wwPDB EM Validation Summary Report (i)

Jan 18, 2024 – 08:37 pm GMT

PDB ID	:	8Q7N
EMDB ID	:	EMD-18225
Title	:	cryo-EM structure of the human spliceosomal B complex protomer (tri-snRNP core region)
Authors	:	Zhang, Z.; Kumar, V.; Dybkov, O.; Will, C.L.; Urlaub, H.; Stark, H.; Luehrmann, R.
Deposited on	:	2023-08-16
Resolution	:	3.10 Å(reported)

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

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

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

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

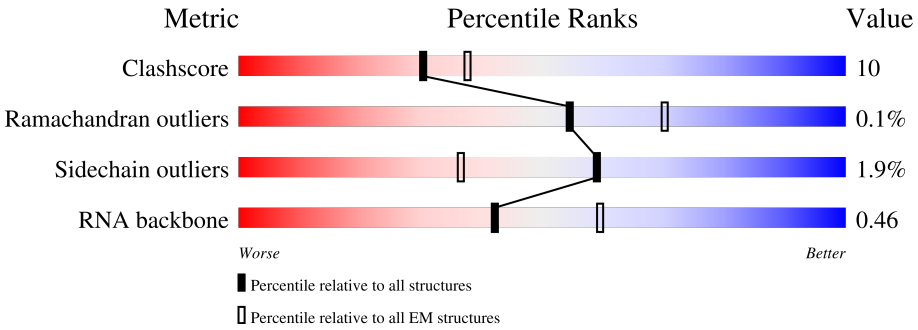
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	5	117	21% 30% 57% 11%
2	6	106	11% 9% 48% 16% 26%
3	7	793	7% 90%
4	C	972	65% 22% 13%
5	D	142	75% 24%
6	I	312	44% 15% 41%
7	K	439	5% 26% 5% 69%

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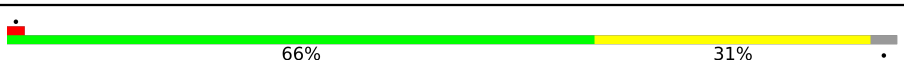
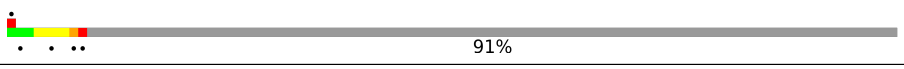
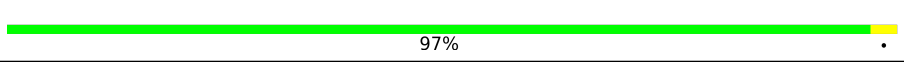
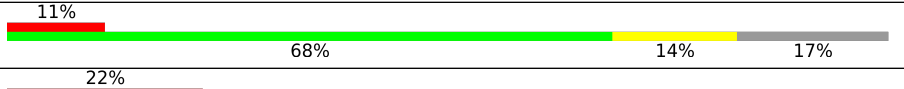
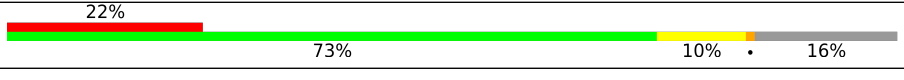
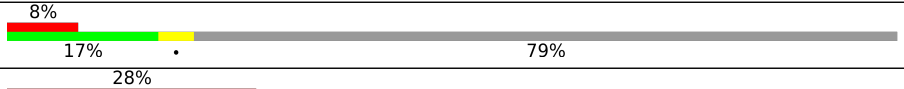
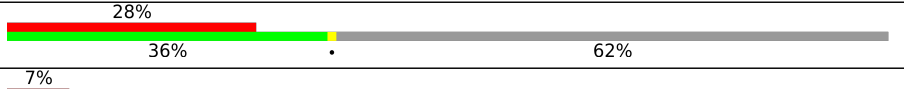
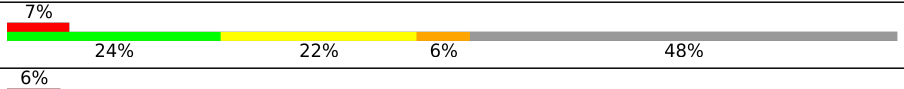
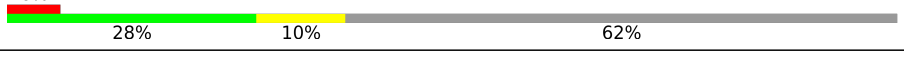
Mol	Chain	Length	Quality of chain
8	M	128	
9	Q	144	
10	X	376	
11	Z	347	
12	r	199	
13	s	73	
14	L	499	
15	F	522	
16	N	941	
17	A	2335	
18	S	800	
19	T	1098	
20	4	145	
21	J	683	

2 Entry composition (i)

There are 21 unique types of molecules in this entry. The entry contains 55463 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 U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	5	115	2420	1084	403	818	115	0	0

- Molecule 2 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	6	78	1670	747	309	536	78	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	7	81	650	405	115	128	2	0	0

- Molecule 4 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	C	843	6649	4250	1117	1249	33	0	0

- Molecule 5 is a protein called Thioredoxin-like protein 4A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	D	141	1170	751	194	215	10	0	0

- Molecule 6 is a protein called Pre-mRNA-splicing factor 38A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	I	184	1521	978	256	277	10	0	0

- Molecule 7 is a protein called Microfibrillar-associated protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	135	Total	C	N	O	S	0	0
			922	577	166	177	2		

- Molecule 8 is a protein called NHP2-like protein 1, N-terminally processed.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	M	124	Total	C	N	O	S	0	0
			962	608	171	178	5		

- Molecule 9 is a protein called Protein BUD31 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Q	142	Total	C	N	O	S	0	0
			1174	738	216	209	11		

- Molecule 10 is a protein called WW domain-binding protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	81	Total	C	N	O	S	0	0
			668	419	120	125	4		

- Molecule 11 is a RNA chain called MINX pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Z	31	Total	C	N	O	P	0	0
			664	297	124	212	31		

- Molecule 12 is a protein called Zinc finger matrin-type protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	r	89	Total	C	N	O	S	0	0
			728	452	137	132	7		

- Molecule 13 is a protein called Ubiquitin-like protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	s	73	Total	C	N	O	S	0	0
			600	383	103	110	4		

- Molecule 14 is a protein called U4/U6 small nuclear ribonucleoprotein Prp31.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	L	373	Total	C	N	O	S	0	0
			2853	1777	520	544	12		

- Molecule 15 is a protein called U4/U6 small nuclear ribonucleoprotein Prp4.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	F	431	Total	C	N	O	S	0	0
			3415	2142	621	632	20		

- Molecule 16 is a protein called Pre-mRNA-processing factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	N	791	Total	C	N	O	S	0	0
			4613	2822	892	894	5		

- Molecule 17 is a protein called Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	A	2234	Total	C	N	O	S	0	0
			17494	11122	3130	3172	70		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	171	Total	C	N	O	S	0	0
			1386	855	258	271	2		

- Molecule 19 is a protein called Transcription elongation regulator 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	412	Total	C	N	O	S	0	0
			2268	1363	452	452	1		

- Molecule 20 is a RNA chain called U4 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	4	76	Total	C	N	O	P	0	0
			1610	720	277	537	76		

- Molecule 21 is a protein called U4/U6 small nuclear ribonucleoprotein Prp3.

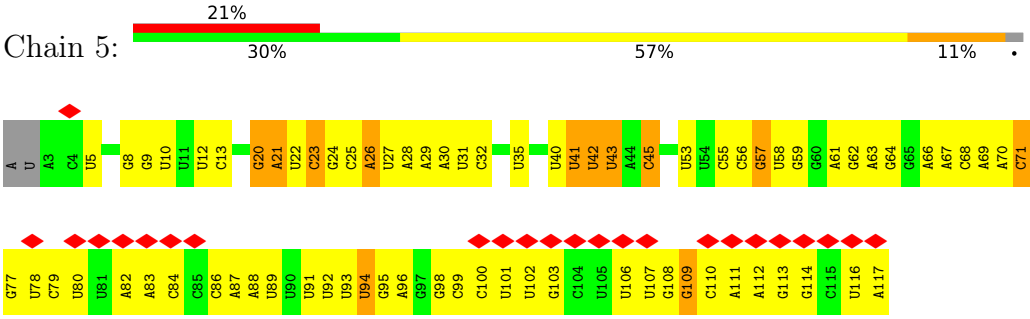
Mol	Chain	Residues	Atoms					AltConf	Trace
21	J	260	Total	C	N	O	S	0	0
			2026	1273	382	363	8		

3 Residue-property plots (i)

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

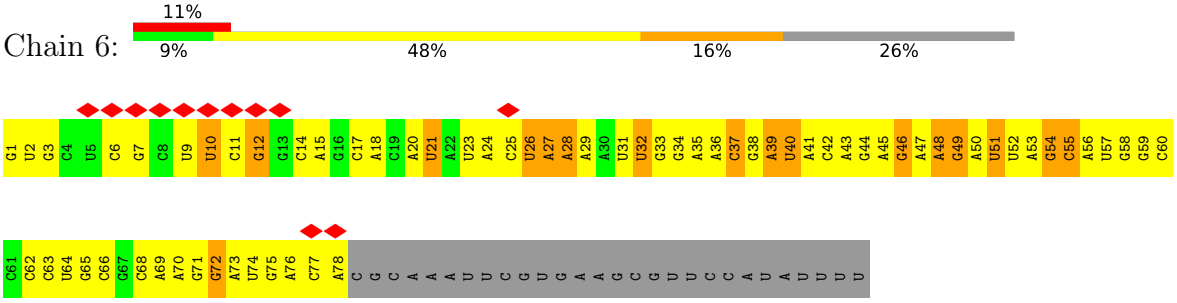
• Molecule 1: U5 snRNA

Chain 5:



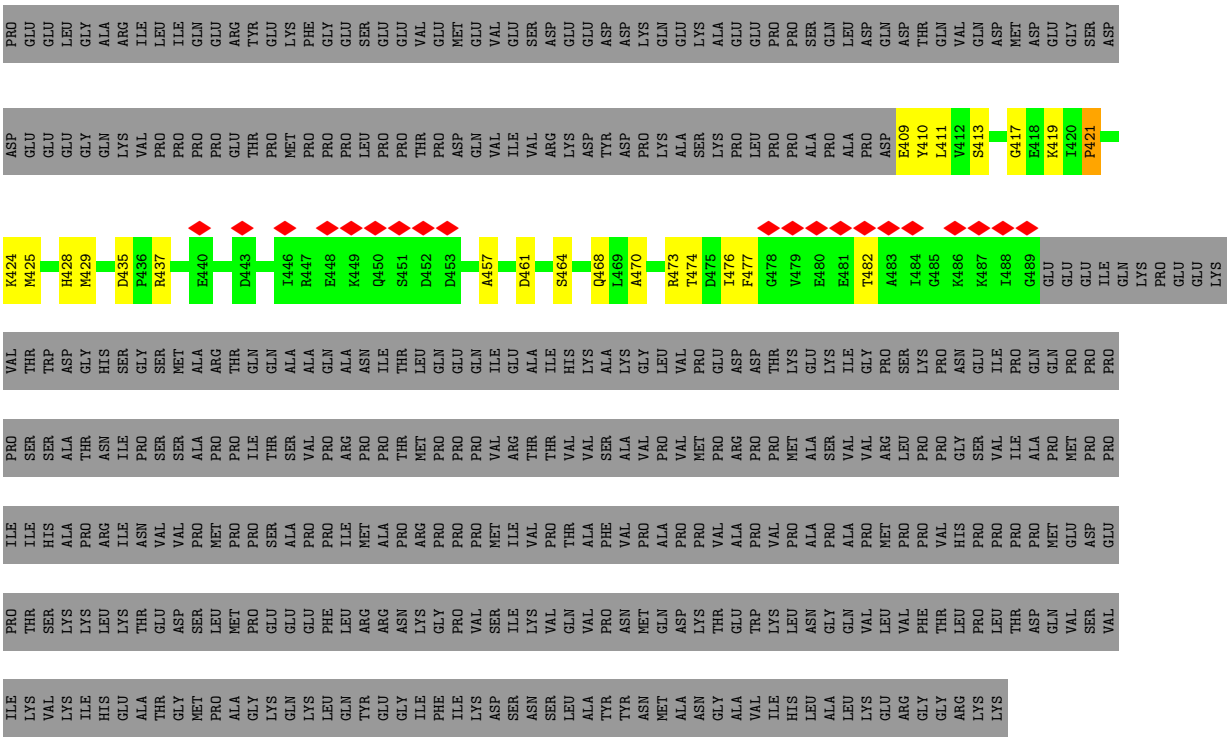
• Molecule 2: U6 snRNA

Chain 6:



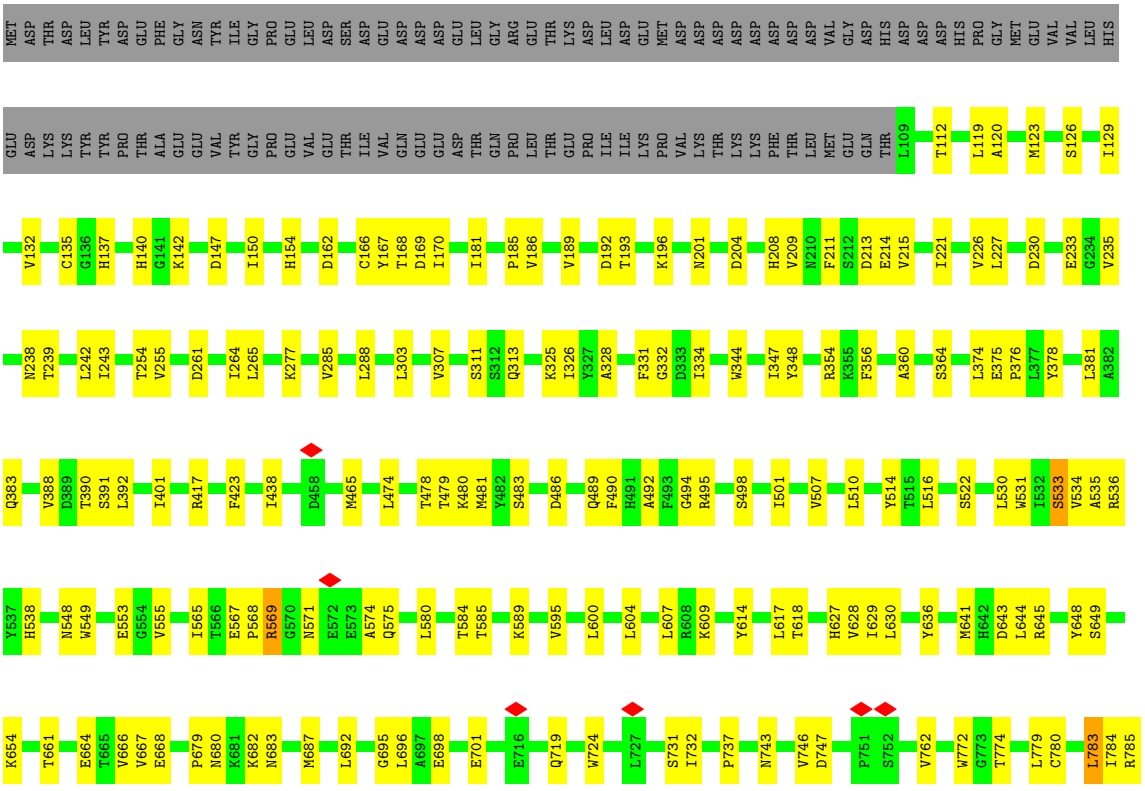
• Molecule 3: Splicing factor 3A subunit 1

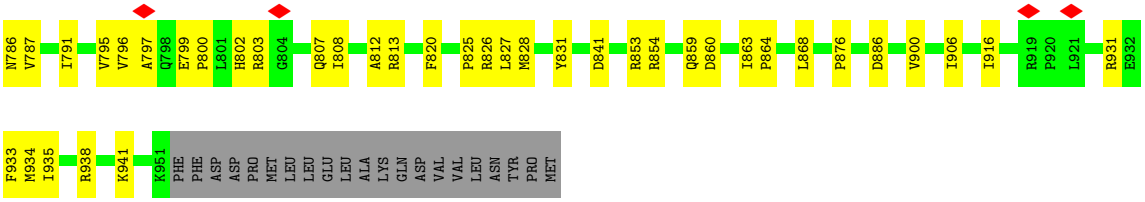
Chain 7:



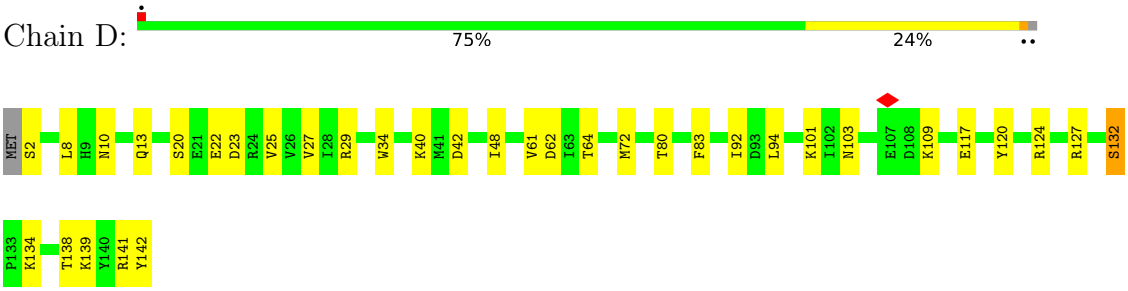
• Molecule 4: 116 kDa U5 small nuclear ribonucleoprotein component

Chain C:

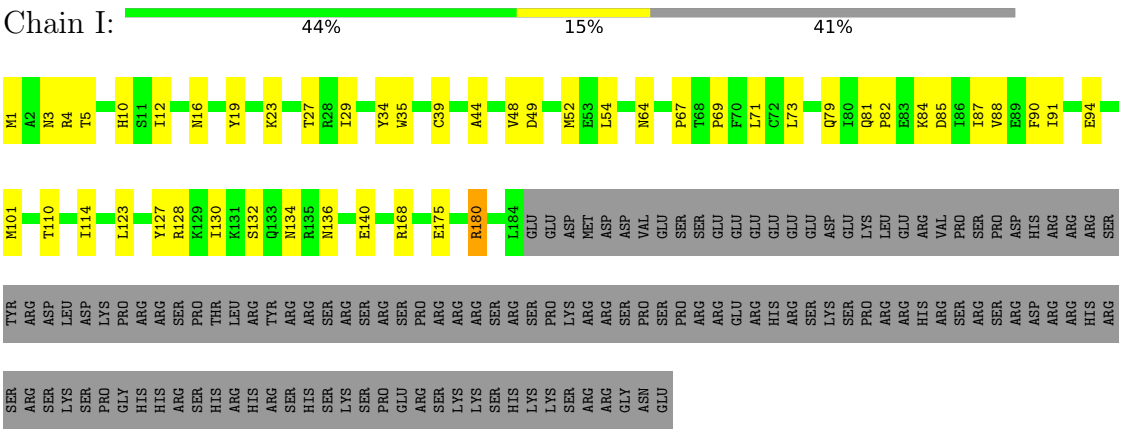




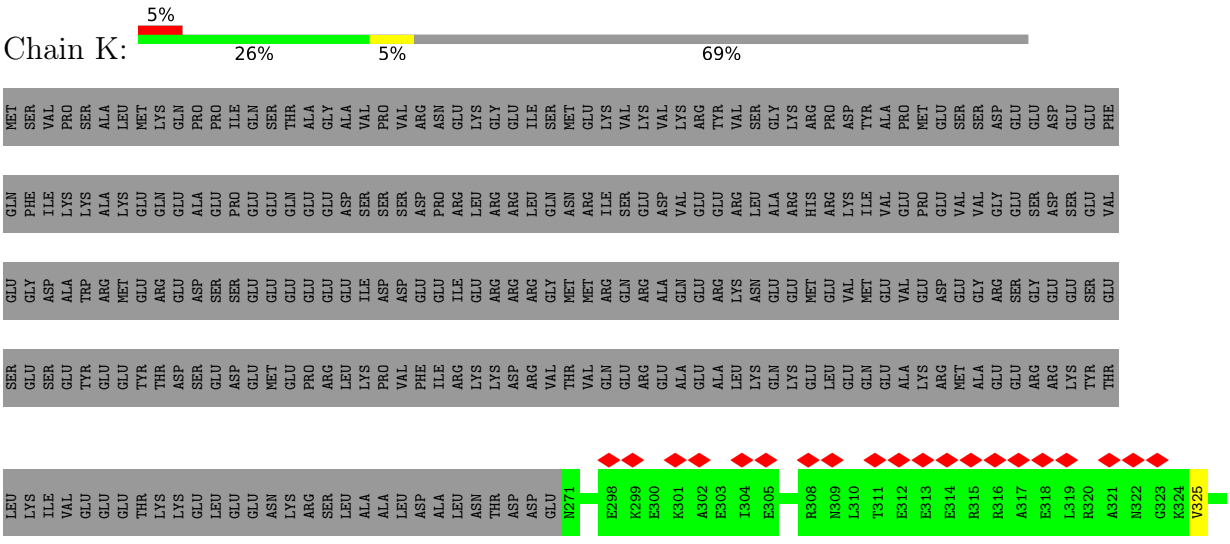
• Molecule 5: Thioredoxin-like protein 4A

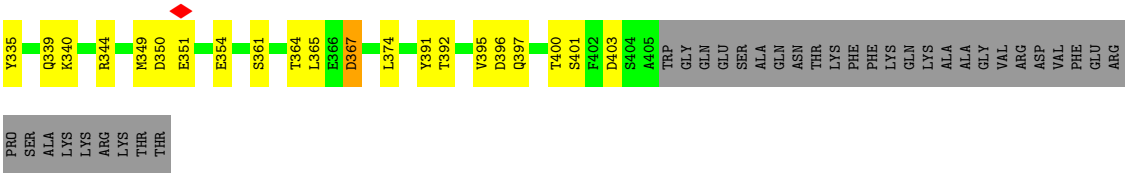


• Molecule 6: Pre-mRNA-splicing factor 38A



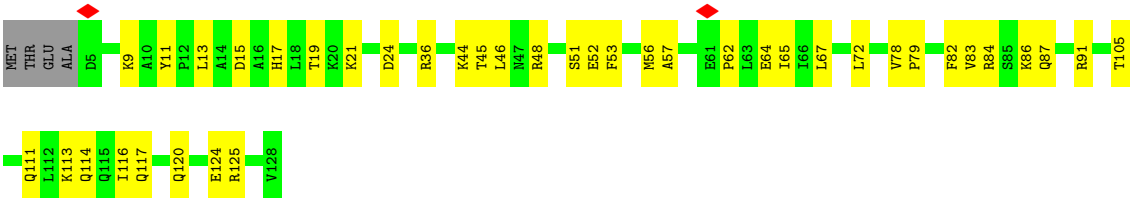
• Molecule 7: Microfibrillar-associated protein 1





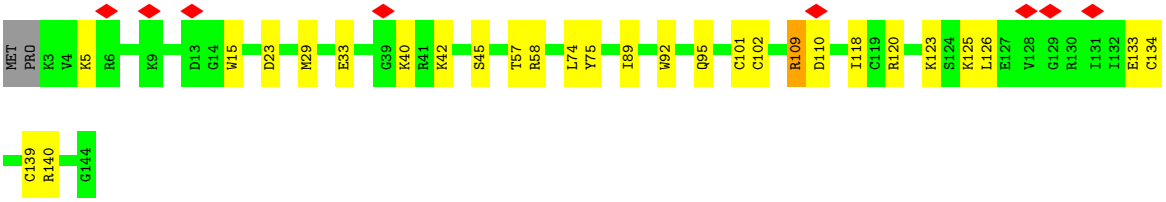
• Molecule 8: NHP2-like protein 1, N-terminally processed

Chain M:



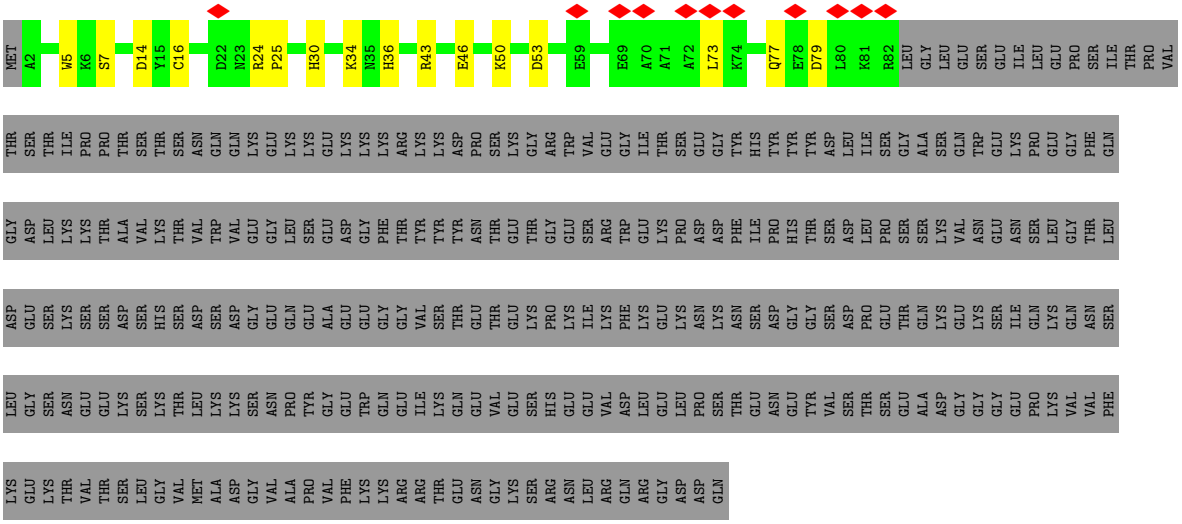
• Molecule 9: Protein BUD31 homolog

Chain Q:



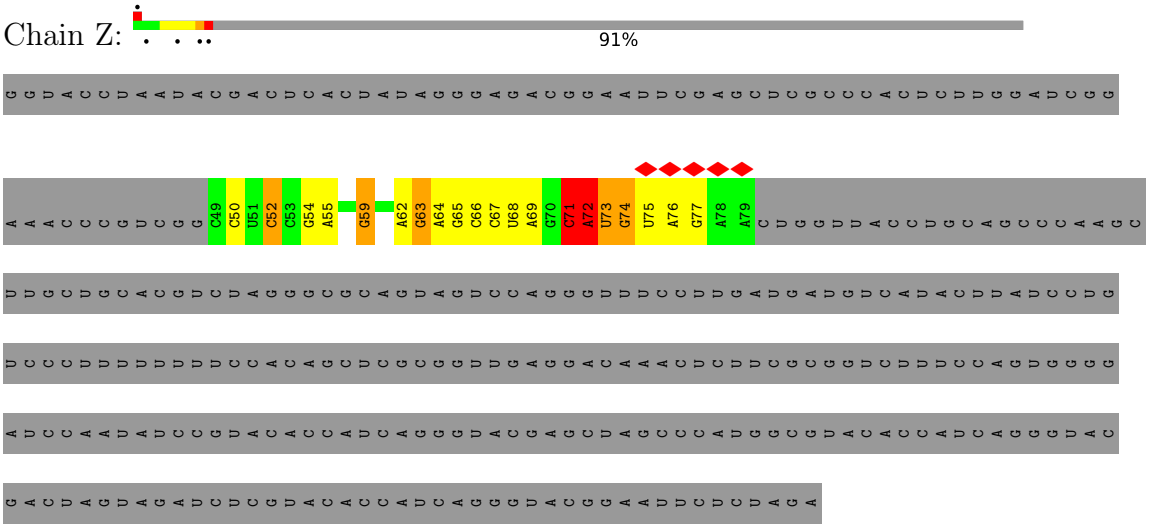
• Molecule 10: WW domain-binding protein 4

Chain X:



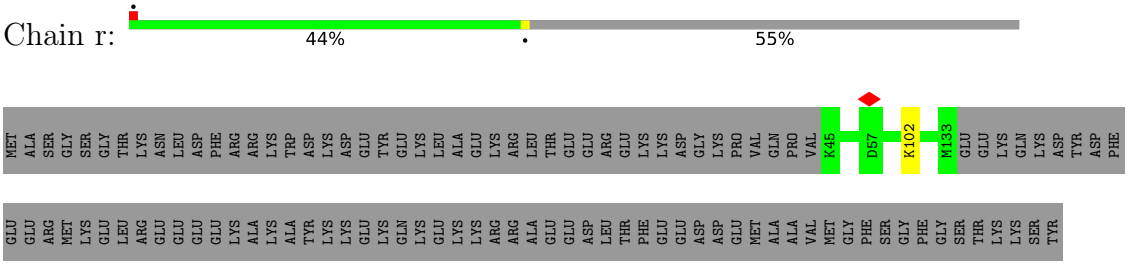
• Molecule 11: MINX pre-mRNA

Chain Z:



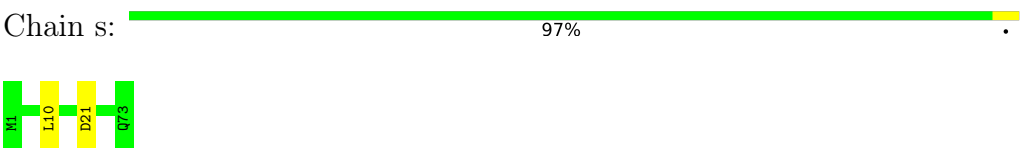
• Molecule 12: Zinc finger matrin-type protein 2

Chain r:



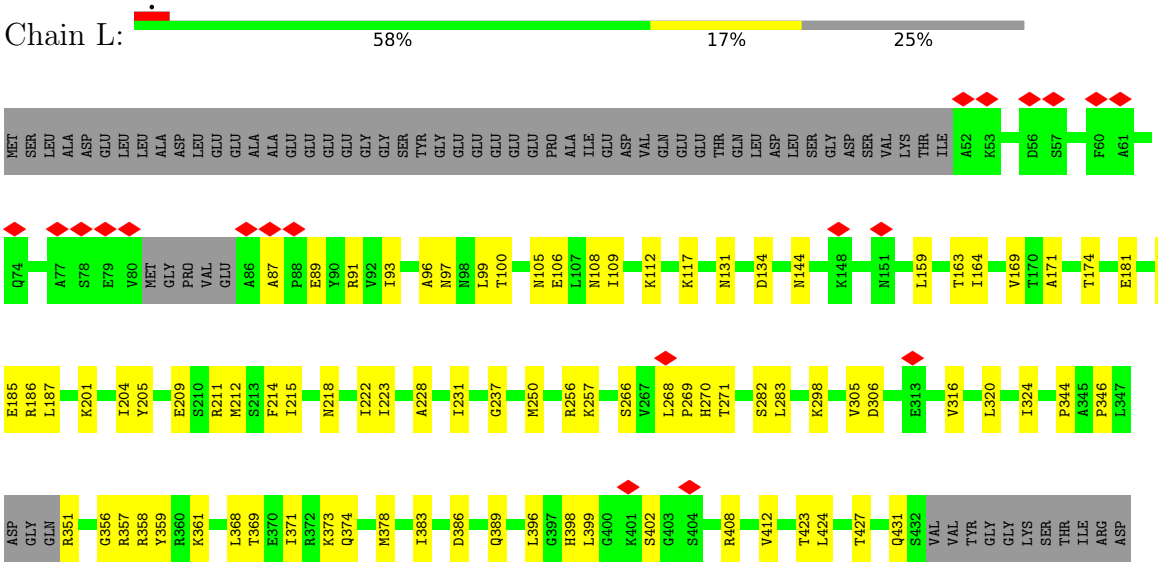
• Molecule 13: Ubiquitin-like protein 5

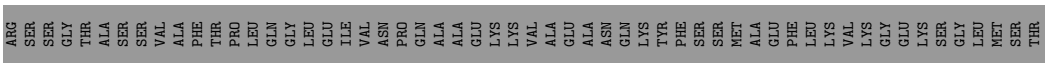
Chain s:



• Molecule 14: U4/U6 small nuclear ribonucleoprotein Prp31

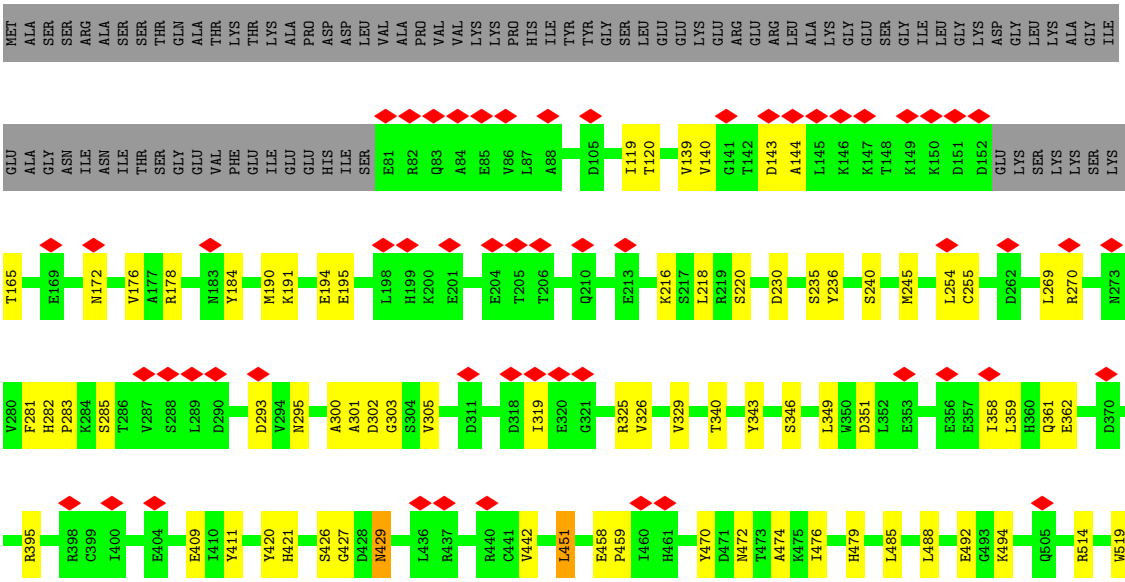
Chain L:





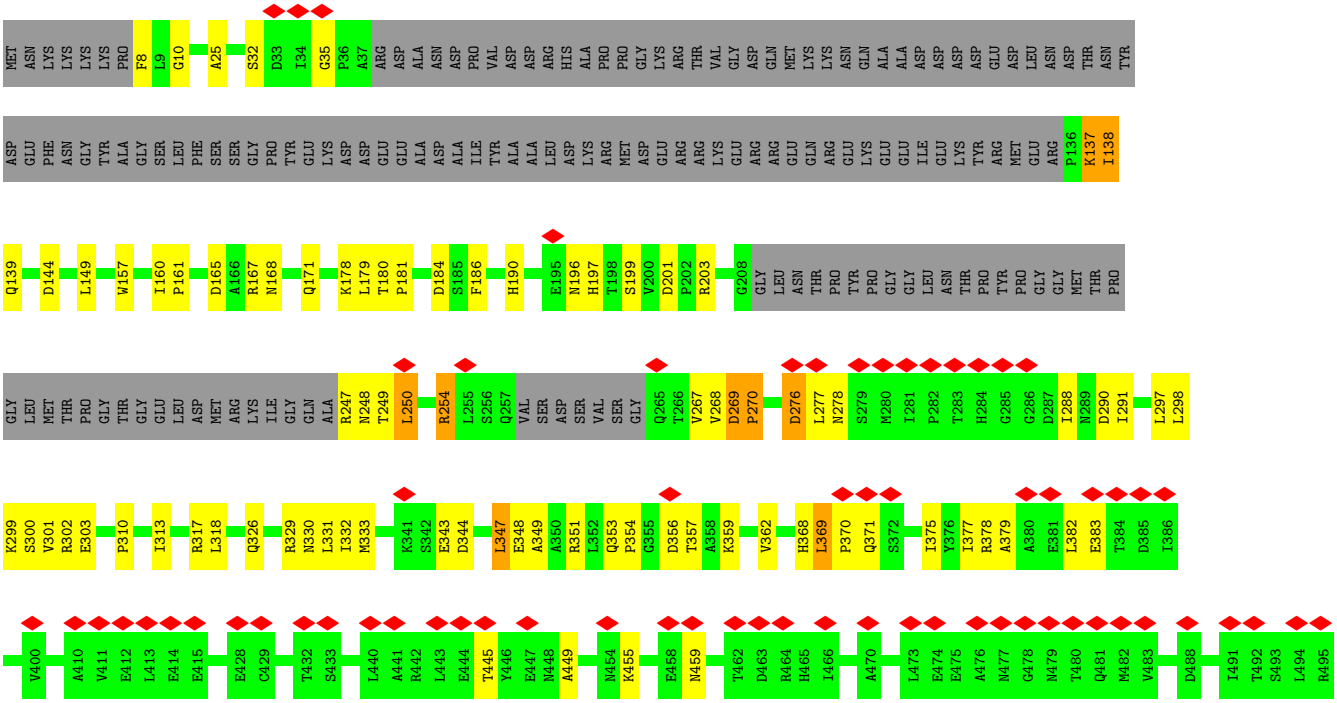
• Molecule 15: U4/U6 small nuclear ribonucleoprotein Prp4

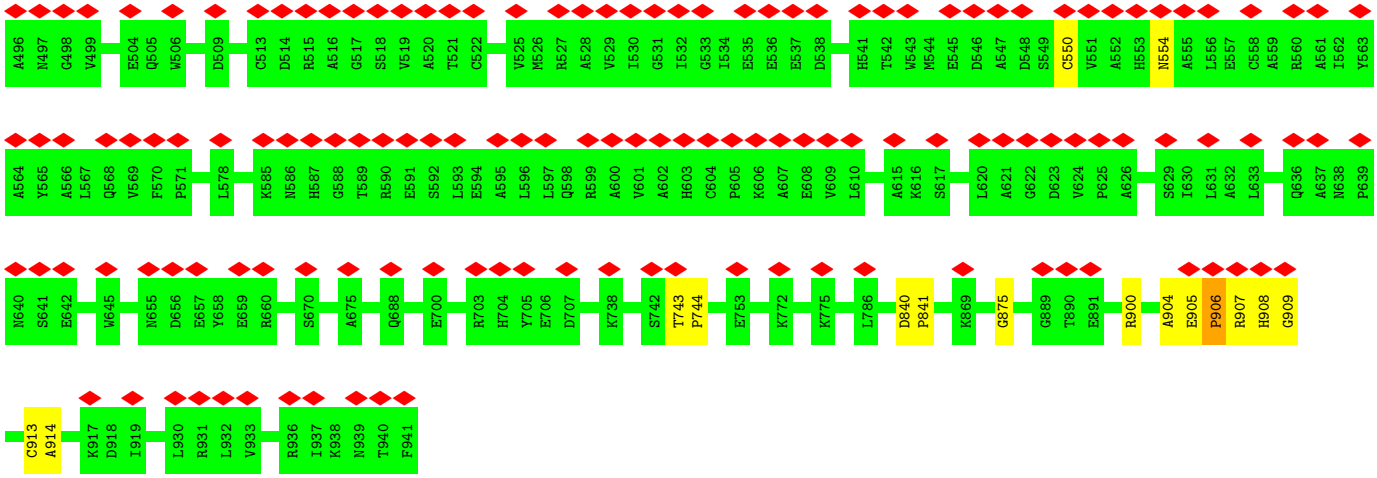
Chain F:



• Molecule 16: Pre-mRNA-processing factor 6

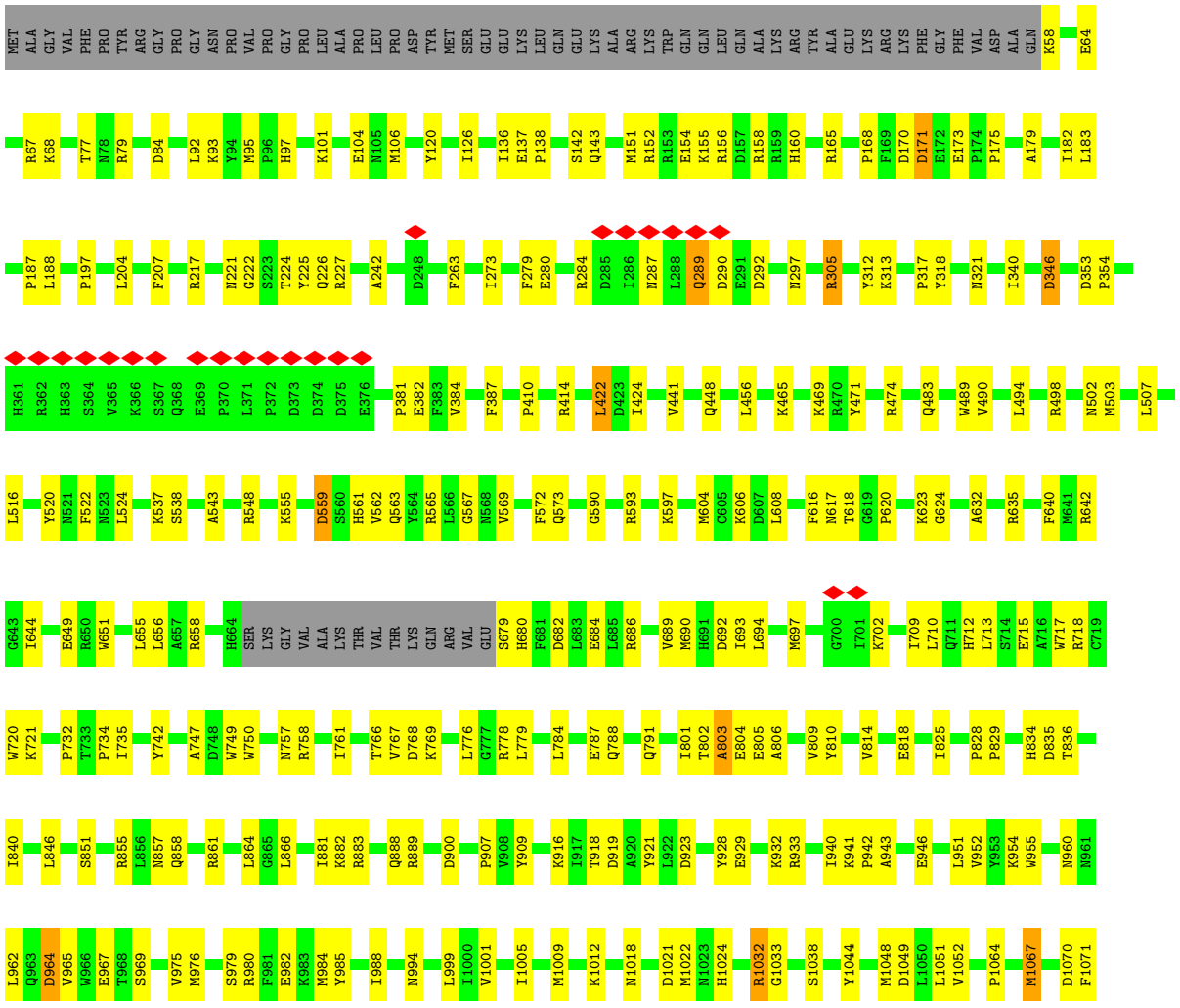
Chain N:

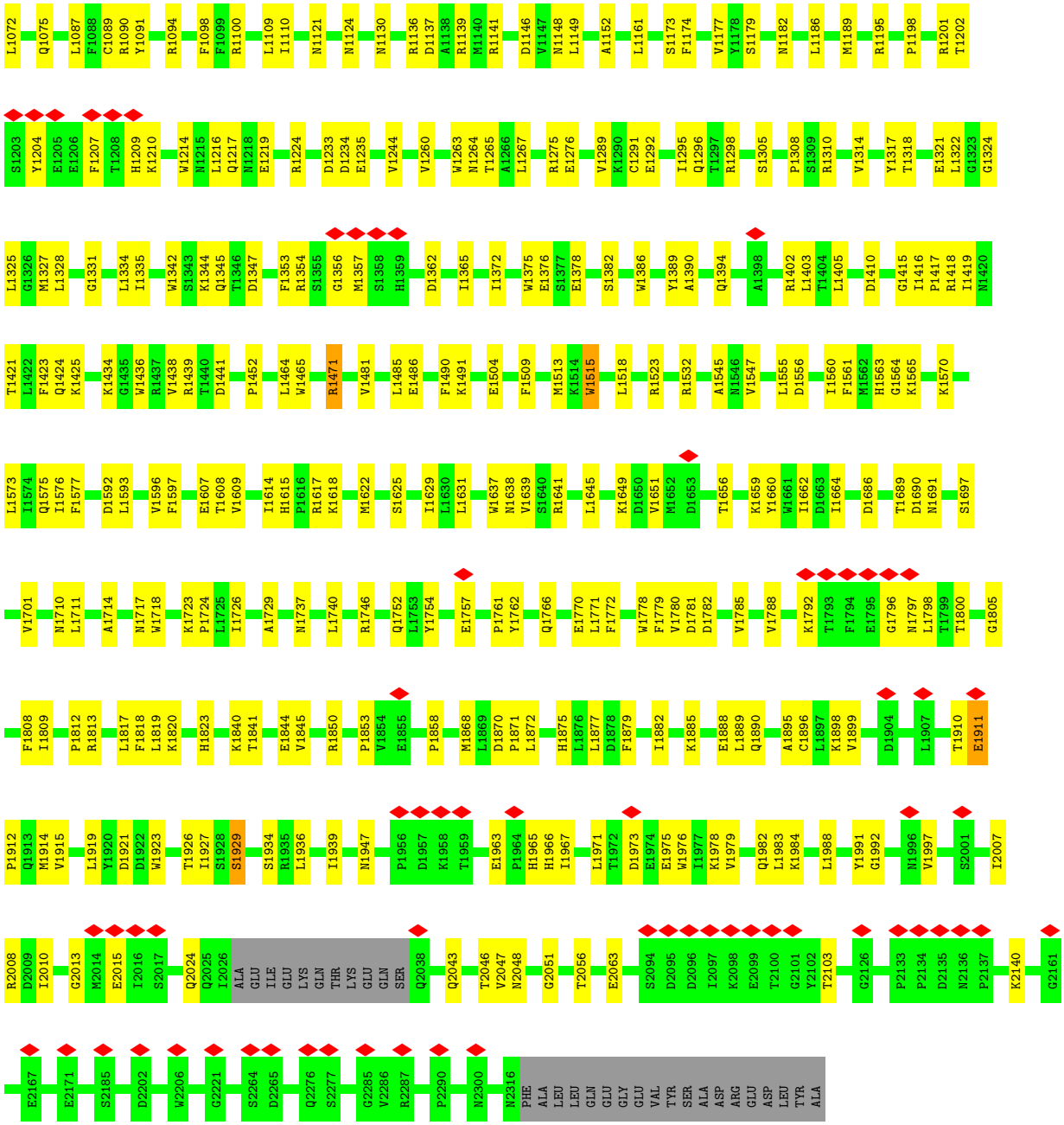




• Molecule 17: Pre-mRNA-processing-splicing factor 8

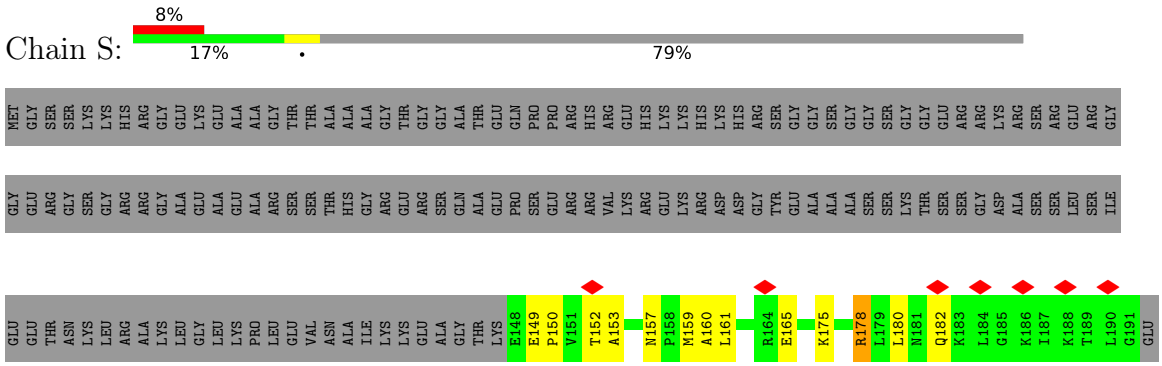
Chain A:

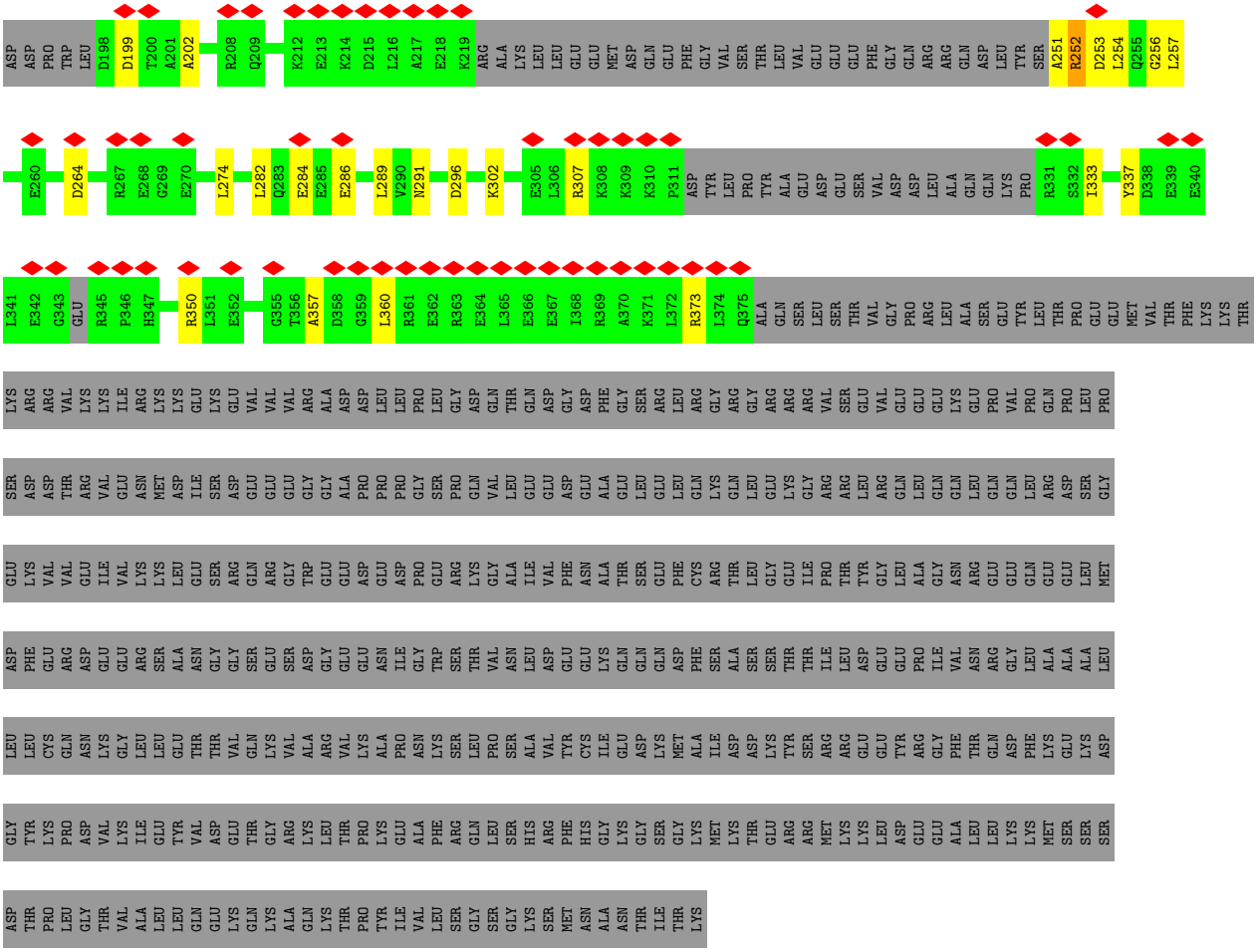




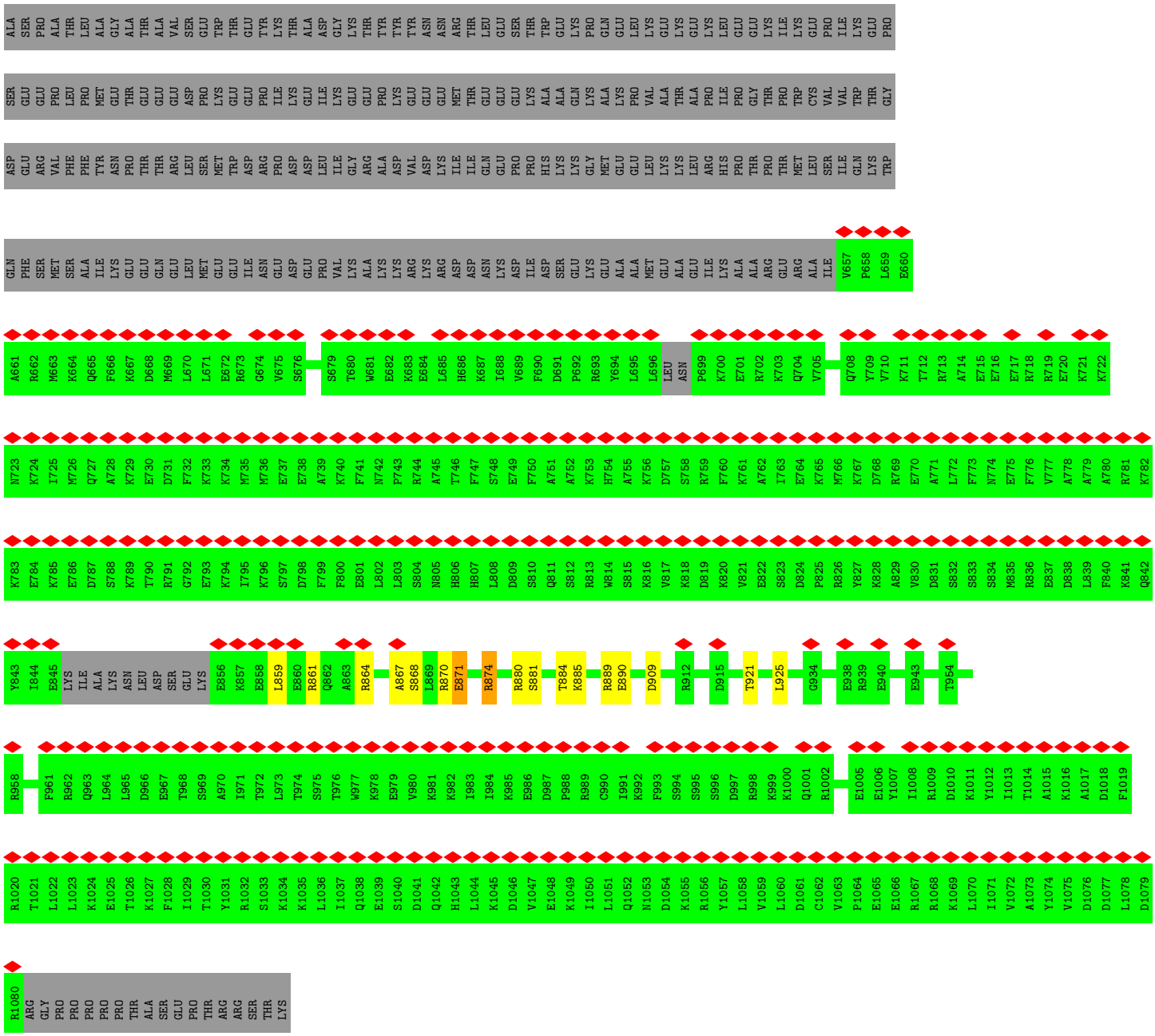
• Molecule 18: U4/U6.U5 tri-snRNP-associated protein 1

Chain S:



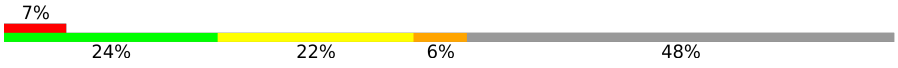


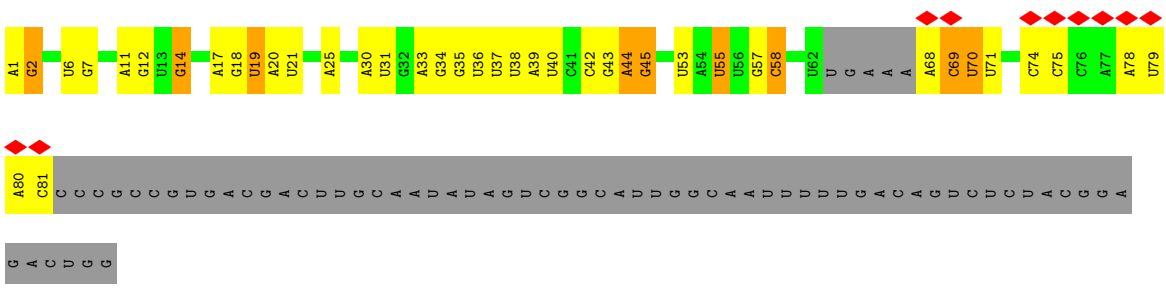
• Molecule 19: Transcription elongation regulator 1



• Molecule 20: U4 snRNA

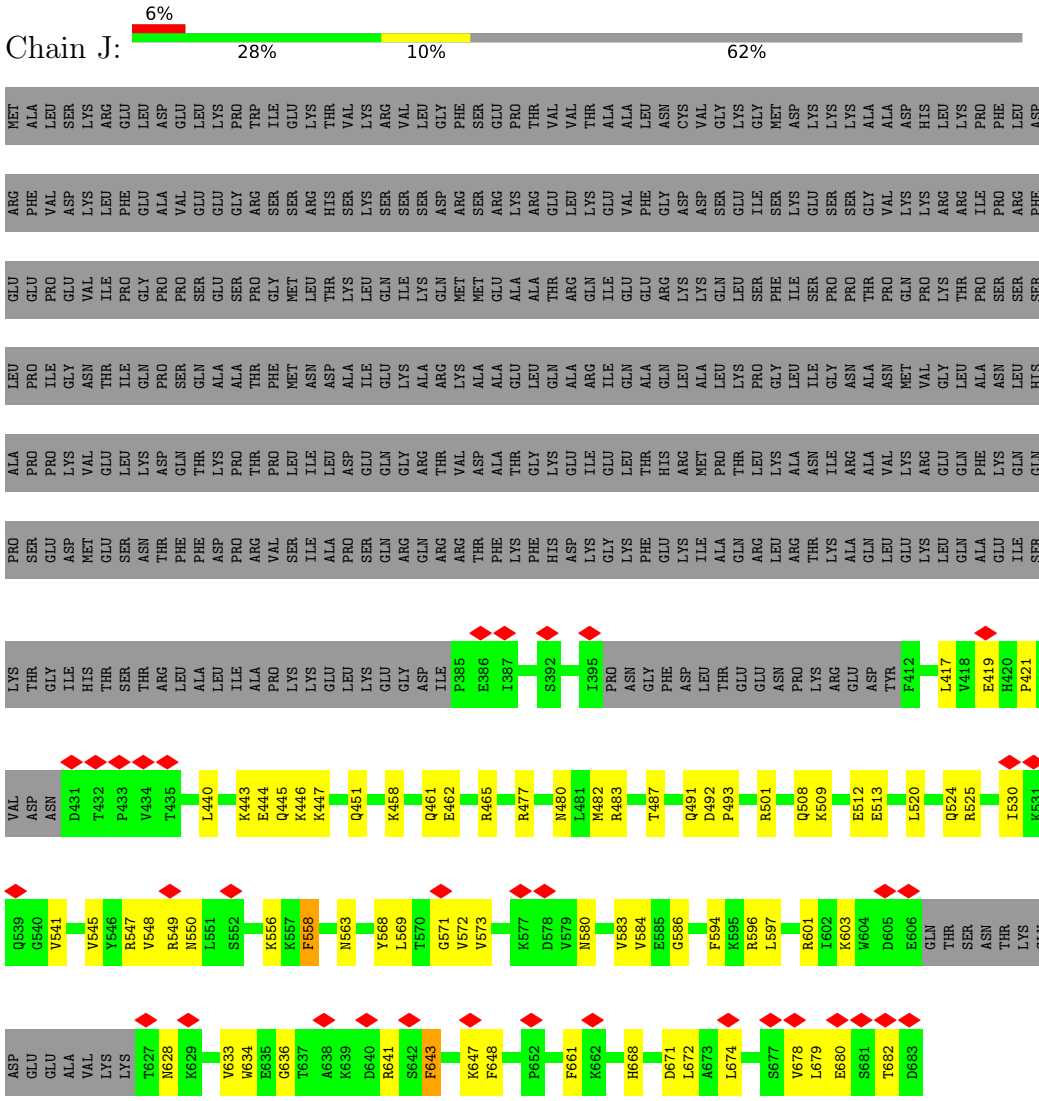
Chain 4:





• Molecule 21: U4/U6 small nuclear ribonucleoprotein Prp3

Chain J:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	251564	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	48	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.240	Depositor
Minimum map value	-0.112	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	603.2, 603.2, 603.2	wwPDB
Map dimensions	520, 520, 520	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.16, 1.16, 1.16	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	5	0.28	0/2698	0.81	0/4195
2	6	0.32	0/1870	0.84	0/2913
3	7	0.44	1/659 (0.2%)	0.78	3/884 (0.3%)
4	C	0.28	0/6798	0.49	0/9234
5	D	0.30	0/1199	0.48	0/1620
6	I	0.29	0/1551	0.51	0/2090
7	K	0.28	0/938	0.50	0/1275
8	M	0.26	0/974	0.51	0/1316
9	Q	0.28	0/1199	0.52	0/1605
10	X	0.26	0/681	0.43	0/906
11	Z	0.37	0/743	0.93	5/1156 (0.4%)
12	r	0.28	0/736	0.57	0/978
13	s	0.31	0/610	0.50	0/819
14	L	0.27	0/2890	0.50	0/3893
15	F	0.25	0/3497	0.50	1/4735 (0.0%)
16	N	0.25	0/4666	0.51	3/6450 (0.0%)
17	A	0.29	0/17943	0.50	2/24236 (0.0%)
18	S	0.26	0/1392	0.52	0/1853
19	T	0.23	0/2274	0.42	0/3145
20	4	0.34	0/1796	0.87	7/2792 (0.3%)
21	J	0.26	0/2058	0.52	0/2762
All	All	0.28	1/57172 (0.0%)	0.57	21/78857 (0.0%)

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
13	s	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	7	421	PRO	CG-CD	-6.85	1.28	1.50

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	7	421	PRO	CA-N-CD	-13.71	92.31	111.50
16	N	270	PRO	CA-N-CD	-13.36	92.79	111.50
3	7	421	PRO	N-CD-CG	-8.44	90.53	103.20
20	4	70	U	C2-N1-C1'	7.82	127.08	117.70
17	A	1853	PRO	CA-N-CD	-7.28	101.31	111.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	s	10	LEU	Peptide

5.2 Too-close contacts (i)

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	5	2420	0	1226	42	0
2	6	1670	0	844	68	0
3	7	650	0	655	15	0
4	C	6649	0	6671	137	0
5	D	1170	0	1141	31	0
6	I	1521	0	1544	30	0
7	K	922	0	727	20	0
8	M	962	0	1012	29	0
9	Q	1174	0	1182	19	0
10	X	668	0	661	11	0
11	Z	664	0	337	20	0
12	r	728	0	757	0	0
13	s	600	0	613	0	0
14	L	2853	0	2840	58	0
15	F	3415	0	3337	50	0
16	N	4613	0	3231	85	0
17	A	17494	0	16691	412	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	S	1386	0	1429	27	0
19	T	2268	0	1282	18	0
20	4	1610	0	815	21	0
21	J	2026	0	2048	56	0
All	All	55463	0	49043	995	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 10.

The worst 5 of 995 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)
3:7:429:MET:HG3	8:M:91:ARG:HH12	1.35	0.89
21:J:545:VAL:HG12	21:J:583:VAL:HG23	1.57	0.85
3:7:410:TYR:HB3	3:7:419:LYS:HE2	1.63	0.81
17:A:1308:PRO:HB3	17:A:1547:VAL:HG23	1.64	0.79
4:C:193:THR:HG23	4:C:325:LYS:HD2	1.65	0.78

There are no symmetry-related clashes.

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	7	79/793 (10%)	73 (92%)	6 (8%)	0	100	100
4	C	841/972 (86%)	809 (96%)	32 (4%)	0	100	100
5	D	139/142 (98%)	137 (99%)	2 (1%)	0	100	100
6	I	182/312 (58%)	175 (96%)	7 (4%)	0	100	100
7	K	133/439 (30%)	118 (89%)	15 (11%)	0	100	100
8	M	122/128 (95%)	118 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	Q	140/144 (97%)	133 (95%)	7 (5%)	0	100	100
10	X	79/376 (21%)	76 (96%)	3 (4%)	0	100	100
12	r	87/199 (44%)	85 (98%)	2 (2%)	0	100	100
13	s	71/73 (97%)	65 (92%)	6 (8%)	0	100	100
14	L	367/499 (74%)	344 (94%)	22 (6%)	1 (0%)	41	73
15	F	427/522 (82%)	416 (97%)	11 (3%)	0	100	100
16	N	783/941 (83%)	690 (88%)	91 (12%)	2 (0%)	41	73
17	A	2228/2335 (95%)	2099 (94%)	128 (6%)	1 (0%)	100	100
18	S	161/800 (20%)	157 (98%)	4 (2%)	0	100	100
19	T	406/1098 (37%)	395 (97%)	11 (3%)	0	100	100
21	J	252/683 (37%)	244 (97%)	8 (3%)	0	100	100
All	All	6497/10456 (62%)	6134 (94%)	359 (6%)	4 (0%)	54	83

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
17	A	803	ALA
16	N	138	ILE
16	N	906	PRO
14	L	344	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	7	71/709 (10%)	71 (100%)	0	100	100
4	C	745/866 (86%)	738 (99%)	7 (1%)	78	91
5	D	129/130 (99%)	126 (98%)	3 (2%)	50	77
6	I	167/293 (57%)	162 (97%)	5 (3%)	41	71
7	K	66/395 (17%)	63 (96%)	3 (4%)	27	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
8	M	108/111 (97%)	105 (97%)	3 (3%)	43 73
9	Q	128/130 (98%)	125 (98%)	3 (2%)	50 77
10	X	69/333 (21%)	66 (96%)	3 (4%)	29 62
12	r	84/181 (46%)	83 (99%)	1 (1%)	71 88
13	s	66/66 (100%)	65 (98%)	1 (2%)	65 85
14	L	297/424 (70%)	292 (98%)	5 (2%)	60 83
15	F	367/442 (83%)	364 (99%)	3 (1%)	81 92
16	N	208/792 (26%)	199 (96%)	9 (4%)	29 62
17	A	1800/2108 (85%)	1769 (98%)	31 (2%)	60 83
18	S	149/681 (22%)	143 (96%)	6 (4%)	31 65
19	T	57/956 (6%)	54 (95%)	3 (5%)	22 54
21	J	208/599 (35%)	204 (98%)	4 (2%)	57 81
All	All	4719/9216 (51%)	4629 (98%)	90 (2%)	59 81

5 of 90 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	A	642	ARG
17	A	1691	ASN
17	A	834	HIS
17	A	1344	LYS
17	A	1929	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
17	A	1615	HIS
21	J	508	GLN
16	N	368	HIS
17	A	680	HIS
17	A	1296	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	5	114/117 (97%)	43 (37%)	2 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	Z	30/347 (8%)	10 (33%)	1 (3%)
2	6	77/106 (72%)	27 (35%)	4 (5%)
20	4	74/145 (51%)	23 (31%)	0
All	All	295/715 (41%)	103 (34%)	7 (2%)

5 of 103 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	5	5	U
1	5	8	G
1	5	9	G
1	5	10	U
1	5	20	G

5 of 7 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	6	39	A
2	6	52	U
11	Z	72	A
2	6	77	C
2	6	25	C

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

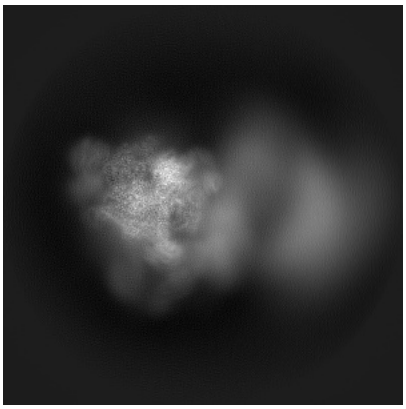
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-18225. These allow visual inspection of the internal detail of the map and identification of artifacts.

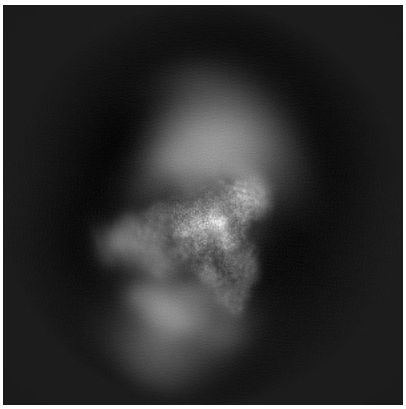
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

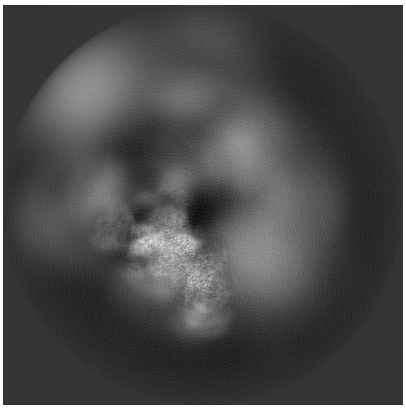
6.1.1 Primary map



X

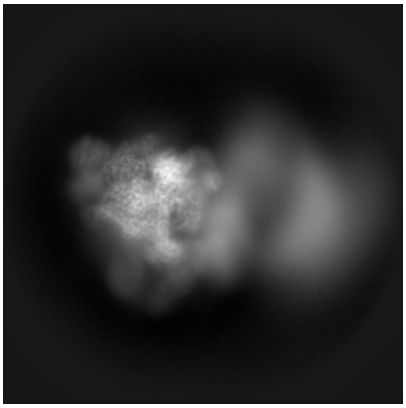


Y

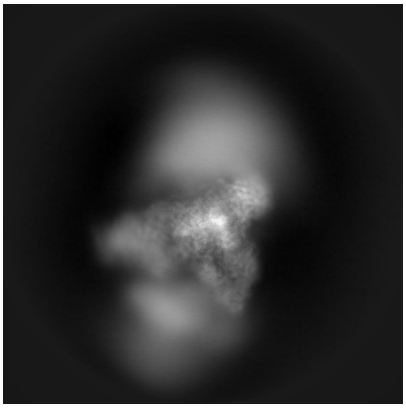


Z

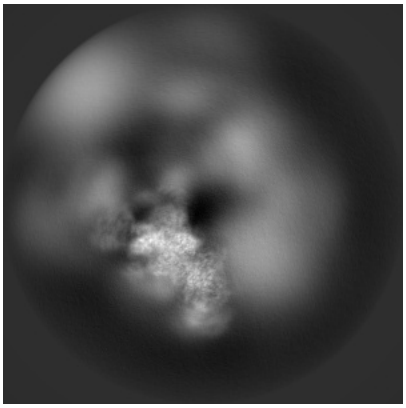
6.1.2 Raw map



X



Y

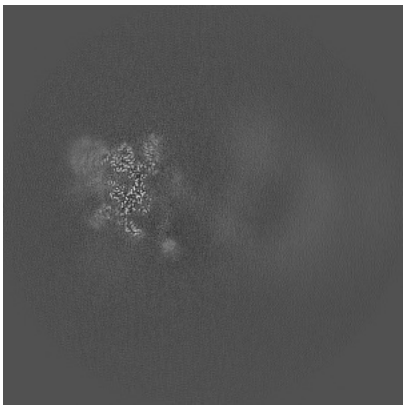


Z

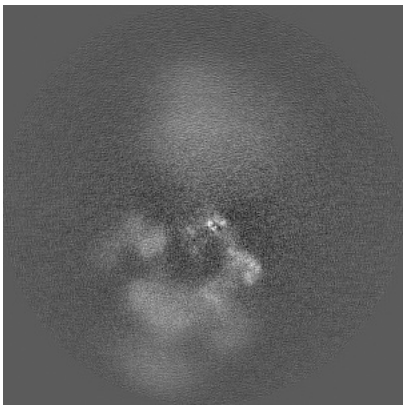
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

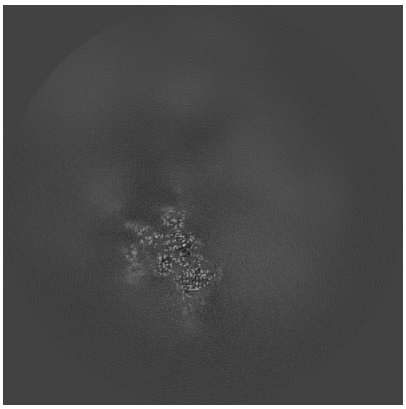
6.2.1 Primary map



X Index: 260

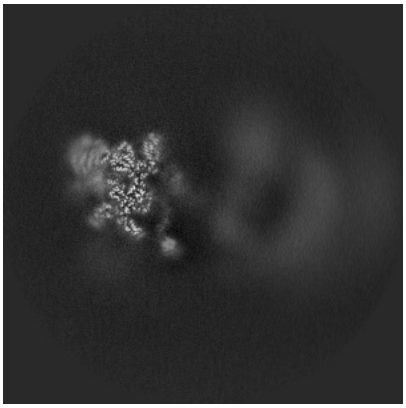


Y Index: 260

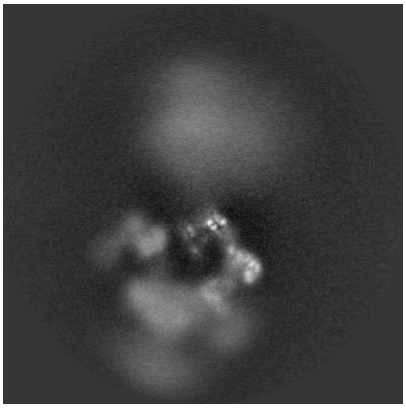


Z Index: 260

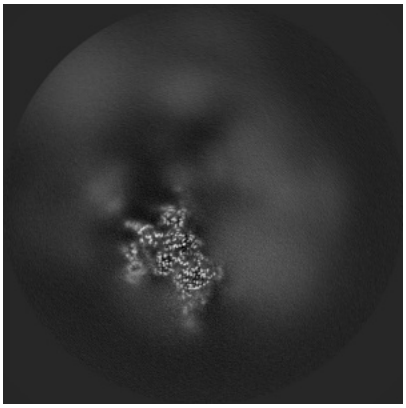
6.2.2 Raw map



X Index: 260



Y Index: 260

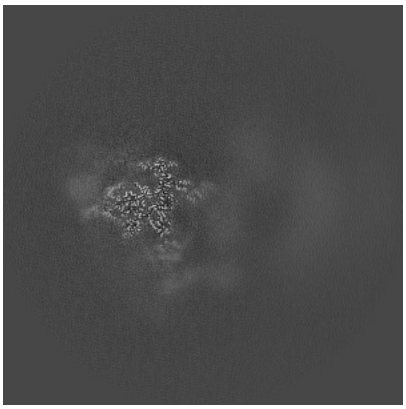


Z Index: 260

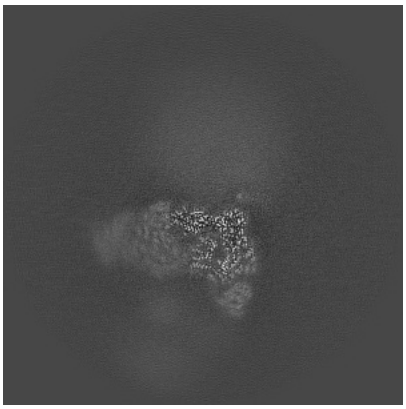
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

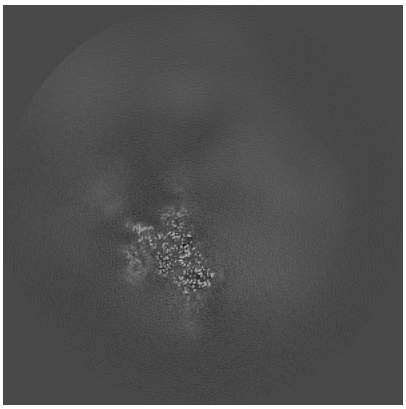
6.3.1 Primary map



X Index: 239

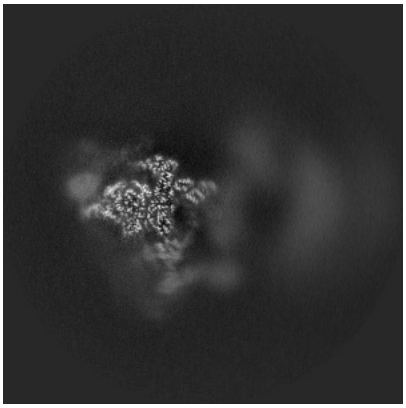


Y Index: 211



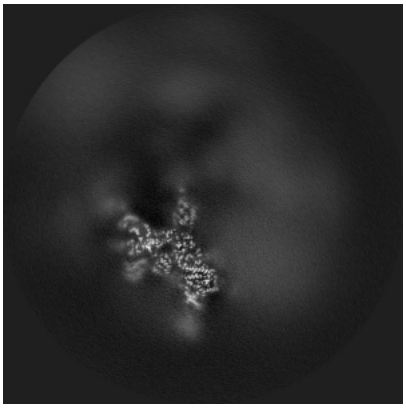
Z Index: 262

6.3.2 Raw map



X Index: 238

Y Index: 212

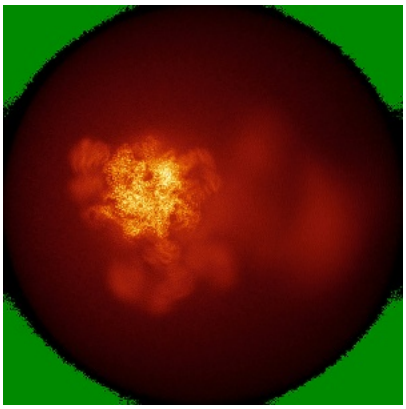


Z Index: 270

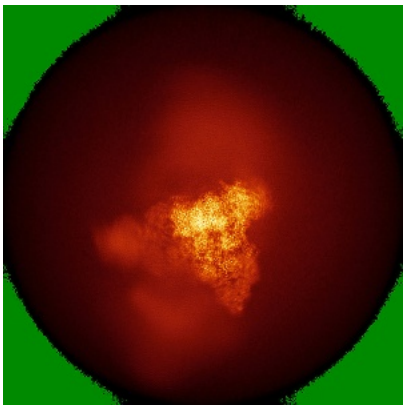
The images above show the largest variance slices of the map in three orthogonal directions.

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

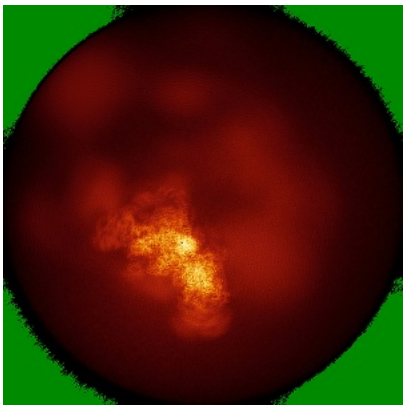
6.4.1 Primary map



X

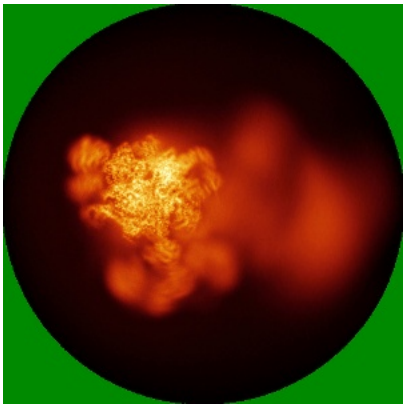


Y

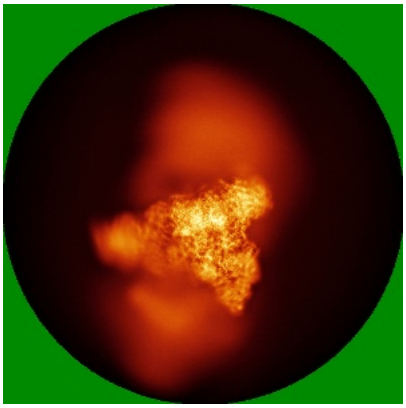


Z

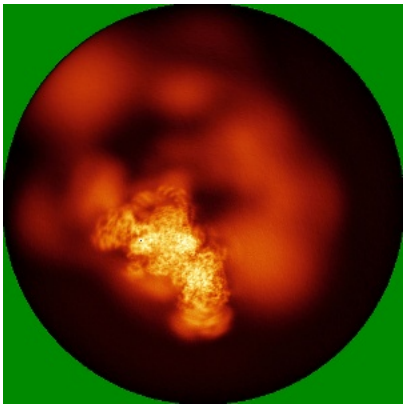
6.4.2 Raw map



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.

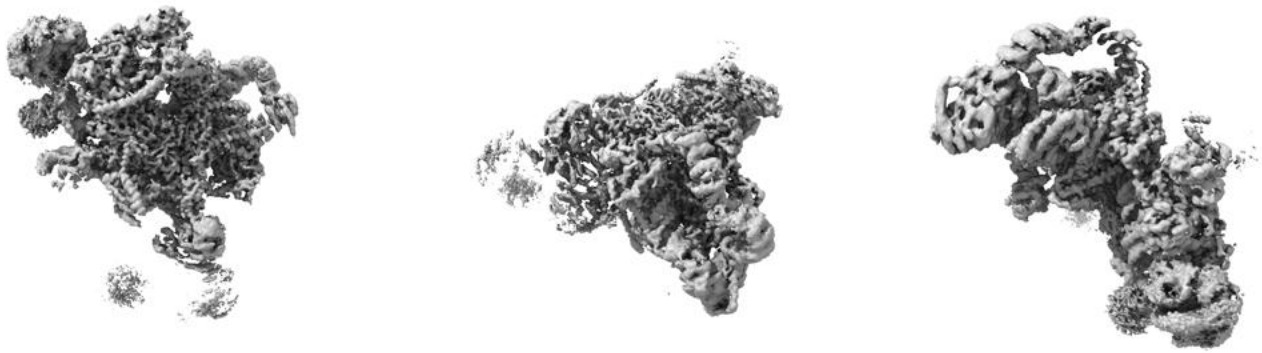
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. 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



X Y Z

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.

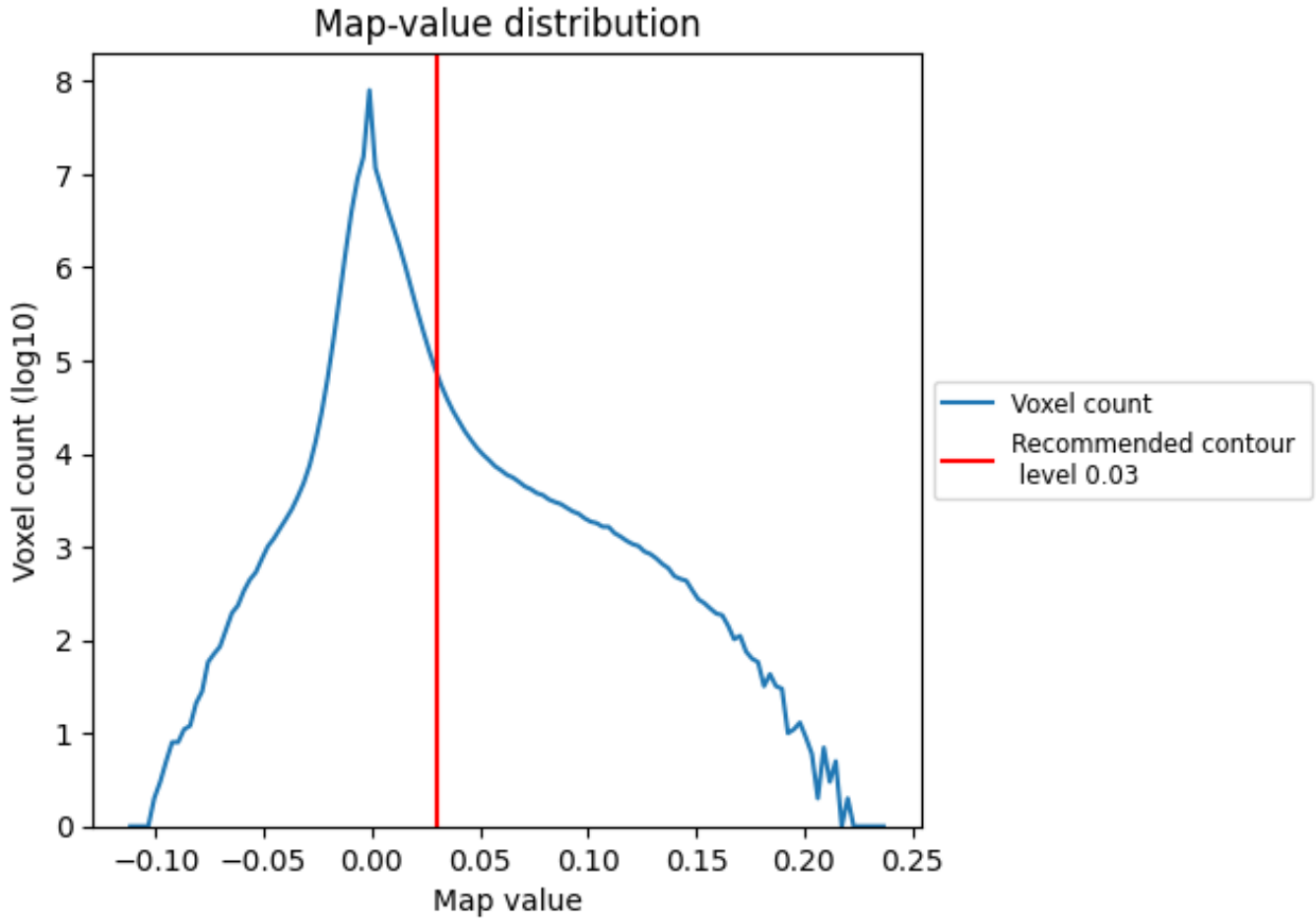
6.6 Mask visualisation (i)

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

7 Map analysis

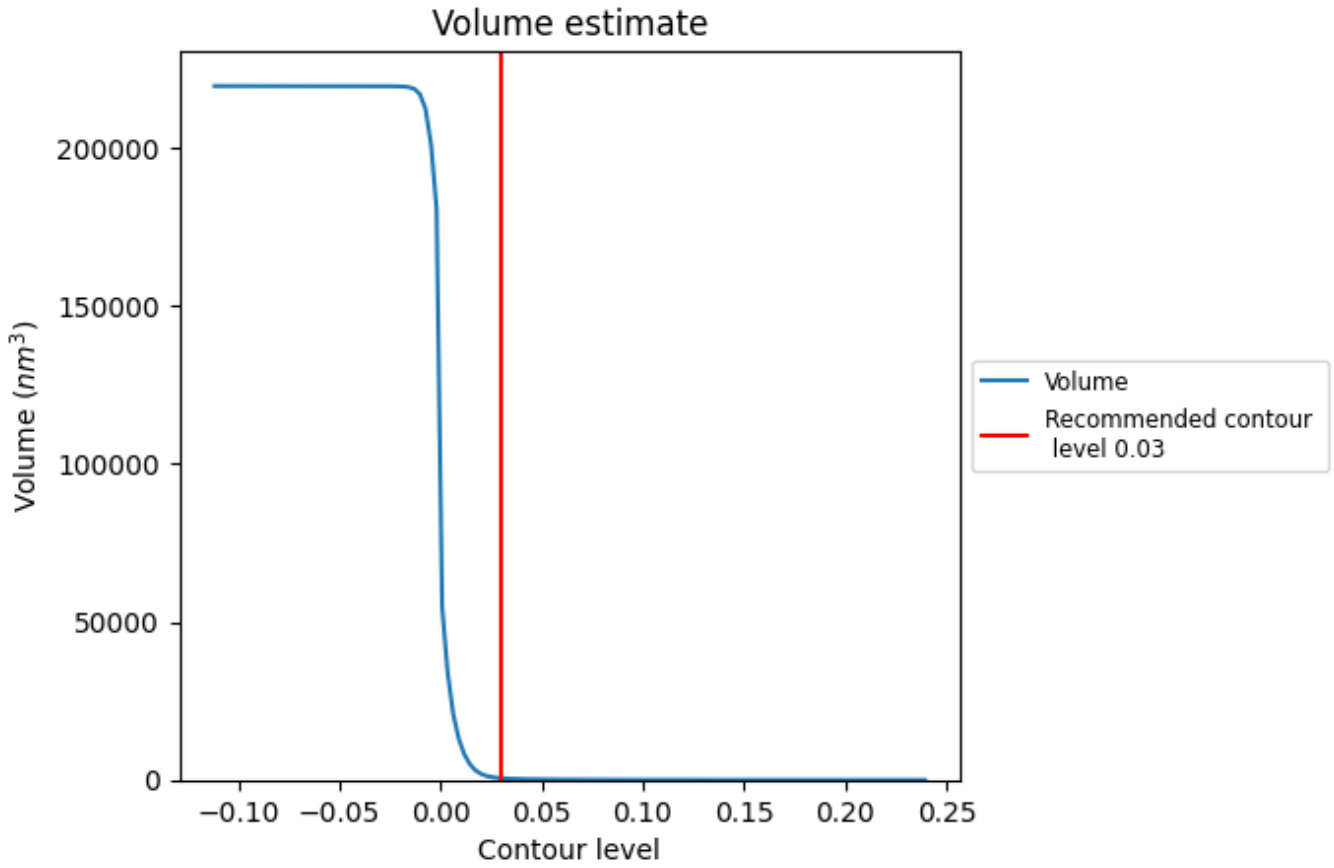
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

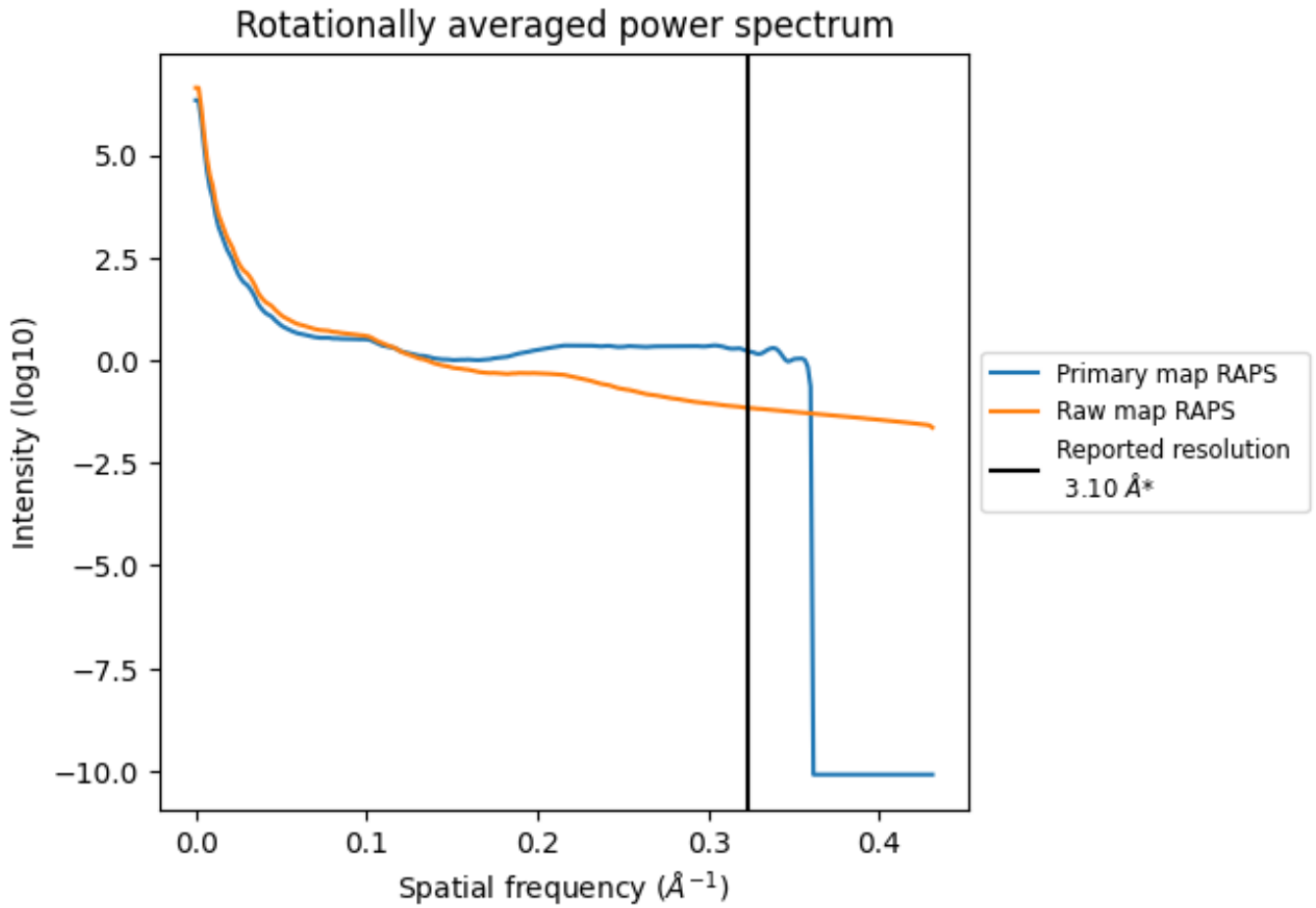
7.2 Volume estimate (i)



The volume at the recommended contour level is 551 nm^3; this corresponds to an approximate mass of 498 kDa.

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

7.3 Rotationally averaged power spectrum (i)

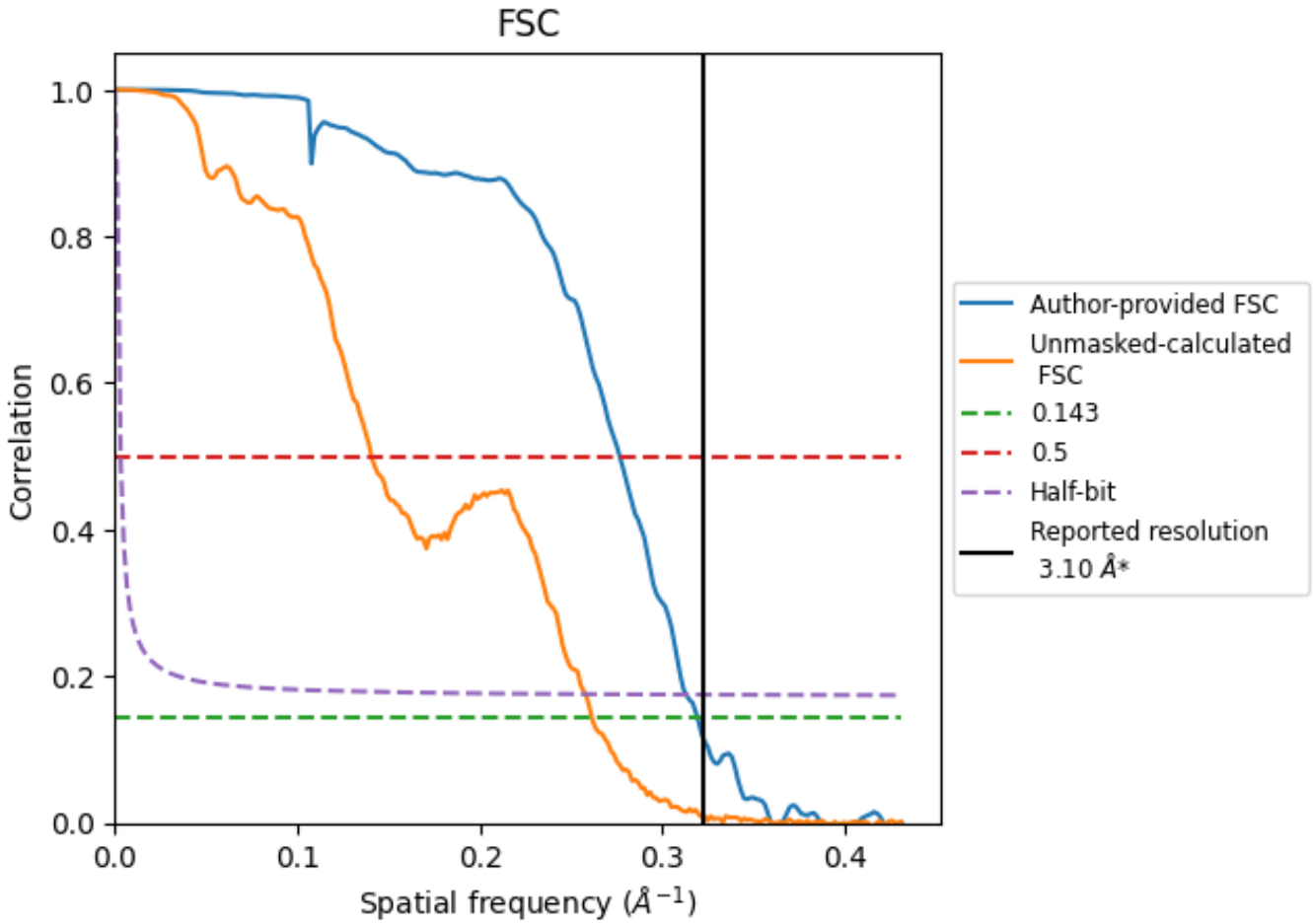


*Reported resolution corresponds to spatial frequency of 0.323 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8.2 Resolution estimates (i)

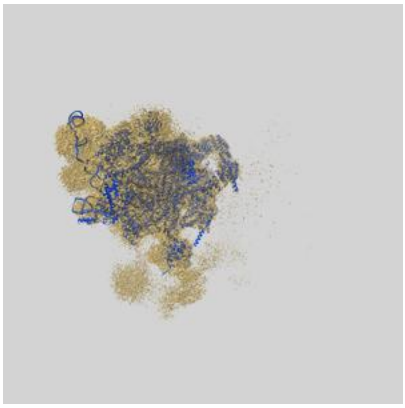
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.13	3.61	3.19
Unmasked-calculated*	3.82	7.11	3.88

*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 3.82 differs from the reported value 3.1 by more than 10 %

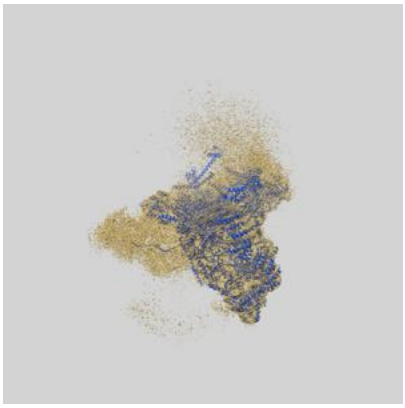
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-18225 and PDB model 8Q7N. Per-residue inclusion information can be found in section 3 on page 8.

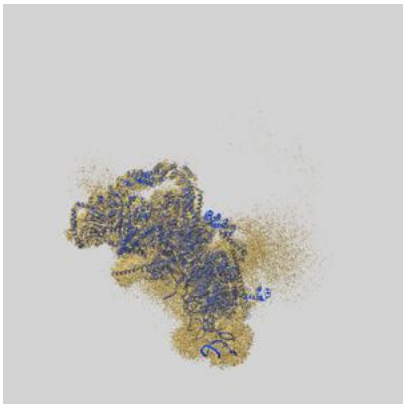
9.1 Map-model overlay



X



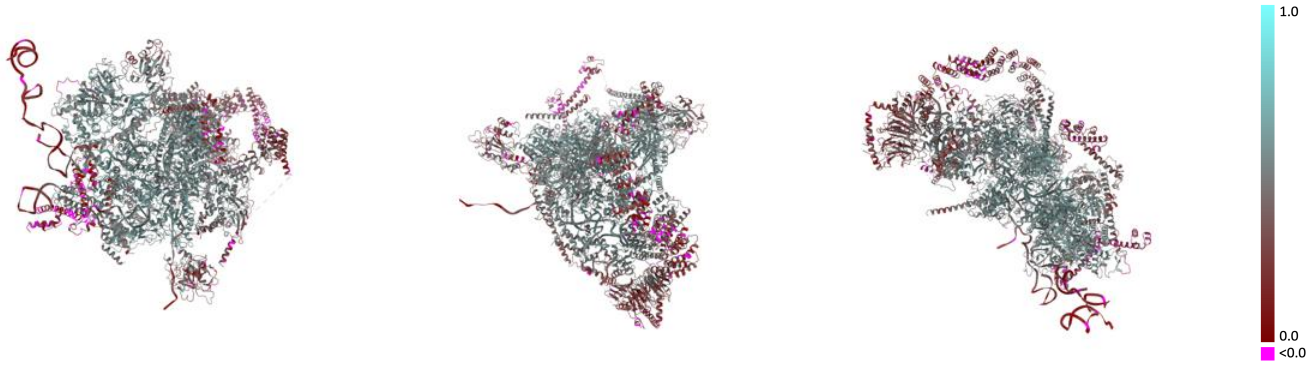
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03 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.

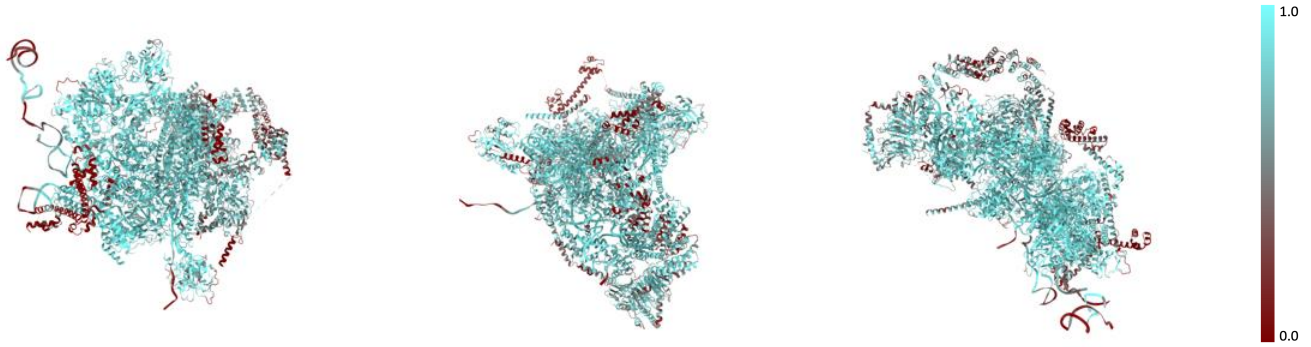
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

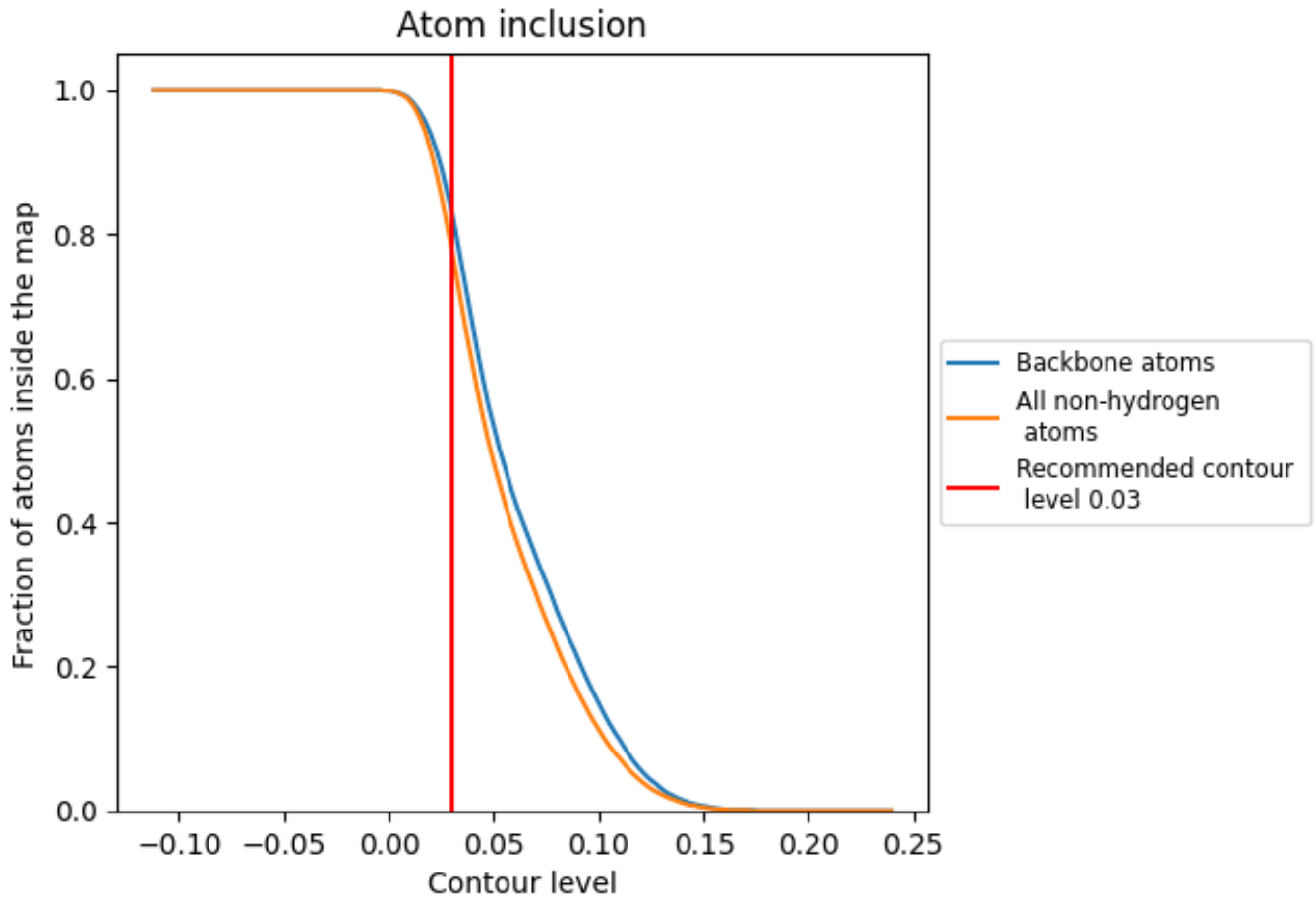
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).

9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 78% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7790	0.4630
4	0.8300	0.4830
5	0.7120	0.3330
6	0.7780	0.3980
7	0.6570	0.4320
A	0.8720	0.5440
C	0.8710	0.5230
D	0.9240	0.5820
F	0.6850	0.3050
I	0.8870	0.5570
J	0.6610	0.3710
K	0.7770	0.4980
L	0.8080	0.4770
M	0.8280	0.5040
N	0.6650	0.3380
Q	0.8280	0.4810
S	0.4750	0.3750
T	0.2830	0.2320
X	0.6840	0.4570
Z	0.8090	0.4740
r	0.8230	0.5160
s	0.9220	0.5950