



## wwPDB EM Validation Summary Report ⓘ

Oct 13, 2024 – 09:35 am BST

PDB ID : 6G90  
EMDB ID : EMD-4364  
Title : Prespliceosome structure provides insight into spliceosome assembly and regulation (map A2)  
Authors : Plaschka, C.; Lin, P.-C.; Charenton, C.; Nagai, K.  
Deposited on : 2018-04-10  
Resolution : 4.00 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

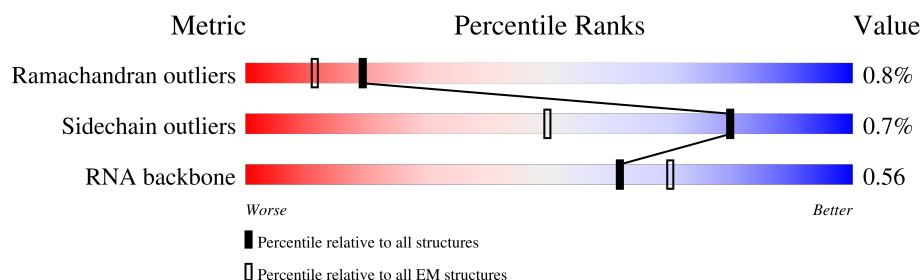
EMDB validation analysis : 0.0.1.dev113  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

# 1 Overall quality at a glance

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

The reported resolution of this entry is 4.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	1	407	<div> <div>17%</div> <div>59%</div> <div>16%</div> <div>5%</div> <div>20%</div> </div>
2	2	143	<div> <div>100%</div> <div>36%</div> <div>52%</div> <div>10%</div> </div>
3	A	298	<div> <div>33%</div> <div>67%</div> </div>
4	B	300	<div> <div>38%</div> <div>62%</div> <div>36%</div> </div>
5	C	231	<div> <div>9%</div> <div>73%</div> <div>23%</div> </div>
6	D	629	<div> <div>13%</div> <div>79%</div> <div>19%</div> </div>
7	E	544	<div> <div>6%</div> <div>91%</div> <div>8%</div> </div>
8	F	523	<div> <div>30%</div> <div>67%</div> </div>

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Mol	Chain	Length	Quality of chain
9	G	492	
10	H	261	
11	I	38	
12	J	620	
13	O	971	
14	P	1361	
15	Q	435	
16	R	213	
17	S	107	
18	T	530	
19	U	266	
20	V	280	
21	W	238	
22	X	51	
23	Y	111	
24	Z	85	
25	b	196	
25	s	196	
26	d	101	
26	v	101	
27	e	94	
27	w	94	
28	f	86	
28	x	86	
29	g	77	

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Mol	Chain	Length	Quality of chain
29	y	77	
30	h	146	
30	t	146	
31	i	110	
31	u	110	

## 2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 65050 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 U1 snRNA,U1 snRNA,U1 snRNA,U1 snRNA,U1 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	327	Total	C	N	O	P	0	0
			6625	2951	1072	2275	327		

- Molecule 2 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	143	Total	C	N	O	P	0	0
			3025	1352	513	1017	143		

- Molecule 3 is a protein called U1 small nuclear ribonucleoprotein A,U1 small nuclear ribonucleoprotein A,U1 small nuclear ribonucleoprotein A,U1 small nuclear ribonucleoprotein A,U1 small nuclear ribonucleoprotein A.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	A	99	Total	C	N	O	0	0
			492	294	99	99		

- Molecule 4 is a protein called U1 small nuclear ribonucleoprotein 70 kDa homolog,U1 small nuclear ribonucleoprotein 70 kDa homolog,U1 small nuclear ribonucleoprotein 70 kDa homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	193	Total	C	N	O	S	0	0
			1450	929	261	258	2		

- Molecule 5 is a protein called U1 small nuclear ribonucleoprotein C.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	177	Total	C	N	O	S	0	0
			1323	832	246	240	5		

- Molecule 6 is a protein called Pre-mRNA-processing factor 39.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	509	Total	C	N	O	S	0	0
			3462	2188	608	659	7		

- Molecule 7 is a protein called U1 small nuclear ribonucleoprotein component PRP42.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	E	541	Total	C	N	O	S	0	0
			4574	2996	723	836	19		

- Molecule 8 is a protein called Protein NAM8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	F	175	Total	C	N	O	S	0	0
			1337	840	232	255	10		

- Molecule 9 is a protein called 56 kDa U1 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	G	216	Total	C	N	O	S	0	0
			1684	1098	274	301	11		

- Molecule 10 is a protein called Protein LUC7,Protein LUC7,Protein LUC7.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	H	158	Total	C	N	O	S	0	0
			1083	675	198	201	9		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	83	VAL	GLU	conflict	UNP Q07508
H	84	GLU	VAL	conflict	UNP Q07508

- Molecule 11 is a RNA chain called Yeast UBC4 pre-mRNA (mutant).

Mol	Chain	Residues	Atoms					AltConf	Trace
11	I	38	Total	C	N	O	P	0	0
			789	355	132	264	38		

- Molecule 12 is a protein called U1 small nuclear ribonucleoprotein component SNU71.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	J	42	Total	C	N	O	0	0
			324	210	55	59		

- Molecule 13 is a protein called U2 snRNP component HSH155.

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

- Molecule 14 is a protein called Pre-mRNA-splicing factor RSE1.

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

- Molecule 15 is a protein called Cold sensitive U2 snRNA suppressor 1.

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

- Molecule 16 is a protein called Protein HSH49.

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

- Molecule 17 is a protein called Pre-mRNA-splicing factor RDS3.

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

- Molecule 18 is a protein called Pre-mRNA-splicing factor PRP9.

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

- Molecule 19 is a protein called Pre-mRNA-splicing factor PRP11,Pre-mRNA-splicing factor PRP11,Pre-mRNA-splicing factor PRP11.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	196	Total	C	N	O	S	0	0
			1489	934	258	291	6		

- Molecule 20 is a protein called Pre-mRNA-splicing factor PRP21.

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

- Molecule 21 is a protein called U2 small nuclear ribonucleoprotein A'.

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

- Molecule 22 is a protein called Unknown.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	X	51	Total	C	N	O		
			255	153	51	51	0	0

- Molecule 23 is a protein called U2 small nuclear ribonucleoprotein B'.

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

- Molecule 24 is a protein called RDS3 complex subunit 10.

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

- Molecule 25 is a protein called Small nuclear ribonucleoprotein-associated protein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	b	121	Total	C	N	O	S	0	0
			972	613	183	173	3		
25	s	65	Total	C	N	O	S	0	0
			518	331	91	93	3		

- Molecule 26 is a protein called Small nuclear ribonucleoprotein Sm D3.



Mol	Chain	Residues	Atoms					AltConf	Trace
26	d	93	Total	C	N	O	S	0	0
			714	453	125	133	3		
26	v	82	Total	C	N	O	S	0	0
			632	402	109	119	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	e	77	Total	C	N	O	S	0	0
			600	395	96	106	3		
27	w	77	Total	C	N	O	S	0	0
			602	396	95	108	3		

- Molecule 28 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	f	73	Total	C	N	O	S	0	0
			585	376	102	106	1		
28	x	73	Total	C	N	O	S	0	0
			585	376	102	106	1		

- Molecule 29 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	g	72	Total	C	N	O	S	0	0
			556	352	97	105	2		
29	y	75	Total	C	N	O	S	0	0
			577	363	100	112	2		

- Molecule 30 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	h	107	Total	C	N	O	S	0	0
			834	525	149	157	3		
30	t	72	Total	C	N	O	S	0	0
			569	364	99	104	2		

- Molecule 31 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	i	99	Total	C	N	O	S	0	0
			805	514	148	139	4		

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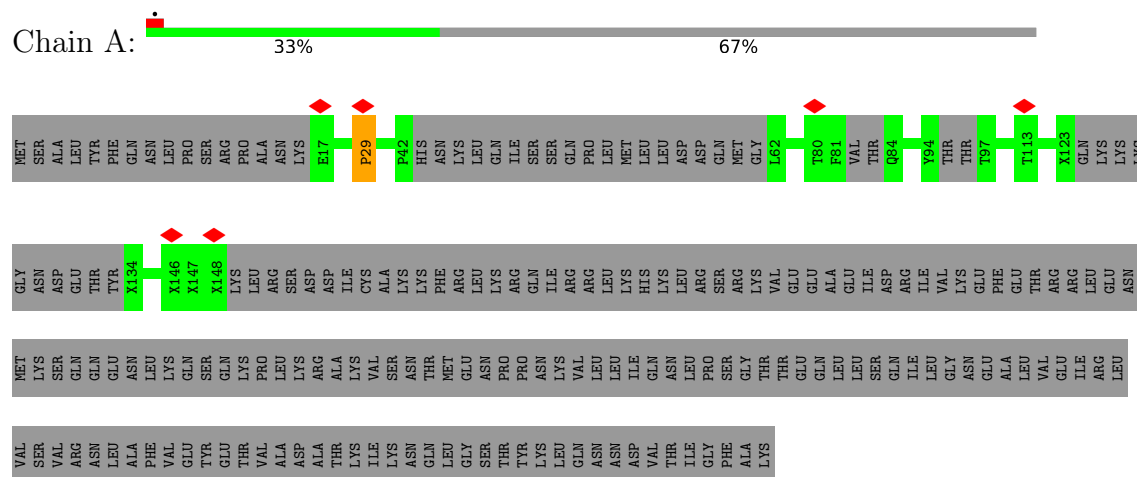
Mol	Chain	Residues	Atoms					AltConf	Trace
31	u	92	Total	C	N	O	S	0	0
			752	481	136	131	4		

- Molecule 32 is ZINC ION (three-letter code: ZN) (formula: Zn).

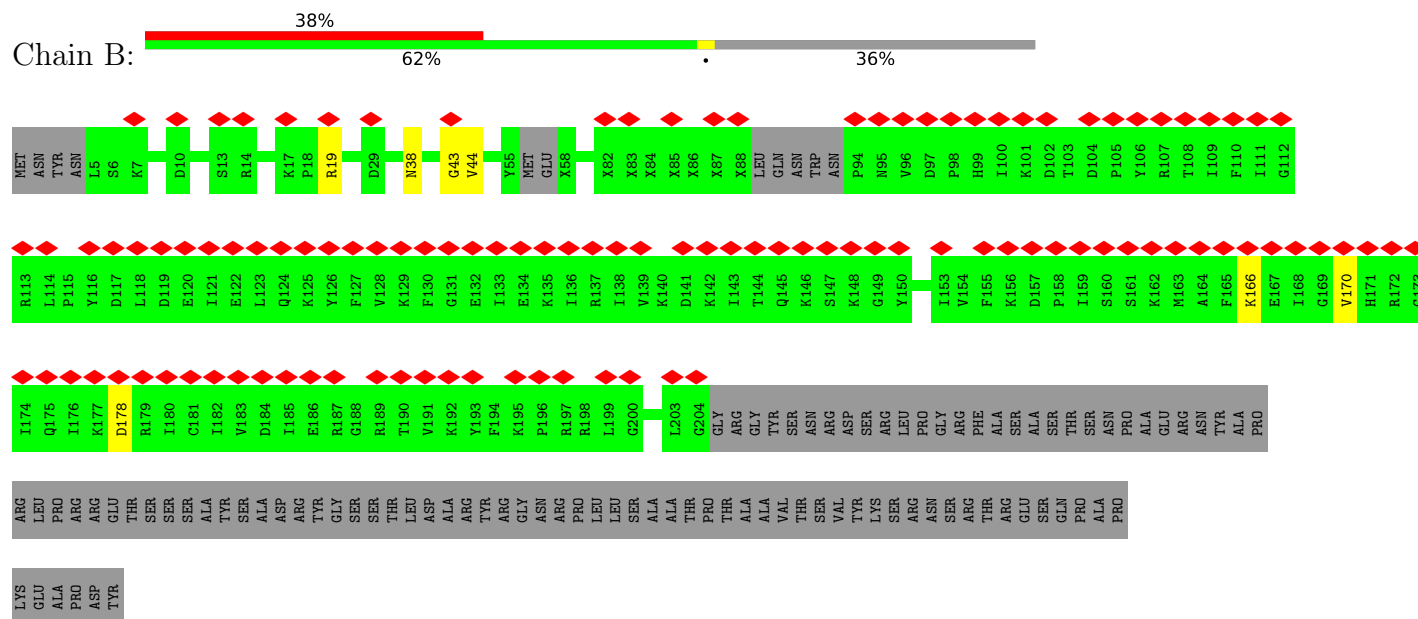
Mol	Chain	Residues	Atoms		AltConf
32	C	1	Total	Zn	0
			1	1	
32	H	2	Total	Zn	0
			2	2	
32	S	3	Total	Zn	0
			3	3	
32	T	2	Total	Zn	0
			2	2	
32	U	1	Total	Zn	0
			1	1	



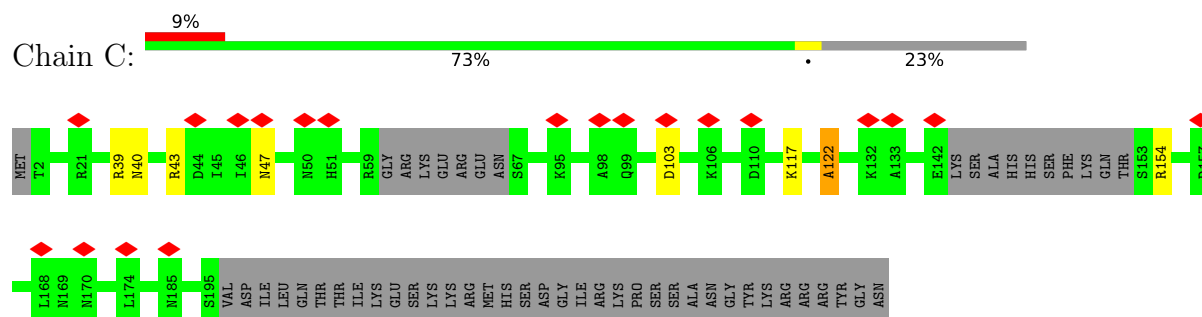
- Molecule 3: U1 small nuclear ribonucleoprotein A,U1 small nuclear ribonucleoprotein A,U1 small nuclear ribonucleoprotein A,U1 small nuclear ribonucleoprotein A,U1 small nuclear ribonucleoprotein A



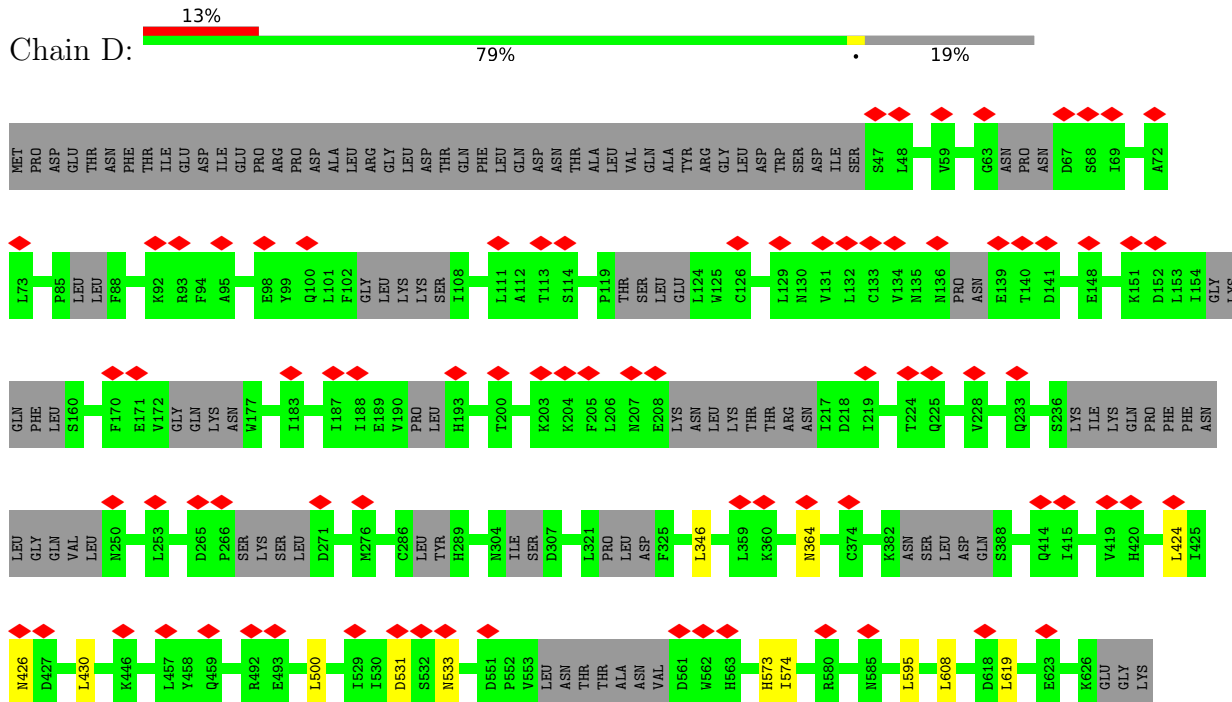
- Molecule 4: U1 small nuclear ribonucleoprotein 70 kDa homolog,U1 small nuclear ribonucleoprotein 70 kDa homolog,U1 small nuclear ribonucleoprotein 70 kDa homolog



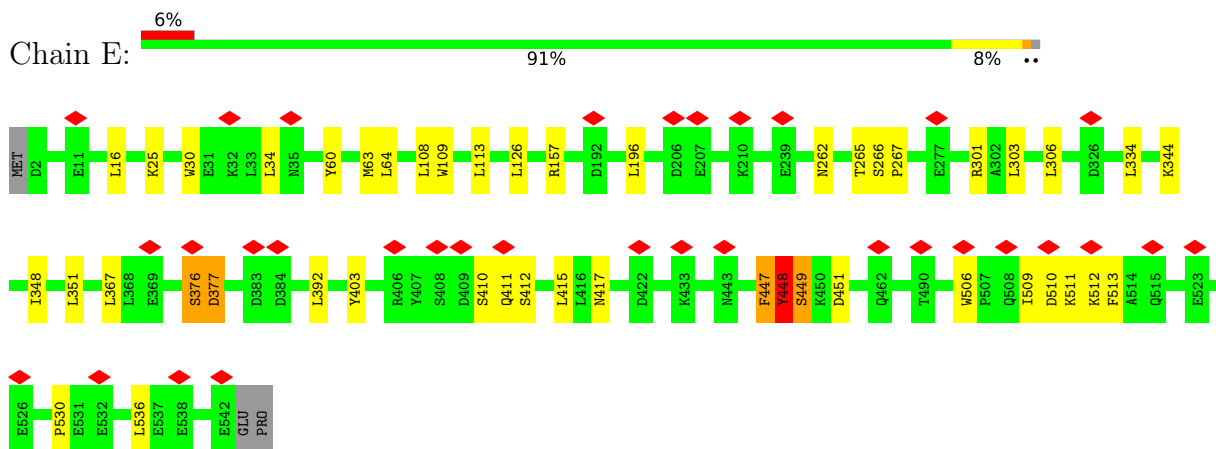
- Molecule 5: U1 small nuclear ribonucleoprotein C



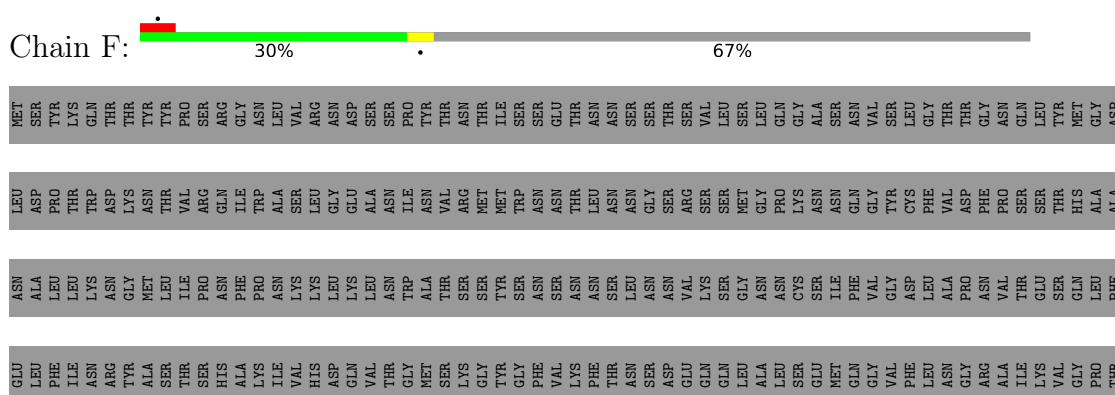
- Molecule 6: Pre-mRNA-processing factor 39



- Molecule 7: U1 small nuclear ribonucleoprotein component PRP42



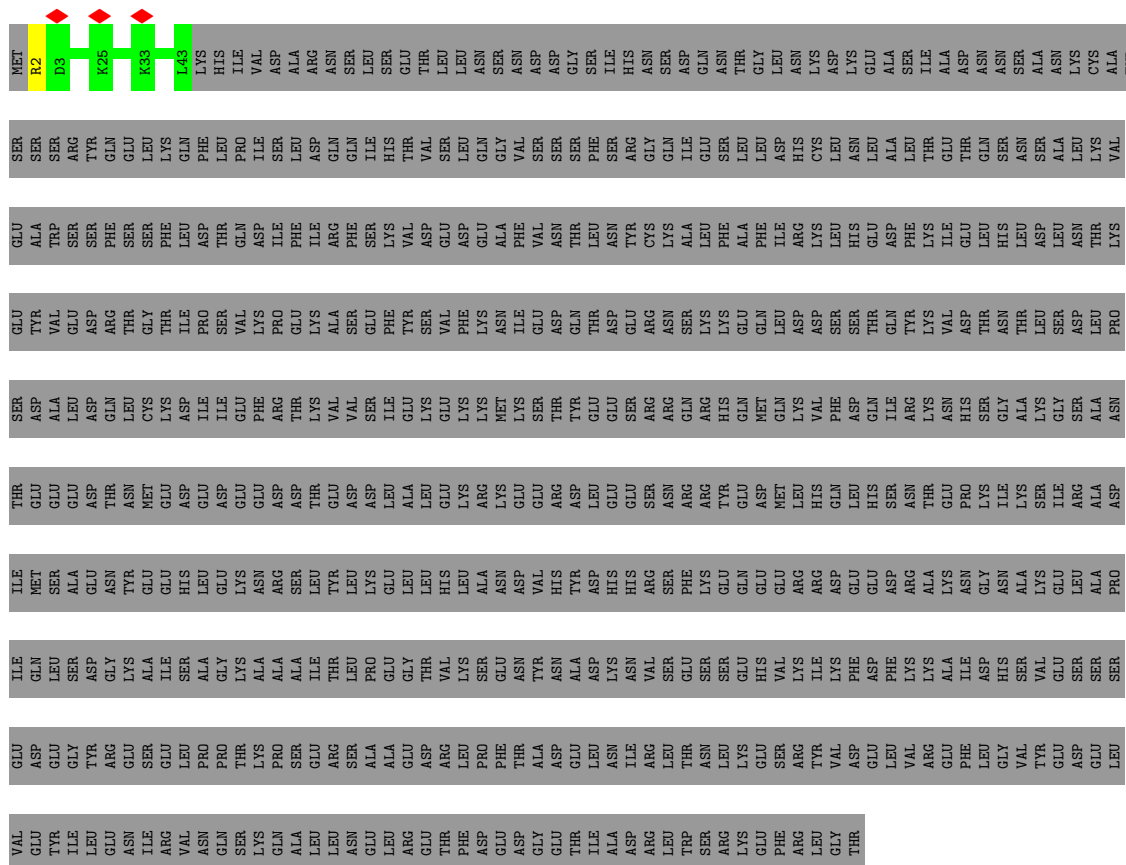
- Molecule 8: Protein NAM8

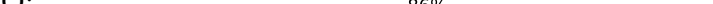


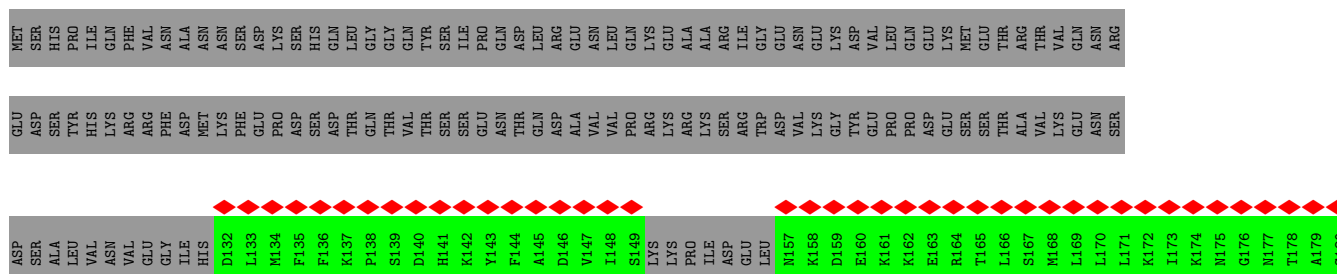




- Chain J:  7% 93%



- Chain O:  86% 86% 14%







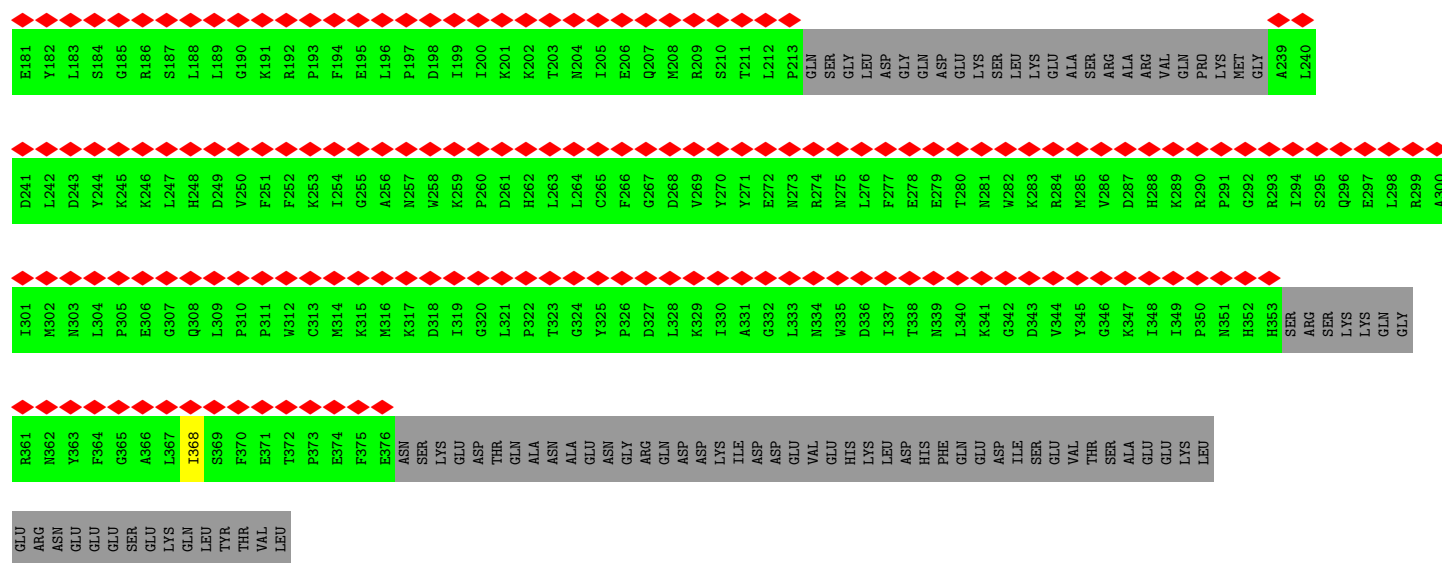
● Molecule 14: Pre-mRNA-splicing factor RSE1

Chain P:

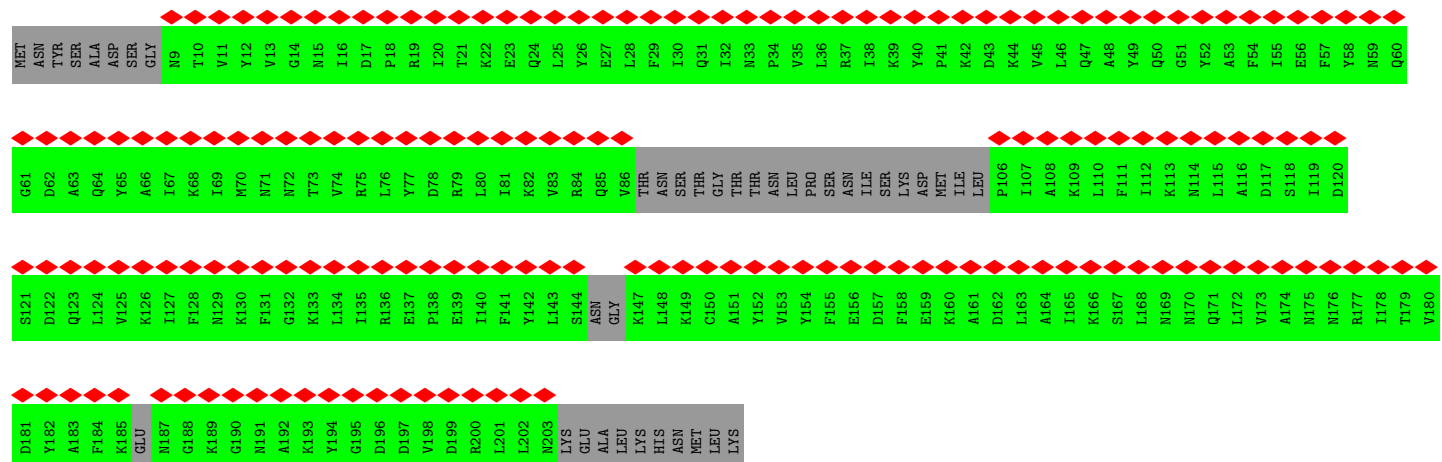
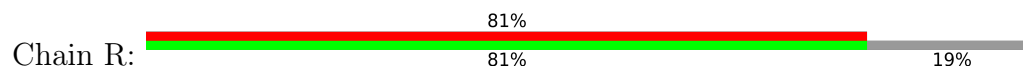


MET	TRP	GLY	GLY	GLY	LYS	MET	ALA	VAL	VAL	SER	LEU	SER	PRO	HIS	THR	ALA	LYS	MET	ARG	LYS	PHE	GLY	GLN	ALA	SER	SER	THR	THR	MET	THR	TYR	ASP	GLY	LEU	LYS	ARG	GLU	ALA	ARG	ARG	THR	ARG	SER	ASP	HIS	ASN	ILE	THR	MET	VAL	ASP	K54	D55	D56	E57	L58	Y59	L60																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
Y61	H62	L63	L63	T64	L65	K66	K67	Q68	T69	N70	F71	H72	V73	S74	C75	I76	G77	H78	F79	V80	D81	L82	E83	A84	G85	S86	K87	R88	E89	Q90	S91	Q92	L93	C94	V95	A96	T97	E98	T99	H100	L101	E102	L103	Y104	D105	T106	A107	D108	G109	E110	L111	K112	L113	I114	A115	K116	F117	Q118	N119	L120																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										

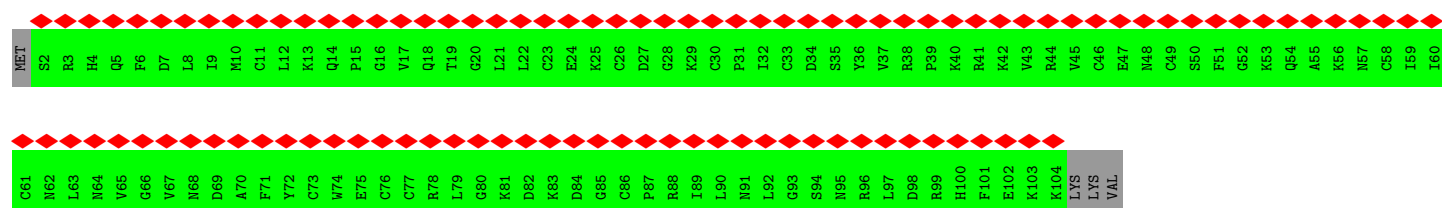




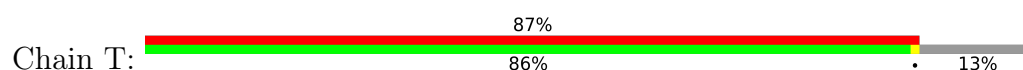
• Molecule 16: Protein HSH49



• Molecule 17: Pre-mRNA-splicing factor RDS3




• Molecule 18: Pre-mRNA-splicing factor PRP9



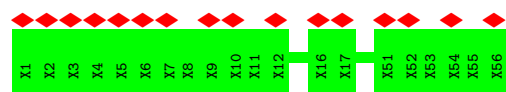
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Y421	R422	C423	E424	I425	C426	S427	N428	K429	V430	Y431	N432	G433	R434	R435	T436	F437	E438	R439	H440	F441	N442	E443	E444	R445	H446	I447	Y448	H449	L450	R451	C452	L453	G454	I455	E456	F457	S458	S459	V460	F461	K462	G463	I464	T465	K466	I467	K468	E469	A470	Q471	E472	L473	W474	K475	N476	M477	Q478	GLY	GLN
Y361	E362	A363	P364	A365	Y366	D367	S368	T369	E370	K371	E372	G373	A374	E375	Q376	V377	D378	GLY	GLU	GLN	ARG	ASP	GLY	GLN	LEU	GLU	GLU	HIS	LEU	SER	GLY	LYS	PHE	ASP	MET	PRO	LEU	PRO	GLY	ASP	GLY	PRO	M407	P408	Y409	W410	L411	Y412	K413	L414	H415	G416	L417	D418	R419	E420			
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K121	E122	L123	K124	M125	E126	D127	E128	M129	F130	E131	L132	D133	I134	M135	S136	I137	K138	D139	K140	Y141	A142	L143	F144	S145	S146	S147	S148	D149	P150	S151	R152	R153	T154	M155	I156	L157	S158	D159	R160	A161	R162	D163	L164	D165	L166	M167	E168	I169	F170	T171	R172	D173	E174	Q175	Y176	G177	E178	I179	M180
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M1	N2	L3	L4	E5	T6	R7	R8	S9	L10	L11	E12	E13	M14	E15	I16	I17	E18	M19	A20	I21	A22	E23	R24	I25	Q26	R27	N28	P29	E30	L31	Y32	Y33	H34	Y35	I36	Q37	E38	S39	S40	K41	V42	F43	P44	D45	T46	K47	L48	P49	R50	S51	S52	L53	T54	A55	E56	N57	K58	I59	V60

- Molecule 19: Pre-mRNA-splicing factor PRP11,Pre-mRNA-splicing factor PRP11,Pre-mRNA-splicing factor PRP11

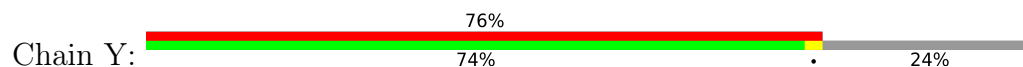
Chain U: 

MET	ASN	TYR	LEU	GLU	GLY	VAL	SER	LYS	LYS	GLY	GLY	ILE	ALA	SER	GLU	SER	GLN	PHE	ASN	LEU	GLN	ARG	ARG	LYS	GLU	VAL	GLU	SER	LEU	L34	S35	K36	G37	E38	N39	P41	Y42	T43	F44	Q45	D46	E47	LYS	ASP	ASP	Q51	V52	R53	S54	N55	P56	Y57	I58	Y59	K60				
N61	H62	S63	G64	K65	L66	V67	C68	R69	L70	C71	H72	T73	M74	H75	M76	S77	W78	S79	S80	W81	E82	R83	H84	L85	G86	G87	K88	R89	H90	G91	L92	N93	V94	L95	R96	R97	G98	I99	S100	I101	E102	K103	S104	S105	LEU	GLY	ARG	GLU	GLY	GLN	THR	THR	HIS	X115	X116	X117	X118	X119	X120
X121	X122	X123	X124	X125	X126	X127	X128	X129	X130	X131	X132	X133	X134	X135	X136	VAL	CYS	LYS	ILE	ALA	THR	VAL	LYS	ASN	PRO	LYS	ASN	G149	S150	V151	G152	L153	A154	I155	Q156	V157	N158	Y159	S160	S161	E162	V163	K164	E165	N166	S167	V168	D169	S170	D171	D172	K173	A174	K175	V176	P177	P178	L179	I180

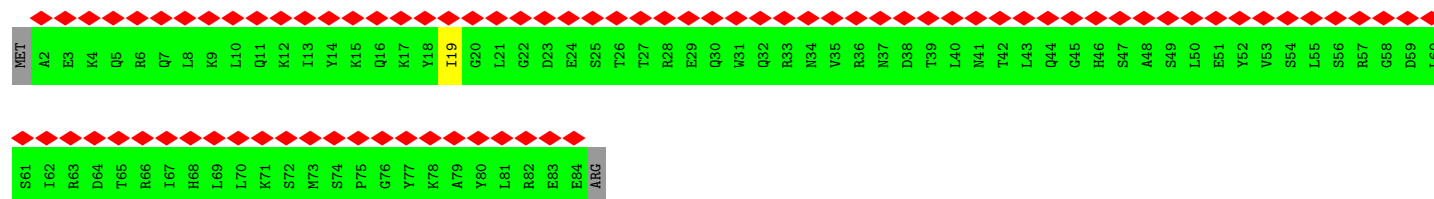




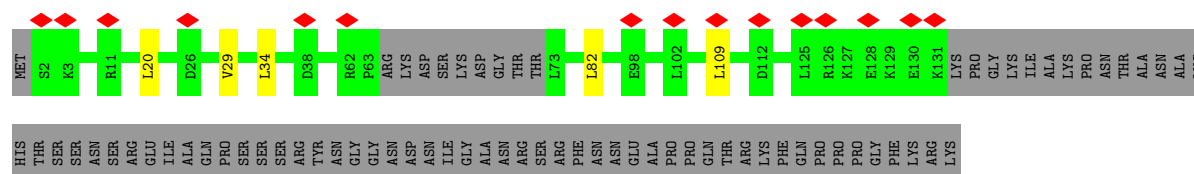
- Molecule 23: U2 small nuclear ribonucleoprotein B''



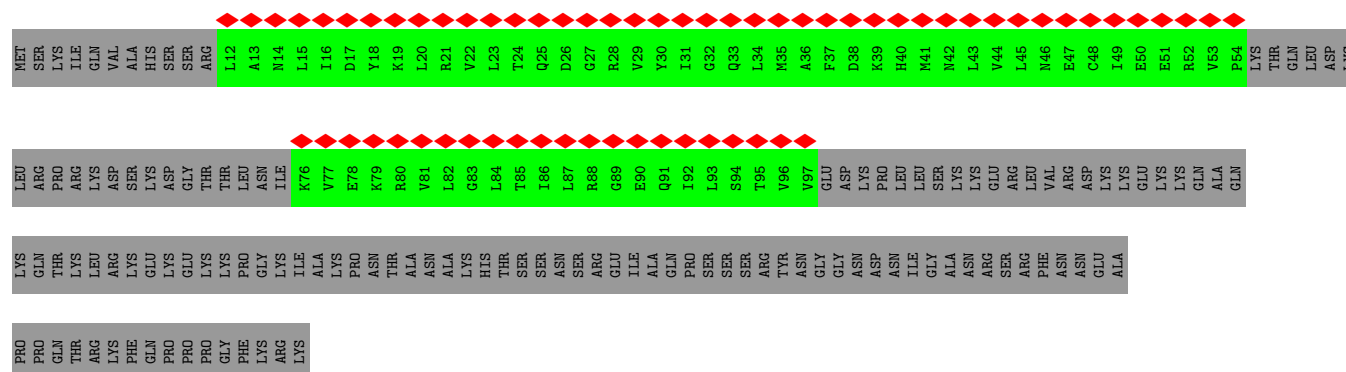
- Molecule 24: RDS3 complex subunit 10




- Molecule 25: Small nuclear ribonucleoprotein-associated protein B

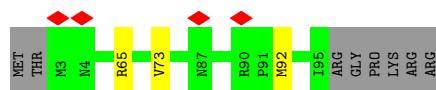


- Molecule 25: Small nuclear ribonucleoprotein-associated protein B




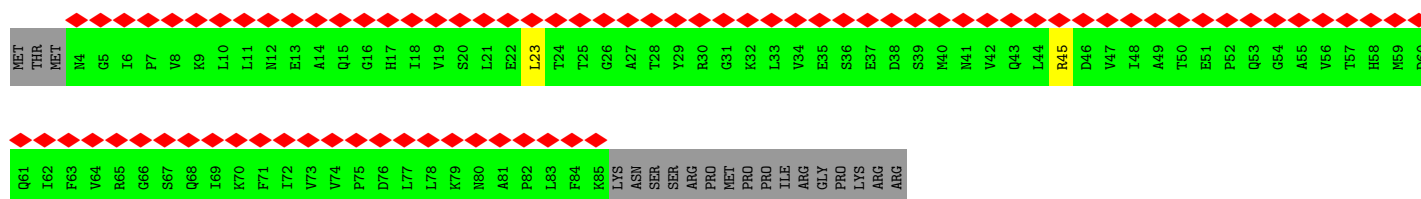
- Molecule 26: Small nuclear ribonucleoprotein Sm D3

Chain d:  89% 8%




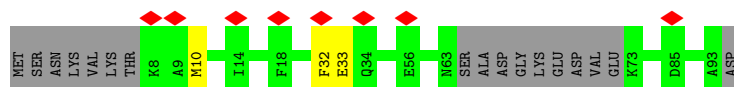
- Molecule 26: Small nuclear ribonucleoprotein Sm D3

Chain v:  81% 79% 19%




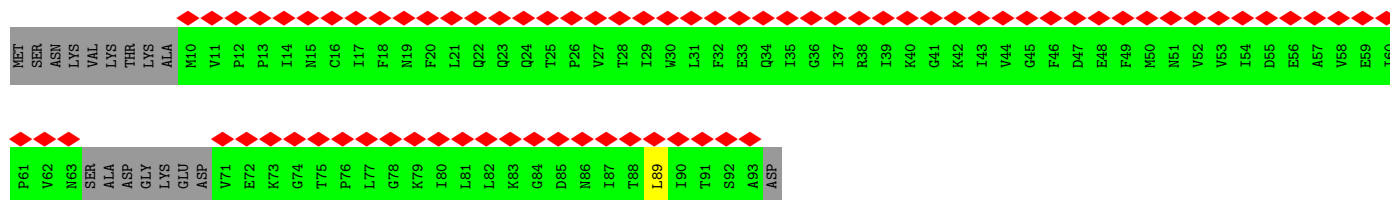
- Molecule 27: Small nuclear ribonucleoprotein E

Chain e:  9% 79% 18%




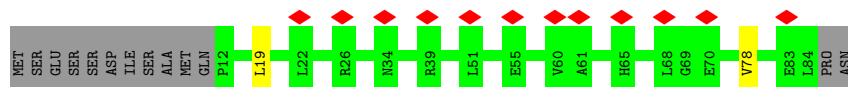
- Molecule 27: Small nuclear ribonucleoprotein E

Chain w:  82% 81% 18%




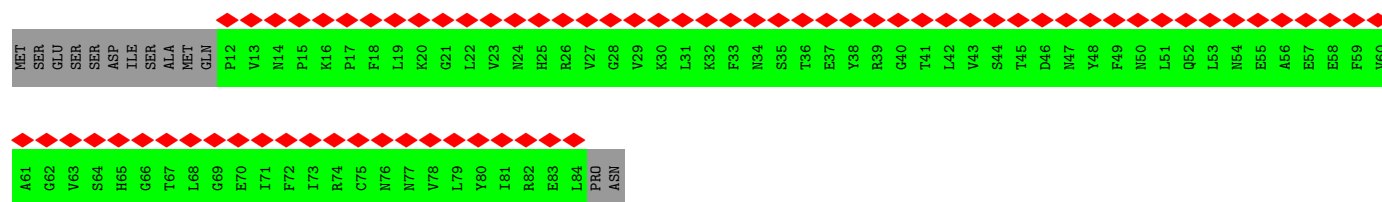
- Molecule 28: Small nuclear ribonucleoprotein F

Chain f:  14% 83% 15%

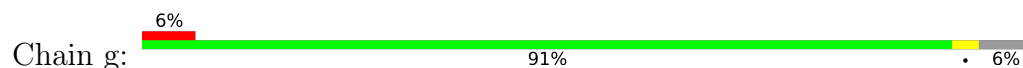


- Molecule 28: Small nuclear ribonucleoprotein F

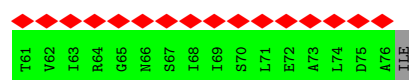
Chain x:  85% 85% 15%



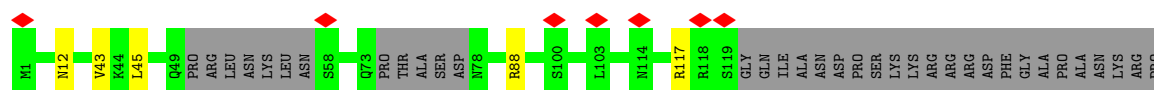
• Molecule 29: Small nuclear ribonucleoprotein G



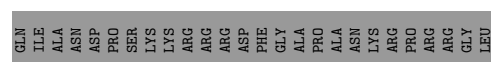
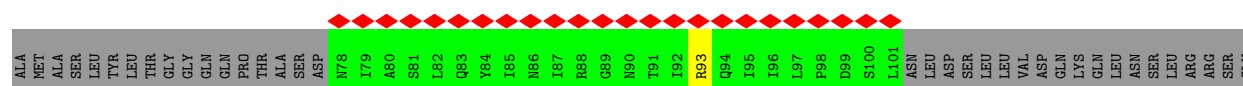
• Molecule 29: Small nuclear ribonucleoprotein G



• Molecule 30: Small nuclear ribonucleoprotein Sm D1

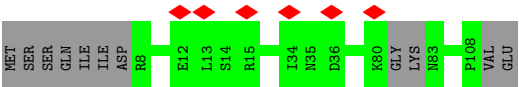
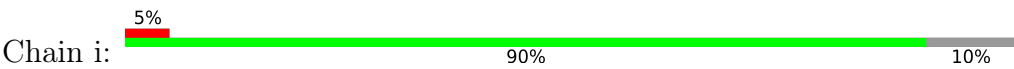


• Molecule 30: Small nuclear ribonucleoprotein Sm D1

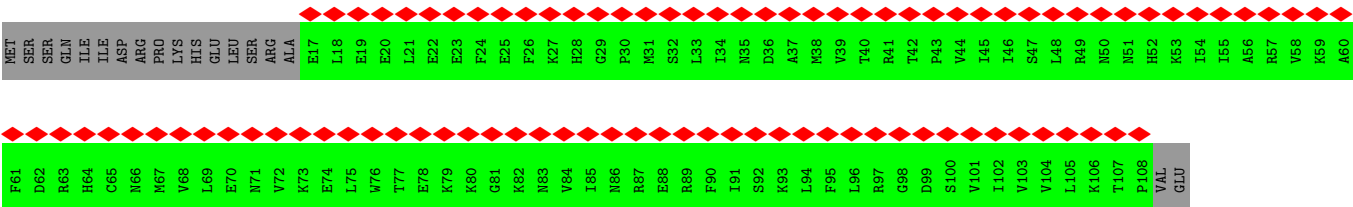
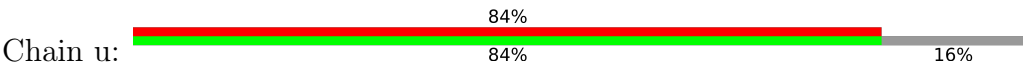


• Molecule 31: Small nuclear ribonucleoprotein Sm D2





• Molecule 31: Small nuclear ribonucleoprotein Sm D2



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	153556	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 ( $e^-/\text{\AA}^2$ )	43	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	105000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.152	Depositor
Minimum map value	-0.083	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0369	Depositor
Map size (Å)	632.8, 632.8, 632.8	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.13, 1.13, 1.13	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1	0.76	0/6890	1.31	72/10700 (0.7%)
2	2	1.40	52/3302 (1.6%)	1.72	120/5123 (2.3%)
3	A	0.28	0/388	0.60	1/535 (0.2%)
4	B	0.45	0/1325	0.79	2/1784 (0.1%)
5	C	0.57	0/1348	0.76	2/1825 (0.1%)
6	D	0.51	0/3499	0.71	7/4772 (0.1%)
7	E	0.77	4/4688 (0.1%)	0.94	26/6331 (0.4%)
8	F	0.65	0/1361	0.89	3/1843 (0.2%)
9	G	0.58	0/1716	0.74	1/2314 (0.0%)
10	H	0.49	0/816	0.69	0/1094
11	I	0.48	0/878	0.93	0/1357
12	J	0.50	0/331	0.78	0/448
13	O	0.28	0/6745	0.45	0/9157
14	P	0.30	1/9623 (0.0%)	0.53	1/13041 (0.0%)
15	Q	0.27	0/1835	0.46	0/2480
16	R	0.26	0/1453	0.42	0/1954
17	S	0.29	0/827	0.46	0/1105
18	T	0.27	0/3992	0.41	0/5346
19	U	0.24	0/1403	0.40	0/1889
20	V	0.24	0/1105	0.36	0/1475
21	W	0.41	0/1406	0.69	4/1905 (0.2%)
23	Y	0.30	0/692	0.54	0/923
24	Z	0.28	0/694	0.47	0/929
25	b	0.65	1/978 (0.1%)	0.93	4/1306 (0.3%)
25	s	0.39	0/521	0.62	0/701
26	d	0.68	1/726 (0.1%)	0.83	1/984 (0.1%)
26	v	0.43	0/641	0.65	2/868 (0.2%)
27	e	0.58	0/610	0.79	0/826
27	w	0.40	0/612	0.61	1/830 (0.1%)
28	f	0.63	1/597 (0.2%)	0.89	2/807 (0.2%)
28	x	0.42	0/597	0.63	0/807
29	g	0.63	0/559	0.83	0/751

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
29	y	0.26	0/582	0.49	0/785
30	h	0.52	0/839	0.77	2/1132 (0.2%)
30	t	0.42	0/574	0.68	1/777 (0.1%)
31	i	0.57	0/818	0.75	0/1099
31	u	0.40	0/764	0.57	0/1026
All	All	0.57	60/65735 (0.1%)	0.84	252/91029 (0.3%)

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
2	2	0	1
4	B	0	3
5	C	0	3
6	D	0	5
7	E	0	12
8	F	0	8
9	G	0	1
10	H	0	1
14	P	0	2
18	T	0	1
21	W	0	1
27	e	0	1
29	g	0	1
30	h	0	1
All	All	0	41

The worst 5 of 60 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1149	G	O3'-P	24.38	1.90	1.61
2	2	143	G	O3'-P	18.83	1.83	1.61
2	2	1161	U	O3'-P	-15.58	1.42	1.61
2	2	143	G	C3'-O3'	15.30	1.63	1.42
2	2	1092	A	O3'-P	-14.80	1.43	1.61

The worst 5 of 252 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	144	G	C4'-C3'-O3'	-16.52	74.71	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1162	U	C5'-C4'-O4'	14.81	126.87	109.10
2	2	1093	C	P-O5'-C5'	14.80	144.59	120.90
2	2	1147	A	C5'-C4'-C3'	-14.18	93.31	116.00
2	2	1092	A	C2'-C3'-O3'	14.12	140.56	109.50

There are no chirality outliers.

5 of 41 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	2	141	A	Sidechain
4	B	166	LYS	Peptide
4	B	170	VAL	Peptide
4	B	43	GLY	Peptide
5	C	103	ASP	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	
3	A	72/298 (24%)	59 (82%)	12 (17%)	1 (1%)	9	40
4	B	158/300 (53%)	135 (85%)	22 (14%)	1 (1%)	22	58
5	C	171/231 (74%)	152 (89%)	18 (10%)	1 (1%)	22	58
6	D	475/629 (76%)	435 (92%)	37 (8%)	3 (1%)	22	58
7	E	539/544 (99%)	482 (89%)	44 (8%)	13 (2%)	5	31
8	F	165/523 (32%)	142 (86%)	17 (10%)	6 (4%)	3	24
9	G	204/492 (42%)	186 (91%)	18 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	H	94/261 (36%)	89 (95%)	5 (5%)	0	100	100
12	J	40/620 (6%)	34 (85%)	6 (15%)	0	100	100
13	O	829/971 (85%)	788 (95%)	41 (5%)	0	100	100
14	P	1170/1361 (86%)	1059 (90%)	104 (9%)	7 (1%)	22	58
15	Q	214/435 (49%)	202 (94%)	11 (5%)	1 (0%)	25	61
16	R	165/213 (78%)	162 (98%)	3 (2%)	0	100	100
17	S	101/107 (94%)	88 (87%)	13 (13%)	0	100	100
18	T	454/530 (86%)	416 (92%)	38 (8%)	0	100	100
19	U	168/266 (63%)	143 (85%)	24 (14%)	1 (1%)	22	58
20	V	123/280 (44%)	112 (91%)	11 (9%)	0	100	100
21	W	168/238 (71%)	129 (77%)	28 (17%)	11 (6%)	1	16
23	Y	82/111 (74%)	76 (93%)	5 (6%)	1 (1%)	11	43
24	Z	81/85 (95%)	76 (94%)	4 (5%)	1 (1%)	11	43
25	b	117/196 (60%)	108 (92%)	9 (8%)	0	100	100
25	s	61/196 (31%)	58 (95%)	3 (5%)	0	100	100
26	d	91/101 (90%)	87 (96%)	4 (4%)	0	100	100
26	v	80/101 (79%)	77 (96%)	3 (4%)	0	100	100
27	e	73/94 (78%)	68 (93%)	4 (6%)	1 (1%)	9	40
27	w	73/94 (78%)	72 (99%)	1 (1%)	0	100	100
28	f	71/86 (83%)	66 (93%)	5 (7%)	0	100	100
28	x	71/86 (83%)	69 (97%)	2 (3%)	0	100	100
29	g	68/77 (88%)	61 (90%)	6 (9%)	1 (2%)	8	40
29	y	73/77 (95%)	64 (88%)	6 (8%)	3 (4%)	2	22
30	h	101/146 (69%)	97 (96%)	4 (4%)	0	100	100
30	t	68/146 (47%)	67 (98%)	1 (2%)	0	100	100
31	i	95/110 (86%)	90 (95%)	5 (5%)	0	100	100
31	u	90/110 (82%)	89 (99%)	1 (1%)	0	100	100
All	All	6605/10115 (65%)	6038 (91%)	515 (8%)	52 (1%)	19	53

5 of 52 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	D	426	ASN

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Mol	Chain	Res	Type
6	D	608	LEU
7	E	448	TYR
8	F	325	THR
8	F	385	SER

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	B	136/236 (58%)	135 (99%)	1 (1%)	81	86
5	C	127/214 (59%)	124 (98%)	3 (2%)	44	63
6	D	266/603 (44%)	266 (100%)	0	100	100
7	E	515/519 (99%)	512 (99%)	3 (1%)	84	88
8	F	148/451 (33%)	144 (97%)	4 (3%)	40	60
9	G	175/448 (39%)	174 (99%)	1 (1%)	84	88
10	H	84/183 (46%)	83 (99%)	1 (1%)	67	78
12	J	34/568 (6%)	33 (97%)	1 (3%)	37	58
13	O	739/867 (85%)	738 (100%)	1 (0%)	92	94
14	P	1093/1244 (88%)	1093 (100%)	0	100	100
15	Q	192/391 (49%)	192 (100%)	0	100	100
16	R	154/189 (82%)	154 (100%)	0	100	100
17	S	93/97 (96%)	93 (100%)	0	100	100
18	T	429/492 (87%)	424 (99%)	5 (1%)	67	78
19	U	158/216 (73%)	157 (99%)	1 (1%)	84	88
20	V	118/259 (46%)	116 (98%)	2 (2%)	56	72
21	W	161/219 (74%)	151 (94%)	10 (6%)	15	38
23	Y	76/100 (76%)	75 (99%)	1 (1%)	65	77
24	Z	75/77 (97%)	75 (100%)	0	100	100
25	b	108/176 (61%)	108 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	s	58/176 (33%)	58 (100%)	0	100	100
26	d	81/89 (91%)	80 (99%)	1 (1%)	67	78
26	v	71/89 (80%)	71 (100%)	0	100	100
27	e	68/83 (82%)	67 (98%)	1 (2%)	60	75
27	w	69/83 (83%)	69 (100%)	0	100	100
28	f	65/77 (84%)	65 (100%)	0	100	100
28	x	65/77 (84%)	65 (100%)	0	100	100
29	g	62/66 (94%)	62 (100%)	0	100	100
29	y	64/66 (97%)	64 (100%)	0	100	100
30	h	96/129 (74%)	94 (98%)	2 (2%)	48	66
30	t	67/129 (52%)	67 (100%)	0	100	100
31	i	90/103 (87%)	90 (100%)	0	100	100
31	u	85/103 (82%)	85 (100%)	0	100	100
All	All	5822/8819 (66%)	5784 (99%)	38 (1%)	80	86

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
21	W	36	LEU
27	e	10	MET
21	W	41	GLU
21	W	160	THR
30	h	117	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 99 such sidechains are listed below:

Mol	Chain	Res	Type
14	P	1117	HIS
18	T	415	HIS
14	P	1203	HIS
16	R	50	GLN
21	W	99	GLN

### 5.3.3 RNA ⓘ



Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	281/407 (69%)	66 (23%)	12 (4%)
11	I	35/38 (92%)	8 (22%)	2 (5%)
2	2	136/143 (95%)	46 (33%)	25 (18%)
All	All	452/588 (76%)	120 (26%)	39 (8%)

5 of 120 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	8	C
1	1	11	U
1	1	12	A
1	1	17	A
1	1	21	G

5 of 39 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	2	1122	U
2	2	1144	U
2	2	1123	C
2	2	1138	G
11	I	77	C

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

5 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	1	5	1	18,21,22	1.47	2 (11%)	22,30,33	1.25	2 (9%)
2	PSU	2	35	11,2	18,21,22	1.06	1 (5%)	22,30,33	1.72	5 (22%)
2	PSU	2	42	11,2	18,21,22	1.09	1 (5%)	22,30,33	1.72	4 (18%)
2	PSU	2	44	11,2	18,21,22	1.03	1 (5%)	22,30,33	1.66	4 (18%)
1	PSU	1	6	11,1	18,21,22	1.35	1 (5%)	22,30,33	1.21	2 (9%)

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	1	5	1	-	0/7/25/26	0/2/2/2
2	PSU	2	35	11,2	-	0/7/25/26	0/2/2/2
2	PSU	2	42	11,2	-	0/7/25/26	0/2/2/2
2	PSU	2	44	11,2	-	0/7/25/26	0/2/2/2
1	PSU	1	6	11,1	-	0/7/25/26	0/2/2/2

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	5	PSU	C2-N1	4.33	1.42	1.36
1	1	6	PSU	C2-N1	3.91	1.42	1.36
2	2	42	PSU	C6-C5	3.50	1.39	1.35
2	2	35	PSU	C6-C5	3.33	1.39	1.35
2	2	44	PSU	C6-C5	3.25	1.39	1.35

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	42	PSU	C4-N3-C2	-4.58	119.74	126.34
2	2	35	PSU	C4-N3-C2	-4.47	119.90	126.34
2	2	42	PSU	N1-C2-N3	4.38	120.09	115.13
2	2	35	PSU	N1-C2-N3	4.36	120.07	115.13
2	2	44	PSU	N1-C2-N3	4.32	120.02	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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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
2	2	10
1	1	4
11	I	2
10	H	2
22	X	1

The worst 5 of 19 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	10:A	O3'	51:C	P	64.91
1	1	440:N	O3'	516:U	P	49.12
1	1	325:A	O3'	378:N	P	48.87
1	2	122:A	O3'	139:G	P	46.36
1	1	532:U	O3'	538:C	P	25.27

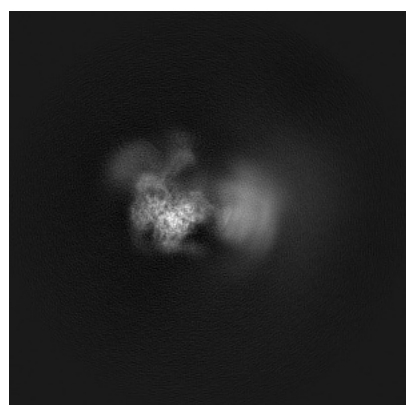
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4364. These allow visual inspection of the internal detail of the map and identification of artifacts.

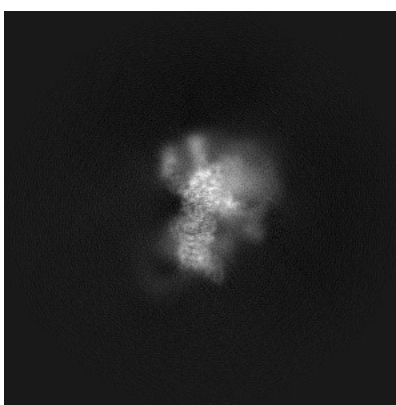
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

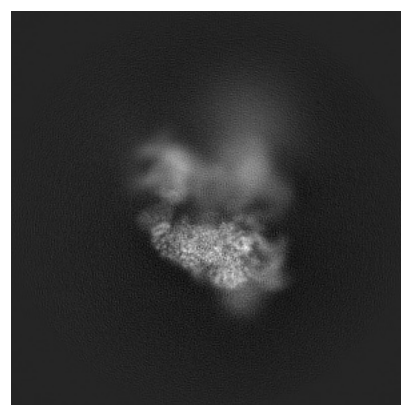
#### 6.1.1 Primary map



X



Y

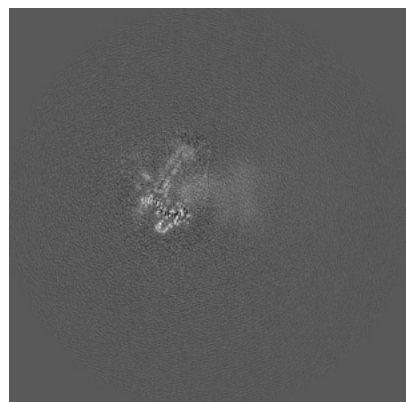


Z

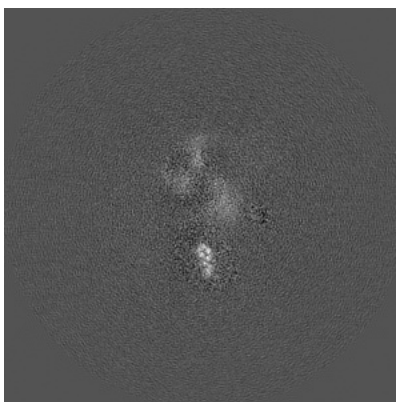
The images above show the map projected in three orthogonal directions.

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

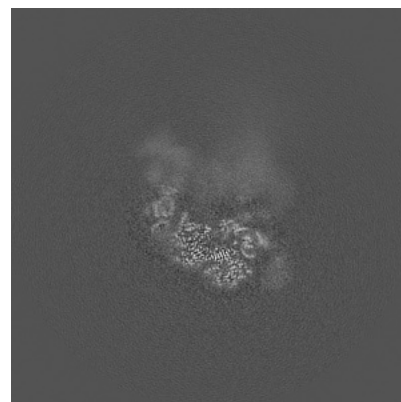
#### 6.2.1 Primary map



X Index: 280



Y Index: 280

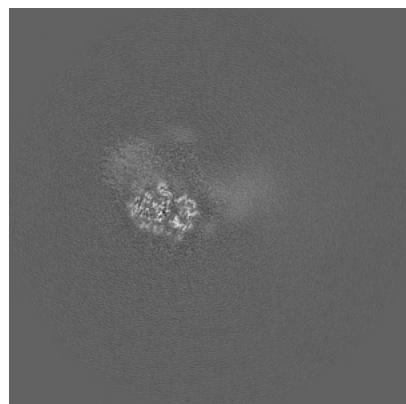


Z Index: 280

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

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

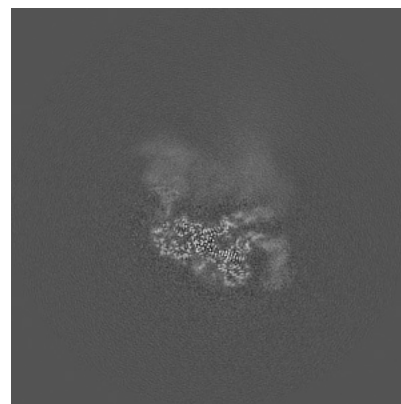
### 6.3.1 Primary map



X Index: 303



Y Index: 225

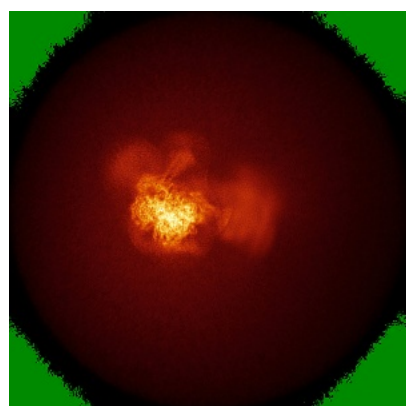


Z Index: 271

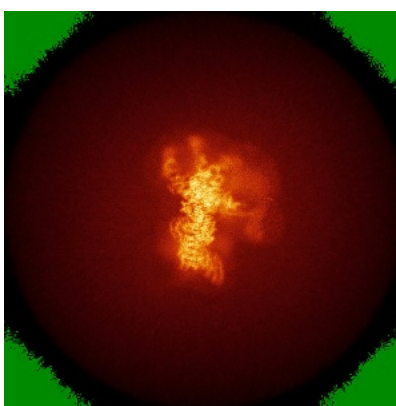
The images above show the largest variance slices of the map in three orthogonal directions.

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

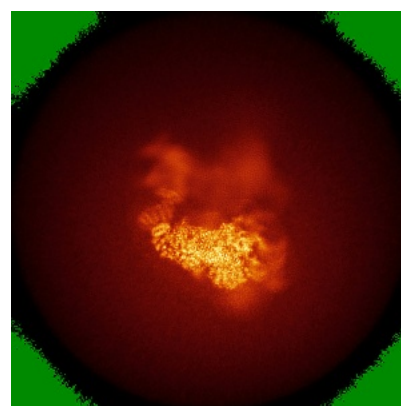
### 6.4.1 Primary map



X



Y

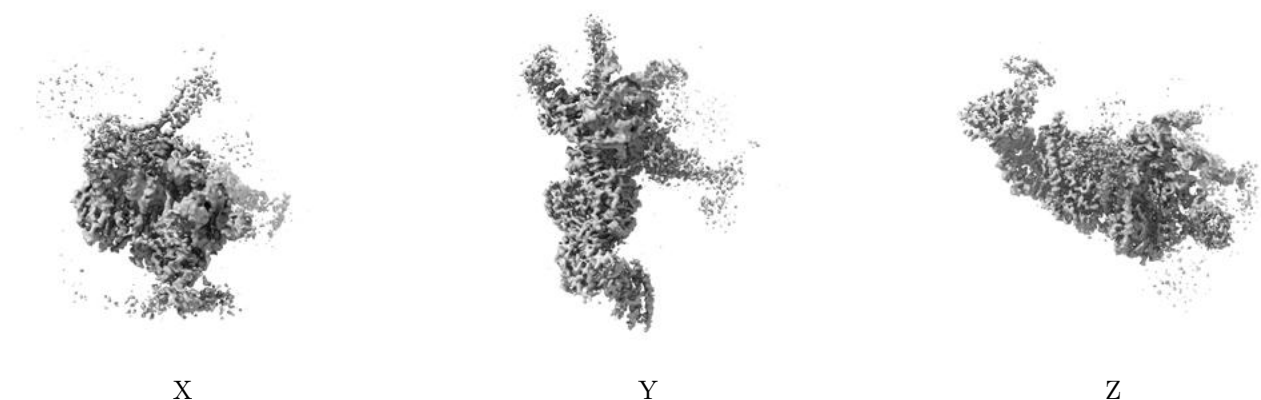


Z

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

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0369. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

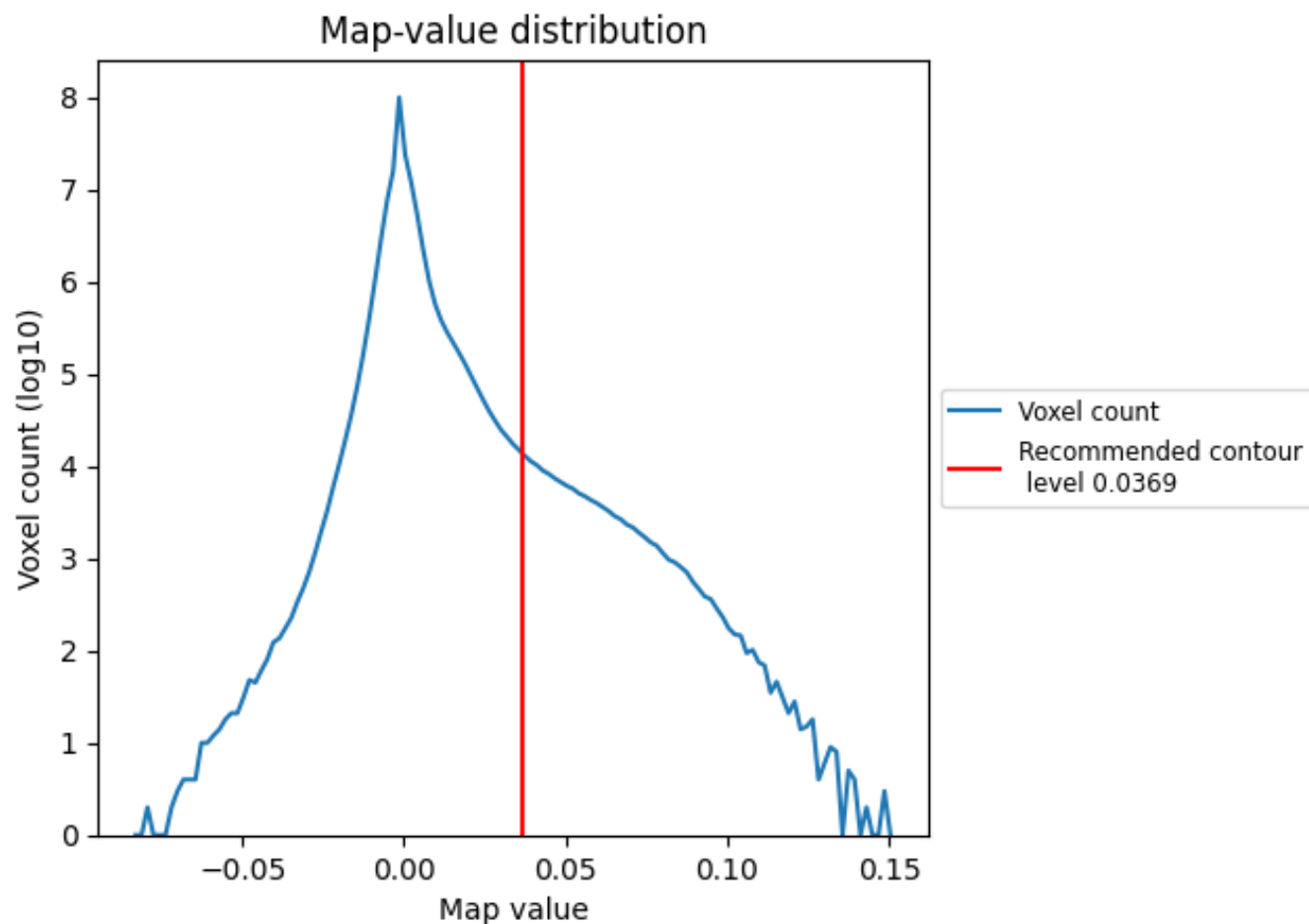
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

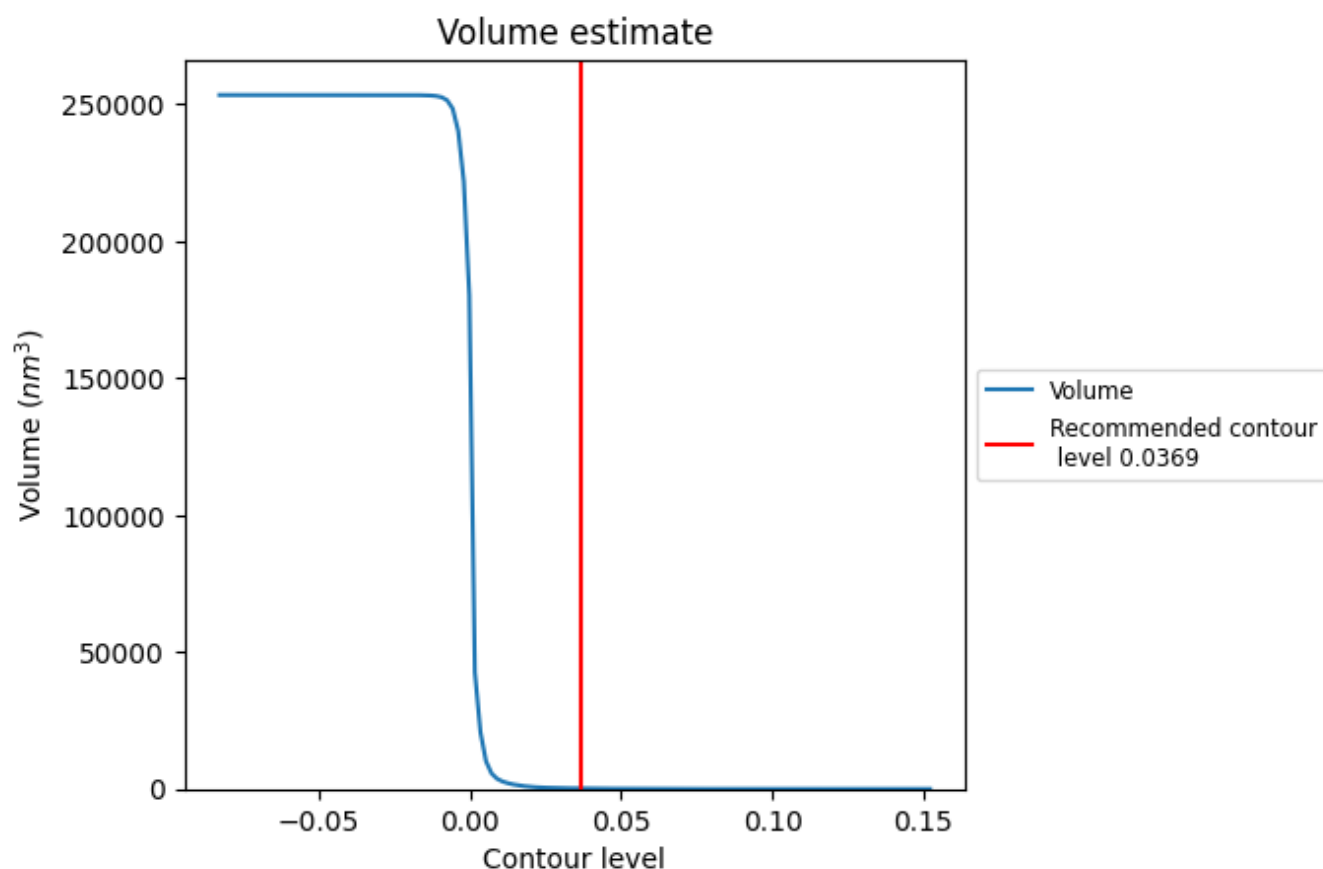
This section contains the results of statistical analysis of the map.

### 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](#)

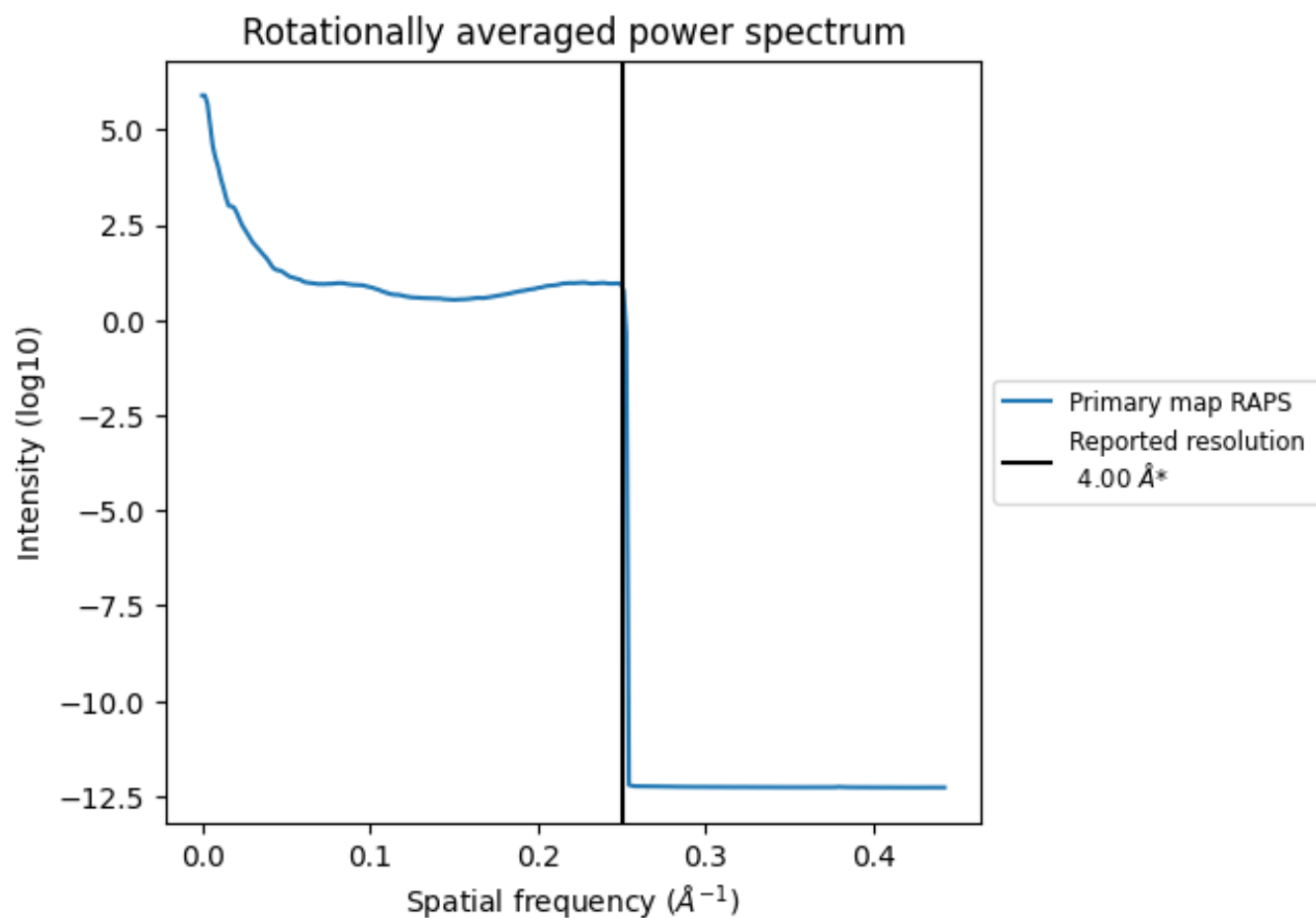


The volume at the recommended contour level is 189  $\text{nm}^3$ ; this corresponds to an approximate mass of 171 kDa.

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 0.250 Å<sup>-1</sup>

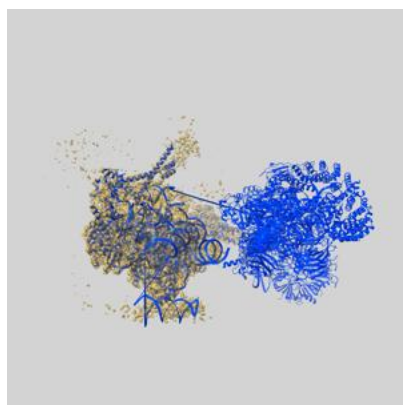
## 8 Fourier-Shell correlation

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

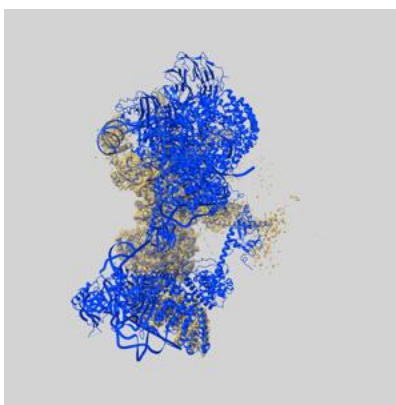
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4364 and PDB model 6G90. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

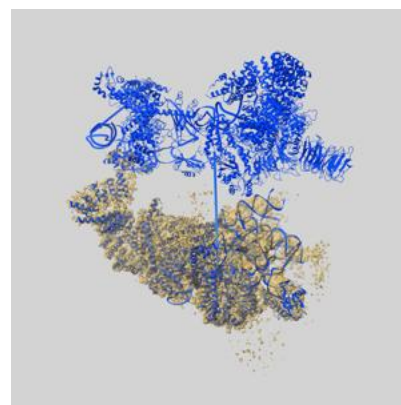
### 9.1 Map-model overlay [i](#)



X



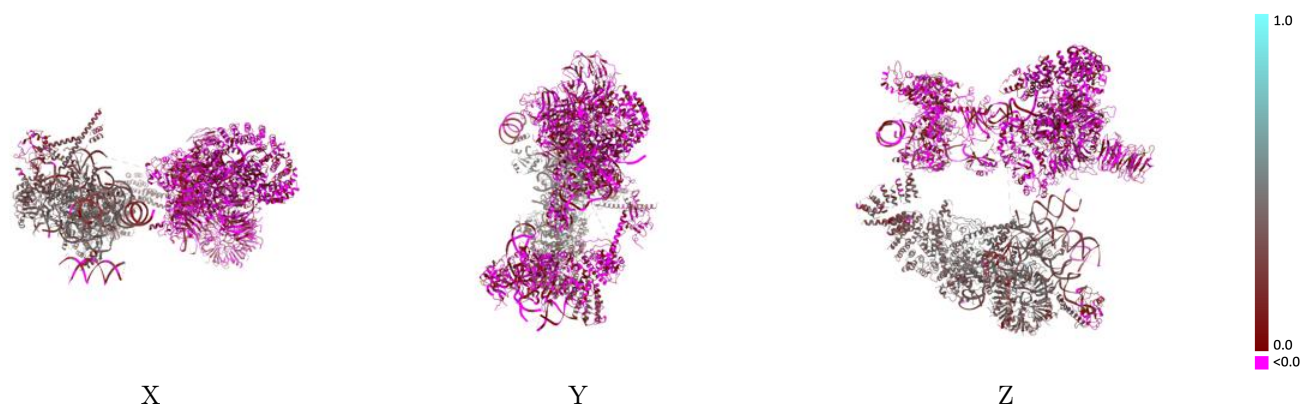
Y



Z

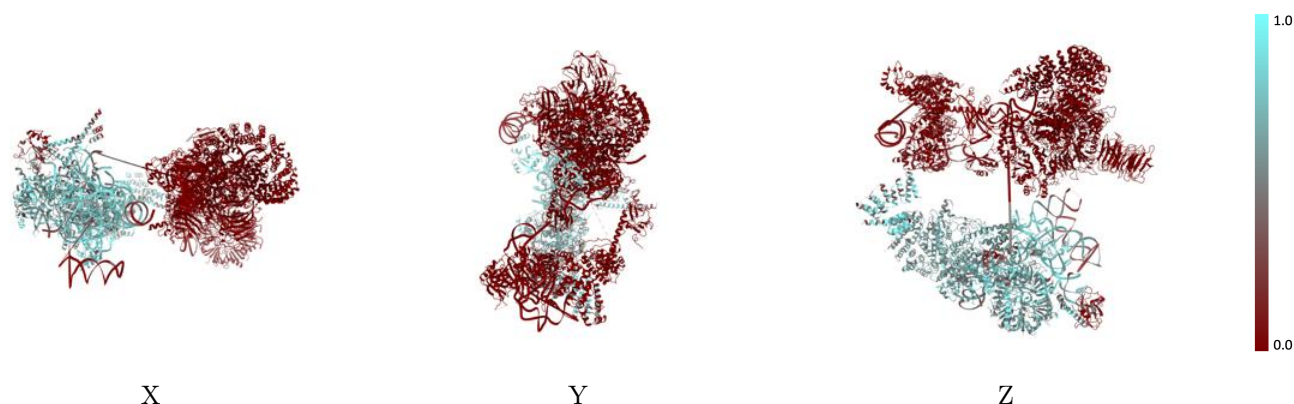
The images above show the 3D surface view of the map at the recommended contour level 0.0369 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



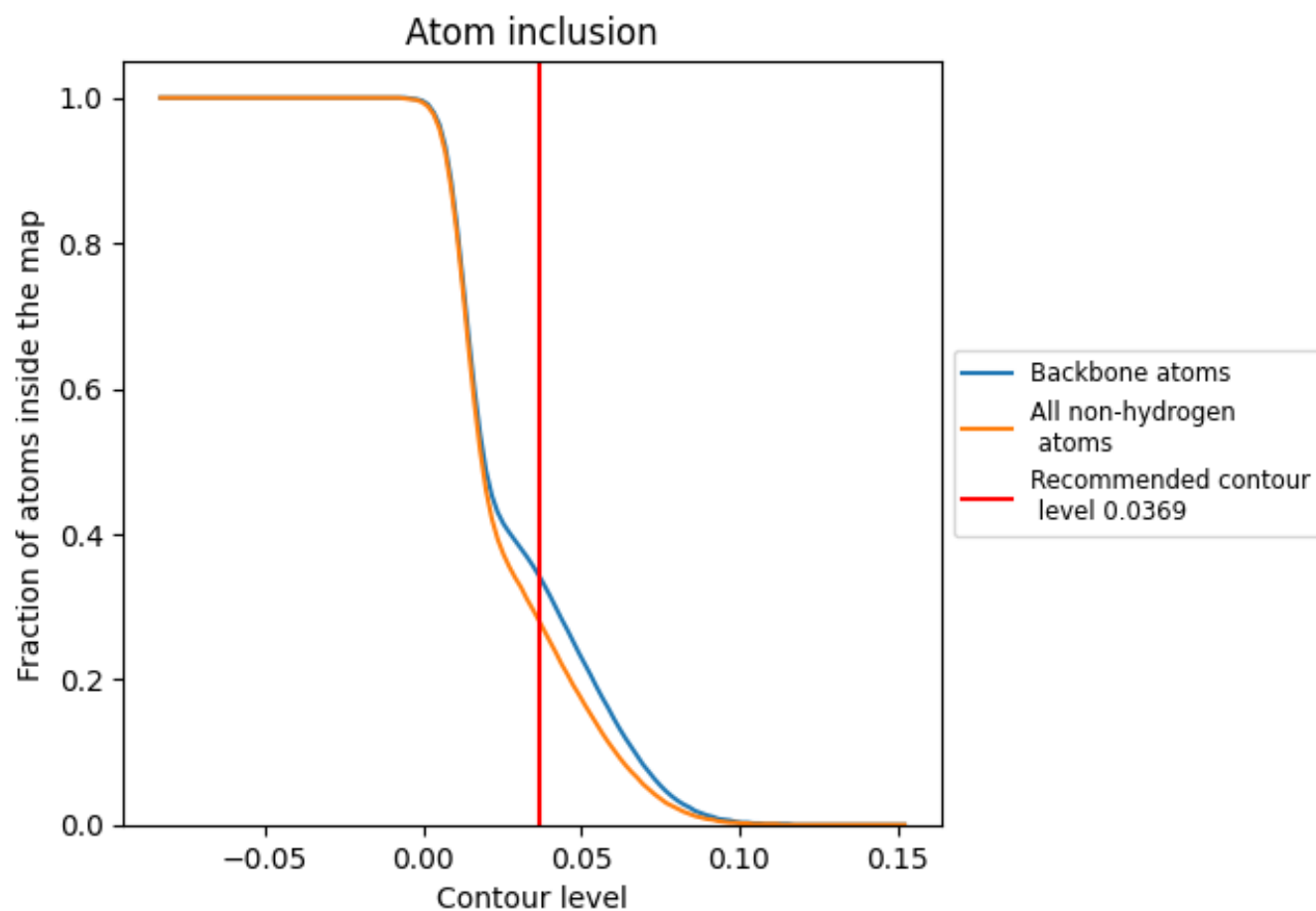
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0369).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 34% of all backbone atoms, 28% 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 (0.0369) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.2790	 0.1520
1	 0.6780	 0.2970
2	 0.0000	 0.0010
A	 0.7990	 0.3950
B	 0.3390	 0.1890
C	 0.6650	 0.4050
D	 0.6580	 0.3440
E	 0.6800	 0.3970
F	 0.6370	 0.3920
G	 0.6570	 0.3800
H	 0.5710	 0.3040
I	 0.2190	 0.0990
J	 0.7040	 0.4150
O	 0.0000	 -0.0020
P	 0.0000	 0.0010
Q	 0.0000	 -0.0020
R	 0.0000	 0.0120
S	 0.0000	 0.0090
T	 0.0000	 0.0070
U	 0.0000	 0.0040
V	 0.0000	 -0.0060
W	 0.0310	 0.0250
X	 0.6120	 0.3000
Y	 0.0210	 0.0230
Z	 0.0000	 0.0080
b	 0.6260	 0.4070
d	 0.6770	 0.4380
e	 0.6250	 0.3770
f	 0.6290	 0.3320
g	 0.6440	 0.4250
h	 0.6390	 0.3970
i	 0.6240	 0.3460
s	 0.0000	 -0.0080
t	 0.0000	 -0.0400
u	 0.0000	 0.0300



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Chain	Atom inclusion	Q-score
v	 0.0000	 0.0160
w	 0.0000	 -0.0150
x	 0.0000	 0.0370
y	 0.0000	 0.0090