wwPDB EM Validation Summary Report (i)

May 15, 2023 – 06:43 pm BST

PDB ID	:	5NRL
EMDB ID	:	EMD-3683
Title	:	Structure of a pre-catalytic spliceosome.
Authors	:	Plaschka, C.; Lin, P.-C.; Nagai, K.
Deposited on	:	2017-04-24
Resolution	:	7.20 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 (i) 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 (1)) were used in the production of this report:

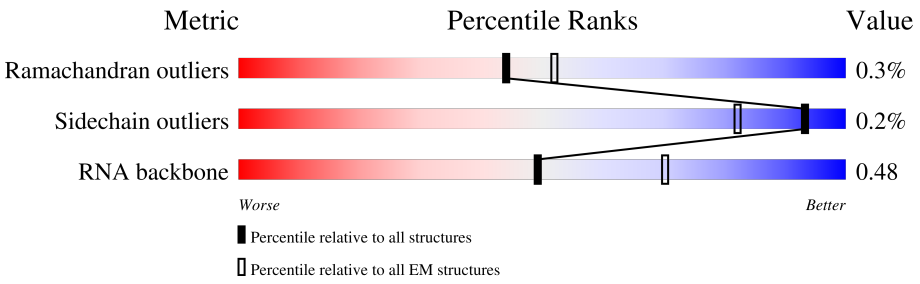
EMDB validation analysis	:	0.0.1.dev50
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 7.20 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	2	1175	9%; 5%, 6%, •, 87%
2	3	89	31%; 87%, 13%
3	4	160	•; 46%, 24%, •, 29%
4	5	214	7%; 48%, 31%, 21%
5	6	112	•; 53%, 32%, 15%
6	7	115	26%; 57%, 43%
7	8	109	20%; 59%, 41%
8	A	2413	5%; 92%, 8%

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Mol	Chain	Length	Quality of chain
9	B	2163	19% 78% 21%
10	C	1008	84% 16%
11	D	143	8% 99%
12	E	587	7% 21% 79%
13	F	494	5% 83% 16%
14	G	469	8% 79% 21%
15	H	465	92% 8%
16	I	95	21% 9% 69%
17	J	899	5% 88% 11%
18	K	126	8% 98%
19	L	194	56% 44%
20	M	242	7% 71% 28%
21	N	291	5% 29% 71%
22	O	971	21% 86% 14%
23	P	1361	26% 86% 13%
24	Q	435	21% 50% 49%
25	R	213	37% 81% 19%
26	S	107	16% 96%
27	T	530	77% 86% 13%
28	U	266	55% 73% 26%
29	V	280	45% 45% 55%
30	W	238	71% 62% 8% 29%
31	X	111	14% 27% 73%
32	Y	111	76% 74% 24%
33	Z	85	20% 96%

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Mol	Chain	Length	Quality of chain
34	a	95	23% 94% 5%
35	b	196	7% 36% 64%
35	k	196	16% 36% 64%
35	s	196	36% 36% 64%
36	d	101	12% 82% 18%
36	n	101	50% 79% 19%
36	v	101	81% 79% 19%
37	e	94	16% 82% 18%
37	p	94	31% 81% 18%
37	w	94	82% 81% 18%
38	f	86	20% 84% 16%
38	q	86	30% 85% 15%
38	x	86	85% 85% 15%
39	g	77	17% 92% 8%
39	r	77	66% 94%
39	y	77	97% 94%
40	h	146	7% 55% 45%
40	l	146	38% 66% 32%
40	t	146	49% 49% 51%
41	i	110	14% 84% 16%
41	m	110	35% 84% 16%
41	u	110	84% 84% 16%
42	j	187	18% 40% 60%
43	o	93	17% 81% 19%
44	z	86	34% 86% 14%

2 Entry composition (i)

There are 46 unique types of molecules in this entry. The entry contains 118701 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	2	155	3275	1464	552	1104	155	0	0

- Molecule 2 is a protein called U6 snRNA-associated Sm-like protein LSm3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	3	77	611	382	105	121	3	0	0

- Molecule 3 is a RNA chain called U4 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	4	114	2423	1084	419	806	114	0	0

- Molecule 4 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	5	170	3615	1618	640	1188	169	0	0

- Molecule 5 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	6	95	2019	904	355	665	95	0	0

- Molecule 6 is a protein called U6 snRNA-associated Sm-like protein LSm7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	7	66	504	325	85	91	3	0	0

- Molecule 7 is a protein called U6 snRNA-associated Sm-like protein LSm8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	8	64	498	320	86	90	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	A	2216	18122	11661	3103	3294	64	0	0

- Molecule 9 is a protein called Pre-mRNA-splicing helicase BRR2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	B	1699	13607	8720	2269	2564	54	1	0

- Molecule 10 is a protein called Pre-mRNA-splicing factor SNU114.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	C	850	6784	4392	1129	1237	26	0	0

- Molecule 11 is a protein called Spliceosomal protein DIB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	D	142	1164	736	202	215	11	0	0

- Molecule 12 is a protein called 66 kDa U4/U6.U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	E	124	825	501	153	170	1	0	0

- Molecule 13 is a protein called Pre-mRNA-processing factor 31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	F	413	3238	2064	578	584	12	0	0

- Molecule 14 is a protein called U4/U6 small nuclear ribonucleoprotein PRP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	G	372	2835	1786	523	512	14	0	0

- Molecule 15 is a protein called U4/U6 small nuclear ribonucleoprotein PRP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	H	429	3396	2120	609	653	14	0	0

- Molecule 16 is a RNA chain called Yeast UBC4 gene for ubiquitin-conjugating enzyme.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
16	I	29	600	271	95	205	29	0	0

- Molecule 17 is a protein called Pre-mRNA-splicing factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	J	800	6485	4151	1106	1201	27	0	0

- Molecule 18 is a protein called 13 kDa ribonucleoprotein-associated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	K	124	936	597	161	174	4	0	0

- Molecule 19 is a protein called 23 kDa U4/U6.U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	L	109	882	570	150	159	3	0	0

- Molecule 20 is a protein called Pre-mRNA-splicing factor 38.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	M	174	1407	915	236	249	7	0	0

- Molecule 21 is a protein called Pre-mRNA-splicing factor SPP381.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
21	N	85	425	255	85	85	0	0

- Molecule 22 is a protein called U2 snRNP component HSH155.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	O	833	6612	4258	1121	1192	41	0	0

- Molecule 23 is a protein called Pre-mRNA-splicing factor RSE1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	P	1186	9437	6034	1589	1763	51	0	0

- Molecule 24 is a protein called Cold sensitive U2 snRNA suppressor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	Q	220	1786	1157	307	313	9	0	0

- Molecule 25 is a protein called Protein HSH49.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	R	173	1429	930	239	258	2	0	0

- Molecule 26 is a protein called Pre-mRNA-splicing factor RDS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	S	103	814	503	154	143	14	0	0

- Molecule 27 is a protein called Pre-mRNA-splicing factor PRP9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	T	462	3915	2487	677	735	16	0	0

- Molecule 28 is a protein called Pre-mRNA-splicing factor PRP11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	U	196	1488	933	258	291	6	0	0

- Molecule 29 is a protein called Pre-mRNA-splicing factor PRP21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	V	127	1084	689	193	196	6	0	0

- Molecule 30 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	W	170	1383	866	253	257	7	0	0

- Molecule 31 is a protein called Unknown.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
31	X	30	150	90	30	30	0	0

- Molecule 32 is a protein called U2 small nuclear ribonucleoprotein B".

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	Y	84	683	439	119	122	3	0	0

- Molecule 33 is a protein called RDS3 complex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	Z	83	685	424	129	131	1	0	0

- Molecule 34 is a protein called U6 snRNA-associated Sm-like protein LSm2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	a	90	735	469	124	139	3	0	0

- Molecule 35 is a protein called Small nuclear ribonucleoprotein-associated protein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	b	70	563	360	98	102	3	0	0
35	k	70	563	360	98	102	3	0	0
35	s	70	563	360	98	102	3	0	0

- Molecule 36 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	d	83	641	408	111	120	2	0	0
36	n	82	632	402	109	119	2	0	0
36	v	82	632	402	109	119	2	0	0

- Molecule 37 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	e	77	602	396	95	108	3	0	0
37	p	77	602	396	95	108	3	0	0
37	w	77	602	396	95	108	3	0	0

- Molecule 38 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	f	72	578	371	101	105	1	0	0
38	q	73	585	376	102	106	1	0	0
38	x	73	585	376	102	106	1	0	0

- Molecule 39 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	g	71	549	345	96	106	2	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	r	75	577	363	100	112	2	0	0
39	y	75	577	363	100	112	2	0	0

- Molecule 40 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	h	80	630	402	108	118	2	0	0
40	l	99	751	475	137	137	2	0	0
40	t	72	569	364	99	104	2	0	0

- Molecule 41 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	i	92	752	481	136	131	4	0	0
41	m	92	752	481	136	131	4	0	0
41	u	92	752	481	136	131	4	0	0

- Molecule 42 is a protein called U6 snRNA-associated Sm-like protein LSm4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	j	74	588	381	96	108	3	0	0

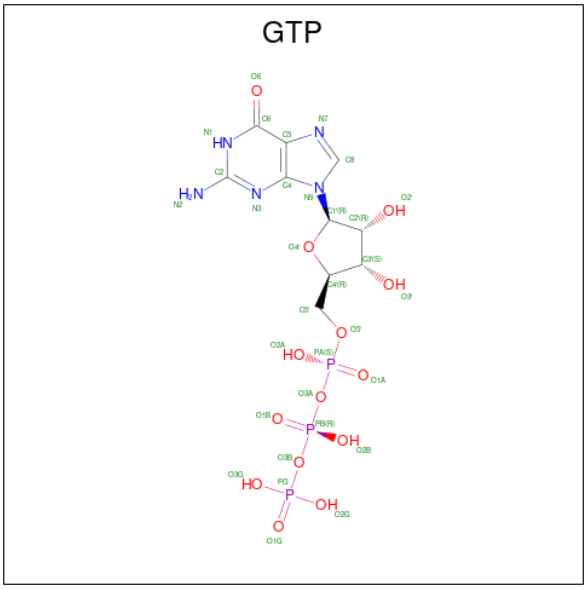
- Molecule 43 is a protein called U6 snRNA-associated Sm-like protein LSm5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	o	75	588	378	98	110	2	0	0

- Molecule 44 is a protein called U6 snRNA-associated Sm-like protein LSm6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	z	74	577	364	95	116	2	0	0

- Molecule 45 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	
45	C	1	32	10	5	14	3	0

- Molecule 46 is ZINC ION (three-letter code: ZN) (formula: Zn).

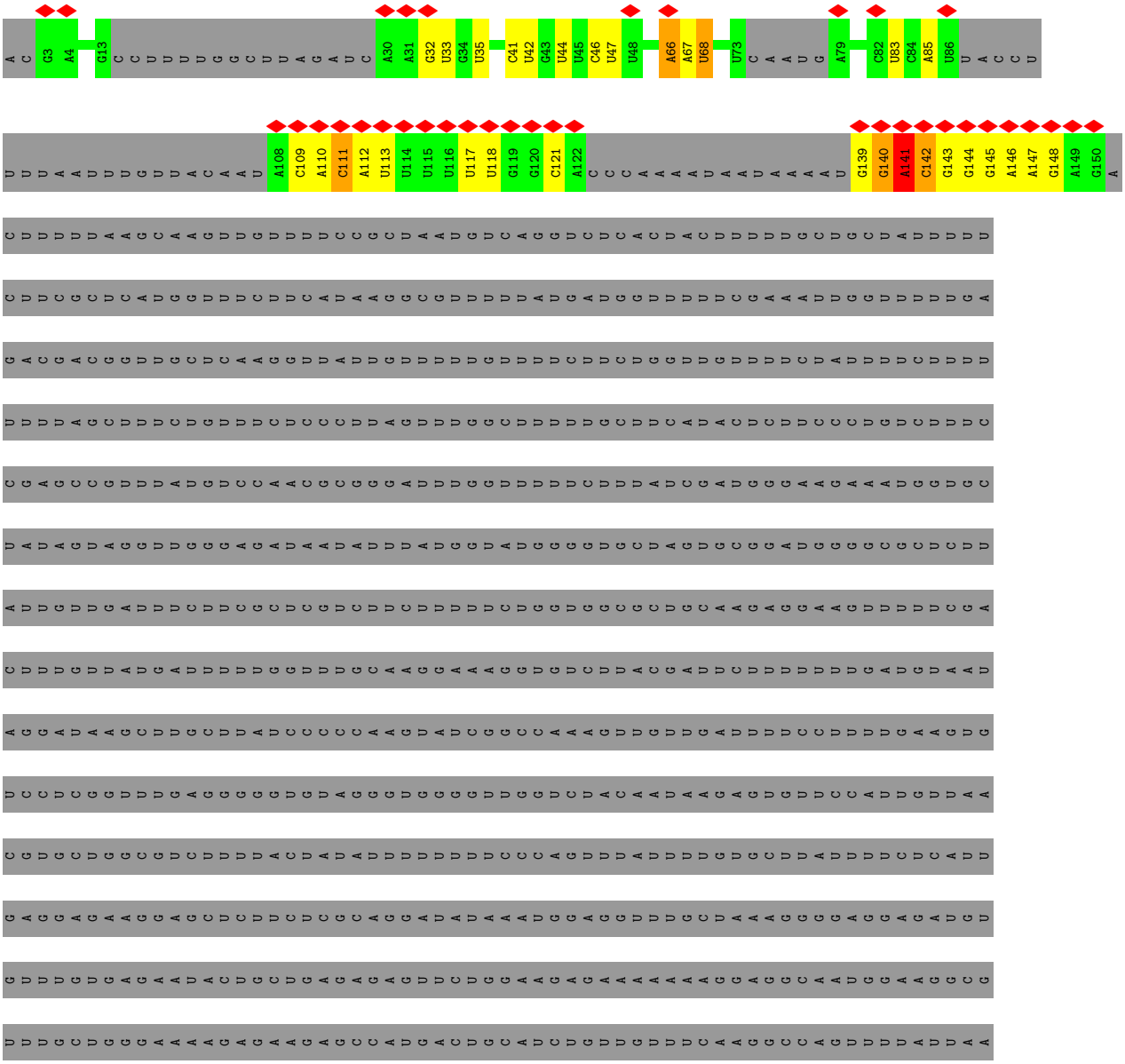
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
46	L	1	1	1	0
46	S	3	3	3	0
46	T	2	2	2	0
46	U	1	1	1	0

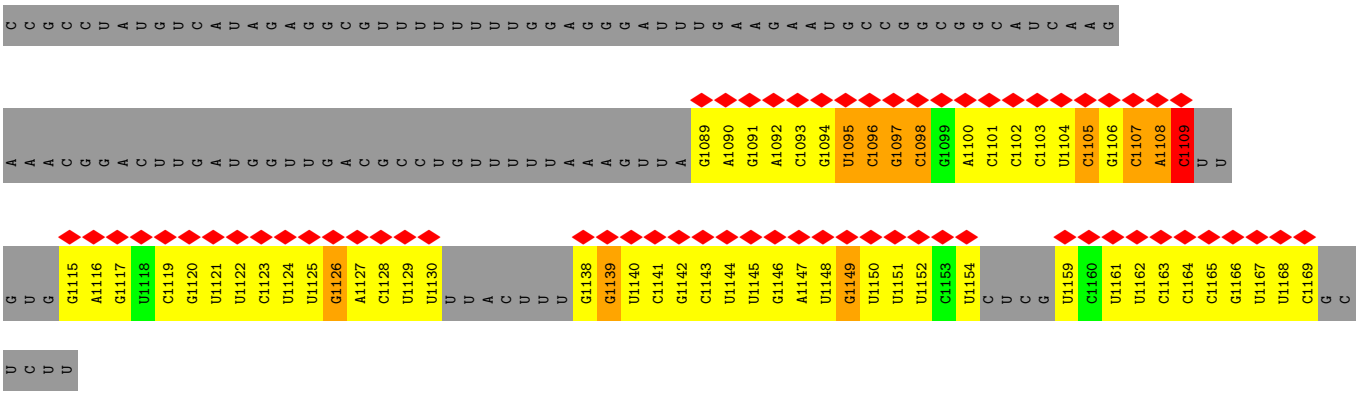
3 Residue-property plots (i)

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: U2 snRNA

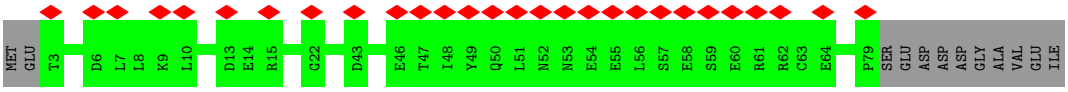
Chain 2:





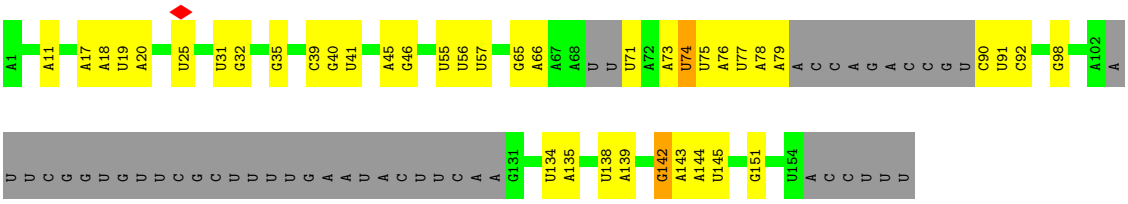
• Molecule 2: U6 snRNA-associated Sm-like protein LSm3

Chain 3:



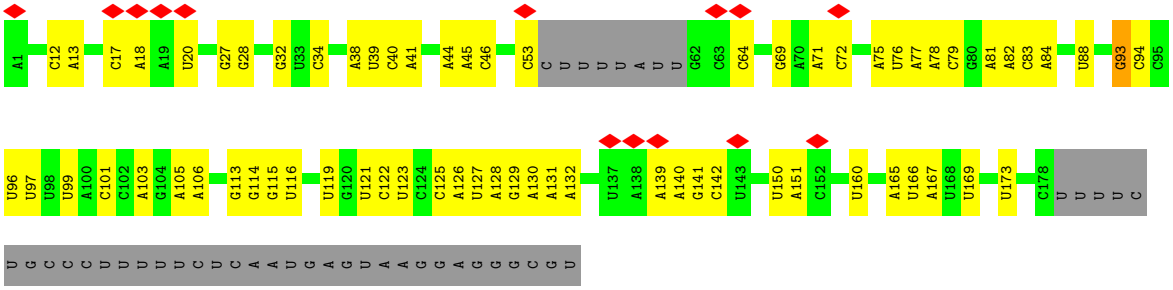
• Molecule 3: U4 snRNA

Chain 4:



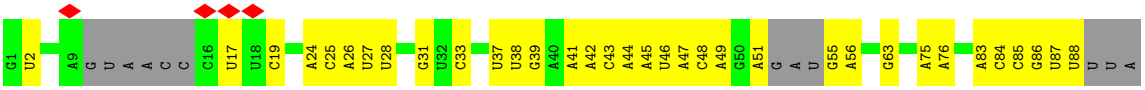
• Molecule 4: U5 snRNA

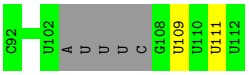
Chain 5:



• Molecule 5: U6 snRNA

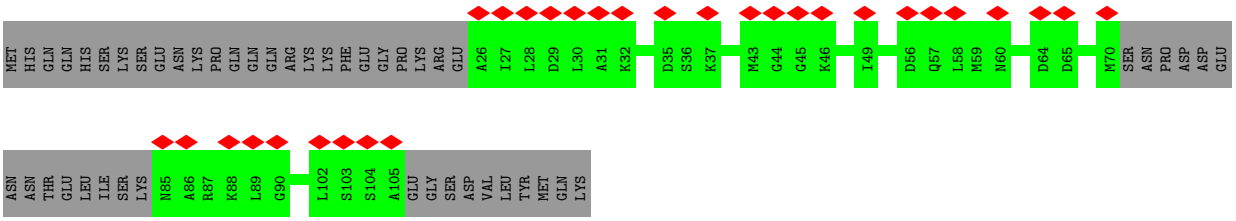
Chain 6:





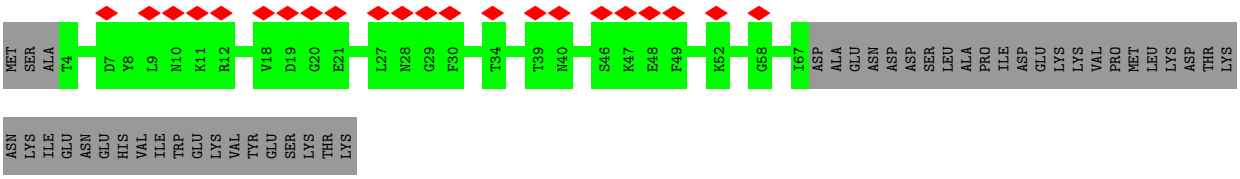
• Molecule 6: U6 snRNA-associated Sm-like protein LSm7

Chain 7:



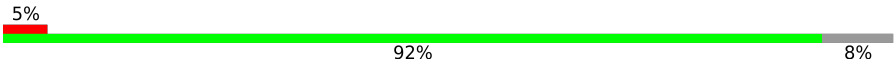
• Molecule 7: U6 snRNA-associated Sm-like protein LSm8

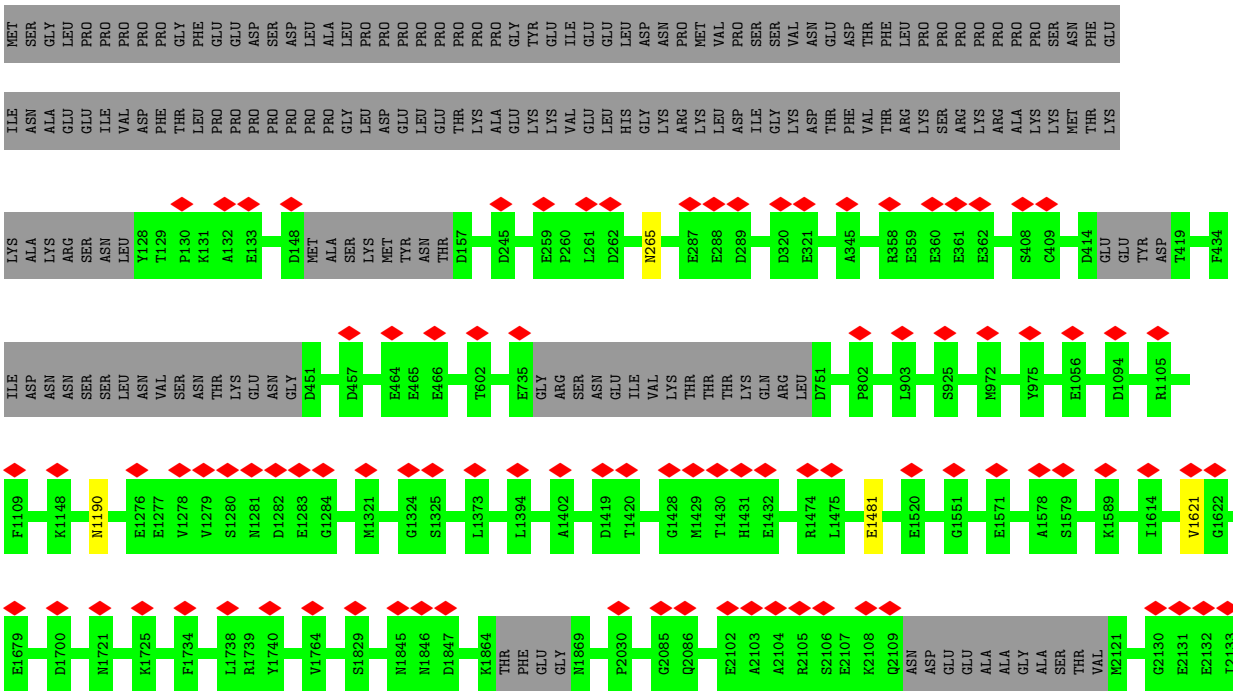
Chain 8:

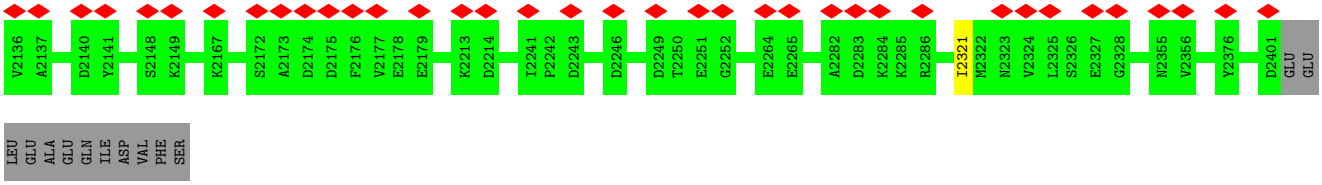


• Molecule 8: Pre-mRNA-splicing factor 8

Chain A:

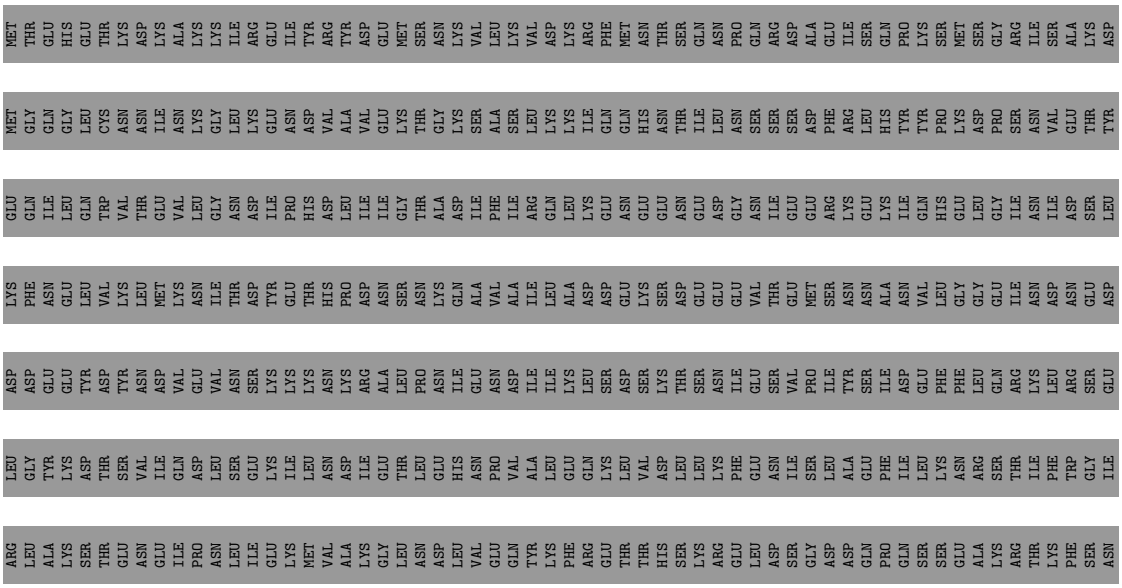


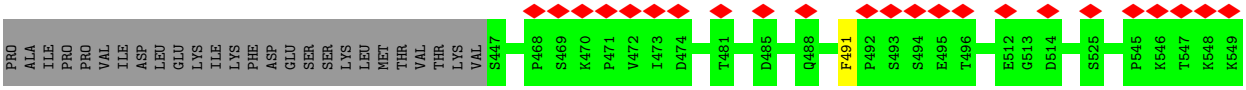


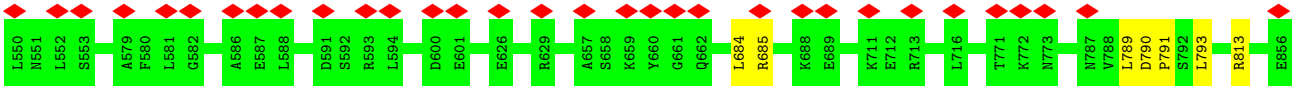


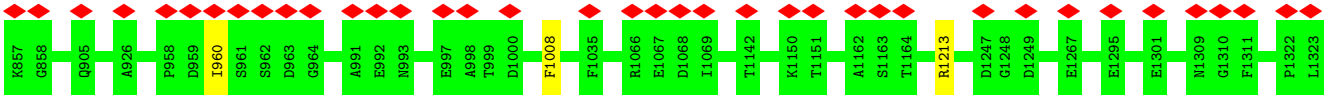
• Molecule 9: Pre-mRNA-splicing helicase BRR2

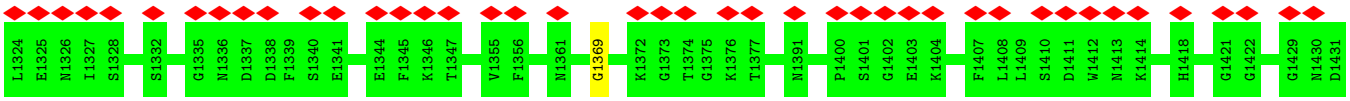
Chain B:

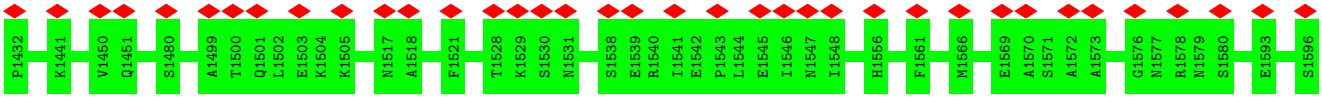


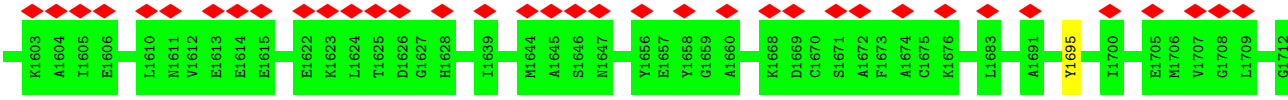


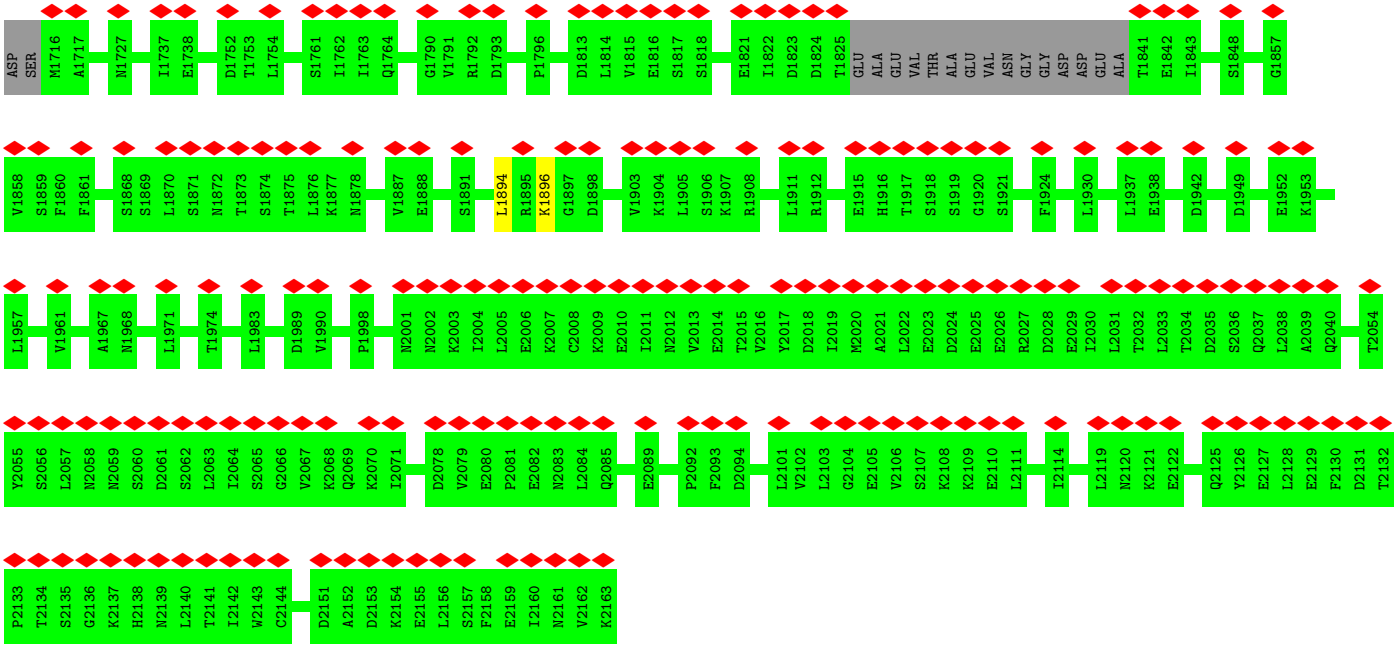






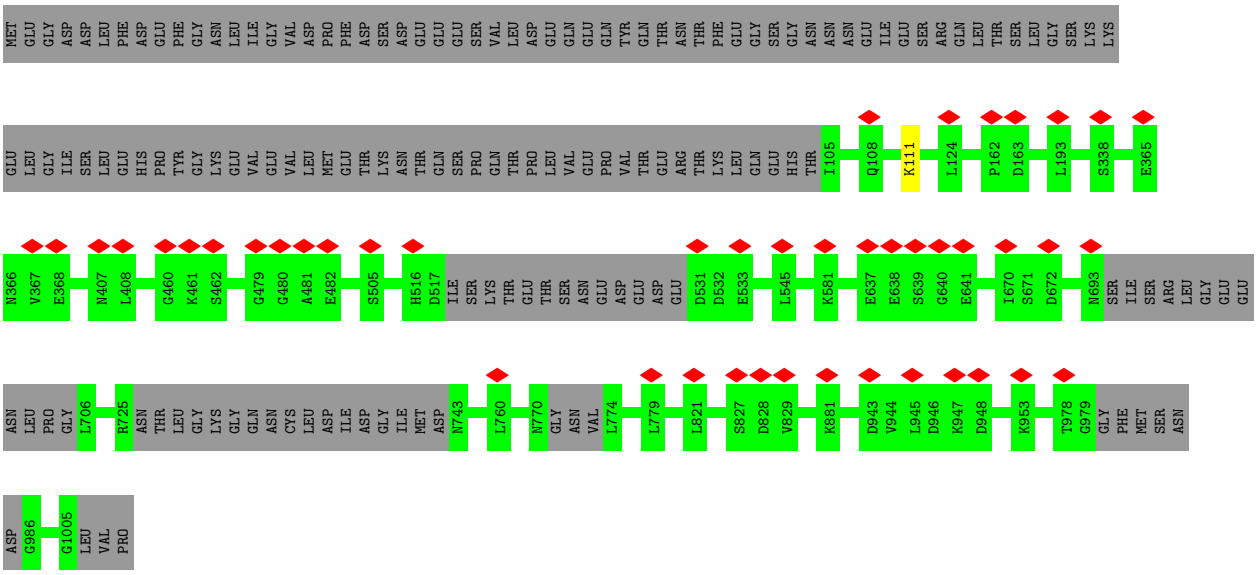






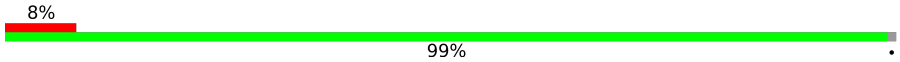
- Molecule 10: Pre-mRNA-splicing factor SNU114

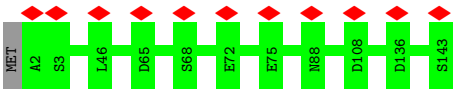
Chain C:



- Molecule 11: Spliceosomal protein DIB1

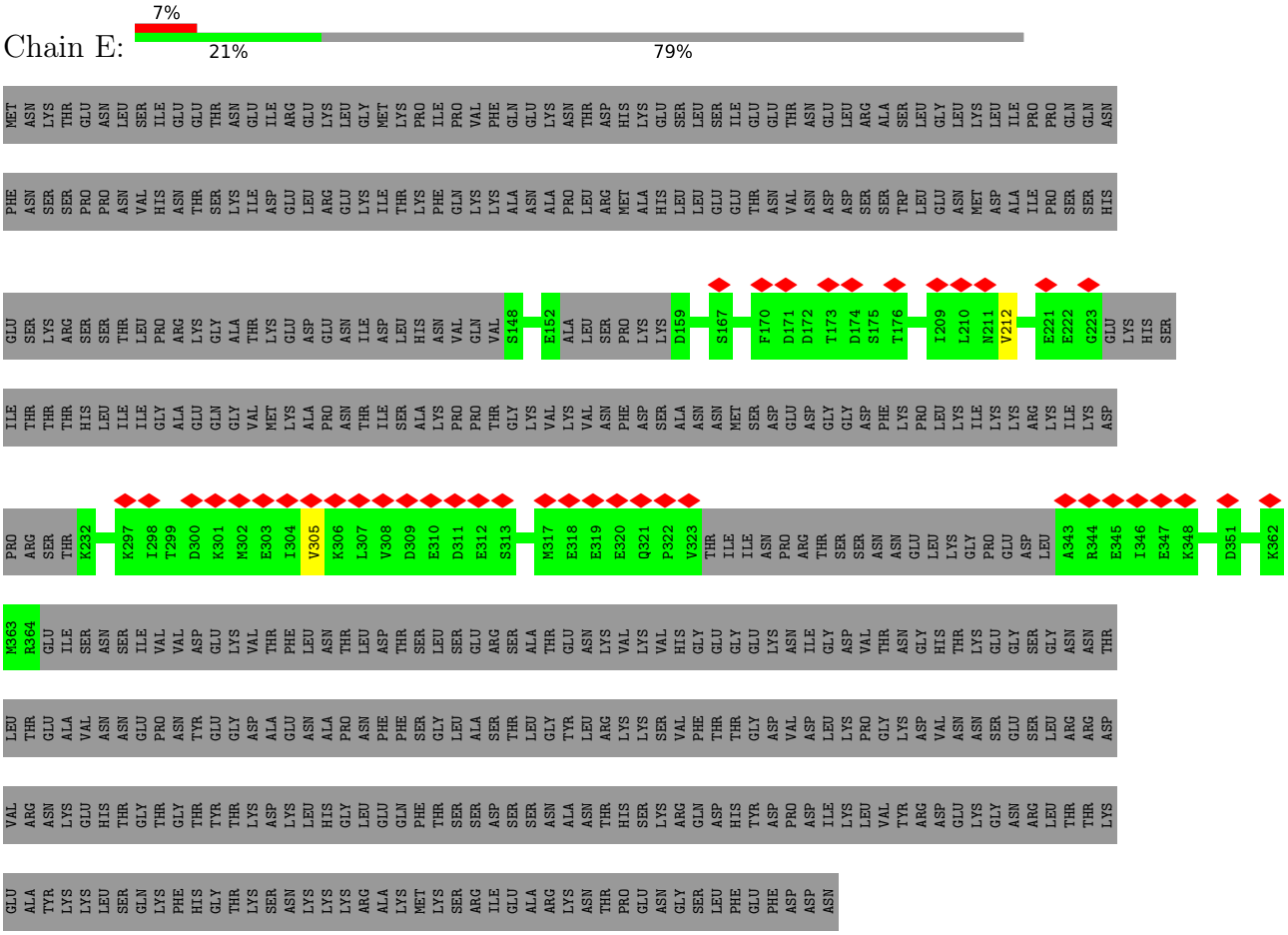
Chain D:





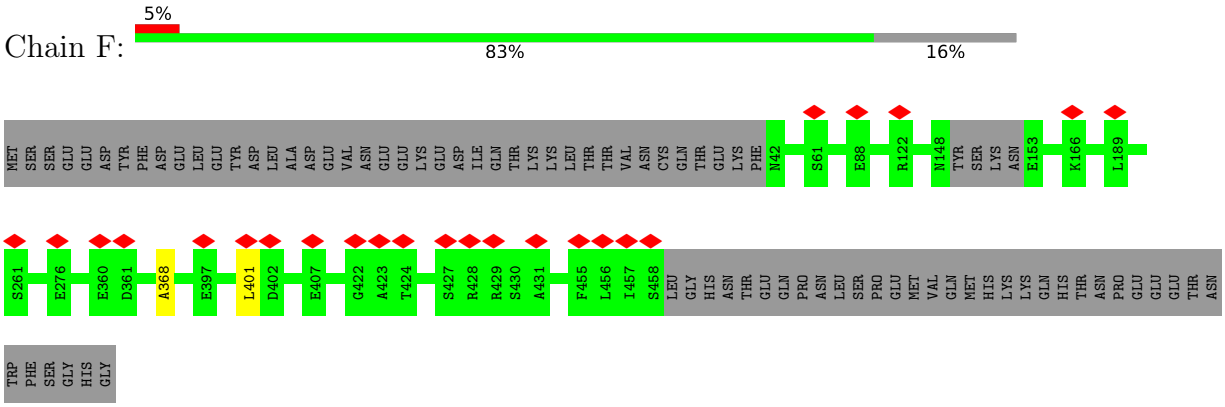
- Molecule 12: 66 kDa U4/U6.U5 small nuclear ribonucleoprotein component

Chain E:



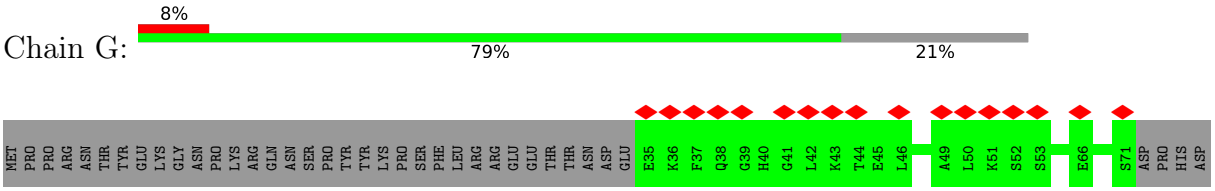
- Molecule 13: Pre-mRNA-processing factor 31

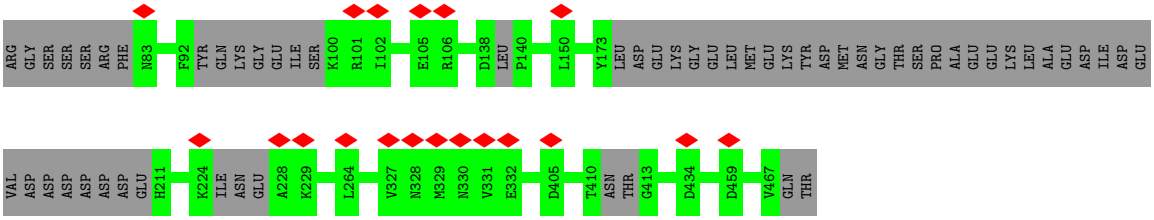
Chain F:



- Molecule 14: U4/U6 small nuclear ribonucleoprotein PRP3

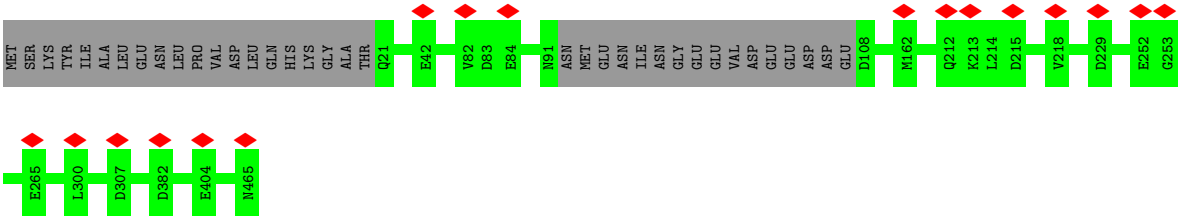
Chain G:





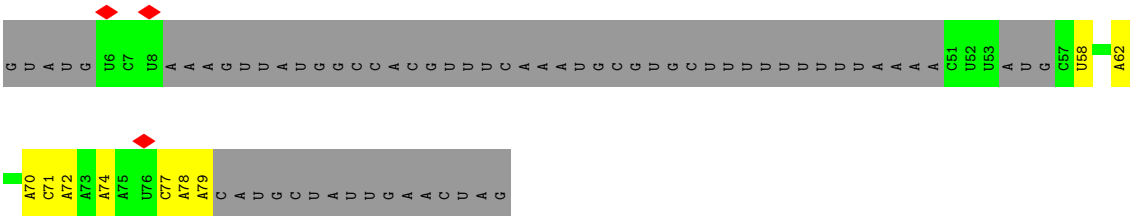
• Molecule 15: U4/U6 small nuclear ribonucleoprotein PRP4

Chain H:



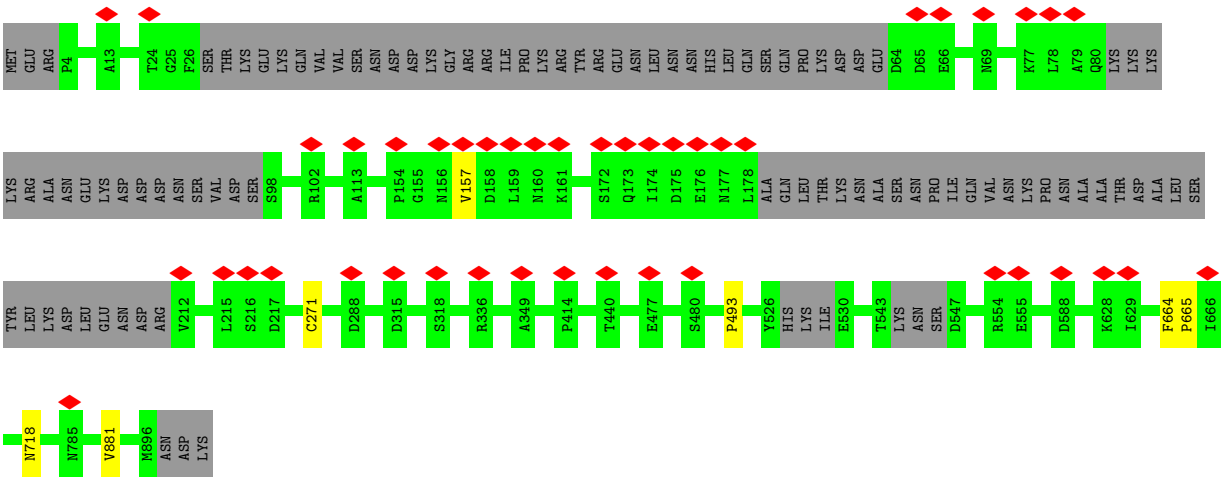
• Molecule 16: Yeast UBC4 gene for ubiquitin-conjugating enzyme

Chain I:



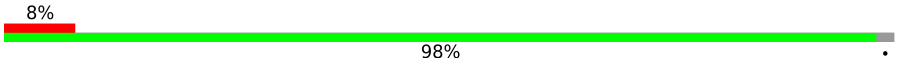
• Molecule 17: Pre-mRNA-splicing factor 6

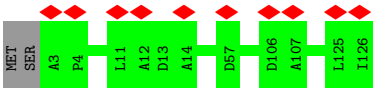
Chain J:



• Molecule 18: 13 kDa ribonucleoprotein-associated protein

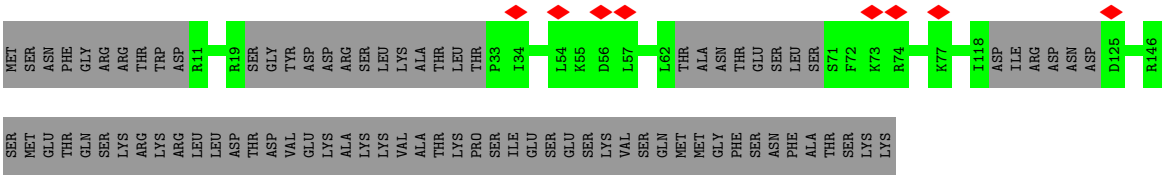
Chain K:





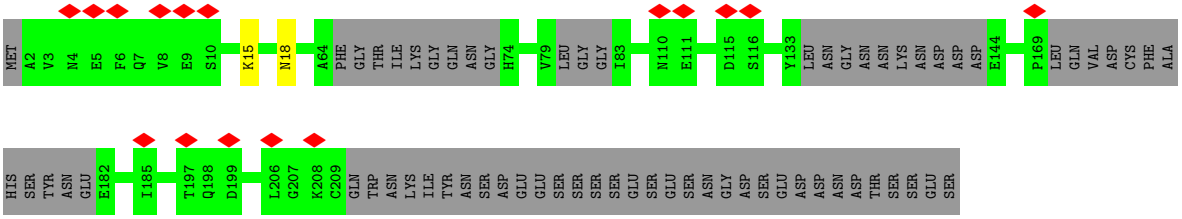
• Molecule 19: 23 kDa U4/U6.U5 small nuclear ribonucleoprotein component

Chain L:



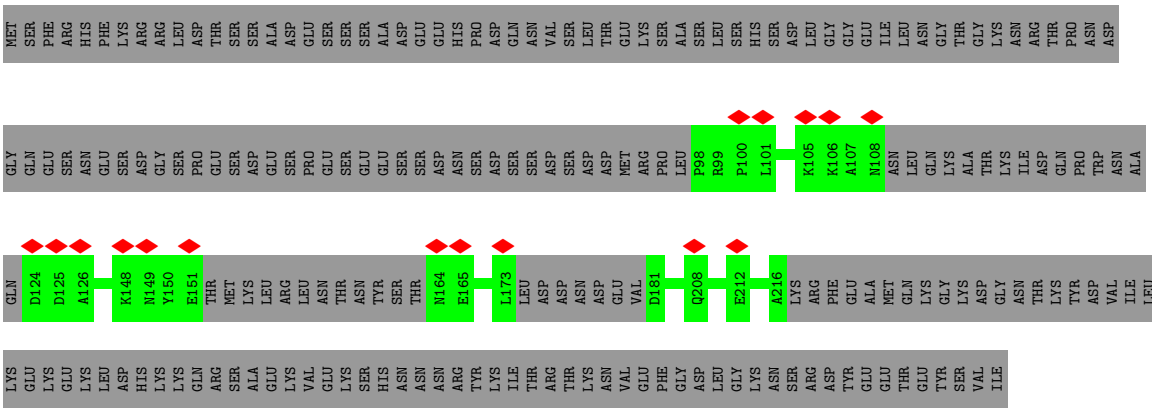
• Molecule 20: Pre-mRNA-splicing factor 38

Chain M:



• Molecule 21: Pre-mRNA-splicing factor SPP381

Chain N:

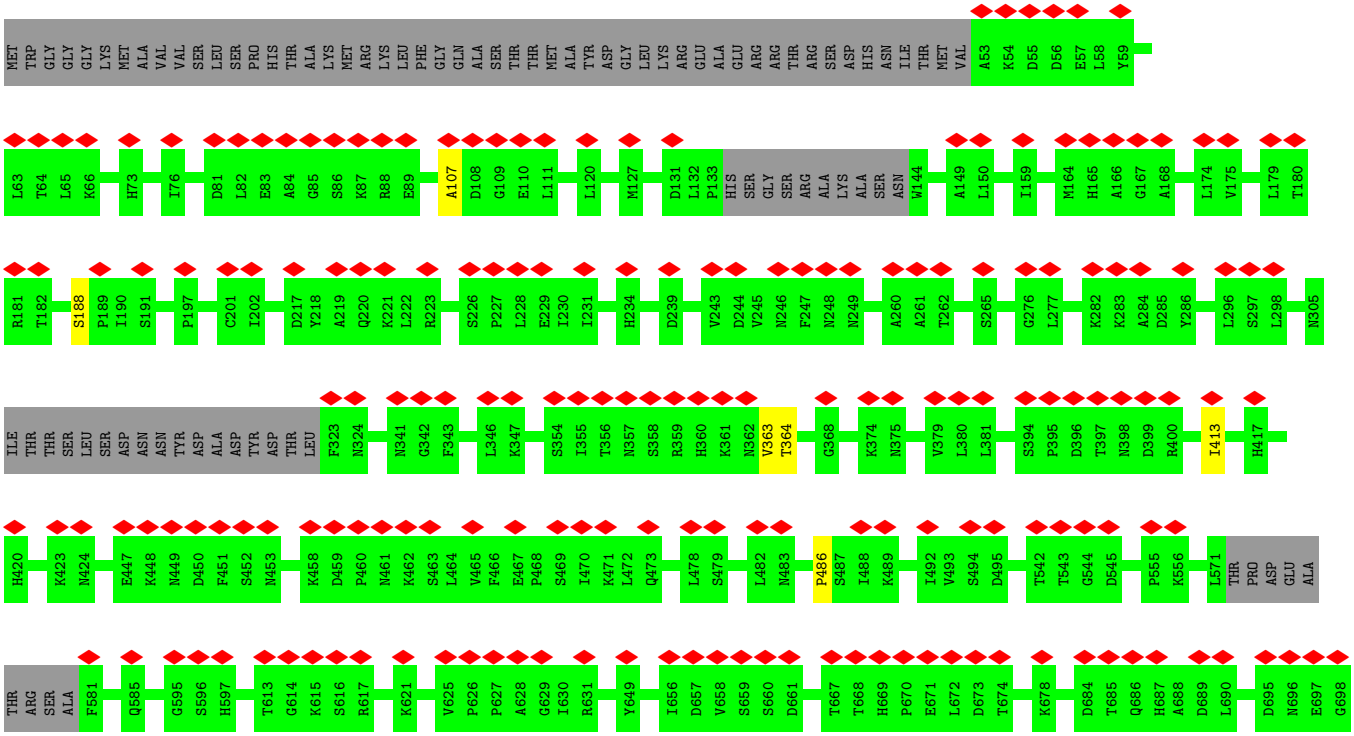


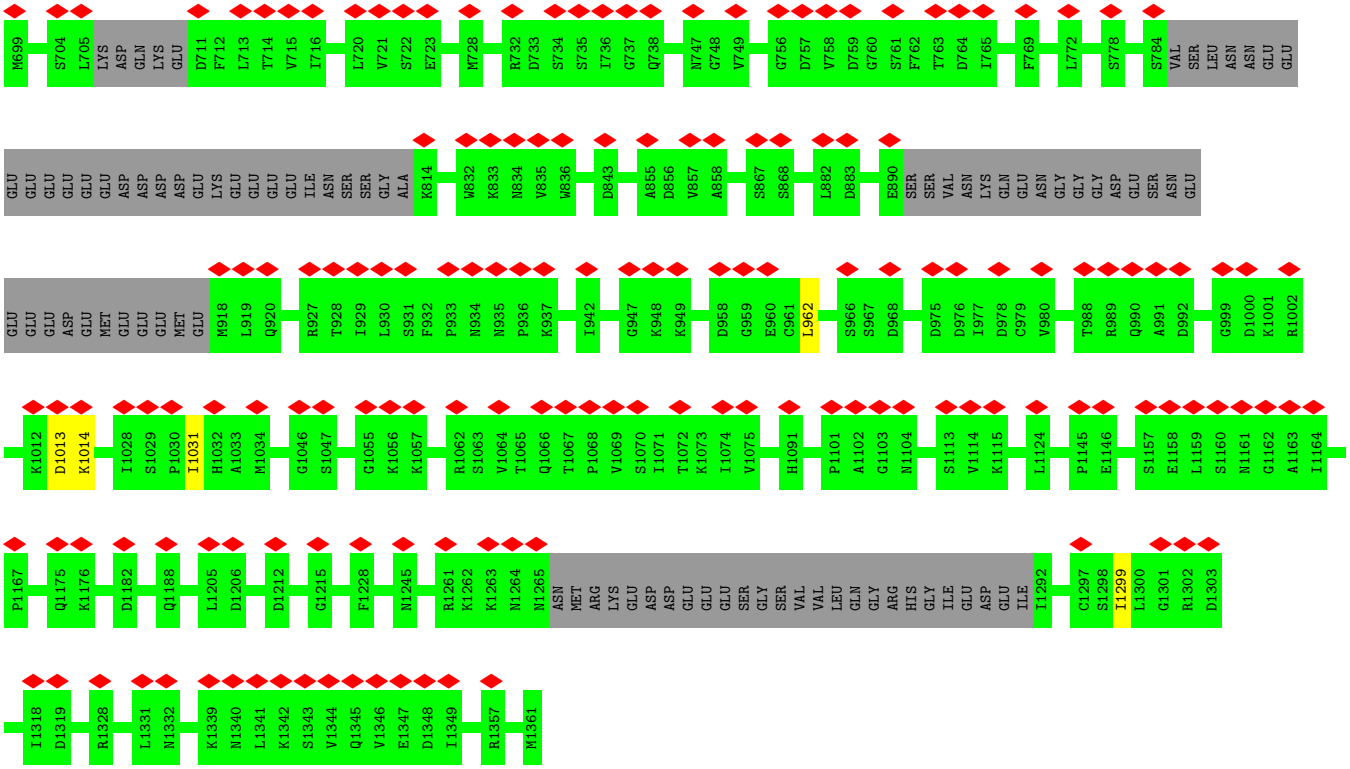
• Molecule 22: U2 snRNP component HSH155

Chain O:

- Molecule 23: Pre-mRNA-splicing factor RSE1

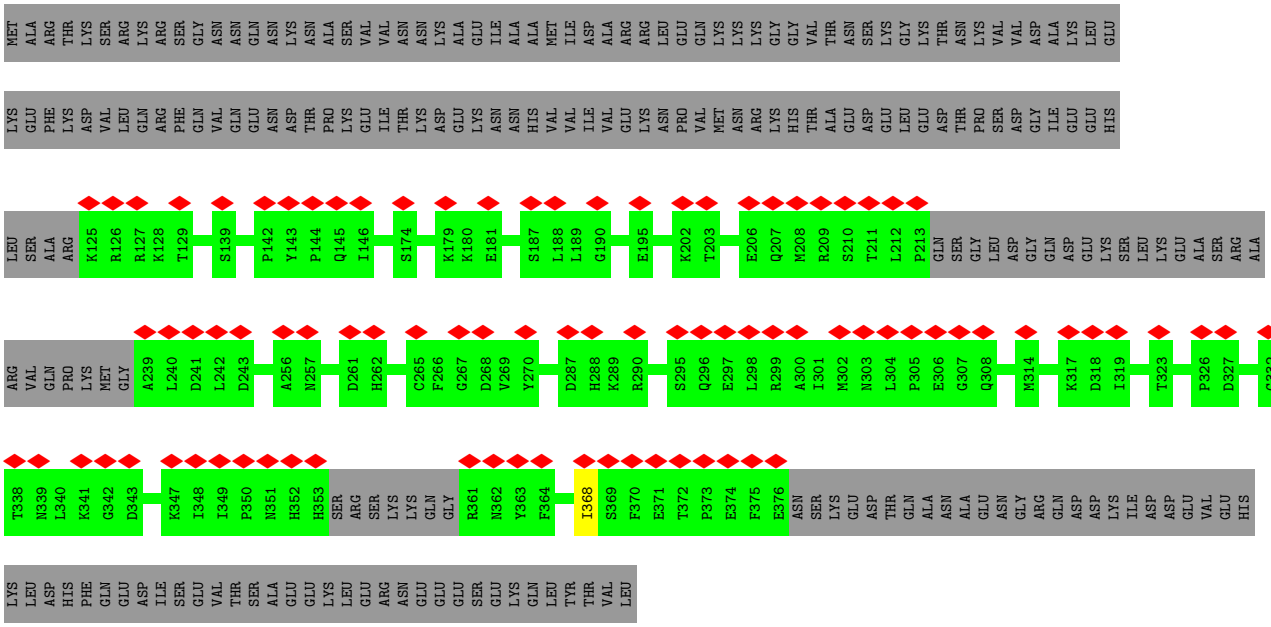
Chain P:





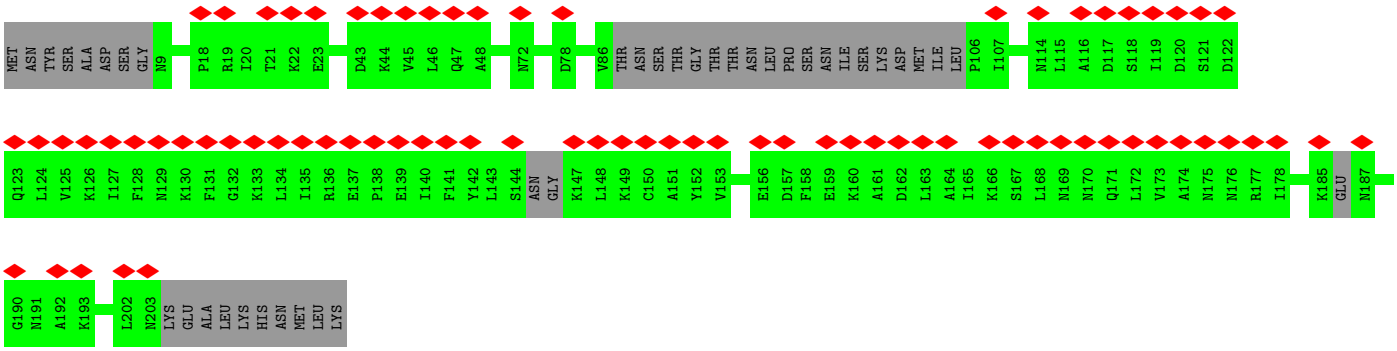
- Molecule 24: Cold sensitive U2 snRNA suppressor 1

Chain Q:



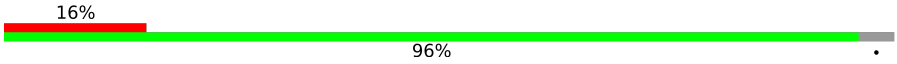
- Molecule 25: Protein HSH49

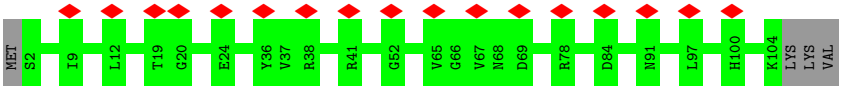
Chain R:



- Molecule 26: Pre-mRNA-splicing factor RDS3

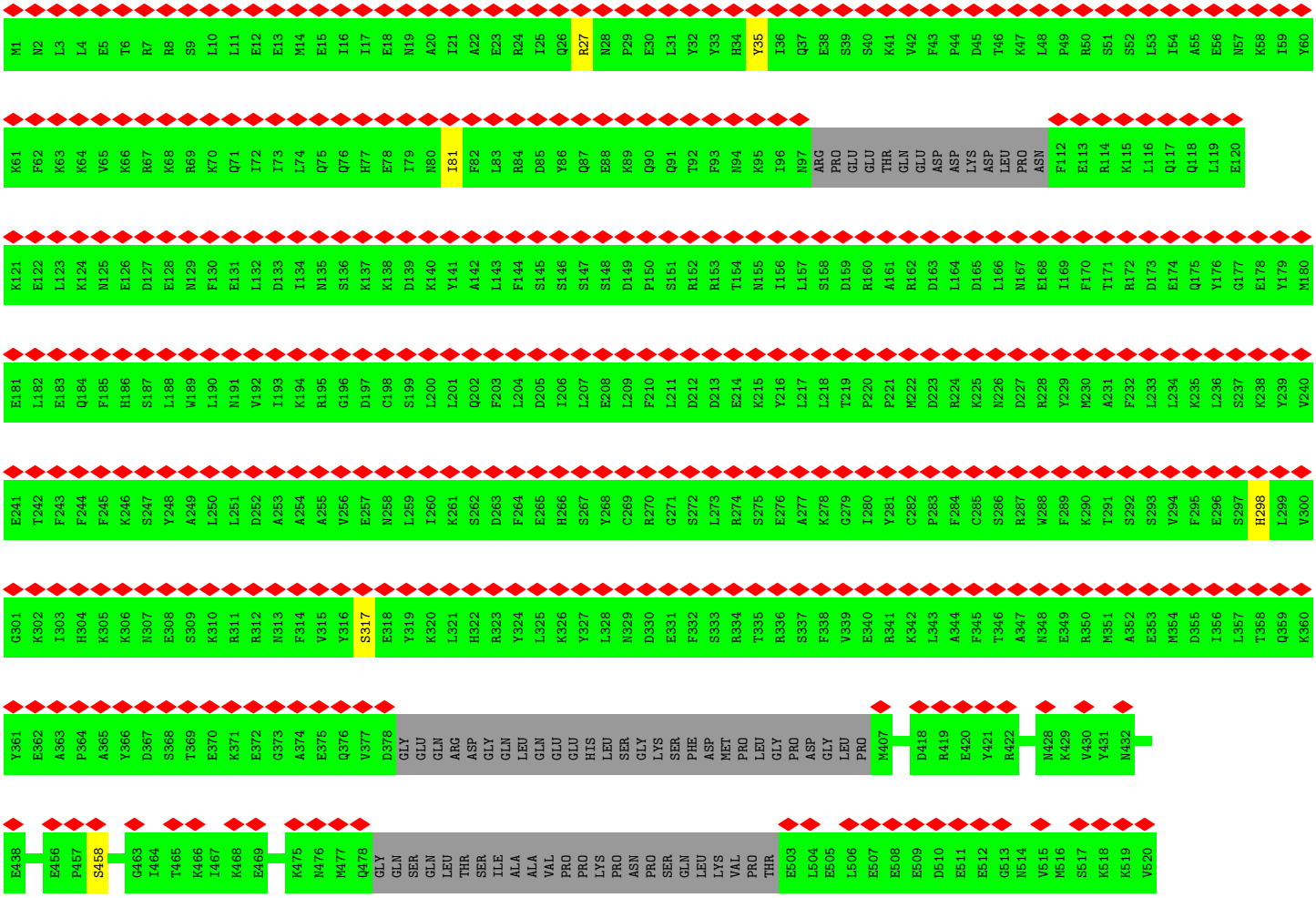
Chain S:

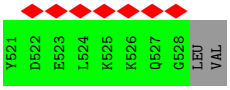




- Molecule 27: Pre-mRNA-splicing factor PRP9

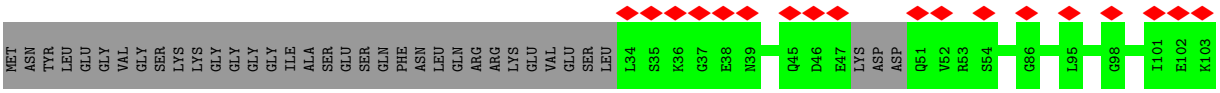
Chain T:

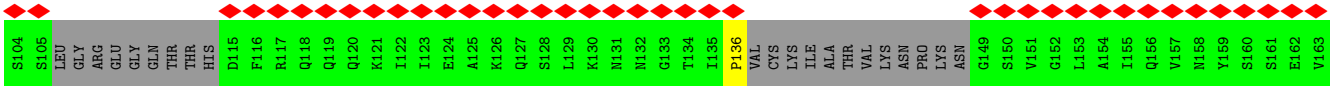


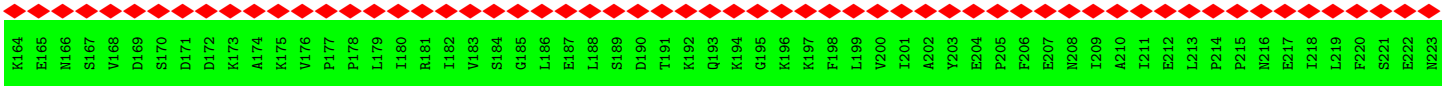


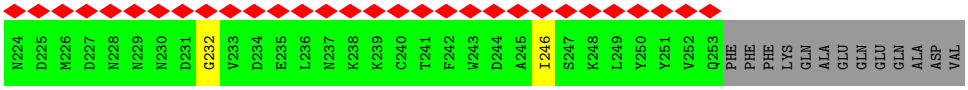
- Molecule 28: Pre-mRNA-splicing factor PRP11

Chain U:



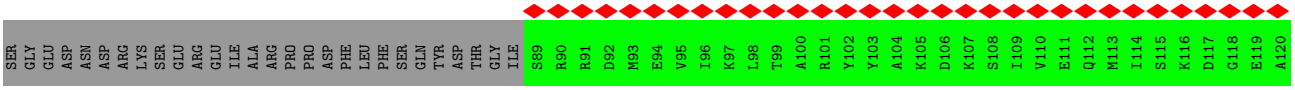


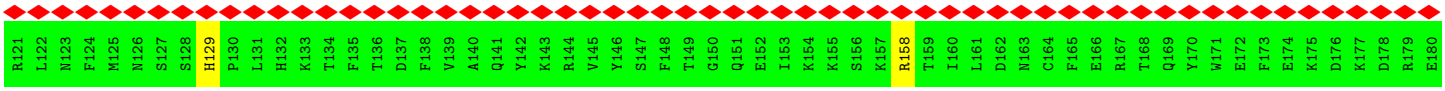




- Molecule 29: Pre-mRNA-splicing factor PRP21

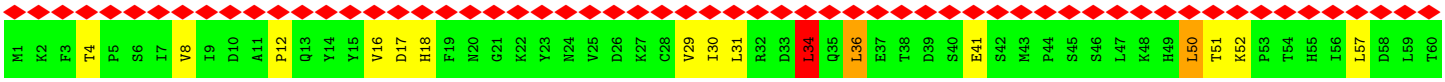
Chain V:

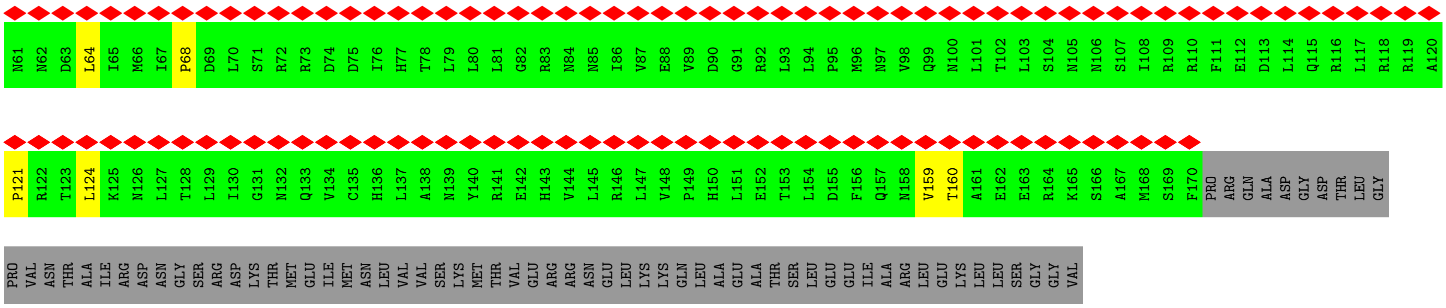




- Molecule 30: U2 small nuclear ribonucleoprotein A'

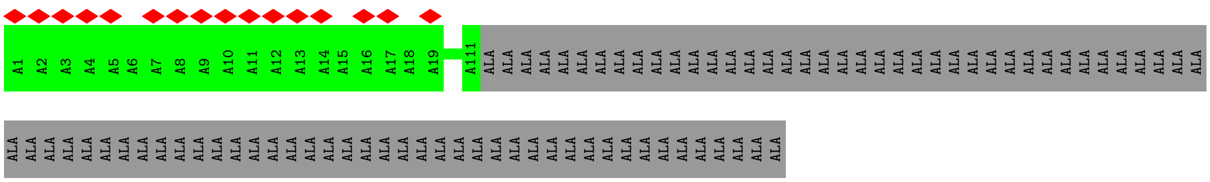
Chain W:





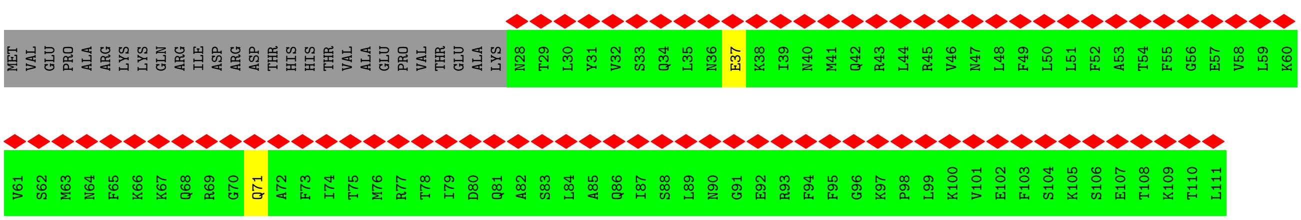
• Molecule 31: Unknown

Chain X:

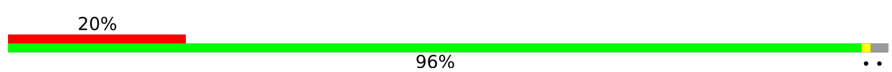


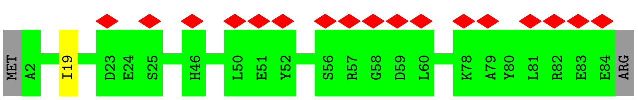
• Molecule 32: U2 small nuclear ribonucleoprotein B"

Chain Y:

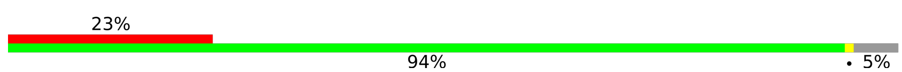


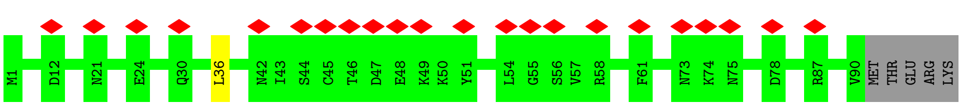
• Molecule 33: RDS3 complex subunit 10

Chain Z:




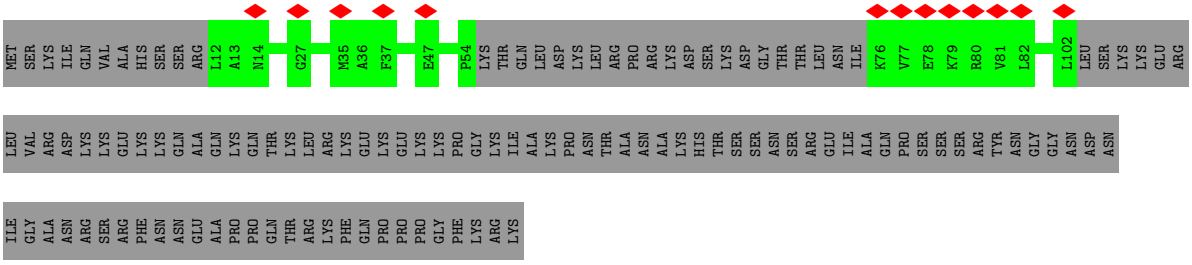
• Molecule 34: U6 snRNA-associated Sm-like protein LSm2

Chain a:




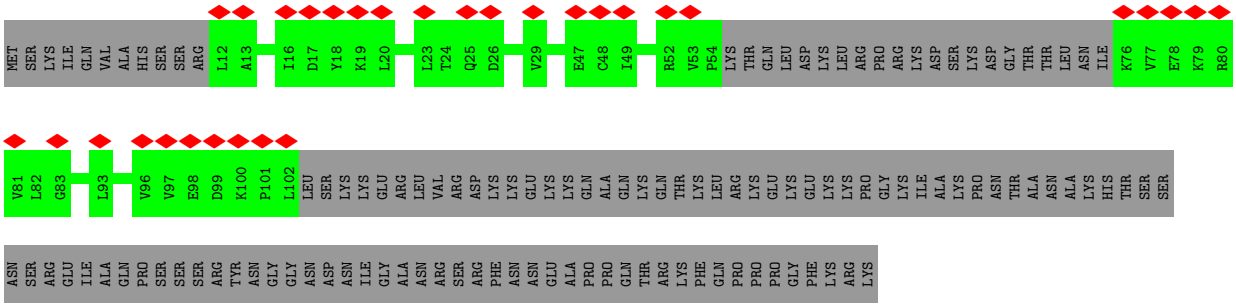
• Molecule 35: Small nuclear ribonucleoprotein-associated protein B

Chain b:



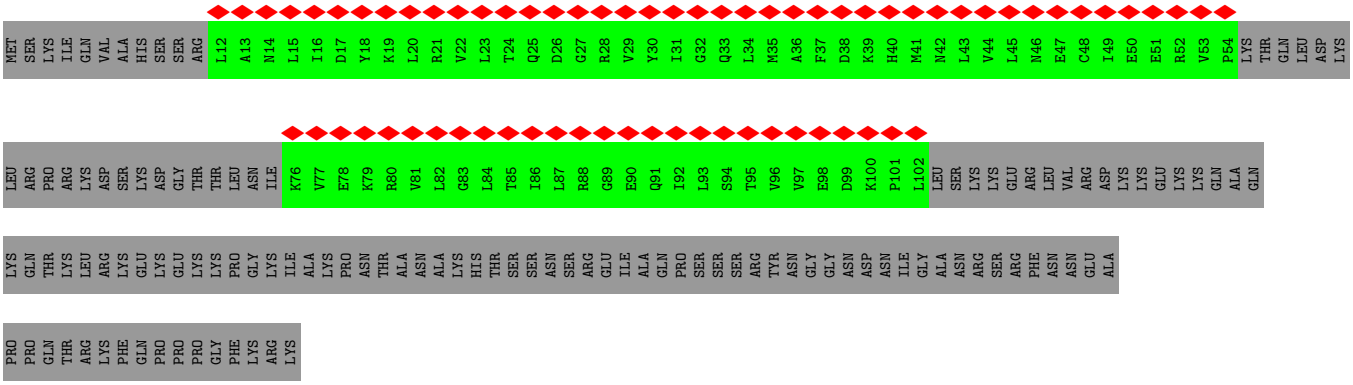
• Molecule 35: Small nuclear ribonucleoprotein-associated protein B

Chain k:



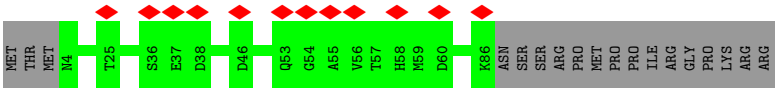
• Molecule 35: Small nuclear ribonucleoprotein-associated protein B

Chain s:



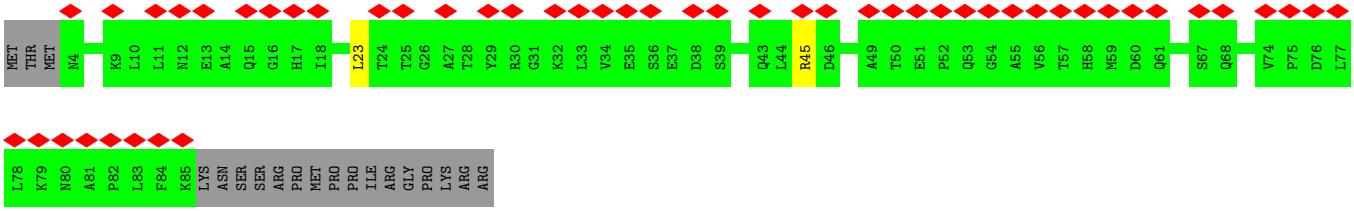
• Molecule 36: Small nuclear ribonucleoprotein Sm D3

Chain d:



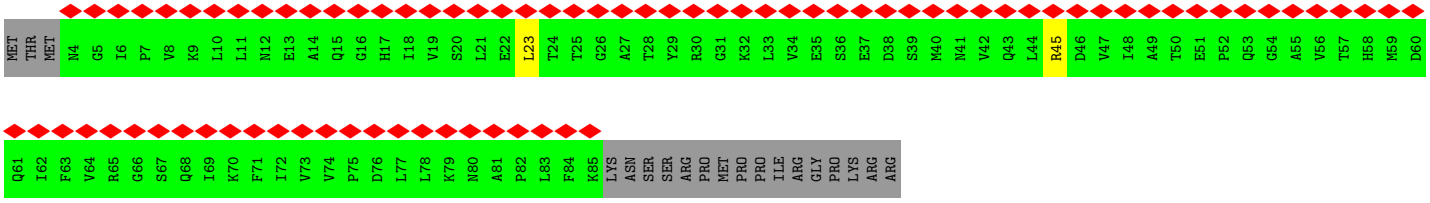
• Molecule 36: Small nuclear ribonucleoprotein Sm D3

Chain n:



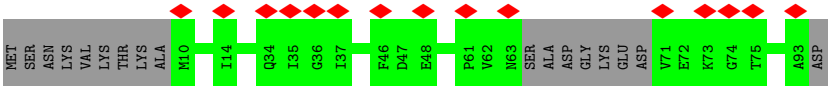
- Molecule 36: Small nuclear ribonucleoprotein Sm D3

Chain v:



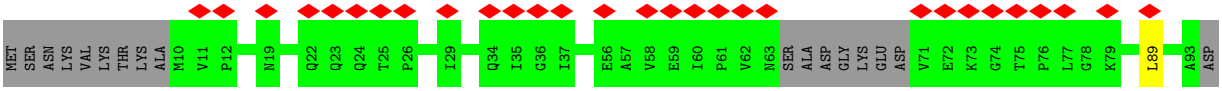
- Molecule 37: Small nuclear ribonucleoprotein E

Chain e:



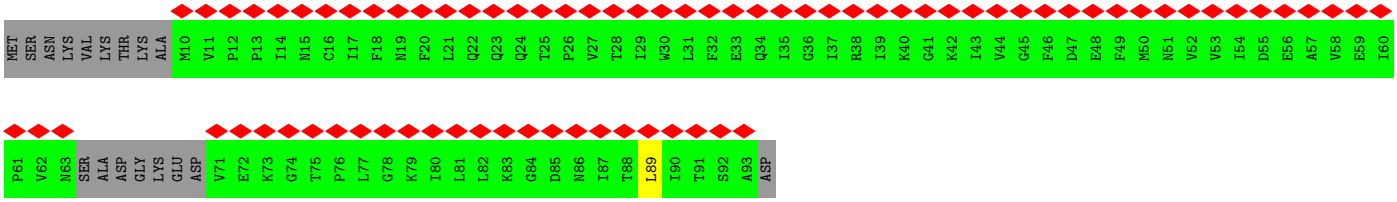
- Molecule 37: Small nuclear ribonucleoprotein E

Chain p:



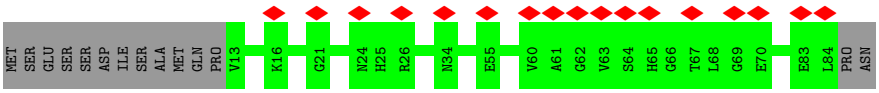
- Molecule 37: Small nuclear ribonucleoprotein E

Chain w:



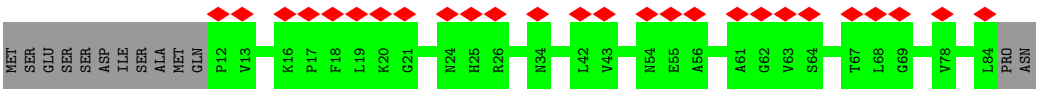
- Molecule 38: Small nuclear ribonucleoprotein F

Chain f:



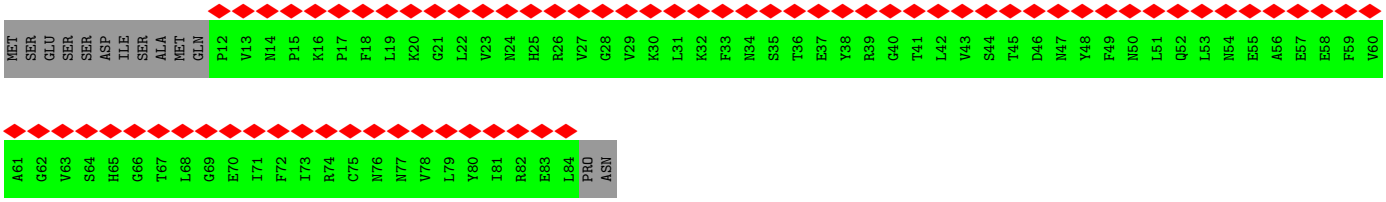
• Molecule 38: Small nuclear ribonucleoprotein F

Chain q:



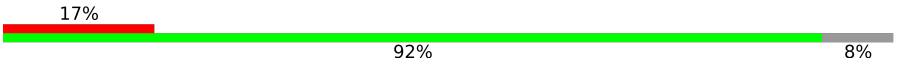
• Molecule 38: Small nuclear ribonucleoprotein F

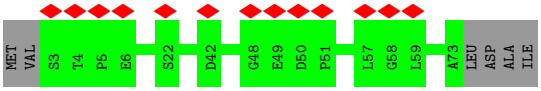
Chain x:



• Molecule 39: Small nuclear ribonucleoprotein G

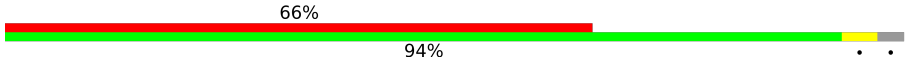
Chain g:

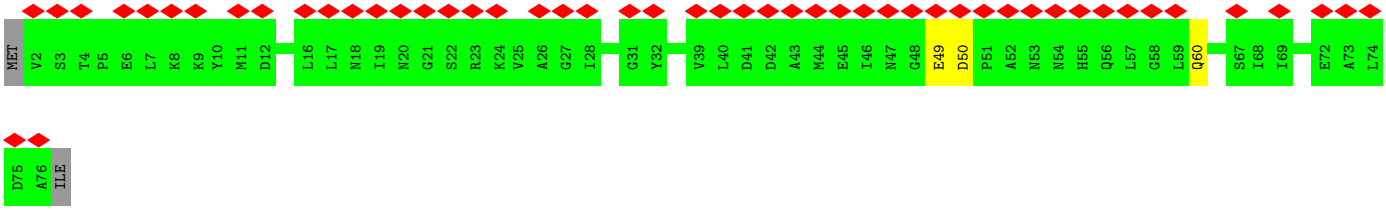




• Molecule 39: Small nuclear ribonucleoprotein G

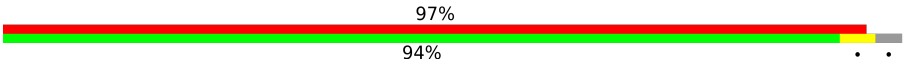
Chain r:

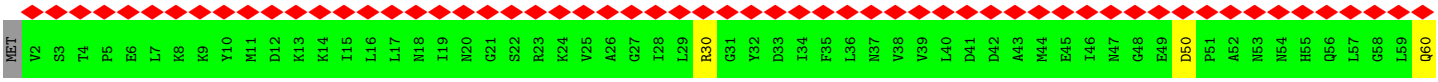


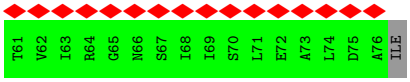


• Molecule 39: Small nuclear ribonucleoprotein G

Chain y:

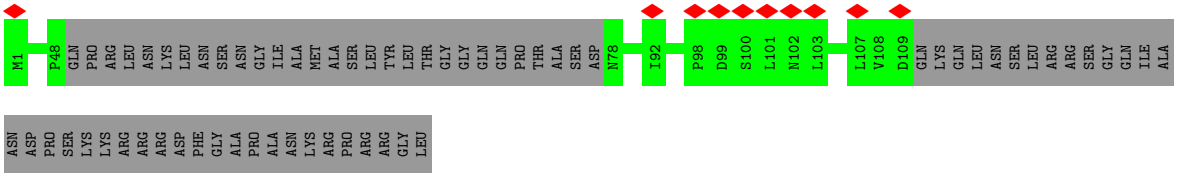






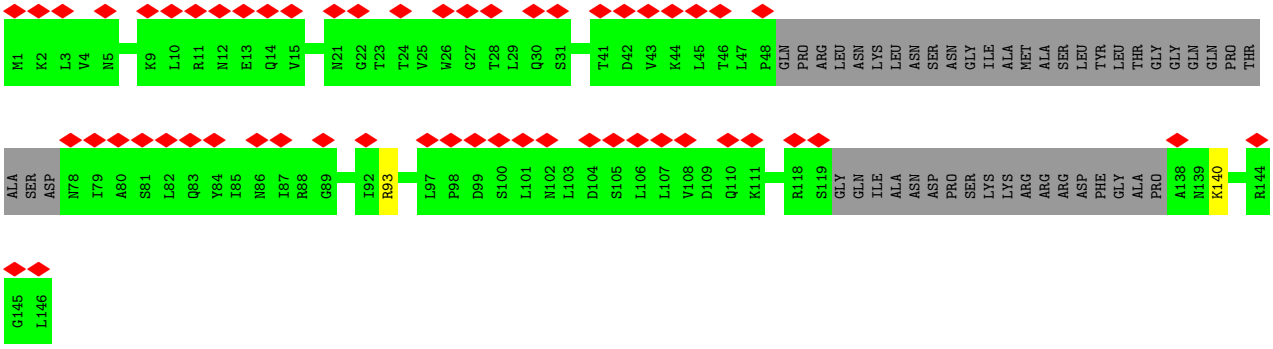
• Molecule 40: Small nuclear ribonucleoprotein Sm D1

Chain h:



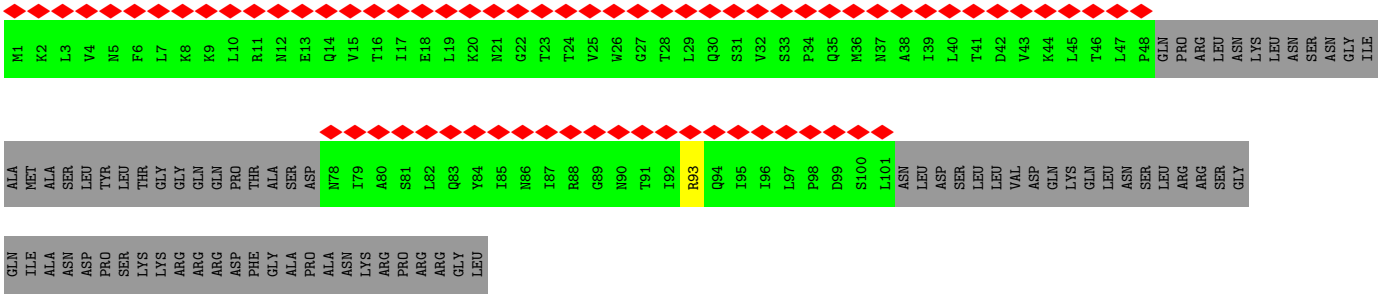
• Molecule 40: Small nuclear ribonucleoprotein Sm D1

Chain l:



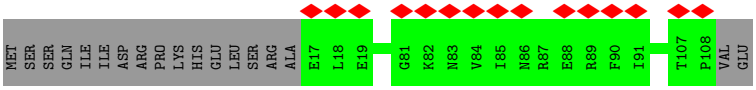
• Molecule 40: Small nuclear ribonucleoprotein Sm D1

Chain t:



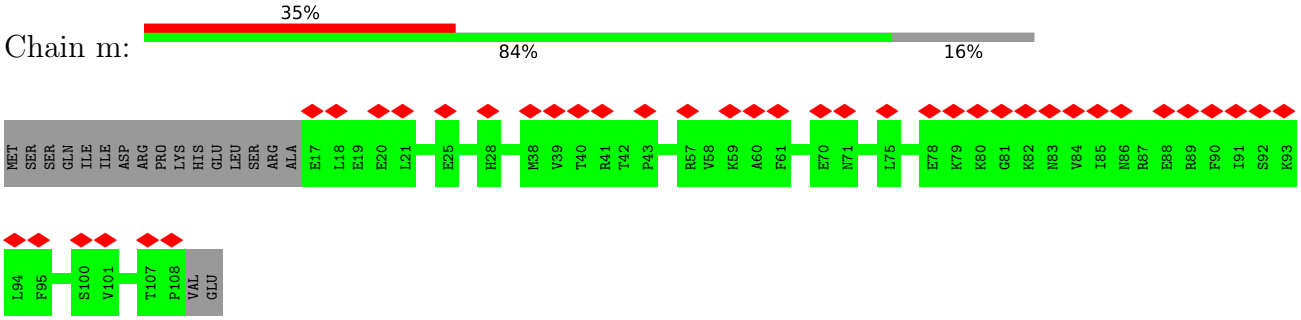
• Molecule 41: Small nuclear ribonucleoprotein Sm D2

Chain i:



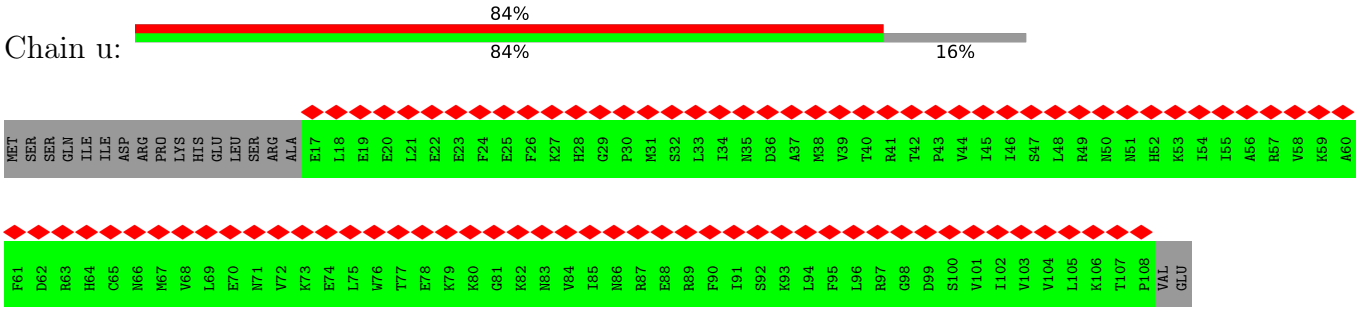
• Molecule 41: Small nuclear ribonucleoprotein Sm D2

Chain m:



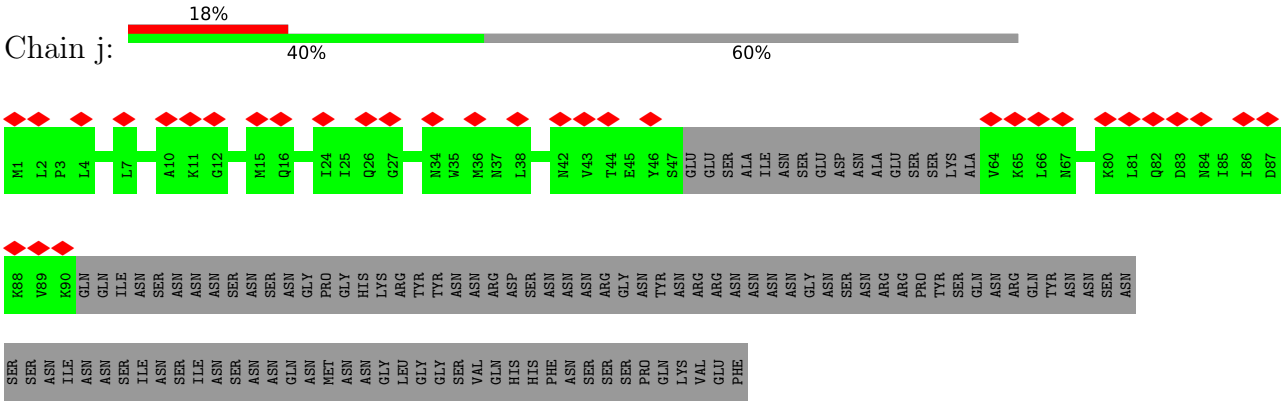
- Molecule 41: Small nuclear ribonucleoprotein Sm D2

Chain u:



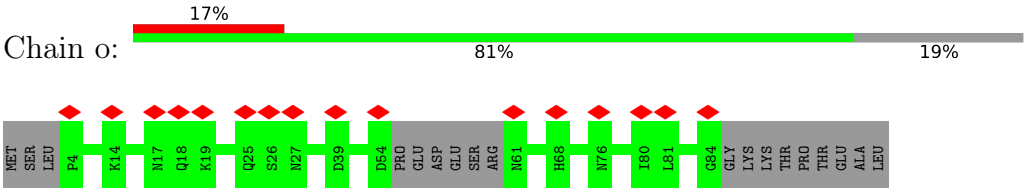
- Molecule 42: U6 snRNA-associated Sm-like protein LSm4

Chain j:



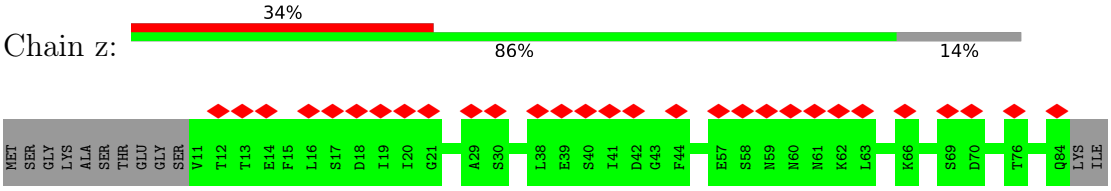
- Molecule 43: U6 snRNA-associated Sm-like protein LSm5

Chain o:



- Molecule 44: U6 snRNA-associated Sm-like protein LSm6

Chain z:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	9559	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 ($e^-/Å^2$)	56	Depositor
Minimum defocus (nm)	350	Depositor
Maximum defocus (nm)	5300	Depositor
Magnification	81000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.080	Depositor
Minimum map value	-0.019	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0258	Depositor
Map size (Å)	686.39996, 686.39996, 686.39996	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.43, 1.43, 1.43	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: GTP, PSU, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	2	1.35	52/3579 (1.5%)	1.69	123/5551 (2.2%)
2	3	0.25	0/617	0.45	0/836
3	4	0.45	4/2705 (0.1%)	0.95	10/4204 (0.2%)
4	5	0.42	1/4039 (0.0%)	0.90	6/6284 (0.1%)
5	6	0.24	0/2253	0.83	3/3497 (0.1%)
6	7	0.24	0/505	0.44	0/675
7	8	0.24	0/501	0.45	0/673
8	A	0.29	0/18580	0.46	1/25189 (0.0%)
9	B	0.40	1/13905 (0.0%)	0.62	6/18852 (0.0%)
10	C	0.32	0/6928	0.47	0/9377
11	D	0.28	0/1185	0.46	0/1596
12	E	0.24	0/822	0.40	0/1109
13	F	0.27	0/3292	0.45	1/4432 (0.0%)
14	G	0.29	0/2885	0.45	0/3882
15	H	0.27	0/3455	0.49	0/4663
16	I	0.28	0/665	0.82	0/1024
17	J	0.26	0/6613	0.43	0/8942
18	K	0.26	0/949	0.45	0/1292
19	L	0.25	0/899	0.44	0/1204
20	M	0.24	0/1430	0.44	0/1927
21	N	0.22	0/421	0.29	0/583
22	O	0.28	0/6745	0.45	0/9157
23	P	0.30	1/9623 (0.0%)	0.53	1/13041 (0.0%)
24	Q	0.27	0/1835	0.46	0/2480
25	R	0.26	0/1453	0.42	0/1954
26	S	0.29	0/827	0.46	0/1105
27	T	0.27	0/3992	0.41	0/5346
28	U	0.25	0/1511	0.41	1/2038 (0.0%)
29	V	0.24	0/1105	0.36	0/1475
30	W	0.42	0/1406	0.69	4/1905 (0.2%)
31	X	0.25	0/148	0.39	0/204
32	Y	0.30	0/692	0.54	0/923

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	Z	0.28	0/694	0.47	0/929
34	a	0.26	0/745	0.51	1/1005 (0.1%)
35	b	0.29	0/567	0.47	0/762
35	k	0.41	0/567	0.61	0/762
35	s	0.40	0/567	0.63	0/762
36	d	0.30	0/650	0.50	0/879
36	n	0.41	0/641	0.65	2/868 (0.2%)
36	v	0.43	0/641	0.65	2/868 (0.2%)
37	e	0.26	0/612	0.44	0/830
37	p	0.39	0/612	0.59	1/830 (0.1%)
37	w	0.40	0/612	0.61	1/830 (0.1%)
38	f	0.27	0/589	0.46	0/796
38	q	0.39	0/597	0.62	0/807
38	x	0.42	0/597	0.63	0/807
39	g	0.25	0/554	0.53	0/746
39	r	0.32	0/582	0.63	0/785
39	y	0.26	0/582	0.49	0/785
40	h	0.25	0/635	0.48	0/861
40	l	0.38	0/756	0.70	1/1023 (0.1%)
40	t	0.41	0/574	0.68	1/777 (0.1%)
41	i	0.25	0/764	0.44	0/1026
41	m	0.38	0/764	0.57	0/1026
41	u	0.40	0/764	0.57	0/1026
42	j	0.25	0/594	0.42	0/802
43	o	0.24	0/595	0.41	0/806
44	z	0.24	0/584	0.43	0/787
All	All	0.39	59/122004 (0.0%)	0.62	165/167605 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	2	0	2
8	A	0	2
9	B	0	4
17	J	0	2
20	M	0	2
23	P	0	2
27	T	0	1
30	W	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
39	r	0	1
All	All	0	17

The worst 5 of 59 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1149	G	O3'-P	24.35	1.90	1.61
1	2	143	G	O3'-P	18.92	1.83	1.61
4	5	105	A	O3'-P	18.04	1.82	1.61
1	2	1161	U	O3'-P	-15.56	1.42	1.61
1	2	143	G	C3'-O3'	15.28	1.63	1.42

The worst 5 of 165 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	144	G	C4'-C3'-O3'	-16.52	74.71	109.40
1	2	1093	C	P-O5'-C5'	14.80	144.59	120.90
1	2	1162	U	C5'-C4'-O4'	14.80	126.86	109.10
1	2	1147	A	C5'-C4'-C3'	-14.15	93.35	116.00
1	2	1092	A	C2'-C3'-O3'	14.11	140.53	109.50

There are no chirality outliers.

5 of 17 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	2	1109	C	Sidechain
1	2	141	A	Sidechain
8	A	1190	ASN	Peptide
8	A	1481	GLU	Peptide
9	B	684	LEU	Peptide

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	
2	3	75/89 (84%)	74 (99%)	1 (1%)	0	100	100
6	7	62/115 (54%)	62 (100%)	0	0	100	100
7	8	62/109 (57%)	61 (98%)	1 (2%)	0	100	100
8	A	2202/2413 (91%)	2095 (95%)	105 (5%)	2 (0%)	51	86
9	B	1694/2163 (78%)	1631 (96%)	60 (4%)	3 (0%)	47	81
10	C	838/1008 (83%)	785 (94%)	52 (6%)	1 (0%)	51	86
11	D	140/143 (98%)	126 (90%)	14 (10%)	0	100	100
12	E	114/587 (19%)	103 (90%)	9 (8%)	2 (2%)	8	40
13	F	409/494 (83%)	387 (95%)	21 (5%)	1 (0%)	47	81
14	G	358/469 (76%)	335 (94%)	23 (6%)	0	100	100
15	H	425/465 (91%)	398 (94%)	27 (6%)	0	100	100
17	J	788/899 (88%)	722 (92%)	61 (8%)	5 (1%)	25	66
18	K	122/126 (97%)	121 (99%)	1 (1%)	0	100	100
19	L	101/194 (52%)	94 (93%)	7 (7%)	0	100	100
20	M	164/242 (68%)	141 (86%)	23 (14%)	0	100	100
21	N	77/291 (26%)	76 (99%)	1 (1%)	0	100	100
22	O	829/971 (85%)	789 (95%)	40 (5%)	0	100	100
23	P	1170/1361 (86%)	1059 (90%)	104 (9%)	7 (1%)	25	66
24	Q	214/435 (49%)	202 (94%)	11 (5%)	1 (0%)	29	69
25	R	165/213 (78%)	162 (98%)	3 (2%)	0	100	100
26	S	101/107 (94%)	88 (87%)	13 (13%)	0	100	100
27	T	454/530 (86%)	416 (92%)	38 (8%)	0	100	100
28	U	188/266 (71%)	159 (85%)	28 (15%)	1 (0%)	29	69
29	V	123/280 (44%)	112 (91%)	11 (9%)	0	100	100
30	W	168/238 (71%)	129 (77%)	28 (17%)	11 (6%)	1	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	X	26/111 (23%)	26 (100%)	0	0	100	100
32	Y	82/111 (74%)	76 (93%)	5 (6%)	1 (1%)	13	50
33	Z	81/85 (95%)	76 (94%)	4 (5%)	1 (1%)	13	50
34	a	88/95 (93%)	81 (92%)	7 (8%)	0	100	100
35	b	66/196 (34%)	61 (92%)	5 (8%)	0	100	100
35	k	66/196 (34%)	62 (94%)	4 (6%)	0	100	100
35	s	66/196 (34%)	62 (94%)	4 (6%)	0	100	100
36	d	81/101 (80%)	79 (98%)	2 (2%)	0	100	100
36	n	80/101 (79%)	77 (96%)	3 (4%)	0	100	100
36	v	80/101 (79%)	77 (96%)	3 (4%)	0	100	100
37	e	73/94 (78%)	71 (97%)	2 (3%)	0	100	100
37	p	73/94 (78%)	72 (99%)	1 (1%)	0	100	100
37	w	73/94 (78%)	72 (99%)	1 (1%)	0	100	100
38	f	70/86 (81%)	67 (96%)	3 (4%)	0	100	100
38	q	71/86 (83%)	68 (96%)	3 (4%)	0	100	100
38	x	71/86 (83%)	69 (97%)	2 (3%)	0	100	100
39	g	69/77 (90%)	63 (91%)	6 (9%)	0	100	100
39	r	73/77 (95%)	66 (90%)	5 (7%)	2 (3%)	5	31
39	y	73/77 (95%)	64 (88%)	6 (8%)	3 (4%)	3	22
40	h	76/146 (52%)	75 (99%)	1 (1%)	0	100	100
40	l	93/146 (64%)	89 (96%)	3 (3%)	1 (1%)	14	52
40	t	68/146 (47%)	67 (98%)	1 (2%)	0	100	100
41	i	90/110 (82%)	90 (100%)	0	0	100	100
41	m	90/110 (82%)	89 (99%)	1 (1%)	0	100	100
41	u	90/110 (82%)	89 (99%)	1 (1%)	0	100	100
42	j	70/187 (37%)	67 (96%)	3 (4%)	0	100	100
43	o	71/93 (76%)	66 (93%)	5 (7%)	0	100	100
44	z	72/86 (84%)	70 (97%)	2 (3%)	0	100	100
All	All	13125/17406 (75%)	12318 (94%)	765 (6%)	42 (0%)	44	77

5 of 42 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
17	J	881	VAL
23	P	1299	ILE
24	Q	368	ILE
30	W	34	LEU
30	W	52	LYS

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	
2	3	71/81 (88%)	71 (100%)	0	100	100
6	7	56/103 (54%)	56 (100%)	0	100	100
7	8	56/99 (57%)	56 (100%)	0	100	100
8	A	1982/2182 (91%)	1982 (100%)	0	100	100
9	B	1525/1955 (78%)	1523 (100%)	2 (0%)	93	97
10	C	761/910 (84%)	761 (100%)	0	100	100
11	D	131/132 (99%)	131 (100%)	0	100	100
12	E	60/534 (11%)	60 (100%)	0	100	100
13	F	354/445 (80%)	354 (100%)	0	100	100
14	G	267/436 (61%)	267 (100%)	0	100	100
15	H	377/410 (92%)	377 (100%)	0	100	100
17	J	708/813 (87%)	708 (100%)	0	100	100
18	K	102/104 (98%)	102 (100%)	0	100	100
19	L	92/179 (51%)	92 (100%)	0	100	100
20	M	154/224 (69%)	154 (100%)	0	100	100
22	O	739/867 (85%)	738 (100%)	1 (0%)	93	97
23	P	1093/1244 (88%)	1093 (100%)	0	100	100
24	Q	192/391 (49%)	192 (100%)	0	100	100
25	R	154/189 (82%)	154 (100%)	0	100	100
26	S	93/97 (96%)	93 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	T	429/492 (87%)	424 (99%)	5 (1%)	71	83
28	U	158/236 (67%)	157 (99%)	1 (1%)	86	92
29	V	118/259 (46%)	116 (98%)	2 (2%)	60	78
30	W	161/219 (74%)	151 (94%)	10 (6%)	18	43
32	Y	76/100 (76%)	75 (99%)	1 (1%)	69	81
33	Z	75/77 (97%)	75 (100%)	0	100	100
34	a	85/91 (93%)	85 (100%)	0	100	100
35	b	64/176 (36%)	64 (100%)	0	100	100
35	k	64/176 (36%)	64 (100%)	0	100	100
35	s	64/176 (36%)	64 (100%)	0	100	100
36	d	72/89 (81%)	72 (100%)	0	100	100
36	n	71/89 (80%)	71 (100%)	0	100	100
36	v	71/89 (80%)	71 (100%)	0	100	100
37	e	69/83 (83%)	69 (100%)	0	100	100
37	p	69/83 (83%)	69 (100%)	0	100	100
37	w	69/83 (83%)	69 (100%)	0	100	100
38	f	64/77 (83%)	64 (100%)	0	100	100
38	q	65/77 (84%)	65 (100%)	0	100	100
38	x	65/77 (84%)	65 (100%)	0	100	100
39	g	61/66 (92%)	61 (100%)	0	100	100
39	r	64/66 (97%)	64 (100%)	0	100	100
39	y	64/66 (97%)	64 (100%)	0	100	100
40	h	75/129 (58%)	75 (100%)	0	100	100
40	l	81/129 (63%)	81 (100%)	0	100	100
40	t	67/129 (52%)	67 (100%)	0	100	100
41	i	85/103 (82%)	85 (100%)	0	100	100
41	m	85/103 (82%)	85 (100%)	0	100	100
41	u	85/103 (82%)	85 (100%)	0	100	100
42	j	64/172 (37%)	64 (100%)	0	100	100
43	o	66/84 (79%)	66 (100%)	0	100	100
44	z	66/75 (88%)	66 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	11739/15369 (76%)	11717 (100%)	22 (0%)	93 96

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
30	W	31	LEU
30	W	41	GLU
30	W	36	LEU
30	W	50	LEU
27	T	298	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 193 such sidechains are listed below:

Mol	Chain	Res	Type
22	O	853	HIS
24	Q	288	HIS
22	O	908	GLN
23	P	609	HIS
27	T	167	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	147/1175 (12%)	47 (31%)	25 (17%)
16	I	26/95 (27%)	8 (30%)	2 (7%)
3	4	110/160 (68%)	33 (30%)	6 (5%)
4	5	166/214 (77%)	61 (36%)	8 (4%)
5	6	91/112 (81%)	33 (36%)	8 (8%)
All	All	540/1756 (30%)	182 (33%)	49 (9%)

5 of 182 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	33	U
1	2	41	C
1	2	46	C
1	2	47	U
1	2	66	A

5 of 49 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	4	91	U
4	5	114	G
3	4	134	U
4	5	40	C
4	5	130	A

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

3 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	$\#\|Z\| > 2$
1	PSU	2	35	1,16	18,21,22	1.07	1 (5%)	22,30,33	1.73	4 (18%)
1	PSU	2	44	1,16	18,21,22	1.03	1 (5%)	22,30,33	1.65	4 (18%)
1	PSU	2	42	1,16	18,21,22	1.08	1 (5%)	22,30,33	1.73	4 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	2	35	1,16	-	0/7/25/26	0/2/2/2
1	PSU	2	44	1,16	-	0/7/25/26	0/2/2/2
1	PSU	2	42	1,16	-	0/7/25/26	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	42	PSU	C6-C5	3.46	1.39	1.35
1	2	35	PSU	C6-C5	3.35	1.39	1.35
1	2	44	PSU	C6-C5	3.22	1.39	1.35

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	42	PSU	C4-N3-C2	-4.57	119.75	126.34
1	2	35	PSU	C4-N3-C2	-4.49	119.87	126.34
1	2	42	PSU	N1-C2-N3	4.43	120.14	115.13
1	2	35	PSU	N1-C2-N3	4.37	120.08	115.13
1	2	44	PSU	N1-C2-N3	4.28	119.98	115.13

There are no chirality outliers.

There are no torsion outliers.

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 8 ligands modelled in this entry, 7 are monoatomic - leaving 1 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	$\#\|Z\| > 2$
45	GTP	C	1101	-	26,34,34	1.19	2 (7%)	32,54,54	1.66	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
45	GTP	C	1101	-	-	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)
45	C	1101	GTP	C5-C6	-4.24	1.38	1.47
45	C	1101	GTP	C2-N3	2.11	1.38	1.33

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	C	1101	GTP	PB-O3B-PG	-4.88	116.09	132.83
45	C	1101	GTP	PA-O3A-PB	-3.57	120.59	132.83
45	C	1101	GTP	C5-C6-N1	3.39	119.93	113.95
45	C	1101	GTP	C2-N1-C6	-2.98	119.61	125.10
45	C	1101	GTP	C8-N7-C5	2.94	108.60	102.99

There are no chirality outliers.

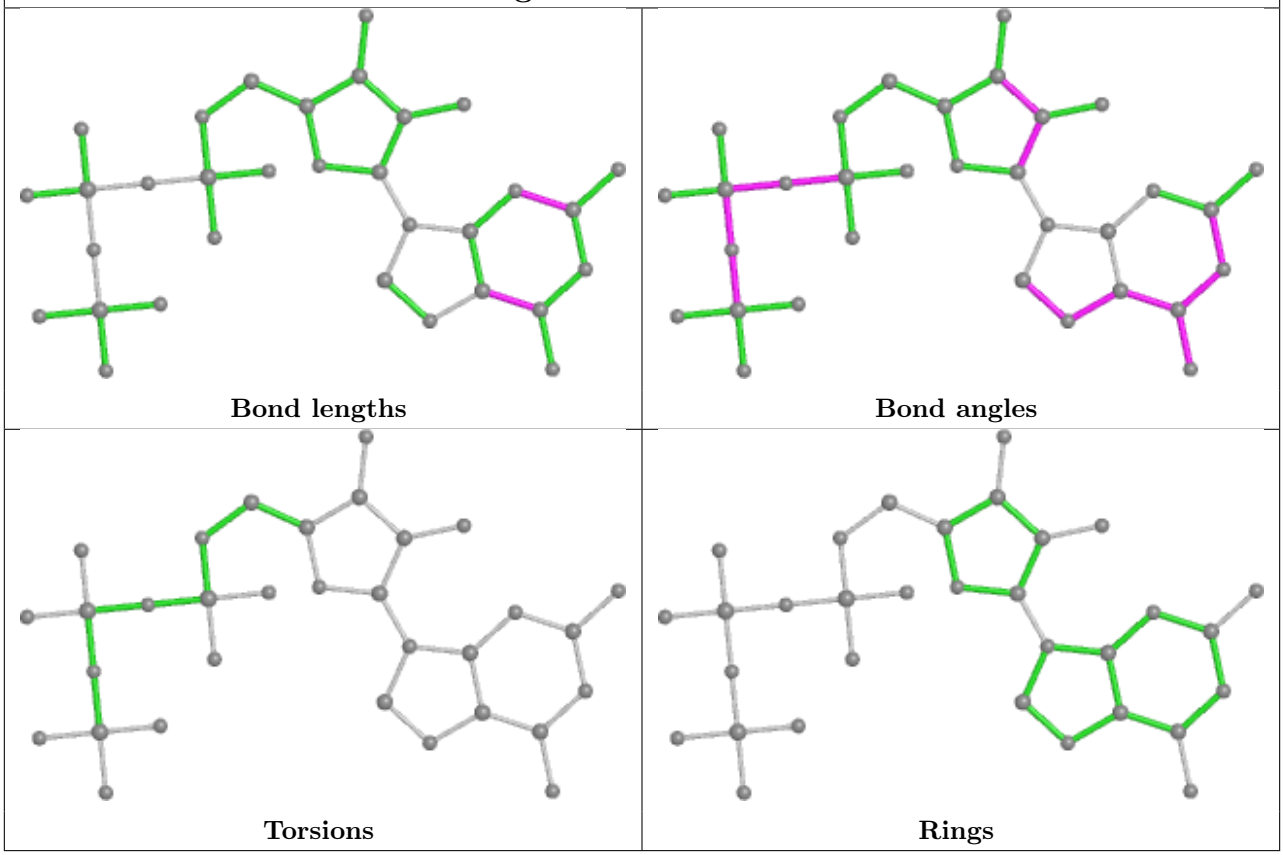
There are no torsion outliers.

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 GTP C 1101



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	5	3
1	2	3
12	E	1
31	X	1

The worst 5 of 8 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	236:SER	C	297:LYS	N	126.30
1	X	19:ALA	C	101:ALA	N	56.70
1	5	72:C	O3'	73:U	P	3.93

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	42:A	O3'	43:G	P	3.10
1	2	1149:G	O3'	1150:U	P	1.90

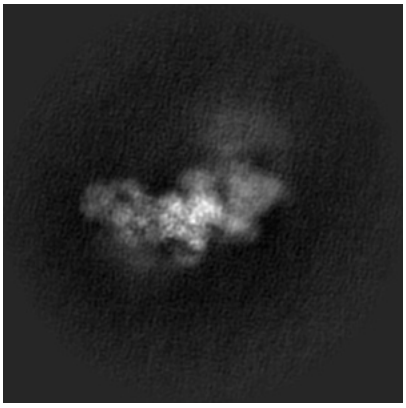
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-3683. These allow visual inspection of the internal detail of the map and identification of artifacts.

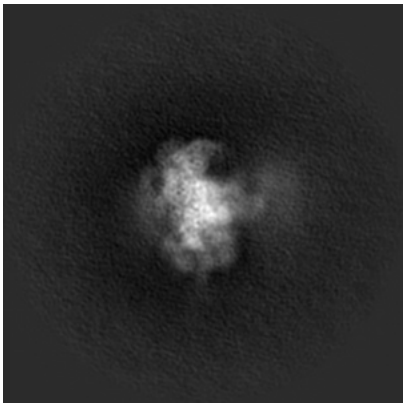
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

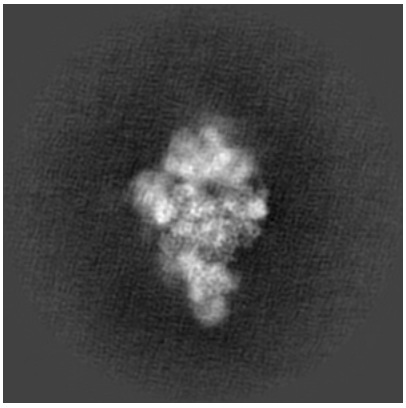
6.1.1 Primary map



X



Y

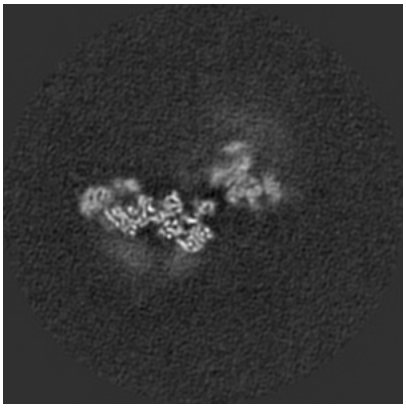


Z

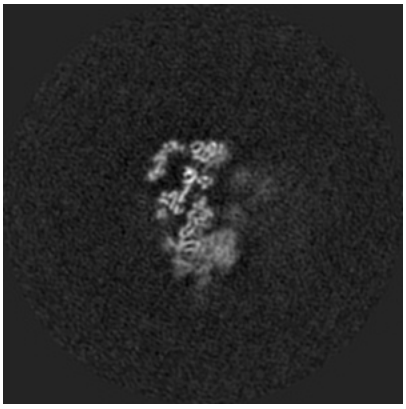
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

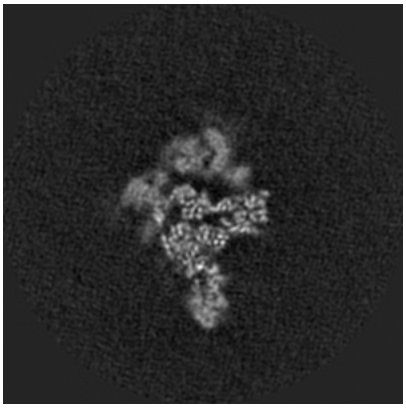
6.2.1 Primary map



X Index: 240



Y Index: 240

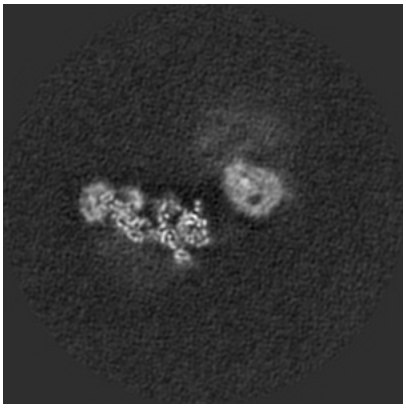


Z Index: 240

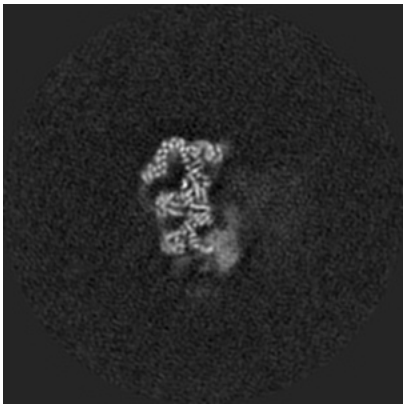
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

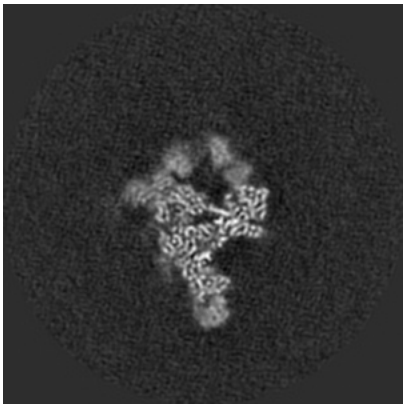
6.3.1 Primary map



X Index: 253



Y Index: 232

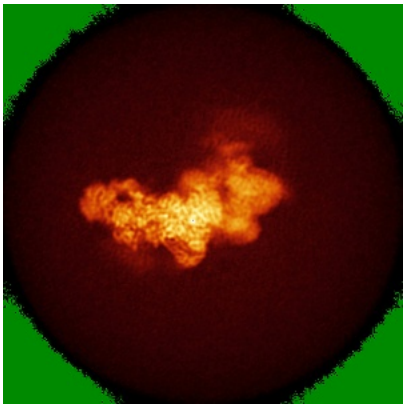


Z Index: 232

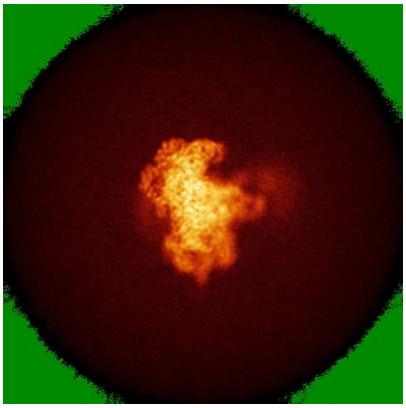
The images above show the largest variance slices of the map in three orthogonal directions.

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

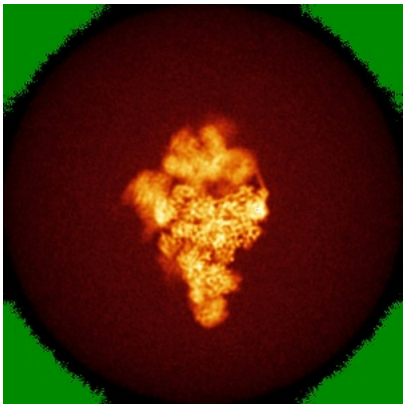
6.4.1 Primary map



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

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0258. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

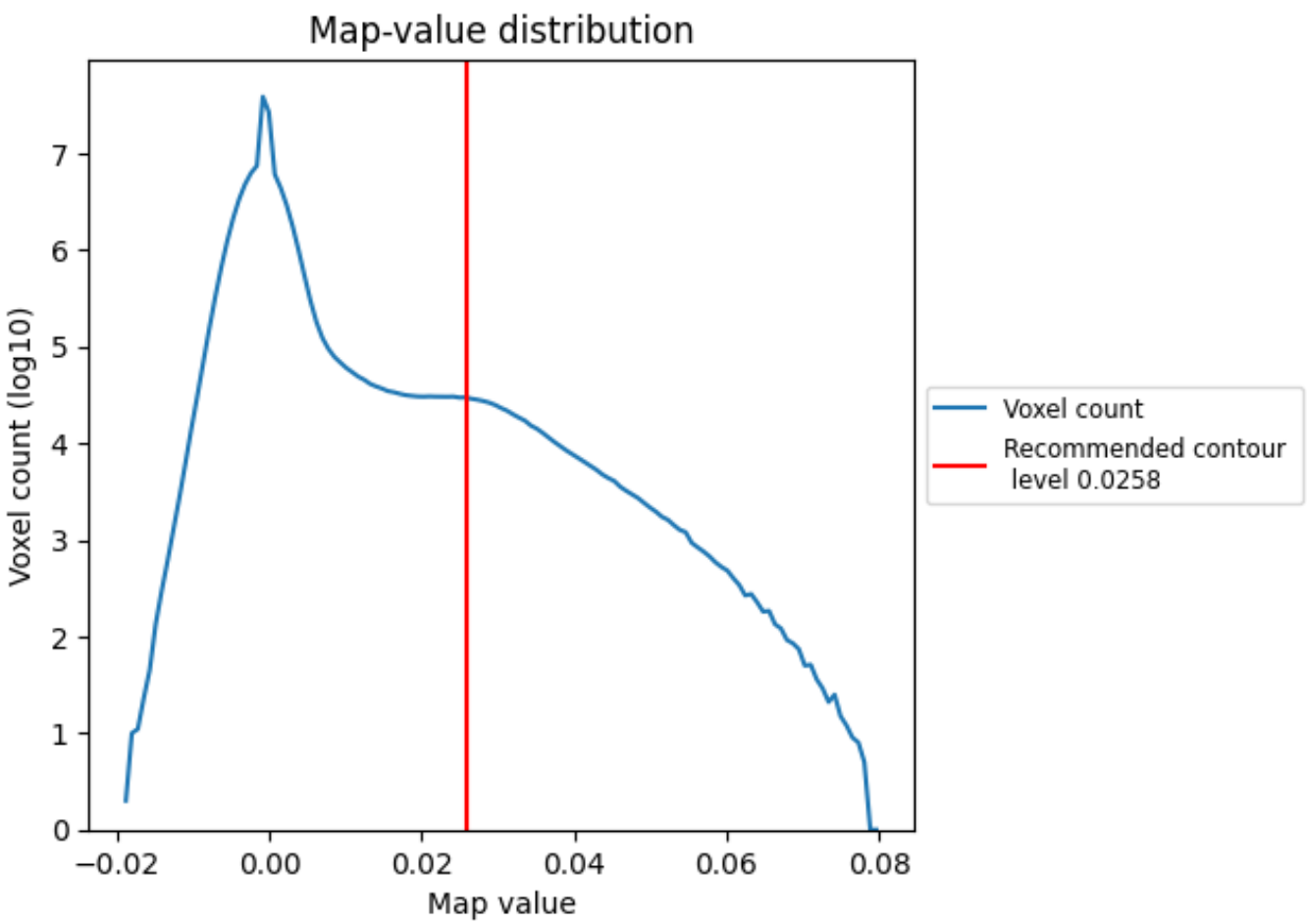
6.6 Mask visualisation (i)

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

7 Map analysis (i)

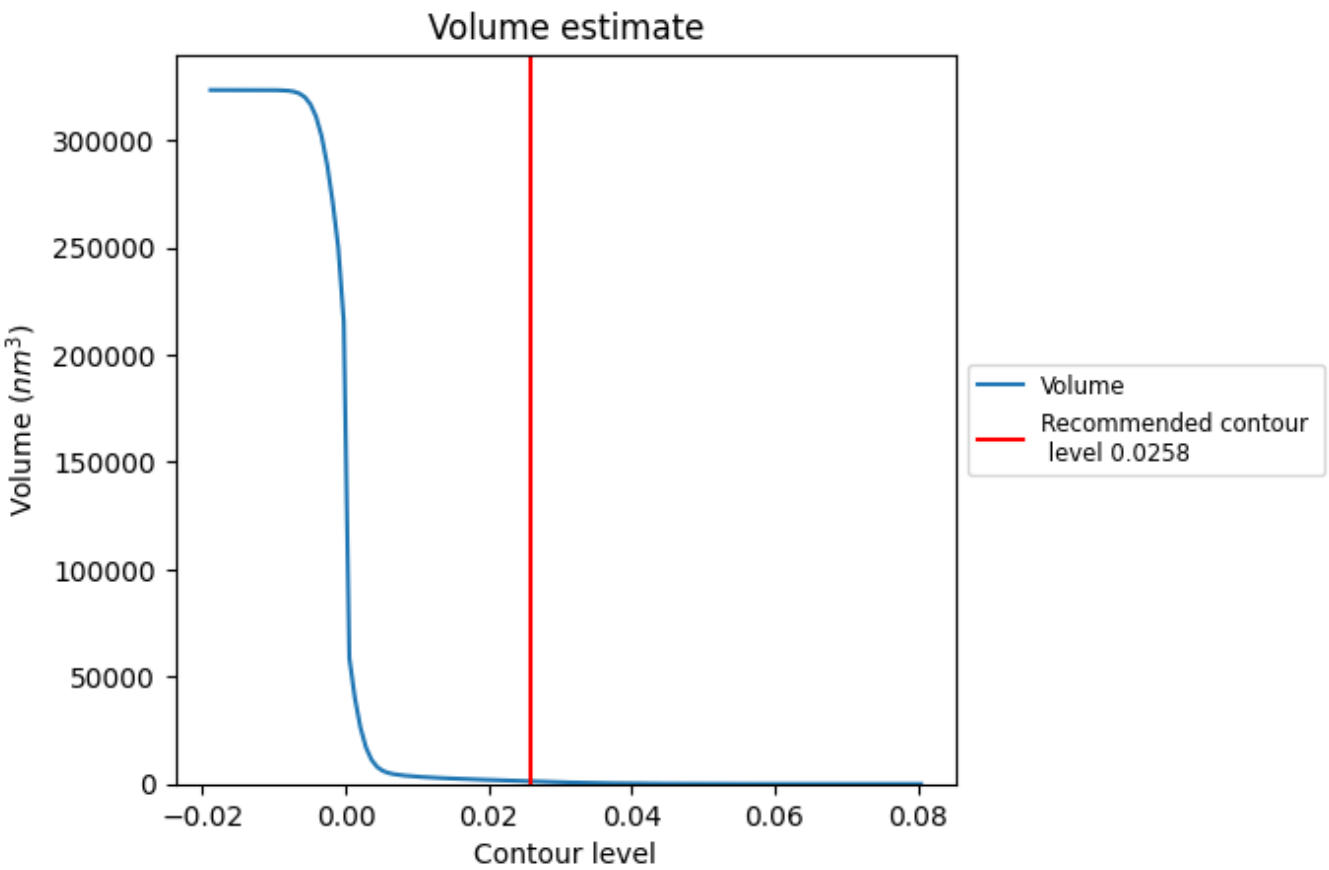
This section contains the results of statistical analysis of the map.

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.

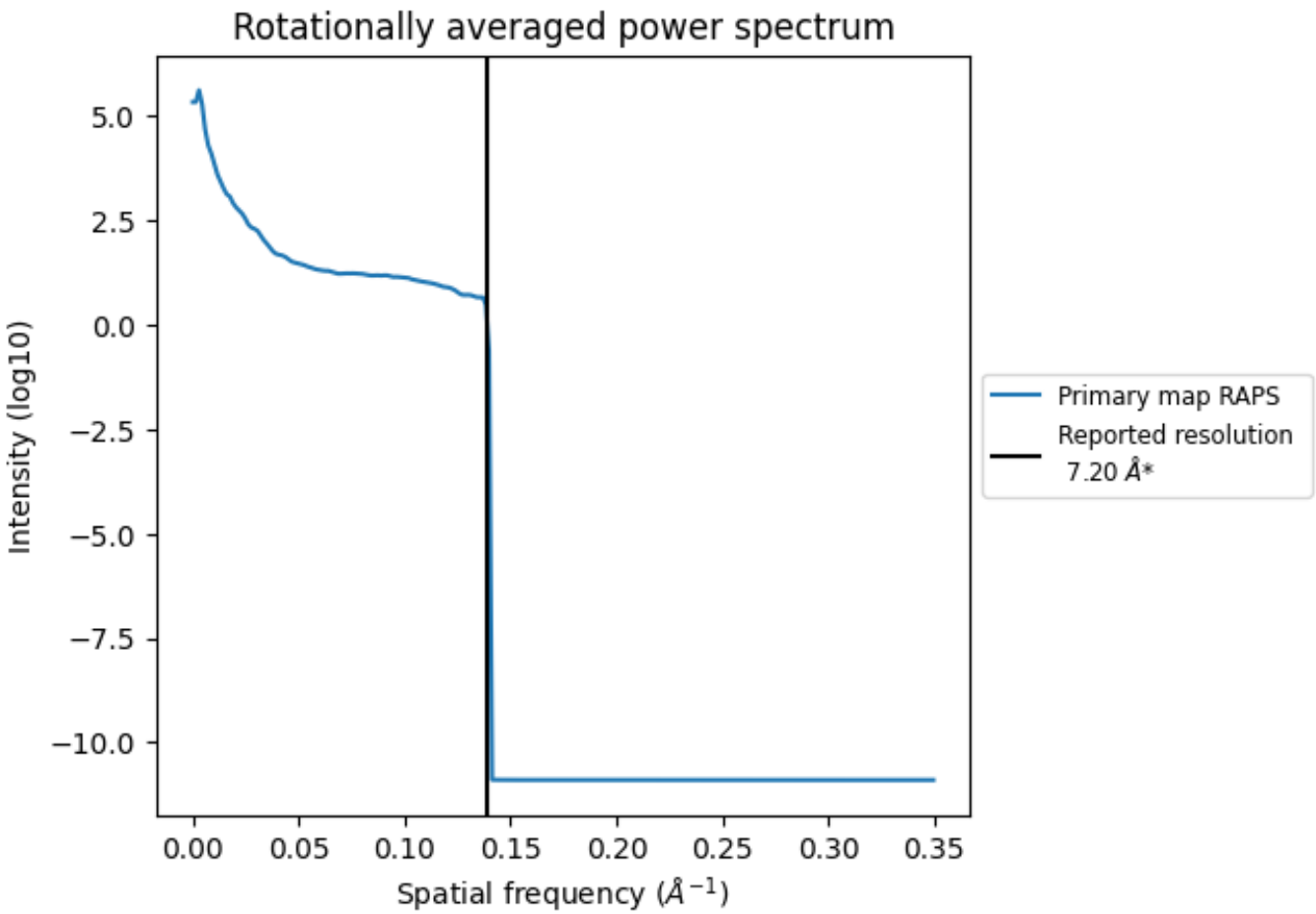
7.2 Volume estimate (i)



The volume at the recommended contour level is 1240 nm^3; this corresponds to an approximate mass of 1120 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 0.139 Å^{-1}

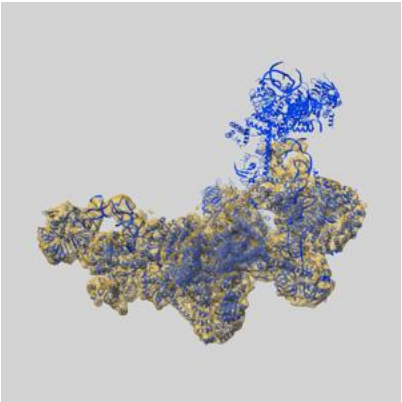
8 Fourier-Shell correlation (i)

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

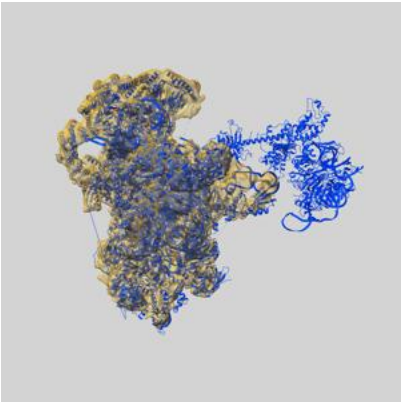
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-3683 and PDB model 5NRL. Per-residue inclusion information can be found in section 3 on page 13.

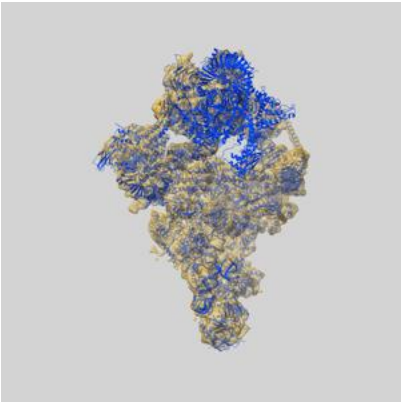
9.1 Map-model overlay (i)



X



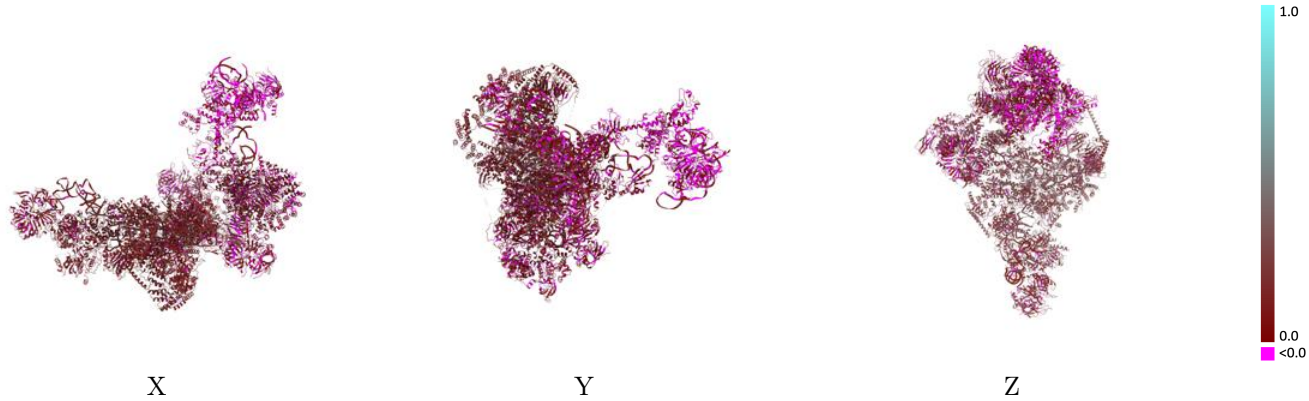
Y



Z

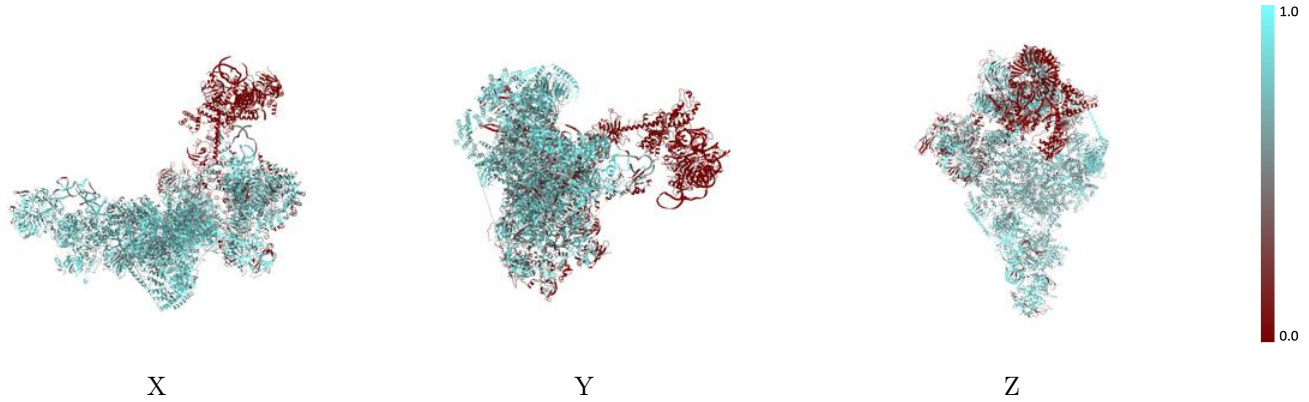
The images above show the 3D surface view of the map at the recommended contour level 0.0258 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



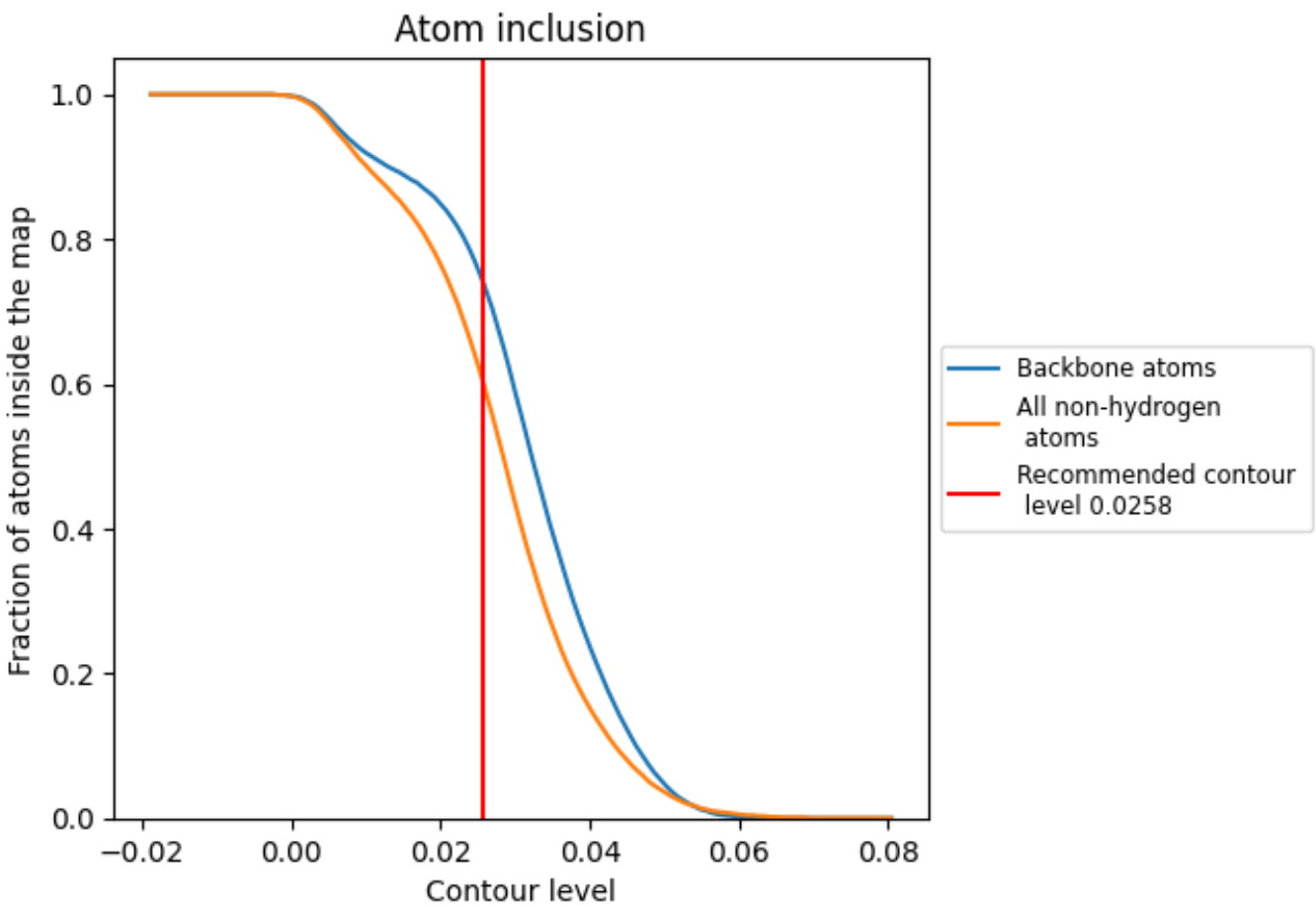
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0258).

9.4 Atom inclusion (i)



At the recommended contour level, 74% of all backbone atoms, 60% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0258) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5990	0.1170
2	0.2760	0.0470
3	0.5440	0.0880
4	0.9080	0.1920
5	0.8050	0.1610
6	0.8490	0.1950
7	0.5250	0.0490
8	0.5600	0.0820
A	0.7100	0.1500
B	0.6040	0.1240
C	0.7390	0.1500
D	0.6650	0.1440
E	0.5550	0.1590
F	0.7210	0.1670
G	0.7410	0.1600
H	0.7760	0.1380
I	0.7900	0.1290
J	0.7460	0.1600
K	0.6930	0.1580
L	0.7210	0.1510
M	0.7060	0.1400
N	0.7880	0.2460
O	0.6550	0.1020
P	0.6160	0.0950
Q	0.5210	0.1160
R	0.4630	0.0960
S	0.7310	0.0980
T	0.1060	0.0240
U	0.2500	0.0420
V	0.0000	0.0440
W	0.0000	-0.0000
X	0.5070	0.2310
Y	0.0000	0.0080
Z	0.6490	0.1080
a	0.6180	0.0880

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Chain	Atom inclusion	Q-score
b	0.6820	0.1200
d	0.6500	0.1270
e	0.6880	0.1190
f	0.6930	0.1170
g	0.6540	0.1230
h	0.7060	0.1050
i	0.7160	0.1360
j	0.5100	0.0780
k	0.4970	0.0340
l	0.3620	0.0730
m	0.4950	0.0640
n	0.3060	0.0440
o	0.6960	0.0800
p	0.5580	0.0620
q	0.5850	0.0790
r	0.3290	0.0510
s	0.0000	0.0010
t	0.0000	0.0150
u	0.0000	-0.0050
v	0.0000	-0.0080
w	0.0000	0.0040
x	0.0000	-0.0260
y	0.0000	-0.0010
z	0.5740	0.0700