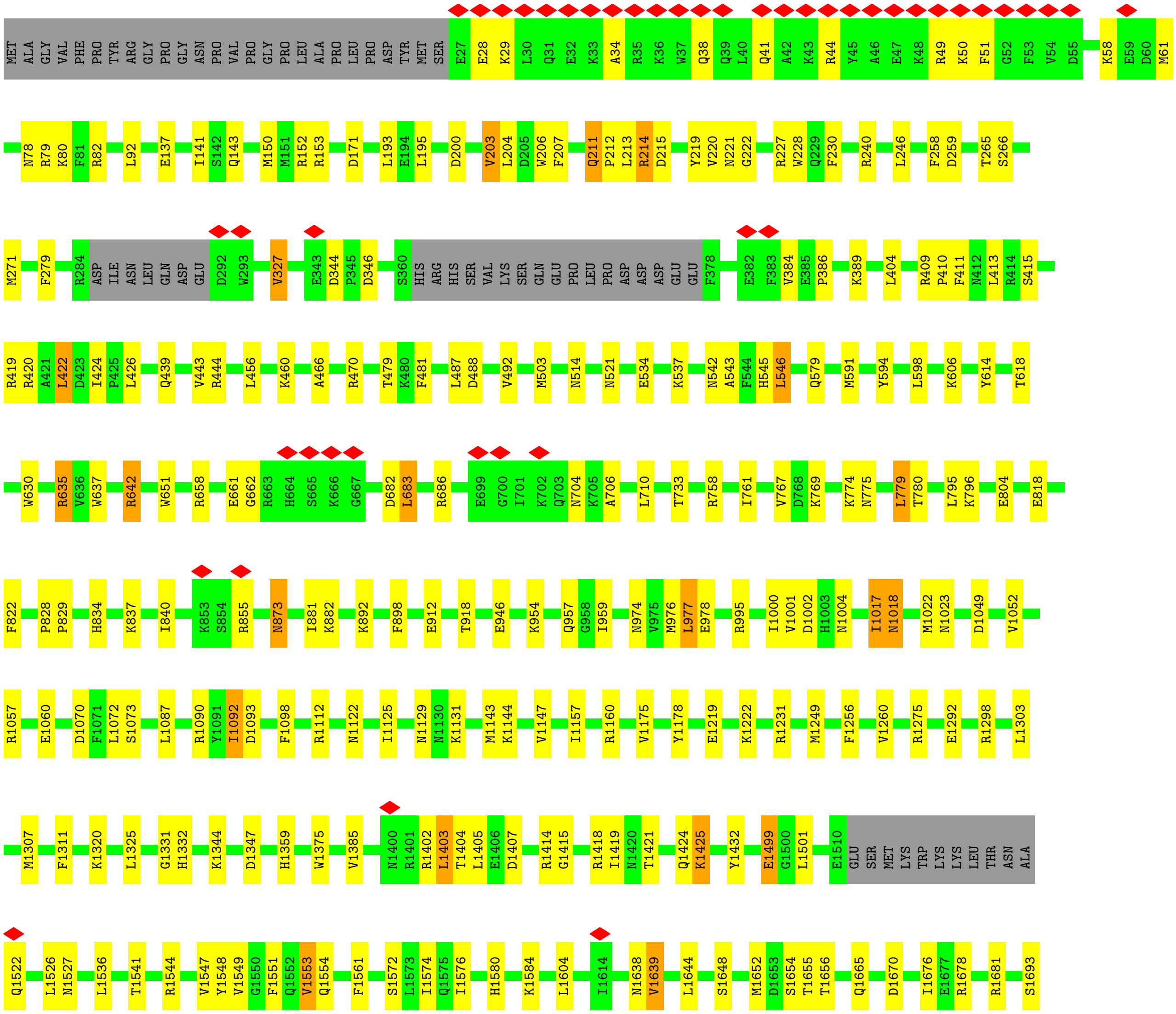
Mol	Chain	Residues	Atoms		AltConf
49	C	3	Total 3	O 3	0

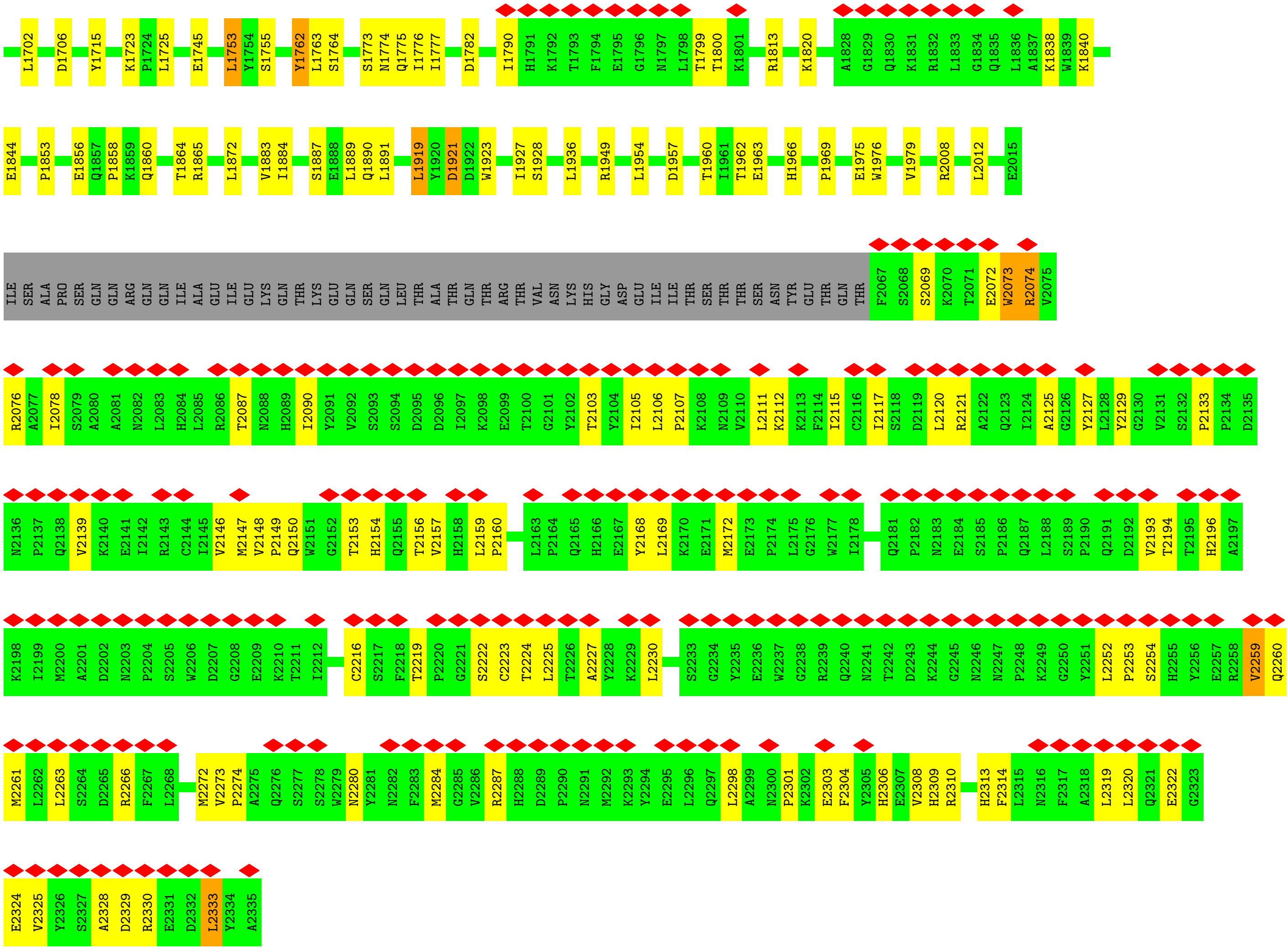
3 Residue-property plots ⓘ

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: Pre-mRNA-processing-splicing factor 8

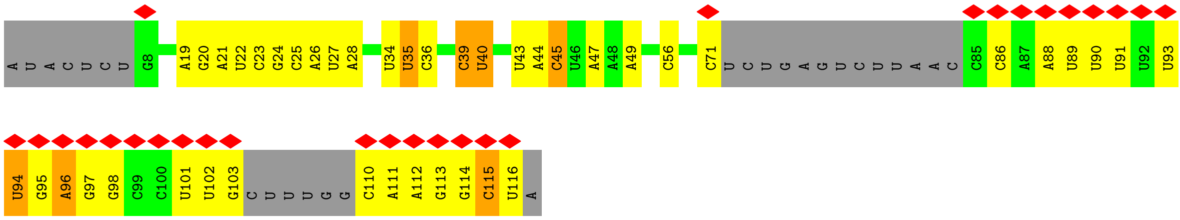
Chain A:





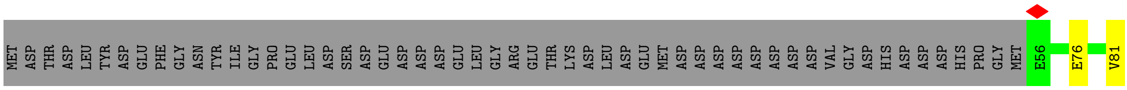
- Molecule 2: U5 snRNA

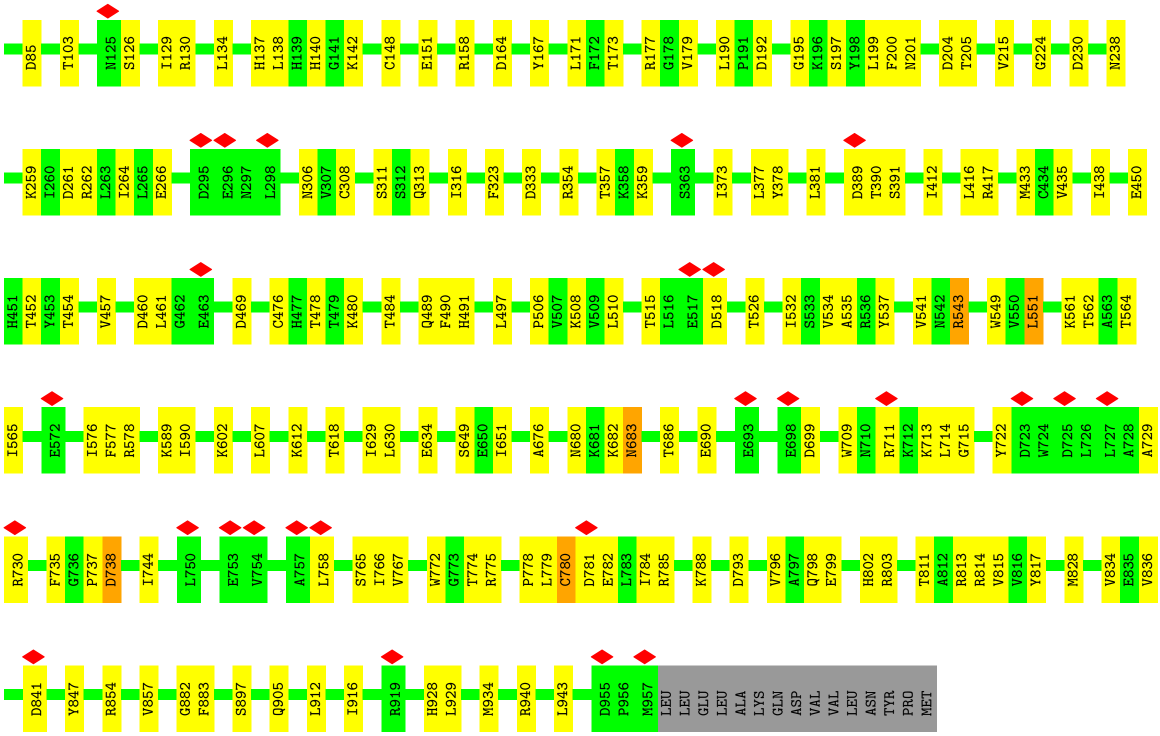
Chain B:



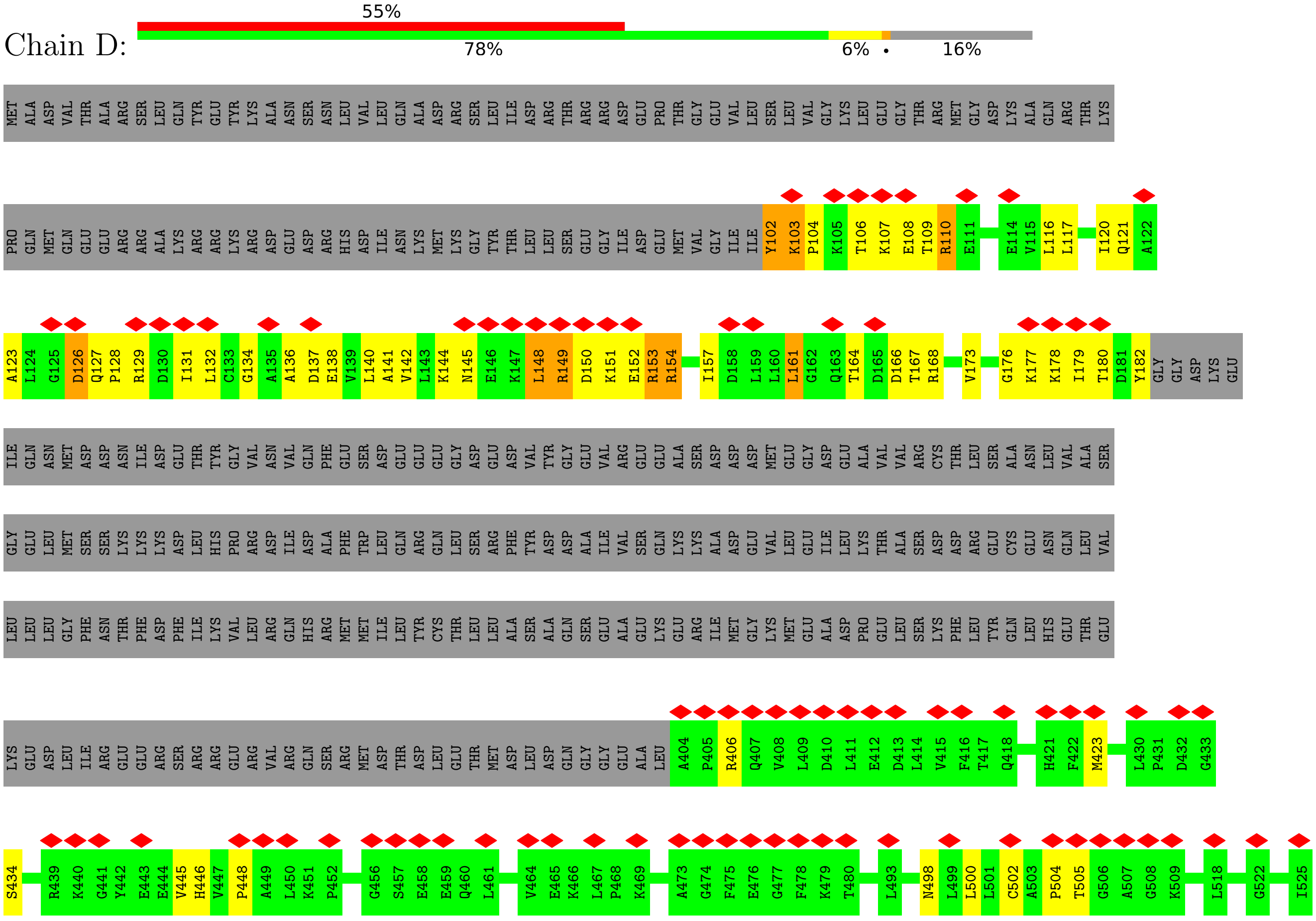
- Molecule 3: 116 kDa U5 small nuclear ribonucleoprotein component

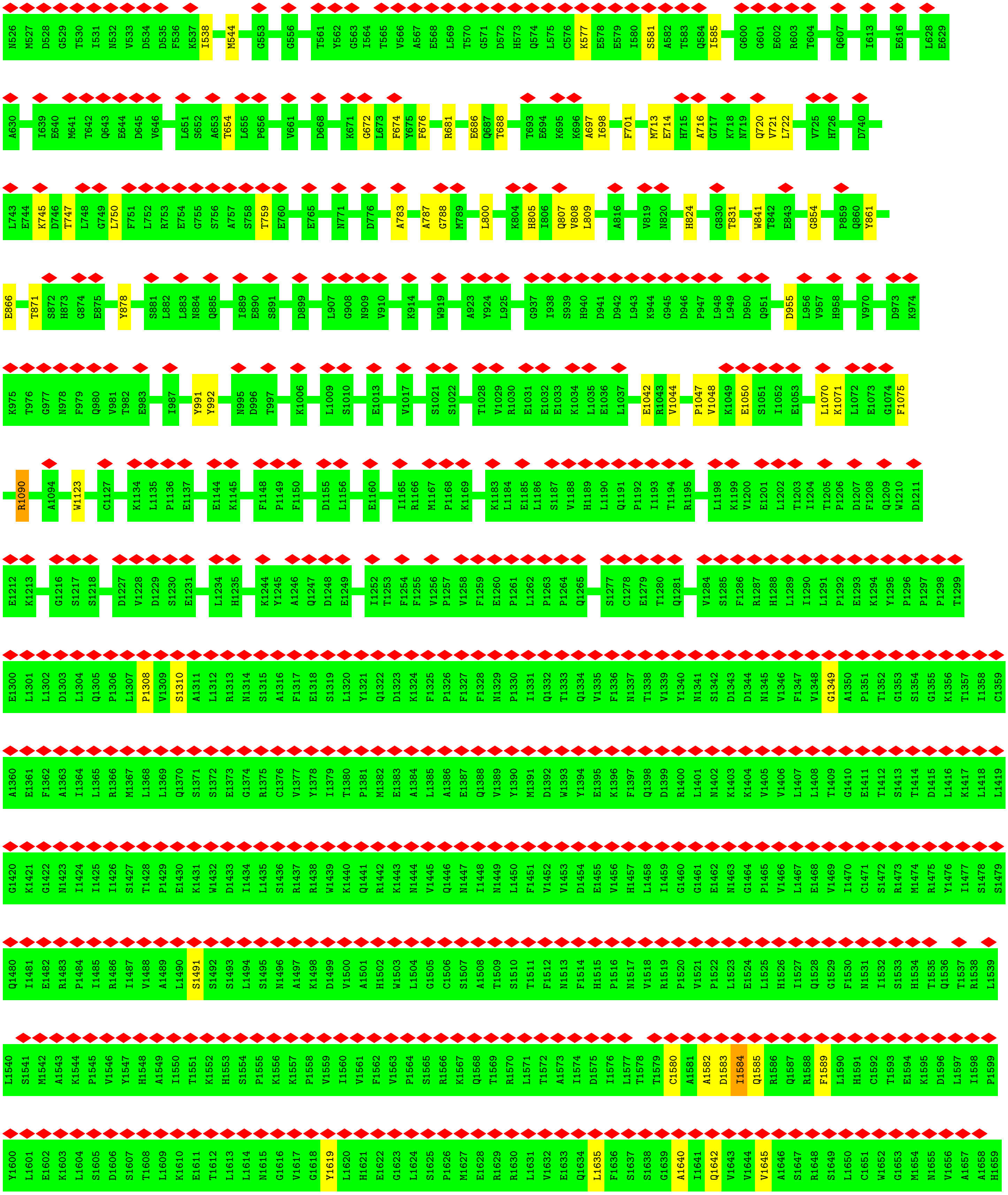
Chain C:





- Molecule 4: U5 small nuclear ribonucleoprotein 200 kDa helicase

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A630 I639 E640 M641 T642 Q643 E644 D645 V646 L651 S652 A653 T654 L655 P656 V661 D668 K671 G672 L673 F674 Y675 F676 R681 E686 Q687 T688 T693 E694 K695 K696 A697 I698 F701 M713 E714 H715 A716 G717 K718 N719 Q720 V721 L722 V725 H726 D740
L743 E744 K745 D746 T747 L748 G749 L750 F751 L752 R753 E754 G755 S756 A757 S758 T759 E760 E765 N771 D776 A783 A787 G788 M789 L800 K804 H805 I806 Q807 V808 L809 A816 V819 N820 H824 G830 T831 W841 T842 E843 G854 P859 Q860 Y861
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A1360 E1361 F1362 A1363 I1364 L1365 R1366 M1367 L1368 L1369 Q1370 S1371 S1372 E1373 G1374 R1375 C1376 V1377 Y1378 I1379 T1380 P1381 M1382 E1383 A1384 L1385 A1386 E1387 Q1388 V1389 Y1390 M1391 D1392 W1393 Y1394 E1395 K1396 F1397 Q1398 D1399 R1400 L1401 N1402 K1403 K1404 V1405 V1406 L1407 L1408 T1409 G1410 E1411 T1412 S1413 T1414 D1415 L1416 K1417 L1418 L1419
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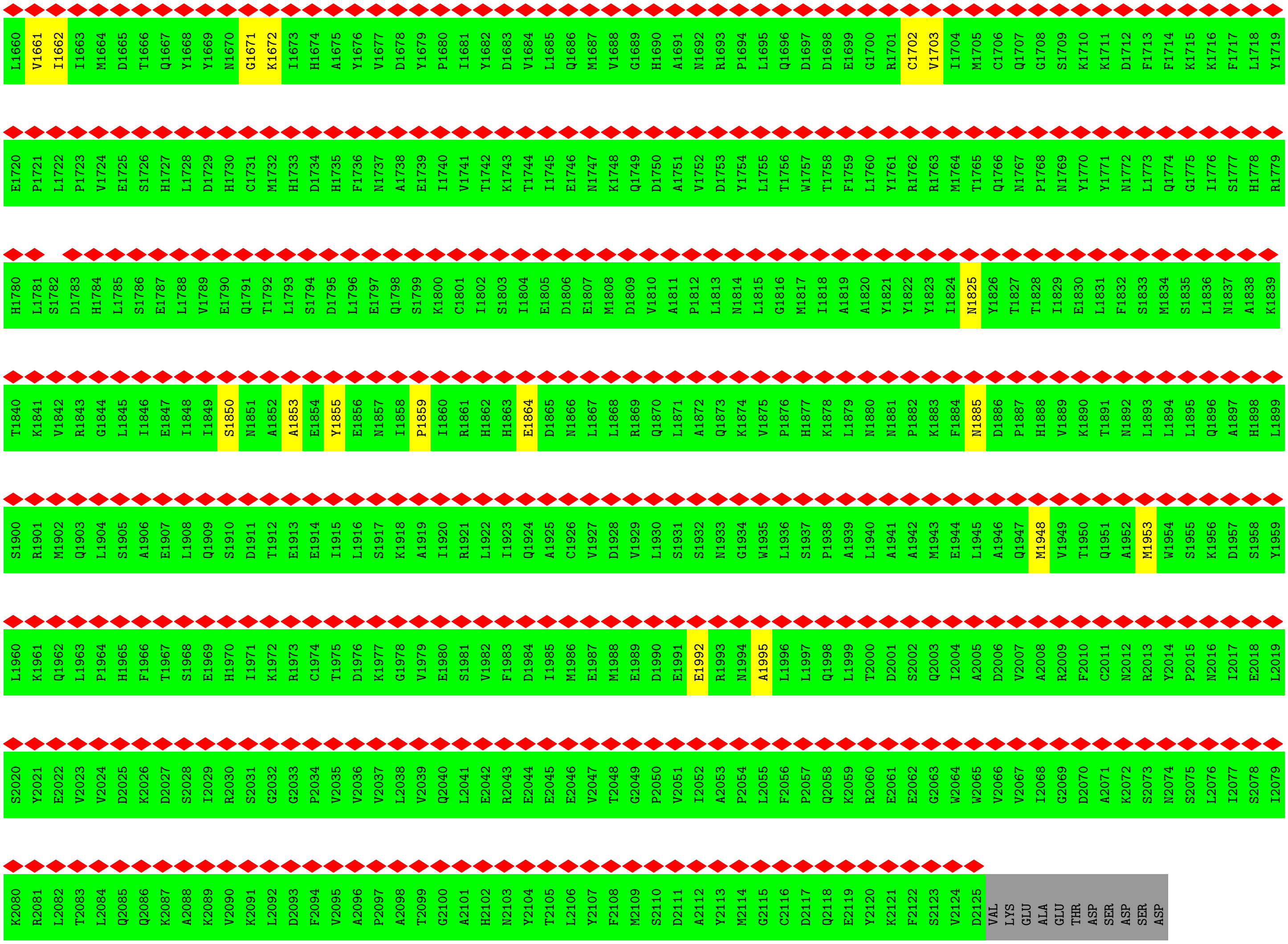
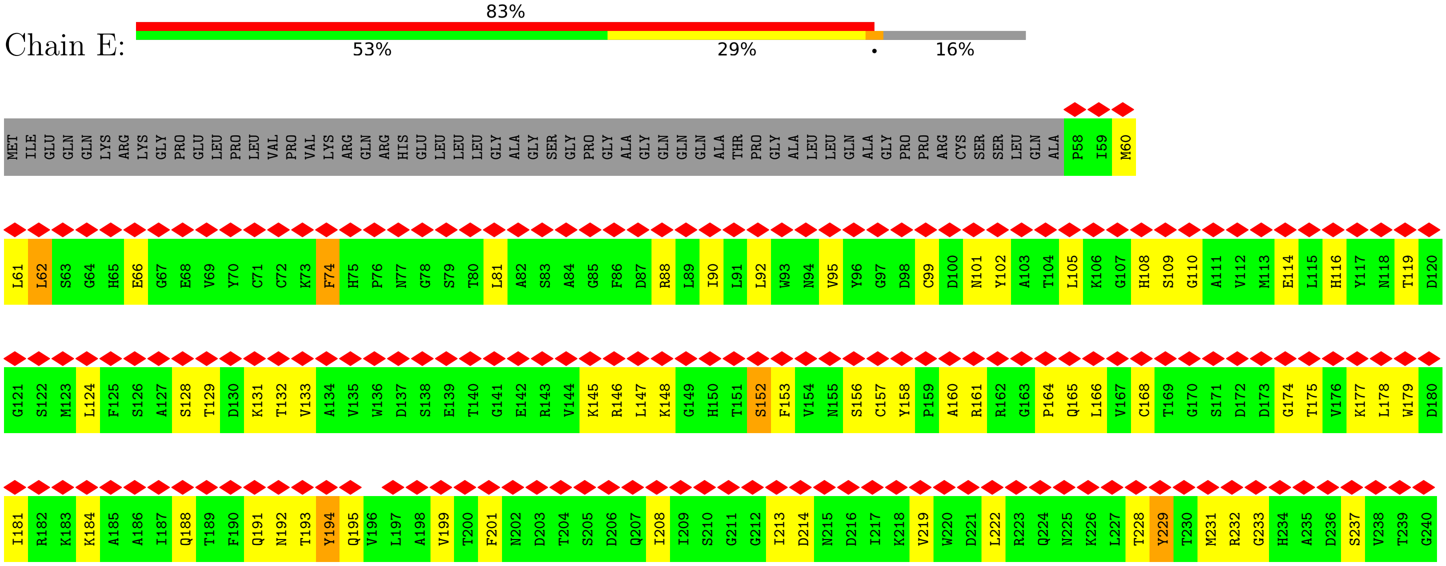
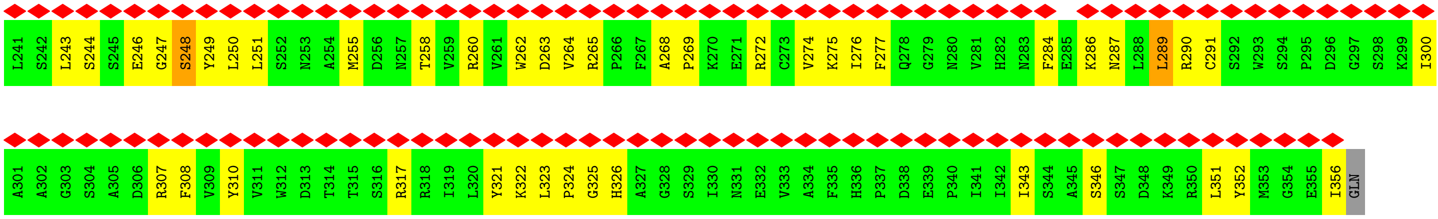


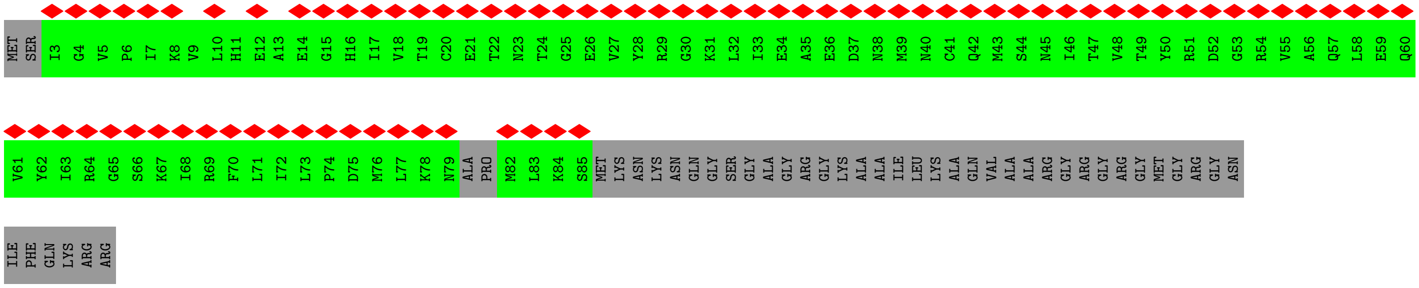
- Molecule 5: U5 small nuclear ribonucleoprotein 40 kDa protein





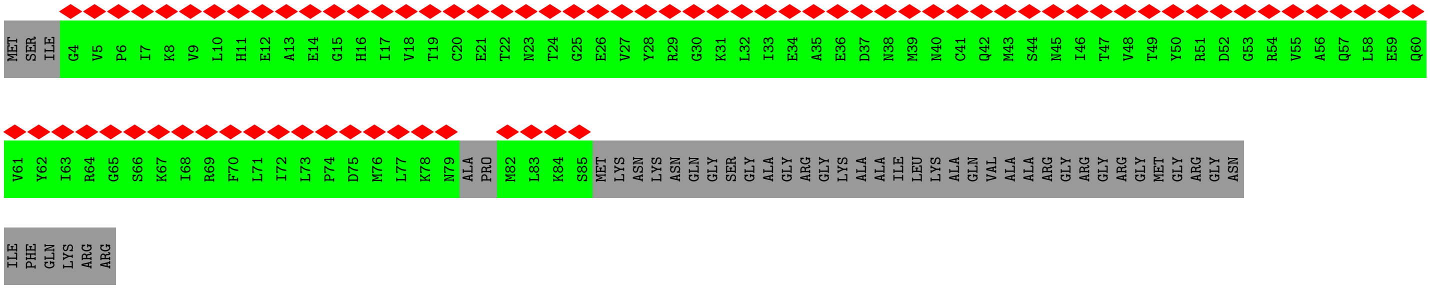
- Molecule 6: Small nuclear ribonucleoprotein Sm D3

Chain a:



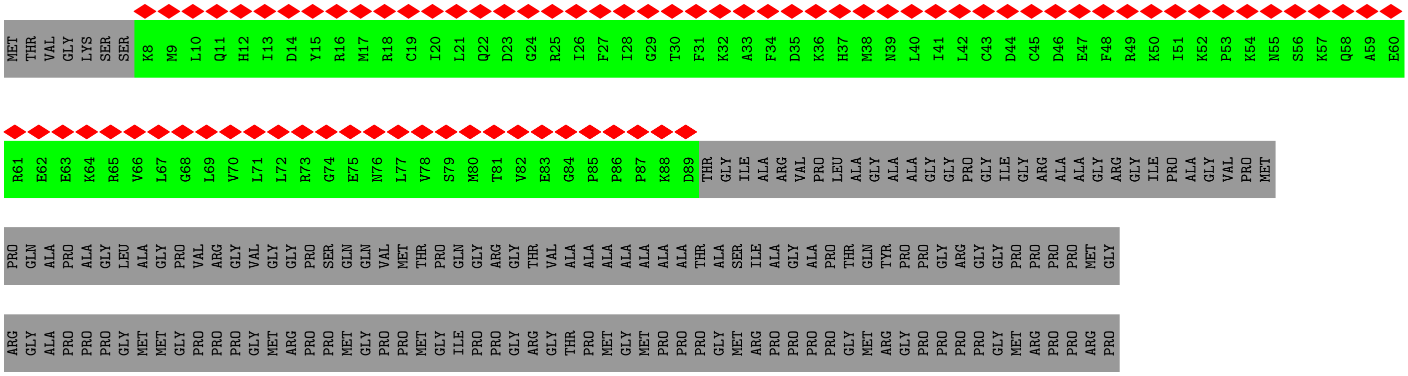
- Molecule 6: Small nuclear ribonucleoprotein Sm D3

Chain h:



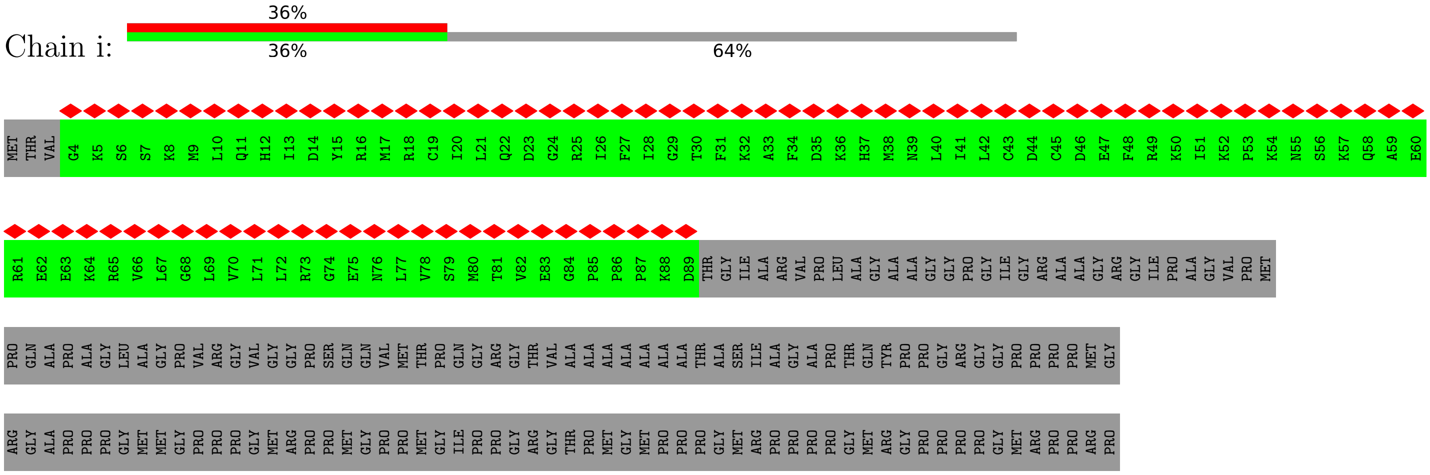
- Molecule 7: Small nuclear ribonucleoprotein-associated proteins B and B’

Chain b:



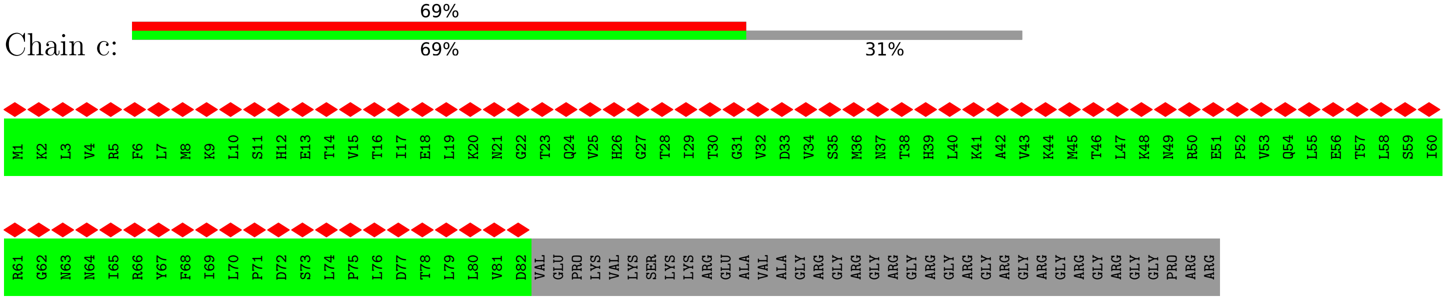
- Molecule 7: Small nuclear ribonucleoprotein-associated proteins B and B’

Chain i:



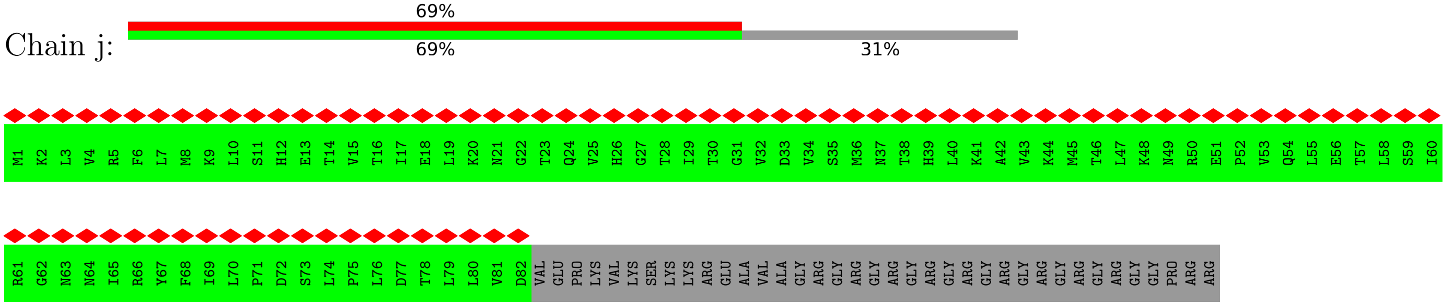
- Molecule 8: Small nuclear ribonucleoprotein Sm D1

Chain c:



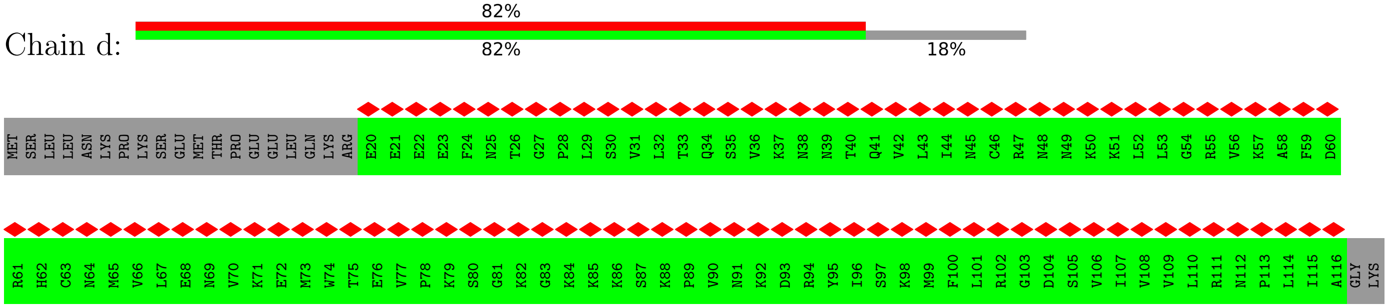
- Molecule 8: Small nuclear ribonucleoprotein Sm D1

Chain j:



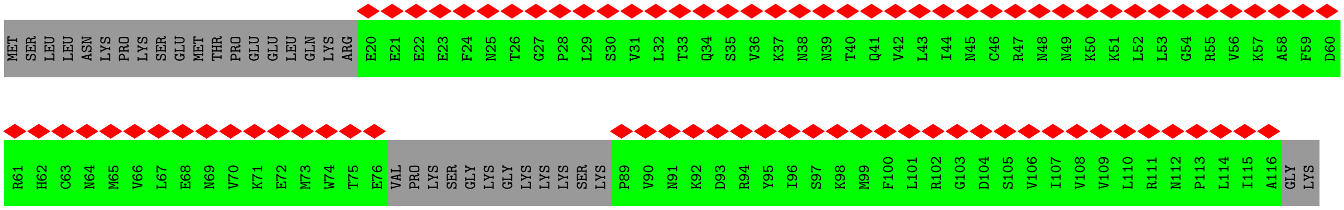
- Molecule 9: Small nuclear ribonucleoprotein Sm D2

Chain d:



- Molecule 9: Small nuclear ribonucleoprotein Sm D2

Chain k:



- Molecule 10: Small nuclear ribonucleoprotein F

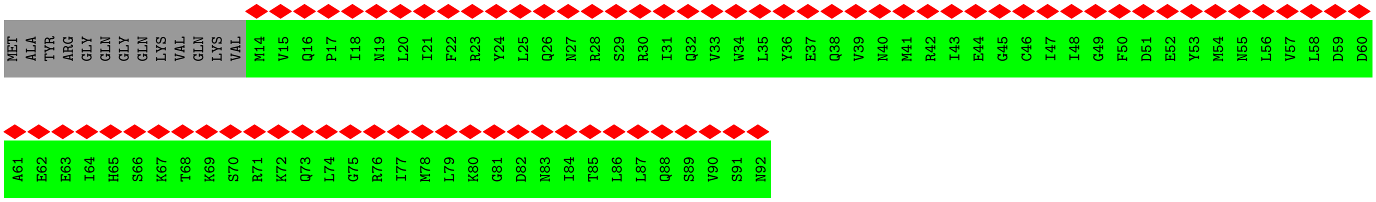
Chain f:

- Molecule 10: Small nuclear ribonucleoprotein F

Chain m:

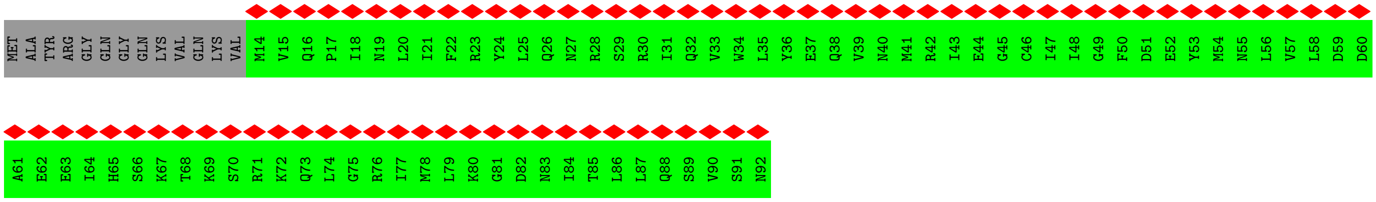
- Molecule 11: Small nuclear ribonucleoprotein E

Chain e:

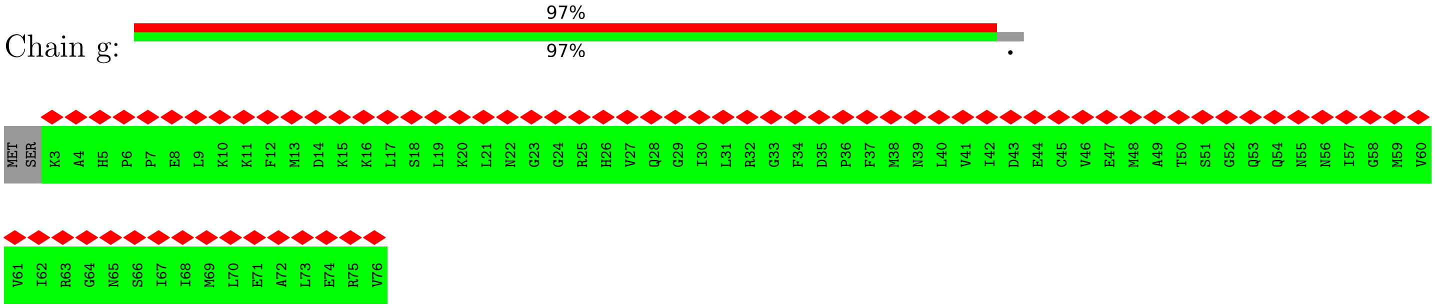


- Molecule 11: Small nuclear ribonucleoprotein E

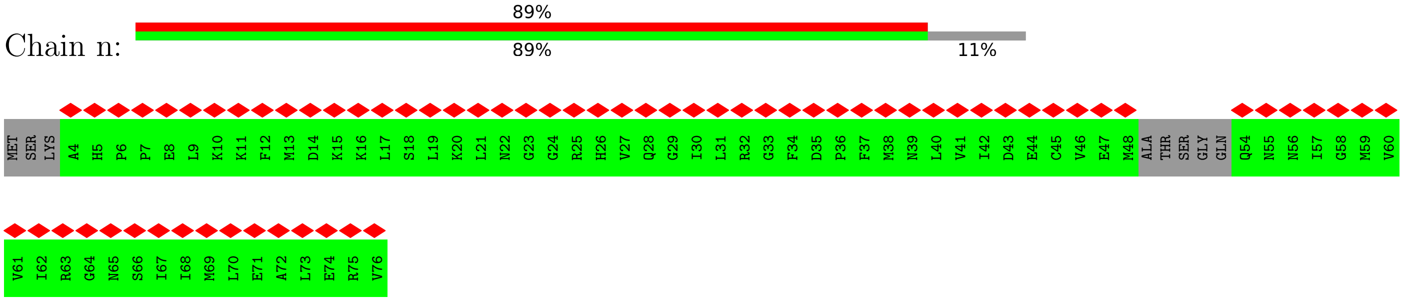
Chain l:



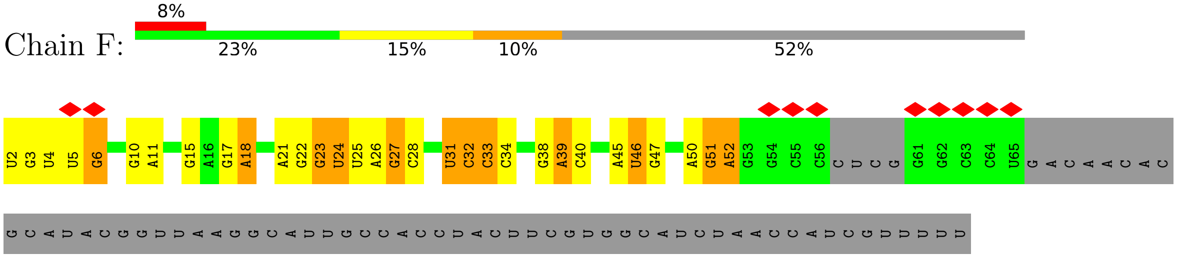
- Molecule 12: Small nuclear ribonucleoprotein G



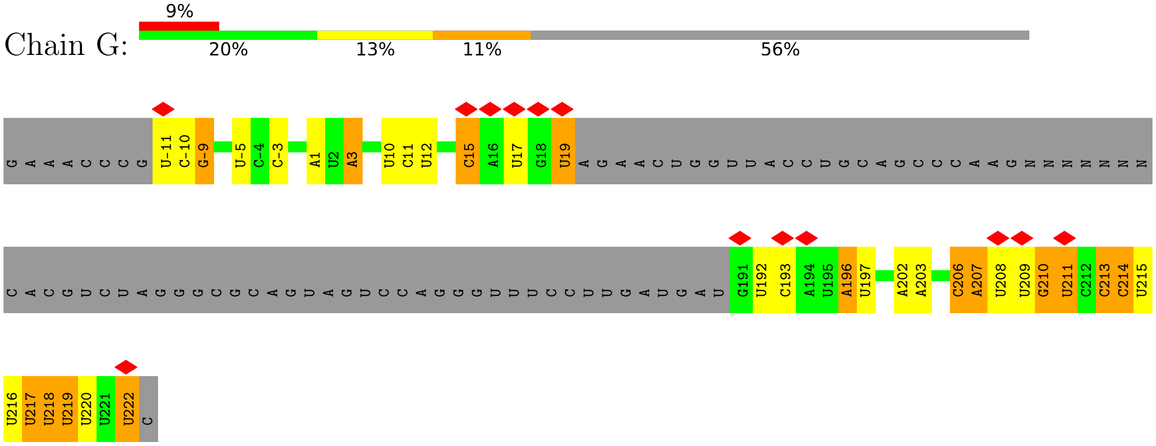
- Molecule 12: Small nuclear ribonucleoprotein G



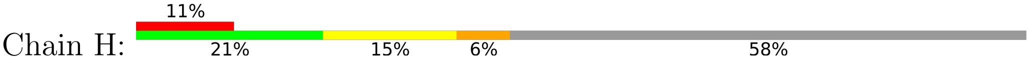
- Molecule 13: U6atac snRNA

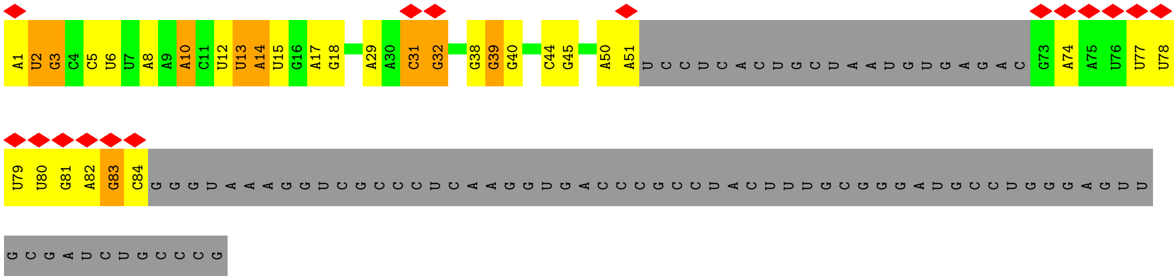


- Molecule 14: pre-mRNA



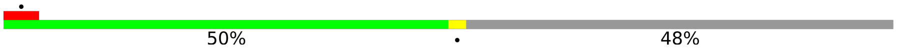
- Molecule 15: U12 snRNA

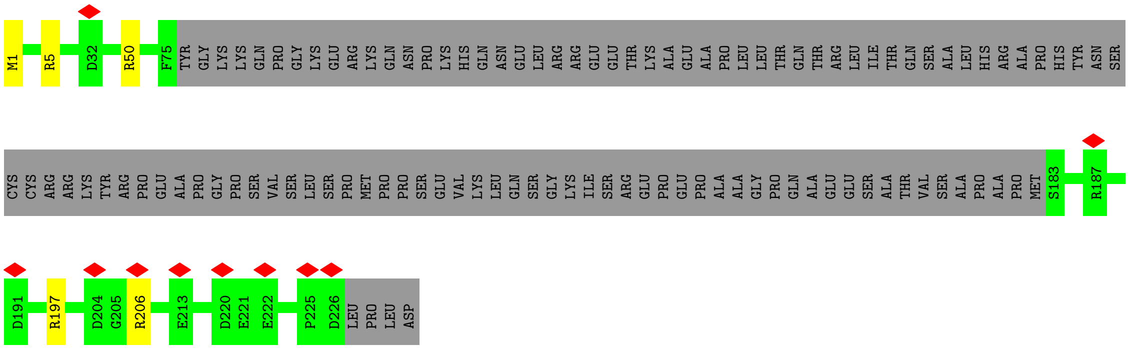




• Molecule 16: Sodium channel modifier 1

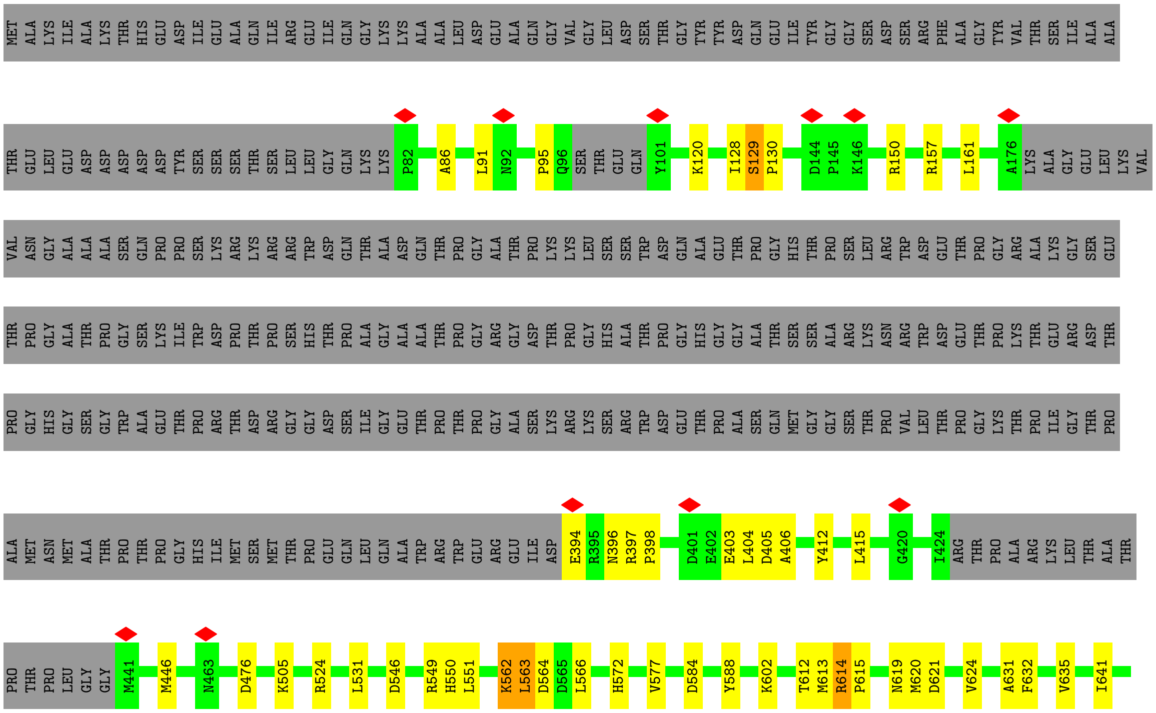
Chain v:

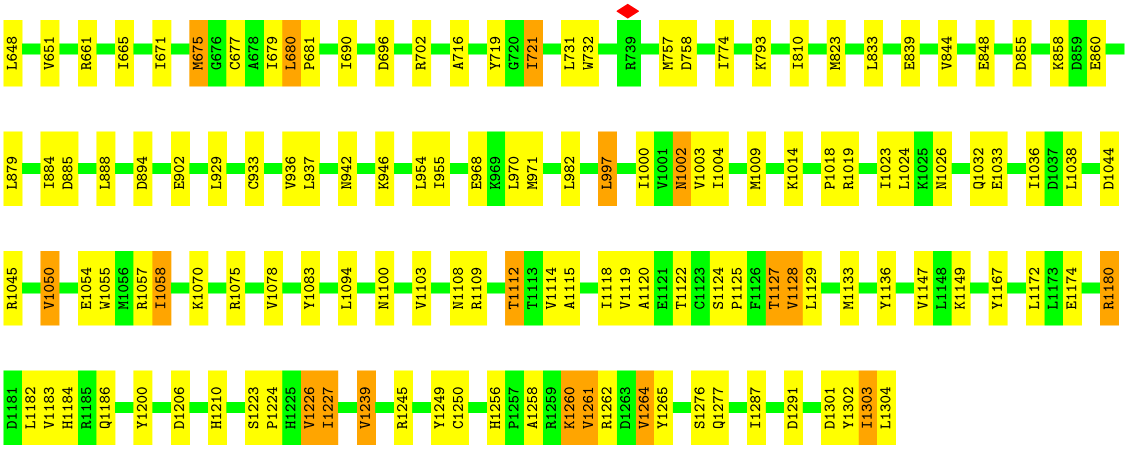




• Molecule 17: Splicing factor 3B subunit 1

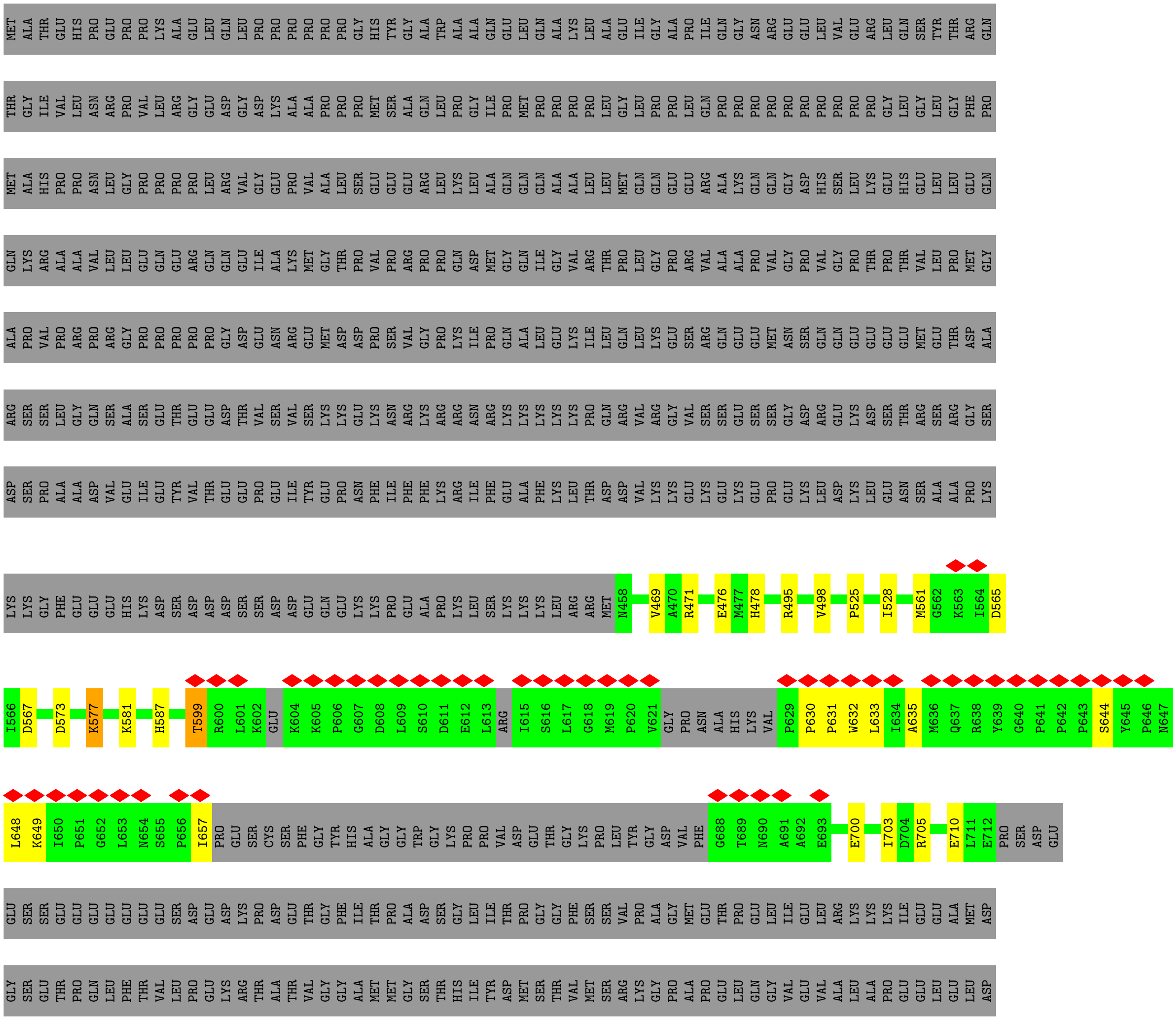
Chain 1:



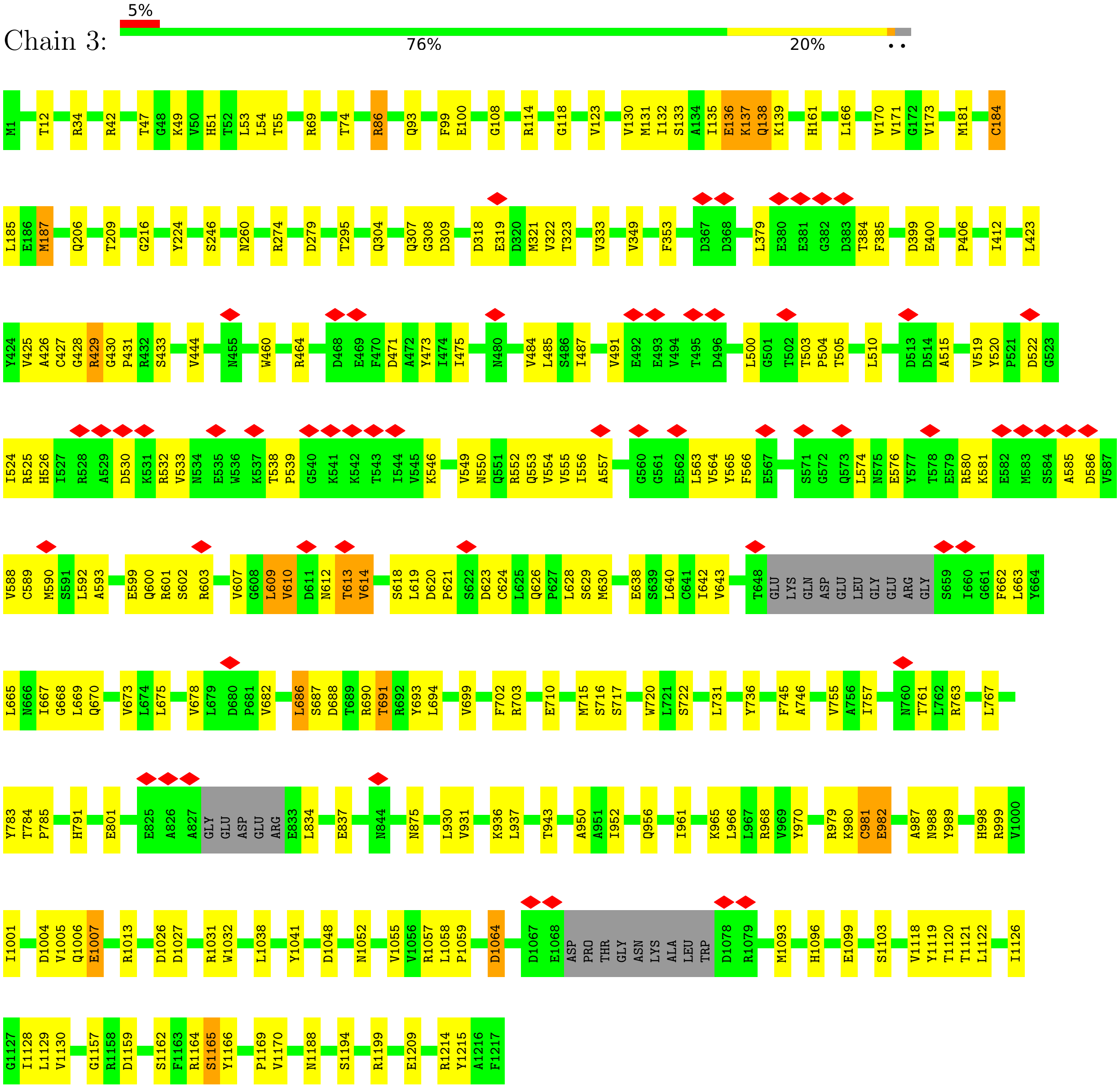


- Molecule 18: Splicing factor 3B subunit 2

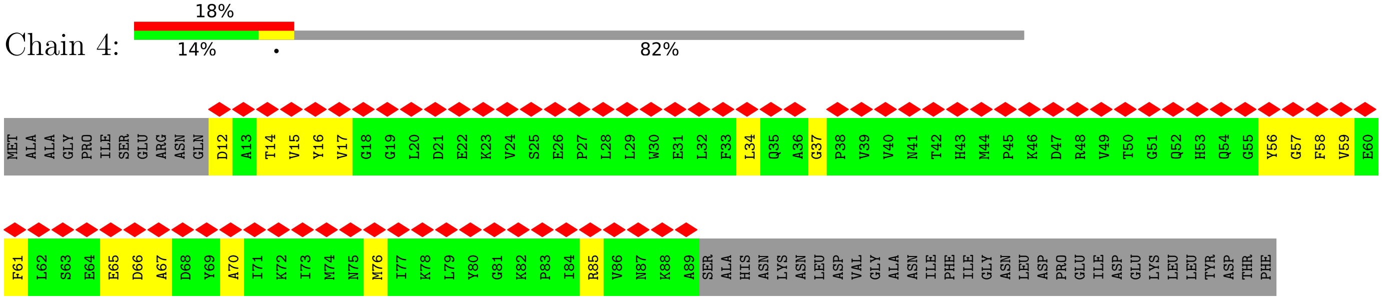
Chain 2:

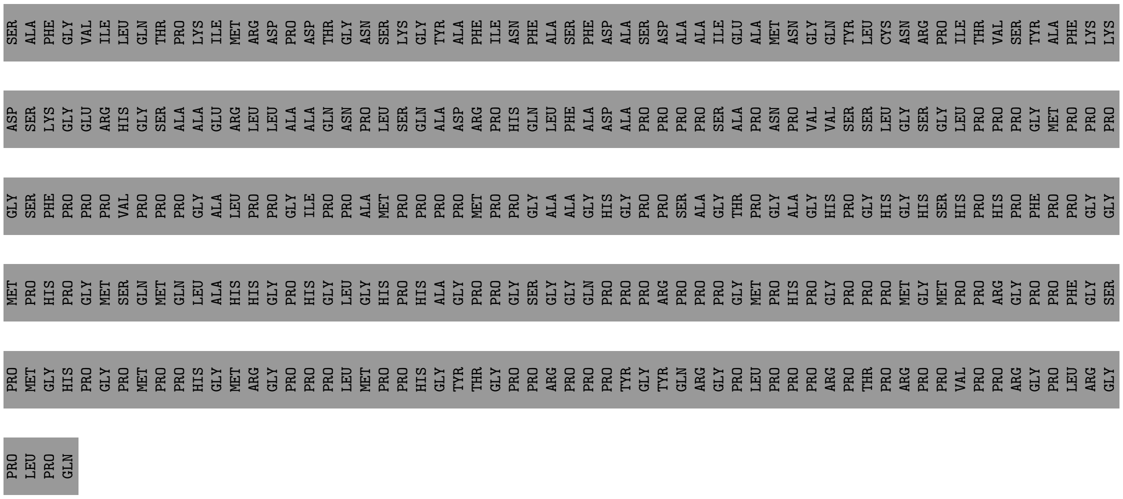


- Molecule 19: Splicing factor 3B subunit 3

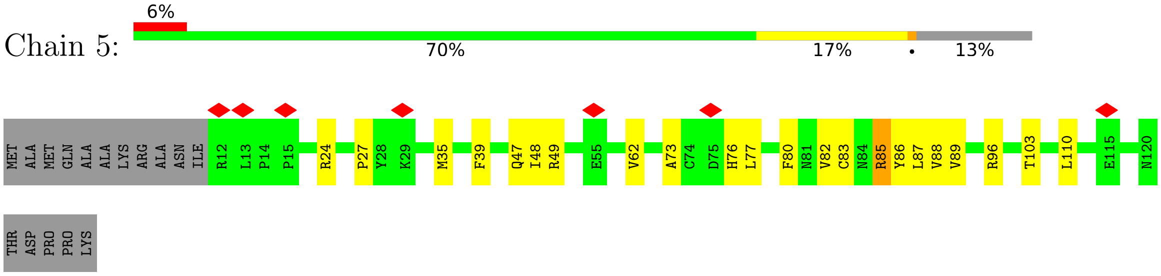


- Molecule 20: Splicing factor 3B subunit 4

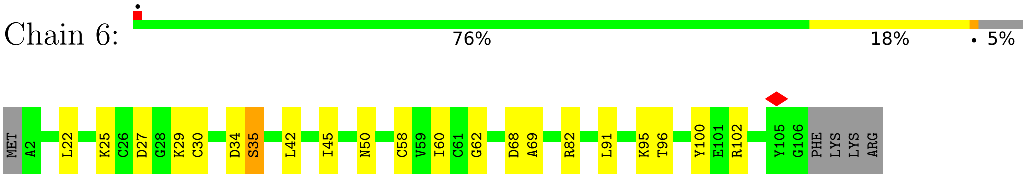




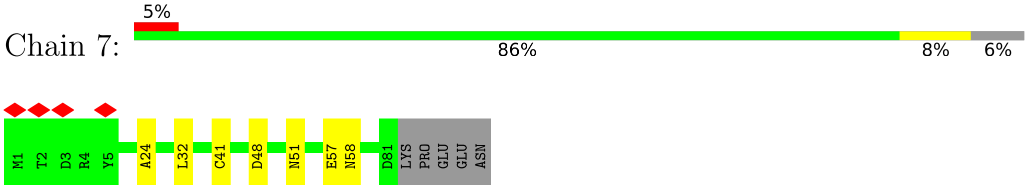
- Molecule 21: Splicing factor 3B subunit 6



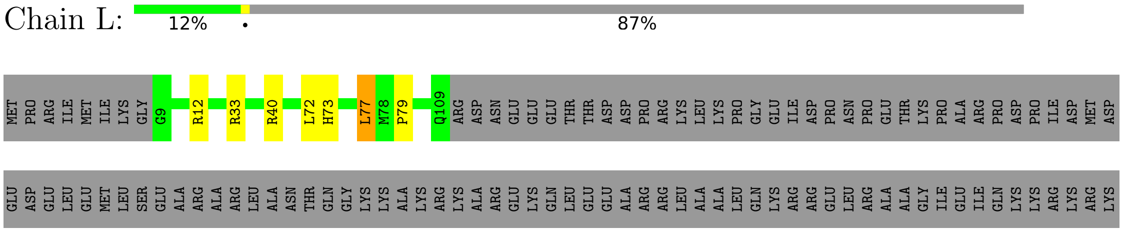
- Molecule 22: PHD finger-like domain-containing protein 5A

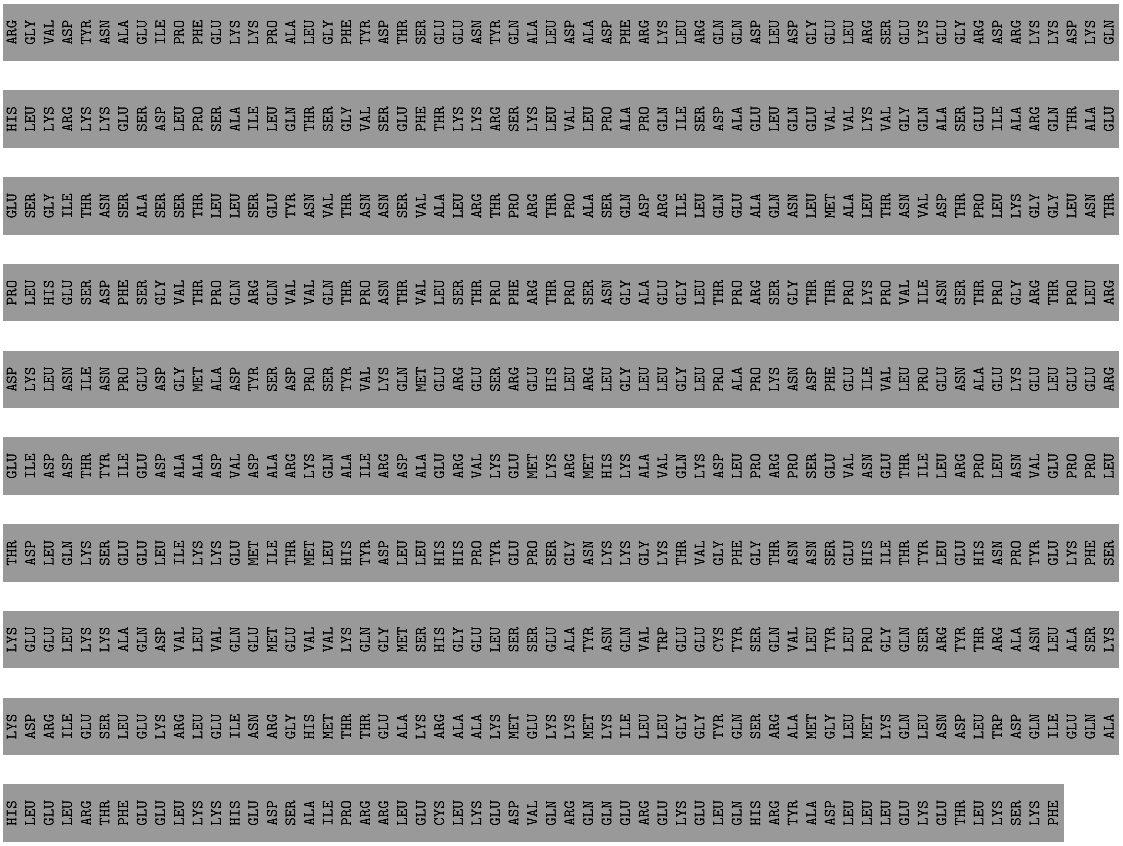


- Molecule 23: Splicing factor 3B subunit 5

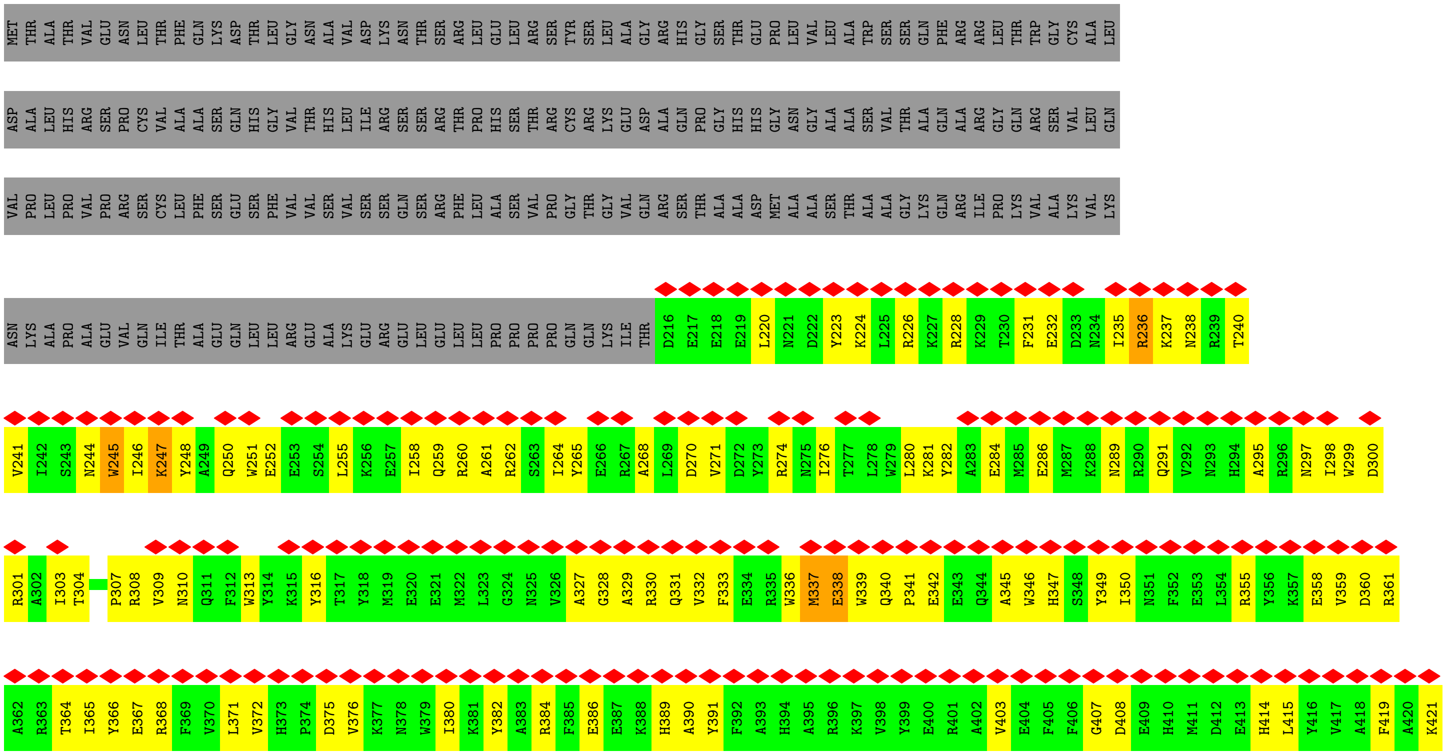


- Molecule 24: Cell division cycle 5-like protein

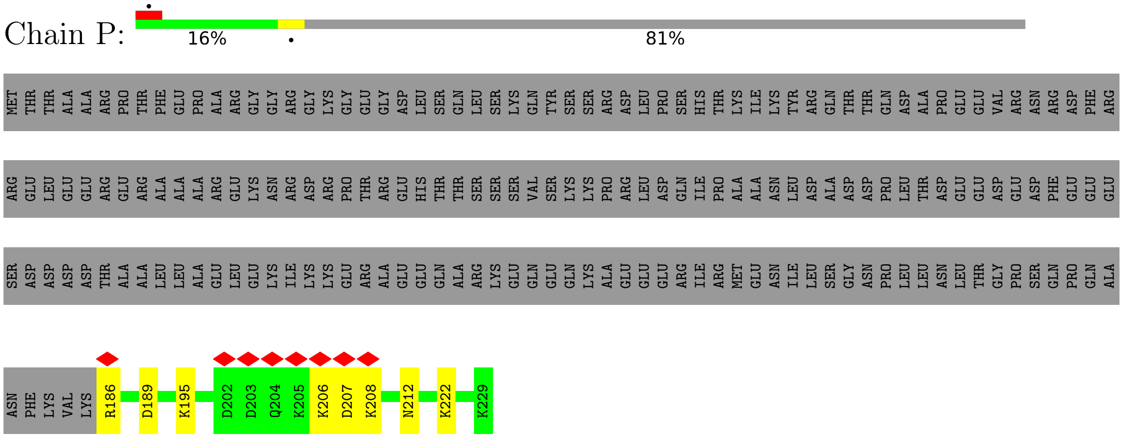




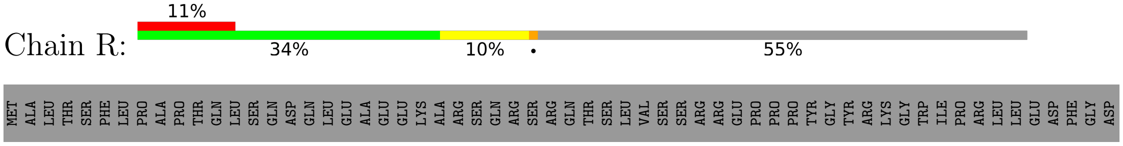
- Molecule 25: Crooked neck-like protein 1

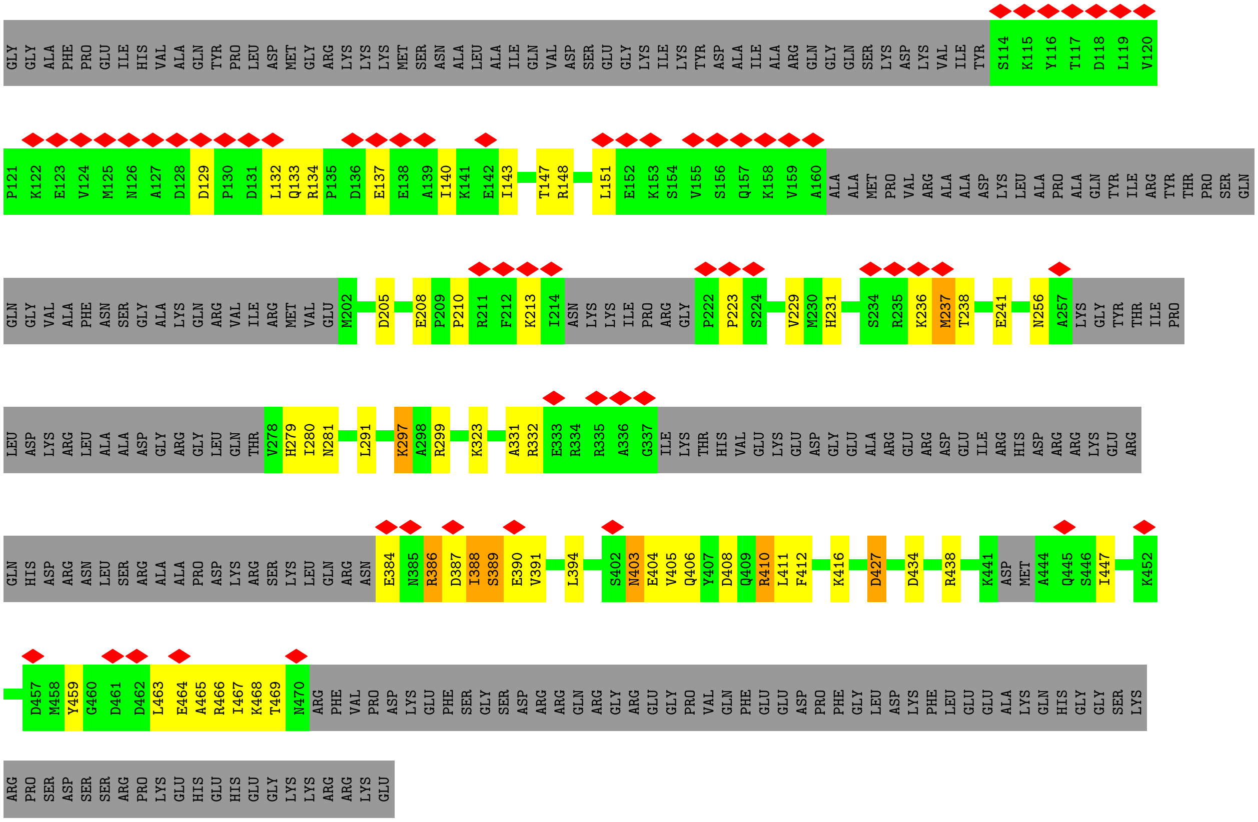


- Molecule 26: Spliceosome-associated protein CWC15 homolog



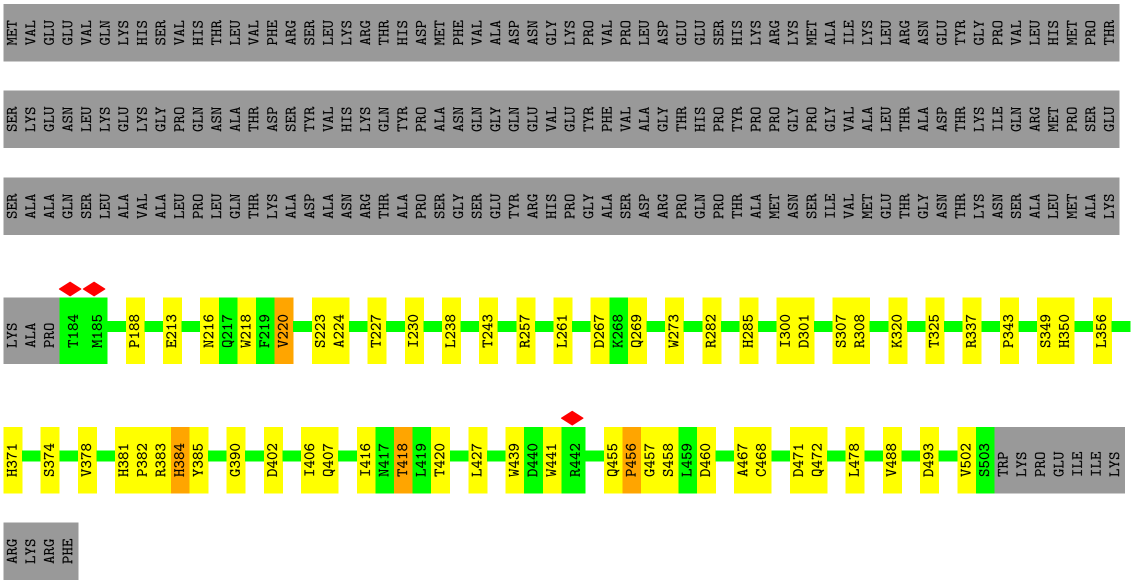
- Molecule 27: SNW domain-containing protein 1





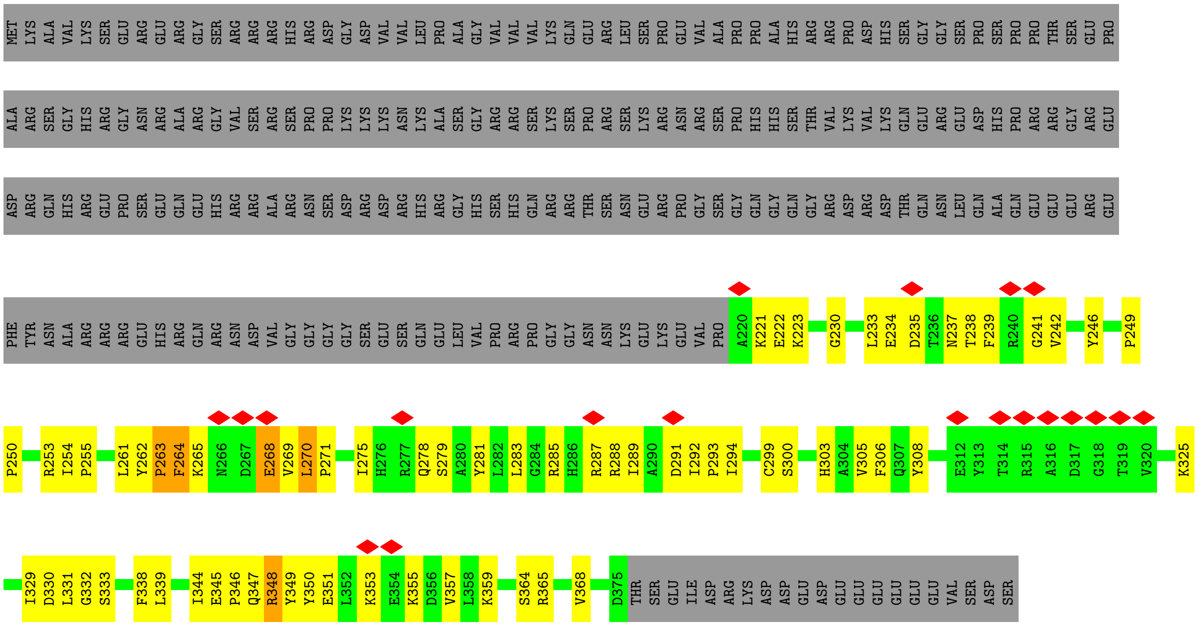
- Molecule 28: Pleiotropic regulator 1

Chain T:



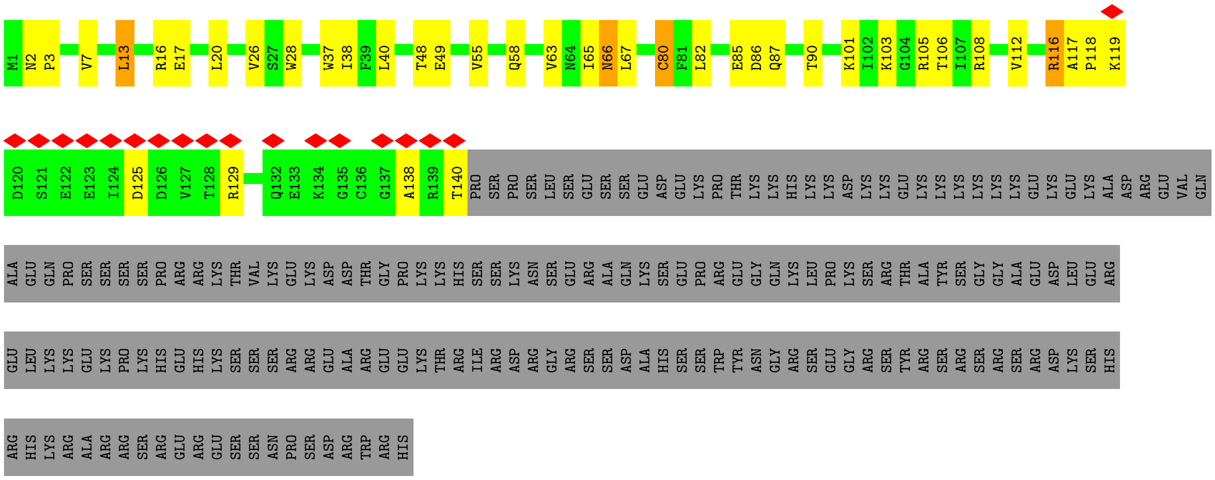
- Molecule 29: Smad nuclear-interacting protein 1

Chain X:



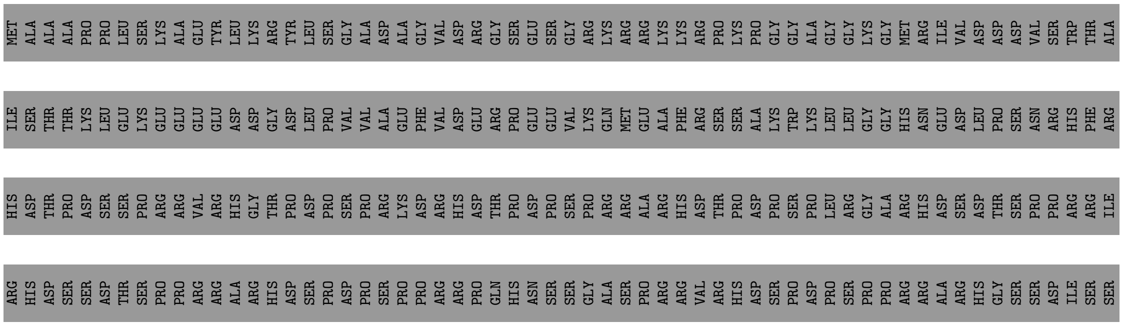
- Molecule 30: RNA-binding motif protein, X-linked 2

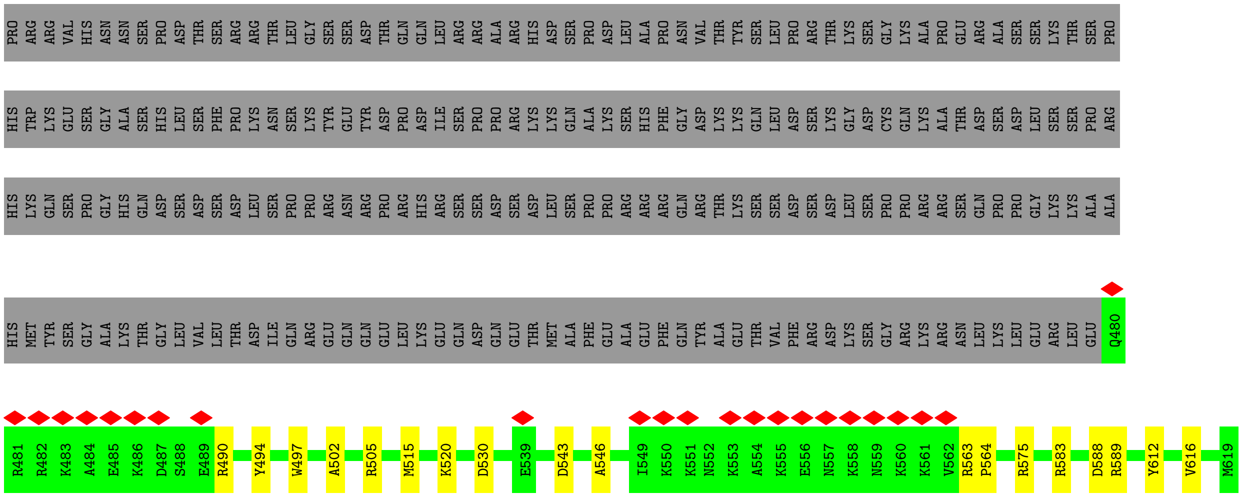
Chain Y:



- Molecule 31: BUD13 homolog

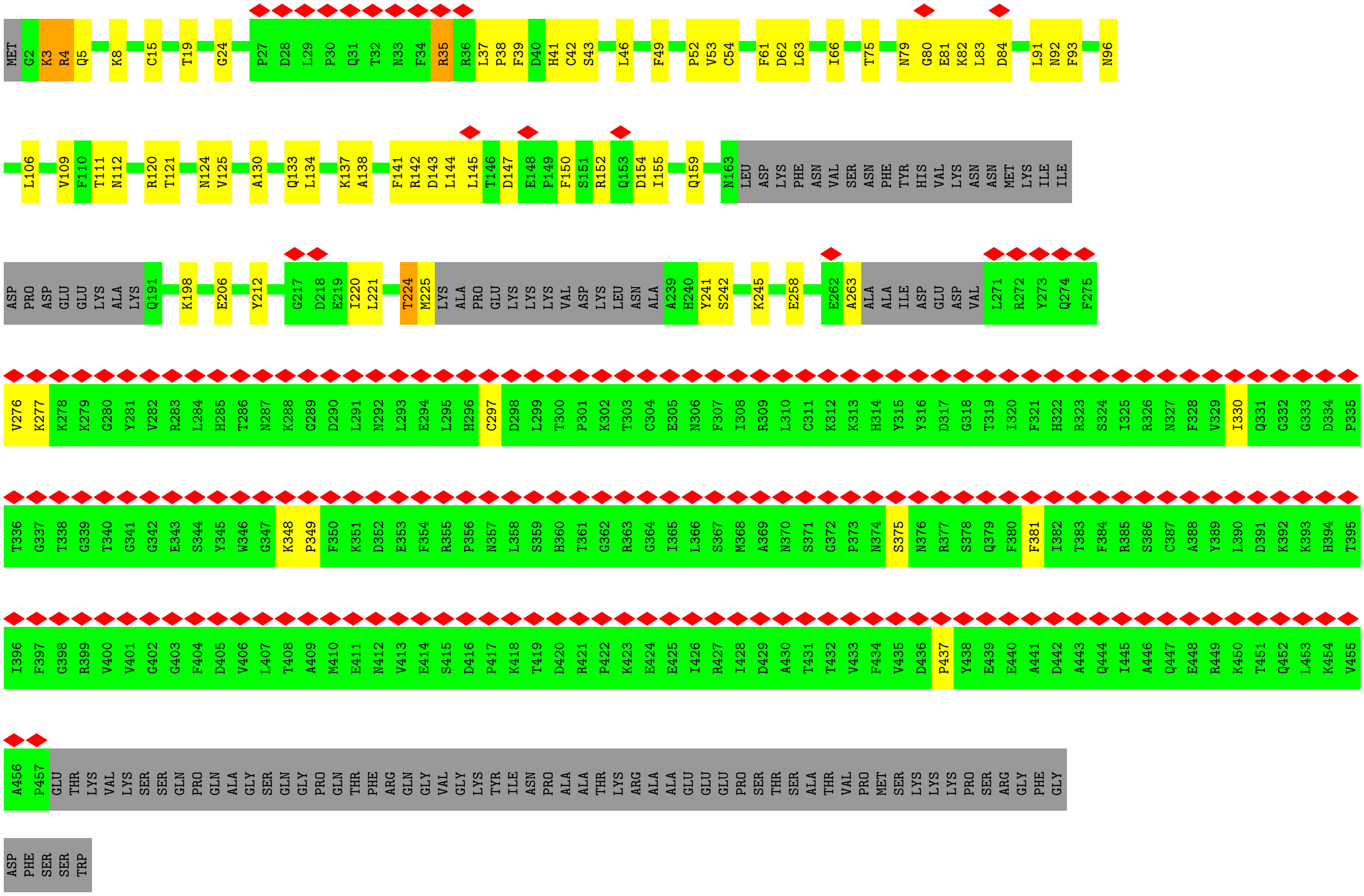
Chain Z:





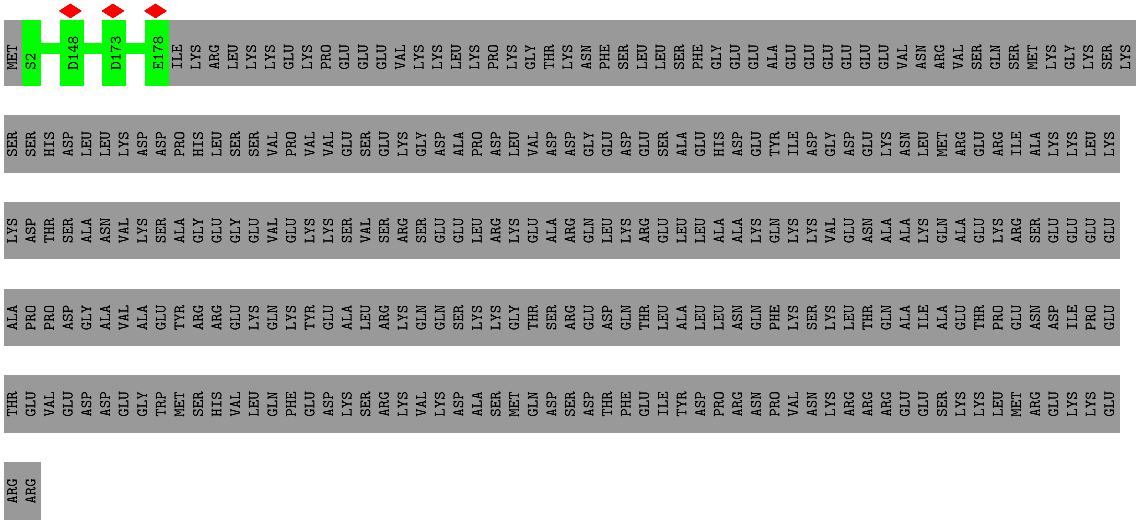
- Molecule 32: RING-type E3 ubiquitin-protein ligase PPIL2

Chain 9:

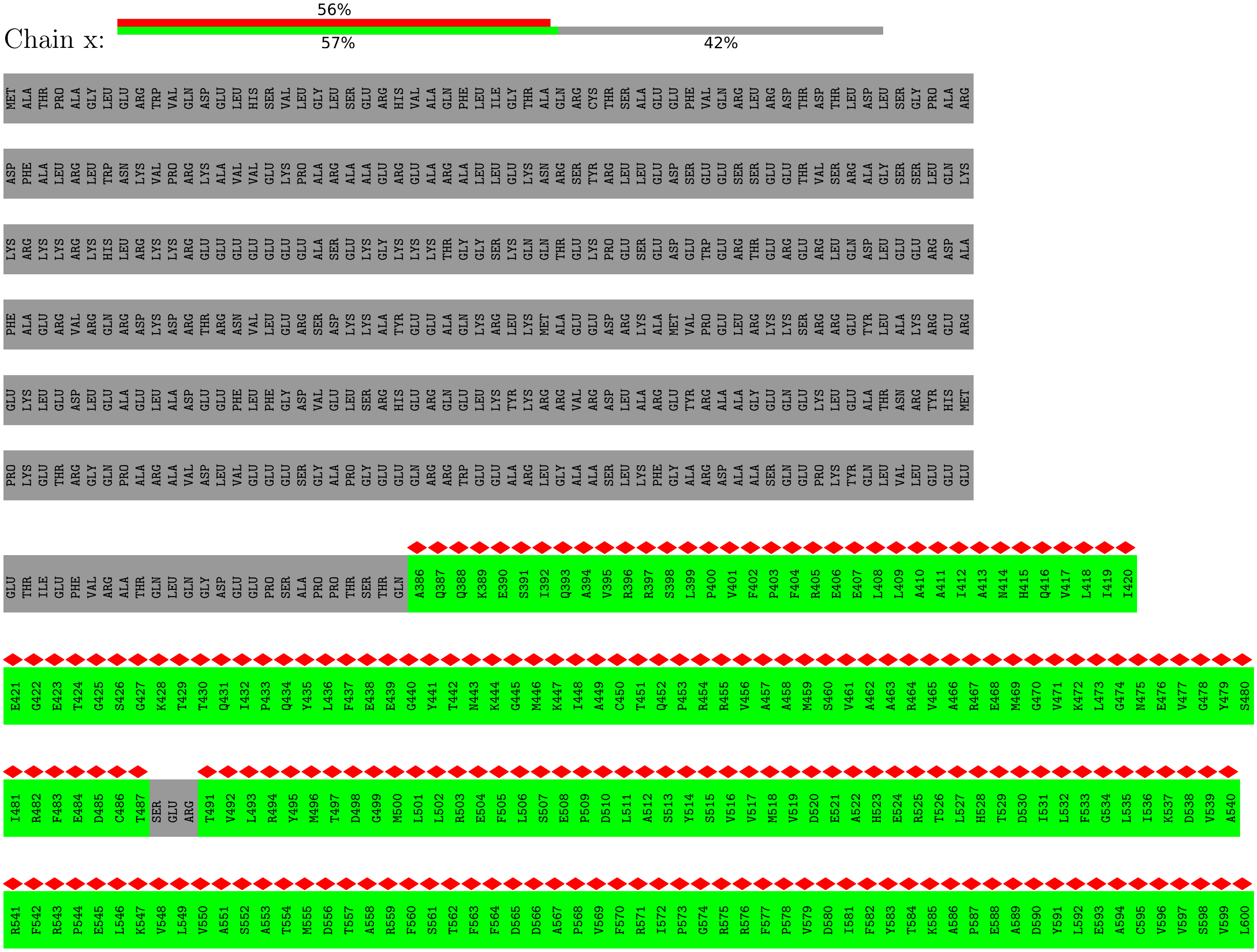


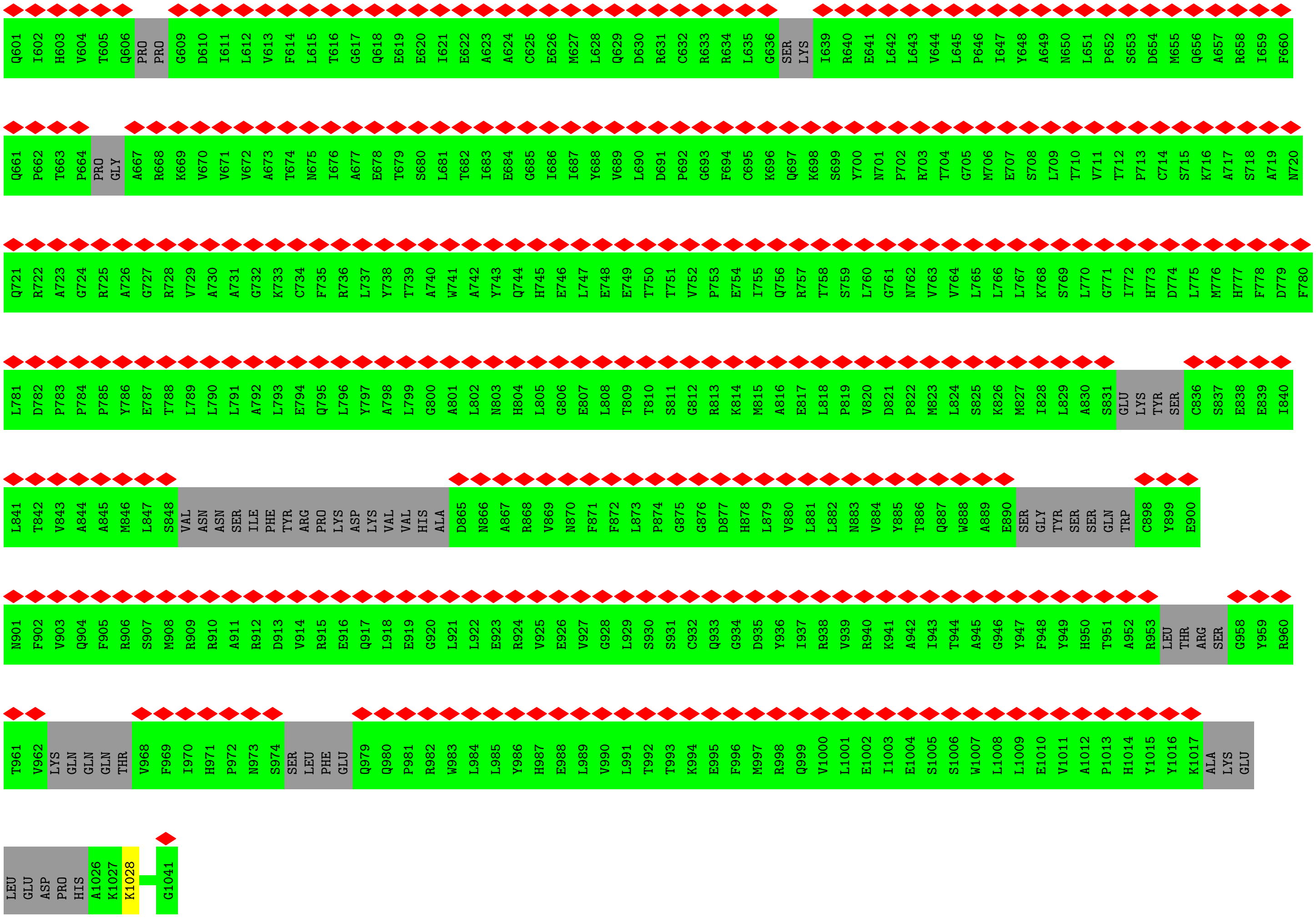
- Molecule 33: Peptidyl-prolyl cis-trans isomerase CWC27 homolog

Chain z:



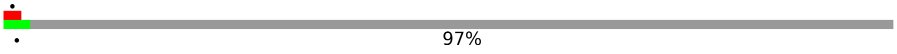
• Molecule 34: Pre-mRNA-splicing factor ATP-dependent RNA helicase DHX16

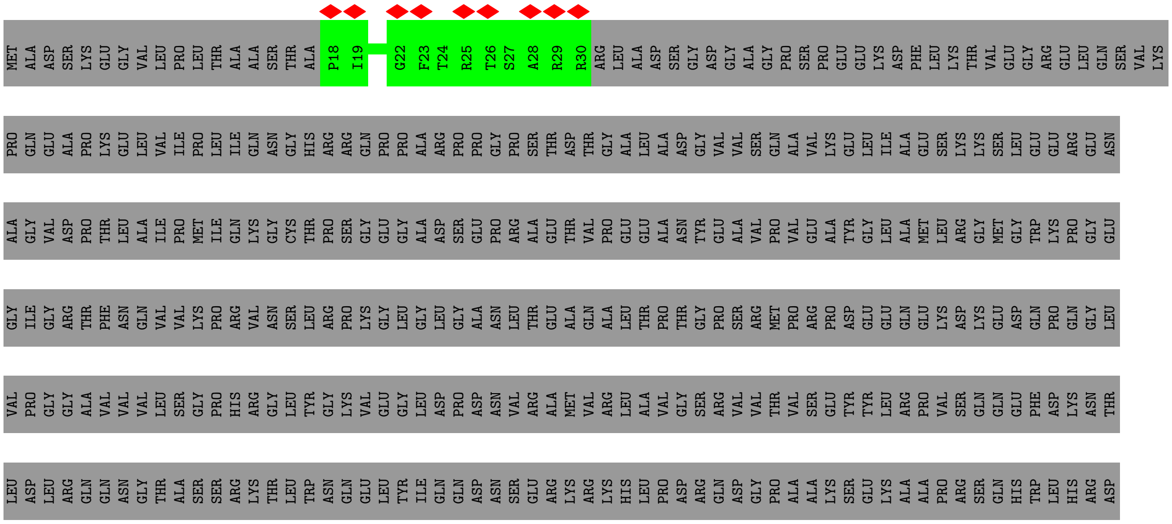


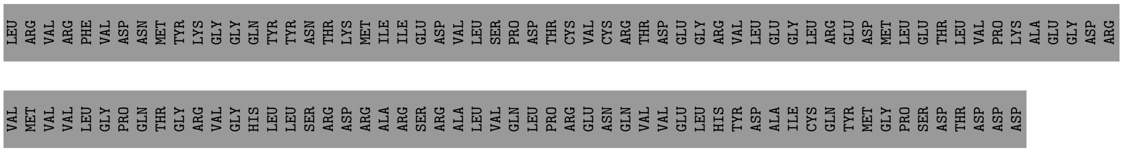


• Molecule 35: G-patch domain and KOW motifs-containing protein

Chain y:

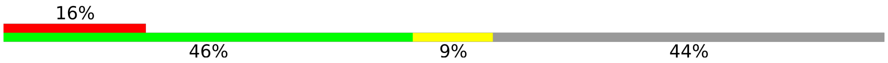


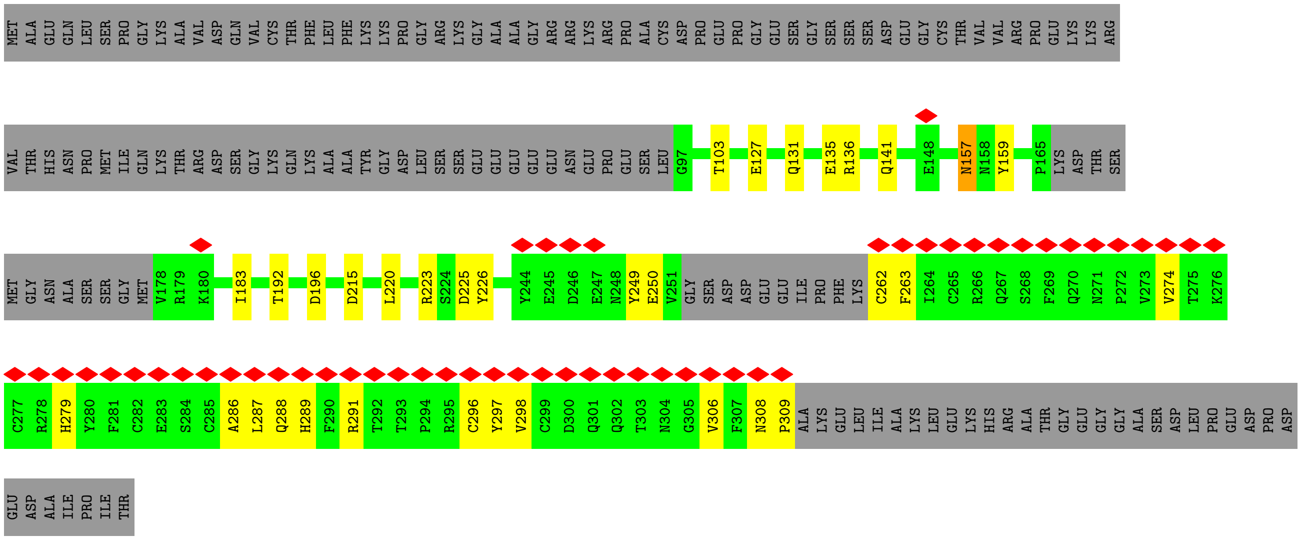




- Molecule 36: RING finger protein 113A

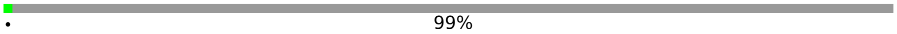
Chain M:

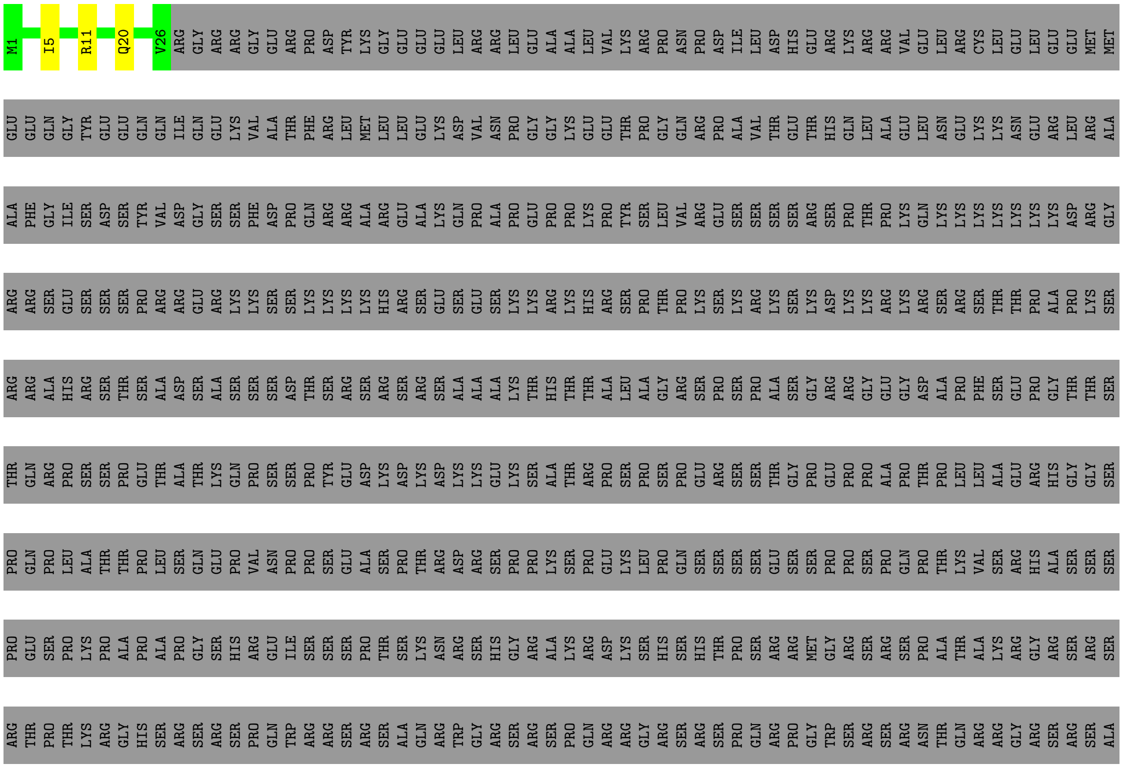


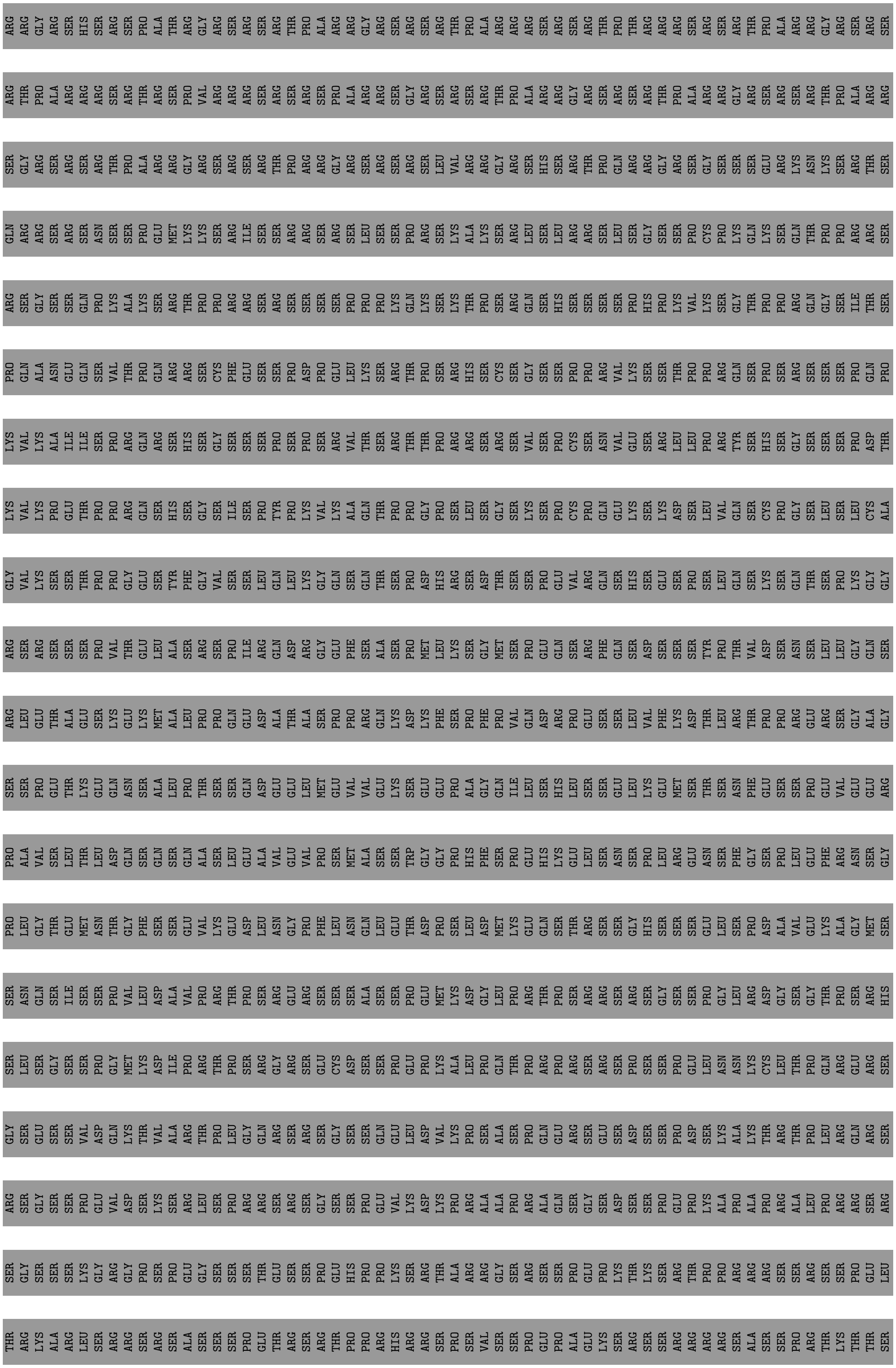


- Molecule 37: Serine/arginine repetitive matrix protein 2

Chain U:



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

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

GLN SER ARG ILE ALA LEU ALA LEU THR ALA ILE SER LEU GLY THR ALA ARG PRO PRO PRO SER MET SER ALA ALA GLY LEU ALA ALA ARG MET SER GLN VAL PRO ALA PRO VAL PRO LEU MET SER LEU ARG THR ALA PRO ALA ALA ASN LEU ALA SER ARG ILE PRO ALA ALA SER ALA

ALA ALA MET ASN LEU ALA SER ALA ARG THR PRO ALA ILE PRO THR ALA VAL ASN LEU ALA ASP SER ARG THR PRO ALA ALA ALA ALA MET ASN LEU ALA SER PRO ARG THR ALA VAL ALA PRO SER ALA VAL ASN LEU ALA ASP PRO ARG THR PRO THR ALA PRO ALA VAL ASN LEU

ALA GLY ALA ARG THR PRO ALA ALA LEU ALA ALA LEU SER LEU THR GLY SER GLY THR PRO PRO THR ALA ALA ASN TYR PRO SER SER SER ARG THR PRO GLN ALA PRO ALA SER ALA ASN LEU VAL GLY PRO ARG SER ALA HIS ALA THR ALA PRO VAL ASN ILE ALA GLY SER ARG THR

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ARG MET THR SER GLU ARG ALA PRO SER PRO SER SER ARG MET GLY GLN ALA PRO SER GLN SER LEU LEU PRO PRO ALA GLN ASP GLN PRO ARG SER PRO VAL PRO SER ALA PHE SER ASP GLN SER ARG CYS LEU ILE ALA GLN THR THR PRO VAL ALA GLY SER GLN SER LEU SER SER

GLY ALA VAL ALA THR THR THR SER SER ALA GLY ASP HIS ASN GLY MET LEU SER VAL PRO ALA PRO GLY VAL PRO HIS SER ASP VAL GLY GLU PRO PRO ALA SER THR GLY ALA GLN GLN PRO SER ALA LEU ALA ALA LEU GLN PRO ALA LYS GLU ARG ARG SER SER SER SER SER SER

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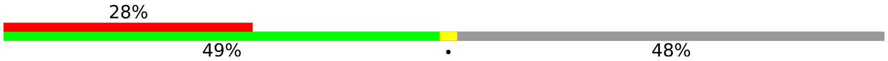
GLY SER ARG ARG GLY GLN ARG GLY ASP SER ARG SER PRO SER HIS LYS ARG ARG ARG GLU THR PRO SER PRO ARG PRO MET ARG HIS ARG SER SER ARG SER PRO

- Molecule 38: Pre-mRNA-splicing factor CWC22 homolog

Chain V:



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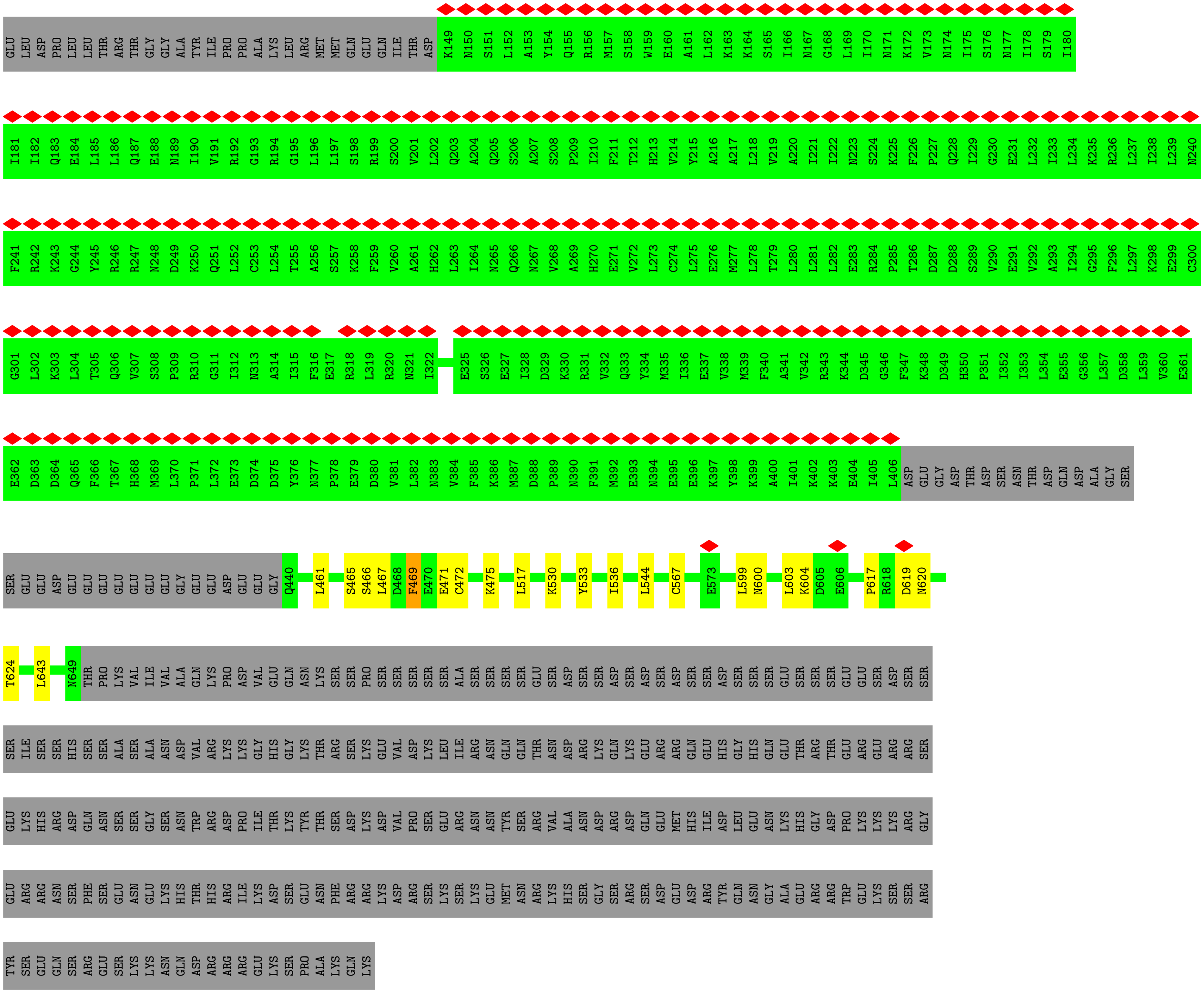
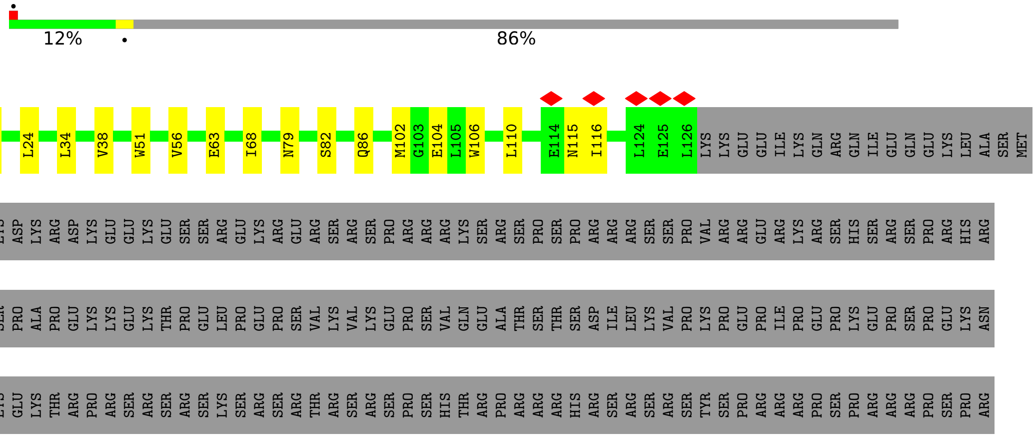
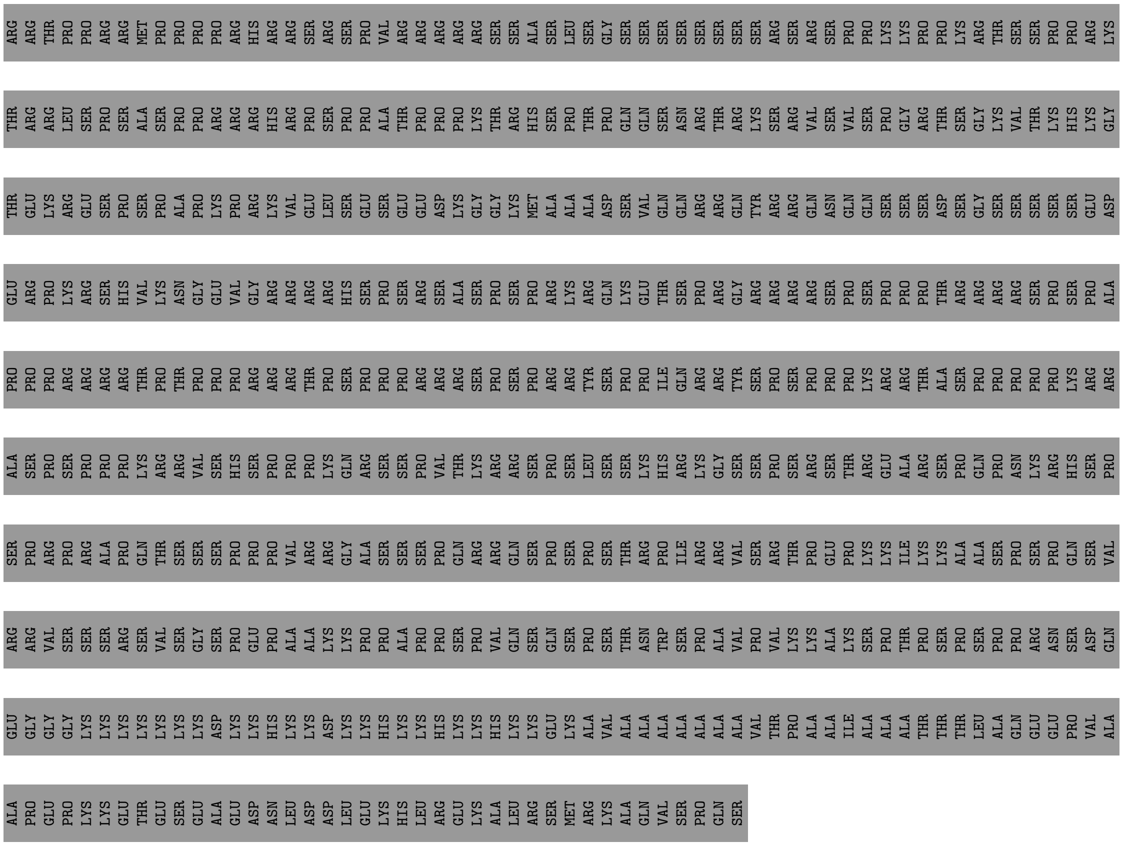
SER TYR ASP SER SER MET GLU SER ARG ASN ARG ASP ARG GLU LYS ARG ARG GLU ARG GLU ARG ASP THR ASP ARG LYS ARG SER ARG LYS SER PRO SER PRO GLY ARG ARG ASN PRO GLU THR SER VAL THR GLN SER SER SER ALA GLN ASP GLU PRO ALA THR LYS LYS LYS LYS ASP



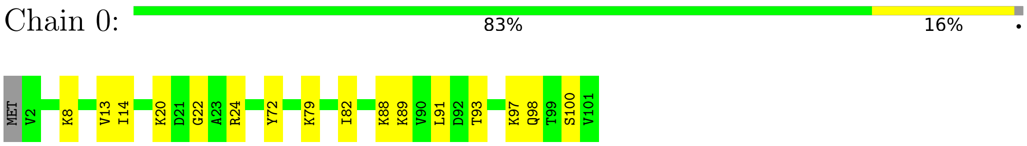
- Molecule 39: Serine/arginine repetitive matrix protein 1

Chain 8:

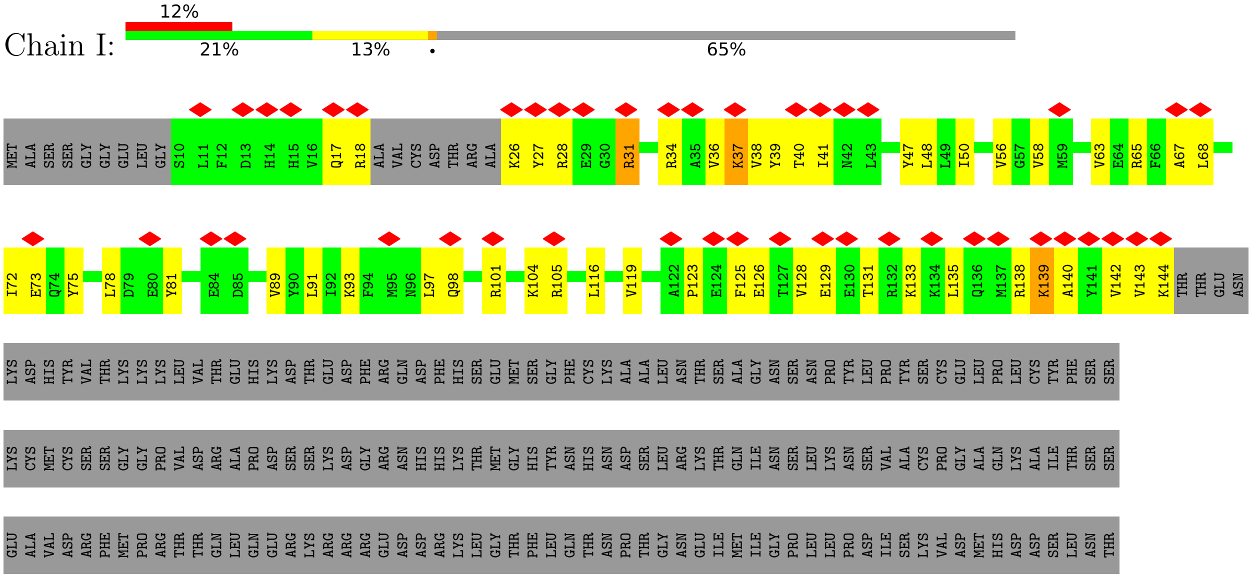




- Molecule 40: Cysteine-rich PDZ-binding protein



- Molecule 41: RNA-binding protein 48



- Molecule 42: Armadillo repeat-containing protein 7

Chain K:

4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	101443	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 $(e^-/\text{Å}^2)$	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.134	Depositor
Minimum map value	-0.056	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.014	Depositor
Map size (Å)	644.52, 644.52, 644.52	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0742, 1.0742, 1.0742	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: K, SEP, GTP, IHP, TPO, G5J, MG, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	1.19	1/18863 (0.0%)	0.77	0/25599
2	B	0.51	0/2115	0.92	0/3284
3	C	1.03	1/7287 (0.0%)	0.79	0/9902
4	D	0.32	0/9225	0.58	0/12826
5	E	0.60	0/2390	0.75	0/3238
6	a	0.43	0/397	0.58	0/549
6	h	0.47	0/390	0.62	0/539
7	b	0.50	0/404	0.72	0/561
7	i	0.50	0/421	0.73	0/583
8	c	0.58	0/405	0.73	0/563
8	j	0.57	0/405	0.73	0/563
9	d	0.66	0/479	0.82	0/666
9	k	0.67	0/420	0.81	0/583
10	f	0.75	0/360	0.82	0/497
10	m	0.75	0/360	0.81	0/497
11	e	0.65	0/390	0.80	0/542
11	l	0.64	0/390	0.81	0/542
12	g	0.54	0/362	0.71	0/501
12	n	0.54	0/332	0.73	0/458
13	F	0.43	0/1449	0.77	0/2257
14	G	0.31	0/1445	0.71	0/2238
15	H	0.45	0/1511	0.72	0/2351
16	v	0.94	0/984	0.66	0/1326
17	1	1.13	0/8025	0.79	0/10859
18	2	1.01	0/1710	0.70	0/2306
19	3	1.03	0/9531	0.74	0/12931
20	4	0.60	0/382	0.70	0/529
21	5	0.88	0/925	0.71	0/1247
22	6	1.15	0/825	0.77	0/1106
23	7	1.29	0/688	0.85	0/930
24	L	1.26	0/864	0.78	0/1165
25	J	0.35	0/3494	0.52	0/4743

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
26	P	1.18	0/391	0.72	0/517
27	R	0.78	0/1954	0.58	0/2622
28	T	1.28	0/2574	0.84	0/3511
29	X	0.31	0/1304	0.52	0/1760
30	Y	1.05	0/1113	0.72	0/1501
31	Z	1.08	0/1153	0.70	0/1548
32	9	0.57	0/2732	0.60	0/3733
33	z	1.09	0/1434	0.76	0/1941
34	x	0.37	0/2996	0.49	0/4142
35	y	0.25	0/107	0.47	0/141
36	M	1.03	0/1609	0.70	0/2164
37	U	0.91	0/196	0.66	0/265
38	V	0.88	0/3042	0.70	0/4152
39	8	0.95	0/1028	0.75	0/1379
40	0	1.01	0/782	0.68	0/1043
41	I	0.42	0/1083	0.53	0/1454
42	K	0.29	0/1333	0.50	0/1826
All	All	0.91	2/102059 (0.0%)	0.72	0/140180

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	204	ASP	C-N	-5.74	1.20	1.34
1	A	279	PHE	C-N	-5.65	1.21	1.34

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	18354	0	18178	381	0
2	B	1898	0	963	36	0
3	C	7125	0	7130	122	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	9215	0	4458	170	0
5	E	2337	0	2272	194	0
6	a	399	0	173	0	0
6	h	392	0	168	0	0
7	b	405	0	170	0	0
7	i	422	0	177	0	0
8	c	406	0	170	0	0
8	j	406	0	170	0	0
9	d	480	0	200	0	0
9	k	422	0	175	0	0
10	f	361	0	158	0	0
10	m	361	0	158	0	0
11	e	391	0	163	0	0
11	l	391	0	163	0	0
12	g	363	0	160	0	0
12	n	334	0	143	0	0
13	F	1294	0	650	41	0
14	G	1303	0	667	46	0
15	H	1350	0	679	30	0
16	v	963	0	945	0	0
17	1	7879	0	8044	165	0
18	2	1674	0	1580	23	0
19	3	9352	0	9273	220	0
20	4	383	0	173	24	0
21	5	906	0	913	31	0
22	6	811	0	788	20	0
23	7	669	0	631	6	0
24	L	843	0	852	15	0
25	J	3457	0	2537	157	0
26	P	384	0	382	10	0
27	R	1923	0	1889	117	0
28	T	2507	0	2451	41	0
29	X	1271	0	1252	92	0
30	Y	1095	0	1083	59	0
31	Z	1129	0	1077	20	0
32	9	2691	0	2121	91	0
33	z	1400	0	1344	0	0
34	x	3007	0	1453	0	0
35	y	105	0	107	0	0
36	M	1572	0	1483	36	0
37	U	193	0	196	3	0
38	V	3008	0	2291	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	8	1011	0	1035	17	0
40	0	770	0	778	28	0
41	I	1062	0	1067	67	0
42	K	1314	0	1177	100	0
43	A	36	0	6	0	0
44	C	32	0	12	3	0
45	C	1	0	0	0	0
45	F	4	0	0	0	0
46	F	2	0	0	0	0
47	F	33	0	0	3	0
48	0	2	0	0	0	0
48	6	3	0	0	0	0
48	M	1	0	0	0	0
48	v	1	0	0	0	0
49	C	3	0	0	0	0
All	All	99906	0	84285	2086	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 12.

The worst 5 of 2086 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)
17:1:641:ILE:HD11	17:1:675:MET:CE	1.58	1.34
20:4:14:THR:HA	20:4:59:VAL:O	1.32	1.30
25:J:337:MET:HE2	25:J:346:TRP:CH2	1.69	1.26
5:E:62:LEU:HD12	5:E:351:LEU:CD1	1.66	1.26
5:E:62:LEU:CD1	5:E:351:LEU:HD12	1.68	1.23

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	2213/2335 (95%)	2146 (97%)	66 (3%)	1 (0%)	100	100
3	C	900/972 (93%)	862 (96%)	38 (4%)	0	100	100
4	D	1799/2136 (84%)	1710 (95%)	84 (5%)	5 (0%)	41	71
5	E	297/357 (83%)	278 (94%)	19 (6%)	0	100	100
6	a	77/126 (61%)	76 (99%)	1 (1%)	0	100	100
6	h	76/126 (60%)	74 (97%)	2 (3%)	0	100	100
7	b	80/240 (33%)	78 (98%)	2 (2%)	0	100	100
7	i	84/240 (35%)	82 (98%)	2 (2%)	0	100	100
8	c	80/119 (67%)	77 (96%)	3 (4%)	0	100	100
8	j	80/119 (67%)	77 (96%)	3 (4%)	0	100	100
9	d	95/118 (80%)	91 (96%)	4 (4%)	0	100	100
9	k	81/118 (69%)	78 (96%)	3 (4%)	0	100	100
10	f	72/86 (84%)	68 (94%)	4 (6%)	0	100	100
10	m	72/86 (84%)	68 (94%)	4 (6%)	0	100	100
11	e	77/92 (84%)	76 (99%)	1 (1%)	0	100	100
11	l	77/92 (84%)	76 (99%)	1 (1%)	0	100	100
12	g	72/76 (95%)	70 (97%)	2 (3%)	0	100	100
12	n	64/76 (84%)	62 (97%)	2 (3%)	0	100	100
16	v	115/230 (50%)	113 (98%)	2 (2%)	0	100	100
17	1	977/1304 (75%)	961 (98%)	16 (2%)	0	100	100
18	2	206/895 (23%)	198 (96%)	8 (4%)	0	100	100
19	3	1184/1217 (97%)	1136 (96%)	48 (4%)	0	100	100
20	4	76/424 (18%)	71 (93%)	5 (7%)	0	100	100
21	5	107/125 (86%)	104 (97%)	3 (3%)	0	100	100
22	6	103/110 (94%)	98 (95%)	5 (5%)	0	100	100
23	7	79/86 (92%)	78 (99%)	1 (1%)	0	100	100
24	L	99/802 (12%)	93 (94%)	6 (6%)	0	100	100
25	J	483/848 (57%)	447 (92%)	36 (8%)	0	100	100
26	P	42/229 (18%)	37 (88%)	5 (12%)	0	100	100
27	R	229/536 (43%)	219 (96%)	10 (4%)	0	100	100
28	T	318/514 (62%)	310 (98%)	8 (2%)	0	100	100
29	X	154/396 (39%)	137 (89%)	16 (10%)	1 (1%)	25	58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	Y	138/322 (43%)	135 (98%)	3 (2%)	0	100	100
31	Z	138/619 (22%)	137 (99%)	1 (1%)	0	100	100
32	9	401/520 (77%)	382 (95%)	18 (4%)	1 (0%)	47	78
33	z	175/472 (37%)	169 (97%)	6 (3%)	0	100	100
34	x	575/1041 (55%)	554 (96%)	21 (4%)	0	100	100
35	y	11/476 (2%)	11 (100%)	0	0	100	100
36	M	185/343 (54%)	172 (93%)	13 (7%)	0	100	100
37	U	24/2752 (1%)	24 (100%)	0	0	100	100
38	V	464/908 (51%)	457 (98%)	7 (2%)	0	100	100
39	8	124/904 (14%)	124 (100%)	0	0	100	100
40	0	98/101 (97%)	98 (100%)	0	0	100	100
41	I	124/367 (34%)	120 (97%)	4 (3%)	0	100	100
42	K	186/198 (94%)	183 (98%)	2 (1%)	1 (0%)	29	61
All	All	13111/24253 (54%)	12617 (96%)	485 (4%)	9 (0%)	54	82

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	1584	ILE
4	D	1864	GLU
1	A	1092	ILE
29	X	263	PRO
42	K	127	PRO

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	
1	A	1979/2108 (94%)	1924 (97%)	55 (3%)	43	76
3	C	798/866 (92%)	787 (99%)	11 (1%)	67	89
4	D	76/1908 (4%)	62 (82%)	14 (18%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	255/300 (85%)	245 (96%)	10 (4%)	32	66
16	v	104/199 (52%)	99 (95%)	5 (5%)	25	58
17	1	854/1103 (77%)	820 (96%)	34 (4%)	31	65
18	2	163/776 (21%)	158 (97%)	5 (3%)	40	74
19	3	1031/1050 (98%)	997 (97%)	34 (3%)	38	72
21	5	97/109 (89%)	96 (99%)	1 (1%)	76	92
22	6	90/95 (95%)	87 (97%)	3 (3%)	38	72
23	7	72/77 (94%)	72 (100%)	0	100	100
24	L	87/709 (12%)	86 (99%)	1 (1%)	73	92
25	J	203/751 (27%)	197 (97%)	6 (3%)	41	75
26	P	42/203 (21%)	41 (98%)	1 (2%)	49	79
27	R	206/459 (45%)	194 (94%)	12 (6%)	20	50
28	T	273/441 (62%)	268 (98%)	5 (2%)	59	85
29	X	134/349 (38%)	127 (95%)	7 (5%)	23	55
30	Y	117/291 (40%)	113 (97%)	4 (3%)	37	71
31	Z	110/545 (20%)	108 (98%)	2 (2%)	59	85
32	9	195/456 (43%)	190 (97%)	5 (3%)	46	77
33	z	152/416 (36%)	152 (100%)	0	100	100
34	x	14/897 (2%)	13 (93%)	1 (7%)	14	40
35	y	11/397 (3%)	11 (100%)	0	100	100
36	M	168/294 (57%)	165 (98%)	3 (2%)	59	85
37	U	21/2432 (1%)	20 (95%)	1 (5%)	25	58
38	V	193/838 (23%)	190 (98%)	3 (2%)	62	86
39	8	111/831 (13%)	111 (100%)	0	100	100
40	0	86/87 (99%)	84 (98%)	2 (2%)	50	80
41	I	112/326 (34%)	108 (96%)	4 (4%)	35	69
42	K	119/171 (70%)	108 (91%)	11 (9%)	9	27
All	All	7873/19484 (40%)	7633 (97%)	240 (3%)	44	75

5 of 240 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	1	1127	THR

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Mol	Chain	Res	Type
38	V	469	PHE
19	3	295	THR
37	U	20	GLN
42	K	136	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
40	0	98	GLN
39	8	88	ASN
19	3	51	HIS
30	Y	66	ASN
17	1	1252	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
13	F	58/124 (46%)	14 (24%)	3 (5%)
14	G	62/142 (43%)	22 (35%)	5 (8%)
15	H	61/150 (40%)	14 (22%)	0
2	B	87/117 (74%)	21 (24%)	2 (2%)
All	All	268/533 (50%)	71 (26%)	10 (3%)

5 of 71 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	20	G
2	B	21	A
2	B	22	U
2	B	24	G
2	B	25	C

5 of 10 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
14	G	213	C
14	G	217	U
14	G	219	U
13	F	31	U
13	F	51	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	$\#\|Z\| > 2$
19	TPO	3	613	19	8,10,11	0.89	0	10,14,16	1.61	2 (20%)
17	SEP	1	129	17	8,9,10	1.07	1 (12%)	8,12,14	1.70	3 (37%)

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
19	TPO	3	613	19	-	2/9/11/13	-
17	SEP	1	129	17	-	4/5/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	1	129	SEP	P-O1P	2.12	1.57	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	3	613	TPO	P-OG1-CB	-4.43	109.83	123.21
17	1	129	SEP	P-OG-CB	-2.83	110.49	118.30
19	3	613	TPO	O-C-CA	-2.22	118.95	124.78
17	1	129	SEP	O3P-P-OG	2.17	112.52	106.73
17	1	129	SEP	OG-CB-CA	2.09	110.18	108.14

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	1	129	SEP	N-CA-CB-OG
17	1	129	SEP	CB-OG-P-O1P
17	1	129	SEP	CB-OG-P-O2P
17	1	129	SEP	CB-OG-P-O3P
19	3	613	TPO	O-C-CA-CB

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	3	613	TPO	1	0
17	1	129	SEP	2	0

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 17 ligands modelled in this entry, 14 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	$\#\|Z\| > 2$
44	GTP	C	1500	45	26,34,34	2.33	11 (42%)	32,54,54	1.91	9 (28%)
47	G5J	F	207	13	25,35,35	0.92	1 (4%)	31,55,55	1.41	3 (9%)
43	IHP	A	3000	-	36,36,36	1.12	3 (8%)	54,60,60	1.06	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
44	GTP	C	1500	45	-	4/18/38/38	0/3/3/3
47	G5J	F	207	13	-	6/21/41/41	0/3/3/3
43	IHP	A	3000	-	-	1/30/54/54	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	C	1500	GTP	C5-C6	-6.29	1.34	1.47
44	C	1500	GTP	C5-C4	-3.87	1.33	1.43
44	C	1500	GTP	C2'-C1'	-3.54	1.48	1.53
44	C	1500	GTP	O4'-C4'	-2.59	1.39	1.45
44	C	1500	GTP	C6-N1	-2.44	1.34	1.37

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	C	1500	GTP	C5-C6-N1	4.60	122.07	113.95
47	F	207	G5J	PG-O3B-PB	-4.55	117.21	132.83
44	C	1500	GTP	C2-N1-C6	-4.29	117.20	125.10
47	F	207	G5J	PB-O3A-PA	-3.93	119.34	132.83
43	A	3000	IHP	C5-C6-C1	-3.74	102.23	110.41

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
44	C	1500	GTP	O4'-C4'-C5'-O5'
47	F	207	G5J	C5'-O5'-PA-O3A
47	F	207	G5J	O4'-C4'-C5'-O5'
47	F	207	G5J	C3'-C4'-C5'-O5'
44	C	1500	GTP	C3'-C4'-C5'-O5'

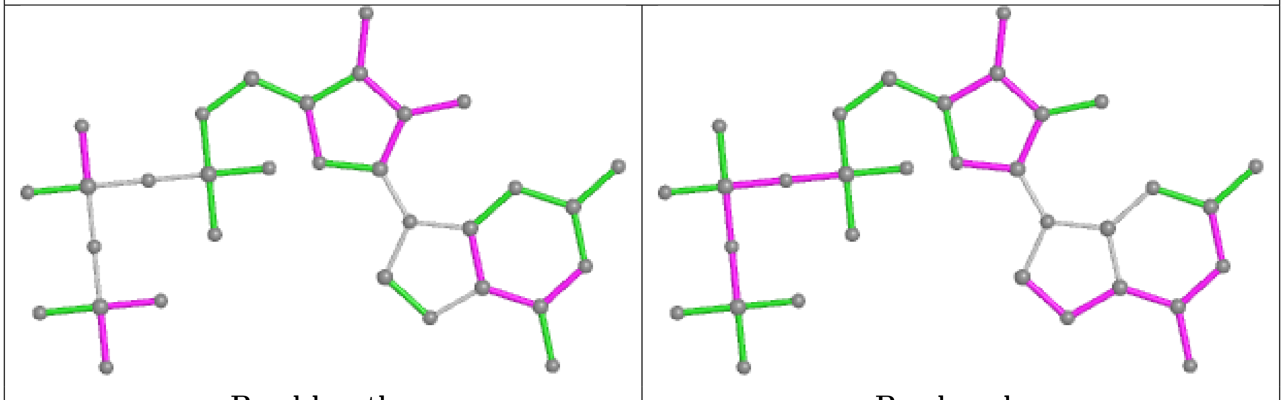
There are no ring outliers.

2 monomers are involved in 6 short contacts:

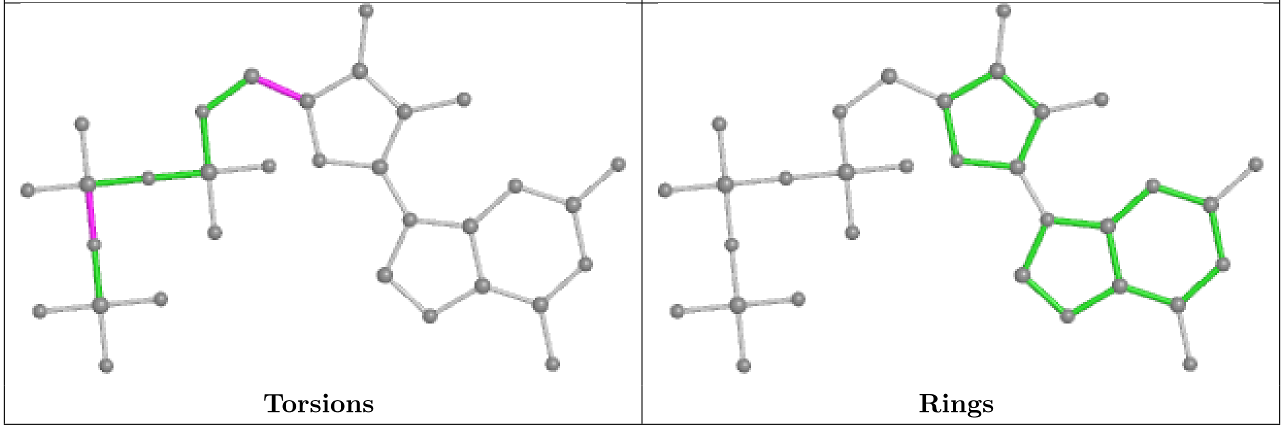
Mol	Chain	Res	Type	Clashes	Symm-Clashes
44	C	1500	GTP	3	0
47	F	207	G5J	3	0

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

Ligand GTP C 1500

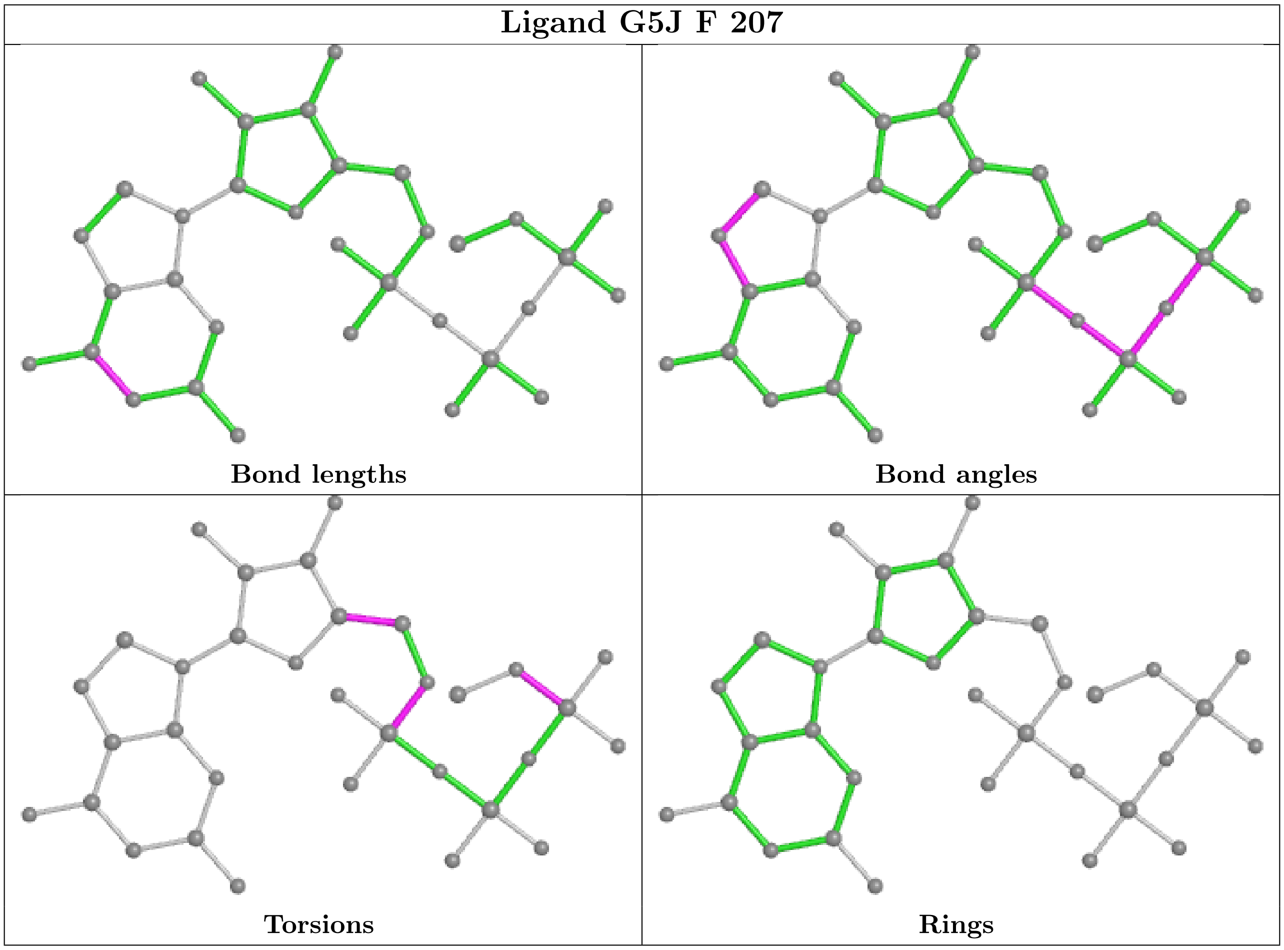


Bond lengths **Bond angles**



Torsions **Rings**

Ligand G5J F 207



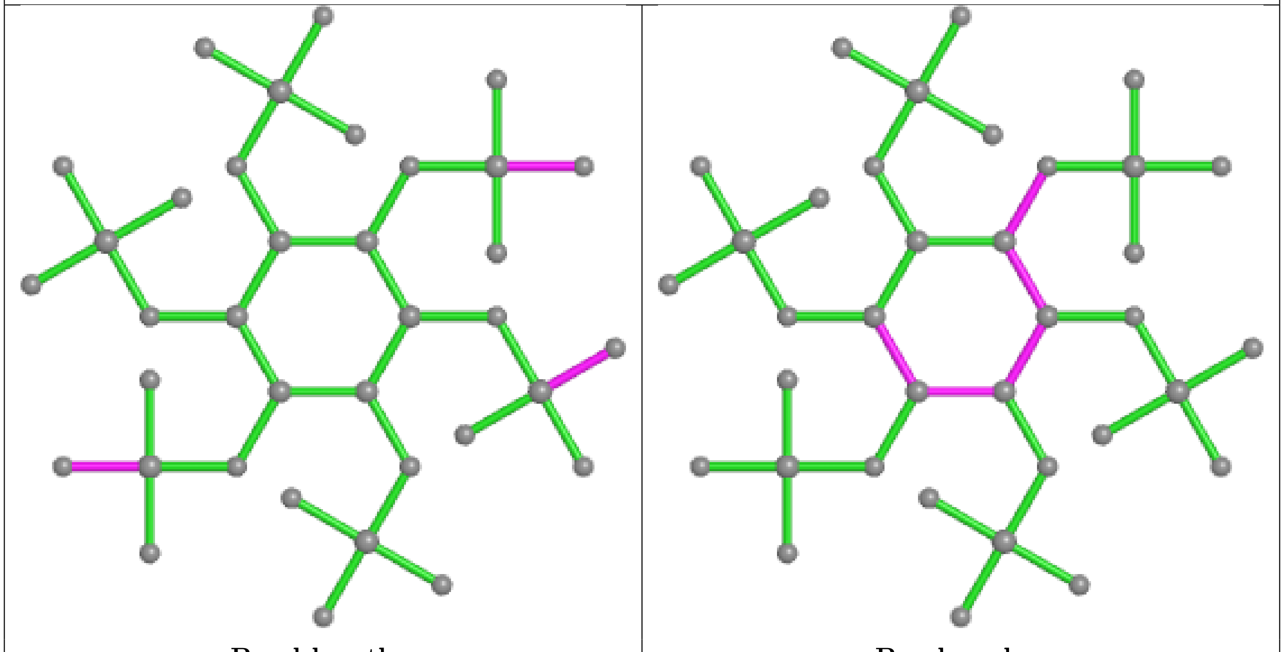
Bond lengths

Bond angles

Torsions

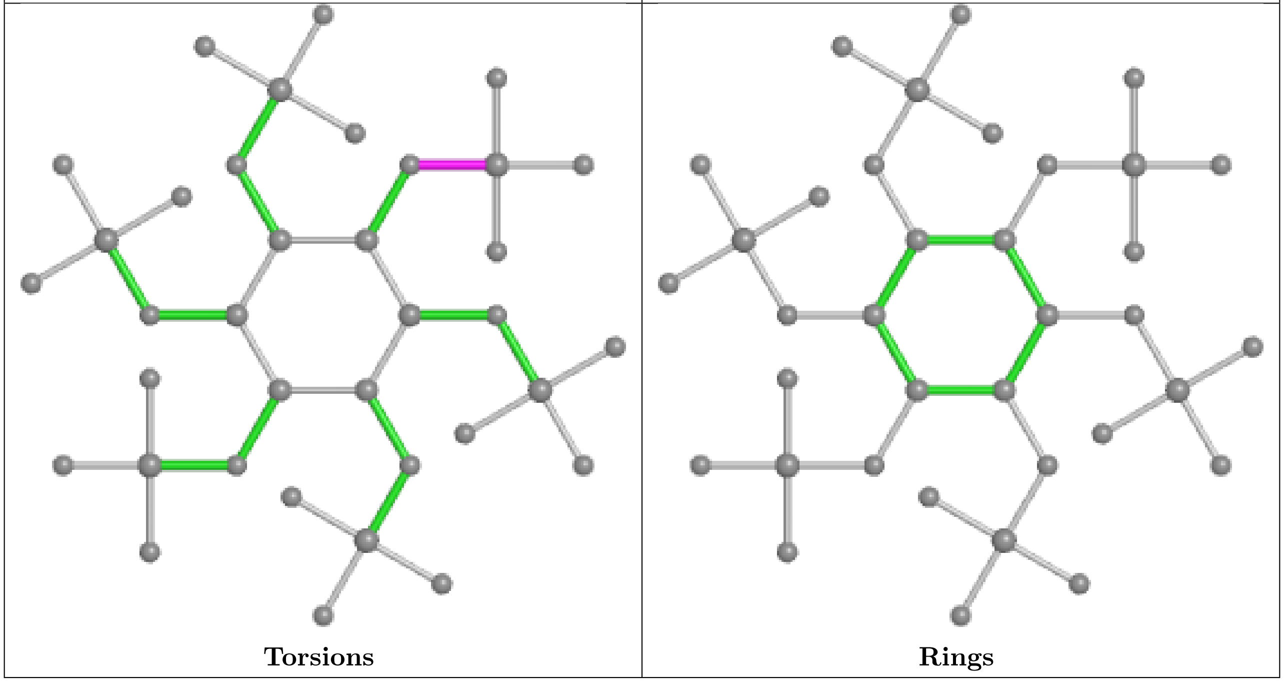
Rings

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.

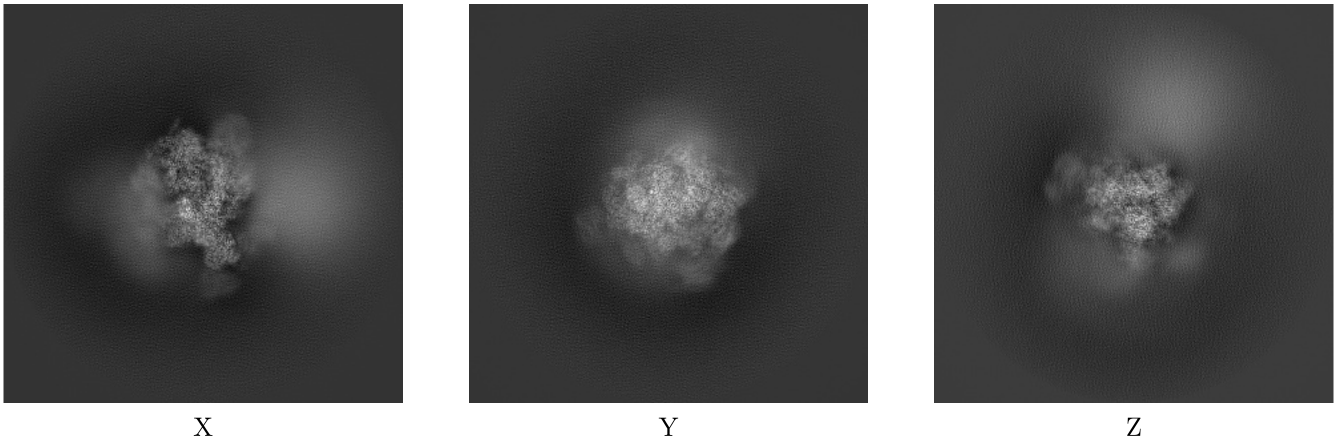
6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-30875. 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

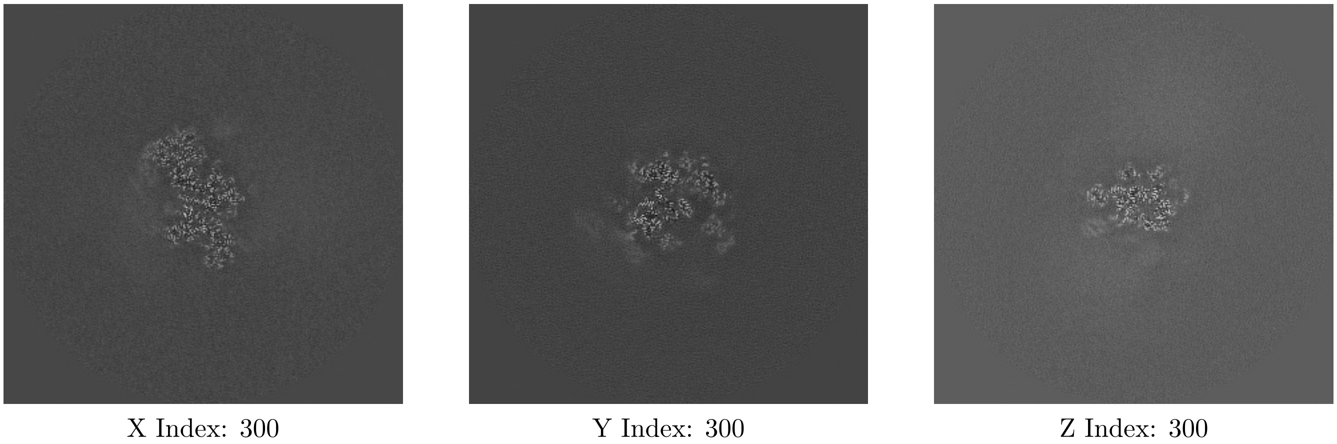


X Y Z

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

6.2 Central slices ⓘ

6.2.1 Primary map

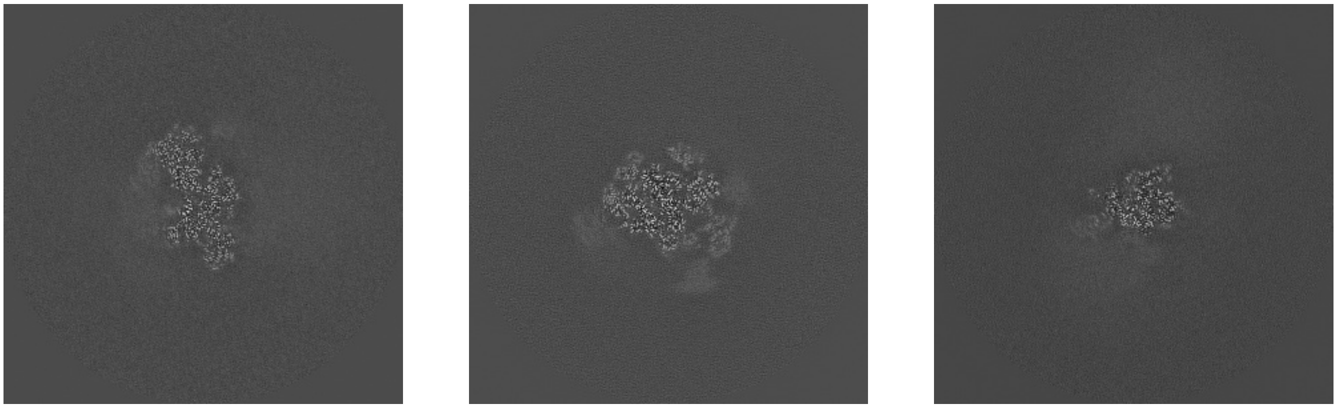


X Index: 300 Y Index: 300 Z Index: 300

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: 304 Y Index: 316 Z Index: 284

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

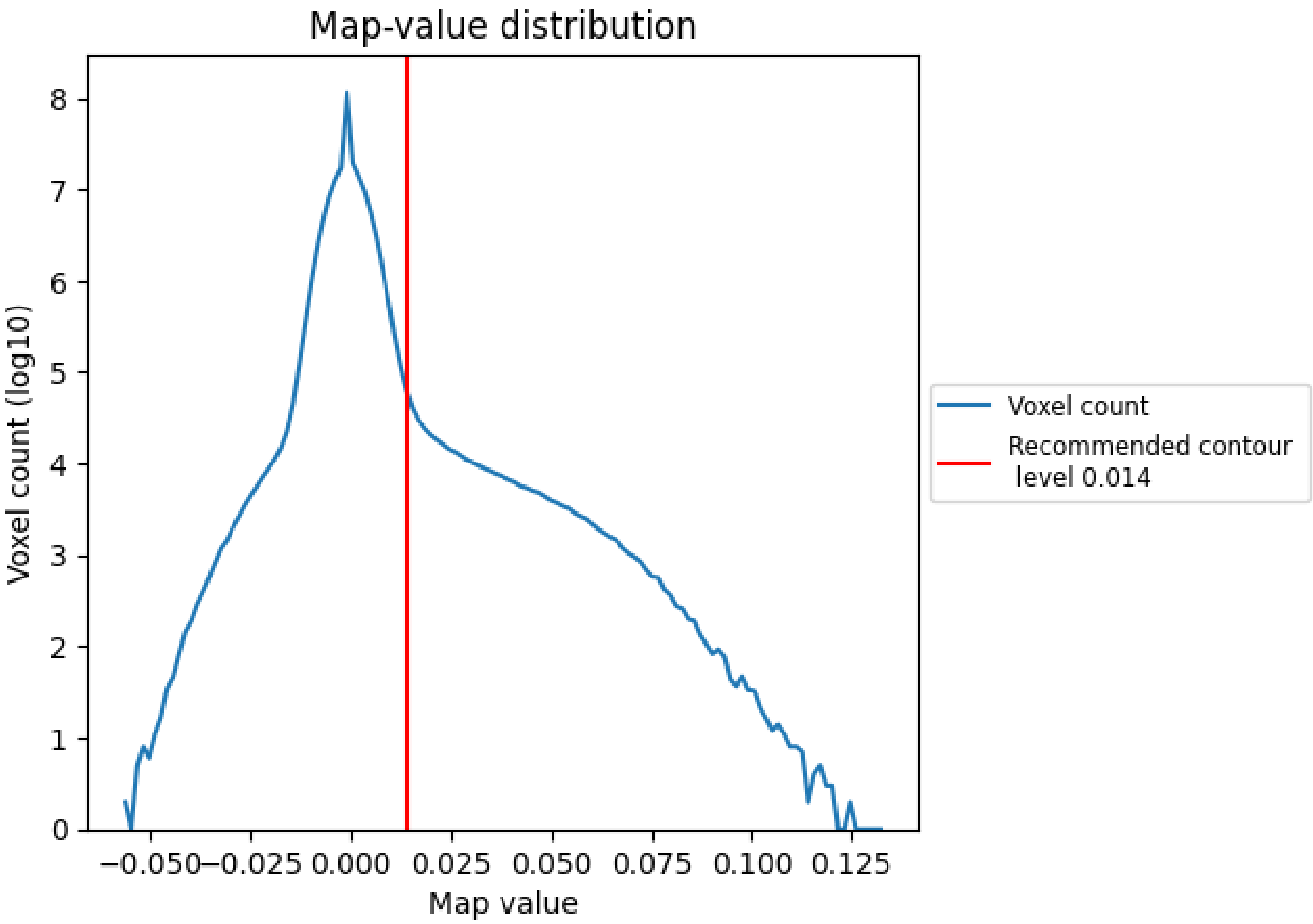
6.5 Mask visualisation ⓘ

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

7 Map analysis ⓘ

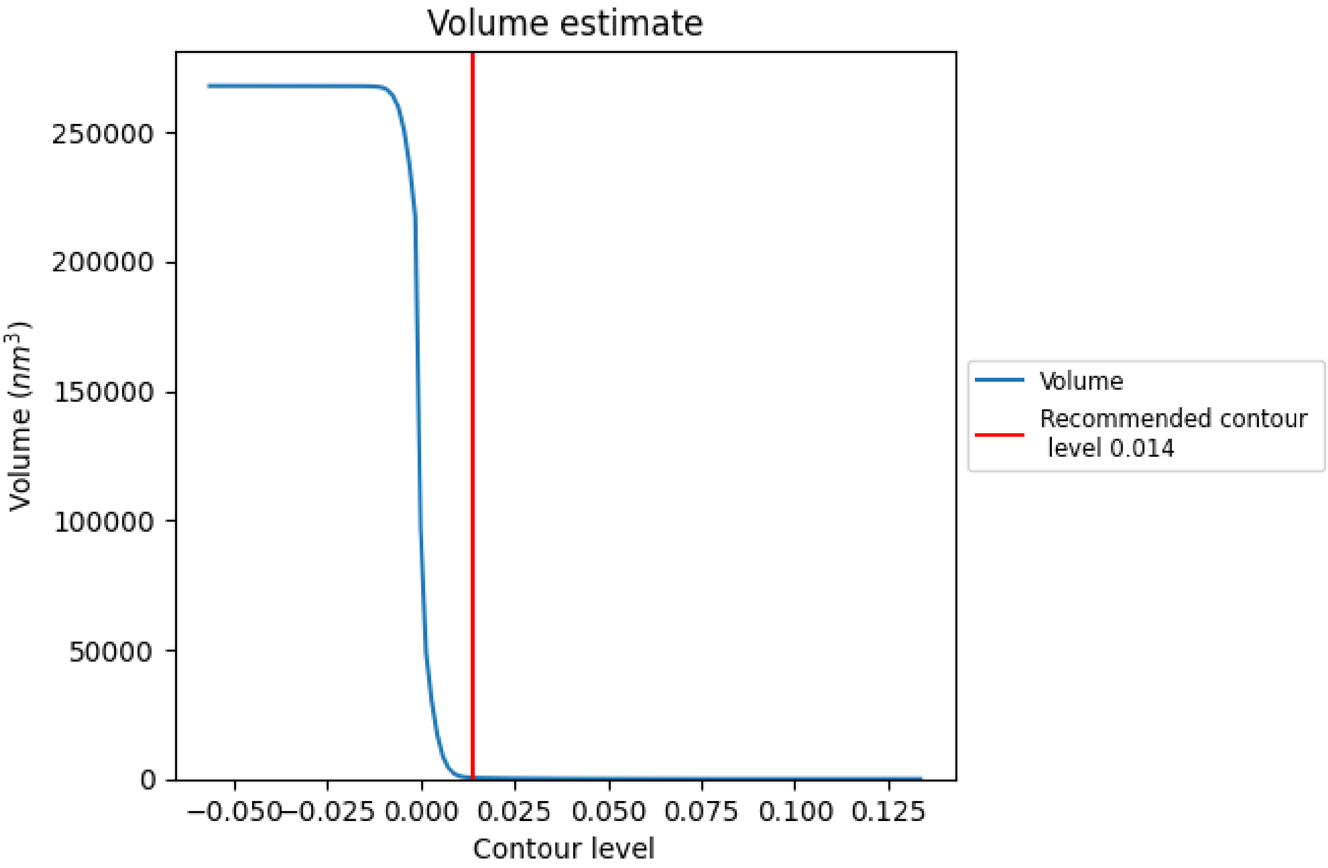
This section contains the results of statistical analysis of the map.

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.

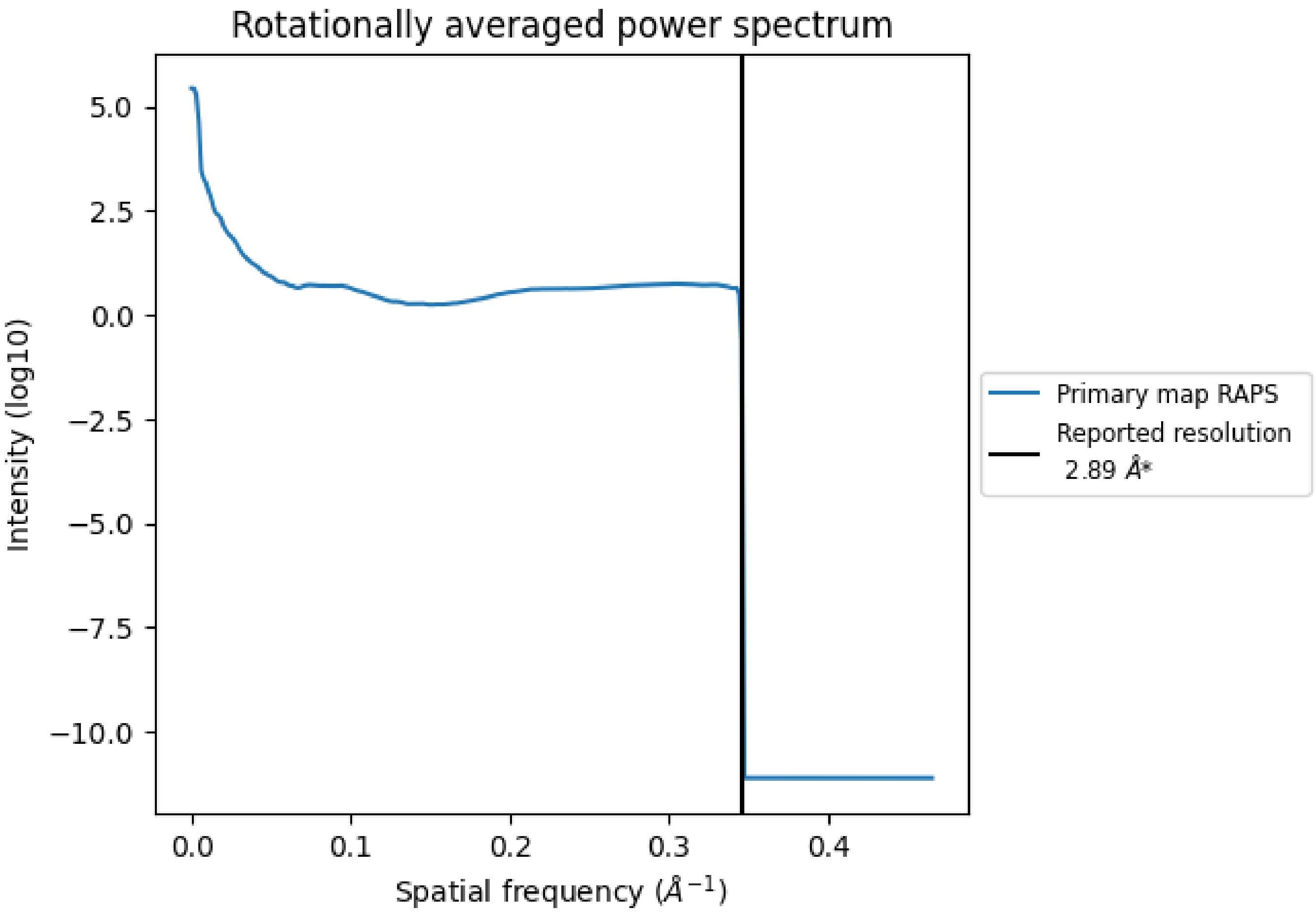
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 486 nm^3; this corresponds to an approximate mass of 439 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 0.346 Å^{-1}

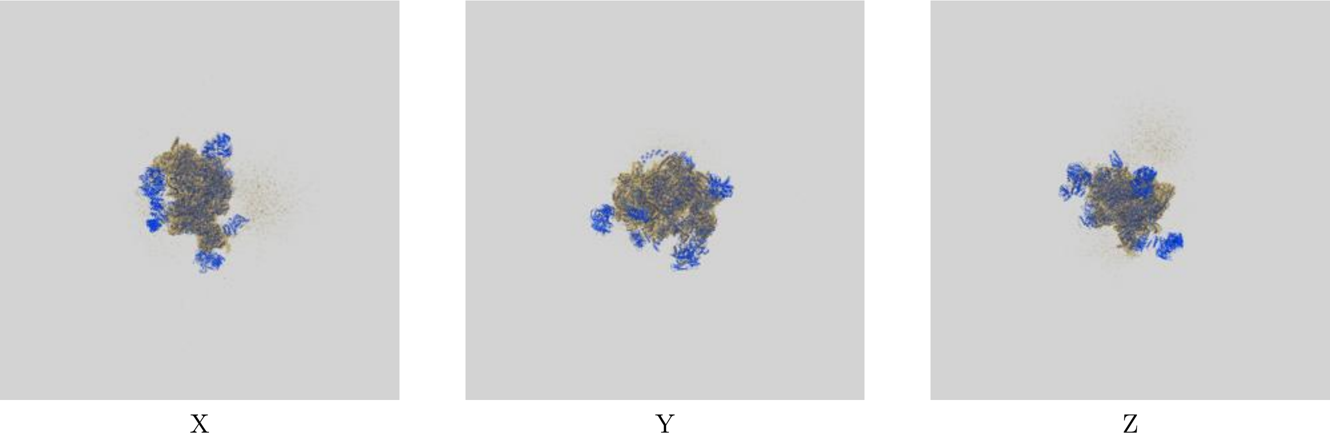
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-30875 and PDB model 7DVQ. Per-residue inclusion information can be found in section 3 on page 14.

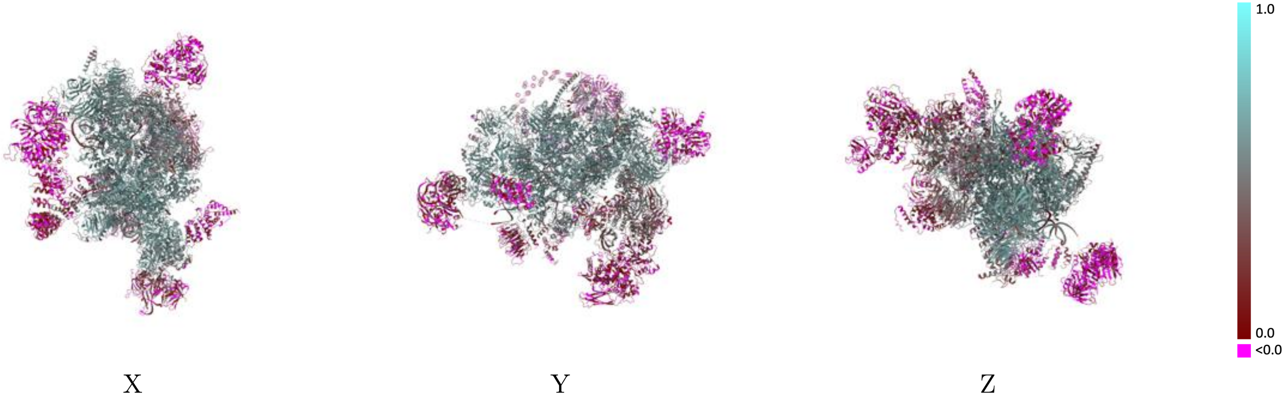
9.1 Map-model overlay ⓘ



X Y Z

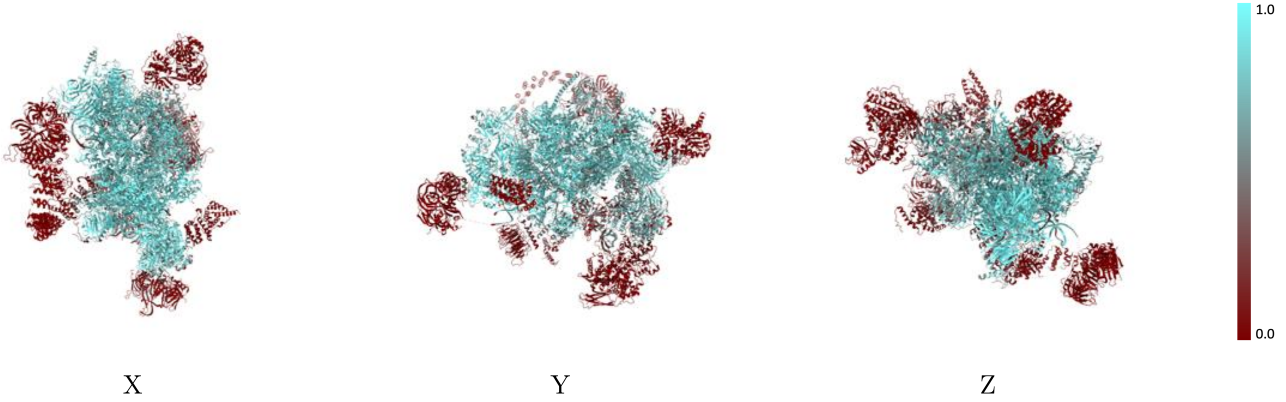
The images above show the 3D surface view of the map at the recommended contour level 0.014 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model ⓘ



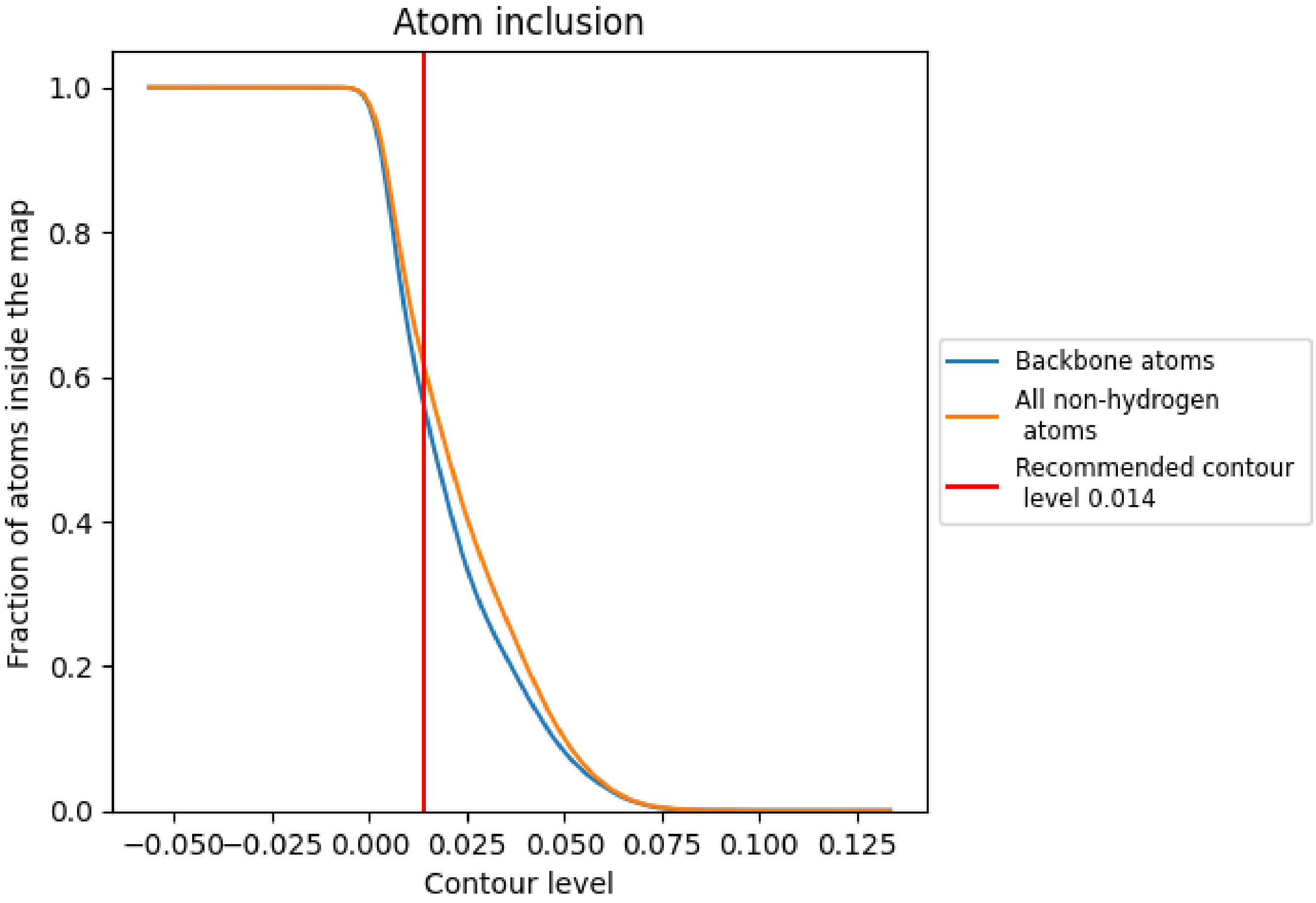
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.014).

9.4 Atom inclusion ⓘ



At the recommended contour level, 56% of all backbone atoms, 62% 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 (0.014) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6163	0.4320
0	0.8643	0.6050
1	0.8839	0.5900
2	0.7176	0.5030
3	0.8243	0.5400
4	0.0496	0.0180
5	0.7477	0.5010
6	0.9243	0.6120
7	0.8853	0.5890
8	0.8132	0.5490
9	0.5004	0.3510
A	0.8242	0.5630
B	0.6312	0.4010
C	0.8441	0.5630
D	0.3162	0.2360
E	0.0328	0.1220
F	0.7787	0.4750
G	0.7183	0.4570
H	0.6704	0.4050
I	0.4985	0.3360
J	0.0754	0.2170
K	0.1662	0.1400
L	0.8976	0.5950
M	0.6271	0.4630
P	0.7406	0.5350
R	0.6326	0.5000
T	0.9425	0.6110
U	0.9251	0.6080
V	0.4995	0.3300
X	0.6767	0.4420
Y	0.8184	0.5610
Z	0.7386	0.5420
a	0.0877	0.2650
b	0.0321	0.1610
c	0.0197	0.0820

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Chain	Atom inclusion	Q-score
d	🟥 0.0146	🟥 0.0700
e	🟥 0.0077	🟥 0.0930
f	🟥 0.0055	🟥 0.0620
g	🟥 0.0138	🟫 0.1750
h	🟥 0.0000	🟪 -0.0340
i	🟥 0.0024	🟪 -0.0230
j	🟥 0.0000	🟥 0.0510
k	🟥 0.0024	🟥 0.0090
l	🟥 0.0026	🟪 -0.0030
m	🟥 0.0028	🟥 0.0080
n	🟥 0.0030	🟪 -0.0330
v	🟦 0.8135	⬜ 0.5130
x	🟥 0.0323	🟥 0.0370
y	🟫 0.3030	🟫 0.2890
z	🟦 0.8916	⬜ 0.5800