



wwPDB EM Validation Summary Report ⓘ

Mar 27, 2026 – 10:43 AM UTC

PDB ID : 6QDV / pdb_00006qdv
EMDB ID : EMD-4525
Title : Human post-catalytic P complex spliceosome
Authors : Fica, S.M.; Oubridge, C.; Wilkinson, M.E.; Newman, A.J.; Nagai, K.
Deposited on : 2019-01-03
Resolution : 3.30 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

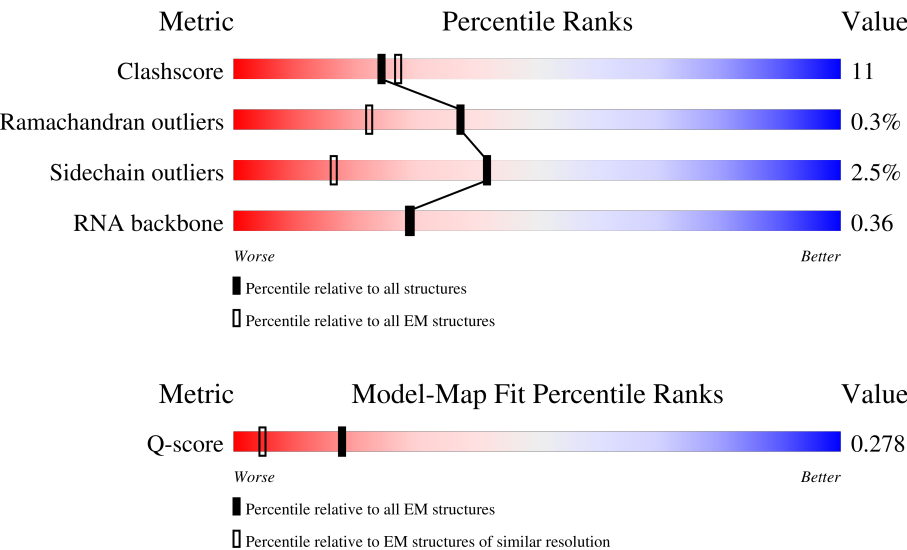
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 3.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	15087 (2.80 - 3.80)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	2	189	38% 35%23%5%37%
2	5	116	9% 35%23%6%35%
3	6	106	12% 38%42%11%8%

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Mol	Chain	Length	Quality of chain
4	7	390	
5	8	91	
6	9	144	
7	A	2335	
8	B	1722	
9	C	899	
10	D	123	
11	E	14	
12	F	122	
13	G	60	
14	H	908	
15	I	113	
16	J	320	
17	K	295	
18	L	144	
19	M	289	
20	N	306	
21	O	802	
22	P	229	
23	R	26	
24	S	848	
25	T	855	
26	U	1485	
27	V	1220	
28	W	162	

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Mol	Chain	Length	Quality of chain
29	Y	92	
30	Z	30	
31	b	82	
31	k	82	
32	c	586	
33	d	84	
33	n	84	
34	e	81	
34	p	81	
35	f	72	
35	q	72	
36	g	73	
36	r	73	
37	h	80	
37	l	80	
38	i	164	
39	j	118	
39	m	118	
40	o	513	
41	s	225	
42	t	504	
42	u	504	
42	v	504	
42	w	504	
43	y	144	

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Mol	Chain	Length	Quality of chain
44	z	34	100% 82% 18%

2 Entry composition

There are 50 unique types of molecules in this entry. The entry contains 121152 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	120	Total	C	N	O	P	0	0
			2535	1135	428	852	120		

- Molecule 2 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	5	75	Total	C	N	O	P	0	0
			1579	708	264	532	75		

- Molecule 3 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	6	97	Total	C	N	O	P	0	0
			2075	928	381	669	97		

- Molecule 4 is a protein called Eukaryotic initiation factor 4A-III, N-terminally processed.

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

- Molecule 5 is a protein called RNA-binding protein 8A.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	8	91	Total	C	N	O	S	0	0
			730	463	122	142	3		

- Molecule 6 is a protein called Protein mago nashi homolog 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	9	144	Total	C	N	O	S	0	0
			1196	772	200	221	3		

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	SER	deletion	UNP Q15029

- Molecule 10 is a protein called PRKR-interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D	123	Total	C	N	O	S	0	0
			1013	635	193	180	5		

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

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

- Molecule 12 is a protein called Cactin.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	654	ALA	GLU	conflict	UNP Q8WUQ7

- Molecule 13 is a protein called Protein FAM32A.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G	60	Total	C	N	O	S	0	0
			504	314	96	92	2		

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

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

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

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

- Molecule 16 is a protein called Pleiotropic regulator 1.

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

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

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

- Molecule 18 is a protein called Protein BUD31 homolog.

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	143	ALA	THR	conflict	UNP Q9NW64
M	144	ALA	SER	conflict	UNP Q9NW64
M	145	ALA	ASP	conflict	UNP Q9NW64
M	146	ALA	MET	conflict	UNP Q9NW64

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	N	306	Total	C	N	O	S	0	0
			2394	1501	422	457	14		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	?	-	ALA	deletion	UNP Q96DI7

- Molecule 21 is a protein called Cell division cycle 5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	O	441	Total	C	N	O	S	0	0
			3416	2116	648	639	13		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Y	92	Total	C	N	O	S	0	0
			745	480	130	130	5		

- Molecule 30 is a protein called NF-kappa-B-activating protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Z	30	Total	C	N	O	S	0	0
			230	140	43	45	2		

- Molecule 31 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	b	68	Total	C	N	O	S	0	0
			545	347	95	96	7		
31	k	82	Total	C	N	O	S	0	0
			664	419	121	117	7		

- Molecule 32 is a protein called Pre-mRNA-splicing factor SLU7.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	c	269	Total	C	N	O	S	0	0
			2215	1392	397	418	8		

- Molecule 33 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	d	84	Total	C	N	O	S	0	0
			658	412	116	124	6		
33	n	83	Total	C	N	O	S	0	0
			652	409	115	122	6		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms					AltConf	Trace
42	w	118	Total	C	N	O	S	0	0
			938	586	167	181	4		

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

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

- Molecule 44 is a protein called Replication stress response regulator SDE2.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	z	34	Total	C	N	O	S	0	0
			280	166	59	53	2		

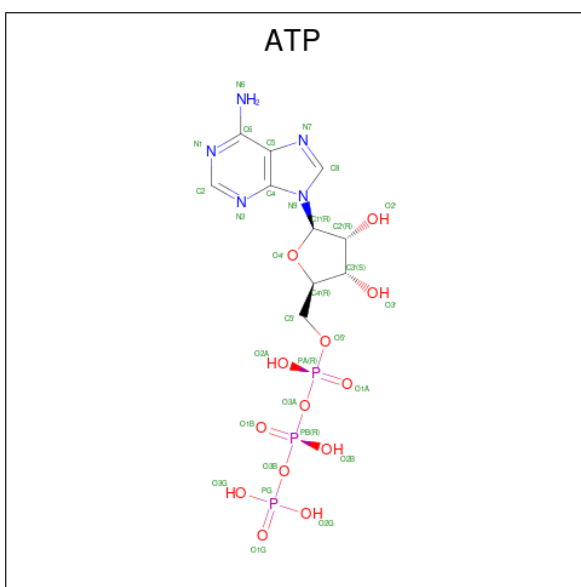
- Molecule 45 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 46 is POTASSIUM ION (CCD ID: K) (formula: K).

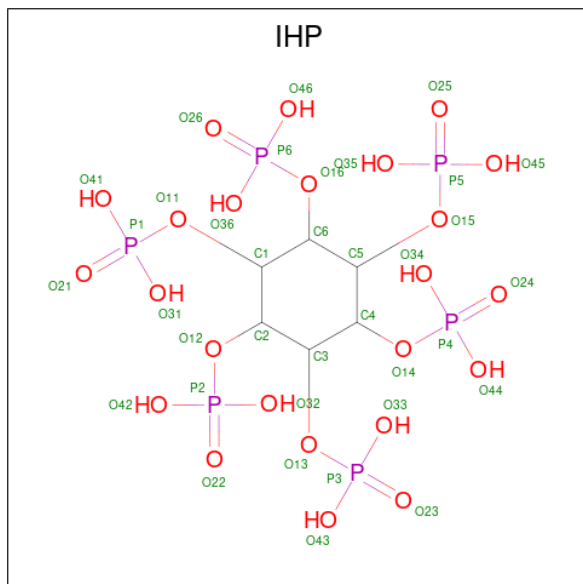
Mol	Chain	Residues	Atoms		AltConf
46	6	1	Total	K	0
			1	1	

- Molecule 47 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).

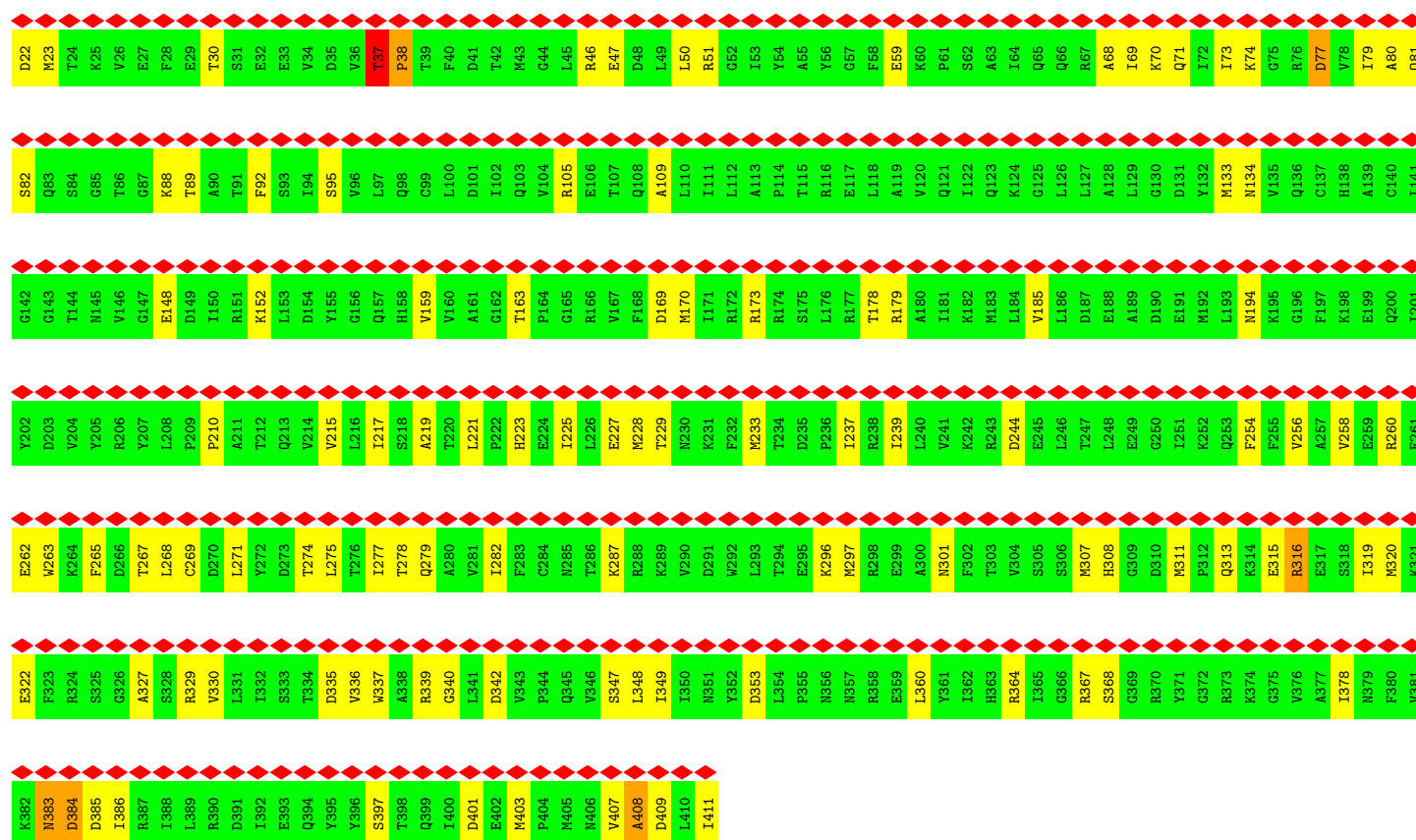


Mol	Chain	Residues	Atoms		AltConf
49	L	3	Total 3	Zn 3	0
49	M	3	Total 3	Zn 3	0
49	c	1	Total 1	Zn 1	0

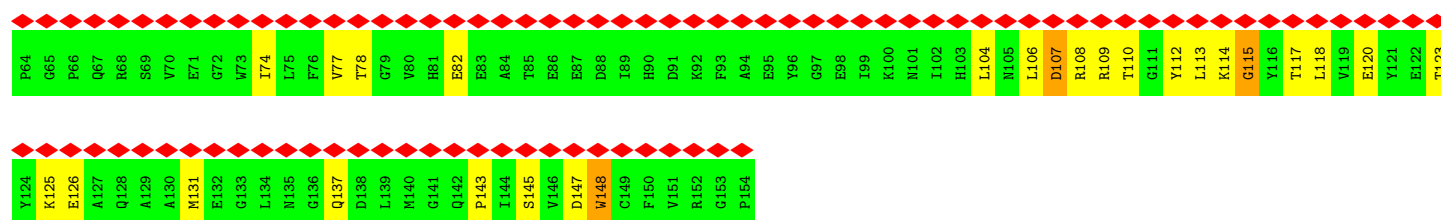
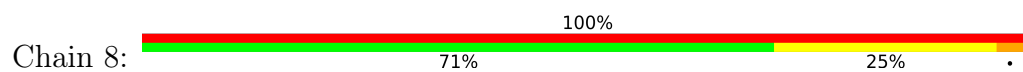
- Molecule 50 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: $C_6H_{18}O_{24}P_6$).



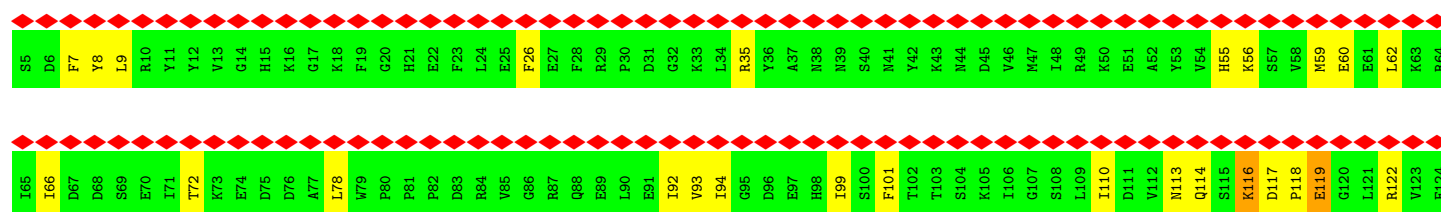
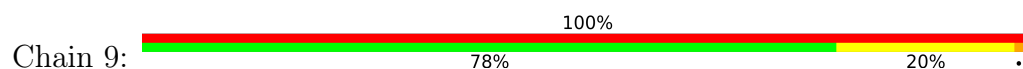
Mol	Chain	Residues	Atoms				AltConf
50	c	1	Total 36	C 6	O 24	P 6	0

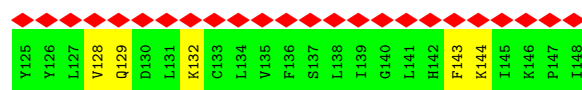


• Molecule 5: RNA-binding protein 8A

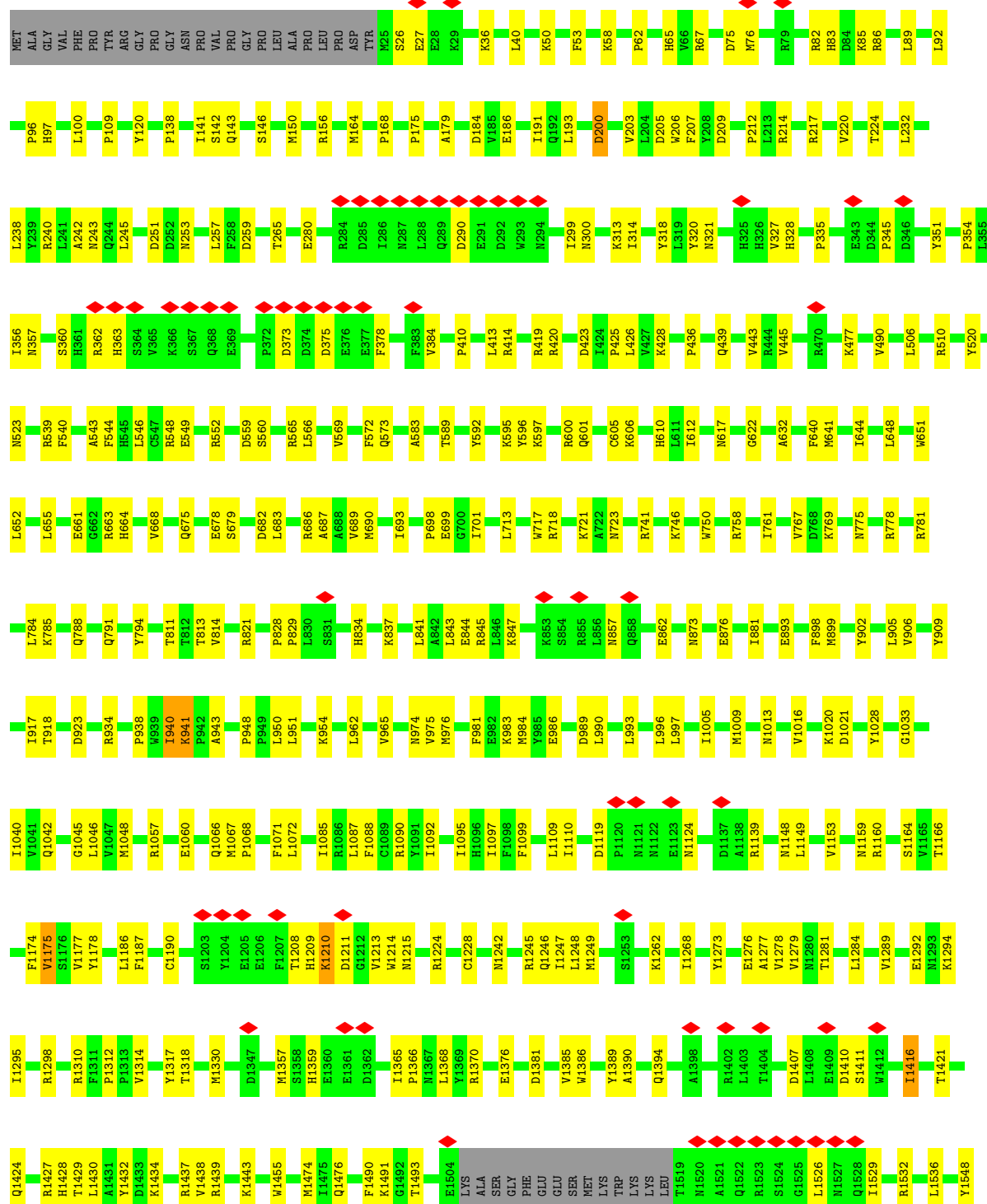


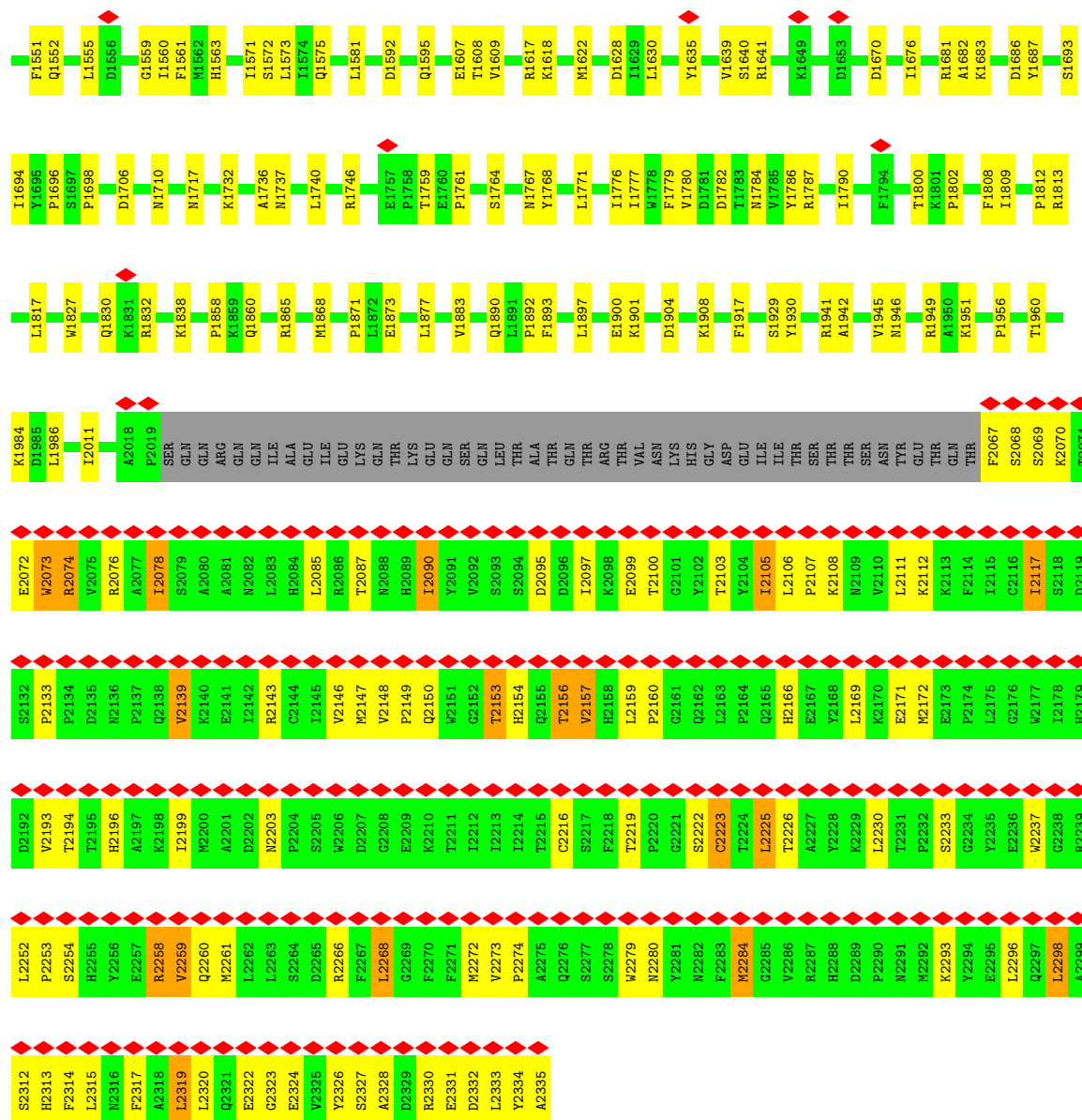
• Molecule 6: Protein mago nashi homolog 2



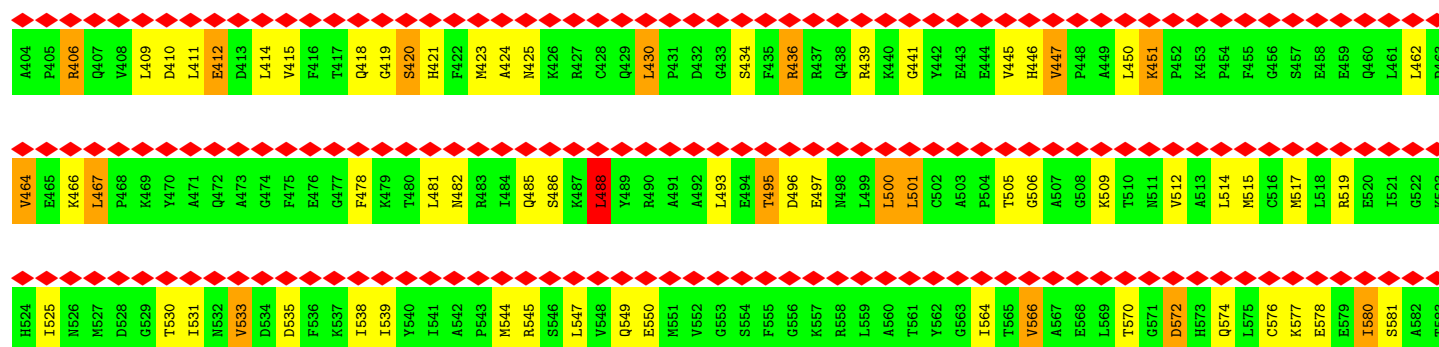


• Molecule 7: Pre-mRNA-processing-splicing factor 8





● Molecule 8: U5 small nuclear ribonucleoprotein 200 kDa helicase



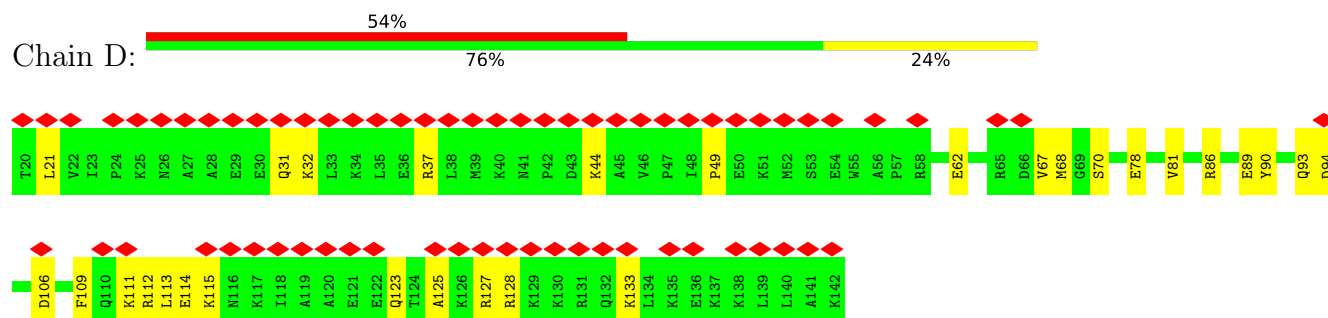
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L1184	E1185	L1186	S1187	V1188	H1189	L1190	Q1191	P1192	I1193	T1194	L1195	R1196	T1197	L1198	K1199	V1200	E1201	L1202	T1203	I1204	T1205	P1206	F1207	F1208	Q1209	W1210	D1211	E1212	K1213	V1214	H1215	G1216	S1217	S1218	E1219	A1220	F1221	W1222	L1223	L1224	V1225	E1226	D1227	V1228	K1229	S1230	E1231	V1232	L1233	L1234	H1235	H1236	E1237	Y1238	H1239	L1240	L1241	K1242	A1243	
Q1124	S1125	M1126	C1127	P1128	L1129	R1130	Q1131	F1132	L1133	K1134	L1135	P1136	E1137	E1138	V1139	V1140	K1141	K1142	I1143	E1144	K1145	K1146	M1147	F1148	P1149	F1150	E1151	R1152	L1153	Y1154	D1155	L1156	N1157	H1158	N1159	E1160	I1161	G1162	E1163	L1164	T1165	R1166	M1167	P1168	K1169	M1170	G1171	K1172	T1173	I1174	H1175	K1176	Y1177	V1178	H1179	L1180	F1181	P1182	K1183	
L1064	A1065	F1066	I1067	S1068	Q1069	L1070	K1071	L1072	E1073	G1074	F1075	A1076	L1077	M1078	A1079	D1080	M1081	V1082	Y1083	V1084	T1085	Q1086	S1087	A1088	G1089	R1090	L1091	M1092	R1093	A1094	I1095	F1096	E1097	I1098	V1099	L1100	N1101	R1102	G1103	W1104	A1105	Q1106	L1107	T1108	D1109	K1110	T1111	L1112	N1113	L1114	C1115	K1116	M1117	I1118	D1119	K1120	M1121	W1122		
L1004	L1005	K944	P1007	T1008	L1009	S1010	E1011	L1012	E1013	L1014	F1015	R1016	V1017	F1018	S1019	L1020	S1021	S1022	E1023	F1024	K1025	N1026	I1027	T1028	V1029	R1030	E1031	E1032	A1033	K1034	L1035	E1036	L1037	Q1038	K1039	L1040	L1041	E1042	R1043	V1044	P1045	L1046	I1047	V1048	K1049	E1050	S1051	L1052	E1053	E1054	P1055	S1056	A1057	K1058	T1059	N1060	V1061	L1062	L1063	
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A2098	L2038	G1978	K1918	T1858	Q1798	A1738	D1678	G1618	P1558	K1498	R1438	I1378
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Q2100	Q2040	E1980	I1920	I1860	K1800	I1740	P1680	L1620	I1560	V1500	K1440	T1380
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I2079	L2019	L2019	V1959	L1899	T1840	R1779	Y1719	H1659	P1599	L1539	S1479	L1419
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L2082	E2022	E2022	Q1962	M1902	V1842	S1782	L1722	T1662	E1602	M1542	E1482	G1422
T2083	V2023	V2023	L1963	N1903	R1843	S1783	P1723	T1663	K1603	A1543	R1483	W1423

• Molecule 9: 116 kDa U5 small nuclear ribonucleoprotein component



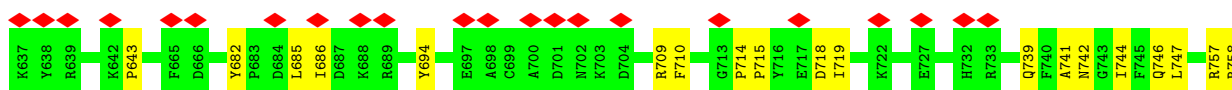
• Molecule 10: PRKR-interacting protein 1



• Molecule 11: Ligated exons: MINX mRNA



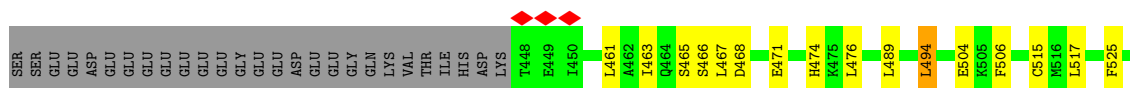
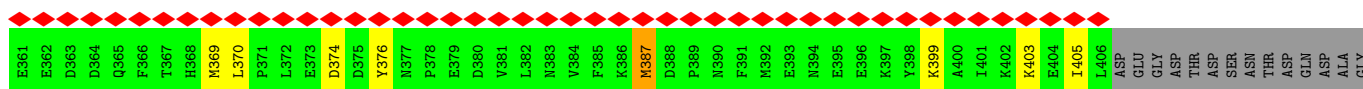
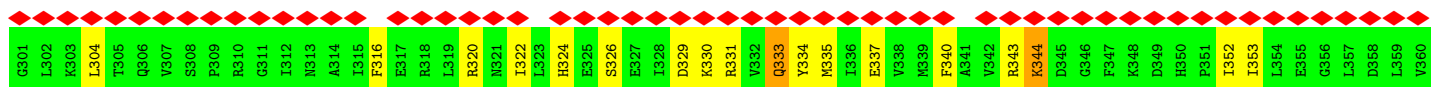
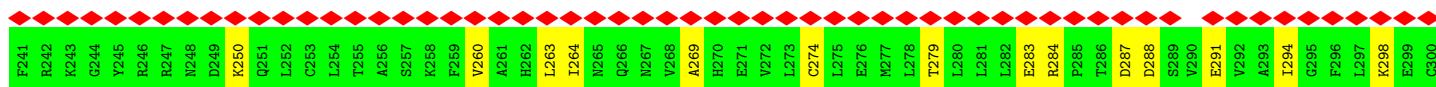
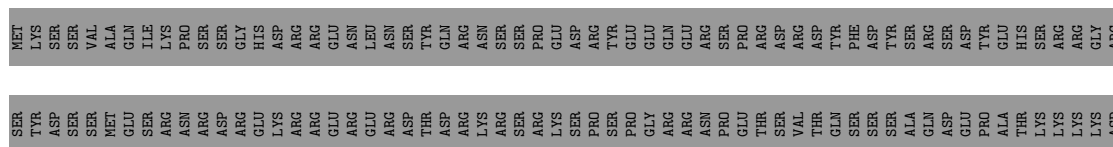
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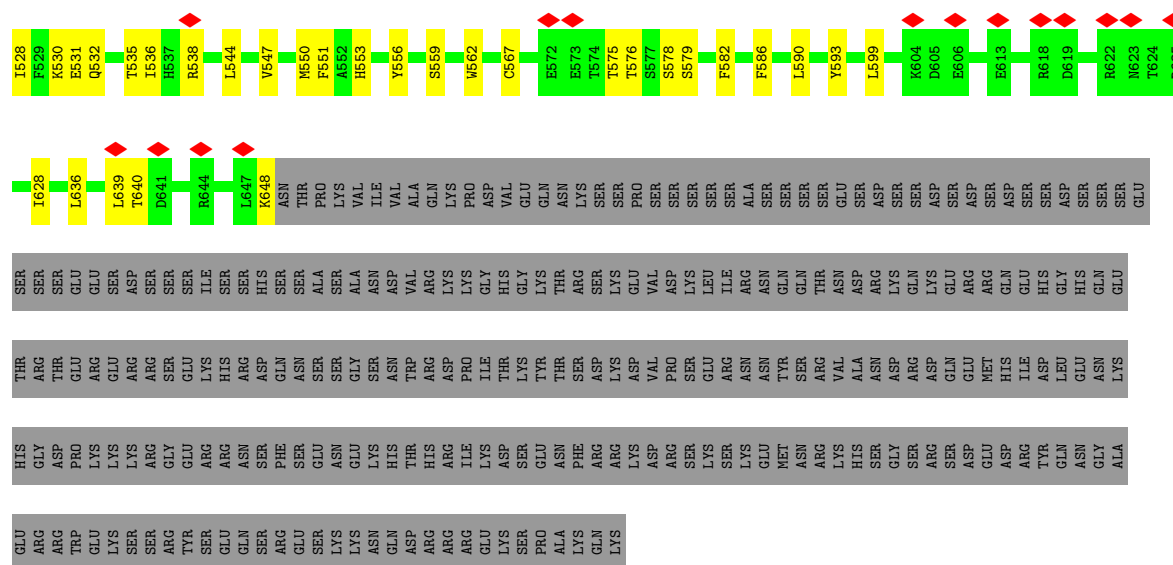


Chain G:

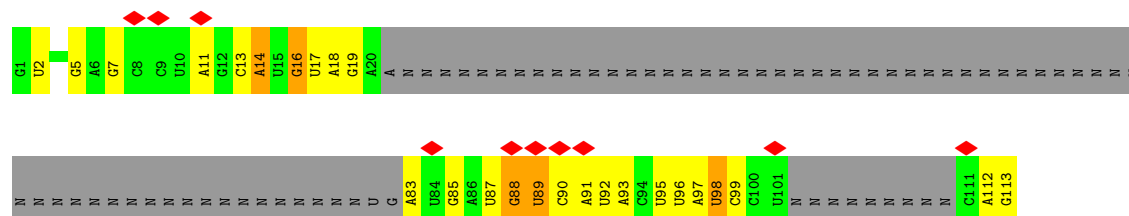


Chain H: 30% 39% 11% 49%

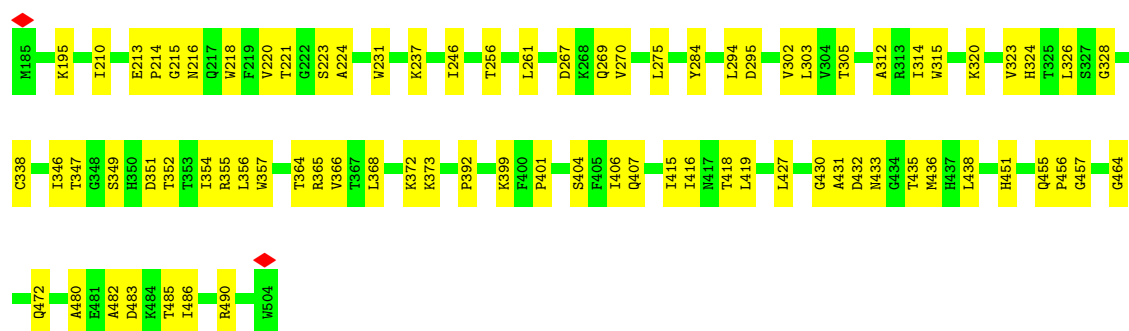
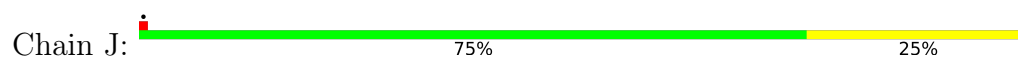




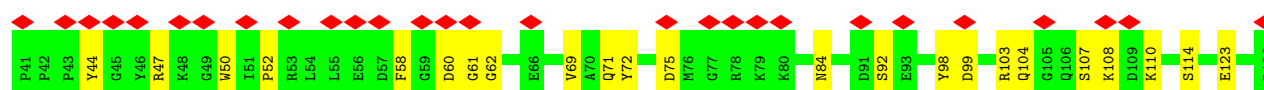
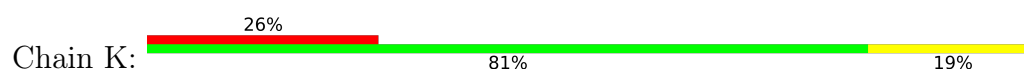
• Molecule 15: Intron lariat: MINX RNA

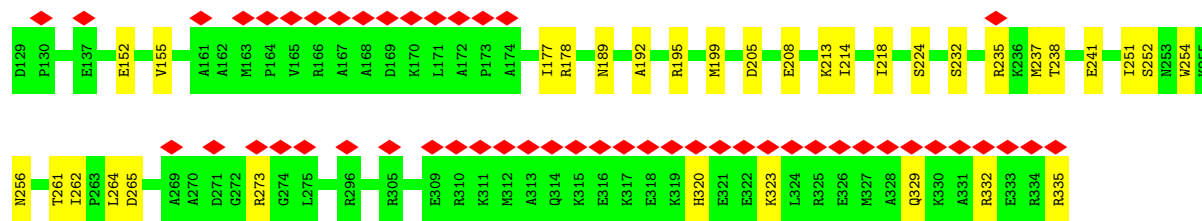


• Molecule 16: Pleiotropic regulator 1

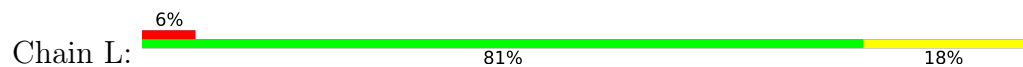


• Molecule 17: SNW domain-containing protein 1

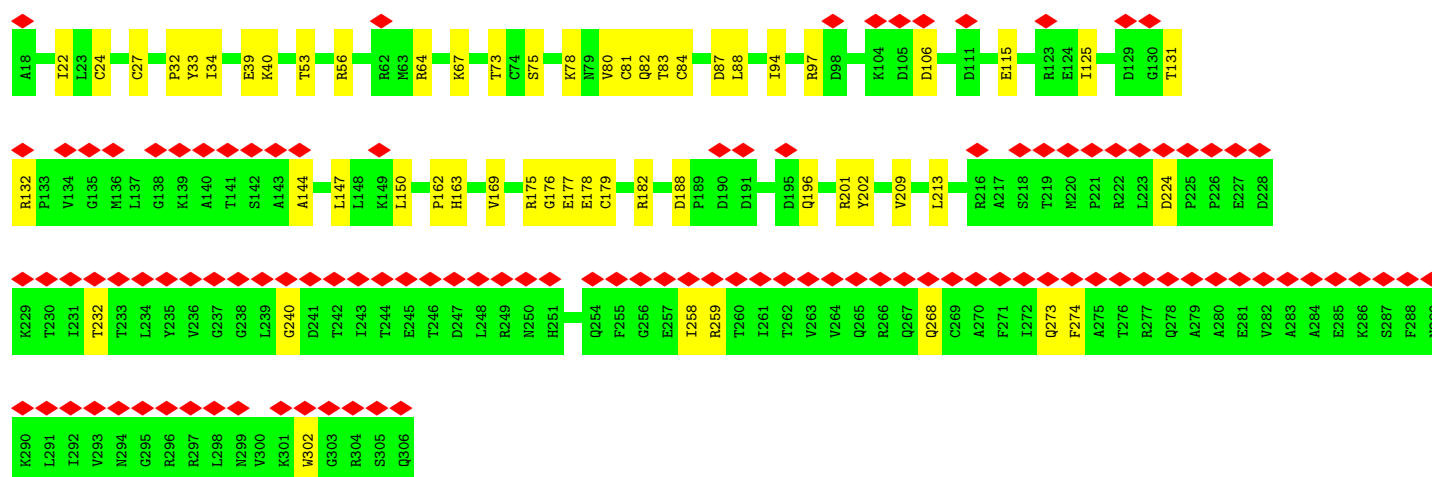
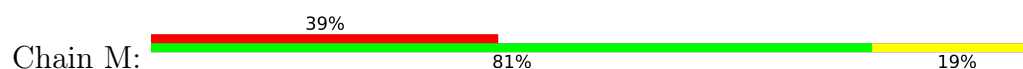




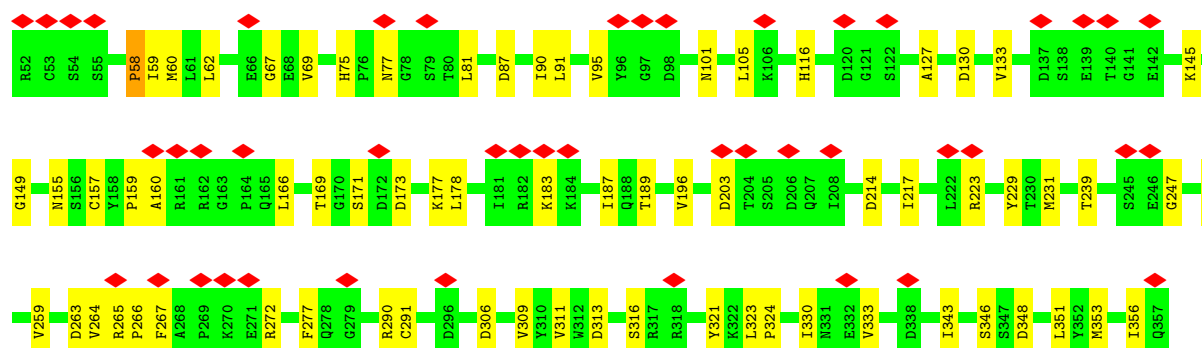
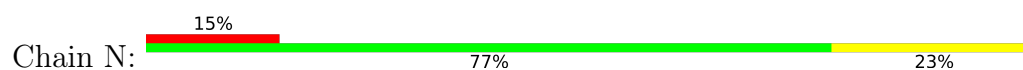
- Molecule 18: Protein BUD31 homolog



- Molecule 19: Pre-mRNA-splicing factor RBM22



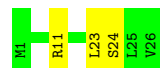
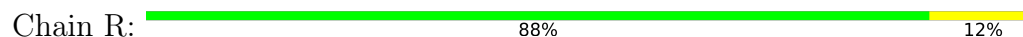
- Molecule 20: U5 small nuclear ribonucleoprotein 40 kDa protein



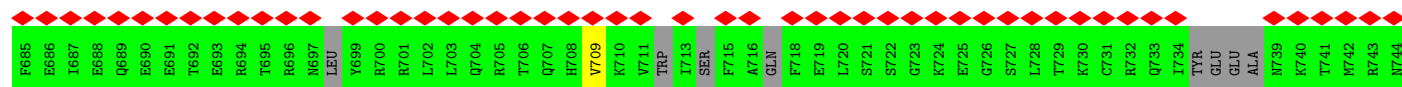
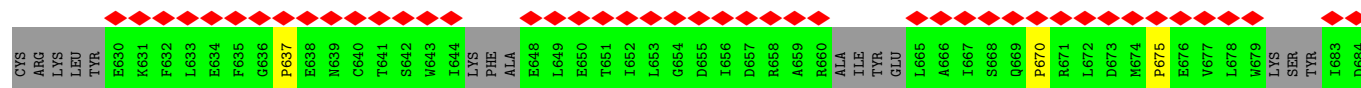
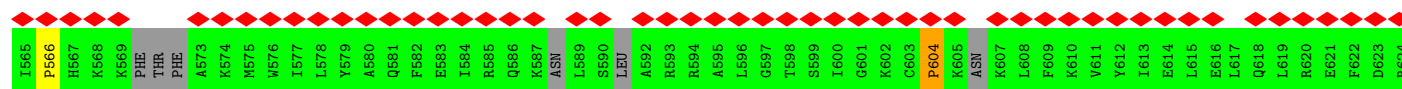
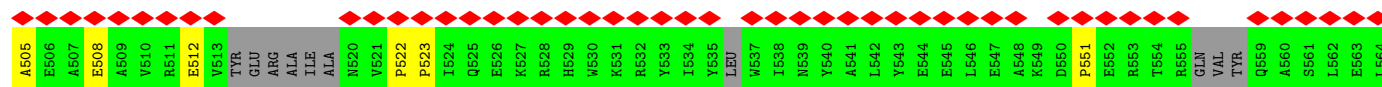
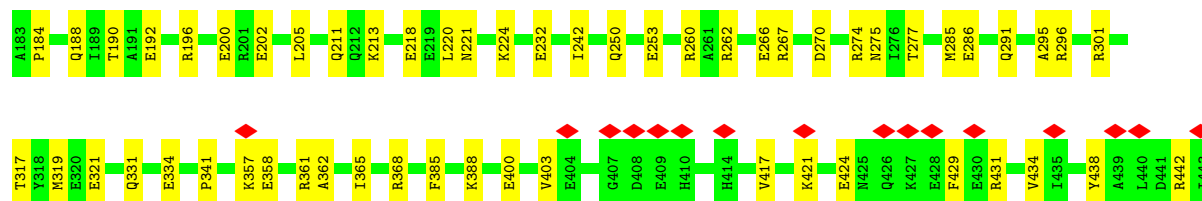
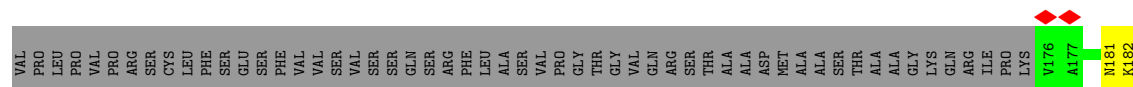
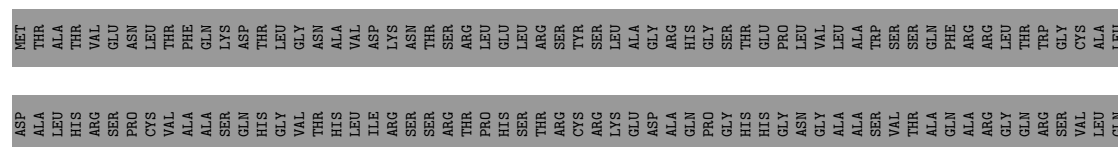
- Molecule 21: Cell division cycle 5-like protein



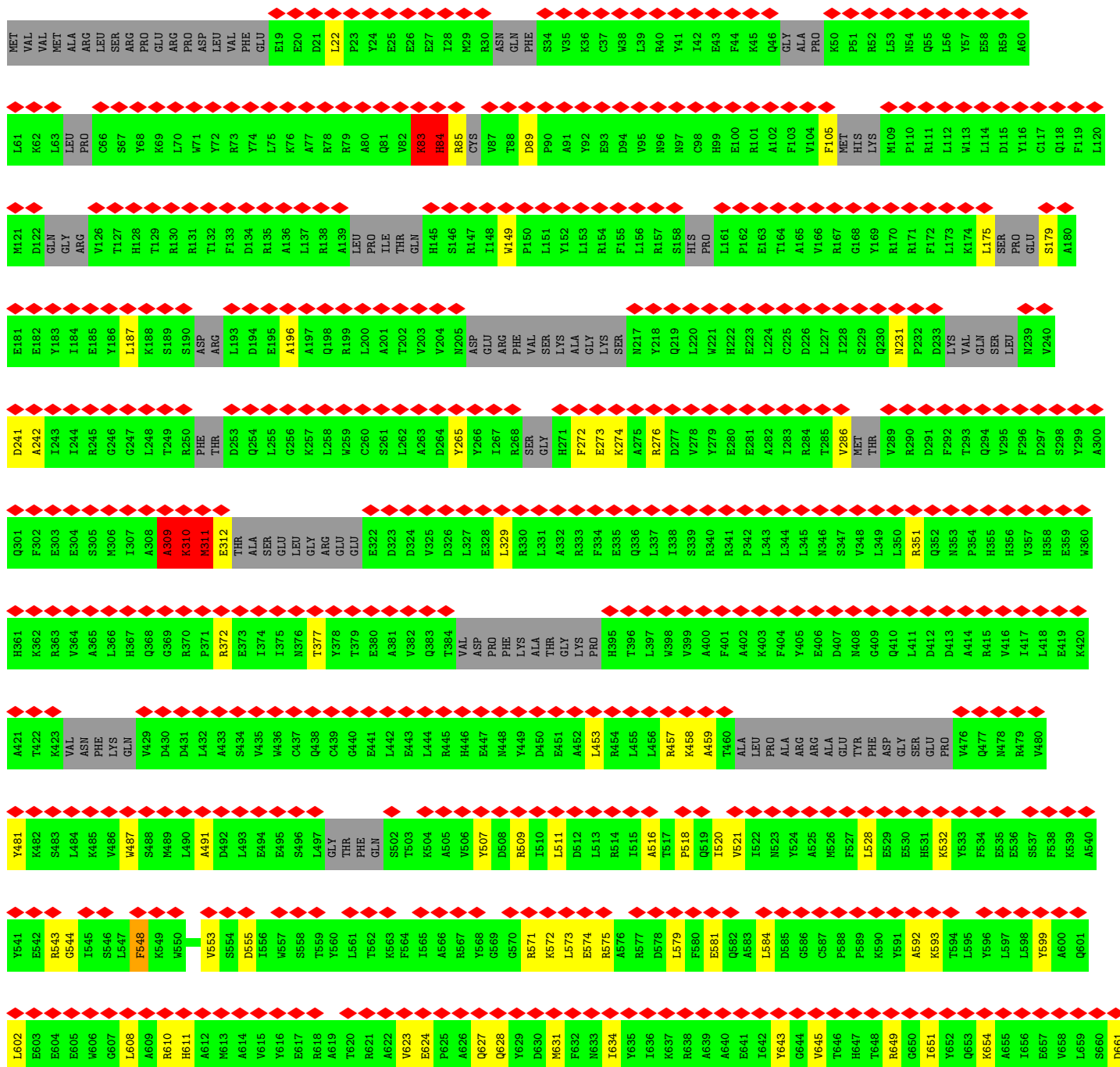
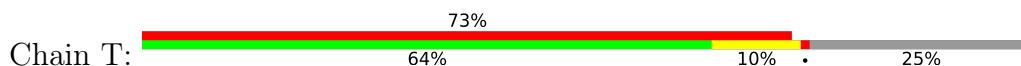
- Molecule 23: Serine/arginine repetitive matrix protein 2



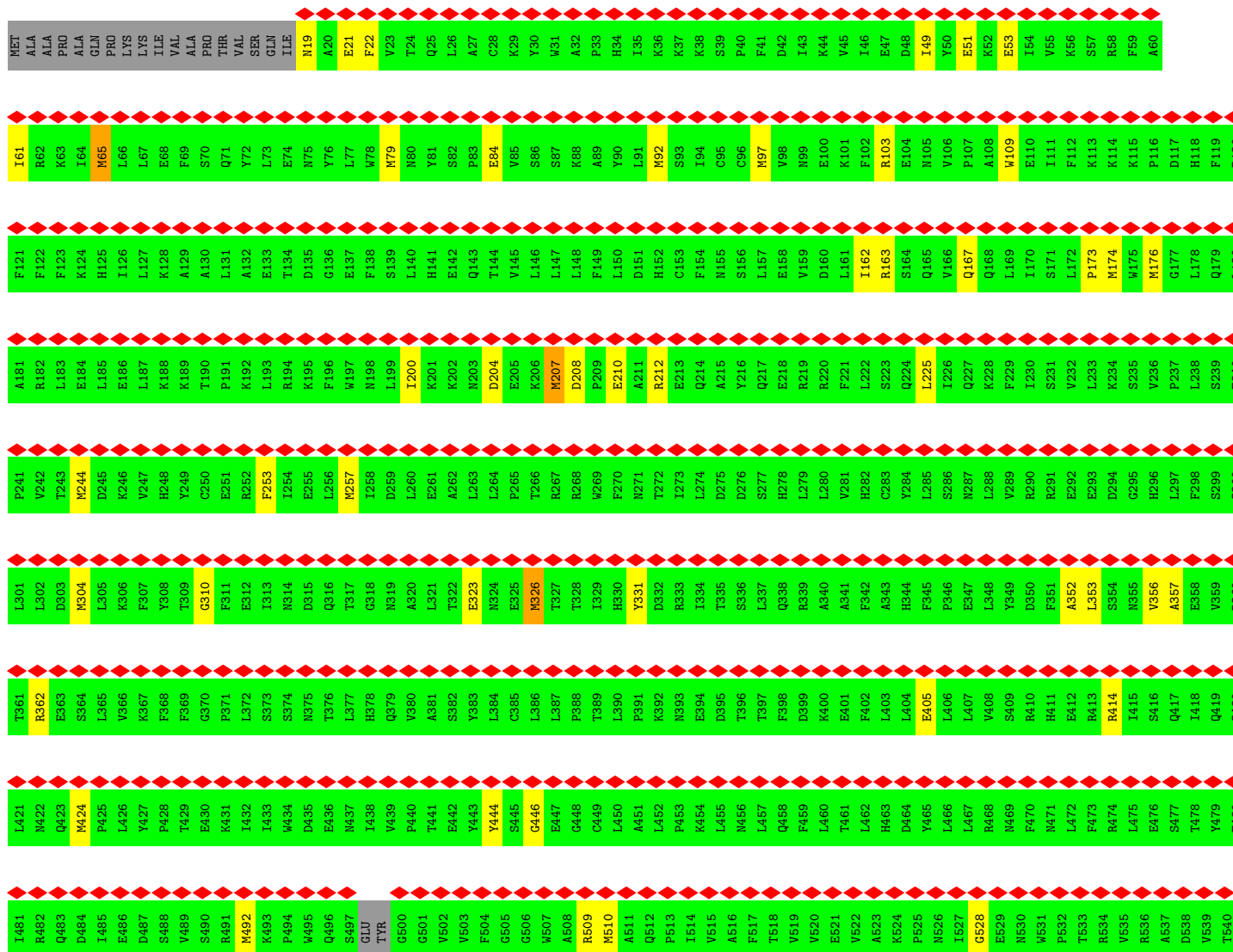
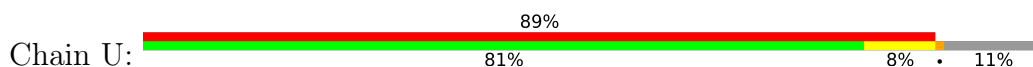
- Molecule 24: Crooked neck-like protein 1



- Molecule 25: Pre-mRNA-splicing factor SYF1



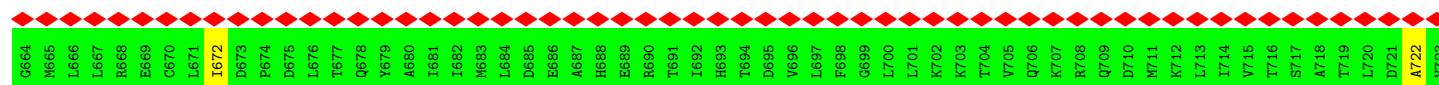
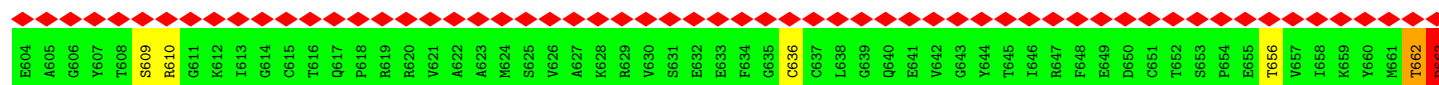
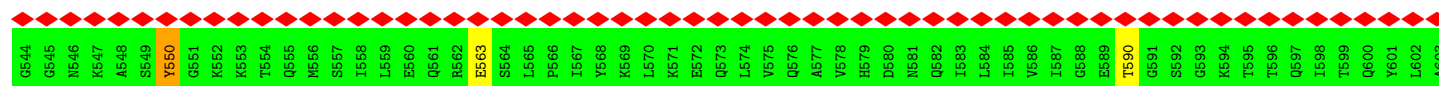
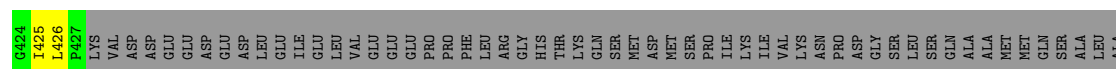
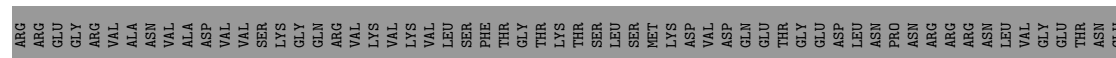
- Molecule 26: Intron-binding protein aquarius

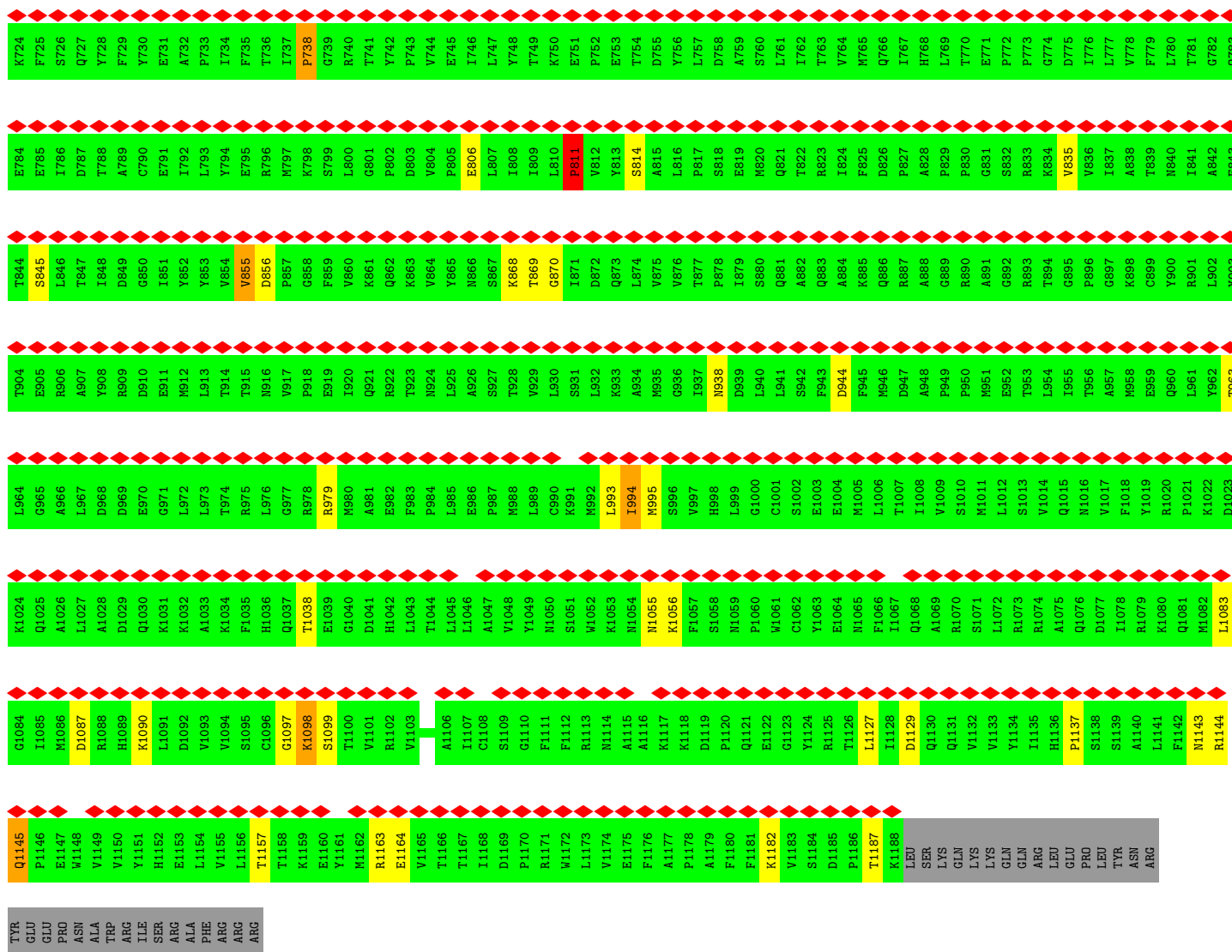


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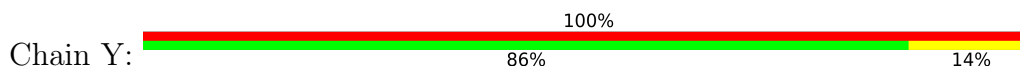
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- Molecule 27: ATP-dependent RNA helicase DHX8



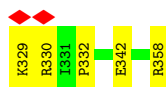
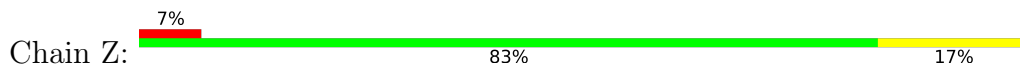


- Molecule 29: U2 small nuclear ribonucleoprotein B''

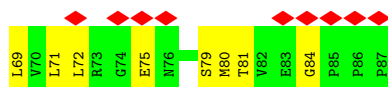
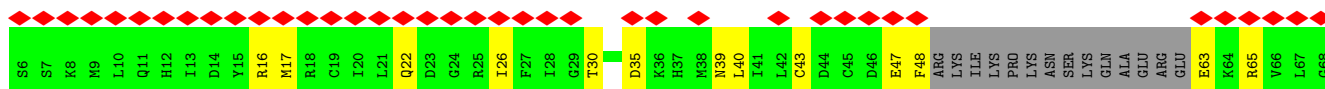




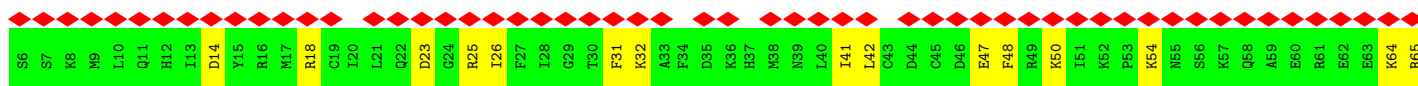
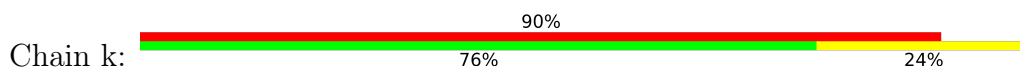
• Molecule 30: NF-kappa-B-activating protein



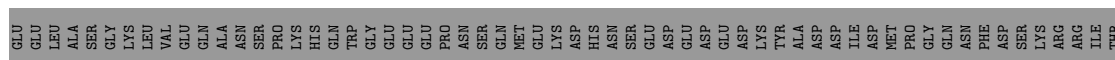
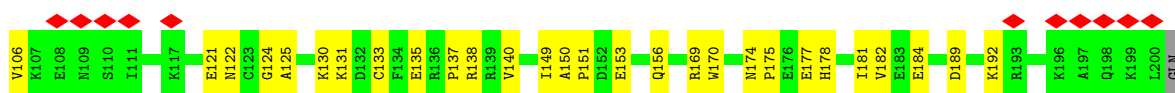
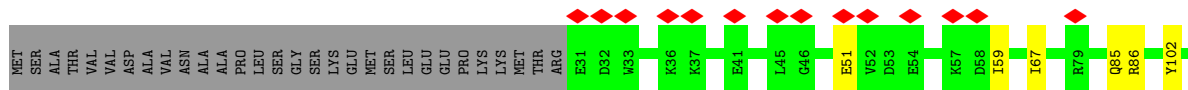
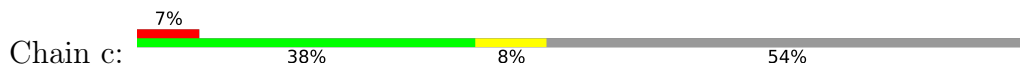
• Molecule 31: Small nuclear ribonucleoprotein-associated proteins B and B'

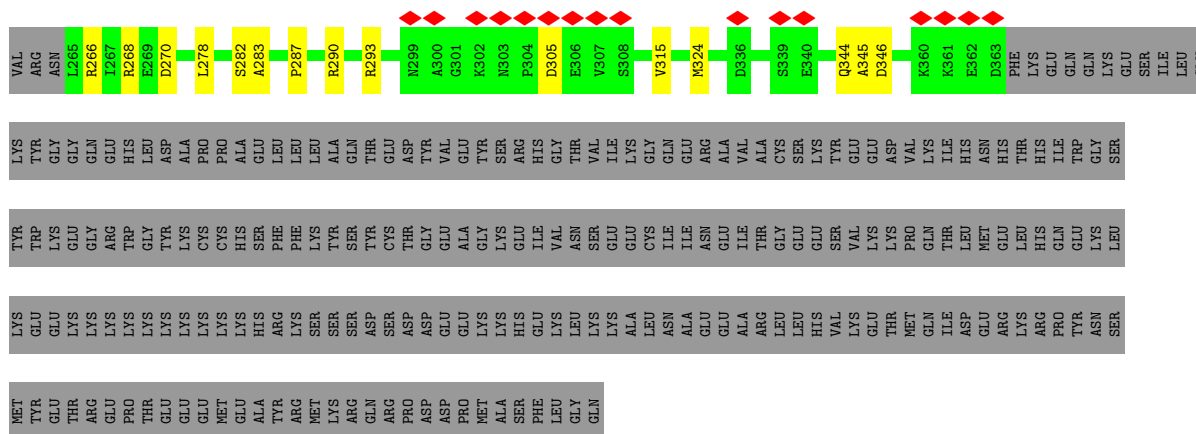


• Molecule 31: Small nuclear ribonucleoprotein-associated proteins B and B'

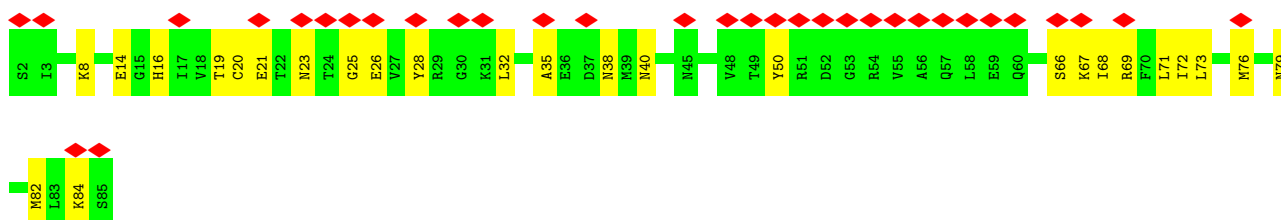
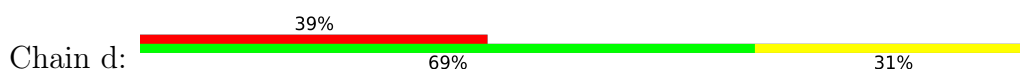


• Molecule 32: Pre-mRNA-splicing factor SLU7

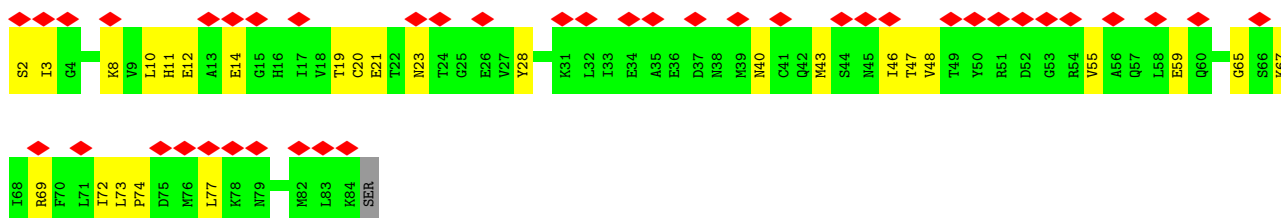




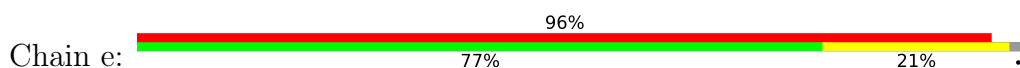
• Molecule 33: Small nuclear ribonucleoprotein Sm D3



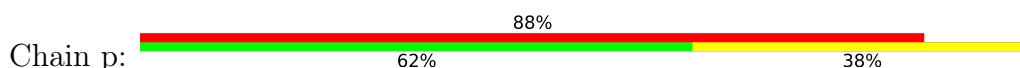
• Molecule 33: Small nuclear ribonucleoprotein Sm D3

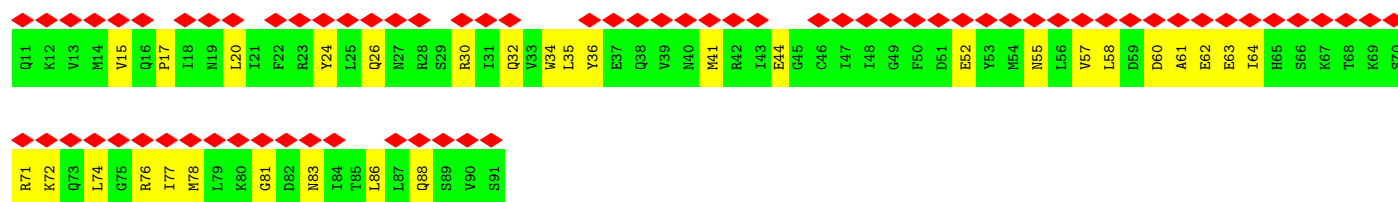


• Molecule 34: Small nuclear ribonucleoprotein E

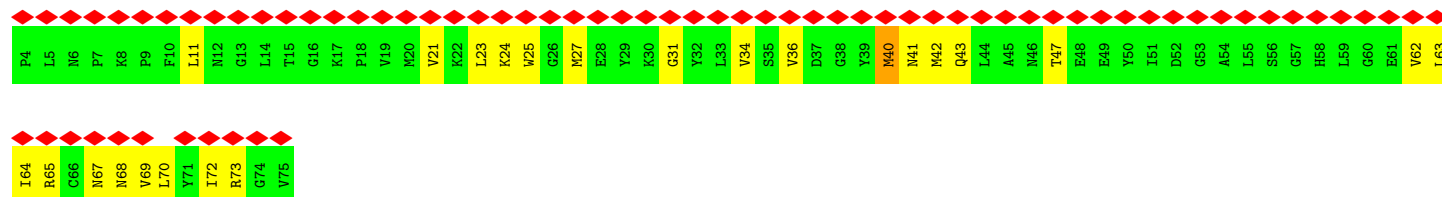


• Molecule 34: Small nuclear ribonucleoprotein E

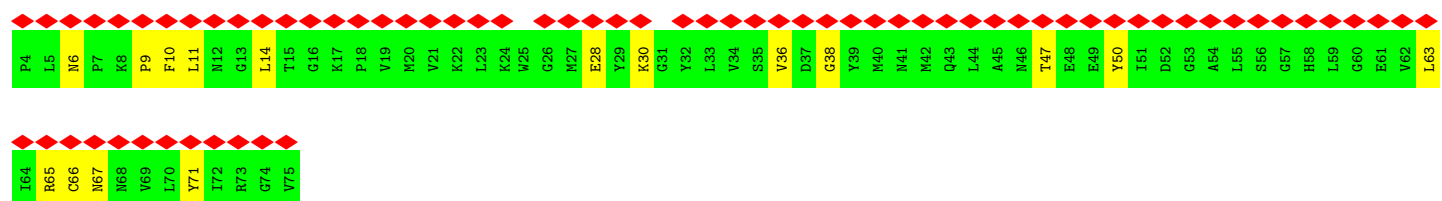
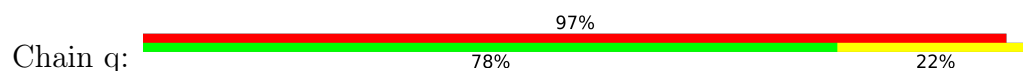




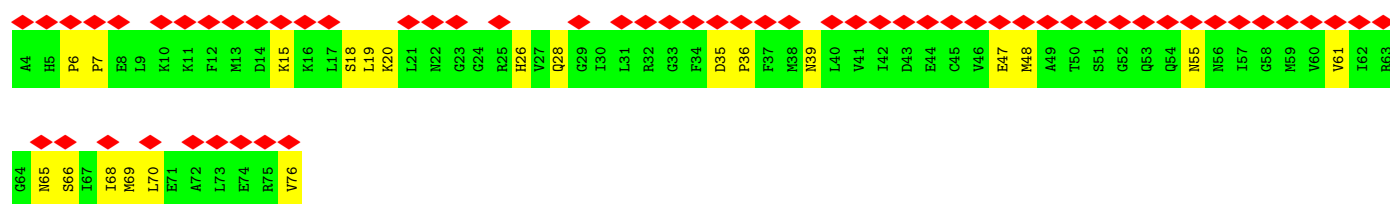
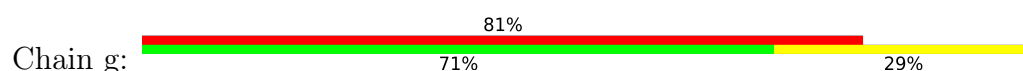
• Molecule 35: Small nuclear ribonucleoprotein F



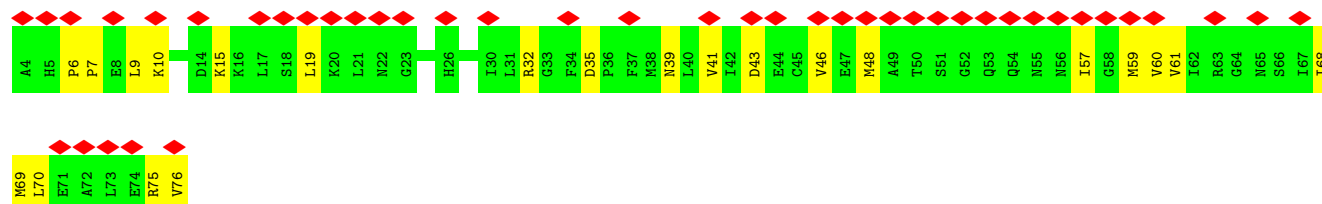
• Molecule 35: Small nuclear ribonucleoprotein F



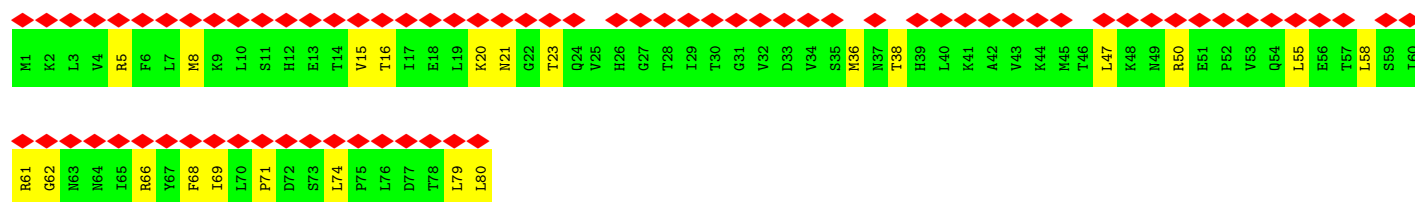
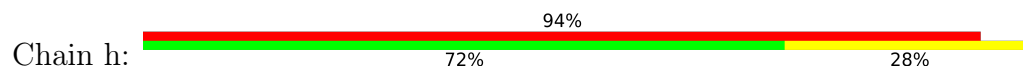
• Molecule 36: Small nuclear ribonucleoprotein G



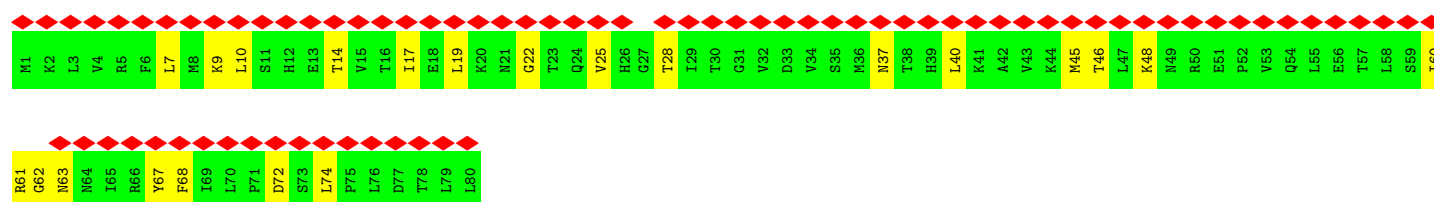
• Molecule 36: Small nuclear ribonucleoprotein G



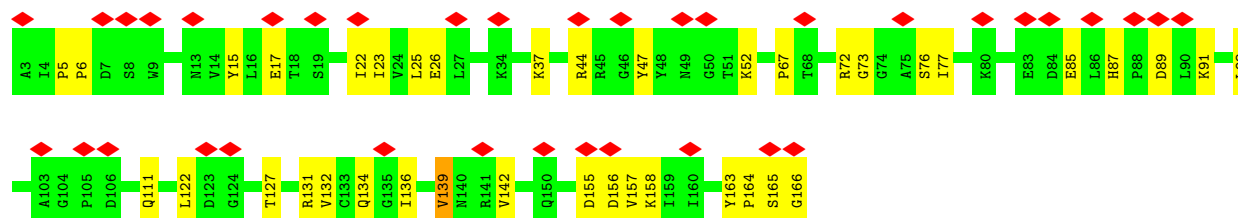
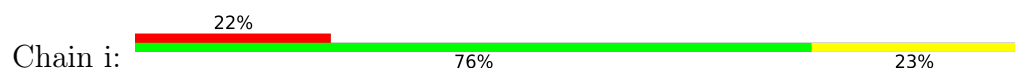
- Molecule 37: Small nuclear ribonucleoprotein Sm D1



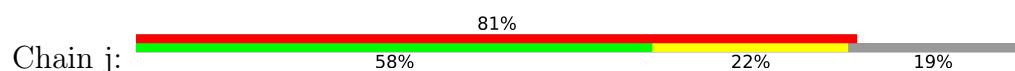
- Molecule 37: Small nuclear ribonucleoprotein Sm D1



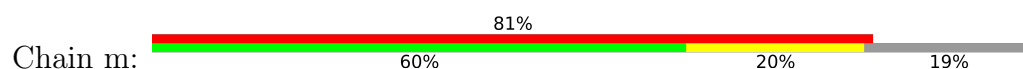
- Molecule 38: Peptidyl-prolyl cis-trans isomerase-like 1



- Molecule 39: Small nuclear ribonucleoprotein Sm D2

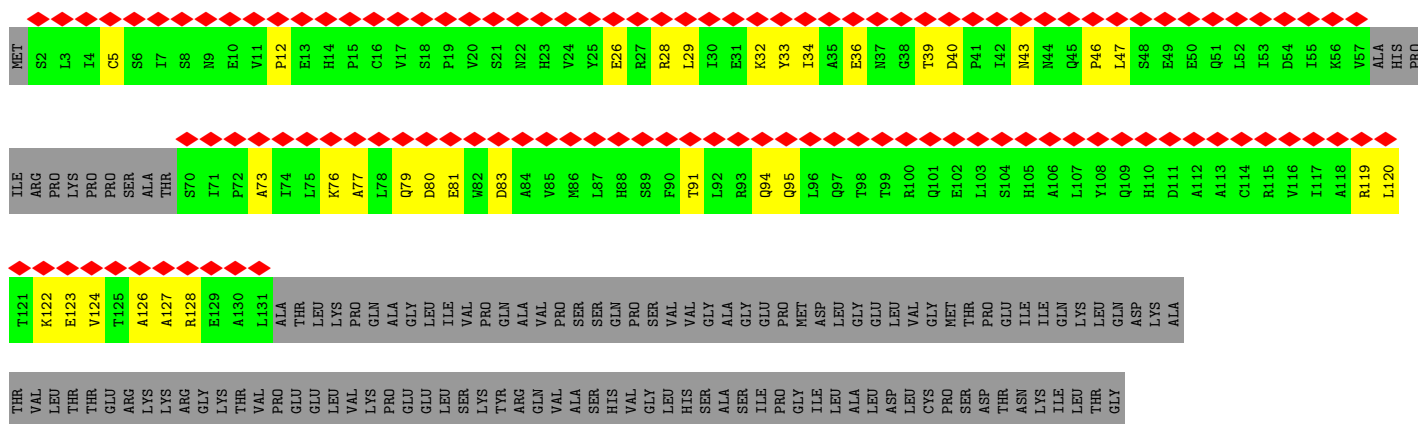


- Molecule 39: Small nuclear ribonucleoprotein Sm D2



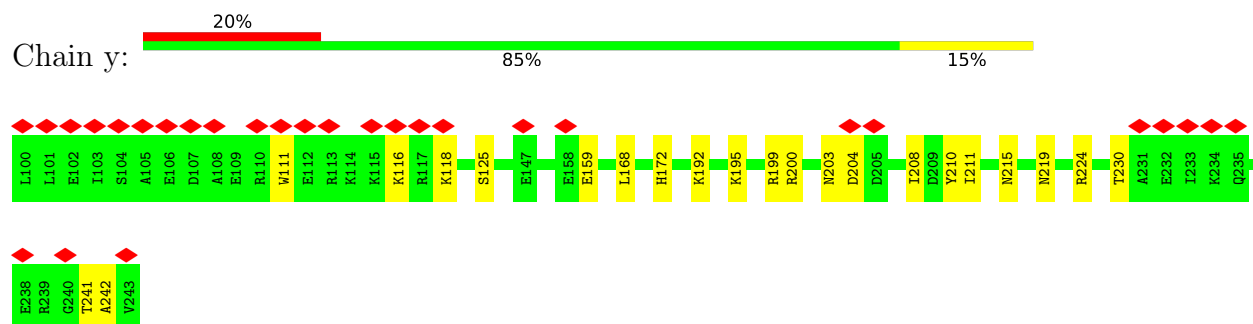




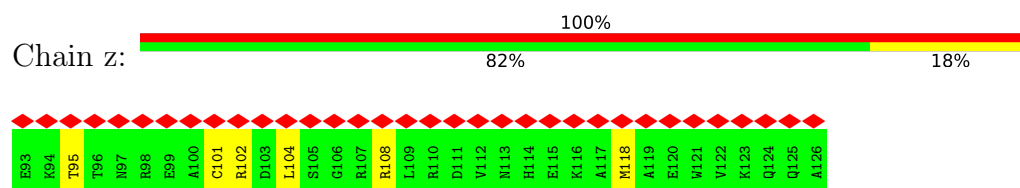


VAL	VAL	LEU	ASP	VAL	GLY
ALA	ALA	ARG	GLY	VAL	ASP
ALA	ALA	ARG	GLY	VAL	ASP
PHE	PHE	LYS	LEU	ALA	LYS
GLY	GLY	LEU	PHE	ILE	ASN
HIS	HIS	LYS	GLY	HIS	VAL
HIS	HIS	ASN	GLY	GLU	VAL
ALA	ALA	PHE	THR	SER	VAL
LYS	LYS	LYS	GLY	ALA	VAL
PHE	PHE	THR	THR	VAL	PHE
ILE	ILE	LEU	MET	THR	ASP
ALA	ALA	GLN	ASP	GLY	LYS
SER	SER	LEU	SER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

- Molecule 43: Pre-mRNA-splicing factor SYF2



- Molecule 44: Replication stress response regulator SDE2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	103860	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	53	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	135000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.177	Depositor
Minimum map value	-0.101	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.024	Depositor
Map size (Å)	492.00003, 492.00003, 492.00003	wwPDB
Map dimensions	410, 410, 410	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2, 1.2, 1.2	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	2	0.29	0/2827	0.47	0/4393
2	5	0.32	0/1760	0.50	0/2733
3	6	0.28	0/2323	0.44	0/3619
4	7	0.45	0/3179	1.00	14/4291 (0.3%)
5	8	0.40	0/748	0.98	4/1012 (0.4%)
6	9	0.40	0/1225	0.84	3/1648 (0.2%)
7	A	0.42	1/19172 (0.0%)	0.69	11/26014 (0.0%)
8	B	0.47	0/14140	0.92	27/19159 (0.1%)
9	C	0.33	0/7277	0.67	0/9887
10	D	0.31	0/1030	0.66	0/1371
11	E	0.34	0/329	0.52	0/510
12	F	0.30	1/1129 (0.1%)	0.55	0/1525
13	G	0.24	0/513	0.58	0/683
14	H	0.37	0/3779	0.68	0/5087
15	I	0.22	0/971	0.49	0/1504
16	J	0.42	0/2592	0.68	0/3535
17	K	0.31	0/2387	0.65	0/3205
18	L	0.34	0/1214	0.68	0/1627
19	M	0.30	0/2366	0.61	0/3193
20	N	0.25	0/2448	0.60	0/3316
21	O	0.29	0/3457	0.57	0/4627
22	P	0.28	0/902	0.63	1/1201 (0.1%)
23	R	0.39	0/196	0.49	0/265
24	S	0.40	0/4013	0.77	8/5432 (0.1%)
25	T	0.56	0/4031	1.35	21/5500 (0.4%)
26	U	0.57	71/11155 (0.6%)	0.70	3/15095 (0.0%)
27	V	0.81	0/3000	1.61	20/3777 (0.5%)
28	W	0.27	0/1299	0.64	0/1761
29	Y	0.33	0/759	0.50	0/1016
30	Z	0.25	0/232	0.60	0/307
31	b	0.29	0/553	0.59	0/739
31	k	0.44	0/674	0.59	0/899

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	c	0.29	0/2268	0.61	0/3052
33	d	0.36	0/666	0.67	0/897
33	n	0.47	0/660	0.70	0/889
34	e	0.27	0/659	0.61	0/885
34	p	0.46	0/677	0.69	0/908
35	f	0.25	0/574	0.62	0/775
35	q	0.42	0/574	0.65	0/775
36	g	0.32	0/575	0.62	0/768
36	r	0.46	0/575	0.66	0/768
37	h	0.25	0/642	0.57	0/867
37	l	0.41	0/642	0.60	0/867
38	i	0.24	0/1304	0.57	0/1767
39	j	0.23	0/784	0.62	0/1053
39	m	0.39	0/784	0.65	0/1053
40	o	0.31	0/4265	0.66	0/5761
41	s	0.33	0/1423	0.65	0/1914
42	t	0.28	0/1004	0.56	0/1365
42	u	0.28	0/953	0.59	0/1295
42	v	0.31	0/1004	0.59	0/1365
42	w	0.26	0/953	0.57	0/1295
43	y	0.28	0/1241	0.63	0/1662
44	z	0.44	0/282	0.68	0/375
All	All	0.42	73/124189 (0.1%)	0.76	112/169287 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
7	A	0	4
8	B	0	1
9	C	0	2
17	K	0	1
18	L	0	2
25	T	0	5
27	V	0	15
35	f	0	1
41	s	0	3
All	All	0	34

The worst 5 of 73 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	U	867	MET	SD-CE	6.53	1.95	1.79
26	U	1093	MET	SD-CE	6.47	1.95	1.79
26	U	79	MET	SD-CE	6.41	1.95	1.79
26	U	1368	MET	SD-CE	6.41	1.95	1.79
26	U	176	MET	SD-CE	6.41	1.95	1.79

The worst 5 of 112 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	T	84	HIS	O-C-N	-12.04	109.67	122.07
25	T	83	LYS	O-C-N	-11.98	109.73	122.07
25	T	309	ALA	O-C-N	-11.96	109.76	122.07
25	T	311	MET	O-C-N	-11.95	109.76	122.07
25	T	310	LYS	O-C-N	-11.93	109.78	122.07

There are no chirality outliers.

5 of 34 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	A	1210	LYS	Peptide
7	A	1416	ILE	Peptide
7	A	1635	TYR	Peptide
7	A	940	ILE	Peptide
8	B	430	LEU	Peptide

5.2 Too-close contacts [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	2	2535	0	1281	48	0
2	5	1579	0	800	18	0
3	6	2075	0	1048	31	0
4	7	3130	0	3172	114	0
5	8	730	0	690	28	0
6	9	1196	0	1182	34	0
7	A	18655	0	18541	564	0
8	B	13846	0	13981	437	0
9	C	7116	0	7127	178	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	D	1013	0	1058	40	0
11	E	296	0	153	3	0
12	F	1084	0	1022	11	0
13	G	504	0	509	22	0
14	H	3713	0	3745	166	0
15	I	872	0	442	21	0
16	J	2523	0	2469	51	0
17	K	2360	0	2406	50	0
18	L	1188	0	1192	20	0
19	M	2318	0	2310	43	0
20	N	2394	0	2329	99	0
21	O	3416	0	3293	134	0
22	P	888	0	865	13	0
23	R	193	0	196	6	0
24	S	3965	0	3156	79	0
25	T	4003	0	2869	85	0
26	U	10885	0	10852	73	0
27	V	2995	0	991	102	0
28	W	1282	0	1305	26	0
29	Y	745	0	767	10	0
30	Z	230	0	229	3	0
31	b	545	0	557	16	0
31	k	664	0	690	20	0
32	c	2215	0	2165	39	0
33	d	658	0	675	32	0
33	n	652	0	670	36	0
34	e	651	0	671	12	0
34	p	669	0	692	26	0
35	f	562	0	574	22	0
35	q	562	0	574	12	0
36	g	568	0	590	15	0
36	r	568	0	590	33	0
37	h	634	0	680	14	0
37	l	634	0	680	16	0
38	i	1270	0	1244	27	0
39	j	774	0	802	20	0
39	m	774	0	802	17	0
40	o	4157	0	4060	140	0
41	s	1402	0	1379	39	0
42	t	988	0	994	27	0
42	u	938	0	938	25	0
42	v	988	0	994	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	w	938	0	938	20	0
43	y	1218	0	1194	21	0
44	z	280	0	276	24	0
45	6	5	0	0	0	0
45	7	1	0	0	0	0
45	C	1	0	0	0	0
46	6	1	0	0	0	0
47	7	31	0	12	2	0
48	C	32	0	12	2	0
49	L	3	0	0	0	0
49	M	3	0	0	0	0
49	c	1	0	0	0	0
50	c	36	0	6	1	0
All	All	121152	0	113439	2491	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 11.

The worst 5 of 2491 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)
7:A:1067:MET:HE3	27:V:413:LYS:CD	1.29	1.60
7:A:1067:MET:CE	27:V:413:LYS:HG2	1.27	1.59
27:V:393:ARG:HB3	27:V:1145:GLN:C	1.26	1.59
7:A:1067:MET:CE	27:V:413:LYS:CG	1.75	1.57
7:A:2333:LEU:CD2	8:B:545:ARG:CG	1.75	1.56

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	
4	7	388/390 (100%)	376 (97%)	9 (2%)	3 (1%)	16	45
5	8	89/91 (98%)	87 (98%)	1 (1%)	1 (1%)	11	39
6	9	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
7	A	2244/2335 (96%)	2105 (94%)	139 (6%)	0	100	100
8	B	1720/1722 (100%)	1633 (95%)	84 (5%)	3 (0%)	43	71
9	C	897/899 (100%)	828 (92%)	67 (8%)	2 (0%)	43	71
10	D	121/123 (98%)	116 (96%)	5 (4%)	0	100	100
12	F	120/122 (98%)	107 (89%)	13 (11%)	0	100	100
13	G	58/60 (97%)	56 (97%)	2 (3%)	0	100	100
14	H	455/908 (50%)	440 (97%)	15 (3%)	0	100	100
16	J	318/320 (99%)	303 (95%)	15 (5%)	0	100	100
17	K	291/295 (99%)	271 (93%)	20 (7%)	0	100	100
18	L	142/144 (99%)	134 (94%)	8 (6%)	0	100	100
19	M	287/289 (99%)	271 (94%)	16 (6%)	0	100	100
20	N	304/306 (99%)	283 (93%)	19 (6%)	2 (1%)	18	49
21	O	429/802 (54%)	416 (97%)	12 (3%)	1 (0%)	43	71
22	P	100/229 (44%)	97 (97%)	3 (3%)	0	100	100
23	R	24/26 (92%)	17 (71%)	7 (29%)	0	100	100
24	S	531/848 (63%)	500 (94%)	28 (5%)	3 (1%)	21	52
25	T	597/855 (70%)	584 (98%)	12 (2%)	1 (0%)	43	71
26	U	1308/1485 (88%)	1283 (98%)	25 (2%)	0	100	100
27	V	709/1220 (58%)	617 (87%)	60 (8%)	32 (4%)	2	13
28	W	160/162 (99%)	147 (92%)	13 (8%)	0	100	100
29	Y	90/92 (98%)	88 (98%)	2 (2%)	0	100	100
30	Z	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
31	b	64/82 (78%)	62 (97%)	2 (3%)	0	100	100
31	k	80/82 (98%)	74 (92%)	6 (8%)	0	100	100
32	c	265/586 (45%)	248 (94%)	17 (6%)	0	100	100
33	d	82/84 (98%)	77 (94%)	5 (6%)	0	100	100
33	n	81/84 (96%)	76 (94%)	5 (6%)	0	100	100
34	e	77/81 (95%)	75 (97%)	2 (3%)	0	100	100
34	p	79/81 (98%)	77 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	f	70/72 (97%)	69 (99%)	1 (1%)	0	100	100
35	q	70/72 (97%)	69 (99%)	1 (1%)	0	100	100
36	g	71/73 (97%)	68 (96%)	3 (4%)	0	100	100
36	r	71/73 (97%)	69 (97%)	2 (3%)	0	100	100
37	h	78/80 (98%)	76 (97%)	2 (3%)	0	100	100
37	l	78/80 (98%)	75 (96%)	3 (4%)	0	100	100
38	i	162/164 (99%)	149 (92%)	13 (8%)	0	100	100
39	j	91/118 (77%)	87 (96%)	4 (4%)	0	100	100
39	m	91/118 (77%)	86 (94%)	5 (6%)	0	100	100
40	o	511/513 (100%)	465 (91%)	45 (9%)	1 (0%)	43	71
41	s	161/225 (72%)	148 (92%)	13 (8%)	0	100	100
42	t	121/504 (24%)	118 (98%)	3 (2%)	0	100	100
42	u	114/504 (23%)	113 (99%)	1 (1%)	0	100	100
42	v	121/504 (24%)	119 (98%)	2 (2%)	0	100	100
42	w	114/504 (23%)	113 (99%)	1 (1%)	0	100	100
43	y	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
44	z	32/34 (94%)	30 (94%)	2 (6%)	0	100	100
All	All	14378/18759 (77%)	13605 (95%)	724 (5%)	49 (0%)	37	65

5 of 49 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	7	383	ASN
8	B	957	VAL
8	B	1584	ILE
20	N	59	ILE
27	V	531	MET

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	7	345/345 (100%)	338 (98%)	7 (2%)	48	68
5	8	76/76 (100%)	75 (99%)	1 (1%)	61	74
6	9	132/132 (100%)	131 (99%)	1 (1%)	73	79
7	A	2033/2108 (96%)	1989 (98%)	44 (2%)	45	66
8	B	1541/1541 (100%)	1346 (87%)	195 (13%)	4	18
9	C	799/799 (100%)	794 (99%)	5 (1%)	78	81
10	D	106/106 (100%)	106 (100%)	0	100	100
12	F	110/110 (100%)	110 (100%)	0	100	100
13	G	54/55 (98%)	54 (100%)	0	100	100
14	H	410/838 (49%)	404 (98%)	6 (2%)	57	72
16	J	276/276 (100%)	274 (99%)	2 (1%)	76	80
17	K	246/247 (100%)	246 (100%)	0	100	100
18	L	130/130 (100%)	129 (99%)	1 (1%)	73	79
19	M	254/254 (100%)	253 (100%)	1 (0%)	84	84
20	N	263/263 (100%)	262 (100%)	1 (0%)	84	84
21	O	322/709 (45%)	320 (99%)	2 (1%)	78	81
22	P	94/203 (46%)	94 (100%)	0	100	100
23	R	21/21 (100%)	21 (100%)	0	100	100
24	S	275/751 (37%)	275 (100%)	0	100	100
25	T	213/749 (28%)	209 (98%)	4 (2%)	50	68
26	U	1202/1336 (90%)	1196 (100%)	6 (0%)	81	83
27	V	31/1085 (3%)	29 (94%)	2 (6%)	15	43
28	W	139/147 (95%)	138 (99%)	1 (1%)	76	80
29	Y	81/82 (99%)	81 (100%)	0	100	100
30	Z	25/25 (100%)	25 (100%)	0	100	100
31	b	62/75 (83%)	62 (100%)	0	100	100
31	k	75/75 (100%)	75 (100%)	0	100	100
32	c	236/520 (45%)	234 (99%)	2 (1%)	73	79
33	d	74/74 (100%)	74 (100%)	0	100	100
33	n	73/74 (99%)	73 (100%)	0	100	100
34	e	74/76 (97%)	74 (100%)	0	100	100
34	p	76/76 (100%)	76 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	f	61/61 (100%)	61 (100%)	0	100	100
35	q	61/61 (100%)	61 (100%)	0	100	100
36	g	63/63 (100%)	62 (98%)	1 (2%)	55	72
36	r	63/63 (100%)	61 (97%)	2 (3%)	34	60
37	h	75/75 (100%)	75 (100%)	0	100	100
37	l	75/75 (100%)	75 (100%)	0	100	100
38	i	133/133 (100%)	132 (99%)	1 (1%)	73	79
39	j	91/110 (83%)	91 (100%)	0	100	100
39	m	91/110 (83%)	91 (100%)	0	100	100
40	o	451/451 (100%)	448 (99%)	3 (1%)	76	80
41	s	152/196 (78%)	152 (100%)	0	100	100
42	t	111/435 (26%)	111 (100%)	0	100	100
42	u	106/435 (24%)	106 (100%)	0	100	100
42	v	111/435 (26%)	111 (100%)	0	100	100
42	w	106/435 (24%)	106 (100%)	0	100	100
43	y	129/129 (100%)	129 (100%)	0	100	100
44	z	29/29 (100%)	29 (100%)	0	100	100
All	All	11756/16654 (71%)	11468 (98%)	288 (2%)	42	65

5 of 288 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	B	2027	ASP
36	r	43	ASP
8	B	2077	ILE
16	J	323	VAL
8	B	750	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 197 such sidechains are listed below:

Mol	Chain	Res	Type
25	T	744	GLN
35	f	41	ASN
26	U	355	ASN
28	W	43	GLN

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Mol	Chain	Res	Type
39	j	39	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	117/189 (61%)	30 (25%)	5 (4%)
11	E	14/14 (100%)	5 (35%)	1 (7%)
15	I	39/113 (34%)	19 (48%)	2 (5%)
2	5	73/116 (62%)	24 (32%)	2 (2%)
3	6	96/106 (90%)	37 (38%)	5 (5%)
All	All	339/538 (63%)	115 (33%)	15 (4%)

5 of 115 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	16	U
1	2	17	U
1	2	19	G
1	2	20	G
1	2	24	A

5 of 15 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	6	5	U
15	I	90	C
3	6	33	G
15	I	95	U
3	6	58	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	SEP	K	232	17	8,9,10	1.63	1 (12%)	7,12,14	1.17	1 (14%)
17	SEP	K	224	17	8,9,10	1.60	1 (12%)	7,12,14	0.88	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
17	SEP	K	232	17	-	3/6/8/10	-
17	SEP	K	224	17	-	0/6/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	K	232	SEP	P-O1P	3.53	1.61	1.50
17	K	224	SEP	P-O1P	3.49	1.61	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	K	232	SEP	OG-CB-CA	2.46	110.54	108.14

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	K	232	SEP	CB-OG-P-O2P
17	K	232	SEP	CB-OG-P-O3P
17	K	232	SEP	CB-OG-P-O1P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
50	IHP	c	601	-	36,36,36	0.75	0	60,60,60	1.01	3 (5%)
47	ATP	7	702	45	32,33,33	1.22	4 (12%)	48,52,52	1.84	8 (16%)
48	GTP	C	1500	45	33,34,34	0.94	0	50,54,54	1.59	9 (18%)

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
50	IHP	c	601	-	-	6/30/54/54	0/1/1/1
47	ATP	7	702	45	-	0/22/38/38	0/3/3/3
48	GTP	C	1500	45	-	5/22/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	7	702	ATP	C4-N9	-3.20	1.31	1.37
47	7	702	ATP	PB-O3B	2.75	1.62	1.59
47	7	702	ATP	C5-N7	-2.12	1.35	1.39
47	7	702	ATP	PA-O3A	2.01	1.61	1.59

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	7	702	ATP	C5-C4-N3	-6.38	117.93	126.72
48	C	1500	GTP	C5-C4-N3	-4.88	120.63	128.39
48	C	1500	GTP	C2-N3-C4	4.56	120.16	112.30
47	7	702	ATP	N3-C2-N1	-4.16	122.29	128.58
47	7	702	ATP	N3-C4-N9	4.08	134.10	127.17

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
48	C	1500	GTP	C5'-O5'-PA-O3A
48	C	1500	GTP	C5'-O5'-PA-O1A
48	C	1500	GTP	C5'-O5'-PA-O2A
48	C	1500	GTP	C3'-C4'-C5'-O5'
48	C	1500	GTP	O4'-C4'-C5'-O5'

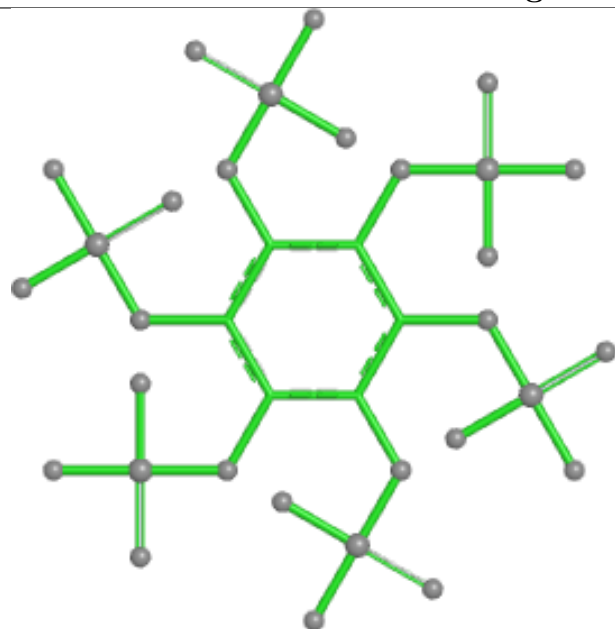
There are no ring outliers.

3 monomers are involved in 5 short contacts:

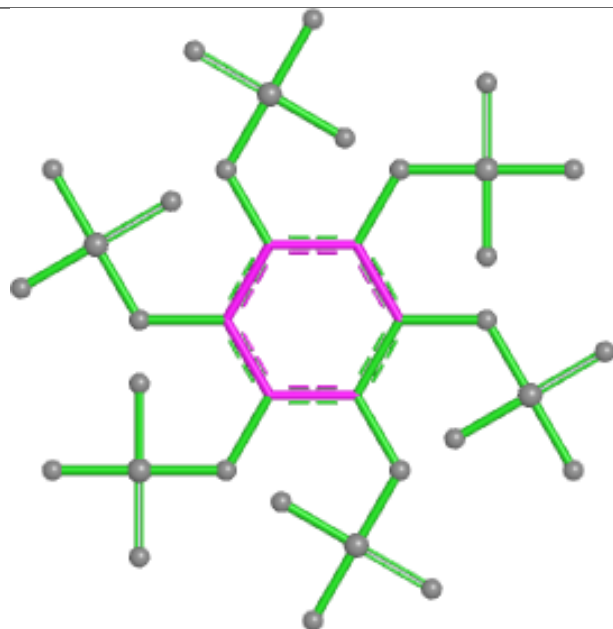
Mol	Chain	Res	Type	Clashes	Symm-Clashes
50	c	601	IHP	1	0
47	7	702	ATP	2	0
48	C	1500	GTP	2	0

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 than 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.

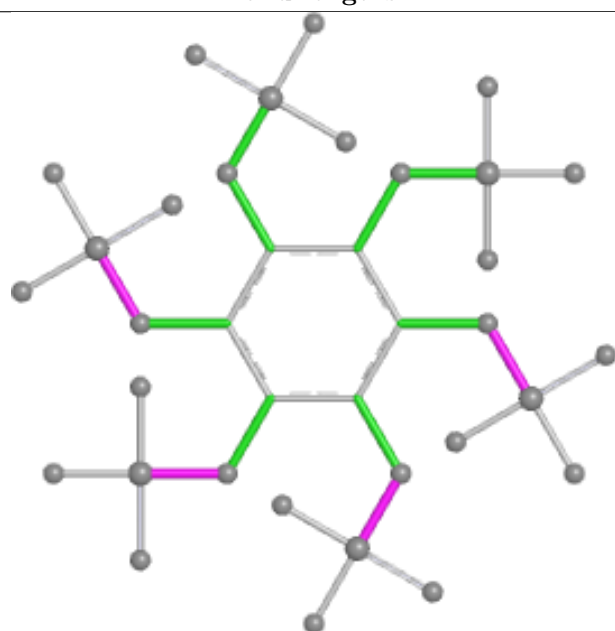
Ligand IHP c 601



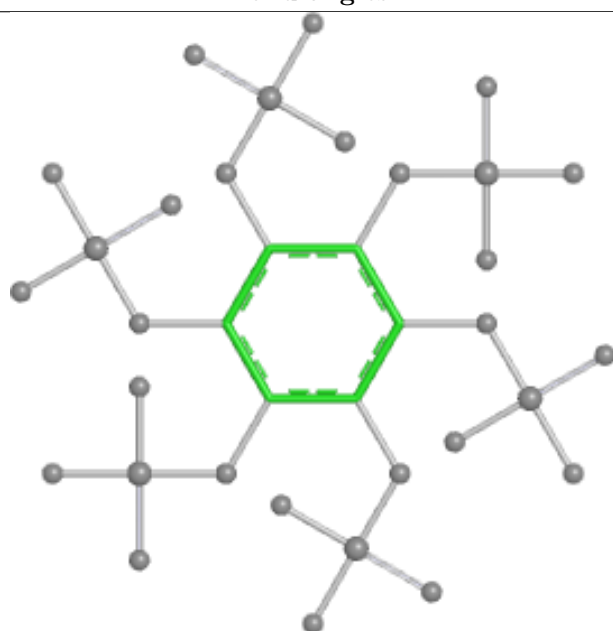
Bond lengths



Bond angles

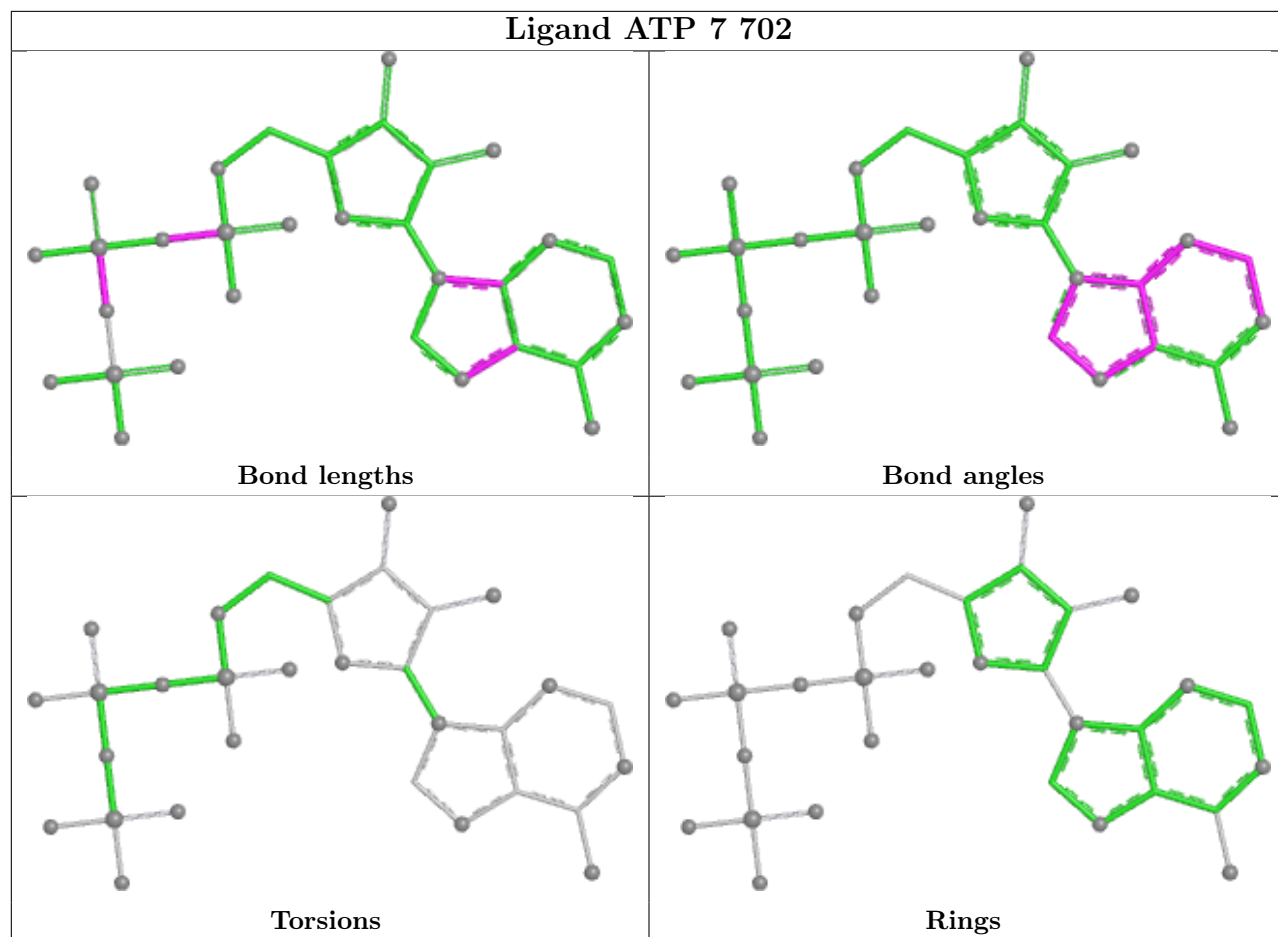


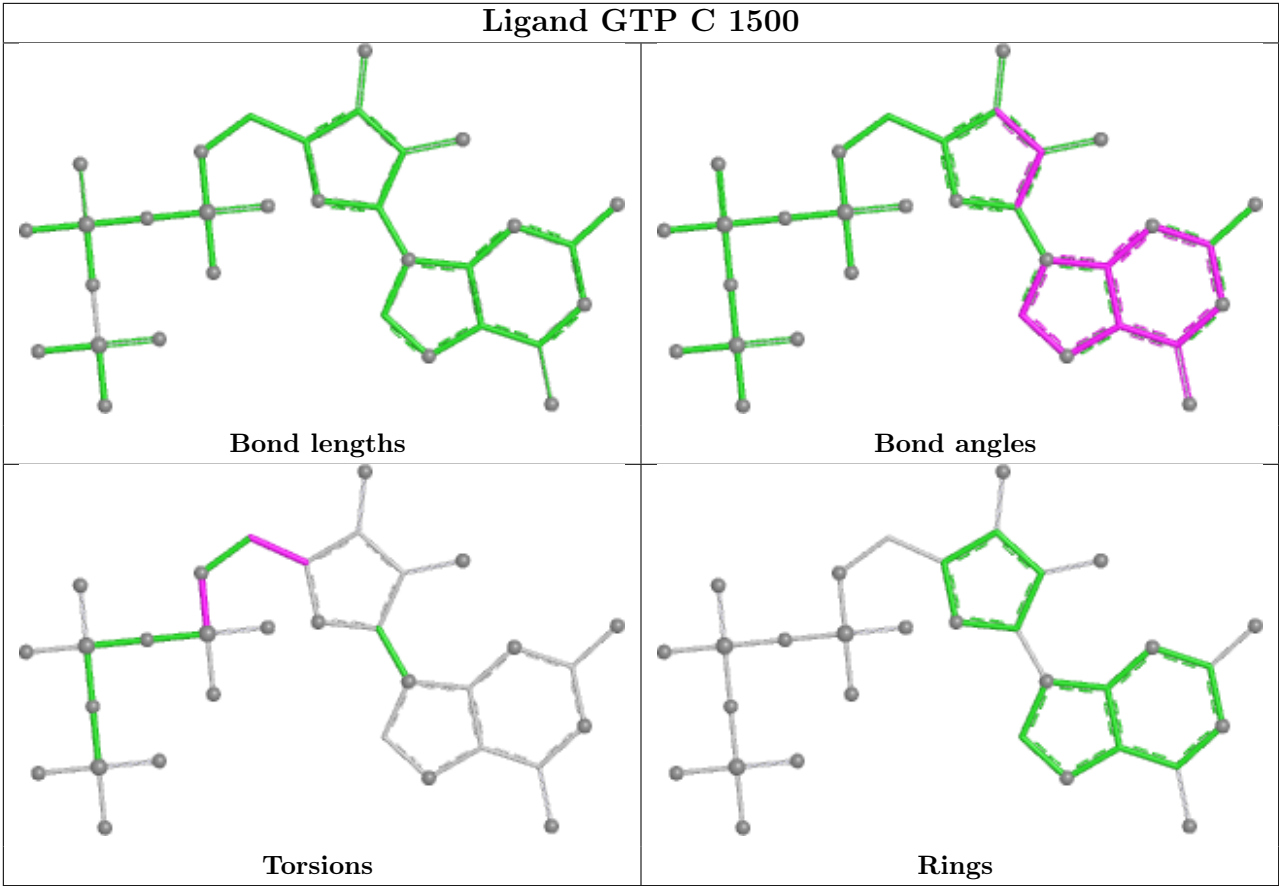
Torsions



Rings

Ligand ATP 7 702





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
15	I	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	83:A	O3'	84:U	P	83.48

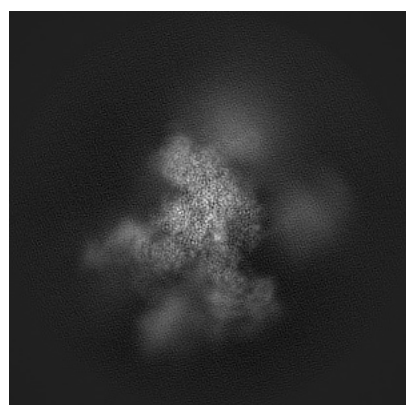
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4525. These allow visual inspection of the internal detail of the map and identification of artifacts.

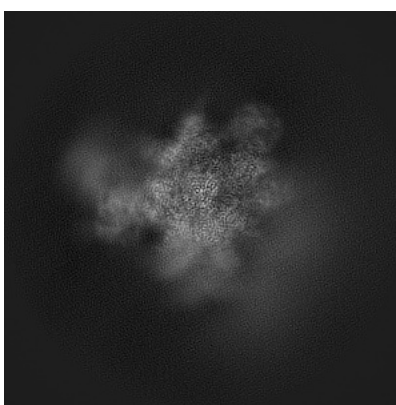
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

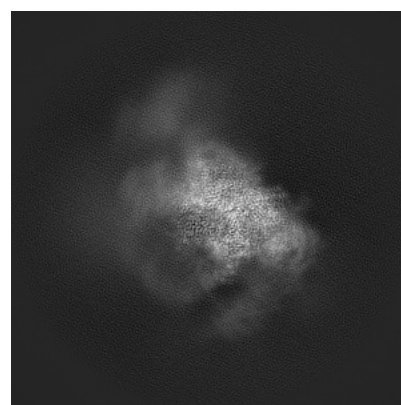
6.1.1 Primary map



X



Y

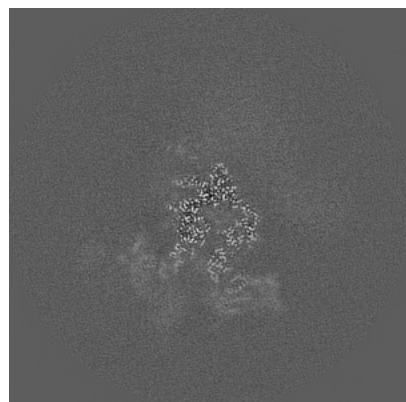


Z

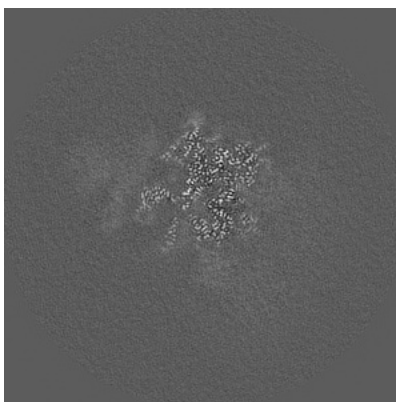
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

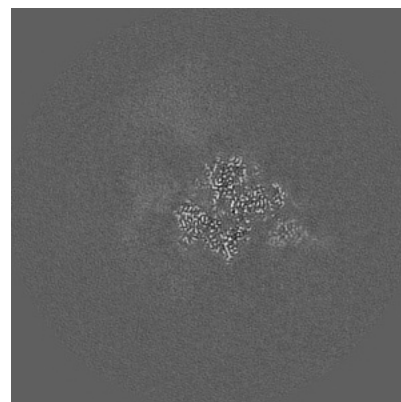
6.2.1 Primary map



X Index: 205



Y Index: 205

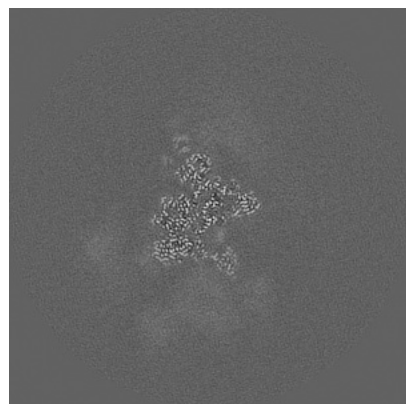


Z Index: 205

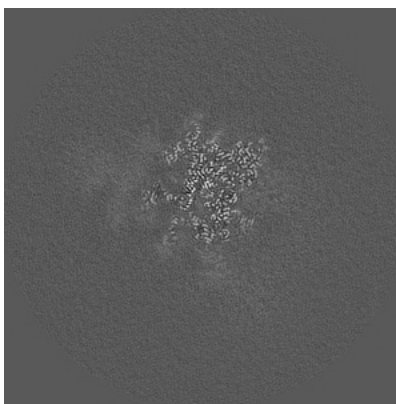
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

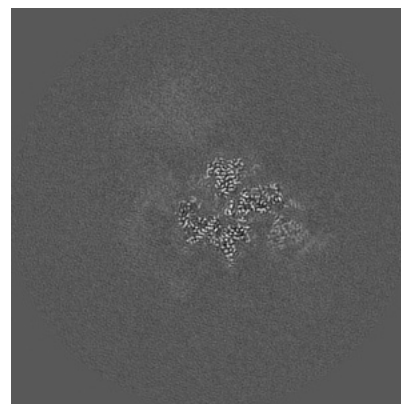
6.3.1 Primary map



X Index: 231



Y Index: 203

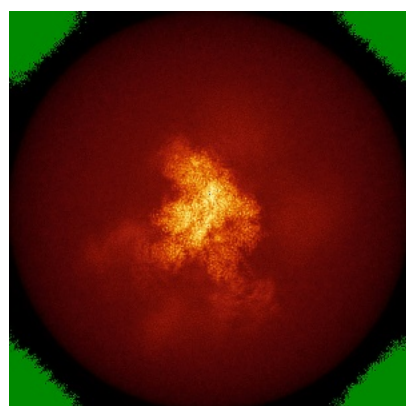


Z Index: 202

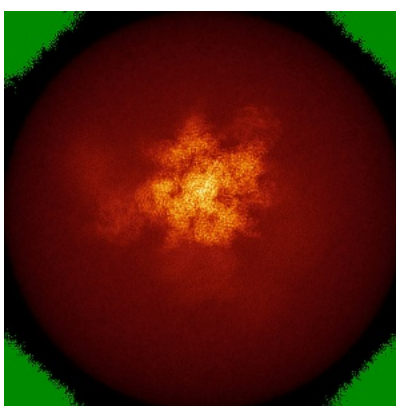
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

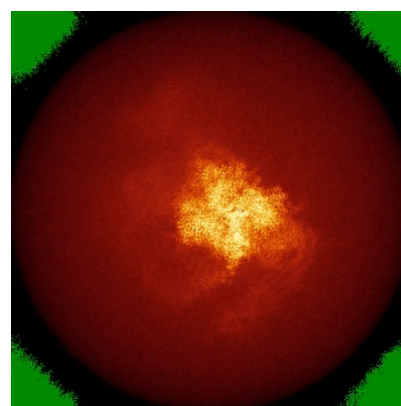
6.4.1 Primary map



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



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

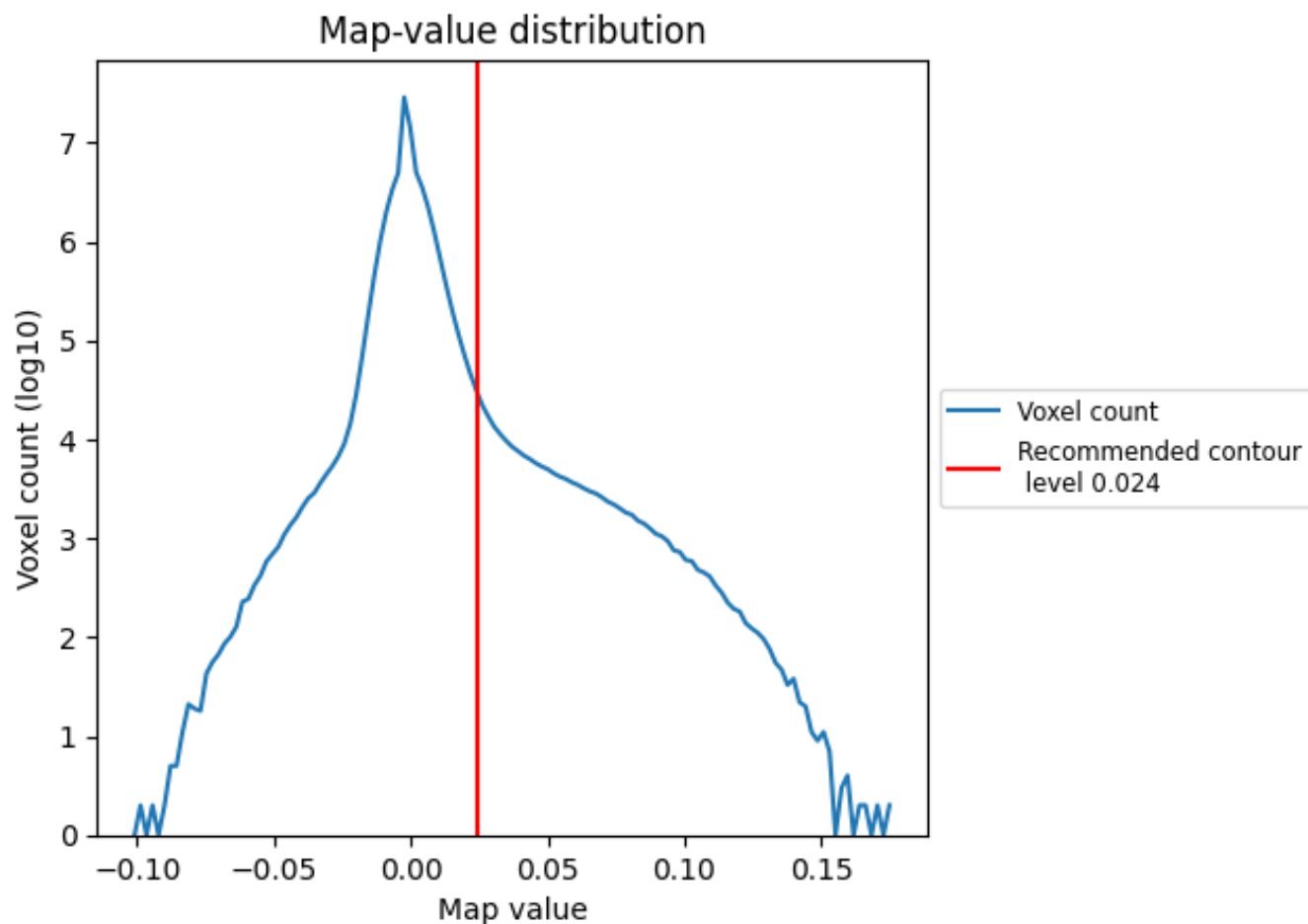
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

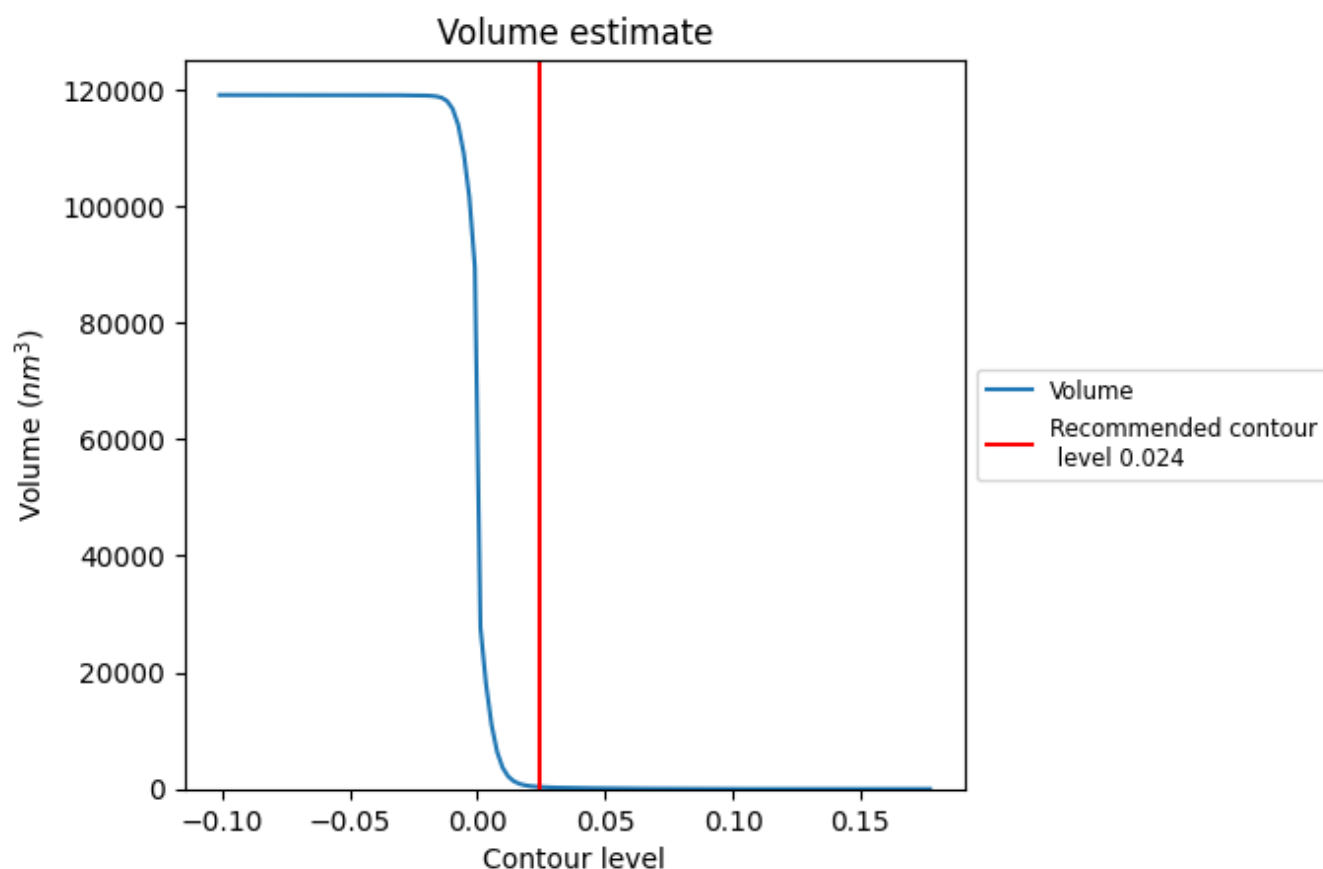
This section contains the results of statistical analysis of the map.

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.

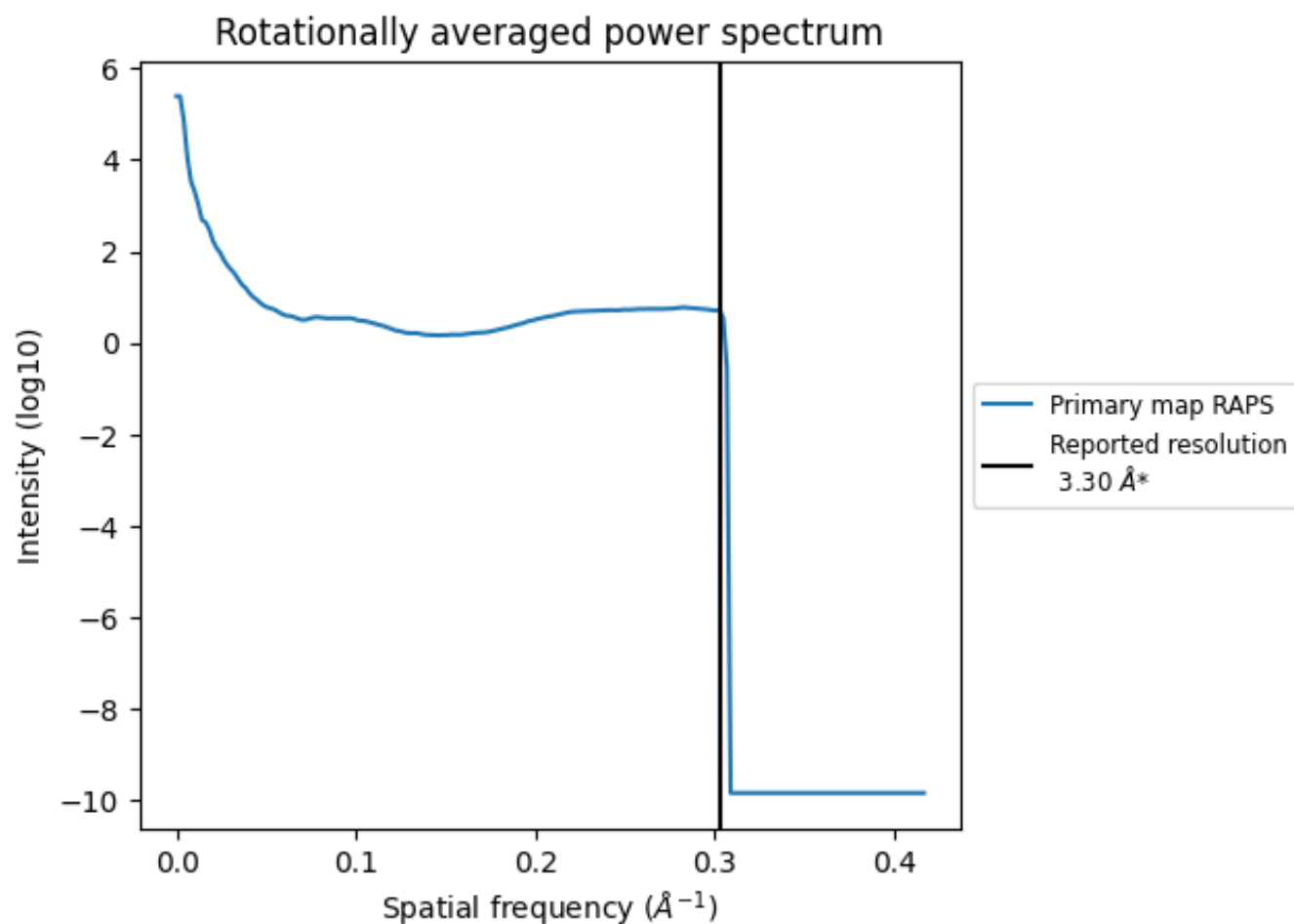
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 356 nm³; this corresponds to an approximate mass of 321 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

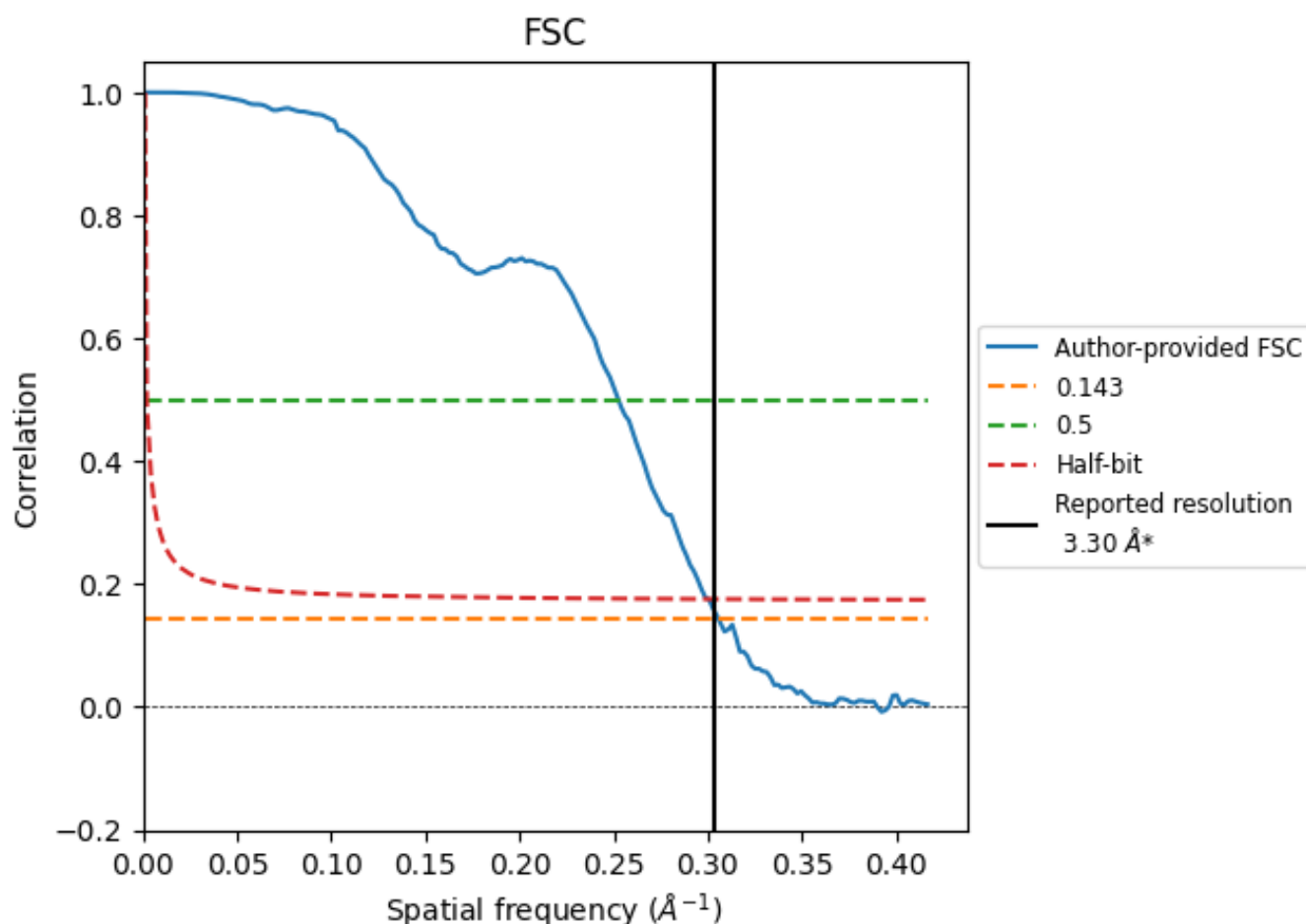


*Reported resolution corresponds to spatial frequency of 0.303 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

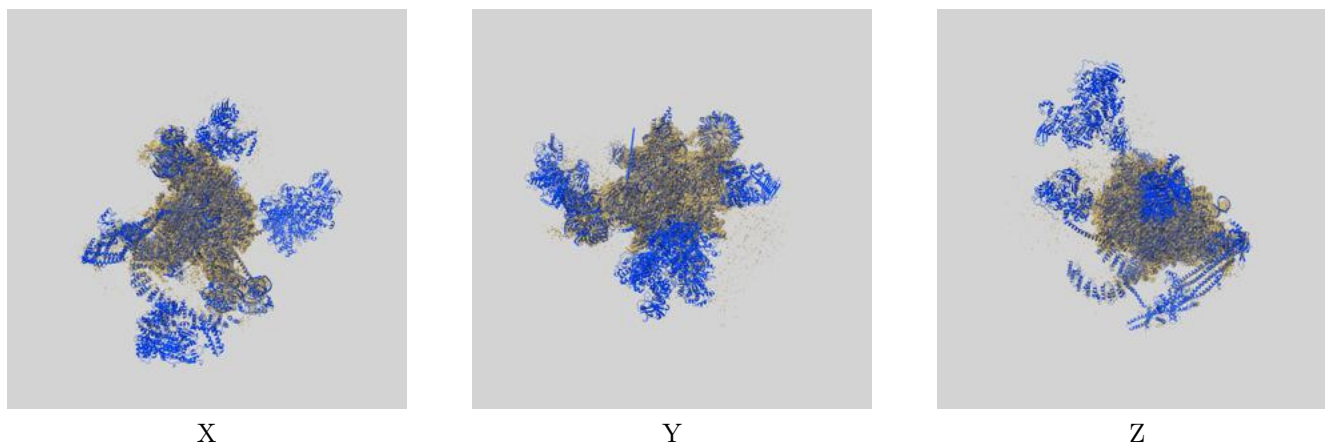
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.27	3.96	3.33
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

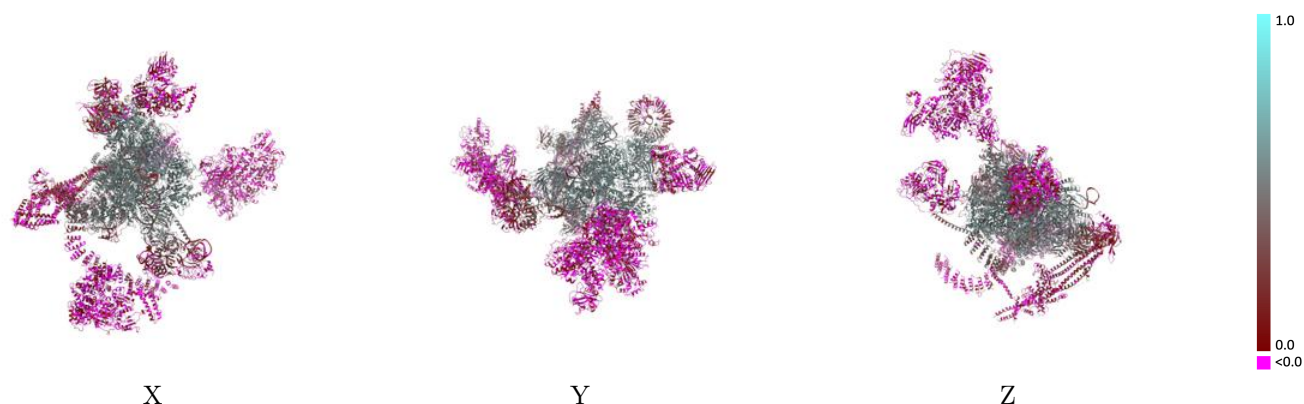
This section contains information regarding the fit between EMDB map EMD-4525 and PDB model 6QDV. Per-residue inclusion information can be found in [section 3](#) on [page 16](#).

9.1 Map-model overlay [i](#)



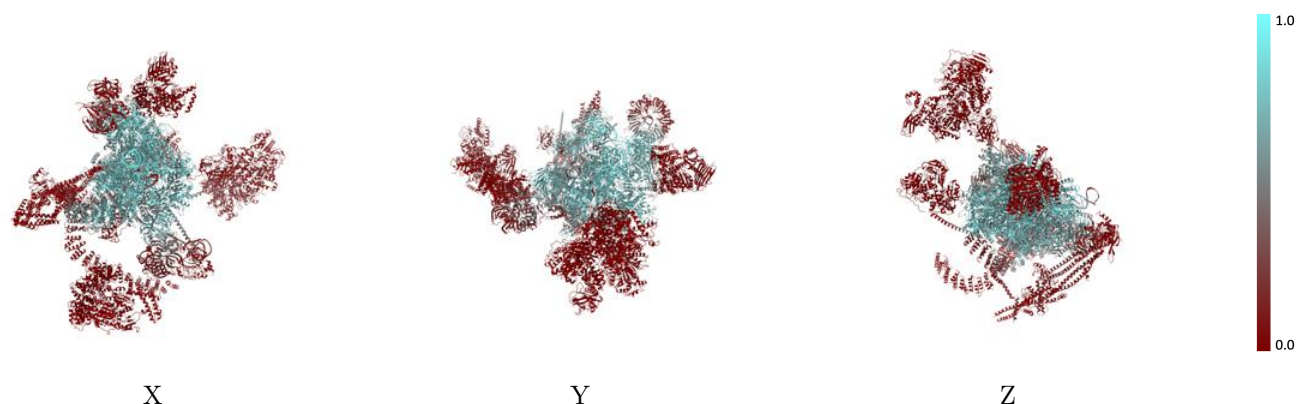
The images above show the 3D surface view of the map at the recommended contour level 0.024 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



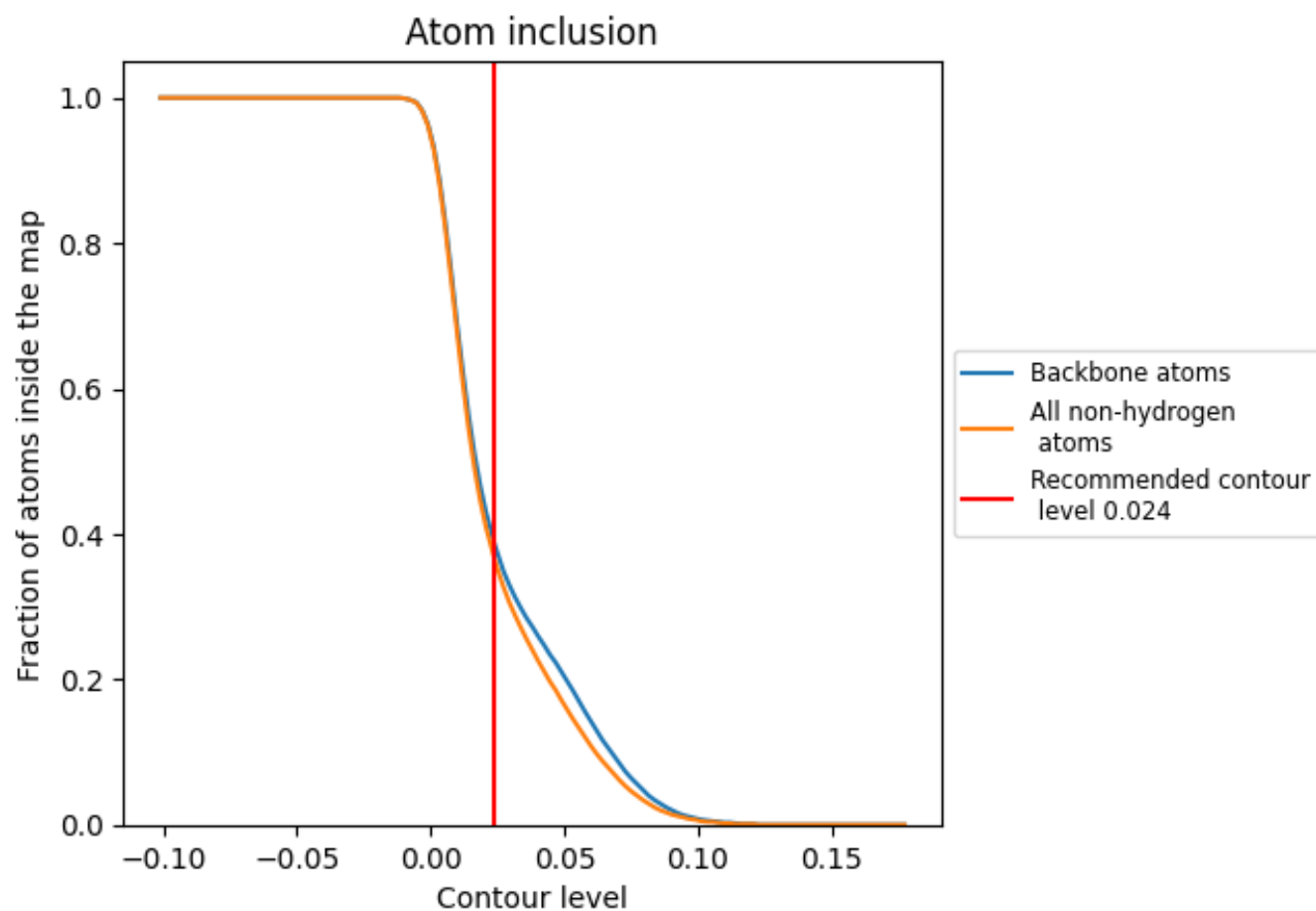
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.024).

9.4 Atom inclusion [i](#)



At the recommended contour level, 38% of all backbone atoms, 36% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.024) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3640	 0.2780
2	 0.4150	 0.2640
5	 0.7510	 0.4540
6	 0.7380	 0.4570
7	 0.0050	 0.0600
8	 0.0000	 -0.0230
9	 0.0000	 0.0230
A	 0.6840	 0.4780
B	 0.0010	 0.0020
C	 0.6850	 0.5010
D	 0.4080	 0.3490
E	 0.8410	 0.5300
F	 0.6280	 0.4670
G	 0.5770	 0.5060
H	 0.3250	 0.2530
I	 0.6040	 0.3950
J	 0.8350	 0.5600
K	 0.5780	 0.4700
L	 0.7400	 0.5240
M	 0.5150	 0.4410
N	 0.6240	 0.4720
O	 0.4300	 0.3550
P	 0.6530	 0.5150
R	 0.8340	 0.5500
S	 0.4420	 0.3340
T	 0.0660	 0.1560
U	 0.0010	 -0.0010
V	 0.0730	 0.0630
W	 0.0210	 0.0440
Y	 0.0480	 0.0930
Z	 0.6520	 0.5040
b	 0.2810	 0.2660
c	 0.6520	 0.4960
d	 0.4340	 0.3790
e	 0.0740	 0.1380



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Chain	Atom inclusion	Q-score
f	 0.0420	 0.1010
g	 0.2160	 0.2880
h	 0.1070	 0.1720
i	 0.5730	 0.4500
j	 0.0500	 0.0950
k	 0.2060	 0.2370
l	 0.1230	 0.1500
m	 0.0610	 0.0830
n	 0.3690	 0.3190
o	 0.6620	 0.4960
p	 0.2240	 0.2290
q	 0.1140	 0.1190
r	 0.3480	 0.3330
s	 0.0730	 0.1200
t	 0.0260	 0.0690
u	 0.0160	 0.0240
v	 0.0240	 0.1160
w	 0.0100	 0.0760
y	 0.6400	 0.4900
z	 0.0110	 0.1960