wwPDB EM Validation Summary Report

Nov 13, 2024 – 12:45 PM JST

PDB ID	:	5XJC
EMDB ID	:	EMD-6721
Title	:	Cryo-EM structure of the human spliceosome just prior to exon ligation at 3.6 angstrom
Authors	:	Zhang, X.; Yan, C.; Hang, J.; Finci, I.L.; Lei, J.; Shi, Y.
Deposited on	:	2017-04-30
Resolution	:	3.60 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:

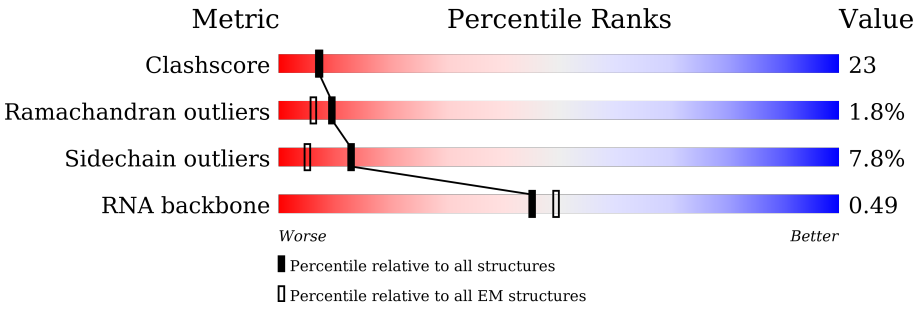
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance

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

The reported resolution of this entry is 3.60 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	A	2335	22% 70% 22%
2	B	117	24% 36% 24% 10% 28%
3	C	972	26% 55% 26% 8% 11%
4	D	2136	81% 52% 25% 19%
5	E	357	42% 62% 18% 16%
6	F	107	28% 32% 24% 34% 9%
7	G	275	20% 10% 16% 69%

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Mol	Chain	Length	Quality of chain
8	H	188	59% 14% 20% 38% 26%
9	I	855	66% 60% 5% 34%
10	J	848	42% 57% 7% 33%
11	K	225	68% 53% 12% 32%
12	L	802	35% 39% 14% 43%
13	M	243	20% 16% 27% 10% 47%
14	N	144	11% 62% 32% 6%
15	O	420	32% 33% 33% 32%
16	P	229	20% 25% 16% 6% 52%
17	Q	1485	89% 81% 8% 11%
18	R	536	19% 19% 20% 8% 51%
19	S	166	68% 61% 28% 5%
20	T	514	38% 19% 39%
21	U	2752	99%
22	V	908	45% 30% 17% 50%
23	W	579	33% 27% 40% 17% 14%
24	X	184	37% 36% 12% 50%
25	Y	1220	57% 54% 42%
26	Z	586	18% 21% 18% 59%
27	a	126	64% 64% 36%
27	h	126	64% 64% 36%
28	b	231	37% 36% 63%
28	i	231	37% 36% 63%
29	c	119	69% 67% 31%
29	j	119	68% 67% 31%

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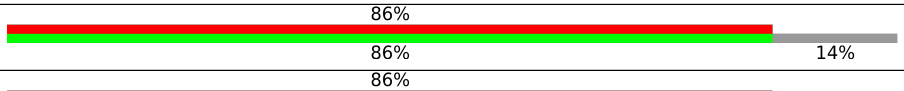
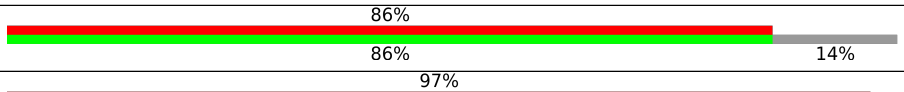
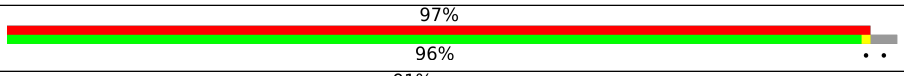
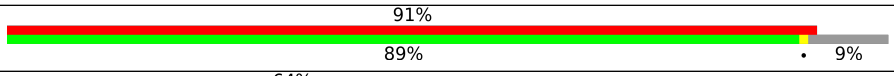
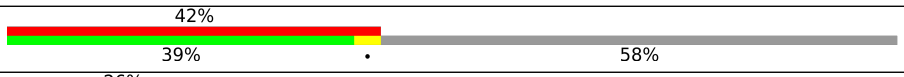
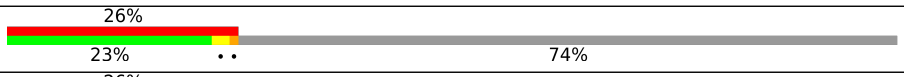
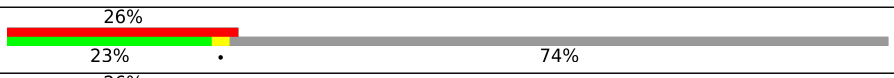
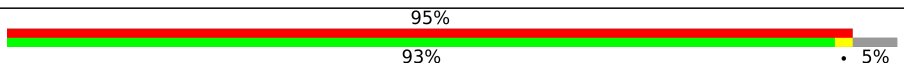
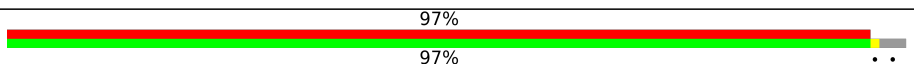
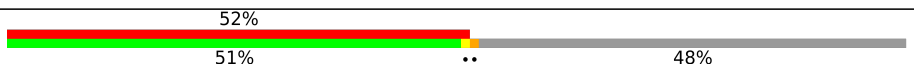
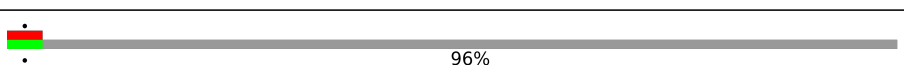
Mol	Chain	Length	Quality of chain
30	d	118	
30	k	118	
31	f	86	
31	m	86	
32	e	92	
32	l	92	
33	g	76	
33	n	76	
34	o	255	
35	p	225	
36	q	504	
36	r	504	
36	s	504	
36	t	504	
37	u	411	
38	v	148	
39	w	174	
40	x	703	

2 Entry composition (i)

There are 46 unique types of molecules in this entry. The entry contains 116421 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	2253	18633	11997	3253	3302	81	0	0

- Molecule 2 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	84	1768	792	295	597	84	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	862	6798	4347	1138	1281	32	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	1722	13846	8848	2369	2557	72	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	2338	1470	410	445	13	0	0

- Molecule 6 is a RNA chain called U6 snRNA.

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

- Molecule 7 is a RNA chain called pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	84	Total	C	N	O	P	0	0
			1551	686	222	560	83		

- Molecule 8 is a RNA chain called Homo sapiens small nuclear RNA (U2) gene.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	140	Total	C	N	O	P	0	0
			2966	1326	510	990	140		

- Molecule 9 is a protein called Pre-mRNA-splicing factor SYF1.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	I	566	Total	C	N	O	0	0
			2792	1660	566	566		

- Molecule 10 is a protein called Crooked neck-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	571	Total	C	N	O	S	0	0
			3829	2385	720	718	6		

- Molecule 11 is a protein called Pre-mRNA-splicing factor SPF27.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	152	Total	C	N	O	S	0	0
			980	612	177	189	2		

- Molecule 12 is a protein called Cell division cycle 5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	454	Total	C	N	O	S	0	0
			3205	2001	604	594	6		

- Molecule 13 is a protein called Pre-mRNA-splicing factor SYF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	130	Total	C	N	O	S	0	0
			1098	684	204	208	2		

- Molecule 14 is a protein called Protein BUD31 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	143	Total	C	N	O	S	0	0
			1184	746	217	209	12		

- Molecule 15 is a protein called Pre-mRNA-splicing factor RBM22.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	285	Total	C	N	O	S	0	0
			2296	1442	408	426	20		

- Molecule 16 is a protein called Spliceosome-associated protein CWC15 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	110	Total	C	N	O	S	0	0
			929	569	182	176	2		

- Molecule 17 is a protein called Intron-binding protein aquarius.

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

- Molecule 18 is a protein called SNW domain-containing protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	R	261	Total	C	N	O	P	S	0	0
			2073	1300	373	386	2	12		

- Molecule 19 is a protein called Peptidyl-prolyl cis-trans isomerase-like 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	159	Total	C	N	O	S	0	0
			1236	787	215	227	7		

- Molecule 20 is a protein called Pleiotropic regulator 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	313	Total	C	N	O	S	0	0
			2461	1554	447	452	8		

- Molecule 21 is a protein called Serine/arginine repetitive matrix protein 2.

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

- Molecule 22 is a protein called Pre-mRNA-splicing factor CWC22 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	452	Total	C	N	O	S	0	0
			3419	2198	593	613	15		

- Molecule 23 is a protein called Pre-mRNA-processing factor 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	496	Total	C	N	O	S	0	0
			4023	2560	697	742	24		

- Molecule 24 is a protein called PRKR-interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	92	Total	C	N	O	S	0	0
			701	432	133	132	4		

- Molecule 25 is a protein called ATP-dependent RNA helicase DHX8.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	420	THR	ASP	conflict	UNP Q14562

- Molecule 26 is a protein called Pre-mRNA-splicing factor SLU7.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	242	Total	C	N	O	S	0	0
			1999	1260	357	374	8		

- Molecule 27 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	a	81	Total	C	N	O	S	0	0
			640	401	113	120	6		
27	h	81	Total	C	N	O	S	0	0
			633	397	112	118	6		

- Molecule 28 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	b	86	Total	C	N	O	S	0	0
			690	434	126	123	7		
28	i	86	Total	C	N	O	S	0	0
			690	434	126	123	7		

- Molecule 29 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c	82	Total	C	N	O	S	0	0
			649	413	113	119	4		
29	j	82	Total	C	N	O	S	0	0
			649	413	113	119	4		

- Molecule 30 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d	97	Total	C	N	O	S	0	0
			776	488	143	140	5		
30	k	85	Total	C	N	O	S	0	0
			688	432	125	126	5		

- Molecule 31 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	74	Total	C	N	O	S	0	0
			576	373	95	103	5		
31	m	74	Total	C	N	O	S	0	0
			576	373	95	103	5		

- Molecule 32 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	e	79	Total	C	N	O	S	0	0
			652	412	116	119	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
32	l	79	Total	C	N	O	S	0	0
			652	412	116	119	5		

- Molecule 33 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	g	74	Total	C	N	O	S	0	0
			577	364	104	103	6		
33	n	69	Total	C	N	O	S	0	0
			542	345	97	94	6		

- Molecule 34 is a protein called U2 small nuclear ribonucleoprotein A'.

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

- Molecule 35 is a protein called U2 small nuclear ribonucleoprotein B".

Mol	Chain	Residues	Atoms					AltConf	Trace
35	p	94	Total	C	N	O	S	0	0
			760	488	135	132	5		

- Molecule 36 is a protein called Pre-mRNA-processing factor 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	q	132	Total	C	N	O	S	0	0
			918	581	156	178	3		
36	r	131	Total	C	N	O	S	0	0
			901	572	149	177	3		
36	s	132	Total	C	N	O	S	0	0
			917	581	156	177	3		
36	t	131	Total	C	N	O	S	0	0
			906	575	152	176	3		

- Molecule 37 is a protein called Eukaryotic initiation factor 4A-III.

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

- Molecule 38 is a protein called Protein mago nashi homolog 2.

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

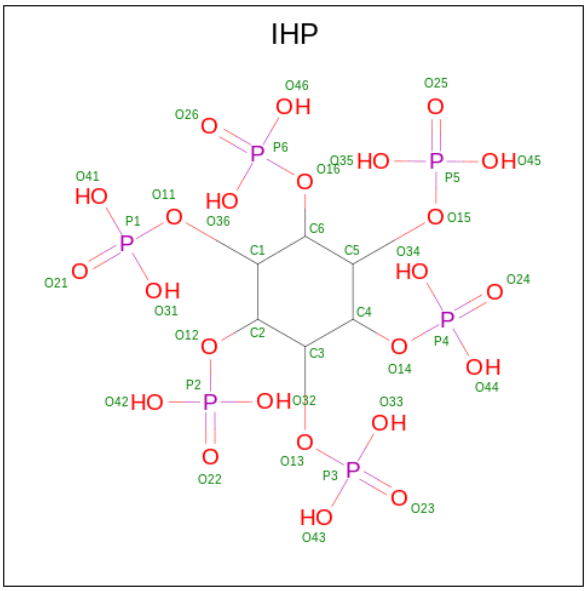
- Molecule 39 is a protein called RNA-binding protein 8A.

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

- Molecule 40 is a protein called Protein CASC3.

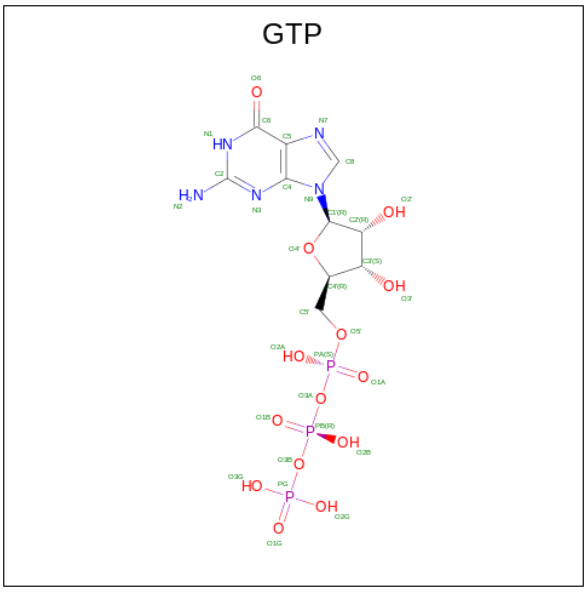
Mol	Chain	Residues	Atoms				AltConf	Trace
40	x	25	Total	C	N	O	0	0
			216	136	39	41		

- Molecule 41 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$).



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

- Molecule 42 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

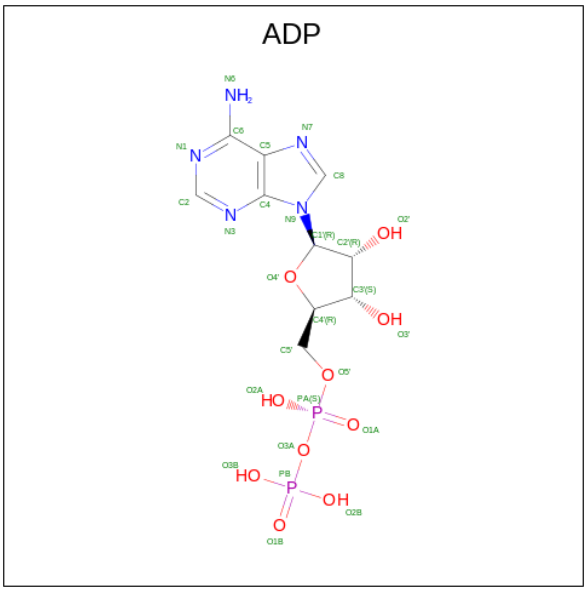


Mol	Chain	Residues	Atoms					AltConf
42	C	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 43 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
43	C	1	Total	Mg	0
			1	1	
43	D	1	Total	Mg	0
			1	1	
43	F	6	Total	Mg	0
			6	6	
43	Q	2	Total	Mg	0
			2	2	
43	u	1	Total	Mg	0
			1	1	

- Molecule 44 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

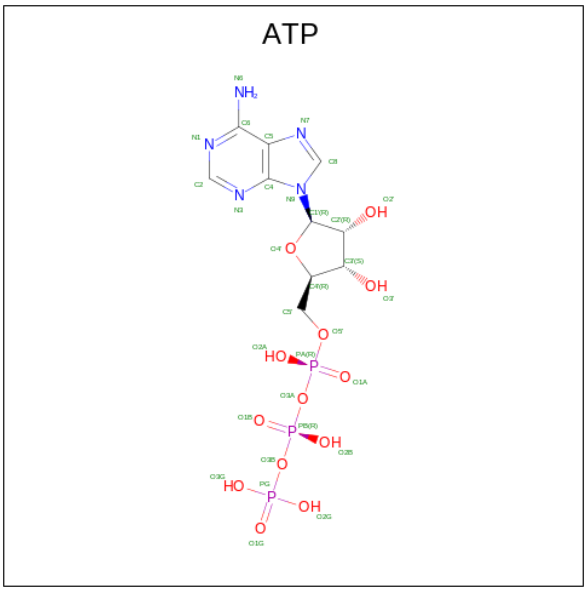


Mol	Chain	Residues	Atoms					AltConf
44	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
44	D	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 45 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
45	N	3	Total	Zn	0
			3	3	
45	O	3	Total	Zn	0
			3	3	
45	Z	1	Total	Zn	0
			1	1	

- Molecule 46 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



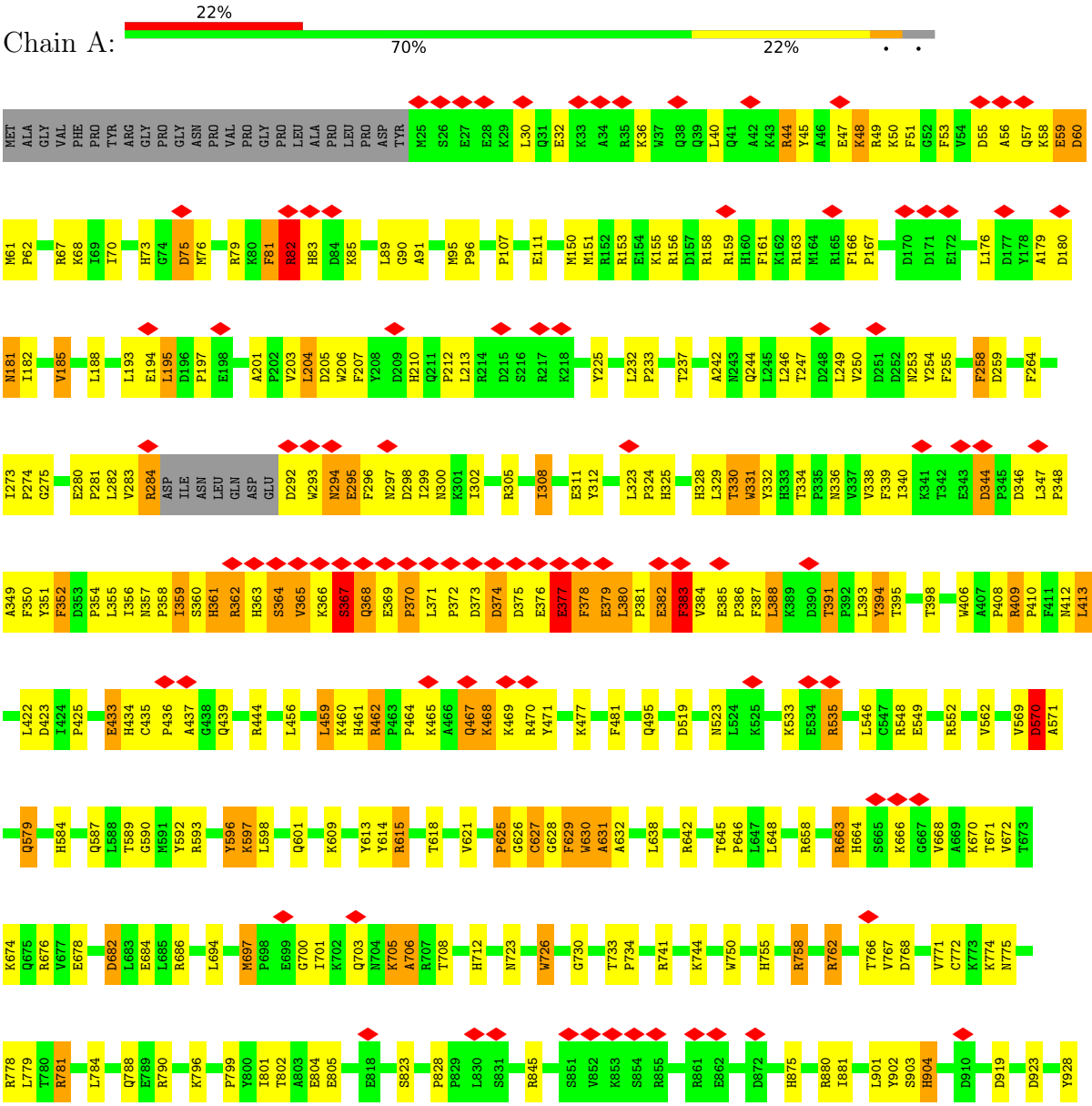
Mol	Chain	Residues	Atoms					AltConf
46	Q	1	Total	C	N	O	P	0
			31	10	5	13	3	
46	u	1	Total	C	N	O	P	0
			31	10	5	13	3	

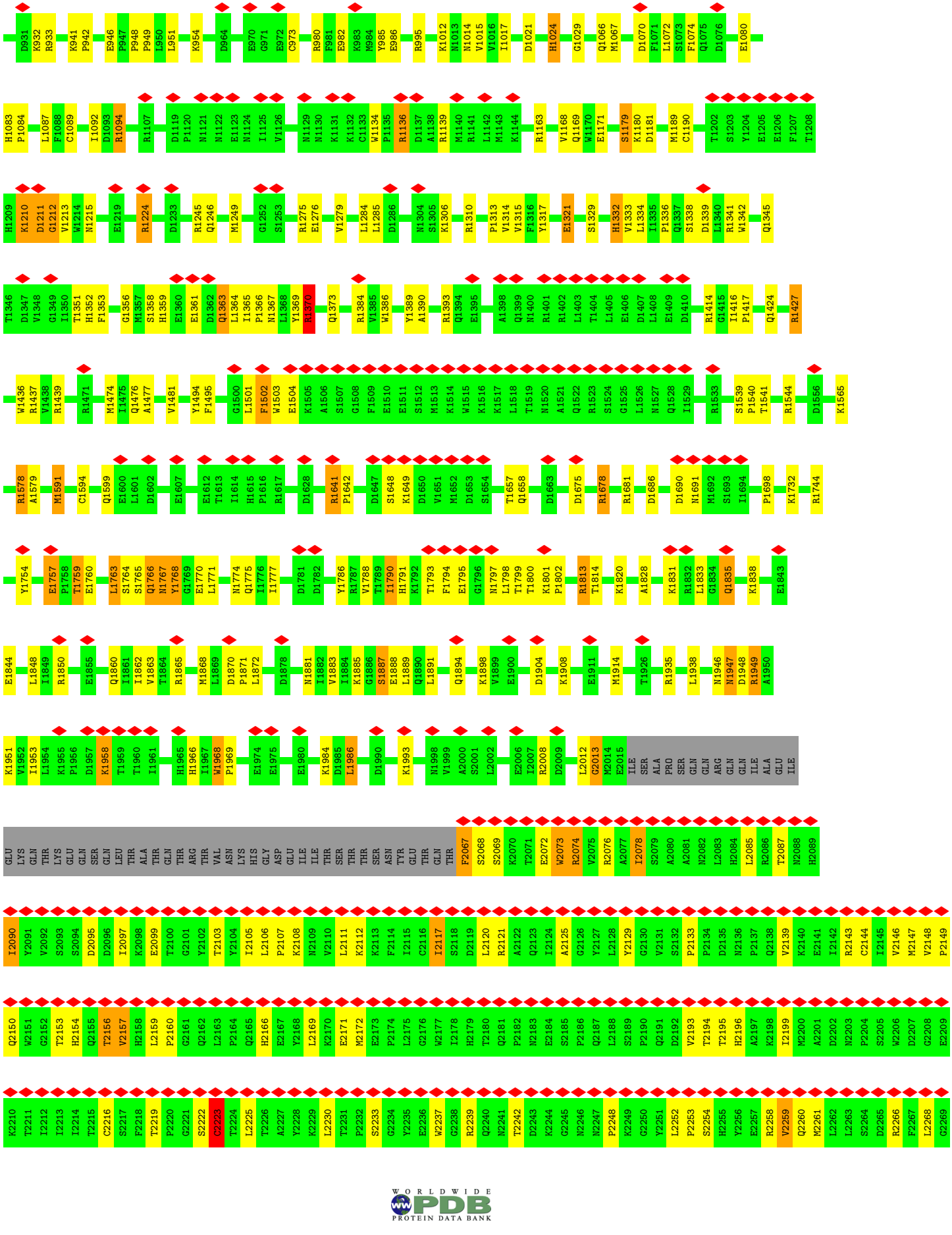
3 Residue-property plots (i)

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:

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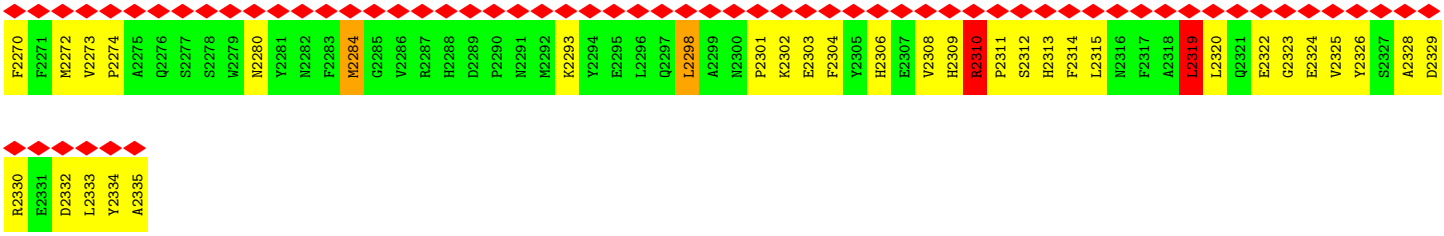

• Molecule 2: U5 snRNA

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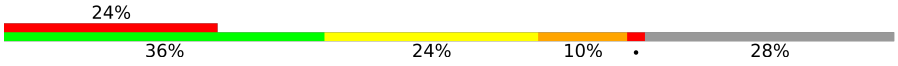
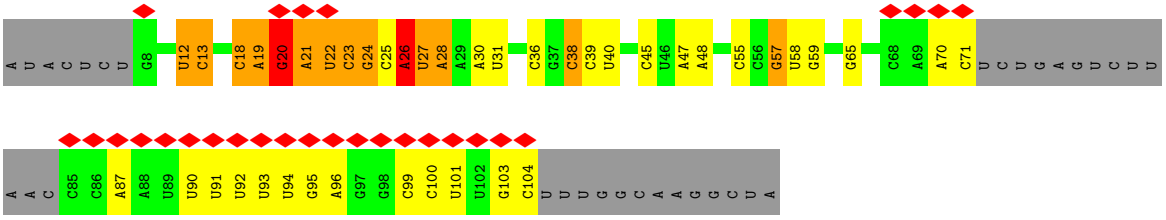
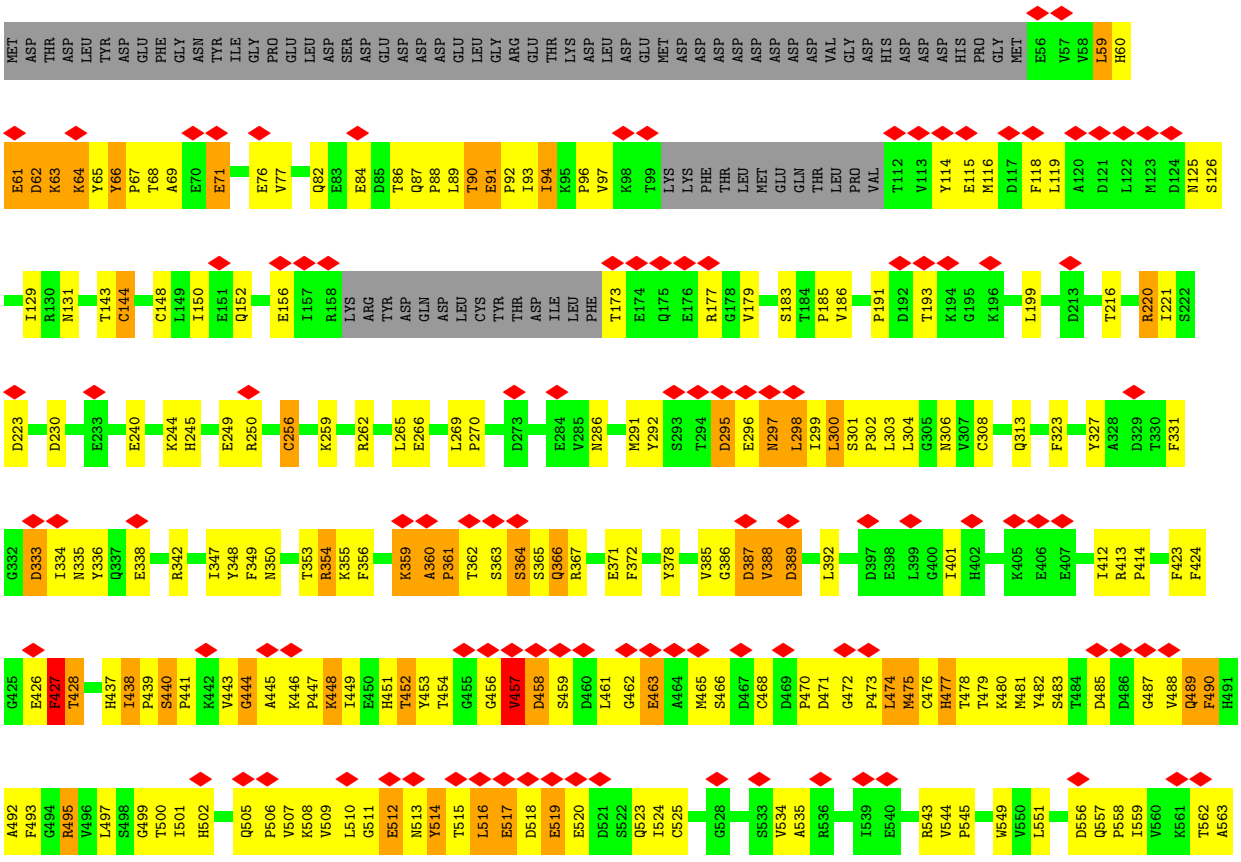
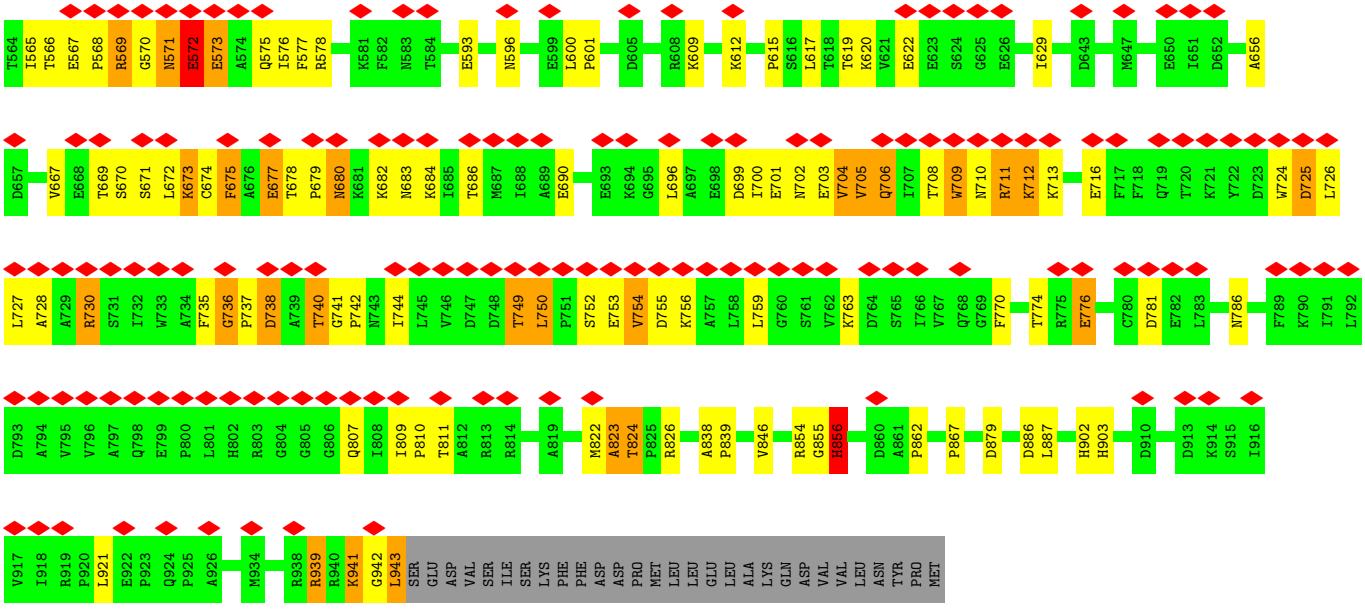




• Molecule 3: 116 kDa U5 small nuclear ribonucleoprotein component

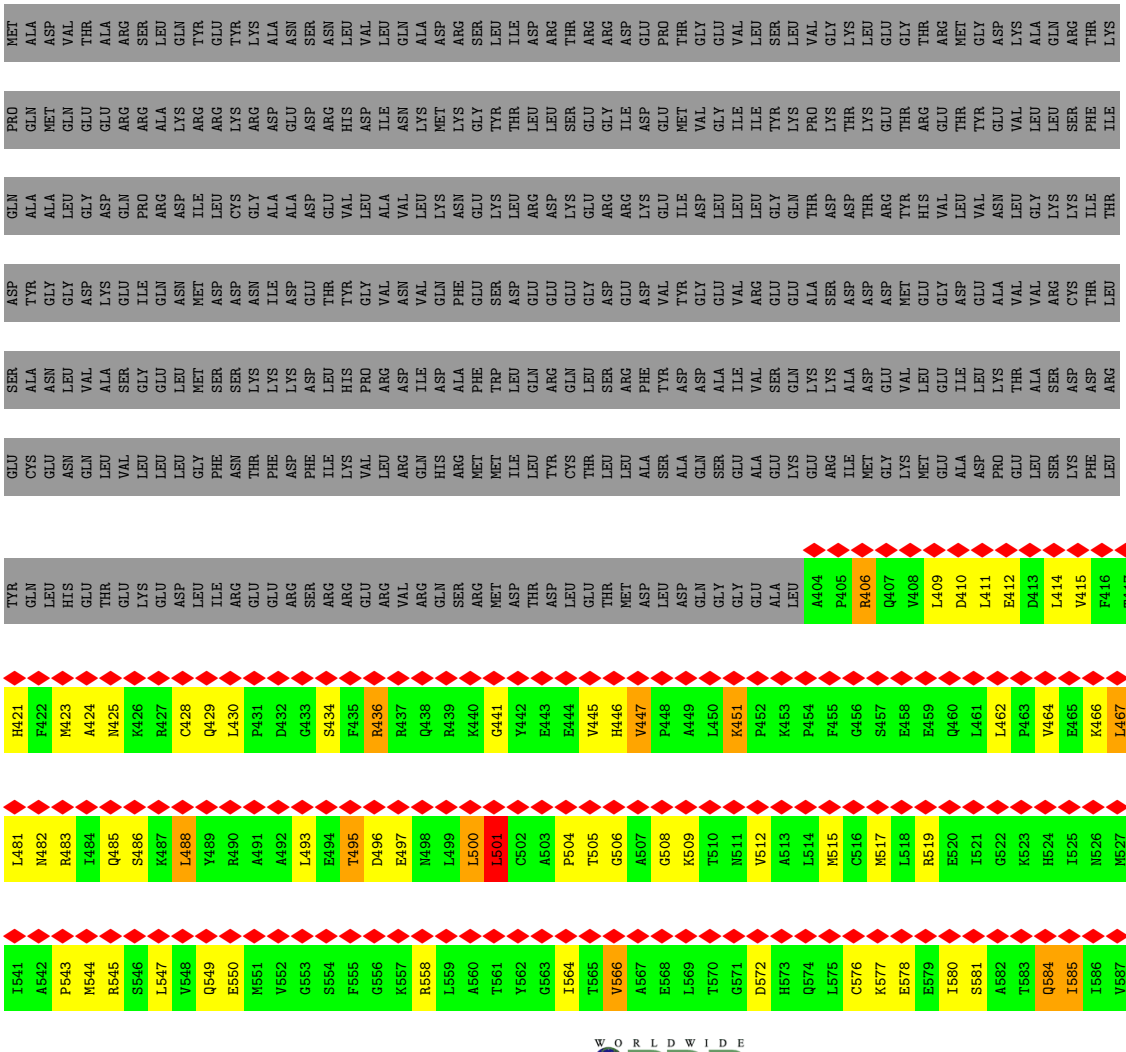
Chain C:

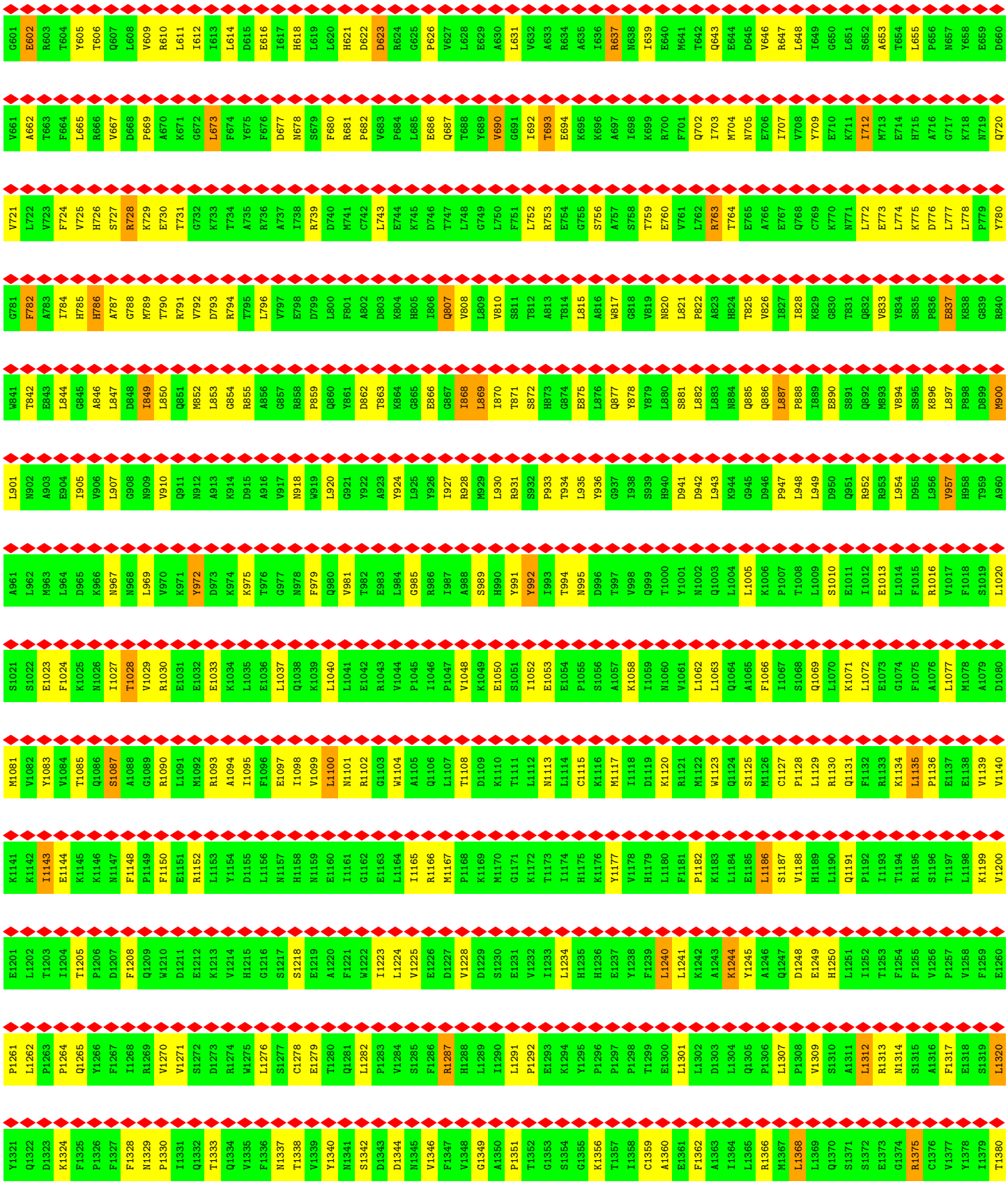




• Molecule 4: U5 small nuclear ribonucleoprotein 200 kDa helicase

Chain D:

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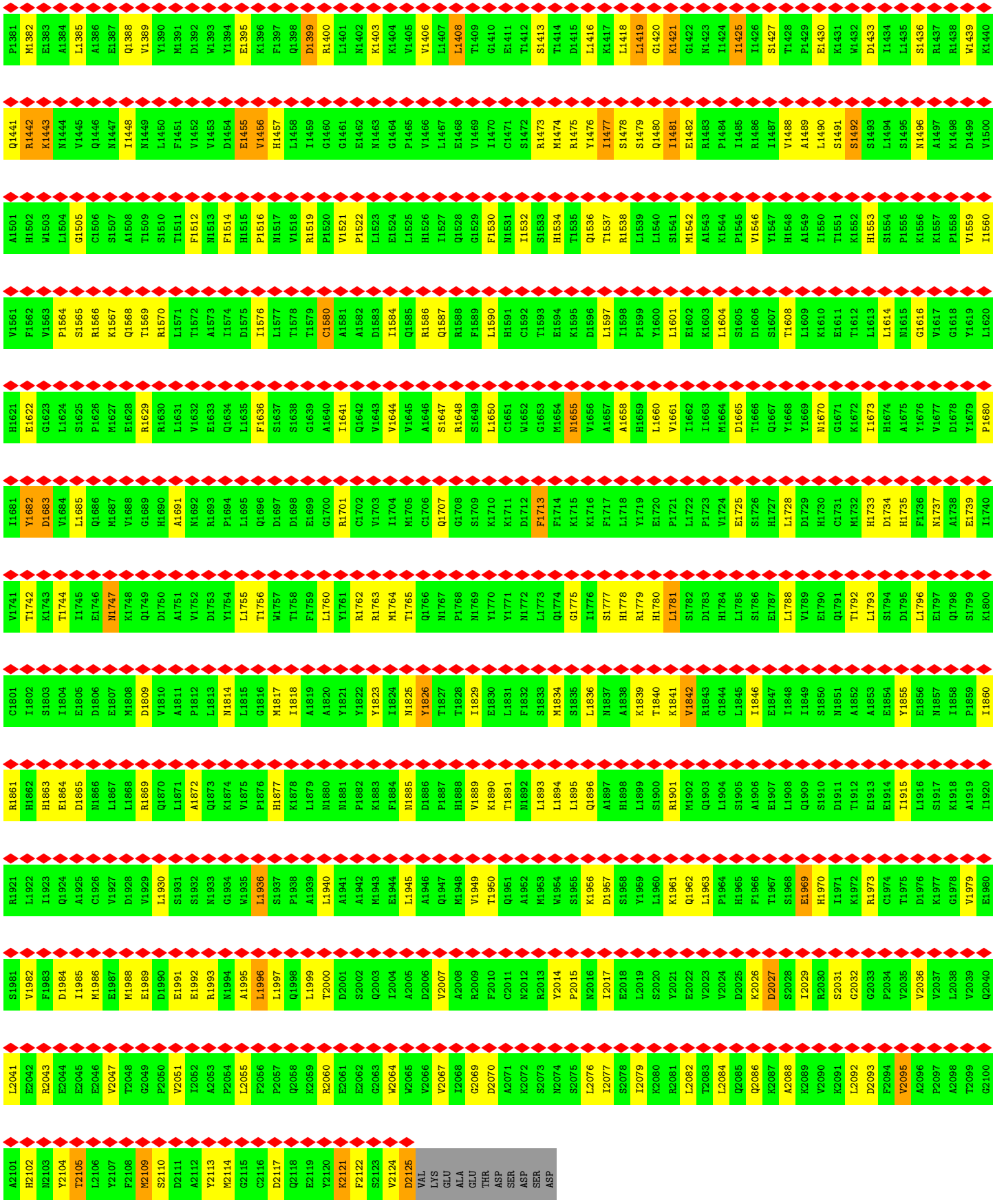
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• Molecule 5: U5 small nuclear ribonucleoprotein 40 kDa protein

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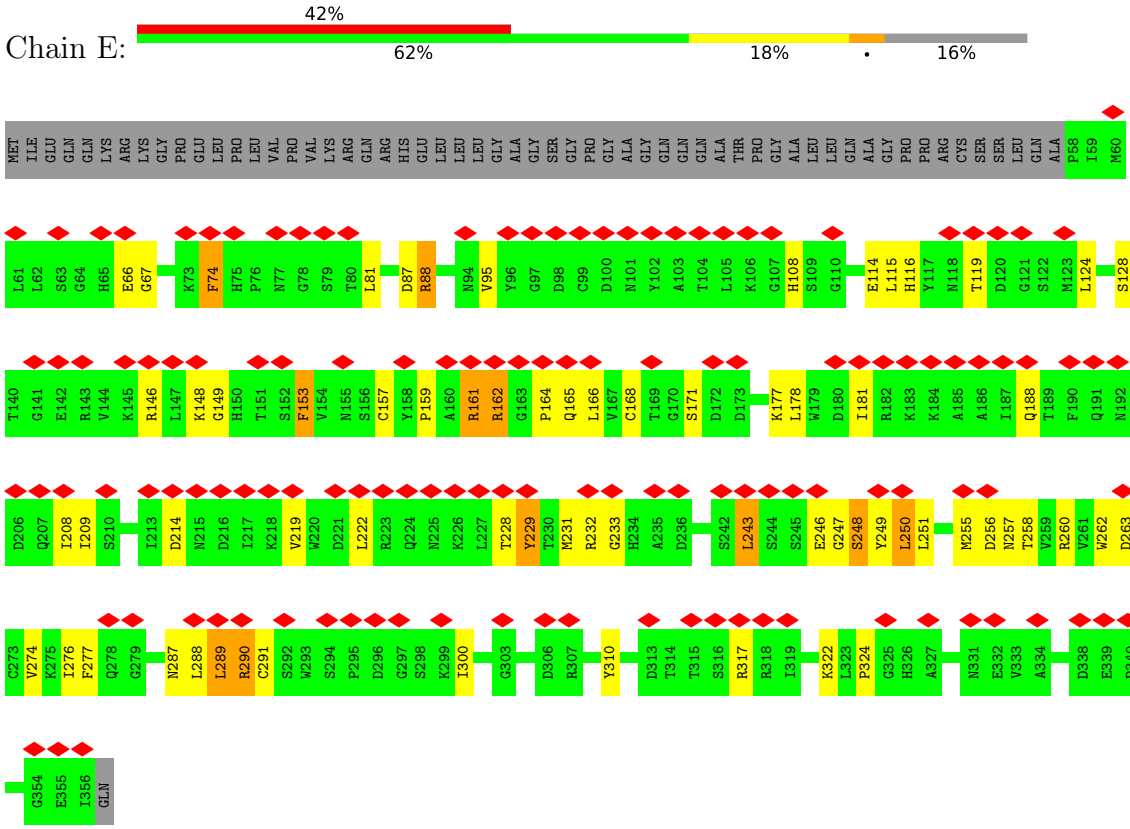
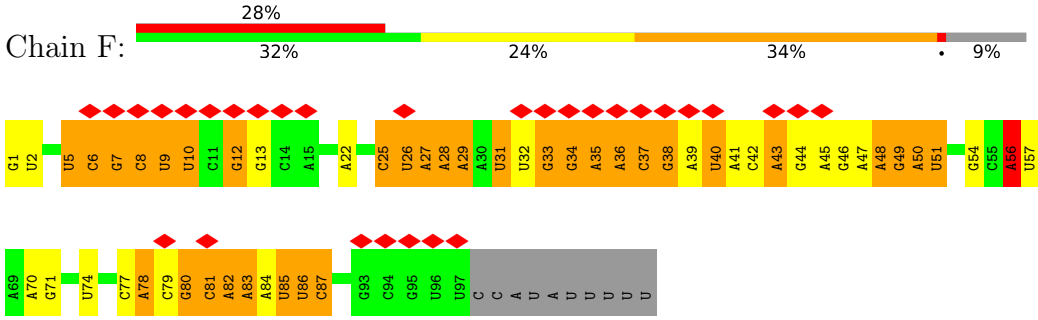


• Molecule 6: U6 snRNA

Chain F:



• Molecule 7: pre-mRNA

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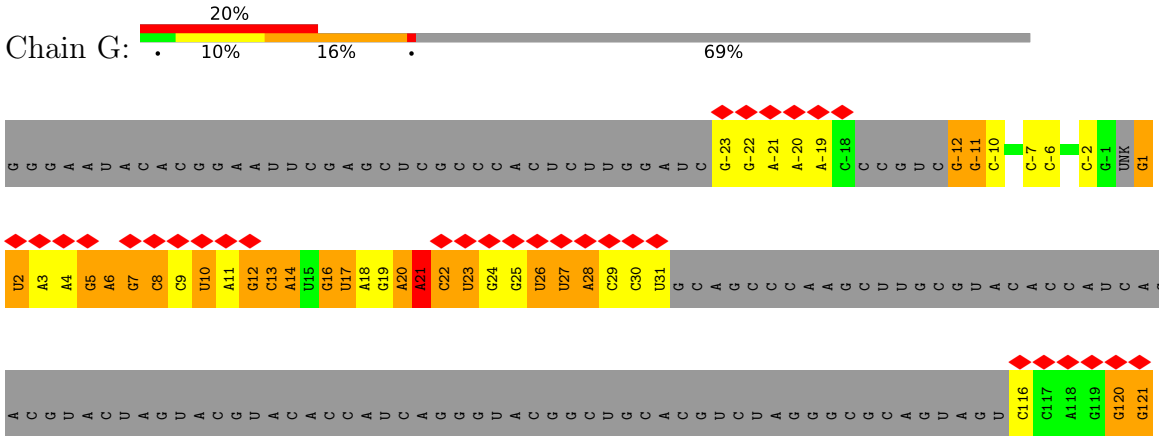
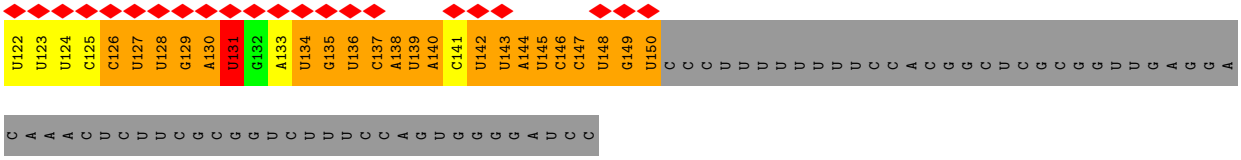
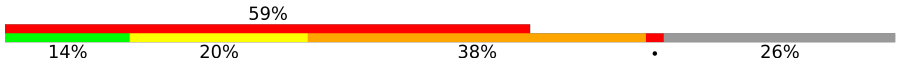
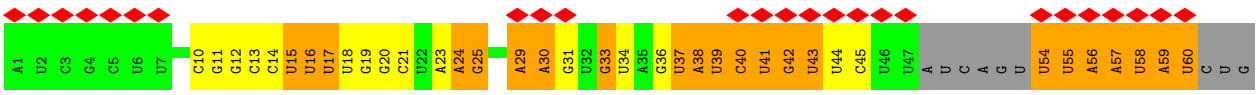


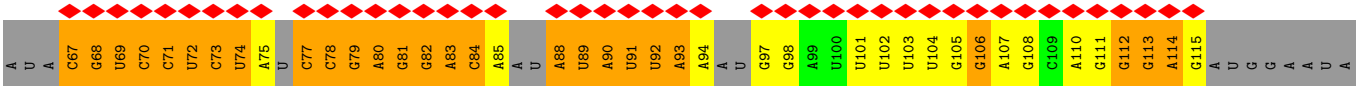


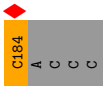
• Molecule 8: Homo sapiens small nuclear RNA (U2) gene

Chain H:



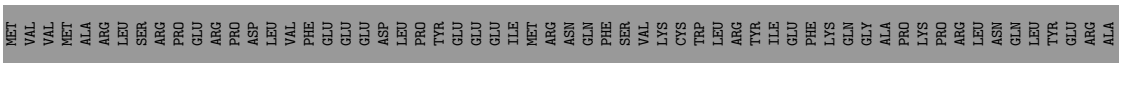


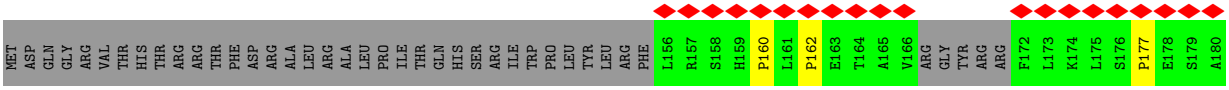


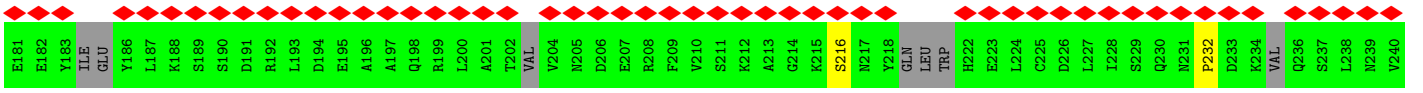


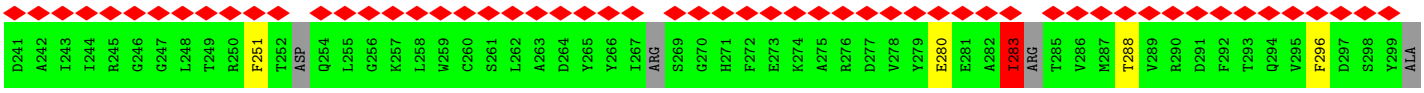
• Molecule 9: Pre-mRNA-splicing factor SYF1

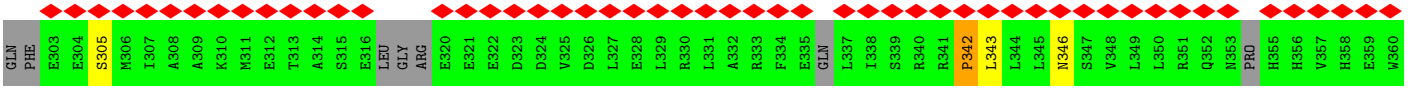
Chain I:

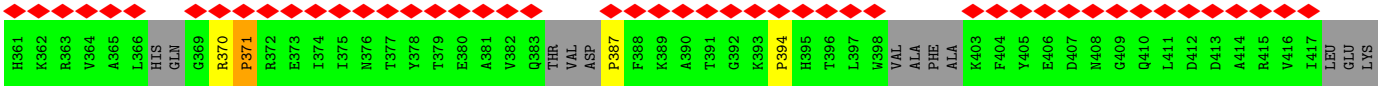


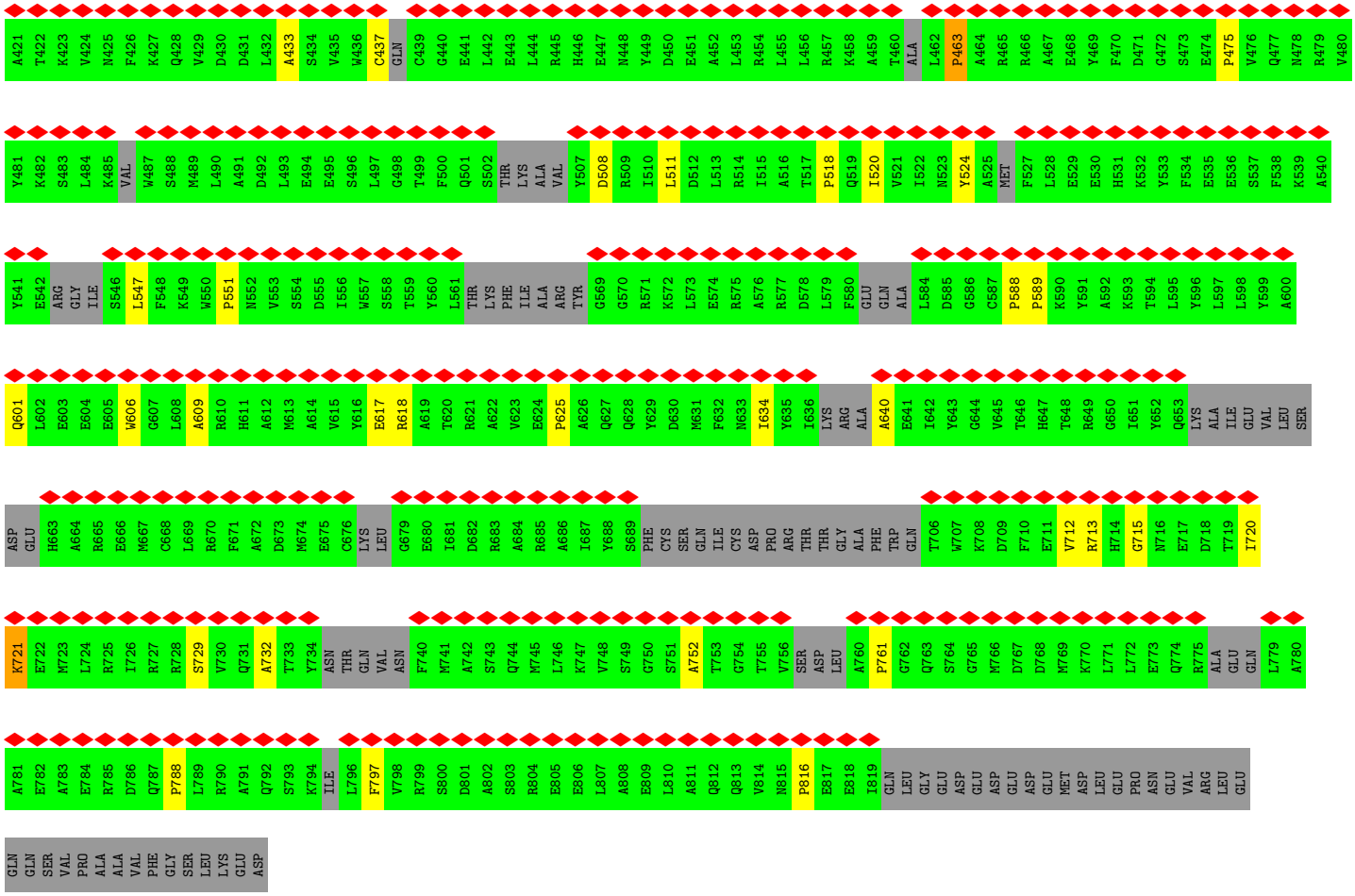




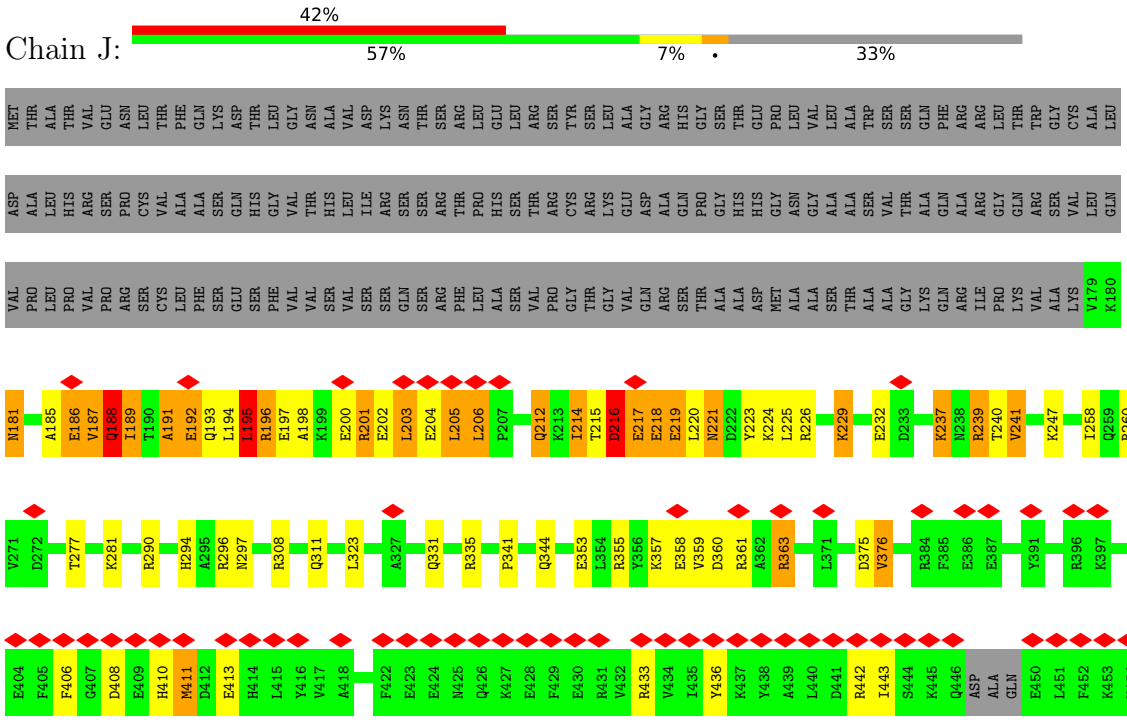


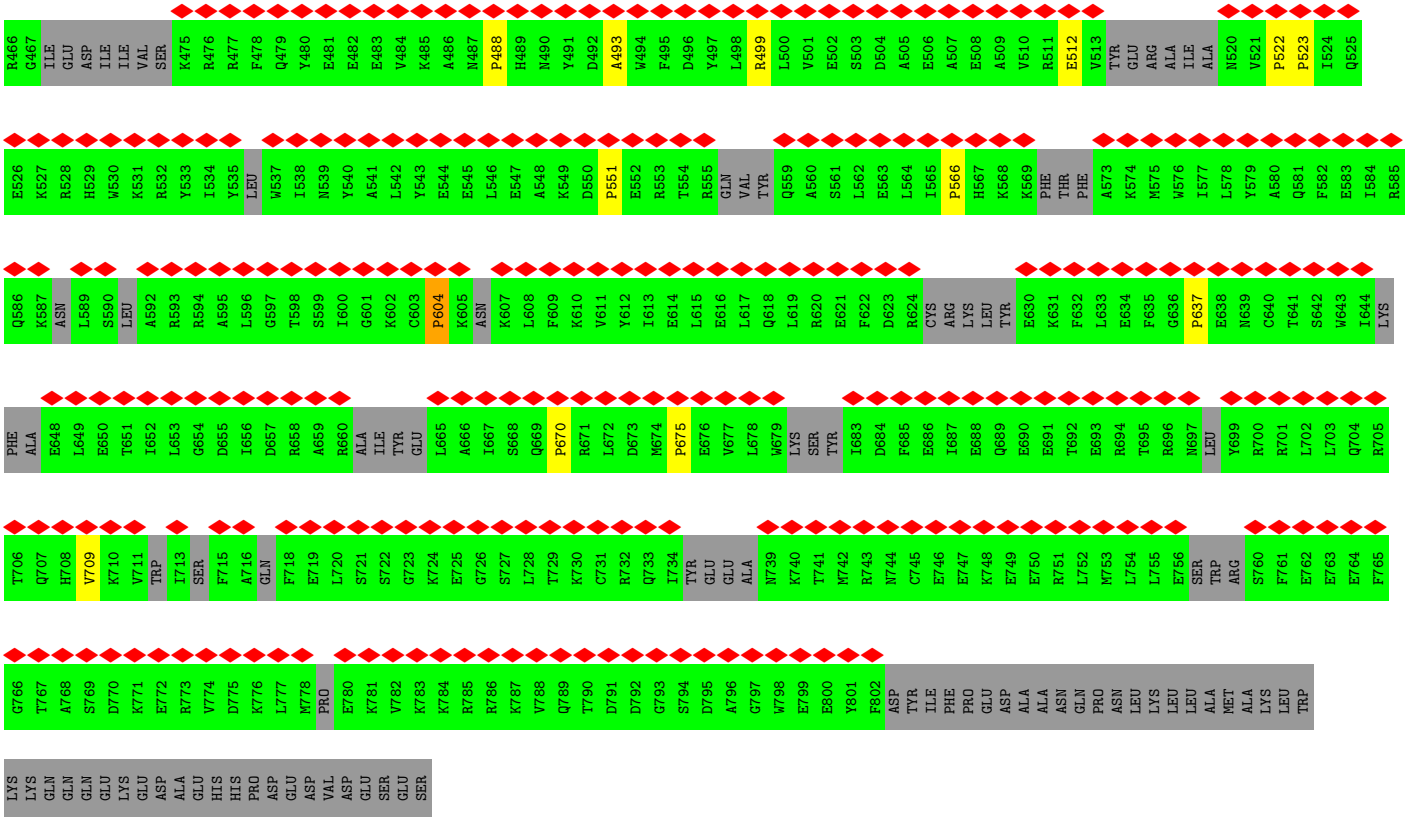






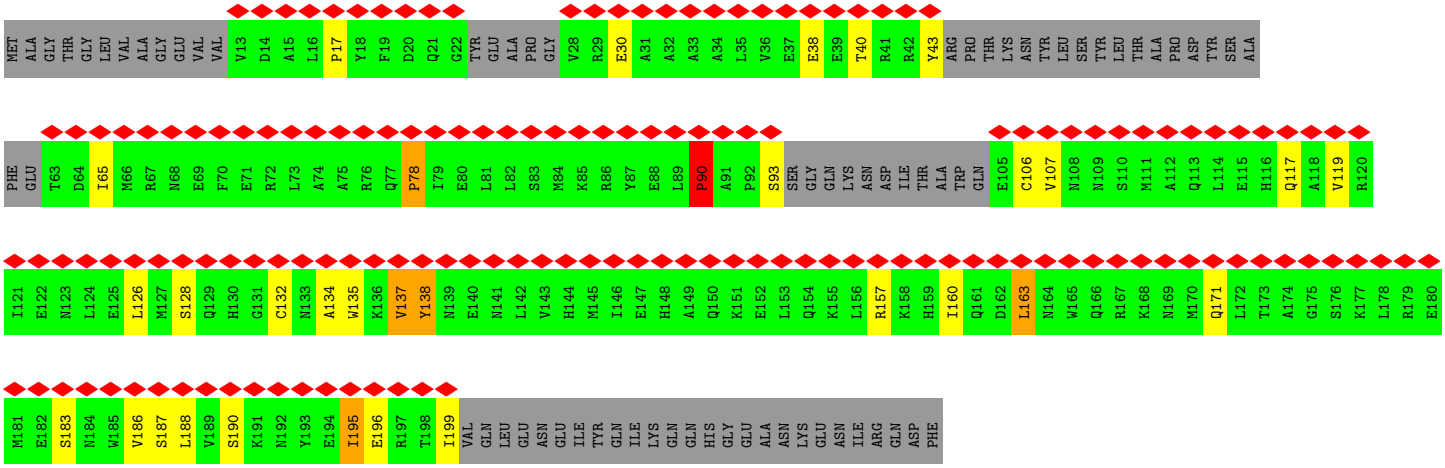
• Molecule 10: Crooked neck-like protein 1





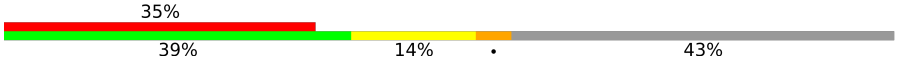
• Molecule 11: Pre-mRNA-splicing factor SPF27

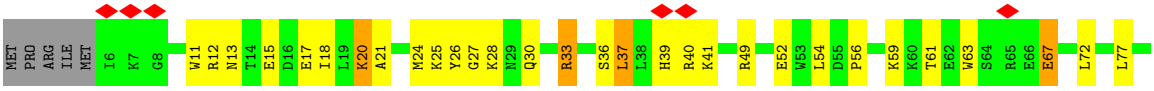
Chain K:

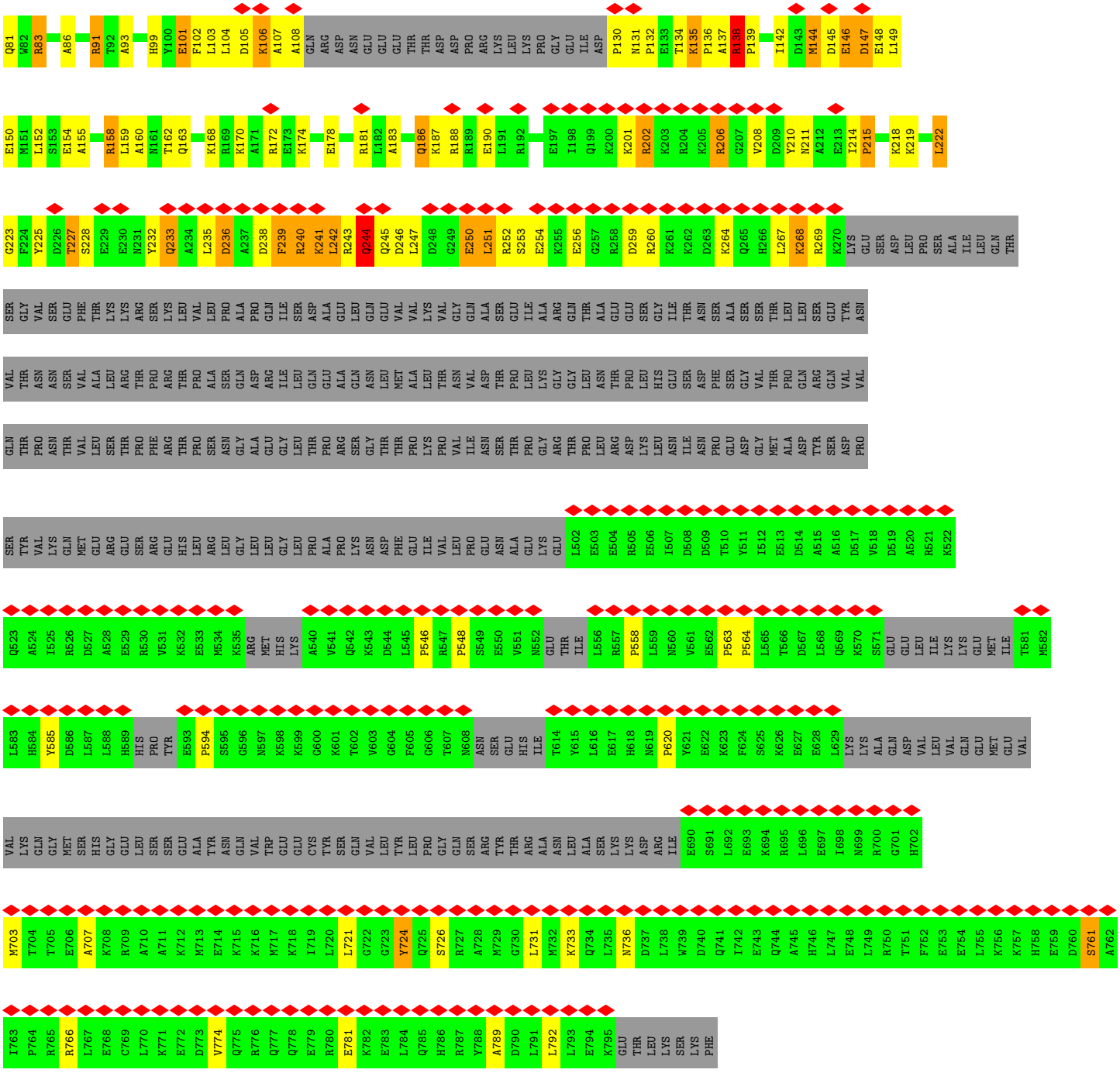


• Molecule 12: Cell division cycle 5-like protein

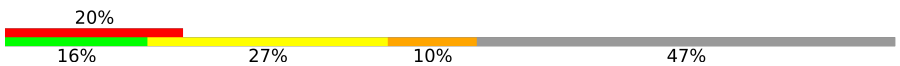
Chain L:

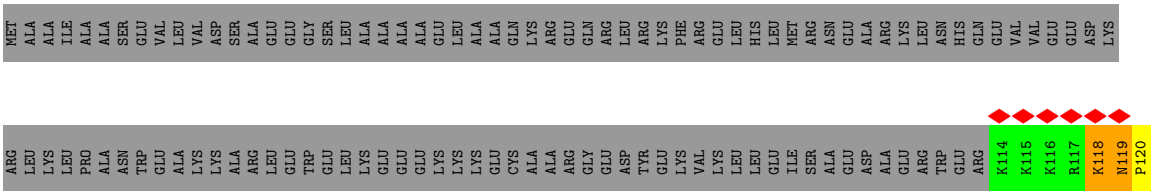


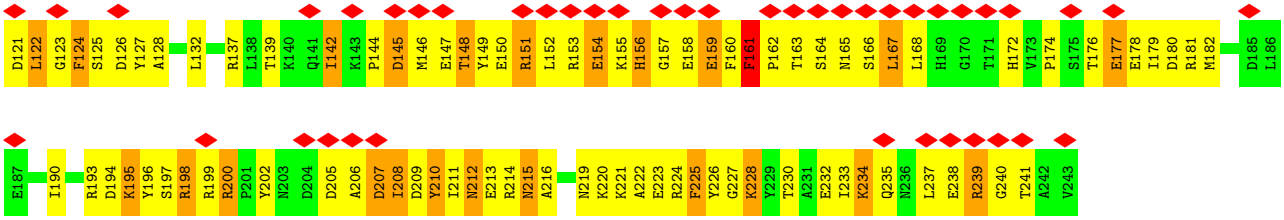




• Molecule 13: Pre-mRNA-splicing factor SYF2

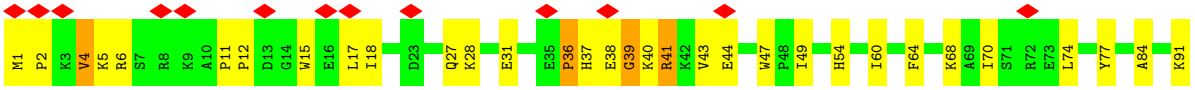






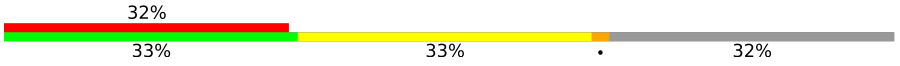
• Molecule 14: Protein BUD31 homolog

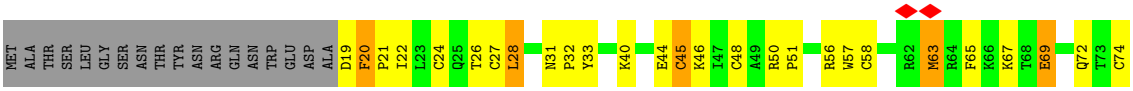
Chain N:

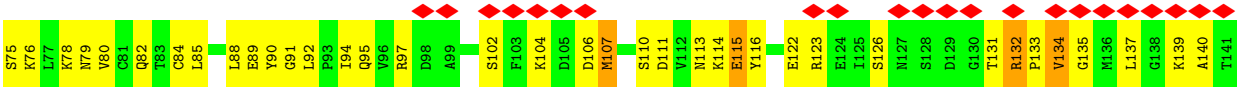


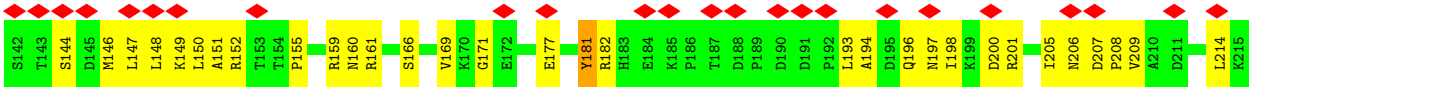
• Molecule 15: Pre-mRNA-splicing factor RBM22

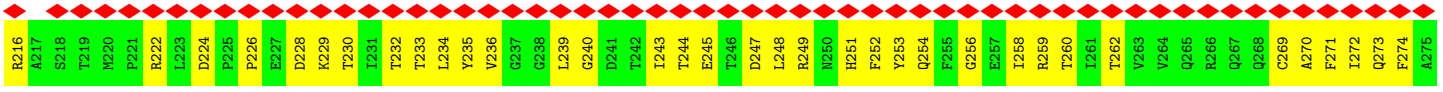
Chain O:

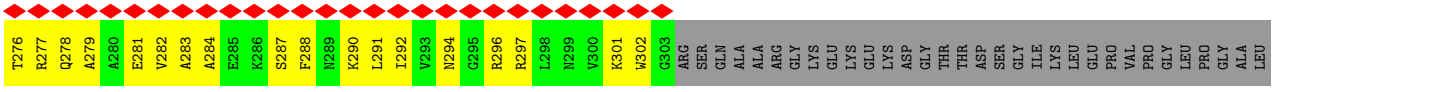


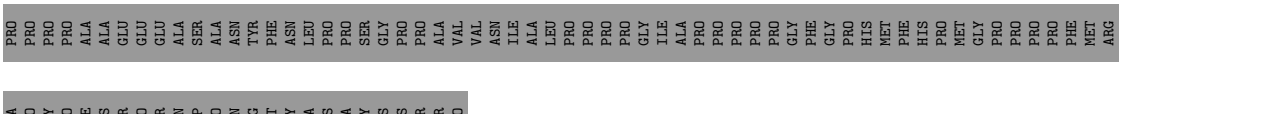


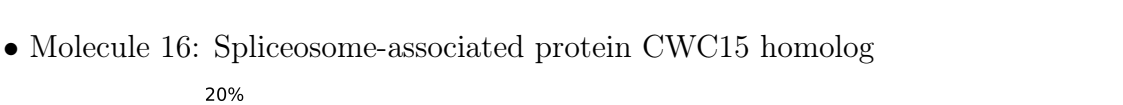






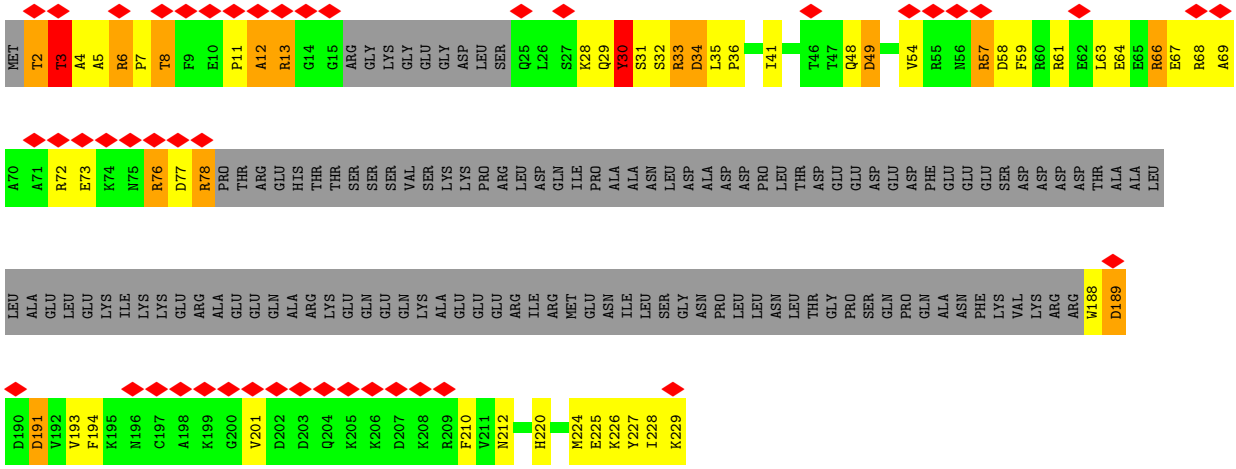






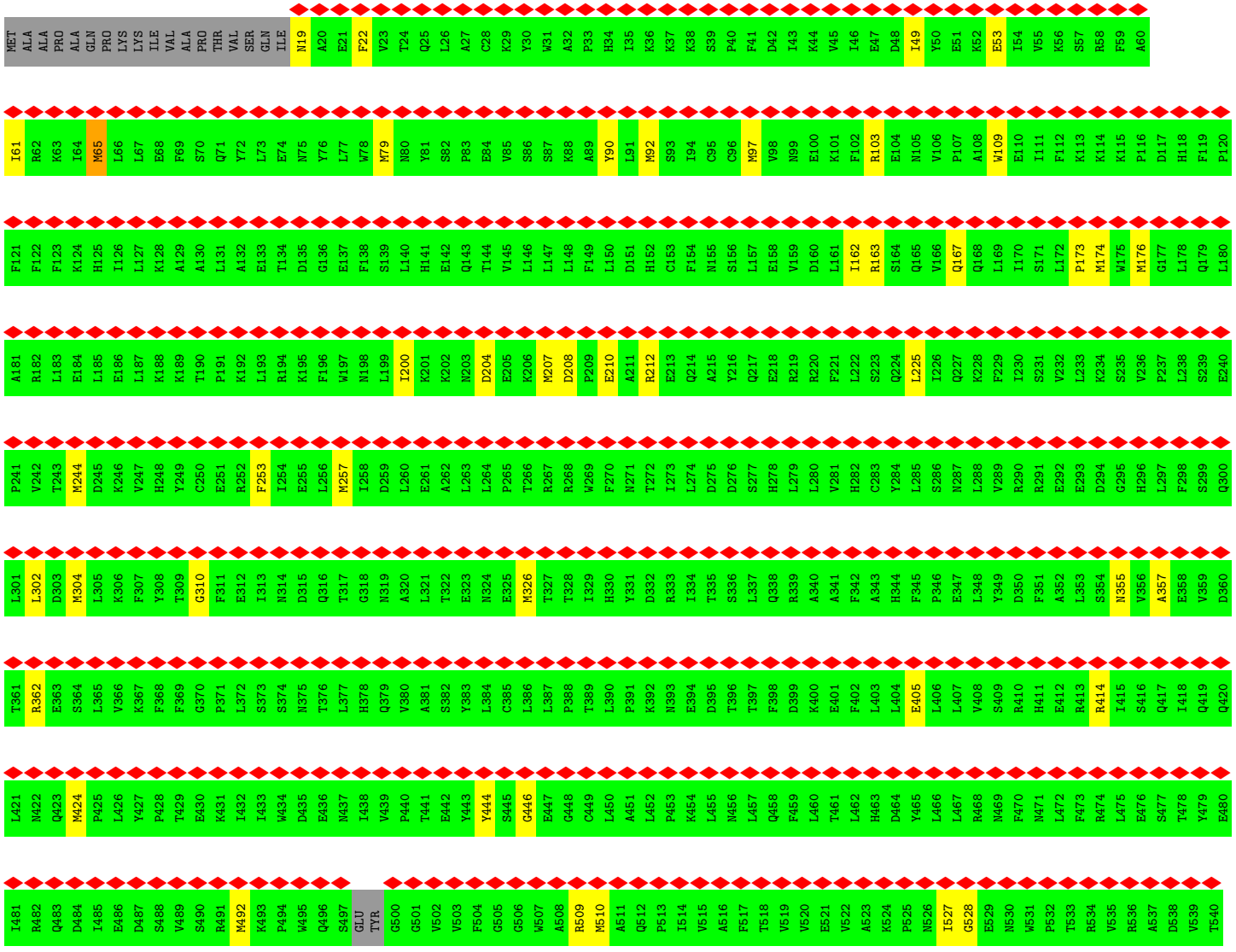
• Molecule 16: Spliceosome-associated protein CWC15 homolog

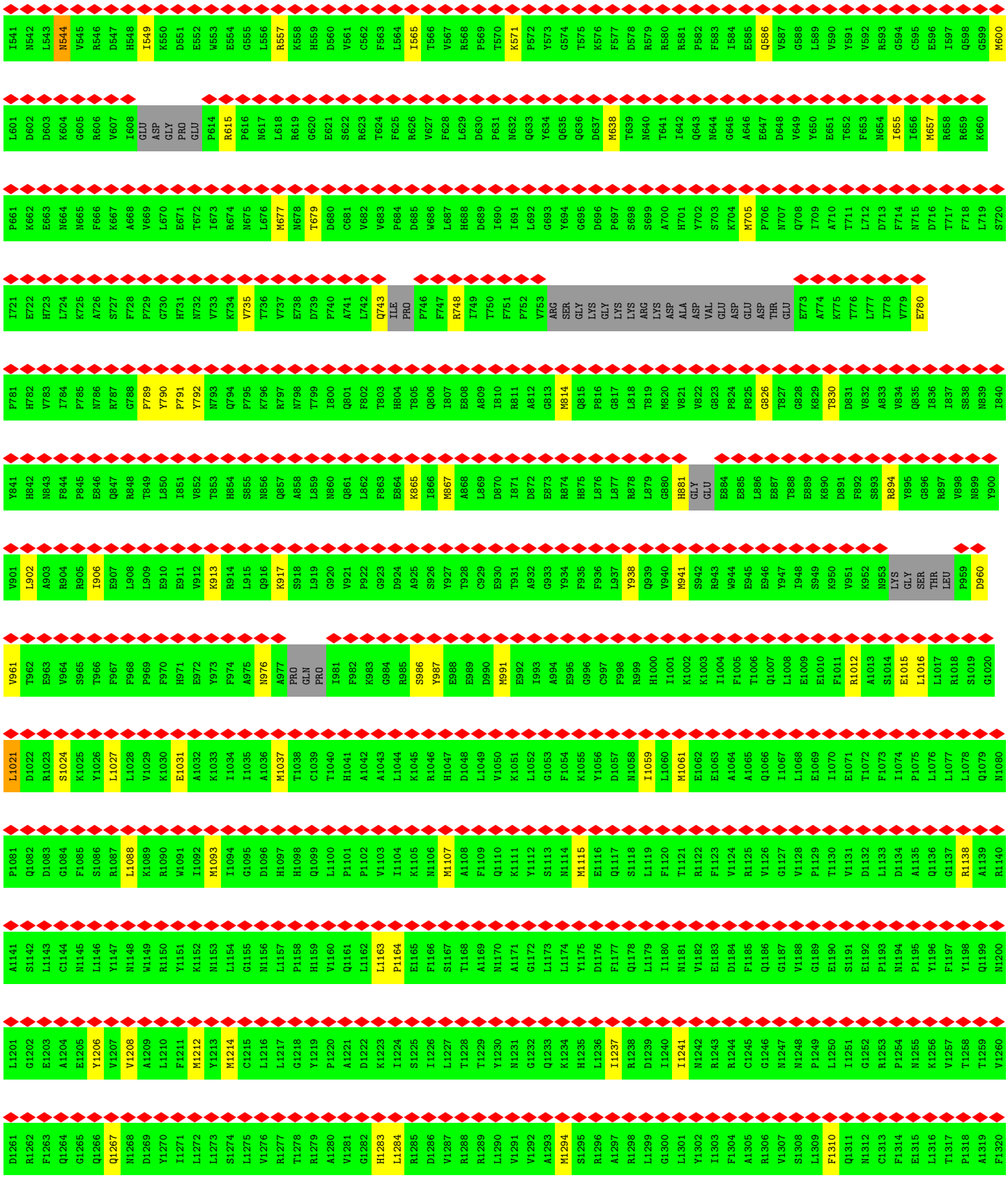
Chain P:



• Molecule 17: Intron-binding protein aquarius

Chain Q:

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L601 D602 D603 K604 G605 R606 V607 I608 GLU ASP GLY PRO GLU P614 R615 P616 N617 L618 R619 G620 E621 S622 R623 T624 F625 R626 V627 F628 L629 D630 P631 N632 Q633 Y634 Q635 Q636 D637 M638 T639 N640 T641 I642 Q643 N644 G645 A646 E647 D648 V649 Y650 E661 T652 F653 N654 I655 I656 M657 R658 R659 K660
P661 K662 E663 N664 N665 F666 K667 A668 V669 L670 E671 T672 I673 R674 N675 L676 M677 N678 T679 D680 C681 V682 V683 P684 D685 W686 L687 H688 D689 I690 I691 L692 G693 Y694 G695 D696 P697 S698 S699 A700 H701 Y702 S703 K704 M705 P706 N707 Q708 I709 A710 T711 L712 D713 F714 N715 D716 T717 F718 L719 S720
I721 E722 H723 L724 K725 A726 S727 F728 P729 G730 H731 N732 V733 K734 V735 T736 V737 E738 D739 P740 A741 L742 Q743 ILE PRO P746 F747 R748 I749 T750 F751 P752 V753 ARG SER GLY LYS GLY LYS LYS ARG LYS ASP ALA ASP VAL GLU ASP GLU ASP THR GLU E773 A774 K775 T776 L777 I778 V779 E780
P781 H782 V783 I784 P785 N786 R787 G788 P789 Y790 P791 Y792 N793 Q794 P795 K796 R797 N798 T799 I800 Q801 F802 T803 H804 T805 Q806 I807 E808 A809 I810 R811 A812 G813 M814 Q815 P816 G817 L818 T819 M820 V821 V822 G823 P824 P825 G826 T827 G828 K829 T830 D831 V832 A833 V834 Q835 I836 I837 S838 N839 I840
Y841 H842 N843 F844 P845 E846 Q847 R848 T849 L850 I851 V852 T853 H854 S855 N856 Q857 A858 L859 N860 Q861 L862 F863 E864 K865 I866 M867 A868 L869 D870 I871 D872 E873 R874 H875 L876 L877 R878 L879 G880 H881 GLY GLU E884 E885 L886 E887 T888 E889 K890 D891 F892 S893 R894 Y895 G896 R897 V898 N899 Y900
V901 L902 A903 R904 R905 I906 E907 L908 L909 E910 E911 V912 K913 R914 L915 Q916 K917 S918 L919 G920 V921 P922 G923 D924 A925 S926 Y927 T928 C929 E930 T931 A932 G933 Y934 F935 F936 L937 Y938 Q939 V940 M941 S942 R943 W944 E945 E946 Y947 I948 S949 K950 V951 K952 N953 LYS GLY SER THR LEU P959 D960
V961 T962 E963 V964 S965 T966 F967 F968 P969 F970 H971 E972 Y973 F974 A975 N976 A977 PRO GLN PRO I981 F982 K983 G984 R985 S986 Y987 E988 E989 D990 M991 E992 I993 A994 E995 G996 C997 F998 R999 H1000 I1001 K1002 K1003 I1004 F1005 T1006 Q1007 L1008 E1009 E1010 F1011 R1012 A1013 S1014 E1015 L1016 L1017 R1018 S1019 G1020
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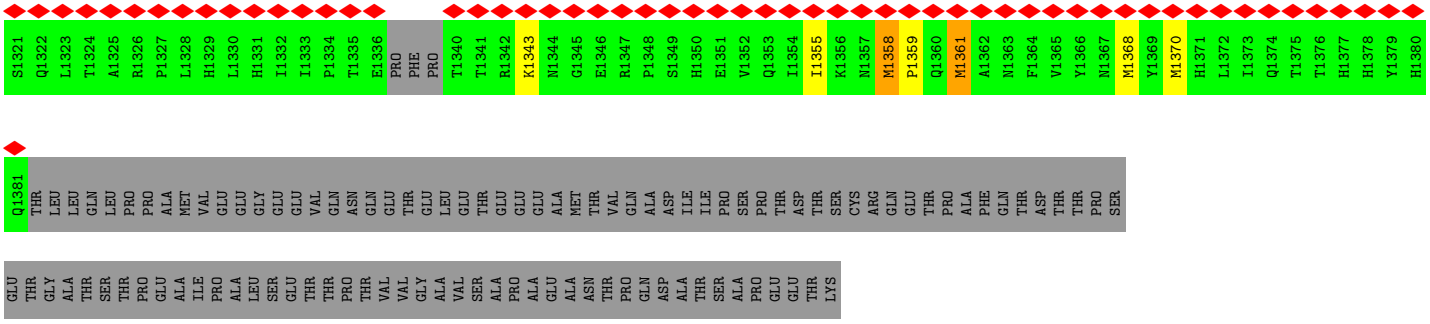
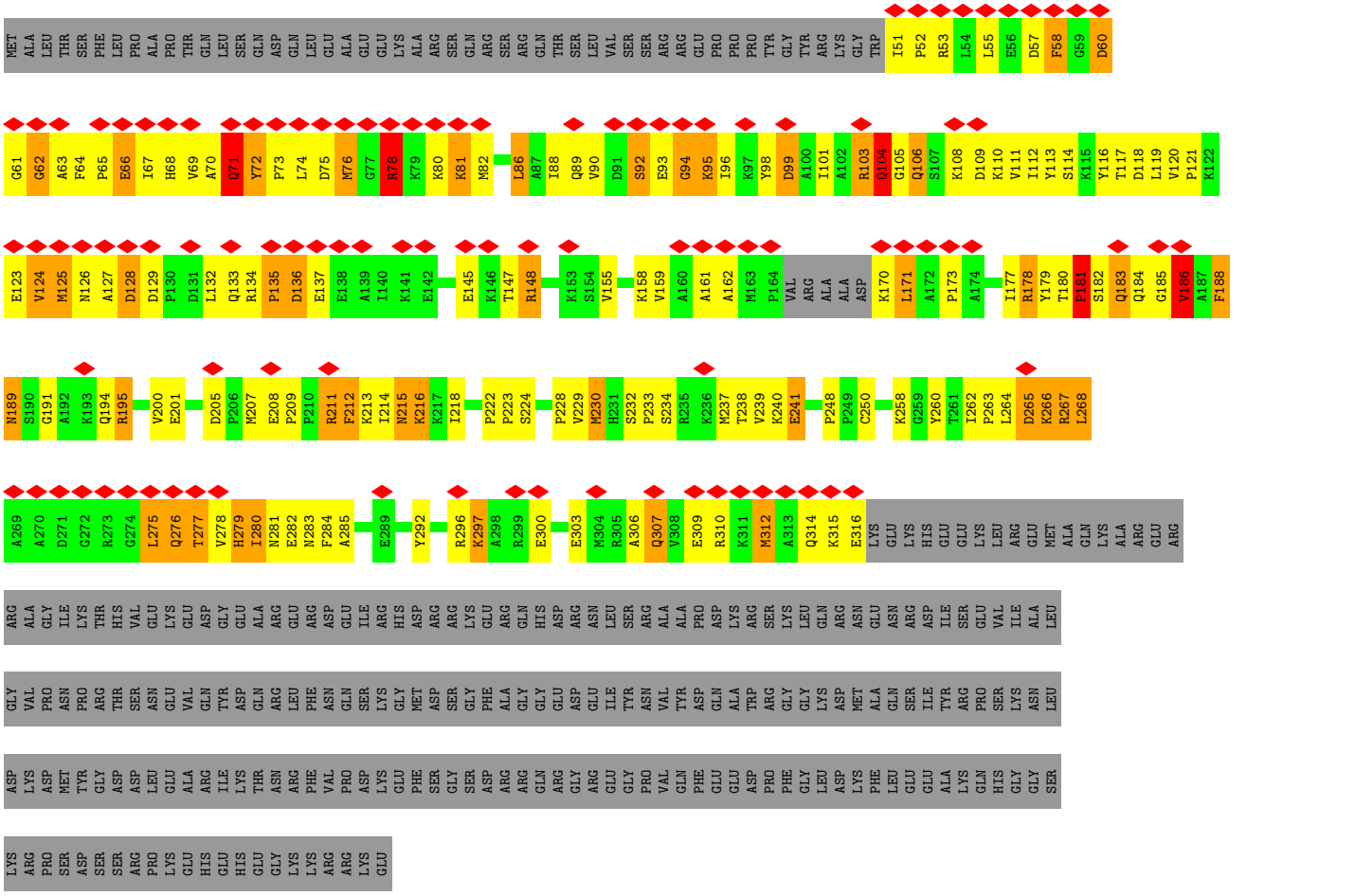
A1141 S1142 L1143 C1144 N1145 L1146 Y1147 N1148 W1149 R1150 Y1151 K1152 N1153 L1154 G1155 N1156 L1157 P1158 H1159 V1160 Q1161 L1162 L1163 P1164 E1165 F1166 S1167 T1168 A1169 N1170 A1171 G1172 L1173 L1174 Y1175 D1176 F1177 Q1178 L1179 I1180 N1181 V1182 E1183 D1184 F1185 Q1186 G1187 V1188 G1189 E1190 S1191 E1192 P1193 N1194 P1195 Y1196 F1197 Y1198 Q1199 N1200
L1201 G1202 E1203 A1204 E1205 Y1206 Y1207 V1208 A1209 L1210 F1211 M1212 Y1213 M1214 C1215 L1216 L1217 G1218 Y1219 P1220 A1221 D1222 K1223 I1224 S1225 I1226 L1227 T1228 T1229 Y1230 N1231 G1232 Q1233 K1234 H1235 L1236 I1237 R1238 D1239 I1240 I1241 N1242 R1243 R1244 C1245 G1246 N1247 N1248 P1249 L1250 I1251 G1252 R1253 P1254 N1255 K1256 V1257 T1258 T1259 V1260
D1261 R1262 F1263 Q1264 G1265 Q1266 Q1267 N1268 D1269 Y1270 I1271 L1272 L1273 S1274 L1275 V1276 R1277 T1278 R1279 A1280 V1281 G1282 H1283 L1284 R1285 D1286 V1287 R1288 R1289 L1290 V1291 V1292 A1293 M1294 S1295 R1296 A1297 R1298 L1299 G1300 L1301 Y1302 I1303 F1304 A1305 R1306 V1307 S1308 L1309 F1310 Q1311 N1312 C1313 F1314 E1315 L1316 T1317 P1318 A1319 F1320



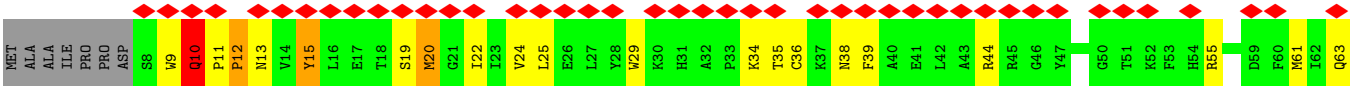
• Molecule 18: SNW domain-containing protein 1

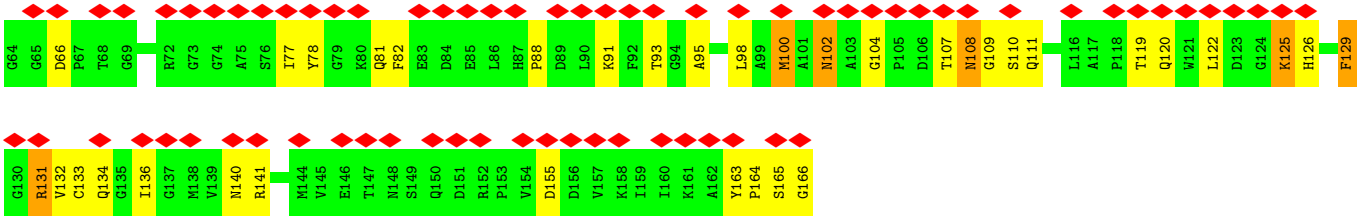
Chain R:



• Molecule 19: Peptidyl-prolyl cis-trans isomerase-like 1

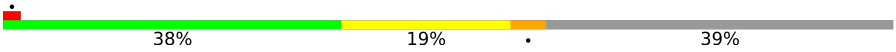
Chain S:

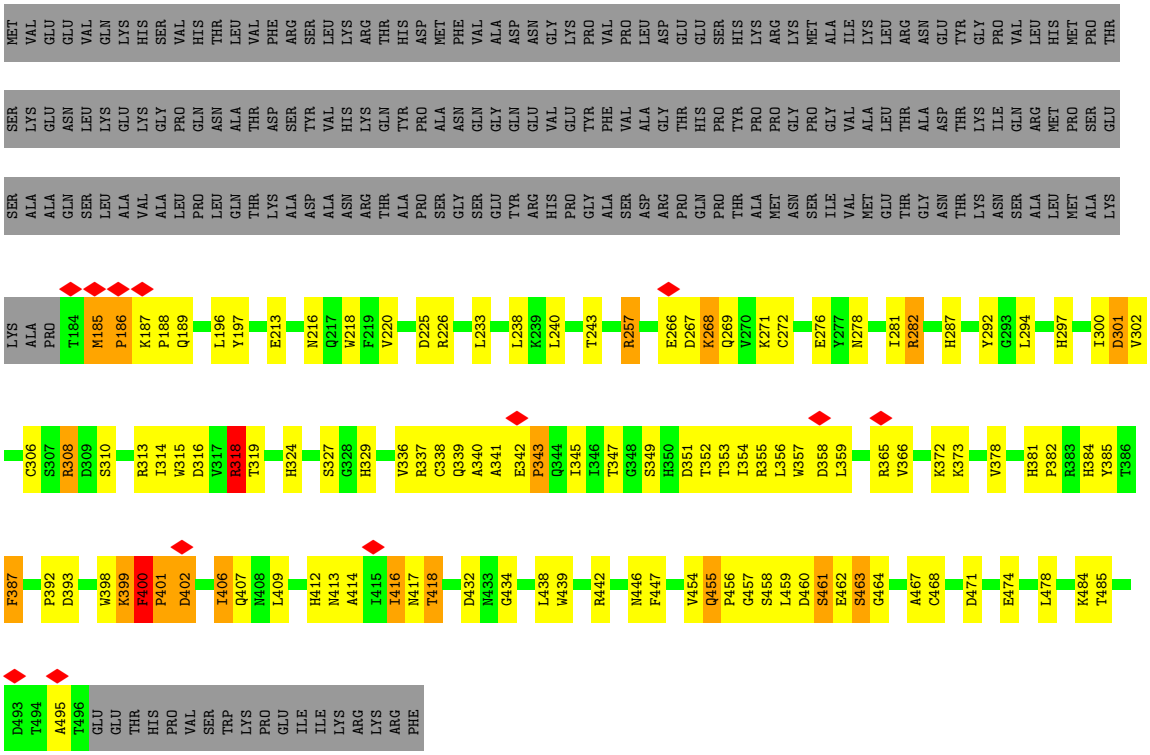




• Molecule 20: Pleiotropic regulator 1

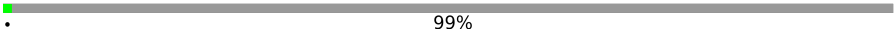
Chain T:

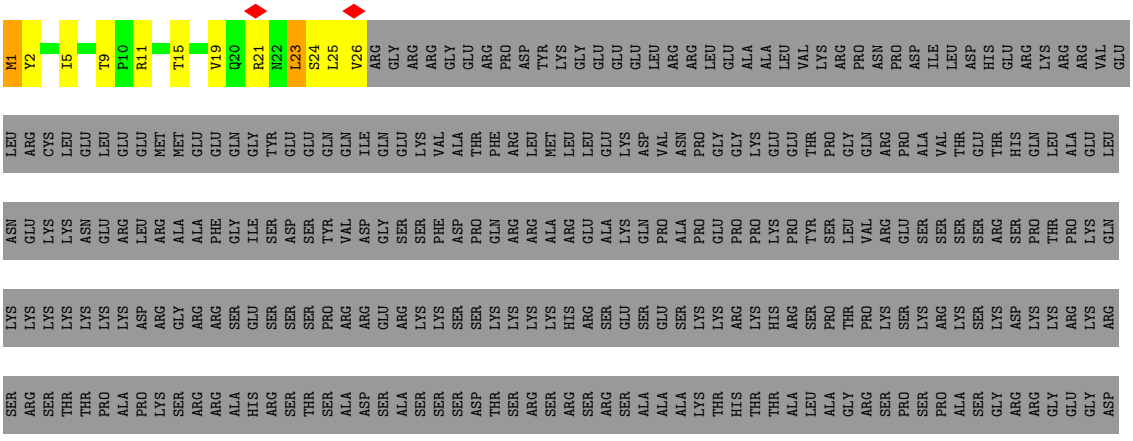


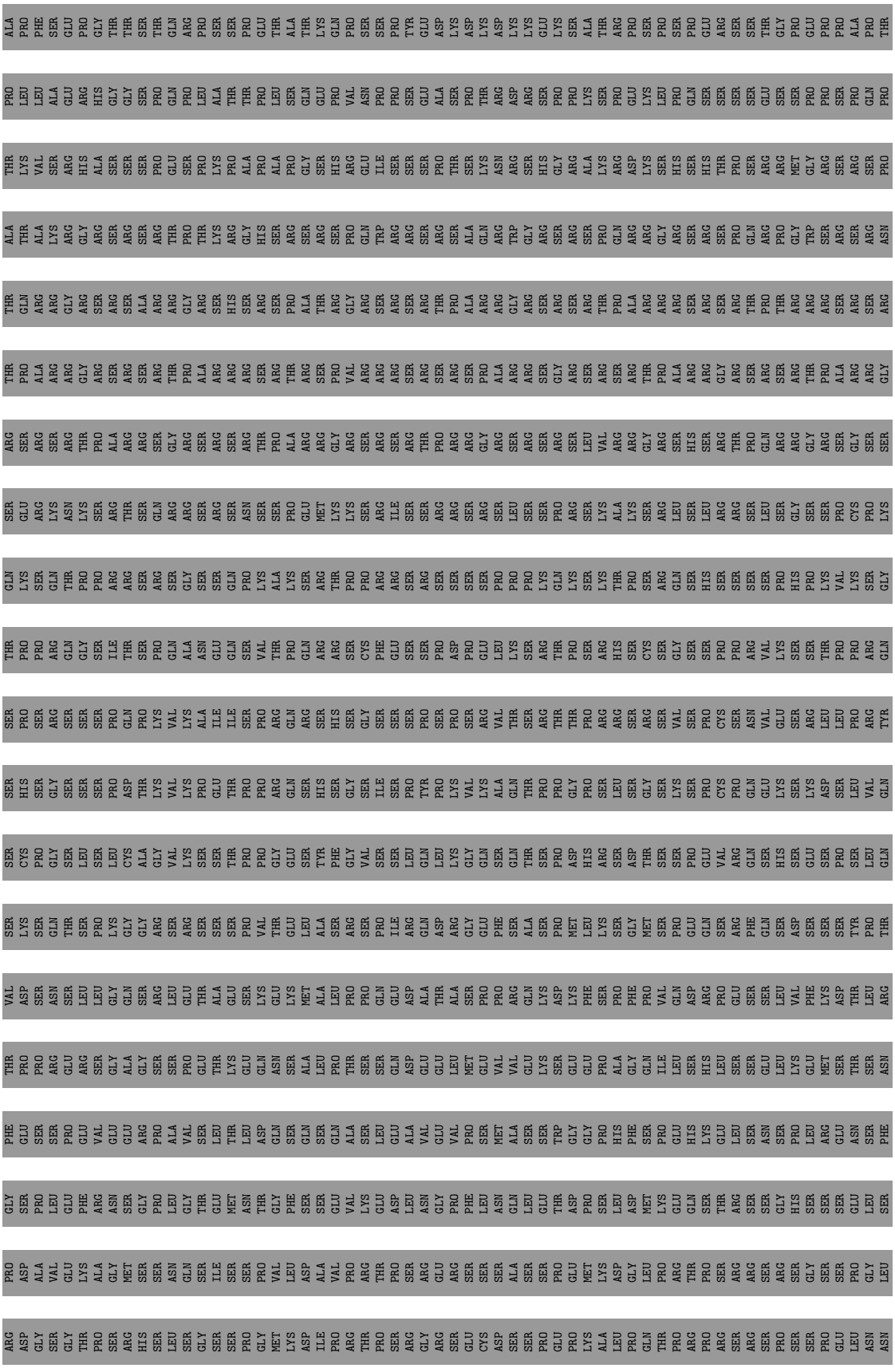


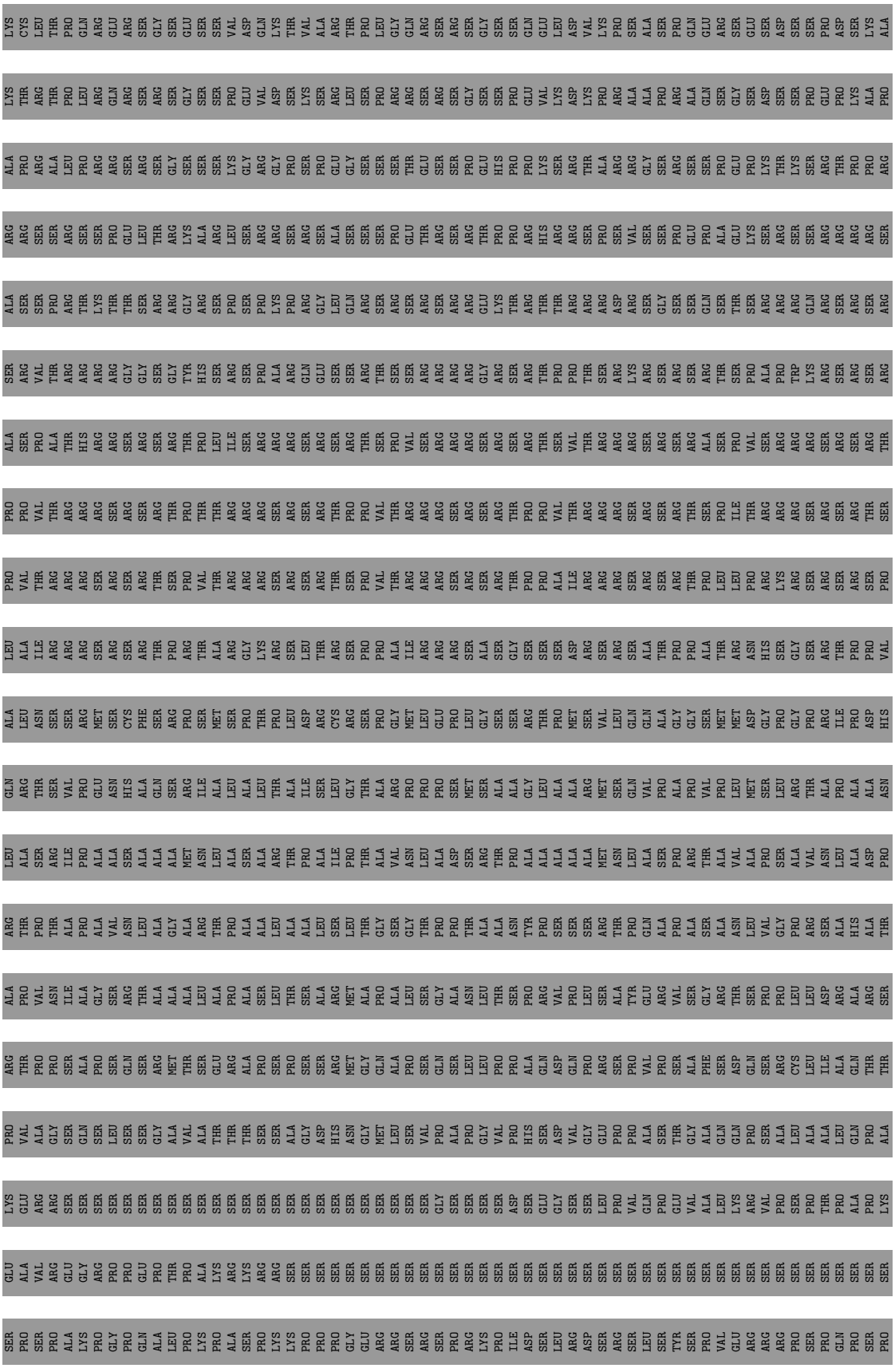
• Molecule 21: Serine/arginine repetitive matrix protein 2

Chain U:

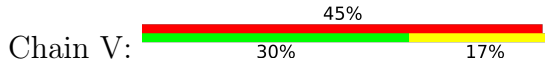


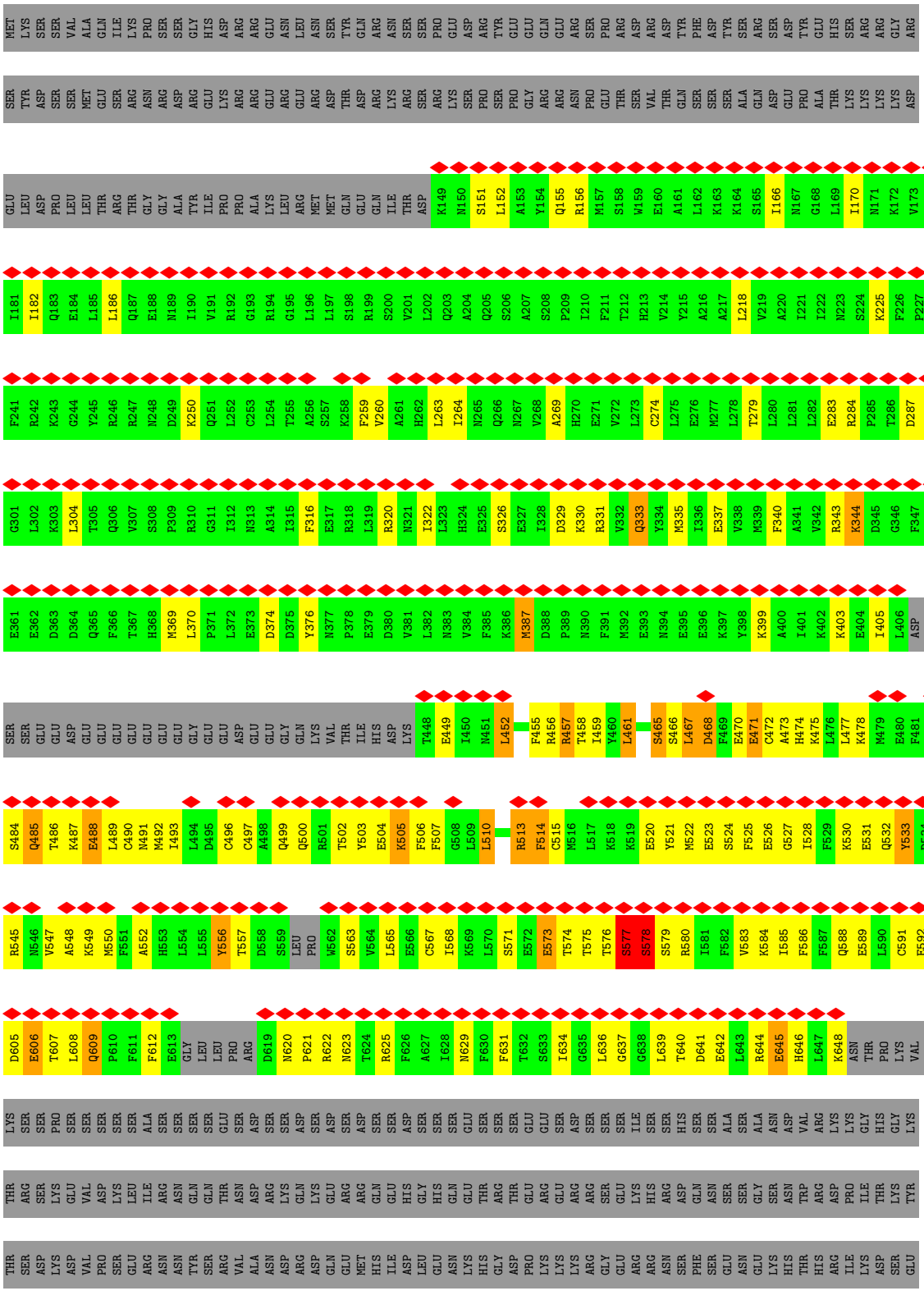


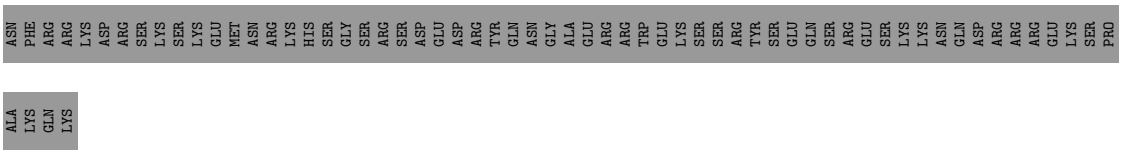




• Molecule 22: Pre-mRNA-splicing factor CWC22 homolog

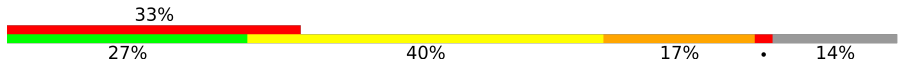


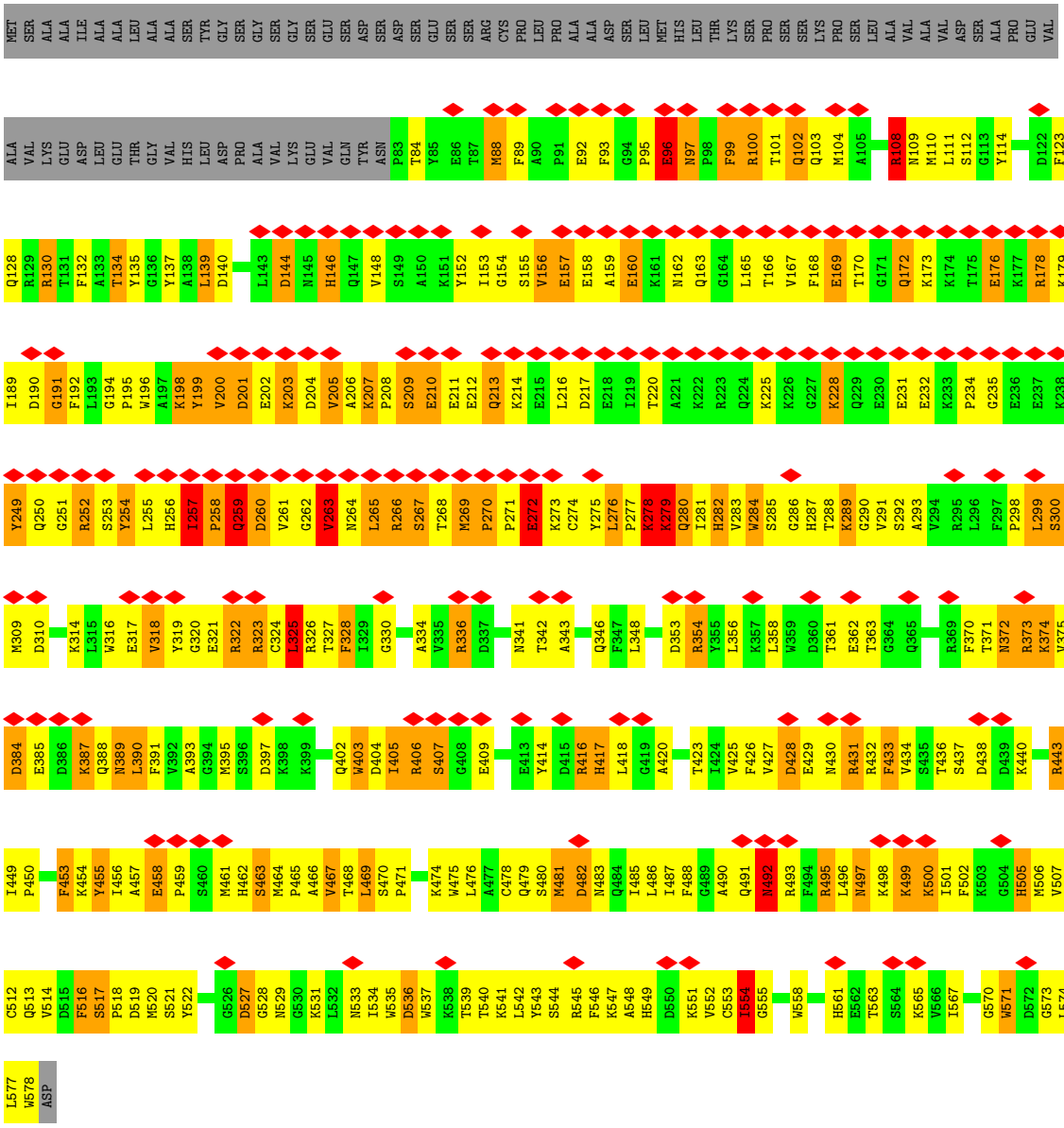




• Molecule 23: Pre-mRNA-processing factor 17

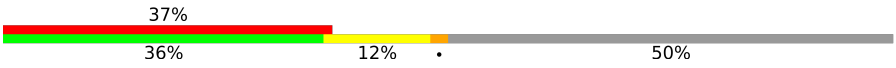
Chain W:

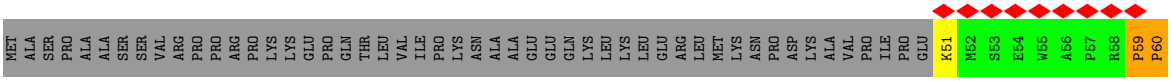


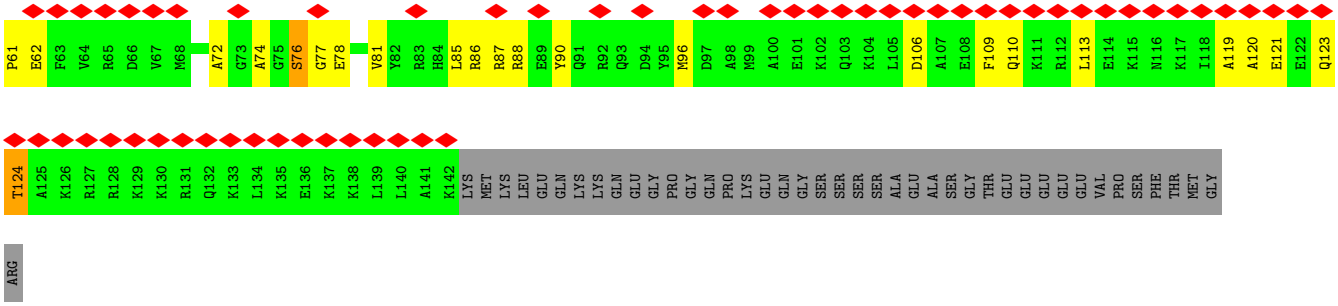


• Molecule 24: PRKR-interacting protein 1

Chain X:

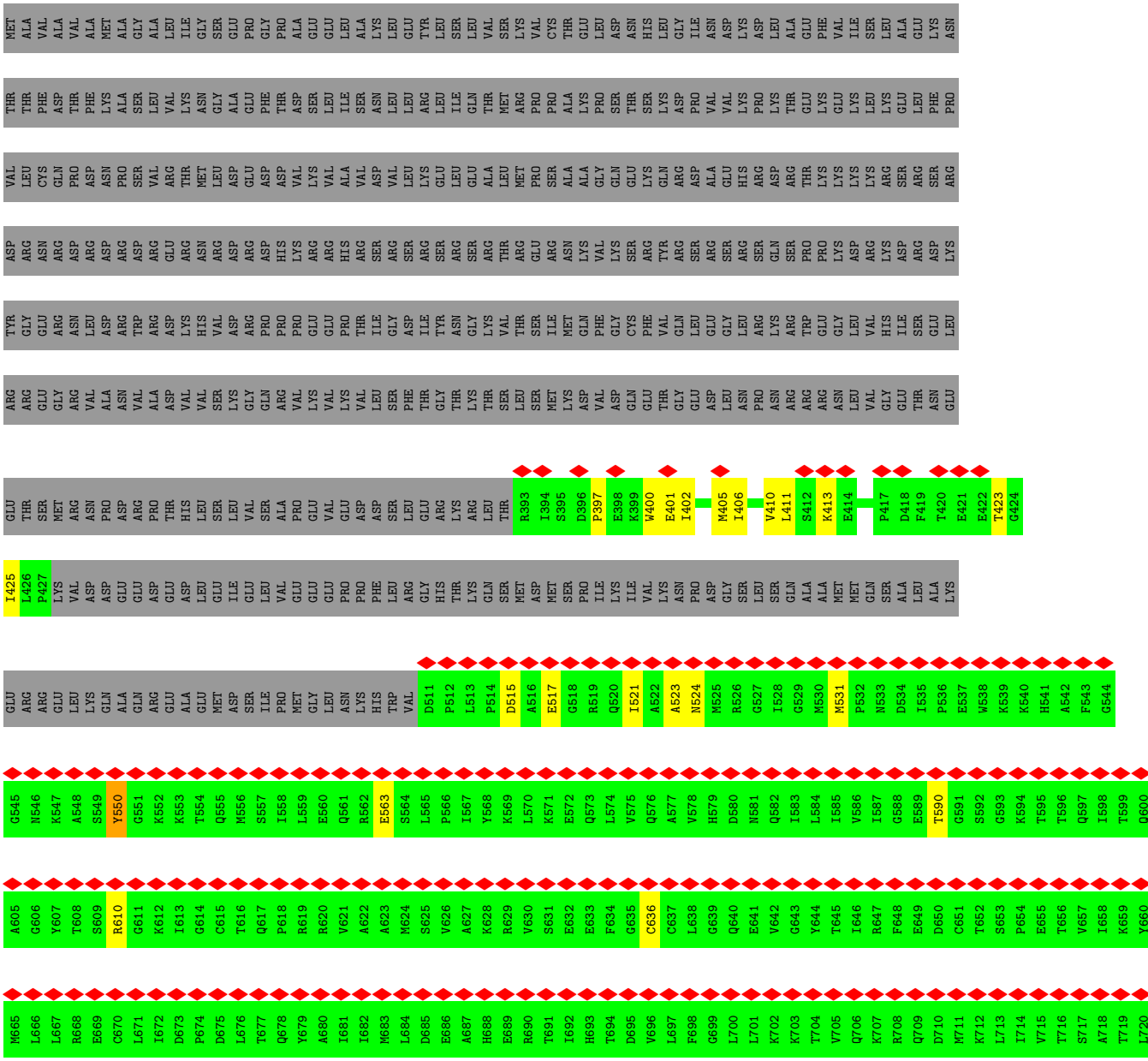


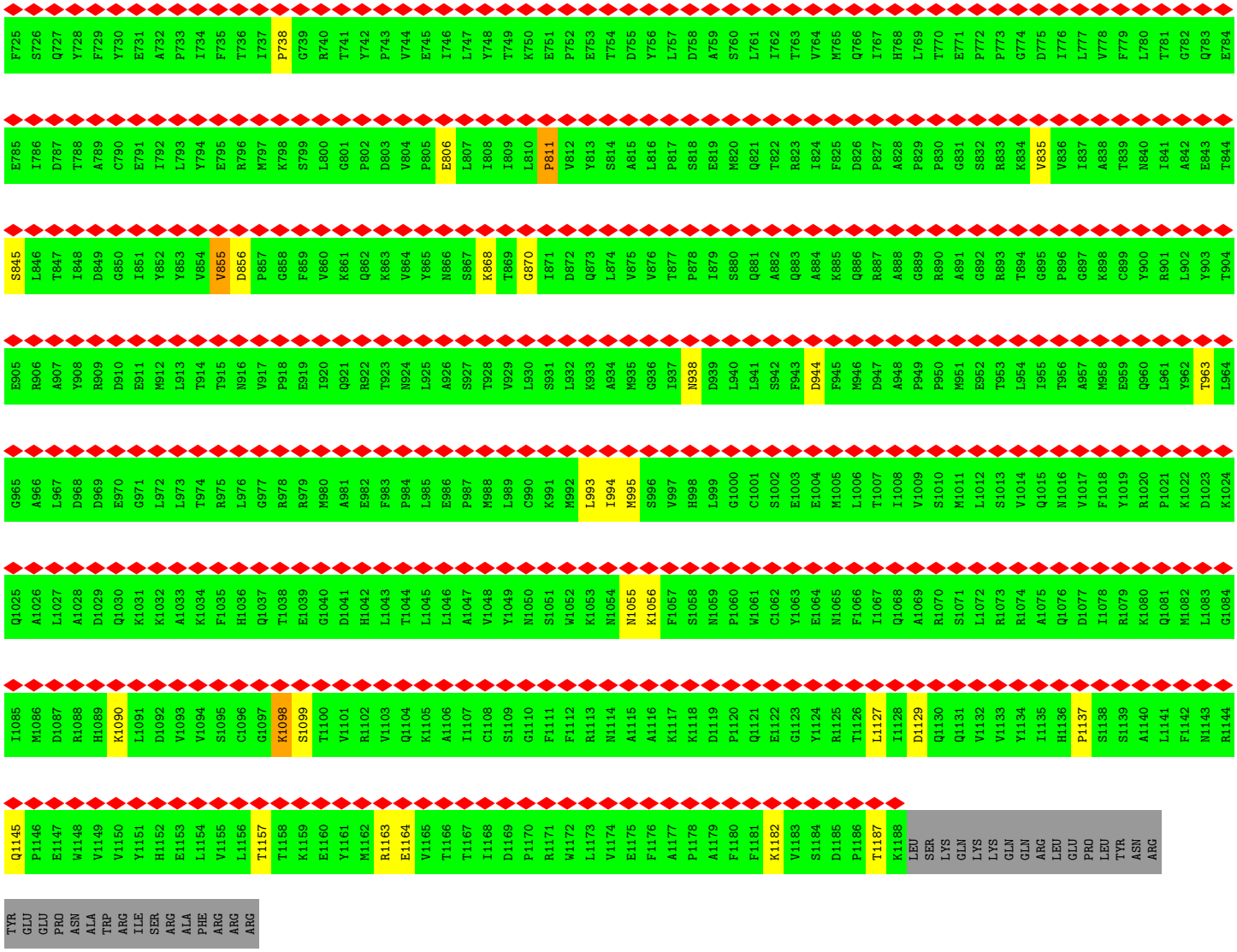




• Molecule 25: ATP-dependent RNA helicase DHX8

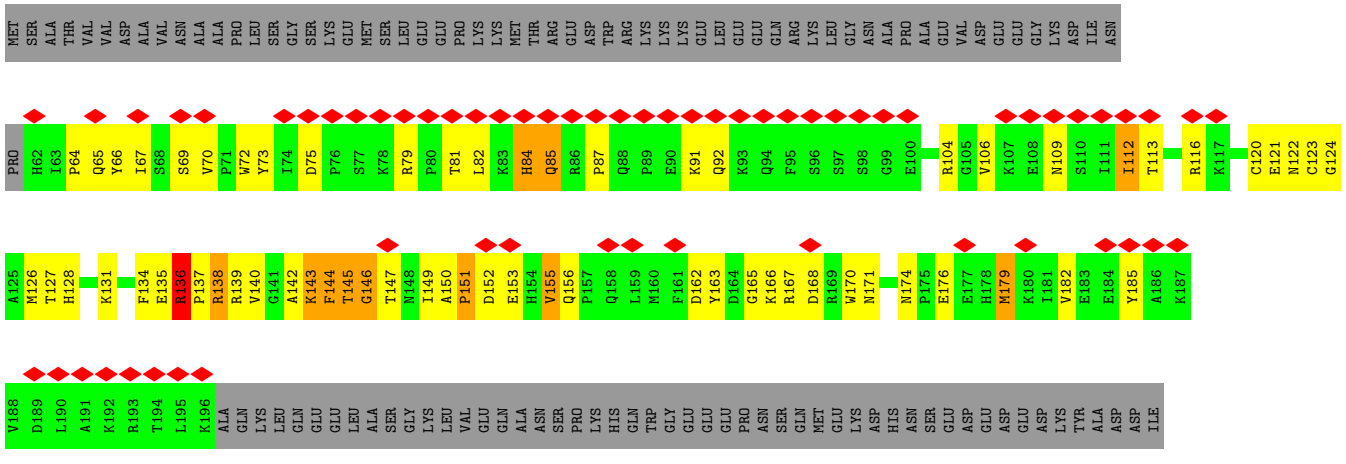
Chain Y:

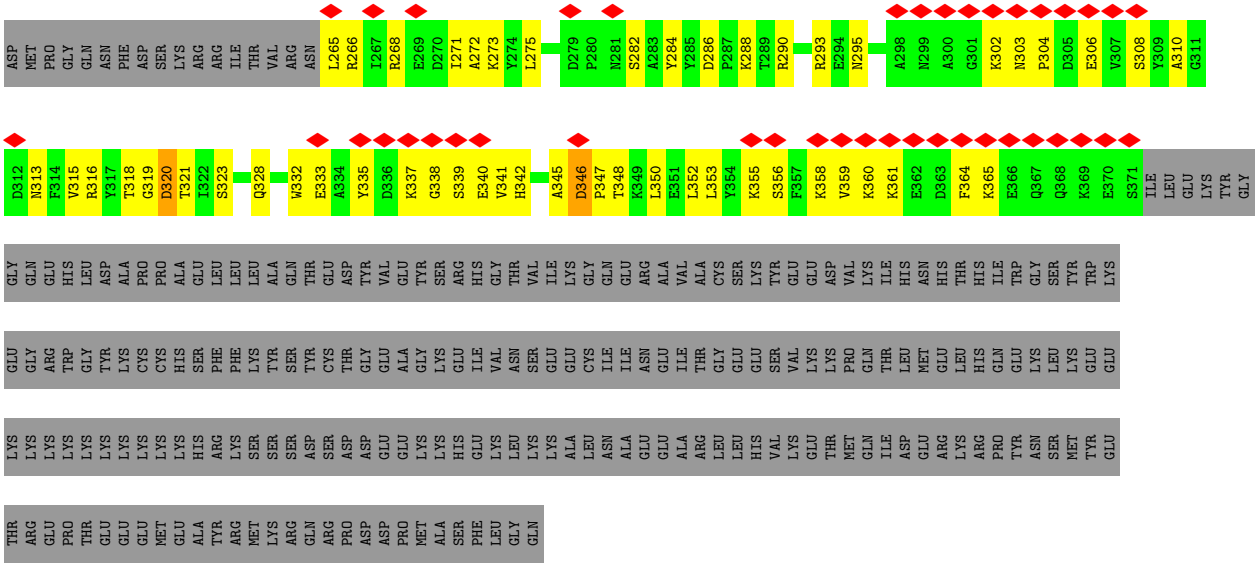


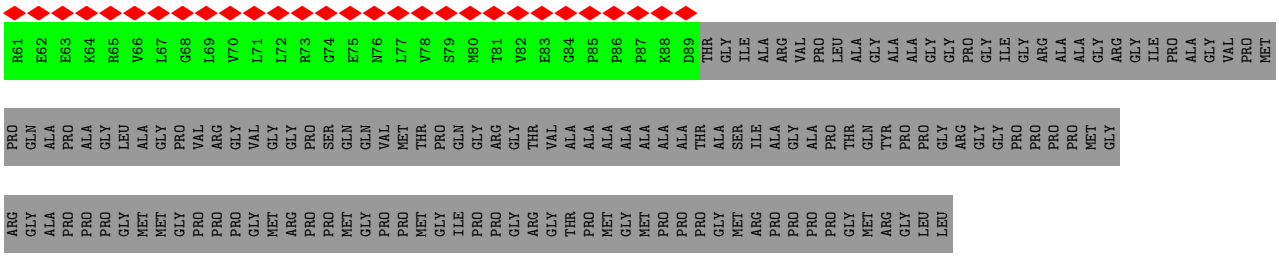


• Molecule 26: Pre-mRNA-splicing factor SLU7

Chain Z:

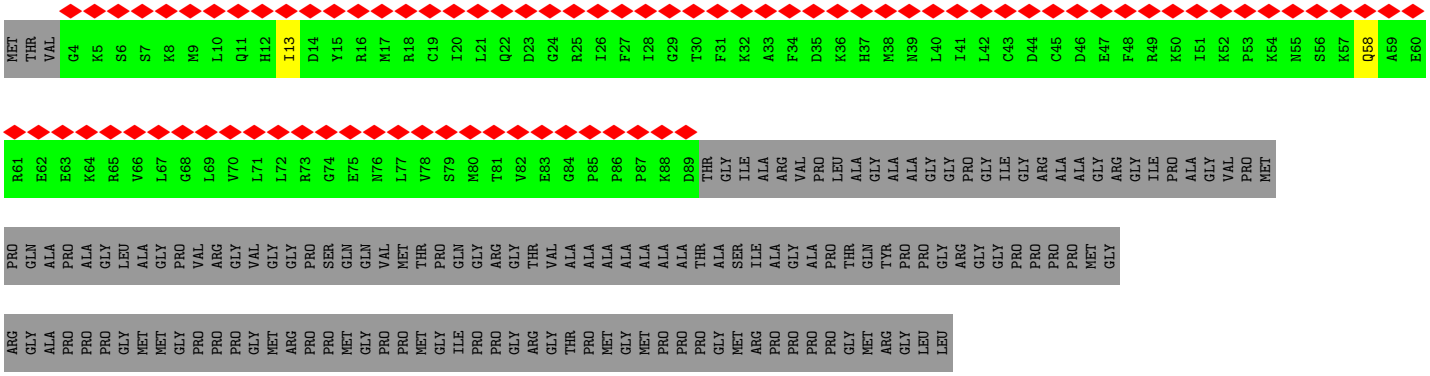






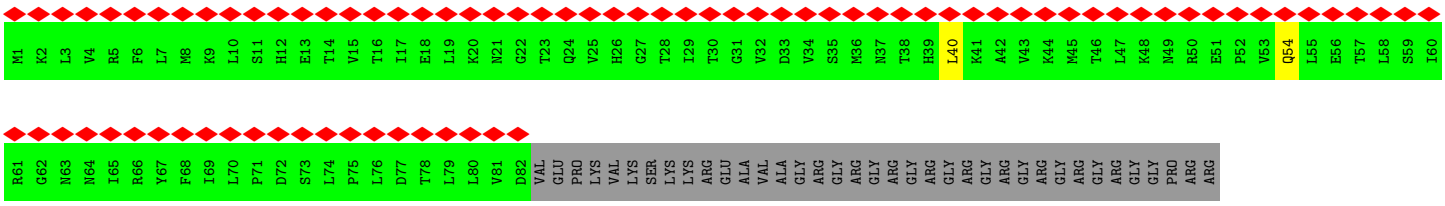
• Molecule 28: Small nuclear ribonucleoprotein-associated proteins B and B'

Chain i:



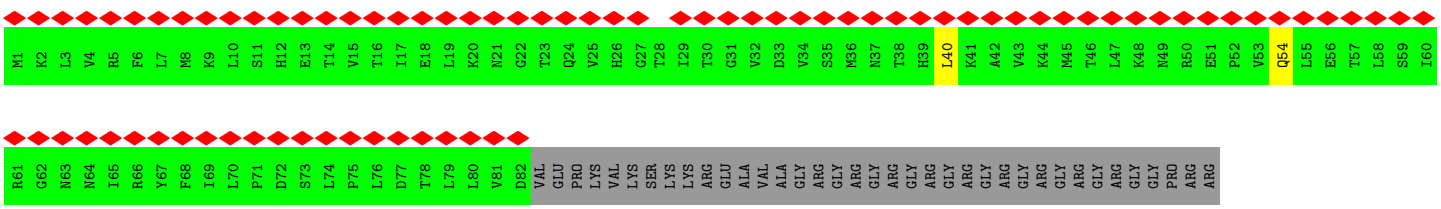
• Molecule 29: Small nuclear ribonucleoprotein Sm D1

Chain c:



• Molecule 29: Small nuclear ribonucleoprotein Sm D1

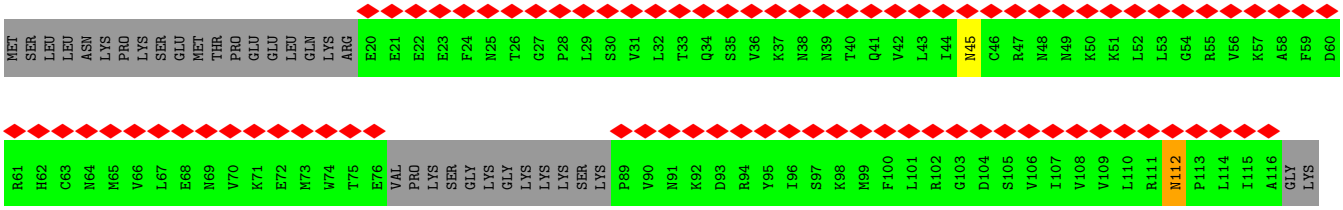
Chain j:



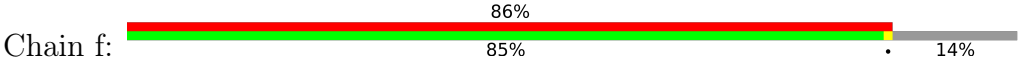
• Molecule 30: Small nuclear ribonucleoprotein Sm D2

Chain d:

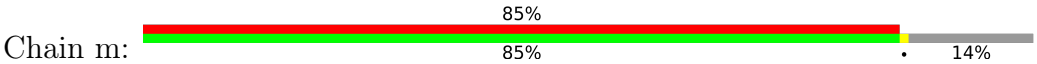
• Molecule 30: Small nuclear ribonucleoprotein Sm D2



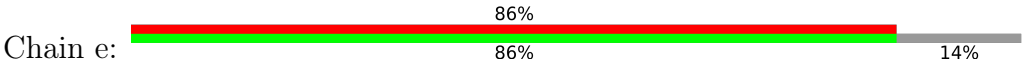
• Molecule 31: Small nuclear ribonucleoprotein F

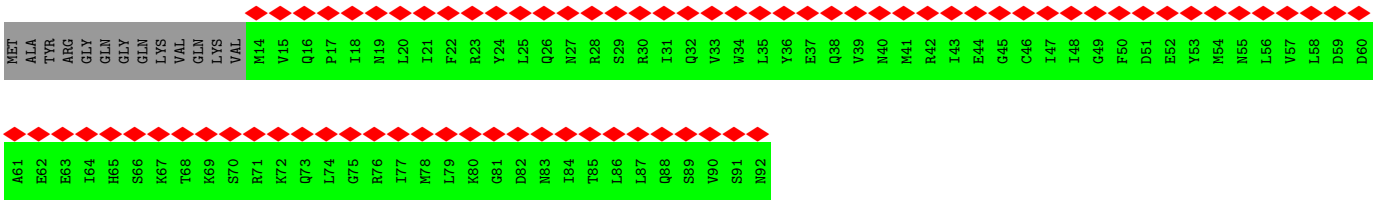


• Molecule 31: Small nuclear ribonucleoprotein F



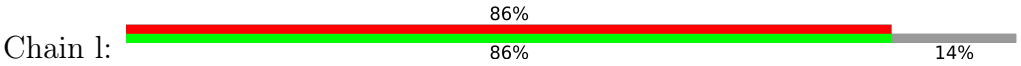
• Molecule 32: Small nuclear ribonucleoprotein E

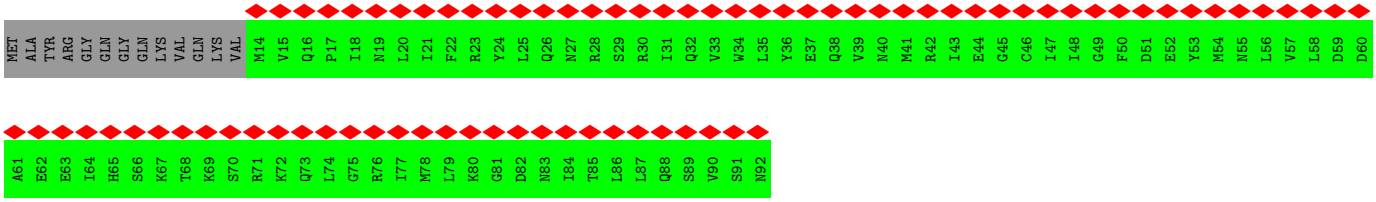




• Molecule 32: Small nuclear ribonucleoprotein E

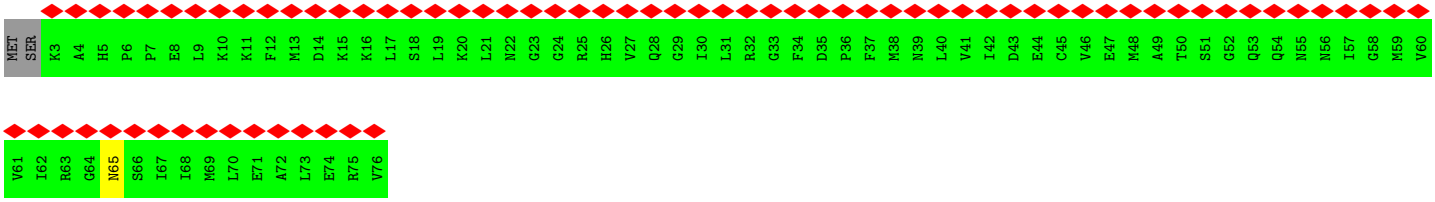
Chain l:





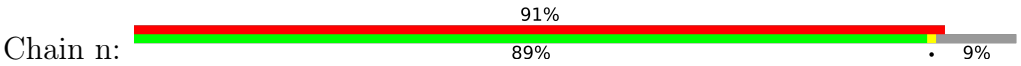
• Molecule 33: Small nuclear ribonucleoprotein G

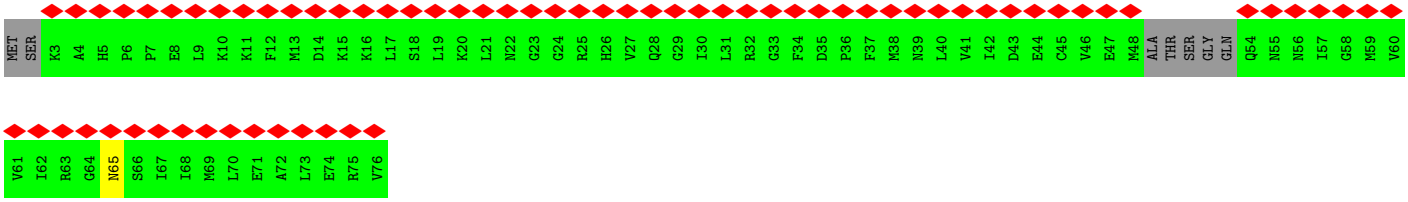
Chain g:



• Molecule 33: Small nuclear ribonucleoprotein G

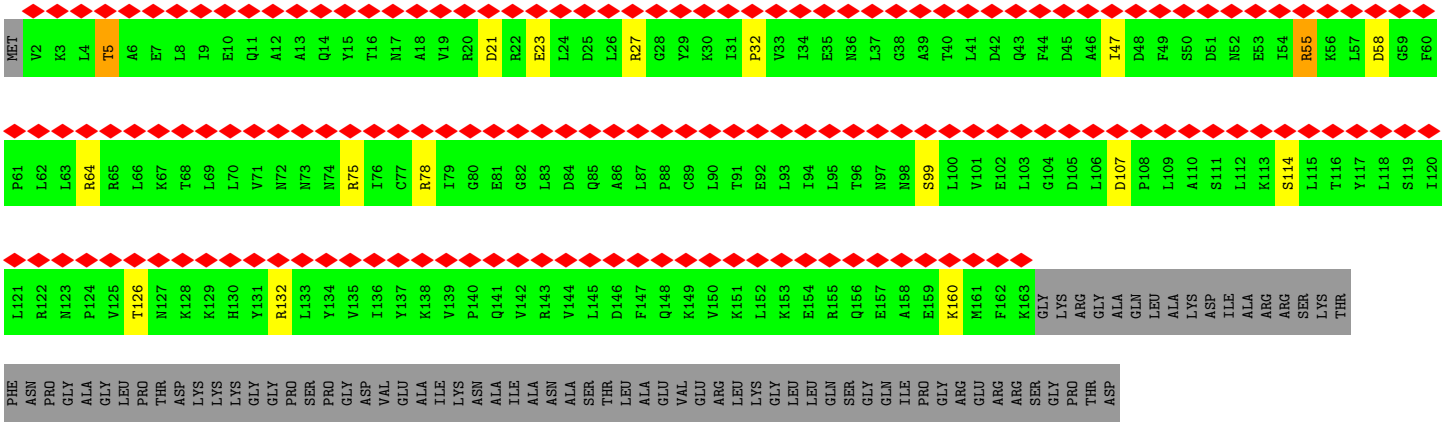
Chain n:



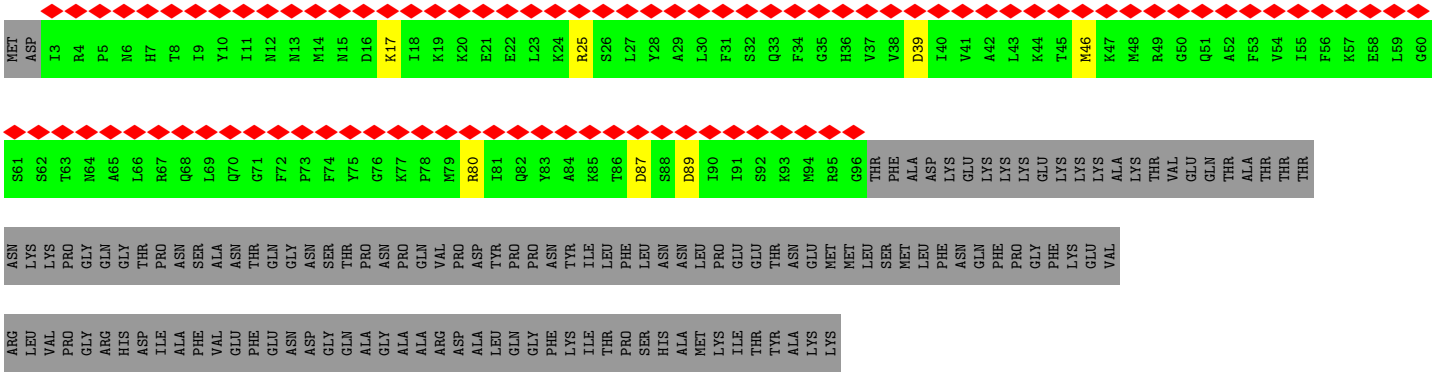


• Molecule 34: U2 small nuclear ribonucleoprotein A'

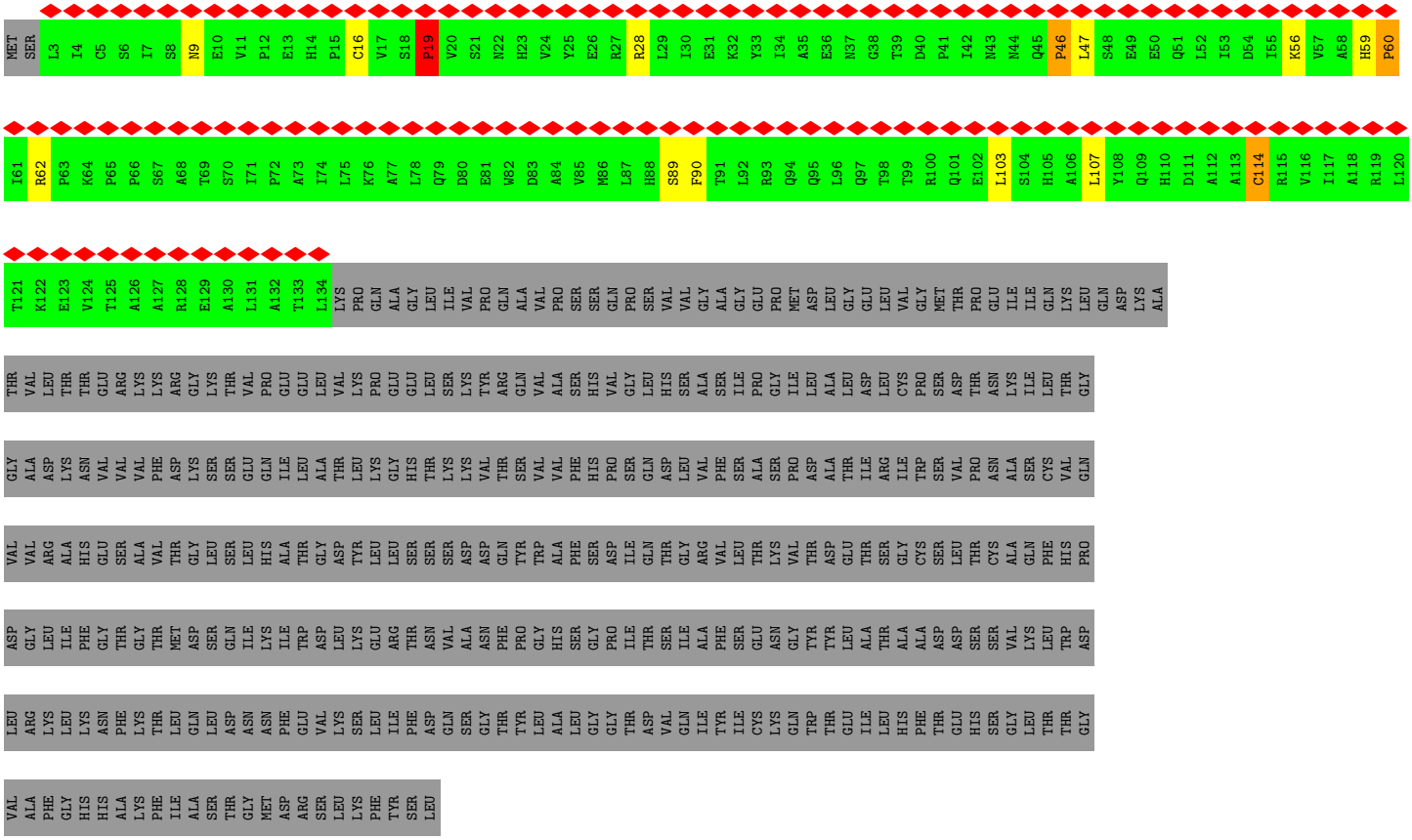
Chain o:



• Molecule 35: U2 small nuclear ribonucleoprotein B"

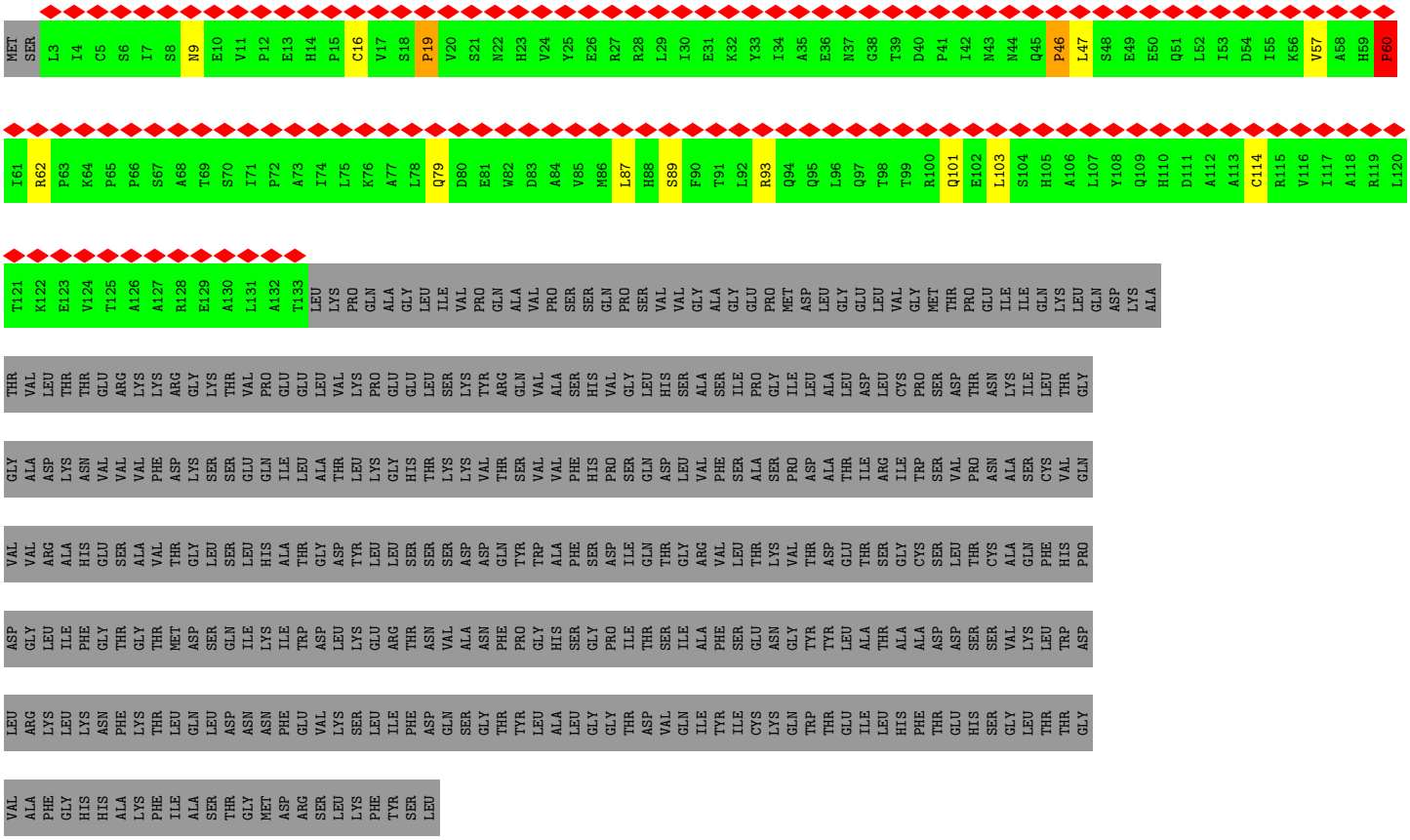


• Molecule 36: Pre-mRNA-processing factor 19



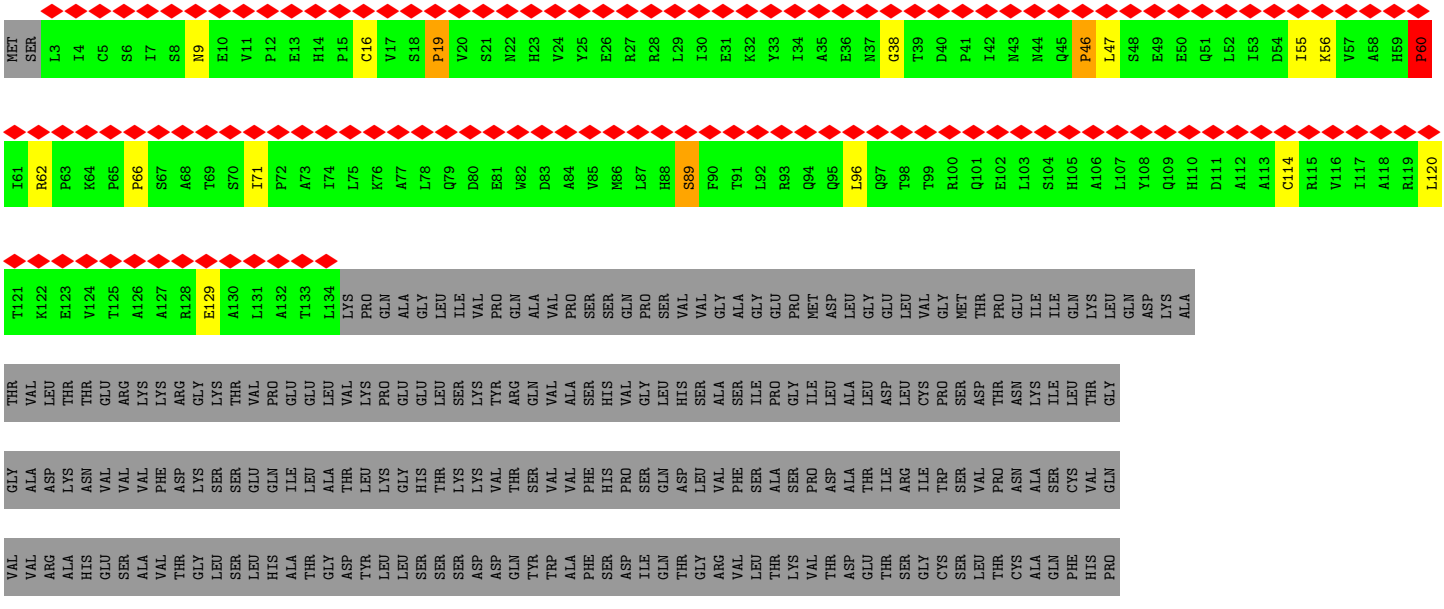
• Molecule 36: Pre-mRNA-processing factor 19

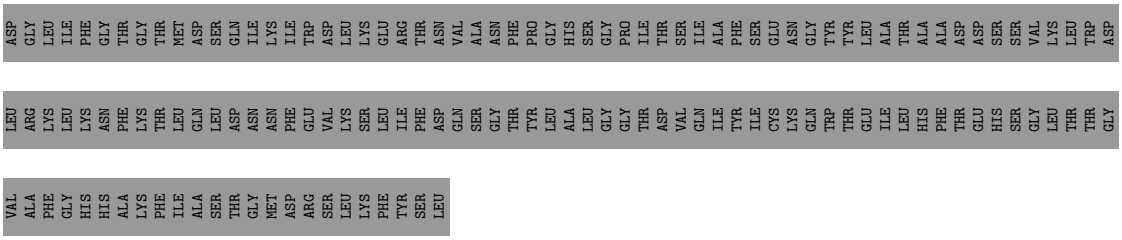
Chain r:



• Molecule 36: Pre-mRNA-processing factor 19

Chain s:



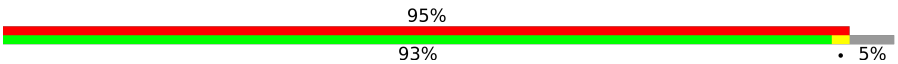


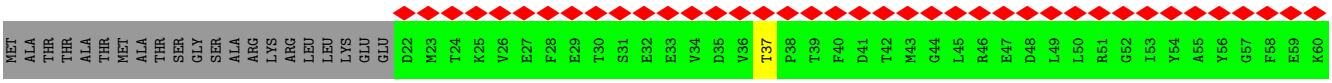
• Molecule 36: Pre-mRNA-processing factor 19

Chain t:

• Molecule 37: Eukaryotic initiation factor 4A-III

Chain u:





I181 K182 M183 L184 V185 L186 D187 E188 A189 D190 E191 M192 L193 N194 K195 G196 F197 K198 E199 Q200 I201 Y202 D203 V204 Y205 R206 Y207 L208 P209 P210 A211 T212 Q213 V214 V215 L216 I217 S218 A219 T220 L221 P222 H223 E224 I225 L226 E227 M228 T229 N230 K231 F232 M233 T234 D235 P236 I237 R238 I239 L240

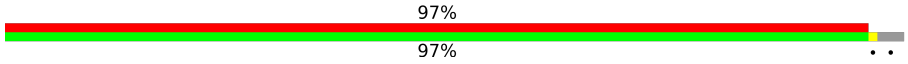
V241 K242 R243 D244 E245 L246 T247 L248 E249 G250 I251 K252 Q253 F254 F255 V256 A257 V258 E259 R260 E261 E262 W263 K264 F265 D266 T267 L268 C269 D270 L271 Y272 D273 T274 L275 T276 I277 T278 Q279 A280 V281 I282 F283 C284 N285 T286 K287 R288 K289 V290 D291 W292 L293 T294 E295 K296 M297 R298 E299 A300

N301 F302 T303 V304 S305 S306 M307 H308 G309 D310 M311 P312 Q313 K314 E315 R316 E317 S318 I319 M320 K321 E322 F323 R324 S325 G326 A327 S328 R329 V330 L331 I332 S333 T334 D335 V336 W337 A338 R339 G340 L341 D342 V343 P344 Q345 V346 S347 L348 I349 I350 N351 Y352 D353 L354 P355 N356 N357 R358 E359 L360

Y361 I362 H363 R364 I365 G366 R367 S368 G369 R370 Y371 G372 R373 K374 G375 V376 A377 I378 N379 F380 V381 K382 N383 D384 D385 I386 R387 I388 L389 R390 D391 I392 E393 Q394 Y395 Y396 S397 T398 Q399 I400 D401 E402 M403 P404 M405 N406 V407 A408 D409 L410 I411

- Molecule 38: Protein mago nashi homolog 2

Chain v:



MET ALA VAL ALA S5 D6 F7 Y8 L9 R10 Y11 Y12 V13 G14 H15 K16 G17 K18 F19 G20 H21 E22 F23 L24 E25 F26 E27 F28 R29 P30 D31 G32 K33 L34 R35 Y36 A37 N38 N39 S40 N41 Y42 K43 N44 D45 V46 M47 I48 R49 K50 E51 A52 Y53 V54 H55 K56 S57 V58 M59 E60

E61 L62 K63 R64 I65 I66 D67 D68 S69 E70 I71 T72 K73 E74 D75 D76 A77 L78 W79 P80 P81 P82 D83 R84 V85 G86 R87 Q88 E89 L90 E91 I92 V93 I94 G95 D96 E97 H98 I99 S100 F101 T102 T103 S104 K105 I106 G107 S108 L109 I110 D111 V112 N113 Q114 S115 K116 D117 P118 E119 G120

L121 R122 V123 F124 Y125 Y126 L127 V128 Q129 D130 L131 K132 C133 L134 V135 F136 S137 L138 I139 G140 L141 H142 F143 K144 I145 K146 P147 I148

- Molecule 39: RNA-binding protein 8A

Chain w:

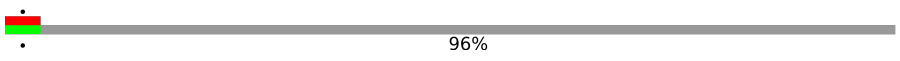
MET ALA ASP VAL LEU ASP LEU HIS GLU ALA GLY GLY GLU ASP PHE ALA MET ASP GLU ASP GLY ASP GLU SER ILE HIS LYS LEU LYS GLU LYS ALA LYS LYS ARG LYS GLY ARG GLY PHE GLY SER GLU GLU GLY SER ARG ALA ARG MET ARG GLU ASP TYR ASP SER VAL GLU GLN ASP

GLY ASP GLU P64 G65 P66 Q67 R68 S69 V70 E71 G72 W73 I74 L75 F76 V77 T78 G79 V80 H81 E82 E83 A84 T85 E86 E87 D88 I89 H90 D91 K92 F93 A94 E95 Y96 G97 E98 I99 K100 N101 I102 H103 L104 N105 L106 D107 R108 R109 T110 G111 Y112 L113 K114 G115 Y116 T117 L118 V119 E120

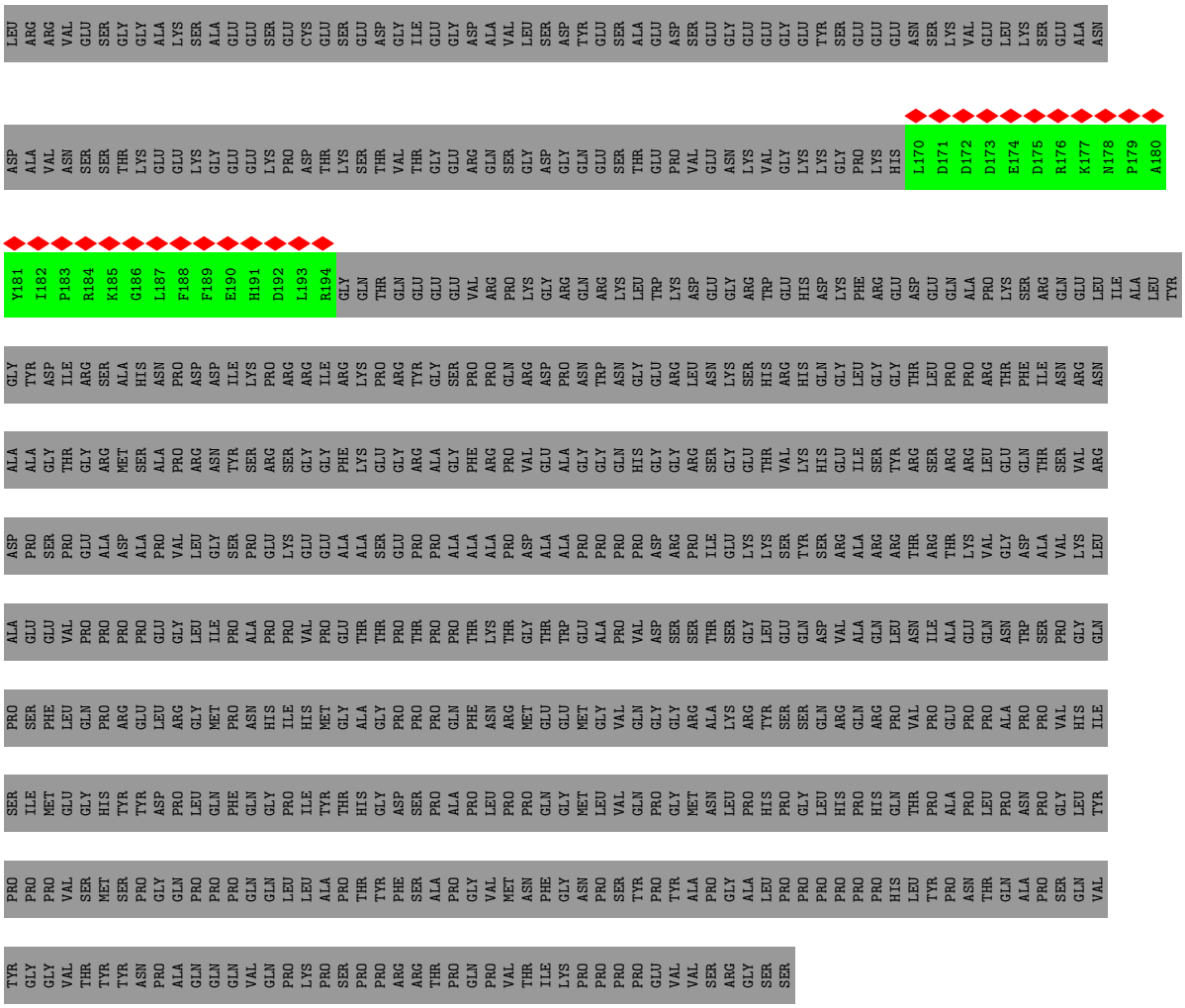
Y121 E122 T123 Y124 K125 E126 A127 Q128 A129 A130 M131 E132 G133 L134 N135 G136 Q137 D138 L139 M140 G141 Q142 P143 I144 S145 V146 D147 W148 C149 F150 V151 R152 G153 P154 PRO LYS GLY LYS ARG ARG GLY GLY ARG ARG ARG SER ARG SER PRO ASP ARG ARG ARG ARG

- Molecule 40: Protein CASC3

Chain x:



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


LEU ARG ARG VAL GLU SER GLY GLY ALA LYS SER ALA GLU GLU SER GLU CYS GLU SER GLU ASP GLY ILE GLU GLY ASP ALA VAL LEU SER ASP TYR GLU SER ALA GLU ASP SER GLU GLY GLU GLU GLY GLU TYR SER GLU GLU GLU ASN SER LYS VAL GLU LEU LYS SER GLU ALA ASN
ASP ALA VAL ASN SER SER THR LYS GLU GLU LYS GLY GLU GLU LYS PRO ASP THR LYS SER THR VAL THR GLY GLU ARG GLN SER GLY ASP GLY GLN GLU SER THR GLU PRO VAL GLU ASN LYS VAL GLY LYS LYS GLY PRO LYS HIS L170 D171 D172 D173 E174 D175 R176 K177 N178 P179 A180
Y181 I182 P183 R184 K185 G186 L187 F188 F189 E190 H191 D192 L193 R194 GLY GLN THR GLN GLU GLU GLU VAL ARG PRO LYS GLY ARG GLN ARG LYS LEU TRP LYS ASP GLU GLY ARG TRP GLU HIS ASP LYS PHE ARG GLU ASP GLU GLN ALA PRO LYS SER ARG GLN GLU LEU ILE ALA LEU TYR
GLY TYR ASP ILE ARG SER ALA HIS ASN PRO ASP ASP ILE LYS PRO ARG ARG ILE ARG LYS PRO ARG TYR GLY SER PRO PRO GLN ARG ASP PRO ASN TRP ASN GLY GLU ARG LEU ASN LYS SER HIS ARG HIS GLN GLY LEU GLY GLY THR LEU PRO PRO ARG THR PHE ILE ASN ARG ASN
ALA ALA GLY THR GLY ARG MET SER ALA PRO ARG ASN TYR SER ARG SER GLY GLY PHE LYS GLU GLY GLY ARG GLY PHE ARG PRO VAL GLU ALA GLY GLY GLN HIS GLY GLY ARG SER GLY GLU THR VAL LYS HIS GLU ILE SER TYR ARG SER ARG ARG LEU GLU GLN THR SER VAL ARG
ASP PRO SER PRO GLU ALA ASP ALA PRO VAL LEU GLY SER PRO GLU LYS GLU GLU ALA ALA SER GLU PRO PRO PRO ALA ALA ALA PRO ASP ALA ALA PRO PRO PRO PRO ASP ARG PRO PRO ILE GLU LYS LYS SER TYR SER ARG ALA ARG ARG THR ARG THR LYS VAL GLY ASP ALA VAL LEU LYS
ALA GLU GLU VAL PRO PRO PRO PRO GLU GLY LEU ILE PRO ALA PRO PRO VAL PRO GLU THR THR PRO THR PRO PRO PRO THR LYS THR GLY THR TRP GLU ALA PRO VAL ASP SER GLY LEU GLU GLN LEU ASN ILE ALA GLU GLN ASN TRP SER PRO GLY GLN
PRO SER PHE LEU GLN PRO ARG GLU LEU ARG GLY MET PRO ASN HIS ILE HIS MET GLY ALA GLY PRO PRO PRO GLN PHE ASN ARG MET GLU GLU MET GLY VAL GLN GLY GLY ARG ALA LYS ARG TYR SER SER GLN ARG GLN ARG PRO VAL PRO GLU PRO PRO PRO ALA PRO VAL HIS ILE
SER ILE MET GLU GLY HIS TYR TYR ASP PRO LEU GLN PHE GLN GLY PRO ILE TYR THR HIS GLY ASP SER PRO ALA PRO LEU PRO PRO GLN GLY MET LEU VAL GLN PRO GLY MET ASN LEU PRO HIS PRO GLY LEU HIS PRO HIS GLN THR PRO ALA PRO LEU PRO ASN PRO GLY LEU TYR
PRO PRO PRO VAL SER MET SER PRO GLY GLN PRO PRO PRO GLN LEU LEU ALA PRO THR TYR PHE SER ALA PRO GLY VAL MET ASN PHE GLY ASN PRO SER TYR PRO TYR ALA PRO GLY ALA LEU PRO PRO PRO PRO PRO HIS LEU TYR PRO ASN THR GLN ALA PRO SER GLN VAL
TYR GLY GLY VAL THR TYR TYR ASN PRO ALA GLN GLN GLN VAL GLN PRO LYS PRO SER PRO PRO ARG ARG THR PRO GLN PRO VAL THR ILE LYS PRO PRO PRO PRO GLU VAL VAL SER ARG GLY SER SER

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	100085	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	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	0.260	Depositor
Minimum map value	-0.149	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.05	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: IHP, ATP, ZN, MG, GTP, ADP, SEP

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	0.71	1/19149 (0.0%)	0.82	12/25983 (0.0%)
2	B	0.61	1/1970 (0.1%)	0.84	4/3060 (0.1%)
3	C	0.58	0/6950	0.80	7/9443 (0.1%)
4	D	0.37	0/14140	0.58	2/19159 (0.0%)
5	E	0.47	0/2392	0.67	0/3242
6	F	0.48	0/2323	0.76	1/3619 (0.0%)
7	G	0.59	6/1720 (0.3%)	0.82	3/2664 (0.1%)
8	H	0.94	26/3305 (0.8%)	1.62	111/5130 (2.2%)
9	I	1.12	1/2760 (0.0%)	0.63	20/3790 (0.5%)
10	J	0.56	0/3870	0.71	12/5252 (0.2%)
11	K	1.35	16/982 (1.6%)	0.69	5/1318 (0.4%)
12	L	0.62	3/3236 (0.1%)	0.75	8/4346 (0.2%)
13	M	0.55	0/1119	0.77	1/1497 (0.1%)
14	N	0.59	0/1210	0.73	1/1622 (0.1%)
15	O	0.62	0/2344	0.76	2/3163 (0.1%)
16	P	0.63	1/943 (0.1%)	0.90	0/1255
17	Q	0.42	35/11155 (0.3%)	0.41	0/15095
18	R	0.60	0/2091	0.86	3/2809 (0.1%)
19	S	0.46	0/1268	0.70	0/1714
20	T	0.82	0/2526	0.91	2/3443 (0.1%)
21	U	0.78	0/196	0.92	0/265
22	V	0.69	10/3462 (0.3%)	0.63	4/4651 (0.1%)
23	W	0.55	0/4128	0.77	6/5572 (0.1%)
24	X	0.46	0/714	0.72	1/959 (0.1%)
25	Y	0.47	0/3000	0.92	0/3777
26	Z	0.58	0/2049	0.73	0/2757
27	a	0.47	0/646	0.68	0/867
27	h	0.47	0/639	0.68	0/857
28	b	0.53	0/700	0.82	0/933
28	i	0.53	0/700	0.82	0/933
29	c	0.56	0/657	0.77	0/888
29	j	0.56	0/657	0.77	0/888

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
30	d	0.69	0/786	0.86	0/1053
30	k	0.69	0/696	0.86	0/935
31	f	0.81	0/588	0.84	0/795
31	m	0.81	0/588	0.84	0/795
32	e	0.61	0/660	0.83	0/886
32	l	0.61	0/660	0.83	0/886
33	g	0.52	0/584	0.78	0/779
33	n	0.53	0/548	0.80	0/729
34	o	0.59	0/1299	1.63	17/1761 (1.0%)
35	p	0.56	0/774	1.35	6/1035 (0.6%)
36	q	1.07	4/929 (0.4%)	0.70	3/1260 (0.2%)
36	r	1.08	4/912 (0.4%)	0.71	3/1239 (0.2%)
36	s	1.06	4/928 (0.4%)	0.72	4/1258 (0.3%)
36	t	1.08	4/917 (0.4%)	0.69	4/1245 (0.3%)
37	u	0.38	0/3179	0.65	0/4291
38	v	0.38	0/1225	0.60	0/1648
39	w	0.36	0/748	0.71	3/1012 (0.3%)
40	x	0.43	0/221	0.66	0/296
All	All	0.63	116/119243 (0.1%)	0.79	245/162854 (0.2%)

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	3
3	C	0	4
4	D	0	1
9	I	0	2
12	L	0	2
14	N	0	2
15	O	0	1
18	R	0	1
20	T	0	2
24	X	0	2
25	Y	0	15
26	Z	0	2
30	d	0	1
30	k	0	1
All	All	0	39

The worst 5 of 116 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	283	ILE	C-N	-55.29	0.06	1.34
11	K	106	CYS	CB-SG	-23.17	1.42	1.82
22	V	591	CYS	CB-SG	-18.62	1.50	1.82
11	K	132	CYS	CB-SG	-17.43	1.52	1.82
36	q	16	CYS	CB-SG	-17.41	1.52	1.82

The worst 5 of 245 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	I	283	ILE	C-N-CA	-16.67	80.03	121.70
34	o	55	ARG	NE-CZ-NH1	15.06	127.83	120.30
34	o	55	ARG	CD-NE-CZ	13.76	142.86	123.60
3	C	939	ARG	NE-CZ-NH1	13.01	126.80	120.30
8	H	167	U	C5-C4-O4	11.89	133.03	125.90

There are no chirality outliers.

5 of 39 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	166	PHE	Peptide
1	A	81	PHE	Peptide
1	A	941	LYS	Peptide
3	C	622	GLU	Peptide
3	C	88	PRO	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	18633	0	18480	806	0
2	B	1768	0	897	43	0
3	C	6798	0	6815	569	0
4	D	13846	0	13985	360	0
5	E	2338	0	2272	148	0
6	F	2075	0	1048	159	0
7	G	1551	0	785	173	0
8	H	2966	0	1505	231	0
9	I	2792	0	1249	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	J	3829	0	2906	138	0
11	K	980	0	741	10	0
12	L	3205	0	2777	206	0
13	M	1098	0	1080	168	0
14	N	1184	0	1189	61	0
15	O	2296	0	2283	187	0
16	P	929	0	910	97	0
17	Q	10885	0	10852	69	0
18	R	2073	0	2115	274	0
19	S	1236	0	1208	131	0
20	T	2461	0	2420	156	0
21	U	193	0	194	17	0
22	V	3419	0	3300	241	0
23	W	4023	0	3938	825	0
24	X	701	0	631	28	0
25	Y	2995	0	992	14	0
26	Z	1999	0	1951	138	0
27	a	640	0	657	0	0
27	h	633	0	645	0	0
28	b	690	0	712	0	0
28	i	690	0	712	0	0
29	c	649	0	693	0	0
29	j	649	0	693	0	0
30	d	776	0	819	0	0
30	k	688	0	709	0	0
31	f	576	0	589	0	0
31	m	576	0	589	0	0
32	e	652	0	668	0	0
32	l	652	0	668	0	0
33	g	577	0	603	0	0
33	n	542	0	568	0	0
34	o	1282	0	1305	0	0
35	p	760	0	783	0	0
36	q	918	0	801	0	0
36	r	901	0	777	0	0
36	s	917	0	798	0	0
36	t	906	0	785	0	0
37	u	3130	0	3172	0	0
38	v	1196	0	1182	0	0
39	w	730	0	690	0	0
40	x	216	0	202	0	0
41	A	36	0	6	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	C	32	0	12	4	0
43	C	1	0	0	0	0
43	D	1	0	0	0	0
43	F	6	0	0	0	0
43	Q	2	0	0	0	0
43	u	1	0	0	0	0
44	D	54	0	24	3	0
45	N	3	0	0	0	0
45	O	3	0	0	0	0
45	Z	1	0	0	0	0
46	Q	31	0	12	0	0
46	u	31	0	12	0	0
All	All	116421	0	106409	4719	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 23.

The worst 5 of 4719 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:264:PHE:CE1	1:A:459:LEU:HD13	1.13	1.65
1:A:264:PHE:CE1	1:A:459:LEU:CD1	1.79	1.64
11:K:163:LEU:CB	11:K:163:LEU:CG	1.81	1.57
9:I:371:PRO:CB	17:Q:357:ALA:CB	1.81	1.53
9:I:511:LEU:CB	9:I:547:LEU:CB	1.80	1.53

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	2247/2335 (96%)	2104 (94%)	107 (5%)	36 (2%)	8 38
3	C	856/972 (88%)	787 (92%)	48 (6%)	21 (2%)	4 29
4	D	1720/2136 (80%)	1632 (95%)	85 (5%)	3 (0%)	44 73
5	E	297/357 (83%)	273 (92%)	17 (6%)	7 (2%)	5 30
9	I	502/855 (59%)	482 (96%)	11 (2%)	9 (2%)	7 35
10	J	530/848 (62%)	482 (91%)	30 (6%)	18 (3%)	3 25
11	K	144/225 (64%)	134 (93%)	6 (4%)	4 (3%)	4 27
12	L	436/802 (54%)	409 (94%)	20 (5%)	7 (2%)	8 38
13	M	128/243 (53%)	118 (92%)	4 (3%)	6 (5%)	2 18
14	N	141/144 (98%)	124 (88%)	13 (9%)	4 (3%)	4 27
15	O	283/420 (67%)	255 (90%)	22 (8%)	6 (2%)	5 33
16	P	104/229 (45%)	91 (88%)	8 (8%)	5 (5%)	2 17
17	Q	1308/1485 (88%)	1283 (98%)	25 (2%)	0	100 100
18	R	255/536 (48%)	229 (90%)	14 (6%)	12 (5%)	2 18
19	S	157/166 (95%)	146 (93%)	8 (5%)	3 (2%)	6 35
20	T	311/514 (60%)	280 (90%)	22 (7%)	9 (3%)	3 27
21	U	24/2752 (1%)	20 (83%)	3 (12%)	1 (4%)	2 20
22	V	444/908 (49%)	418 (94%)	20 (4%)	6 (1%)	9 40
23	W	494/579 (85%)	434 (88%)	31 (6%)	29 (6%)	1 14
24	X	90/184 (49%)	81 (90%)	8 (9%)	1 (1%)	12 45
25	Y	709/1220 (58%)	617 (87%)	60 (8%)	32 (4%)	2 18
26	Z	238/586 (41%)	197 (83%)	30 (13%)	11 (5%)	2 18
27	a	77/126 (61%)	76 (99%)	1 (1%)	0	100 100
27	h	77/126 (61%)	76 (99%)	1 (1%)	0	100 100
28	b	84/231 (36%)	82 (98%)	2 (2%)	0	100 100
28	i	84/231 (36%)	82 (98%)	2 (2%)	0	100 100
29	c	80/119 (67%)	77 (96%)	3 (4%)	0	100 100
29	j	80/119 (67%)	77 (96%)	3 (4%)	0	100 100
30	d	95/118 (80%)	91 (96%)	4 (4%)	0	100 100
30	k	81/118 (69%)	78 (96%)	3 (4%)	0	100 100
31	f	72/86 (84%)	69 (96%)	3 (4%)	0	100 100
31	m	72/86 (84%)	68 (94%)	4 (6%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
32	e	77/92 (84%)	76 (99%)	1 (1%)	0	100 100
32	l	77/92 (84%)	76 (99%)	1 (1%)	0	100 100
33	g	72/76 (95%)	70 (97%)	2 (3%)	0	100 100
33	n	65/76 (86%)	63 (97%)	2 (3%)	0	100 100
34	o	160/255 (63%)	146 (91%)	12 (8%)	2 (1%)	10 41
35	p	92/225 (41%)	90 (98%)	2 (2%)	0	100 100
36	q	130/504 (26%)	119 (92%)	7 (5%)	4 (3%)	3 26
36	r	129/504 (26%)	118 (92%)	9 (7%)	2 (2%)	8 38
36	s	130/504 (26%)	116 (89%)	7 (5%)	7 (5%)	1 15
36	t	129/504 (26%)	116 (90%)	9 (7%)	4 (3%)	3 26
37	u	388/411 (94%)	376 (97%)	9 (2%)	3 (1%)	16 51
38	v	142/148 (96%)	138 (97%)	4 (3%)	0	100 100
39	w	89/174 (51%)	87 (98%)	1 (1%)	1 (1%)	12 45
40	x	23/703 (3%)	22 (96%)	1 (4%)	0	100 100
All	All	13923/24124 (58%)	12985 (93%)	685 (5%)	253 (2%)	9 35

5 of 253 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	82	ARG
1	A	308	ILE
1	A	331	TRP
1	A	346	ASP
1	A	365	VAL

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	2021/2108 (96%)	1881 (93%)	140 (7%)	13 40
3	C	761/866 (88%)	689 (90%)	72 (10%)	7 30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	D	1541/1908 (81%)	1363 (88%)	178 (12%)	4 23
5	E	256/300 (85%)	244 (95%)	12 (5%)	22 51
10	J	241/751 (32%)	219 (91%)	22 (9%)	7 31
11	K	56/196 (29%)	51 (91%)	5 (9%)	8 32
12	L	229/709 (32%)	186 (81%)	43 (19%)	1 8
13	M	117/209 (56%)	81 (69%)	36 (31%)	0 2
14	N	130/130 (100%)	127 (98%)	3 (2%)	45 68
15	O	255/361 (71%)	250 (98%)	5 (2%)	50 72
16	P	99/203 (49%)	80 (81%)	19 (19%)	1 7
17	Q	1202/1336 (90%)	1193 (99%)	9 (1%)	81 90
18	R	219/457 (48%)	167 (76%)	52 (24%)	0 4
19	S	129/134 (96%)	120 (93%)	9 (7%)	12 40
20	T	269/441 (61%)	252 (94%)	17 (6%)	15 44
21	U	21/2432 (1%)	17 (81%)	4 (19%)	1 7
22	V	327/838 (39%)	303 (93%)	24 (7%)	11 38
23	W	436/502 (87%)	324 (74%)	112 (26%)	0 3
24	X	62/157 (40%)	59 (95%)	3 (5%)	21 51
25	Y	31/1085 (3%)	31 (100%)	0	100 100
26	Z	214/520 (41%)	203 (95%)	11 (5%)	20 49
27	a	72/101 (71%)	72 (100%)	0	100 100
27	h	70/101 (69%)	70 (100%)	0	100 100
28	b	77/169 (46%)	75 (97%)	2 (3%)	41 65
28	i	77/169 (46%)	75 (97%)	2 (3%)	41 65
29	c	77/101 (76%)	75 (97%)	2 (3%)	41 65
29	j	77/101 (76%)	75 (97%)	2 (3%)	41 65
30	d	90/110 (82%)	88 (98%)	2 (2%)	47 69
30	k	80/110 (73%)	78 (98%)	2 (2%)	42 66
31	f	63/74 (85%)	62 (98%)	1 (2%)	58 76
31	m	63/74 (85%)	62 (98%)	1 (2%)	58 76
32	e	74/84 (88%)	74 (100%)	0	100 100
32	l	74/84 (88%)	74 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
33	g	64/66 (97%)	63 (98%)	1 (2%)	58 76
33	n	60/66 (91%)	59 (98%)	1 (2%)	56 75
34	o	139/218 (64%)	135 (97%)	4 (3%)	37 63
35	p	82/195 (42%)	79 (96%)	3 (4%)	29 58
36	q	79/435 (18%)	70 (89%)	9 (11%)	4 23
36	r	77/435 (18%)	67 (87%)	10 (13%)	3 19
36	s	77/435 (18%)	69 (90%)	8 (10%)	5 26
36	t	77/435 (18%)	71 (92%)	6 (8%)	10 36
37	u	345/361 (96%)	340 (99%)	5 (1%)	62 79
38	v	132/134 (98%)	131 (99%)	1 (1%)	79 88
39	w	76/143 (53%)	75 (99%)	1 (1%)	65 81
40	x	23/581 (4%)	23 (100%)	0	100 100
All	All	10741/20425 (53%)	9902 (92%)	839 (8%)	13 36

5 of 839 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	L	250	GLU
18	R	186	VAL
36	q	19	PRO
13	M	145	ASP
12	L	247	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 121 such sidechains are listed below:

Mol	Chain	Res	Type
17	Q	393	ASN
28	i	22	GLN
19	S	13	ASN
27	h	60	GLN
37	u	301	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	82/117 (70%)	17 (20%)	4 (4%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
6	F	96/107 (89%)	44 (45%)	14 (14%)
7	G	82/275 (29%)	53 (64%)	10 (12%)
8	H	133/188 (70%)	33 (24%)	8 (6%)
All	All	393/687 (57%)	147 (37%)	36 (9%)

5 of 147 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	12	U
2	B	13	C
2	B	19	A
2	B	20	G
2	B	21	A

5 of 36 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	H	15	U
8	H	168	A
8	H	29	A
8	H	40	C
6	F	50	A

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
18	SEP	R	224	18	8,9,10	0.69	0	8,12,14	1.19	0
18	SEP	R	232	18	8,9,10	0.83	0	8,12,14	1.16	0

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
18	SEP	R	224	18	-	0/5/8/10	-
18	SEP	R	232	18	-	1/5/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	R	232	SEP	N-CA-CB-OG

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	R	224	SEP	1	0
18	R	232	SEP	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 24 ligands modelled in this entry, 18 are monoatomic - leaving 6 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	ADP	D	2202	43	24,29,29	0.95	1 (4%)	29,45,45	1.46	4 (13%)
46	ATP	u	702	43	26,33,33	0.92	1 (3%)	31,52,52	1.55	5 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
42	GTP	C	1500	43	26,34,34	1.09	1 (3%)	32,54,54	1.85	7 (21%)
41	IHP	A	3000	-	36,36,36	0.79	0	54,60,60	1.31	6 (11%)
46	ATP	Q	1501	43	26,33,33	1.73	8 (30%)	31,52,52	1.86	10 (32%)
44	ADP	D	2201	-	24,29,29	0.97	1 (4%)	29,45,45	1.34	4 (13%)

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	ADP	D	2202	43	-	2/12/32/32	0/3/3/3
46	ATP	u	702	43	-	0/18/38/38	0/3/3/3
42	GTP	C	1500	43	-	6/18/38/38	0/3/3/3
41	IHP	A	3000	-	-	9/30/54/54	0/1/1/1
46	ATP	Q	1501	43	-	4/18/38/38	0/3/3/3
44	ADP	D	2201	-	-	8/12/32/32	0/3/3/3

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	Q	1501	ATP	C2'-C1'	-3.69	1.48	1.53
42	C	1500	GTP	C6-N1	-3.56	1.32	1.37
46	Q	1501	ATP	C4-N3	3.49	1.40	1.35
46	Q	1501	ATP	C6-N6	3.32	1.46	1.34
46	Q	1501	ATP	C2'-C3'	-2.76	1.45	1.53

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
46	Q	1501	ATP	PB-O3B-PG	-5.47	114.04	132.83
46	u	702	ATP	PB-O3B-PG	-4.34	117.95	132.83
46	Q	1501	ATP	N3-C2-N1	-4.19	122.13	128.68
42	C	1500	GTP	C5-C6-N1	4.16	121.30	113.95
46	u	702	ATP	N3-C2-N1	-4.10	122.28	128.68

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
41	A	3000	IHP	C4-C5-O15-P5
41	A	3000	IHP	C6-C5-O15-P5
41	A	3000	IHP	C2-O12-P2-O42
42	C	1500	GTP	C5'-O5'-PA-O3A
42	C	1500	GTP	C5'-O5'-PA-O1A

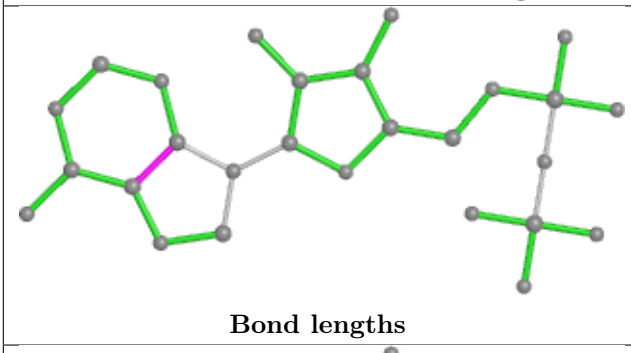
There are no ring outliers.

3 monomers are involved in 11 short contacts:

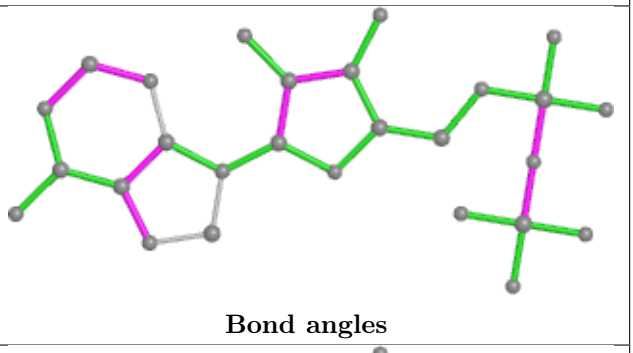
Mol	Chain	Res	Type	Clashes	Symm-Clashes
42	C	1500	GTP	4	0
41	A	3000	IHP	4	0
44	D	2201	ADP	3	0

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.

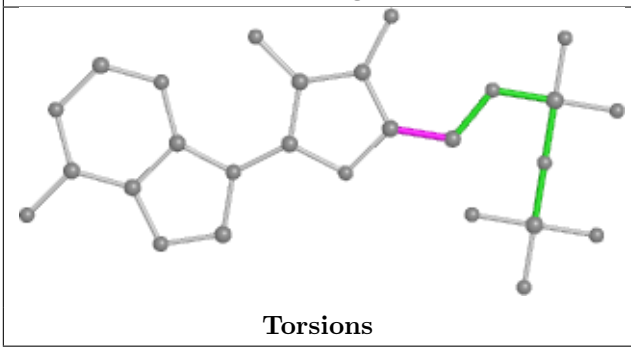
Ligand ADP D 2202



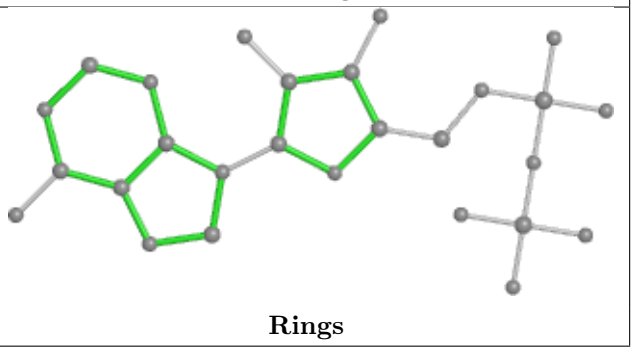
Bond lengths



Bond angles

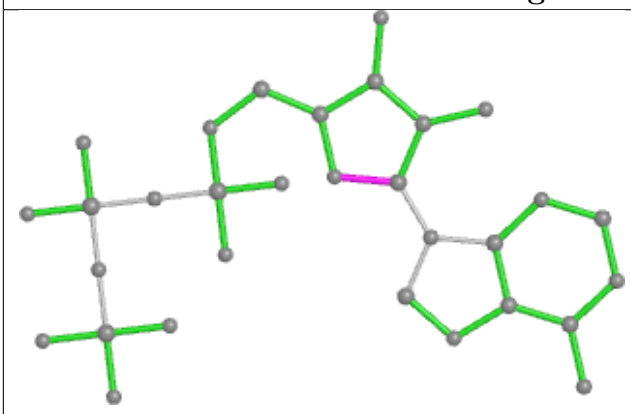


Torsions

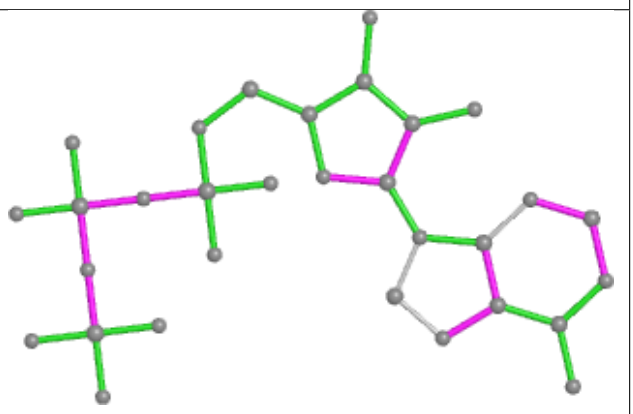


Rings

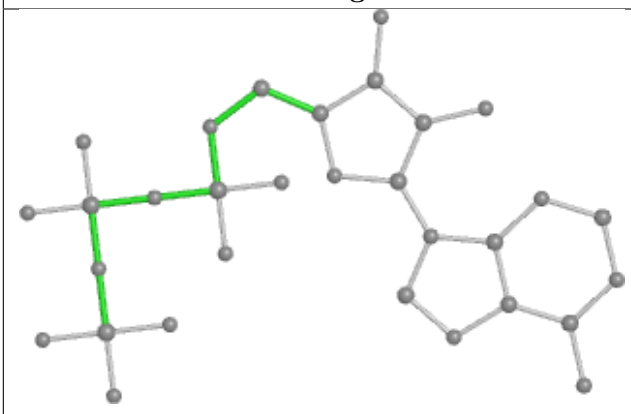
Ligand ATP u 702



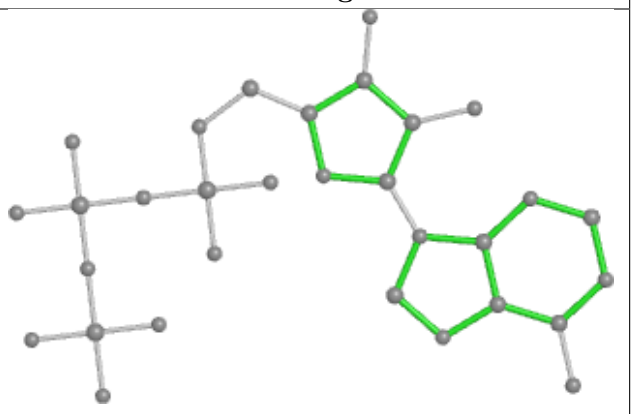
Bond lengths



Bond angles

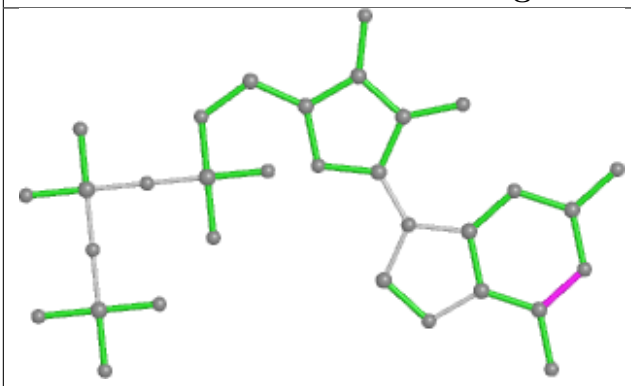


Torsions

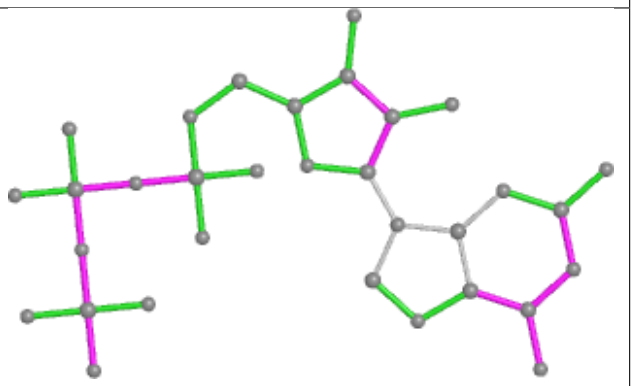


Rings

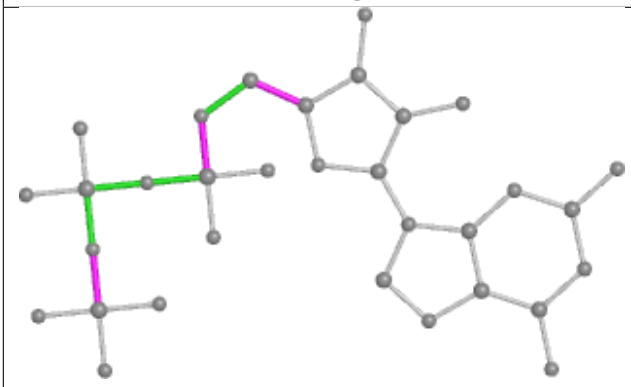
Ligand GTP C 1500



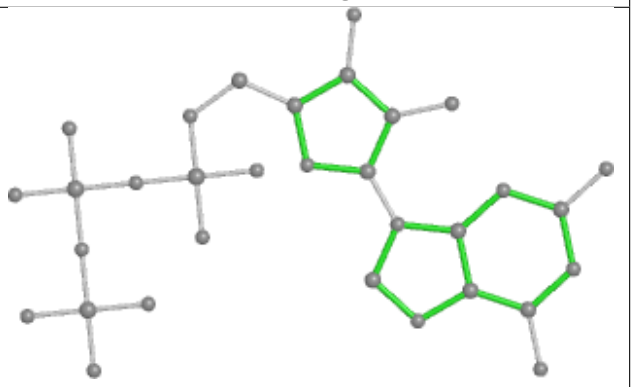
Bond lengths



Bond angles

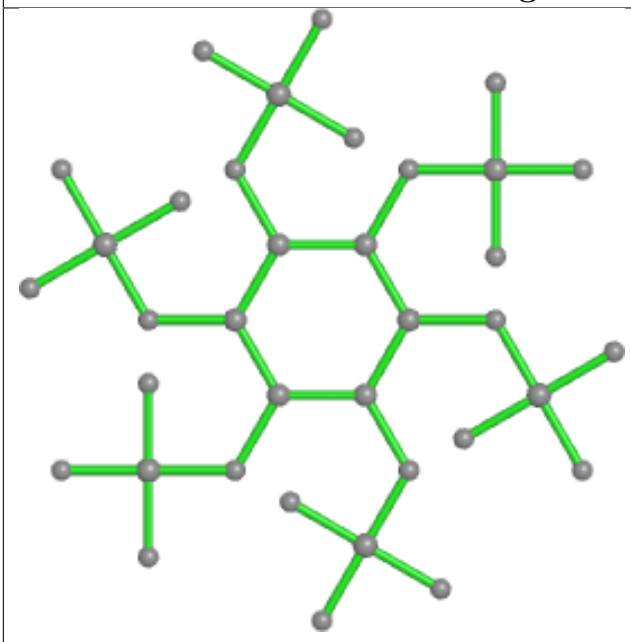


Torsions

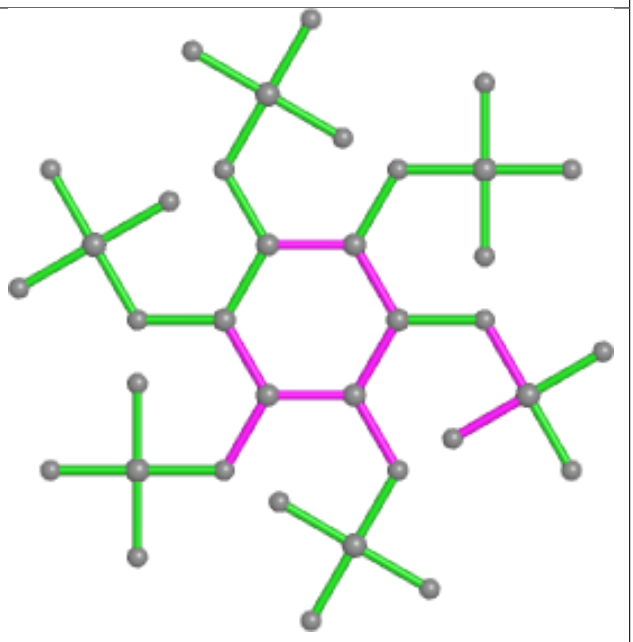


Rings

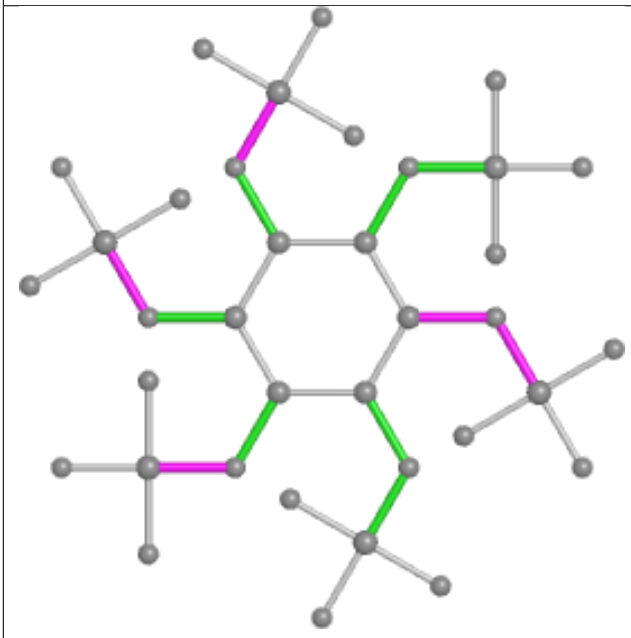
Ligand IHP A 3000



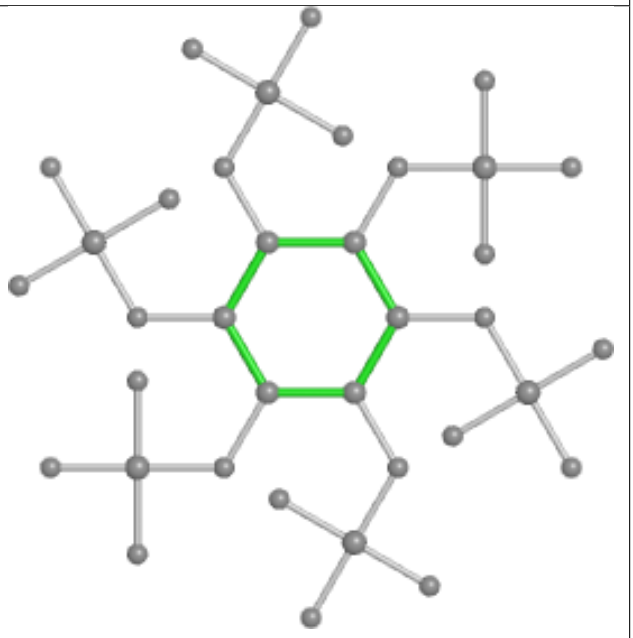
Bond lengths



Bond angles

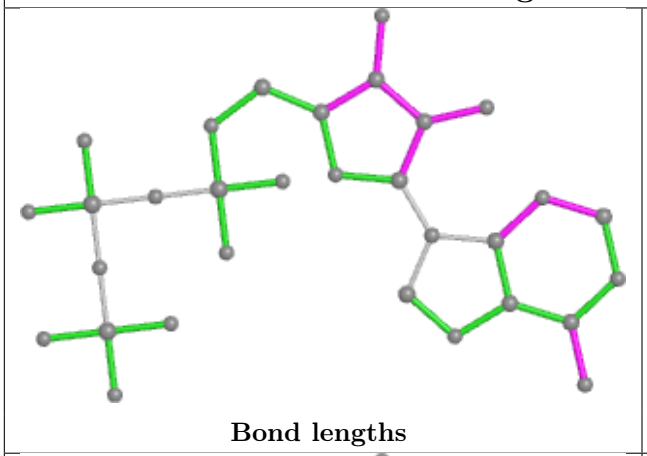


Torsions

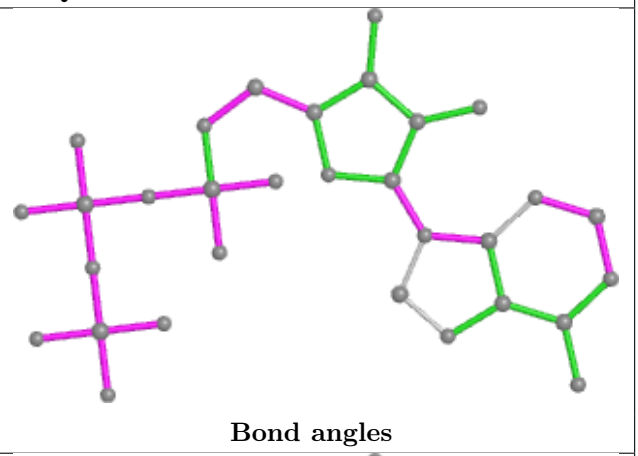


Rings

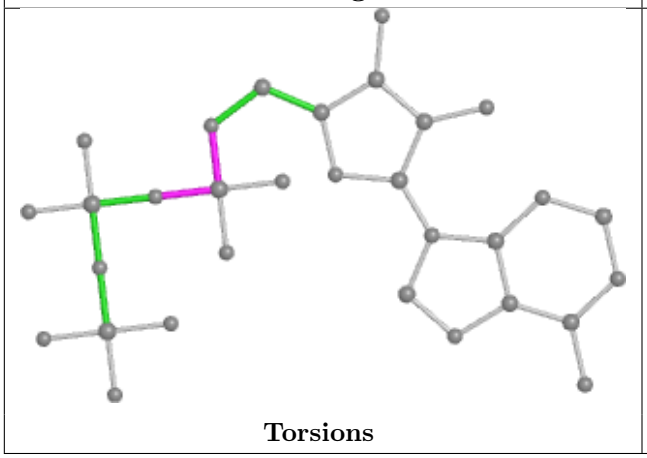
Ligand ATP Q 1501



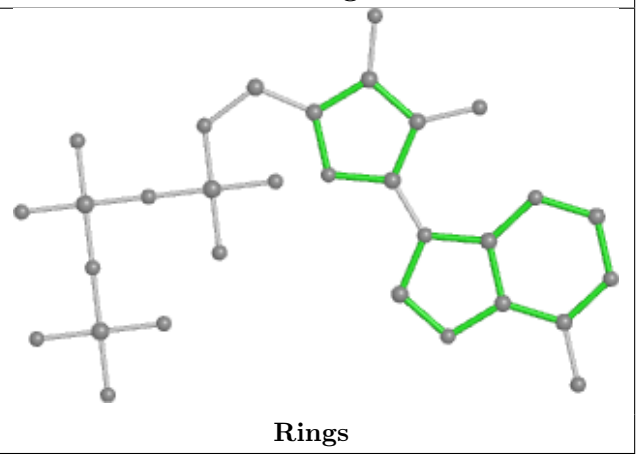
Bond lengths



Bond angles

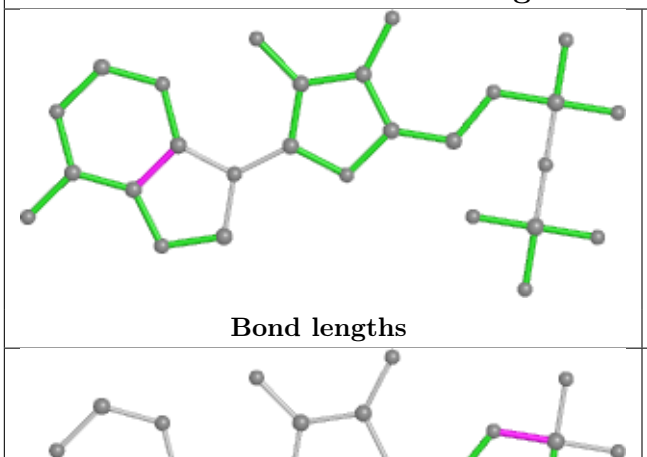


Torsions

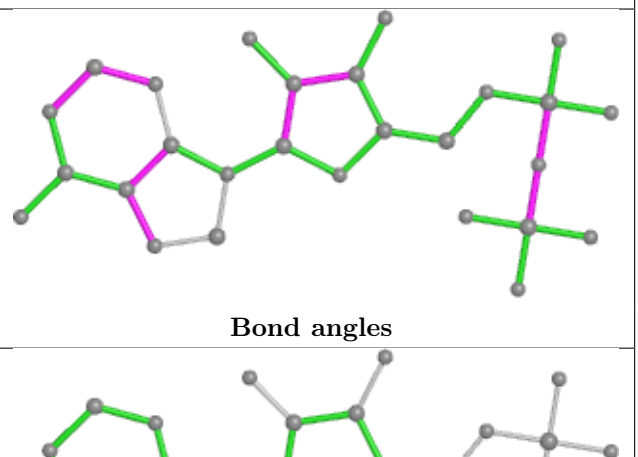


Rings

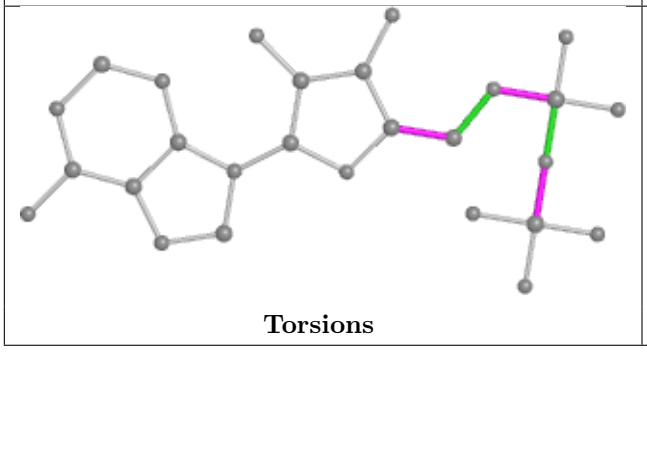
Ligand ADP D 2201



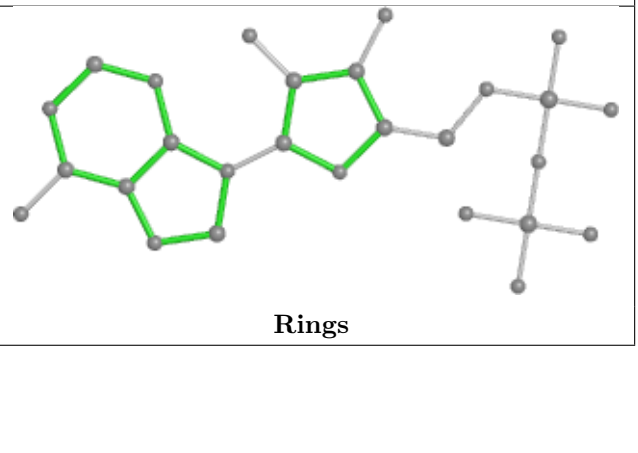
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

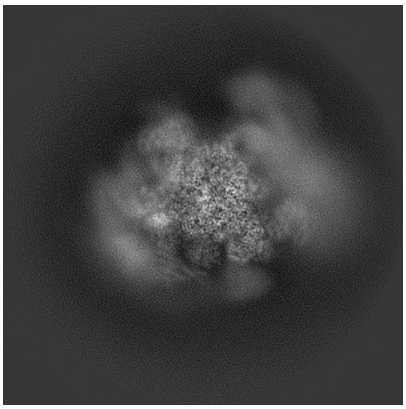
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-6721. These allow visual inspection of the internal detail of the map and identification of artifacts.

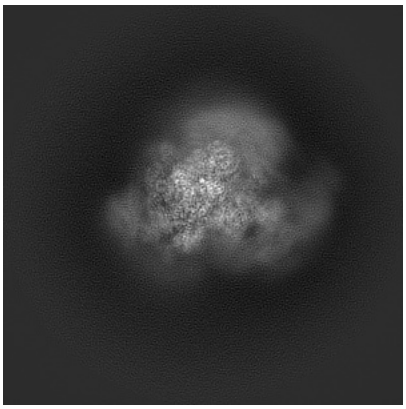
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

6.1.1 Primary map



X



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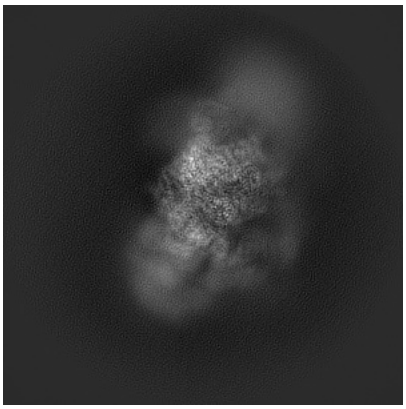
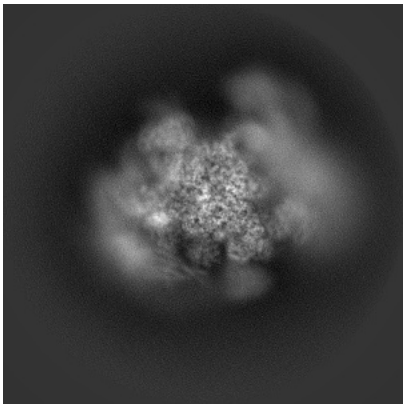


Z

6.1.2 Raw map



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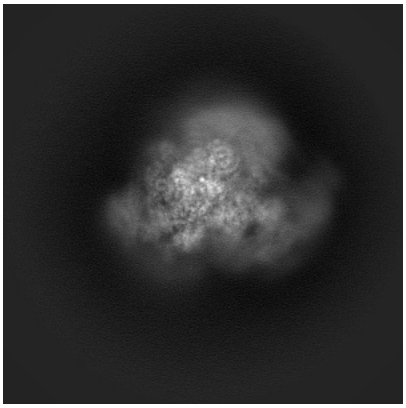

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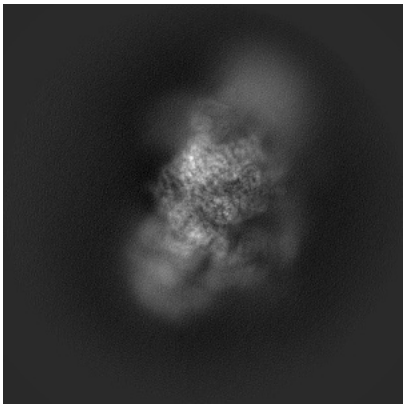
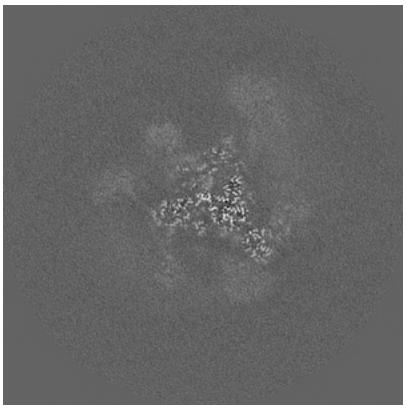


Z

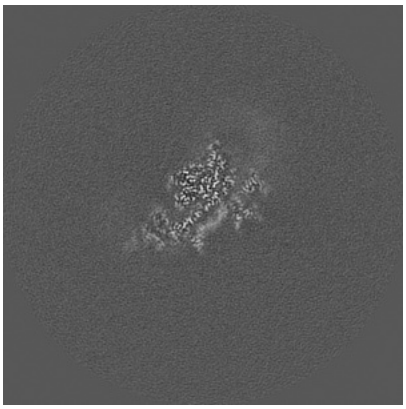
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map



X Index: 200



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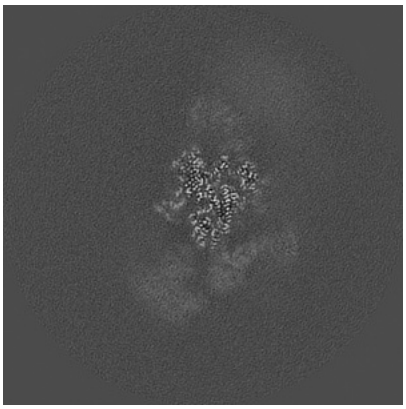
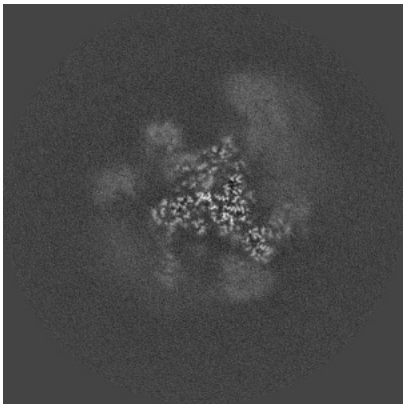
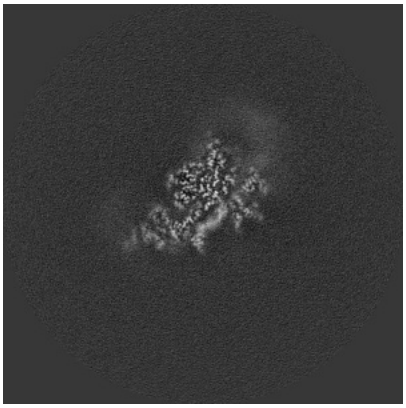


Z Index: 200

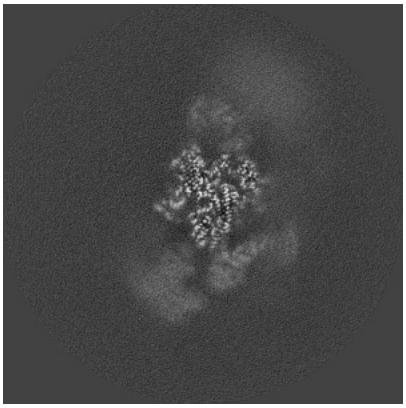
6.2.2 Raw map



X Index: 200



Y Index: 200

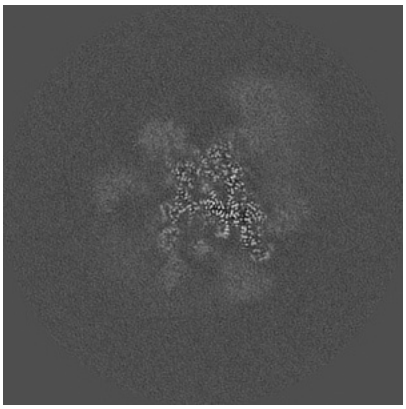


Z Index: 200

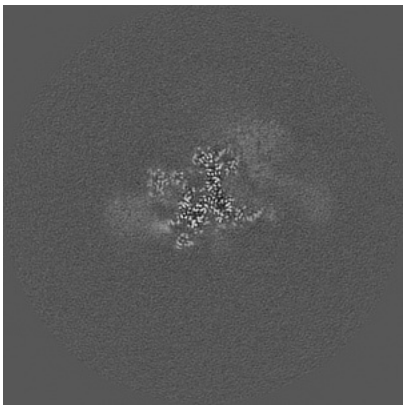
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

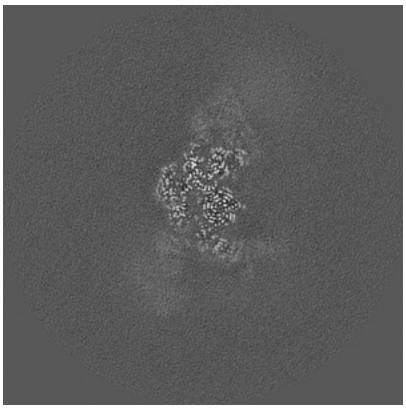
6.3.1 Primary map



X Index: 194

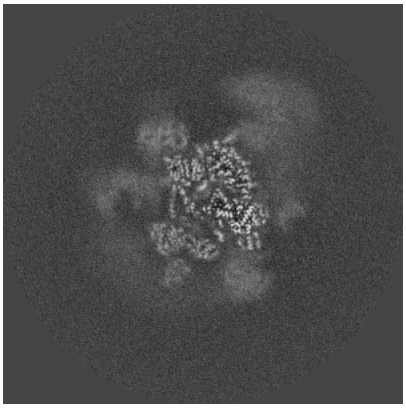


Y Index: 229

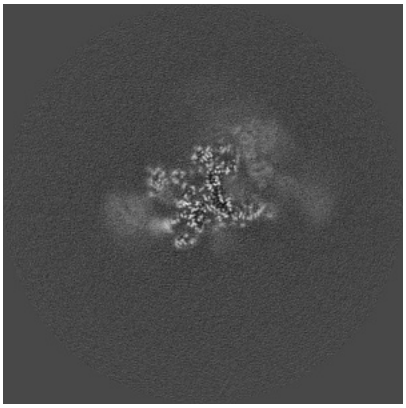


Z Index: 182

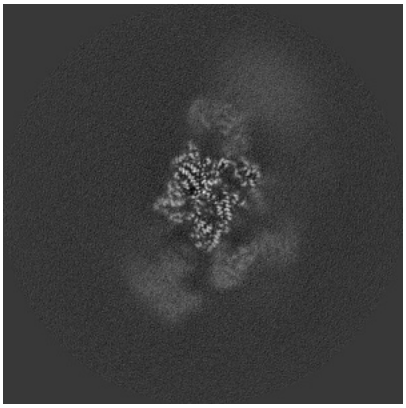
6.3.2 Raw map



X Index: 188



Y Index: 228

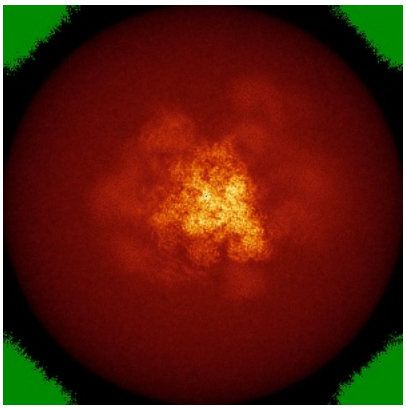


Z Index: 197

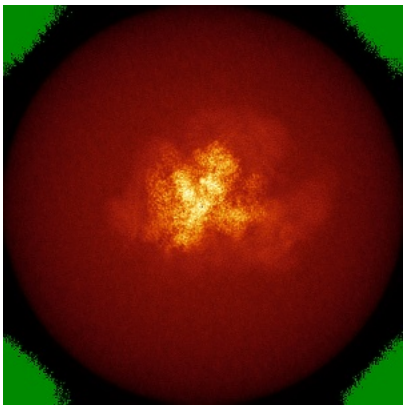
The images above show the largest variance slices of the map in three orthogonal directions.

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

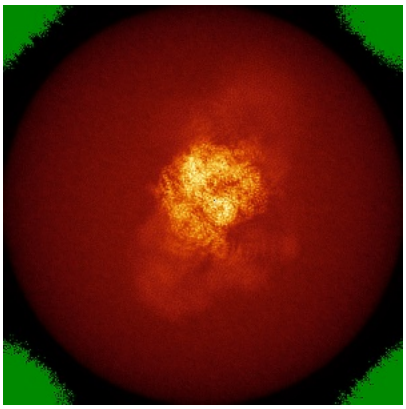
6.4.1 Primary map



X

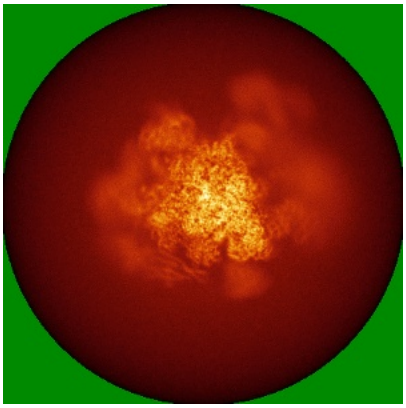


Y

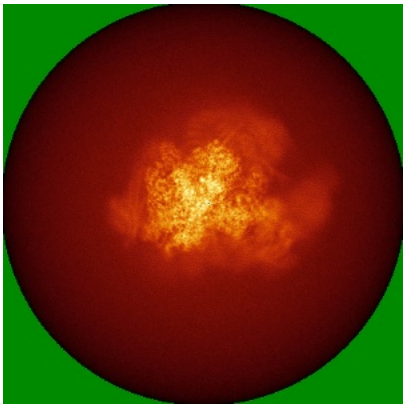


Z

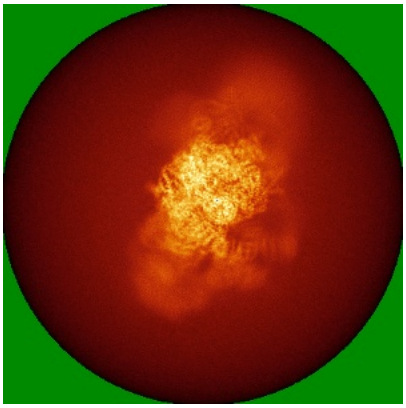
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

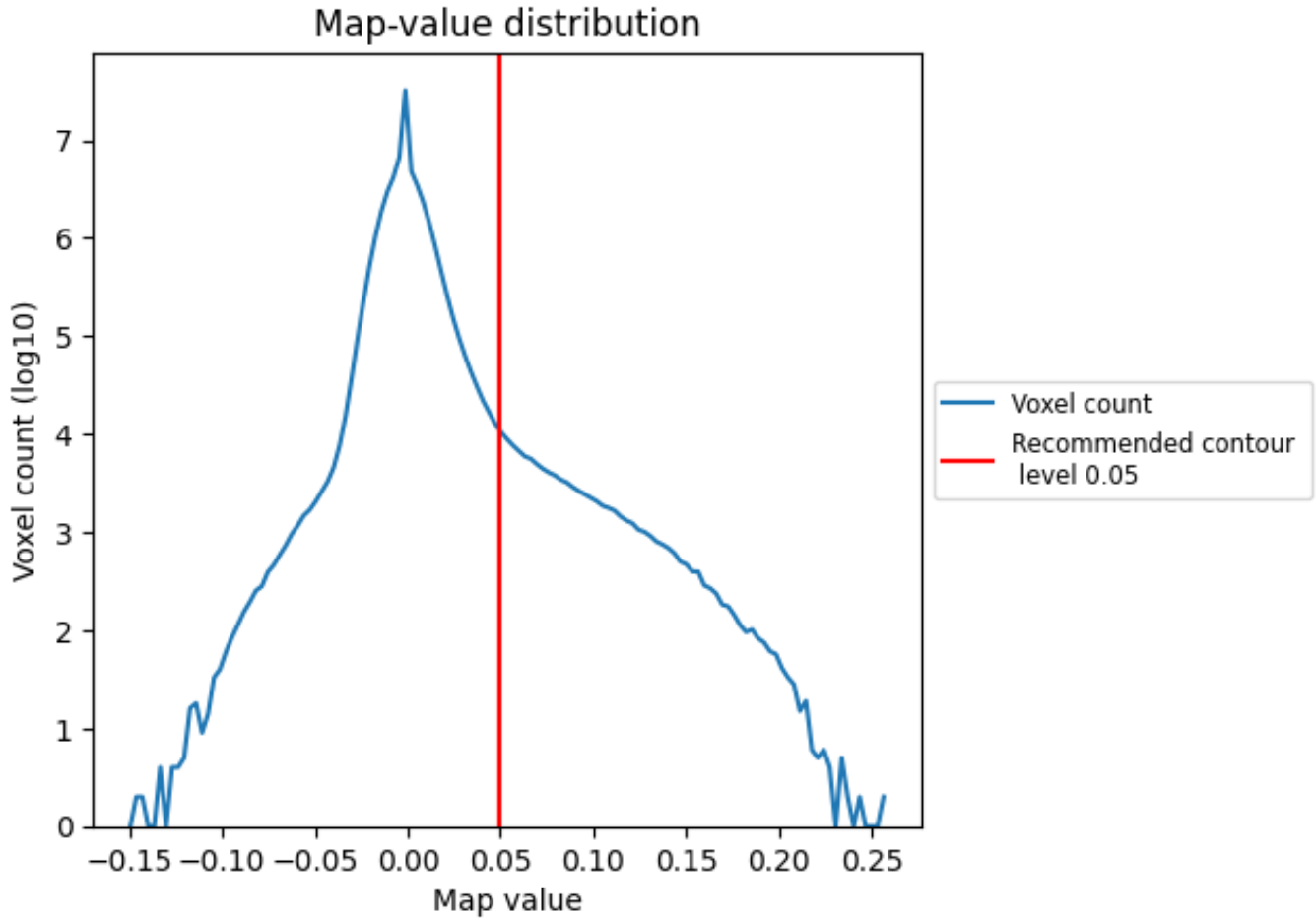
6.6 Mask visualisation (i)

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

7 Map analysis

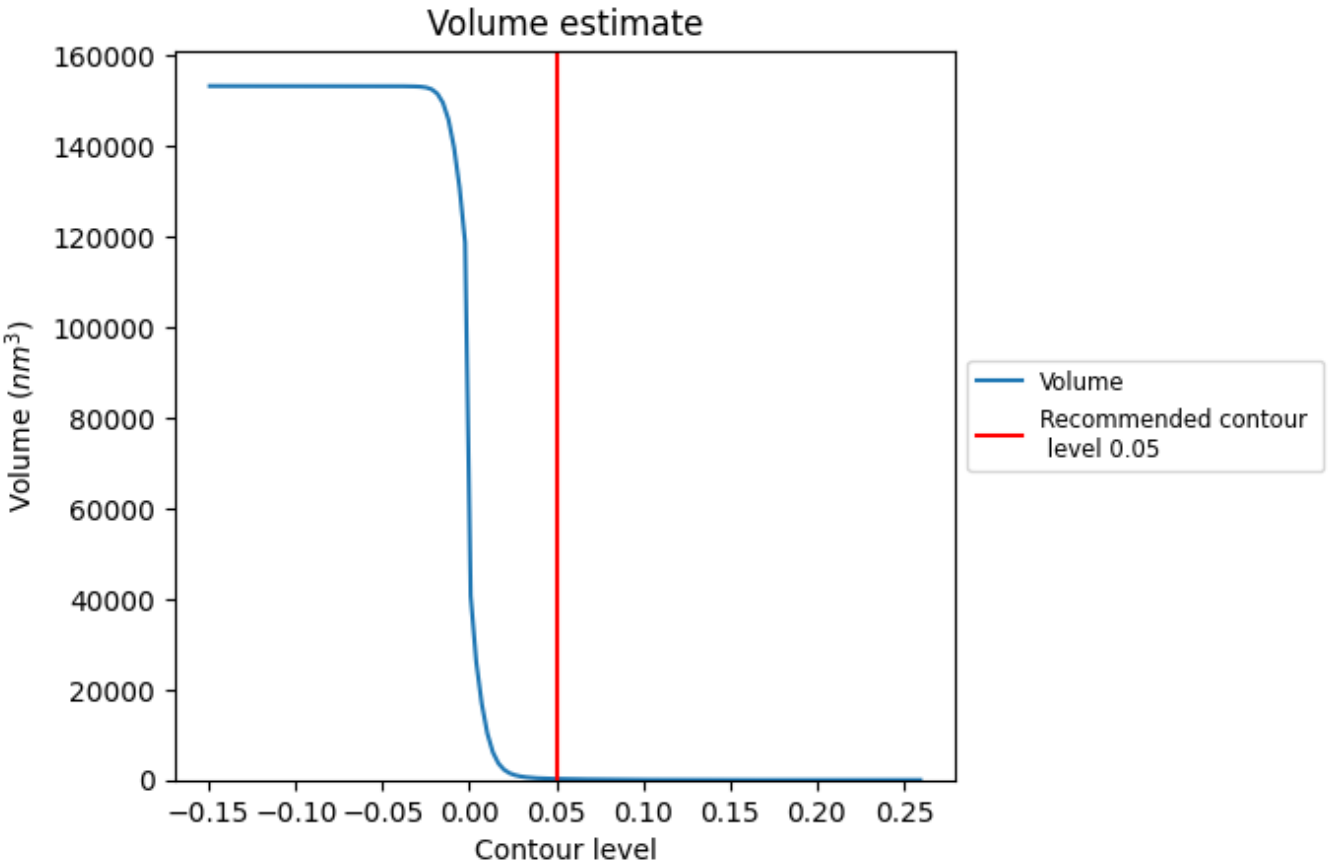
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

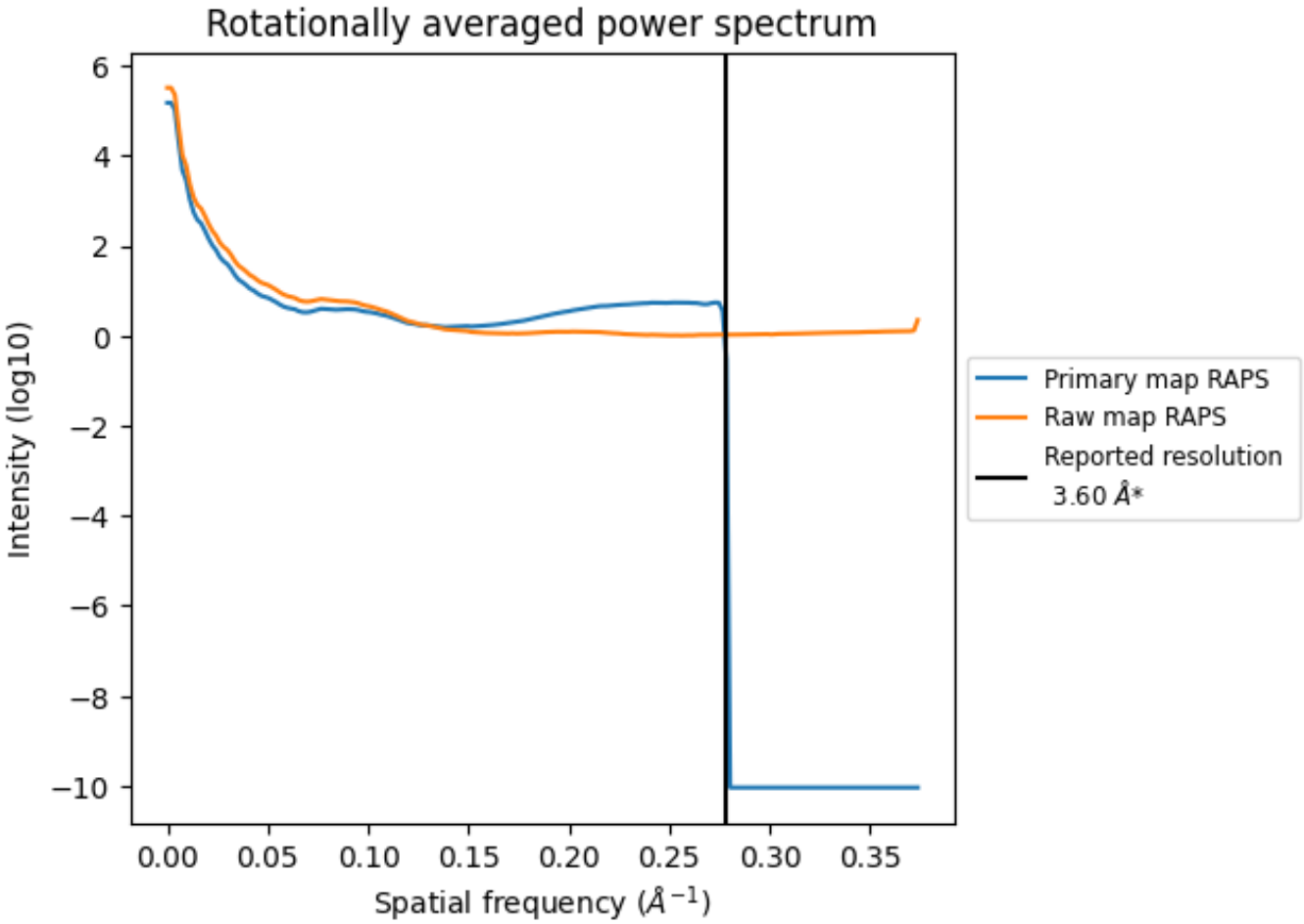
7.2 Volume estimate (i)



The volume at the recommended contour level is 243 nm^3; this corresponds to an approximate mass of 220 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)

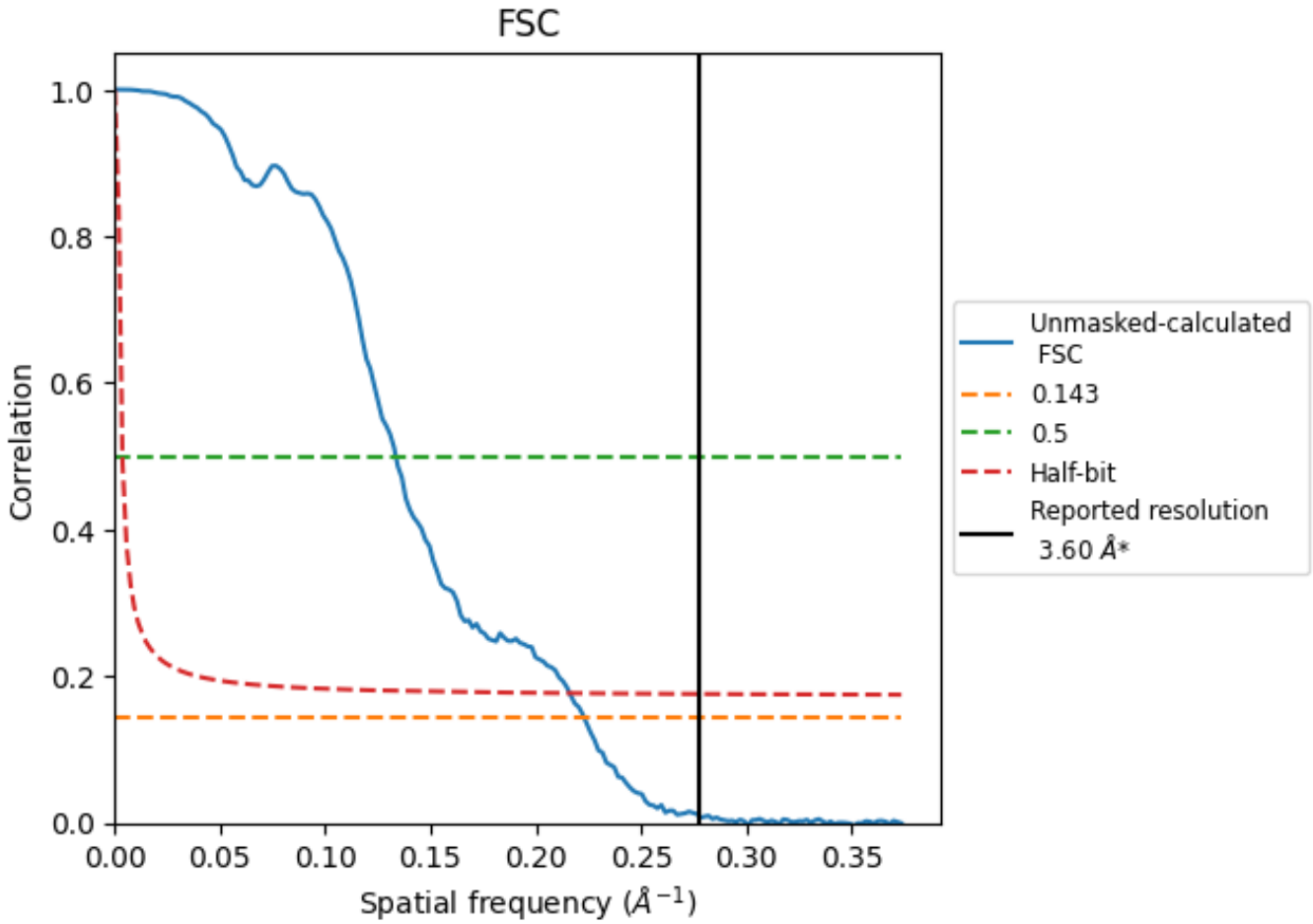


*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

8.2 Resolution estimates (i)

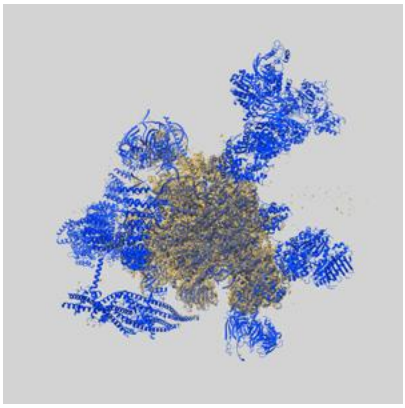
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.48	7.49	4.63

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.48 differs from the reported value 3.6 by more than 10 %

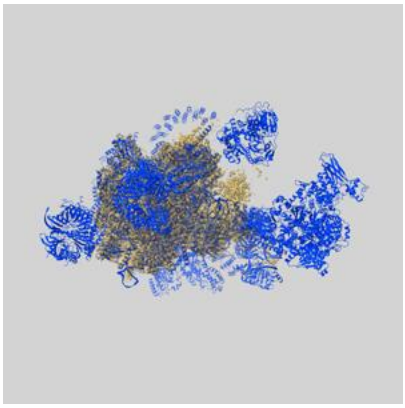
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-6721 and PDB model 5XJC. Per-residue inclusion information can be found in section 3 on page 15.

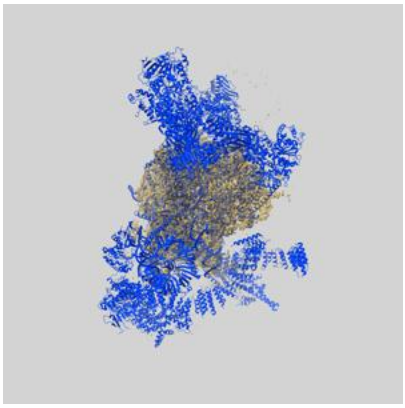
9.1 Map-model overlay



X



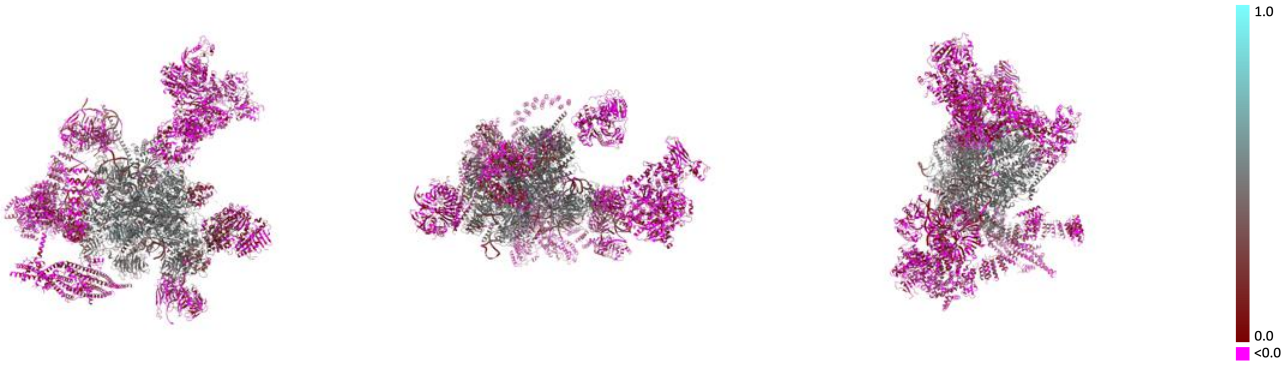
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

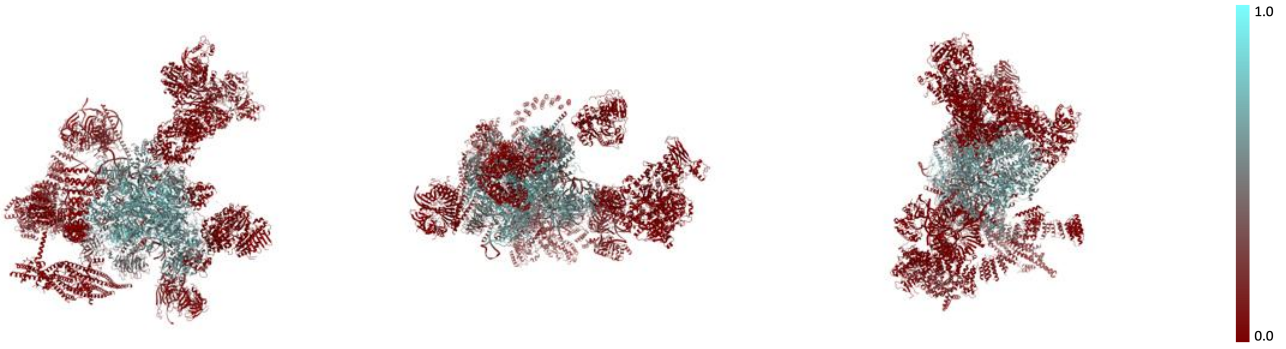
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

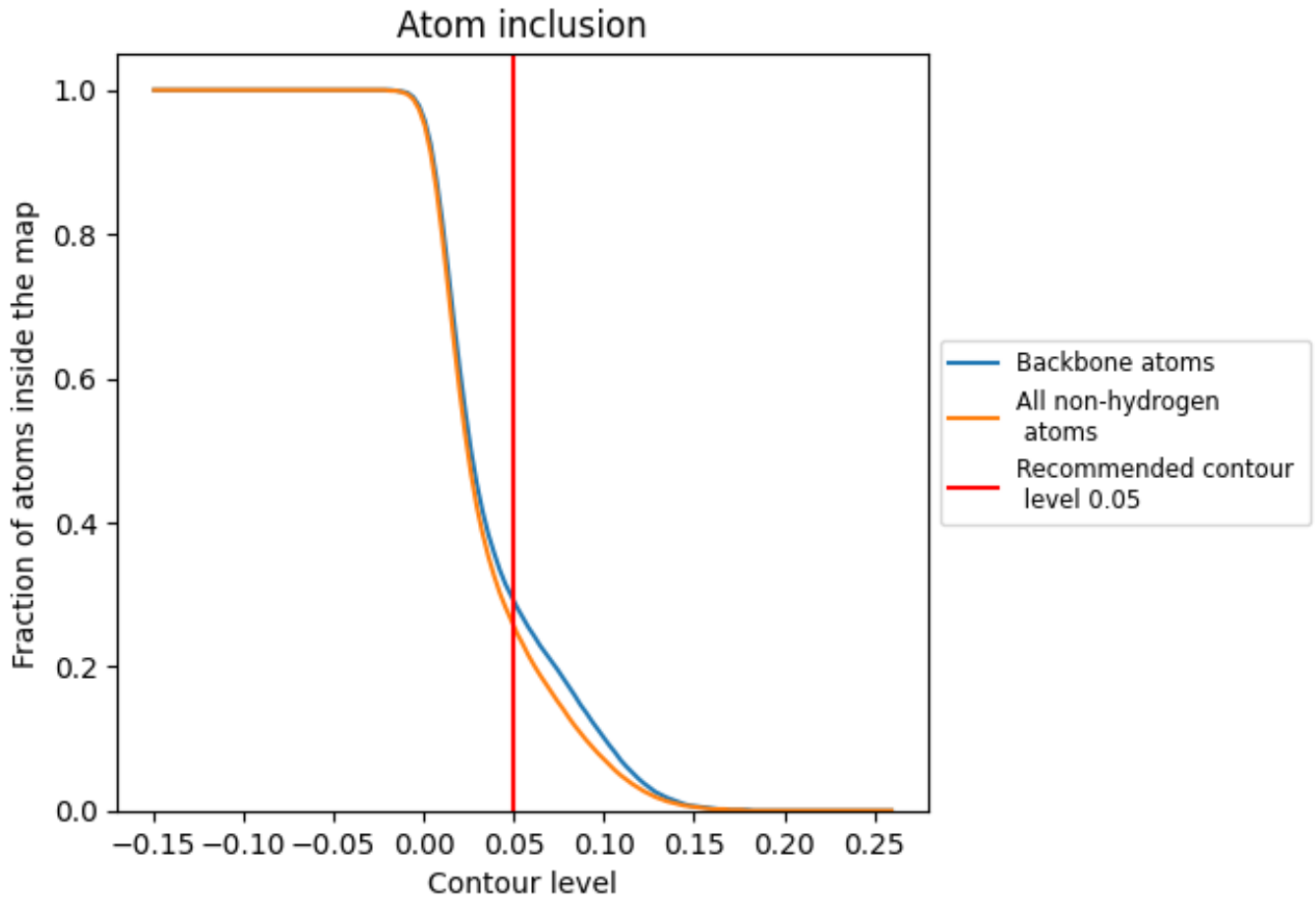
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).

9.4 Atom inclusion (i)



At the recommended contour level, 29% of all backbone atoms, 26% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.2560	0.2200
A	0.5640	0.4190
B	0.5240	0.3110
C	0.5120	0.4170
D	0.0000	0.0040
E	0.3880	0.4040
F	0.6060	0.3820
G	0.3400	0.2520
H	0.2000	0.1500
I	0.0060	0.0560
J	0.3380	0.2840
K	0.0030	0.1110
L	0.3250	0.2780
M	0.4910	0.4280
N	0.6470	0.4810
O	0.4250	0.4380
P	0.4330	0.4200
Q	0.0000	0.0010
R	0.4730	0.4290
S	0.2880	0.3640
T	0.7080	0.5000
U	0.7010	0.5090
V	0.0960	0.1920
W	0.4500	0.4070
X	0.2420	0.3880
Y	0.0400	0.0400
Z	0.4240	0.4540
a	0.0000	0.0300
b	0.0000	0.0130
c	0.0000	-0.0140
d	0.0000	0.0020
e	0.0000	0.0320
f	0.0000	0.0120
g	0.0000	0.0170
h	0.0110	0.0680

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Chain	Atom inclusion	Q-score
i	0.0040	0.0110
j	0.0090	-0.0050
k	0.0040	0.0070
l	0.0050	-0.0070
m	0.0160	0.0990
n	0.0190	0.0720
o	0.0010	0.0030
p	0.0010	0.0030
q	0.0000	-0.0090
r	0.0000	0.0390
s	0.0000	0.0600
t	0.0000	0.0090
u	0.0060	0.1250
v	0.0010	0.0320
w	0.0000	0.0570
x	0.0000	0.0030