



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 10:18 PM UTC

PDB ID : 8QXD / pdb_00008qxd
EMDB ID : EMD-18718
Title : Cryo-EM structure of the cross-exon pre-B complex
Authors : Zhang, Z.; Kumar, V.; Dybkov, O.; Will, C.L.; Zhong, J.; Ludwig, S.; Urlaub, H.; Kastner, B.; Stark, H.; Luehrmann, R.
Deposited on : 2023-10-24
Resolution : 9.60 Å(reported)

This is a Full wwPDB EM Validation 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
MolProbity : 4-5-2 with Phenix2.0
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

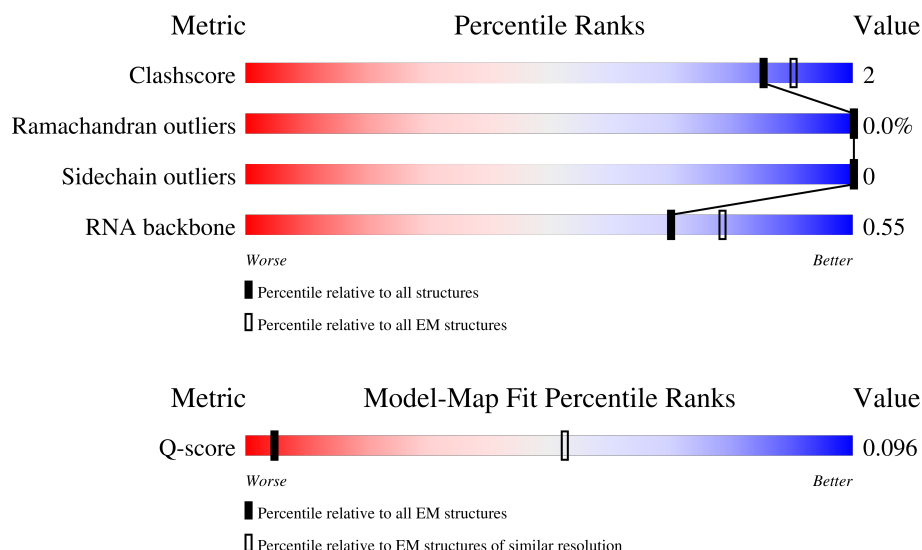
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 9.60 Å.

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



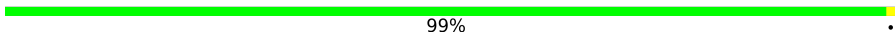
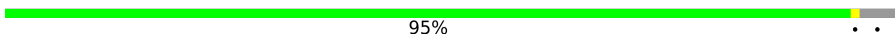
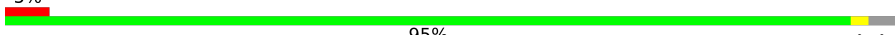
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	185 (9.10 - 10.10)

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	A	2335	 90% 7%
2	B	2136	 93% 6%
3	2	182	 8% 34% 16% 47%

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Mol	Chain	Length	Quality of chain
4	4	144	
5	5	115	
6	6	76	
7	7	793	
8	8	464	
9	C	972	
10	D	142	
11	E	357	
12	F	522	
13	M	128	
14	R	480	
15	U	565	
16	X	155	
17	Z	15	
18	S	800	
19	J	683	
20	K	1007	
21	N	941	
22	G	820	
23	L	499	
24	B4	424	
25	9	501	
26	B2	895	
27	B5	86	
28	B3	1217	

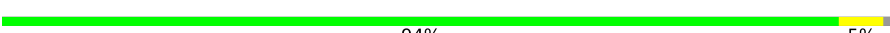
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Mol	Chain	Length	Quality of chain
29	BP	110	
30	B1	1304	
31	B6	125	
32	22	118	
32	42	118	
32	52	118	
33	2B	225	
34	2f	86	
34	4f	86	
34	5f	86	
35	2b	240	
36	23	126	
36	43	126	
36	53	126	
37	2g	76	
38	2e	92	
38	4e	92	
38	5e	92	
39	21	119	
39	41	119	
40	2A	255	
41	4b	82	
42	4g	74	
42	5g	74	
43	5b	86	

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Mol	Chain	Length	Quality of chain
44	51	82	 100%
45	66	80	 6%88%10%
46	67	103	 75%25%
47	62	95	 100%
48	63	102	 13%80%17%
49	68	96	 94%5%
50	64	139	 51%47%
51	65	91	 81%16%

2 Entry composition

There are 51 unique types of molecules in this entry. The entry contains 81571 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	2179	Total	C	N	O	0	0
			11054	6696	2179	2179		

- Molecule 2 is a protein called U5 small nuclear ribonucleoprotein 200 kDa helicase.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	2001	Total	C	N	O	0	0
			10078	6076	2001	2001		

- Molecule 3 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	97	Total	C	N	O	P	0	0
			2051	917	346	691	97		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	97	A	G	conflict	GB 36516

- Molecule 4 is a RNA chain called U4 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	124	Total	C	N	O	P	0	0
			2636	1179	466	868	123		

- Molecule 5 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	104	Total	C	N	O	P	0	0
			2192	983	372	734	103		

- Molecule 6 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	53	Total	C	N	O	P	0	0
			1133	506	203	371	53		

- Molecule 7 is a protein called Splicing factor 3A subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7	136	Total	C	N	O		0	0
			686	414	136	136			

- Molecule 8 is a protein called Splicing factor 3A subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	8	144	Total	C	N	O		0	0
			729	441	144	144			

- Molecule 9 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	852	Total	C	N	O		0	0
			4307	2603	852	852			

- Molecule 10 is a protein called Thioredoxin-like protein 4A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D	141	Total	C	N	O		0	0
			708	426	141	141			

- Molecule 11 is a protein called U5 small nuclear ribonucleoprotein 40 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	E	307	Total	C	N	O		0	0
			1531	917	307	307			

- Molecule 12 is a protein called U4/U6 small nuclear ribonucleoprotein Prp4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F	359	Total	C	N	O		0	0
			1795	1077	359	359			

- Molecule 13 is a protein called NHP2-like protein 1, N-terminally processed.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	123	Total	C	N	O	0	0
			622	376	123	123		

- Molecule 14 is a protein called RNA-binding protein 42.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	R	106	Total	C	N	O	0	0
			531	319	106	106		

- Molecule 15 is a protein called Ubiquitin carboxyl-terminal hydrolase 39.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	U	456	Total	C	N	O	0	0
			2308	1396	456	456		

- Molecule 16 is a protein called U4/U6.U5 small nuclear ribonucleoprotein 27 kDa protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	X	26	Total	C	N	O	0	0
			130	78	26	26		

- Molecule 17 is a RNA chain called pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Z	15	Total	C	N	O	P	0	0
			314	141	51	107	15		

- Molecule 18 is a protein called U4/U6.U5 tri-snRNP-associated protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	S	108	Total	C	N	O	0	0
			539	323	108	108		

- Molecule 19 is a protein called U4/U6 small nuclear ribonucleoprotein Prp3.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	J	196	Total	C	N	O	0	0
			991	599	196	196		

- Molecule 20 is a protein called Serine/threonine-protein kinase PRP4 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	K	322	Total	C	N	O	0	0
			1615	971	322	322		

- Molecule 21 is a protein called Pre-mRNA-processing factor 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	N	801	Total	C	N	O	0	0
			4030	2428	801	801		

- Molecule 22 is a protein called Probable ATP-dependent RNA helicase DDX23.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	G	585	Total	C	N	O	7	0
			2987	1803	592	592		

- Molecule 23 is a protein called U4/U6 small nuclear ribonucleoprotein Prp31.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	L	301	Total	C	N	O	0	0
			1510	908	301	301		

- Molecule 24 is a protein called Splicing factor 3B subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	B4	78	Total	C	N	O	0	0
			391	235	78	78		

- Molecule 25 is a protein called Splicing factor 3A subunit 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	9	383	Total	C	N	O	0	0
			1920	1154	383	383		

- Molecule 26 is a protein called Splicing factor 3B subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	B2	208	Total	C	N	O	0	0
			1072	656	208	208		

- Molecule 27 is a protein called Splicing factor 3B subunit 5.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	B5	69	Total	C	N	O	0	0
			347	209	69	69		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
28	B3	1186	Total	C	N	O	0	0
			5969	3597	1186	1186		

- Molecule 29 is a protein called PHD finger-like domain-containing protein 5A.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	BP	100	Total	C	N	O	0	0
			498	298	100	100		

- Molecule 30 is a protein called Splicing factor 3B subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	B1	870	Total	C	N	O	0	0
			4383	2643	870	870		

- Molecule 31 is a protein called Splicing factor 3B subunit 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	B6	90	Total	C	N	O	0	0
			455	275	90	90		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
32	22	95	Total	C	N	O	0	0
			482	292	95	95		
32	42	92	Total	C	N	O	0	0
			463	279	92	92		
32	52	97	Total	C	N	O	0	0
			388	194	97	97		

- Molecule 33 is a protein called U2 small nuclear ribonucleoprotein B''.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	2B	92	Total	C	N	O	0	0
			461	277	92	92		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
34	2f	72	Total	C	N	O	0	0
			359	215	72	72		
34	4f	72	Total	C	N	O	0	0
			359	215	72	72		
34	5f	74	Total	C	N	O	0	0
			296	148	74	74		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
35	2b	82	Total	C	N	O	0	0
			413	249	82	82		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
36	23	83	Total	C	N	O	0	0
			415	249	83	83		
36	43	83	Total	C	N	O	0	0
			415	249	83	83		
36	53	77	Total	C	N	O	0	0
			308	154	77	77		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
37	2g	73	Total	C	N	O	0	0
			364	218	73	73		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
38	2e	81	Total	C	N	O	0	0
			403	241	81	81		
38	4e	76	Total	C	N	O	0	0
			378	226	76	76		
38	5e	79	Total	C	N	O	0	0
			316	158	79	79		

- Molecule 39 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	21	80	Total	C	N	O	0	0
			402	242	80	80		
39	41	81	Total	C	N	O	0	0
			407	245	81	81		

- Molecule 40 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	2A	162	Total	C	N	O	0	0
			816	492	162	162		

- Molecule 41 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	4b	82	Total	C	N	O	0	0
			413	249	82	82		

- Molecule 42 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	4g	74	Total	C	N	O	0	0
			369	221	74	74		
42	5g	74	Total	C	N	O	0	0
			296	148	74	74		

- Molecule 43 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	5b	86	Total	C	N	O	0	0
			344	172	86	86		

- Molecule 44 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	51	82	Total	C	N	O	0	0
			328	164	82	82		

- Molecule 45 is a protein called U6 snRNA-associated Sm-like protein LSm6.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	66	72	Total	C	N	O	0	0
			357	213	72	72		

- Molecule 46 is a protein called U6 snRNA-associated Sm-like protein LSm7.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	67	77	Total	C	N	O	0	0
			384	230	77	77		

- Molecule 47 is a protein called U6 snRNA-associated Sm-like protein LSm2.

Mol	Chain	Residues	Atoms				AltConf	Trace
47	62	95	Total	C	N	O	0	0
			478	288	95	95		

- Molecule 48 is a protein called U6 snRNA-associated Sm-like protein LSm3.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	63	85	Total	C	N	O	0	0
			429	259	85	85		

- Molecule 49 is a protein called U6 snRNA-associated Sm-like protein LSm8.

Mol	Chain	Residues	Atoms				AltConf	Trace
49	68	95	Total	C	N	O	0	0
			469	279	95	95		

- Molecule 50 is a protein called U6 snRNA-associated Sm-like protein LSm4.

Mol	Chain	Residues	Atoms				AltConf	Trace
50	64	73	Total	C	N	O	0	0
			369	223	73	73		

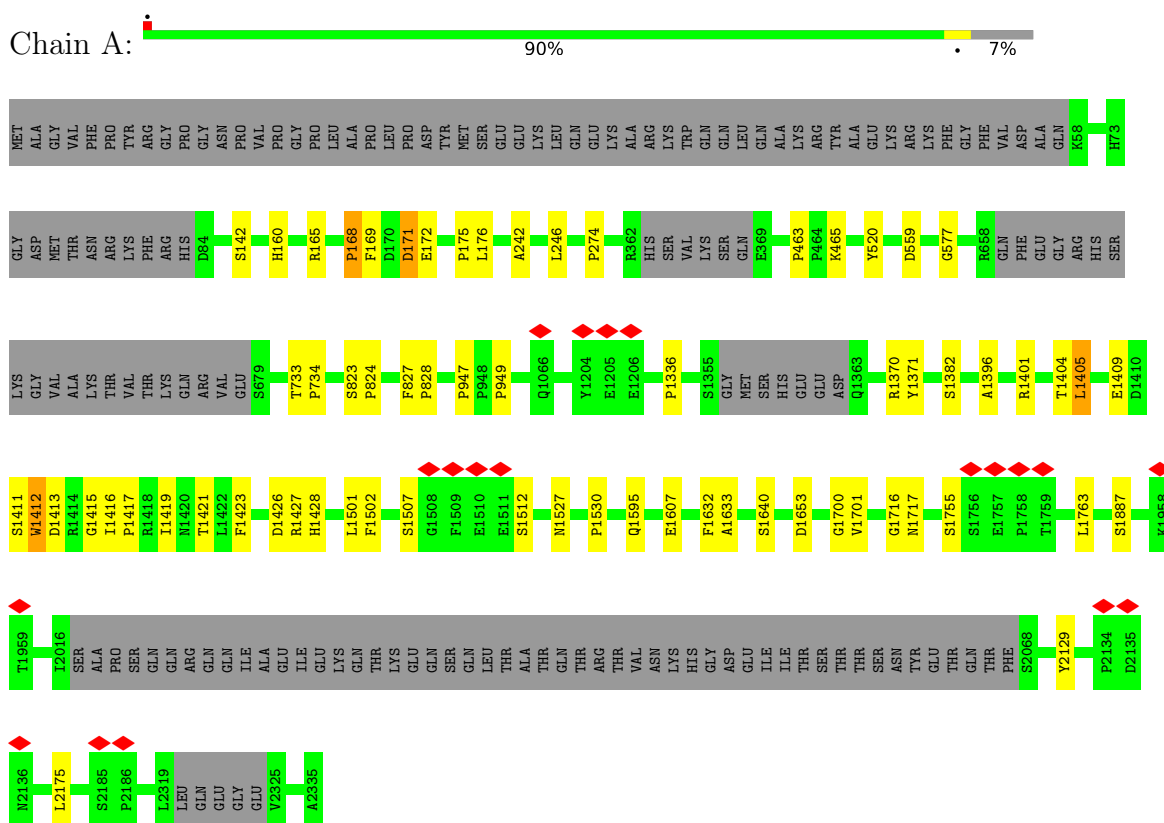
- Molecule 51 is a protein called U6 snRNA-associated Sm-like protein LSm5.

Mol	Chain	Residues	Atoms				AltConf	Trace
51	65	76	Total	C	N	O	0	0
			378	226	76	76		

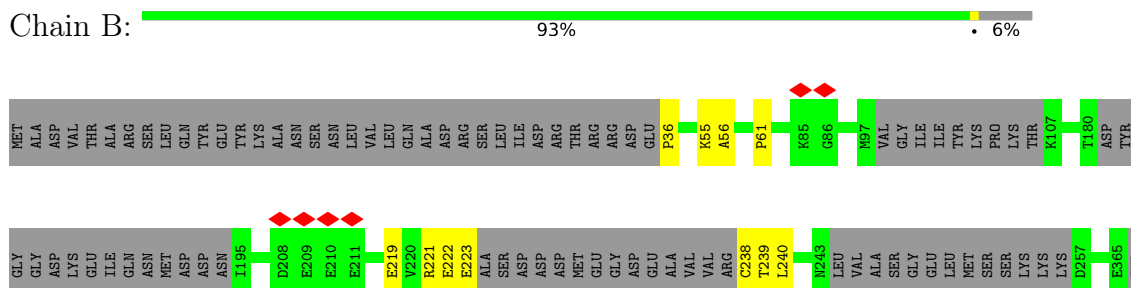
3 Residue-property plots

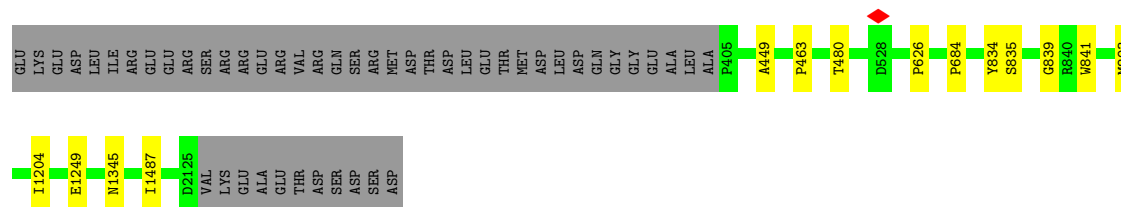
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Pre-mRNA-processing-splicing factor 8

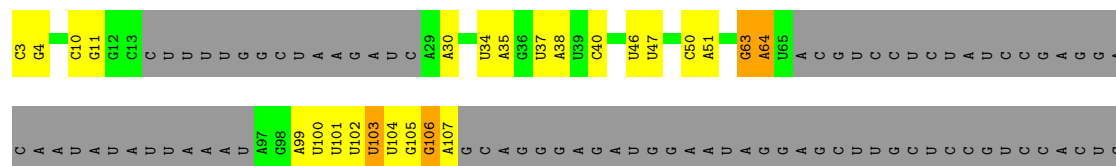
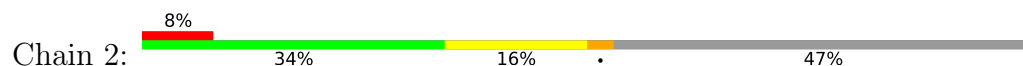


- Molecule 2: U5 small nuclear ribonucleoprotein 200 kDa helicase

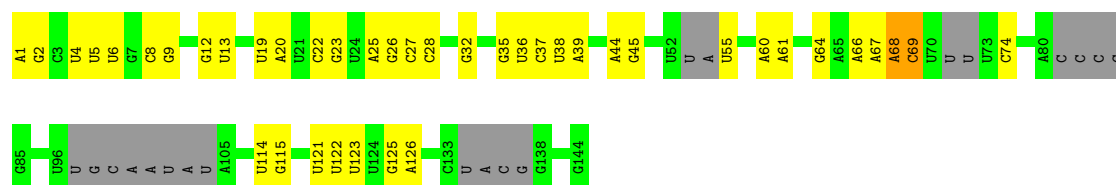




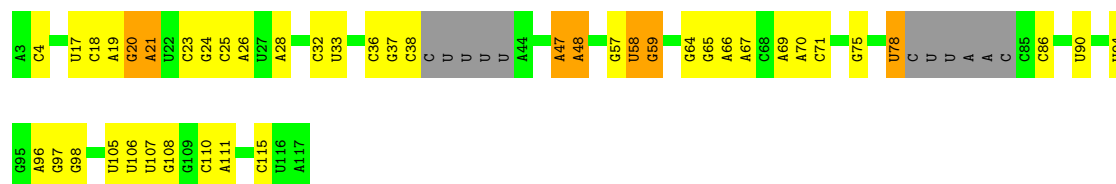
• Molecule 3: U2 snRNA



• Molecule 4: U4 snRNA



• Molecule 5: U5 snRNA



• Molecule 6: U6 snRNA



• Molecule 7: Splicing factor 3A subunit 1



ASP	GLY	SER	VAL	ASN	A126	Q133	K134	R135	K136	L151	ASP	PHE	ILE	ALA
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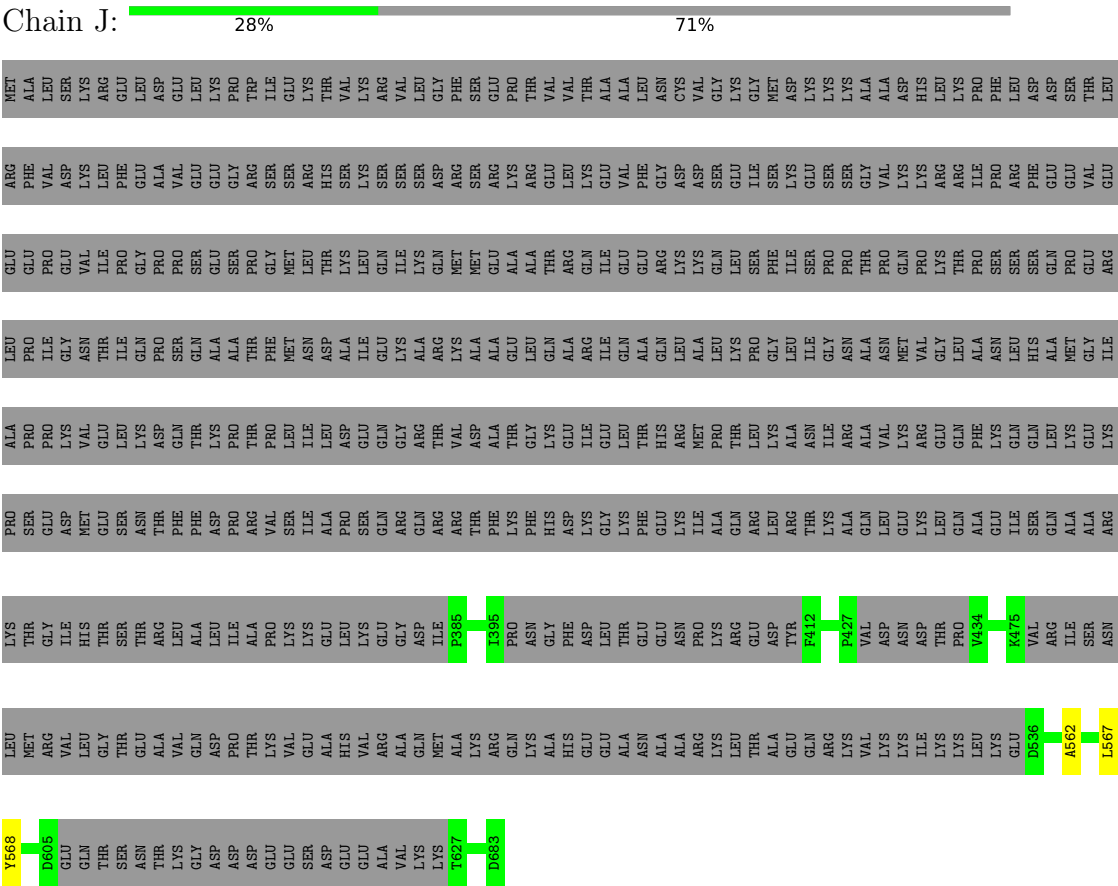
- Chain Z: 93% 7%

G29	A41	U42	C43
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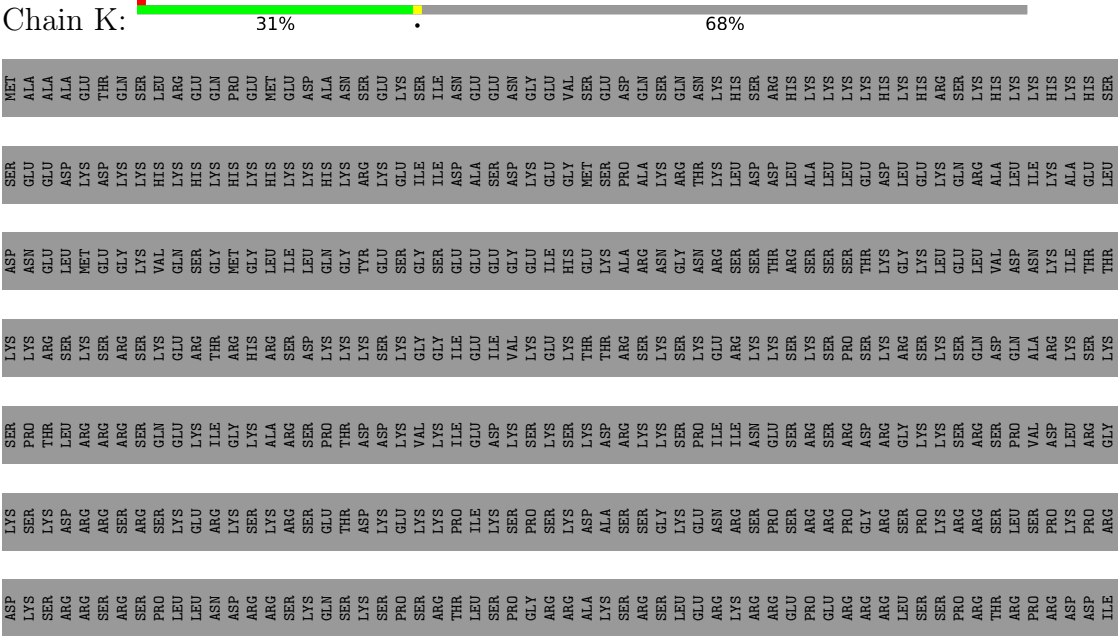
- Chain S: 14% 86%

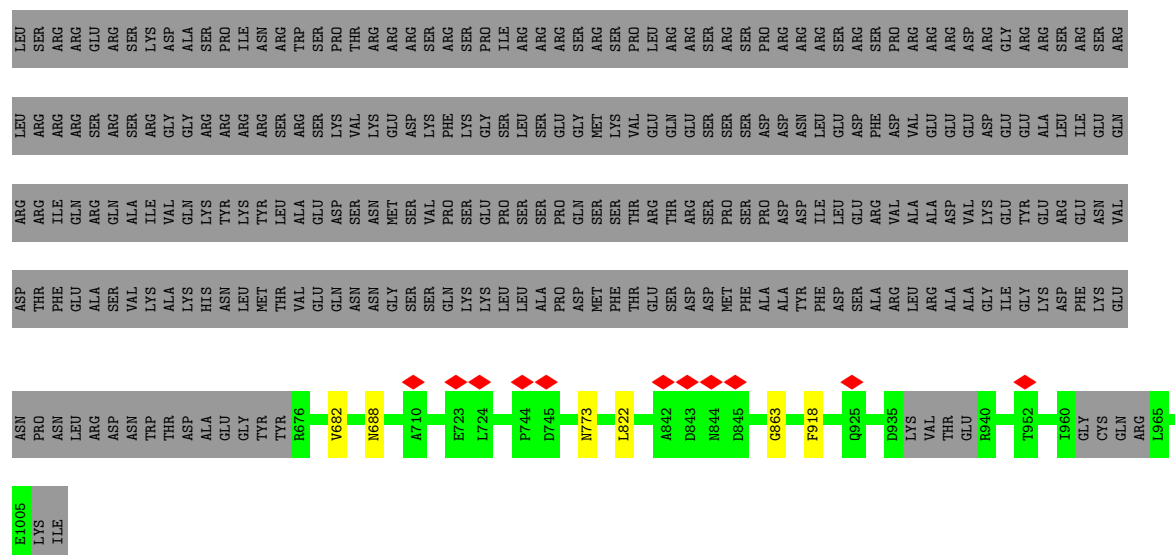
THR	GLN	ASP	PHE	LYS	GLU	T701	T716	T717	T718	T719	T720	T721	T750	T759	SER	SER	SER	ASP	THR	THR	PRO	T766	T774	LYS	GLN	LYS	ALA	GLN	LEU	SER	SER	GLY	LYS	GLY	LYS	THR	THR	THR	LYS
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● Molecule 19: U4/U6 small nuclear ribonucleoprotein Prp3

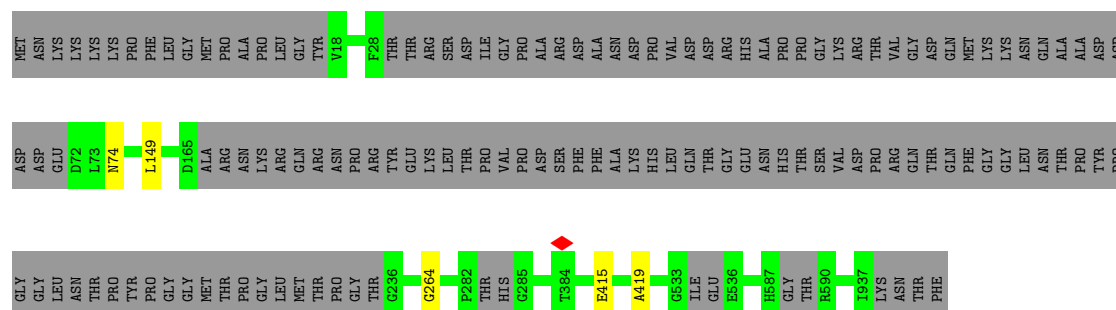
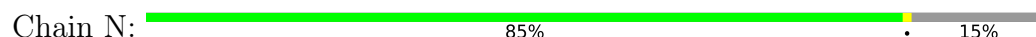


● Molecule 20: Serine/threonine-protein kinase PRP4 homolog

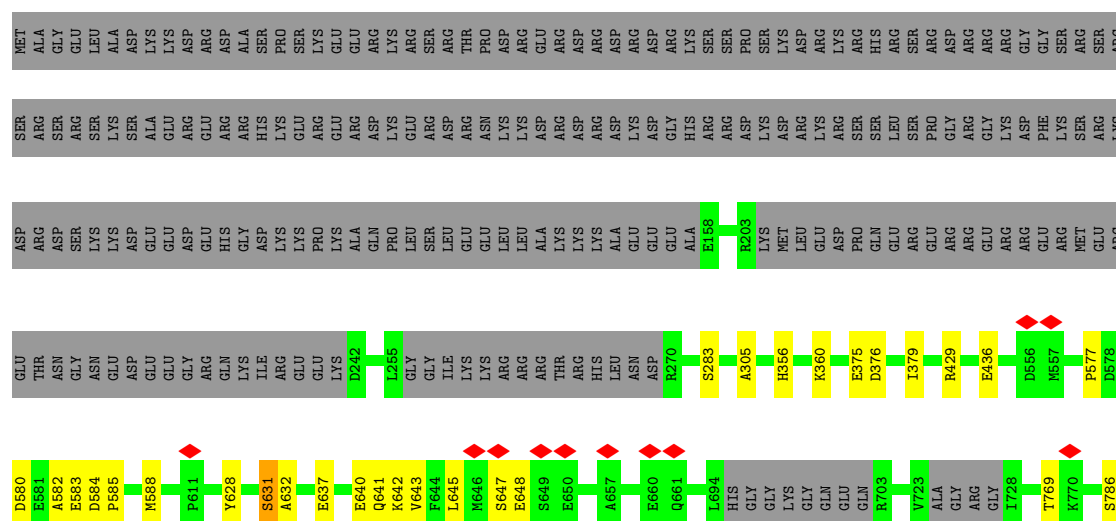


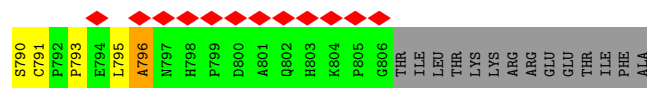


- Molecule 21: Pre-mRNA-processing factor 6



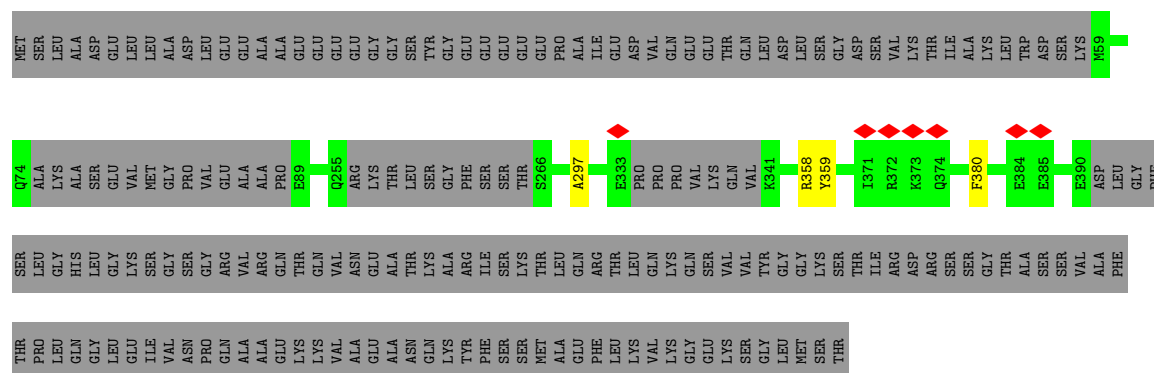
- Molecule 22: Probable ATP-dependent RNA helicase DDX23





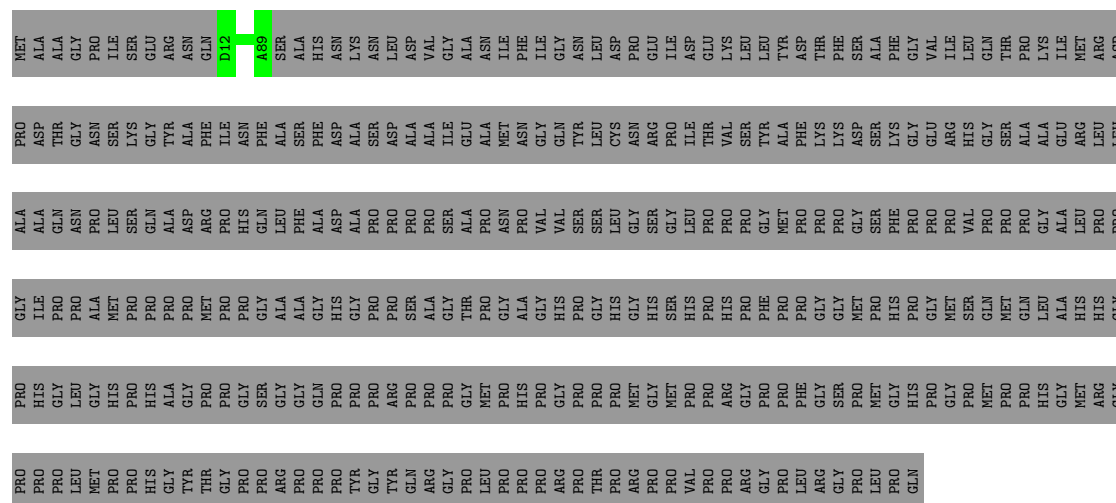
- Molecule 23: U4/U6 small nuclear ribonucleoprotein Prp31

Chain L: 60% 40%



- Molecule 24: Splicing factor 3B subunit 4

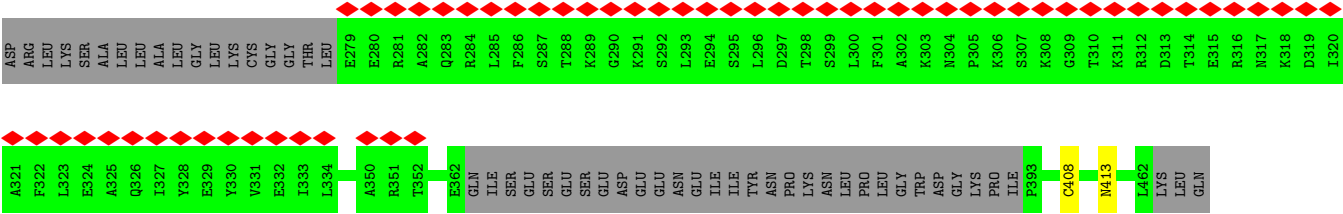
Chain B4: 18% 82%



- Molecule 25: Splicing factor 3A subunit 3

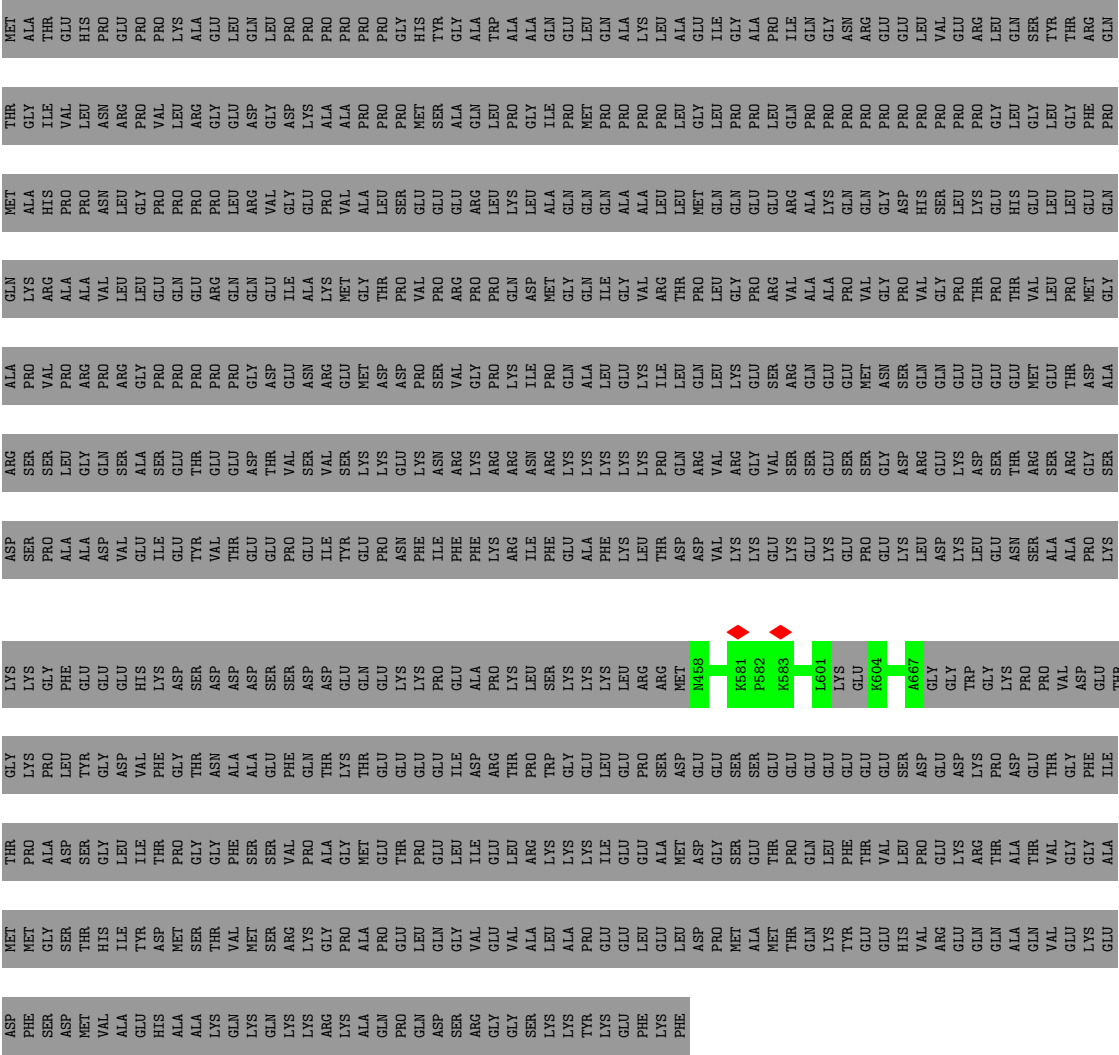
Chain 9: 28% 76% 24%





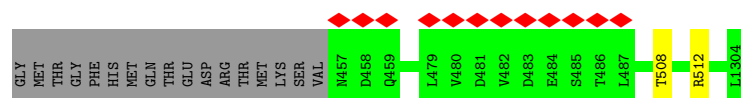
• Molecule 26: Splicing factor 3B subunit 2

Chain B2: 23% 77%



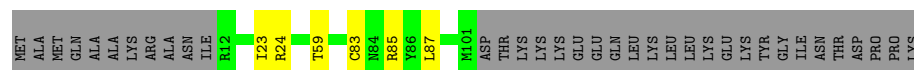
• Molecule 27: Splicing factor 3B subunit 5

Chain B5: 78% 20%



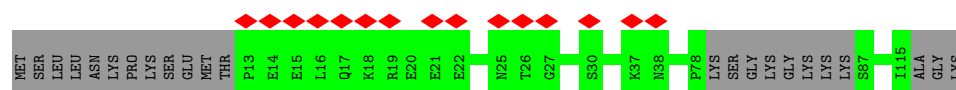
- Molecule 31: Splicing factor 3B subunit 6

Chain B6: 67% 5% 28%



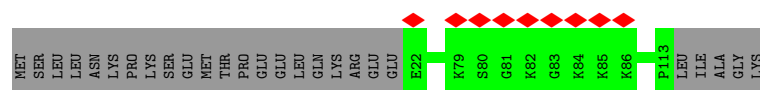
- Molecule 32: Small nuclear ribonucleoprotein Sm D2

Chain 22: 13% 81% 19%



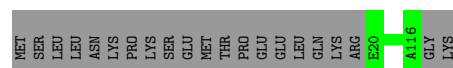
- Molecule 32: Small nuclear ribonucleoprotein Sm D2

Chain 42: 8% 78% 22%



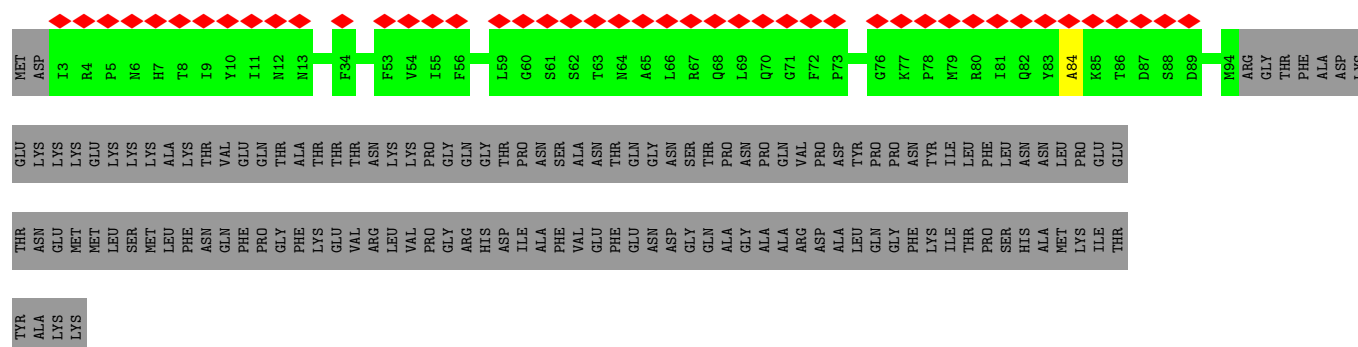
- Molecule 32: Small nuclear ribonucleoprotein Sm D2

Chain 52: 82% 18%

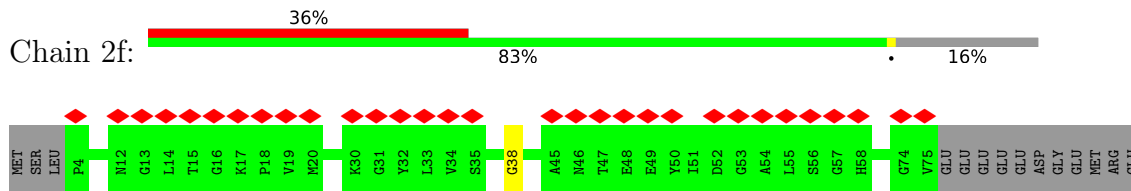


- Molecule 33: U2 small nuclear ribonucleoprotein B''

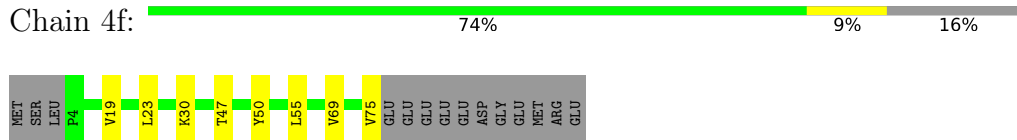
Chain 2B: 20% 40% 59%



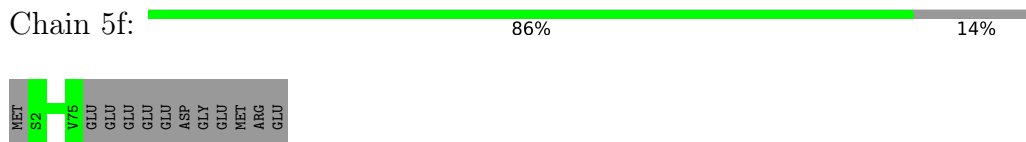
- Molecule 34: Small nuclear ribonucleoprotein F



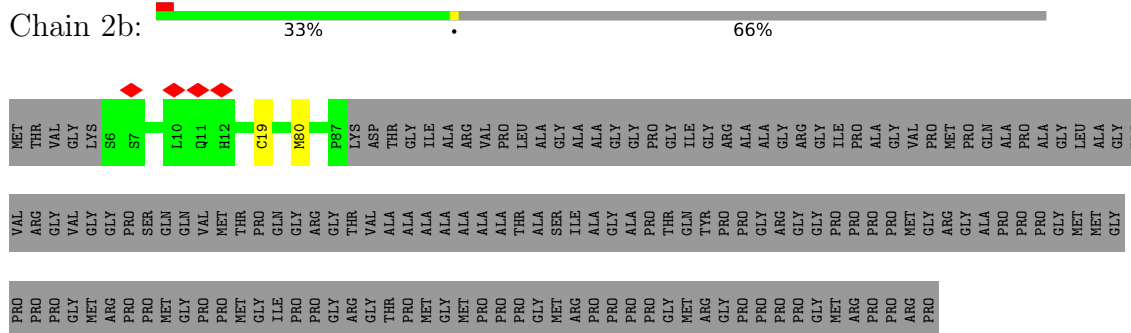
- Molecule 34: Small nuclear ribonucleoprotein F



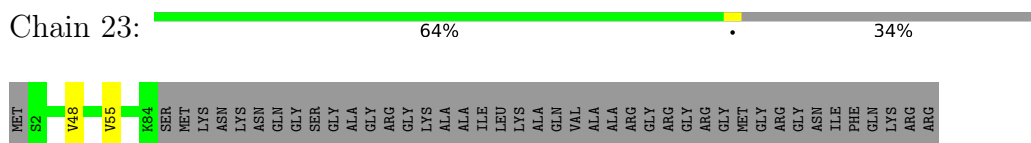
- Molecule 34: Small nuclear ribonucleoprotein F



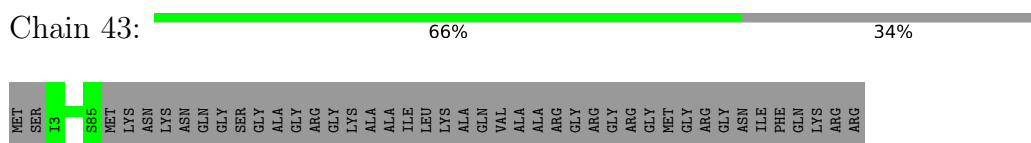
- Molecule 35: Small nuclear ribonucleoprotein-associated proteins B and B'



- Molecule 36: Small nuclear ribonucleoprotein Sm D3



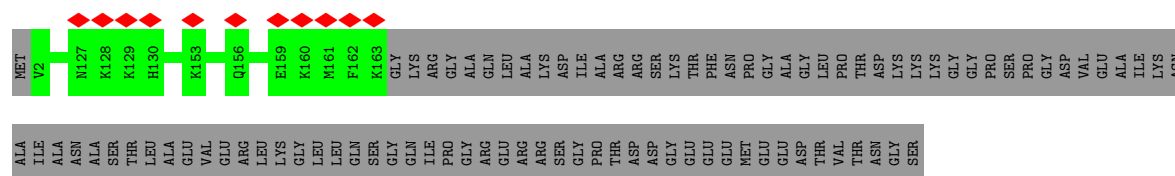
- Molecule 36: Small nuclear ribonucleoprotein Sm D3



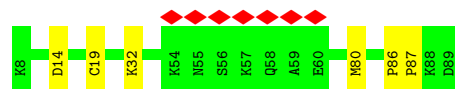
- Molecule 36: Small nuclear ribonucleoprotein Sm D3



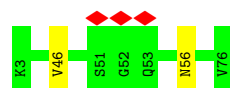




- Molecule 41: Small nuclear ribonucleoprotein-associated proteins B and B'



- Molecule 42: Small nuclear ribonucleoprotein G



- Molecule 42: Small nuclear ribonucleoprotein G



- Molecule 43: Small nuclear ribonucleoprotein-associated proteins B and B'



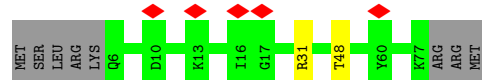
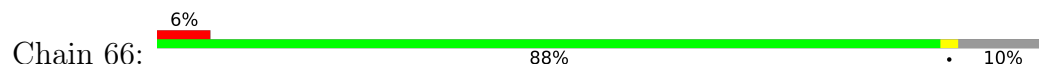
There are no outlier residues recorded for this chain.

- Molecule 44: Small nuclear ribonucleoprotein Sm D1



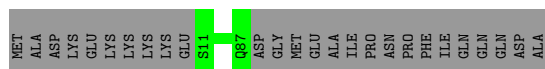
There are no outlier residues recorded for this chain.

- Molecule 45: U6 snRNA-associated Sm-like protein LSm6



- Molecule 46: U6 snRNA-associated Sm-like protein LSm7

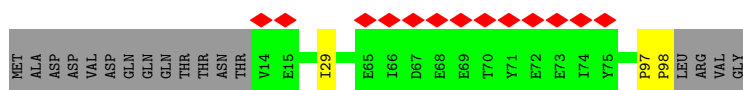
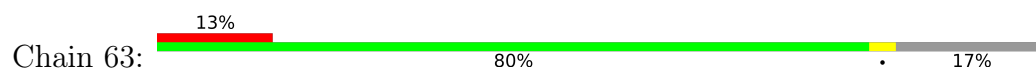




- Molecule 47: U6 snRNA-associated Sm-like protein LSm2



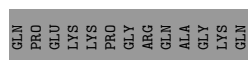
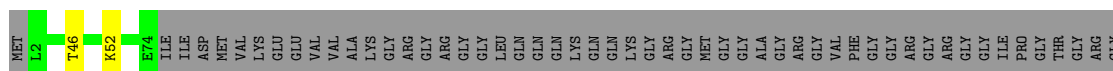
- Molecule 48: U6 snRNA-associated Sm-like protein LSm3



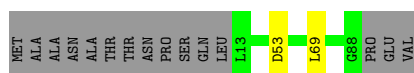
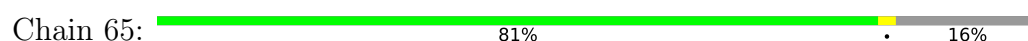
- Molecule 49: U6 snRNA-associated Sm-like protein LSm8



- Molecule 50: U6 snRNA-associated Sm-like protein LSm4



- Molecule 51: U6 snRNA-associated Sm-like protein LSm5



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	279781	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 ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.107	Depositor
Minimum map value	-0.055	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0125	Depositor
Map size (Å)	648.0, 648.0, 648.0	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.7, 2.7, 2.7	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.21	0/11173	0.41	2/15676 (0.0%)
2	B	0.14	0/10156	0.34	0/14217
3	2	0.18	0/2285	0.38	2/3548 (0.1%)
4	4	0.09	0/2941	0.17	0/4569
5	5	0.14	0/2444	0.30	0/3798
6	6	0.09	0/1264	0.16	0/1961
7	7	0.14	0/688	0.32	0/962
8	8	0.15	0/734	0.38	0/1025
9	C	0.16	0/4356	0.36	0/6105
10	D	0.18	0/712	0.43	0/995
11	E	0.15	0/1540	0.38	0/2148
12	F	0.15	0/1809	0.37	0/2525
13	M	0.16	0/627	0.38	0/878
14	R	0.10	0/534	0.26	0/745
15	U	0.18	0/2330	0.41	0/3268
16	X	0.55	0/130	0.73	0/180
17	Z	0.13	0/349	0.25	0/540
18	S	0.12	0/539	0.29	0/746
19	J	0.35	0/997	0.54	0/1389
20	K	0.14	0/1622	0.37	0/2265
21	N	0.16	0/4054	0.36	0/5669
22	G	0.30	0/3012	0.50	2/4213 (0.0%)
23	L	0.16	0/1516	0.39	0/2115
24	B4	0.14	0/394	0.29	0/549
25	9	0.14	0/1928	0.31	0/2692
26	B2	0.15	0/1092	0.35	0/1536
27	B5	0.11	0/349	0.25	0/487
28	B3	0.16	0/6024	0.37	0/8425
29	BP	0.13	0/501	0.37	0/697
30	B1	0.18	0/4421	0.40	0/6190
31	B6	0.12	0/459	0.30	0/642
32	22	0.14	0/485	0.35	0/677
32	42	0.15	0/466	0.41	0/651
32	52	0.11	0/387	0.21	0/482

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	2B	0.11	0/463	0.26	0/646
34	2f	0.16	0/362	0.40	0/502
34	4f	0.16	0/362	0.38	0/502
34	5f	0.10	0/295	0.21	0/367
35	2b	0.12	0/416	0.36	0/581
36	23	0.17	0/417	0.43	0/581
36	43	0.15	0/417	0.35	0/581
36	53	0.09	0/307	0.21	0/382
37	2g	0.14	0/366	0.37	0/509
38	2e	0.13	0/403	0.38	0/561
38	4e	0.14	0/378	0.42	0/526
38	5e	0.09	0/315	0.21	0/392
39	21	0.13	0/404	0.34	0/564
39	41	0.12	0/409	0.35	0/571
40	2A	0.16	0/821	0.41	0/1149
41	4b	0.16	0/416	0.38	0/581
42	4g	0.13	0/371	0.42	0/516
42	5g	0.11	0/295	0.23	0/367
43	5b	0.09	0/343	0.22	0/427
44	51	0.10	0/327	0.21	0/407
45	66	0.15	0/358	0.38	0/497
46	67	0.11	0/386	0.26	0/537
47	62	0.15	0/480	0.40	0/671
48	63	0.14	0/432	0.42	0/604
49	68	0.14	0/469	0.33	0/651
50	64	0.16	0/372	0.38	0/520
51	65	0.13	0/380	0.32	0/528
All	All	0.17	0/83082	0.37	6/117285 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	G	632	ALA	N-CA-C	-7.31	103.39	111.36
3	2	106	G	P-O3'-C3'	5.39	128.28	120.20
22	G	631	SER	N-CA-C	5.37	117.62	110.53
1	A	171	ASP	CB-CA-C	-5.28	110.47	116.54
1	A	1405	LEU	N-CA-C	-5.18	105.75	111.71
3	2	103	U	P-O3'-C3'	5.11	127.87	120.20

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	A	11054	0	5413	62	0
2	B	10078	0	4861	27	0
3	2	2051	0	1038	12	0
4	4	2636	0	1339	19	0
5	5	2192	0	1111	12	0
6	6	1133	0	573	15	0
7	7	686	0	316	0	0
8	8	729	0	356	2	0
9	C	4307	0	2141	12	0
10	D	708	0	328	1	0
11	E	1531	0	747	9	0
12	F	1795	0	891	8	0
13	M	622	0	313	1	0
14	R	531	0	253	0	0
15	U	2308	0	1104	17	0
16	X	130	0	64	2	0
17	Z	314	0	160	0	0
18	S	539	0	265	0	0
19	J	991	0	484	2	0
20	K	1615	0	754	3	0
21	N	4030	0	2054	5	0
22	G	2987	0	1475	27	0
23	L	1510	0	735	4	0
24	B4	391	0	197	0	0
25	9	1920	0	902	2	0
26	B2	1072	0	563	0	0
27	B5	347	0	171	1	0
28	B3	5969	0	2985	15	0
29	BP	498	0	241	0	0
30	B1	4383	0	2195	1	0
31	B6	455	0	227	3	0
32	22	482	0	220	0	0
32	42	463	0	211	0	0
32	52	388	0	102	0	0
33	2B	461	0	218	1	0
34	2f	359	0	179	1	0
34	4f	359	0	179	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	5f	296	0	87	0	0
35	2b	413	0	194	1	0
36	23	415	0	198	1	0
36	43	415	0	198	0	0
36	53	308	0	86	6	0
37	2g	364	0	176	2	0
38	2e	403	0	173	1	0
38	4e	378	0	163	1	0
38	5e	316	0	85	0	0
39	21	402	0	184	0	0
39	41	407	0	183	0	0
40	2A	816	0	386	0	0
41	4b	413	0	194	3	0
42	4g	369	0	178	1	0
42	5g	296	0	84	1	0
43	5b	344	0	93	0	0
44	51	328	0	89	0	0
45	66	357	0	169	1	0
46	67	384	0	178	0	0
47	62	478	0	222	0	0
48	63	429	0	199	2	0
49	68	469	0	220	3	0
50	64	369	0	172	1	0
51	65	378	0	174	1	0
All	All	81571	0	39450	243	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 2.

All (243) 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)
22:G:436:GLU:CB	22:G:631:SER:CB	2.30	1.10
11:E:58:PRO:CA	11:E:354:GLY:HA3	1.84	1.07
11:E:58:PRO:HA	11:E:354:GLY:CA	1.85	1.05
1:A:1404:THR:CA	2:B:219:GLU:HA	1.89	1.03
1:A:1404:THR:HA	2:B:219:GLU:CA	1.90	1.01
1:A:160:HIS:CB	22:G:376:ASP:HA	1.93	0.99
1:A:1404:THR:HA	2:B:219:GLU:HA	0.99	0.99
22:G:637:GLU:HA	22:G:786:SER:HA	1.47	0.96
11:E:58:PRO:HA	11:E:354:GLY:HA3	0.95	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:B3:673:VAL:HA	28:B3:690:ARG:HA	1.52	0.89
28:B3:886:GLU:HA	28:B3:910:ALA:O	1.74	0.88
36:23:48:VAL:O	36:23:55:VAL:HA	1.74	0.86
6:6:72:G:H4'	13:M:111:GLN:O	1.81	0.80
1:A:1595:GLN:CB	16:X:133:GLN:CB	2.61	0.79
3:2:168:A:H3'	3:2:169:C:H6	1.46	0.79
9:C:478:THR:HA	9:C:494:GLY:HA3	1.66	0.78
15:U:205:LEU:H	15:U:245:ASN:HA	1.48	0.77
2:B:1204:ILE:O	2:B:1249:GLU:HA	1.85	0.76
9:C:127:GLU:CB	36:53:15:GLY:O	2.34	0.75
28:B3:699:VAL:HA	28:B3:715:MET:O	1.90	0.72
9:C:118:PHE:HA	36:53:76:MET:O	1.90	0.72
4:4:4:U:H3	6:6:71:G:H1	1.35	0.72
1:A:1640:SER:HA	1:A:1653:ASP:H	1.56	0.71
4:4:32:G:OP2	23:L:297:ALA:HB1	1.90	0.70
15:U:198:THR:HA	15:U:254:LEU:CB	2.22	0.70
22:G:641:GLN:H	22:G:789:SER:HA	1.57	0.69
3:2:168:A:H3'	3:2:169:C:C6	2.27	0.69
9:C:196:LYS:CB	36:53:11:HIS:O	2.42	0.68
4:4:74:C:H42	6:6:35:A:H61	1.39	0.68
1:A:160:HIS:CB	22:G:376:ASP:CA	2.72	0.67
2:B:1345:ASN:HA	2:B:1487:ILE:O	1.95	0.67
1:A:1427:ARG:CB	2:B:223:GLU:HA	2.24	0.66
38:2e:58:LEU:O	38:2e:76:ARG:HA	1.95	0.66
1:A:465:LYS:HA	5:5:20:G:H22	1.61	0.65
15:U:205:LEU:N	15:U:245:ASN:HA	2.11	0.65
1:A:1382:SER:HA	1:A:1415:GLY:HA3	1.79	0.65
1:A:165:ARG:CB	1:A:577:GLY:CA	2.76	0.64
1:A:823:SER:HA	2:B:239:THR:HA	1.80	0.63
11:E:53:SER:HA	11:E:339:GLU:CB	2.28	0.63
11:E:56:GLN:O	11:E:354:GLY:HA2	1.98	0.62
28:B3:427:CYS:O	28:B3:433:SER:HA	1.99	0.62
49:68:38:LEU:O	49:68:59:LEU:HA	2.00	0.61
1:A:465:LYS:HA	5:5:20:G:N2	2.15	0.60
2:B:239:THR:O	21:N:264:GLY:HA3	2.00	0.60
3:2:165:A:H61	33:2B:84:ALA:HB1	1.67	0.60
1:A:1413:ASP:HA	1:A:1419:ILE:N	2.16	0.60
1:A:1428:HIS:CA	2:B:223:GLU:C	2.74	0.59
6:6:47:A:H4'	6:6:48:A:O5'	2.03	0.59
9:C:830:PRO:HG2	9:C:877:ALA:HB3	1.84	0.58
28:B3:990:ILE:HA	28:B3:1004:ASP:HA	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1700:GLY:O	1:A:1717:ASN:N	2.36	0.58
1:A:142:SER:HA	1:A:242:ALA:HB2	1.86	0.58
1:A:1371:TYR:HA	2:B:55:LYS:C	2.29	0.58
1:A:1502:PHE:HA	23:L:380:PHE:H	1.68	0.58
34:4f:19:VAL:HA	34:4f:75:VAL:H	1.69	0.57
1:A:1409:GLU:CB	2:B:61:PRO:HG2	2.35	0.57
2:B:240:LEU:HA	21:N:264:GLY:HA3	1.86	0.57
25:9:408:CYS:O	25:9:413:ASN:HA	2.04	0.56
1:A:1413:ASP:HA	1:A:1419:ILE:H	1.69	0.56
15:U:202:ILE:HA	15:U:251:ASN:CB	2.35	0.56
45:66:31:ARG:O	45:66:48:THR:HA	2.04	0.56
1:A:165:ARG:CB	1:A:577:GLY:HA3	2.36	0.56
31:B6:24:ARG:O	31:B6:87:LEU:HA	2.06	0.56
22:G:429:ARG:CB	22:G:583:GLU:HA	2.36	0.55
22:G:580:ASP:O	22:G:584:ASP:N	2.39	0.55
4:4:68:A:O2'	4:4:69:C:OP1	2.23	0.55
1:A:1763:LEU:H	1:A:1887:SER:HA	1.71	0.54
5:5:21:A:H61	5:5:59:G:N2	2.06	0.54
6:6:74:U:H2'	6:6:75:G:H8	1.72	0.54
1:A:1336:PRO:HG3	2:B:36:PRO:HB2	1.89	0.54
1:A:1428:HIS:N	2:B:223:GLU:C	2.65	0.54
1:A:1371:TYR:HA	2:B:56:ALA:N	2.23	0.54
3:2:63:G:H3'	3:2:64:A:H8	1.72	0.54
15:U:205:LEU:C	15:U:223:GLY:HA3	2.33	0.53
15:U:174:CYS:O	15:U:178:ASN:HA	2.09	0.53
1:A:1607:GLU:N	1:A:1632:PHE:O	2.41	0.53
22:G:643:VAL:CB	22:G:793:PRO:HA	2.39	0.53
28:B3:676:ARG:O	28:B3:687:SER:N	2.42	0.53
31:B6:23:ILE:O	31:B6:59:THR:HA	2.08	0.53
3:2:168:A:H5''	3:2:169:C:H5	1.74	0.53
11:E:240:GLY:HA3	11:E:290:ARG:HA	1.89	0.53
15:U:411:PRO:HG2	15:U:469:THR:HA	1.91	0.53
4:4:64:G:H22	4:4:67:A:H5'	1.72	0.52
5:5:19:A:N3	5:5:21:A:N6	2.57	0.52
15:U:174:CYS:O	15:U:178:ASN:N	2.43	0.52
28:B3:698:PRO:O	28:B3:699:VAL:C	2.51	0.52
5:5:23:C:H2'	5:5:58:U:O2	2.10	0.52
1:A:1501:LEU:HA	1:A:1755:SER:HA	1.92	0.52
9:C:310:SER:HA	9:C:316:ILE:O	2.10	0.51
22:G:577:PRO:C	22:G:579:THR:N	2.66	0.51
6:6:68:C:H2'	6:6:69:A:C8	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:B3:669:LEU:O	28:B3:698:PRO:HA	2.10	0.51
5:5:47:A:O2'	5:5:48:A:O5'	2.28	0.51
12:F:350:TRP:HA	12:F:357:GLU:HA	1.93	0.51
22:G:585:PRO:HA	22:G:588:MET:CB	2.41	0.51
22:G:795:LEU:O	22:G:796:ALA:C	2.54	0.51
12:F:236:TYR:HA	12:F:497:GLY:HA3	1.94	0.50
1:A:1428:HIS:CB	2:B:223:GLU:C	2.85	0.50
4:4:22:C:H2'	4:4:23:G:H8	1.77	0.50
2:B:463:PRO:HA	2:B:480:THR:HA	1.93	0.50
28:B3:336:ALA:HA	28:B3:351:SER:HA	1.94	0.50
1:A:2129:TYR:HA	1:A:2175:LEU:H	1.76	0.50
38:4e:58:LEU:O	38:4e:76:ARG:HA	2.12	0.50
1:A:274:PRO:HB3	22:G:283:SER:HA	1.93	0.50
1:A:1426:ASP:O	1:A:1427:ARG:C	2.54	0.50
4:4:22:C:H2'	4:4:23:G:C8	2.47	0.50
1:A:165:ARG:CB	1:A:577:GLY:HA2	2.42	0.49
22:G:642:LYS:HA	22:G:791:CYS:O	2.11	0.49
4:4:8:C:H2'	4:4:9:G:C8	2.46	0.49
49:68:39:ASP:HA	49:68:59:LEU:H	1.77	0.49
11:E:295:PRO:HG2	11:E:337:PRO:HA	1.94	0.49
22:G:786:SER:O	22:G:787:PRO:C	2.54	0.49
28:B3:1033:VAL:HA	28:B3:1048:ASP:HA	1.95	0.49
22:G:577:PRO:C	22:G:579:THR:H	2.21	0.49
9:C:127:GLU:CB	36:53:15:GLY:HA2	2.43	0.49
15:U:195:PRO:O	15:U:197:PHE:N	2.46	0.48
1:A:1701:VAL:HA	1:A:1716:GLY:HA3	1.94	0.48
1:A:824:PRO:HD2	2:B:238:CYS:O	2.13	0.48
15:U:210:LYS:C	15:U:212:SER:H	2.21	0.48
48:63:29:ILE:HA	48:63:98:PRO:HD3	1.95	0.48
15:U:174:CYS:O	15:U:178:ASN:CA	2.61	0.48
15:U:206:ASP:HA	15:U:222:PRO:O	2.13	0.48
15:U:211:LEU:O	15:U:212:SER:C	2.55	0.48
12:F:281:PHE:HA	12:F:296:LEU:HA	1.95	0.48
4:4:32:G:OP2	23:L:297:ALA:CB	2.60	0.48
12:F:452:VAL:HA	12:F:469:ALA:HA	1.96	0.48
28:B3:785:PRO:HA	28:B3:801:GLU:HA	1.96	0.47
4:4:35:G:H2'	4:4:39:A:H61	1.79	0.47
28:B3:828:GLY:O	28:B3:834:LEU:HA	2.14	0.47
15:U:206:ASP:O	15:U:207:LYS:C	2.58	0.47
51:65:53:ASP:HA	51:65:69:LEU:HA	1.97	0.47
1:A:160:HIS:CB	22:G:376:ASP:C	2.88	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:4:C:N4	5:5:78:U:O2	2.48	0.47
6:6:71:G:H2'	6:6:72:G:H8	1.80	0.47
20:K:682:VAL:HA	20:K:688:ASN:HA	1.96	0.47
15:U:203:ALA:HA	15:U:247:PRO:HB3	1.96	0.46
1:A:1382:SER:CA	1:A:1415:GLY:HA3	2.44	0.46
22:G:645:LEU:C	22:G:647:SER:H	2.23	0.46
3:2:99:A:N6	34:2f:38:GLY:O	2.48	0.46
5:5:110:C:H2'	5:5:111:A:H8	1.80	0.46
10:D:76:TYR:O	21:N:74:ASN:HA	2.16	0.46
42:4g:46:VAL:HA	42:4g:56:ASN:HA	1.98	0.46
1:A:1396:ALA:O	1:A:1401:ARG:N	2.41	0.46
4:4:5:U:H2'	4:4:6:U:C6	2.51	0.46
21:N:415:GLU:O	21:N:419:ALA:N	2.47	0.46
1:A:172:GLU:HA	1:A:520:TYR:H	1.82	0.45
34:4f:23:LEU:HA	34:4f:69:VAL:HA	1.97	0.45
23:L:358:ARG:O	23:L:359:TYR:C	2.59	0.45
4:4:66:A:N6	6:6:47:A:N7	2.65	0.45
1:A:160:HIS:CB	22:G:375:GLU:O	2.64	0.45
12:F:373:PHE:HA	12:F:380:ALA:HA	1.98	0.45
20:K:863:GLY:HA3	20:K:918:PHE:H	1.82	0.45
22:G:577:PRO:O	22:G:579:THR:N	2.50	0.45
22:G:648:GLU:CB	22:G:769:THR:HA	2.47	0.45
1:A:463:PRO:HG2	5:5:20:G:C5	2.52	0.45
4:4:64:G:N2	4:4:67:A:H5'	2.30	0.45
1:A:1507:SER:O	1:A:1512:SER:N	2.50	0.45
5:5:64:G:H2'	5:5:65:G:H8	1.82	0.44
4:4:55:U:H3	6:6:58:G:H1'	1.82	0.44
8:8:147:PRO:HB3	8:8:173:ALA:HB2	1.98	0.44
9:C:118:PHE:CB	36:53:79:ASN:O	2.65	0.44
12:F:234:ILE:HA	12:F:250:CYS:HA	1.99	0.44
1:A:1423:PHE:HA	2:B:221:ARG:H	1.83	0.44
2:B:449:ALA:HB1	2:B:684:PRO:HB2	2.00	0.44
1:A:1405:LEU:O	1:A:1409:GLU:N	2.50	0.44
49:68:35:ASN:HA	49:68:62:VAL:O	2.18	0.44
4:4:12:G:H2'	4:4:13:U:C6	2.53	0.44
22:G:379:ILE:HA	22:G:628:TYR:O	2.17	0.44
4:4:35:G:H2'	4:4:39:A:N6	2.33	0.43
9:C:619:THR:HA	9:C:628:VAL:O	2.18	0.43
22:G:641:GLN:N	22:G:790:SER:H	2.15	0.43
4:4:60:A:H2'	4:4:61:A:C8	2.53	0.43
35:2b:19:CYS:HA	35:2b:80:MET:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1607:GLU:H	1:A:1633:ALA:HA	1.83	0.43
9:C:776:GLU:O	9:C:782:GLU:N	2.51	0.43
1:A:160:HIS:CB	22:G:376:ASP:O	2.65	0.43
8:8:56:CYS:O	8:8:60:LEU:HA	2.18	0.43
12:F:276:VAL:HA	12:F:300:ALA:HA	2.01	0.43
25:9:77:GLY:HA3	25:9:78:PRO:HD3	1.84	0.43
28:B3:667:ILE:O	28:B3:674:LEU:HA	2.18	0.43
5:5:17:U:H2'	5:5:18:C:C6	2.53	0.43
11:E:76:PRO:HA	11:E:337:PRO:HG3	2.01	0.43
11:E:290:ARG:N	11:E:331:ASN:O	2.52	0.43
28:B3:674:LEU:O	28:B3:675:LEU:C	2.60	0.43
50:64:46:THR:HA	50:64:52:LYS:HA	2.01	0.43
6:6:61:C:H2'	6:6:62:C:C6	2.54	0.43
1:A:827:PHE:O	1:A:828:PRO:C	2.62	0.42
15:U:203:ALA:C	15:U:247:PRO:HA	2.44	0.42
37:2g:21:LEU:HA	37:2g:67:ILE:HA	2.01	0.42
1:A:175:PRO:O	1:A:176:LEU:C	2.62	0.42
6:6:76:A:C6	19:J:562:ALA:HB1	2.54	0.42
16:X:135:ARG:O	16:X:136:LYS:C	2.62	0.42
1:A:246:LEU:C	22:G:305:ALA:HB2	2.45	0.42
2:B:834:TYR:HA	2:B:841:TRP:HA	2.01	0.42
5:5:32:C:H2'	5:5:33:U:C6	2.54	0.42
30:B1:508:THR:O	30:B1:512:ARG:N	2.47	0.42
6:6:66:C:H2'	6:6:67:G:C8	2.54	0.42
19:J:567:LEU:O	19:J:568:TYR:C	2.63	0.42
6:6:89:U:H2'	6:6:90:G:H8	1.84	0.42
34:4f:50:TYR:HA	34:4f:55:LEU:HA	2.01	0.42
3:2:168:A:H5''	3:2:169:C:C5	2.53	0.42
1:A:1428:HIS:HA	2:B:223:GLU:C	2.44	0.42
20:K:773:ASN:HA	20:K:822:LEU:HA	2.00	0.42
22:G:356:HIS:O	22:G:360:LYS:N	2.42	0.42
1:A:168:PRO:HB2	1:A:171:ASP:HA	2.02	0.42
3:2:34:U:H2'	3:2:35:A:H8	1.85	0.42
27:B5:78:PRO:HA	27:B5:79:PRO:HD3	1.95	0.42
1:A:947:PRO:HB2	1:A:949:PRO:HD2	2.02	0.42
1:A:1370:ARG:O	2:B:55:LYS:N	2.46	0.42
3:2:151:C:H2'	3:2:152:G:H8	1.84	0.41
4:4:27:C:H2'	4:4:28:C:C6	2.55	0.41
34:4f:30:LYS:O	34:4f:47:THR:HA	2.20	0.41
41:4b:14:ASP:H	41:4b:32:LYS:HA	1.85	0.41
22:G:645:LEU:C	22:G:647:SER:N	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1411:SER:O	1:A:1412:TRP:C	2.62	0.41
37:2g:6:PRO:HA	37:2g:7:PRO:HD3	1.97	0.41
1:A:1527:ASN:O	1:A:1530:PRO:HD2	2.21	0.41
2:B:626:PRO:HG3	2:B:893:MET:HA	2.01	0.41
9:C:196:LYS:CB	36:53:11:HIS:C	2.93	0.41
28:B3:637:PRO:HA	28:B3:669:LEU:HA	2.01	0.41
41:4b:86:PRO:HA	41:4b:87:PRO:HD3	1.93	0.41
1:A:733:THR:N	1:A:734:PRO:HD2	2.36	0.41
1:A:1416:ILE:N	1:A:1417:PRO:HD2	2.36	0.41
1:A:1421:THR:C	1:A:1423:PHE:H	2.29	0.41
3:2:10:C:H2'	3:2:11:G:H8	1.85	0.41
4:4:55:U:N3	6:6:58:G:H1'	2.36	0.41
1:A:1423:PHE:HA	2:B:221:ARG:N	2.35	0.41
2:B:835:SER:O	2:B:839:GLY:N	2.53	0.41
6:6:68:C:H2'	6:6:69:A:H8	1.85	0.41
1:A:1421:THR:C	1:A:1423:PHE:N	2.76	0.40
31:B6:83:CYS:O	31:B6:85:ARG:N	2.52	0.40
42:5g:42:ILE:O	42:5g:59:MET:CA	2.69	0.40
1:A:734:PRO:HB2	21:N:149:LEU:HA	2.03	0.40
9:C:888:ARG:O	9:C:893:GLY:N	2.49	0.40
12:F:259:SER:O	12:F:263:CYS:N	2.54	0.40
1:A:169:PHE:HA	1:A:559:ASP:CB	2.51	0.40
2:B:222:GLU:O	2:B:223:GLU:C	2.64	0.40
3:2:3:C:H2'	3:2:4:G:H8	1.85	0.40
22:G:640:GLU:HA	22:G:789:SER:HA	2.03	0.40
41:4b:19:CYS:HA	41:4b:80:MET:HA	2.02	0.40
3:2:50:C:H2'	3:2:51:A:H8	1.87	0.40
15:U:244:SER:C	15:U:246:VAL:H	2.29	0.40
48:63:97:PRO:HA	48:63:98:PRO:HD3	1.94	0.40

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	A	2165/2335 (93%)	2095 (97%)	68 (3%)	2 (0%)	48	83
2	B	1989/2136 (93%)	1961 (99%)	28 (1%)	0	100	100
7	7	132/793 (17%)	132 (100%)	0	0	100	100
8	8	138/464 (30%)	135 (98%)	3 (2%)	0	100	100
9	C	850/972 (87%)	825 (97%)	25 (3%)	0	100	100
10	D	139/142 (98%)	136 (98%)	3 (2%)	0	100	100
11	E	305/357 (85%)	300 (98%)	5 (2%)	0	100	100
12	F	357/522 (68%)	345 (97%)	12 (3%)	0	100	100
13	M	121/128 (94%)	120 (99%)	1 (1%)	0	100	100
14	R	104/480 (22%)	99 (95%)	5 (5%)	0	100	100
15	U	454/565 (80%)	427 (94%)	26 (6%)	1 (0%)	43	78
16	X	24/155 (16%)	23 (96%)	1 (4%)	0	100	100
18	S	100/800 (12%)	98 (98%)	2 (2%)	0	100	100
19	J	186/683 (27%)	180 (97%)	6 (3%)	0	100	100
20	K	316/1007 (31%)	310 (98%)	6 (2%)	0	100	100
21	N	789/941 (84%)	776 (98%)	13 (2%)	0	100	100
22	G	582/820 (71%)	567 (97%)	13 (2%)	2 (0%)	36	72
23	L	293/499 (59%)	282 (96%)	11 (4%)	0	100	100
24	B4	76/424 (18%)	76 (100%)	0	0	100	100
25	9	377/501 (75%)	369 (98%)	8 (2%)	0	100	100
26	B2	204/895 (23%)	200 (98%)	4 (2%)	0	100	100
27	B5	67/86 (78%)	66 (98%)	1 (2%)	0	100	100
28	B3	1176/1217 (97%)	1144 (97%)	31 (3%)	1 (0%)	48	83
29	BP	98/110 (89%)	96 (98%)	2 (2%)	0	100	100
30	B1	866/1304 (66%)	849 (98%)	17 (2%)	0	100	100
31	B6	88/125 (70%)	85 (97%)	3 (3%)	0	100	100
32	22	91/118 (77%)	91 (100%)	0	0	100	100
32	42	90/118 (76%)	88 (98%)	2 (2%)	0	100	100
32	52	95/118 (80%)	89 (94%)	6 (6%)	0	100	100
33	2B	90/225 (40%)	90 (100%)	0	0	100	100
34	2f	70/86 (81%)	68 (97%)	2 (3%)	0	100	100
34	4f	70/86 (81%)	67 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	5f	72/86 (84%)	71 (99%)	1 (1%)	0	100	100
35	2b	80/240 (33%)	80 (100%)	0	0	100	100
36	23	81/126 (64%)	79 (98%)	2 (2%)	0	100	100
36	43	81/126 (64%)	81 (100%)	0	0	100	100
36	53	75/126 (60%)	73 (97%)	2 (3%)	0	100	100
37	2g	71/76 (93%)	71 (100%)	0	0	100	100
38	2e	79/92 (86%)	79 (100%)	0	0	100	100
38	4e	74/92 (80%)	73 (99%)	1 (1%)	0	100	100
38	5e	77/92 (84%)	75 (97%)	2 (3%)	0	100	100
39	21	78/119 (66%)	76 (97%)	2 (3%)	0	100	100
39	41	79/119 (66%)	78 (99%)	1 (1%)	0	100	100
40	2A	160/255 (63%)	160 (100%)	0	0	100	100
41	4b	80/82 (98%)	79 (99%)	1 (1%)	0	100	100
42	4g	72/74 (97%)	70 (97%)	2 (3%)	0	100	100
42	5g	72/74 (97%)	70 (97%)	2 (3%)	0	100	100
43	5b	84/86 (98%)	80 (95%)	4 (5%)	0	100	100
44	51	80/82 (98%)	73 (91%)	7 (9%)	0	100	100
45	66	70/80 (88%)	70 (100%)	0	0	100	100
46	67	75/103 (73%)	74 (99%)	1 (1%)	0	100	100
47	62	93/95 (98%)	91 (98%)	2 (2%)	0	100	100
48	63	83/102 (81%)	82 (99%)	1 (1%)	0	100	100
49	68	93/96 (97%)	92 (99%)	1 (1%)	0	100	100
50	64	71/139 (51%)	71 (100%)	0	0	100	100
51	65	74/91 (81%)	74 (100%)	0	0	100	100
All	All	14456/21865 (66%)	14111 (98%)	339 (2%)	6 (0%)	100	100

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	U	196	THR
28	B3	699	VAL
22	G	582	ALA
22	G	796	ALA
1	A	1412	TRP

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Mol	Chain	Res	Type
1	A	168	PRO

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	A	126/2108 (6%)	126 (100%)	0	100	100
2	B	84/1908 (4%)	84 (100%)	0	100	100
7	7	4/709 (1%)	4 (100%)	0	100	100
8	8	8/382 (2%)	8 (100%)	0	100	100
9	C	50/866 (6%)	50 (100%)	0	100	100
10	D	5/130 (4%)	5 (100%)	0	100	100
11	E	10/300 (3%)	10 (100%)	0	100	100
12	F	15/442 (3%)	15 (100%)	0	100	100
13	M	6/111 (5%)	6 (100%)	0	100	100
14	R	4/369 (1%)	4 (100%)	0	100	100
15	U	23/511 (4%)	23 (100%)	0	100	100
16	X	1/144 (1%)	1 (100%)	0	100	100
18	S	4/681 (1%)	4 (100%)	0	100	100
19	J	11/599 (2%)	11 (100%)	0	100	100
20	K	10/919 (1%)	10 (100%)	0	100	100
21	N	30/792 (4%)	30 (100%)	0	100	100
22	G	30/721 (4%)	30 (100%)	0	100	100
23	L	10/424 (2%)	10 (100%)	0	100	100
24	B4	4/336 (1%)	4 (100%)	0	100	100
25	9	11/446 (2%)	11 (100%)	0	100	100
26	B2	22/776 (3%)	22 (100%)	0	100	100
27	B5	3/77 (4%)	3 (100%)	0	100	100
28	B3	60/1051 (6%)	60 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	BP	4/95 (4%)	4 (100%)	0	100	100
30	B1	40/1104 (4%)	40 (100%)	0	100	100
31	B6	5/109 (5%)	5 (100%)	0	100	100
32	22	5/110 (4%)	5 (100%)	0	100	100
32	42	4/110 (4%)	4 (100%)	0	100	100
33	2B	3/195 (2%)	3 (100%)	0	100	100
34	2f	4/74 (5%)	4 (100%)	0	100	100
34	4f	4/74 (5%)	4 (100%)	0	100	100
35	2b	4/177 (2%)	4 (100%)	0	100	100
36	23	3/101 (3%)	3 (100%)	0	100	100
36	43	3/101 (3%)	3 (100%)	0	100	100
37	2g	3/66 (4%)	3 (100%)	0	100	100
38	2e	1/84 (1%)	1 (100%)	0	100	100
38	4e	1/84 (1%)	1 (100%)	0	100	100
39	21	3/101 (3%)	3 (100%)	0	100	100
39	41	3/101 (3%)	3 (100%)	0	100	100
40	2A	6/218 (3%)	6 (100%)	0	100	100
41	4b	4/75 (5%)	4 (100%)	0	100	100
42	4g	3/64 (5%)	3 (100%)	0	100	100
45	66	2/70 (3%)	2 (100%)	0	100	100
46	67	3/91 (3%)	3 (100%)	0	100	100
47	62	3/88 (3%)	3 (100%)	0	100	100
48	63	4/94 (4%)	4 (100%)	0	100	100
49	68	1/82 (1%)	1 (100%)	0	100	100
50	64	4/111 (4%)	4 (100%)	0	100	100
51	65	3/80 (4%)	3 (100%)	0	100	100
All	All	654/18461 (4%)	654 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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
17	Z	14/15 (93%)	1 (7%)	0
3	2	93/182 (51%)	19 (20%)	6 (6%)
4	4	119/144 (82%)	19 (15%)	3 (2%)
5	5	101/115 (87%)	29 (28%)	5 (4%)
6	6	50/76 (65%)	4 (8%)	1 (2%)
All	All	377/532 (70%)	72 (19%)	15 (3%)

All (72) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	2	30	A
3	2	38	A
3	2	40	C
3	2	47	U
3	2	63	G
3	2	64	A
3	2	100	U
3	2	101	U
3	2	102	U
3	2	103	U
3	2	104	U
3	2	105	G
3	2	106	G
3	2	107	A
3	2	164	C
3	2	168	A
3	2	170	C
3	2	171	U
3	2	178	A
4	4	2	G
4	4	19	U
4	4	20	A
4	4	25	A
4	4	26	G
4	4	36	U
4	4	37	C
4	4	38	U
4	4	44	A
4	4	45	G
4	4	68	A
4	4	69	C

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Mol	Chain	Res	Type
4	4	114	U
4	4	115	G
4	4	121	U
4	4	122	U
4	4	123	U
4	4	125	G
4	4	126	A
5	5	20	G
5	5	21	A
5	5	25	C
5	5	26	A
5	5	28	A
5	5	36	C
5	5	37	G
5	5	38	C
5	5	47	A
5	5	48	A
5	5	58	U
5	5	59	G
5	5	66	A
5	5	67	A
5	5	69	A
5	5	70	A
5	5	71	C
5	5	75	G
5	5	78	U
5	5	86	C
5	5	90	U
5	5	94	U
5	5	97	G
5	5	98	G
5	5	105	U
5	5	106	U
5	5	107	U
5	5	108	G
5	5	115	C
6	6	48	A
6	6	49	G
6	6	77	C
6	6	106	U
17	Z	41	A

All (15) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	2	37	U
3	2	46	U
3	2	103	U
3	2	106	G
3	2	167	U
3	2	170	C
4	4	1	A
4	4	68	A
4	4	114	U
5	5	24	G
5	5	57	G
5	5	58	U
5	5	96	A
5	5	105	U
6	6	47	A

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

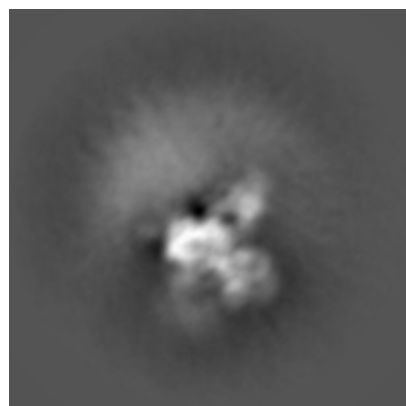
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18718. These allow visual inspection of the internal detail of the map and identification of artifacts.

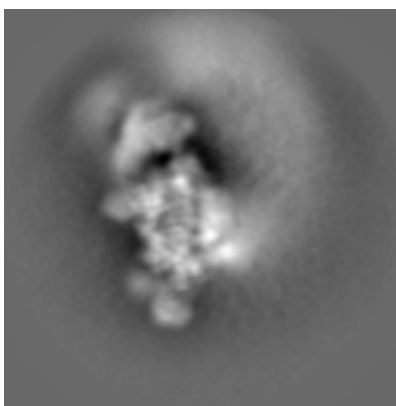
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

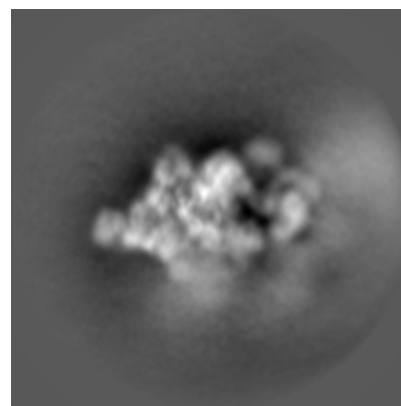
6.1.1 Primary map



X

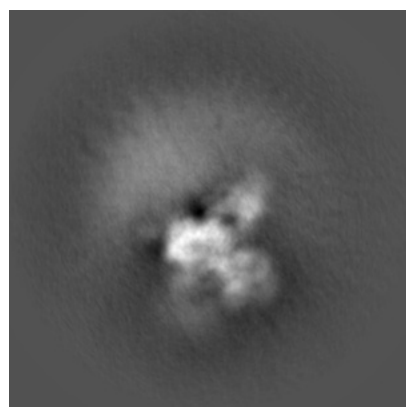


Y

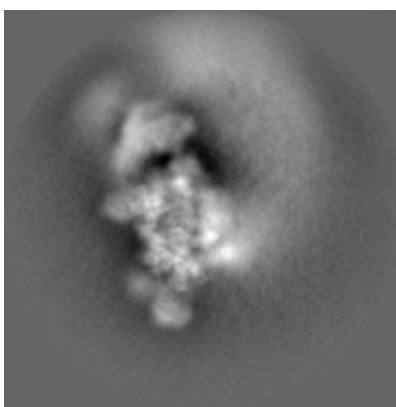


Z

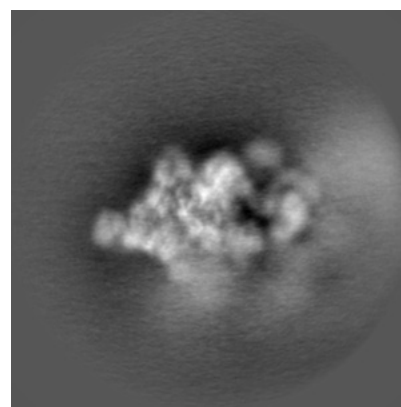
6.1.2 Raw map



X



Y

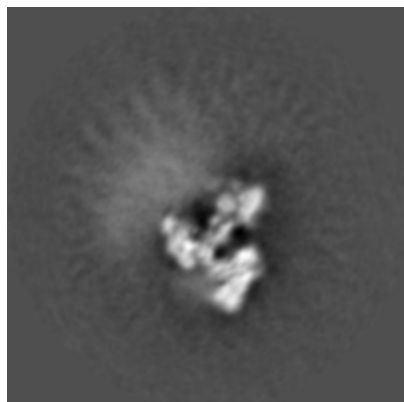


Z

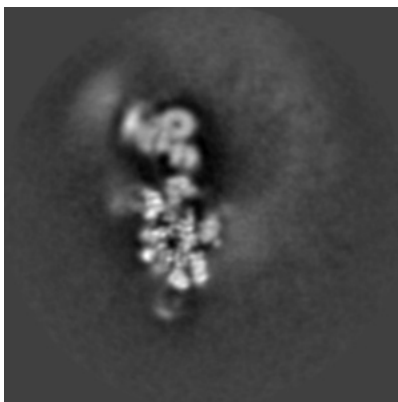
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

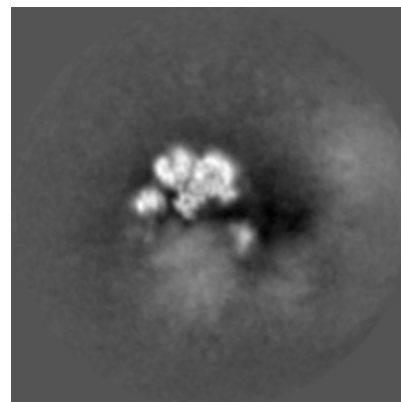
6.2.1 Primary map



X Index: 120

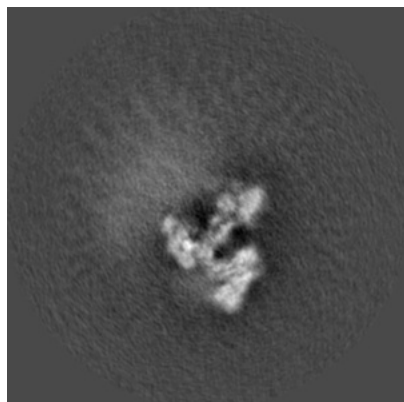


Y Index: 120

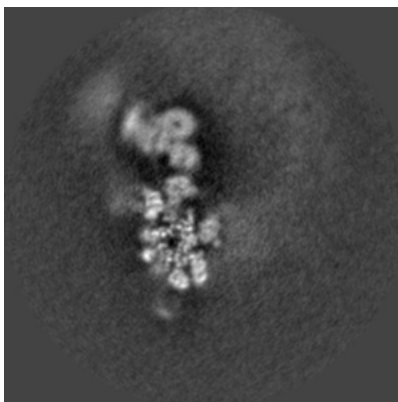


Z Index: 120

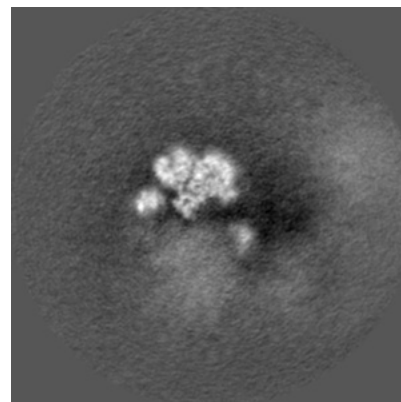
6.2.2 Raw map



X Index: 120



Y Index: 120

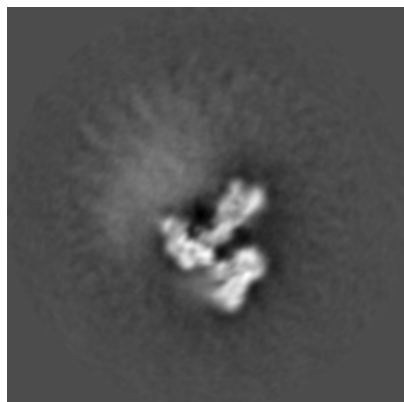


Z Index: 120

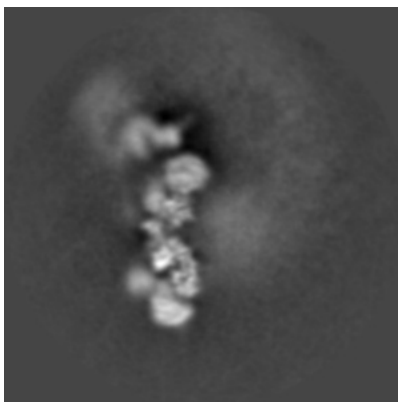
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

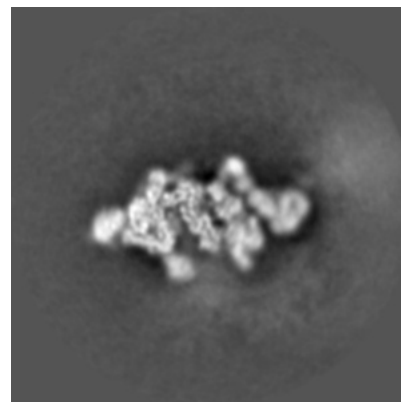
6.3.1 Primary map



X Index: 122

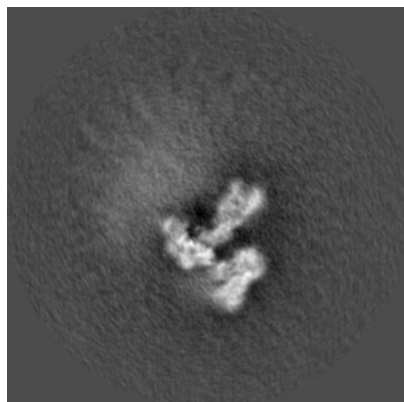


Y Index: 104

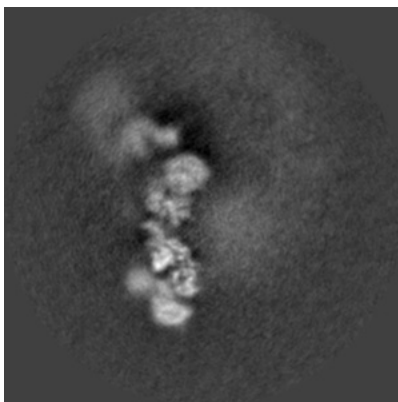


Z Index: 105

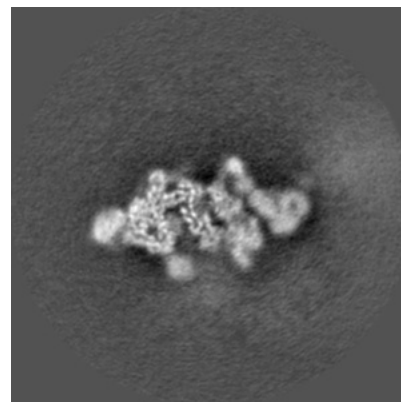
6.3.2 Raw map



X Index: 122



Y Index: 103

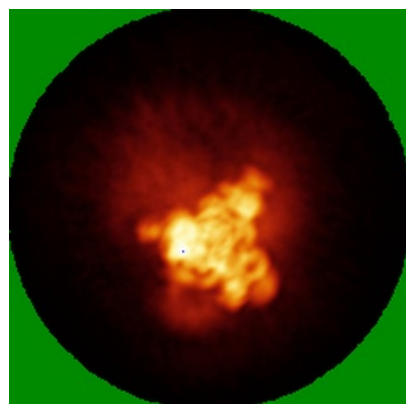


Z Index: 104

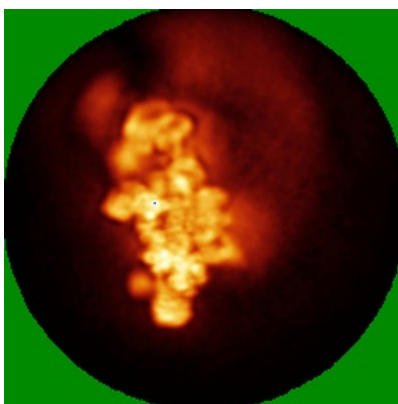
The images above show the largest variance slices of the map in three orthogonal directions.

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

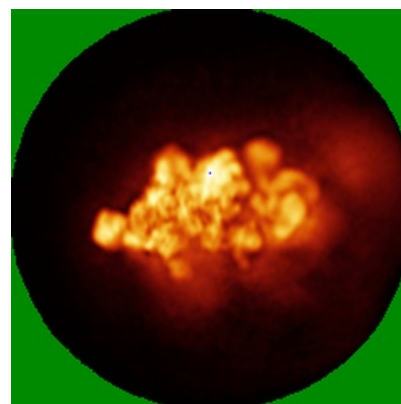
6.4.1 Primary map



X

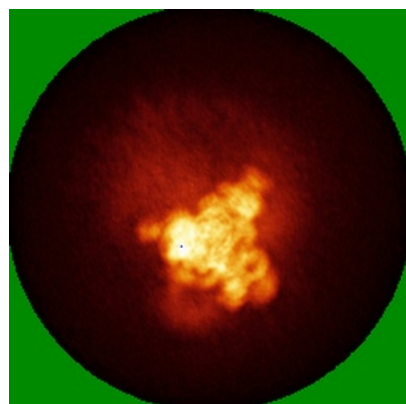


Y

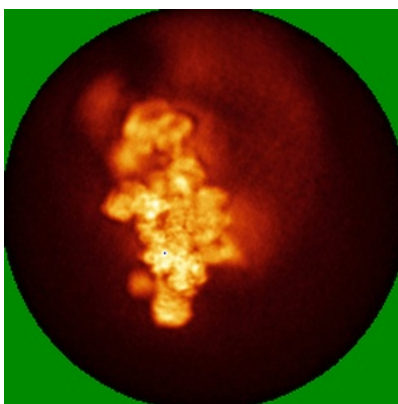


Z

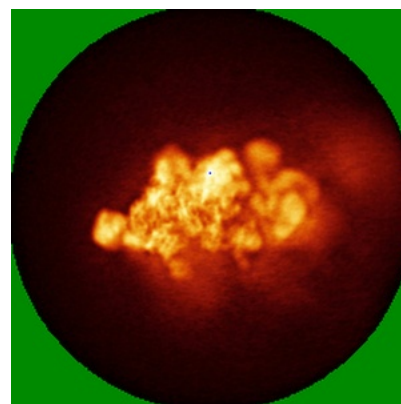
6.4.2 Raw map



X



Y

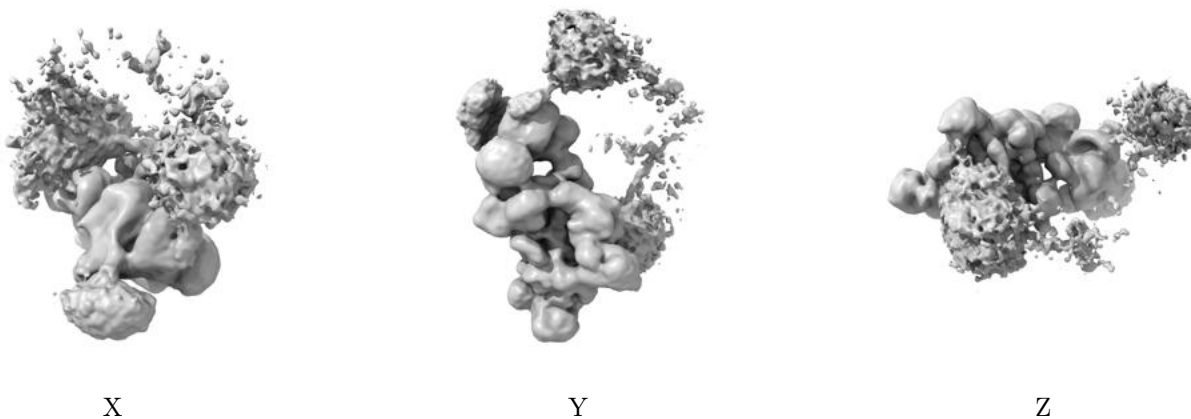


Z

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.

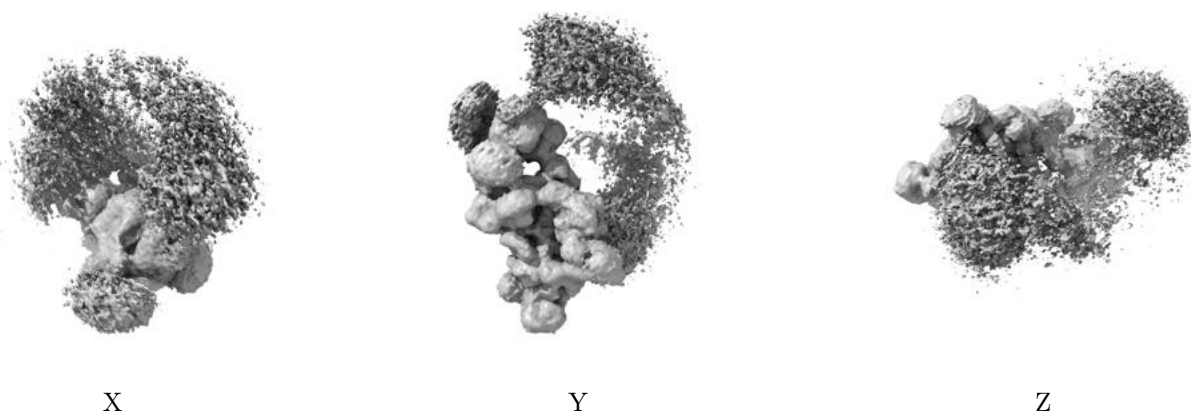
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0125. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

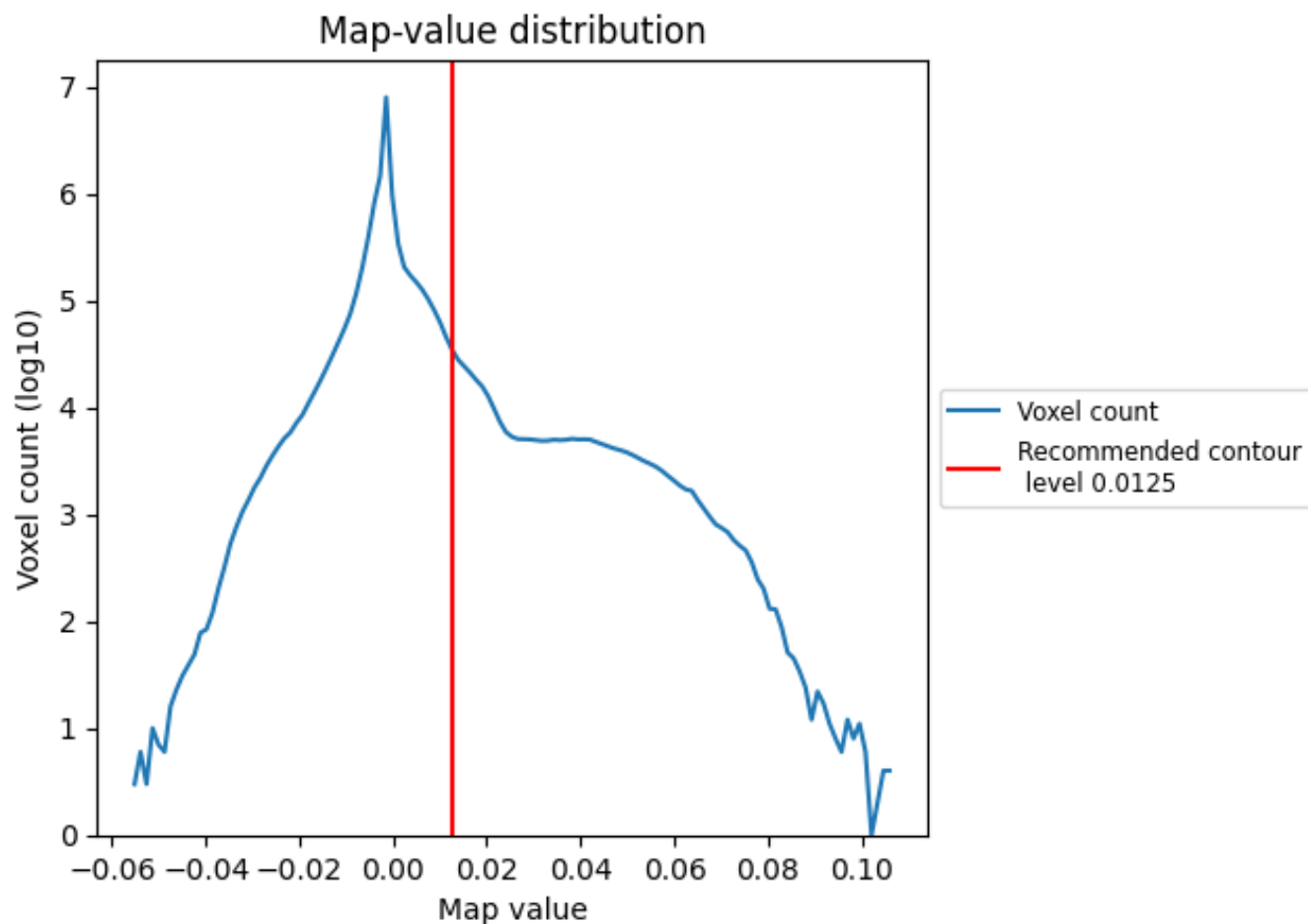
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

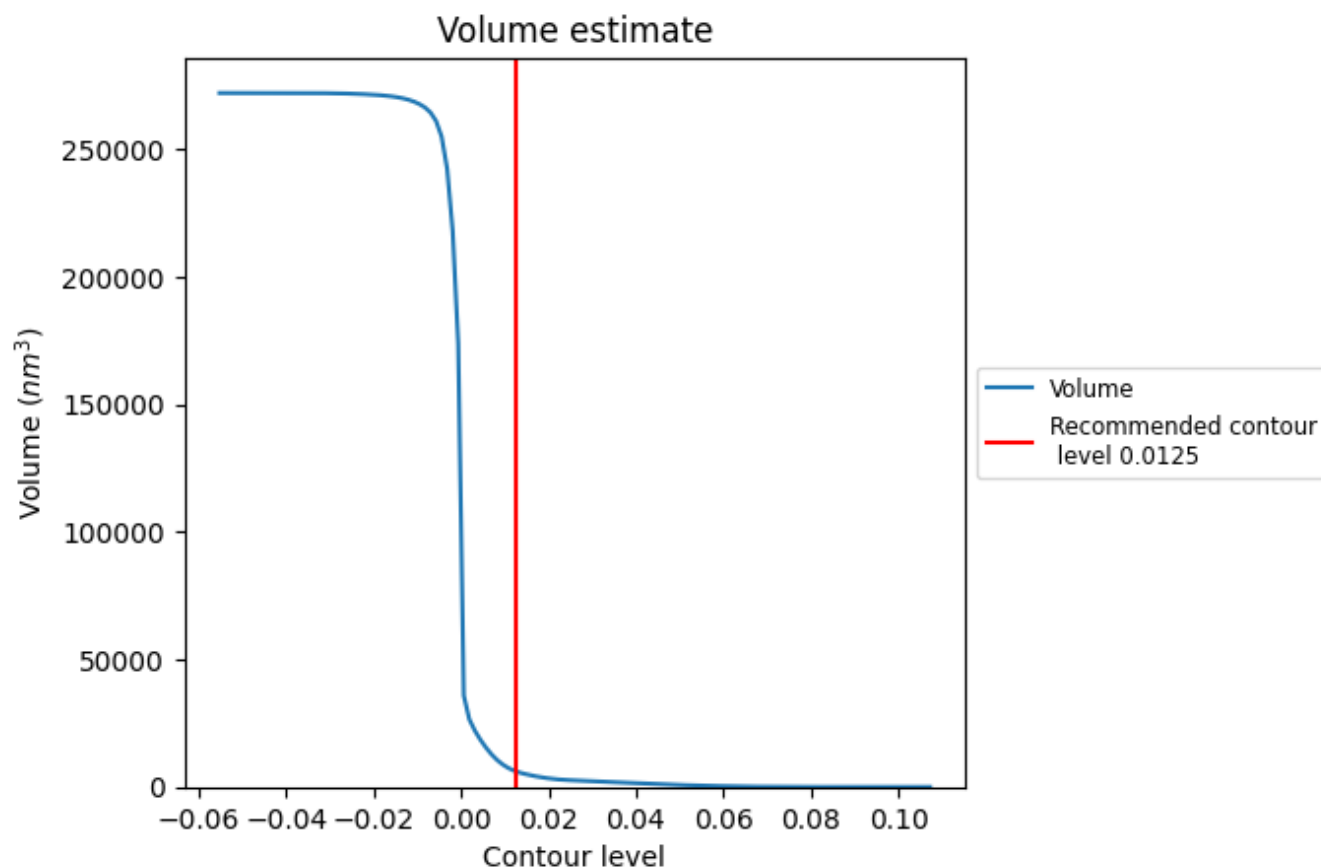
This section contains the results of statistical analysis of the map.

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.

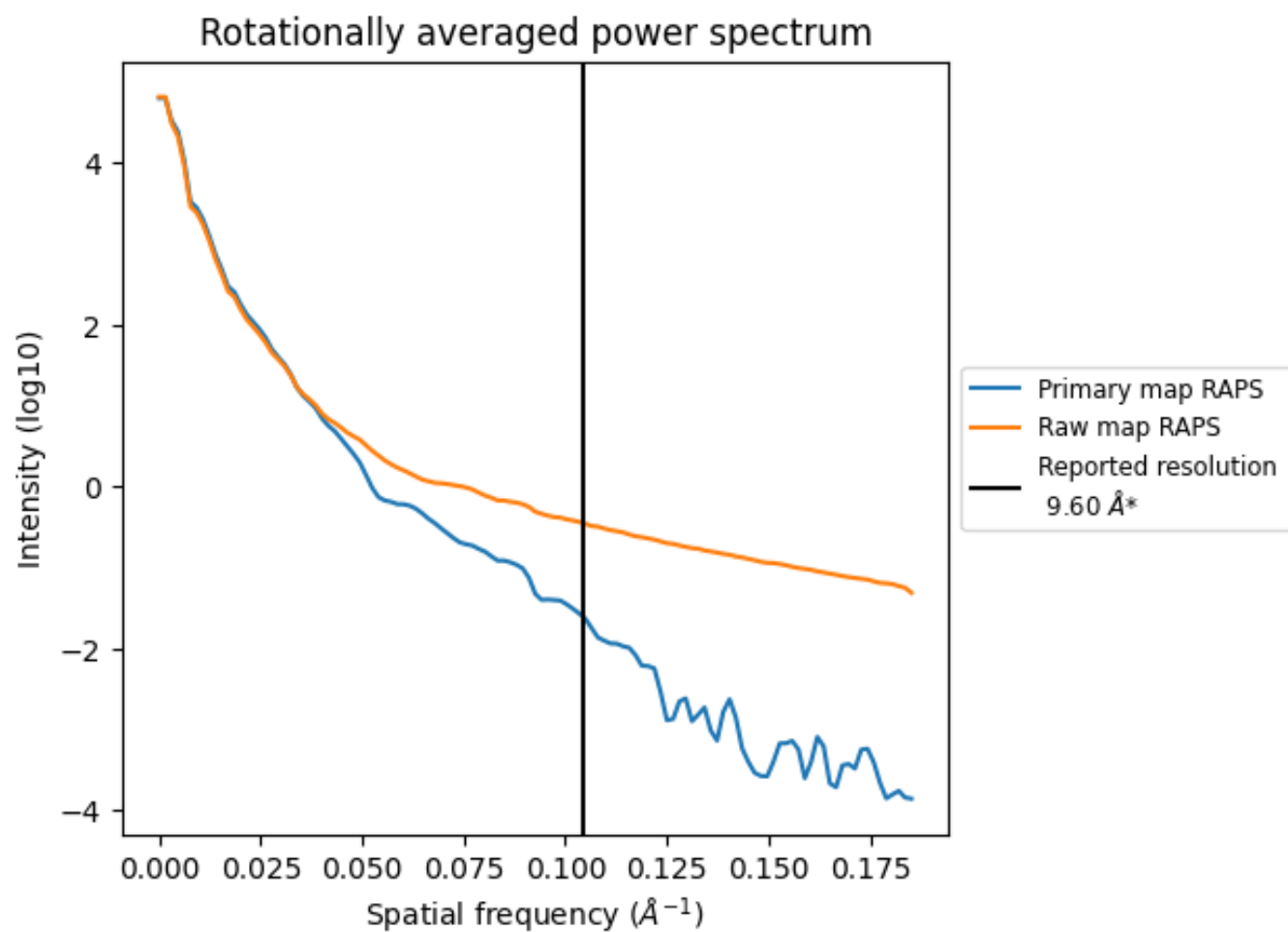
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 6186 nm^3 ; this corresponds to an approximate mass of 5588 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 ⓘ

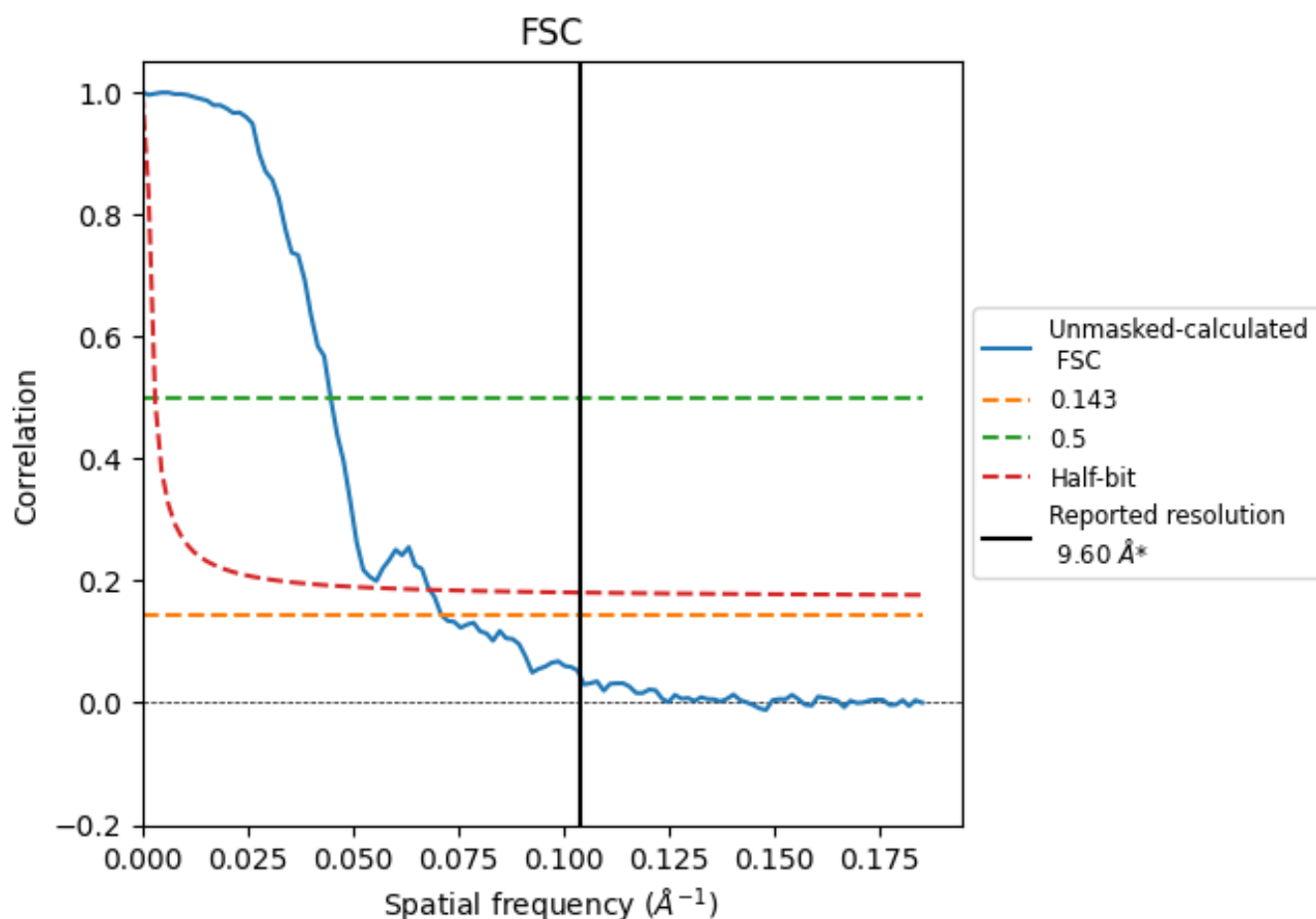


*Reported resolution corresponds to spatial frequency of 0.104 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.104 Å⁻¹

8.2 Resolution estimates [i](#)

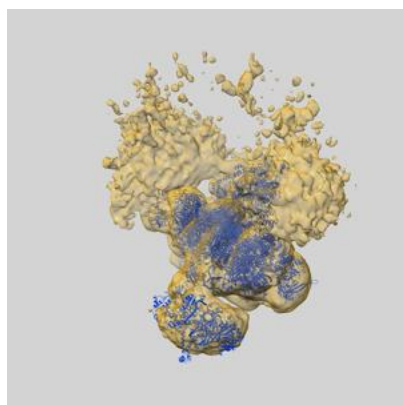
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	9.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	14.06	22.37	14.64

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 14.06 differs from the reported value 9.6 by more than 10 %

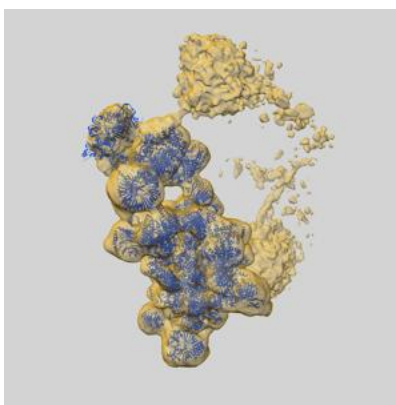
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-18718 and PDB model 8QXD. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

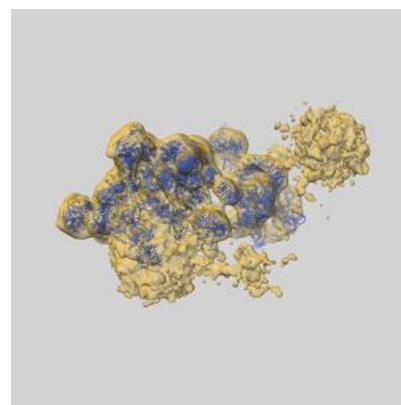
9.1 Map-model overlay [i](#)



X



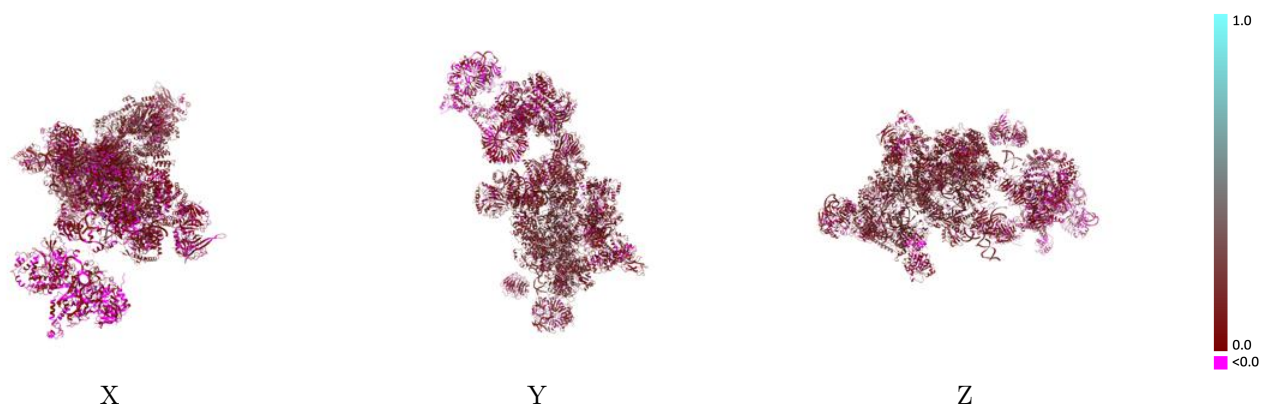
Y



Z

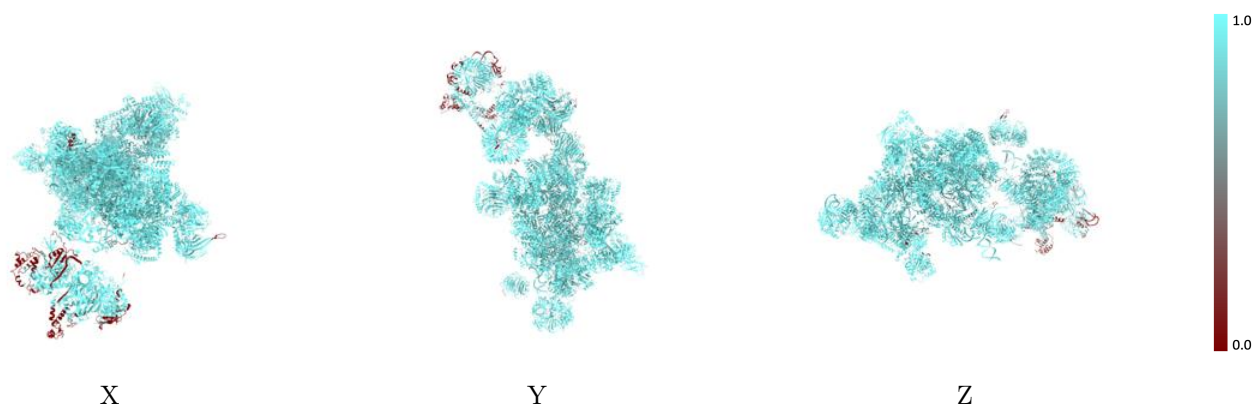
The images above show the 3D surface view of the map at the recommended contour level 0.0125 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



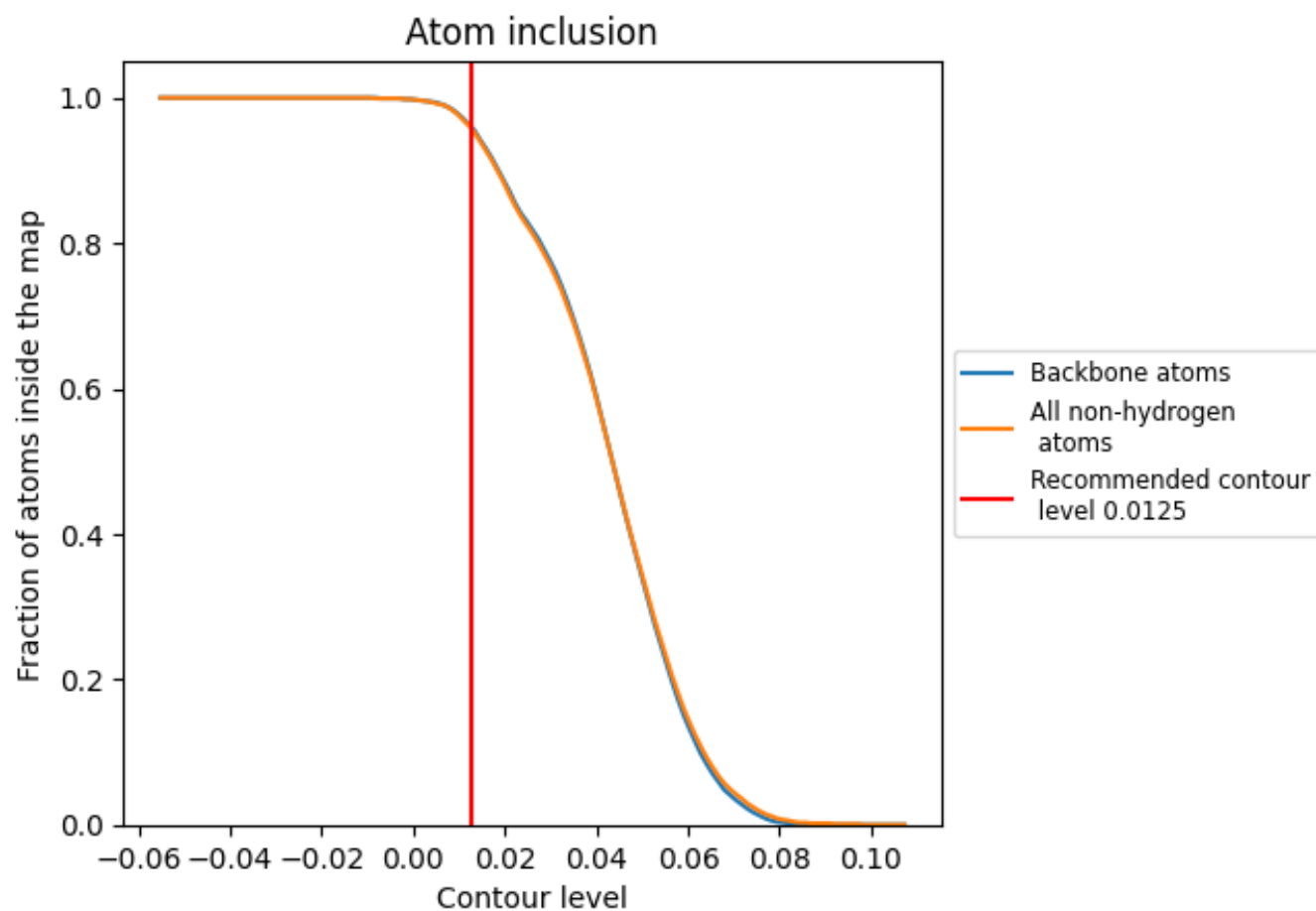
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0125).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 96% 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 (0.0125) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9590	 0.0960
2	 0.8420	 0.0400
21	 1.0000	 0.0600
22	 0.8380	 -0.0230
23	 1.0000	 0.0370
2A	 0.9280	 0.0530
2B	 0.5010	 -0.0010
2b	 0.9540	 -0.0030
2e	 0.7070	 0.0060
2f	 0.5910	 0.0100
2g	 0.9890	 0.0450
4	 0.9910	 0.1240
41	 0.9930	 0.0810
42	 0.9050	 0.0710
43	 1.0000	 0.0580
4b	 0.9200	 0.0540
4e	 1.0000	 0.1100
4f	 0.9920	 0.0980
4g	 0.9760	 0.0880
5	 1.0000	 0.1240
51	 1.0000	 0.1010
52	 1.0000	 0.1160
53	 1.0000	 0.1220
5b	 0.9970	 0.0860
5e	 1.0000	 0.1010
5f	 1.0000	 0.0920
5g	 0.9930	 0.0970
6	 0.9820	 0.1110
62	 0.9920	 0.0460
63	 0.8510	 0.0500
64	 1.0000	 0.0600
65	 0.9970	 0.0500
66	 0.9270	 0.0440
67	 0.9970	 0.0540
68	 1.0000	 0.0240



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Chain	Atom inclusion	Q-score
7	 0.4810	 0.0360
8	 0.8190	 0.0460
9	 0.6310	 0.0270
A	 0.9860	 0.1510
B	 0.9950	 0.1080
B1	 0.9850	 0.0510
B2	 0.9820	 0.0540
B3	 0.9470	 0.0660
B4	 1.0000	 0.0680
B5	 0.9910	 0.0480
B6	 1.0000	 0.0740
BP	 0.9780	 0.0670
C	 0.9990	 0.1440
D	 1.0000	 0.1420
E	 0.9780	 0.0500
F	 1.0000	 0.0980
G	 0.9570	 0.0890
J	 1.0000	 0.1110
K	 0.9640	 0.0860
L	 0.9700	 0.1220
M	 1.0000	 0.1060
N	 0.9980	 0.1220
R	 0.9700	 0.0920
S	 0.9520	 0.0890
U	 0.9960	 0.1540
X	 1.0000	 0.0580
Z	 1.0000	 0.1090