Full wwPDB EM Validation Report ⓘ

Dec 1, 2021 – 01:54 am GMT

PDB ID	:	7OHS
EMDB ID	:	EMD-12907
Title	:	Nog1-TAP associated immature ribosomal particle population F from S. cerevisiae
Authors	:	Milkereit, P.; Poell, G.
Deposited on	:	2021-05-11
Resolution	:	4.38 Å(reported)
Based on initial model	:	6EM1

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

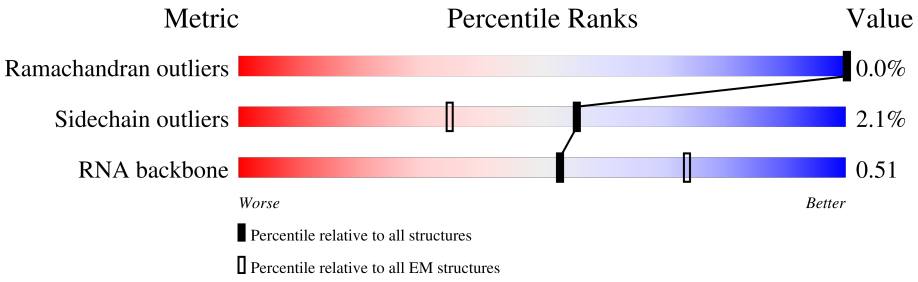
EMDB validation analysis	:	0.0.0.dev97
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance

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

The reported resolution of this entry is 4.38 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	1	3396	38% 11% 50%
2	2	158	75% 18% 7%
3	3	306	8% 55% 43%
4	4	278	8% 77% 22%
5	5	463	11% 82% 17%
6	6	232	16% 11% 72%
7	A	291	19% 48% 51%
8	B	387	11% 85% 14%

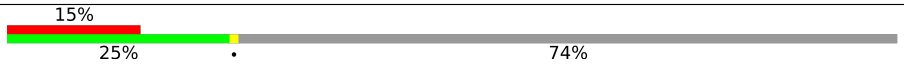
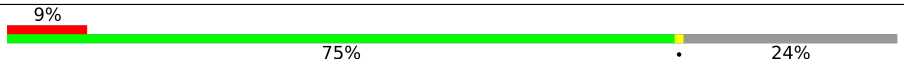
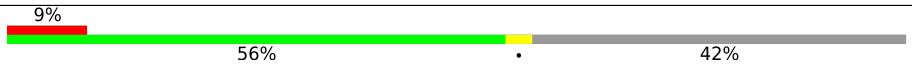
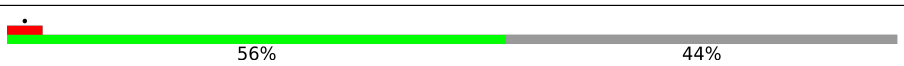
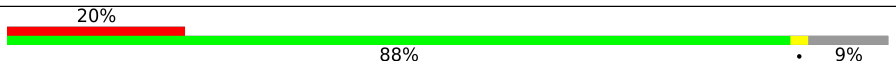
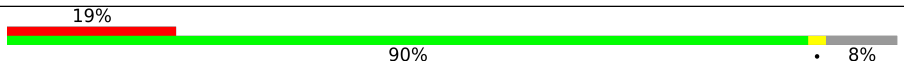
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	C	362	6% 94% 5%
10	D	505	19% 85% 13%
11	E	176	85% 14%
12	F	244	98%
13	G	256	6% 61% 38%
14	H	191	42% 80% 18%
15	K	376	67% 32%
16	L	199	52% 46%
17	M	138	91% 8%
18	N	204	12% 84% 13%
19	O	199	7% 97%
20	P	184	14% 73% 26%
21	Q	186	5% 69% 30%
22	S	172	98%
23	V	137	6% 36% 64%
24	W	236	32% 71% 27%
25	Y	127	97%
26	b	647	37% 63% 35%
27	e	130	17% 93% 5%
28	f	107	6% 99%
29	h	120	95%
30	i	100	9% 68% 30%
31	j	88	81% 19%
32	m	807	20% 80%
33	n	605	6% 53% 45%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	o	220	
35	r	261	
36	t	322	
37	u	199	
38	v	231	
39	x	295	
40	y	245	

2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 175937 atoms, of which 78846 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 25S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
1	1	1697	54624	16232	18261	6602	11832	1697	0	0

- Molecule 2 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
2	2	147	4702	1397	1579	550	1029	147	0	0

- Molecule 3 is a protein called Protein MAK16.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	3	173	2908	901	1474	274	250	9	0	0

- Molecule 4 is a protein called Ribosomal RNA-processing protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	4	217	3744	1208	1891	319	323	3	0	0

- Molecule 5 is a protein called Ribosome biogenesis protein NSA1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	5	385	6170	1957	3115	514	573	11	0	0

- Molecule 6 is a RNA chain called ITS2.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
6	6	65	2061	614	691	228	463	65	0	0

- Molecule 7 is a protein called Ribosome biogenesis protein BRX1.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	A	142	Total	C	H	N	O	S	0	0
			2379	765	1190	215	206	3		

- Molecule 8 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	B	333	Total	C	H	N	O	S	0	0
			5374	1680	2728	490	470	6		

- Molecule 9 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	C	343	Total	C	H	N	O	S	0	0
			5336	1643	2725	499	466	3		

- Molecule 10 is a protein called ATP-dependent RNA helicase HAS1.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	D	437	Total	C	H	N	O	S	0	0
			7106	2247	3620	600	627	12		

- Molecule 11 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	E	151	Total	C	H	N	O	S	0	0
			2497	780	1292	215	209	1		

- Molecule 12 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	F	241	Total	C	H	N	O	S	0	0
			3969	1246	2033	351	338	1		

- Molecule 13 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	G	158	Total	C	H	N	O	S	0	0
			2510	791	1284	208	225	2		

- Molecule 14 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	H	156	Total	C	H	N	O	S	0	0
			2560	800	1311	219	227	3		

- Molecule 15 is a protein called Proteasome-interacting protein CIC1.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	K	257	Total	C	H	N	O	S	0	0
			4230	1337	2157	341	392	3		

- Molecule 16 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	108	Total	C	H	N	O	0	0
			1782	541	918	180	143		

- Molecule 17 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	M	127	Total	C	H	N	O	S	0	0
			2078	638	1086	189	163	2		

- Molecule 18 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	N	177	Total	C	H	N	O	S	0	0
			3079	948	1566	320	244	1		

- Molecule 19 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	O	197	Total	C	H	N	O	S	0	0
			3215	1003	1660	289	262	1		

- Molecule 20 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	P	137	Total	C	H	N	O	0	0
			2139	666	1077	198	198		

- Molecule 21 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	Q	131	Total	C	H	N	O	S	0	0
			2101	645	1092	190	173	1		

- Molecule 22 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	S	170	Total	C	H	N	O	S	0	0
			2904	922	1472	265	242	3		

- Molecule 23 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	V	50	Total	C	H	N	O	S	0	0
			758	241	380	69	66	2		

- Molecule 24 is a protein called Ribosome assembly factor MRT4.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	W	172	Total	C	H	N	O	S	0	0
			2834	906	1429	235	260	4		

- Molecule 25 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	125	Total	C	H	N	O	0	0
			2060	620	1076	191	173		

- Molecule 26 is a protein called Nucleolar GTP-binding protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	b	421	Total	C	H	N	O	S	0	0
			6876	2180	3466	585	627	18		

- Molecule 27 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	e	123	Total	C	H	N	O	S	0	0
			2057	630	1063	201	162	1		

- Molecule 28 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	f	106	Total	C	H	N	O	S	0	0
			1731	540	881	165	144	1		

- Molecule 29 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	h	118	Total	C	H	N	O	S	0	0
			2038	612	1074	185	166	1		

- Molecule 30 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	i	70	Total	C	H	N	O	S	0	0
			1163	343	608	116	95	1		

- Molecule 31 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	j	71	Total	C	H	N	O	S	0	0
			1137	344	571	123	94	5		

- Molecule 32 is a protein called Ribosome biogenesis protein ERB1.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	m	161	Total	C	H	N	O	S	0	0
			2709	867	1347	238	253	4		

- Molecule 33 is a protein called Pescadillo homolog.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	n	331	Total	C	H	N	O	S	0	0
			5472	1771	2764	454	475	8		

- Molecule 34 is a protein called Ribosome biogenesis protein 15.

Mol	Chain	Residues	Atoms						AltConf	Trace
34	o	133	Total	C	H	N	O	S	0	0
			2267	716	1160	198	189	4		

- Molecule 35 is a protein called Ribosome biogenesis protein NSA2.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	r	68	Total	C	H	N	O	S	0	0
			1210	365	617	127	100	1		

- Molecule 36 is a protein called Ribosome biogenesis protein RLP7.

Mol	Chain	Residues	Atoms						AltConf	Trace
36	t	244	Total	C	H	N	O	S	0	0
			3974	1233	2039	345	354	3		

- Molecule 37 is a protein called Ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms						AltConf	Trace
37	u	116	Total	C	H	N	O	S	0	0
			1987	612	1011	200	155	9		

- Molecule 38 is a protein called Nucleolar protein 16.

Mol	Chain	Residues	Atoms						AltConf	Trace
38	v	130	Total	C	H	N	O	S	0	0
			2223	678	1136	211	195	3		

- Molecule 39 is a protein called Ribosome production factor 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
39	x	267	Total	C	H	N	O	S	0	0
			4573	1444	2305	413	407	4		

- Molecule 40 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms						AltConf	Trace
40	y	225	Total	C	H	N	O	S	0	0
			3398	1056	1697	295	343	7		

- Molecule 41 is ZINC ION (three-letter code: ZN) (formula: Zn).

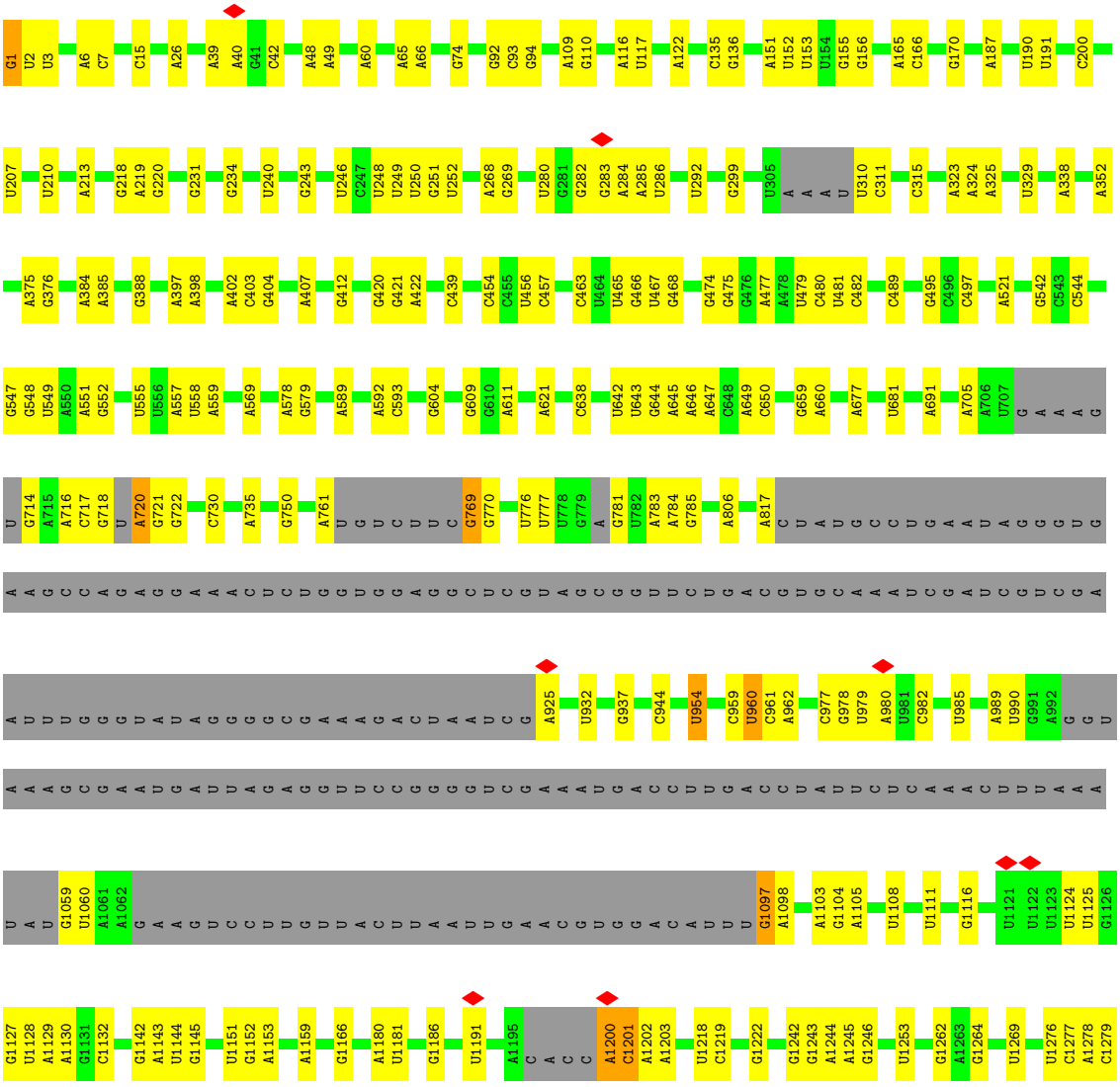
Mol	Chain	Residues	Atoms		AltConf
41	j	1	Total	Zn	0
			1	1	
41	u	1	Total	Zn	0
			1	1	

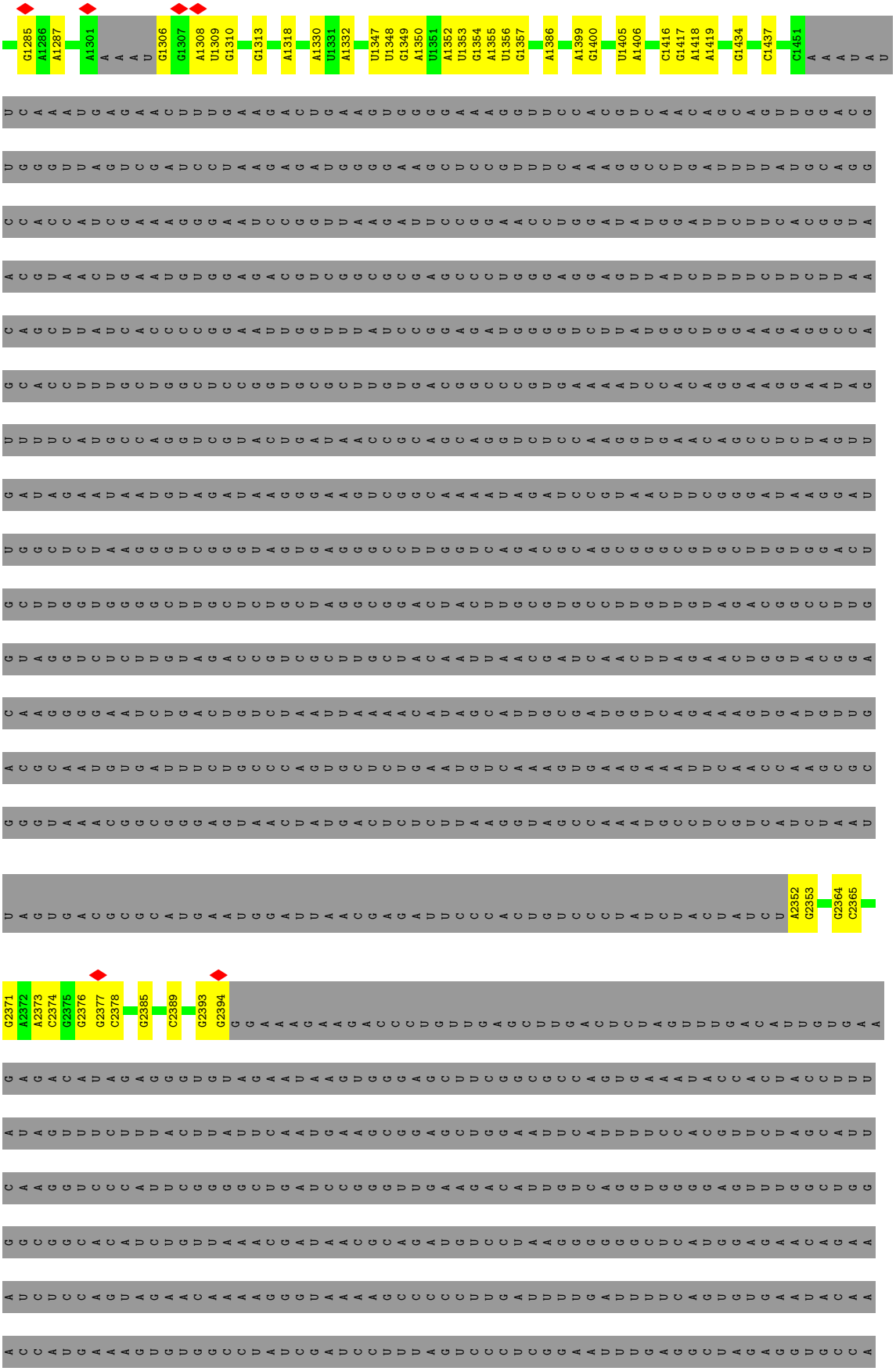
3 Residue-property plots (i)

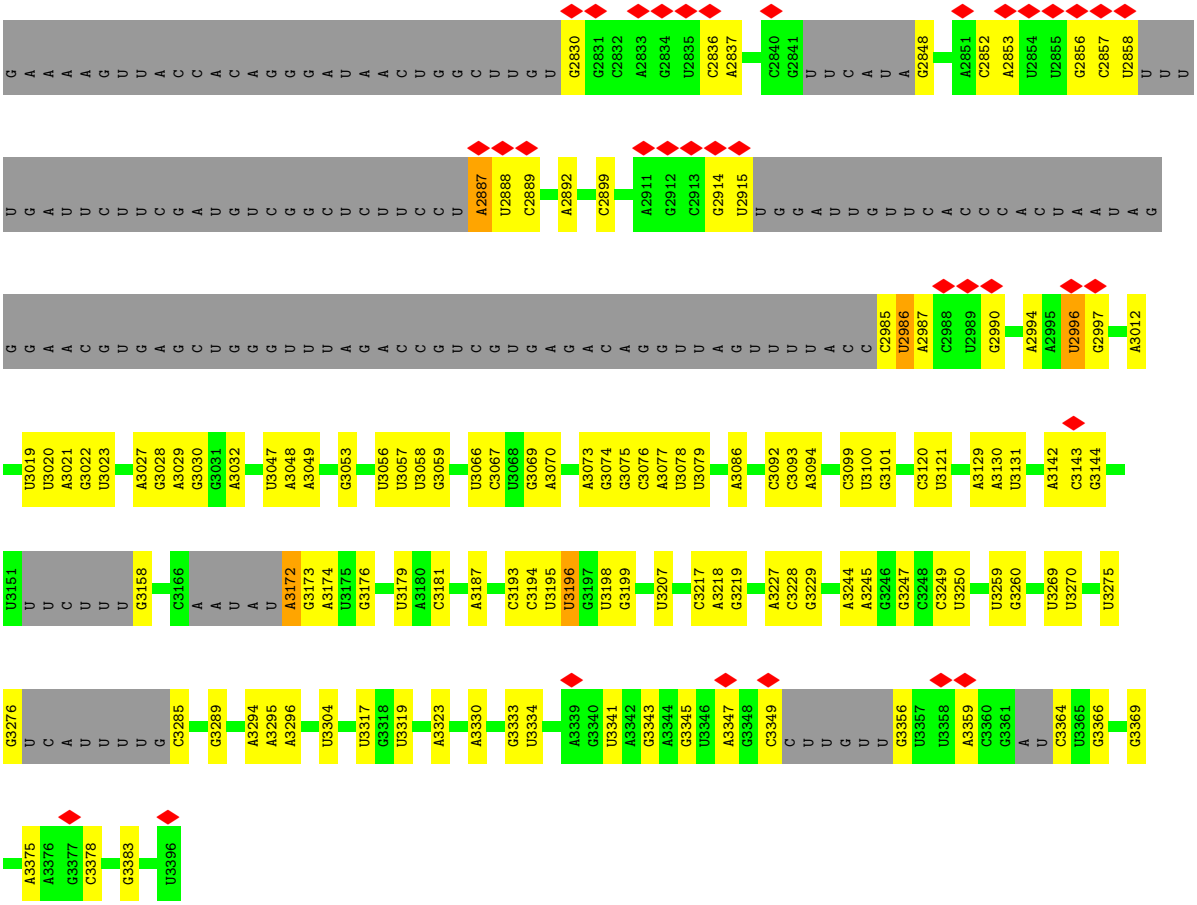
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 25S rRNA

Chain 1:

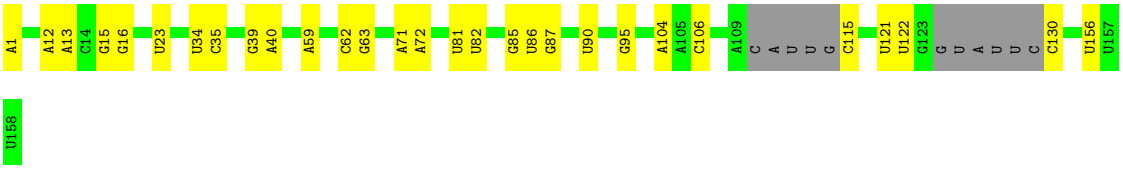



G1285 A1286 A1287 A1301 G1306 G1307 A1308 U1309 G1310 G1313 A1318 A1330 U1331 A1332 U1347 U1348 G1349 A1350 U1351 A1362 U1353 G1354 A1365 U1356 G1357 A1386 A1399 G1400 U1405 A1406 C1416 G1417 A1418 A1419 G1434 C1437 C1451
A2352 G2353 G2364 C2365
G2371 A2372 A2373 C2374 G2375 G2376 G2377 C2378 G2385 C2389 G2393 G2394



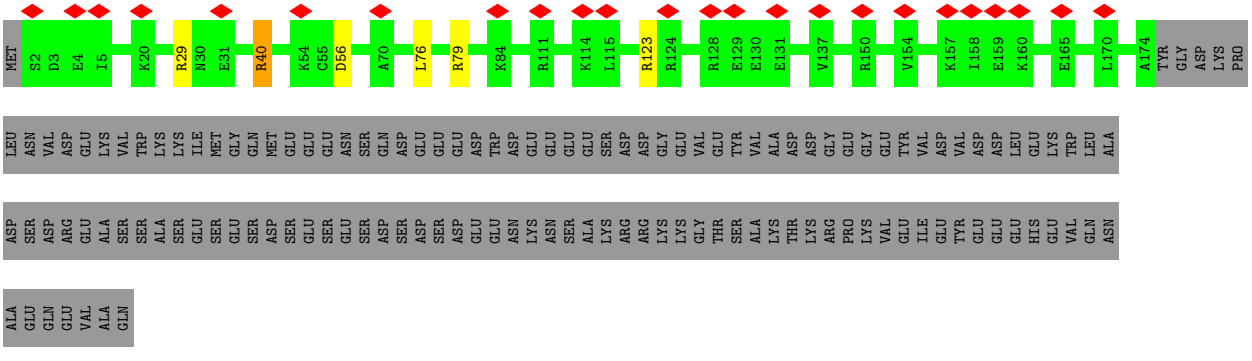
• Molecule 2: 5.8S rRNA

Chain 2:



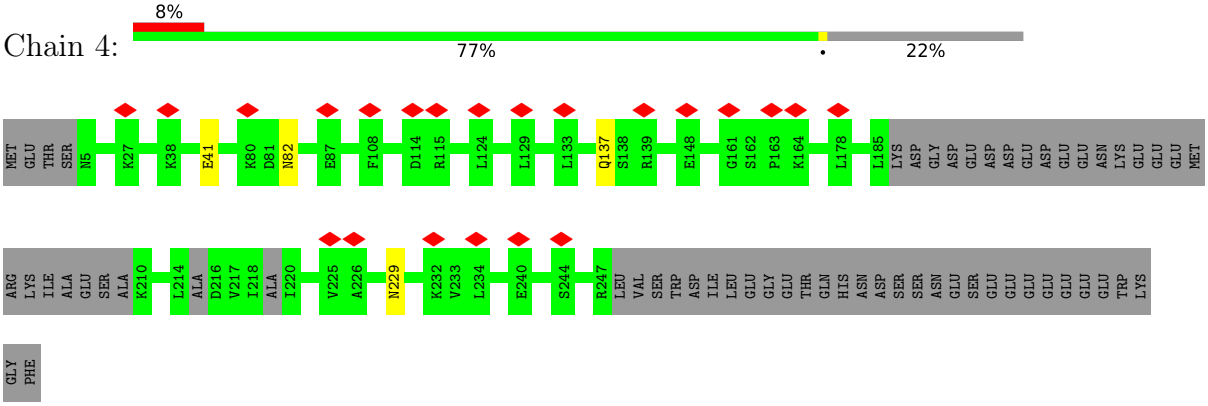
• Molecule 3: Protein MAK16

Chain 3:



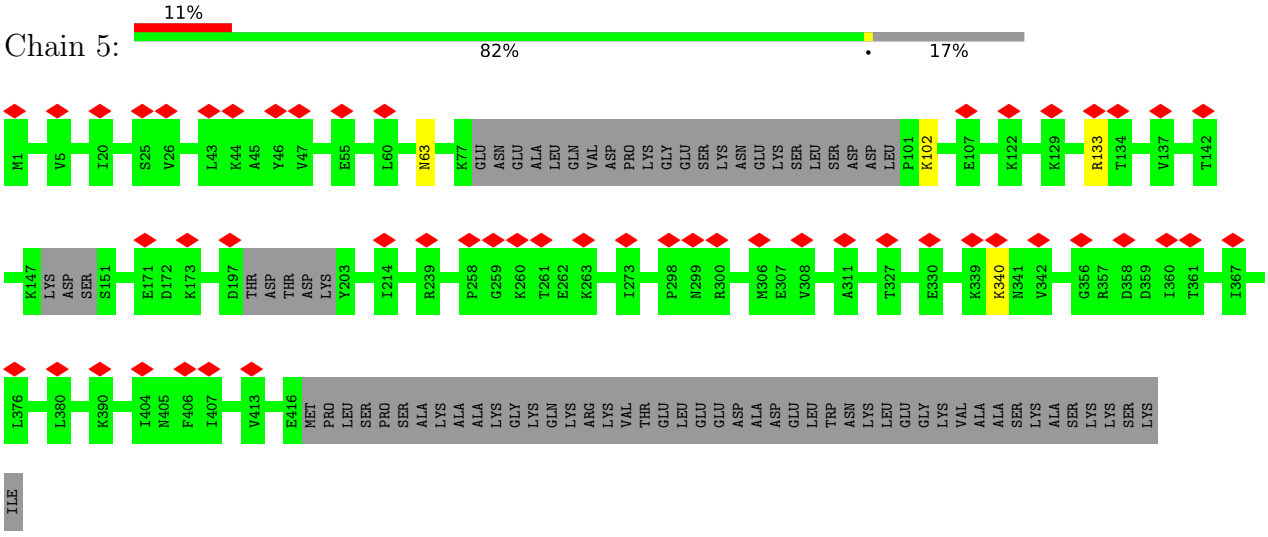
• Molecule 4: Ribosomal RNA-processing protein 1

Chain 4:



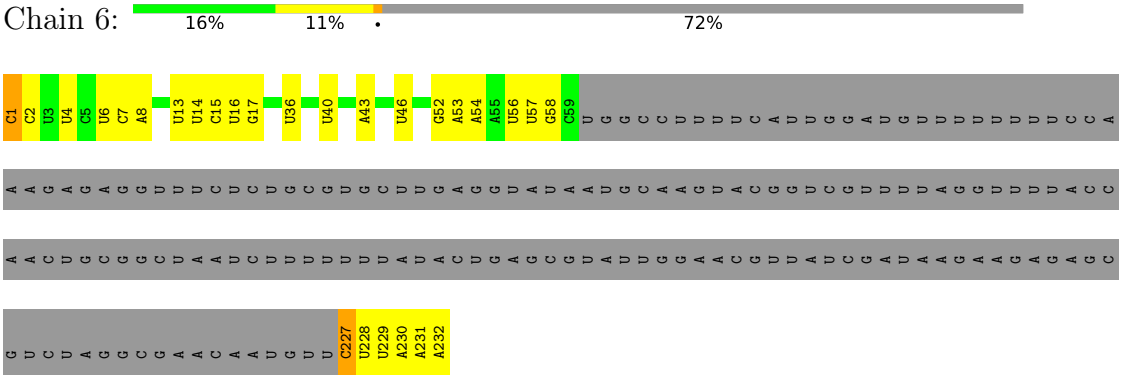
• Molecule 5: Ribosome biogenesis protein NSA1

Chain 5:



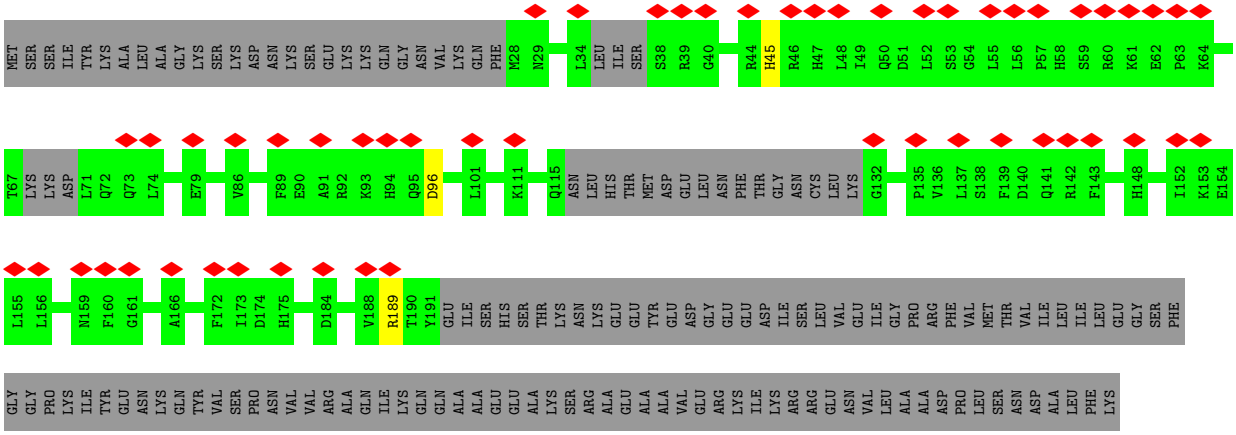
• Molecule 6: ITS2

Chain 6:



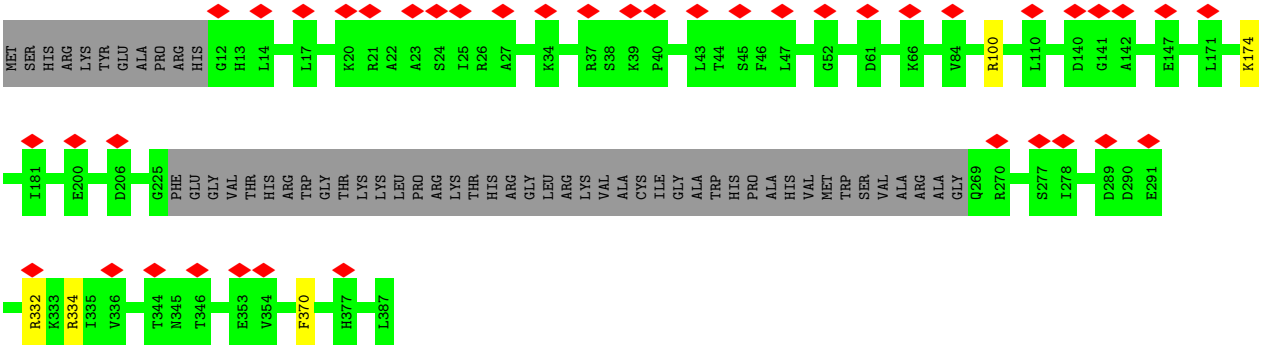
• Molecule 7: Ribosome biogenesis protein BRX1

Chain A:



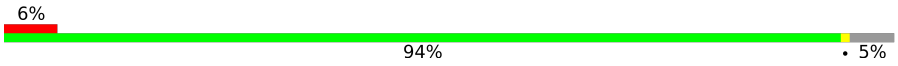
• Molecule 8: 60S ribosomal protein L3

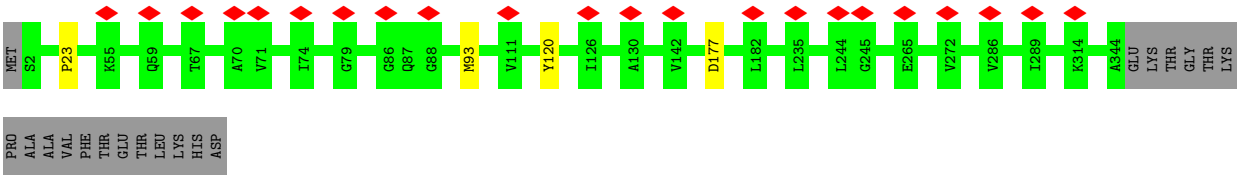
Chain B:



• Molecule 9: 60S ribosomal protein L4-A

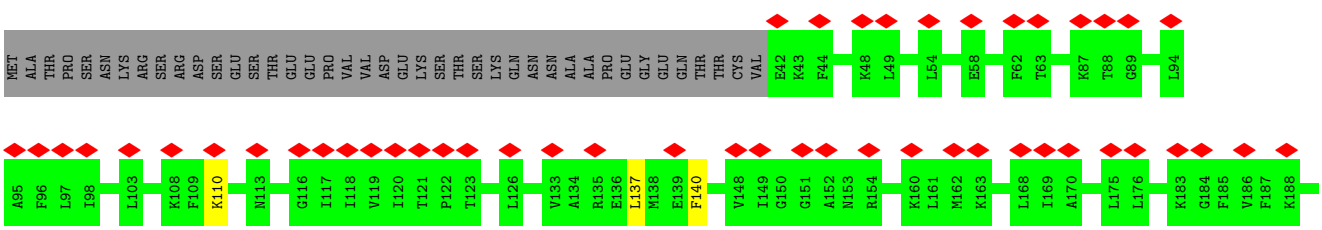
Chain C:

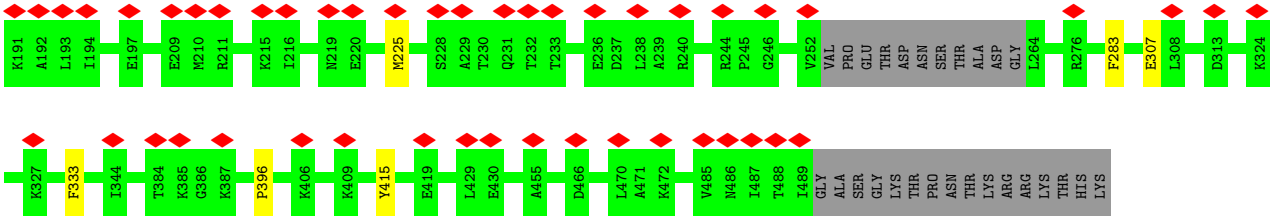




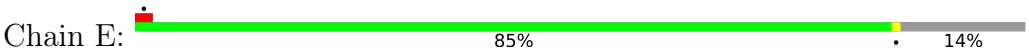
• Molecule 10: ATP-dependent RNA helicase HAS1

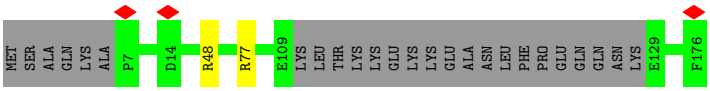
Chain D:



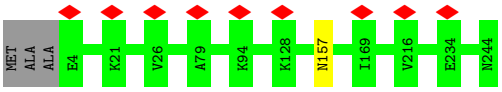


• Molecule 11: 60S ribosomal protein L6-A

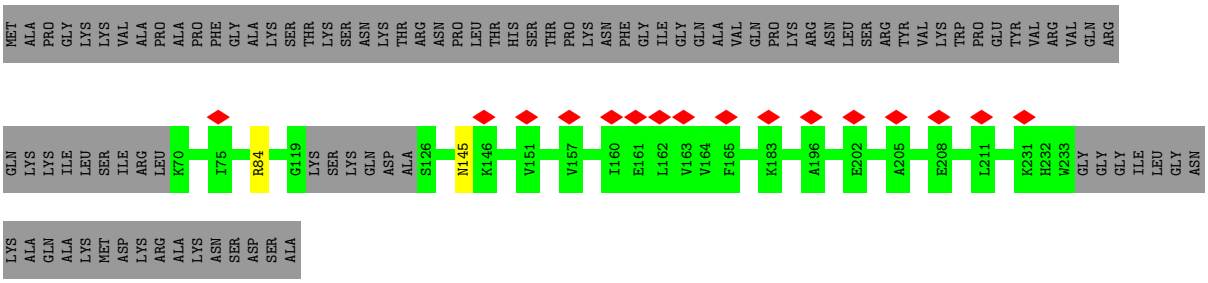




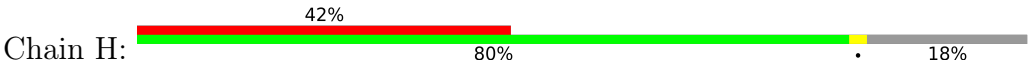
• Molecule 12: 60S ribosomal protein L7-A

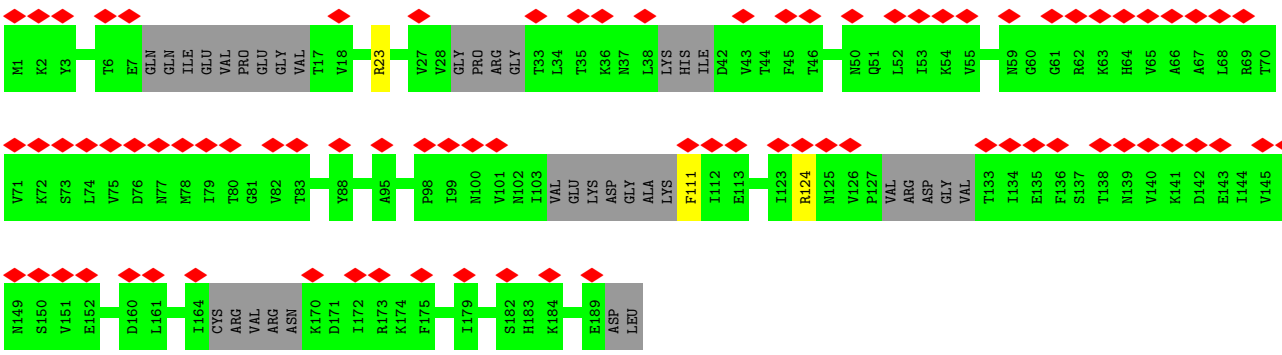


• Molecule 13: 60S ribosomal protein L8-A



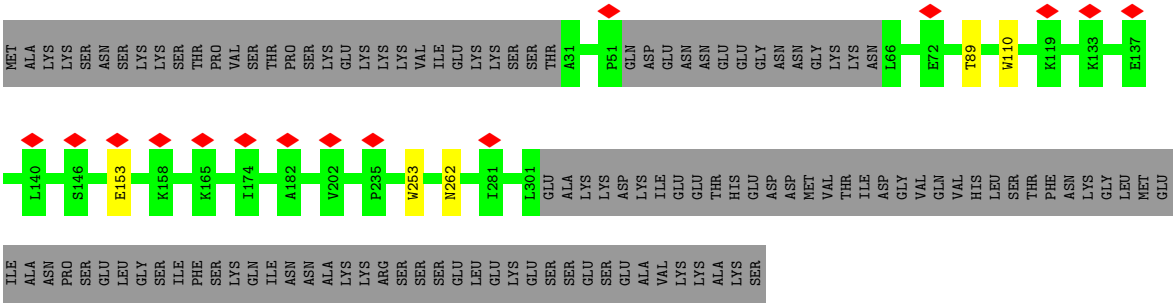
• Molecule 14: 60S ribosomal protein L9-A





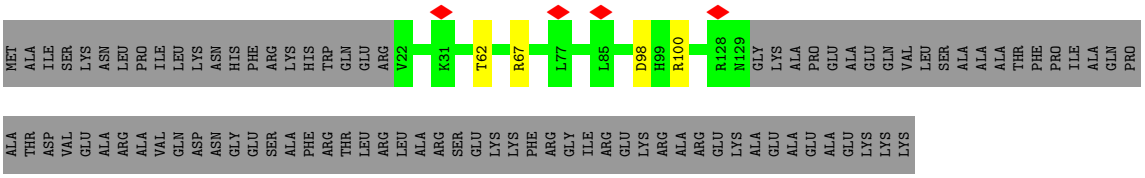
• Molecule 15: Proteasome-interacting protein CIC1

Chain K:



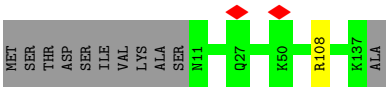
• Molecule 16: 60S ribosomal protein L13-A

Chain L:



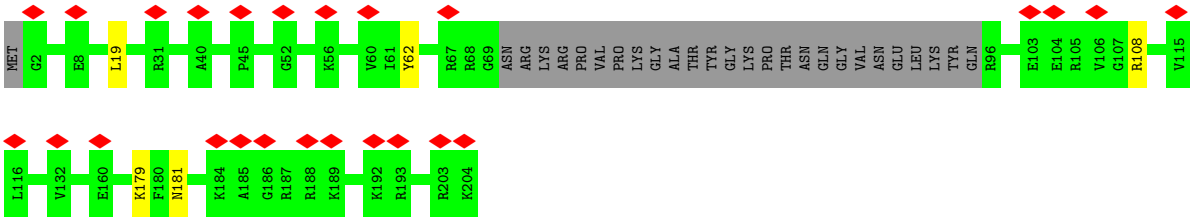
• Molecule 17: 60S ribosomal protein L14-A

Chain M:



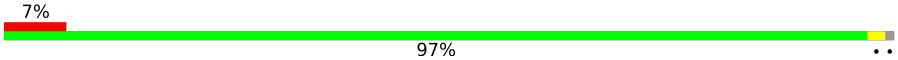
• Molecule 18: 60S ribosomal protein L15-A

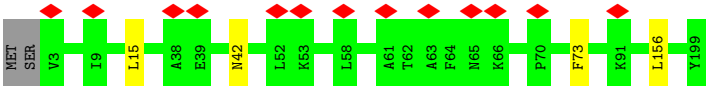
Chain N:



• Molecule 19: 60S ribosomal protein L16-A

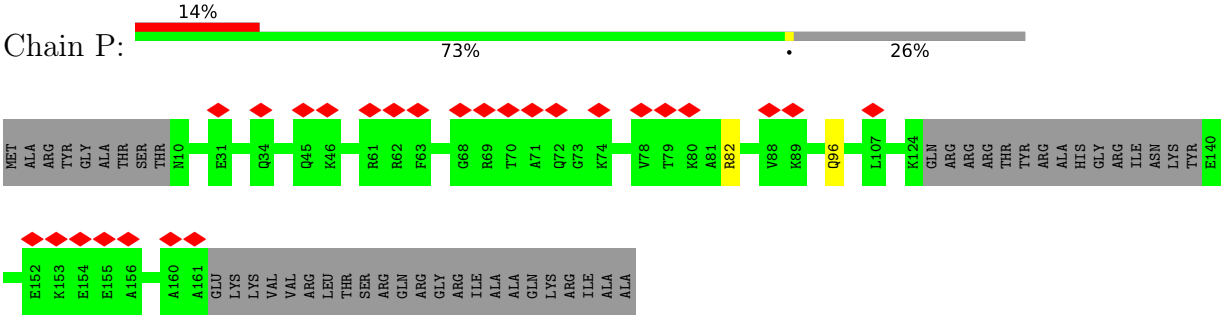
Chain O:





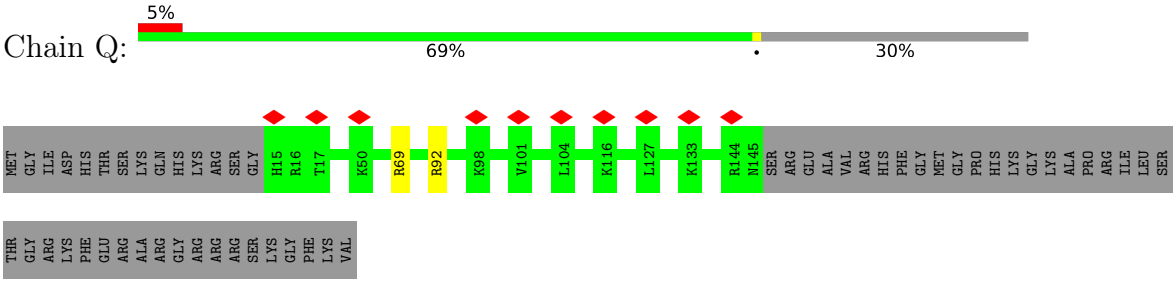
• Molecule 20: 60S ribosomal protein L17-A

Chain P:



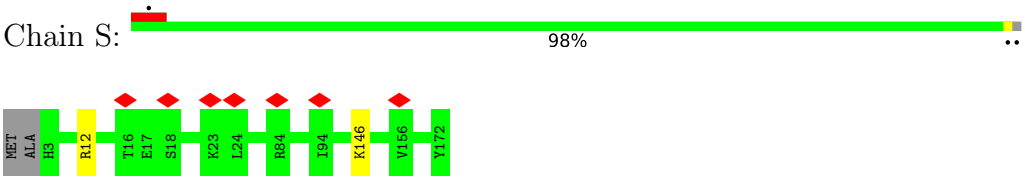
• Molecule 21: 60S ribosomal protein L18-A

Chain Q:



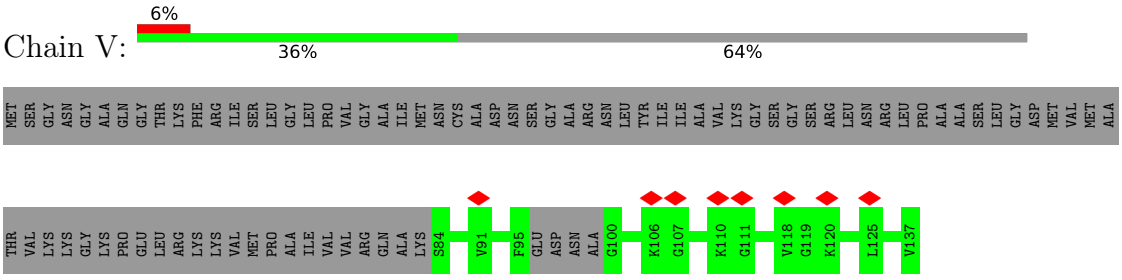
• Molecule 22: 60S ribosomal protein L20-A

Chain S:



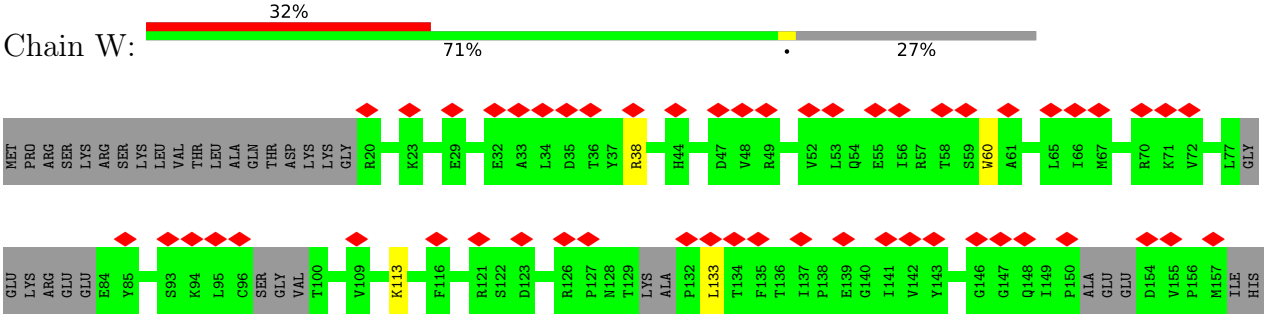
• Molecule 23: 60S ribosomal protein L23-A

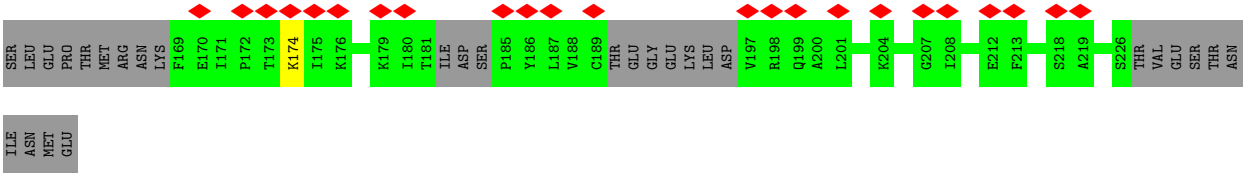
Chain V:



• Molecule 24: Ribosome assembly factor MRT4

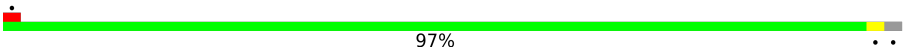
Chain W:

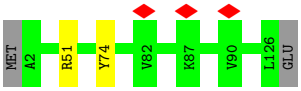




• Molecule 25: 60S ribosomal protein L26-A

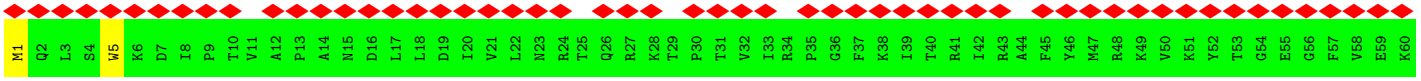
Chain Y:

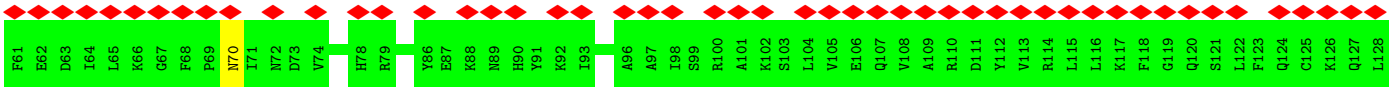


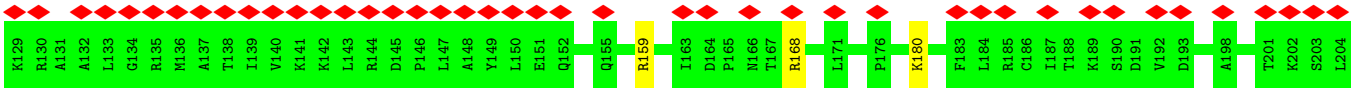


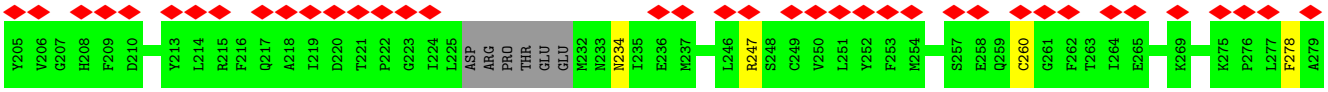
• Molecule 26: Nucleolar GTP-binding protein 1

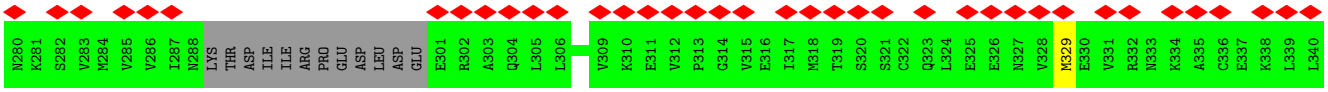
Chain b:

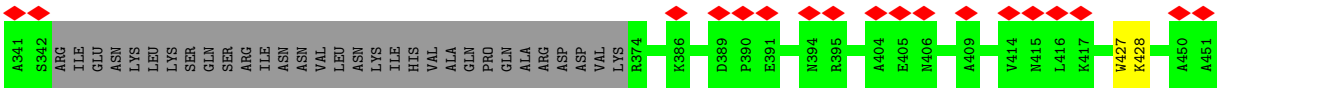


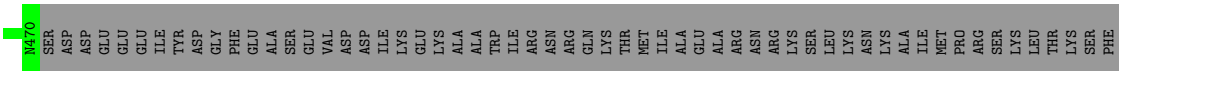


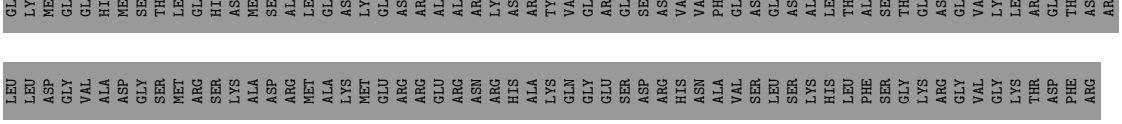






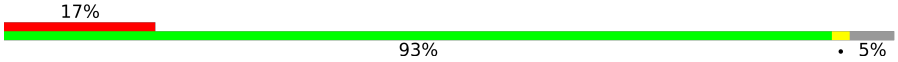


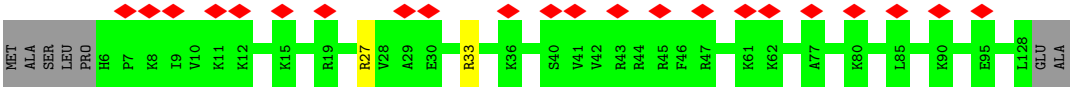




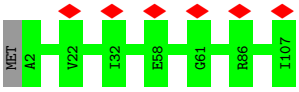
• Molecule 27: 60S ribosomal protein L32

Chain e:

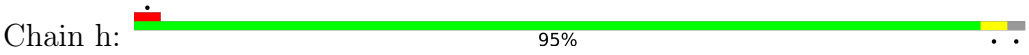


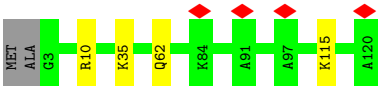


• Molecule 28: 60S ribosomal protein L33-A

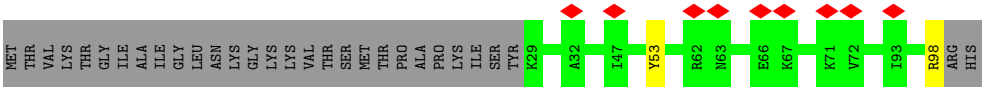


• Molecule 29: 60S ribosomal protein L35-A

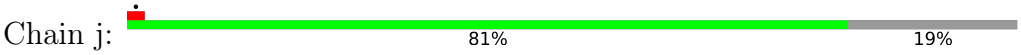


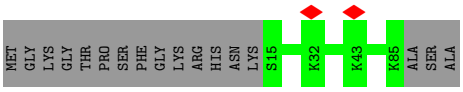


• Molecule 30: 60S ribosomal protein L36-A

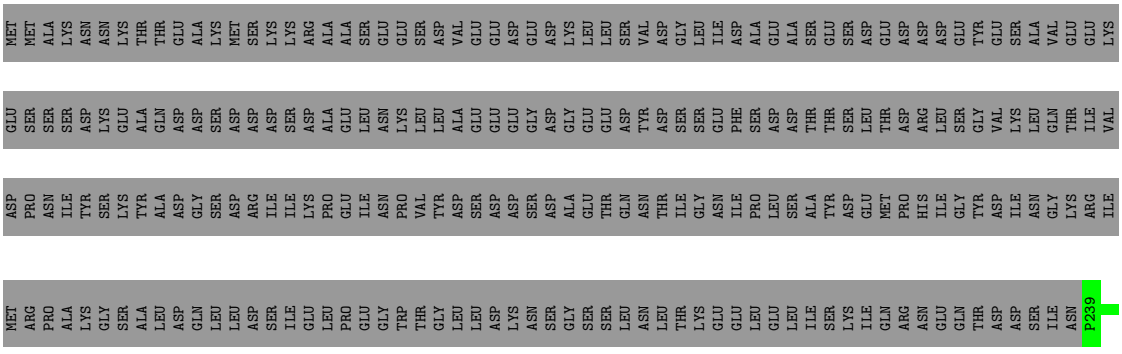


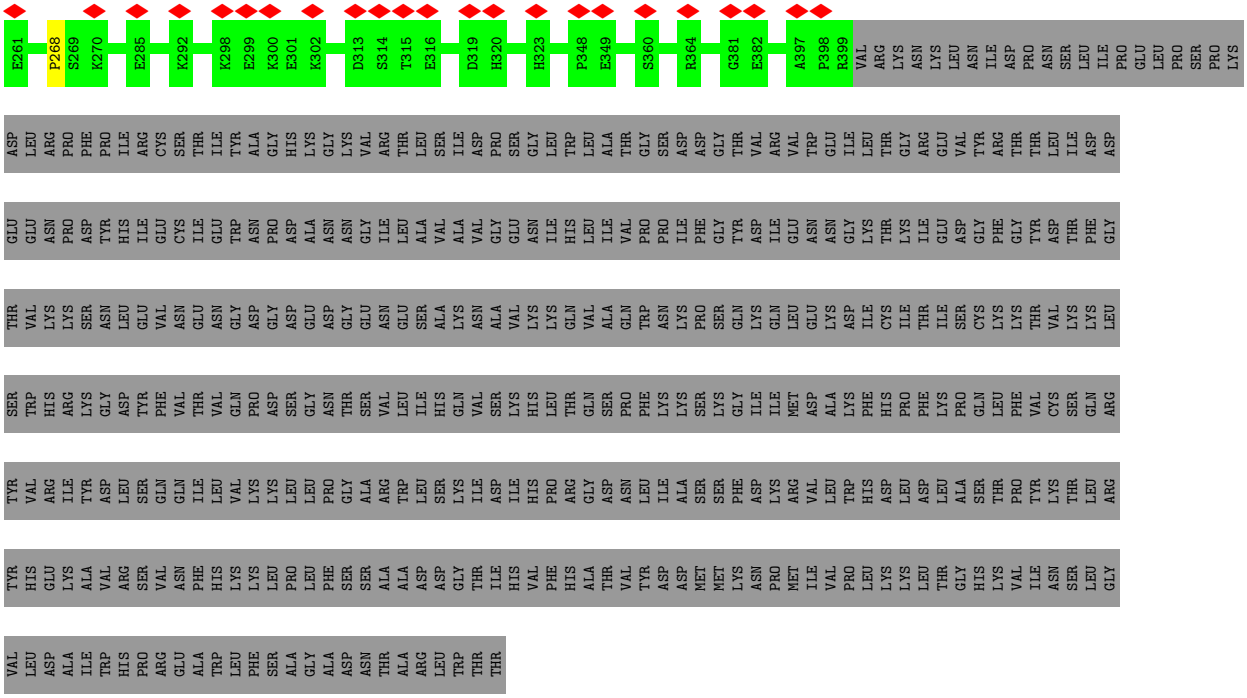
• Molecule 31: 60S ribosomal protein L37-A





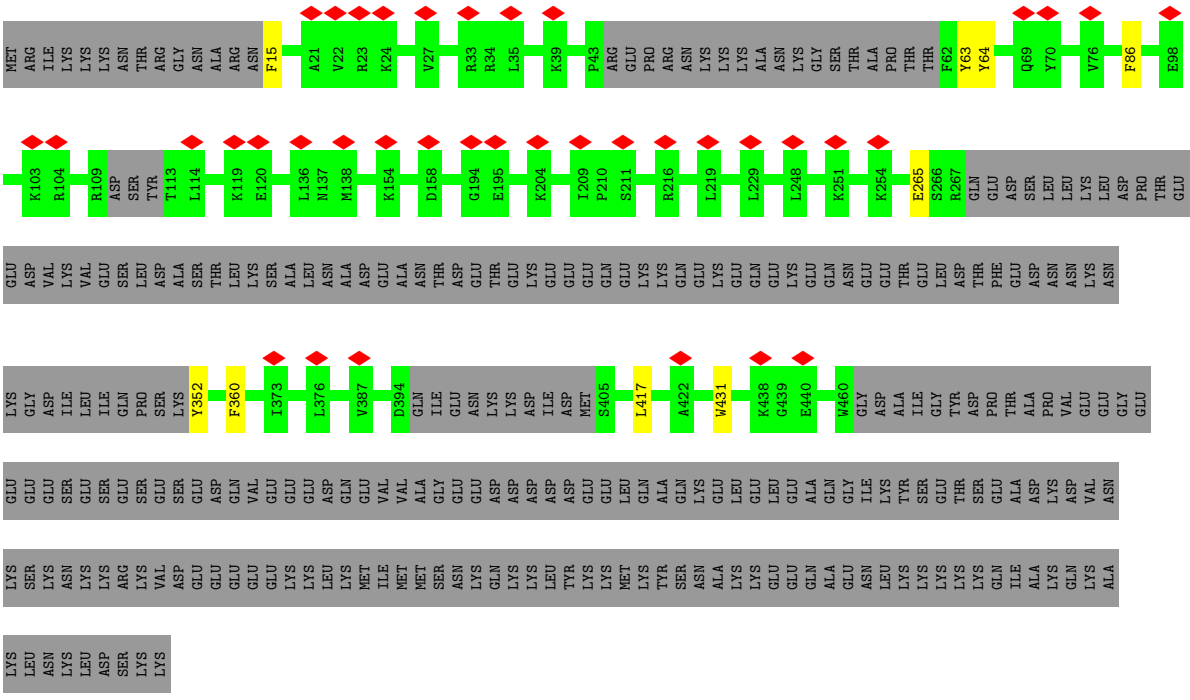
• Molecule 32: Ribosome biogenesis protein ERB1





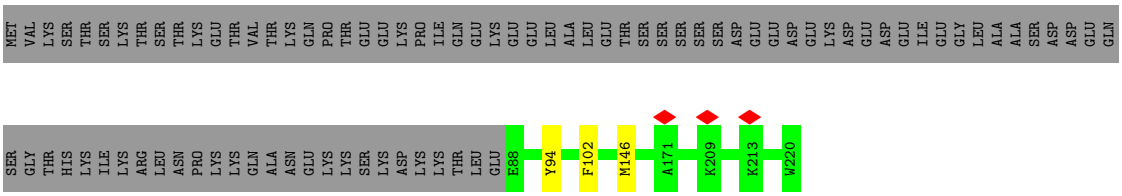
• Molecule 33: Pescadillo homolog

Chain n:

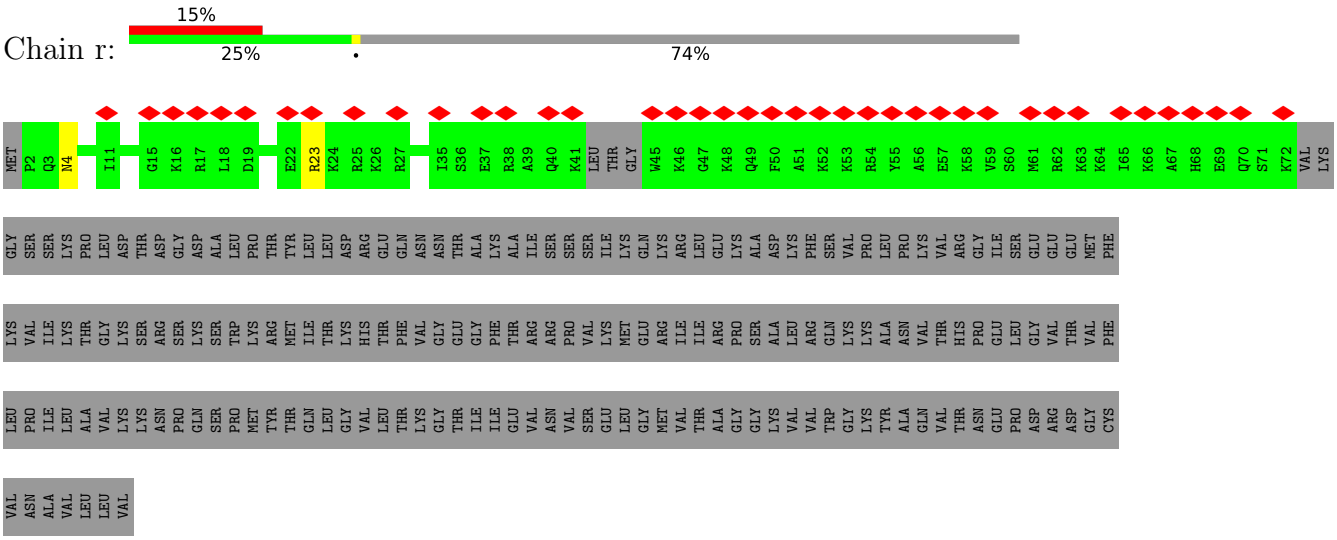


• Molecule 34: Ribosome biogenesis protein 15

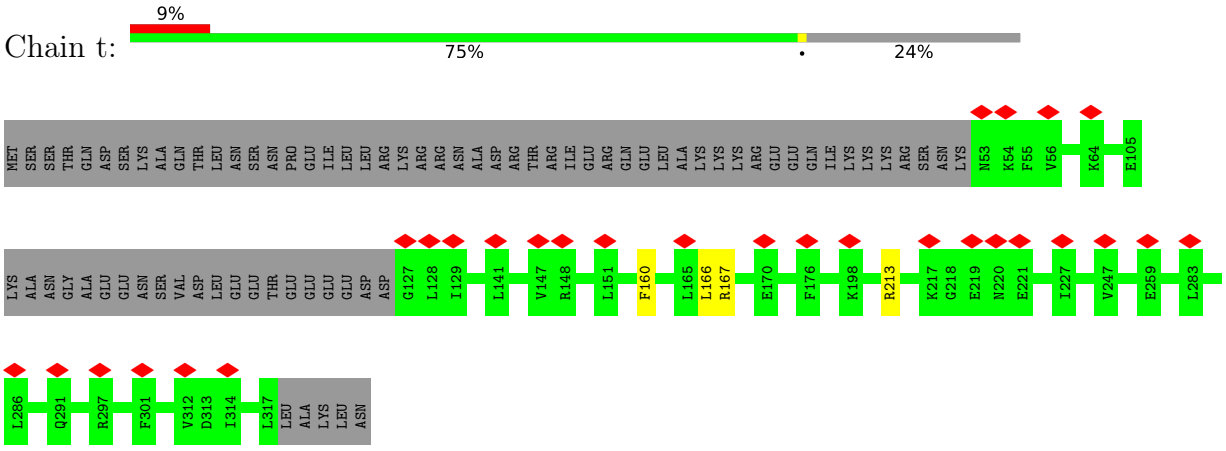
Chain o:



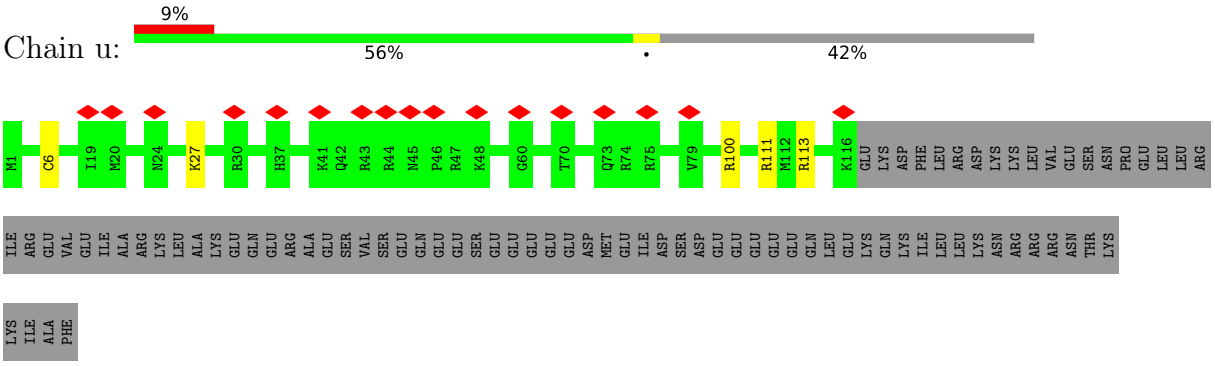
• Molecule 35: Ribosome biogenesis protein NSA2



• Molecule 36: Ribosome biogenesis protein RLP7

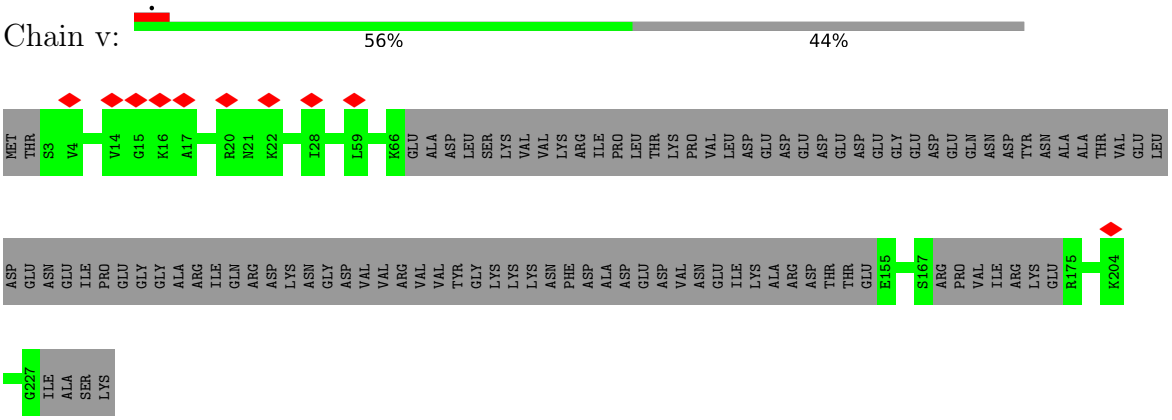


• Molecule 37: Ribosome biogenesis protein RLP24



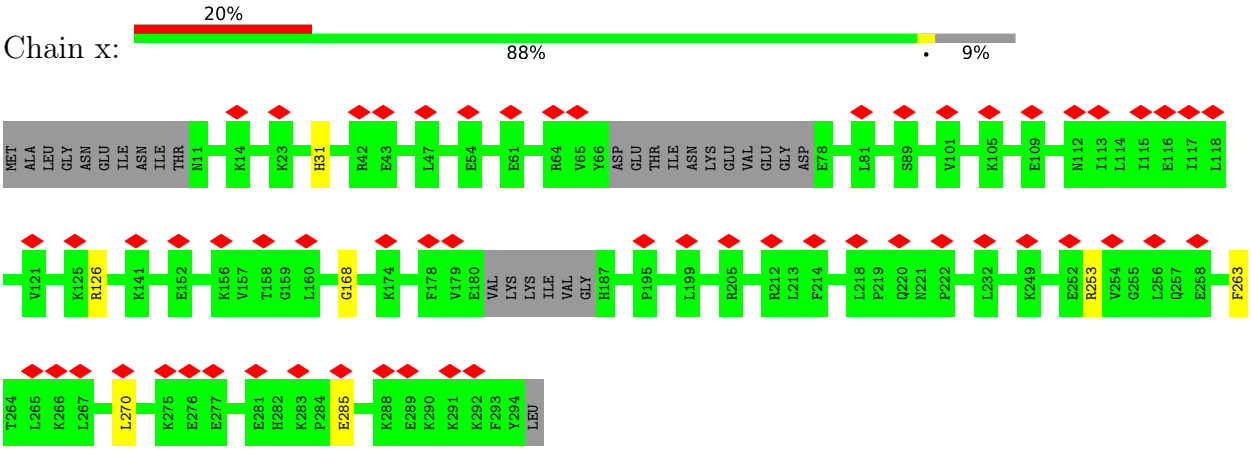
• Molecule 38: Nucleolar protein 16

Chain v:



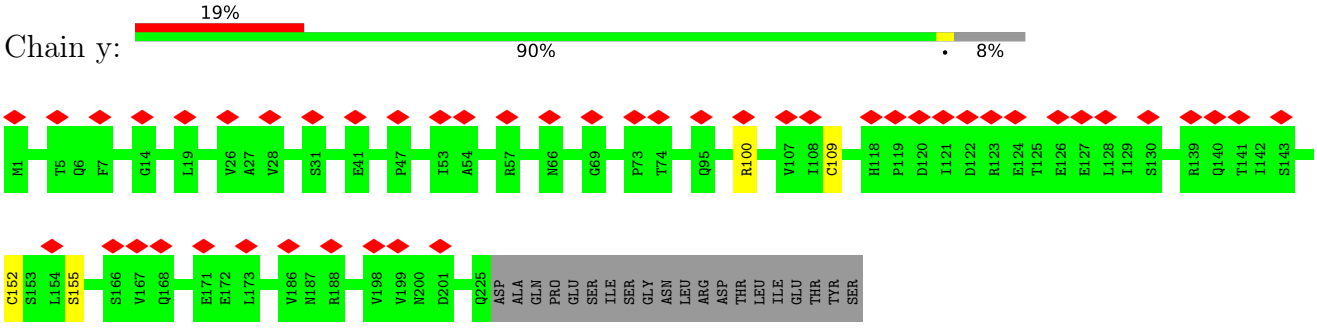
• Molecule 39: Ribosome production factor 1

Chain x:



• Molecule 40: Eukaryotic translation initiation factor 6

Chain y:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	9258	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 ($e^-/Å^2$)	84.67	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.100	Depositor
Minimum map value	-0.032	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.022	Depositor
Map size (Å)	425.40002, 425.40002, 425.40002	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0635, 1.0635, 1.0635	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	1	0.15	0/40695	0.74	33/63419 (0.1%)
2	2	0.16	0/3488	0.76	4/5426 (0.1%)
3	3	0.23	0/1461	0.38	0/1958
4	4	0.24	0/1895	0.39	0/2549
5	5	0.23	0/3109	0.41	0/4187
6	6	0.16	0/1527	0.76	3/2371 (0.1%)
7	A	0.24	0/1220	0.40	0/1646
8	B	0.24	0/2699	0.43	0/3626
9	C	0.24	0/2660	0.41	0/3601
10	D	0.24	0/3552	0.40	0/4789
11	E	0.24	0/1226	0.40	0/1648
12	F	0.24	0/1974	0.38	0/2654
13	G	0.24	0/1247	0.39	0/1688
14	H	0.24	0/1261	0.42	0/1690
15	K	0.24	0/2107	0.40	0/2845
16	L	0.24	0/877	0.39	0/1179
17	M	0.24	0/1007	0.38	0/1355
18	N	0.23	0/1544	0.38	0/2065
19	O	0.24	0/1585	0.38	0/2128
20	P	0.24	0/1080	0.39	0/1455
21	Q	0.24	0/1024	0.41	0/1385
22	S	0.24	0/1468	0.41	0/1973
23	V	0.25	0/386	0.41	0/520
24	W	0.23	0/1428	0.39	0/1918
25	Y	0.23	0/995	0.40	0/1329
26	b	0.24	0/3474	0.38	0/4683
27	e	0.24	0/1014	0.40	0/1356
28	f	0.25	0/868	0.41	0/1168
29	h	0.24	0/973	0.36	0/1294
30	i	0.24	0/558	0.37	0/738
31	j	0.24	0/578	0.41	0/767
32	m	0.23	0/1401	0.39	0/1895

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	n	0.24	0/2774	0.38	0/3751
34	o	0.24	0/1129	0.41	0/1502
35	r	0.22	0/602	0.33	0/787
36	t	0.24	0/1961	0.41	0/2639
37	u	0.24	0/996	0.37	0/1324
38	v	0.23	0/1100	0.37	0/1456
39	x	0.24	0/2313	0.41	0/3100
40	y	0.23	0/1722	0.44	0/2343
All	All	0.20	0/102978	0.59	40/148207 (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
39	x	0	2

There are no bond length outliers.

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	497	C	N3-C2-O2	-7.95	116.33	121.90
1	1	1201	C	C2-N1-C1'	7.77	127.34	118.80
6	6	1	C	OP1-P-OP2	-6.86	109.31	119.60
2	2	130	C	OP1-P-OP2	-6.80	109.40	119.60
1	1	2830	G	OP1-P-OP2	-6.80	109.40	119.60
1	1	3158	G	OP1-P-OP2	-6.79	109.41	119.60
1	1	1059	G	OP1-P-OP2	-6.79	109.41	119.60
1	1	2848	G	OP1-P-OP2	-6.79	109.41	119.60
2	2	115	C	OP1-P-OP2	-6.79	109.42	119.60
1	1	769	G	OP1-P-OP2	-6.79	109.42	119.60
1	1	1097	G	OP1-P-OP2	-6.79	109.42	119.60
1	1	1306	G	OP1-P-OP2	-6.78	109.43	119.60
1	1	714	G	OP1-P-OP2	-6.77	109.45	119.60
1	1	925	A	OP1-P-OP2	-6.76	109.46	119.60
1	1	2985	C	OP1-P-OP2	-6.76	109.46	119.60
1	1	2352	A	OP1-P-OP2	-6.76	109.46	119.60
1	1	310	U	OP1-P-OP2	-6.75	109.47	119.60
1	1	3172	A	OP1-P-OP2	-6.75	109.47	119.60
1	1	1	G	OP1-P-OP2	-6.75	109.48	119.60
1	1	3356	G	OP1-P-OP2	-6.74	109.49	119.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	3364	C	OP1-P-OP2	-6.73	109.50	119.60
1	1	781	G	OP1-P-OP2	-6.73	109.51	119.60
6	6	227	C	OP1-P-OP2	-6.72	109.51	119.60
1	1	3285	C	OP1-P-OP2	-6.72	109.53	119.60
1	1	1200	A	OP1-P-OP2	-6.71	109.53	119.60
1	1	720	A	OP1-P-OP2	-6.71	109.53	119.60
1	1	2887	A	OP1-P-OP2	-6.71	109.54	119.60
2	2	1	A	OP1-P-OP2	-6.70	109.56	119.60
1	1	960	U	C2-N1-C1'	6.33	125.30	117.70
1	1	1201	C	N1-C2-O2	6.15	122.59	118.90
1	1	3196	U	C2-N1-C1'	5.85	124.72	117.70
1	1	2996	U	C2-N1-C1'	5.56	124.37	117.70
1	1	1201	C	C6-N1-C1'	-5.51	114.19	120.80
1	1	2986	U	C2-N1-C1'	5.51	124.31	117.70
1	1	954	U	C2-N1-C1'	5.49	124.28	117.70
2	2	156	U	C2-N1-C1'	5.47	124.26	117.70
1	1	3023	U	C2-N1-C1'	5.31	124.08	117.70
1	1	730	C	N3-C2-O2	-5.24	118.23	121.90
1	1	1201	C	N3-C2-O2	-5.14	118.30	121.90
6	6	1	C	O4'-C1'-N1	5.12	112.30	108.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
39	x	168	GLY	Peptide
39	x	285	GLU	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	3	171/306 (56%)	157 (92%)	13 (8%)	1 (1%)	25	65
4	4	209/278 (75%)	192 (92%)	17 (8%)	0	100	100
5	5	377/463 (81%)	370 (98%)	7 (2%)	0	100	100
7	A	134/291 (46%)	123 (92%)	11 (8%)	0	100	100
8	B	329/387 (85%)	313 (95%)	16 (5%)	0	100	100
9	C	341/362 (94%)	327 (96%)	14 (4%)	0	100	100
10	D	433/505 (86%)	415 (96%)	18 (4%)	0	100	100
11	E	147/176 (84%)	142 (97%)	5 (3%)	0	100	100
12	F	239/244 (98%)	233 (98%)	6 (2%)	0	100	100
13	G	154/256 (60%)	149 (97%)	5 (3%)	0	100	100
14	H	142/191 (74%)	138 (97%)	4 (3%)	0	100	100
15	K	253/376 (67%)	244 (96%)	9 (4%)	0	100	100
16	L	106/199 (53%)	103 (97%)	3 (3%)	0	100	100
17	M	125/138 (91%)	124 (99%)	1 (1%)	0	100	100
18	N	173/204 (85%)	172 (99%)	1 (1%)	0	100	100
19	O	195/199 (98%)	190 (97%)	5 (3%)	0	100	100
20	P	133/184 (72%)	130 (98%)	3 (2%)	0	100	100
21	Q	129/186 (69%)	127 (98%)	2 (2%)	0	100	100
22	S	168/172 (98%)	158 (94%)	10 (6%)	0	100	100
23	V	46/137 (34%)	46 (100%)	0	0	100	100
24	W	156/236 (66%)	152 (97%)	4 (3%)	0	100	100
25	Y	123/127 (97%)	121 (98%)	2 (2%)	0	100	100
26	b	413/647 (64%)	391 (95%)	22 (5%)	0	100	100
27	e	121/130 (93%)	118 (98%)	3 (2%)	0	100	100
28	f	104/107 (97%)	101 (97%)	3 (3%)	0	100	100
29	h	116/120 (97%)	108 (93%)	8 (7%)	0	100	100
30	i	68/100 (68%)	65 (96%)	3 (4%)	0	100	100
31	j	69/88 (78%)	68 (99%)	1 (1%)	0	100	100
32	m	159/807 (20%)	154 (97%)	5 (3%)	0	100	100
33	n	321/605 (53%)	311 (97%)	10 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	o	131/220 (60%)	123 (94%)	8 (6%)	0	100	100
35	r	64/261 (24%)	64 (100%)	0	0	100	100
36	t	240/322 (74%)	222 (92%)	18 (8%)	0	100	100
37	u	114/199 (57%)	113 (99%)	1 (1%)	0	100	100
38	v	124/231 (54%)	121 (98%)	3 (2%)	0	100	100
39	x	261/295 (88%)	236 (90%)	25 (10%)	0	100	100
40	y	223/245 (91%)	217 (97%)	6 (3%)	0	100	100
All	All	6811/9994 (68%)	6538 (96%)	272 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	3	40	ARG

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	3	155/274 (57%)	149 (96%)	6 (4%)	32	57
4	4	203/257 (79%)	199 (98%)	4 (2%)	55	74
5	5	343/410 (84%)	339 (99%)	4 (1%)	71	84
7	A	134/263 (51%)	131 (98%)	3 (2%)	52	71
8	B	280/323 (87%)	275 (98%)	5 (2%)	59	77
9	C	273/289 (94%)	269 (98%)	4 (2%)	65	80
10	D	381/440 (87%)	372 (98%)	9 (2%)	49	69
11	E	131/153 (86%)	129 (98%)	2 (2%)	65	80
12	F	204/205 (100%)	203 (100%)	1 (0%)	88	93
13	G	128/208 (62%)	126 (98%)	2 (2%)	62	79
14	H	142/171 (83%)	139 (98%)	3 (2%)	53	72

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
15	K	238/346 (69%)	233 (98%)	5 (2%)	53 72
16	L	87/159 (55%)	83 (95%)	4 (5%)	27 53
17	M	100/109 (92%)	99 (99%)	1 (1%)	76 86
18	N	153/176 (87%)	148 (97%)	5 (3%)	38 61
19	O	160/162 (99%)	156 (98%)	4 (2%)	47 68
20	P	109/146 (75%)	107 (98%)	2 (2%)	59 77
21	Q	107/151 (71%)	105 (98%)	2 (2%)	57 75
22	S	155/156 (99%)	153 (99%)	2 (1%)	69 82
23	V	39/105 (37%)	39 (100%)	0	100 100
24	W	156/213 (73%)	151 (97%)	5 (3%)	39 62
25	Y	108/110 (98%)	106 (98%)	2 (2%)	57 75
26	b	377/573 (66%)	364 (97%)	13 (3%)	37 61
27	e	106/111 (96%)	104 (98%)	2 (2%)	57 75
28	f	90/91 (99%)	90 (100%)	0	100 100
29	h	104/105 (99%)	100 (96%)	4 (4%)	33 58
30	i	57/82 (70%)	55 (96%)	2 (4%)	36 60
31	j	59/71 (83%)	59 (100%)	0	100 100
32	m	150/723 (21%)	149 (99%)	1 (1%)	84 90
33	n	299/548 (55%)	290 (97%)	9 (3%)	41 63
34	o	118/199 (59%)	115 (98%)	3 (2%)	47 68
35	r	61/229 (27%)	59 (97%)	2 (3%)	38 61
36	t	216/287 (75%)	212 (98%)	4 (2%)	57 75
37	u	101/180 (56%)	96 (95%)	5 (5%)	24 51
38	v	116/205 (57%)	116 (100%)	0	100 100
39	x	252/276 (91%)	247 (98%)	5 (2%)	55 74
40	y	193/211 (92%)	189 (98%)	4 (2%)	53 72
All	All	6085/8717 (70%)	5956 (98%)	129 (2%)	56 72

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	3	29	ARG
3	3	40	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	3	56	ASP
3	3	76	LEU
3	3	79	ARG
3	3	123	ARG
4	4	41	GLU
4	4	82	ASN
4	4	137	GLN
4	4	229	ASN
5	5	63	ASN
5	5	102	LYS
5	5	133	ARG
5	5	340	LYS
7	A	45	HIS
7	A	96	ASP
7	A	189	ARG
8	B	100	ARG
8	B	174	LYS
8	B	332	ARG
8	B	334	ARG
8	B	370	PHE
9	C	23	PRO
9	C	93	MET
9	C	120	TYR
9	C	177	ASP
10	D	110	LYS
10	D	137	LEU
10	D	140	PHE
10	D	225	MET
10	D	283	PHE
10	D	307	GLU
10	D	333	PHE
10	D	396	PRO
10	D	415	TYR
11	E	48	ARG
11	E	77	ARG
12	F	157	ASN
13	G	84	ARG
13	G	145	ASN
14	H	23	ARG
14	H	111	PHE
14	H	124	ARG
15	K	89	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	K	110	TRP
15	K	153	GLU
15	K	253	TRP
15	K	262	ASN
16	L	62	THR
16	L	67	ARG
16	L	98	ASP
16	L	100	ARG
17	M	108	ARG
18	N	19	LEU
18	N	62	TYR
18	N	108	ARG
18	N	179	LYS
18	N	181	ASN
19	O	15	LEU
19	O	42	ASN
19	O	73	PHE
19	O	156	LEU
20	P	82	ARG
20	P	96	GLN
21	Q	69	ARG
21	Q	92	ARG
22	S	12	ARG
22	S	146	LYS
24	W	38	ARG
24	W	60	TRP
24	W	113	LYS
24	W	133	LEU
24	W	174	LYS
25	Y	51	ARG
25	Y	74	TYR
26	b	1	MET
26	b	5	TRP
26	b	70	ASN
26	b	159	ARG
26	b	168	ARG
26	b	180	LYS
26	b	234	ASN
26	b	247	ARG
26	b	260	CYS
26	b	278	PHE
26	b	329	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	b	427	TRP
26	b	428	LYS
27	e	27	ARG
27	e	33	ARG
29	h	10	ARG
29	h	35	LYS
29	h	62	GLN
29	h	115	LYS
30	i	53	TYR
30	i	98	ARG
32	m	268	PRO
33	n	15	PHE
33	n	63	TYR
33	n	64	TYR
33	n	86	PHE
33	n	265	GLU
33	n	352	TYR
33	n	360	PHE
33	n	417	LEU
33	n	431	TRP
34	o	94	TYR
34	o	102	PHE
34	o	146	MET
35	r	4	ASN
35	r	23	ARG
36	t	160	PHE
36	t	166	LEU
36	t	167	ARG
36	t	213	ARG
37	u	6	CYS
37	u	27	LYS
37	u	100	ARG
37	u	111	ARG
37	u	113	ARG
39	x	31	HIS
39	x	126	ARG
39	x	253	ARG
39	x	263	PHE
39	x	270	LEU
40	y	100	ARG
40	y	109	CYS
40	y	152	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
40	y	155	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
3	3	11	ASN
5	5	234	ASN
5	5	269	GLN
8	B	173	GLN
9	C	116	ASN
10	D	300	ASN
10	D	441	GLN
12	F	157	ASN
12	F	186	HIS
14	H	125	ASN
17	M	126	GLN
18	N	57	GLN
19	O	55	HIS
26	b	70	ASN
26	b	234	ASN
26	b	272	HIS
27	e	20	HIS
27	e	35	GLN
27	e	98	HIS
29	h	59	ASN
29	h	62	GLN
32	m	320	HIS
33	n	419	ASN
34	o	130	ASN
36	t	53	ASN
38	v	206	ASN
40	y	79	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	1683/3396 (49%)	361 (21%)	44 (2%)
2	2	144/158 (91%)	24 (16%)	1 (0%)
6	6	65/232 (28%)	24 (36%)	5 (7%)
All	All	1892/3786 (49%)	409 (21%)	50 (2%)

All (409) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	2	U
1	1	3	U
1	1	6	A
1	1	7	C
1	1	15	C
1	1	26	A
1	1	39	A
1	1	40	A
1	1	42	C
1	1	48	A
1	1	49	A
1	1	60	A
1	1	65	A
1	1	66	A
1	1	74	G
1	1	92	G
1	1	93	C
1	1	94	G
1	1	109	A
1	1	110	G
1	1	116	A
1	1	117	U
1	1	122	A
1	1	135	C
1	1	136	G
1	1	151	A
1	1	153	U
1	1	155	G
1	1	156	G
1	1	165	A
1	1	166	C
1	1	170	G
1	1	187	A
1	1	190	U
1	1	191	U
1	1	200	C
1	1	207	U
1	1	210	U
1	1	213	A
1	1	218	G
1	1	219	A
1	1	220	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	231	G
1	1	234	G
1	1	240	U
1	1	243	G
1	1	246	U
1	1	248	U
1	1	249	U
1	1	250	U
1	1	251	G
1	1	252	U
1	1	268	A
1	1	269	G
1	1	280	U
1	1	282	G
1	1	283	G
1	1	284	A
1	1	285	A
1	1	286	U
1	1	292	U
1	1	299	G
1	1	311	C
1	1	315	C
1	1	323	A
1	1	325	A
1	1	329	U
1	1	338	A
1	1	352	A
1	1	375	A
1	1	376	G
1	1	384	A
1	1	385	A
1	1	388	G
1	1	397	A
1	1	398	A
1	1	402	A
1	1	403	C
1	1	404	G
1	1	407	A
1	1	412	G
1	1	420	G
1	1	421	G
1	1	422	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	439	C
1	1	454	C
1	1	457	C
1	1	463	C
1	1	465	U
1	1	466	G
1	1	467	U
1	1	468	G
1	1	474	G
1	1	475	G
1	1	477	A
1	1	479	U
1	1	480	C
1	1	481	U
1	1	482	C
1	1	489	C
1	1	495	G
1	1	521	A
1	1	542	G
1	1	544	C
1	1	547	G
1	1	548	G
1	1	549	U
1	1	551	A
1	1	552	G
1	1	555	U
1	1	557	A
1	1	558	U
1	1	559	A
1	1	569	A
1	1	578	A
1	1	579	G
1	1	589	A
1	1	592	A
1	1	593	C
1	1	604	G
1	1	609	G
1	1	611	A
1	1	621	A
1	1	638	C
1	1	642	U
1	1	643	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	644	G
1	1	645	A
1	1	646	A
1	1	647	A
1	1	650	C
1	1	660	A
1	1	677	A
1	1	681	U
1	1	691	A
1	1	705	A
1	1	716	A
1	1	717	C
1	1	718	G
1	1	721	G
1	1	722	G
1	1	735	A
1	1	750	G
1	1	761	A
1	1	770	G
1	1	776	U
1	1	777	U
1	1	783	A
1	1	784	A
1	1	785	G
1	1	806	A
1	1	817	A
1	1	932	U
1	1	937	G
1	1	944	C
1	1	954	U
1	1	959	C
1	1	960	U
1	1	961	C
1	1	962	A
1	1	977	C
1	1	978	G
1	1	979	U
1	1	980	A
1	1	982	C
1	1	985	U
1	1	990	U
1	1	1060	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	1098	A
1	1	1103	A
1	1	1104	G
1	1	1105	A
1	1	1108	U
1	1	1111	U
1	1	1116	G
1	1	1124	U
1	1	1125	U
1	1	1128	U
1	1	1129	A
1	1	1130	A
1	1	1132	C
1	1	1142	G
1	1	1143	A
1	1	1144	U
1	1	1145	G
1	1	1151	U
1	1	1152	G
1	1	1153	A
1	1	1159	A
1	1	1166	G
1	1	1180	A
1	1	1181	U
1	1	1186	G
1	1	1191	U
1	1	1201	C
1	1	1202	A
1	1	1203	A
1	1	1219	C
1	1	1222	G
1	1	1242	G
1	1	1243	G
1	1	1244	A
1	1	1245	A
1	1	1246	G
1	1	1253	U
1	1	1262	G
1	1	1264	G
1	1	1269	U
1	1	1277	C
1	1	1278	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	1279	C
1	1	1285	G
1	1	1287	A
1	1	1308	A
1	1	1309	U
1	1	1310	G
1	1	1313	G
1	1	1318	A
1	1	1330	A
1	1	1332	A
1	1	1348	U
1	1	1349	G
1	1	1350	A
1	1	1352	A
1	1	1353	U
1	1	1354	G
1	1	1355	A
1	1	1356	U
1	1	1357	G
1	1	1386	A
1	1	1399	A
1	1	1400	G
1	1	1406	A
1	1	1417	G
1	1	1418	A
1	1	1419	A
1	1	1434	G
1	1	1437	C
1	1	2353	G
1	1	2365	C
1	1	2371	G
1	1	2373	A
1	1	2374	C
1	1	2376	G
1	1	2378	C
1	1	2385	G
1	1	2389	C
1	1	2393	G
1	1	2394	G
1	1	2836	C
1	1	2837	A
1	1	2852	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	2853	A
1	1	2856	G
1	1	2857	C
1	1	2858	U
1	1	2888	U
1	1	2889	C
1	1	2892	A
1	1	2899	C
1	1	2915	U
1	1	2987	A
1	1	2990	G
1	1	2994	A
1	1	2996	U
1	1	2997	G
1	1	3012	A
1	1	3019	U
1	1	3020	U
1	1	3021	A
1	1	3022	G
1	1	3027	A
1	1	3028	G
1	1	3029	A
1	1	3030	G
1	1	3032	A
1	1	3047	U
1	1	3048	A
1	1	3049	A
1	1	3053	G
1	1	3056	U
1	1	3057	U
1	1	3058	U
1	1	3059	G
1	1	3066	U
1	1	3067	C
1	1	3069	G
1	1	3070	A
1	1	3073	A
1	1	3074	G
1	1	3075	G
1	1	3076	C
1	1	3077	A
1	1	3078	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	3079	U
1	1	3086	A
1	1	3092	C
1	1	3093	C
1	1	3094	A
1	1	3099	C
1	1	3100	U
1	1	3101	G
1	1	3120	C
1	1	3121	U
1	1	3129	A
1	1	3130	A
1	1	3131	U
1	1	3142	A
1	1	3143	C
1	1	3144	G
1	1	3173	G
1	1	3174	A
1	1	3176	G
1	1	3179	U
1	1	3181	C
1	1	3187	A
1	1	3193	C
1	1	3194	C
1	1	3195	U
1	1	3196	U
1	1	3198	U
1	1	3199	G
1	1	3207	U
1	1	3217	C
1	1	3218	A
1	1	3219	G
1	1	3227	A
1	1	3228	C
1	1	3229	G
1	1	3244	A
1	1	3245	A
1	1	3247	G
1	1	3249	C
1	1	3250	U
1	1	3259	U
1	1	3260	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	3270	U
1	1	3275	U
1	1	3276	G
1	1	3289	G
1	1	3294	A
1	1	3295	A
1	1	3296	A
1	1	3304	U
1	1	3317	U
1	1	3319	U
1	1	3323	A
1	1	3330	A
1	1	3333	G
1	1	3334	U
1	1	3341	U
1	1	3343	G
1	1	3345	G
1	1	3347	A
1	1	3349	C
1	1	3359	A
1	1	3366	G
1	1	3369	G
1	1	3375	A
1	1	3378	C
1	1	3383	G
2	2	12	A
2	2	13	A
2	2	15	G
2	2	16	G
2	2	23	U
2	2	34	U
2	2	35	C
2	2	39	G
2	2	40	A
2	2	59	A
2	2	62	C
2	2	63	G
2	2	71	A
2	2	72	A
2	2	81	U
2	2	82	U
2	2	85	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2	86	U
2	2	87	G
2	2	90	U
2	2	95	G
2	2	104	A
2	2	106	C
2	2	122	U
6	6	2	C
6	6	4	U
6	6	6	U
6	6	7	C
6	6	8	A
6	6	13	U
6	6	14	U
6	6	15	C
6	6	16	U
6	6	17	G
6	6	36	U
6	6	40	U
6	6	43	A
6	6	46	U
6	6	52	G
6	6	53	A
6	6	54	A
6	6	56	U
6	6	57	U
6	6	58	G
6	6	228	U
6	6	230	A
6	6	231	A
6	6	232	A

All (50) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	1	G
1	1	93	C
1	1	152	U
1	1	165	A
1	1	324	A
1	1	456	U
1	1	548	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	551	A
1	1	644	G
1	1	649	A
1	1	659	G
1	1	720	A
1	1	769	G
1	1	783	A
1	1	989	A
1	1	1097	G
1	1	1103	A
1	1	1127	G
1	1	1129	A
1	1	1200	A
1	1	1218	U
1	1	1276	U
1	1	1347	U
1	1	1356	U
1	1	1405	U
1	1	1416	C
1	1	2364	G
1	1	2377	G
1	1	2393	G
1	1	2852	C
1	1	2856	G
1	1	2857	C
1	1	2887	A
1	1	2914	G
1	1	2986	U
1	1	3019	U
1	1	3058	U
1	1	3069	G
1	1	3077	A
1	1	3172	A
1	1	3218	A
1	1	3228	C
1	1	3269	U
1	1	3295	A
2	2	121	U
6	6	1	C
6	6	15	C
6	6	56	U
6	6	227	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	6	229	U

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

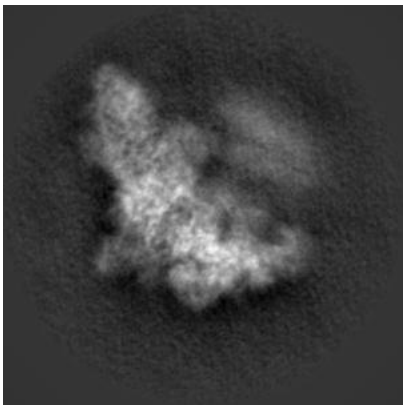
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-12907. These allow visual inspection of the internal detail of the map and identification of artifacts.

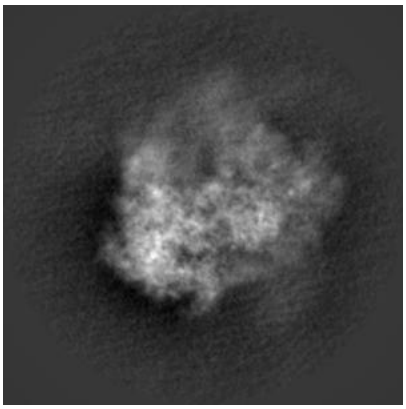
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

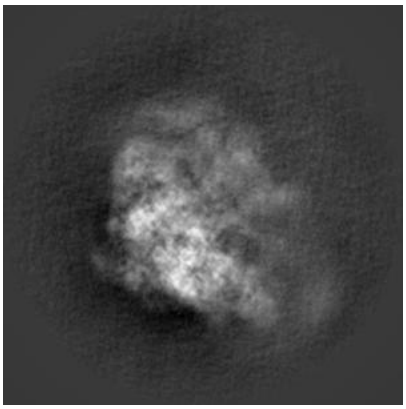
6.1.1 Primary map



X

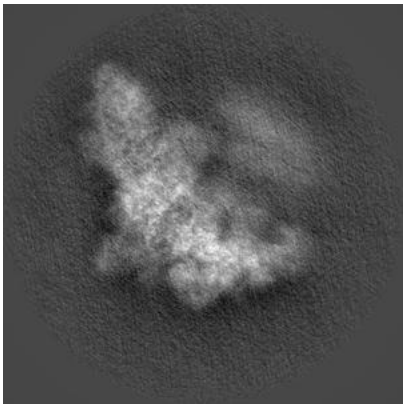


Y

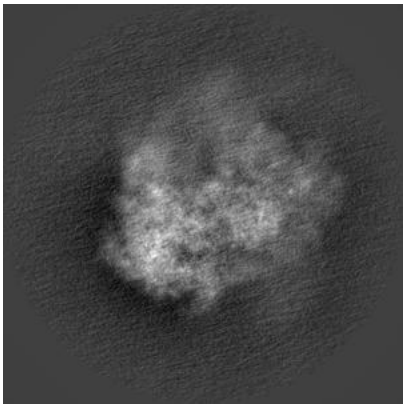


Z

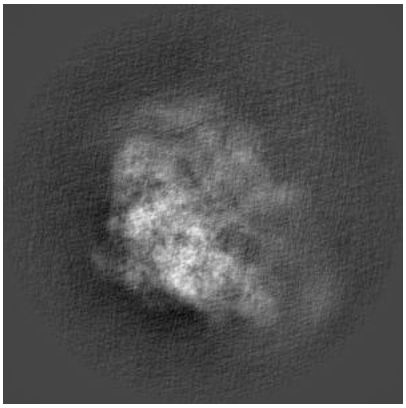
6.1.2 Raw map



X



Y

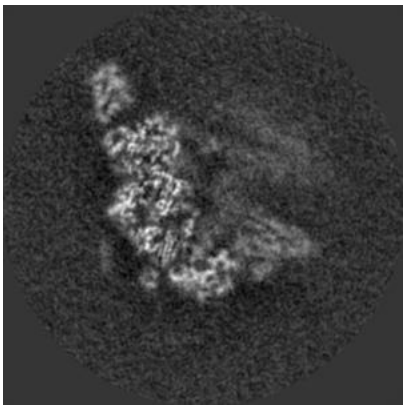


Z

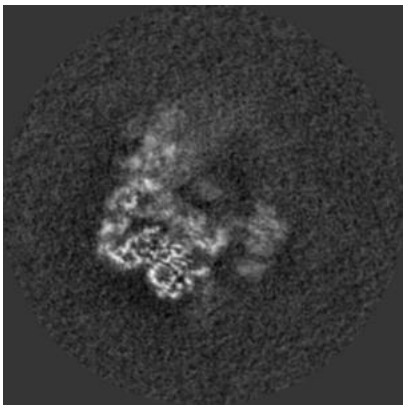
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

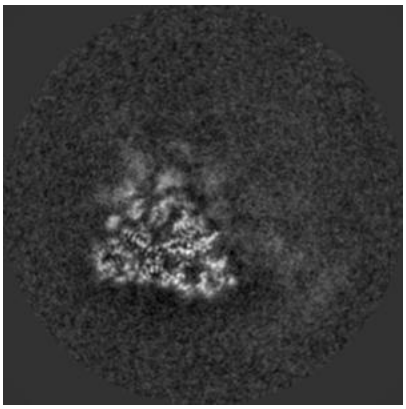
6.2.1 Primary map



X Index: 200

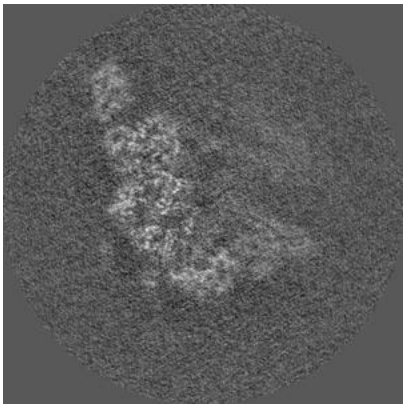


Y Index: 200

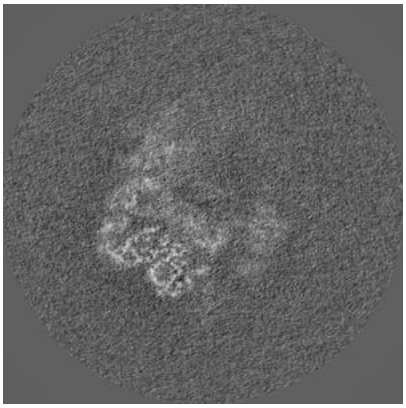


Z Index: 200

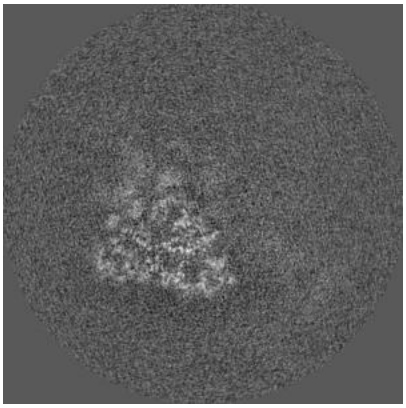
6.2.2 Raw map



X Index: 200



Y Index: 200

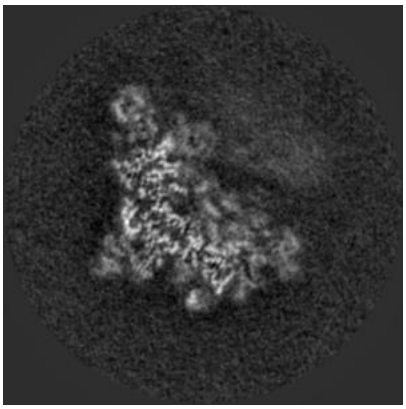


Z Index: 200

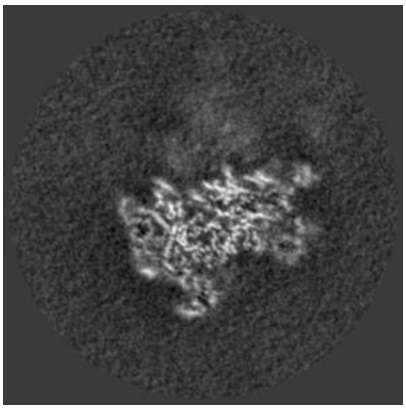
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

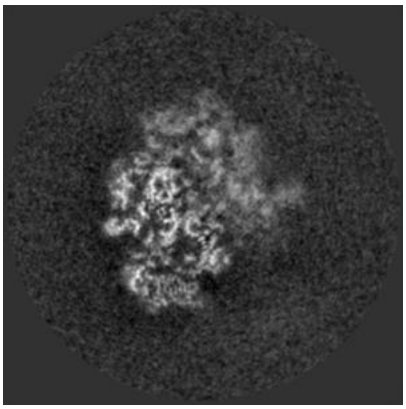
6.3.1 Primary map



X Index: 167

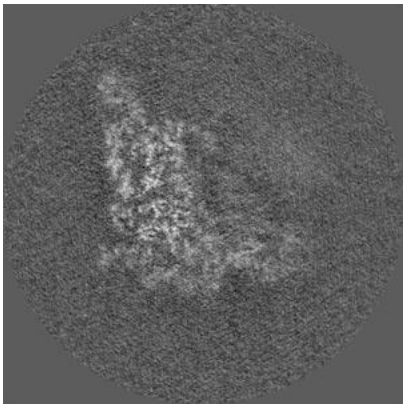


Y Index: 146

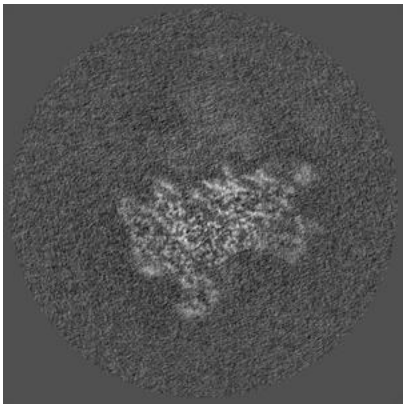


Z Index: 155

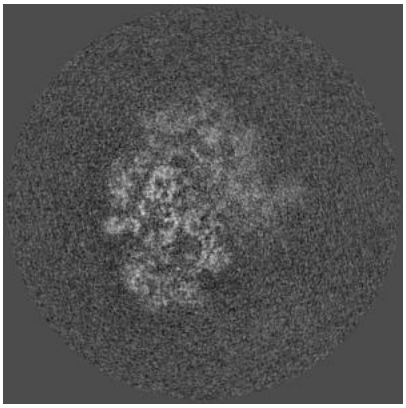
6.3.2 Raw map



X Index: 190



Y Index: 147



Z Index: 155

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

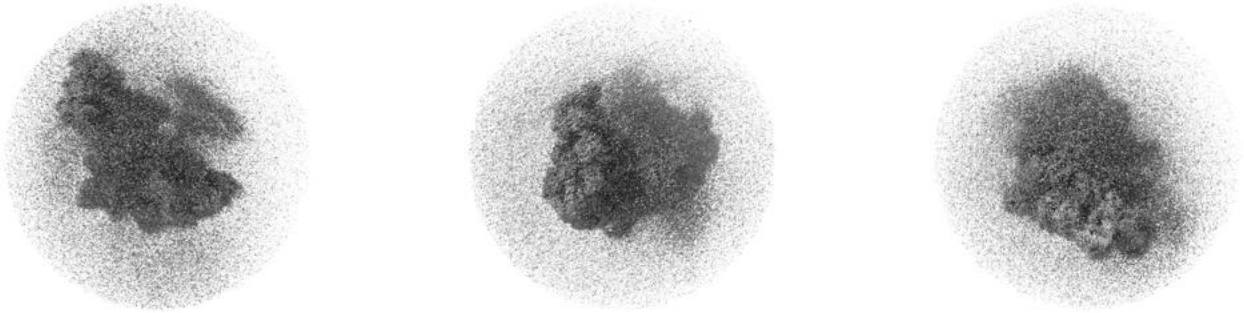
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.022. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

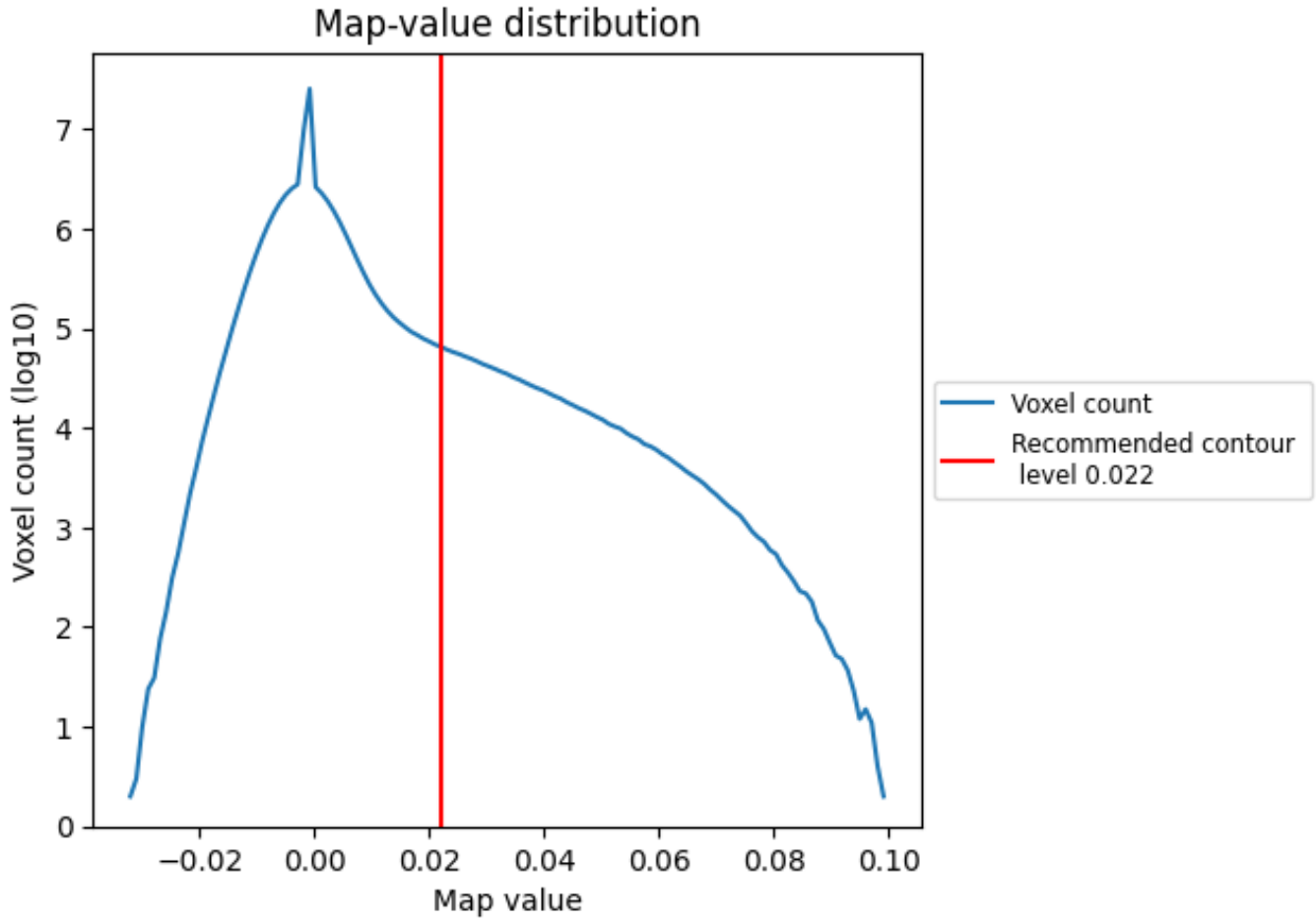
6.5 Mask visualisation (i)

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

7 Map analysis

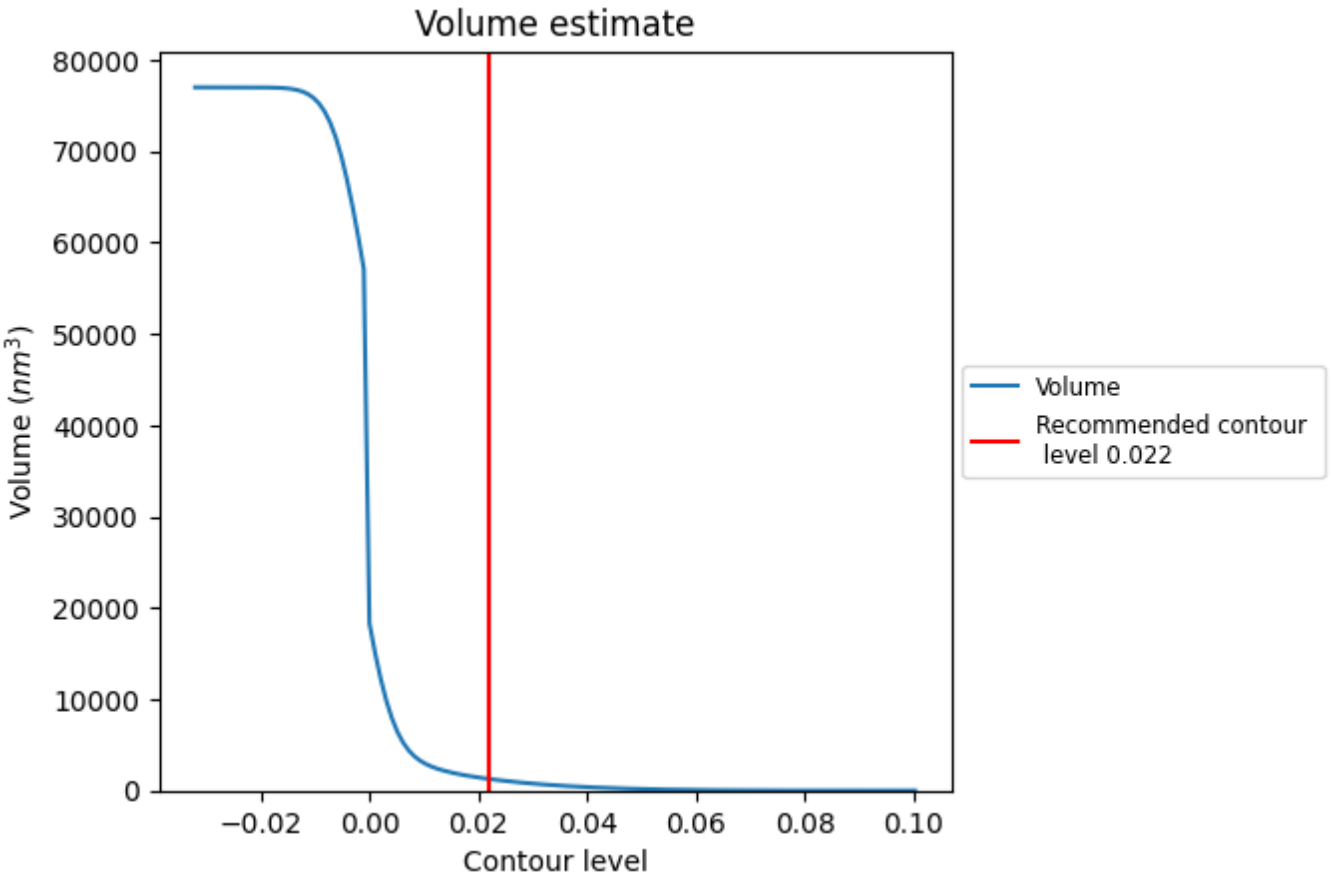
This section contains the results of statistical analysis of the map.

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.

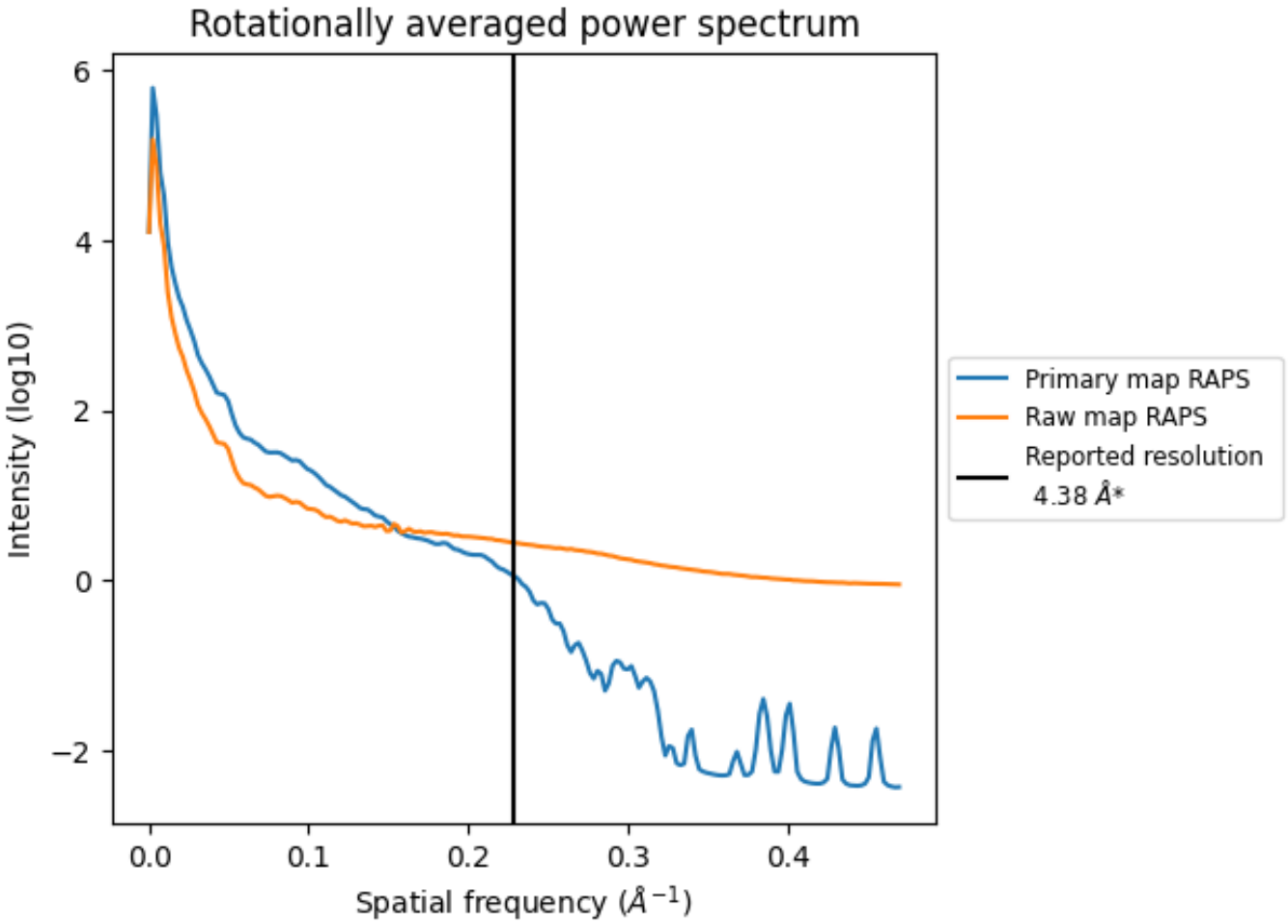
7.2 Volume estimate



The volume at the recommended contour level is 1266 nm^3; this corresponds to an approximate mass of 1144 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)

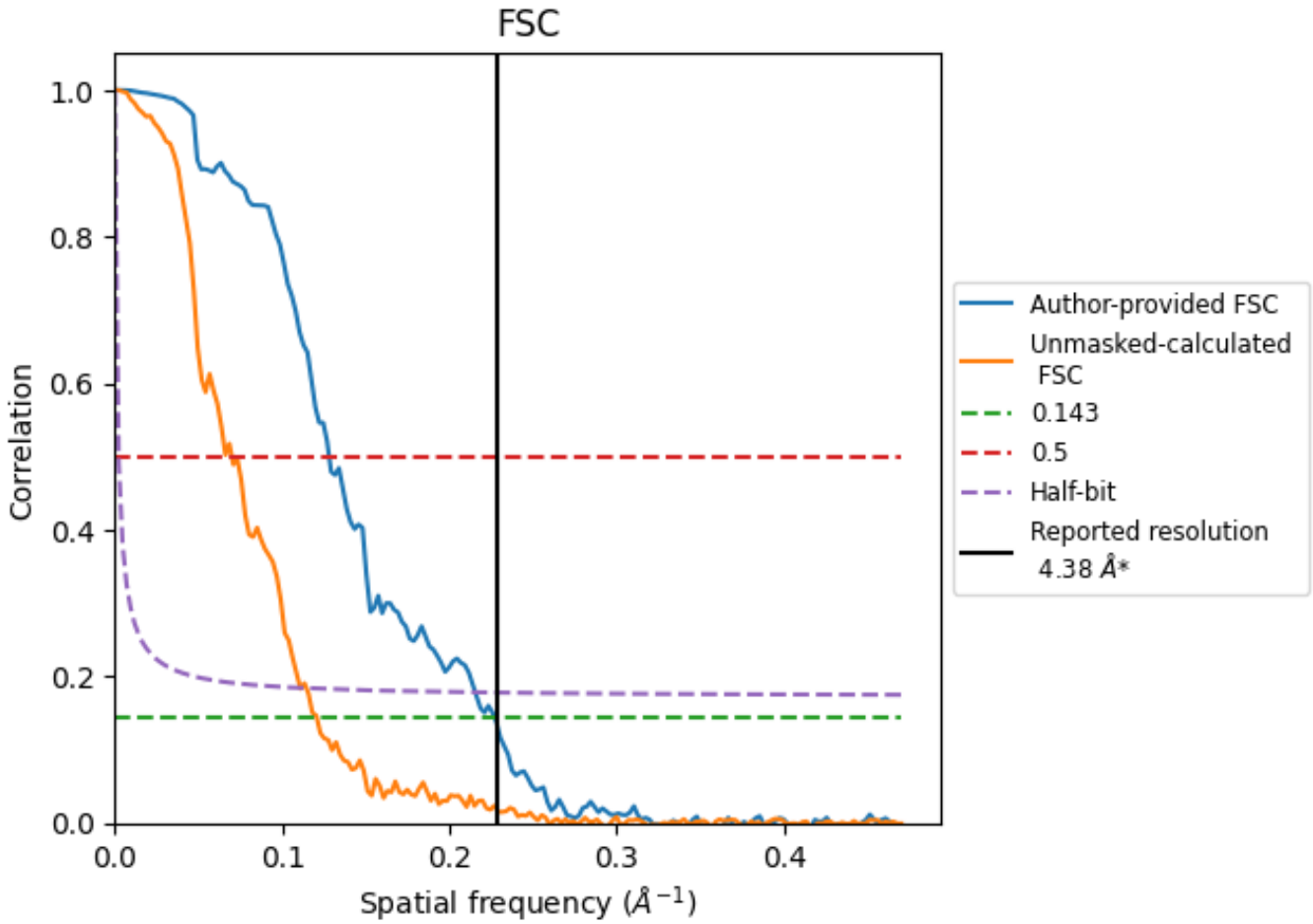


*Reported resolution corresponds to spatial frequency of 0.228 $Å^{-1}$

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 0.228 Å^{-1}

8.2 Resolution estimates (i)

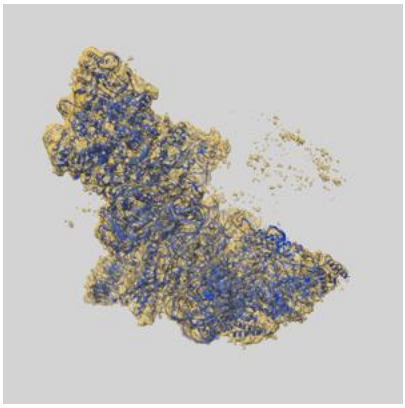
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.38	-	-
Author-provided FSC curve	4.40	7.81	4.64
Unmasked-calculated*	8.28	14.31	9.02

*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 8.28 differs from the reported value 4.38 by more than 10 %

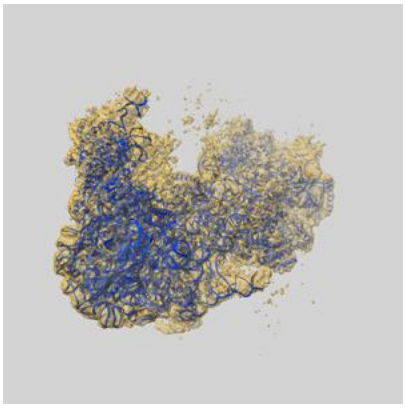
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-12907 and PDB model 7OHS. Per-residue inclusion information can be found in section 3 on page 11.

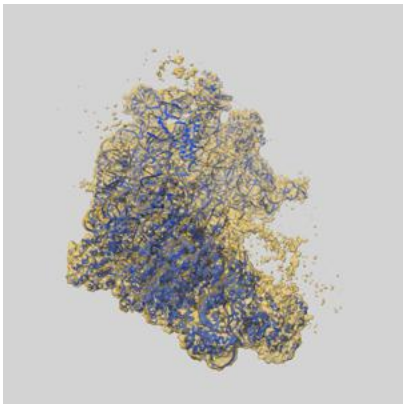
9.1 Map-model overlay



X



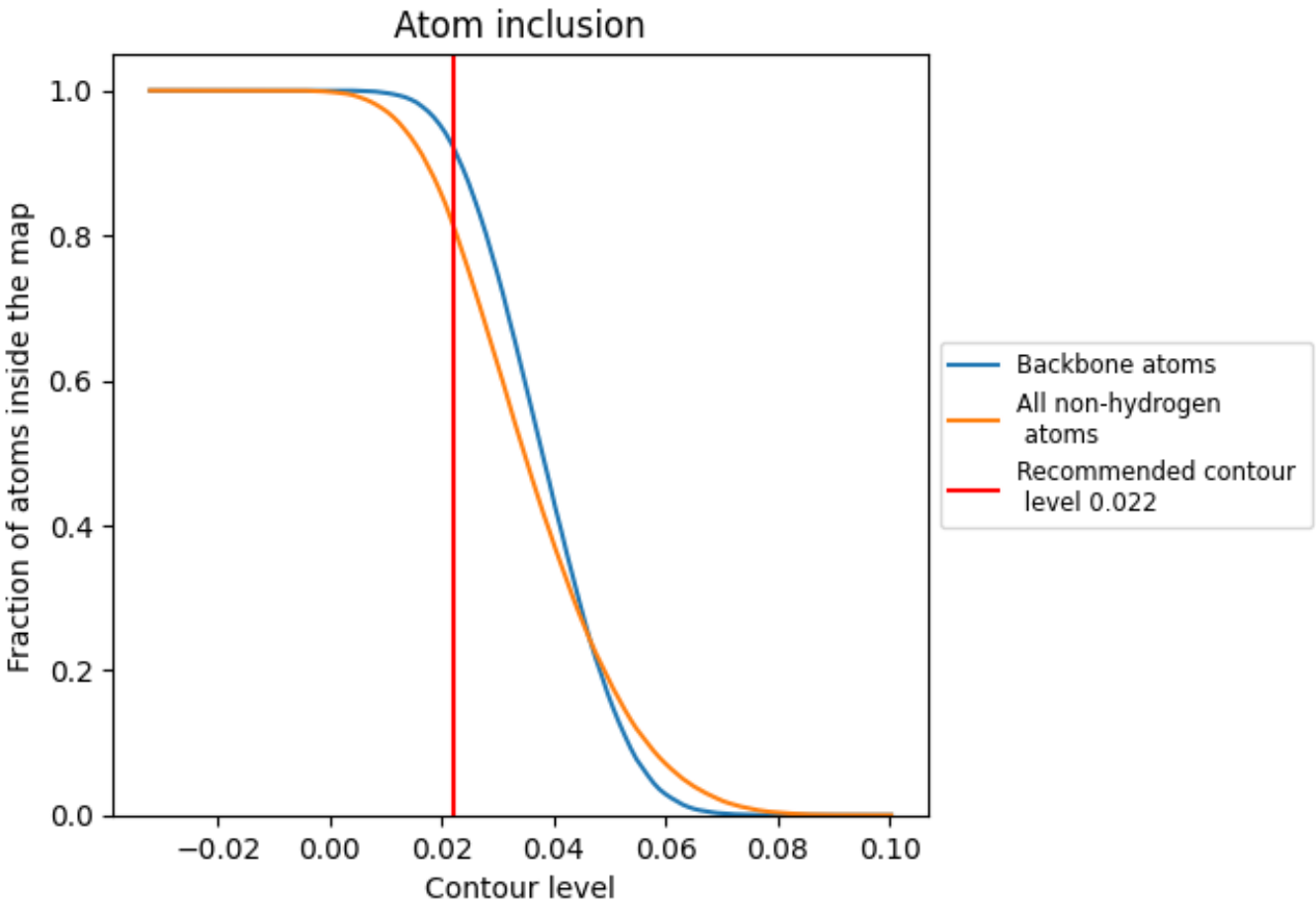
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.022 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 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.