



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 07:24 PM UTC

PDB ID : 7ABG / pdb_00007abg
EMDB ID : EMD-11695
Title : Human pre-Bact-1 spliceosome
Authors : Townsend, C.; Kastner, B.; Leelaram, M.N.; Bertram, K.; Stark, H.;
Luehrmann, R.
Deposited on : 2020-09-07
Resolution : 7.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

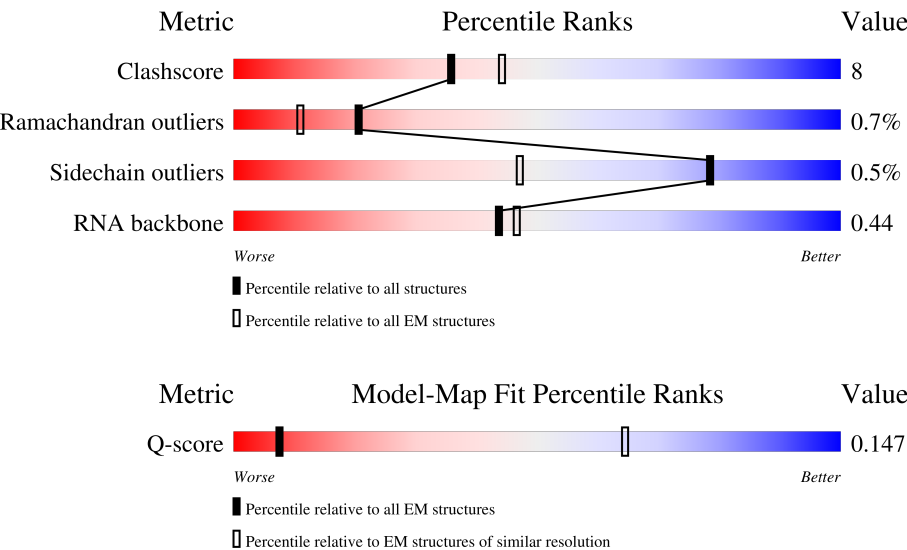
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance i

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

The reported resolution of this entry is 7.80 Å.

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



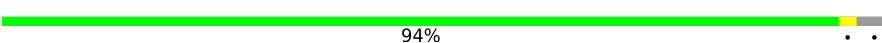
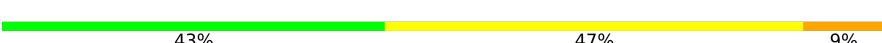
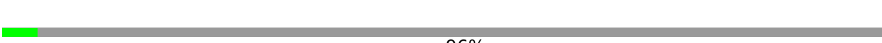
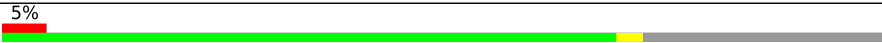
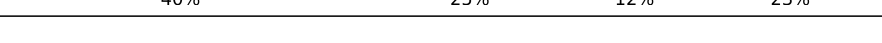
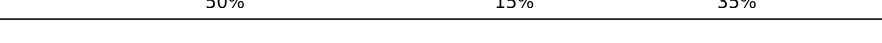
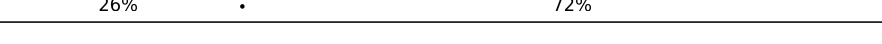
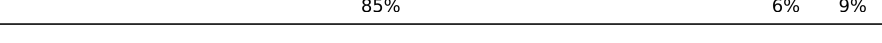
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	370 (7.30 - 8.30)

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

Mol	Chain	Length	Quality of chain
1	A5	790	
2	A2	103	
3	Z	125	

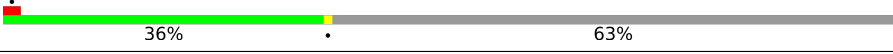
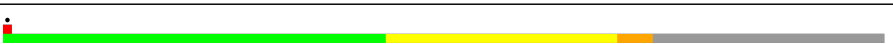
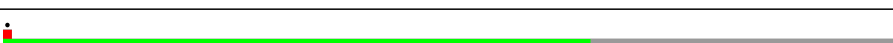
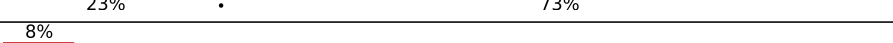
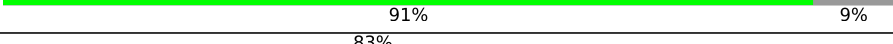
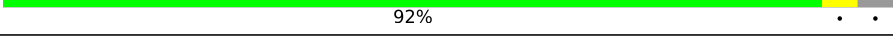
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Mol	Chain	Length	Quality of chain
4	F	464	
5	D	357	
6	W	255	
7	B	225	
8	s	2136	
9	Q	144	
10	A1	156	
11	5	116	
12	L	802	
13	R	229	
14	V	95	
15	9	102	
16	C	139	
17	H	91	
18	J	80	
19	2	188	
20	A3	96	
21	K	439	
22	y	110	
23	G	514	
24	Z	230	
25	A	2335	
26	I	312	
27	P	420	
28	p	793	

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Mol	Chain	Length	Quality of chain
29	4	501	
30	A4	1098	
31	u	1304	
32	T	895	
33	E	1217	
34	w	424	
35	x	86	
36	v	536	
37	0	396	
38	N	199	
39	r	972	
40	Y	904	
41	6	106	
42	A6	248	
43	a	118	
43	h	118	
44	b	86	
44	i	86	
45	f	240	
45	m	240	
46	e	126	
46	l	126	
47	d	76	
47	k	76	
48	c	92	

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Mol	Chain	Length	Quality of chain
48	j	92	
49	g	119	
49	n	119	
50	q	73	
51	X	641	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
53	GTP	r	1500	-	-	X	-

2 Entry composition [i](#)

There are 55 unique types of molecules in this entry. The entry contains 73818 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 Nuclear cap-binding protein subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A5	732	Total	C	N	O	0	0
			3723	2259	732	732		

- Molecule 2 is a protein called U6 snRNA-associated Sm-like protein LSm7.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	A2	79	Total	C	N	O	0	0
			393	235	79	79		

- Molecule 3 is a protein called Splicing factor 3B subunit 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	z	108	Total	C	N	O	0	0
			544	328	108	108		

- Molecule 4 is a protein called Splicing factor 3A subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	F	49	Total	C	N	O	0	0
			242	144	49	49		

- Molecule 5 is a protein called U5 small nuclear ribonucleoprotein 40 kDa protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	D	302	Total	C	N	O	0	0
			1506	902	302	302		

- Molecule 6 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	W	162	Total	C	N	O	0	0
			816	492	162	162		

- Molecule 7 is a protein called U2 small nuclear ribonucleoprotein B”.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	B	169	Total	C	N	O	0	0
			851	513	169	169		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
8	s	1722	Total	C	N	O	0	0
			8688	5244	1722	1722		

- Molecule 9 is a protein called Protein BUD31 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	Q	138	Total	C	N	O	0	0
			695	419	138	138		

- Molecule 10 is a protein called Nuclear cap-binding protein subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	A1	148	Total	C	N	O	0	0
			724	428	148	148		

- Molecule 11 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	5	114	Total	C	N	O	P	0	0
			2397	1074	399	810	114		

- Molecule 12 is a protein called Cell division cycle 5-like protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	L	103	Total	C	N	O	0	0
			517	311	103	103		

- Molecule 13 is a protein called Spliceosome-associated protein CWC15 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	R	9	Total	C	N	O	0	0
			45	27	9	9		

- Molecule 14 is a protein called U6 snRNA-associated Sm-like protein LSm2.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	V	90	Total	C	N	O	0	0
			453	273	90	90		

- Molecule 15 is a protein called U6 snRNA-associated Sm-like protein LSm3.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	9	73	Total	C	N	O	0	0
			369	223	73	73		

- Molecule 16 is a protein called U6 snRNA-associated Sm-like protein LSm4.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	C	80	Total	C	N	O	0	0
			404	244	80	80		

- Molecule 17 is a protein called U6 snRNA-associated Sm-like protein LSm5.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	H	76	Total	C	N	O	0	0
			380	228	76	76		

- Molecule 18 is a protein called U6 snRNA-associated Sm-like protein LSm6.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	J	69	Total	C	N	O	0	0
			342	204	69	69		

- Molecule 19 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	2	145	Total	C	N	O	P	0	0
			3077	1374	533	1025	145		

- Molecule 20 is a protein called U6 snRNA-associated Sm-like protein LSm8.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	A3	62	Total	C	N	O	0	0
			304	180	62	62		

- Molecule 21 is a protein called Microfibrillar-associated protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	K	123	Total	C	N	O	0	0
			614	368	123	123		

- Molecule 22 is a protein called PHD finger-like domain-containing protein 5A.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	y	100	Total	C	N	O	0	0
			498	298	100	100		

- Molecule 23 is a protein called Pleiotropic regulator 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	G	320	Total	C	N	O	0	0
			1604	964	320	320		

- Molecule 24 is a RNA chain called MINX M3 pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Z	47	Total	C	N	O	P	0	0
			998	447	177	327	47		

- Molecule 25 is a protein called Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	A	2174	Total	C	N	O	0	0
			11024	6676	2174	2174		

- Molecule 26 is a protein called Pre-mRNA-splicing factor 38A.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	I	176	Total	C	N	O	0	0
			883	531	176	176		

- Molecule 27 is a protein called Pre-mRNA-splicing factor RBM22.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	P	162	Total	C	N	O	0	0
			825	501	162	162		

- Molecule 28 is a protein called Splicing factor 3A subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	p	60	Total	C	N	O	0	0
			301	181	60	60		

- Molecule 29 is a protein called Splicing factor 3A subunit 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	4	421	Total	C	N	O	0	0
			2110	1268	421	421		

- Molecule 30 is a protein called Transcription elongation regulator 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	A4	405	Total	C	N	O	0	0
			2034	1224	405	405		

- Molecule 31 is a protein called Splicing factor 3B subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	u	836	Total	C	N	O	0	0
			4207	2535	836	836		

- Molecule 32 is a protein called Splicing factor 3B subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	T	183	Total	C	N	O	0	0
			942	576	183	183		

- Molecule 33 is a protein called Splicing factor 3B subunit 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	E	1177	Total	C	N	O	0	0
			5926	3572	1177	1177		

- Molecule 34 is a protein called Splicing factor 3B subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	w	78	Total	C	N	O	0	0
			391	235	78	78		

- Molecule 35 is a protein called Splicing factor 3B subunit 5.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	x	79	Total	C	N	O	0	0
			397	239	79	79		

- Molecule 36 is a protein called SNW domain-containing protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	v	119	Total	C	N	O	0	0
			605	367	119	119		

- Molecule 37 is a protein called Smad nuclear-interacting protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	0	150	Total	C	N	O	0	0
			761	461	150	150		

- Molecule 38 is a protein called Zinc finger matrin-type protein 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	N	56	Total	C	N	O	0	0
			277	165	56	56		

- Molecule 39 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	r	844	Total	C	N	O	0	0
			4265	2577	844	844		

- Molecule 40 is a protein called Serine/arginine repetitive matrix protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	Y	95	Total	C	N	O	0	0
			478	288	95	95		

- Molecule 41 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	6	78	Total	C	N	O	P	0	0
			1672	747	309	538	78		

- Molecule 42 is a protein called Serine/arginine-rich splicing factor 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	A6	74	Total	C	N	O	0	0
			368	220	74	74		

- Molecule 43 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	h	95	Total	C	N	O	0	0
			482	292	95	95		
43	a	78	Total	C	N	O	0	0
			393	237	78	78		

- Molecule 44 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	i	72	Total	C	N	O	0	0
			359	215	72	72		
44	b	73	Total	C	N	O	0	0
			364	218	73	73		

- Molecule 45 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	m	82	Total	C	N	O	0	0
			413	249	82	82		
45	f	64	Total	C	N	O	0	0
			319	191	64	64		

- Molecule 46 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	l	83	Total	C	N	O	0	0
			415	249	83	83		
46	e	78	Total	C	N	O	0	0
			390	234	78	78		

- Molecule 47 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms				AltConf	Trace
47	k	73	Total	C	N	O	0	0
			364	218	73	73		
47	d	69	Total	C	N	O	0	0
			344	206	69	69		

- Molecule 48 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	j	81	Total	C	N	O	0	0
			403	241	81	81		
48	c	78	Total	C	N	O	0	0
			388	232	78	78		

- Molecule 49 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms				AltConf	Trace
49	n	80	Total	C	N	O	0	0
			402	242	80	80		
49	g	93	Total	C	N	O	0	0
			469	283	93	93		

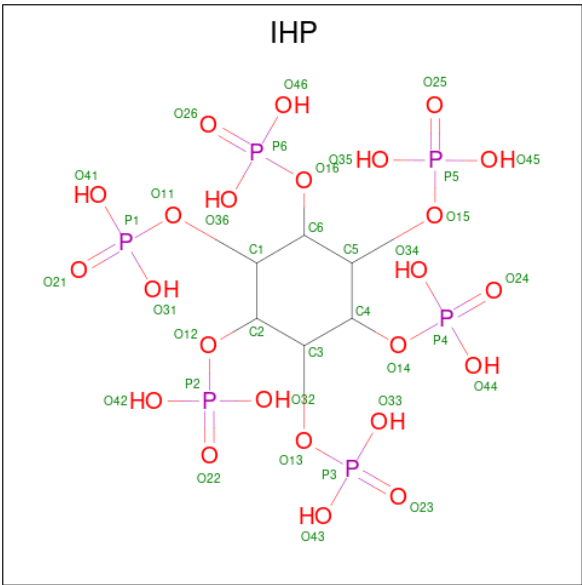
- Molecule 50 is a protein called Ubiquitin-like protein 5.

Mol	Chain	Residues	Atoms				AltConf	Trace
50	q	73	Total	C	N	O	0	0
			360	214	73	73		

- Molecule 51 is a protein called WW domain-binding protein 11.

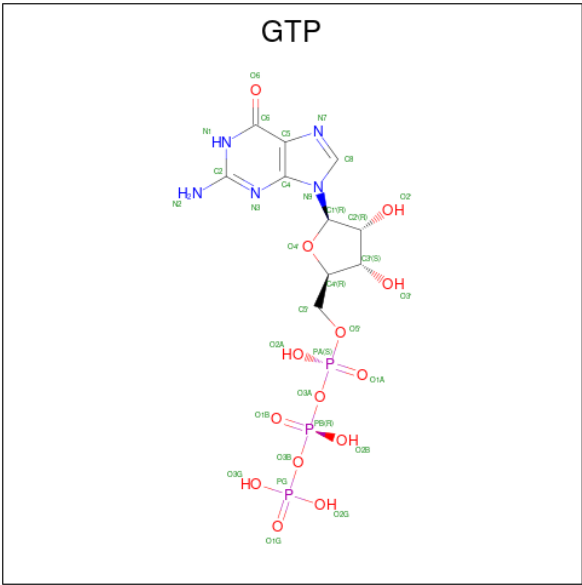
Mol	Chain	Residues	Atoms				AltConf	Trace
51	X	36	Total	C	N	O	0	0
			182	110	36	36		

- Molecule 52 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: $C_6H_{18}O_{24}P_6$).



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

- Molecule 53 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

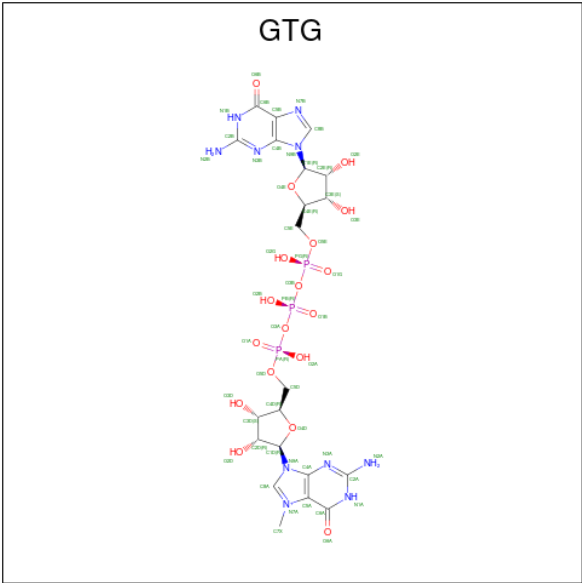


Mol	Chain	Residues	Atoms					AltConf
53	r	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 54 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
54	r	1	Total	Mg	0
			1	1	

- Molecule 55 is 7-METHYL-GUANOSINE-5'-TRIPHOSPHATE-5'-GUANOSINE (CCD ID: GTG) (formula: C₂₁H₃₀N₁₀O₁₈P₃).

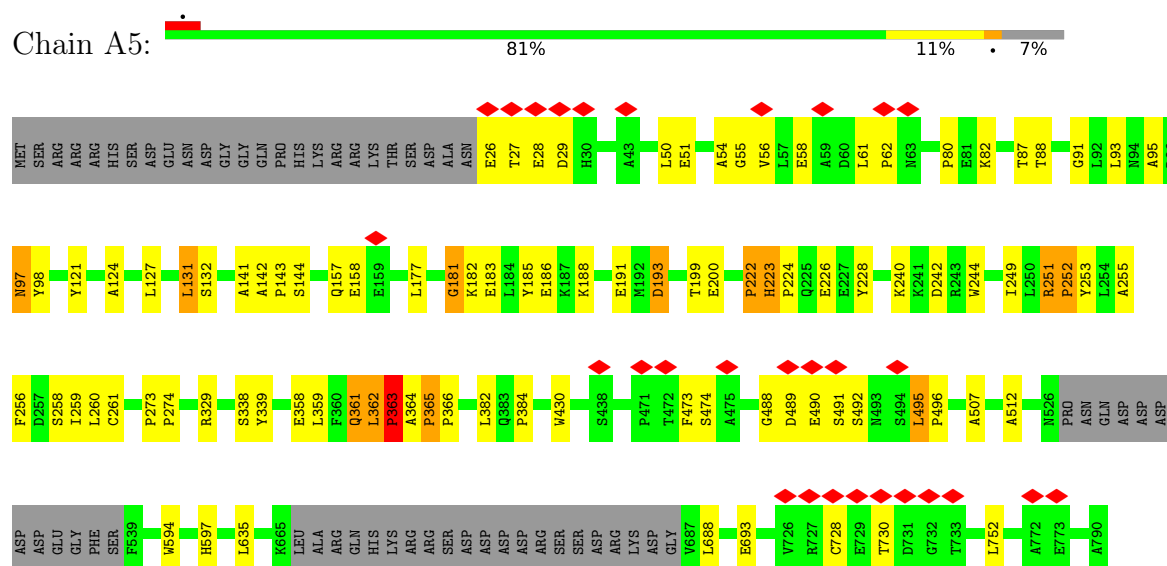


Mol	Chain	Residues	Atoms					AltConf
55	A6	1	Total	C	N	O	P	0
			52	21	10	18	3	

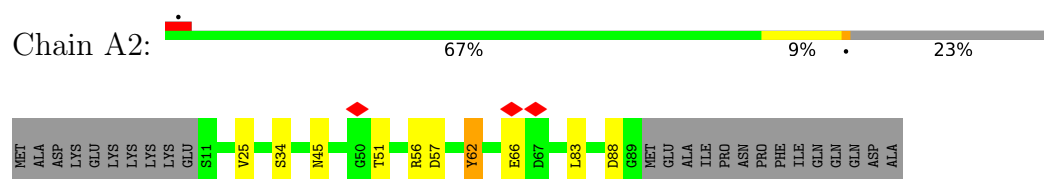
3 Residue-property plots

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

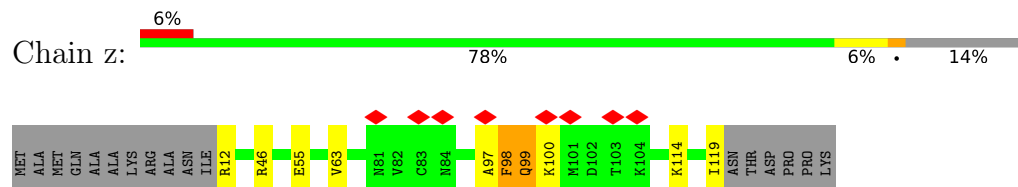
- Molecule 1: Nuclear cap-binding protein subunit 1



- Molecule 2: U6 snRNA-associated Sm-like protein LSm7

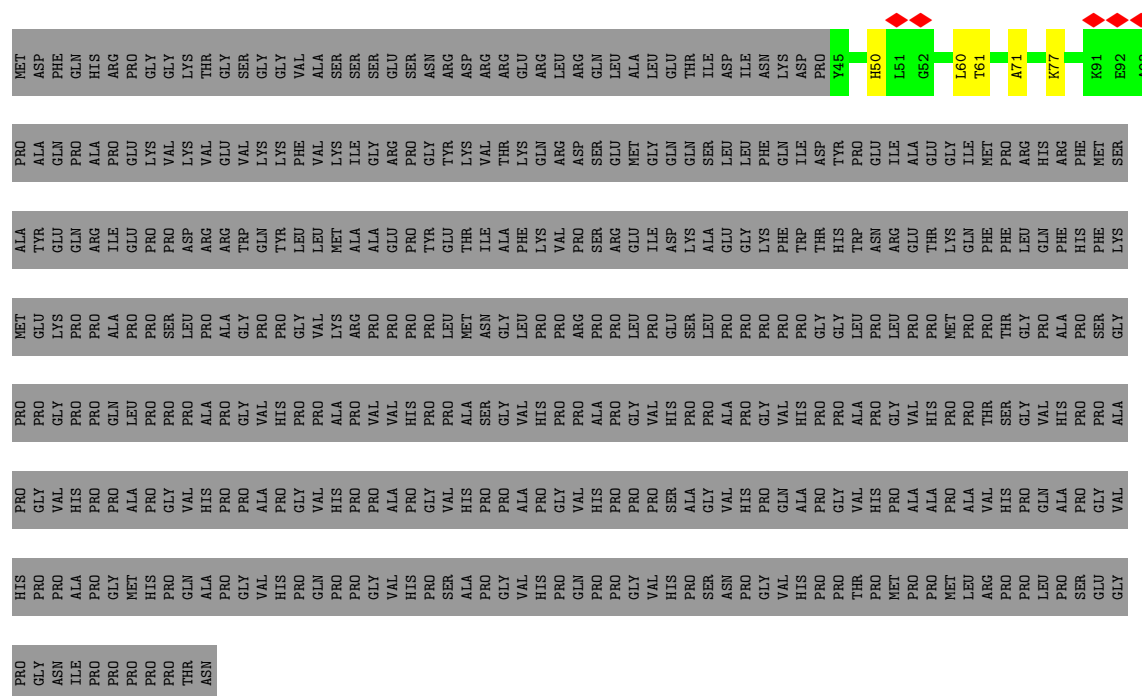


- Molecule 3: Splicing factor 3B subunit 6

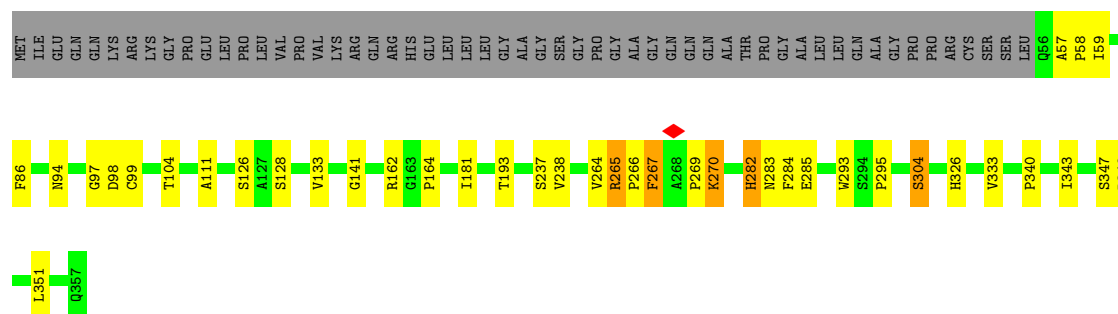


- Molecule 4: Splicing factor 3A subunit 2

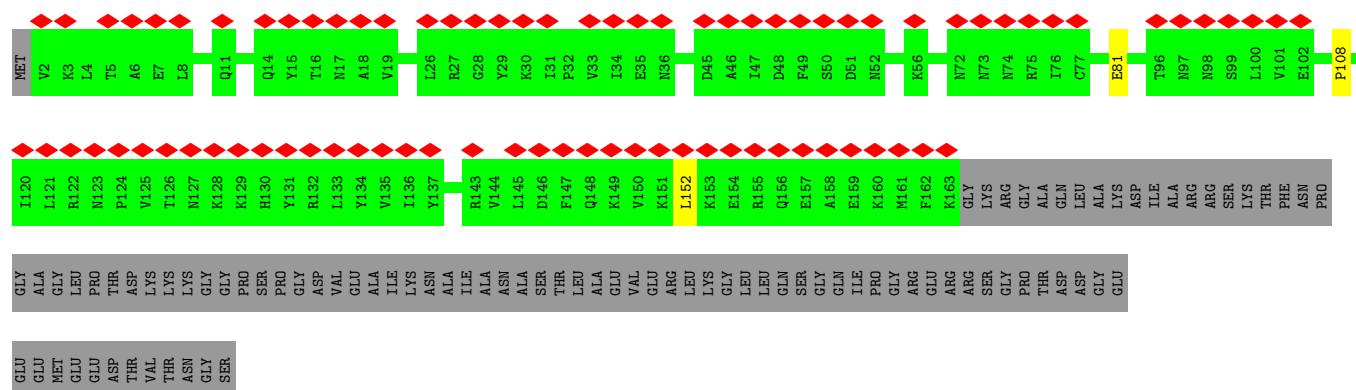




- Molecule 5: U5 small nuclear ribonucleoprotein 40 kDa protein



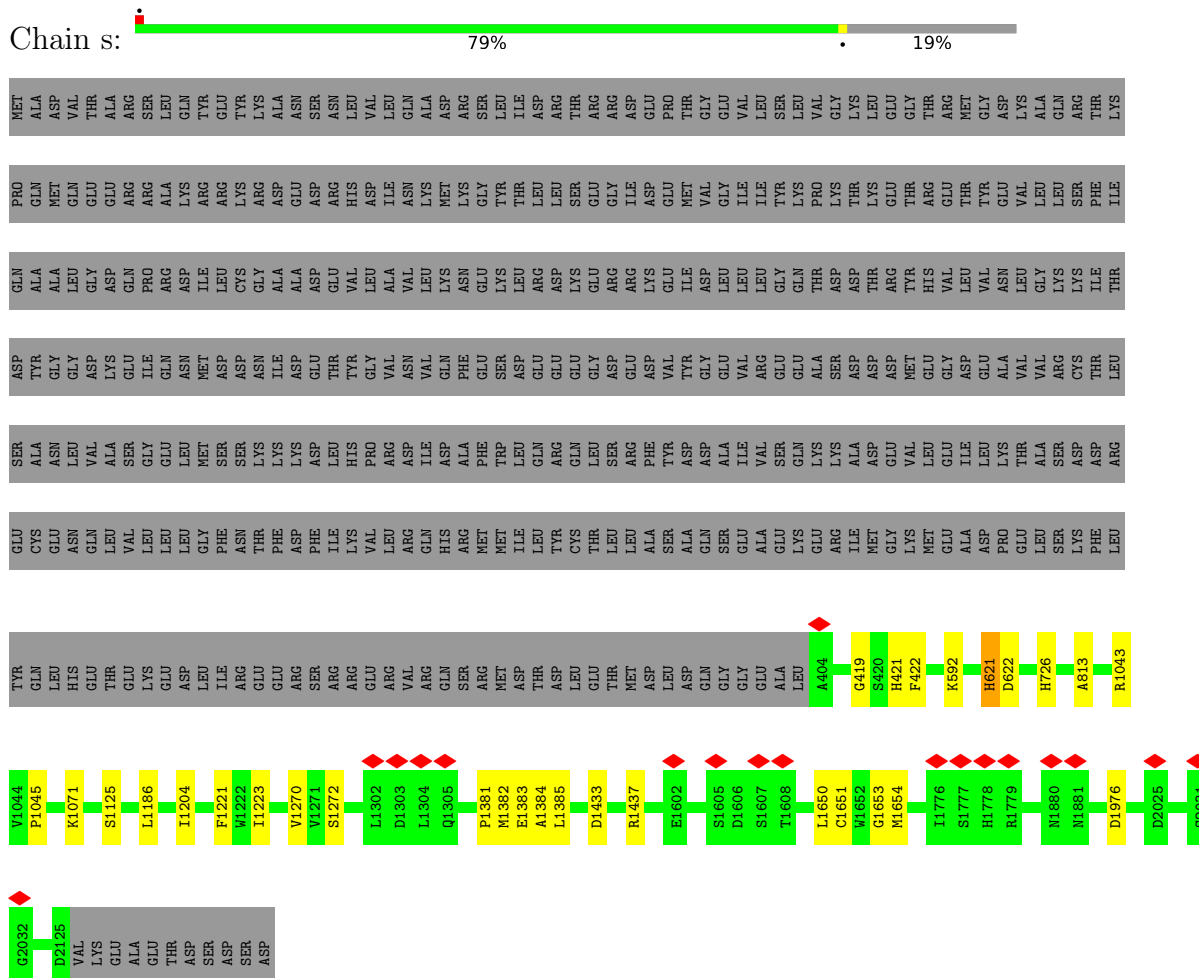
- Molecule 6: U2 small nuclear ribonucleoprotein A'



Chain B:



Chain s:

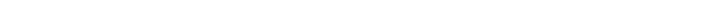


- Molecule 9: Protein BUD31 homolog

[illegible]

- Chain A1:  85% 9% 5%

MET	SER	GLY	GLY	LEU	L6	K7	A8	L9	Q19	Y20	Q23	N29	C40	S48	C81	R99	G126	R127	G128	G132	A153	GLN	ASN	GLN
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- Chain 5:  43% 47% 9%

A83	A88	U89	U90	U91	U92	U93	U94	G95	A96	G97	C98	C99	U100	U101	G107	C108	C109	A110	A111	A116																													
A	U	A3	C4	U5	C6	U7	C8	G9	U10	U11	U12	C13	U14	C15	A19	G20	A21	U22	C23	G24	C25	A26	U27	A28	U35	C36	G37	C38	C39	U40	A44	C45	A48	G57	A61	G65	A66	C68	A69	U72	C73	U74	G75	A76	G77	U78	C79	U80	U81

- Chain L: 12% 87%

MET	PRO	ARG	ILE	MET	ILE	LYS	G8	G9	V10	T14	Y51	L77	A86	P87	R110	ASP	ASN	GLU	GLU	GLU	THR	THR	ASP	ASP	PRO	ARG	LYS	LYS	LEU	PRO	PRO	ASN	ASN	PRO	PRO	GLU	THR	LYS	PRO	ALA	ARG	PRO	PRO	ASP	ILE	ASP	ASP	ASP	ASP	ASP	GLU
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GLU	LEU	MET	SER	GLY	ALA	ARG	ARG	LEU	ARG	ALA	ASN	THR	GLN	GLY	LYS	LYS	ALA	LYS	ARG	LYS	ALA	ARG	GLU	GLU	LYS	LEU	GLU	GLU	ALA	ALA	ARG	ARG	GLN	GLN	LYS	GLY	ILE	GLU	ILE	GLN	LYS	LYS	ARG	LYS	GLY	VAL
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Tyr.	Asn	Ala	Glu	Ile	Pro	Phe	Lys	Lys	Pro	Leu	Ala	Gly	Phe	Tyr	Asp	Thr	Ser	Glu	Glu	Asn	Tyr	Gln	Ala	Leu	Asp	Asp	Phe	Arg	Lys	Leu	Arg	Gln	Gln	Asp	Asp	Leu	Gly	Leu	Glu	Arg	Ser	Lys	Gly	Leu	Glu	Gly	Asp	Asp	Lys	Lys	Lys	Asp	Gln	Lys	Lys
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LYS	LYS	GLU	ASP	LEU	PRO	SER	ALA	LEU	GLN	THR	SER	GLY	VAL	SER	SER	GLU	PHE	LEU	VAL	LYS	LYS	ARG	SER	SER	LYS	LEU	VAL	LEU	PRO	ALA	PRO	GLN	ILE	SER	ASP	GLU	GLU	LEU	GLN	GLU	VAL	VAL	VAL	LYS	GLY	GLY	GLN	ALA	ALA	SER	GLU	ILE	ALA	ALA	ARG	GLN	THR	ALA	GLU	GLU	SER	GLY
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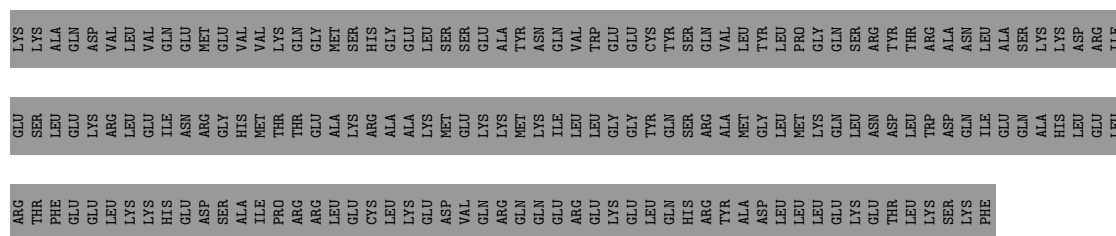
THR	ASN	SER	SER	ALA	SER	SER	THR	LEU	LEU	GLY	TYR	ASN	ASN	VAL	THR	VAL	ASN	ASN	ARG	ARG	PRO	PRO	ALA	ALA	GLN	ASP	ASP	ILE	LEU	LEU	GLN	GLU	ALA	ALA	GLN	ASN	ASN	LEU	MET	ALA	LEU	LEU	THR	THR	THR	VAL	VAL	ASP	THR	PRO	PRO	LEU	LYS	GLY	GLY	LEU	LEU	ASN	HIS
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SER	ASP	PHE	SER	GLY	VAL	THR	PRO	THR	GLN	ARG	GLN	VAL	GLN	VAL	VAL	GLN	THR	PRO	ASN	THR	THR	PRO	PHE	ARG	THR	PRO	PRO	ASN	GLY	ALA	GLU	GLY	LEU	THR	THR	THR	PRO	PRO	LYS	PRO	VAL	VAL	ILE	ASN	THR	SER	THR	PRO	PRO	GLY	GLY	ARG	THR	THR	PRO	LEU	LEU	ARG	ASP	LYS	LEU	LEU
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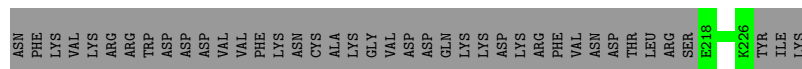
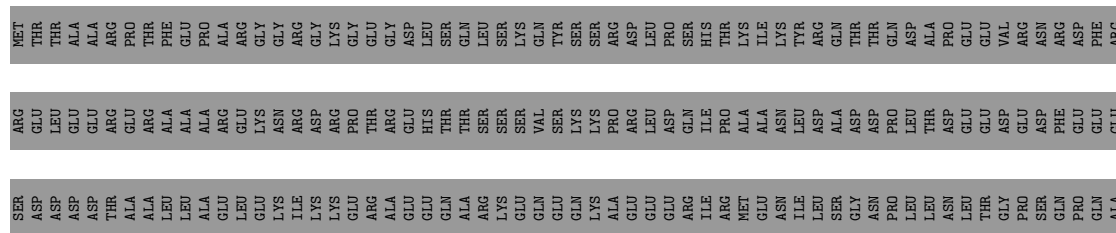
ILE	ASN	PRO	GLU	ASP	GLY	MET	ALA	ASP	TYR	SER	ASP	PRO	PRO	TYR	SER	VAL	LYS	GLN	MET	GLU	ARG	GLU	SER	ARG	GLU	GLU	HIS	LEU	ARG	LEU	GLY	LEU	LEU	GLY	LEU	PRO	ALA	ASN	LYS	PRO	PRO	ASP	PHE	GLU	GLU	ILE	VAL	LEU	PRO	LEU	GLU	GLU	LEU	GLU	GLU	ARG	GLU	ILE	GLU	ASP
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[illegible]

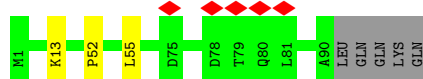
LYS SER GLU GLU LEU LEU ILE LYS LYS LYS MET MET ILE THR MET MET HIS HIS ASP LEU LEU LEU TYR TYR PRO PRO TYR TYR GLU PRO SER SER GLY GLY ASN LYS LYS GLY GLY THR THR VAL VAL GLY PHE GLY GLY THR THR ASN ASN SER SER GLU GLU ILE THR THR TYR TYR LEU LEU GLU LYS PHE SER LYS LYS GLU GLU



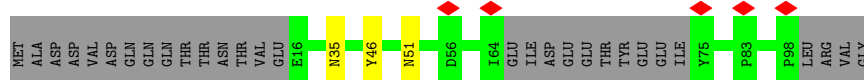
- Molecule 13: Spliceosome-associated protein CWC15 homolog



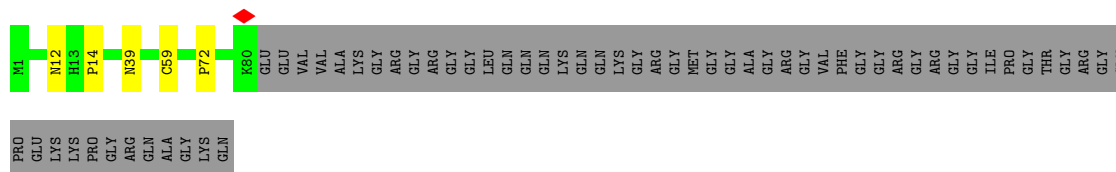
- Molecule 14: U6 snRNA-associated Sm-like protein LSm2



- Molecule 15: U6 snRNA-associated Sm-like protein LSm3



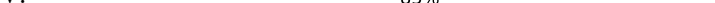
- Molecule 16: U6 snRNA-associated Sm-like protein LSm4

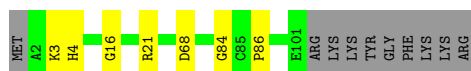


- Molecule 17: U6 snRNA-associated Sm-like protein LSm5



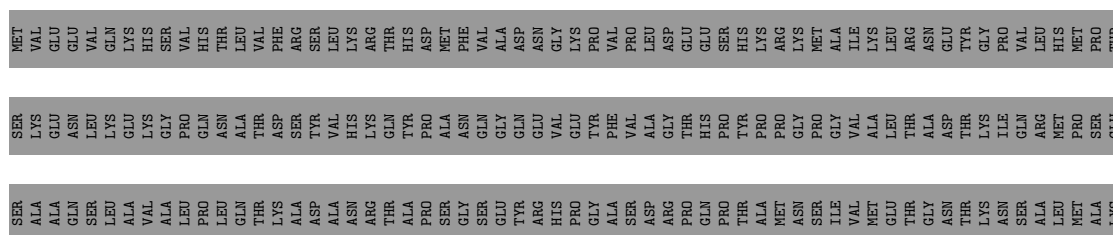
- Molecule 22: PHD finger-like domain-containing protein 5A

Chain y:  85% 6% 9%



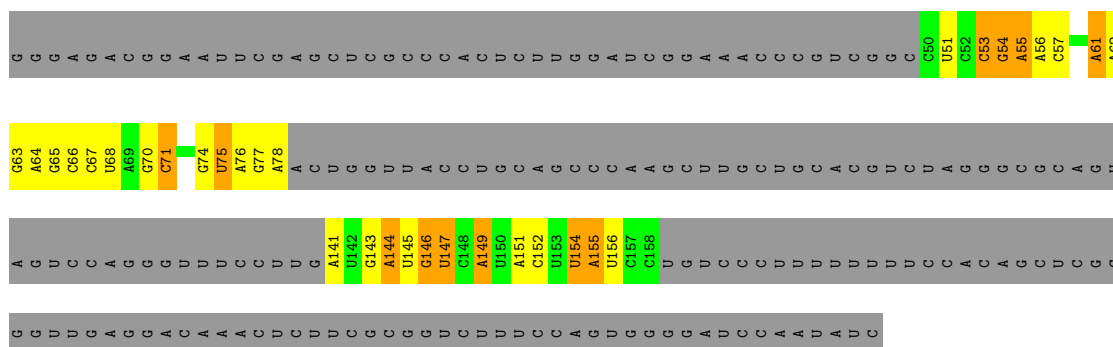
- Molecule 23: Pleiotropic regulator 1

Chain G: 60% .. 38%

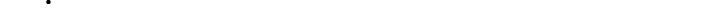


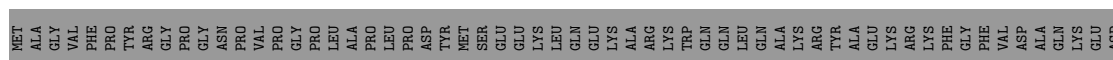
- Molecule 24: MINX M3 pre-mRNA

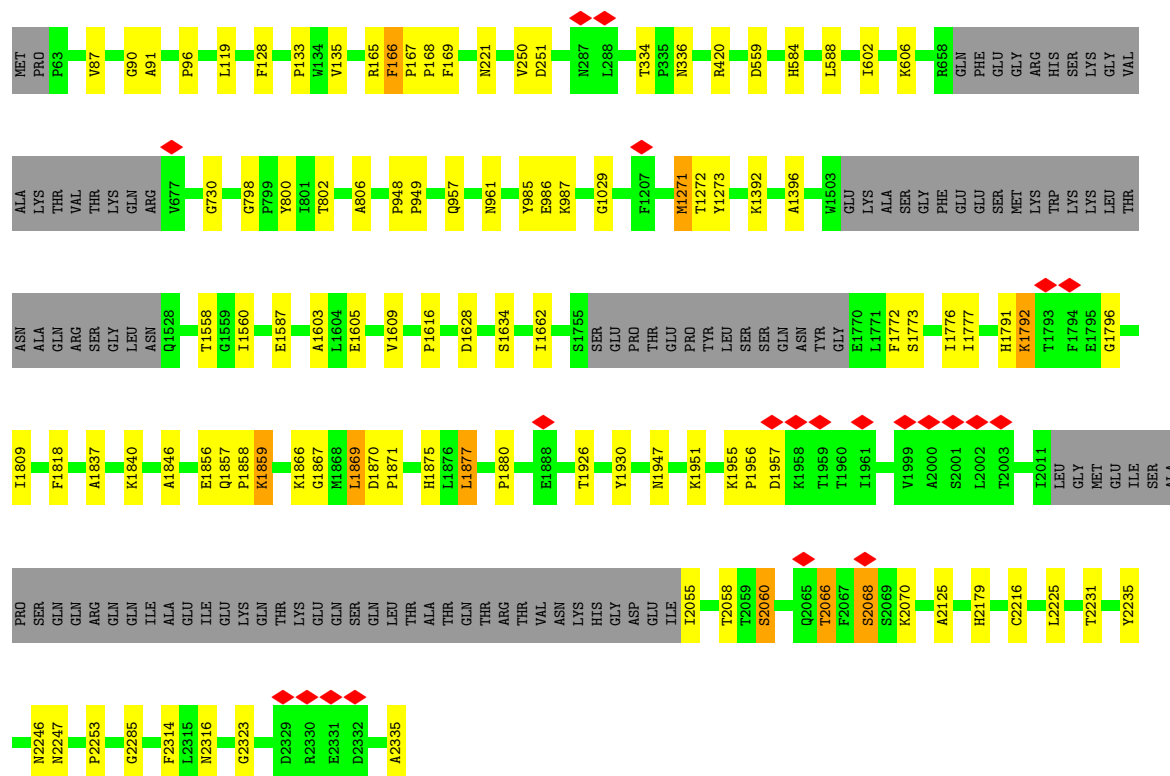
Chain Z:  6% 9% 5% 80%



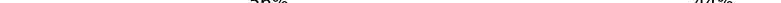
- Molecule 25: Pre-mRNA-processing-splicing factor 8

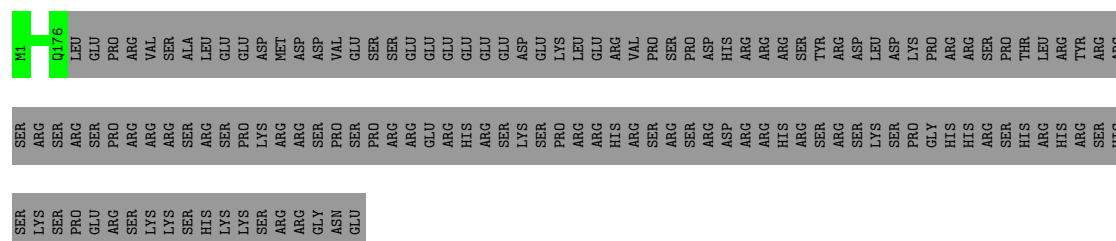
Chain A:  89% 7%



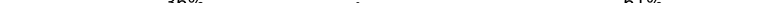


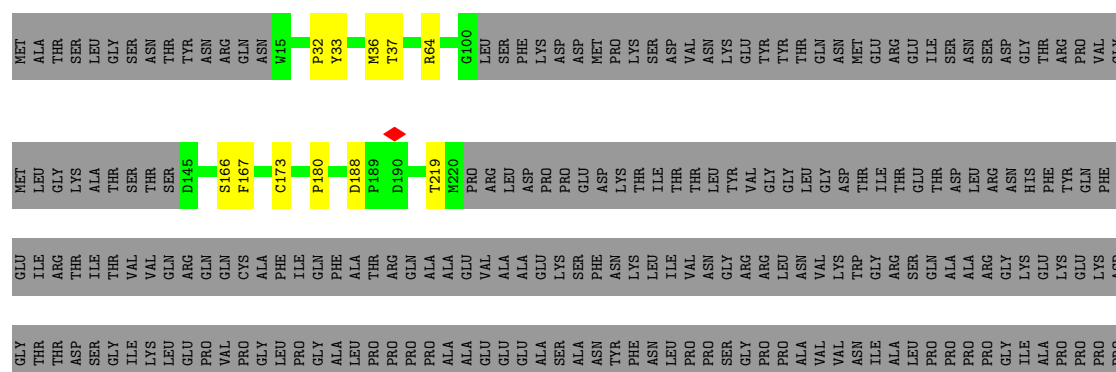
- Molecule 26: Pre-mRNA-splicing factor 38A

Chain I:  56% 44%

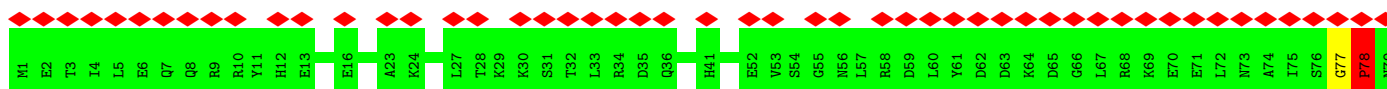
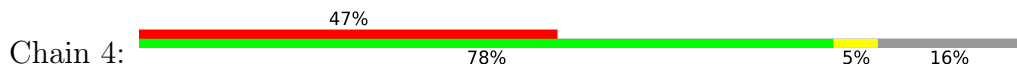


- Molecule 27: Pre-mRNA-splicing factor RBM22

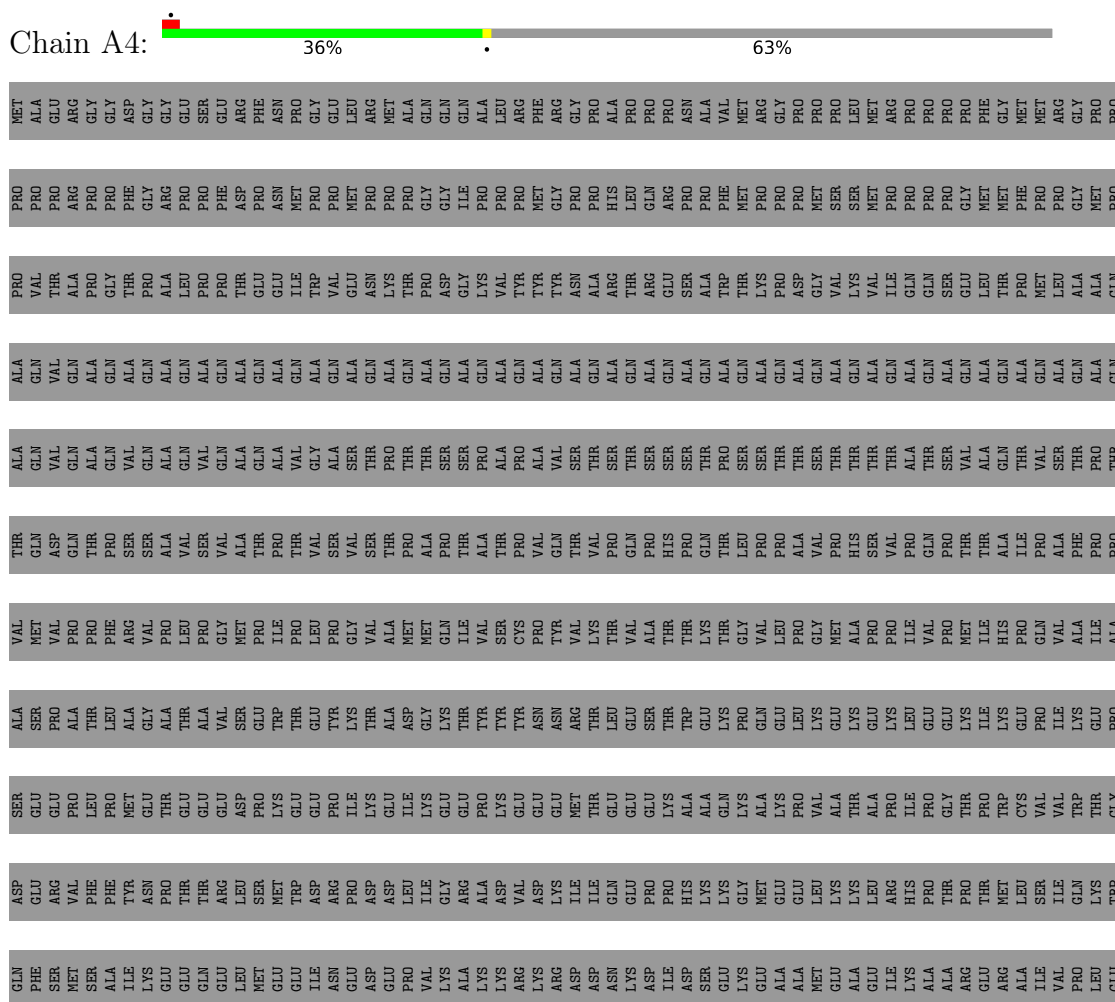
Chain P:  36% 1% 61%



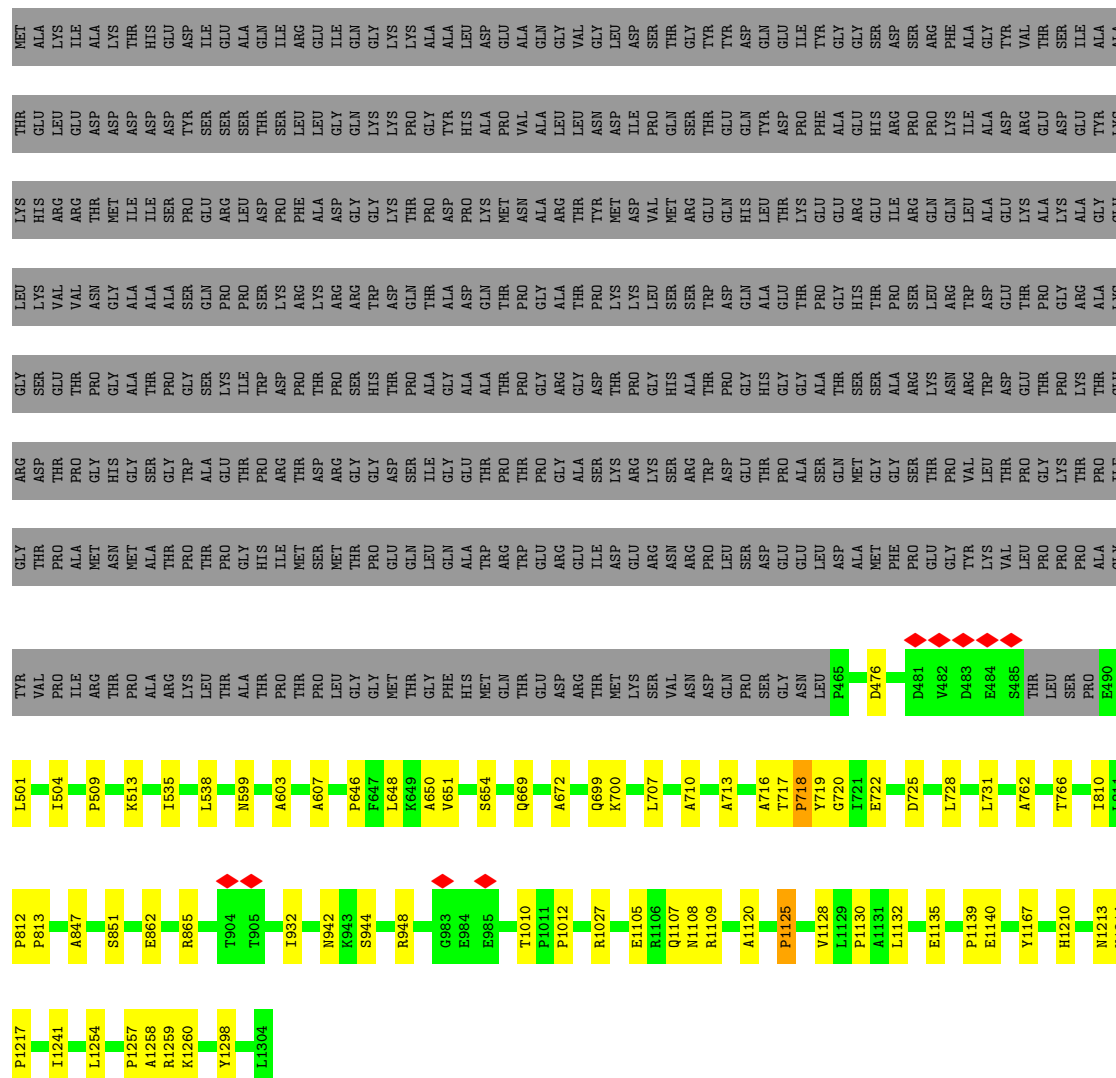
Chain p: 7% 7% 92%



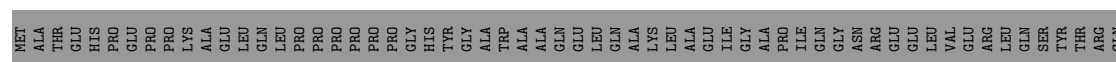
- Molecule 30: Transcription elongation regulator 1



- Molecule 31: Splicing factor 3B subunit 1

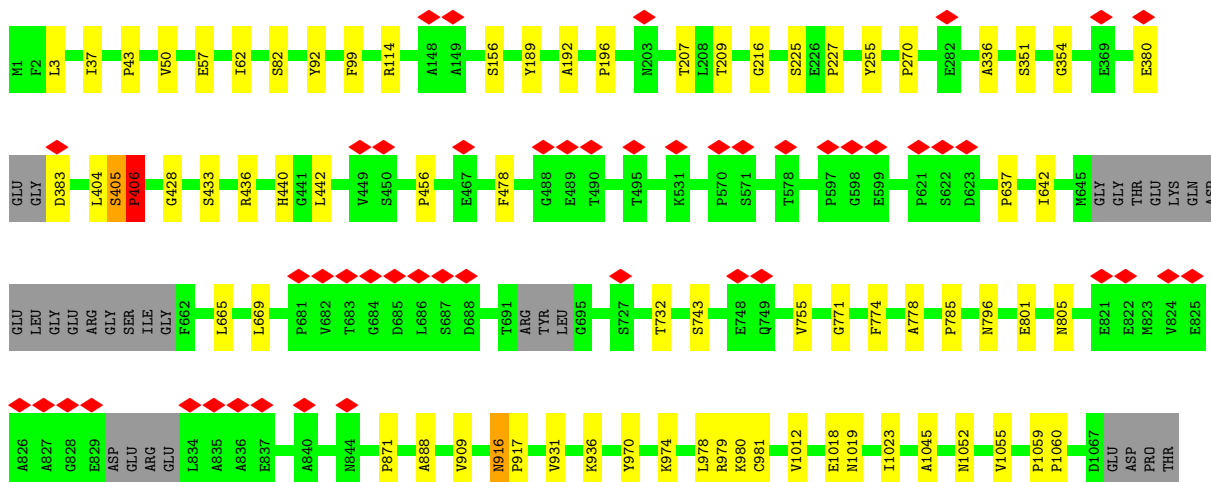
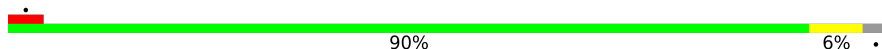


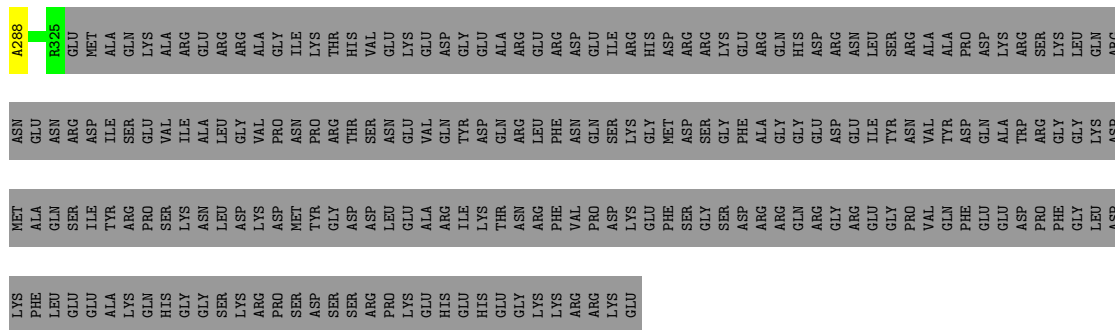
- Molecule 32: Splicing factor 3B subunit 2



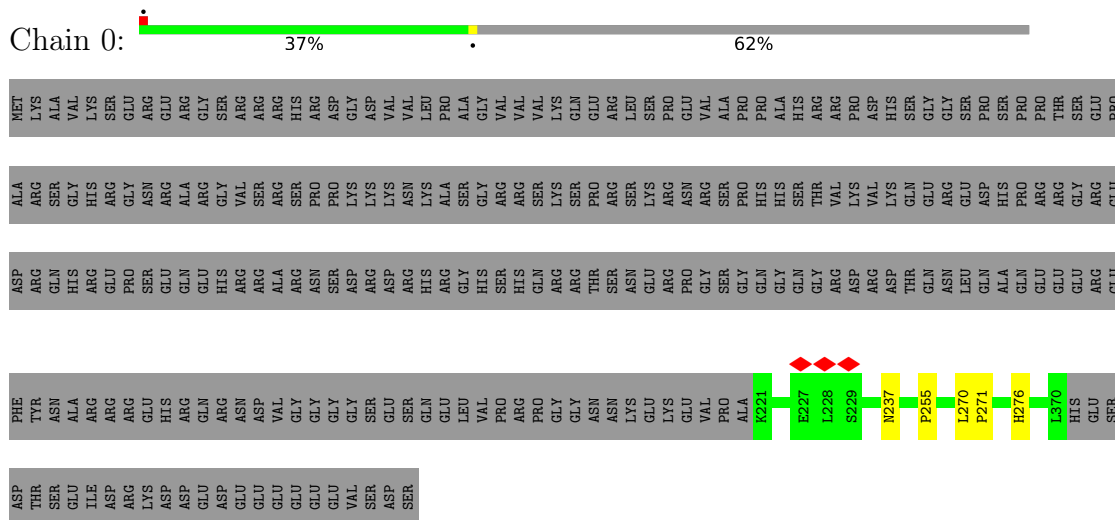
- Molecule 33: Splicing factor 3B subunit 3

Chain E:

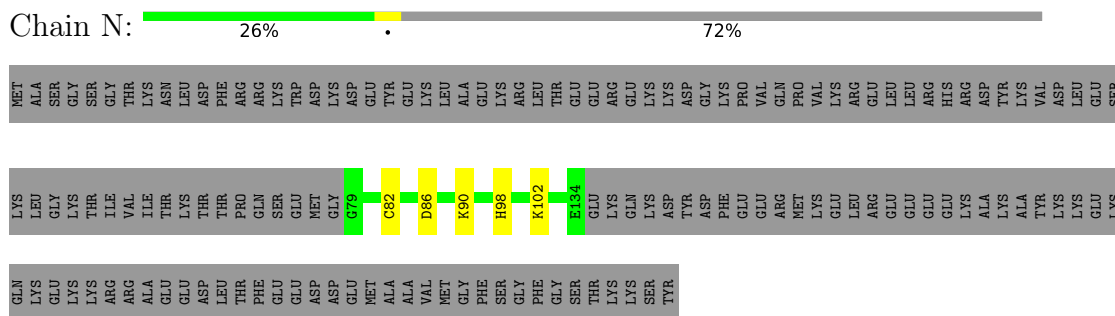




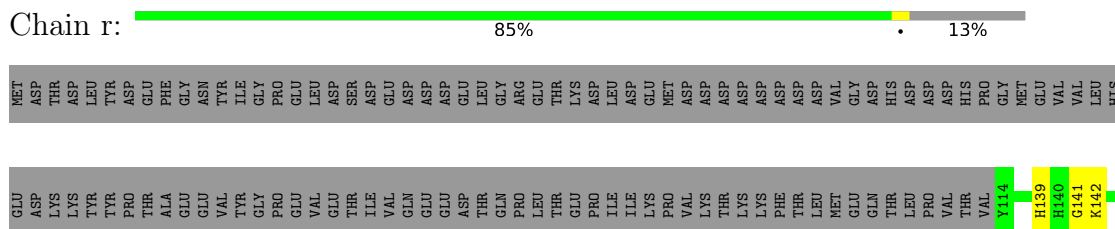
- Molecule 37: Smad nuclear-interacting protein 1

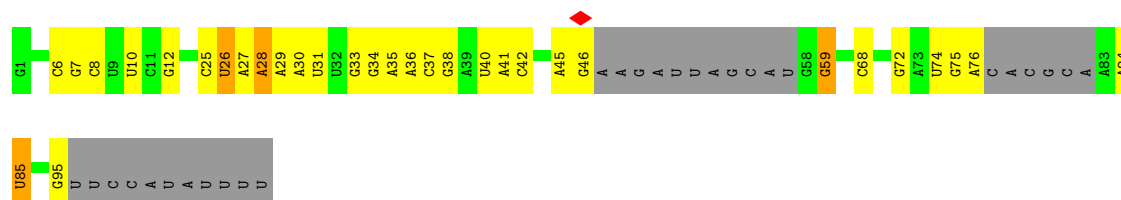


- Molecule 38: Zinc finger matrin-type protein 2



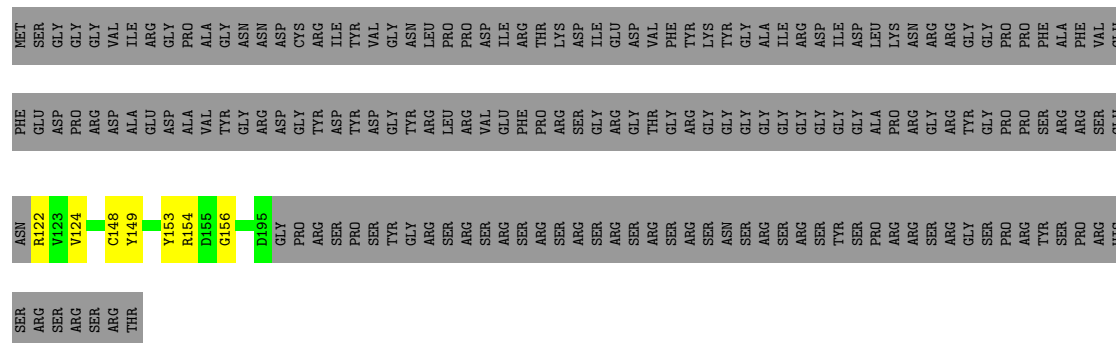
- Molecule 39: 116 kDa U5 small nuclear ribonucleoprotein component





- Molecule 42: Serine/arginine-rich splicing factor 1

Chain A6: 27% 70%



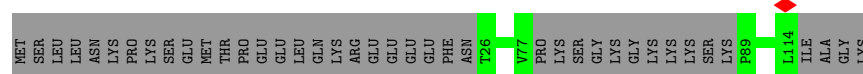
- Molecule 43: Small nuclear ribonucleoprotein Sm D2

Chain h: 9% 77% 19%



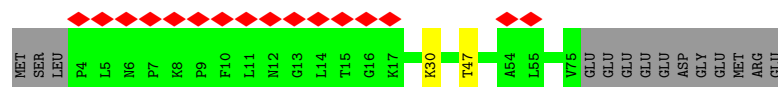
- Molecule 43: Small nuclear ribonucleoprotein Sm D2

Chain a: 66% 34%



- Molecule 44: Small nuclear ribonucleoprotein F

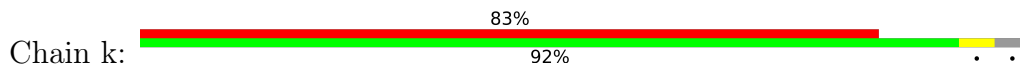
Chain i: 19% 81% 16%



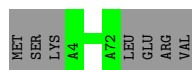
- Molecule 44: Small nuclear ribonucleoprotein F

Chain b: 81% 15%

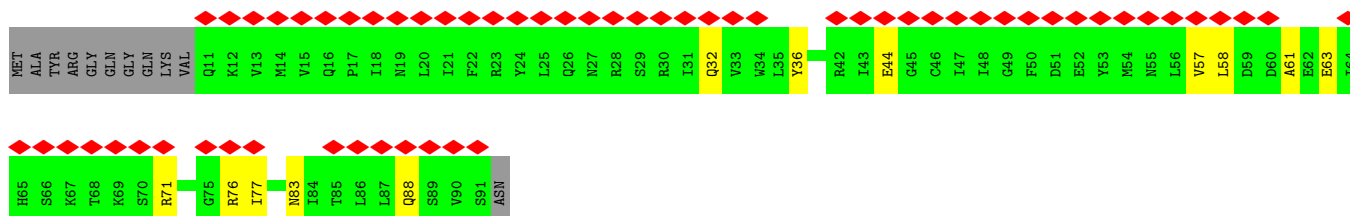
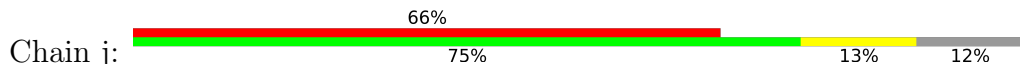
- Molecule 47: Small nuclear ribonucleoprotein G



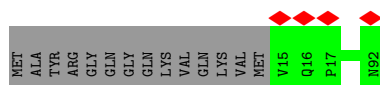
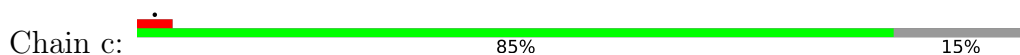
- Molecule 47: Small nuclear ribonucleoprotein G



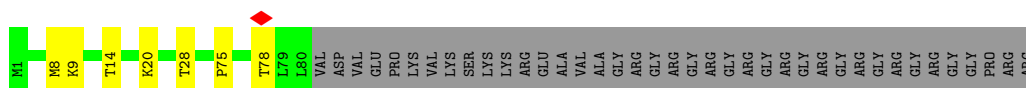
- Molecule 48: Small nuclear ribonucleoprotein E



- Molecule 48: Small nuclear ribonucleoprotein E



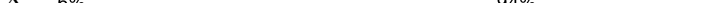
- Molecule 49: Small nuclear ribonucleoprotein Sm D1



- Molecule 49: Small nuclear ribonucleoprotein Sm D1

MET	K2	T16	L19	H26	S35	MET	N37	N40	R59	NG3	NG4	I65	V83	E84	P85	K86	K90	K91	V95	ALA	GLY	ARG	GLY	GLY	ARG	GLY	GLY	ARG	ARG	GLY	ARG	ARG	GLY	ARG	GLY	GLY	PRO	ARG	ARG
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- Chain q: 97%

- Chain X:  6% 94%

[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	84539	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	2.25	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.055	Depositor
Minimum map value	-0.015	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0095	Depositor
Map size ($\text{\AA}$)	445.44, 445.44, 445.44	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.16, 1.16, 1.16	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GTG, 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	A5	0.71	4/3759 (0.1%)	1.29	26/5280 (0.5%)
2	A2	0.96	0/395	1.24	1/549 (0.2%)
3	z	0.35	0/548	0.62	0/766
4	F	0.45	0/241	0.77	0/334
5	D	1.42	3/1515 (0.2%)	1.52	19/2113 (0.9%)
6	W	0.28	0/821	0.69	0/1149
7	B	1.05	0/857	1.23	6/1196 (0.5%)
8	s	0.20	0/8766	0.57	2/12286 (0.0%)
9	Q	0.21	0/700	0.58	0/979
10	A1	0.50	0/723	1.30	7/1001 (0.7%)
11	5	0.19	0/2672	0.34	0/4154
12	L	0.17	0/519	0.61	0/725
13	R	0.07	0/44	0.33	0/60
14	V	0.78	0/455	1.23	0/636
15	9	0.80	0/371	1.28	0/517
16	C	0.77	0/407	1.29	0/569
17	H	0.83	0/382	1.34	1/532 (0.2%)
18	J	0.94	0/343	1.40	4/475 (0.8%)
19	2	0.36	6/3430 (0.2%)	0.65	11/5329 (0.2%)
20	A3	0.87	0/302	1.18	2/416 (0.5%)
21	K	0.12	0/615	0.34	0/858
22	y	0.16	0/501	0.53	0/697
23	G	0.31	0/1616	0.50	2/2258 (0.1%)
24	Z	0.48	6/1114 (0.5%)	0.25	0/1730
25	A	0.27	1/11142 (0.0%)	0.56	1/15633 (0.0%)
26	I	0.20	0/888	0.49	0/1241
27	P	0.63	1/835 (0.1%)	1.18	4/1170 (0.3%)
28	p	0.93	0/301	1.70	2/420 (0.5%)
29	4	0.86	0/2119	1.58	11/2960 (0.4%)
30	A4	0.51	0/2037	0.78	2/2850 (0.1%)
31	u	0.33	0/4241	0.70	9/5935 (0.2%)
32	T	0.84	4/957 (0.4%)	1.10	6/1341 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	E	0.22	0/5980	0.47	2/8363 (0.0%)
34	w	0.99	0/394	1.14	1/549 (0.2%)
35	x	0.64	0/399	0.75	0/557
36	v	0.23	0/607	0.52	0/847
37	0	0.18	0/770	0.51	0/1079
38	N	0.32	0/276	0.56	0/383
39	r	0.20	0/4313	0.48	0/6044
40	Y	0.33	0/481	0.58	0/672
41	6	0.12	0/1870	0.27	0/2909
42	A6	0.32	0/369	0.70	0/513
43	a	0.17	0/394	0.51	0/548
43	h	0.38	0/485	0.71	0/677
44	b	0.20	0/367	0.49	0/509
44	i	0.40	0/362	0.71	0/502
45	f	0.16	0/319	0.42	0/442
45	m	0.40	0/416	0.65	0/581
46	e	0.18	0/392	0.62	0/546
46	l	0.47	0/417	0.78	0/581
47	d	0.22	0/346	0.58	0/481
47	k	0.45	0/366	0.72	0/509
48	c	0.17	0/388	0.51	0/540
48	j	0.42	0/403	0.76	0/561
49	g	0.18	0/471	0.48	0/657
49	n	0.39	0/404	0.66	0/564
50	q	0.23	0/359	0.55	0/498
51	X	0.12	0/182	0.36	0/254
All	All	0.46	25/75146 (0.0%)	0.77	119/106525 (0.1%)

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A5	252	PRO	N-CA	20.75	1.70	1.47
32	T	605	LYS	C-N	14.87	1.50	1.33
27	P	188	ASP	C-N	13.72	1.50	1.33
1	A5	251	ARG	C-N	13.51	1.45	1.33
1	A5	223	HIS	C-N	12.81	1.50	1.33

The worst 5 of 119 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	P	188	ASP	CA-C-N	18.47	138.40	119.56
27	P	188	ASP	C-N-CA	18.47	138.40	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A5	223	HIS	CA-C-N	18.38	138.69	119.76
1	A5	223	HIS	C-N-CA	18.38	138.69	119.76
32	T	605	LYS	CA-C-N	17.34	140.09	119.98

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A5	3723	0	1806	75	0
2	A2	393	0	183	4	0
3	z	544	0	264	9	0
4	F	242	0	118	25	0
5	D	1506	0	737	29	0
6	W	816	0	386	2	0
7	B	851	0	423	7	0
8	s	8688	0	4220	19	0
9	Q	695	0	327	2	0
10	A1	724	0	335	13	0
11	5	2397	0	1216	65	0
12	L	517	0	257	5	0
13	R	45	0	17	0	0
14	V	453	0	212	1	0
15	9	369	0	174	1	0
16	C	404	0	189	2	0
17	H	380	0	172	6	0
18	J	342	0	164	11	0
19	2	3077	0	1559	146	0
20	A3	304	0	137	7	0
21	K	614	0	284	9	0
22	y	498	0	241	10	0
23	G	1604	0	795	22	0
24	Z	998	0	504	54	0
25	A	11024	0	5384	80	0
26	I	883	0	414	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	P	825	0	409	25	0
28	p	301	0	134	0	0
29	4	2110	0	987	51	0
30	A4	2034	0	912	29	0
31	u	4207	0	2103	109	0
32	T	942	0	490	55	0
33	E	5926	0	2964	78	0
34	w	391	0	197	19	0
35	x	397	0	191	11	0
36	v	605	0	311	27	0
37	0	761	0	376	7	0
38	N	277	0	114	3	0
39	r	4265	0	2120	19	0
40	Y	478	0	226	25	0
41	6	1672	0	846	34	0
42	A6	368	0	175	23	0
43	a	393	0	176	0	0
43	h	482	0	220	6	0
44	b	364	0	181	2	0
44	i	359	0	179	1	0
45	f	319	0	144	6	0
45	m	413	0	193	7	0
46	e	390	0	188	3	0
46	l	415	0	198	21	0
47	d	344	0	168	0	0
47	k	364	0	176	12	0
48	c	388	0	167	0	0
48	j	403	0	173	6	0
49	g	469	0	214	9	0
49	n	402	0	184	24	0
50	q	360	0	159	2	0
51	X	182	0	85	0	0
52	A	36	0	6	0	0
53	r	32	0	12	13	0
54	r	1	0	0	0	0
55	A6	52	0	26	11	0
All	All	73818	0	35922	850	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 850 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:91:ALA:HB2	36:v:207:MET:CA	1.21	1.65
1:A5:258:SER:CB	30:A4:766:MET:HA	1.27	1.64
1:A5:258:SER:CB	30:A4:766:MET:CA	1.77	1.63
25:A:1772:PHE:CB	25:A:2246:ASN:CB	1.79	1.60
30:A4:731:ASP:CB	30:A4:759:ARG:CA	1.77	1.59

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	A5	726/790 (92%)	655 (90%)	61 (8%)	10 (1%)	9	40
2	A2	77/103 (75%)	71 (92%)	3 (4%)	3 (4%)	2	19
3	<i>z</i>	106/125 (85%)	92 (87%)	12 (11%)	2 (2%)	6	32
4	F	47/464 (10%)	46 (98%)	0	1 (2%)	5	30
5	D	300/357 (84%)	276 (92%)	17 (6%)	7 (2%)	5	28
6	W	160/255 (63%)	147 (92%)	13 (8%)	0	100	100
7	B	165/225 (73%)	158 (96%)	4 (2%)	3 (2%)	6	34
8	<i>s</i>	1720/2136 (80%)	1660 (96%)	58 (3%)	2 (0%)	48	83
9	Q	136/144 (94%)	114 (84%)	22 (16%)	0	100	100
10	A1	146/156 (94%)	137 (94%)	7 (5%)	2 (1%)	9	40
12	L	101/802 (13%)	97 (96%)	4 (4%)	0	100	100
13	R	7/229 (3%)	7 (100%)	0	0	100	100
14	V	88/95 (93%)	79 (90%)	7 (8%)	2 (2%)	5	28
15	9	69/102 (68%)	66 (96%)	2 (3%)	1 (1%)	9	40
16	C	78/139 (56%)	73 (94%)	4 (5%)	1 (1%)	9	42
17	H	74/91 (81%)	64 (86%)	8 (11%)	2 (3%)	4	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	J	67/80 (84%)	57 (85%)	9 (13%)	1 (2%)	8	40
20	A3	58/96 (60%)	53 (91%)	4 (7%)	1 (2%)	7	36
21	K	121/439 (28%)	98 (81%)	23 (19%)	0	100	100
22	y	98/110 (89%)	96 (98%)	2 (2%)	0	100	100
23	G	318/514 (62%)	292 (92%)	22 (7%)	4 (1%)	9	42
25	A	2164/2335 (93%)	1904 (88%)	239 (11%)	21 (1%)	12	49
26	I	174/312 (56%)	152 (87%)	22 (13%)	0	100	100
27	P	158/420 (38%)	128 (81%)	30 (19%)	0	100	100
28	p	58/793 (7%)	53 (91%)	3 (5%)	2 (3%)	3	21
29	4	415/501 (83%)	369 (89%)	35 (8%)	11 (3%)	4	25
30	A4	399/1098 (36%)	387 (97%)	10 (2%)	2 (0%)	24	63
31	u	832/1304 (64%)	728 (88%)	98 (12%)	6 (1%)	18	56
32	T	175/895 (20%)	159 (91%)	15 (9%)	1 (1%)	21	59
33	E	1165/1217 (96%)	1143 (98%)	19 (2%)	3 (0%)	36	72
34	w	76/424 (18%)	69 (91%)	6 (8%)	1 (1%)	9	42
35	x	77/86 (90%)	68 (88%)	8 (10%)	1 (1%)	9	42
36	v	111/536 (21%)	98 (88%)	13 (12%)	0	100	100
37	0	148/396 (37%)	146 (99%)	2 (1%)	0	100	100
38	N	54/199 (27%)	53 (98%)	1 (2%)	0	100	100
39	r	842/972 (87%)	781 (93%)	61 (7%)	0	100	100
40	Y	93/904 (10%)	90 (97%)	2 (2%)	1 (1%)	11	46
42	A6	72/248 (29%)	61 (85%)	10 (14%)	1 (1%)	9	40
43	a	74/118 (63%)	71 (96%)	3 (4%)	0	100	100
43	h	91/118 (77%)	86 (94%)	5 (6%)	0	100	100
44	b	71/86 (83%)	70 (99%)	1 (1%)	0	100	100
44	i	70/86 (81%)	69 (99%)	1 (1%)	0	100	100
45	f	60/240 (25%)	57 (95%)	3 (5%)	0	100	100
45	m	80/240 (33%)	74 (92%)	6 (8%)	0	100	100
46	e	76/126 (60%)	73 (96%)	3 (4%)	0	100	100
46	l	81/126 (64%)	76 (94%)	5 (6%)	0	100	100
47	d	67/76 (88%)	63 (94%)	4 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	k	71/76 (93%)	69 (97%)	2 (3%)	0	100	100
48	c	76/92 (83%)	70 (92%)	6 (8%)	0	100	100
48	j	79/92 (86%)	77 (98%)	2 (2%)	0	100	100
49	g	89/119 (75%)	83 (93%)	6 (7%)	0	100	100
49	n	78/119 (66%)	75 (96%)	3 (4%)	0	100	100
50	q	71/73 (97%)	65 (92%)	6 (8%)	0	100	100
51	X	34/641 (5%)	34 (100%)	0	0	100	100
All	All	12843/22520 (57%)	11839 (92%)	912 (7%)	92 (1%)	20	56

5 of 92 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A5	188	LYS
1	A5	222	PRO
1	A5	361	GLN
1	A5	362	LEU
3	z	99	GLN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A5	39/724 (5%)	39 (100%)	0	100	100
2	A2	3/91 (3%)	3 (100%)	0	100	100
3	z	5/109 (5%)	5 (100%)	0	100	100
5	D	10/300 (3%)	10 (100%)	0	100	100
6	W	6/218 (3%)	6 (100%)	0	100	100
7	B	8/195 (4%)	8 (100%)	0	100	100
8	s	79/1908 (4%)	79 (100%)	0	100	100
9	Q	6/130 (5%)	6 (100%)	0	100	100
12	L	3/709 (0%)	3 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	V	3/88 (3%)	3 (100%)	0	100	100
15	9	4/94 (4%)	4 (100%)	0	100	100
16	C	4/111 (4%)	4 (100%)	0	100	100
17	H	3/80 (4%)	3 (100%)	0	100	100
18	J	2/70 (3%)	2 (100%)	0	100	100
21	K	2/395 (0%)	2 (100%)	0	100	100
22	y	4/95 (4%)	4 (100%)	0	100	100
23	G	13/441 (3%)	13 (100%)	0	100	100
25	A	123/2108 (6%)	123 (100%)	0	100	100
26	I	6/293 (2%)	6 (100%)	0	100	100
27	P	12/361 (3%)	12 (100%)	0	100	100
28	p	1/709 (0%)	1 (100%)	0	100	100
29	4	12/446 (3%)	11 (92%)	1 (8%)	10	30
30	A4	6/956 (1%)	6 (100%)	0	100	100
31	u	36/1104 (3%)	35 (97%)	1 (3%)	38	60
32	T	19/776 (2%)	19 (100%)	0	100	100
33	E	60/1051 (6%)	59 (98%)	1 (2%)	53	69
34	w	4/336 (1%)	4 (100%)	0	100	100
35	x	3/77 (4%)	3 (100%)	0	100	100
36	v	6/459 (1%)	6 (100%)	0	100	100
37	0	10/349 (3%)	10 (100%)	0	100	100
39	r	49/866 (6%)	49 (100%)	0	100	100
40	Y	4/831 (0%)	4 (100%)	0	100	100
42	A6	2/203 (1%)	2 (100%)	0	100	100
43	a	3/110 (3%)	3 (100%)	0	100	100
43	h	5/110 (4%)	5 (100%)	0	100	100
44	b	4/74 (5%)	4 (100%)	0	100	100
44	i	4/74 (5%)	4 (100%)	0	100	100
45	f	2/177 (1%)	2 (100%)	0	100	100
45	m	4/177 (2%)	4 (100%)	0	100	100
46	e	3/101 (3%)	3 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	l	3/101 (3%)	3 (100%)	0	100	100
47	d	3/66 (4%)	3 (100%)	0	100	100
47	k	3/66 (4%)	3 (100%)	0	100	100
48	c	1/84 (1%)	1 (100%)	0	100	100
48	j	1/84 (1%)	1 (100%)	0	100	100
49	g	4/101 (4%)	4 (100%)	0	100	100
49	n	3/101 (3%)	3 (100%)	0	100	100
51	X	1/554 (0%)	1 (100%)	0	100	100
All	All	591/18663 (3%)	588 (100%)	3 (0%)	78	83

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
29	4	78	PRO
31	u	718	PRO
33	E	406	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	5	113/116 (97%)	40 (35%)	2 (1%)
19	2	139/188 (73%)	29 (20%)	1 (0%)
24	Z	45/230 (19%)	12 (26%)	0
41	6	75/106 (70%)	24 (32%)	0
All	All	372/640 (58%)	105 (28%)	3 (0%)

5 of 105 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	5	8	G
11	5	9	G
11	5	10	U
11	5	15	C
11	5	19	A

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
11	5	26	A
11	5	78	U
19	2	60	U

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
55	GTG	A6	301	-	57,57,57	2.28	18 (31%)	85,90,90	2.70	23 (27%)
52	IHP	A	3001	-	36,36,36	1.58	6 (16%)	60,60,60	0.93	2 (3%)
53	GTP	r	1500	54	33,34,34	1.18	4 (12%)	50,54,54	1.98	9 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	GTG	A6	301	-	-	13/32/64/64	0/6/6/6
52	IHP	A	3001	-	-	3/30/54/54	0/1/1/1
53	GTP	r	1500	54	-	7/22/38/38	0/3/3/3

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	A6	301	GTG	PG-O3B	-7.59	1.51	1.59
55	A6	301	GTG	O4E-C1E	5.99	1.55	1.42
55	A6	301	GTG	O4E-C4E	5.92	1.58	1.45
55	A6	301	GTG	PA-O3A	-4.54	1.54	1.59
55	A6	301	GTG	C5E-C4E	-4.34	1.38	1.51

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	A6	301	GTG	C5E-C4E-C3E	-10.70	76.70	115.21
55	A6	301	GTG	O5E-C5E-C4E	7.31	133.90	108.99
55	A6	301	GTG	C2E-C3E-C4E	7.30	116.72	102.61
55	A6	301	GTG	PG-O5E-C5E	6.71	159.81	121.35
53	r	1500	GTP	C5-C4-N3	-6.55	117.96	128.39

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
52	A	3001	IHP	C1-C2-O12-P2
53	r	1500	GTP	C5'-O5'-PA-O3A
53	r	1500	GTP	C5'-O5'-PA-O1A
53	r	1500	GTP	C5'-O5'-PA-O2A
53	r	1500	GTP	O4'-C4'-C5'-O5'

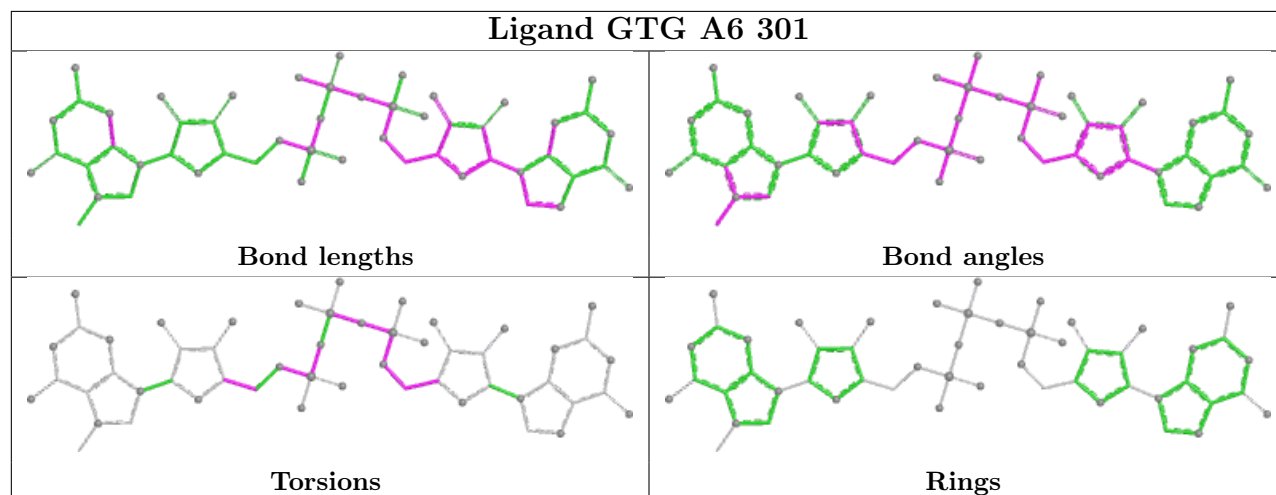
There are no ring outliers.

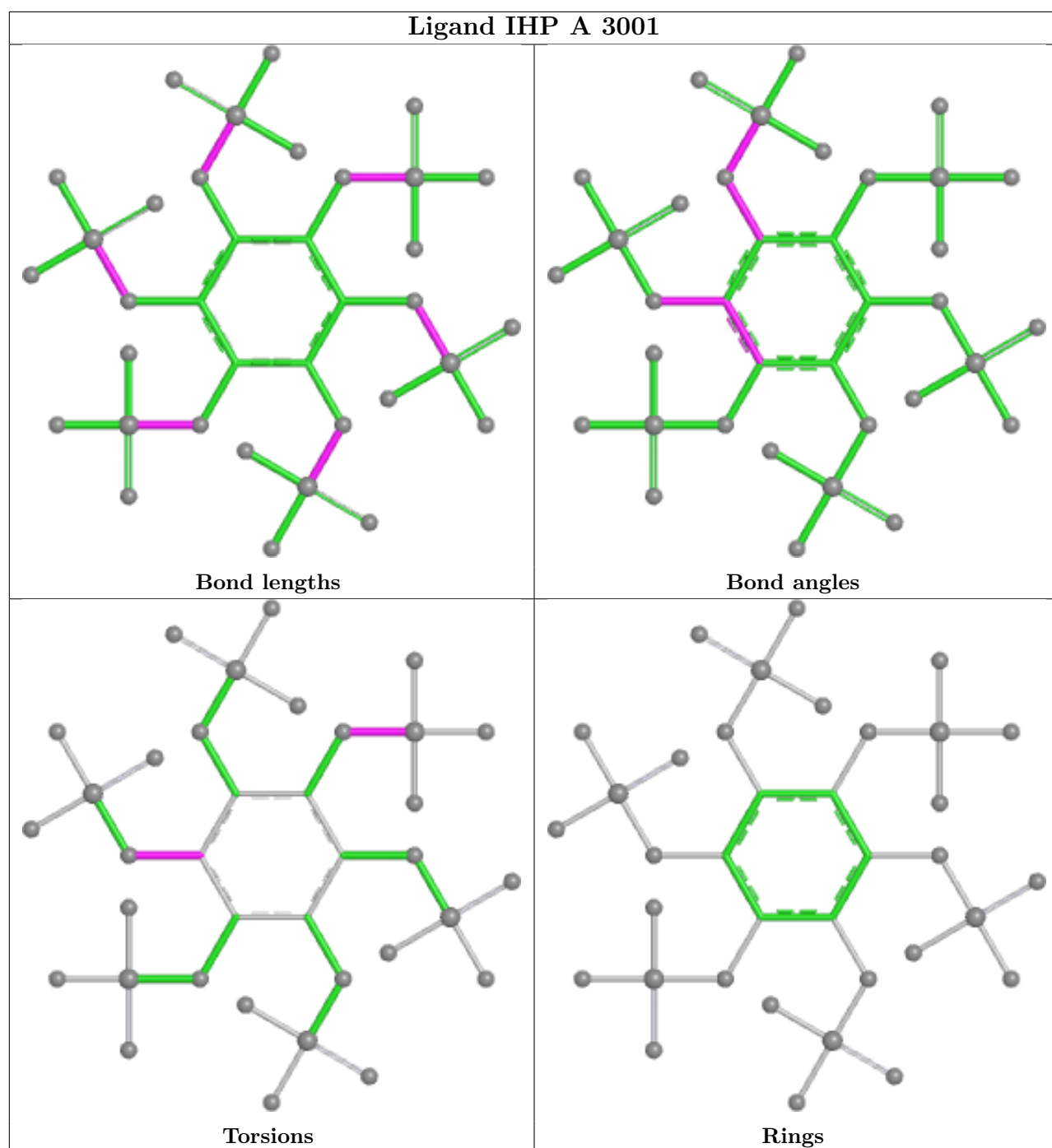
2 monomers are involved in 24 short contacts:

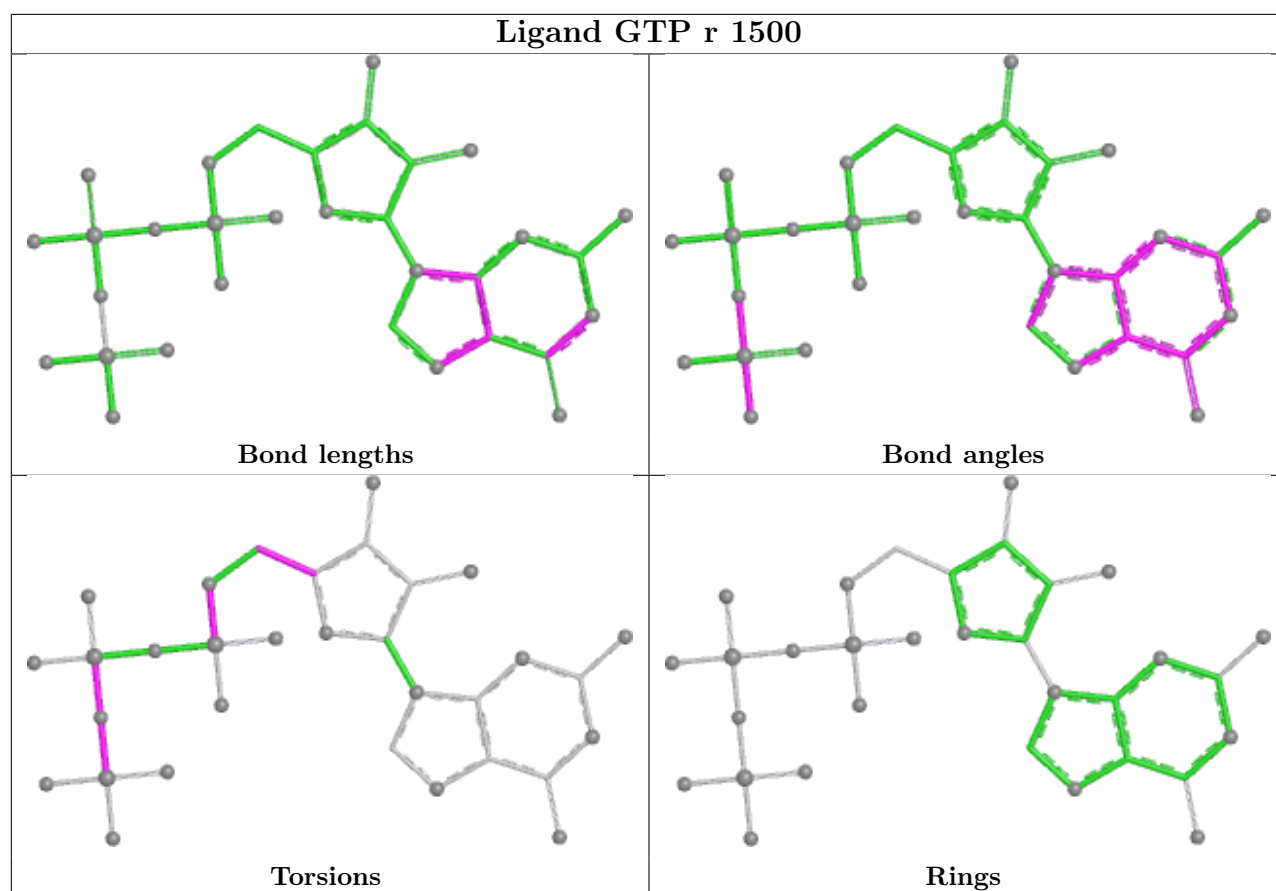
Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	A6	301	GTG	11	0
53	r	1500	GTP	13	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

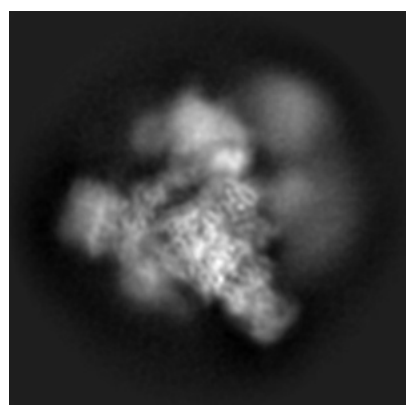
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11695. These allow visual inspection of the internal detail of the map and identification of artifacts.

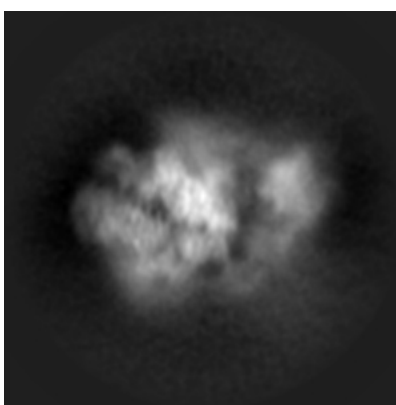
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

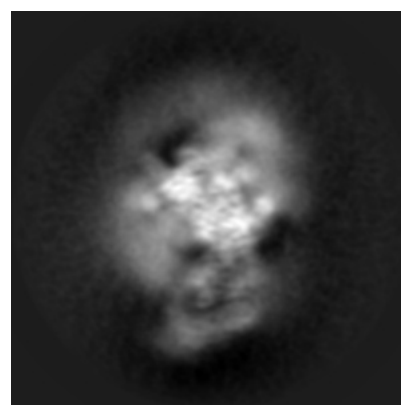
6.1.1 Primary map



X



Y

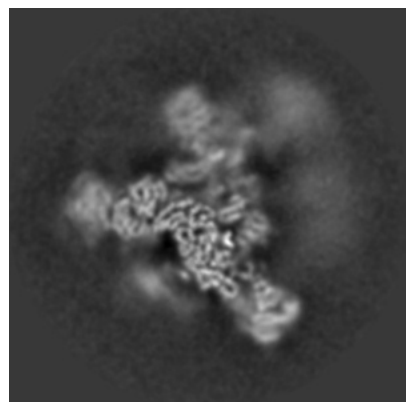


Z

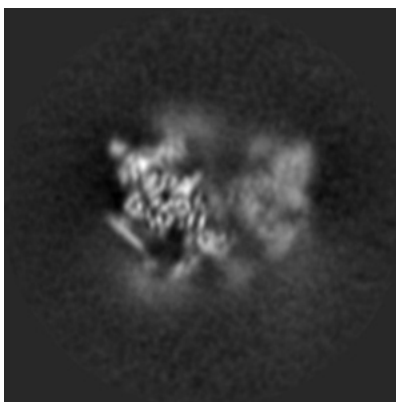
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

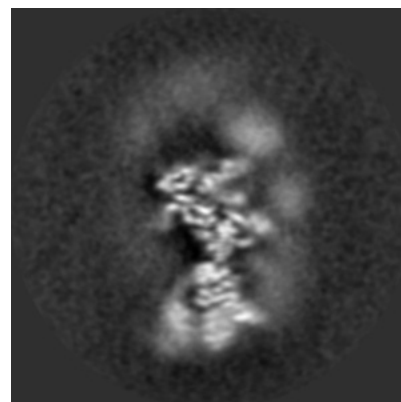
6.2.1 Primary map



X Index: 192



Y Index: 192

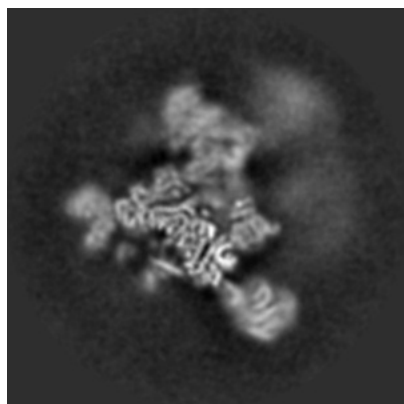


Z Index: 192

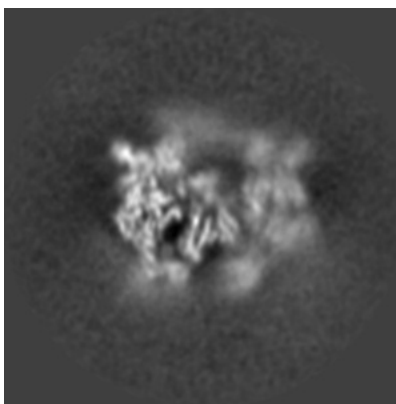
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

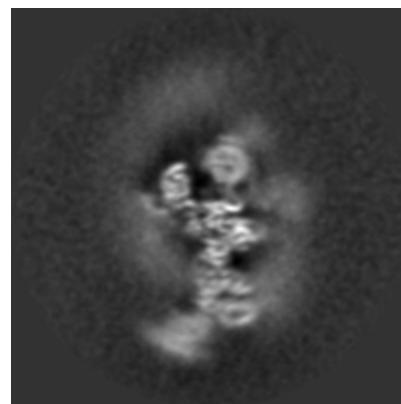
6.3.1 Primary map



X Index: 202



Y Index: 201

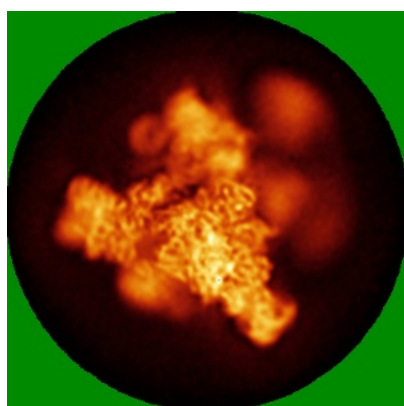


Z Index: 175

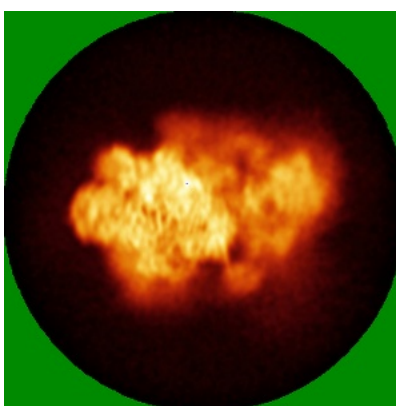
The images above show the largest variance slices of the map in three orthogonal directions.

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

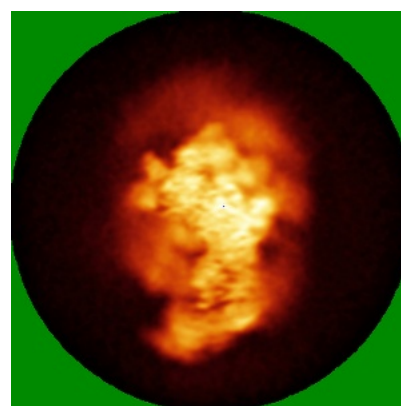
6.4.1 Primary map



X



Y

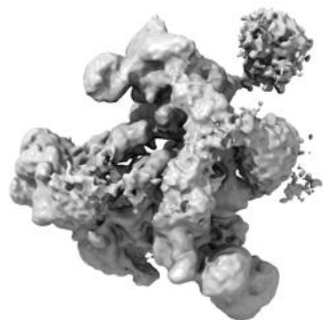


Z

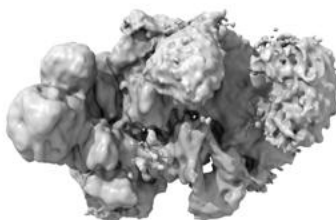
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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 0.0095. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

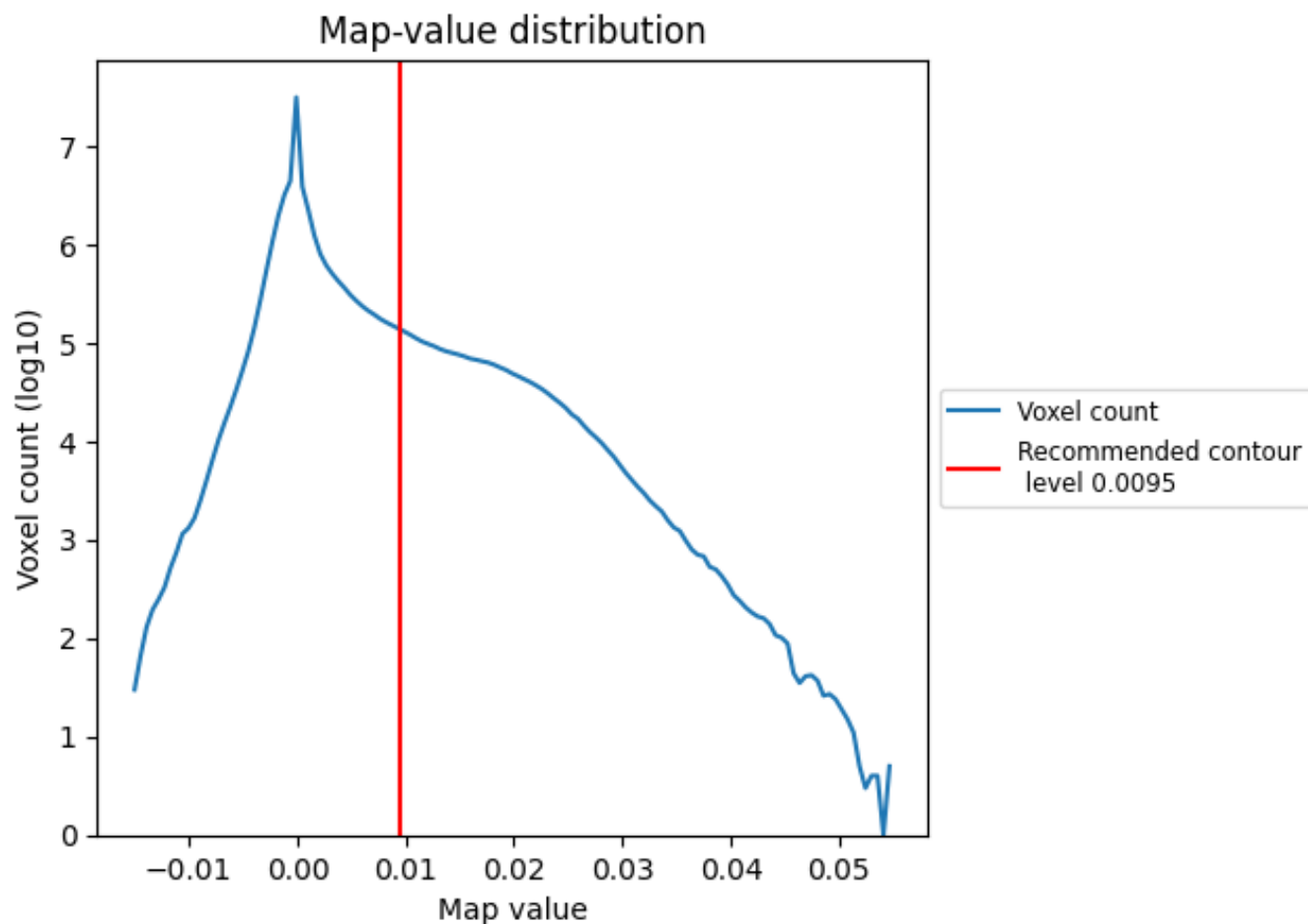
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

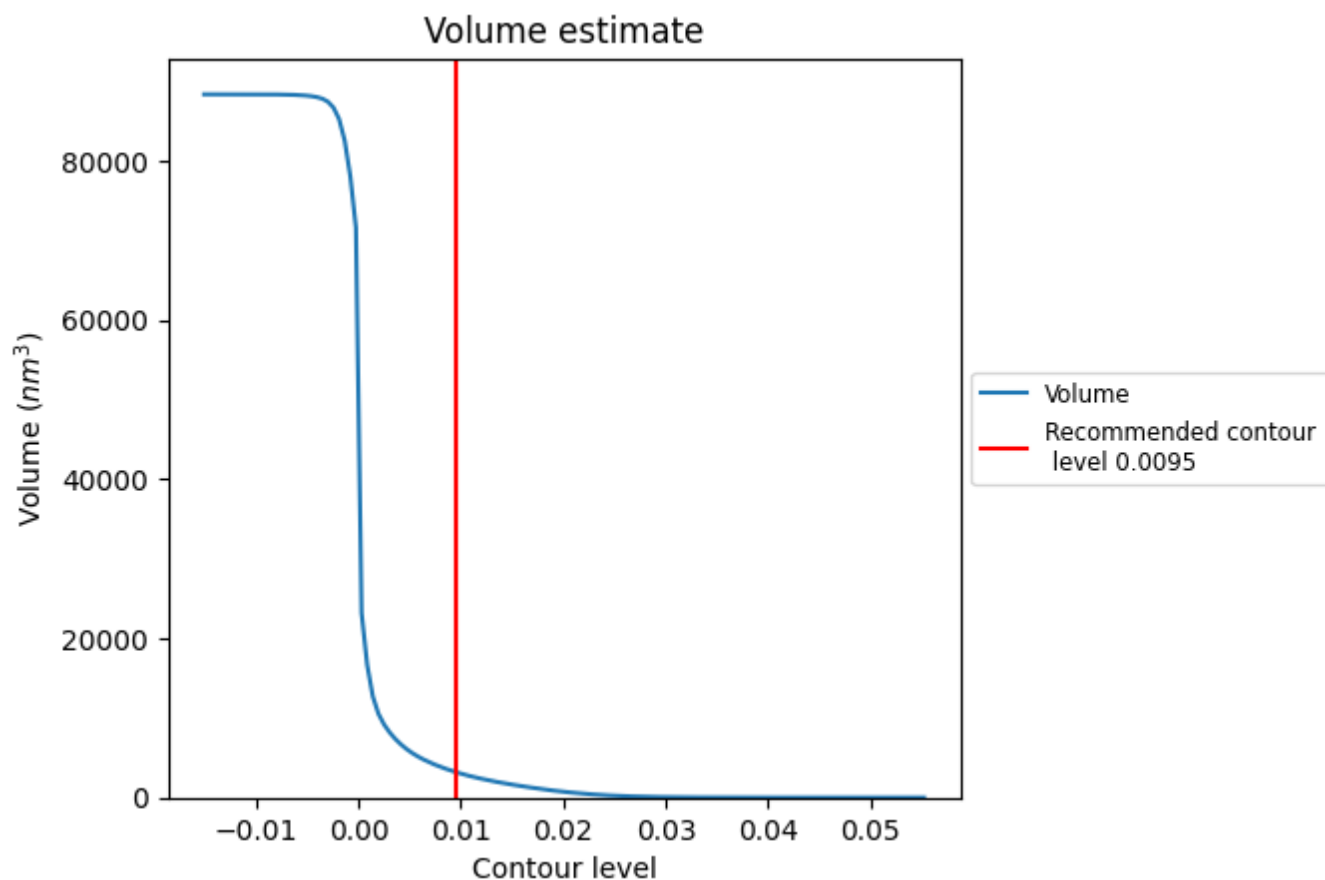
This section contains the results of statistical analysis of the map.

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.

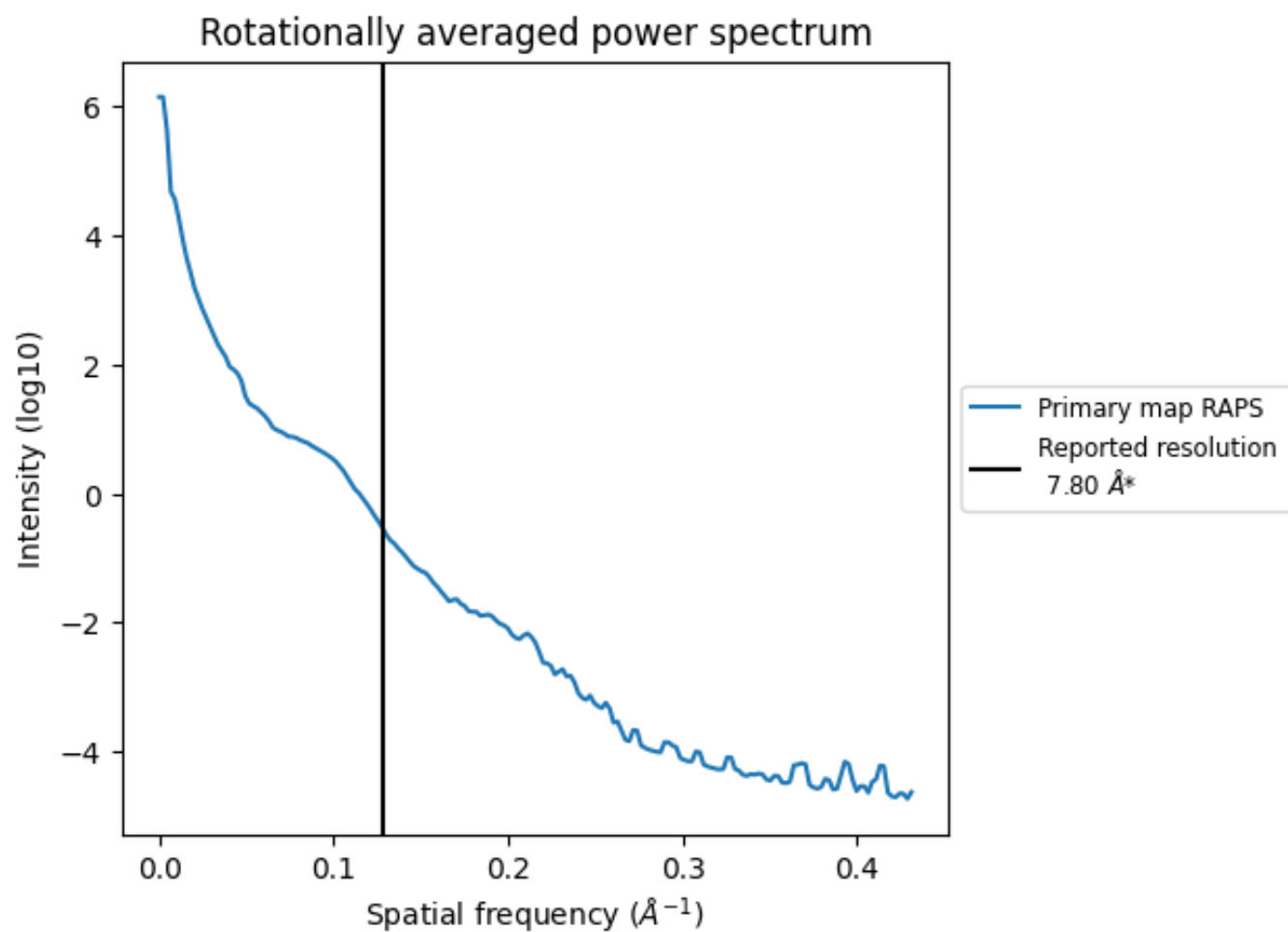
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3218 nm³; this corresponds to an approximate mass of 2907 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.128 Å⁻¹

8 Fourier-Shell correlation

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

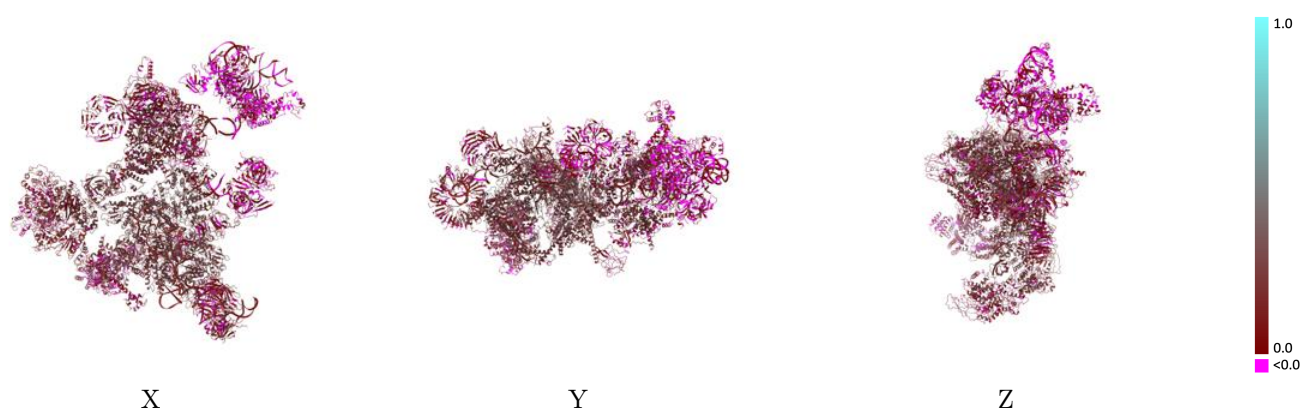
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-11695 and PDB model 7ABG. Per-residue inclusion information can be found in section 3 on page 16.

9.1 Map-model overlay [i](#)

This section was not generated.

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

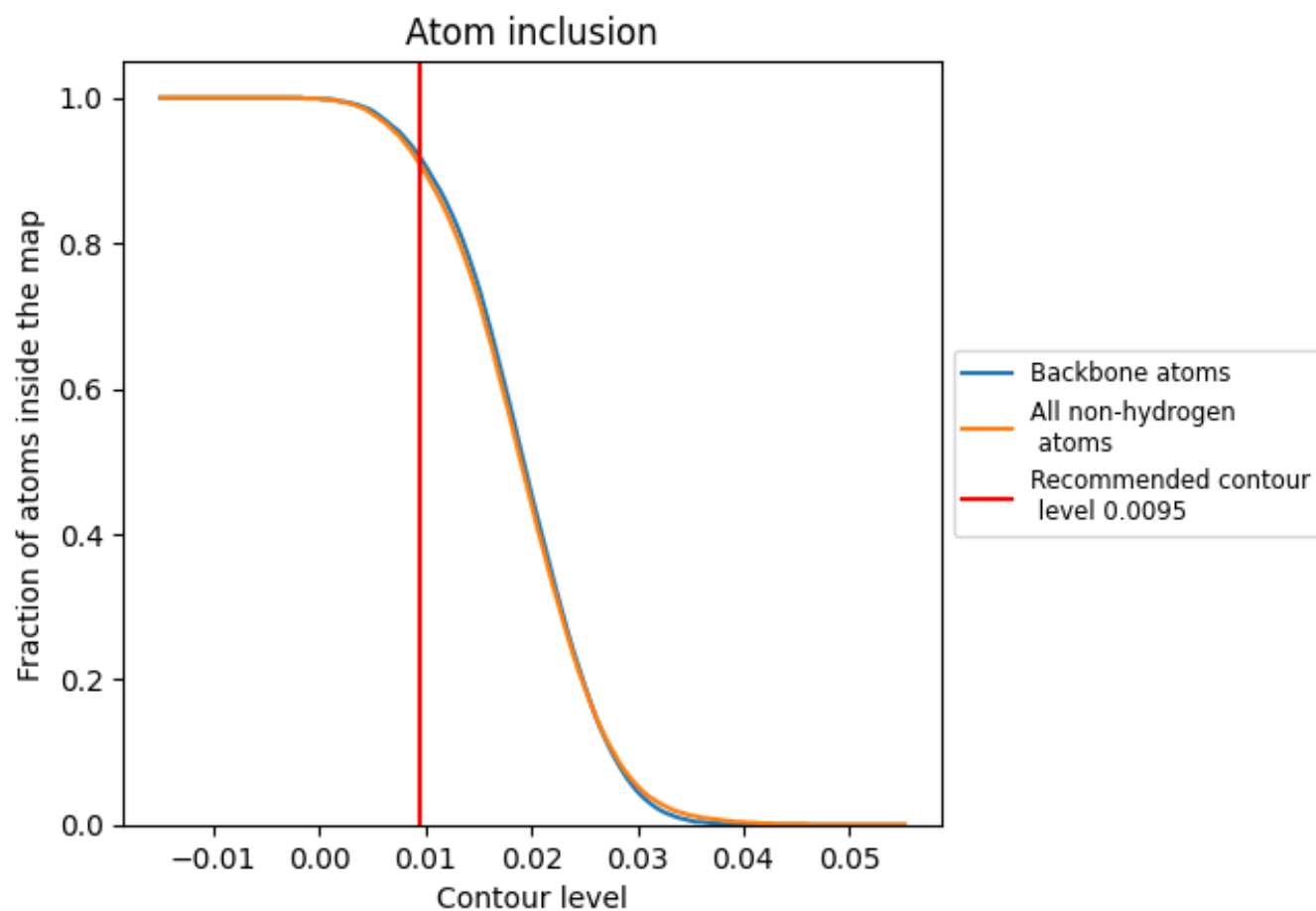


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 91% 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 (0.0095) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9080	 0.1470
0	 0.9720	 0.0750
2	 0.5410	 0.0490
4	 0.4400	 0.0250
5	 0.9880	 0.1780
6	 0.9690	 0.1550
9	 0.9050	 0.0210
A	 0.9870	 0.2520
A1	 0.9970	 0.0610
A2	 0.9620	 0.0650
A3	 1.0000	 0.0740
A4	 0.9420	 0.1610
A5	 0.9620	 0.0740
A6	 1.0000	 0.0640
B	 0.0010	 -0.0040
C	 0.9880	 0.0570
D	 0.9960	 0.0960
E	 0.9520	 0.1080
F	 0.8800	 0.0670
G	 0.9980	 0.1600
H	 0.8580	 0.0370
I	 0.9970	 0.2580
J	 0.9880	 0.0780
K	 0.9940	 0.2720
L	 0.9480	 0.1760
N	 1.0000	 0.2480
P	 0.9960	 0.1760
Q	 0.9990	 0.2290
R	 0.9560	 0.2570
T	 0.9930	 0.1120
V	 0.9450	 0.0510
W	 0.4860	 0.0180
X	 1.0000	 0.2510
Y	 0.9330	 0.1320
Z	 1.0000	 0.1940



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Chain	Atom inclusion	Q-score
a	 0.9900	 0.1530
b	 0.9560	 0.1180
c	 0.9510	 0.1160
d	 0.9940	 0.1820
e	 0.9970	 0.1990
f	 1.0000	 0.1560
g	 0.9700	 0.1360
h	 0.8750	 -0.0140
i	 0.7600	 0.0090
j	 0.2360	 0.0320
k	 0.1320	 0.0160
l	 0.2020	 0.0100
m	 0.7360	 0.0420
n	 0.9730	 0.0000
p	 0.0200	 0.0700
q	 1.0000	 0.2990
r	 0.9980	 0.2390
s	 0.9870	 0.1560
u	 0.9850	 0.1630
v	 0.9350	 0.2120
w	 0.9850	 0.0730
x	 1.0000	 0.1200
y	 0.9940	 0.1280
z	 0.9040	 0.1010