



## wwPDB EM Validation Summary Report ⓘ

Nov 4, 2024 – 02:16 AM JST

PDB ID : 6ICZ  
EMDB ID : EMD-9645  
Title : Cryo-EM structure of a human post-catalytic spliceosome (P complex) at 3.0 angstrom  
Authors : Zhang, X.; Zhan, X.; Yan, C.; Shi, Y.  
Deposited on : 2018-09-07  
Resolution : 3.00 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](mailto: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>.

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

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



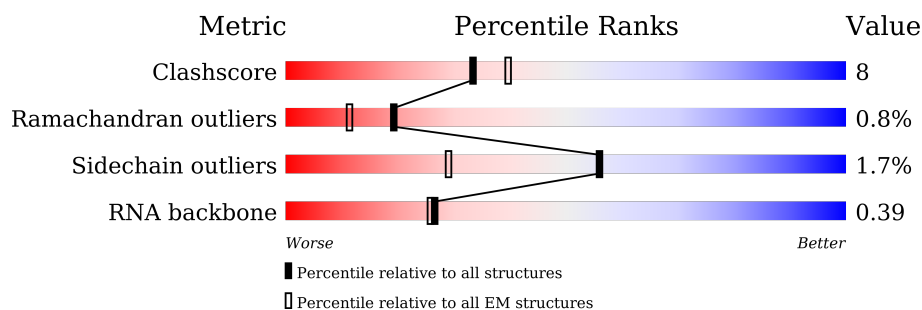
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.00 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




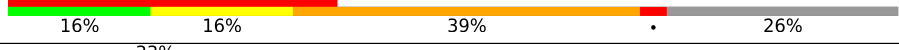

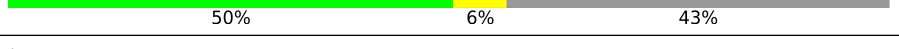
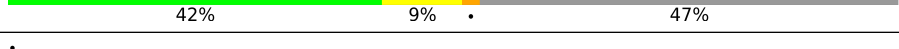
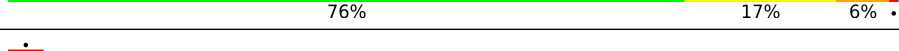
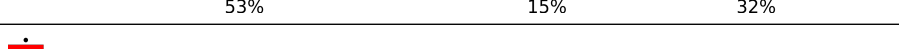
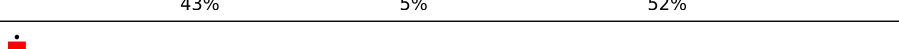
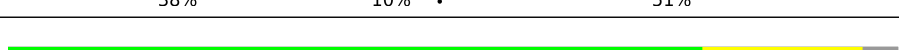
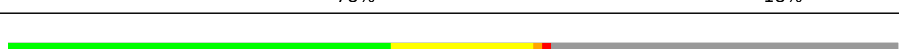

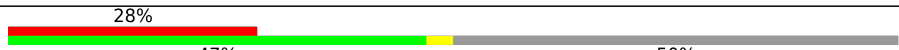
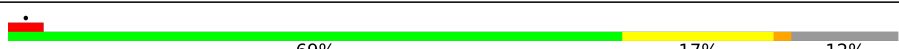





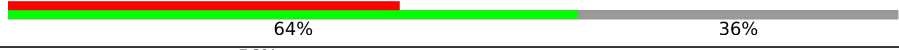




The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey 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	v	148	<div> <div>97%</div> <div>97%</div> <div>.</div> </div>
2	w	174	<div> <div>52%</div> <div>51%</div> <div>48%</div> <div>..</div> </div>
3	u	411	<div> <div>94%</div> <div>93%</div> <div>6%</div> <div>.</div> </div>
4	x	703	<div> <div>96%</div> <div>.</div> </div>
5	A	2335	<div> <div>12%</div> <div>81%</div> <div>15%</div> <div>.</div> </div>
6	B	117	<div> <div>14%</div> <div>26%</div> <div>38%</div> <div>17%</div> <div>17%</div> <div>.</div> </div>
7	C	972	<div> <div>74%</div> <div>17%</div> <div>8%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
8	E	357	
9	F	107	
10	G	273	
11	H	188	
12	J	848	
13	L	802	
14	M	243	
15	N	144	
16	O	420	
17	P	229	
18	R	536	
19	S	166	
20	T	514	
21	U	2752	
22	V	908	
23	W	579	
24	X	184	
25	Z	586	
26	I	855	
27	y	301	
28	Q	1485	
29	a	126	
29	h	126	
30	b	231	
30	i	231	

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Mol	Chain	Length	Quality of chain
31	c	119	
31	j	119	
32	d	118	
32	k	118	
33	f	86	
33	m	86	
34	e	92	
34	l	92	
35	g	76	
35	n	76	
36	o	255	
37	p	225	
38	Y	1220	
39	K	225	
40	q	504	
40	r	504	
40	s	504	
40	t	504	
41	D	2136	



## 2 Entry composition [i](#)

There are 46 unique types of molecules in this entry. The entry contains 97900 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 Protein mago nashi homolog 2.

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

- Molecule 2 is a protein called RNA-binding protein 8A.

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

- Molecule 3 is a protein called Eukaryotic initiation factor 4A-III.

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

- Molecule 4 is a protein called Protein CASC3.

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

- Molecule 5 is a protein called Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	2253	Total	C	N	O	S	0	0
			17837	11432	3157	3177	71		

- Molecule 6 is a RNA chain called U5snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	97	Total	C	N	O	P	0	0
			2040	914	339	690	97		



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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	894	Total	C	N	O	S	0	0
			7066	4520	1178	1334	34		

- Molecule 8 is a protein called U5 small nuclear ribonucleoprotein 40 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	303	Total	C	N	O	S	0	0
			2366	1487	415	451	13		

- Molecule 9 is a RNA chain called U6snRNA.

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

- Molecule 10 is a RNA chain called pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	84	Total	C	N	O	P	0	0
			1549	684	218	563	84		

- Molecule 11 is a RNA chain called U2snRNA.

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

- Molecule 12 is a protein called Crooked neck-like protein 1.

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

- Molecule 13 is a protein called Cell division cycle 5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	454	Total	C	N	O	S	0	0
			3064	1884	596	578	6		

- Molecule 14 is a protein called Pre-mRNA-splicing factor SYF2.



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

- Molecule 15 is a protein called Protein BUD31 homolog.

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

- Molecule 16 is a protein called Pre-mRNA-splicing factor RBM22.

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

- Molecule 17 is a protein called Spliceosome-associated protein CWC15 homolog.

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

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

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

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

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

- Molecule 20 is a protein called Pleiotropic regulator 1.

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

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



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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	452	Total	C	N	O	S	0	0
			2765	1723	508	523	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	508	Total	C	N	O	S	0	0
			4122	2623	714	761	24		

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

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

- Molecule 25 is a protein called Pre-mRNA-splicing factor SLU7.

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

- Molecule 26 is a protein called Pre-mRNA-splicing factor SYF1.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	I	564	Total	C	N	O	0	0
			2782	1654	564	564		

- Molecule 27 is a protein called Peptidyl-prolyl cis-trans isomerase E.

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

- Molecule 28 is a protein called RNA helicase aquarius.



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

- Molecule 29 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	h	81	Total	C	N	O	0	0
			398	236	81	81		
29	a	81	Total	C	N	O	0	0
			399	237	81	81		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
30	i	86	Total	C	N	O	0	0
			424	252	86	86		
30	b	86	Total	C	N	O	0	0
			424	252	86	86		

- Molecule 31 is a protein called Small nuclear ribonucleoprotein Sm D1.

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

- Molecule 32 is a protein called Small nuclear ribonucleoprotein Sm D2.

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
33	m	73	Total	C	N	O	0	0
			356	210	73	73		
33	f	74	Total	C	N	O	0	0
			361	213	74	74		



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

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
35	n	69	Total	C	N	O	0	0
			339	201	69	69		
35	g	74	Total	C	N	O	0	0
			363	215	74	74		

- Molecule 36 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	o	162	Total	C	N	O	0	0
			804	480	162	162		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
37	p	94	Total	C	N	O	0	0
			464	276	94	94		

- Molecule 38 is a protein called ATP-dependent RNA helicase DHX8.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Y	713	Total	C	N	O	S	0	0
			2917	1486	716	714	1		

- Molecule 39 is a protein called Pre-mRNA-splicing factor SPF27.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	K	152	Total	C	N	O	0	0
			757	453	152	152		

- Molecule 40 is a protein called Pre-mRNA-processing factor 19.

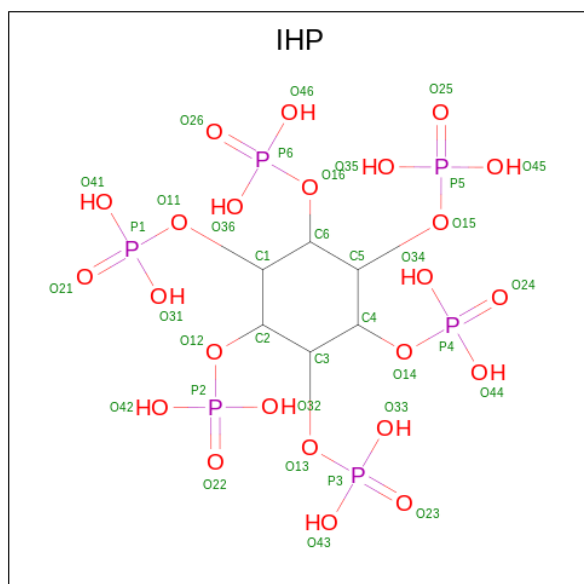


Mol	Chain	Residues	Atoms				AltConf	Trace
40	q	132	Total 659	C 395	N 132	O 132	0	0
40	r	131	Total 654	C 392	N 131	O 131	0	0
40	s	67	Total 335	C 201	N 67	O 67	0	0
40	t	67	Total 335	C 201	N 67	O 67	0	0

- Molecule 41 is a protein called U5 small nuclear ribonucleoprotein 200 kDa helicase.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	D	1722	Total	C	N	O	0	0
			8530	5086	1722	1722		

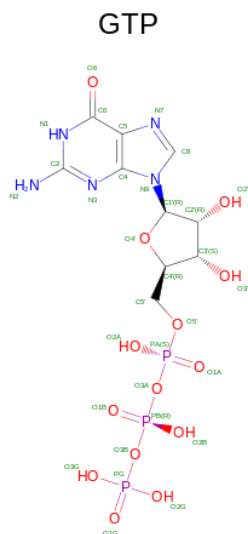
- Molecule 42 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula:  $\text{C}_6\text{H}_{18}\text{O}_{24}\text{P}_6$ ).



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

- Molecule 43 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula:  $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{14}\text{P}_3$ ).





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

- Molecule 44 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

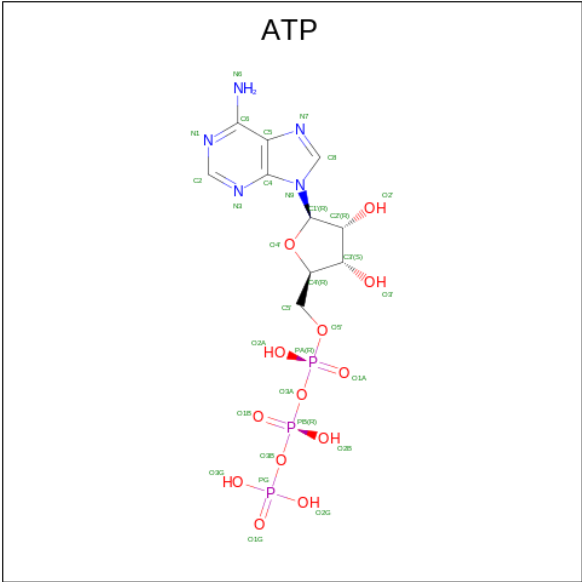
Mol	Chain	Residues	Atoms	AltConf
44	C	1	Total Mg 1 1	0
44	F	6	Total Mg 6 6	0
44	Q	2	Total Mg 2 2	0

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

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

- Molecule 46 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{13}\text{P}_3$ ).





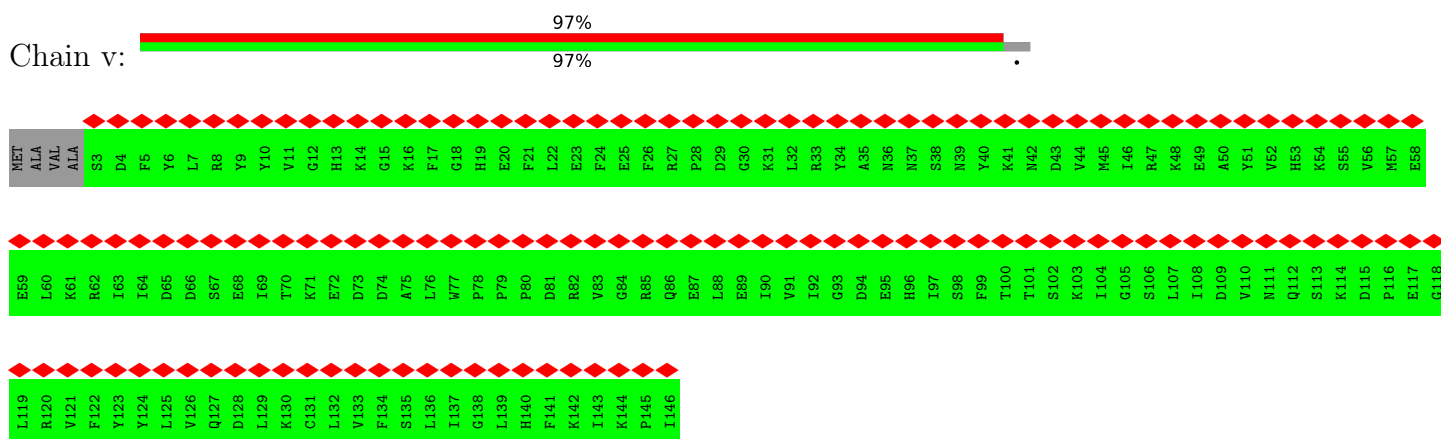
Mol	Chain	Residues	Atoms					AltConf
46	Q	1	Total	C	N	O	P	0
			31	10	5	13	3	



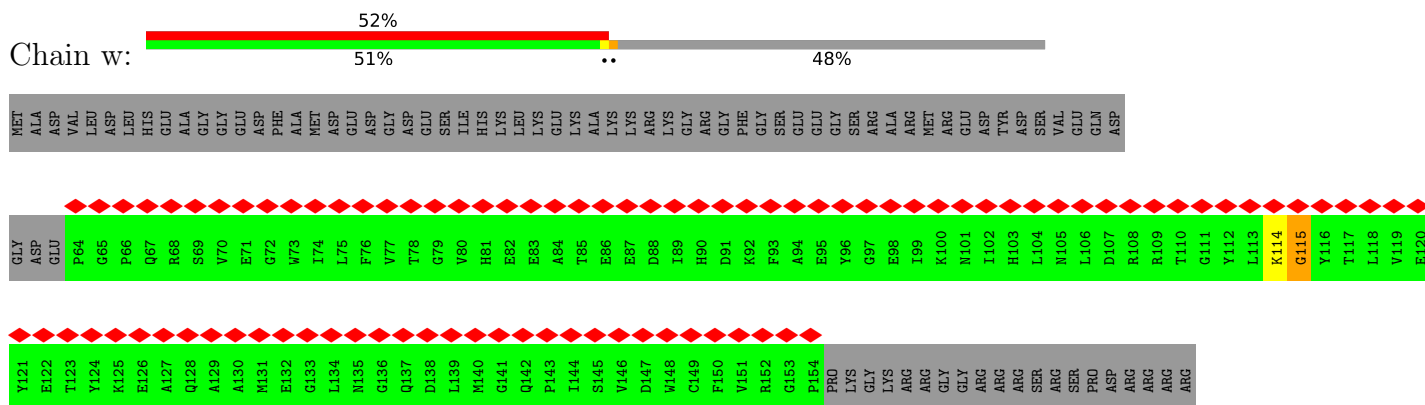
### 3 Residue-property plots

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

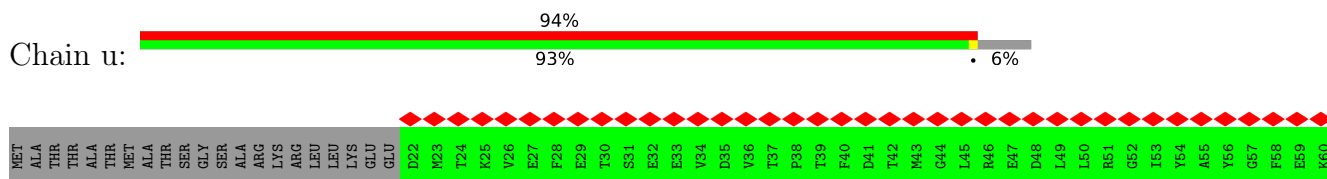
#### • Molecule 1: Protein mago nashi homolog 2



#### • Molecule 2: RNA-binding protein 8A



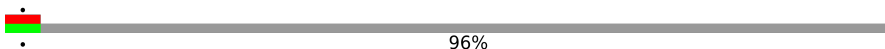
#### • Molecule 3: Eukaryotic initiation factor 4A-III





- Molecule 4: Protein CASC3

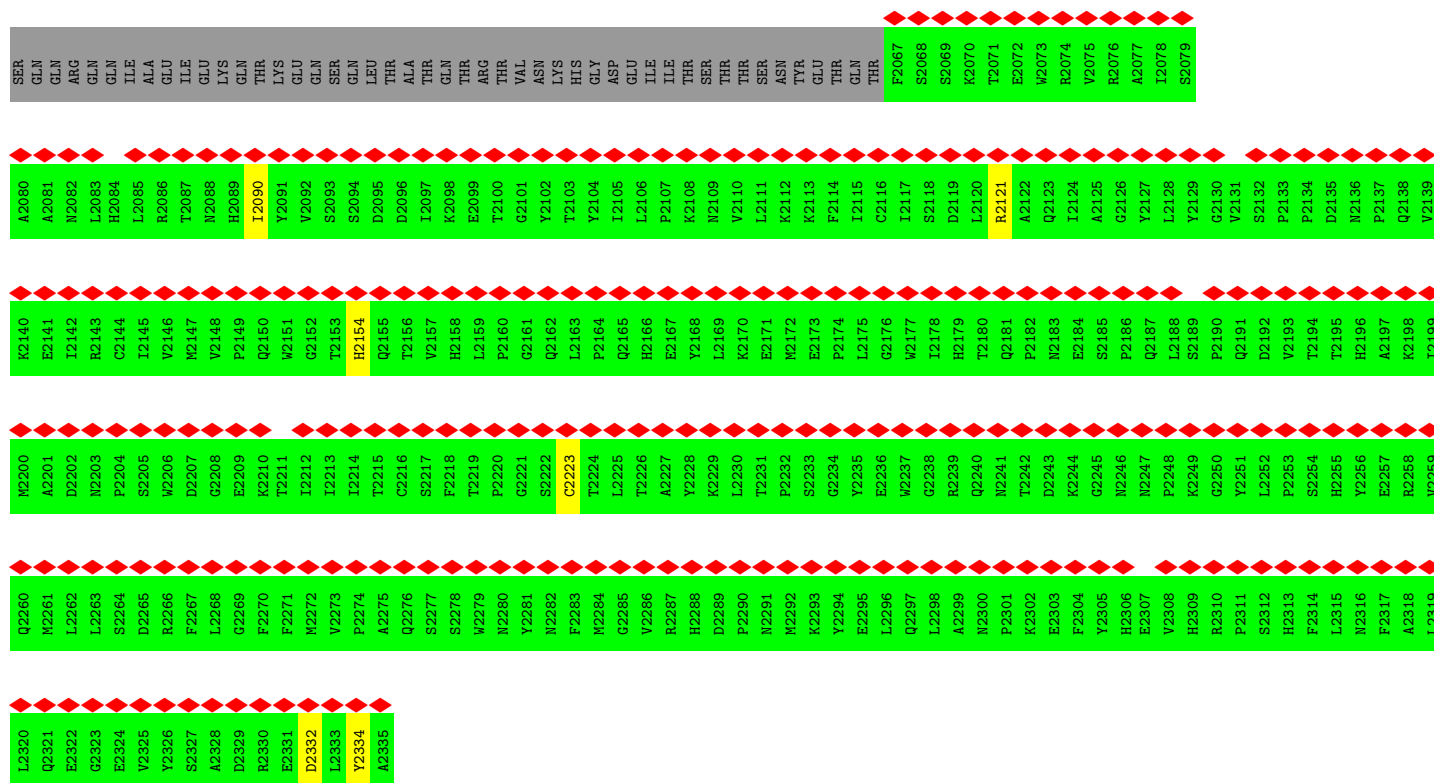
Chain x:

[illegible]

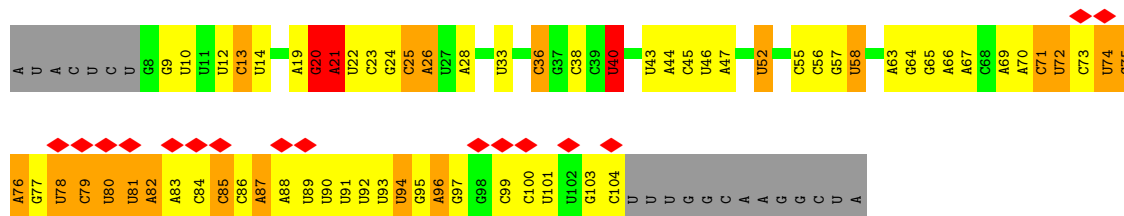
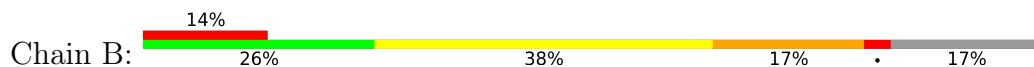




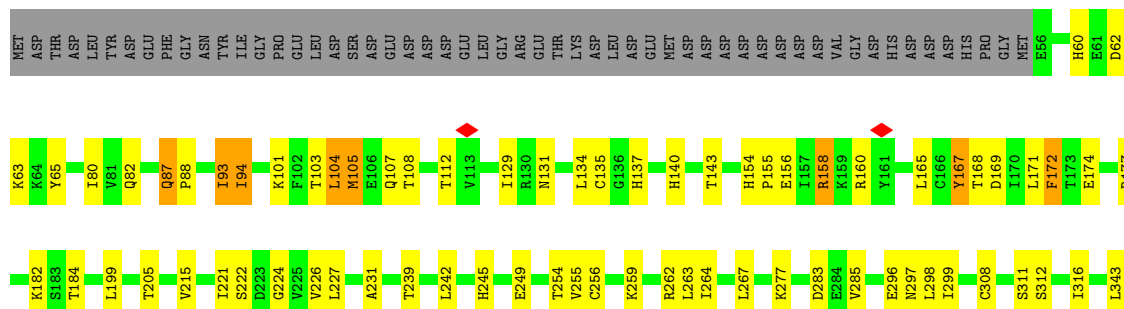
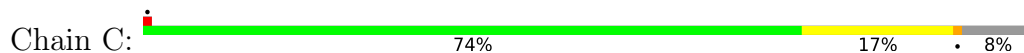




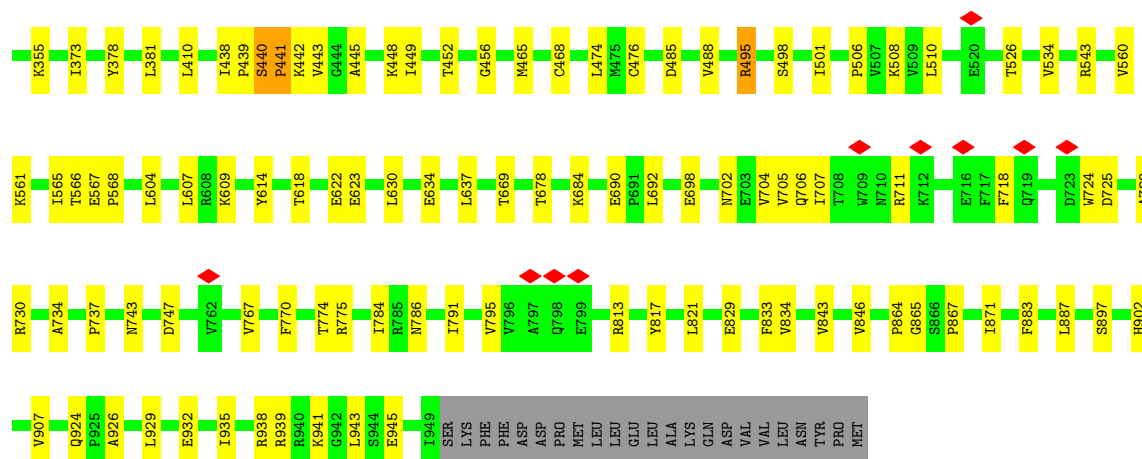
• Molecule 6: U5snRNA



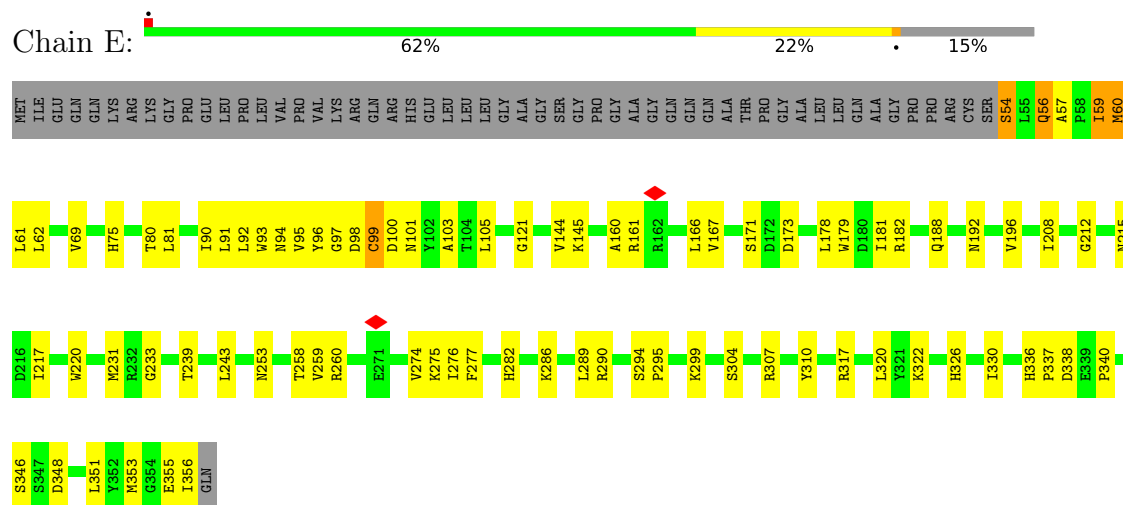
• Molecule 7: 116 kDa U5 small nuclear ribonucleoprotein component



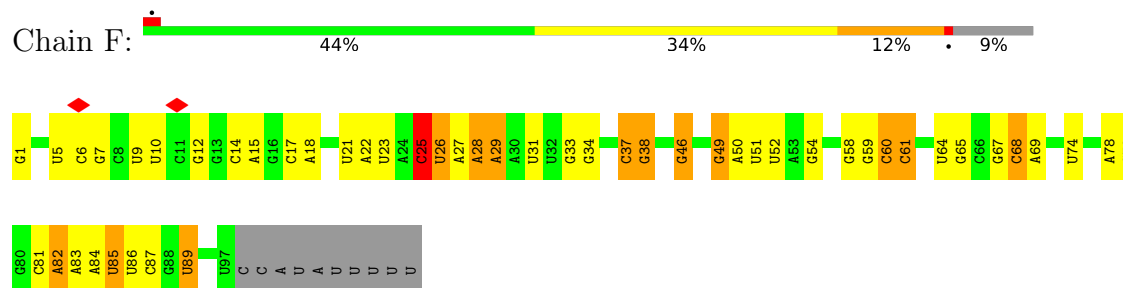




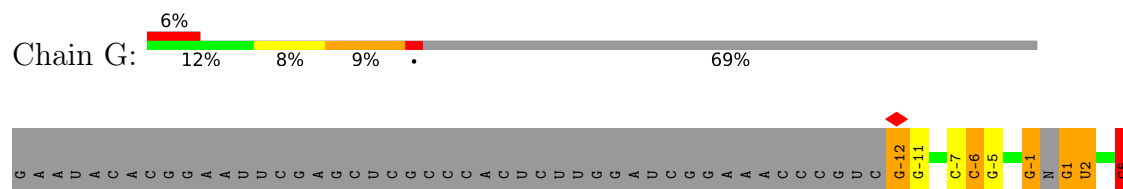
- Molecule 8: U5 small nuclear ribonucleoprotein 40 kDa protein



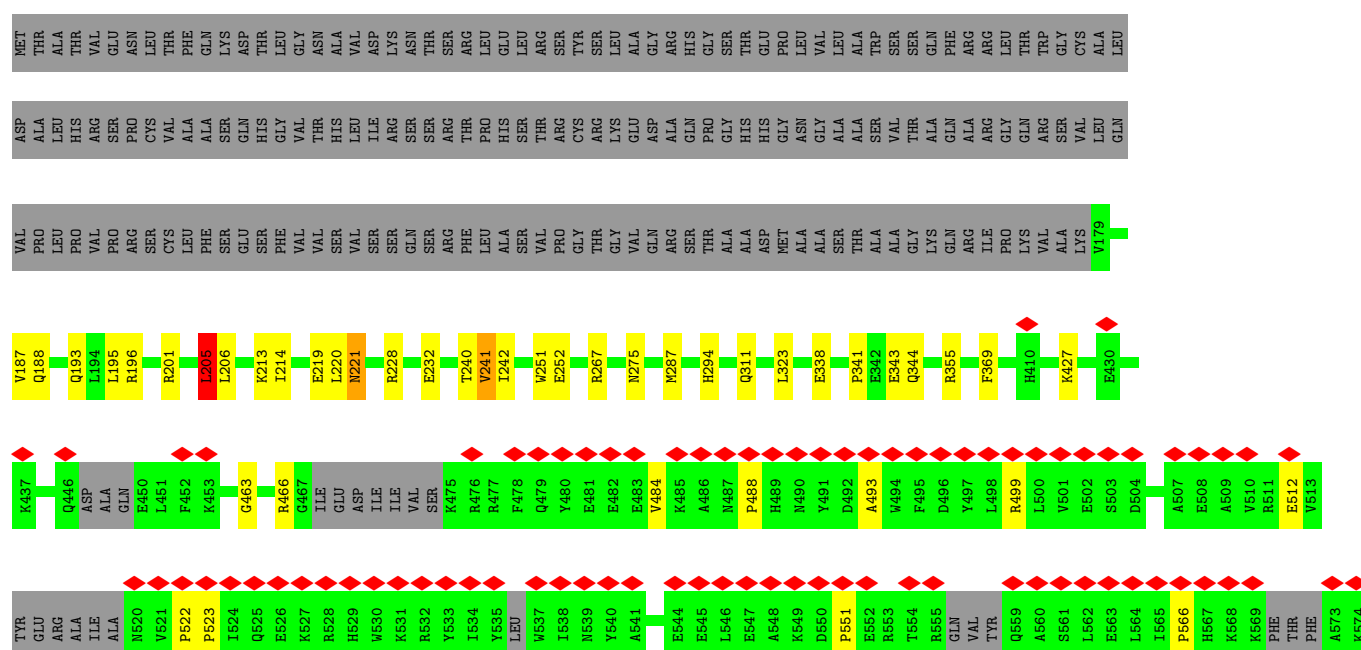
- Molecule 9: U6snRNA



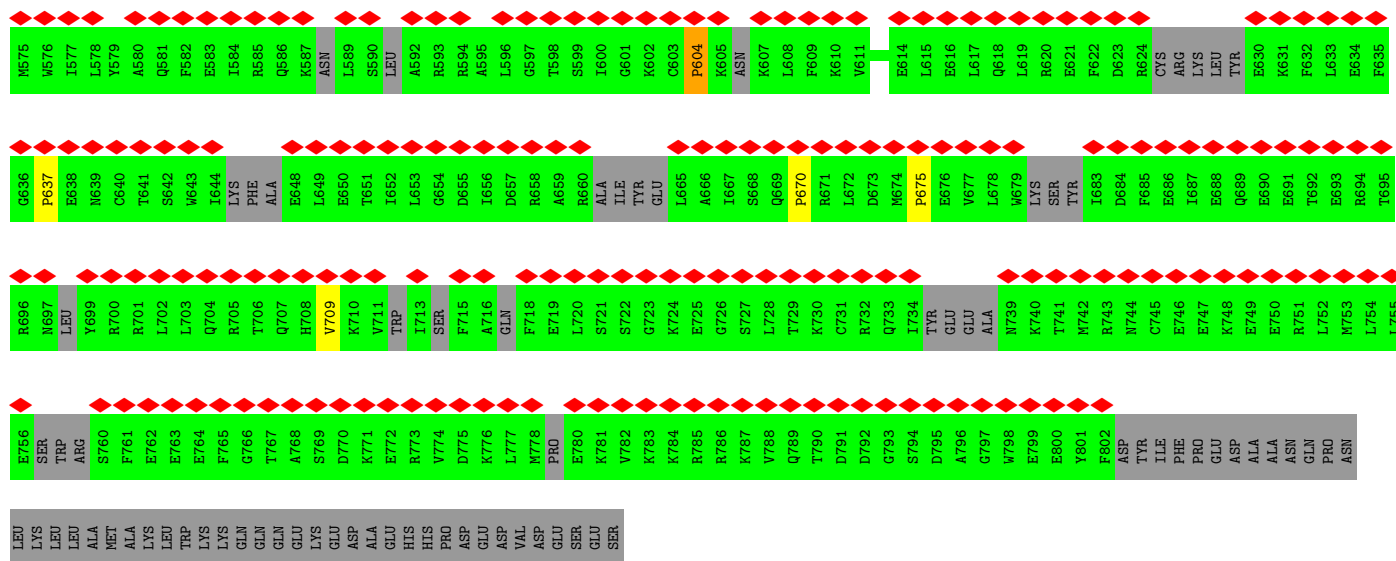
- Molecule 10: pre-mRNA



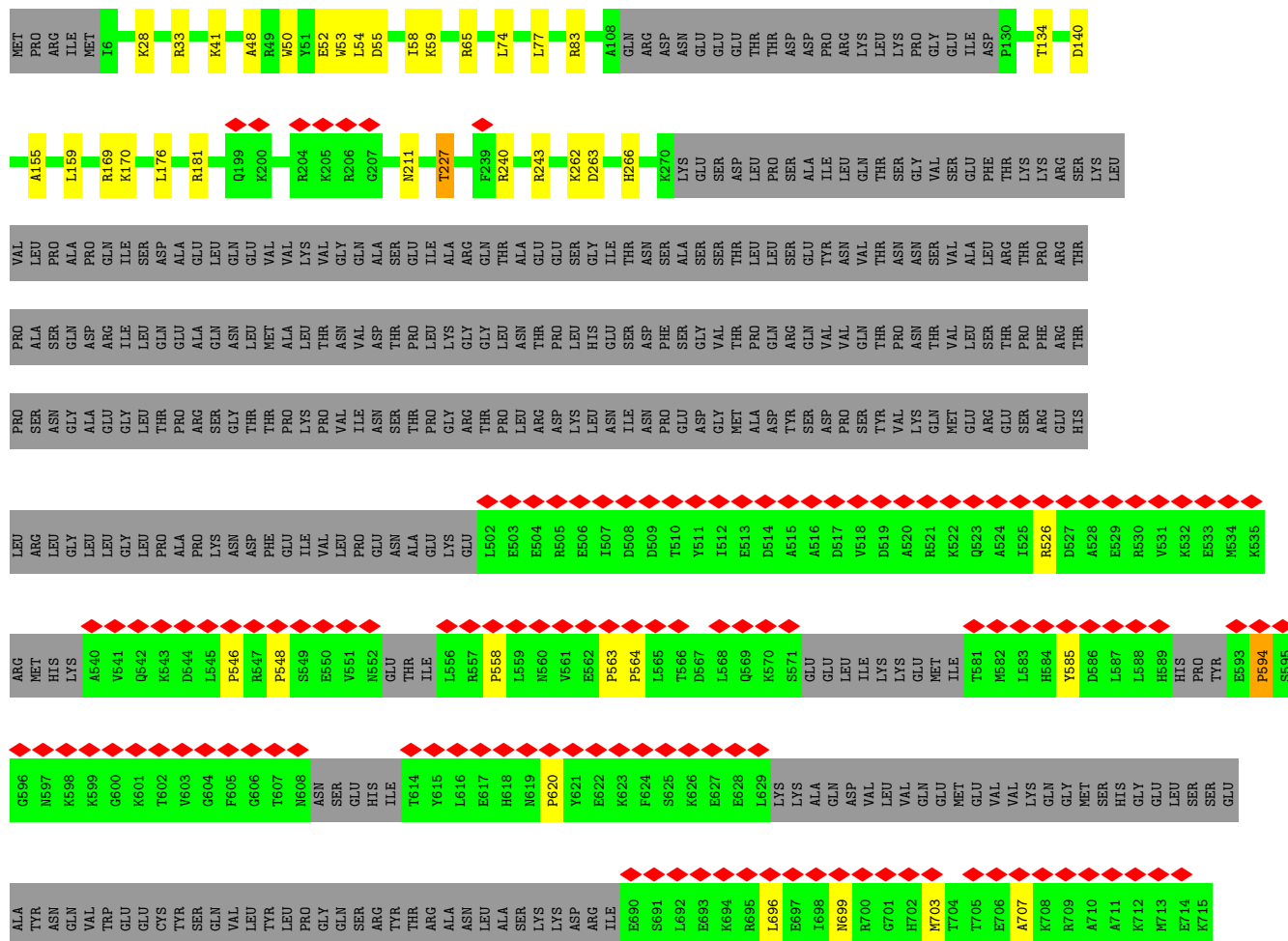




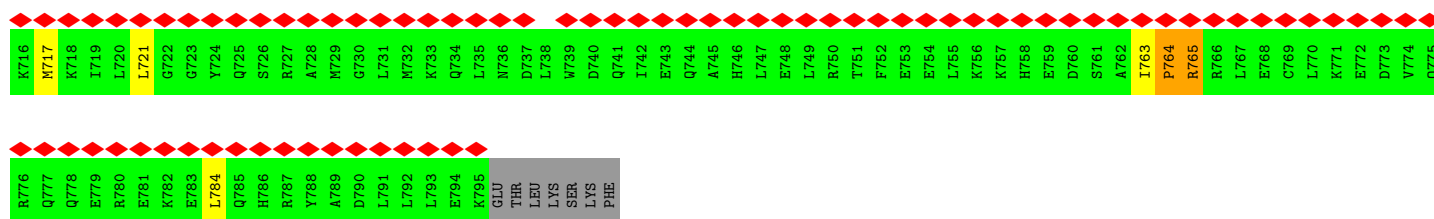




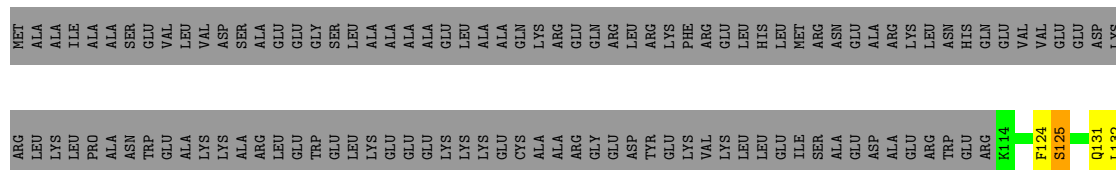
### • Molecule 13: Cell division cycle 5-like protein



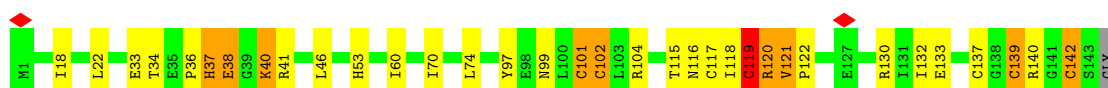




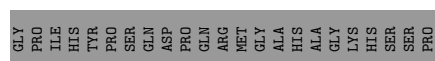
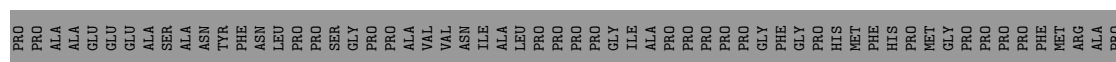
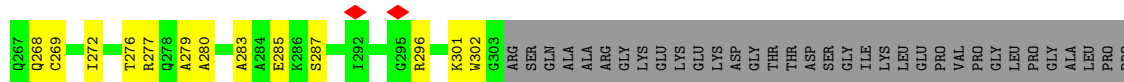
• Molecule 14: Pre-mRNA-splicing factor SYF2



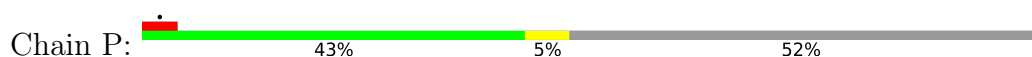
• Molecule 15: Protein BUD31 homolog



• Molecule 16: Pre-mRNA-splicing factor RBM22

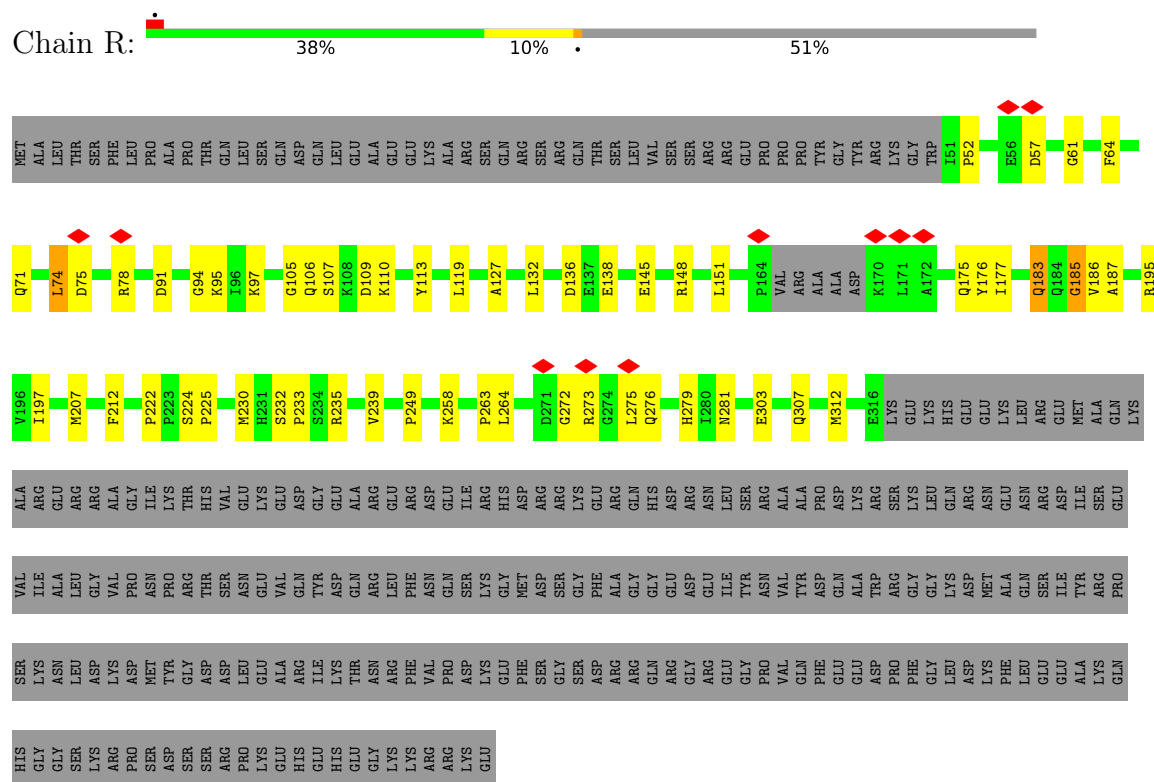


• Molecule 17: Spliceosome-associated protein CWC15 homolog

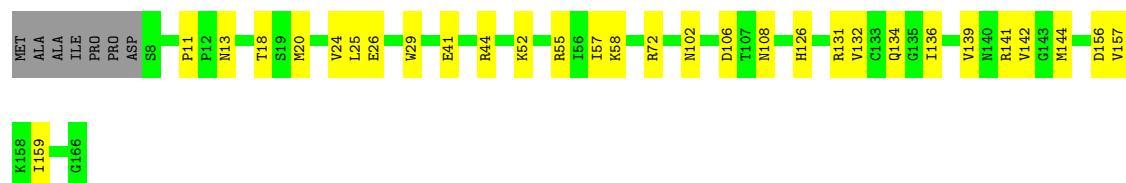
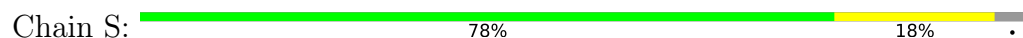




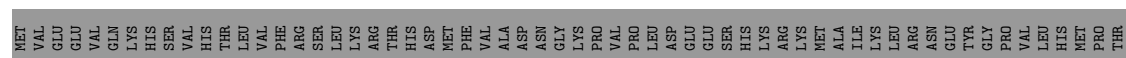
- Molecule 18: SNW domain-containing protein 1



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



- Molecule 20: Pleiotropic regulator 1













[illegible]

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

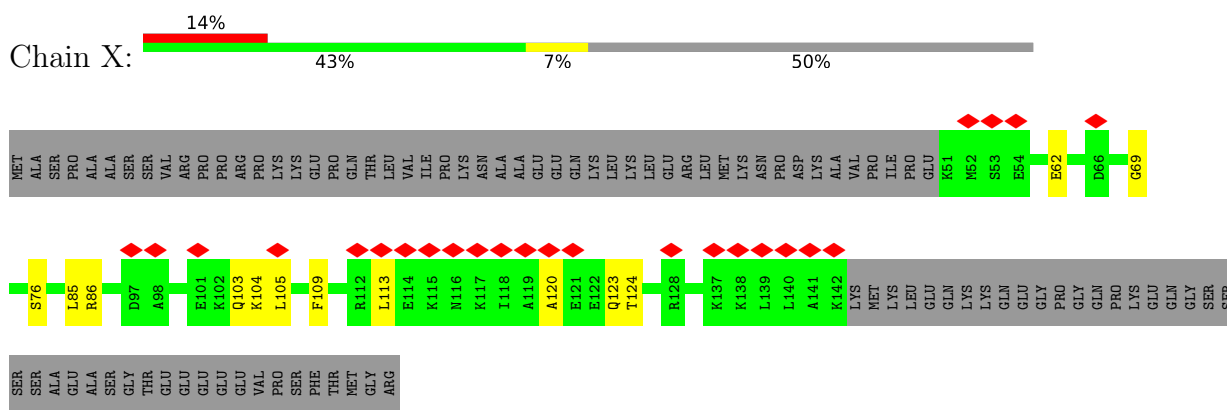


I181	I182	Q183	E184	L185	L186	Q187	E188	N189	I190	V191	R192	G193	R194	G195	L196	L197	S198	R199	S200	L202	Q203	A204	Q205	S206	A207	S208	P209	I210	F211	T212	H213	V214	Y215	A216	A217	L218	V219	A220	I221	I222	N223	S224	K225	F226				
LEU	ASP	PRO	LEU	LEU	THR	ARG	THR	THR	GLY	ALA	PRO	PRO	ALA	LYS	LEU	ARG	MET	GLN	GLU	GLN	ASP	K149	N150	S151	L152	A153	A207	Y154	Q155	R156	M157	S158	W159	E160	A161	L162	K163	K164	S165	I166	N167	G168	L169	I170	N171	K172		
MET	LYS	SER	SER	VAL	ALA	GLN	ILE	LYS	PRO	PRO	ASP	SER	SER	ARG	ARG	GLU	ASN	GLU	LEU	ASN	GLN	LYS	SER	ASP	THR	GLY	GLU	GLN	GLU	ARG	ASN	PRO	GLU	THR	SER	ASP	THR	THR	GLN	SER	ASP	THR	THR	LYS	ARG	LYS	GLY	ASP

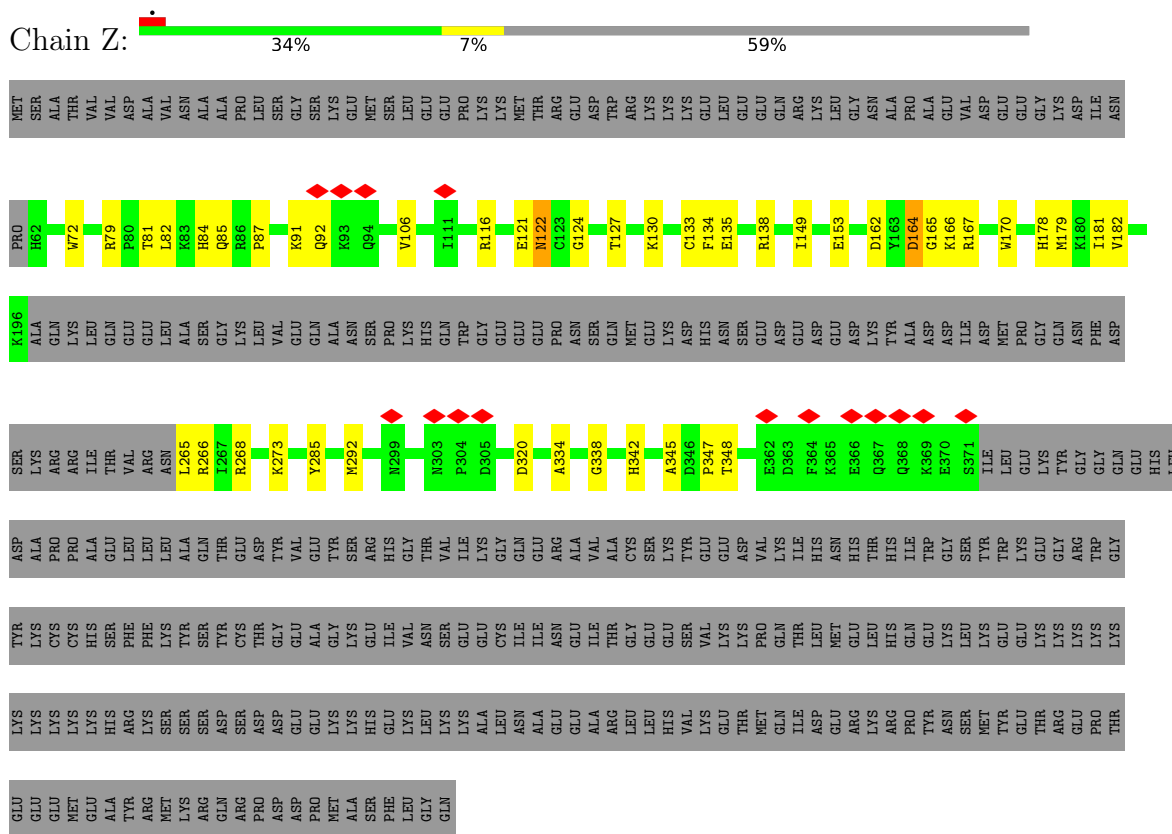




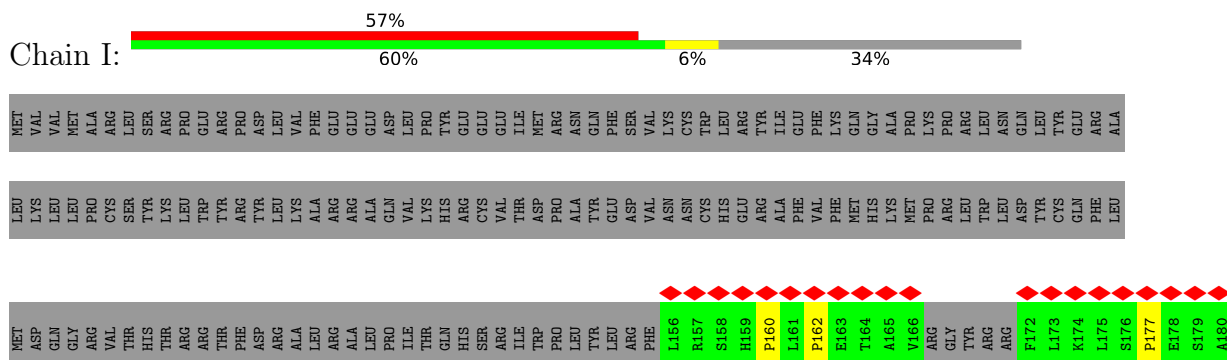




- Molecule 25: Pre-mRNA-splicing factor SLU7



- Molecule 26: Pre-mRNA-splicing factor SYF1











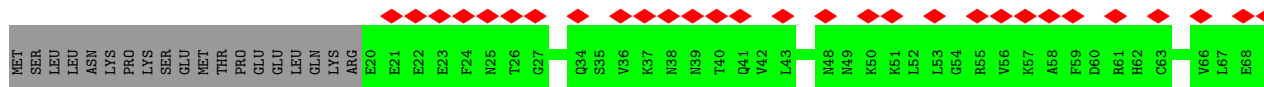


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LEU	LEU	E663	H723	V783	N842	A903	E963	R1023	D1083	L1143	E1203	F1263	L1322	L1322	LEU
LEU	LEU	N664	L724	I784	F844	R904	V964	S1024	G1084	C1144	A1204	Q1264	T1324	T1324	LEU
PRO	PRO	N665	K725	N785	P845	R905	S965	K1025	F1085	M1145	E1205	Q1265	A1325	A1325	PRO
PRO	PRO	F666	K726	N786	E946	I906	T966	Y1026	S1086	L1146	Y1206	Q1267	R1326	R1326	PRO
ALA	ALA	K667	S727	R787	Q947	E907	F967	L1027	R1087	Y1147	V1207	Q1267	P1327	P1327	ALA
MET	MET	A668	F728	G788	R848	L908	F968	L1028	L1088	M1148	V1208	M1268	L1328	L1328	MET
VAL	VAL	V669	F729	R789	T949	L909	P969	K1029	K1089	M1149	A1209	D1269	H1329	H1329	VAL
GLU	GLU	L670	G730	F790	L850	E910	F970	K1030	R1090	R1150	L1210	Y1270	L1330	L1330	GLU
GLY	GLY	E671	H731	P791	I851	E911	H971	E1031	M1091	Y1151	F1211	I1271	H1331	H1331	GLY
GLU	GLU	T672	N732	Y792	V852	V912	E972	K1032	I1092	K1152	M1212	L1272	L1332	L1332	GLU
VAL	VAL	L673	V733	N793	H853	K913	Y973	K1033	M1093	M1153	Y1213	L1273	L1333	L1333	VAL
GLN	GLN	R674	K734	Q794	H854	R914	F974	I1034	I1094	L1154	M1214	S1274	P1334	P1334	GLN
ASN	ASN	N675	V735	P795	S855	L915	A975	I1035	G1095	G1155	C1215	L1275	T1335	T1335	ASN
GLN	GLN	L676	T736	K796	N956	Q916	N976	A1036	D1096	M1156	L1216	V1276	E1336	E1336	GLN
PRO	PRO	M677	V737	Q857	Q917	K917	A977	M1037	H1097	L1157	L1217	R1277	P1336	P1336	PRO
PHE	PHE	N678	E738	N798	A858	S918	T968	T1038	H1098	P1158	G1218	T1278	P1337	P1337	PHE
GLU	GLU	T679	D739	T799	L859	L919	PRO	C1039	Q1099	H1159	Y1219	R1279	PRO	PRO	GLU
LEU	LEU	T679	D739	T799	L859	L919	PRO	C1039	Q1099	H1159	Y1219	R1279	PRO	PRO	LEU
GLU	GLU	D680	P740	I800	N960	G920	I981	T1040	L1100	V1160	P1220	A1280	T1340	T1340	GLU
GLU	GLU	C681	A741	Q801	Q861	V921	F982	H1041	P1101	Q1161	A1221	V1281	T1341	T1341	GLU
GLU	GLU	V682	L742	F802	L862	P922	K983	L1042	P1102	L1162	A1222	G1282	R1342	R1342	GLU
ALA	ALA	V683	Q743	T803	F963	G923	G984	A1043	V1103	L1163	K1223	H1283	K1344	K1344	ALA
MET	MET	P684	PRO	H804	E964	D924	R985	L1044	I1104	P1164	I1224	L1284	G1345	G1345	MET
THR	THR	D685	P746	T805	A925	S926	S986	K1045	M1106	E1165	I1225	D1285	E1346	E1346	THR
VAL	VAL	M686	F747	I807	I966	Y927	Y987	R1046	M1107	F1166	L1227	D1287	P1347	P1347	VAL
GLN	GLN	L687	R748	E808	M967	T928	E988	H1047	A1108	S1167	T1228	V1287	R1348	R1348	GLN
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ASP	ASP	D689	T750	L810	L869	G930	D990	L1049	F1109	A1169	Y1229	R1289	H1350	H1350	ASP
ILE	ILE	I690	F751	I811	D870	E930	M991	V1050	Q1110	M1170	T1230	L1290	H1351	H1351	ILE
PRO	PRO	L692	P752	R811	I871	T931	E992	K1051	K1111	A1171	N1231	V1291	E1352	E1352	PRO
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THR	THR	G695	GLY	Q815	R874	F935	E995	K1055	M1115	L1174	H1235	M1294	I1355	I1355	THR
SER	SER	D696	LYS	Q816	H875	F936	G996	Y1056	E1116	Y1175	H1236	S1295	K1356	K1356	SER
CYS	CYS	P697	LYS	P816	L876	L937	C997	D1057	E1117	D1176	L1237	R1296	I1357	I1357	CYS
GLN	GLN	P697	LYS	G817	L877	T938	F998	L1058	Q1117	F1177	I1238	A1297	M1358	M1358	GLN
GLU	GLU	S699	LYS	L818	R878	Y938	E999	L1059	S1118	Q1178	R1239	L1299	P1359	P1359	GLU
THR	THR	A700	ARG	T819	L879	Q939	H1000	I1060	R999	L1179	D1239	L1299	P1360	P1360	THR
PRO	PRO	H701	ASP	M820	G880	V940	I1001	L1061	F1120	I1180	T1240	G1300	M1361	M1361	PRO
ALA	ALA	Y702	ALA	V821	H891	M941	K1002	M1062	T1121	M1181	I1241	L1301	A1362	A1362	ALA
GLN	GLN	S703	VAL	G823	S942	R943	K1003	E1063	R1122	Y1182	N1242	Y1302	I1363	I1363	GLN
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ASP	ASP	M705	ASP	P825	E885	E945	F1005	A1065	V1124	D1184	R1244	F1304	V1365	V1365	ASP
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PRO	PRO	N707	THR	T827	E887	Y947	Q1007	Q1066	V1126	Q1186	G1246	R1306	Y1367	Y1367	PRO
SER	SER	Q708	GLU	T827	T888	I948	L1008	I1067	G1127	G1187	N1247	V1307	M1368	M1368	SER
LEU	LEU	I709	E773	G828	E889	I948	E1009	L1068	V1128	V1188	P1248	S1308	Y1369	Y1369	LEU
GLU	GLU	A774	A774	K829	E889	S949	E1009	L1069	P1129	G1189	P1249	L1309	M1370	M1370	GLU
THR	THR	K775	K775	T830	K900	K950	F1010	I1070	F1130	E1190	L1250	F1310	H1371	H1371	THR
VAL	VAL	T711	T776	D891	D891	V951	F1011	E1071	V1131	S1191	I1251	Q1311	L1372	L1372	VAL
GLN	GLN	D712	L777	V832	F992	K952	R1012	T1072	D1132	E1192	R1252	M1312	I1373	I1373	GLN
THR	THR	F714	I778	A833	S893	N953	A1013	F1073	L1133	F1193	R1253	C1313	Q1374	Q1374	THR
LEU	LEU	N715	V779	V834	R894	LYS	E1015	T1074	D1134	M1194	P1254	F1314	T1375	T1375	LEU
GLU	GLU	D716	E780	Q835	Y895	GLY	E1016	P1075	A1135	F1195	N1255	E1315	L1376	L1376	GLU
THR	THR	T717	I836	I836	G996	SER	L1016	L1076	Q1136	Y1196	K1256	L1316	H1377	H1377	THR
GLN	GLN	S838	I837	I837	R897	THR	L1017	L1077	G1137	F1197	V1257	T1317	H1378	H1378	GLN
LEU	LEU	L719	S838	S838	R897	LEU	R1018	L1078	R1138	Y1198	T1258	P1318	Y1379	Y1379	LEU
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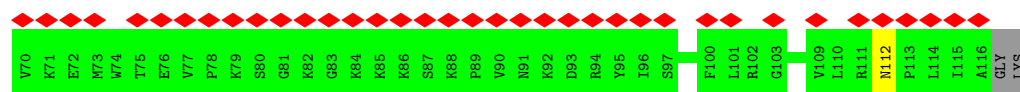




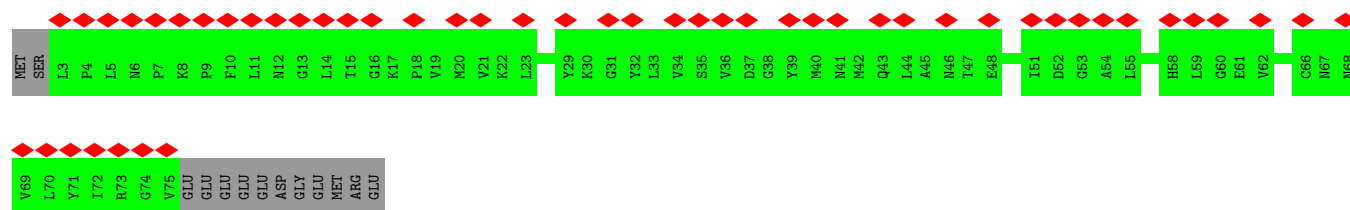
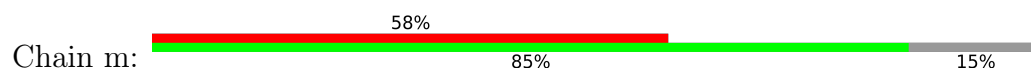




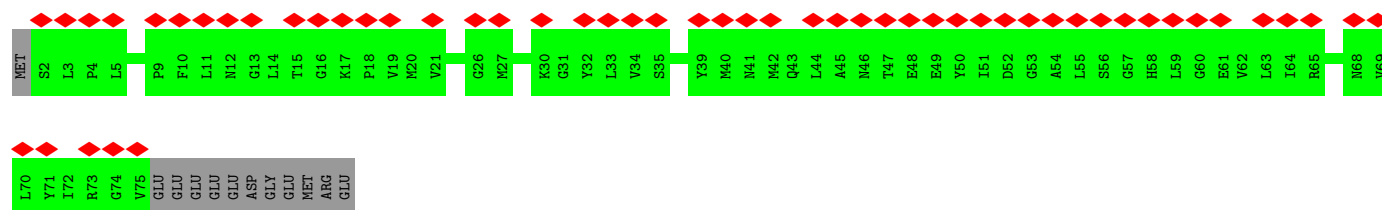
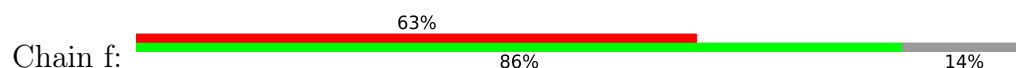




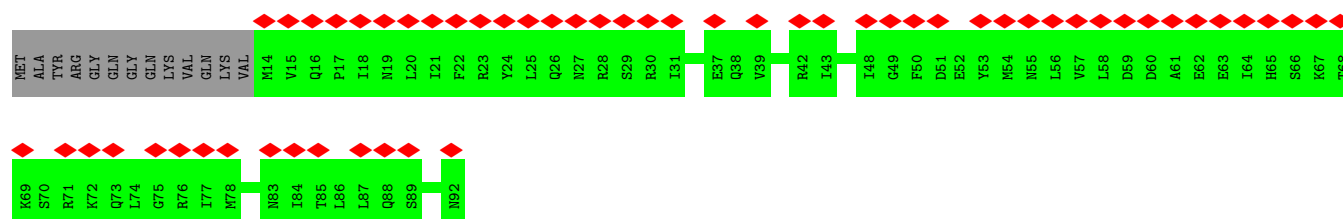
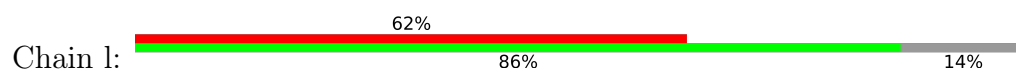
• Molecule 33: Small nuclear ribonucleoprotein F



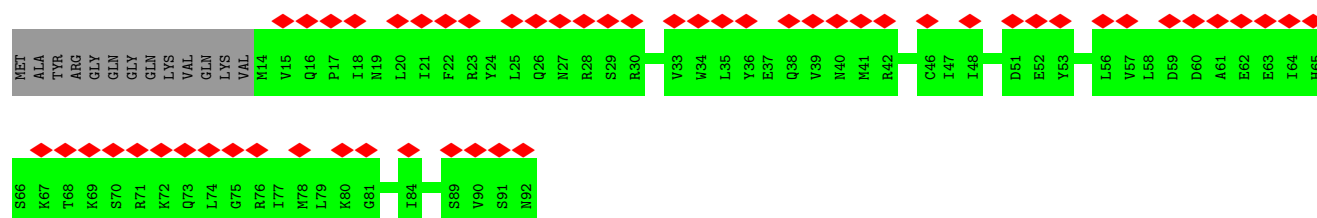
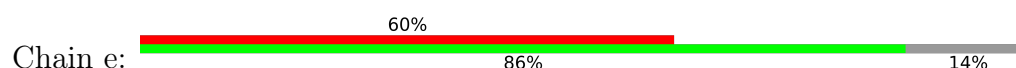
• Molecule 33: Small nuclear ribonucleoprotein F



• Molecule 34: Small nuclear ribonucleoprotein E



• Molecule 34: Small nuclear ribonucleoprotein E



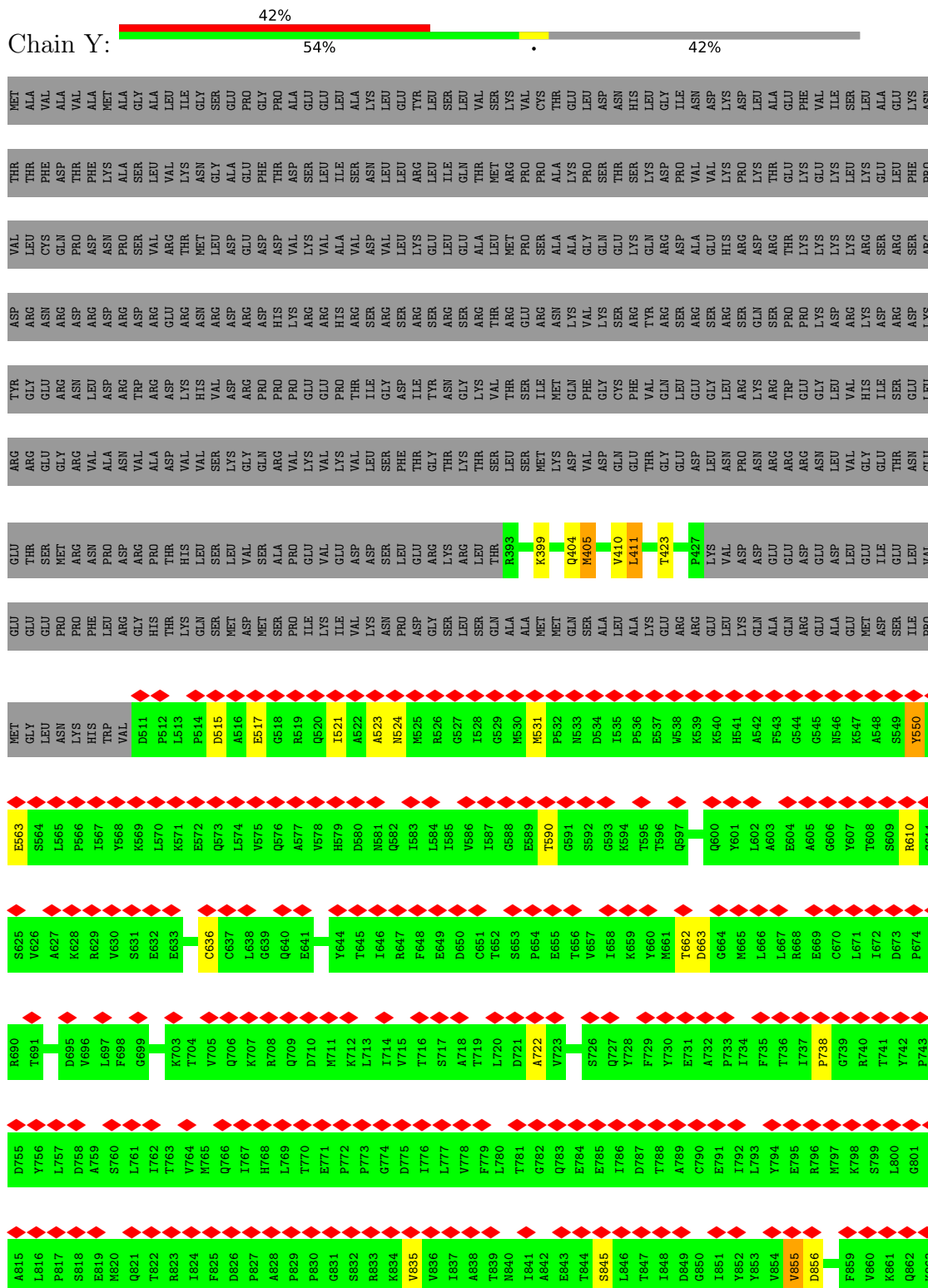
• Molecule 35: Small nuclear ribonucleoprotein G



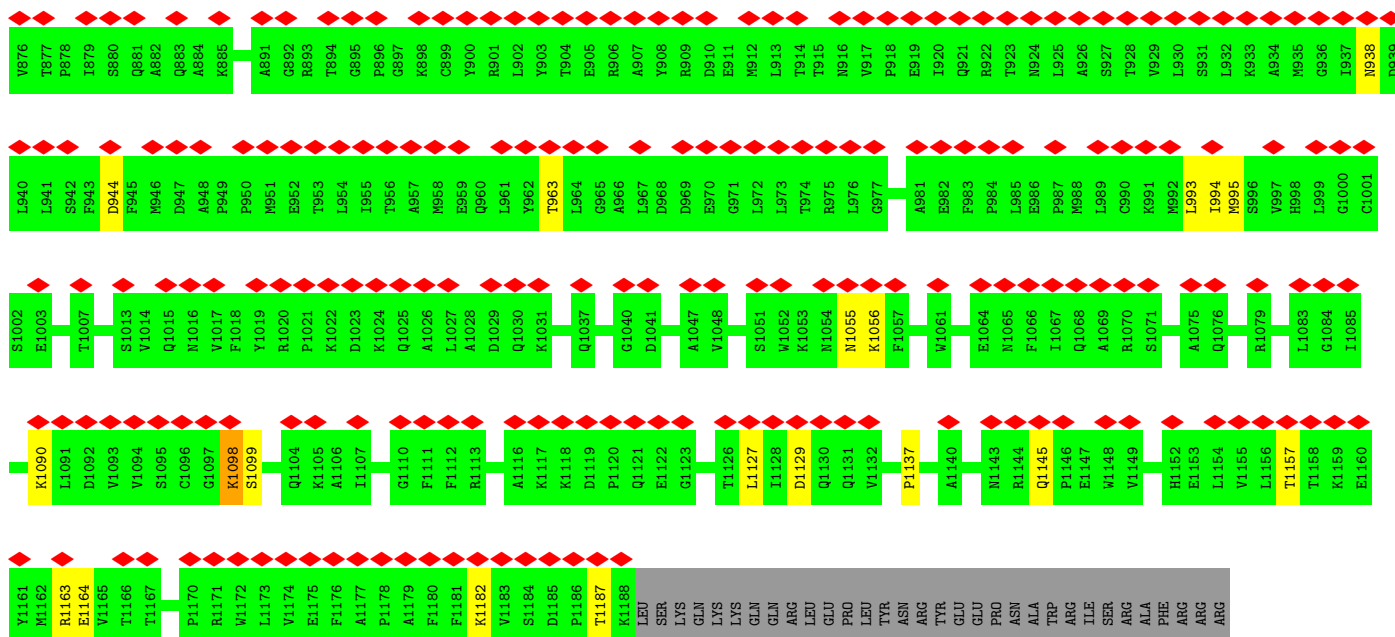




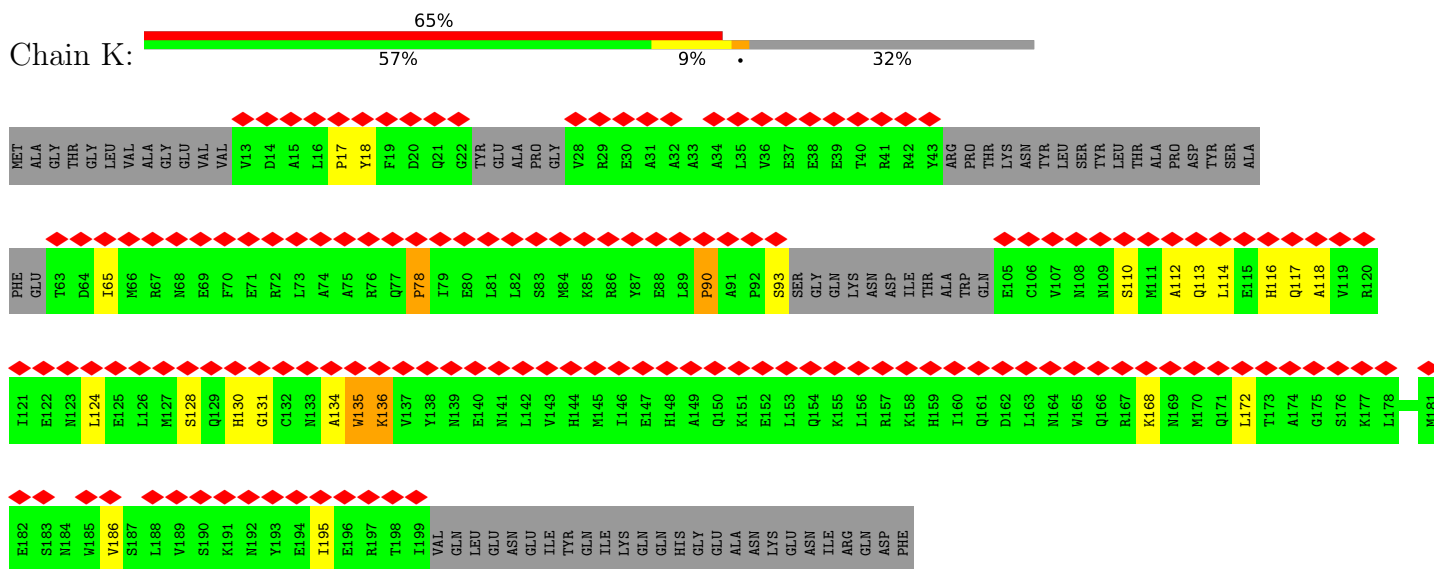
- Molecule 38: ATP-dependent RNA helicase DHX8



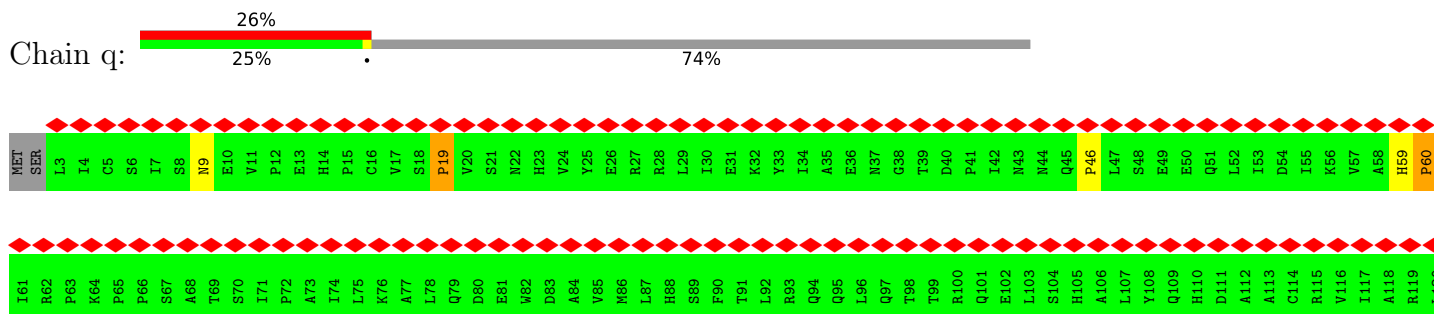




• Molecule 39: Pre-mRNA-splicing factor SPF27

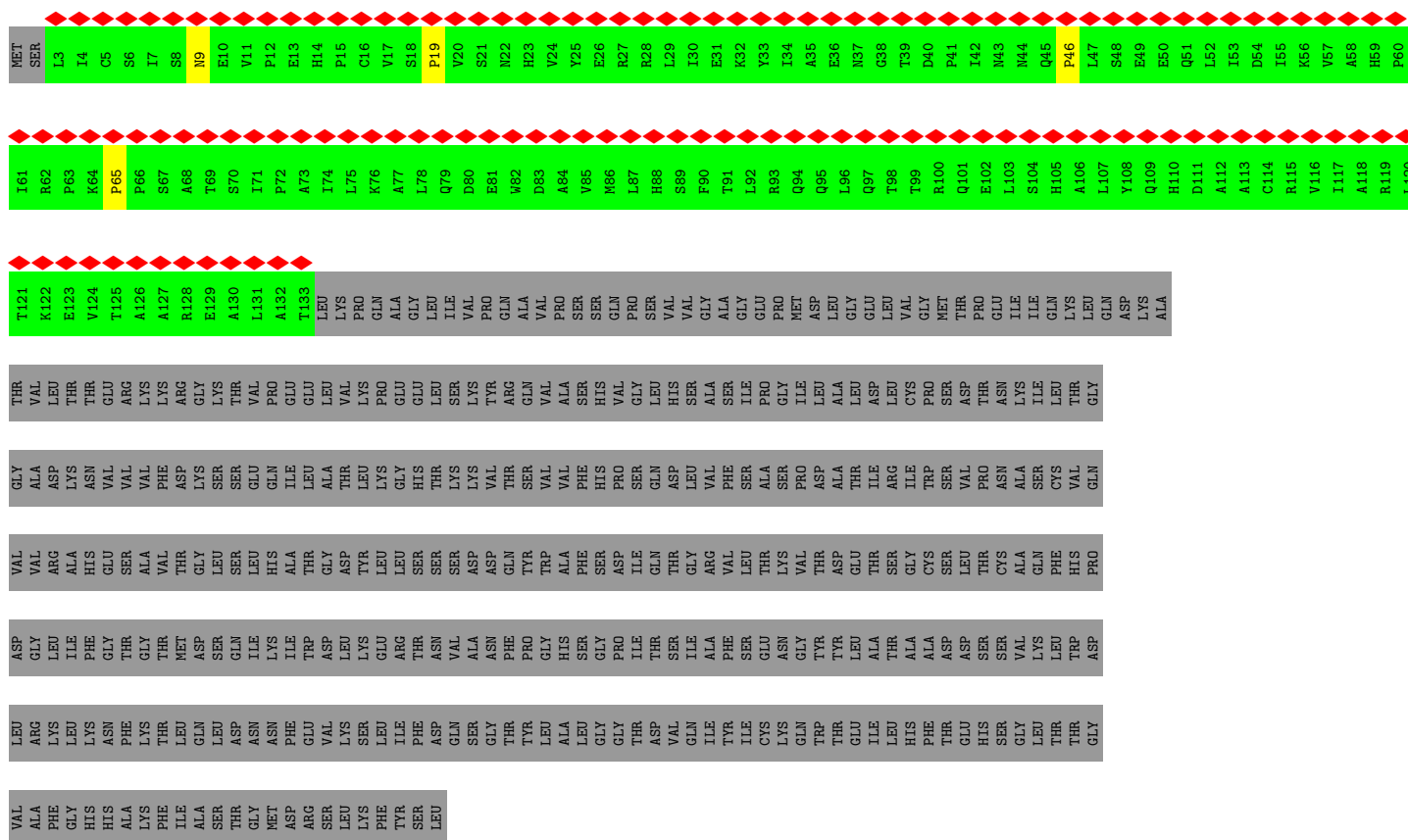


• Molecule 40: Pre-mRNA-processing factor 19





- Molecule 40: Pre-mRNA-processing factor 19



- Molecule 40: Pre-mRNA-processing factor 19











A1501	Q1441	P1381	Y1321	P1261	E1201	K1141	M1081	S1021	A961	L901	W841	G781
H1502	R1442	M1382	Q1322	L1262	L1202	K1142	V1082	S1022	L962	N902	T842	F782
W1503	K1443	E1383	D1323	P1263	T1203	I1143	Y1083	E1023	M963	N903	E843	A783
L1504	N1444	A1384	K1324	P1264	I1204	E1144	V1084	F1024	L964	E904	L844	I784
G1505	V1445	L1385	F1325	K1265	T1205	K1145	T1085	N1025	D965	I905	G845	H785
C1506	Q1446	A1386	P1326	Y1266	P1206	K1146	Q1086	K1026	K966	V906	A846	H786
S1507	L1447	E1387	F1327	F1267	D1207	N1147	S1087	I1027	N967	L907	L847	A787
A1508	T1448	Q1388	F1328	I1268	F1208	F1148	A1088	T1028	N968	G908	D848	G788
T1509	N1449	L1389	N1329	A1269	Q1209	F1149	L1089	V1029	L969	N909	I849	M789
S1510	L1450	Y1390	P1330	W1210	W1210	F1150	R1090	R1030	V970	V910	L850	T790
T1511	F1451	M1391	I1331	D1211	D1211	E1151	L1091	E1031	K971	Q911	Q851	R791
F1512	V1452	D1392	Q1332	S1272	E1212	R1152	M1092	E1032	Y972	N912	M852	V792
M1513	P1453	W1393	T1333	K1213	K1213	L1153	R1093	E1033	D973	N913	L853	D793
F1514	D1454	Y1394	Q1334	V1214	V1214	Y1154	A1094	K1034	K974	K914	G854	R794
H1515	E1455	E1395	V1335	H1215	H1215	D1155	I1095	L1035	K975	D915	R855	T795
P1516	V1456	K1396	F1336	G1216	G1216	L1156	F1096	E1036	T976	A916	A856	L796
M1517	H1457	F1397	S1277	S1217	S1217	N1157	E1097	L1037	G977	V917	G857	V797
V1518	L1458	Q1398	T1338	S1218	S1218	H1158	I1098	Q1038	N978	N918	R858	E798
R1519	I1459	D1399	V1339	E1219	E1219	M1159	V1099	K1039	F979	W919	P859	D799
P1520	G1460	R1400	Y1340	A1220	A1220	E1160	L1100	L1040	Q980	L920	Q860	L800
V1521	G1461	L1401	N1341	F1221	F1221	I1161	M1101	L1041	Y981	G921	Y861	F801
P1522	E1462	M1402	S1342	W1222	W1222	G1162	I1102	E1042	T982	Y922	D862	A802
L1523	N1463	K1403	D1343	I1223	I1223	E1163	G1103	R1043	E983	A923	T863	D803
E1524	G1464	K1404	D1344	L1224	L1224	L1164	W1104	V1044	L984	Y924	K864	K804
L1525	P1465	V1405	N1345	V1225	V1225	I1165	A1105	P1045	G985	L925	G865	H805
H1526	V1466	V1406	V1346	E1226	E1226	R1166	Q1106	I1046	R986	Y926	G866	I806
I1527	L1467	L1407	F1347	D1227	D1227	M1167	L1107	P1047	I987	I927	G867	Q807
Q1528	E1468	L1408	V1348	V1228	V1228	P1168	T1108	V1048	A988	R928	I868	V808
G1529	V1469	T1409	G1349	D1229	D1229	K1169	I1109	E1049	S989	M929	L869	L809
F1530	L1470	G1410	I1290	S1230	S1230	M1170	K1110	E1050	H990	L930	I870	V810
M1531	C1471	E1411	P1351	E1231	E1231	G1171	T1111	S1051	Y991	R931	T871	S811
I1532	S1472	T1412	T1352	V1232	V1232	K1172	I1112	E1052	Y992	S932	S872	T812
S1533	R1473	S1413	G1353	I1233	I1233	T1173	M1113	E1053	I993	P933	H873	A813
H1534	M1474	T1414	S1354	L1234	L1234	L1174	L1114	E1054	T994	T934	G874	T814
T1535	R1475	D1415	G1355	H1235	H1235	H1175	C1115	P1055	N995	L935	E875	L815
Q1536	Y1476	L1416	K1356	H1236	H1236	K1176	K1116	S1056	D996	Y936	L876	A816
T1537	I1477	K1417	T1357	E1237	E1237	Y1177	M1117	A1057	T997	G937	G877	W817
R1538	S1478	L1418	I1358	V1238	V1238	V1178	I1118	K1058	V998	I938	Y878	G818
L1539	S1479	L1419	C1359	F1239	F1239	H1179	D1119	I1059	Q999	S939	Y879	V819
L1540	Q1480	G1420	A1360	L1240	L1240	L1180	K1120	N1060	T1000	H940	L880	N820
S1541	I1481	K1421	E1361	L1241	L1241	F1181	R1121	V1061	Y1001	D941	S881	L821
M1542	E1482	G1422	F1362	K1242	K1242	P1182	M1122	L1062	I1002	D942	L882	P822
A1543	R1483	N1423	A1363	A1243	A1243	K1183	W1123	L1063	Q1003	L943	L883	A823
K1544	P1484	I1424	I1364	K1244	K1244	L1184	Q1124	Q1064	L1004	K944	N884	H824
P1545	I1485	L1425	L1365	Y1245	Y1245	E1185	S1125	A1065	L1005	G945	Q885	T825
V1546	R1486	I1426	P1366	A1246	A1246	L1186	M1126	F1066	K1006	D946	Q886	V826
Y1547	I1487	S1427	M1367	Q1247	Q1247	S1187	C1127	I1067	P1007	P947	L887	I827
H1548	V1488	T1428	L1368	D1248	D1248	V1188	P1128	S1068	T1008	L948	P888	I828
A1549	L1489	P1429	L1369	E1249	E1249	H1189	L1129	Q1069	L949	L949	I889	K829
I1550	L1490	E1430	Q1370	H1250	H1250	L1190	R1130	L1070	S1010	D950	E890	G830
T1551	S1491	K1431	S1371	L1251	L1251	Q1191	Q1131	K1071	E1011	Q951	S891	T831
K1552	S1492	W1432	S1372	I1252	I1252	P1192	F1132	L1072	I1012	R952	Q892	Q832
H1553	S1493	D1433	E1373	T1253	T1253	L1193	R1133	E1073	R953	L953	M893	R833
S1554	L1494	I1434	G1374	F1254	F1254	T1194	K1134	G1074	L1014	L954	V894	Y834
P1555	S1495	L1435	R1375	F1255	F1255	R1195	L1135	F1075	F1015	D955	S895	S835
K1556	N1496	S1436	C1376	V1256	V1256	S1196	P1136	A1076	R1016	L956	K896	P836
L1557	A1497	R1437	V1377	P1257	P1257	T1197	E1137	L1077	V1017	V957	L897	E837
P1558	L1498	L1438	Y1378	E1258	E1258	L1198	E1138	L1078	F1018	V958	P898	K838
V1559	D1499	W1439	I1379	F1259	F1259	K1199	V1139	A1079	S1019	T959	D899	G839
I1560	V1500	L1320	T1380	E1260	E1260	V1200	V1140	L1080	L1020	A960	M900	R840







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	143320	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 ( $e^-/\text{\AA}^2$ )	45	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.552	Depositor
Minimum map value	-0.288	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.03	Depositor
Map size ( $\text{\AA}$ )	535.2, 535.2, 535.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.338, 1.338, 1.338	Depositor



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, GTP, ZN, ATP, IHP, 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	v	0.30	0/710	0.65	0/987
2	w	0.30	0/444	0.78	2/614 (0.3%)
3	u	0.32	0/1906	0.69	0/2653
4	x	0.34	0/123	0.70	0/170
5	A	0.53	0/18287	0.65	7/24842 (0.0%)
6	B	0.77	1/2274 (0.0%)	1.17	25/3535 (0.7%)
7	C	2.14	9/7225 (0.1%)	0.78	12/9818 (0.1%)
8	E	0.34	0/2420	0.64	0/3281
9	F	0.95	0/2323	1.23	19/3619 (0.5%)
10	G	0.57	0/1716	1.23	21/2656 (0.8%)
11	H	0.95	24/3305 (0.7%)	1.55	96/5130 (1.9%)
12	J	0.46	0/3870	0.61	13/5252 (0.2%)
13	L	0.41	0/3091	0.59	7/4178 (0.2%)
14	M	0.41	0/1119	0.63	1/1497 (0.1%)
15	N	1.19	6/1210 (0.5%)	0.87	2/1622 (0.1%)
16	O	0.47	0/2344	0.62	1/3163 (0.0%)
17	P	0.46	0/943	0.61	0/1255
18	R	0.47	0/2091	0.66	1/2809 (0.0%)
19	S	0.35	0/1268	0.59	1/1714 (0.1%)
20	T	0.65	1/2526 (0.0%)	0.82	3/3443 (0.1%)
21	U	0.34	0/196	0.63	0/265
22	V	0.31	0/2784	0.54	3/3791 (0.1%)
23	W	0.40	0/4230	0.69	3/5713 (0.1%)
24	X	0.32	0/714	0.53	2/959 (0.2%)
25	Z	0.37	0/2049	0.61	1/2757 (0.0%)
26	I	0.38	0/2749	0.56	16/3773 (0.4%)
27	y	0.25	0/389	0.62	0/540
28	Q	0.22	0/6565	0.42	0/9143
29	a	0.48	0/397	0.62	0/549
29	h	0.47	0/396	0.61	0/547
30	b	0.51	0/423	0.72	0/587
30	i	0.50	0/423	0.73	0/587



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
31	c	0.57	0/405	0.73	0/563
31	j	0.57	0/405	0.73	0/563
32	d	0.68	0/479	0.85	0/666
32	k	0.70	0/420	0.85	0/583
33	f	0.75	0/360	0.81	0/497
33	m	0.76	0/355	0.81	0/490
34	e	0.65	0/390	0.80	0/542
34	l	0.62	0/390	0.80	0/542
35	g	0.54	0/362	0.71	0/501
35	n	0.50	0/337	0.70	0/465
36	o	0.64	0/803	1.49	4/1119 (0.4%)
37	p	0.61	0/463	1.25	0/643
38	Y	0.46	0/2917	0.92	0/3670
39	K	0.40	1/753 (0.1%)	0.55	3/1046 (0.3%)
40	q	0.35	0/658	0.58	3/919 (0.3%)
40	r	0.33	0/653	0.56	2/912 (0.2%)
40	s	0.27	0/334	0.37	0/466
40	t	0.31	0/334	0.38	0/466
41	D	0.33	0/8529	0.59	0/11891
All	All	0.76	42/99857 (0.0%)	0.77	248/137993 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
5	A	0	6
7	C	0	7
8	E	0	1
11	H	0	1
12	J	0	3
14	M	0	1
16	O	0	1
17	P	0	1
18	R	0	2
20	T	0	3
23	W	0	3
25	Z	0	2
32	d	0	1
32	k	0	1
38	Y	0	15

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Mol	Chain	#Chirality outliers	#Planarity outliers
41	D	0	1
All	All	0	49

The worst 5 of 42 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	172	PHE	CE1-CZ	84.80	2.98	1.37
7	C	172	PHE	CE2-CZ	79.82	2.89	1.37
7	C	172	PHE	CD1-CE1	78.14	2.95	1.39
7	C	172	PHE	CD2-CE2	76.95	2.93	1.39
7	C	172	PHE	CG-CD1	47.98	2.10	1.38

The worst 5 of 248 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	104	LEU	CA-CB-CG	18.46	157.76	115.30
7	C	104	LEU	CB-CG-CD1	16.32	138.75	111.00
7	C	104	LEU	CB-CG-CD2	15.04	136.56	111.00
11	H	167	U	C5-C4-O4	11.93	133.06	125.90
7	C	172	PHE	CD1-CG-CD2	9.95	131.24	118.30

There are no chirality outliers.

5 of 49 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	A	1070	ASP	Peptide
5	A	1091	TYR	Peptide
5	A	1209	HIS	Peptide
5	A	851	SER	Peptide
5	A	941	LYS	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	v	711	0	299	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	w	445	0	203	0	0
3	u	1907	0	845	0	0
4	x	124	0	51	0	0
5	A	17837	0	17053	235	0
6	B	2040	0	1034	51	0
7	C	7066	0	7084	130	0
8	E	2366	0	2303	65	0
9	F	2075	0	1048	27	0
10	G	1549	0	784	51	0
11	H	2966	0	1505	227	0
12	J	3829	0	2907	38	0
13	L	3064	0	2521	40	0
14	M	1098	0	1082	25	0
15	N	1184	0	1189	41	0
16	O	2296	0	2284	36	0
17	P	929	0	910	6	0
18	R	2073	0	2119	36	0
19	S	1236	0	1210	23	0
20	T	2461	0	2420	69	0
21	U	193	0	196	4	0
22	V	2765	0	1955	17	0
23	W	4122	0	4031	109	0
24	X	701	0	631	30	0
25	Z	1999	0	1951	35	0
26	I	2782	0	1245	52	0
27	y	390	0	190	0	0
28	Q	6562	0	2836	5	0
29	a	399	0	173	0	0
29	h	398	0	172	0	0
30	b	424	0	179	0	0
30	i	424	0	179	0	0
31	c	406	0	170	0	0
31	j	406	0	170	0	0
32	d	480	0	200	0	0
32	k	422	0	175	0	0
33	f	361	0	158	0	0
33	m	356	0	156	0	0
34	e	391	0	163	0	0
34	l	391	0	163	0	0
35	g	363	0	160	0	0
35	n	339	0	145	0	0
36	o	804	0	350	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	p	464	0	205	0	0
38	Y	2917	0	857	9	0
39	K	757	0	338	19	0
40	q	659	0	296	0	0
40	r	654	0	294	0	0
40	s	335	0	168	0	0
40	t	335	0	168	0	0
41	D	8530	0	3747	8	0
42	A	36	0	6	3	0
43	C	32	0	12	2	0
44	C	1	0	0	0	0
44	F	6	0	0	0	0
44	Q	2	0	0	0	0
45	N	3	0	0	0	0
45	O	3	0	0	0	0
45	Z	1	0	0	0	0
46	Q	31	0	12	0	0
All	All	97900	0	70702	1177	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 8.

The worst 5 of 1177 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:C:104:LEU:CG	7:C:104:LEU:CD1	1.74	1.61
12:J:466:ARG:CB	26:I:607:GLY:HA2	1.44	1.47
8:E:56:GLN:NE2	8:E:97:GLY:HA2	1.35	1.40
7:C:172:PHE:CD1	7:C:172:PHE:CG	2.10	1.39
7:C:172:PHE:CG	7:C:172:PHE:CD2	2.10	1.39

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	v	142/148 (96%)	138 (97%)	4 (3%)	0	100	100
2	w	89/174 (51%)	87 (98%)	1 (1%)	1 (1%)	12	44
3	u	384/411 (93%)	372 (97%)	9 (2%)	3 (1%)	16	51
4	x	23/703 (3%)	22 (96%)	1 (4%)	0	100	100
5	A	2247/2335 (96%)	2091 (93%)	147 (6%)	9 (0%)	30	66
7	C	892/972 (92%)	798 (90%)	90 (10%)	4 (0%)	30	66
8	E	301/357 (84%)	273 (91%)	28 (9%)	0	100	100
12	J	530/848 (62%)	491 (93%)	32 (6%)	7 (1%)	10	39
13	L	436/802 (54%)	405 (93%)	27 (6%)	4 (1%)	14	49
14	M	128/243 (53%)	124 (97%)	3 (2%)	1 (1%)	16	51
15	N	141/144 (98%)	126 (89%)	13 (9%)	2 (1%)	9	37
16	O	283/420 (67%)	260 (92%)	22 (8%)	1 (0%)	30	66
17	P	104/229 (45%)	86 (83%)	15 (14%)	3 (3%)	3	20
18	R	255/536 (48%)	229 (90%)	24 (9%)	2 (1%)	16	51
19	S	157/166 (95%)	148 (94%)	9 (6%)	0	100	100
20	T	311/514 (60%)	281 (90%)	23 (7%)	7 (2%)	5	26
21	U	24/2752 (1%)	23 (96%)	1 (4%)	0	100	100
22	V	444/908 (49%)	429 (97%)	14 (3%)	1 (0%)	44	77
23	W	506/579 (87%)	441 (87%)	60 (12%)	5 (1%)	13	46
24	X	90/184 (49%)	84 (93%)	6 (7%)	0	100	100
25	Z	238/586 (41%)	214 (90%)	24 (10%)	0	100	100
26	I	498/855 (58%)	481 (97%)	10 (2%)	7 (1%)	9	37
27	y	77/301 (26%)	75 (97%)	2 (3%)	0	100	100
28	Q	1308/1485 (88%)	1282 (98%)	26 (2%)	0	100	100
29	a	77/126 (61%)	76 (99%)	1 (1%)	0	100	100
29	h	77/126 (61%)	76 (99%)	1 (1%)	0	100	100
30	b	84/231 (36%)	82 (98%)	2 (2%)	0	100	100
30	i	84/231 (36%)	82 (98%)	2 (2%)	0	100	100
31	c	80/119 (67%)	77 (96%)	3 (4%)	0	100	100
31	j	80/119 (67%)	77 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	d	95/118 (80%)	91 (96%)	4 (4%)	0	100	100
32	k	81/118 (69%)	78 (96%)	3 (4%)	0	100	100
33	f	72/86 (84%)	69 (96%)	3 (4%)	0	100	100
33	m	71/86 (83%)	68 (96%)	3 (4%)	0	100	100
34	e	77/92 (84%)	76 (99%)	1 (1%)	0	100	100
34	l	77/92 (84%)	76 (99%)	1 (1%)	0	100	100
35	g	72/76 (95%)	70 (97%)	2 (3%)	0	100	100
35	n	65/76 (86%)	59 (91%)	4 (6%)	2 (3%)	3	19
36	o	160/255 (63%)	146 (91%)	12 (8%)	2 (1%)	10	39
37	p	92/225 (41%)	90 (98%)	2 (2%)	0	100	100
38	Y	709/1220 (58%)	616 (87%)	61 (9%)	32 (4%)	2	12
39	K	144/225 (64%)	129 (90%)	8 (6%)	7 (5%)	2	10
40	q	130/504 (26%)	119 (92%)	7 (5%)	4 (3%)	3	19
40	r	129/504 (26%)	119 (92%)	8 (6%)	2 (2%)	8	34
40	s	65/504 (13%)	62 (95%)	2 (3%)	1 (2%)	8	36
40	t	65/504 (13%)	64 (98%)	0	1 (2%)	8	36
41	D	1720/2136 (80%)	1633 (95%)	84 (5%)	3 (0%)	44	77
All	All	13914/24425 (57%)	12995 (93%)	808 (6%)	111 (1%)	19	51

5 of 111 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	u	383	ASN
15	N	36	PRO
18	R	233	PRO
20	T	343	PRO
20	T	458	SER

### 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	
5	A	1795/2108 (85%)	1780 (99%)	15 (1%)	79	90
7	C	793/866 (92%)	786 (99%)	7 (1%)	75	89
8	E	259/300 (86%)	254 (98%)	5 (2%)	52	79
12	J	241/751 (32%)	239 (99%)	2 (1%)	79	90
13	L	208/709 (29%)	204 (98%)	4 (2%)	52	79
14	M	117/209 (56%)	113 (97%)	4 (3%)	32	66
15	N	130/130 (100%)	124 (95%)	6 (5%)	23	56
16	O	255/361 (71%)	250 (98%)	5 (2%)	50	78
17	P	99/203 (49%)	98 (99%)	1 (1%)	73	88
18	R	219/457 (48%)	212 (97%)	7 (3%)	34	67
19	S	129/134 (96%)	129 (100%)	0	100	100
20	T	269/441 (61%)	261 (97%)	8 (3%)	36	69
21	U	21/2432 (1%)	20 (95%)	1 (5%)	21	55
22	V	140/838 (17%)	136 (97%)	4 (3%)	37	70
23	W	447/502 (89%)	434 (97%)	13 (3%)	37	70
24	X	62/157 (40%)	57 (92%)	5 (8%)	9	34
25	Z	214/520 (41%)	210 (98%)	4 (2%)	52	79
38	Y	8/1085 (1%)	5 (62%)	3 (38%)	0	0
All	All	5406/12203 (44%)	5312 (98%)	94 (2%)	56	81

5 of 94 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
20	T	339	GLN
23	W	252	ARG
20	T	344	GLN
22	V	458	THR
23	W	322	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 64 such sidechains are listed below:

Mol	Chain	Res	Type
23	W	103	GLN
23	W	462	HIS
7	C	548	ASN
7	C	297	ASN

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Mol	Chain	Res	Type
23	W	492	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	G	82/273 (30%)	44 (53%)	7 (8%)
11	H	133/188 (70%)	45 (33%)	9 (6%)
6	B	96/117 (82%)	46 (47%)	8 (8%)
9	F	96/107 (89%)	33 (34%)	6 (6%)
All	All	407/685 (59%)	168 (41%)	30 (7%)

5 of 168 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	B	9	G
6	B	10	U
6	B	13	C
6	B	19	A
6	B	20	G

5 of 30 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
10	G	-12	G
11	H	106	G
10	G	21	A
11	H	168	A
11	H	100	U

## 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
18	SEP	R	232	18	8,9,10	1.47	1 (12%)	8,12,14	2.47	2 (25%)
18	SEP	R	224	18	8,9,10	0.81	0	8,12,14	1.48	1 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	SEP	R	232	18	-	1/5/8/10	-
18	SEP	R	224	18	-	1/5/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	R	232	SEP	P-O1P	3.18	1.60	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	R	232	SEP	P-OG-CB	-5.11	104.21	118.30
18	R	232	SEP	OG-CB-CA	4.37	112.39	108.14
18	R	224	SEP	OG-CB-CA	-2.59	105.63	108.14

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	R	232	SEP	N-CA-CB-OG
18	R	224	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 19 ligands modelled in this entry, 16 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
46	ATP	Q	1501	44	26,33,33	1.73	8 (30%)	31,52,52	1.87	10 (32%)
42	IHP	A	3000	-	36,36,36	0.83	0	54,60,60	1.05	2 (3%)
43	GTP	C	1500	44	26,34,34	1.34	3 (11%)	32,54,54	1.51	7 (21%)

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
46	ATP	Q	1501	44	-	4/18/38/38	0/3/3/3
42	IHP	A	3000	-	-	7/30/54/54	0/1/1/1
43	GTP	C	1500	44	-	4/18/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	C	1500	GTP	C5-C6	-4.30	1.38	1.47
46	Q	1501	ATP	C2'-C1'	-3.61	1.48	1.53
46	Q	1501	ATP	C4-N3	3.59	1.40	1.35
46	Q	1501	ATP	C6-N6	3.25	1.45	1.34
46	Q	1501	ATP	C2'-C3'	-2.78	1.45	1.53

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	Q	1501	ATP	PB-O3B-PG	-5.52	113.89	132.83
46	Q	1501	ATP	N3-C2-N1	-4.26	122.02	128.68
43	C	1500	GTP	C5-C6-N1	3.52	120.18	113.95
43	C	1500	GTP	C8-N7-C5	3.16	109.00	102.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	C	1500	GTP	C2-N1-C6	-3.07	119.44	125.10

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
42	A	3000	IHP	C2-O12-P2-O22
42	A	3000	IHP	C6-O16-P6-O26
43	C	1500	GTP	PB-O3B-PG-O3G
46	Q	1501	ATP	C5'-O5'-PA-O1A
46	Q	1501	ATP	C5'-O5'-PA-O2A

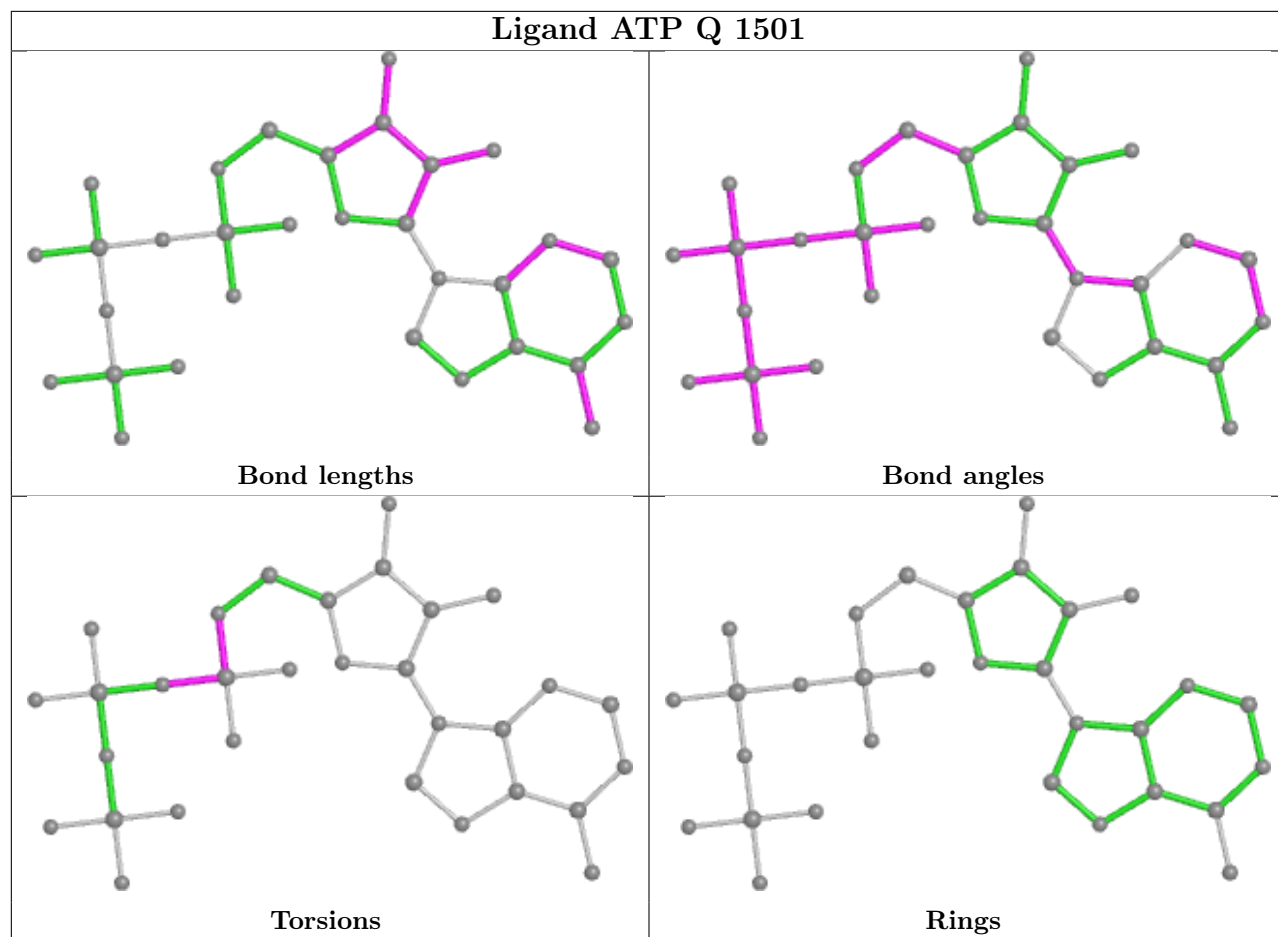
There are no ring outliers.

2 monomers are involved in 5 short contacts:

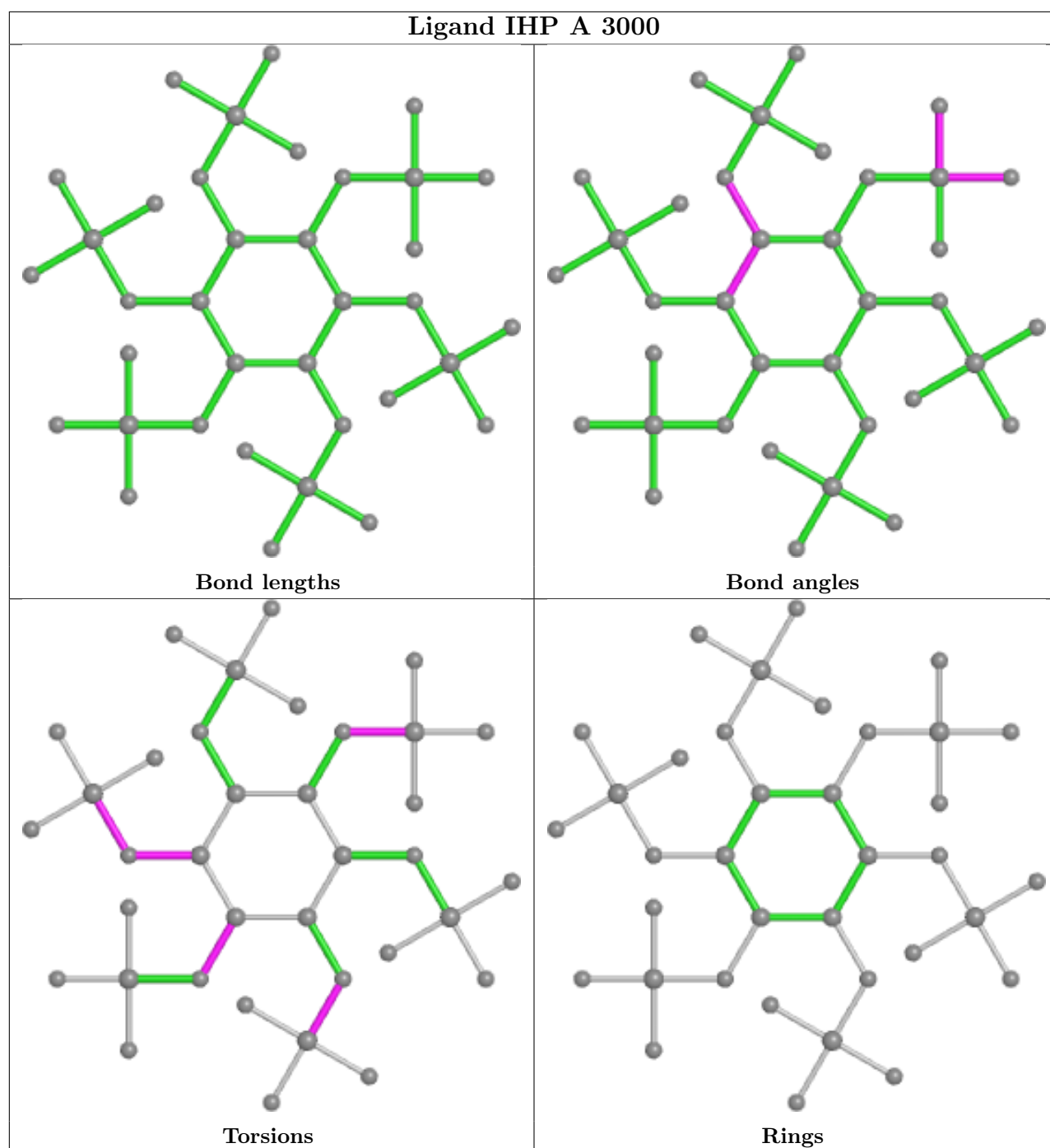
Mol	Chain	Res	Type	Clashes	Symm-Clashes
42	A	3000	IHP	3	0
43	C	1500	GTP	2	0

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.

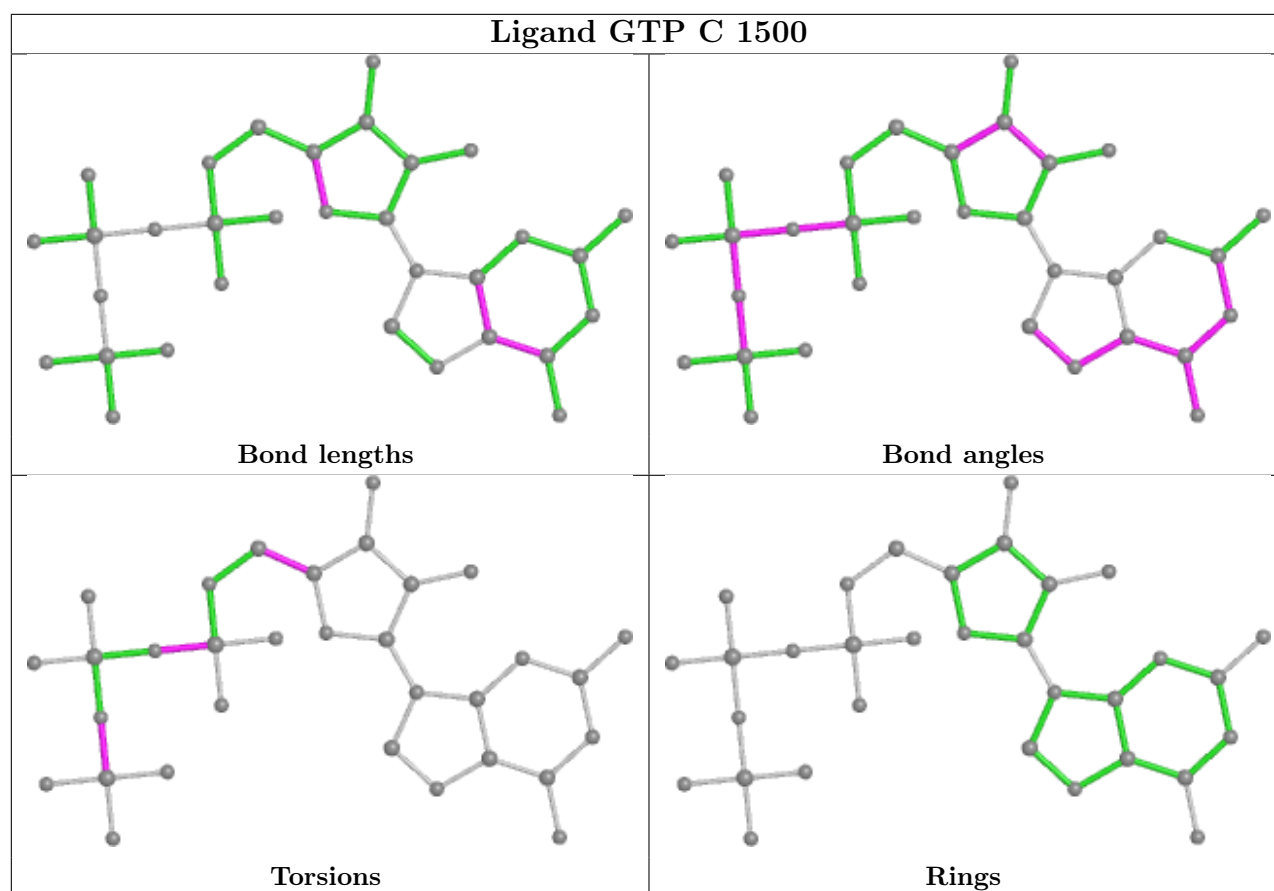












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



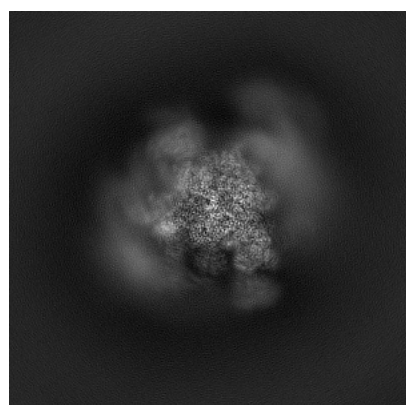
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9645. These allow visual inspection of the internal detail of the map and identification of artifacts.

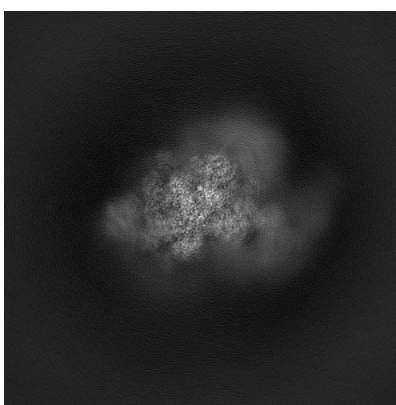
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

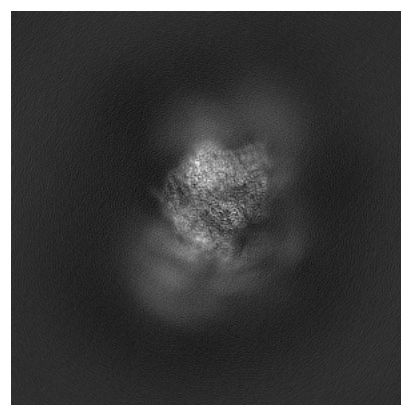
#### 6.1.1 Primary map



X



Y

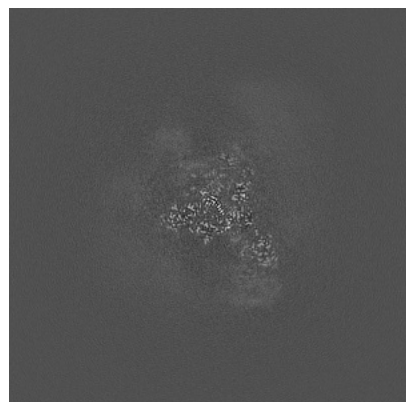


Z

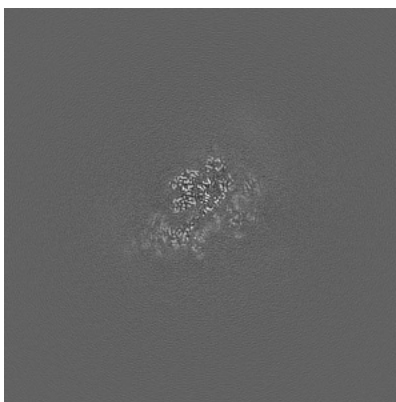
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

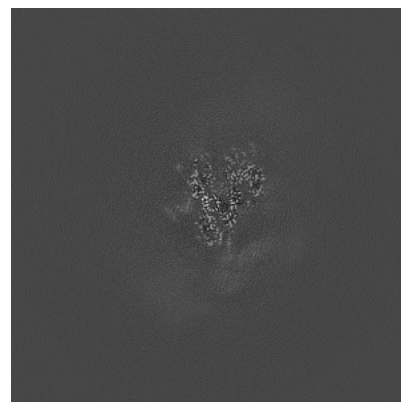
#### 6.2.1 Primary map



X Index: 200



Y Index: 200



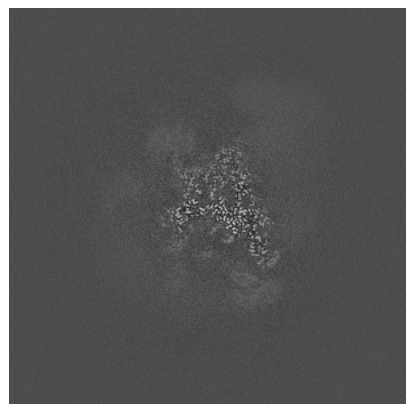
Z Index: 200



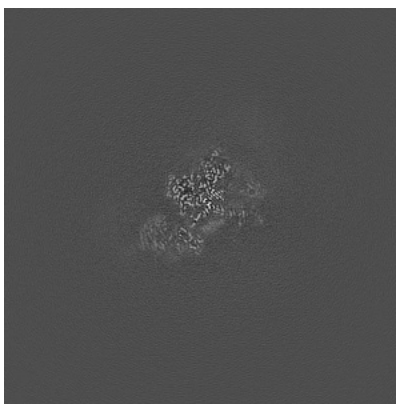
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

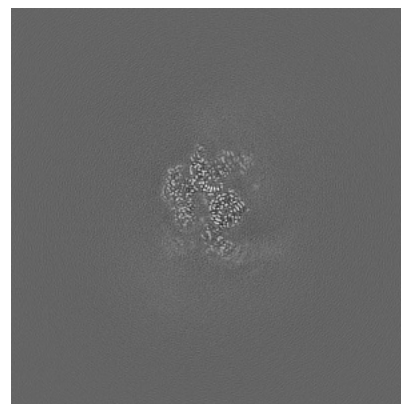
### 6.3.1 Primary map



X Index: 193



Y Index: 205

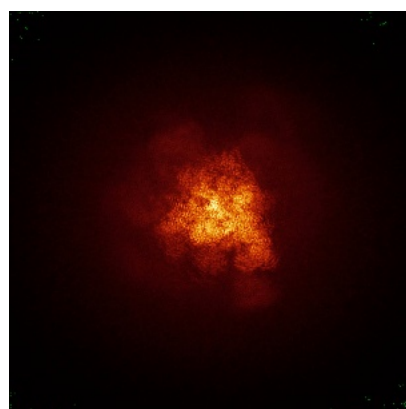


Z Index: 180

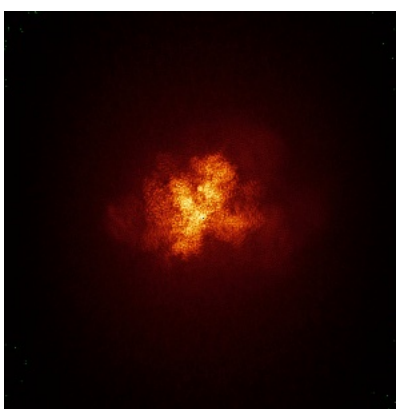
The images above show the largest variance slices of the map in three orthogonal directions.

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

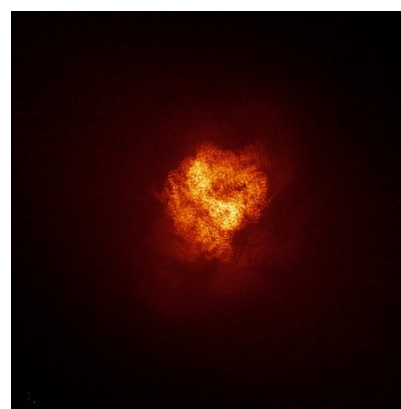
### 6.4.1 Primary map



X



Y



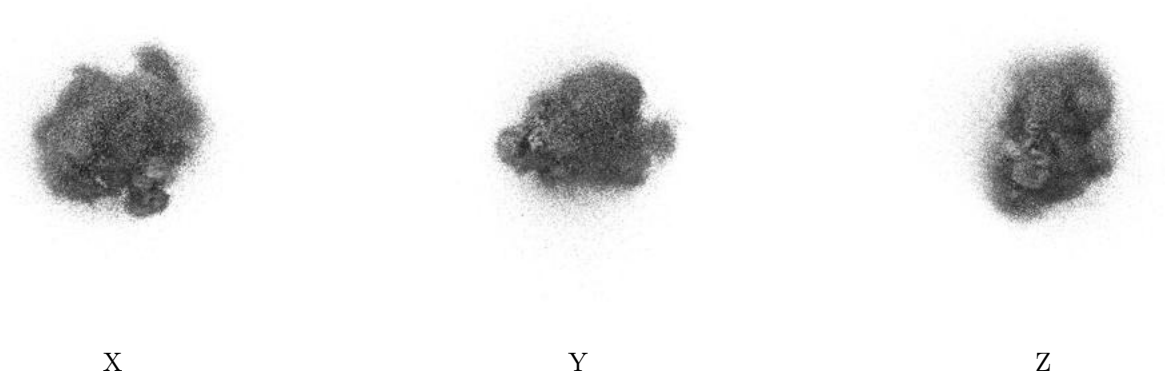
Z

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 0.03. 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](#)

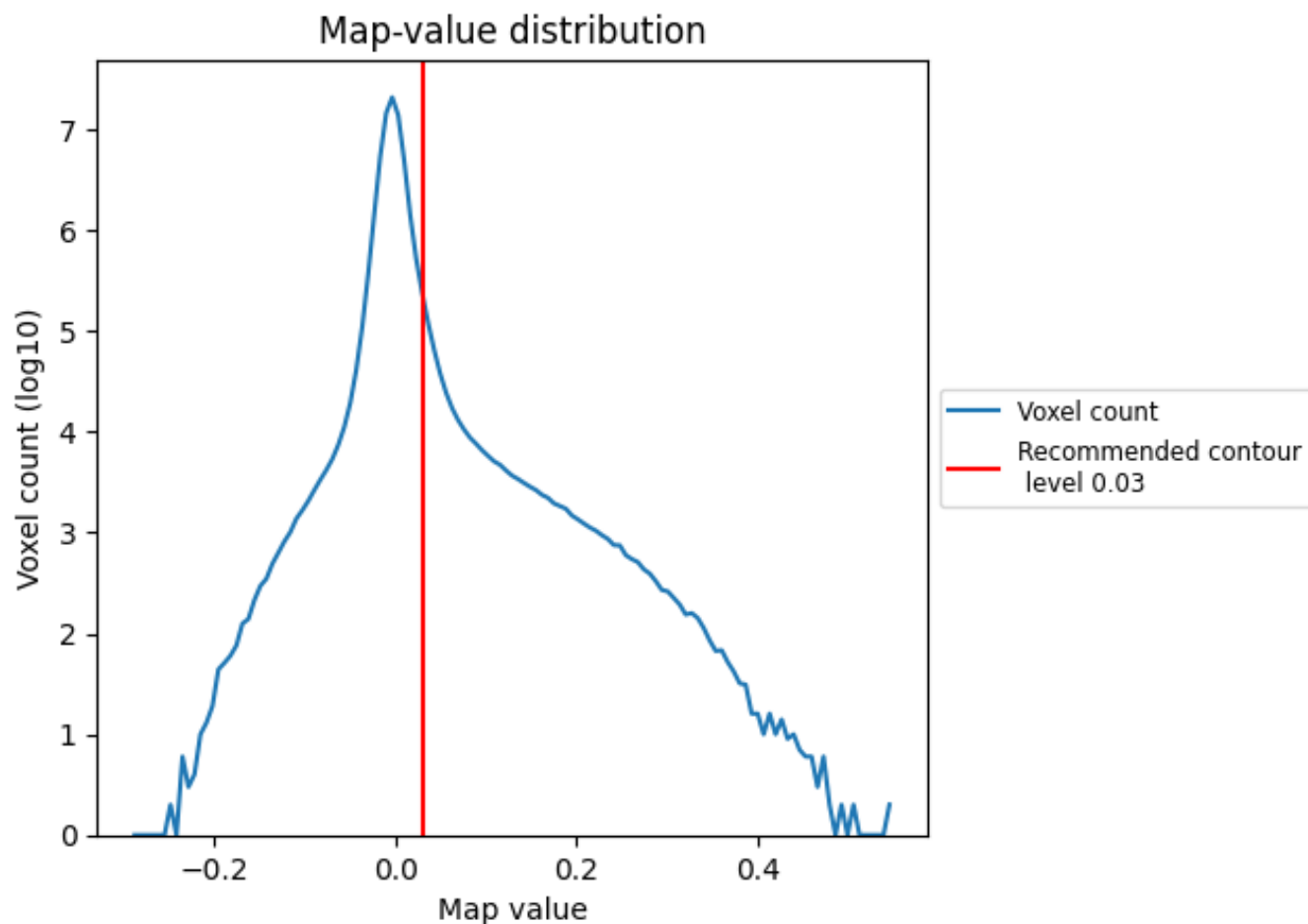
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

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

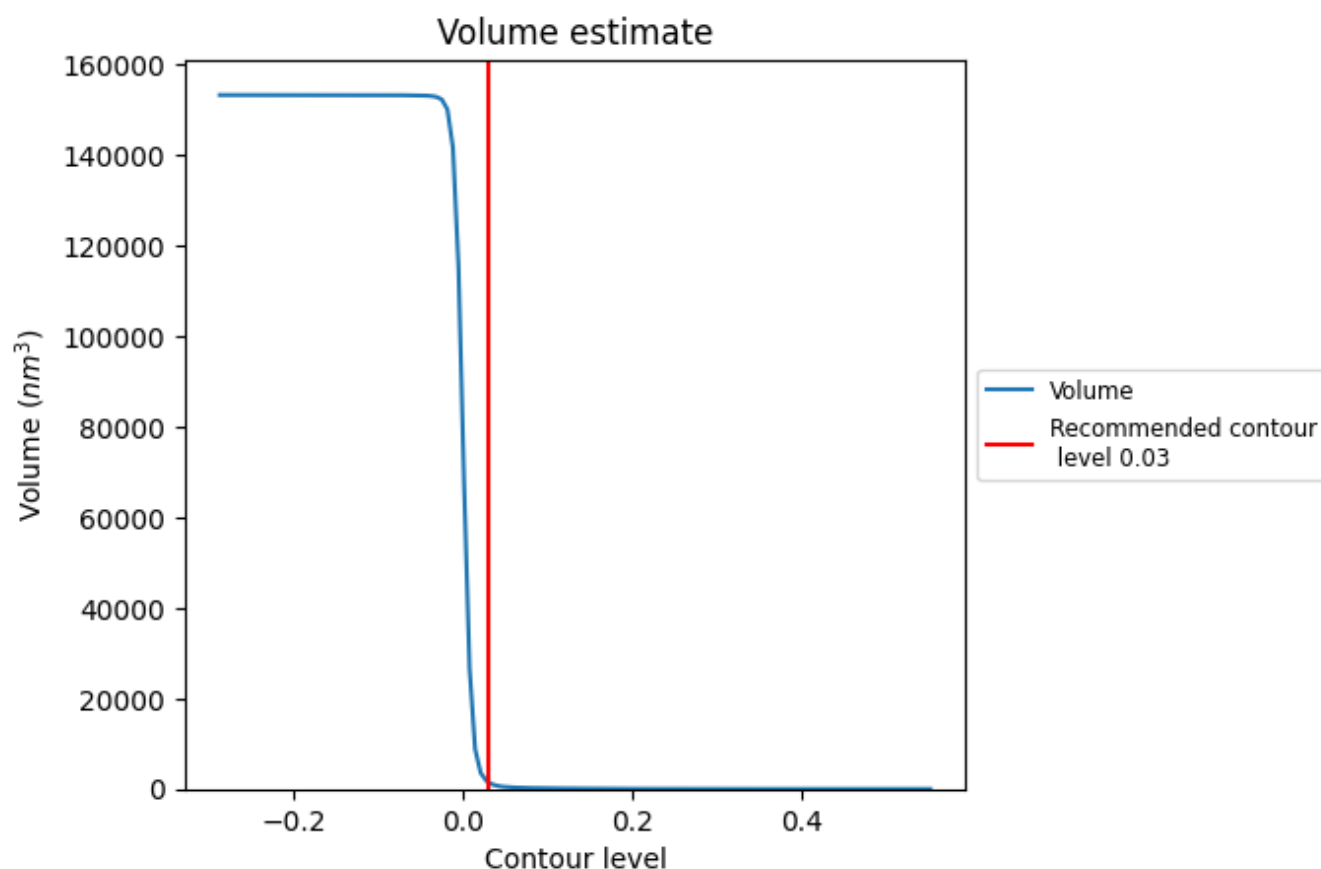
### 7.1 Map-value distribution [i](#)



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](#)

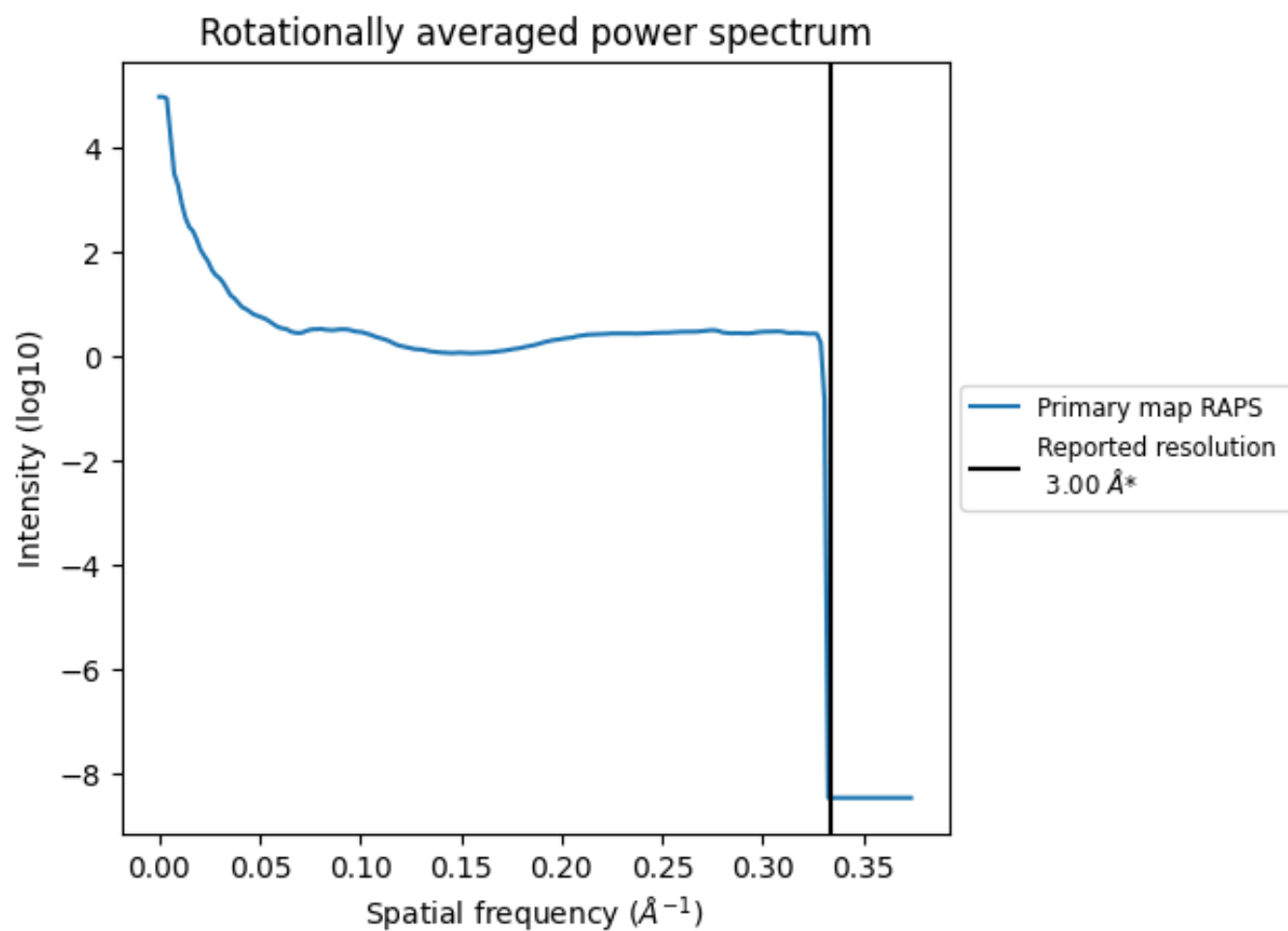


The volume at the recommended contour level is 1504 nm<sup>3</sup>; this corresponds to an approximate mass of 1358 kDa.

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 0.333 Å<sup>-1</sup>



## 8 Fourier-Shell correlation

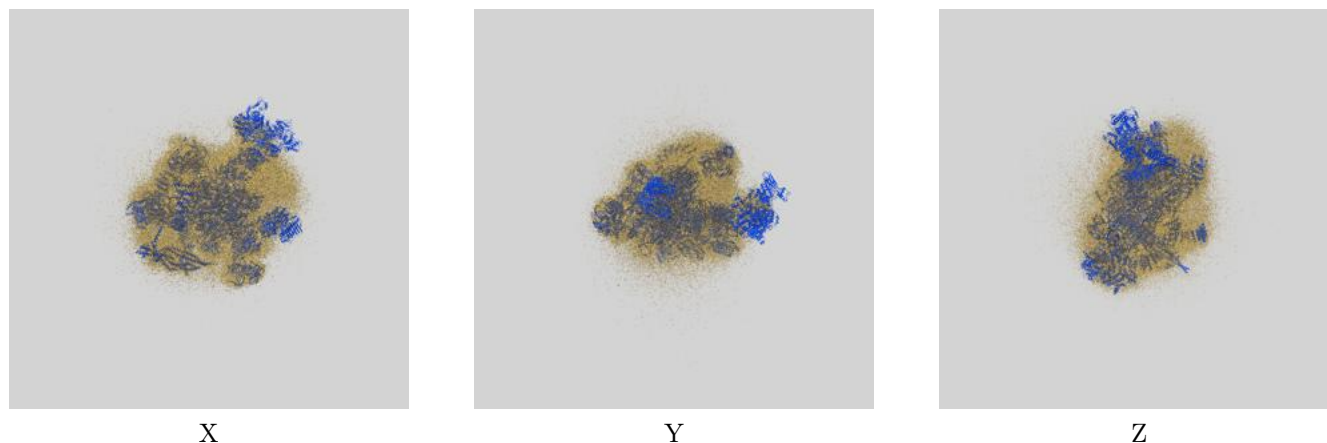
This section was not generated. No FSC curve or half-maps provided.



## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-9645 and PDB model 6ICZ. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

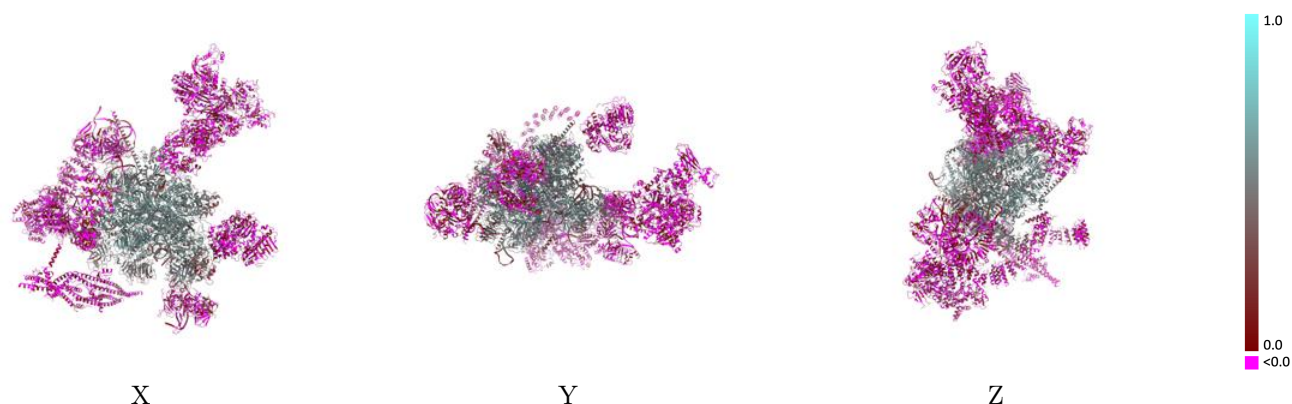
### 9.1 Map-model overlay [i](#)



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

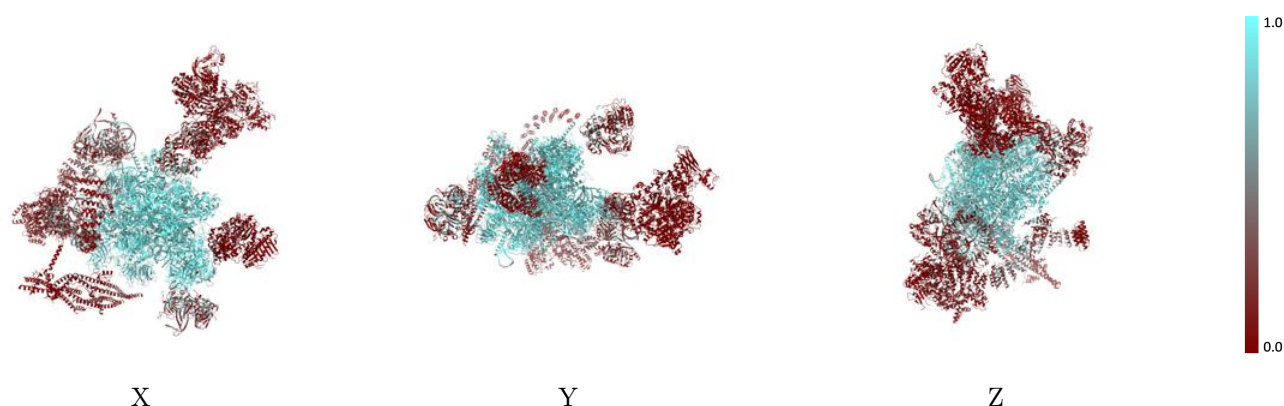


## 9.2 Q-score mapped to coordinate model [i](#)



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.

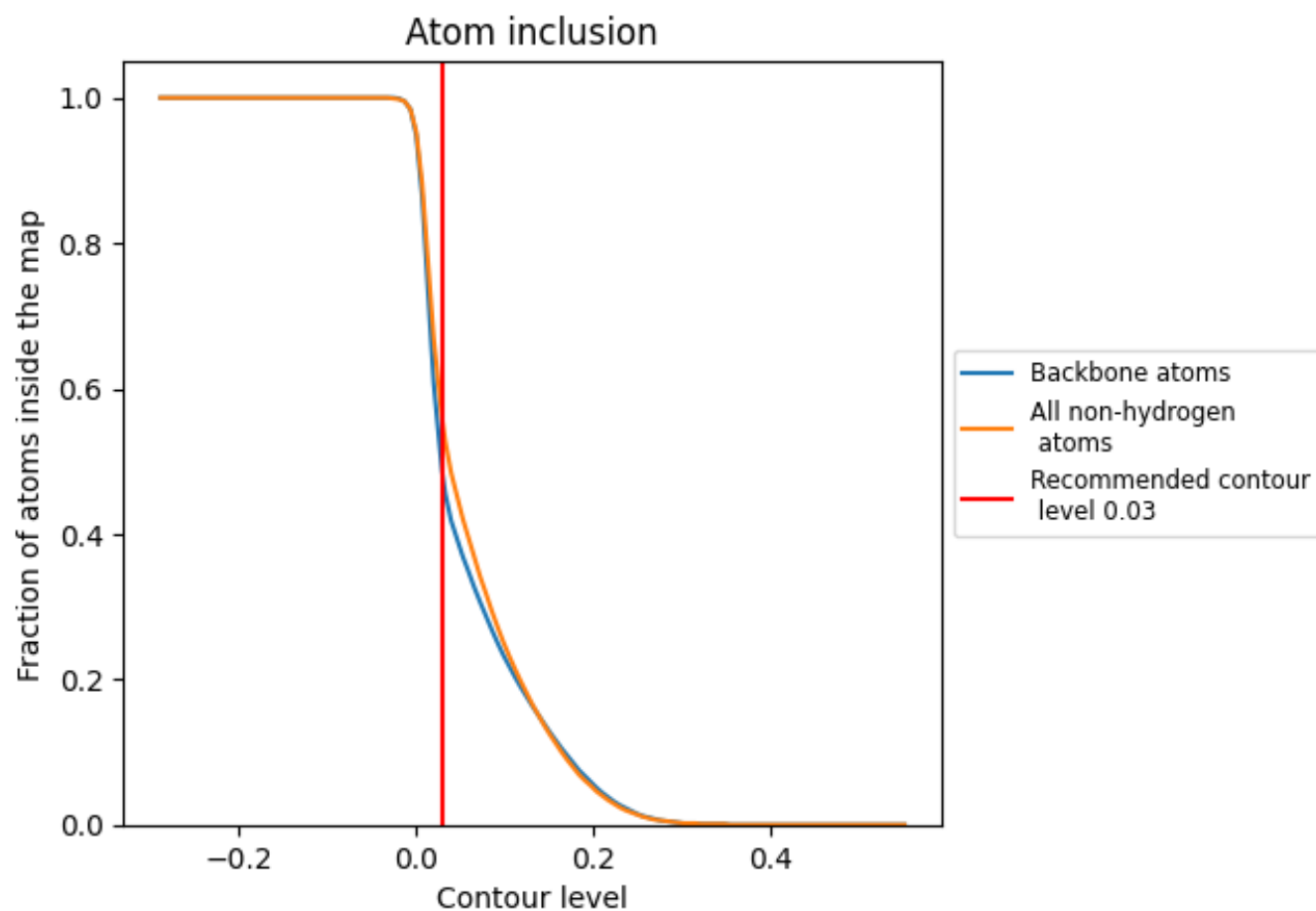
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.03).



## 9.4 Atom inclusion [i](#)









































































At the recommended contour level, 49% of all backbone atoms, 56% of all non-hydrogen atoms, are inside the map.



## 9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.03) and Q-score for the entire model and for each chain.



































Chain	Atom inclusion	Q-score
All	 0.5600	 0.2840
A	 0.8720	 0.5070
B	 0.7660	 0.3530
C	 0.8960	 0.4650
D	 0.0170	 0.0020
E	 0.8600	 0.4140
F	 0.9330	 0.4850
G	 0.7650	 0.3440
H	 0.4880	 0.1340
I	 0.2180	 0.0190
J	 0.5970	 0.3190
K	 0.1120	 -0.0060
L	 0.6000	 0.3280
M	 0.8730	 0.4830
N	 0.9350	 0.5390
O	 0.8170	 0.4200
P	 0.8340	 0.4750
Q	 0.0290	 0.0020
R	 0.8770	 0.4780
S	 0.8670	 0.4200
T	 0.9650	 0.5840
U	 0.8240	 0.5200
V	 0.4890	 0.2780
W	 0.8310	 0.4190
X	 0.5930	 0.3250
Y	 0.2630	 0.0450
Z	 0.7970	 0.4390
a	 0.3460	 0.0120
b	 0.3260	 0.0300
c	 0.2930	 0.0150
d	 0.3210	 0.0150
e	 0.3220	 0.0560
f	 0.3020	 0.0360
g	 0.3000	 0.0160
h	 0.1990	 -0.0100



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Chain	Atom inclusion	Q-score
i	 0.2030	 0.0080
j	 0.3640	 0.0370
k	 0.2940	 -0.0060
l	 0.3040	 0.0530
m	 0.3820	 0.0410
n	 0.2270	 -0.0020
o	 0.1490	 0.0120
p	 0.2390	 -0.0180
q	 0.0430	 -0.0060
r	 0.0690	 0.0010
s	 0.1190	 0.0440
t	 0.0570	 -0.0170
u	 0.0290	 -0.0080
v	 0.0010	 0.0100
w	 0.0000	 0.0450
x	 0.0000	 0.0520
y	 0.1870	 -0.0070