wwPDB EM Validation Summary Report (i)

Jun 10, 2025 – 11:54 PM JST

PDB ID	:	7W59 / pdb_00007w59
EMDB ID	:	EMD-32317
Title	:	The cryo-EM structure of human pre-C*-I complex
Authors	:	Zhan, X.; Lu, Y.; Shi, Y.
Deposited on	:	2021-11-29
Resolution	:	3.60 Å(reported)

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

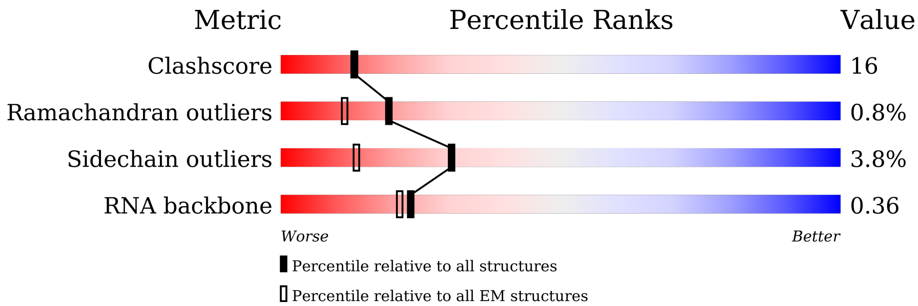
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.60 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	• / 61% 19% • • 15%
2	C	972	69% 18% • 11%
3	E	357	59% 23% • 16%
4	4	46	9% 11% • • 72%
5	G	174	9% / 6% 10% 24% 7% 53%
6	J	848	• / 58% 8% • 33%
7	L	802	• / 46% 7% • 46%

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Mol	Chain	Length	Quality of chain
8	M	243	• 44% 9% 47%
9	N	144	• 77% 16% • • •
10	O	420	• 52% 16% 32%
11	P	229	• 36% 10% • • 51%
12	R	536	• 37% 10% 5% 48%
13	S	166	• 70% 23% • •
14	T	514	37% 18% • • 39%
15	U	2752	• 97%
16	V	908	21% 47% • 50%
17	W	579	• 65% 21% •• 12%
18	B	117	• 36% 22% 10% • 28%
19	F	107	• 31% 24% 34% • 9%
20	H	188	6% 13% 22% 37% • 26%
21	b	240	6% 29% 12% • 58%
21	i	240	14% 28% 8% 64%
22	X	254	6% 12% 9% • 73%
23	I	855	• 58% 12% •• 28%
24	y	301	• 24% • 74%
25	Y	1220	41% 51% • 45%
26	a	126	5% 52% 13% 36%
26	h	126	12% 52% 13% 36%
27	c	119	• 59% 10% 31%
27	j	119	21% 58% 11% 31%
28	d	118	14% 49% 31% • 18%
28	k	118	24% 43% 28% • 28%

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Mol	Chain	Length	Quality of chain
29	f	86	16% / 60% 26% 14%
29	m	86	10% / 57% 29% 14%
30	e	92	16% / 64% 22% 14%
30	l	92	23% / 65% 20% 15%
31	g	76	29% / 74% 22% • •
31	n	76	8% / 62% 28% • 9%
32	v	146	99% / 92% 6% •
33	w	174	52% / 47% 5% • 48%
34	u	411	81% / 89% 5% 6%
35	x	703	• / • 96%
36	Q	1485	35% / 85% • • 11%
37	o	255	24% / 38% 22% • 36%
38	p	225	• / 32% 8% • 58%
39	q	504	10% / 24% • 74%
39	r	504	• / 24% • 74%
39	s	504	13% / 22% • • 74%
39	t	504	15% / 24% • 74%
40	K	225	• / 63% 5% • 31%

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

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

2 Entry composition (i)

There are 45 unique types of molecules in this entry. The entry contains 92315 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	1984	16449	10601	2879	2899	70	0	0

- Molecule 2 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	862	6798	4347	1138	1281	32	0	0

- Molecule 3 is a protein called U5 small nuclear ribonucleoprotein 40 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	E	299	2338	1470	410	445	13	0	0

- Molecule 4 is a RNA chain called pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	4	13	276	123	50	90	13	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	G	82	1510	666	210	552	82	0	0

- Molecule 6 is a protein called Crooked neck-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	J	568	3814	2376	717	715	6	0	0

- Molecule 7 is a protein called Cell division cycle 5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	L	437	Total 3015	C 1859	N 584	O 565	S 7	0	0

- Molecule 8 is a protein called Pre-mRNA-splicing factor SYF2.

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

- Molecule 9 is a protein called Protein BUD31 homolog.

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

- Molecule 10 is a protein called Pre-mRNA-splicing factor RBM22.

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

- Molecule 11 is a protein called Spliceosome-associated protein CWC15 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	P	113	Total 953	C 583	N 189	O 179	S 2	0	0

- Molecule 12 is a protein called SNW domain-containing protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	R	280	Total 2243	C 1401	N 411	O 416	P 2	S 13	0	0

- Molecule 13 is a protein called Peptidyl-prolyl cis-trans isomerase-like 1.

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

- Molecule 14 is a protein called Pleiotropic regulator 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	T	312	Total 2454	C 1550	N 446	O 450	S 8	0	0

- Molecule 15 is a protein called Serine/arginine repetitive matrix protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	U	72	Total 422	C 257	N 82	O 82	S 1	0	0

- Molecule 16 is a protein called Pre-mRNA-splicing factor CWC22 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	V	452	Total 2632	C 1639	N 492	O 495	S 6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	W	509	Total 4129	C 2628	N 715	O 762	S 24	0	0

- Molecule 18 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	B	84	Total 1768	C 792	N 295	O 597	P 84	0	0

- Molecule 19 is a RNA chain called U6 snRNA.

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

- Molecule 20 is a RNA chain called U2 snRNA.

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

- Molecule 21 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	b	102	Total 786	C 492	N 148	O 139	S 7	0	0
21	i	86	Total 690	C 434	N 126	O 123	S 7	0	0

- Molecule 22 is a protein called PSME3-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	X	69	Total 616	C 380	N 111	O 124	S 1	0	0

- Molecule 23 is a protein called Pre-mRNA-splicing factor SYF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	I	617	Total 3845	C 2380	N 721	O 733	S 11	0	0

- Molecule 24 is a protein called Peptidyl-prolyl cis-trans isomerase E.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	y	79	Total 390	C 232	N 79	O 79	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	667	Total 3431	C 2057	N 680	O 693	S 1	4	0

- Molecule 26 is a protein called Small nuclear ribonucleoprotein Sm D3.

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

- Molecule 27 is a protein called Small nuclear ribonucleoprotein Sm D1.

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

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

- Molecule 28 is a protein called Small nuclear ribonucleoprotein Sm D2.

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

- Molecule 29 is a protein called Small nuclear ribonucleoprotein F.

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

- Molecule 30 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	79	Total 652	C 412	N 116	O 119	S 5	0	0
30	l	78	Total 644	C 407	N 115	O 118	S 4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	g	74	Total 577	C 364	N 104	O 103	S 6	0	0
31	n	69	Total 538	C 342	N 96	O 94	S 6	0	0

- Molecule 32 is a protein called Protein mago nashi homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	v	144	Total 711	C 423	N 144	O 144	0	0

- Molecule 33 is a protein called RNA-binding protein 8A.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	w	91	Total 445	C 263	N 91	O 91	0	0

- Molecule 34 is a protein called Eukaryotic initiation factor 4A-III.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	u	386	Total 1907	C 1135	N 386	O 386	0	0

- Molecule 35 is a protein called Protein CASC3.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	x	25	Total 124	C 74	N 25	O 25	0	0

- Molecule 36 is a protein called RNA helicase aquarius.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	Q	1322	Total 6562	C 3918	N 1322	O 1322	4	0

- Molecule 37 is a protein called U2 small nuclear ribonucleoprotein A'.

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

- Molecule 38 is a protein called U2 small nuclear ribonucleoprotein B".

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

- Molecule 39 is a protein called Pre-mRNA-processing factor 19.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	q	132	Total 659	C 395	N 132	O 132	0	0
39	r	131	Total 654	C 392	N 131	O 131	0	0
39	s	132	Total 659	C 395	N 132	O 132	0	0

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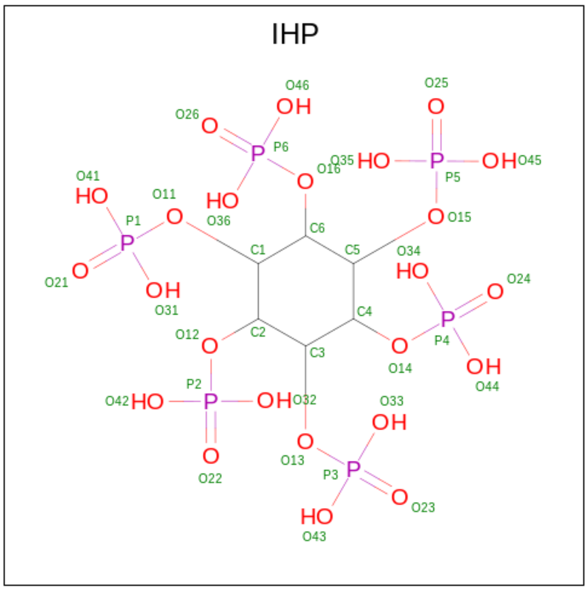
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
39	t	131	654	392	131	131	0	0

- Molecule 40 is a protein called Pre-mRNA-splicing factor SPF27.

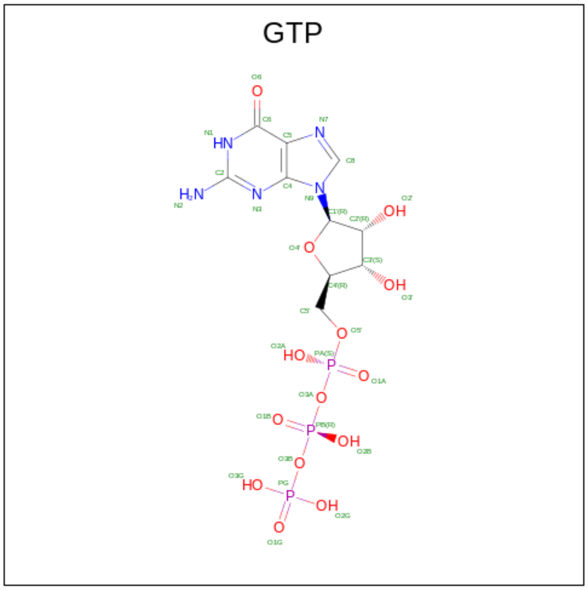
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
40	K	155	772	462	155	155	0	0

- Molecule 41 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: $C_6H_{18}O_{24}P_6$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 42 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



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

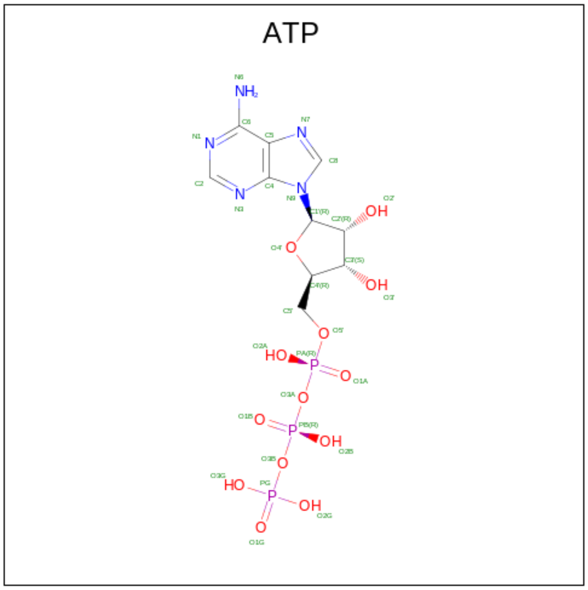
- Molecule 43 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 44 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
44	N	3	Total Zn 3 3	0
44	O	3	Total Zn 3 3	0

- Molecule 45 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).

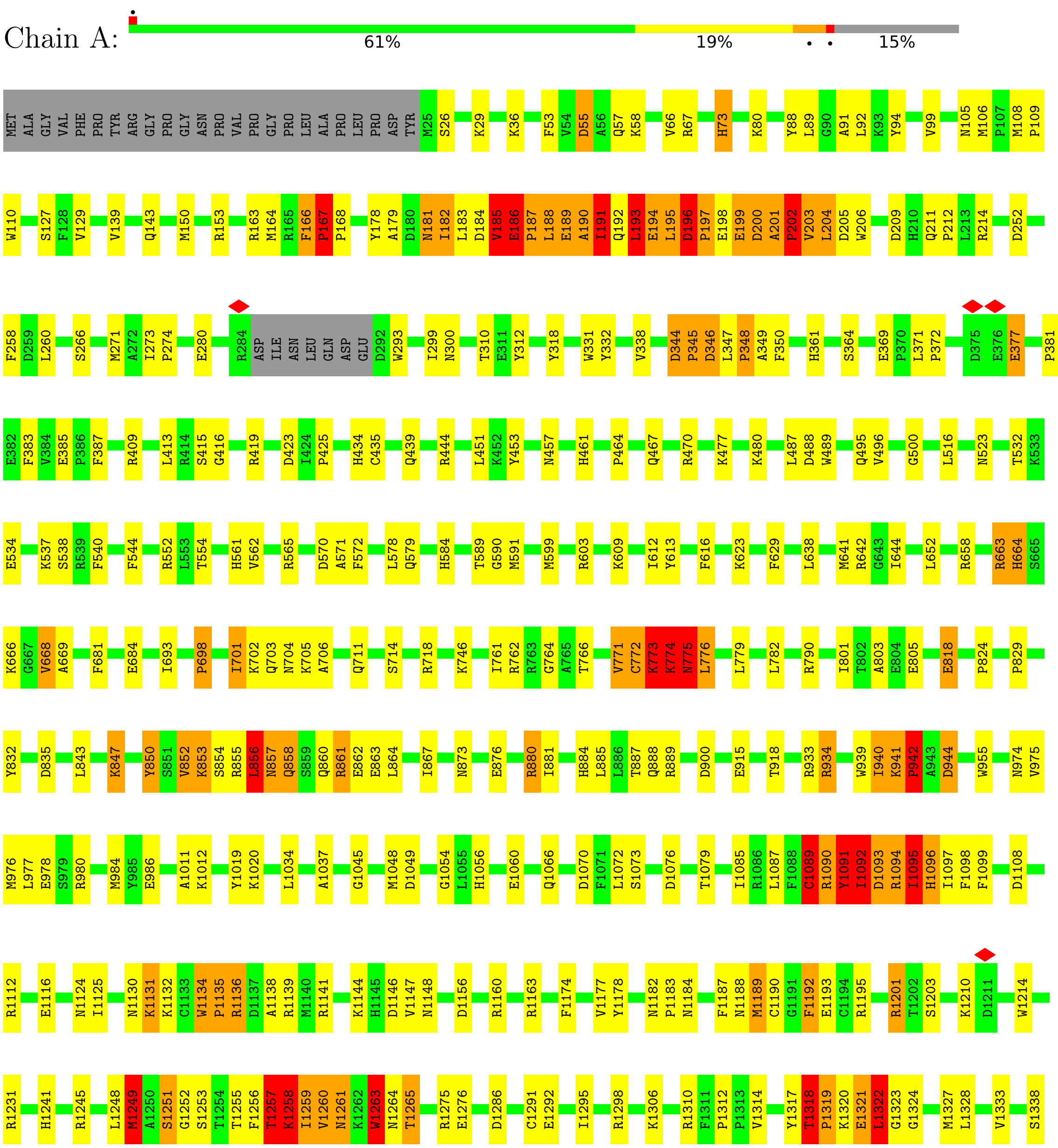


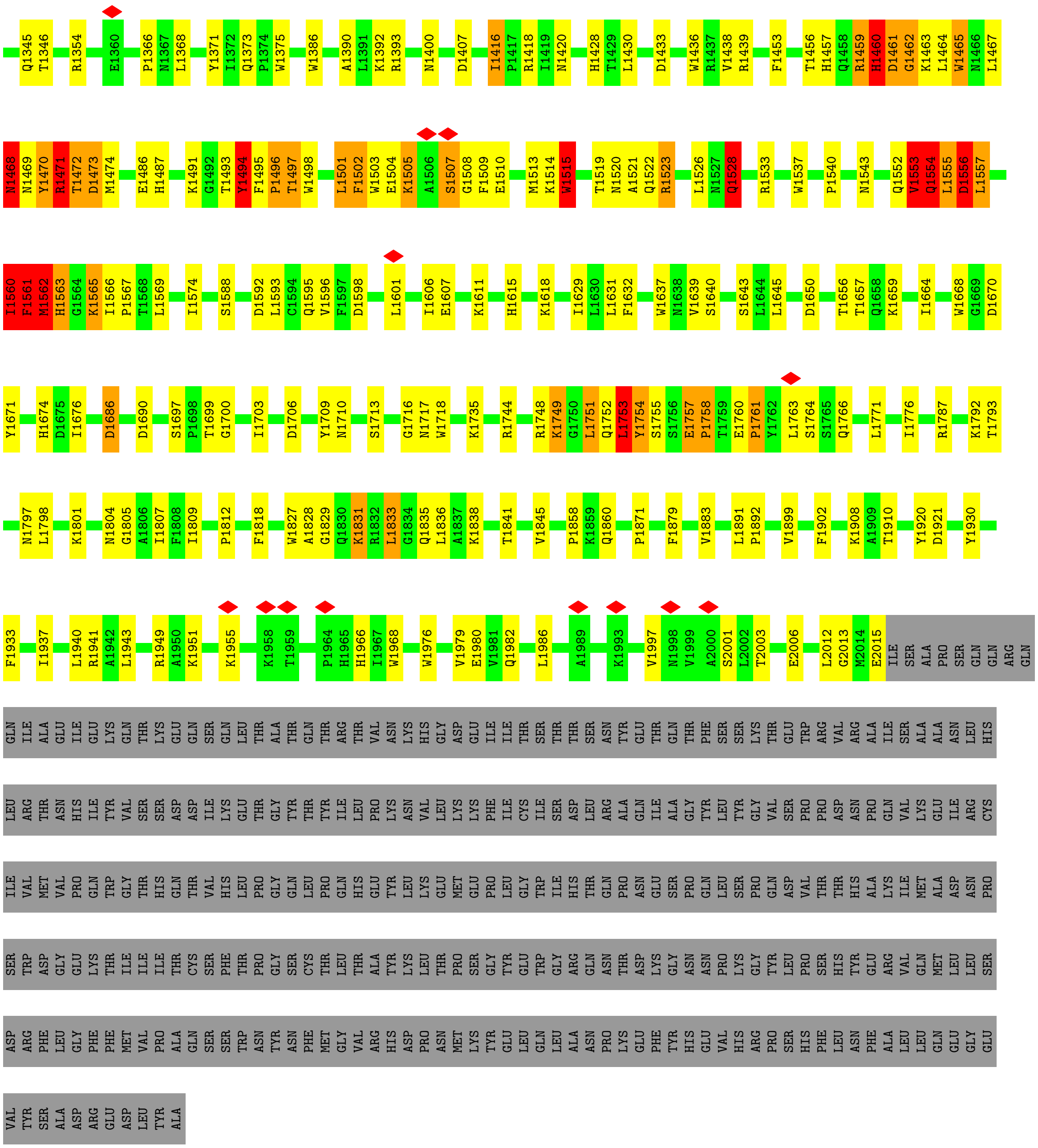
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
45	Q	1	31	10	5	13	3	0

3 Residue-property plots (i)

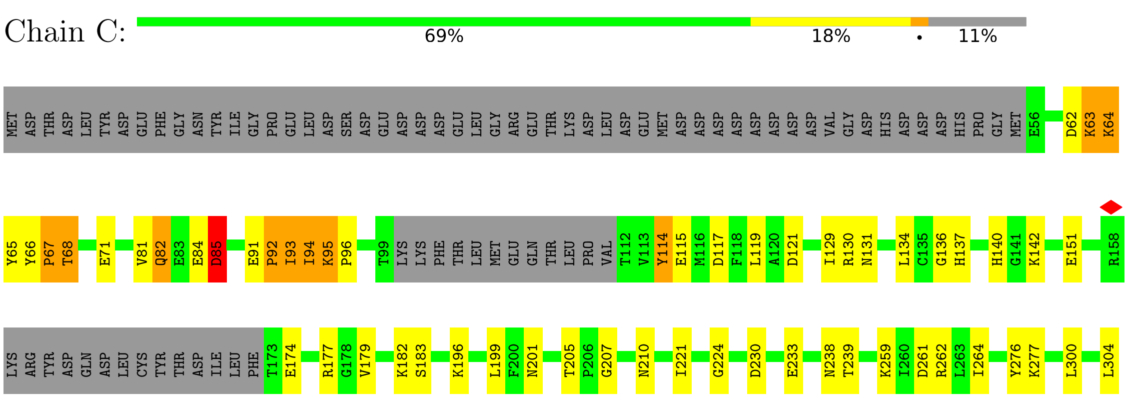
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

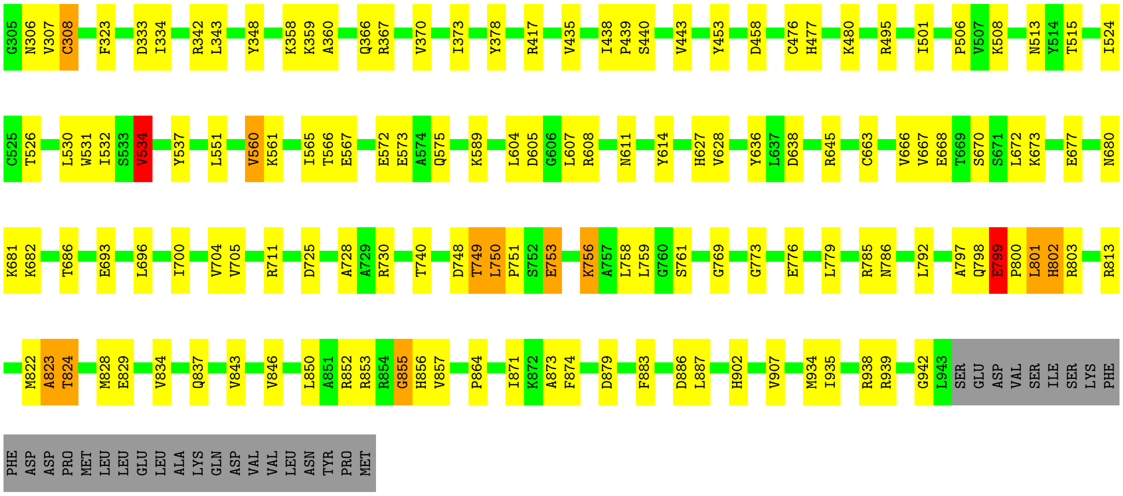
- Molecule 1: Pre-mRNA-processing-splicing factor 8



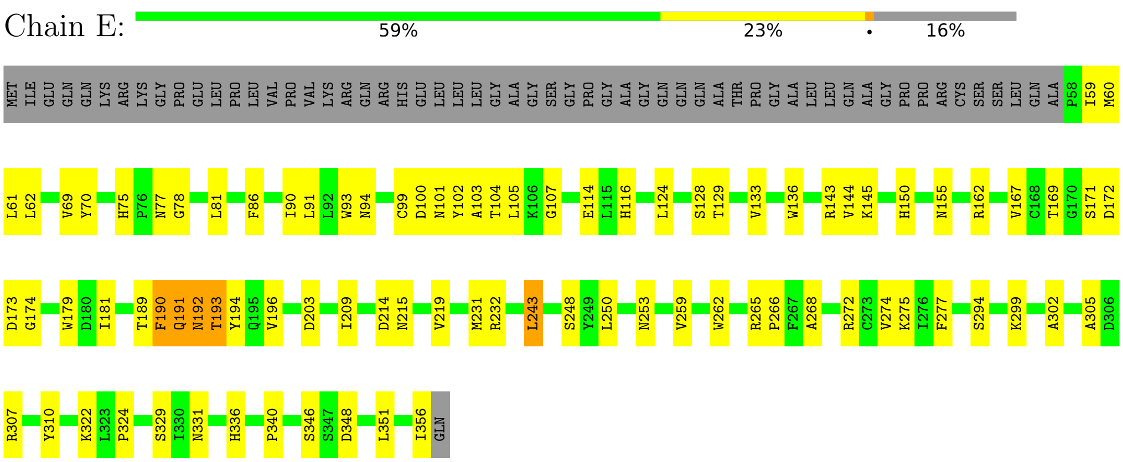


• Molecule 2: 116 kDa U5 small nuclear ribonucleoprotein component



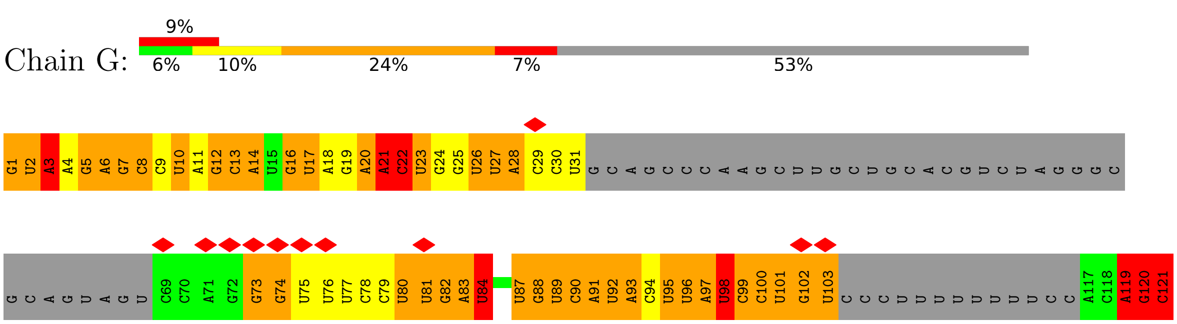


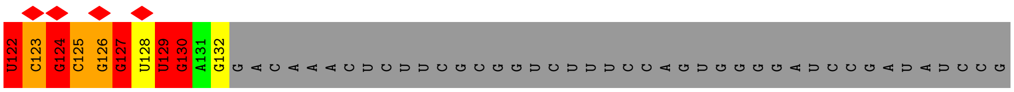
• Molecule 3: U5 small nuclear ribonucleoprotein 40 kDa protein



• Molecule 4: pre-mRNA

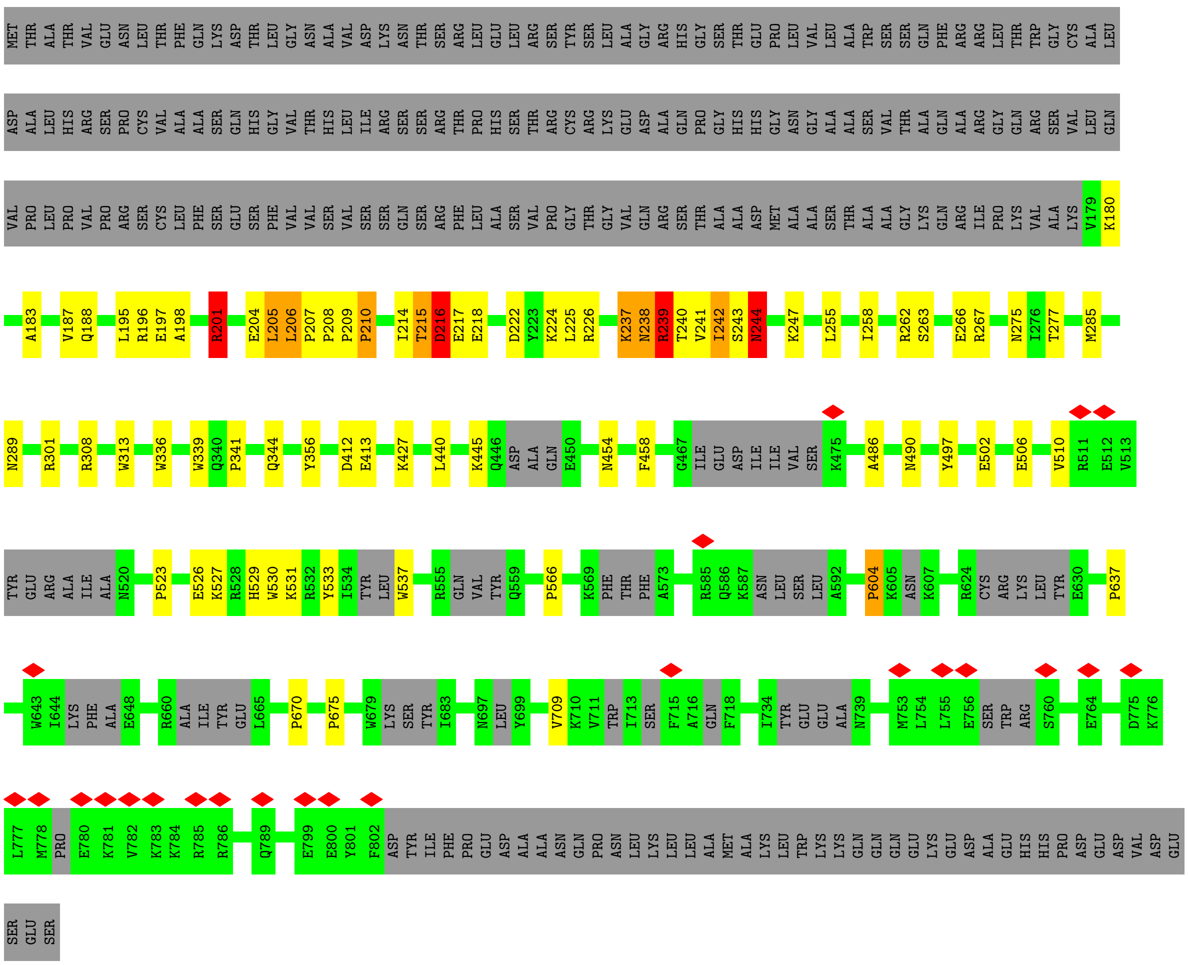
• Molecule 5: pre-mRNA





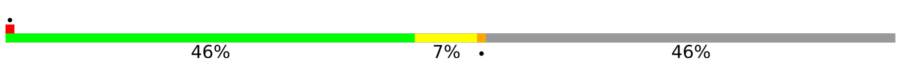
- Molecule 6: Crooked neck-like protein 1

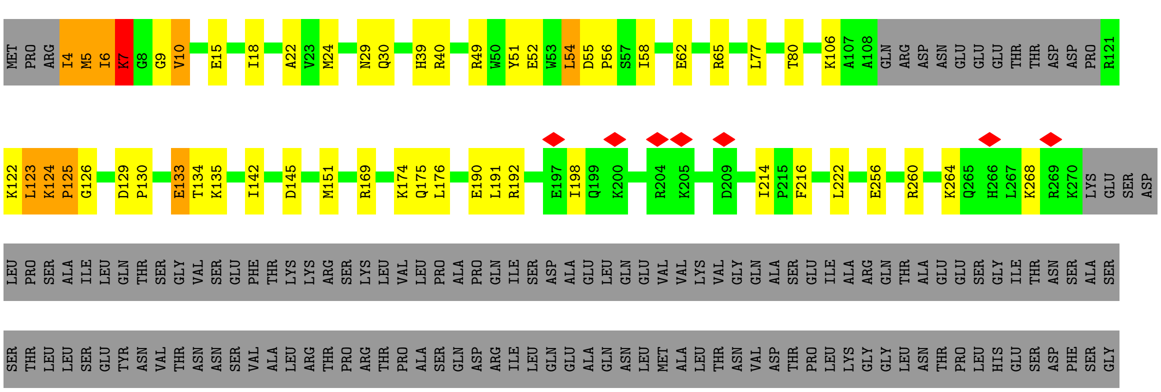
Chain J:

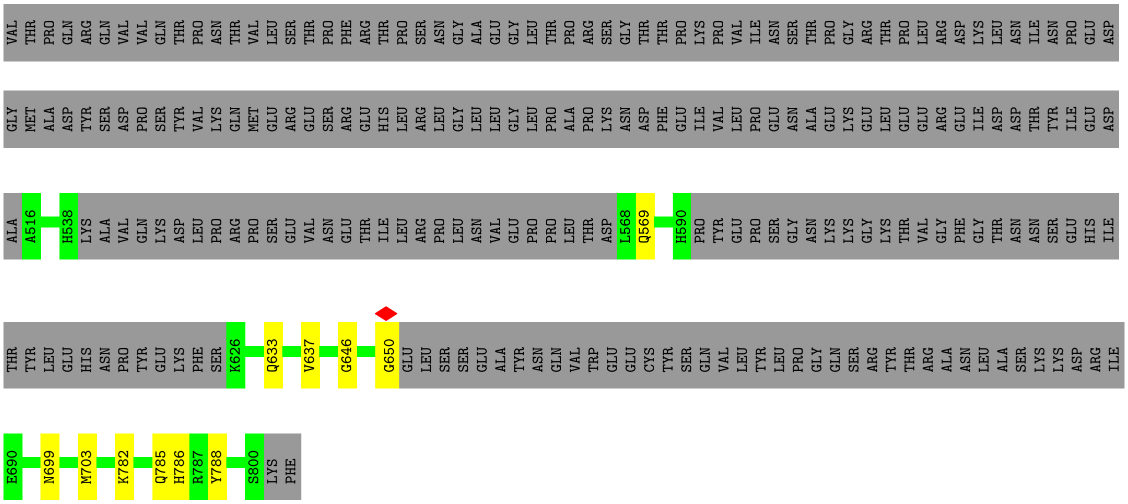


- Molecule 7: Cell division cycle 5-like protein

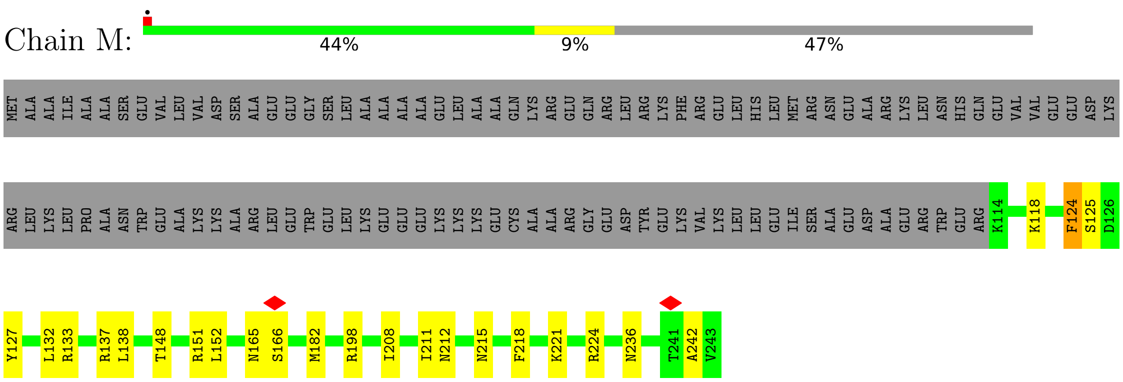
Chain L:



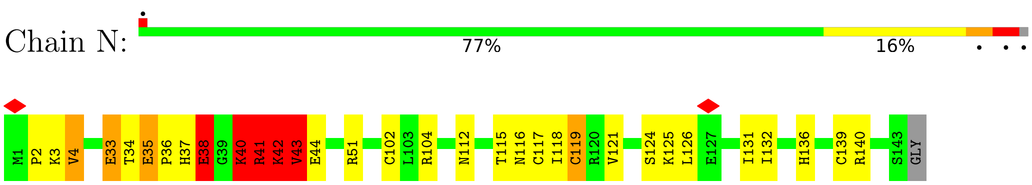




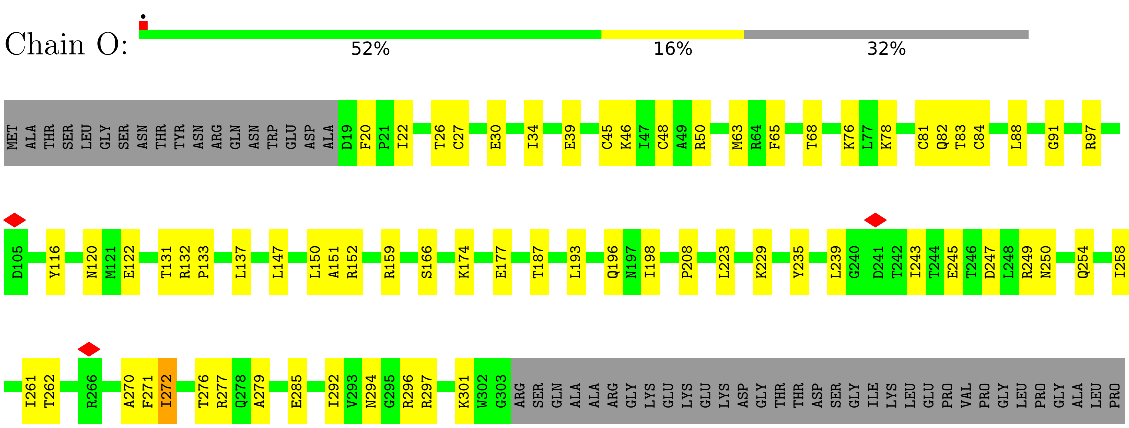
- Molecule 8: Pre-mRNA-splicing factor SYF2

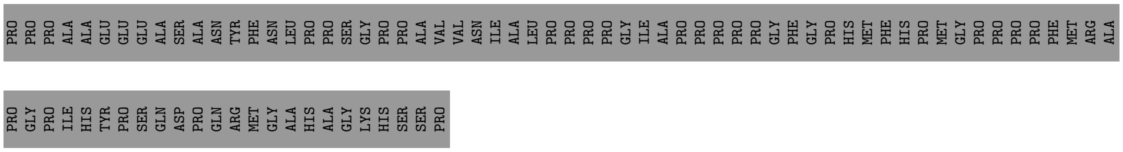


- Molecule 9: Protein BUD31 homolog

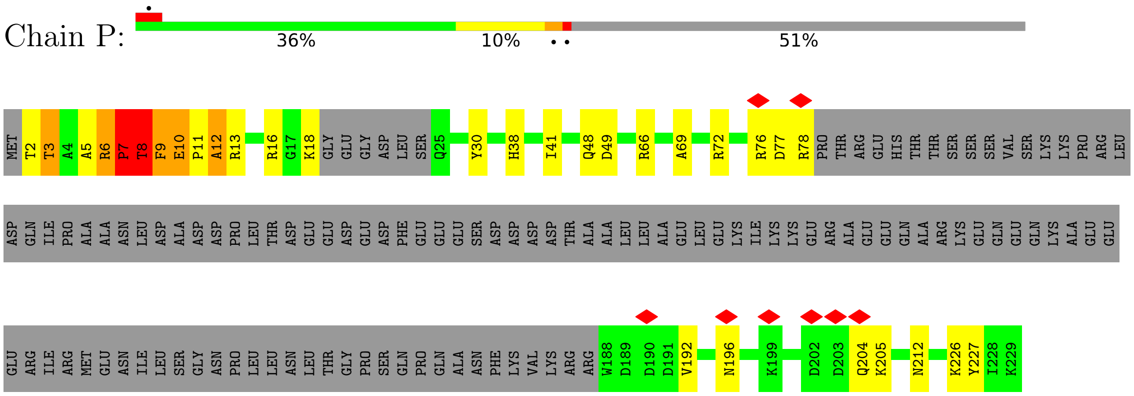


- Molecule 10: Pre-mRNA-splicing factor RBM22

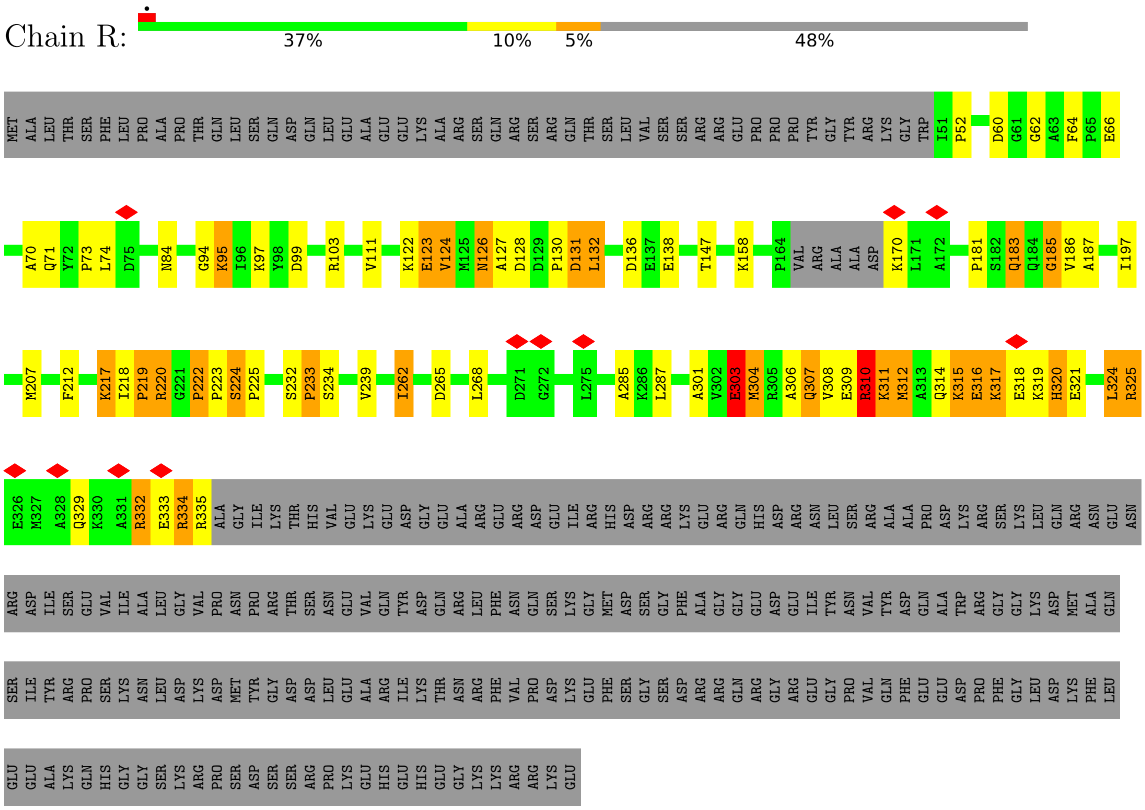




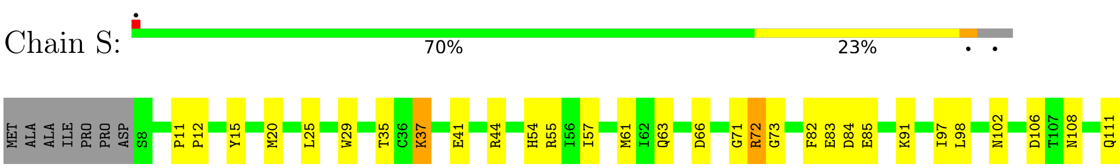
- Molecule 11: Spliceosome-associated protein CWC15 homolog

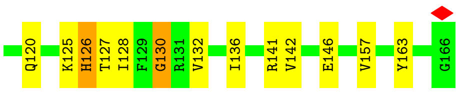


- Molecule 12: SNW domain-containing protein 1



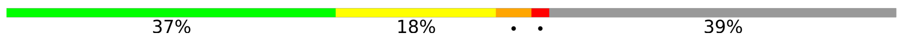
- Molecule 13: Peptidyl-prolyl cis-trans isomerase-like 1

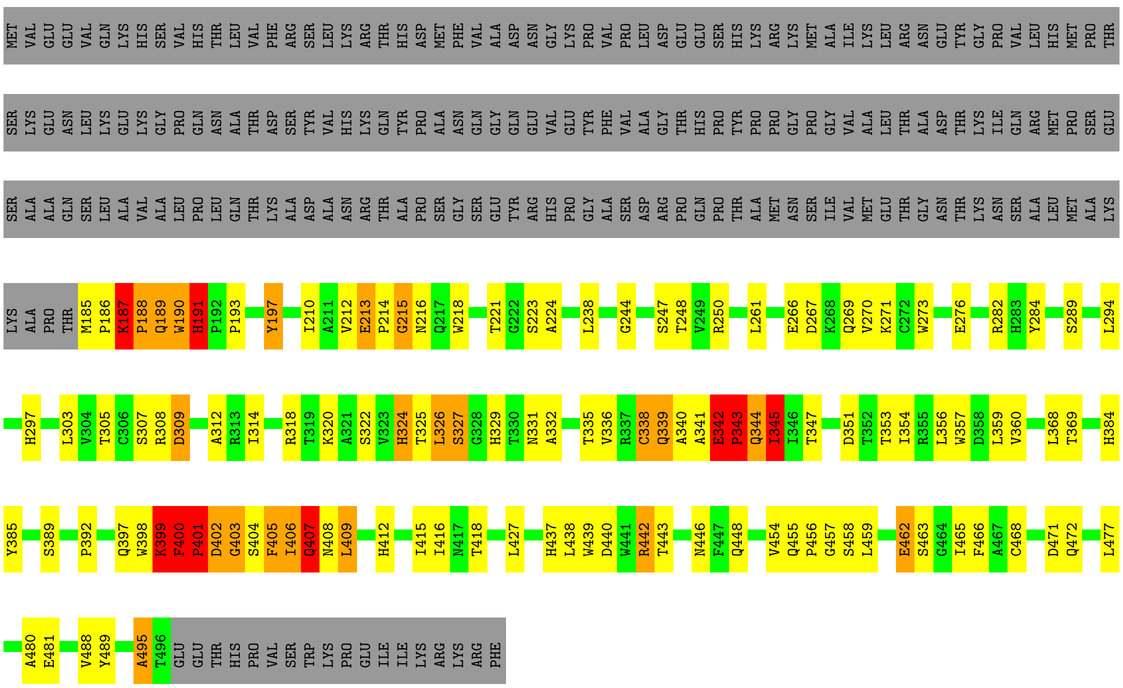




• Molecule 14: Pleiotropic regulator 1

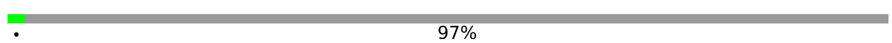
Chain T:

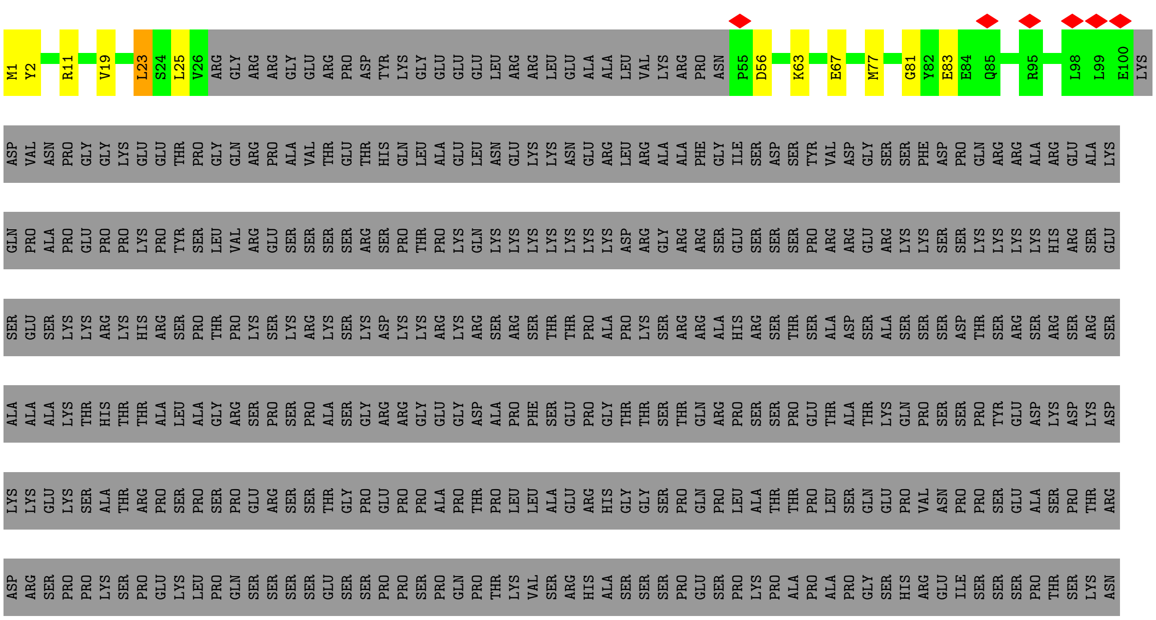


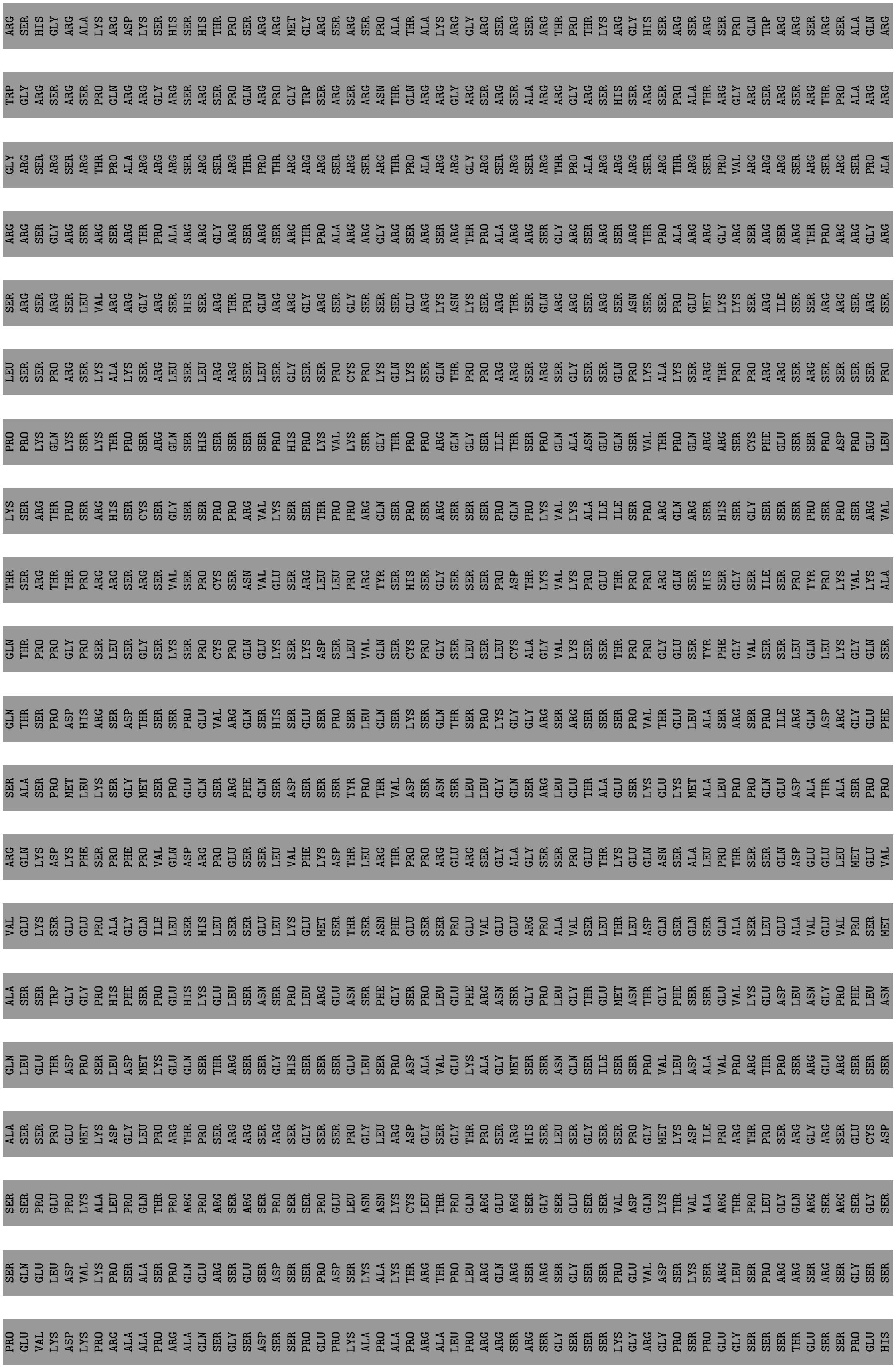


• Molecule 15: Serine/arginine repetitive matrix protein 2

Chain U:



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LEU SER SER PRO ARG SER LYS ALA LYS SER ARG LEU SER LEU ARG ARG SER LEU SER GLY SER SER PRO CYS PRO LYS GLN LYS SER GLN THR PRO PRO ARG ARG SER ARG SER GLY SER SER GLN PRO LYS ALA LYS SER ARG THR PRO PRO ARG ARG SER ARG SER SER SER SER PRO
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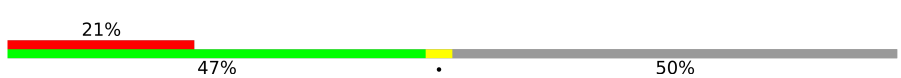
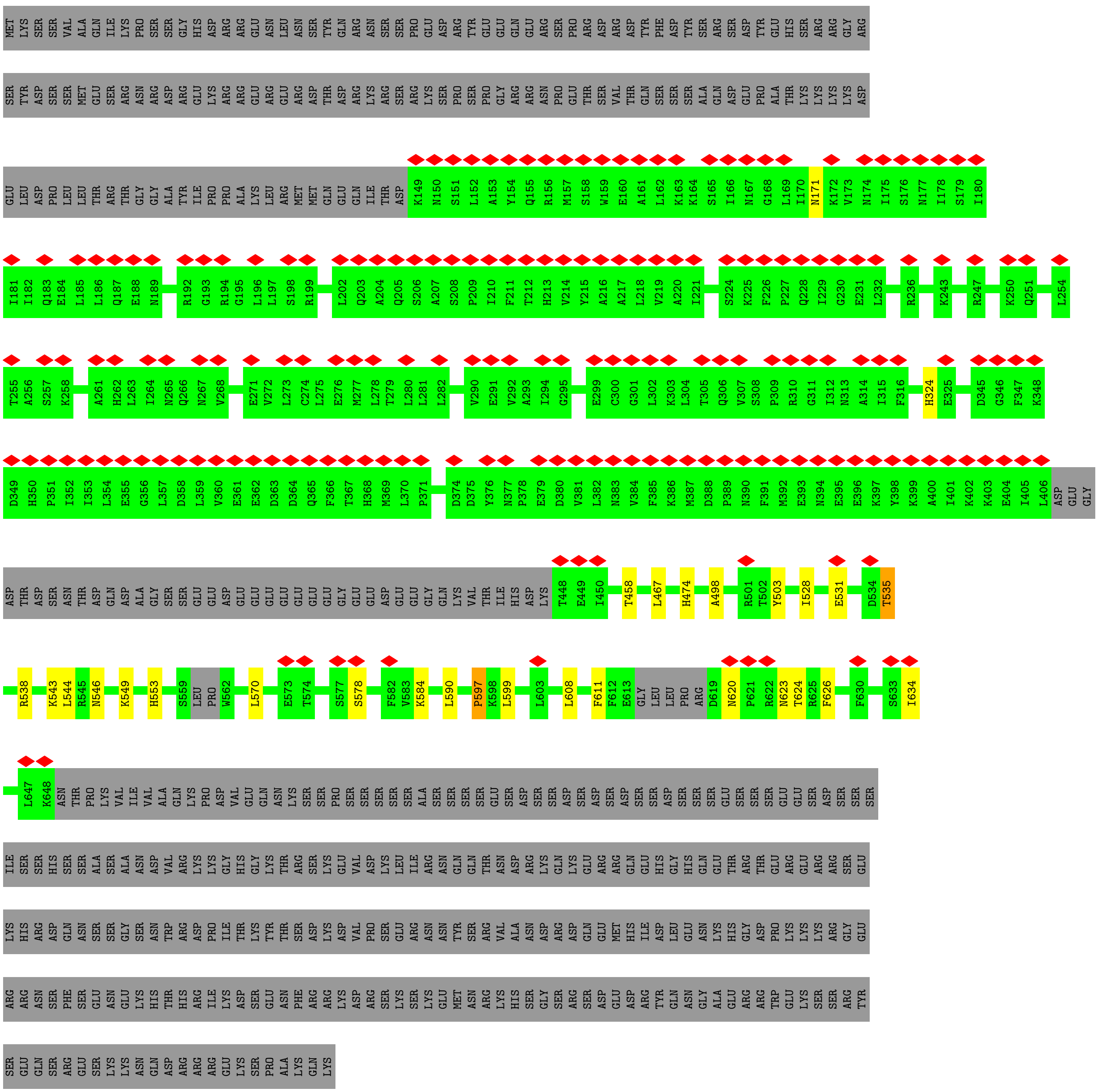
ARG PRO MET ARG HIS ARG SER SER ARG SER PRO

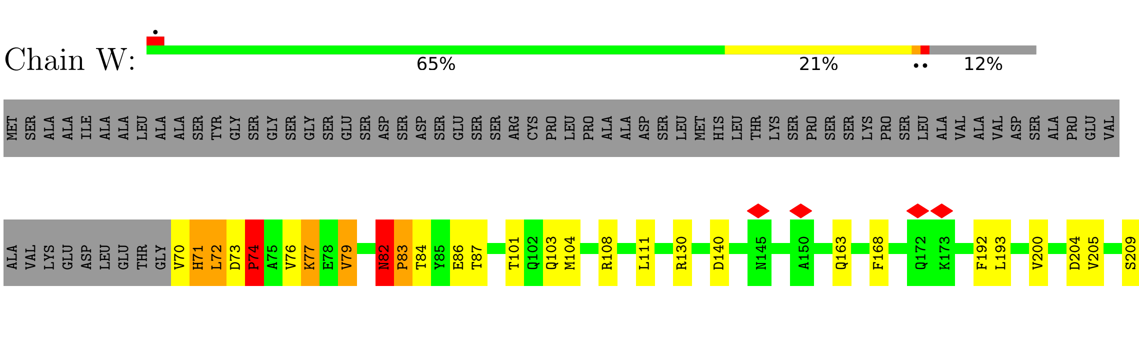
• Molecule 16: Pre-mRNA-splicing factor CWC22 homolog

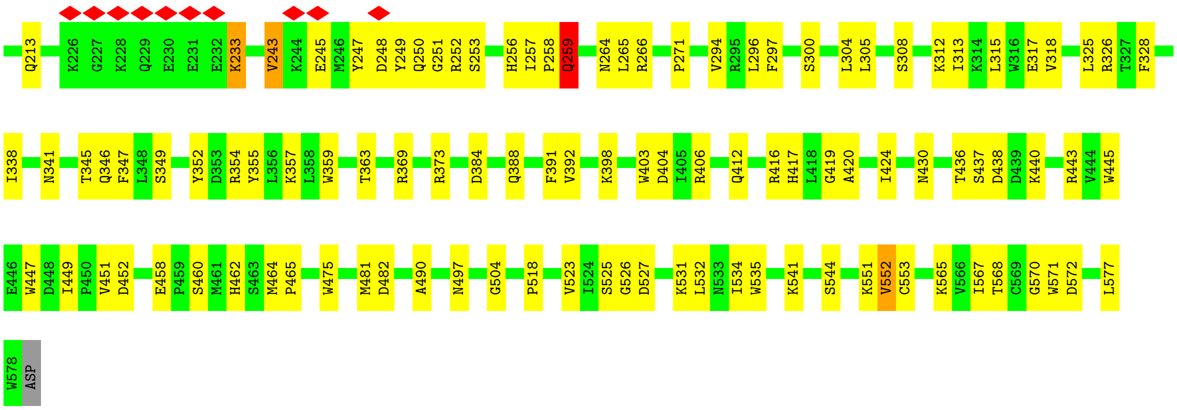
Chain V:





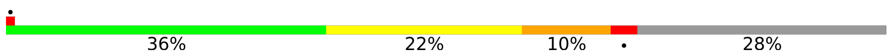
• Molecule 17: Pre-mRNA-processing factor 17

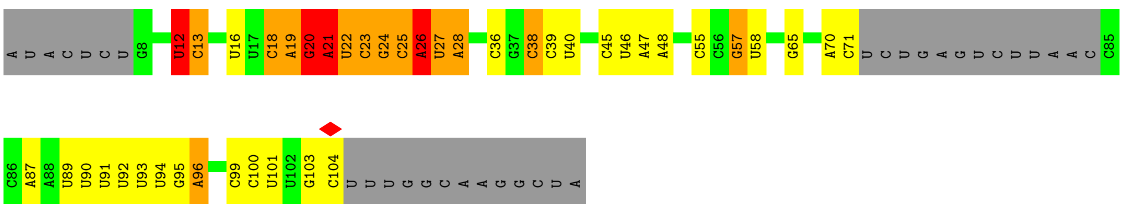




• Molecule 18: U5 snRNA

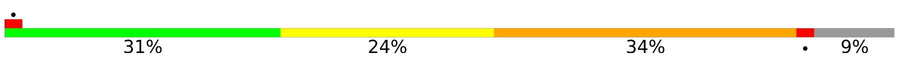
Chain B:

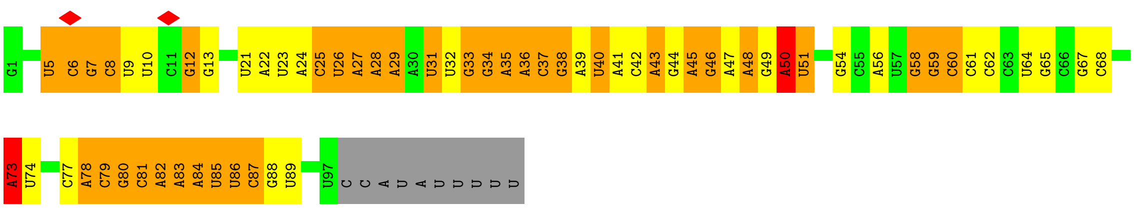




• Molecule 19: U6 snRNA

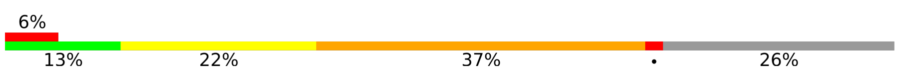
Chain F:

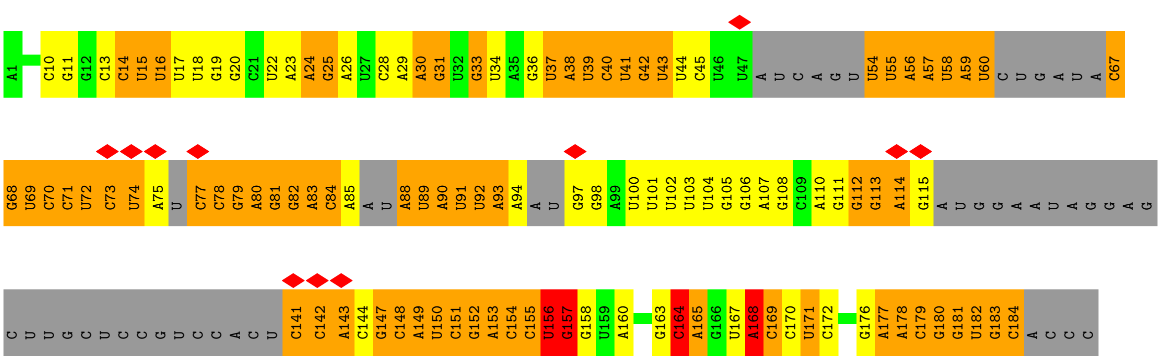




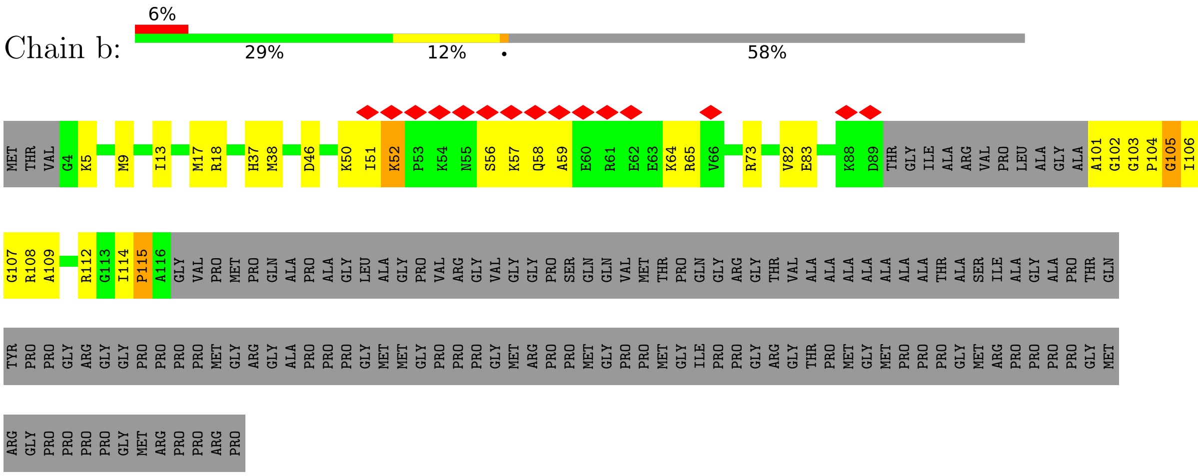
• Molecule 20: U2 snRNA

Chain H:

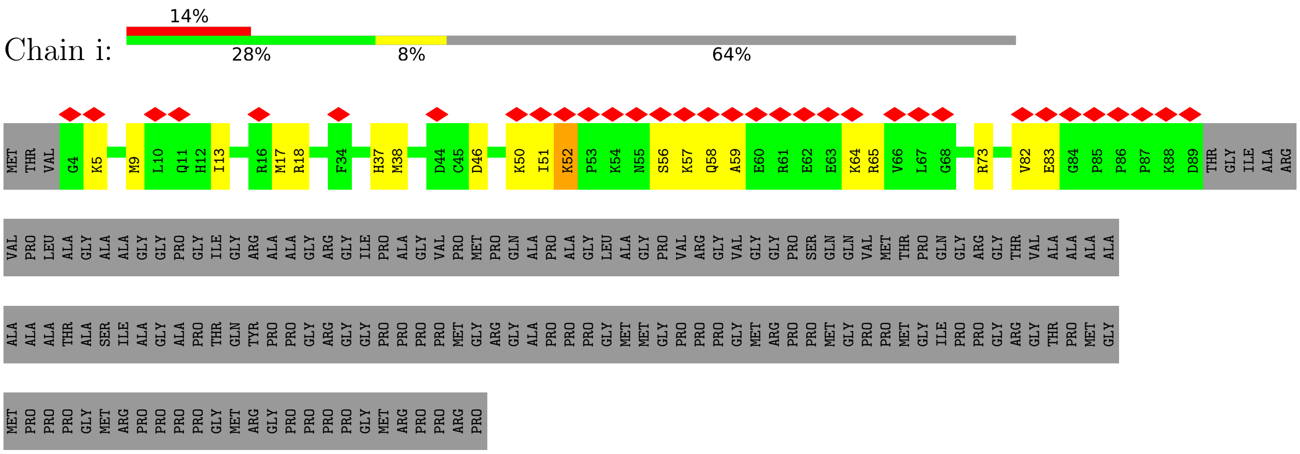




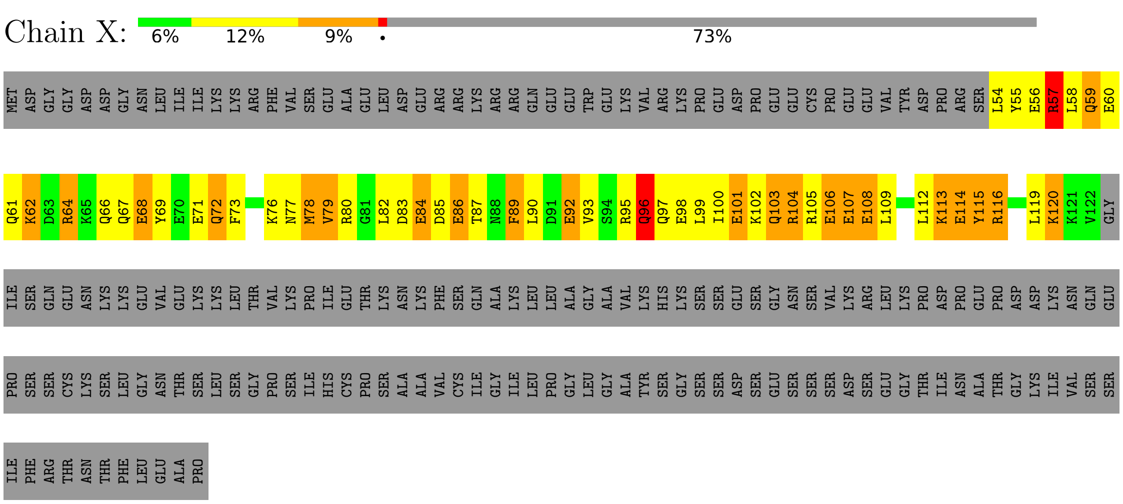
• Molecule 21: Small nuclear ribonucleoprotein-associated proteins B and B’



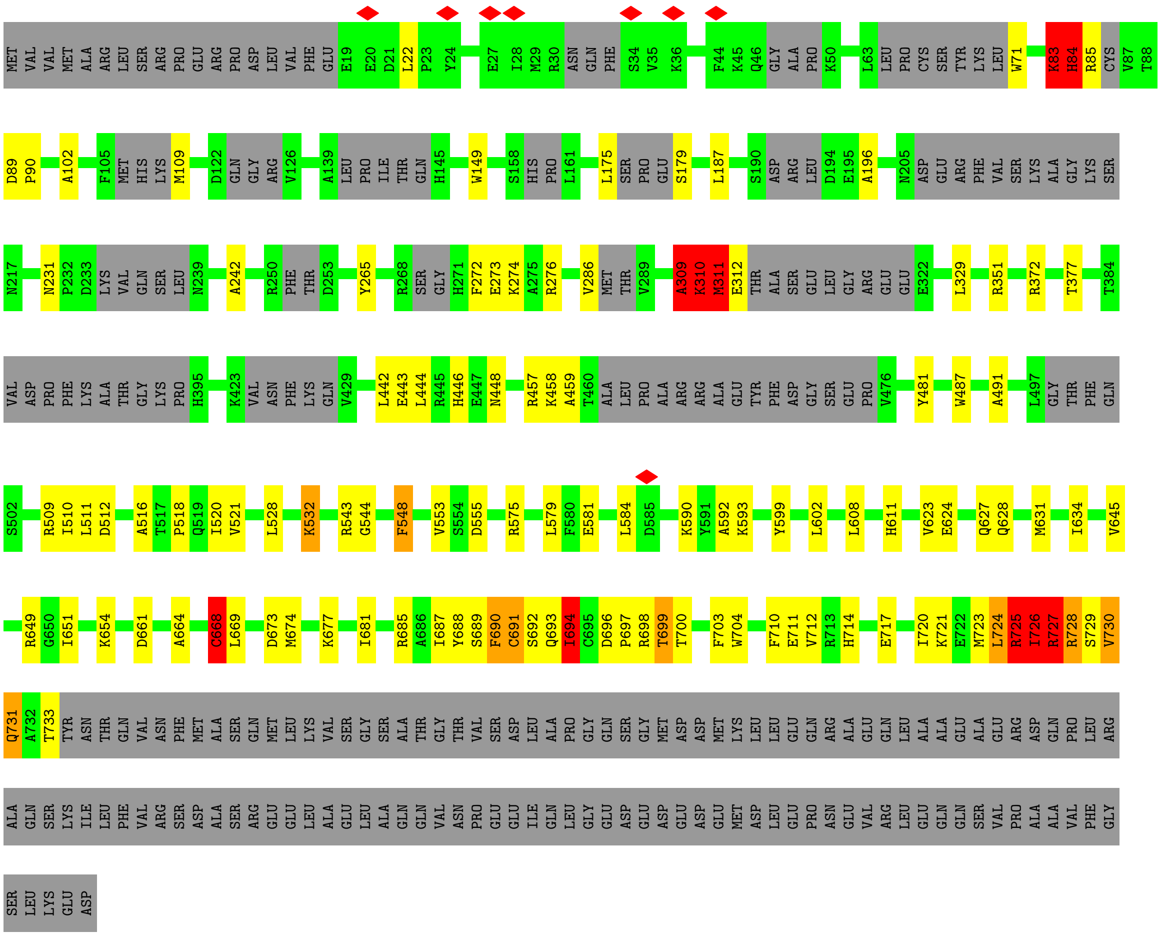
• Molecule 21: Small nuclear ribonucleoprotein-associated proteins B and B’



• Molecule 22: PSME3-interacting protein

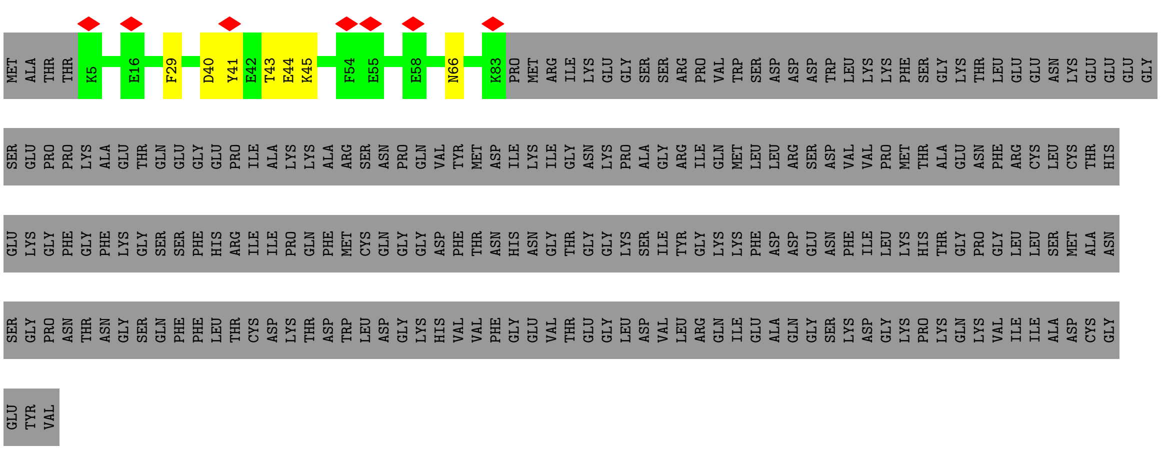


• Molecule 23: Pre-mRNA-splicing factor SYF1

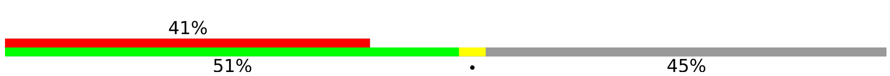


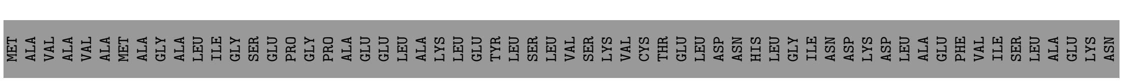
- Molecule 24: Peptidyl-prolyl cis-trans isomerase E

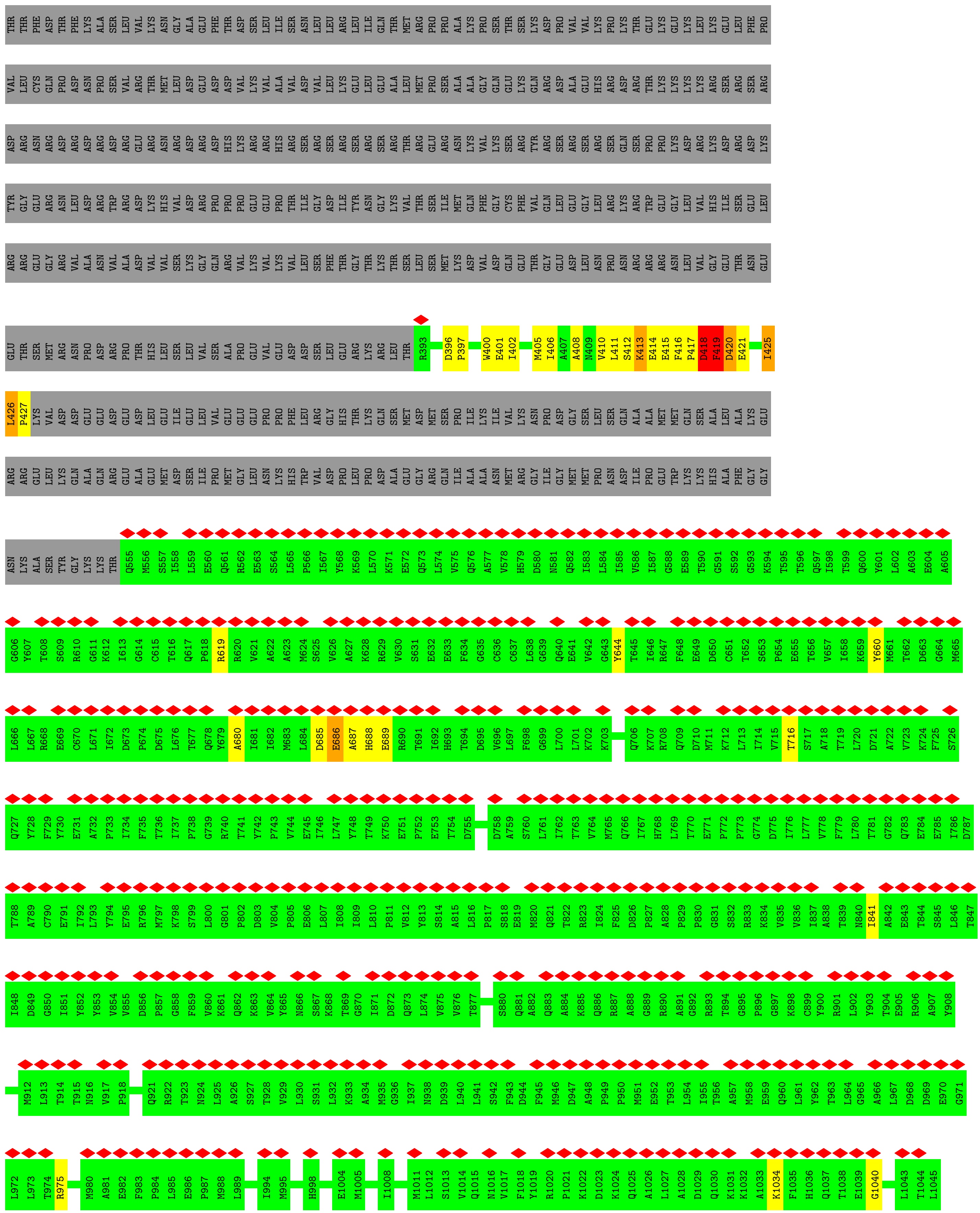
Chain y: 



- Molecule 25: ATP-dependent RNA helicase DHX8

Chain Y: 

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VAL LEU CYS GLN PRO ASP ASN PRO SER VAL ARG THR MET LEU ASP GLU ASP ASP VAL LYS VAL ALA VAL ASP VAL LEU LYS GLU LEU GLU ALA LEU MET PRO SER ALA ALA GLY GLN GLU LYS GLN ARG ASP ALA GLU HIS ARG ASP ARG THR LYS LYS LYS LYS ARG SER ARG SER ARG
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L426 P427 LYS VAL ASP ASP GLU GLU ASP GLU ASP LEU GLU ILE GLU LEU VAL GLU GLU GLU PRO PRO PHE LEU ARG GLY HIS THR LYS GLN SER MET ASP MET SER PRO ILE LYS ILE VAL LYS ASN PRO ASP GLY SER LEU SER GLN ALA ALA MET MET GLN SER ALA LEU ALA LYS GLU
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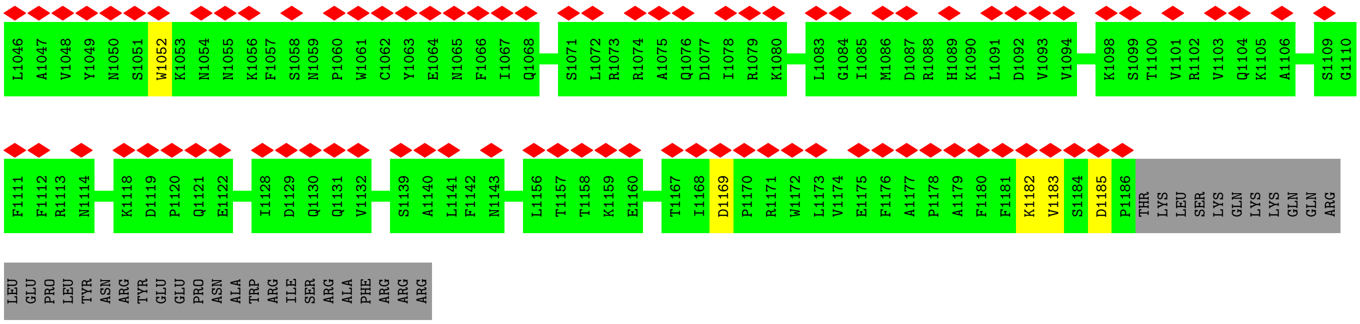
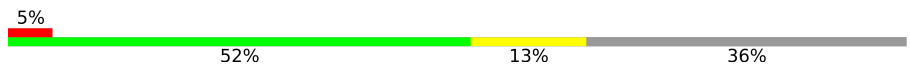
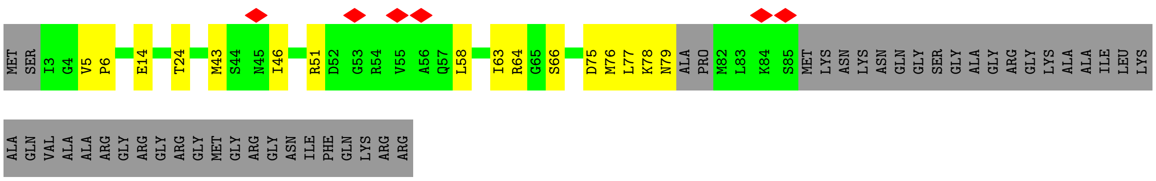
M912 L913 T914 T915 N916 V917 P918 Q921 R922 T923 N924 L925 A926 S927 T928 V929 L930 S931 L932 K933 A934 M935 G936 I937 N938 D939 L940 L941 S942 F943 D944 F945 M946 D947 A948 P949 P950 M951 E952 T953 L954 I955 T956 A957 M958 E959 Q960 L961 Y962 T963 L964 G965 A966 L967 D968 D969 E970 G971
L972 L973 T974 R975 M980 A981 E982 F983 P984 L985 E986 P987 M988 L989 I994 M995 H998 E1004 M1005 I1008 M1011 L1012 S1013 V1014 Q1015 N1016 V1017 F1018 Y1019 R1020 P1021 K1022 D1023 K1024 Q1025 A1026 L1027 A1028 D1029 Q1030 K1031 K1032 A1033 K1034 F1035 H1036 Q1037 T1038 E1039 G1040 L1043 T1044 L1045



• Molecule 26: Small nuclear ribonucleoprotein Sm D3

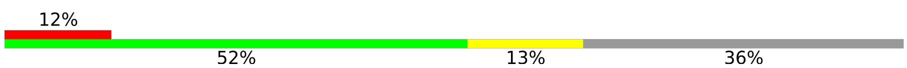
Chain a:

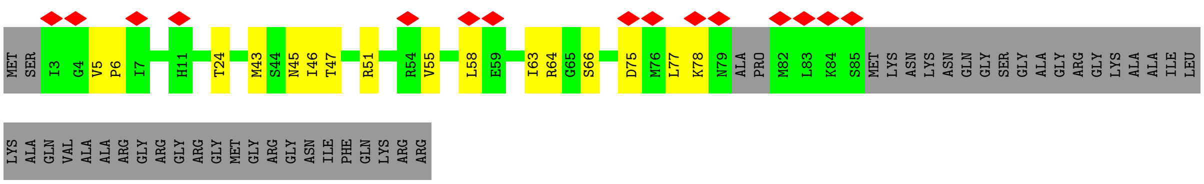




• Molecule 26: Small nuclear ribonucleoprotein Sm D3

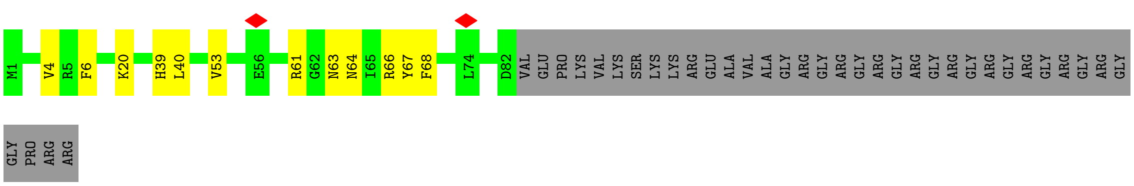
Chain h:





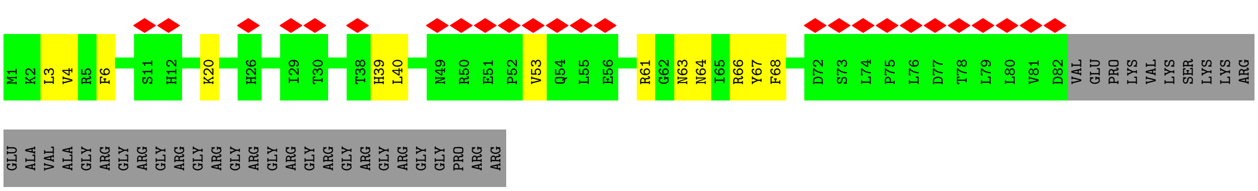
• Molecule 27: Small nuclear ribonucleoprotein Sm D1

Chain c:

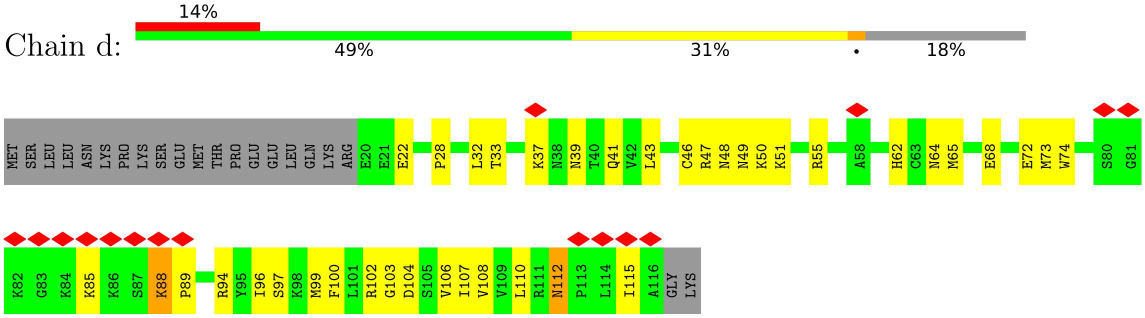


• Molecule 27: Small nuclear ribonucleoprotein Sm D1

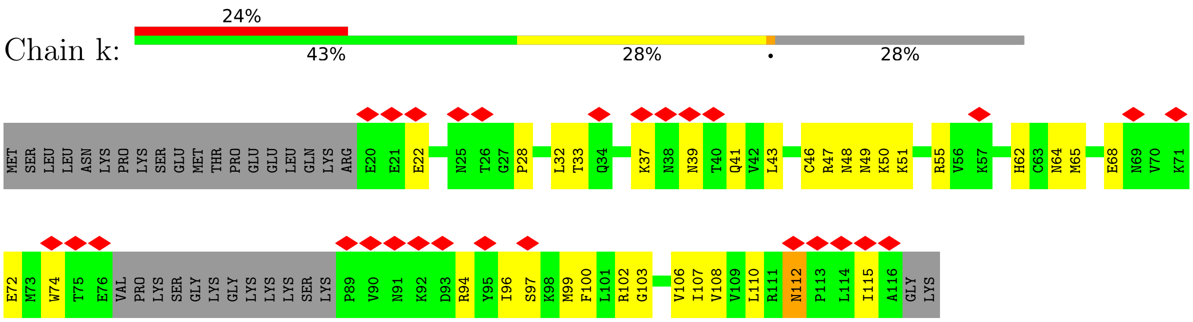
Chain j:



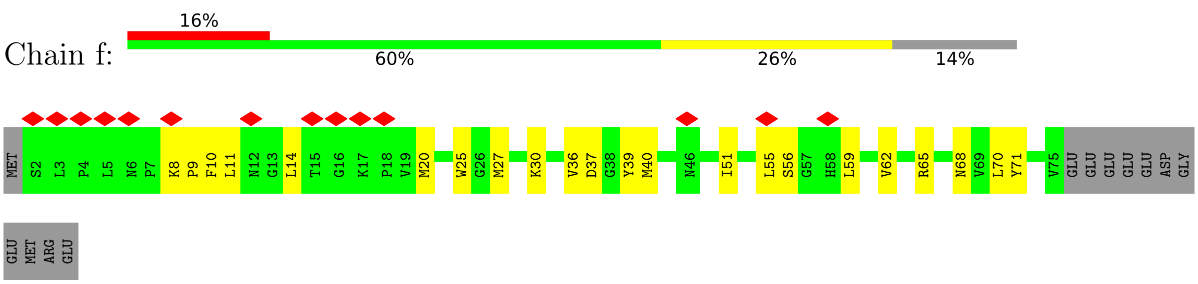
- Molecule 28: Small nuclear ribonucleoprotein Sm D2



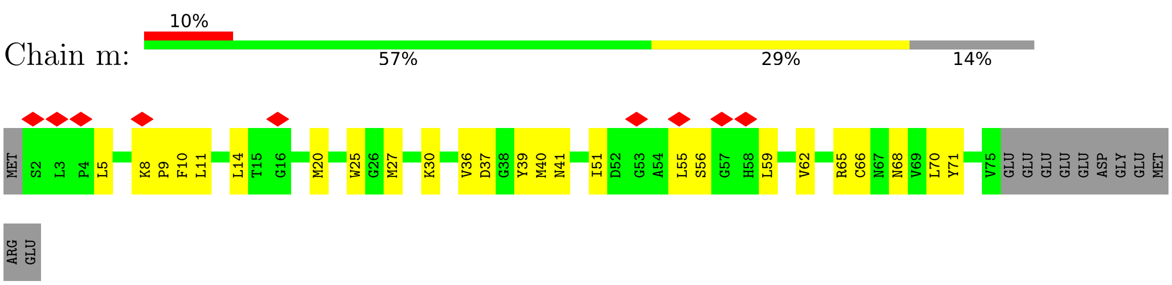
- Molecule 28: Small nuclear ribonucleoprotein Sm D2



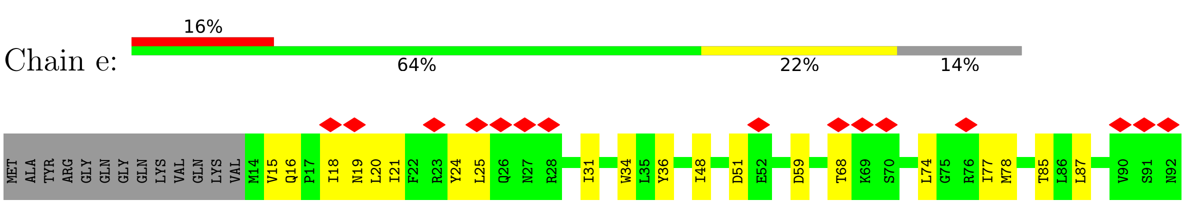
- Molecule 29: Small nuclear ribonucleoprotein F



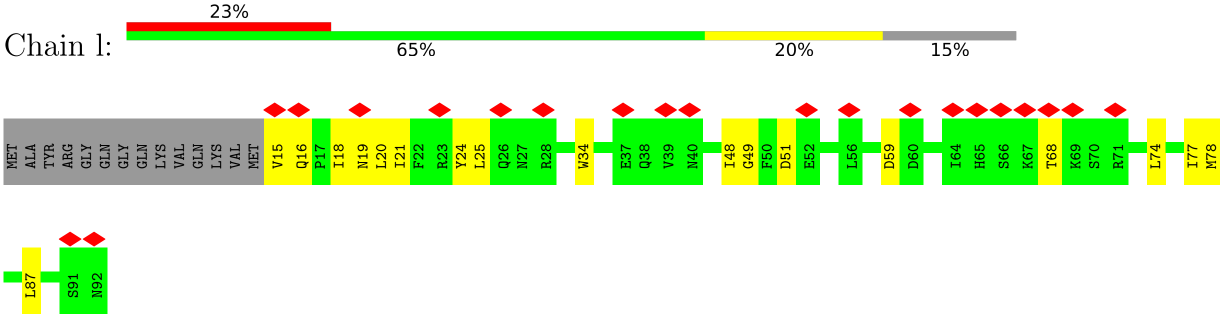
- Molecule 29: Small nuclear ribonucleoprotein F



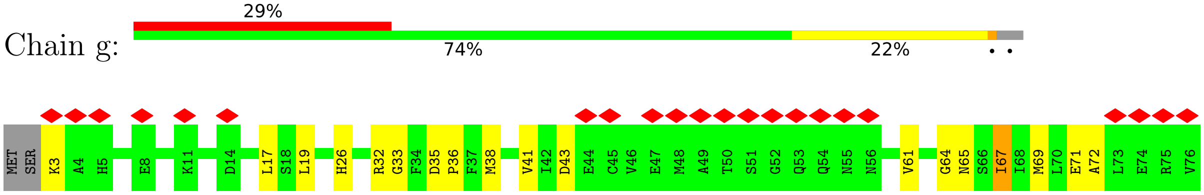
- Molecule 30: Small nuclear ribonucleoprotein E



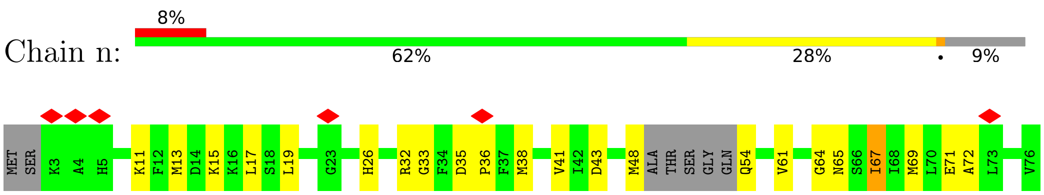
- Molecule 30: Small nuclear ribonucleoprotein E



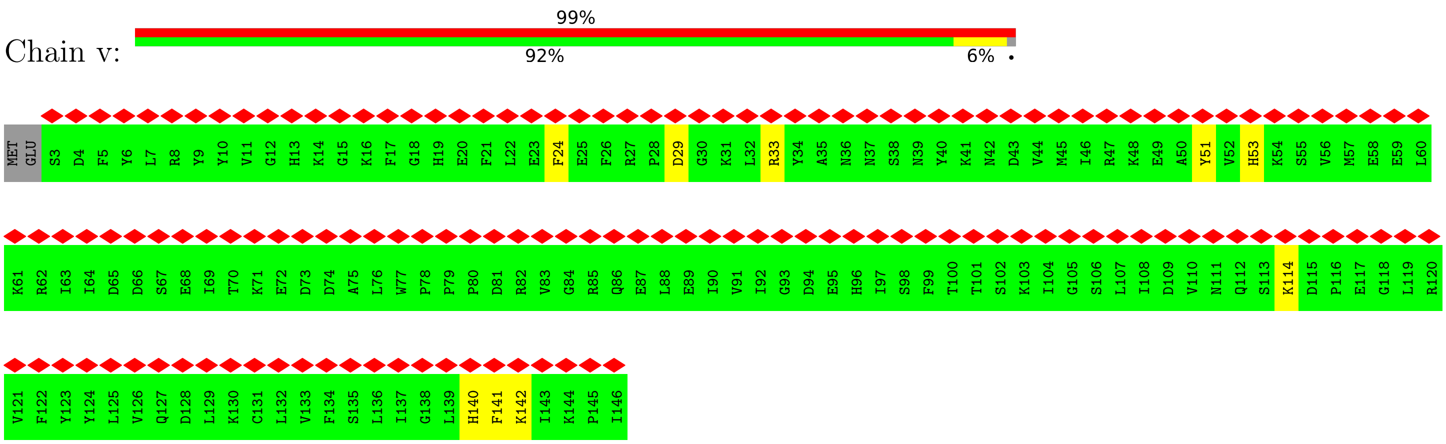
- Molecule 31: Small nuclear ribonucleoprotein G



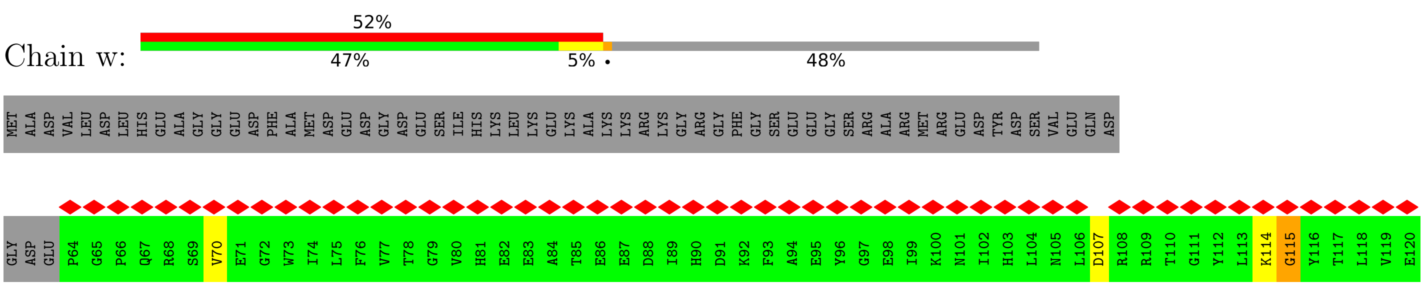
- Molecule 31: Small nuclear ribonucleoprotein G

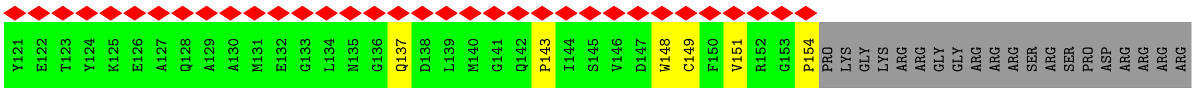


- Molecule 32: Protein mago nashi homolog



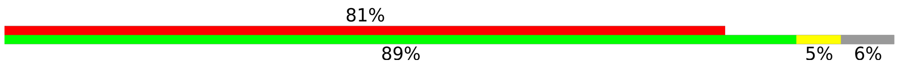
- Molecule 33: RNA-binding protein 8A

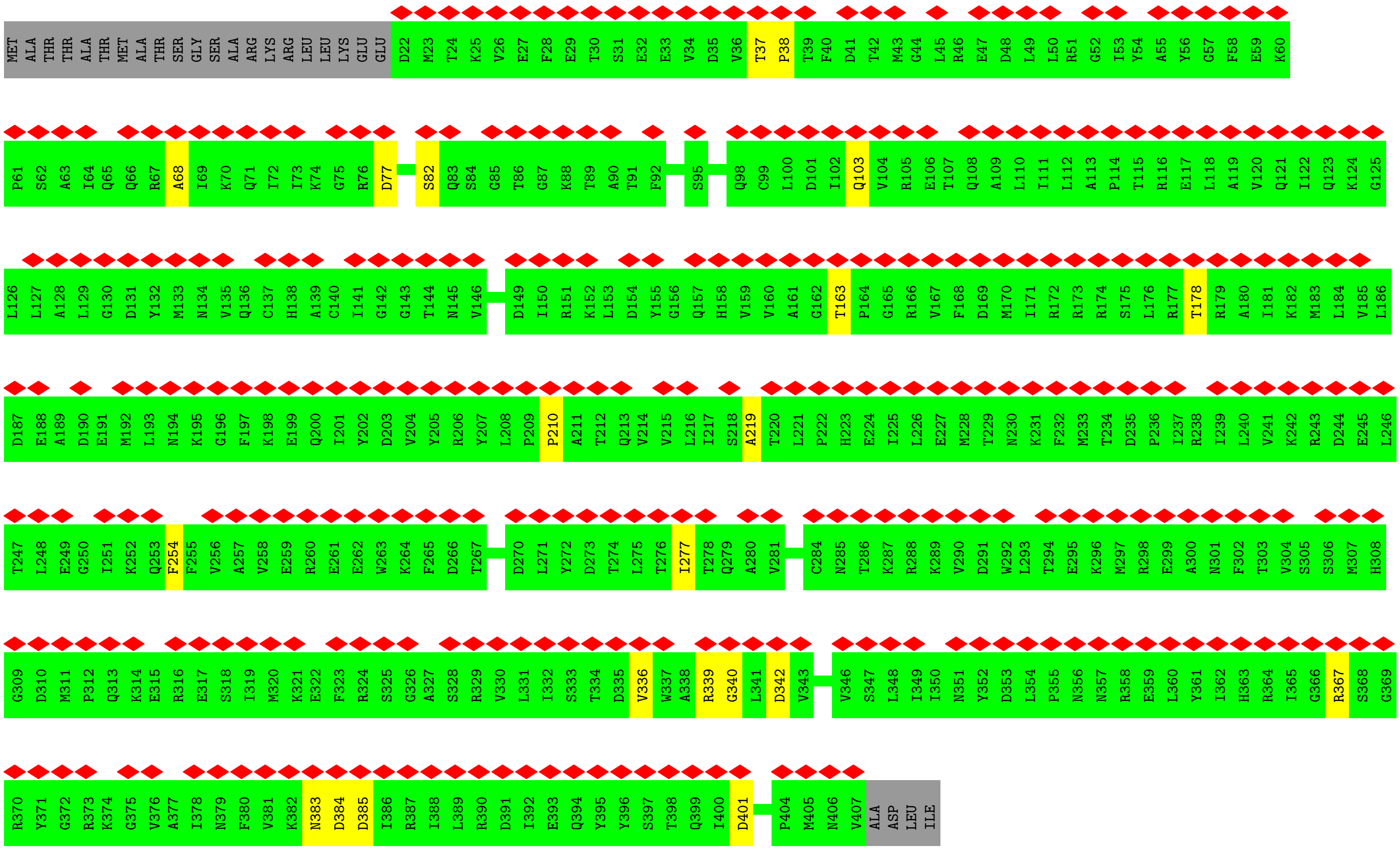




• Molecule 34: Eukaryotic initiation factor 4A-III

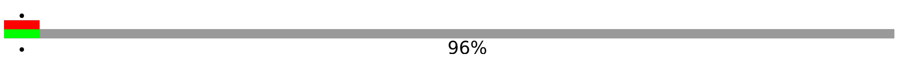
Chain u:

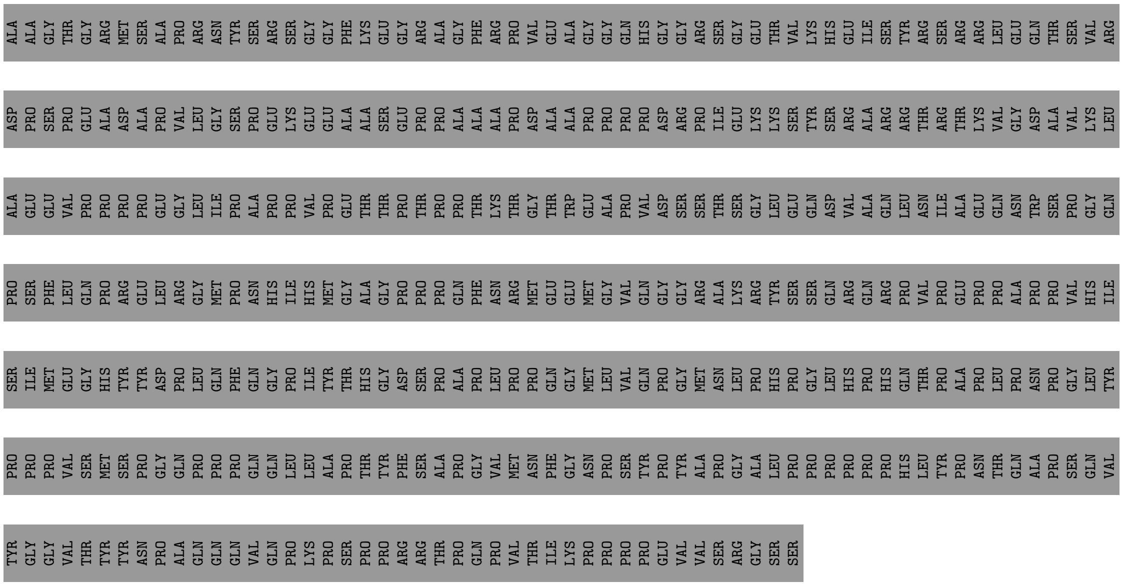




• Molecule 35: Protein CASC3

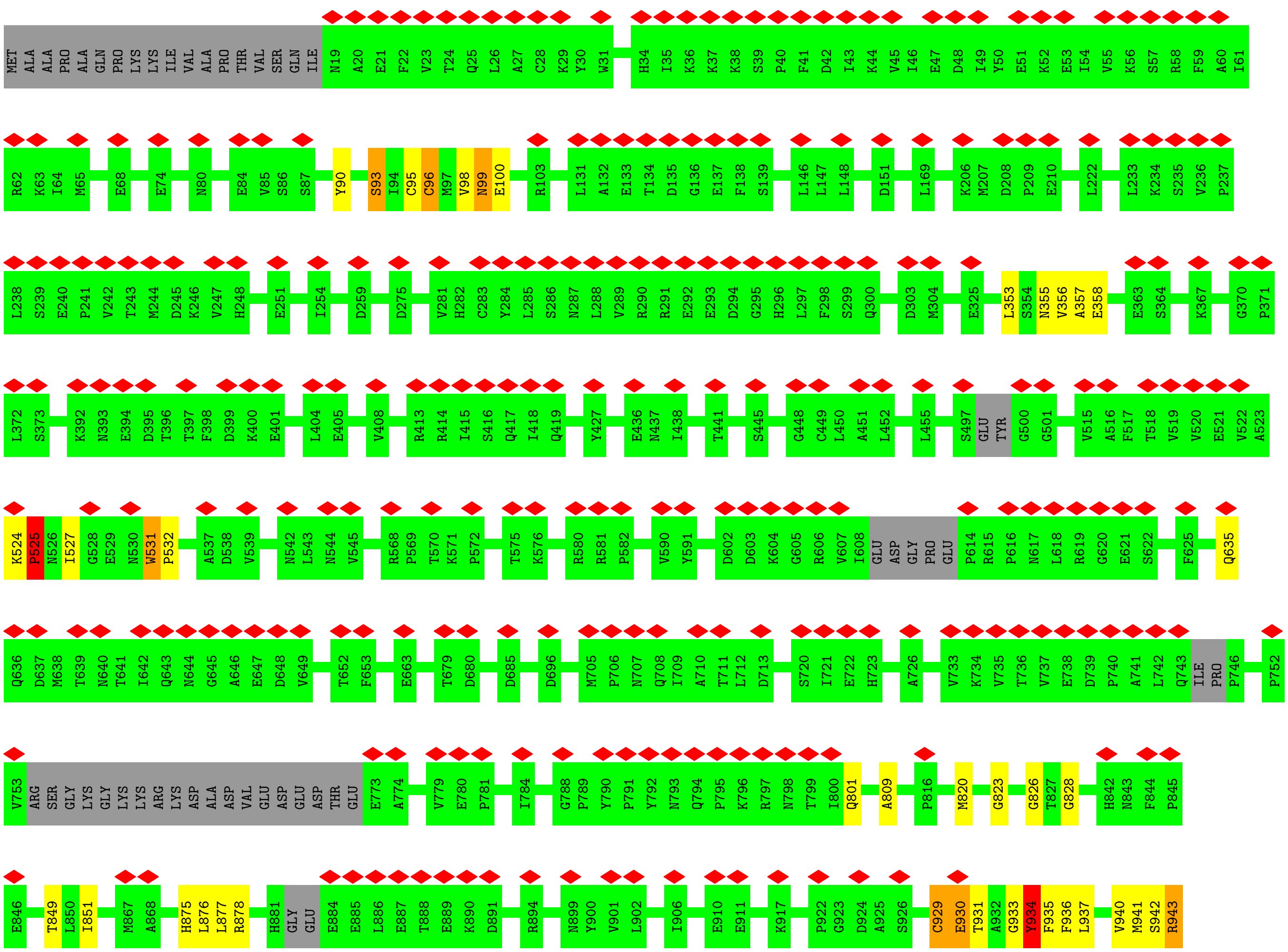
Chain x:

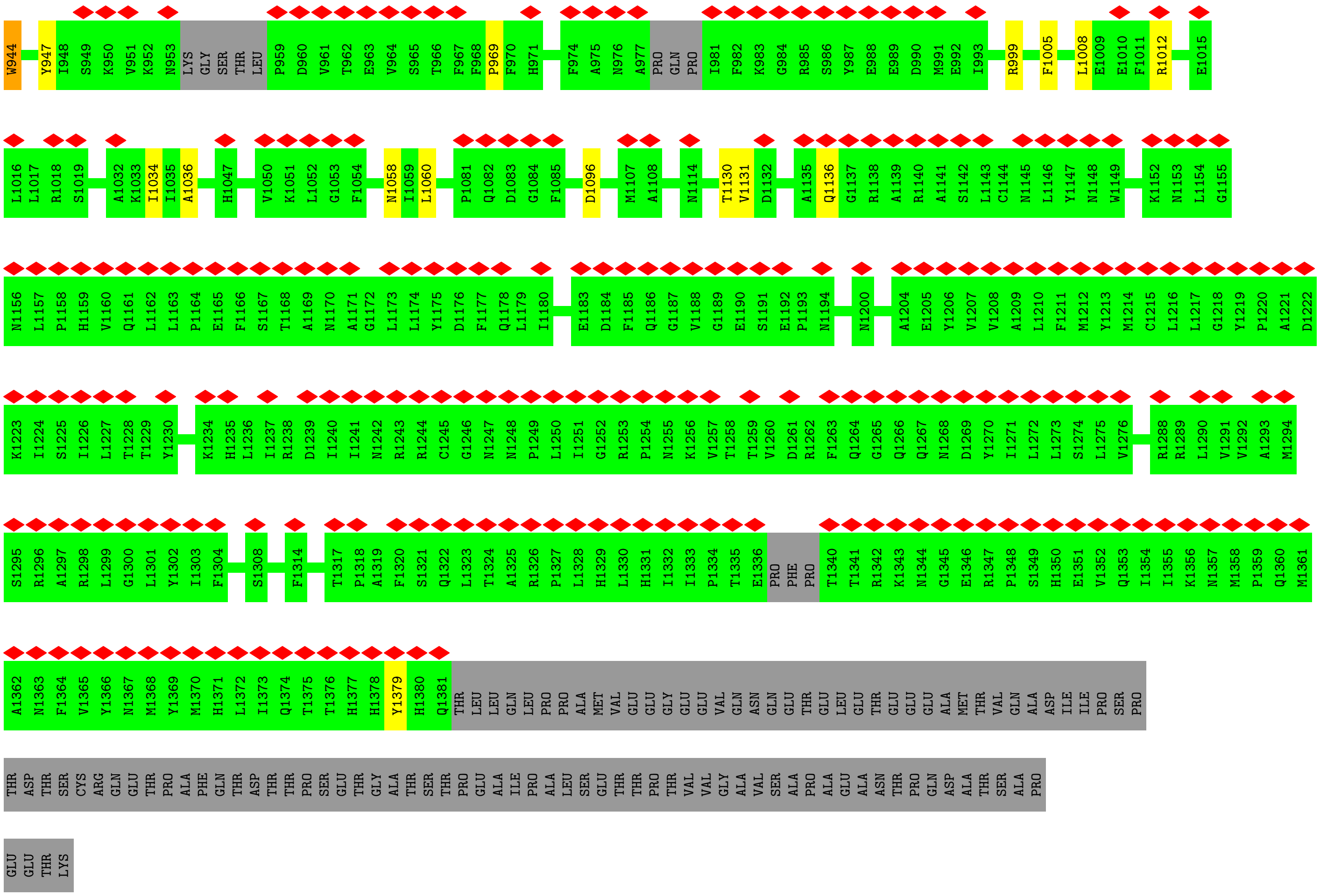




- Molecule 36: RNA helicase aquarius

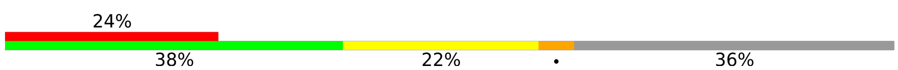
Chain Q:

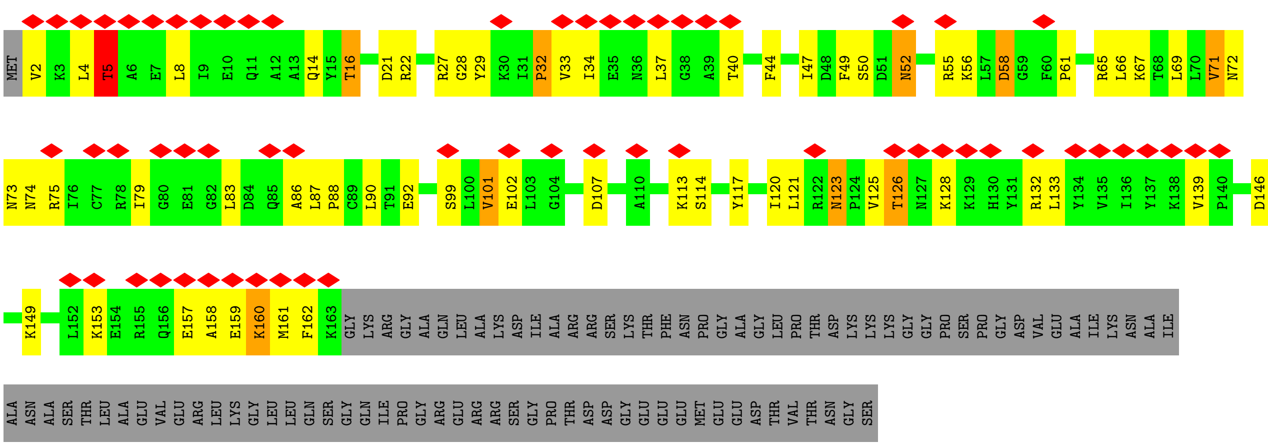




- Molecule 37: U2 small nuclear ribonucleoprotein A'

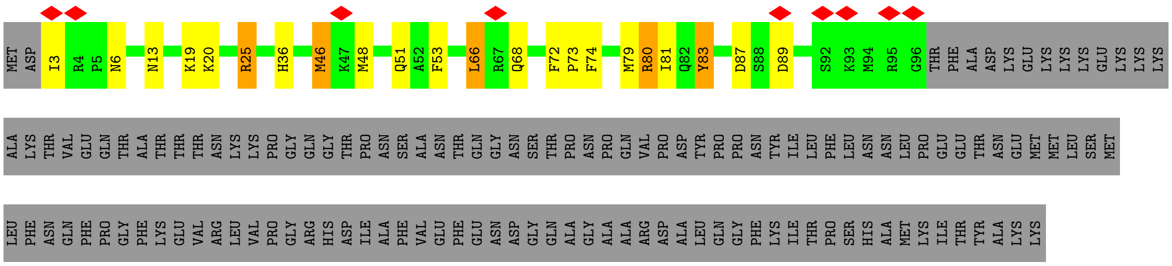
Chain o:





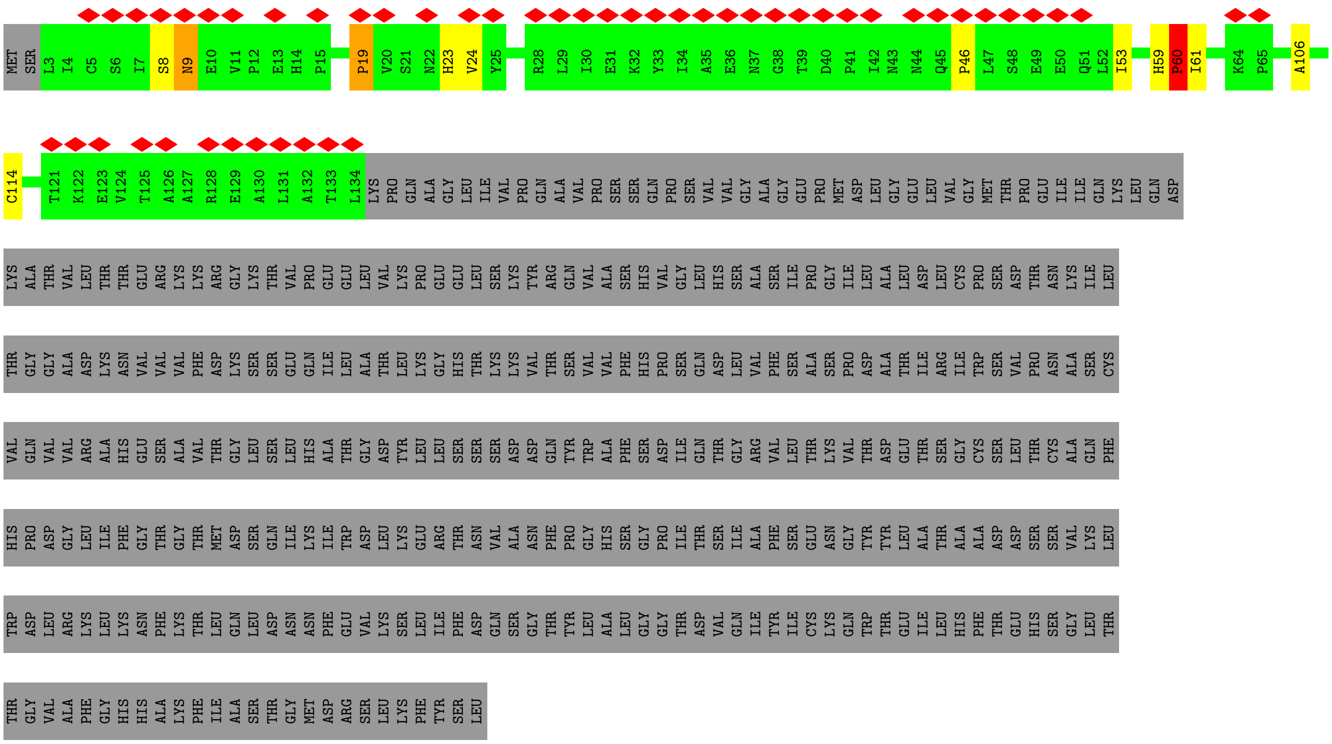
- Molecule 38: U2 small nuclear ribonucleoprotein B"

Chain p:



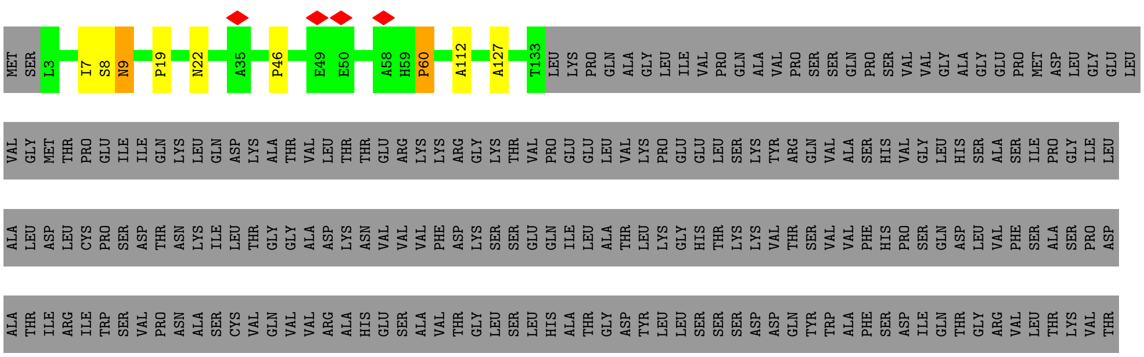
• Molecule 39: Pre-mRNA-processing factor 19

Chain q:



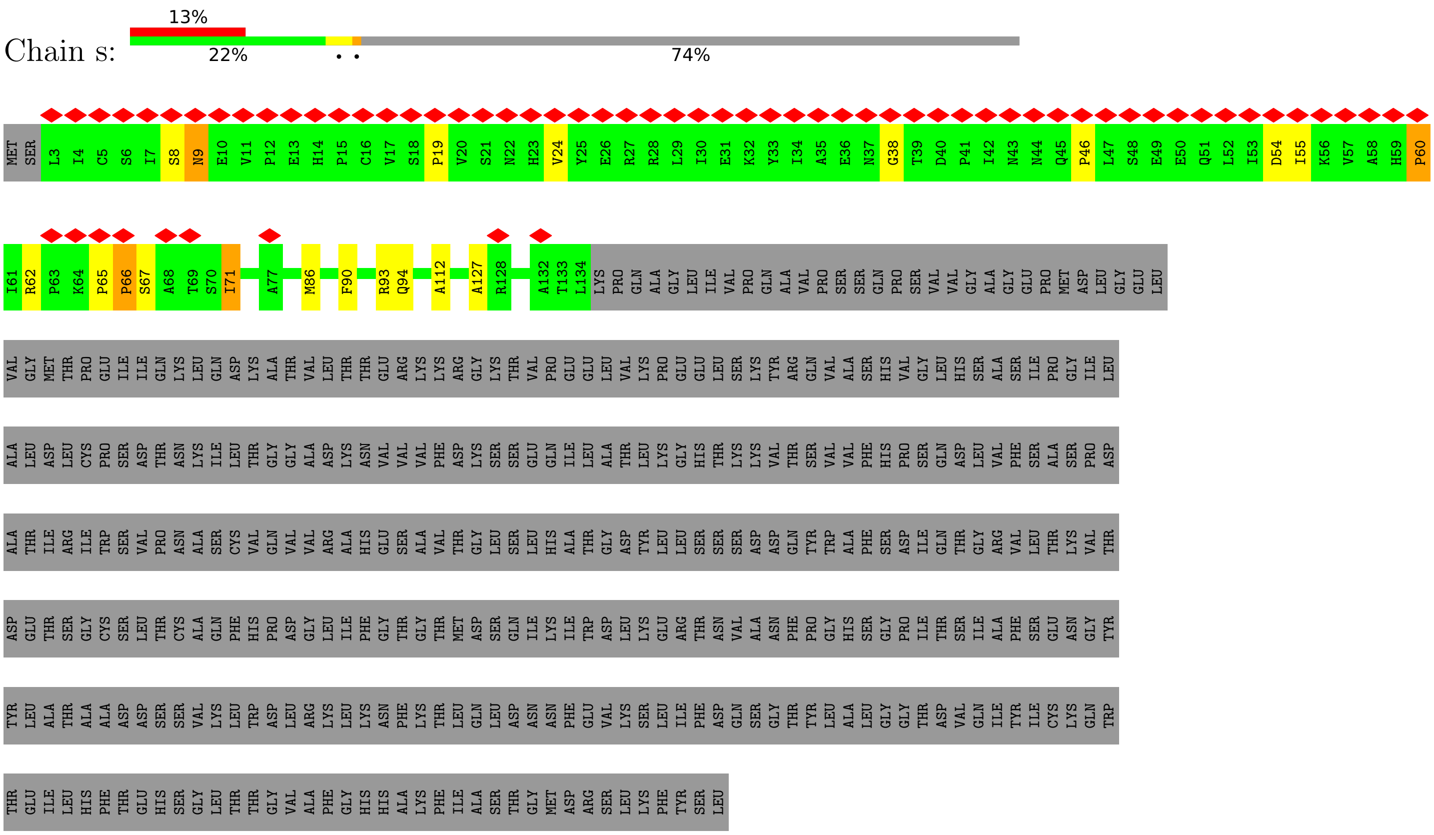
• Molecule 39: Pre-mRNA-processing factor 19

Chain r:



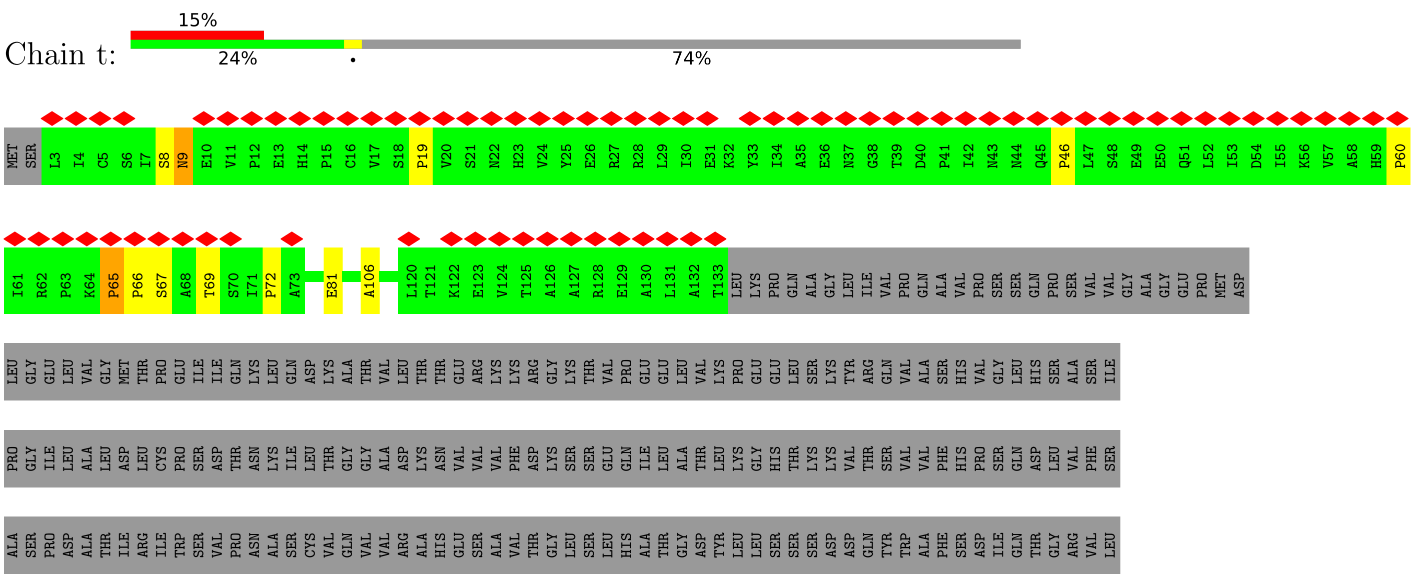
- Molecule 39: Pre-mRNA-processing factor 19

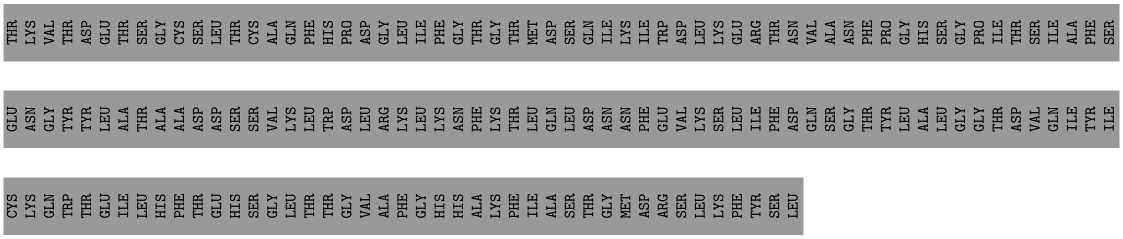
Chain s:



- Molecule 39: Pre-mRNA-processing factor 19

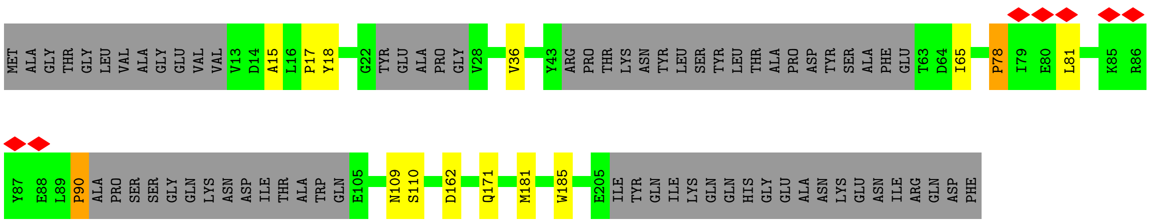
Chain t:





• Molecule 40: Pre-mRNA-splicing factor SPF27

Chain K:



4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	192274	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.470	Depositor
Minimum map value	-1.736	Depositor
Average map value	0.012	Depositor
Map value standard deviation	0.092	Depositor
Recommended contour level	0.38	Depositor
Map size (Å)	535.2, 535.2, 535.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.338, 1.338, 1.338	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, ATP, IHP, GTP, 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	0.92	74/16897 (0.4%)	1.12	132/22917 (0.6%)
2	C	0.64	6/6950 (0.1%)	0.95	28/9443 (0.3%)
3	E	0.54	0/2392	0.83	7/3242 (0.2%)
4	4	0.72	0/307	1.00	3/476 (0.6%)
5	G	0.62	2/1674 (0.1%)	1.43	39/2594 (1.5%)
6	J	0.64	7/3856 (0.2%)	0.92	21/5234 (0.4%)
7	L	0.50	0/3046	0.81	10/4115 (0.2%)
8	M	0.47	0/1119	0.78	2/1497 (0.1%)
9	N	0.78	0/1210	1.00	9/1622 (0.6%)
10	O	0.53	0/2344	0.80	2/3163 (0.1%)
11	P	0.72	1/967 (0.1%)	1.19	8/1285 (0.6%)
12	R	0.83	5/2262 (0.2%)	1.21	19/3031 (0.6%)
13	S	0.52	1/1268 (0.1%)	0.82	2/1714 (0.1%)
14	T	1.15	20/2519 (0.8%)	1.36	35/3433 (1.0%)
15	U	0.50	0/424	0.85	2/582 (0.3%)
16	V	0.42	0/2642	0.82	0/3602
17	W	0.47	0/4237	0.92	11/5723 (0.2%)
18	B	0.60	2/1970 (0.1%)	0.82	6/3060 (0.2%)
19	F	0.48	0/2323	0.82	3/3619 (0.1%)
20	H	0.85	26/3305 (0.8%)	1.41	60/5130 (1.2%)
21	b	0.77	0/797	1.05	4/1062 (0.4%)
21	i	0.73	0/700	1.03	4/933 (0.4%)
22	X	1.12	1/621 (0.2%)	2.08	17/822 (2.1%)
23	I	0.62	0/3871	1.45	30/5283 (0.6%)
24	y	0.49	0/389	1.05	0/540
25	Y	1.00	1/3436 (0.0%)	1.52	26/4774 (0.5%)
26	a	0.66	0/646	0.85	0/867
26	h	0.65	0/639	0.86	0/857
27	c	0.74	0/657	0.98	0/888
27	j	0.74	0/657	0.98	0/888
28	d	0.94	1/786 (0.1%)	1.10	2/1053 (0.2%)
28	k	0.95	0/696	1.07	1/935 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
29	f	1.04	1/588 (0.2%)	1.08	0/795
29	m	1.04	1/588 (0.2%)	1.08	0/795
30	e	0.84	0/660	1.06	1/886 (0.1%)
30	l	0.85	0/652	1.06	0/876
31	g	0.71	0/584	0.95	1/779 (0.1%)
31	n	0.70	0/544	0.96	1/725 (0.1%)
32	v	0.47	0/710	1.03	3/987 (0.3%)
33	w	0.47	0/444	1.21	4/614 (0.7%)
34	u	0.51	0/1906	1.20	13/2653 (0.5%)
35	x	0.53	0/123	1.12	0/170
36	Q	0.53	8/6565 (0.1%)	1.07	34/9143 (0.4%)
37	o	0.81	0/1299	2.05	54/1761 (3.1%)
38	p	0.77	0/774	1.71	12/1035 (1.2%)
39	q	0.62	0/658	1.04	3/919 (0.3%)
39	r	0.57	0/653	0.99	3/912 (0.3%)
39	s	0.60	0/658	1.11	4/919 (0.4%)
39	t	0.62	0/653	0.94	3/912 (0.3%)
40	K	0.56	1/768 (0.1%)	0.95	2/1067 (0.2%)
All	All	0.73	158/94434 (0.2%)	1.12	621/130332 (0.5%)

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	15
2	C	0	5
6	J	0	3
9	N	0	3
10	O	0	1
11	P	0	3
12	R	0	6
17	W	0	1
23	I	0	5
28	d	0	1
28	k	0	1
36	Q	0	1
All	All	0	45

The worst 5 of 158 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	92	PRO	N-CA	16.17	1.67	1.47
36	Q	525	PRO	N-CA	15.81	1.67	1.47
1	A	345	PRO	N-CA	15.55	1.68	1.47
14	T	191	HIS	C-N	13.26	1.49	1.33
1	A	942	PRO	C-O	-13.00	1.07	1.24

The worst 5 of 621 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	344	ASP	CA-C-N	20.68	142.03	119.28
1	A	344	ASP	C-N-CA	20.68	142.03	119.28
1	A	856	LEU	CA-C-N	17.52	155.00	121.54
1	A	856	LEU	C-N-CA	17.52	155.00	121.54
36	Q	531	TRP	CA-C-N	17.41	141.60	119.84

There are no chirality outliers.

5 of 45 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	186	GLU	Mainchain
1	A	196	ASP	Mainchain
1	A	377	GLU	Peptide
1	A	55	ASP	Peptide
1	A	73	HIS	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	16449	0	16375	659	0
2	C	6798	0	6815	184	0
3	E	2338	0	2275	81	0
4	4	276	0	142	16	0
5	G	1510	0	760	206	0
6	J	3814	0	2902	58	0
7	L	3015	0	2570	92	0
8	M	1098	0	1082	32	0
9	N	1184	0	1190	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	O	2296	0	2284	75	0
11	P	953	0	939	46	0
12	R	2243	0	2298	86	0
13	S	1236	0	1210	42	0
14	T	2454	0	2413	149	0
15	U	422	0	291	13	0
16	V	2632	0	1734	21	0
17	W	4129	0	4040	133	0
18	B	1768	0	897	66	0
19	F	2075	0	1048	182	0
20	H	2966	0	1505	279	0
21	b	786	0	811	48	0
21	i	690	0	712	15	0
22	X	616	0	605	140	0
23	I	3845	0	2729	192	0
24	y	390	0	190	12	0
25	Y	3431	0	1662	47	0
26	a	640	0	657	15	0
26	h	633	0	645	15	0
27	c	649	0	693	10	0
27	j	649	0	693	13	0
28	d	776	0	819	32	0
28	k	688	0	709	29	0
29	f	576	0	589	21	0
29	m	576	0	589	22	0
30	e	652	0	668	20	0
30	l	644	0	659	23	0
31	g	577	0	603	15	0
31	n	538	0	557	25	0
32	v	711	0	299	6	0
33	w	445	0	203	6	0
34	u	1907	0	845	5	0
35	x	124	0	51	0	0
36	Q	6562	0	2836	61	0
37	o	1282	0	1305	28	0
38	p	760	0	783	12	0
39	q	659	0	296	19	0
39	r	654	0	294	8	0
39	s	659	0	296	20	0
39	t	654	0	294	10	0
40	K	772	0	342	11	0
41	A	36	0	6	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	C	32	0	12	2	0
43	C	1	0	0	0	0
43	F	6	0	0	0	0
43	Q	2	0	0	0	0
44	N	3	0	0	0	0
44	O	3	0	0	0	0
45	Q	31	0	12	5	0
All	All	92315	0	75234	2699	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 16.

The worst 5 of 2699 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)
23:I:265:TYR:CB	23:I:274:LYS:CB	1.84	1.53
36:Q:943:ARG:CB	36:Q:969:PRO:CB	1.82	1.53
36:Q:525:PRO:N	36:Q:525:PRO:CA	1.67	1.52
1:A:345:PRO:N	1:A:345:PRO:CA	1.68	1.46
14:T:297:HIS:CE1	14:T:340:ALA:HB2	1.51	1.45

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	1980/2335 (85%)	1807 (91%)	160 (8%)	13 (1%)	19	53
2	C	856/972 (88%)	790 (92%)	64 (8%)	2 (0%)	44	73
3	E	297/357 (83%)	276 (93%)	20 (7%)	1 (0%)	37	67
6	J	529/848 (62%)	491 (93%)	31 (6%)	7 (1%)	10	41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	L	425/802 (53%)	408 (96%)	15 (4%)	2 (0%)	25	59
8	M	128/243 (53%)	117 (91%)	11 (9%)	0	100	100
9	N	141/144 (98%)	125 (89%)	14 (10%)	2 (1%)	9	40
10	O	283/420 (67%)	259 (92%)	23 (8%)	1 (0%)	30	63
11	P	107/229 (47%)	88 (82%)	16 (15%)	3 (3%)	4	27
12	R	274/536 (51%)	247 (90%)	23 (8%)	4 (2%)	8	39
13	S	157/166 (95%)	148 (94%)	9 (6%)	0	100	100
14	T	310/514 (60%)	278 (90%)	25 (8%)	7 (2%)	5	31
15	U	68/2752 (2%)	60 (88%)	8 (12%)	0	100	100
16	V	444/908 (49%)	431 (97%)	12 (3%)	1 (0%)	44	73
17	W	507/579 (88%)	433 (85%)	68 (13%)	6 (1%)	11	43
21	b	98/240 (41%)	93 (95%)	2 (2%)	3 (3%)	3	26
21	i	84/240 (35%)	82 (98%)	2 (2%)	0	100	100
22	X	67/254 (26%)	64 (96%)	3 (4%)	0	100	100
23	I	575/855 (67%)	562 (98%)	11 (2%)	2 (0%)	37	67
24	y	77/301 (26%)	74 (96%)	1 (1%)	2 (3%)	4	28
25	Y	667/1220 (55%)	642 (96%)	23 (3%)	2 (0%)	37	67
26	a	77/126 (61%)	76 (99%)	1 (1%)	0	100	100
26	h	77/126 (61%)	76 (99%)	1 (1%)	0	100	100
27	c	80/119 (67%)	77 (96%)	3 (4%)	0	100	100
27	j	80/119 (67%)	77 (96%)	3 (4%)	0	100	100
28	d	95/118 (80%)	91 (96%)	4 (4%)	0	100	100
28	k	81/118 (69%)	78 (96%)	3 (4%)	0	100	100
29	f	72/86 (84%)	69 (96%)	3 (4%)	0	100	100
29	m	72/86 (84%)	69 (96%)	3 (4%)	0	100	100
30	e	77/92 (84%)	76 (99%)	1 (1%)	0	100	100
30	l	76/92 (83%)	75 (99%)	1 (1%)	0	100	100
31	g	72/76 (95%)	70 (97%)	2 (3%)	0	100	100
31	n	65/76 (86%)	63 (97%)	2 (3%)	0	100	100
32	v	142/146 (97%)	138 (97%)	4 (3%)	0	100	100
33	w	89/174 (51%)	87 (98%)	1 (1%)	1 (1%)	12	45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	u	384/411 (93%)	372 (97%)	9 (2%)	3 (1%)	16	51
35	x	23/703 (3%)	22 (96%)	1 (4%)	0	100	100
36	Q	1308/1485 (88%)	1278 (98%)	27 (2%)	3 (0%)	44	73
37	o	160/255 (63%)	146 (91%)	12 (8%)	2 (1%)	10	41
38	p	92/225 (41%)	90 (98%)	2 (2%)	0	100	100
39	q	130/504 (26%)	117 (90%)	7 (5%)	6 (5%)	2	18
39	r	129/504 (26%)	118 (92%)	9 (7%)	2 (2%)	8	38
39	s	130/504 (26%)	114 (88%)	8 (6%)	8 (6%)	1	13
39	t	129/504 (26%)	116 (90%)	9 (7%)	4 (3%)	3	26
40	K	147/225 (65%)	139 (95%)	5 (3%)	3 (2%)	6	34
All	All	11861/21789 (54%)	11109 (94%)	662 (6%)	90 (1%)	19	51

5 of 90 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	167	PRO
1	A	857	ASN
1	A	942	PRO
1	A	1831	LYS
6	J	217	GLU

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	1780/2108 (84%)	1705 (96%)	75 (4%)	25	54
2	C	761/866 (88%)	746 (98%)	15 (2%)	50	72
3	E	256/300 (85%)	254 (99%)	2 (1%)	79	88
6	J	241/751 (32%)	236 (98%)	5 (2%)	48	71
7	L	218/709 (31%)	211 (97%)	7 (3%)	34	61
8	M	117/209 (56%)	116 (99%)	1 (1%)	75	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	N	130/130 (100%)	122 (94%)	8 (6%)	15	44
10	O	255/361 (71%)	253 (99%)	2 (1%)	79	88
11	P	101/203 (50%)	96 (95%)	5 (5%)	20	49
12	R	236/457 (52%)	213 (90%)	23 (10%)	6	29
13	S	129/134 (96%)	127 (98%)	2 (2%)	58	76
14	T	268/441 (61%)	250 (93%)	18 (7%)	13	41
15	U	21/2432 (1%)	19 (90%)	2 (10%)	7	30
16	V	98/838 (12%)	95 (97%)	3 (3%)	35	62
17	W	448/502 (89%)	435 (97%)	13 (3%)	37	63
21	b	83/177 (47%)	80 (96%)	3 (4%)	30	59
21	i	77/177 (44%)	74 (96%)	3 (4%)	27	57
22	X	68/230 (30%)	45 (66%)	23 (34%)	0	1
23	I	198/749 (26%)	183 (92%)	15 (8%)	11	37
25	Y	32/1085 (3%)	26 (81%)	6 (19%)	1	8
26	a	72/101 (71%)	72 (100%)	0	100	100
26	h	70/101 (69%)	70 (100%)	0	100	100
27	c	77/101 (76%)	75 (97%)	2 (3%)	41	65
27	j	77/101 (76%)	75 (97%)	2 (3%)	41	65
28	d	90/110 (82%)	89 (99%)	1 (1%)	70	83
28	k	80/110 (73%)	79 (99%)	1 (1%)	65	81
29	f	63/74 (85%)	61 (97%)	2 (3%)	34	61
29	m	63/74 (85%)	61 (97%)	2 (3%)	34	61
30	e	74/84 (88%)	74 (100%)	0	100	100
30	l	73/84 (87%)	73 (100%)	0	100	100
31	g	64/66 (97%)	63 (98%)	1 (2%)	58	76
31	n	59/66 (89%)	58 (98%)	1 (2%)	56	75
37	o	139/218 (64%)	133 (96%)	6 (4%)	25	54
38	p	82/195 (42%)	79 (96%)	3 (4%)	29	58
All	All	6600/14344 (46%)	6348 (96%)	252 (4%)	30	57

5 of 252 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	P	3	THR
23	I	733	THR
13	S	37	LYS
23	I	730	VAL
21	i	58	GLN

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

Mol	Chain	Res	Type
6	J	275	ASN
31	g	65	ASN
12	R	133	GLN
30	e	65	HIS
31	n	65	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
18	B	82/117 (70%)	17 (20%)	4 (4%)
19	F	96/107 (89%)	46 (47%)	16 (16%)
20	H	133/188 (70%)	34 (25%)	10 (7%)
4	4	13/46 (28%)	8 (61%)	3 (23%)
5	G	80/174 (45%)	63 (78%)	19 (23%)
All	All	404/632 (63%)	168 (41%)	52 (12%)

5 of 168 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	4	-12	G
4	4	-11	G
4	4	-10	C
4	4	-9	C
4	4	-7	C

5 of 52 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
19	F	25	C
19	F	50	A
20	H	156	U
19	F	26	U

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Mol	Chain	Res	Type
19	F	35	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	$\#\|Z\| > 2$
12	SEP	R	224	12	8,9,10	1.69	3 (37%)	8,12,14	2.06	3 (37%)
12	SEP	R	232	12	8,9,10	1.55	1 (12%)	8,12,14	1.71	2 (25%)

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
12	SEP	R	224	12	-	0/5/8/10	-
12	SEP	R	232	12	-	1/5/8/10	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	R	232	SEP	P-O1P	3.39	1.61	1.50
12	R	224	SEP	P-OG	-2.84	1.51	1.60
12	R	224	SEP	CB-CA	-2.13	1.45	1.52
12	R	224	SEP	P-O2P	-2.05	1.46	1.54

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	R	224	SEP	OG-CB-CA	-4.52	103.74	108.14
12	R	232	SEP	P-OG-CB	-4.07	107.09	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	R	232	SEP	OG-CB-CA	2.34	110.42	108.14
12	R	224	SEP	O3P-P-O2P	2.30	116.42	107.64
12	R	224	SEP	O3P-P-OG	-2.14	101.03	106.73

There are no chirality outliers.

All (1) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
42	GTP	C	1500	43	26,34,34	1.50	3 (11%)	32,54,54	1.95	7 (21%)
45	ATP	Q	1501	43	26,33,33	1.72	8 (30%)	31,52,52	1.85	10 (32%)
41	IHP	A	3000	-	36,36,36	0.72	0	54,60,60	1.05	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
42	GTP	C	1500	43	-	1/18/38/38	0/3/3/3
45	ATP	Q	1501	43	-	4/18/38/38	0/3/3/3
41	IHP	A	3000	-	-	3/30/54/54	0/1/1/1

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	C	1500	GTP	C5-C6	-4.84	1.37	1.47
45	Q	1501	ATP	C2'-C1'	-3.63	1.48	1.53
45	Q	1501	ATP	C4-N3	3.47	1.40	1.35
45	Q	1501	ATP	C6-N6	3.34	1.46	1.34
45	Q	1501	ATP	C2'-C3'	-2.76	1.45	1.53

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	C	1500	GTP	PA-O3A-PB	-5.63	113.49	132.83
45	Q	1501	ATP	PB-O3B-PG	-5.46	114.08	132.83
42	C	1500	GTP	PB-O3B-PG	-4.37	117.82	132.83
45	Q	1501	ATP	N3-C2-N1	-4.17	122.16	128.68
42	C	1500	GTP	C5-C6-N1	3.72	120.52	113.95

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
41	A	3000	IHP	C3-O13-P3-O43
42	C	1500	GTP	O4'-C4'-C5'-O5'
45	Q	1501	ATP	C5'-O5'-PA-O1A
45	Q	1501	ATP	C5'-O5'-PA-O2A
41	A	3000	IHP	C3-C4-O14-P4

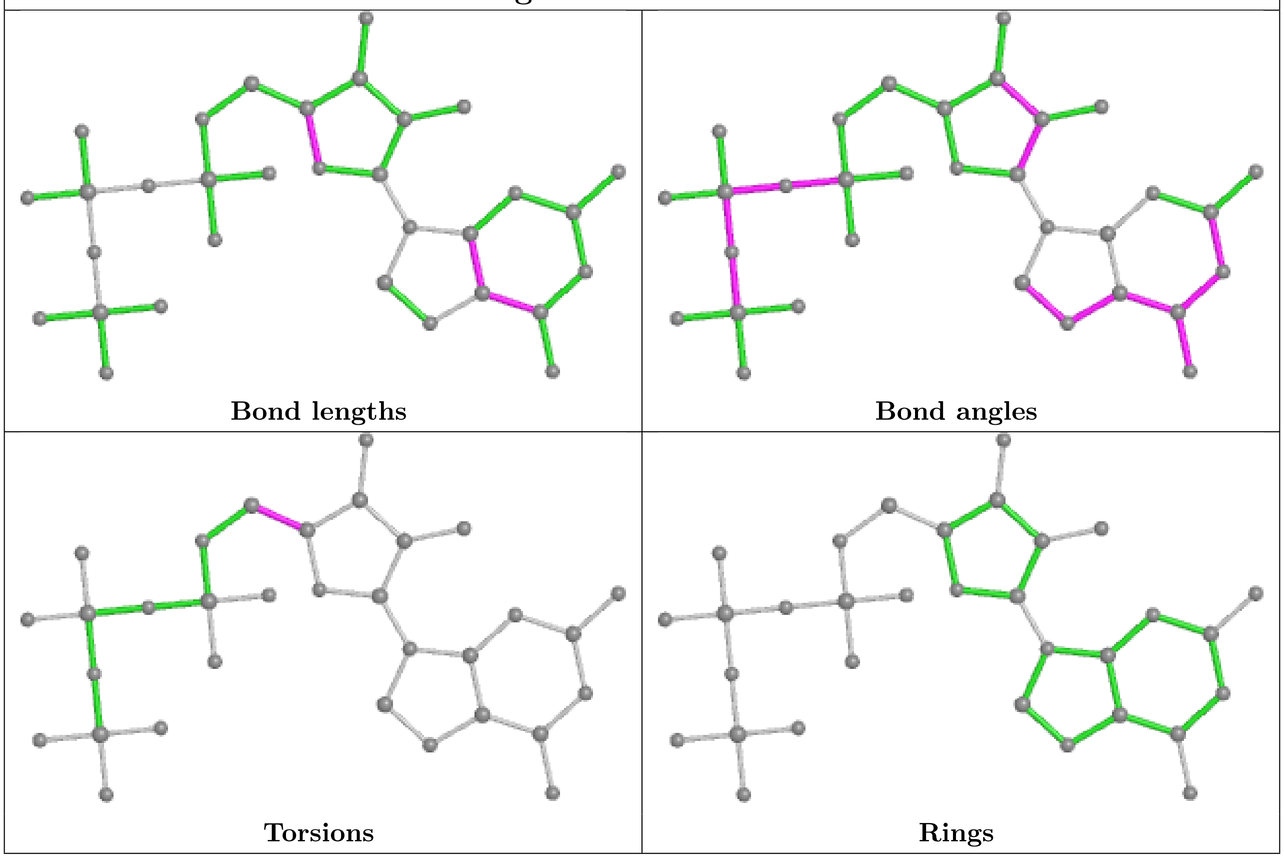
There are no ring outliers.

3 monomers are involved in 16 short contacts:

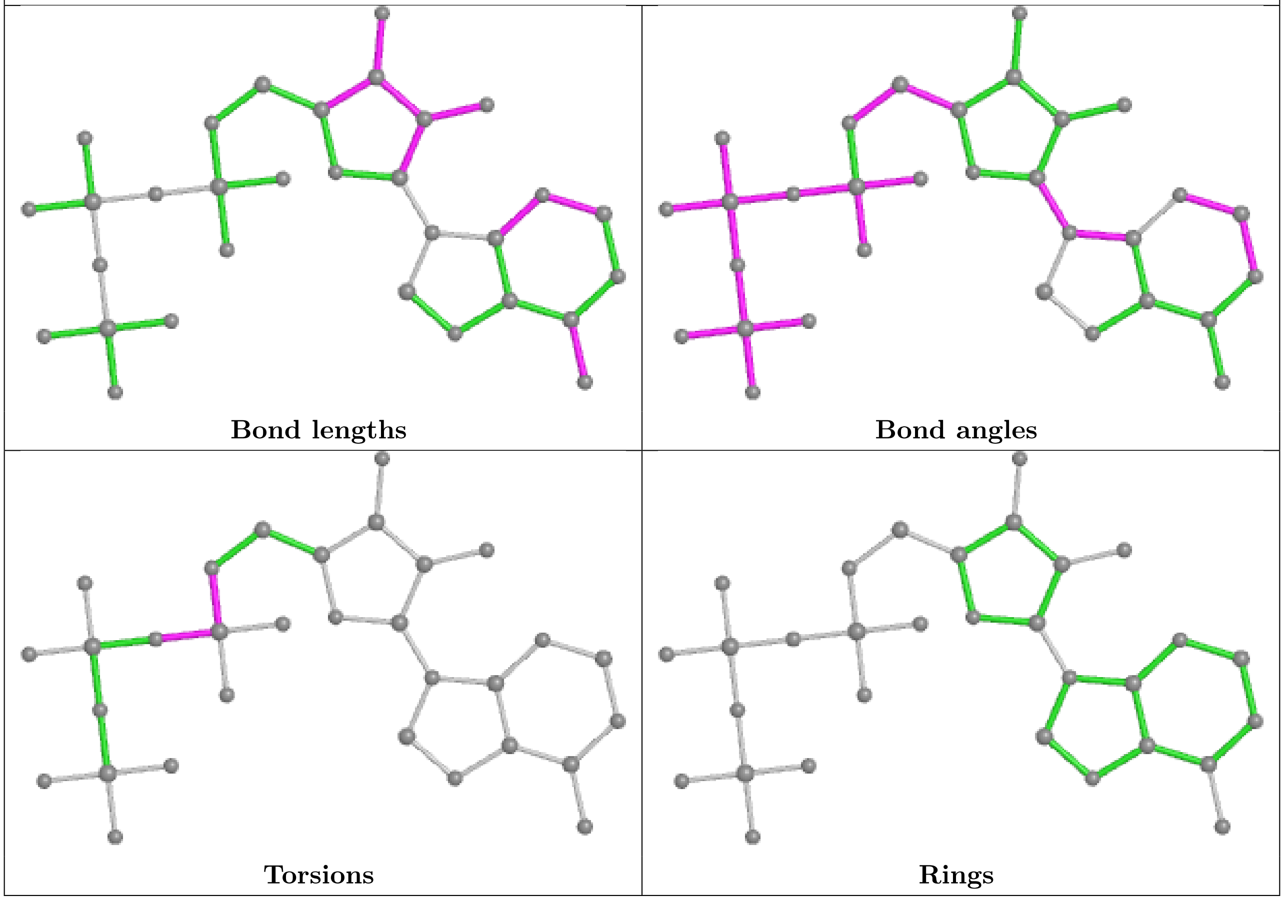
Mol	Chain	Res	Type	Clashes	Symm-Clashes
42	C	1500	GTP	2	0
45	Q	1501	ATP	5	0
41	A	3000	IHP	9	0

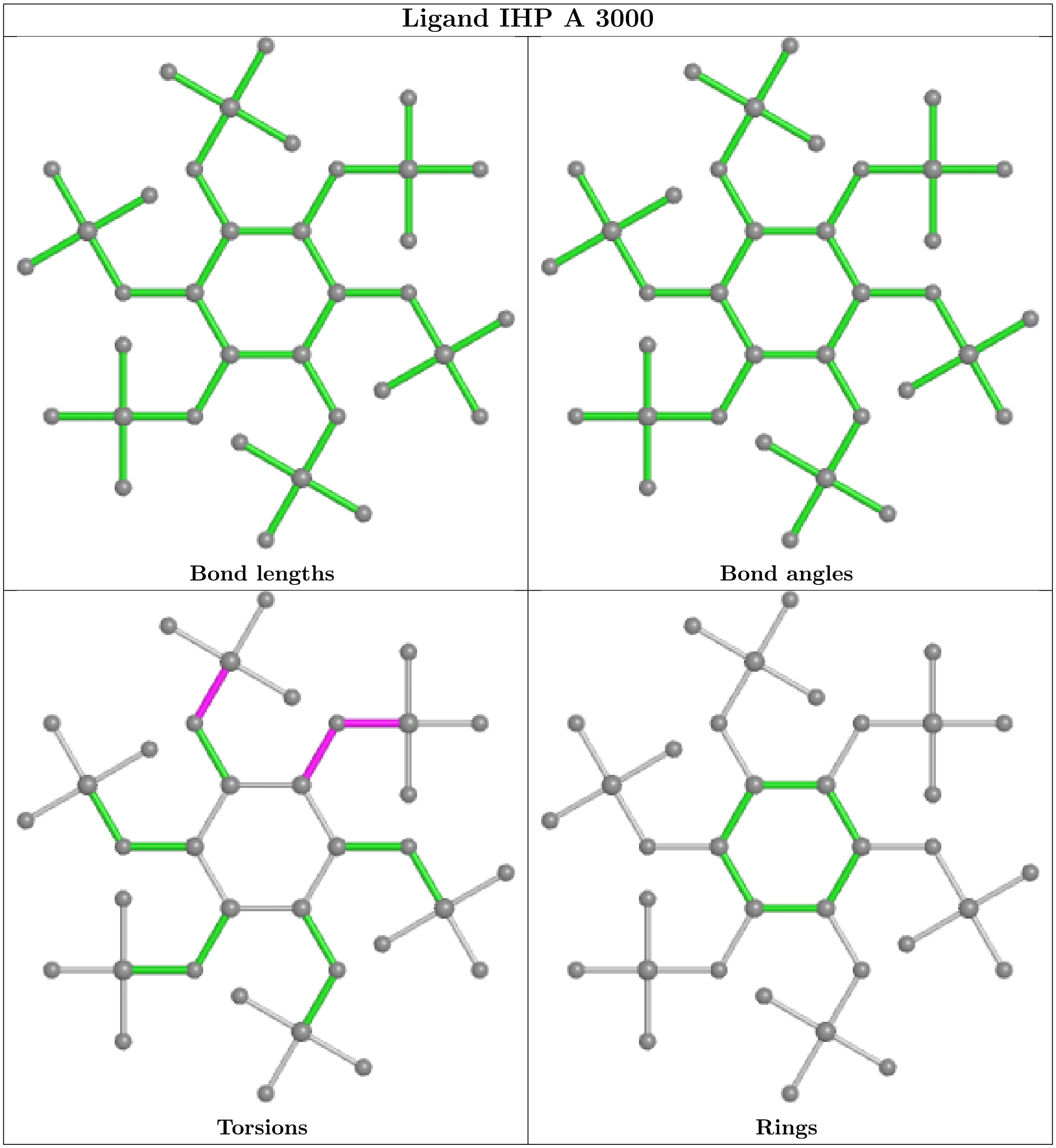
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand GTP C 1500



Ligand ATP Q 1501





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.

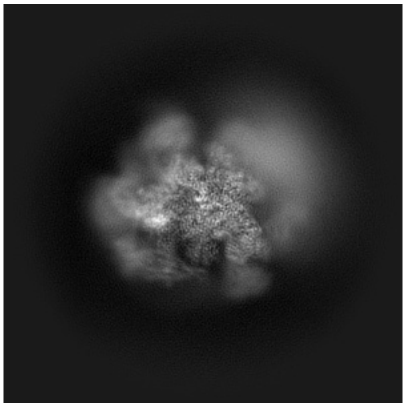
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-32317. These allow visual inspection of the internal detail of the map and identification of artifacts.

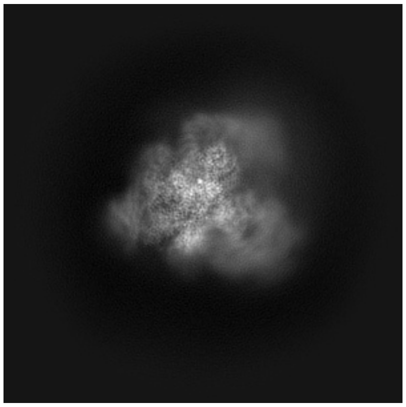
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

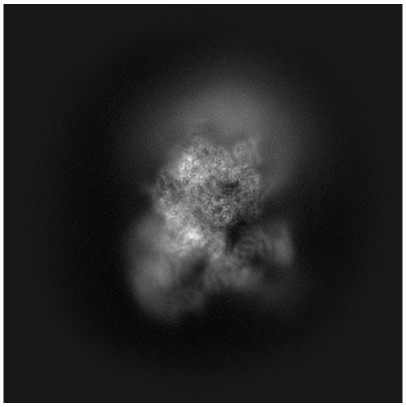
6.1.1 Primary map



X



Y

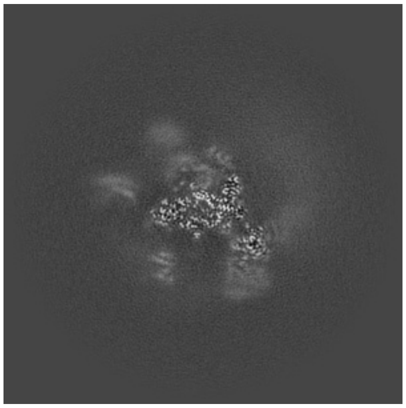


Z

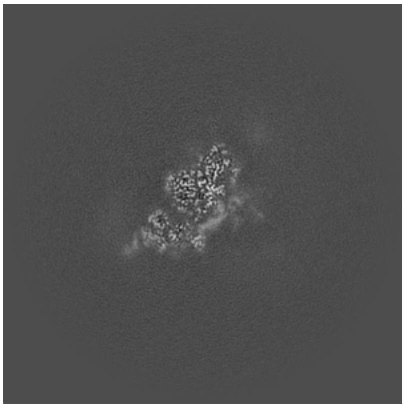
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map



X Index: 200



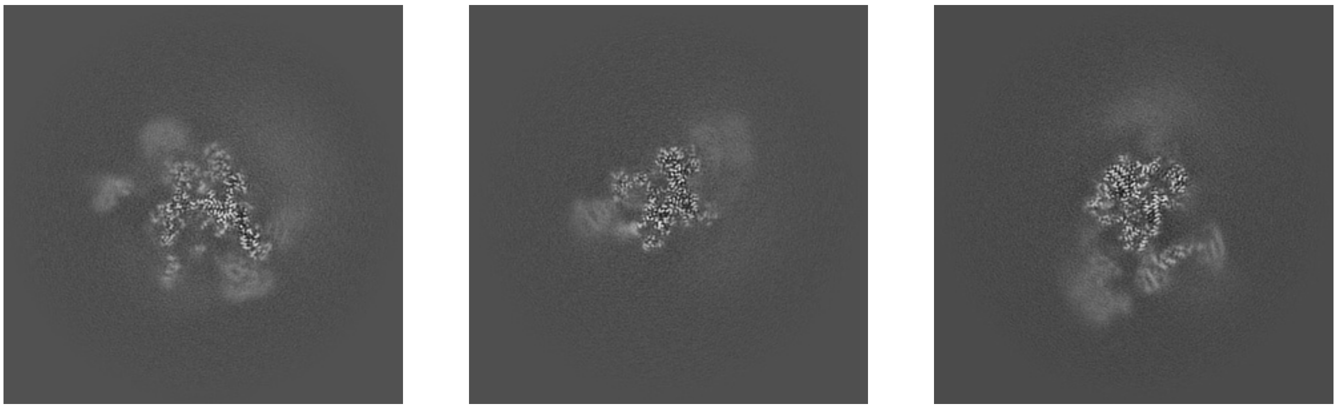
Y Index: 200

Z Index: 200

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

6.3 Largest variance slices

6.3.1 Primary map

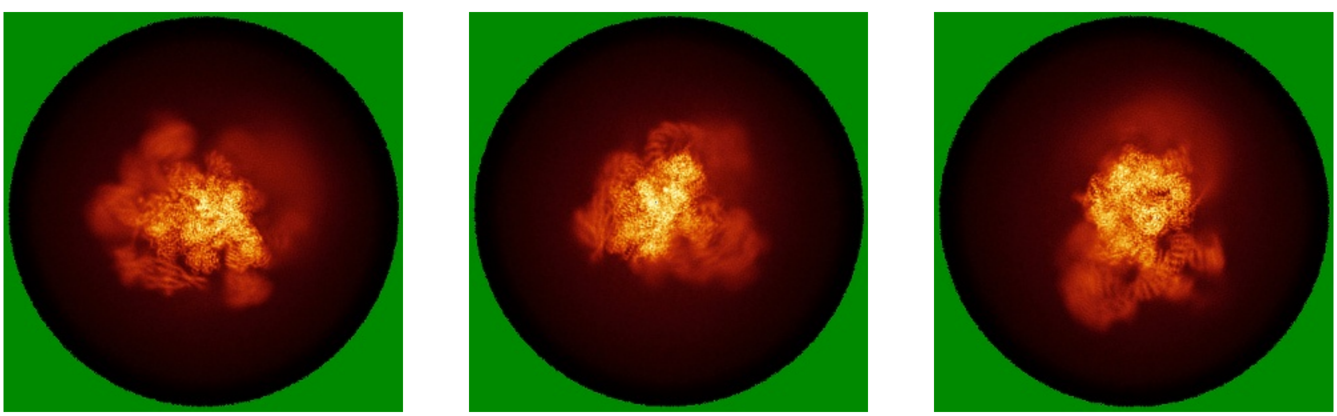


X Index: 193 Y Index: 227 Z Index: 197

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

6.4 Orthogonal standard-deviation projections (False-color)

6.4.1 Primary map



X Y Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.38. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

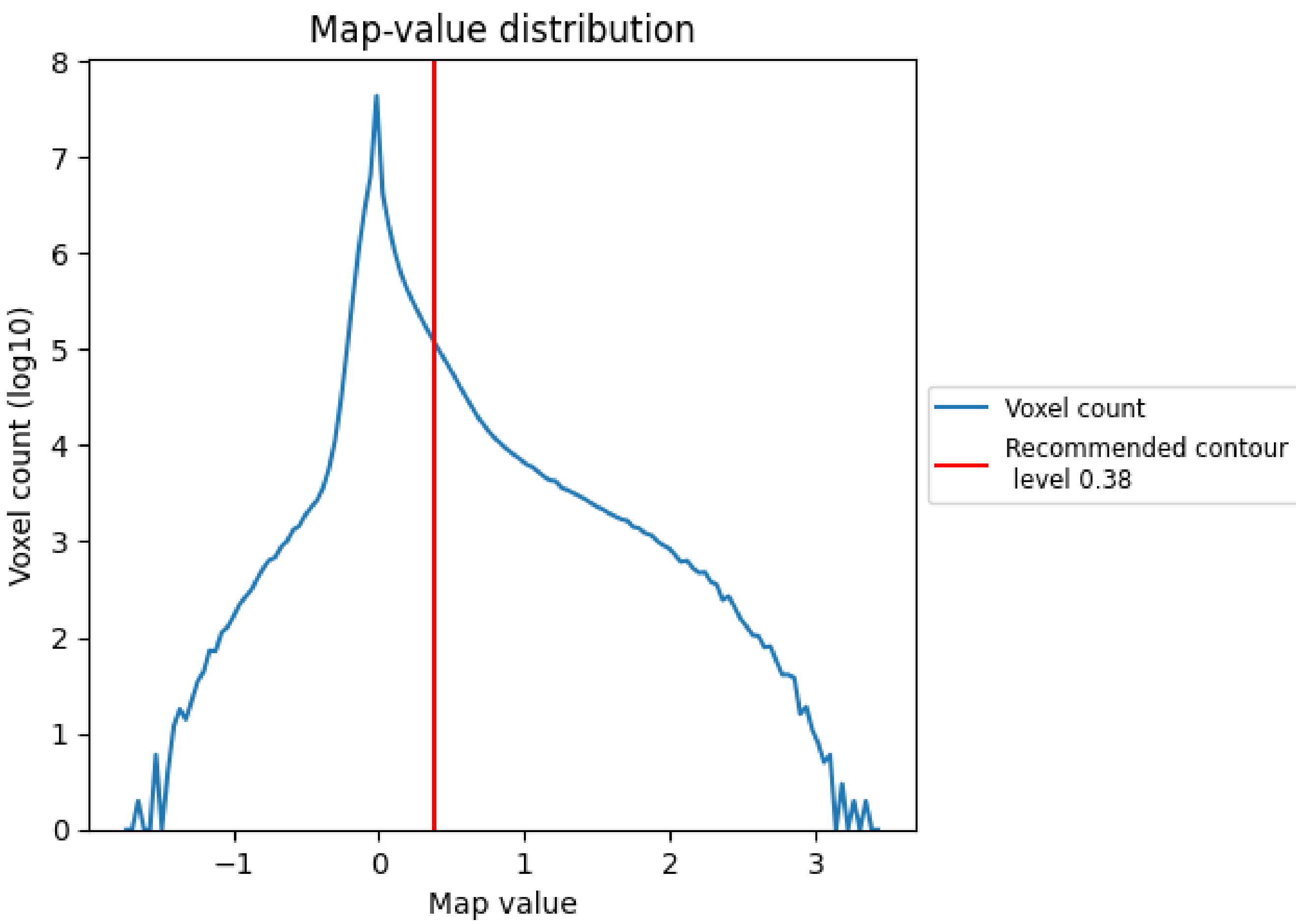
6.6 Mask visualisation (i)

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

7 Map analysis (i)

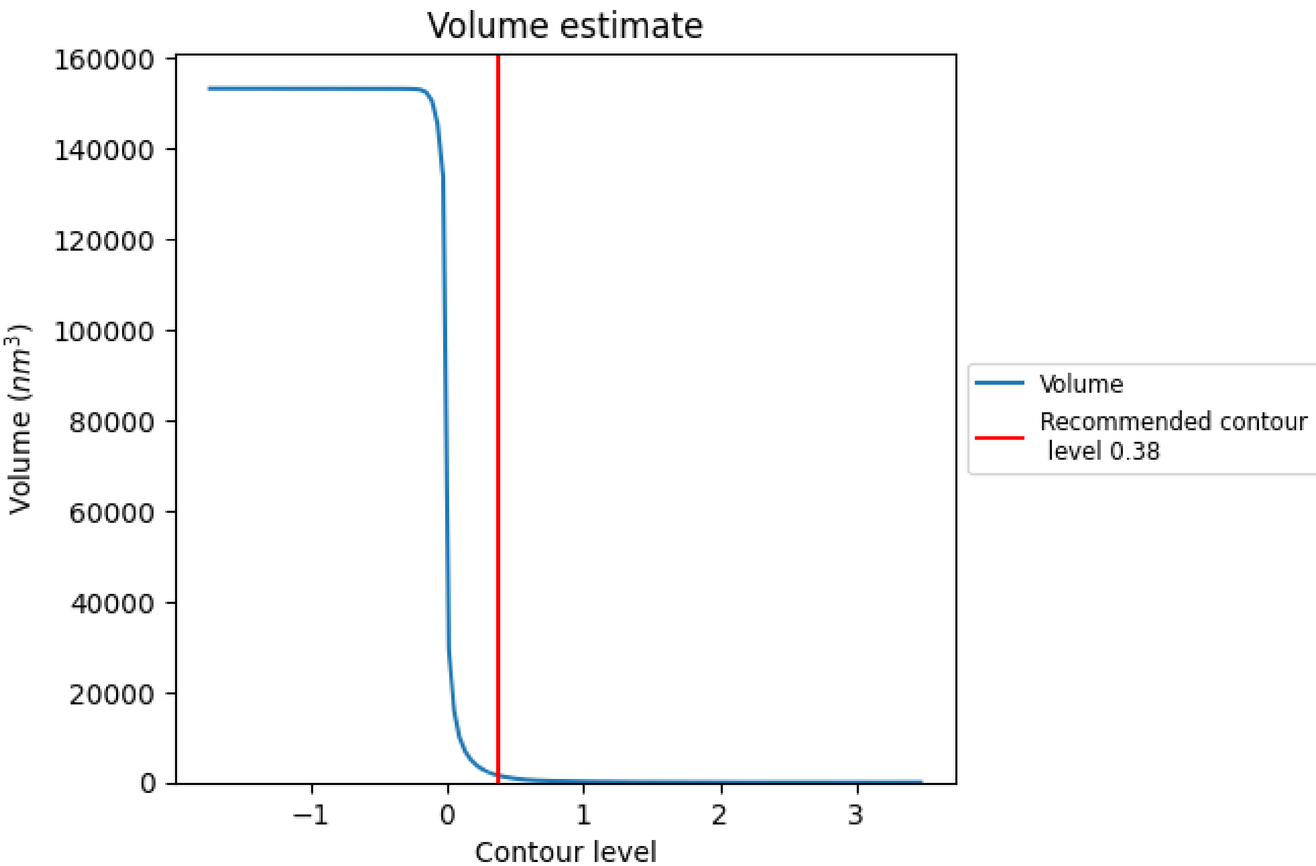
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

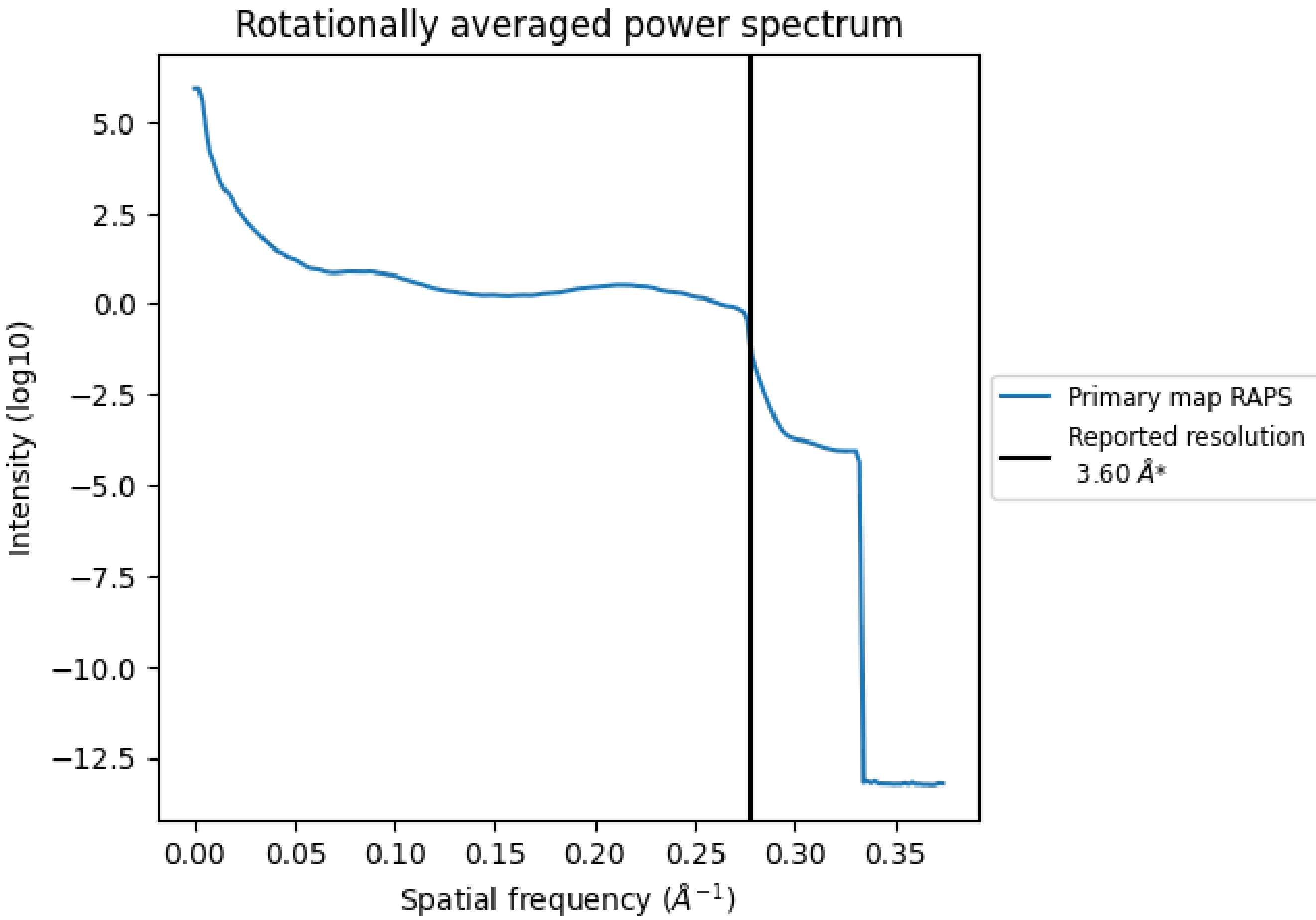
7.2 Volume estimate (i)



The volume at the recommended contour level is 1511 nm^3; this corresponds to an approximate mass of 1365 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}

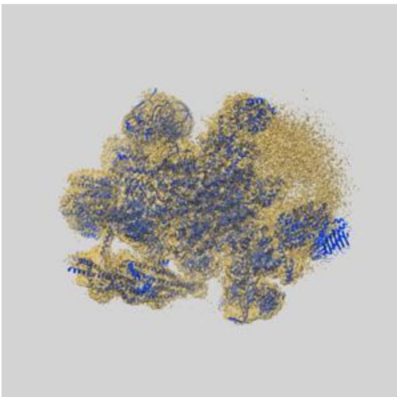
8 Fourier-Shell correlation (i)

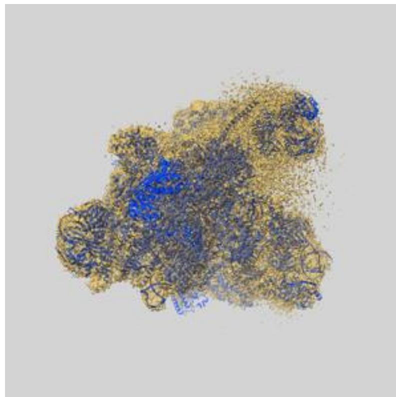
This section was not generated. No FSC curve or half-maps provided.

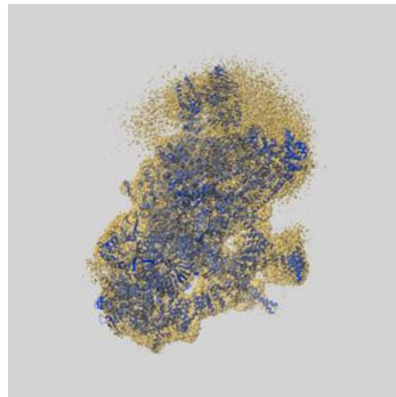
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-32317 and PDB model 7W59. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay (i)

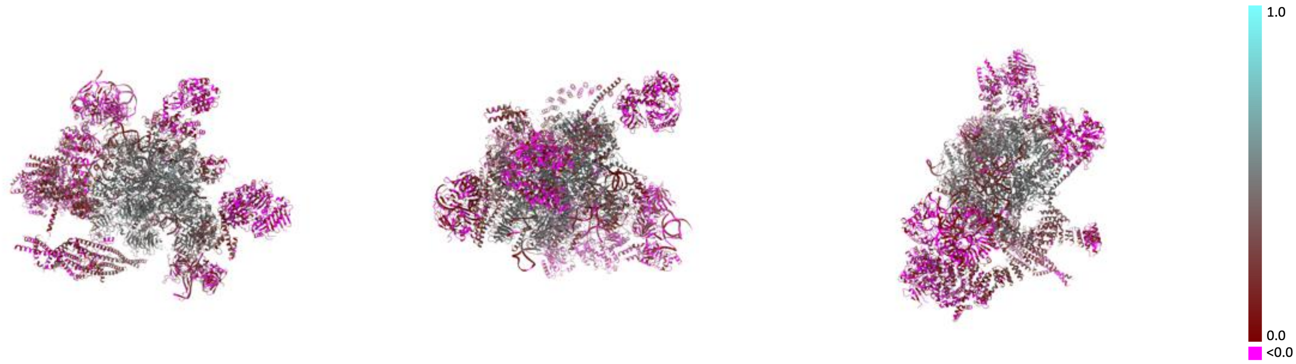

X


Y


Z

The images above show the 3D surface view of the map at the recommended contour level 0.38 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

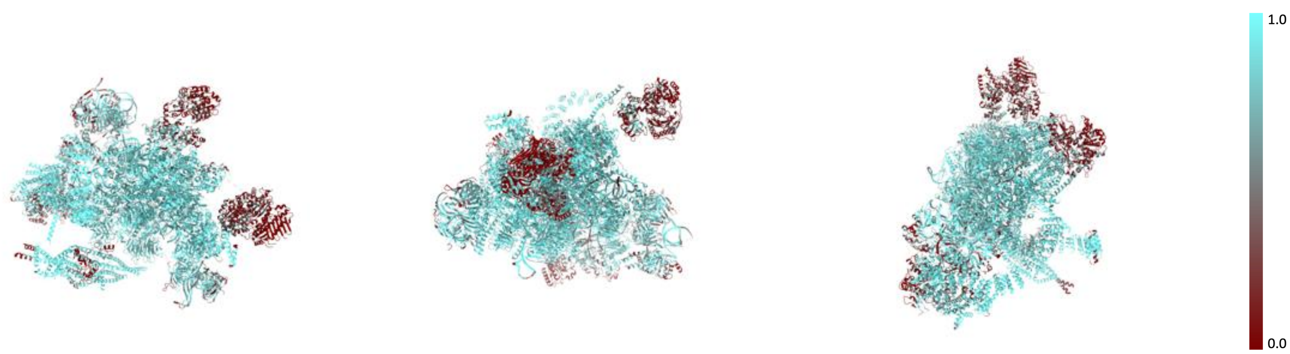
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

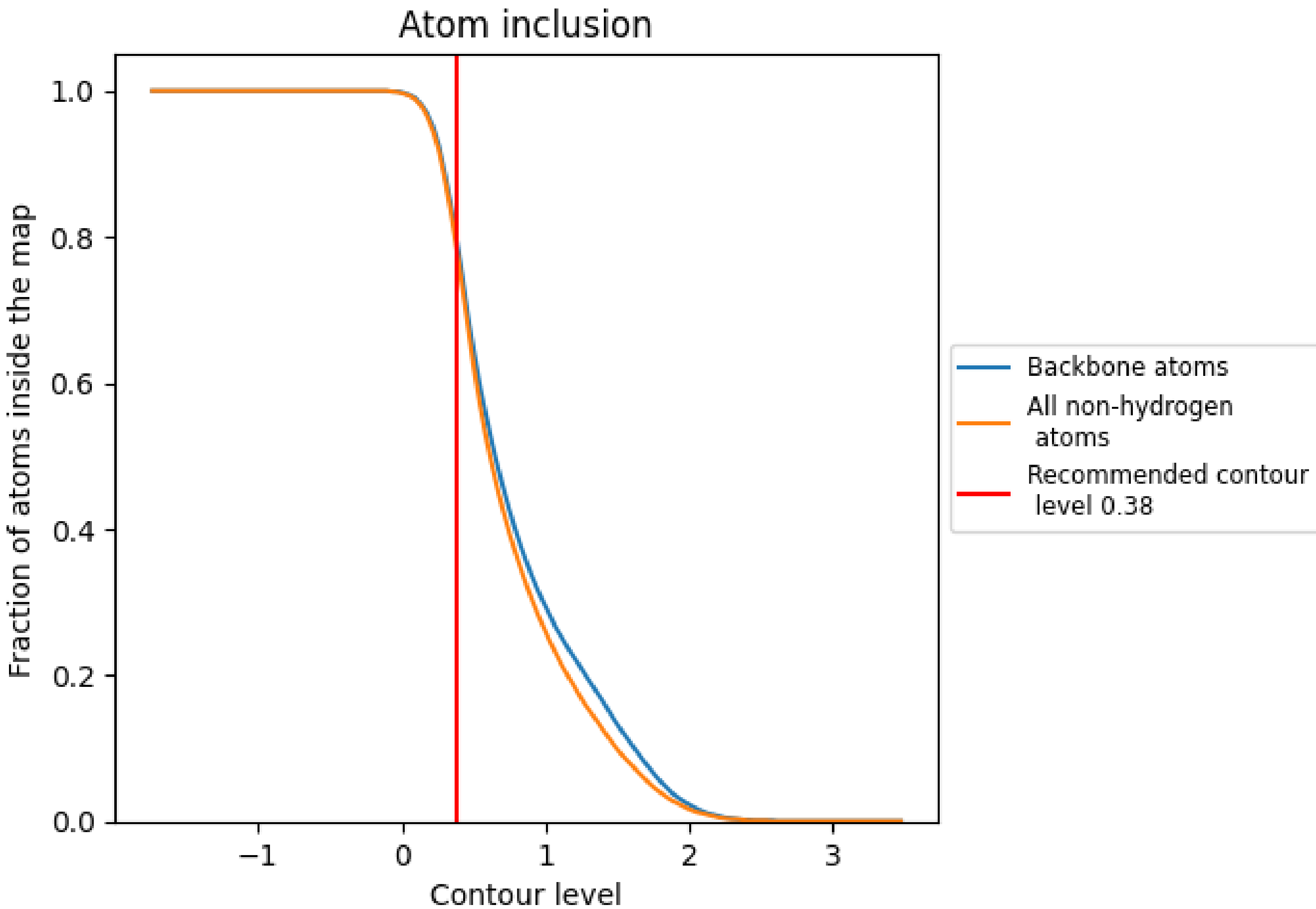
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.38).

9.4 Atom inclusion (i)



At the recommended contour level, 80% of all backbone atoms, 78% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.38) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7840	0.2680
4	0.9930	0.4660
A	0.9080	0.4360
B	0.9410	0.3070
C	0.9120	0.4070
E	0.9420	0.4320
F	0.9510	0.3510
G	0.7400	0.1590
H	0.7980	0.1190
I	0.9150	0.2190
J	0.9070	0.3200
K	0.9470	0.1950
L	0.8990	0.3480
M	0.8760	0.4000
N	0.9380	0.4560
O	0.8940	0.3870
P	0.8340	0.4200
Q	0.5800	0.0360
R	0.8750	0.4190
S	0.9270	0.4120
T	0.9660	0.5060
U	0.8800	0.3190
V	0.5730	0.1630
W	0.8580	0.3230
X	0.9320	0.4390
Y	0.2980	0.0460
a	0.7690	0.1890
b	0.7540	0.1470
c	0.8630	0.0820
d	0.7680	0.0280
e	0.6850	0.1080
f	0.7670	0.0650
g	0.5850	0.0950
h	0.7070	0.0390
i	0.5380	0.0180

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Chain	Atom inclusion	Q-score
j	0.6140	0.0150
k	0.6200	0.0240
l	0.7020	0.0070
m	0.7990	0.0160
n	0.7580	0.0690
o	0.5350	0.0260
p	0.7860	0.0300
q	0.6090	0.0490
r	0.9330	0.1960
s	0.4960	0.1310
t	0.4140	0.0610
u	0.1990	0.0220
v	0.0070	-0.0000
w	0.0130	-0.0170
x	0.0650	0.0020
y	0.8000	0.1020