wwPDB EM Validation Summary Report ⓘ

Nov 14, 2022 – 03:17 PM JST

PDB ID	:	6J6H
EMDB ID	:	EMD-0687
Title	:	Cryo-EM structure of the yeast B*-a1 complex at an average resolution of 3.6 angstrom
Authors	:	Wan, R.; Bai, R.; Yan, C.; Lei, J.; Shi, Y.
Deposited on	:	2019-01-15
Resolution	:	3.60 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

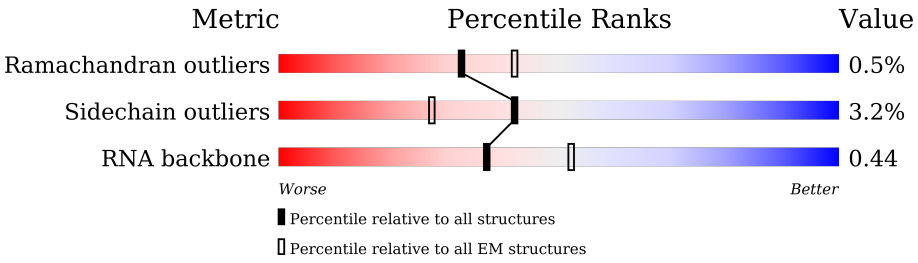
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance

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

The reported resolution of this entry is 3.60 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	A	2413	8% 77% · 21%
2	C	1008	90% · 9%
3	J	135	20% 80%
4	O	451	78% · 21%
5	P	379	6% 54% · 46%
6	Q	364	78% · 20%
7	R	339	76% · 23%
8	S	175	5% 39% · 60%

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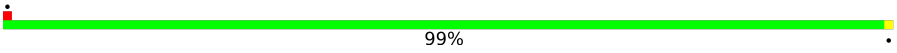
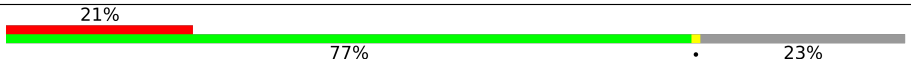
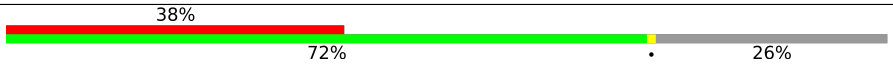
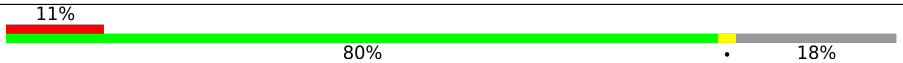
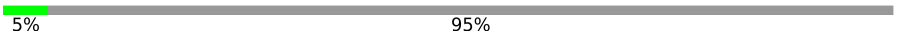
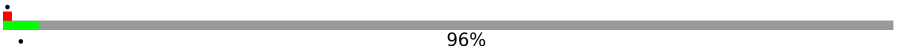
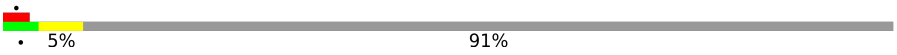
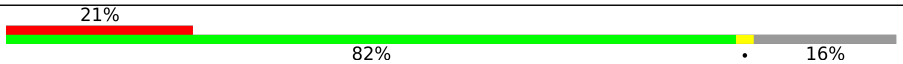
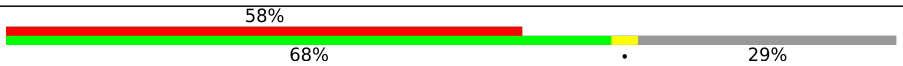
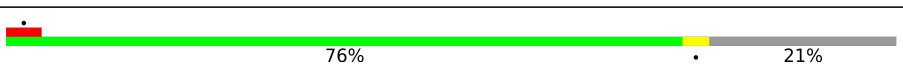
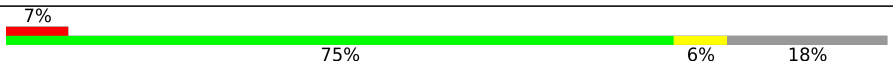
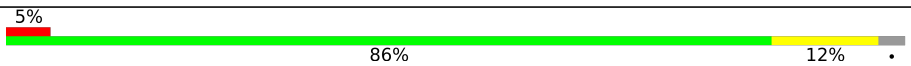
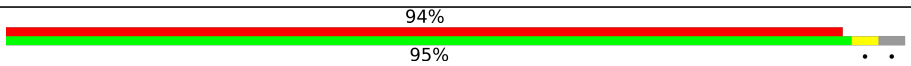
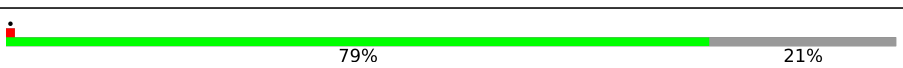
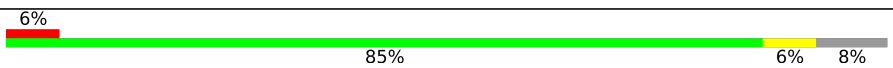
Mol	Chain	Length	Quality of chain
9	T	157	
10	Z	577	
11	c	590	
12	d	687	
13	I	215	
14	n	455	
15	H	235	
16	B	679	
17	D	214	
18	E	112	
19	L	1175	
20	v	859	
21	a	111	
22	b	238	
23	t	175	
24	i	94	
24	u	94	
25	m	146	
25	z	146	
26	j	77	
26	x	77	
27	h	86	
27	w	86	
28	e	110	
28	g	110	

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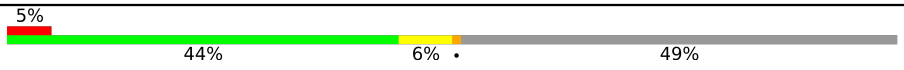
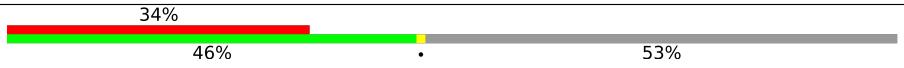
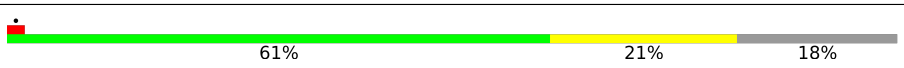
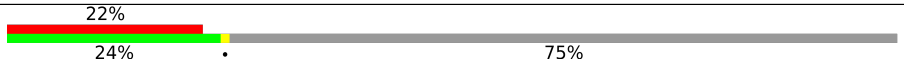
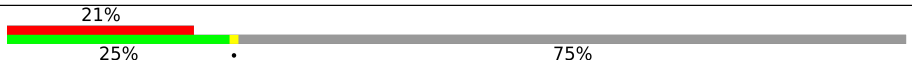
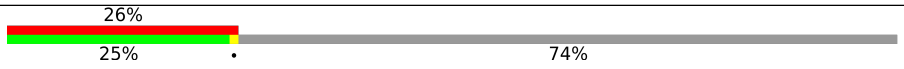
Mol	Chain	Length	Quality of chain
29	k	196	
29	s	196	
30	l	101	
30	y	101	
31	o	503	
31	p	503	
31	q	503	
31	r	503	

2 Entry composition (i)

There are 35 unique types of molecules in this entry. The entry contains 76847 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Pre-mRNA-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1913	15793	10154	2714	2868	57	0	0

- Molecule 2 is a protein called Pre-mRNA-splicing factor SNU114.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	920	7348	4733	1223	1362	30	0	0

- Molecule 3 is a protein called Pre-mRNA-splicing factor CWC21.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	J	27	190	112	38	40	0	0

- Molecule 4 is a protein called Pre-mRNA-splicing factor PRP46.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	O	357	2810	1777	493	530	10	0	0

- Molecule 5 is a protein called Pre-mRNA-processing protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	P	205	1608	1003	294	304	7	0	0

- Molecule 6 is a protein called Pre-mRNA-splicing factor SLT11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	Q	292	2301	1461	399	426	15	0	0

- Molecule 7 is a protein called Pre-mRNA-splicing factor CWC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	R	261	Total	C	N	O	S	0	0
			2089	1320	369	388	12		

- Molecule 8 is a protein called Pre-mRNA-splicing factor CWC15.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	S	70	Total	C	N	O	S	0	0
			567	355	113	98	1		

- Molecule 9 is a protein called Pre-mRNA-splicing factor BUD31.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	T	157	Total	C	N	O	S	0	0
			1291	808	240	232	11		

- Molecule 10 is a protein called Pre-mRNA-splicing factor CWC22.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Z	447	Total	C	N	O	S	0	0
			3651	2343	602	688	18		

- Molecule 11 is a protein called Pre-mRNA-splicing factor CEF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	c	436	Total	C	N	O	S	0	0
			2978	1843	552	575	8		

- Molecule 12 is a protein called Pre-mRNA-splicing factor CLF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	d	566	Total	C	N	O	S	0	0
			3881	2433	707	732	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	102	Total	C	N	O	S	0	0
			822	504	152	165	1		

- Molecule 14 is a protein called Pre-mRNA-processing factor 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	n	23	Total	C	N	O	P	0	0
			199	122	41	35	1		

- Molecule 15 is a protein called Pre-mRNA-splicing factor ISY1.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	H	9	Total	C	N	O	0	0
			94	65	17	12		

- Molecule 16 is a RNA chain called ACT1 pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	B	60	Total	C	N	O	P	0	0
			1266	567	213	426	60		

- Molecule 17 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	D	179	Total	C	N	O	P	0	0
			3795	1699	660	1258	178		

- Molecule 18 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	E	103	Total	C	N	O	P	0	0
			2192	982	391	716	103		

- Molecule 19 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	L	209	Total	C	N	O	P	0	0
			4405	1972	737	1487	209		

- Molecule 20 is a protein called Pre-mRNA-splicing factor SYF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	v	722	Total	C	N	O	S	0	0
			4625	2893	825	895	12		

- Molecule 21 is a protein called U2 small nuclear ribonucleoprotein B".

Mol	Chain	Residues	Atoms				AltConf	Trace
21	a	84	Total 416	C 248	N 84	O 84	0	0

- Molecule 22 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	b	169	Total 841	C 503	N 169	O 169	0	0

- Molecule 23 is a protein called Pre-mRNA-splicing factor SNT309.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	t	156	Total 926	C 585	N 160	O 180	S 1	0	0

- Molecule 24 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	u	74	Total 526	C 346	N 87	O 90	S 3	0	0
24	i	74	Total 541	C 358	N 90	O 90	S 3	0	0

- Molecule 25 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	m	119	Total 917	C 575	N 163	O 176	S 3	0	0
25	z	108	Total 824	C 521	N 142	O 158	S 3	0	0

- Molecule 26 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	j	75	Total 552	C 350	N 98	O 103	S 1	0	0
26	x	75	Total 552	C 350	N 98	O 103	S 1	0	0

- Molecule 27 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	h	68	Total	C	N	O	S	0	0
			518	337	96	84	1		
27	w	68	Total	C	N	O	S	0	0
			518	337	96	84	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	g	101	Total	C	N	O	S	0	0
			785	504	149	128	4		
28	e	101	Total	C	N	O	S	0	0
			785	504	149	128	4		

- Molecule 29 is a protein called Small nuclear ribonucleoprotein-associated protein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	k	100	Total	C	N	O	S	0	0
			809	514	150	142	3		
29	s	93	Total	C	N	O	S	0	0
			749	476	138	132	3		

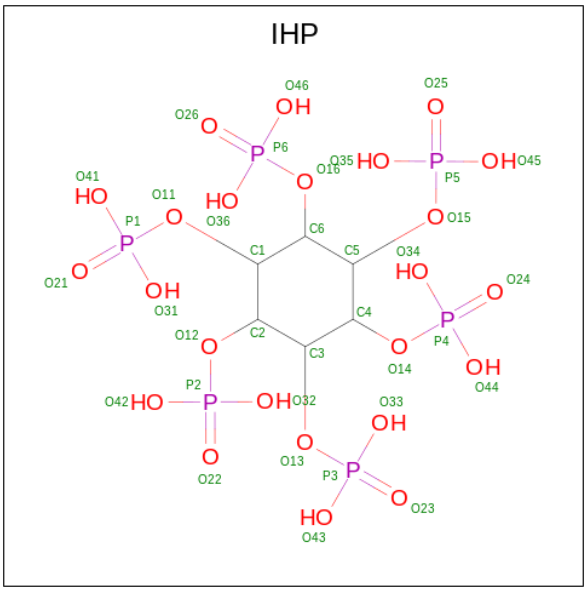
- Molecule 30 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	l	83	Total	C	N	O	S	0	0
			641	408	111	120	2		
30	y	81	Total	C	N	O	S	0	0
			616	394	107	113	2		

- Molecule 31 is a protein called Pre-mRNA-processing factor 19.

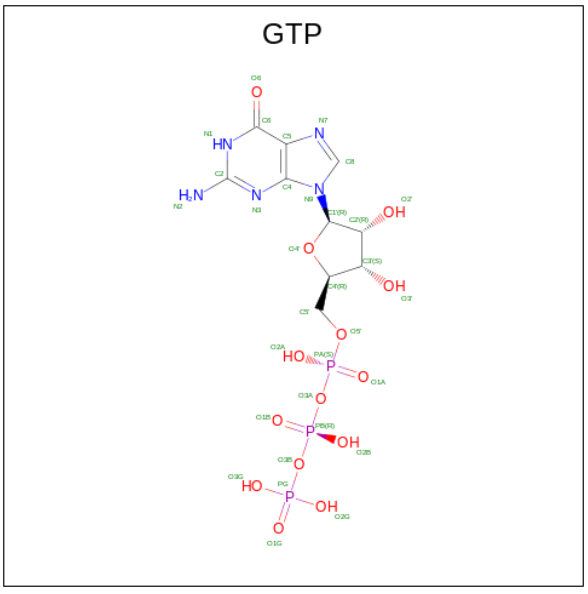
Mol	Chain	Residues	Atoms					AltConf	Trace
31	r	125	Total	C	N	O	S	0	0
			823	521	133	167	2		
31	p	128	Total	C	N	O	S	0	0
			843	532	136	173	2		
31	q	129	Total	C	N	O	S	0	0
			850	537	137	174	2		
31	o	126	Total	C	N	O	S	0	0
			830	525	134	169	2		

- Molecule 32 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$).



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

- Molecule 33 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

- Molecule 34 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
34	C	1	Total Mg 1 1	0
34	E	5	Total Mg 5 5	0

- Molecule 35 is ZINC ION (three-letter code: ZN) (formula: Zn).

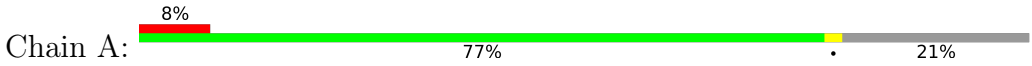
Mol	Chain	Residues	Atoms	AltConf
35	Q	2	Total Zn 2 2	0
35	R	1	Total Zn 1 1	0
35	T	3	Total Zn 3 3	0

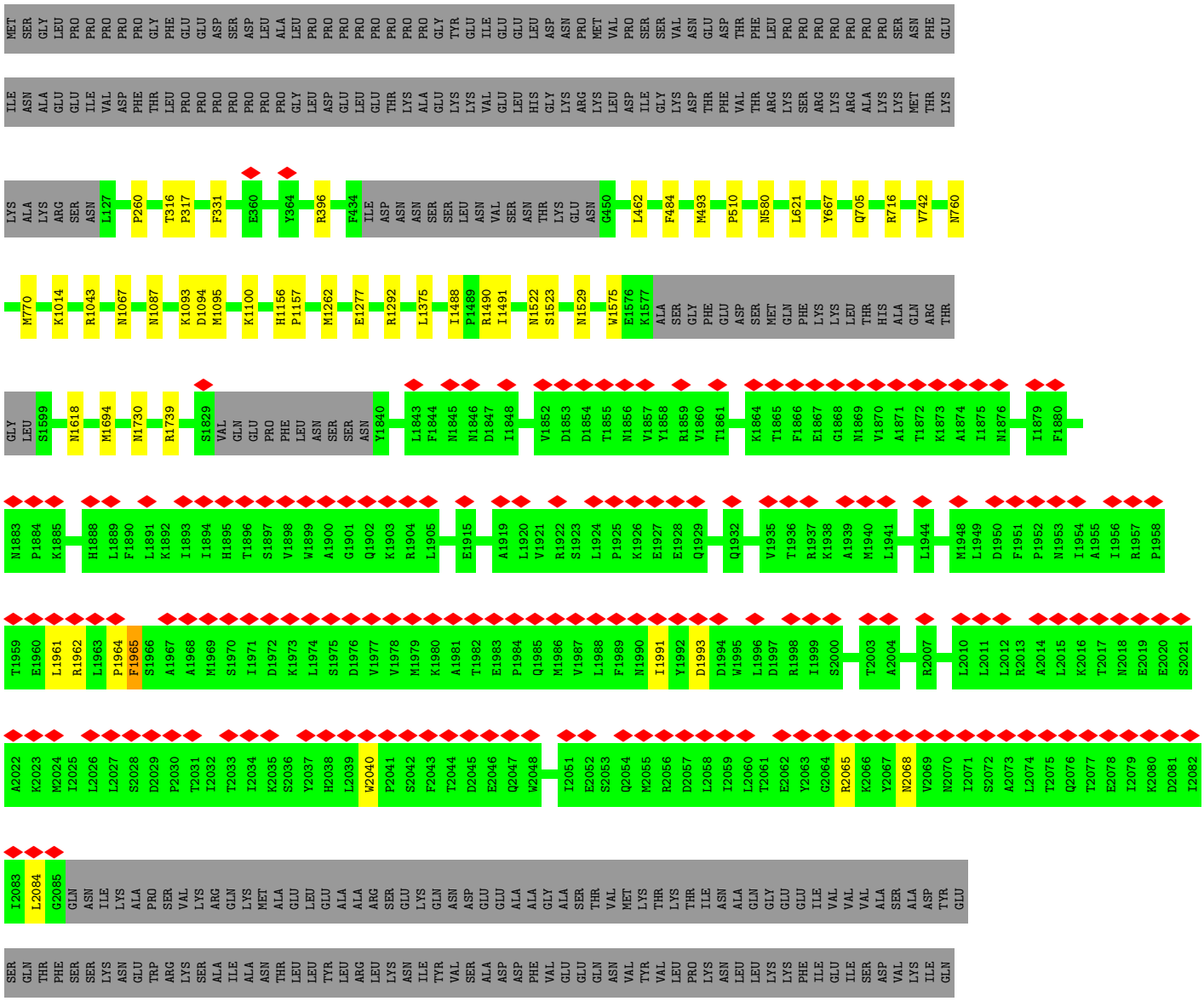
3 Residue-property plots (i)

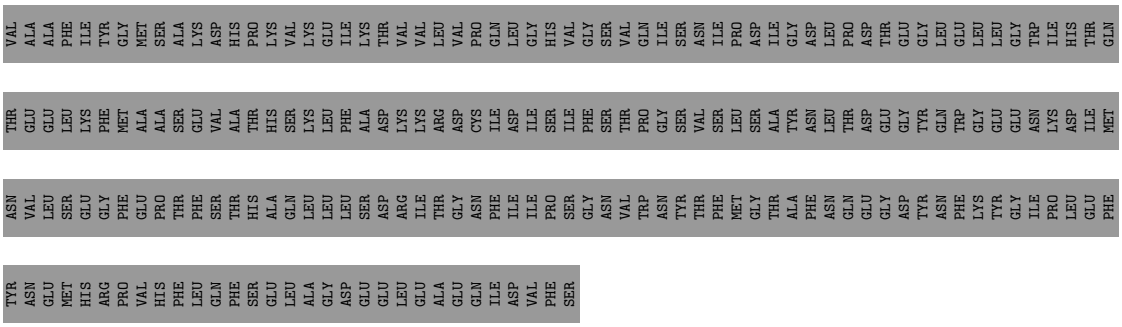
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Pre-mRNA-splicing factor 8

Chain A:

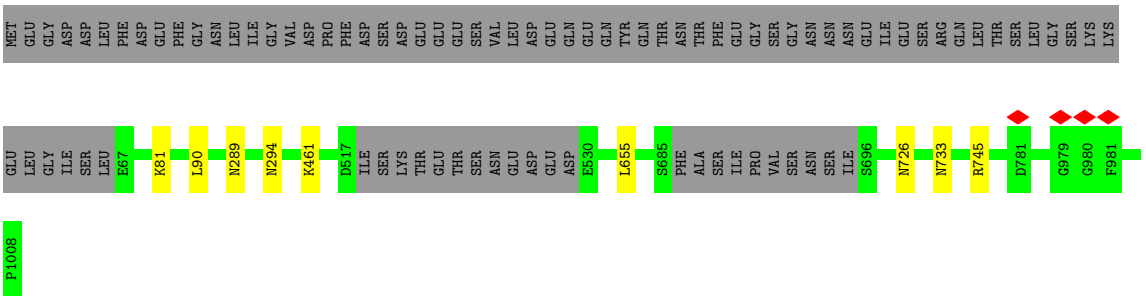






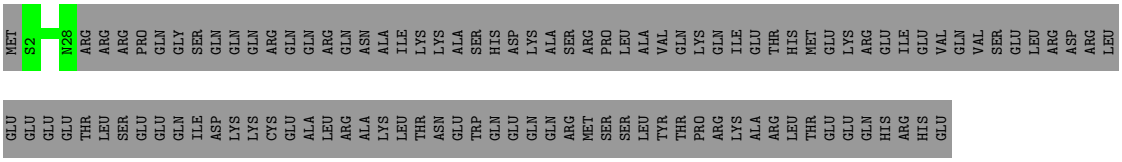
• Molecule 2: Pre-mRNA-splicing factor SNU114

Chain C:



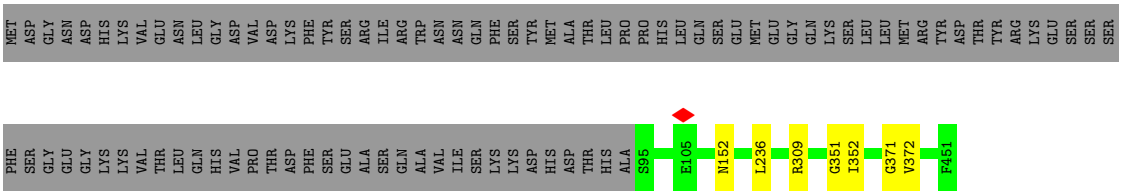
• Molecule 3: Pre-mRNA-splicing factor CWC21

Chain J:



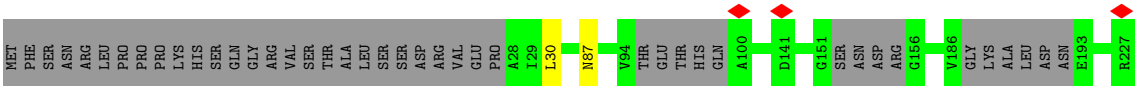
• Molecule 4: Pre-mRNA-splicing factor PRP46

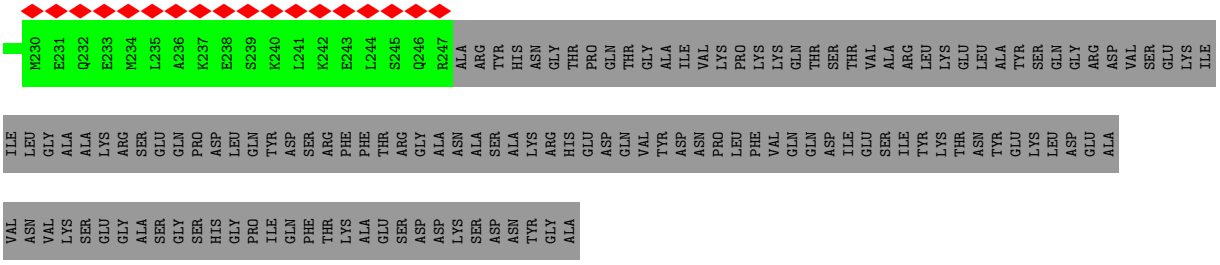
Chain O:



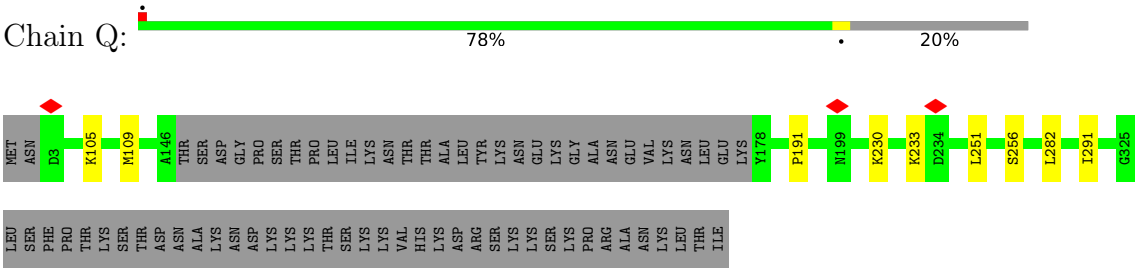
• Molecule 5: Pre-mRNA-processing protein 45

Chain P:

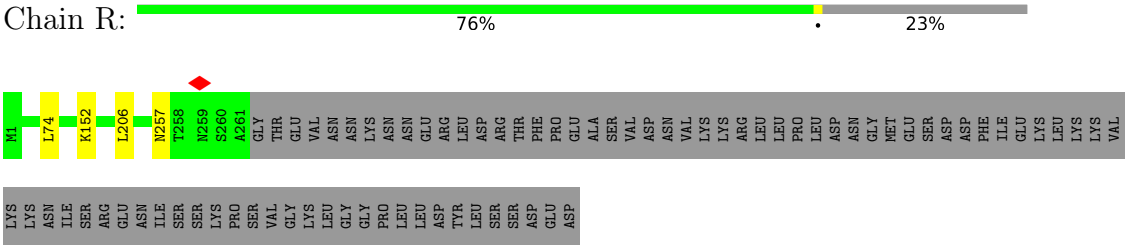




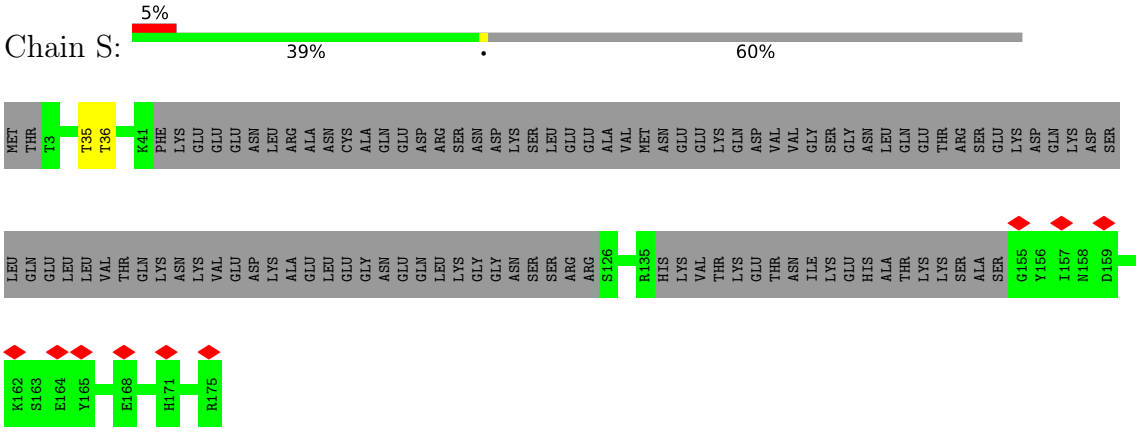
• Molecule 6: Pre-mRNA-splicing factor SLT11



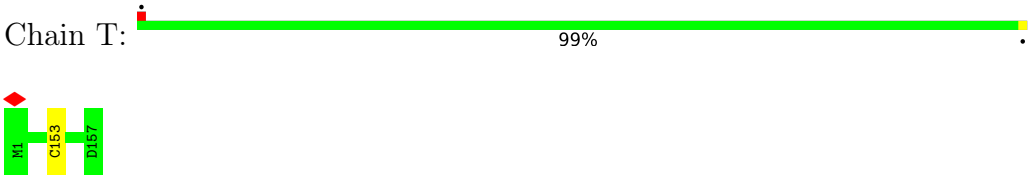
• Molecule 7: Pre-mRNA-splicing factor CWC2



• Molecule 8: Pre-mRNA-splicing factor CWC15

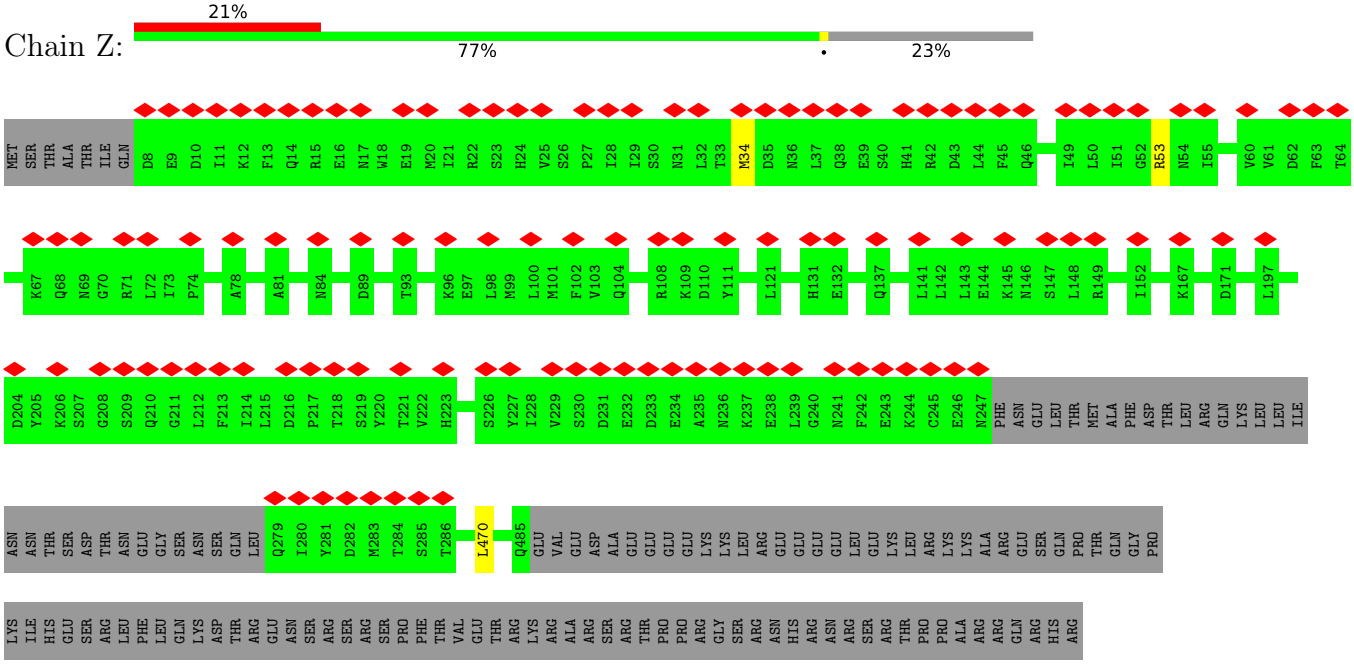


• Molecule 9: Pre-mRNA-splicing factor BUD31



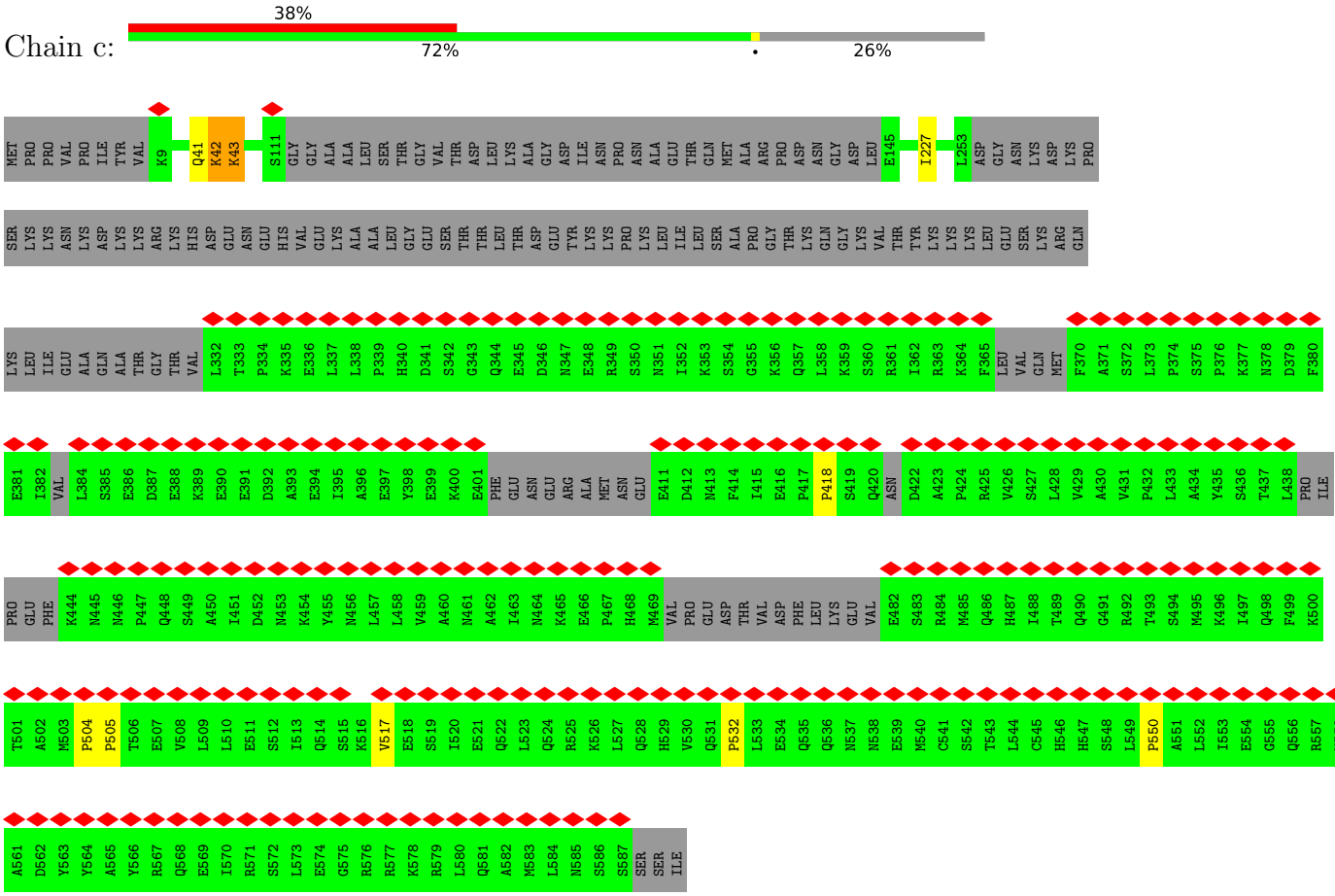
• Molecule 10: Pre-mRNA-splicing factor CWC22

Chain Z:



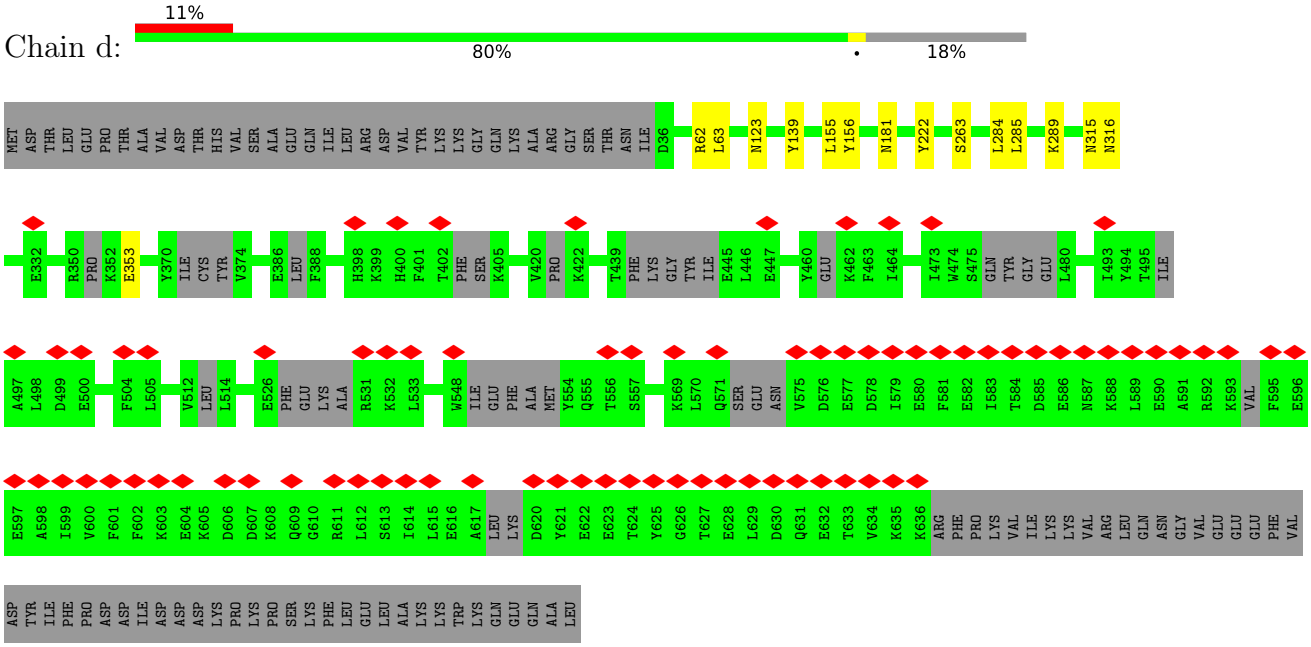
• Molecule 11: Pre-mRNA-splicing factor CEF1

Chain c:



• Molecule 12: Pre-mRNA-splicing factor CLF1

Chain d:



• Molecule 13: Pre-mRNA-splicing factor SYF2

Chain I:

• Molecule 14: Pre-mRNA-processing factor 17

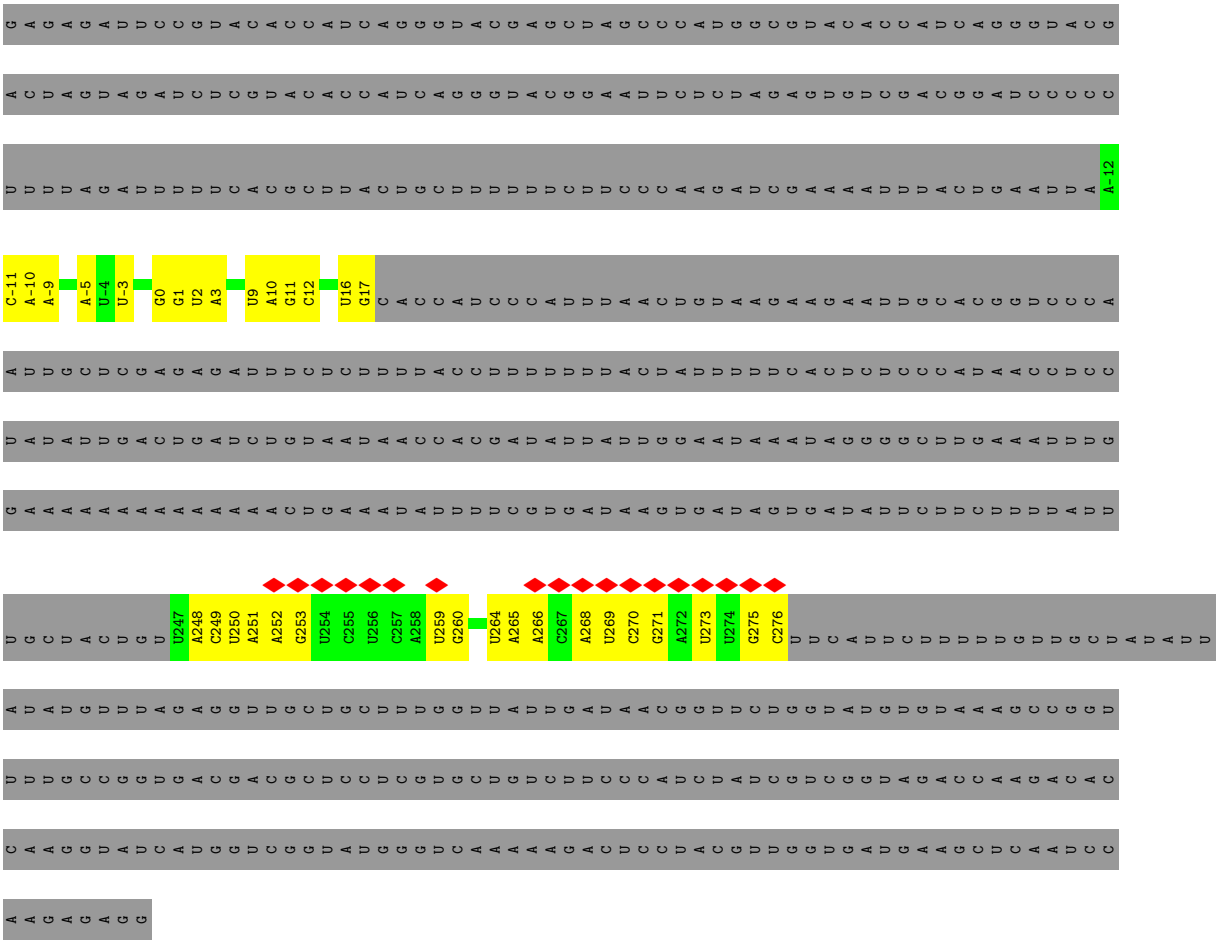
Chain n:

• Molecule 15: Pre-mRNA-splicing factor ISY1

Chain H: 96%

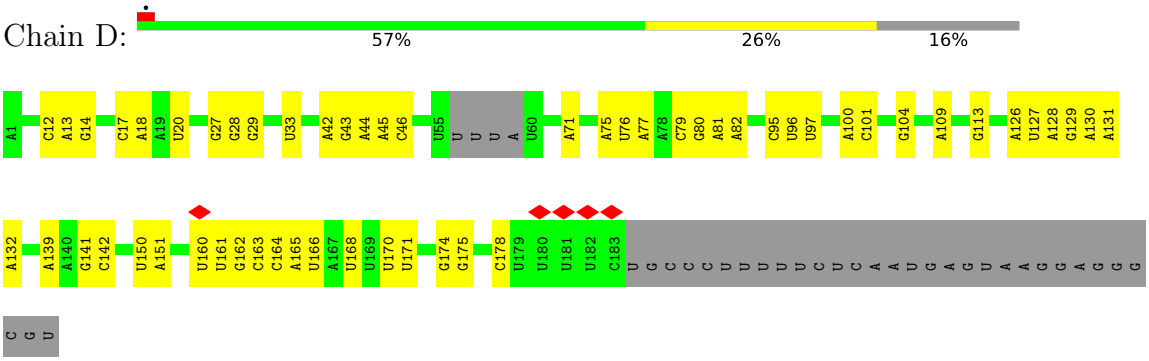
• Molecule 16: ACT1 pre-mRNA

Chain B: 5% 91%



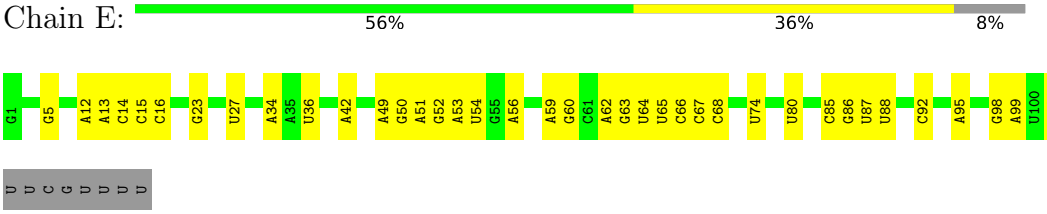
• Molecule 17: U5 snRNA

Chain D:



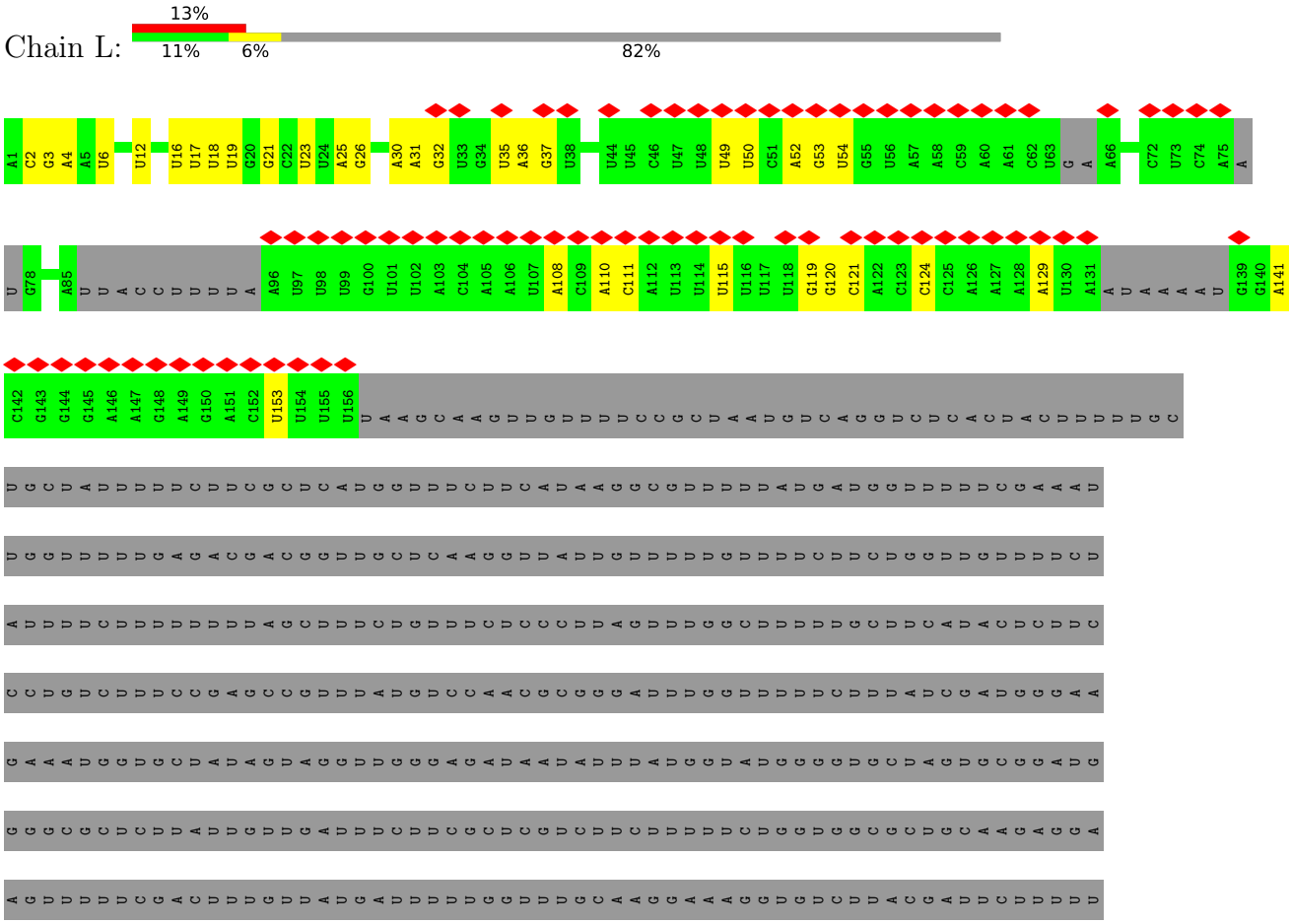
• Molecule 18: U6 snRNA

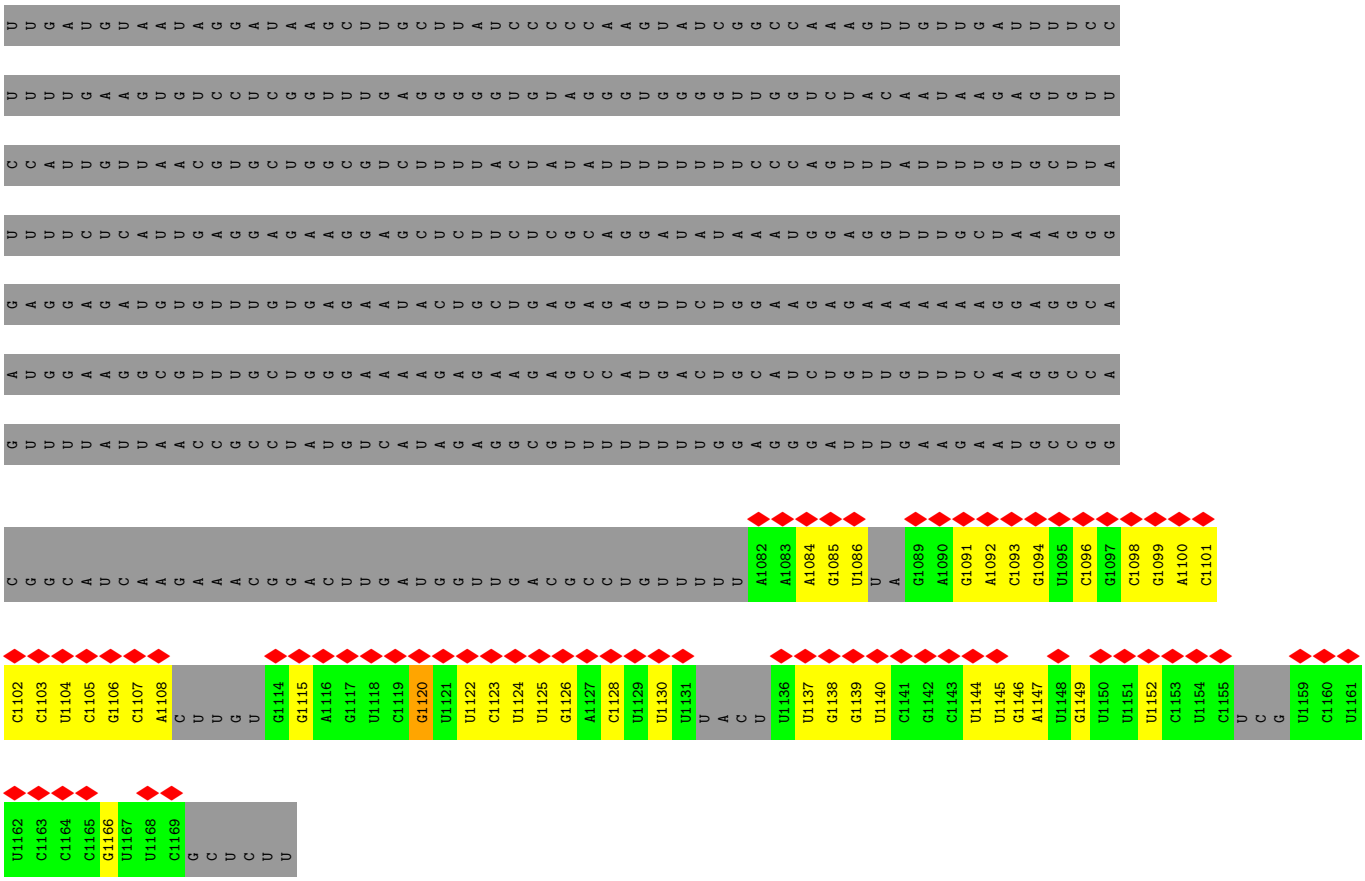
Chain E:



• Molecule 19: U2 snRNA

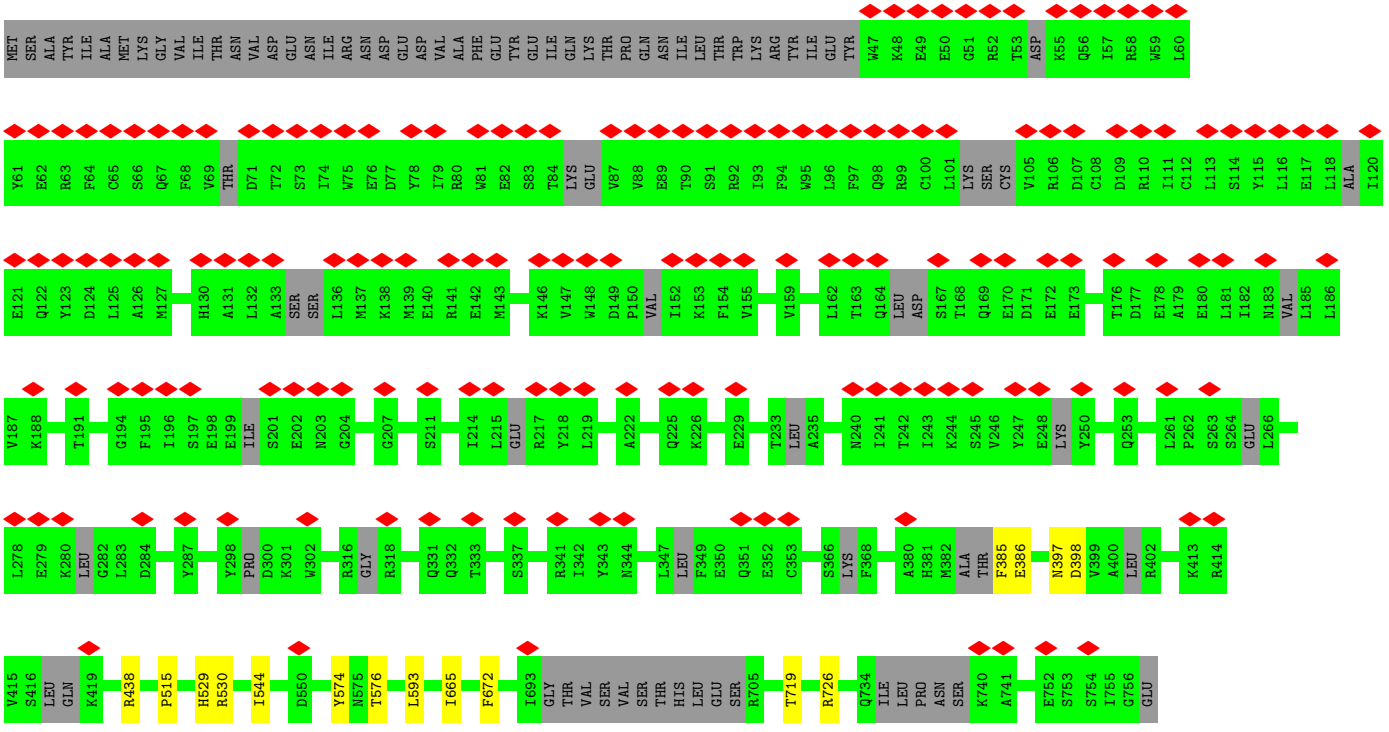
Chain L:

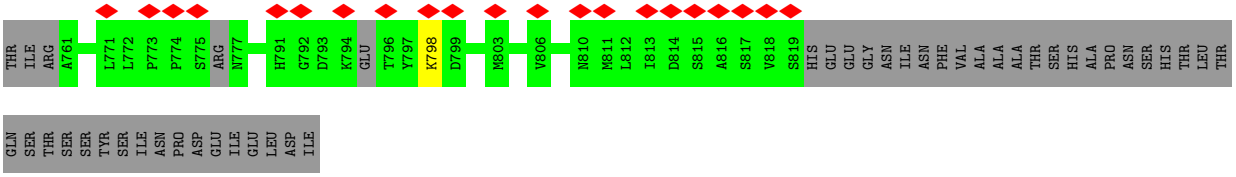




• Molecule 20: Pre-mRNA-splicing factor SYF1

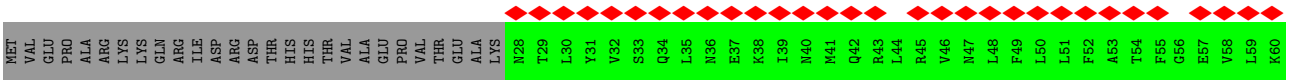
Chain v:

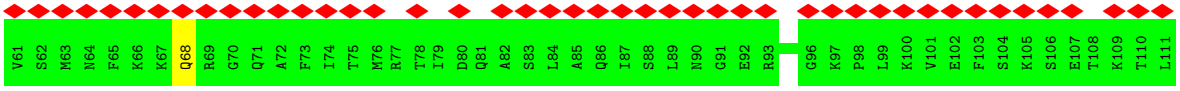




• Molecule 21: U2 small nuclear ribonucleoprotein B"

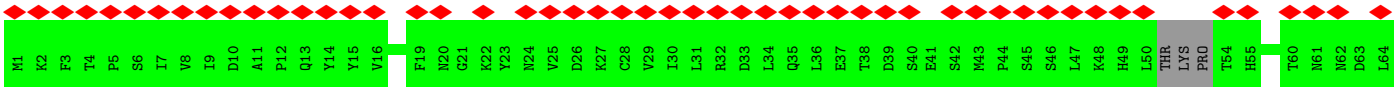
Chain a:

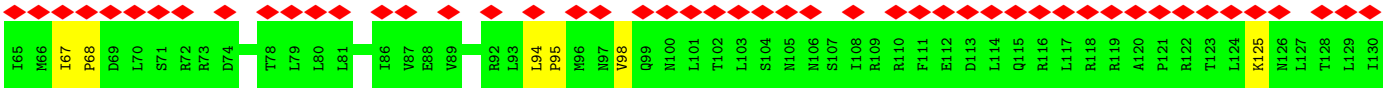


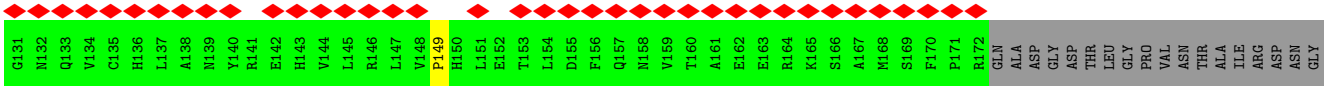


• Molecule 22: U2 small nuclear ribonucleoprotein A'

Chain b:

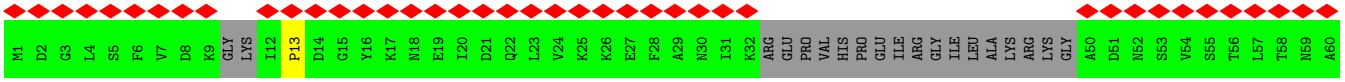


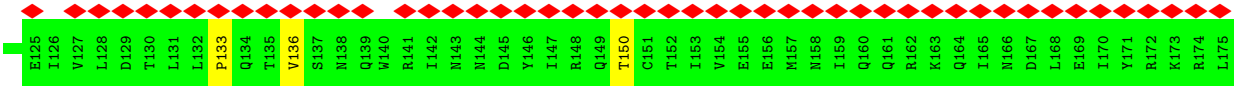




• Molecule 23: Pre-mRNA-splicing factor SNT309

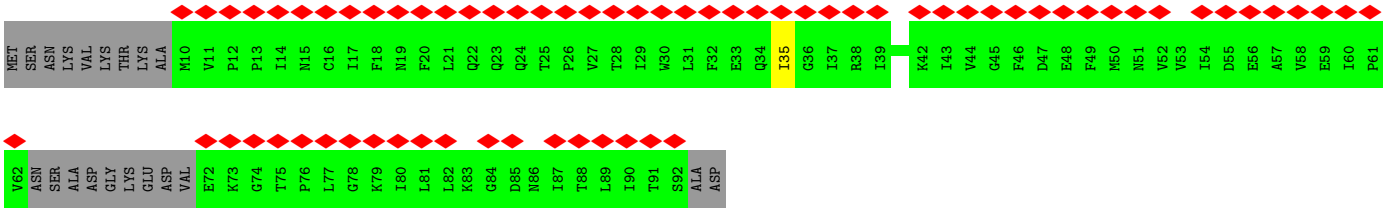
Chain t:





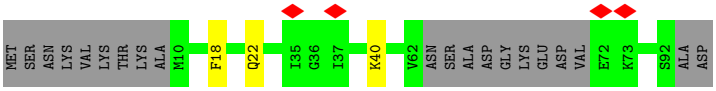
• Molecule 24: Small nuclear ribonucleoprotein E

Chain u:



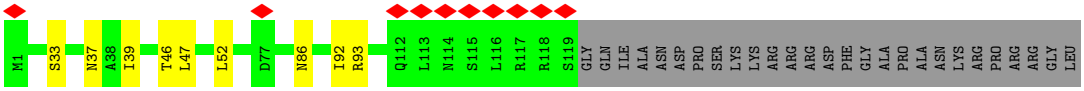
• Molecule 24: Small nuclear ribonucleoprotein E

Chain i:



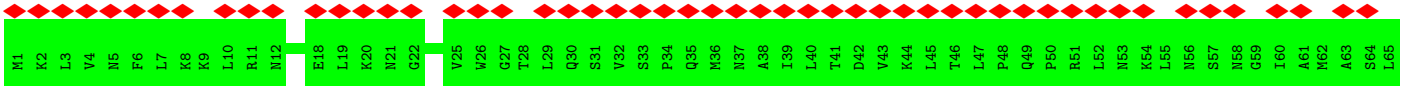
• Molecule 25: Small nuclear ribonucleoprotein Sm D1

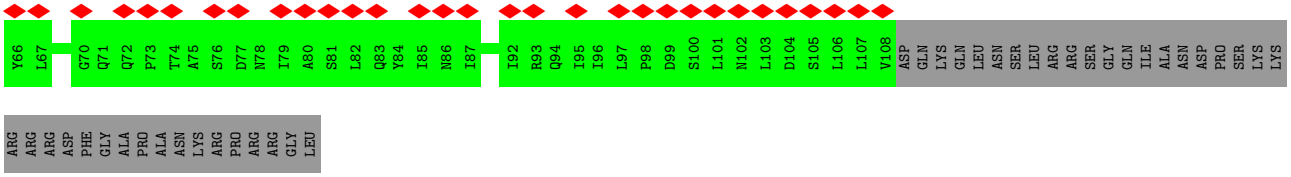
Chain m:



• Molecule 25: Small nuclear ribonucleoprotein Sm D1

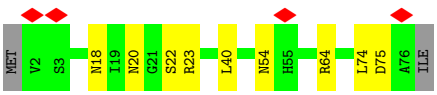
Chain z:





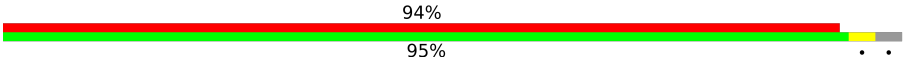
• Molecule 26: Small nuclear ribonucleoprotein G

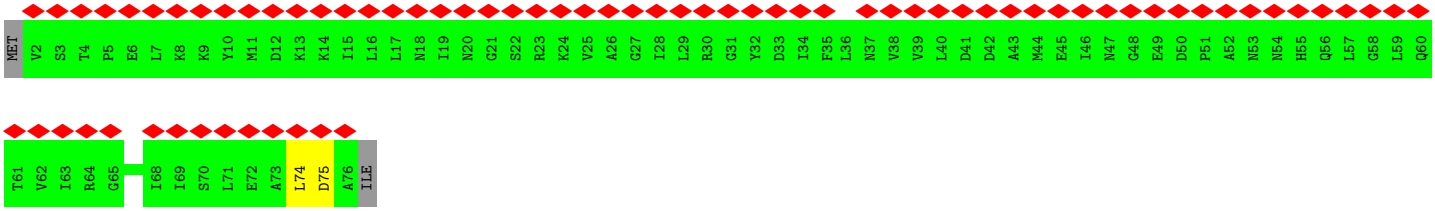
Chain j:



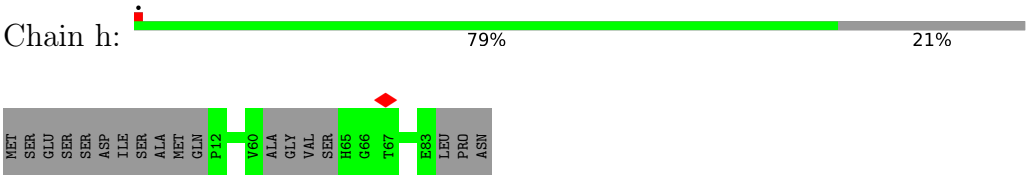
• Molecule 26: Small nuclear ribonucleoprotein G

Chain x:

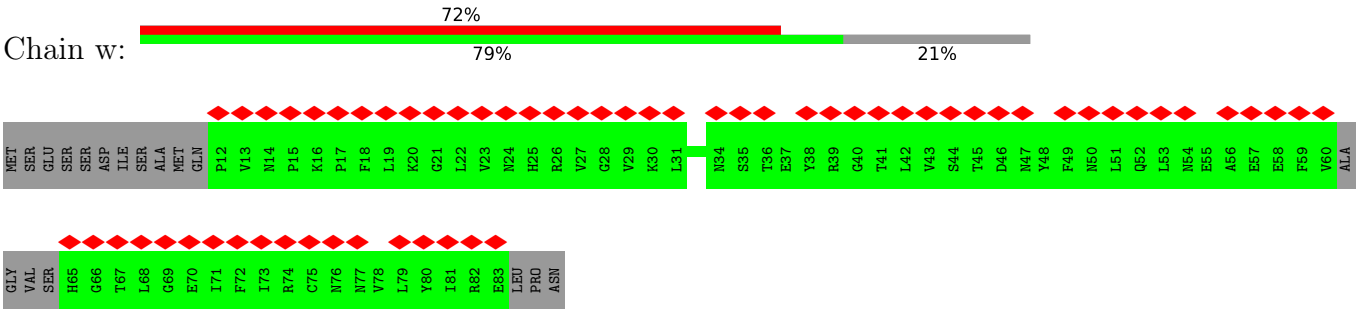




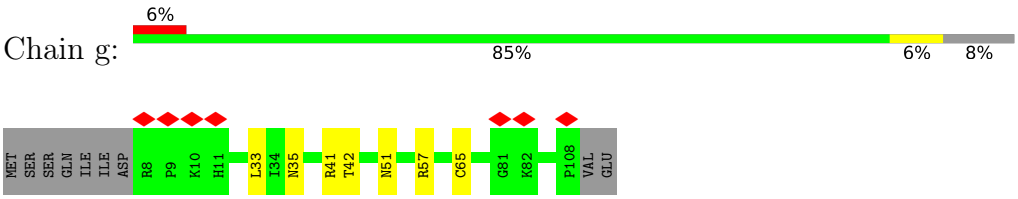
• Molecule 27: Small nuclear ribonucleoprotein F



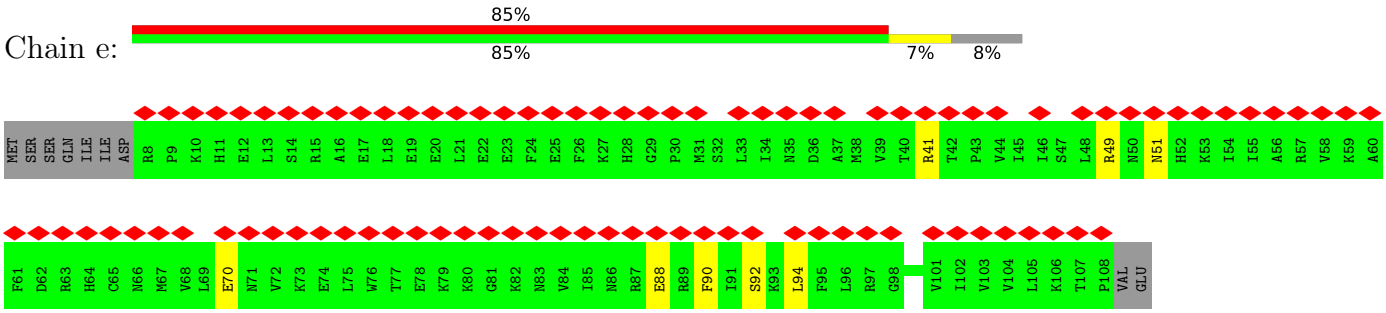
• Molecule 27: Small nuclear ribonucleoprotein F



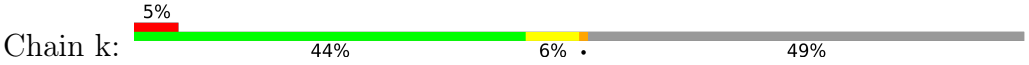
• Molecule 28: Small nuclear ribonucleoprotein Sm D2

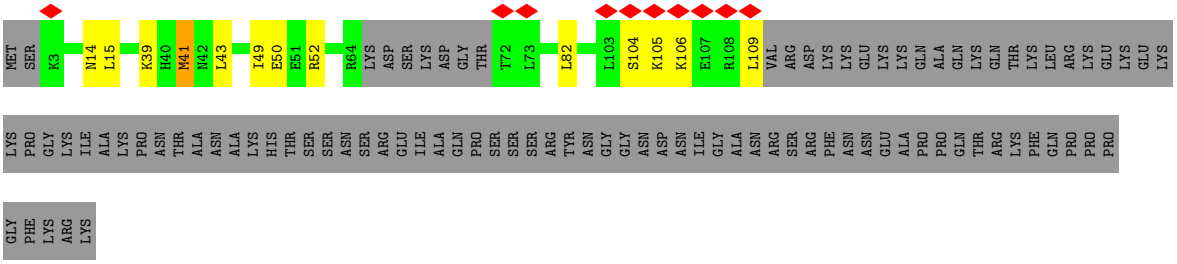


• Molecule 28: Small nuclear ribonucleoprotein Sm D2



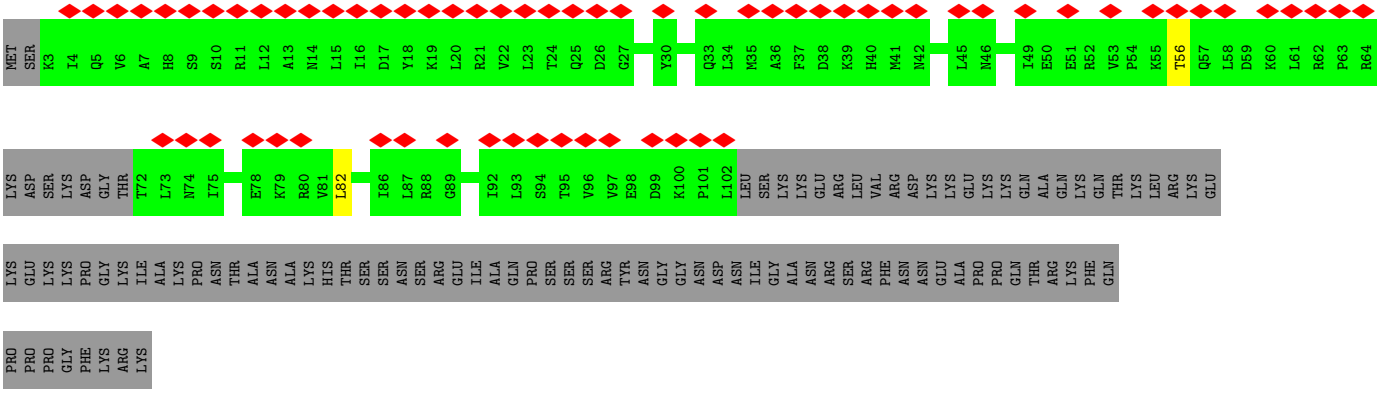
• Molecule 29: Small nuclear ribonucleoprotein-associated protein B





• Molecule 29: Small nuclear ribonucleoprotein-associated protein B

Chain s:

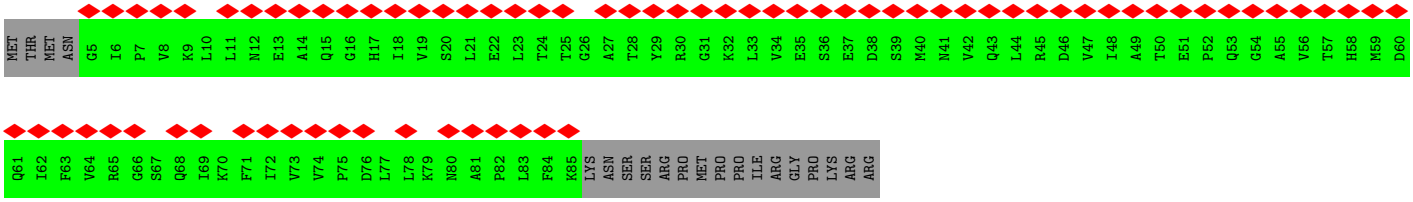


• Molecule 30: Small nuclear ribonucleoprotein Sm D3

Chain l:

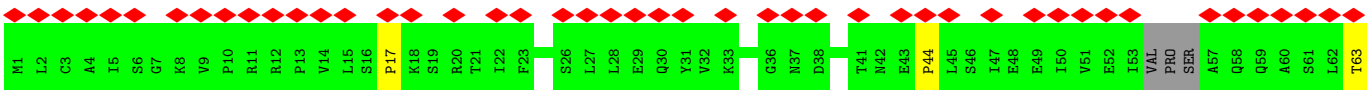
• Molecule 30: Small nuclear ribonucleoprotein Sm D3

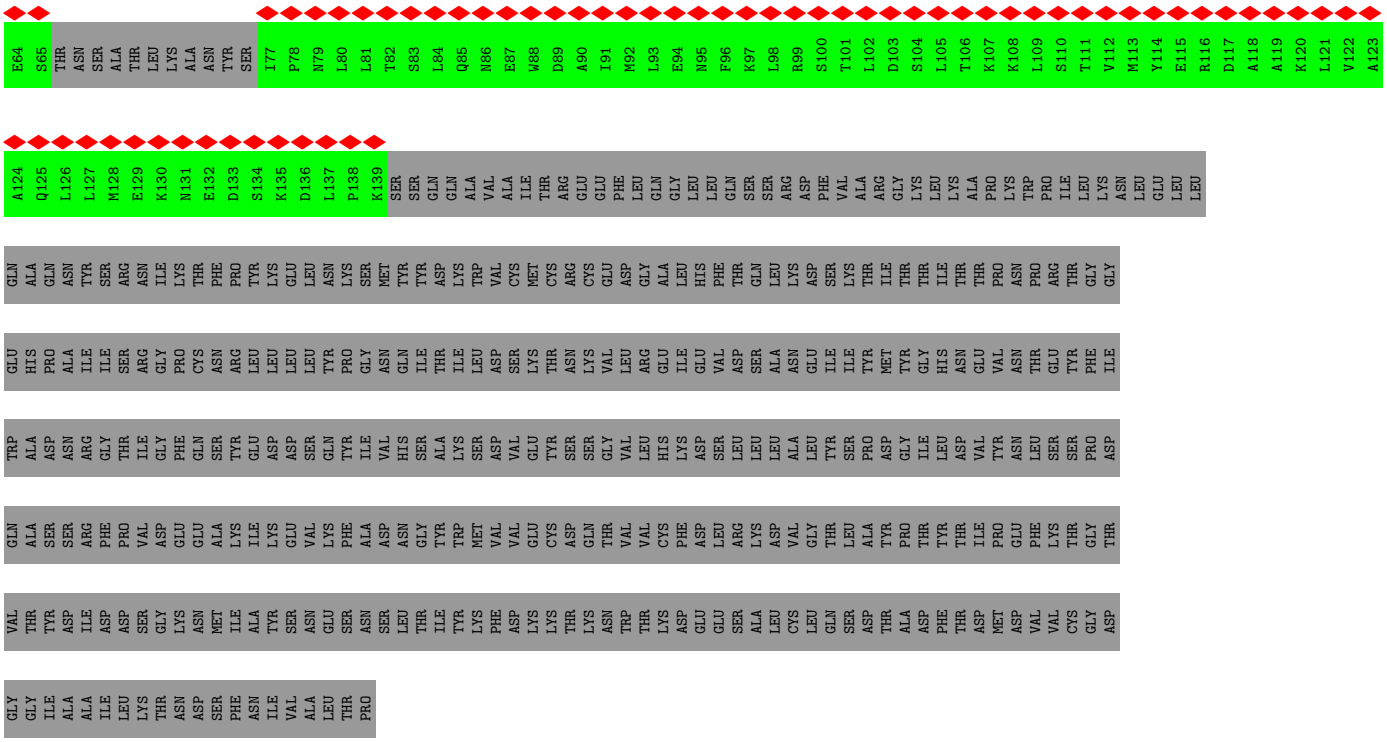
Chain y:



• Molecule 31: Pre-mRNA-processing factor 19

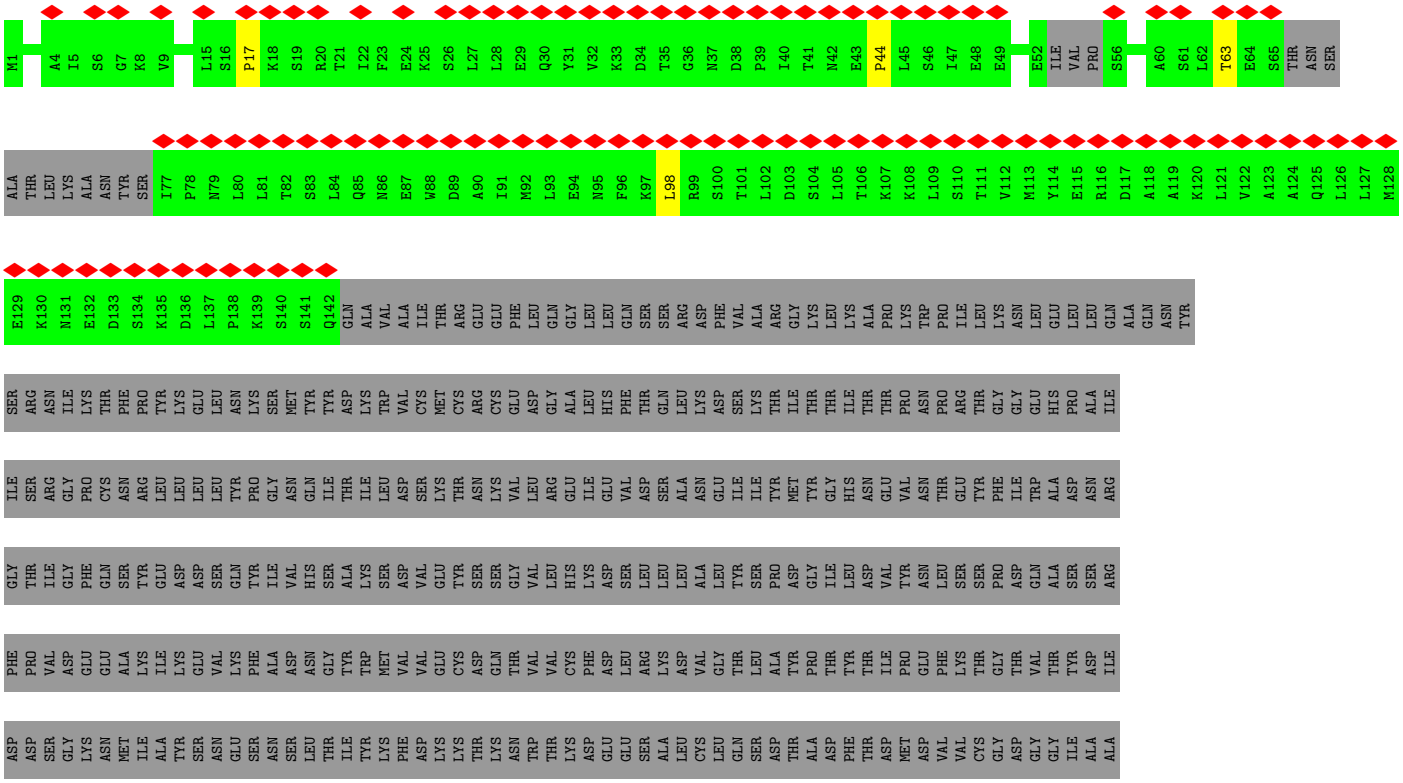
Chain r:



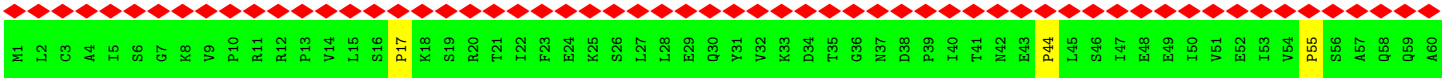


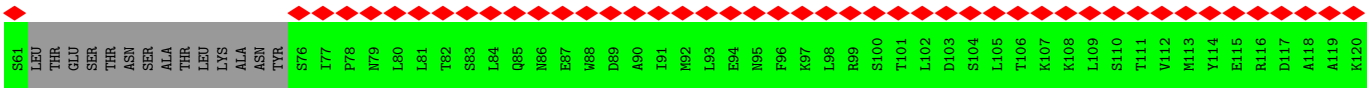
• Molecule 31: Pre-mRNA-processing factor 19

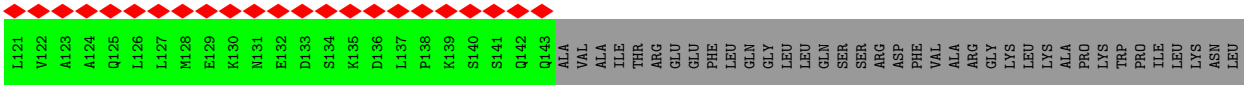
Chain p:



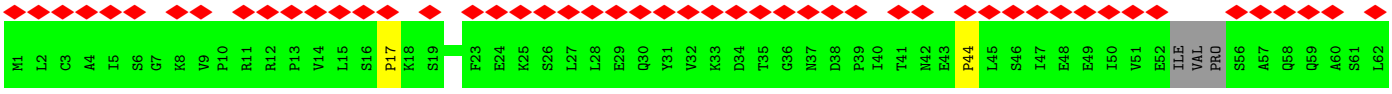
• Molecule 31: Pre-mRNA-processing factor 19

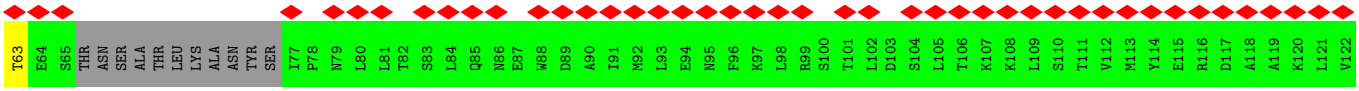


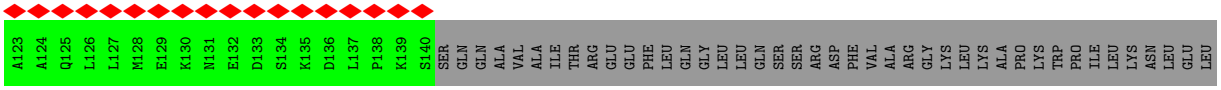




• Molecule 31: Pre-mRNA-processing factor 19







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

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

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

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

ASP GLY GLY ILE ALA ALA ILE LEU LYS THR ASN ASP SER PHE ASN ILE VAL ALA LEU THR PRO

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	555036	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	49.3	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	0.255	Depositor
Minimum map value	-0.117	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.024	Depositor
Map size (Å)	532.0, 532.0, 532.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.33, 1.33, 1.33	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.47	0/16198	0.58	0/21958
2	C	0.46	0/7503	0.59	0/10159
3	J	0.39	0/191	0.56	0/254
4	O	0.53	0/2872	0.61	0/3902
5	P	0.38	0/1629	0.51	0/2194
6	Q	0.36	0/2339	0.61	0/3154
7	R	0.42	0/2135	0.56	0/2871
8	S	0.31	0/581	0.52	0/776
9	T	0.49	0/1315	0.58	0/1759
10	Z	0.32	0/3712	0.53	0/5004
11	c	0.32	0/2996	0.44	0/4033
12	d	0.33	0/3931	0.48	0/5356
13	I	0.33	0/826	0.46	0/1097
14	n	0.39	0/194	0.50	0/256
15	H	0.33	0/98	0.35	0/130
16	B	0.57	0/1411	0.99	0/2191
17	D	0.68	0/4239	0.87	0/6598
18	E	0.70	0/2452	0.81	0/3817
19	L	0.37	1/4904 (0.0%)	0.77	0/7607
20	v	0.42	0/4662	0.51	0/6358
21	a	0.42	0/415	0.56	0/577
22	b	0.68	0/839	0.70	0/1169
23	t	0.29	0/924	0.42	0/1244
24	i	0.29	0/551	0.50	0/750
24	u	0.29	0/535	0.48	0/730
25	m	0.35	0/926	0.55	0/1257
25	z	0.30	0/833	0.53	0/1134
26	j	0.45	0/557	0.54	0/756
26	x	0.34	0/557	0.51	0/756
27	h	0.28	0/529	0.50	0/715
27	w	0.28	0/529	0.50	0/715
28	e	0.38	0/799	0.52	0/1078

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
28	g	0.40	0/799	0.55	0/1078
29	k	0.41	0/815	0.60	0/1092
29	s	0.35	0/755	0.59	0/1014
30	l	0.49	0/650	0.57	0/879
30	y	0.31	0/625	0.50	0/847
31	o	0.28	0/835	0.50	0/1126
31	p	0.25	0/848	0.51	0/1143
31	q	0.30	0/856	0.52	0/1155
31	r	0.29	0/828	0.54	0/1117
All	All	0.45	1/79193 (0.0%)	0.61	0/109806

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	L	1120	G	O3'-P	-5.54	1.54	1.61

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1905/2413 (79%)	1826 (96%)	68 (4%)	11 (1%)	25	64
2	C	914/1008 (91%)	881 (96%)	33 (4%)	0	100	100
3	J	25/135 (18%)	23 (92%)	2 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	O	355/451 (79%)	315 (89%)	36 (10%)	4 (1%)	14 53
5	P	197/379 (52%)	192 (98%)	5 (2%)	0	100 100
6	Q	288/364 (79%)	264 (92%)	22 (8%)	2 (1%)	22 61
7	R	259/339 (76%)	248 (96%)	10 (4%)	1 (0%)	34 71
8	S	64/175 (37%)	63 (98%)	1 (2%)	0	100 100
9	T	155/157 (99%)	147 (95%)	8 (5%)	0	100 100
10	Z	443/577 (77%)	427 (96%)	16 (4%)	0	100 100
11	c	418/590 (71%)	396 (95%)	19 (4%)	3 (1%)	22 61
12	d	534/687 (78%)	513 (96%)	18 (3%)	3 (1%)	25 64
13	I	98/215 (46%)	97 (99%)	1 (1%)	0	100 100
14	n	21/455 (5%)	21 (100%)	0	0	100 100
15	H	7/235 (3%)	7 (100%)	0	0	100 100
20	v	666/859 (78%)	642 (96%)	22 (3%)	2 (0%)	41 75
21	a	82/111 (74%)	78 (95%)	3 (4%)	1 (1%)	13 51
22	b	165/238 (69%)	138 (84%)	20 (12%)	7 (4%)	3 25
23	t	150/175 (86%)	145 (97%)	4 (3%)	1 (1%)	22 61
24	i	70/94 (74%)	67 (96%)	3 (4%)	0	100 100
24	u	70/94 (74%)	67 (96%)	3 (4%)	0	100 100
25	m	117/146 (80%)	111 (95%)	6 (5%)	0	100 100
25	z	106/146 (73%)	100 (94%)	6 (6%)	0	100 100
26	j	73/77 (95%)	67 (92%)	5 (7%)	1 (1%)	11 48
26	x	73/77 (95%)	65 (89%)	7 (10%)	1 (1%)	11 48
27	h	64/86 (74%)	60 (94%)	4 (6%)	0	100 100
27	w	64/86 (74%)	61 (95%)	3 (5%)	0	100 100
28	e	99/110 (90%)	95 (96%)	3 (3%)	1 (1%)	15 55
28	g	99/110 (90%)	93 (94%)	4 (4%)	2 (2%)	7 41
29	k	96/196 (49%)	90 (94%)	5 (5%)	1 (1%)	15 55
29	s	89/196 (45%)	83 (93%)	6 (7%)	0	100 100
30	l	81/101 (80%)	79 (98%)	0	2 (2%)	5 36
30	y	79/101 (78%)	75 (95%)	4 (5%)	0	100 100
31	o	120/503 (24%)	115 (96%)	5 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	p	122/503 (24%)	118 (97%)	4 (3%)	0	100	100
31	q	125/503 (25%)	116 (93%)	9 (7%)	0	100	100
31	r	119/503 (24%)	112 (94%)	7 (6%)	0	100	100
All	All	8412/13195 (64%)	7997 (95%)	372 (4%)	43 (0%)	32	68

5 of 43 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1575	TRP
1	A	1965	PHE
4	O	372	VAL
12	d	181	ASN
12	d	353	GLU

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1737/2182 (80%)	1695 (98%)	42 (2%)	49	75
2	C	830/910 (91%)	821 (99%)	9 (1%)	73	88
3	J	21/121 (17%)	21 (100%)	0	100	100
4	O	312/397 (79%)	309 (99%)	3 (1%)	76	88
5	P	175/328 (53%)	173 (99%)	2 (1%)	73	88
6	Q	265/332 (80%)	258 (97%)	7 (3%)	46	74
7	R	224/296 (76%)	221 (99%)	3 (1%)	69	86
8	S	57/151 (38%)	55 (96%)	2 (4%)	36	68
9	T	141/141 (100%)	140 (99%)	1 (1%)	84	93
10	Z	417/538 (78%)	414 (99%)	3 (1%)	84	93
11	c	214/525 (41%)	205 (96%)	9 (4%)	30	63
12	d	274/633 (43%)	262 (96%)	12 (4%)	28	63
13	I	92/193 (48%)	90 (98%)	2 (2%)	52	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
14	n	19/412 (5%)	19 (100%)	0	100 100
15	H	9/216 (4%)	9 (100%)	0	100 100
20	v	294/786 (37%)	279 (95%)	15 (5%)	24 58
23	t	39/165 (24%)	26 (67%)	13 (33%)	0 2
24	i	55/83 (66%)	52 (94%)	3 (6%)	21 57
24	u	52/83 (63%)	51 (98%)	1 (2%)	57 80
25	m	106/129 (82%)	97 (92%)	9 (8%)	10 41
25	z	95/129 (74%)	95 (100%)	0	100 100
26	j	56/66 (85%)	48 (86%)	8 (14%)	3 21
26	x	56/66 (85%)	55 (98%)	1 (2%)	59 81
27	h	51/77 (66%)	51 (100%)	0	100 100
27	w	51/77 (66%)	51 (100%)	0	100 100
28	e	82/103 (80%)	75 (92%)	7 (8%)	10 41
28	g	82/103 (80%)	77 (94%)	5 (6%)	18 53
29	k	92/176 (52%)	79 (86%)	13 (14%)	3 21
29	s	85/176 (48%)	83 (98%)	2 (2%)	49 75
30	l	72/89 (81%)	53 (74%)	19 (26%)	0 4
30	y	68/89 (76%)	68 (100%)	0	100 100
31	o	60/451 (13%)	57 (95%)	3 (5%)	24 59
31	p	62/451 (14%)	58 (94%)	4 (6%)	17 51
31	q	62/451 (14%)	59 (95%)	3 (5%)	25 60
31	r	60/451 (13%)	57 (95%)	3 (5%)	24 59
All	All	6367/11576 (55%)	6163 (97%)	204 (3%)	42 70

5 of 204 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
23	t	100	THR
28	g	41	ARG
31	q	44	PRO
23	t	111	VAL
25	m	86	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 96 such sidechains are listed below:

Mol	Chain	Res	Type
11	c	31	HIS
25	m	30	GLN
12	d	79	HIS
20	v	397	ASN
26	j	18	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
16	B	58/679 (8%)	32 (55%)	7 (12%)
17	D	177/214 (82%)	53 (29%)	8 (4%)
18	E	102/112 (91%)	39 (38%)	5 (4%)
19	L	199/1175 (16%)	73 (36%)	9 (4%)
All	All	536/2180 (24%)	197 (36%)	29 (5%)

5 of 197 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
16	B	-11	C
16	B	-10	A
16	B	-9	A
16	B	-5	A
16	B	-3	U

5 of 29 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
17	D	150	U
19	L	1107	C
18	E	49	A
19	L	1092	A
18	E	23	G

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

1 non-standard protein/DNA/RNA residue is 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	$\#\|Z\| > 2$
14	SEP	n	73	14	8,9,10	0.63	0	8,12,14	0.60	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
14	SEP	n	73	14	-	4/5/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	n	73	SEP	N-CA-CB-OG
14	n	73	SEP	CB-OG-P-O1P
14	n	73	SEP	CB-OG-P-O2P
14	n	73	SEP	CB-OG-P-O3P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 12 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
32	IHP	A	3000	-	36,36,36	0.76	0	54,60,60	0.53	0
33	GTP	C	1500	34	26,34,34	0.94	2 (7%)	32,54,54	0.68	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
32	IHP	A	3000	-	-	10/30/54/54	0/1/1/1
33	GTP	C	1500	34	-	0/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	C	1500	GTP	C5-C6	-2.61	1.42	1.47
33	C	1500	GTP	C8-N7	-2.02	1.31	1.35

There are no bond angle outliers.

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	A	3000	IHP	C2-C1-O11-P1
32	A	3000	IHP	C6-C1-O11-P1
32	A	3000	IHP	C6-O16-P6-O26
32	A	3000	IHP	C1-O11-P1-O31
32	A	3000	IHP	C6-O16-P6-O36

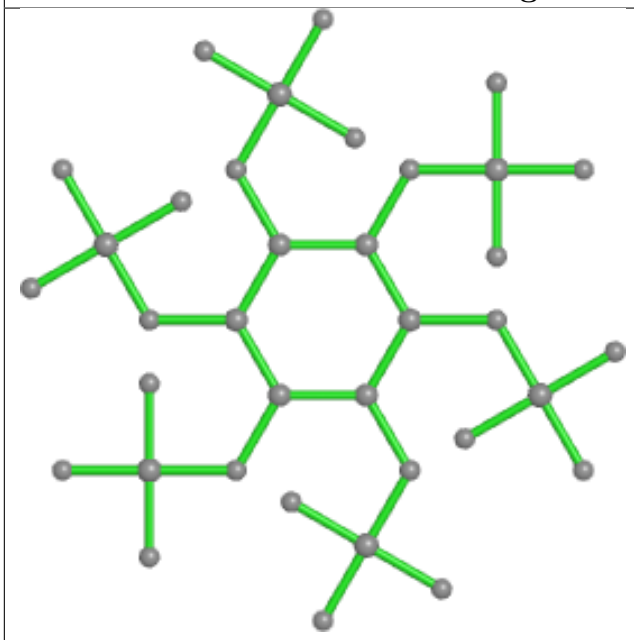
There are no ring outliers.

No monomer is involved in short contacts.

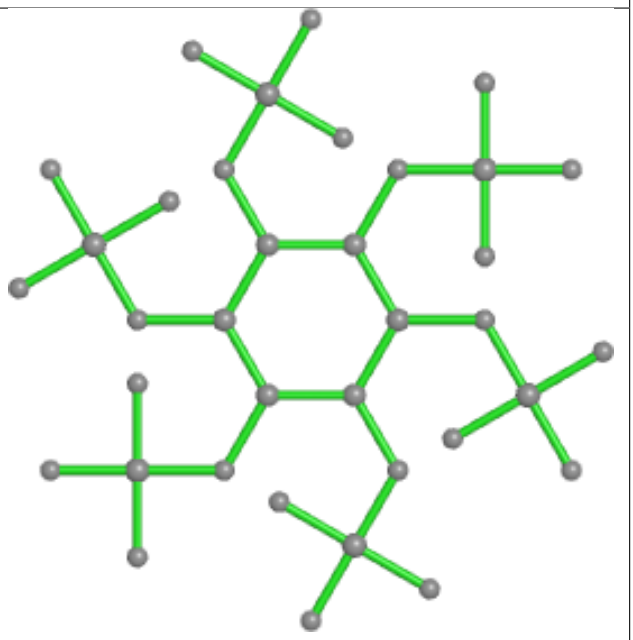
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

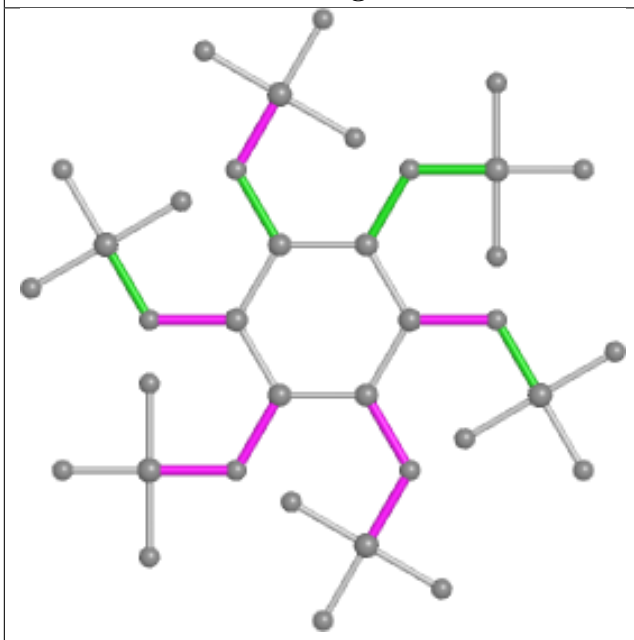
Ligand IHP A 3000



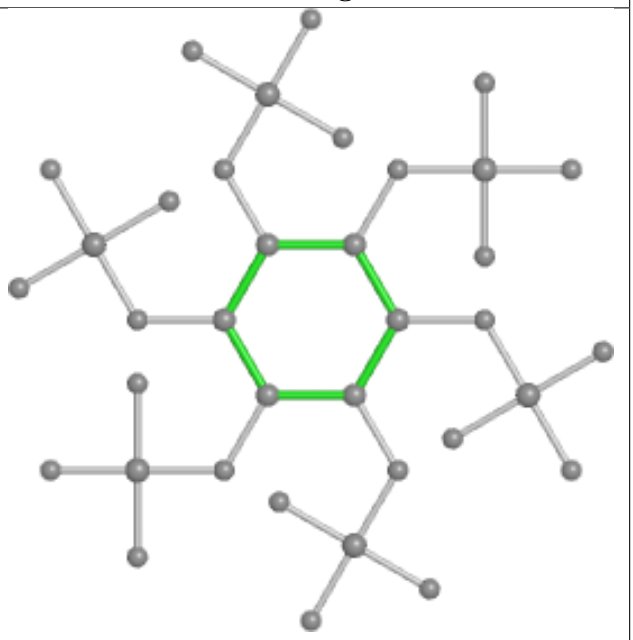
Bond lengths



Bond angles

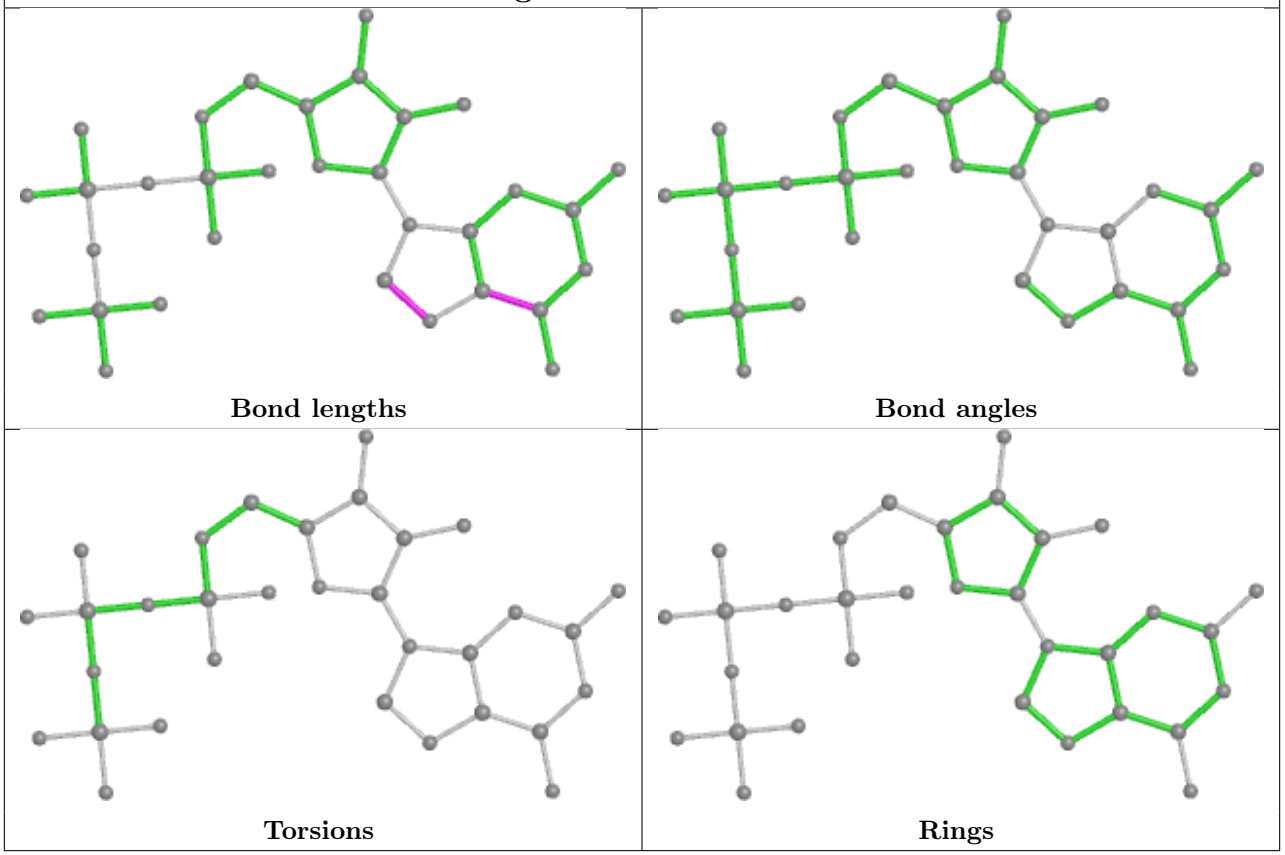


Torsions



Rings

Ligand GTP C 1500



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

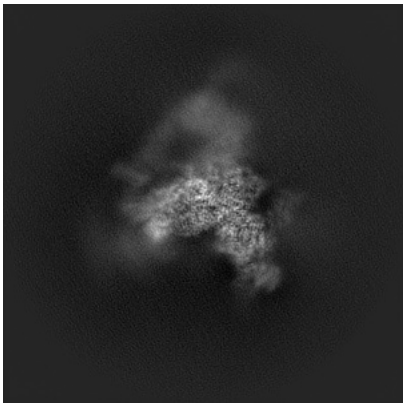
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-0687. These allow visual inspection of the internal detail of the map and identification of artifacts.

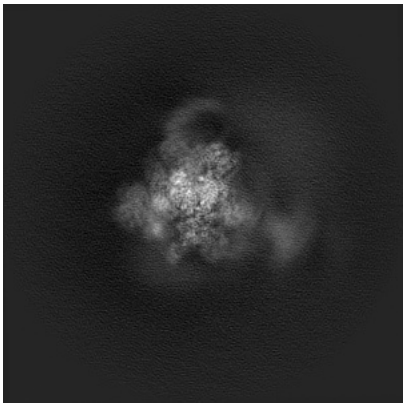
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

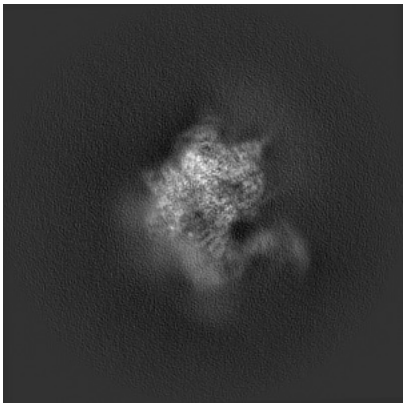
6.1.1 Primary map



X



Y

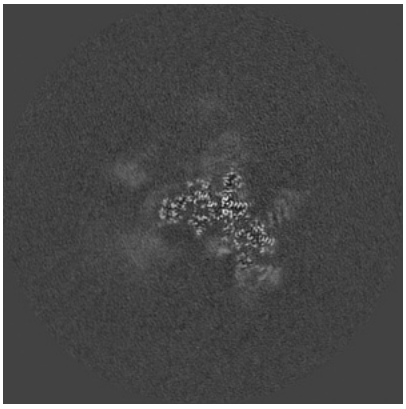


Z

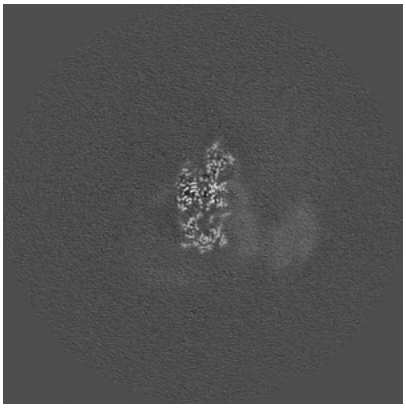
The images above show the map projected in three orthogonal directions.

6.2 Central slices

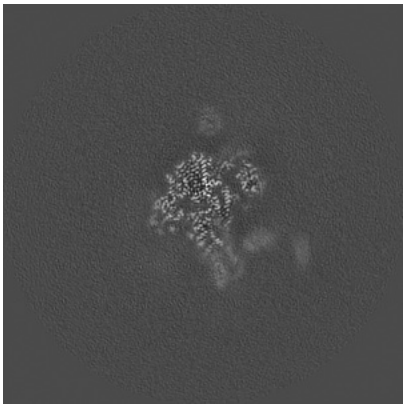
6.2.1 Primary map



X Index: 200



Y Index: 200

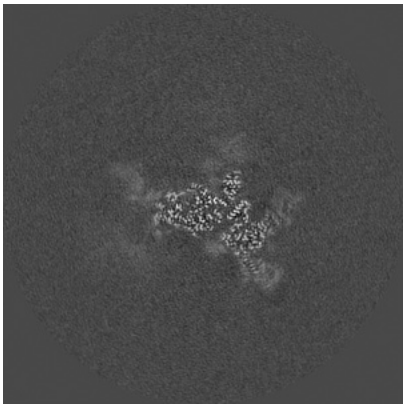


Z Index: 200

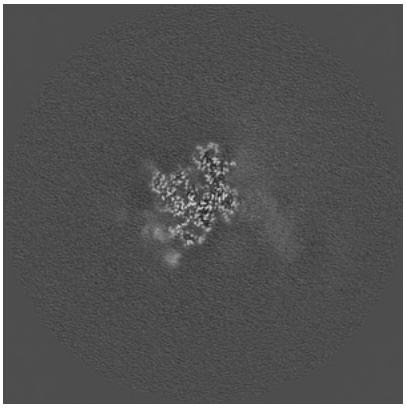
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

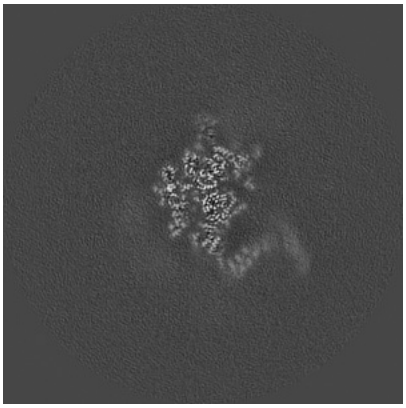
6.3.1 Primary map



X Index: 207



Y Index: 228



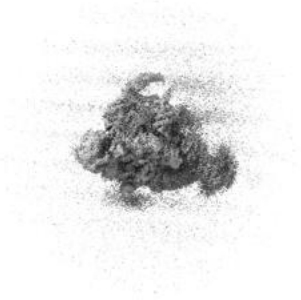
Z Index: 186

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y

Z

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

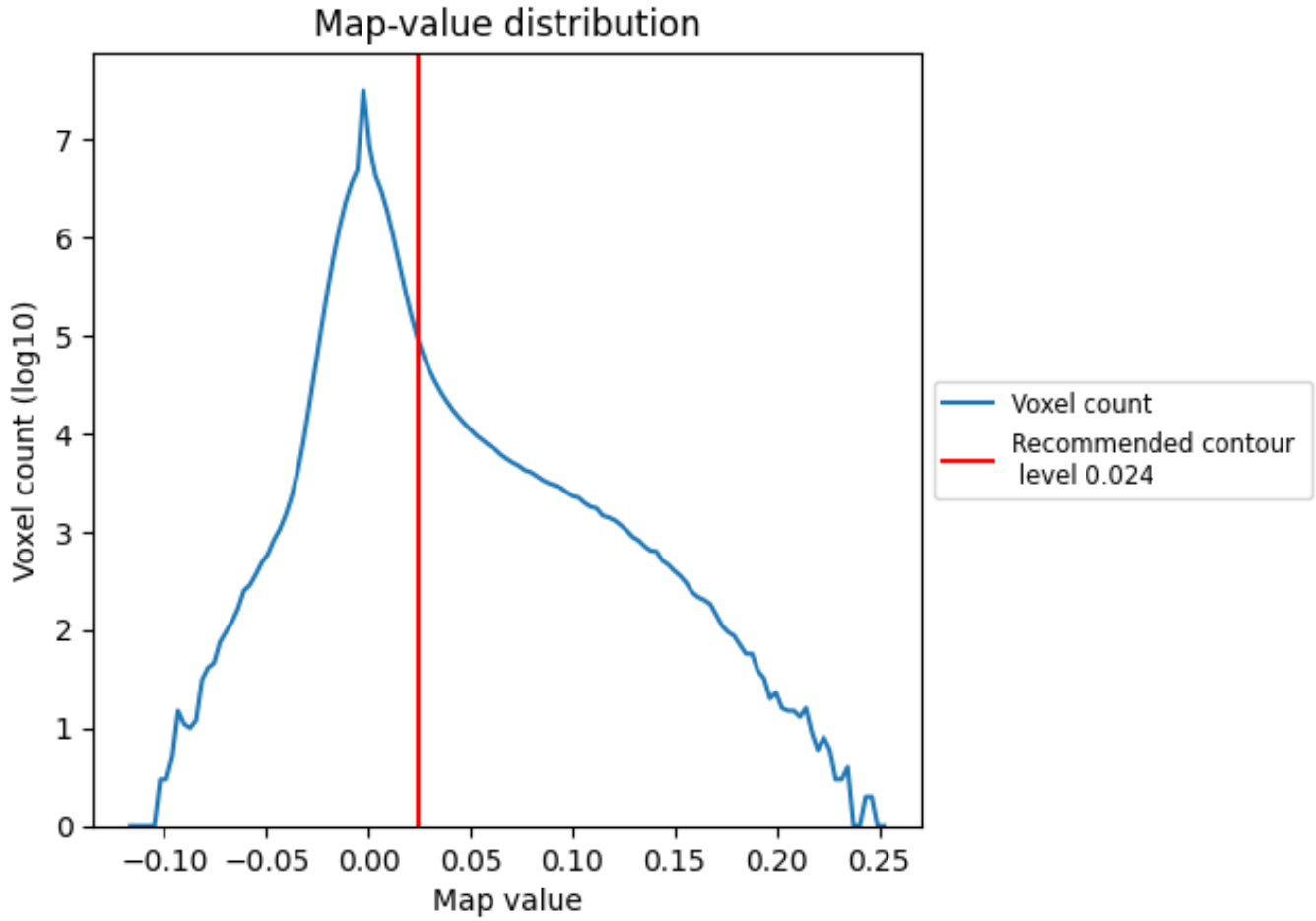
6.5 Mask visualisation (i)

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

7 Map analysis

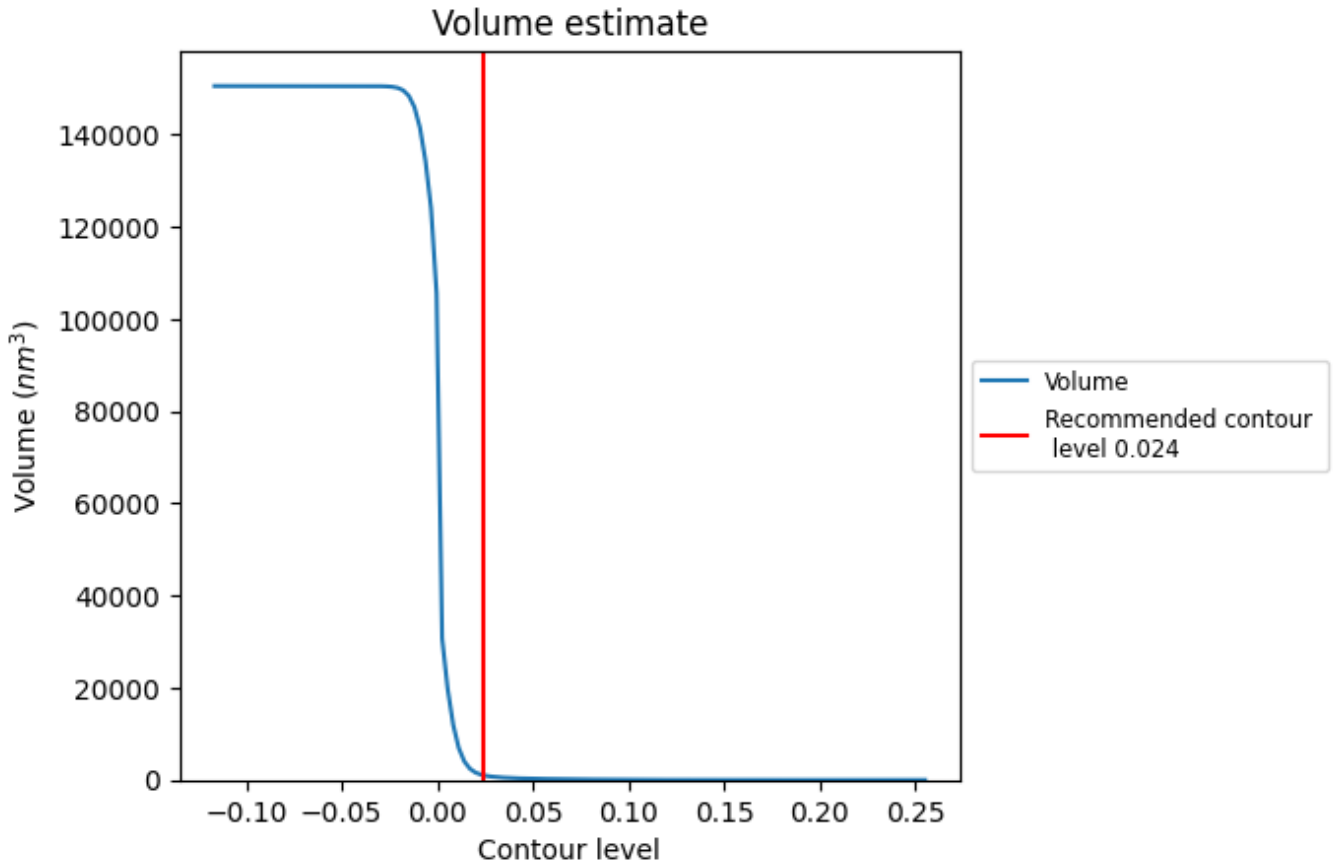
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

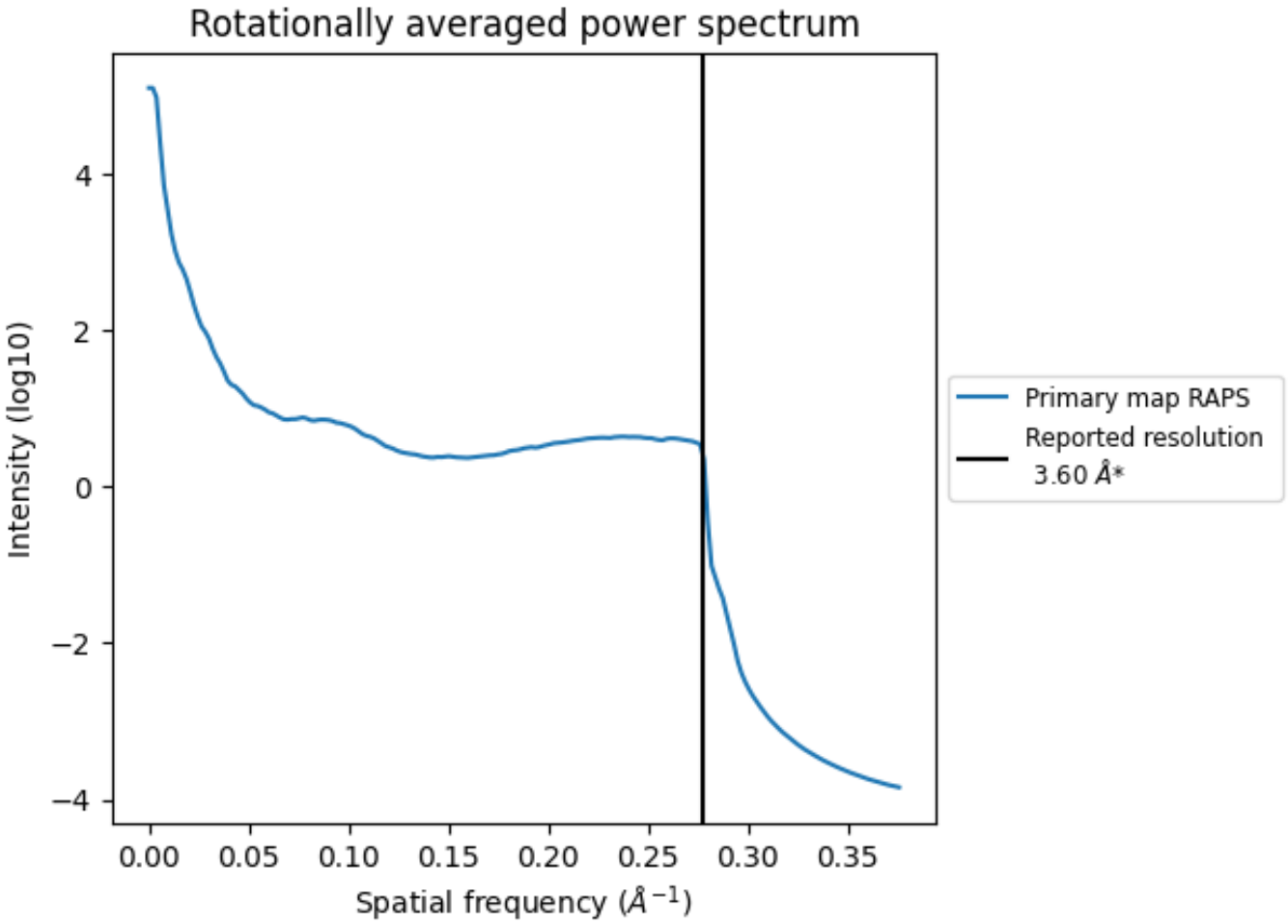
7.2 Volume estimate (i)



The volume at the recommended contour level is 1055 nm^3; this corresponds to an approximate mass of 953 kDa.

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

7.3 Rotationally averaged power spectrum (i)



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

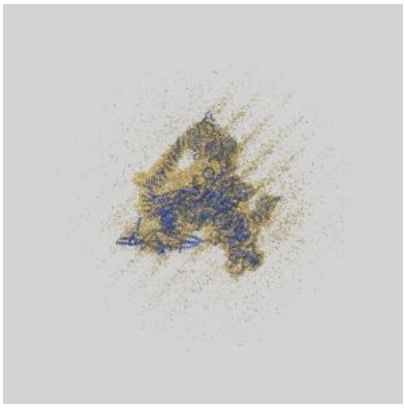
8 Fourier-Shell correlation (i)

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

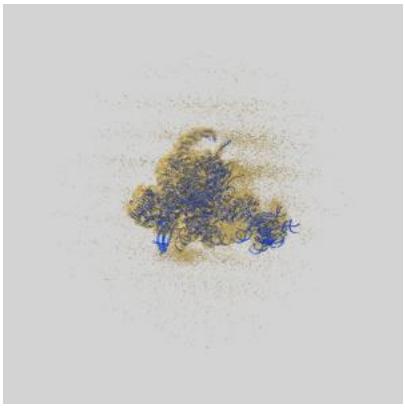
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-0687 and PDB model 6J6H. Per-residue inclusion information can be found in section 3 on page 12.

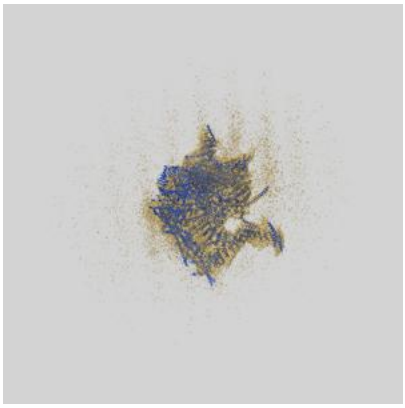
9.1 Map-model overlay



X



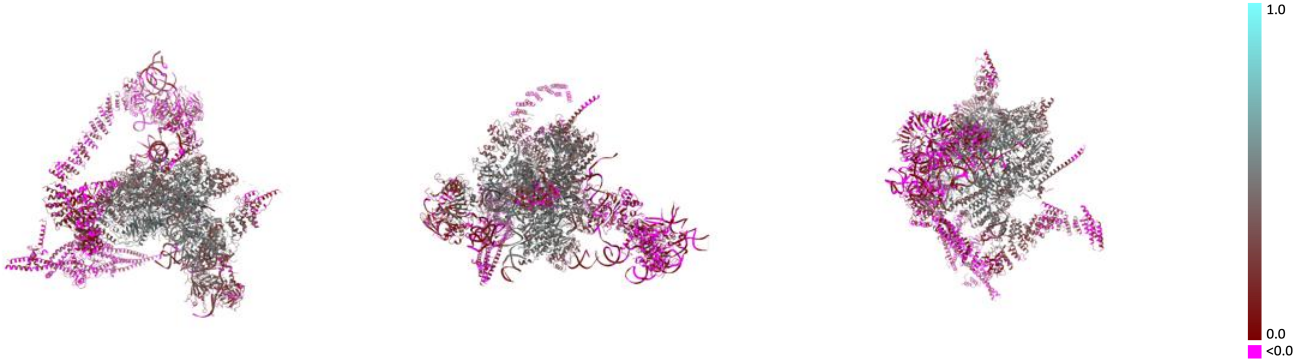
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.024 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.

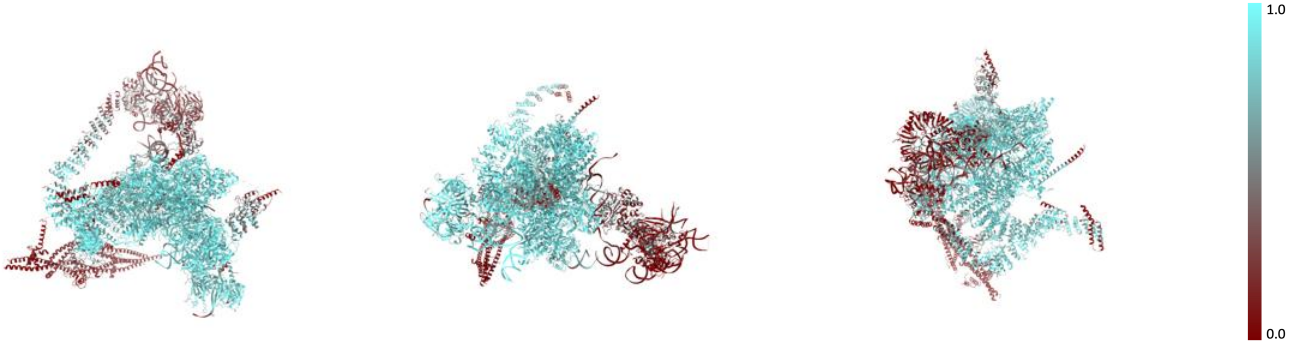
9.2 Q-score mapped to coordinate model



X Y Z

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

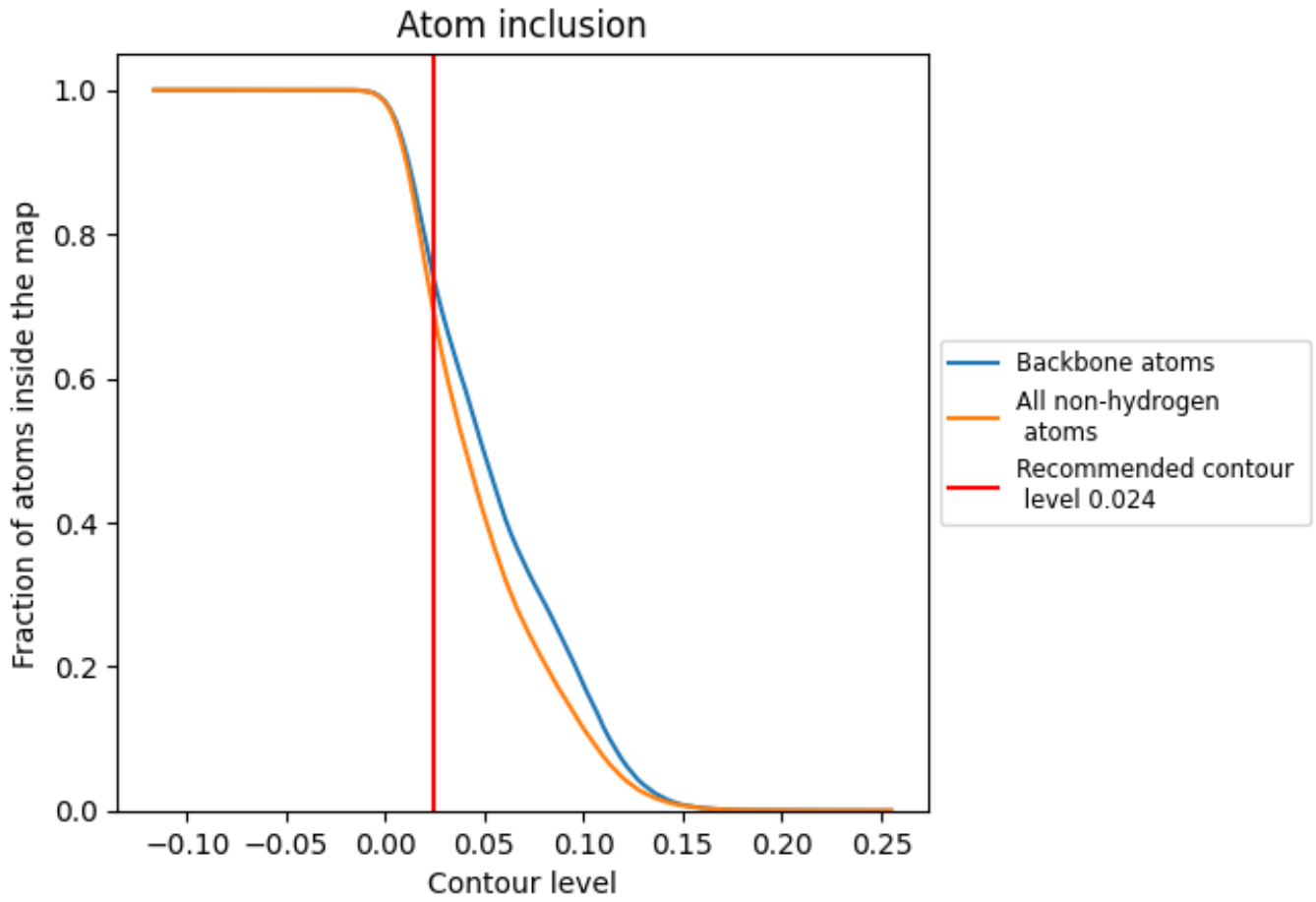
9.3 Atom inclusion mapped to coordinate model



X Y Z

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

9.4 Atom inclusion (i)



At the recommended contour level, 74% of all backbone atoms, 70% 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	0.6969	0.2830
A	0.8376	0.4070
B	0.5972	0.1860
C	0.9097	0.4340
D	0.9265	0.2930
E	0.9795	0.4190
H	0.4889	0.0520
I	0.8189	0.3750
J	0.8235	0.4640
L	0.3183	0.0850
O	0.9343	0.4800
P	0.7828	0.3760
Q	0.8445	0.3440
R	0.9053	0.4250
S	0.7245	0.4160
T	0.9300	0.4620
Z	0.6185	0.2660
a	0.1611	-0.0220
b	0.2675	0.0140
c	0.5118	0.2380
d	0.8191	0.2660
e	0.1510	0.0360
g	0.7734	0.1370
h	0.8718	0.1560
i	0.8271	0.1680
j	0.8254	0.2710
k	0.7541	0.2690
l	0.8502	0.3730
m	0.7124	0.1760
n	0.9683	0.4070
o	0.1320	0.0040
p	0.1418	0.0180
q	0.0165	0.0040
r	0.1111	-0.0050
s	0.2804	0.0030

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Chain	Atom inclusion	Q-score
t	0.0768	0.0120
u	0.0914	0.0460
v	0.7023	0.1310
w	0.1538	0.0330
x	0.0515	0.0520
y	0.1117	0.0000
z	0.2417	0.0270