wwPDB EM Validation Summary Report ⓘ

Jun 21, 2023 – 11:52 pm BST

PDB ID	:	8AZW
EMDB ID	:	EMD-15773
Title	:	Cryo-EM structure of the plant 60S subunit
Authors	:	Smirnova, J.; Loerke, J.; Kleinau, G.; Schmidt, A.; Buerger, J.; Meyer, E.H.; Mielke, T.; Scheerer, P.; Bock, R.; Spahn, C.M.T.; Zoschke, R.
Deposited on	:	2022-09-06
Resolution	:	2.14 Å(reported)

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

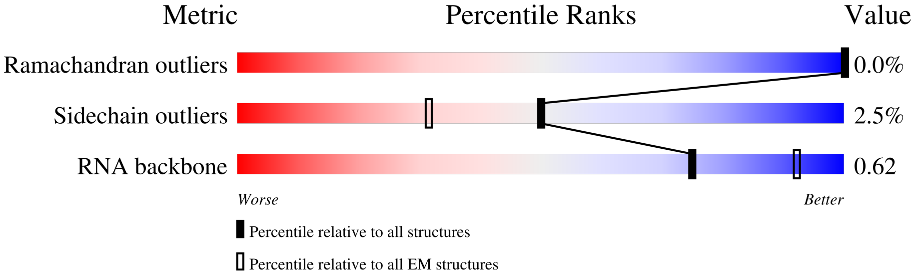
EMDB validation analysis	:	0.0.1.dev50
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

1 Overall quality at a glance ⓘ

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

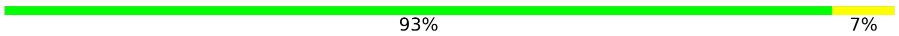
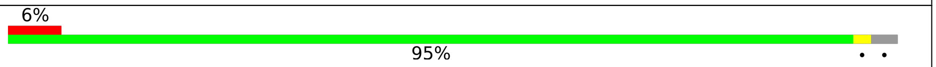
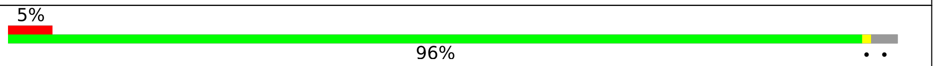
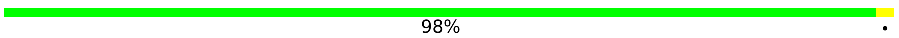
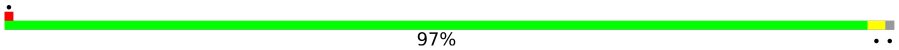
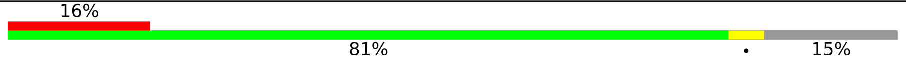
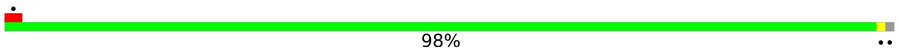
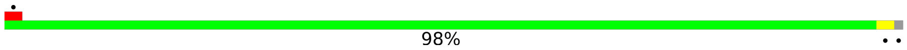
The reported resolution of this entry is 2.14 Å.

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	C	119	
2	D	206	
3	E	134	
4	F	204	
5	G	187	
6	H	214	
7	I	178	
8	J	164	

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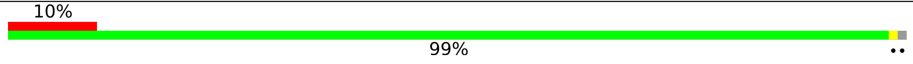
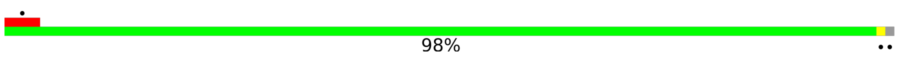
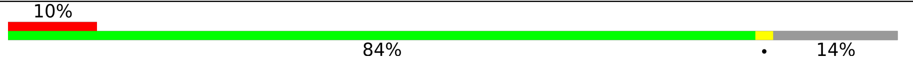
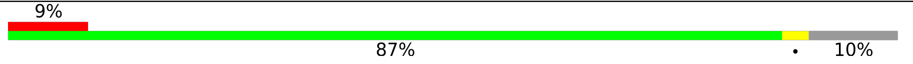
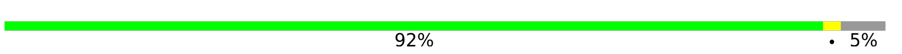
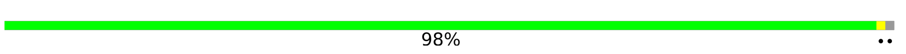
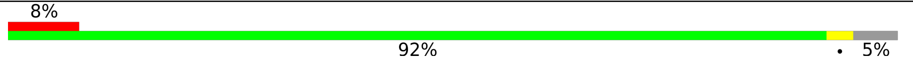
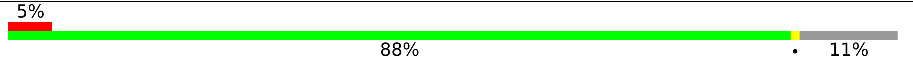
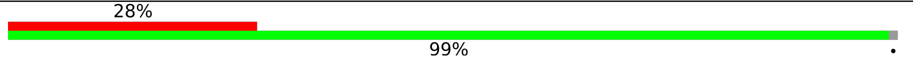
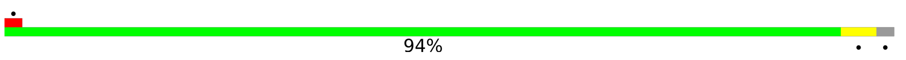
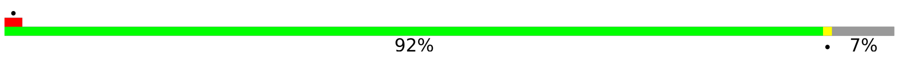
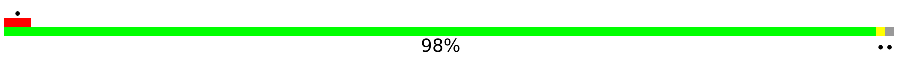
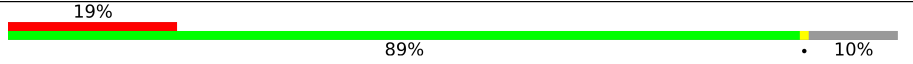
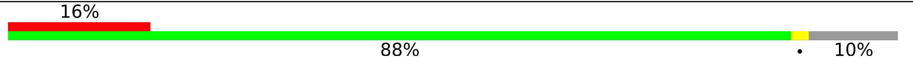
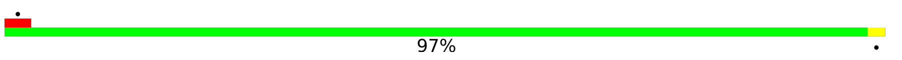
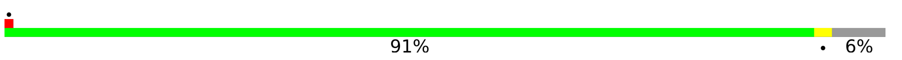
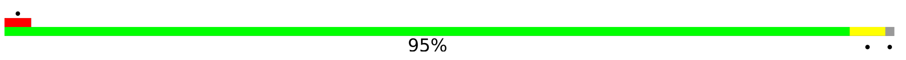
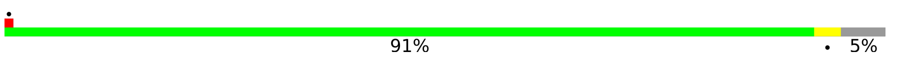
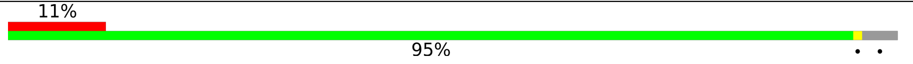
Mol	Chain	Length	Quality of chain
9	K	127	
10	L	164	
11	M	135	
12	N	143	
13	O	61	
14	P	113	
15	Q	120	
16	R	133	
17	S	112	
18	T	120	
19	U	110	
20	V	95	
21	W	69	
22	X	51	
23	Y	128	
24	p	25	
25	Z	105	
26	a	92	
27	b	230	
28	c	258	
29	d	206	
30	e	140	
31	f	148	
32	g	221	
33	h	301	

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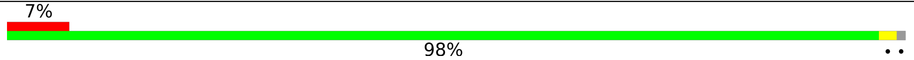
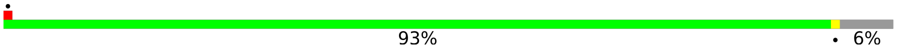
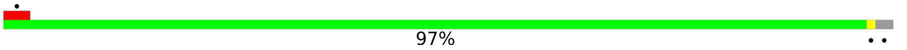
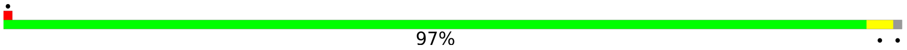
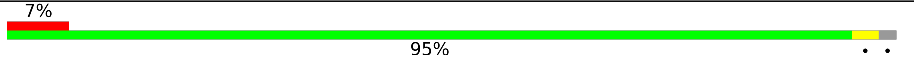
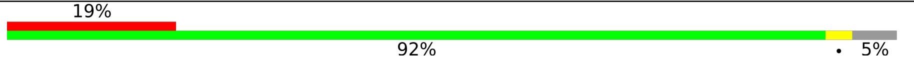
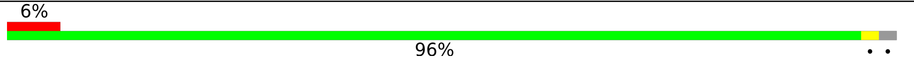
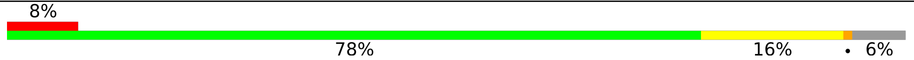
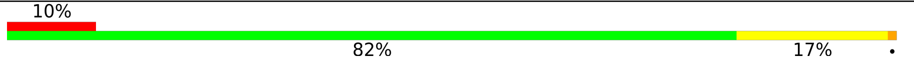
Mol	Chain	Length	Quality of chain
34	j	175	
35	k	154	
36	m	146	
37	n	123	
38	o	260	
39	q	242	
40	r	389	
41	s	405	
42	t	181	
43	u	194	
44	l	24	
45	A	3390	
46	B	163	

2 Entry composition

There are 52 unique types of molecules in this entry. The entry contains 223261 atoms, of which 92404 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 5S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
1	C	119	3823	1133	1285	457	829	119	0	0

- Molecule 2 is a protein called eL13 (60S ribosomal protein L13).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	D	200	3296	1007	1691	324	270	4	0	0

- Molecule 3 is a protein called eL14 (60S ribosomal protein L14).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	E	130	2206	678	1150	196	179	3	0	0

- Molecule 4 is a protein called eL15 (60S ribosomal protein L15).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	F	203	3469	1071	1768	350	277	3	0	0

- Molecule 5 is a protein called eL18 (60S ribosomal protein L18).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	G	186	3042	931	1580	283	245	3	0	0

- Molecule 6 is a protein called eL19 (60S ribosomal protein L19).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	H	182	3181	946	1652	327	247	9	0	0

- Molecule 7 is a protein called eL20 (60S ribosomal protein L18a).

Mol	Chain	Residues	Atoms						AltConf	Trace
7	I	177	Total	C	H	N	O	S	0	0
			3061	969	1556	277	251	8		

- Molecule 8 is a protein called eL21 (60S ribosomal protein L21).

Mol	Chain	Residues	Atoms						AltConf	Trace
8	J	163	Total	C	H	N	O	S	0	0
			2672	823	1366	255	224	4		

- Molecule 9 is a protein called eL22 (60S ribosomal protein L22).

Mol	Chain	Residues	Atoms						AltConf	Trace
9	K	99	Total	C	H	N	O	S	0	0
			1653	515	845	141	150	2		

- Molecule 10 is a protein called eL24 (60S ribosomal protein L24).

Mol	Chain	Residues	Atoms						AltConf	Trace
10	L	62	Total	C	H	N	O	S	0	0
			1079	341	553	101	81	3		

- Molecule 11 is a protein called eL27 (60S ribosomal protein L27).

Mol	Chain	Residues	Atoms						AltConf	Trace
11	M	134	Total	C	H	N	O	S	0	0
			2283	708	1184	206	183	2		

- Molecule 12 is a protein called eL28 (60S ribosomal protein L28).

Mol	Chain	Residues	Atoms						AltConf	Trace
12	N	142	Total	C	H	N	O	S	0	0
			2298	701	1187	207	201	2		

- Molecule 13 is a protein called eL29 (60S ribosomal protein L29).

Mol	Chain	Residues	Atoms						AltConf	Trace
13	O	49	Total	C	H	N	O	S	0	0
			831	250	419	95	66	1		

- Molecule 14 is a protein called eL30 (60S ribosomal protein L30).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
14	P	97	1526	475	781	130	135	5	0	0

- Molecule 15 is a protein called eL31 (60S ribosomal protein L31).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
15	Q	108	1809	549	934	168	156	2	0	0

- Molecule 16 is a protein called eL32 (60S ribosomal protein L32).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
16	R	126	2151	655	1115	207	169	5	0	0

- Molecule 17 is a protein called eL33 (60S ribosomal protein L35a).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
17	S	111	1832	571	932	171	153	5	0	0

- Molecule 18 is a protein called eL34 (60S ribosomal protein L34).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
18	T	114	1939	579	1013	193	153	1	0	0

- Molecule 19 is a protein called eL36 (60S ribosomal protein L36).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
19	U	98	1650	489	868	162	129	2	0	0

- Molecule 20 is a protein called eL37 (60S ribosomal protein L37).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
20	V	86	1427	429	726	155	112	5	0	0

- Molecule 21 is a protein called eL38 (60S ribosomal protein L38).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
21	W	68	1160	358	602	99	98	3	0	0

- Molecule 22 is a protein called eL39 (60S ribosomal protein L39).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
22	X	50	928	286	480	96	64	2	0	0

- Molecule 23 is a protein called eL40 (60S ribosomal protein L40).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
23	Y	51	881	262	460	88	65	6	0	0

- Molecule 24 is a protein called eL41 (60S ribosomal protein L41).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
24	p	25	527	145	289	62	28	3	0	0

- Molecule 25 is a protein called eL42 (60S ribosomal protein L42).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
25	Z	98	1629	494	842	157	131	5	0	0

- Molecule 26 is a protein called eL43 (60S ribosomal protein L37a).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
26	a	91	1453	443	745	136	124	5	0	0

- Molecule 27 is a protein called eL6 (60S ribosomal protein L6).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
27	b	208	3360	1046	1749	290	271	4	0	0

- Molecule 28 is a protein called eL8 (60S ribosomal protein L7a).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
28	c	233	3907	1206	2028	347	319	7	0	0

- Molecule 29 is a protein called uL13 (60S ribosomal protein L13a).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
29	d	205	3414	1046	1774	318	268	8	0	0

- Molecule 30 is a protein called uL14 (60S ribosomal protein L23).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
30	e	131	2029	623	1044	183	170	9	0	0

- Molecule 31 is a protein called uL15 (60S ribosomal protein L27a).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
31	f	147	2361	740	1200	228	190	3	0	0

- Molecule 32 is a protein called uL16 (60S ribosomal protein L10).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
32	g	209	3397	1058	1726	329	273	11	0	0

- Molecule 33 is a protein called uL18 (60S ribosomal protein L5).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
33	h	288	4715	1481	2374	426	429	5	0	0

- Molecule 34 is a protein called uL22 (60S ribosomal protein L17).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
34	j	154	2515	775	1270	246	219	5	0	0

- Molecule 35 is a protein called uL23 (60S ribosomal protein L23a).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
35	k	117	1980	609	1030	170	169	2	0	0

- Molecule 36 is a protein called uL24 (60S ribosomal protein L26).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
36	m	126	2124	634	1103	209	175	3	0	0

- Molecule 37 is a protein called uL29 (60S ribosomal protein L35).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
37	n	122	2140	642	1141	191	165	1	0	0

- Molecule 38 is a protein called uL2 (60S ribosomal protein L8).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
38	o	245	3791	1174	1911	381	315	10	0	0

- Molecule 39 is a protein called uL30 (60S ribosomal protein L7).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
39	q	238	4016	1256	2058	359	339	4	0	0

- Molecule 40 is a protein called uL3 (60S ribosomal protein L3).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
40	r	386	6327	1981	3223	578	530	15	0	0

- Molecule 41 is a protein called uL4 (60S ribosomal protein L4).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
41	s	398	6324	1956	3227	583	548	10	0	0

- Molecule 42 is a protein called uL5 (60S ribosomal protein L11).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
42	t	172	2836	882	1444	259	244	7	0	0

- Molecule 43 is a protein called uL6 (60S ribosomal protein L9).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
43	u	191	3124	963	1604	276	276	5	0	0

- Molecule 44 is a protein called nascent chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
44	l	4	29	12	9	4	4	0	0

- Molecule 45 is a RNA chain called 25S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
45	A	3196	103169	30602	34651	12456	22264	3196	0	0

- Molecule 46 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
46	B	163	5243	1555	1763	627	1135	163	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	85	U	C	conflict	GB 1782605526

- Molecule 47 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
47	C	4	4	4	0
47	V	1	1	1	0
47	e	1	1	1	0
47	j	1	1	1	0

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Mol	Chain	Residues	Atoms	AltConf
47	q	1	Total Mg 1 1	0
47	r	2	Total Mg 2 2	0
47	A	50	Total Mg 50 50	0

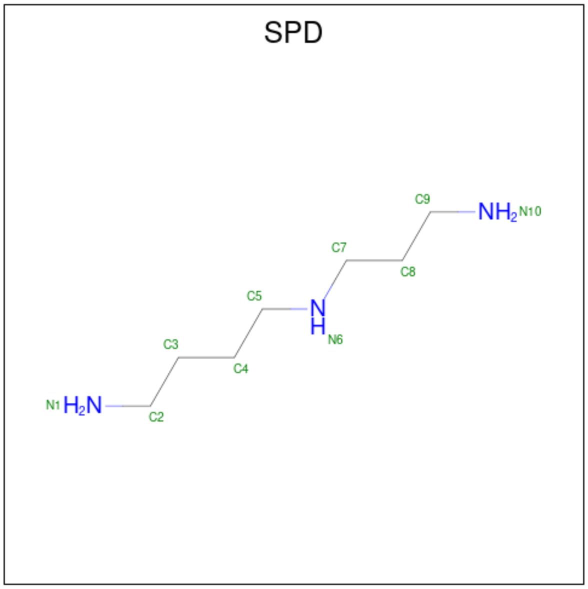
- Molecule 48 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
48	D	1	Total K 1 1	0
48	R	1	Total K 1 1	0
48	T	1	Total K 1 1	0
48	Z	1	Total K 1 1	0
48	f	1	Total K 1 1	0
48	g	1	Total K 1 1	0
48	o	2	Total K 2 2	0
48	r	1	Total K 1 1	0
48	A	83	Total K 83 83	0
48	B	2	Total K 2 2	0

- Molecule 49 is ZINC ION (three-letter code: ZN) (formula: Zn).

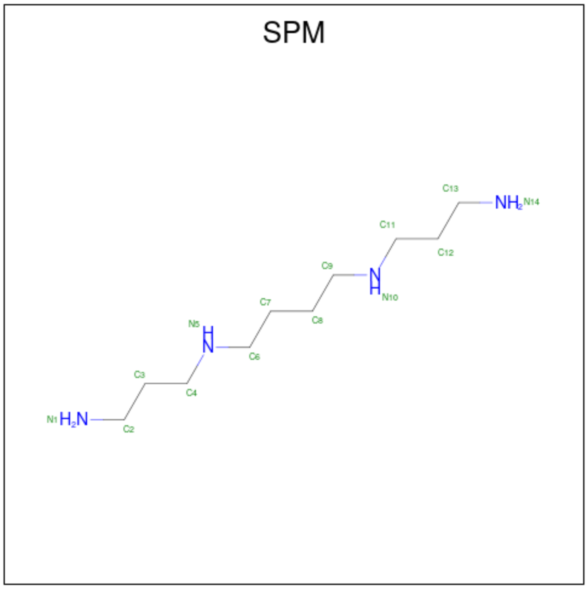
Mol	Chain	Residues	Atoms	AltConf
49	V	1	Total Zn 1 1	0
49	Y	1	Total Zn 1 1	0
49	Z	1	Total Zn 1 1	0
49	a	1	Total Zn 1 1	0

- Molecule 50 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).



Mol	Chain	Residues	Atoms	AltConf
50	A	1	Total C N 10 7 3	0

- Molecule 51 is SPERMINE (three-letter code: SPM) (formula: $C_{10}H_{26}N_4$).



Mol	Chain	Residues	Atoms	AltConf
51	A	1	Total C H N 40 10 26 4	0
51	A	1	Total C H N 40 10 26 4	0

- Molecule 52 is water.

Mol	Chain	Residues	Atoms	AltConf
52	C	88	Total O 88 88	0
52	D	47	Total O 47 47	0
52	F	105	Total O 105 105	0
52	G	53	Total O 53 53	0
52	H	11	Total O 11 11	0
52	I	13	Total O 13 13	0
52	J	27	Total O 27 27	0
52	M	2	Total O 2 2	0
52	N	8	Total O 8 8	0
52	O	26	Total O 26 26	0
52	Q	3	Total O 3 3	0
52	R	42	Total O 42 42	0
52	S	5	Total O 5 5	0
52	T	12	Total O 12 12	0
52	U	3	Total O 3 3	0
52	V	30	Total O 30 30	0
52	W	1	Total O 1 1	0
52	X	6	Total O 6 6	0
52	Y	2	Total O 2 2	0
52	Z	25	Total O 25 25	0
52	a	6	Total O 6 6	0

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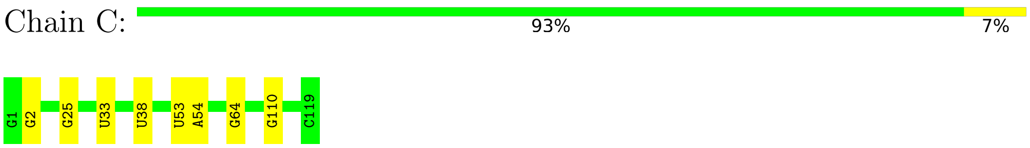
Mol	Chain	Residues	Atoms	AltConf
52	b	1	Total O 1 1	0
52	c	10	Total O 10 10	0
52	d	12	Total O 12 12	0
52	e	13	Total O 13 13	0
52	f	41	Total O 41 41	0
52	g	16	Total O 16 16	0
52	h	19	Total O 19 19	0
52	j	15	Total O 15 15	0
52	k	16	Total O 16 16	0
52	m	8	Total O 8 8	0
52	n	17	Total O 17 17	0
52	o	56	Total O 56 56	0
52	q	27	Total O 27 27	0
52	r	27	Total O 27 27	0
52	s	66	Total O 66 66	0
52	t	1	Total O 1 1	0
52	u	2	Total O 2 2	0
52	A	3376	Total O 3376 3376	0
52	B	168	Total O 168 168	0

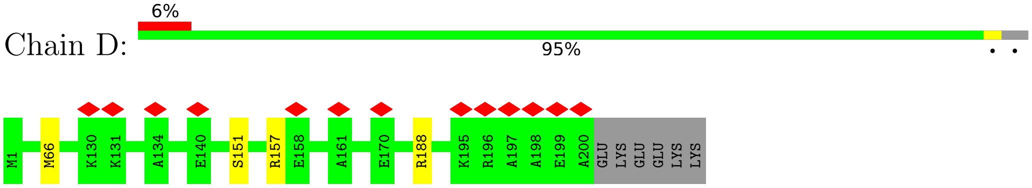
3 Residue-property plots ⓘ

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

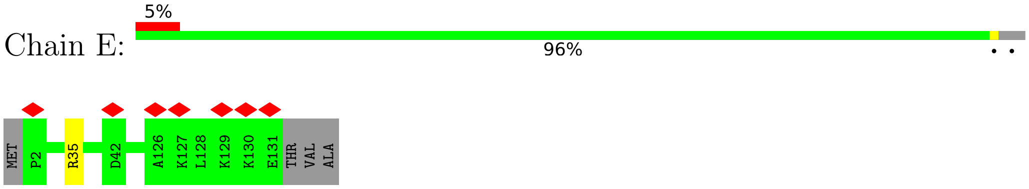
- Molecule 1: 5S rRNA



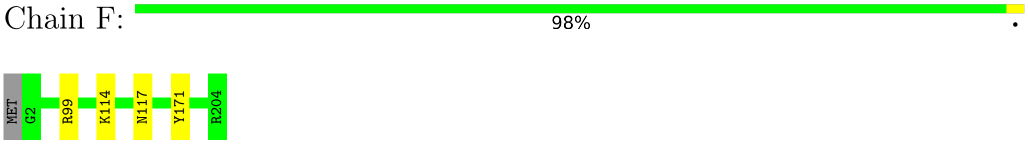
- Molecule 2: eL13 (60S ribosomal protein L13)



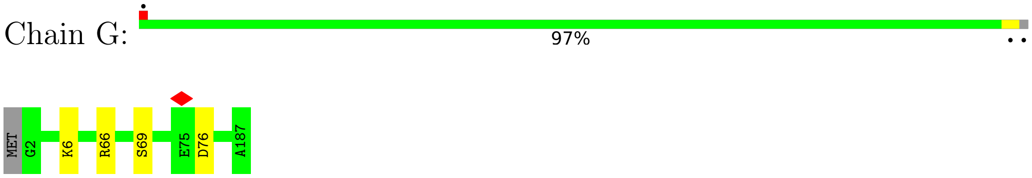
- Molecule 3: eL14 (60S ribosomal protein L14)



- Molecule 4: eL15 (60S ribosomal protein L15)

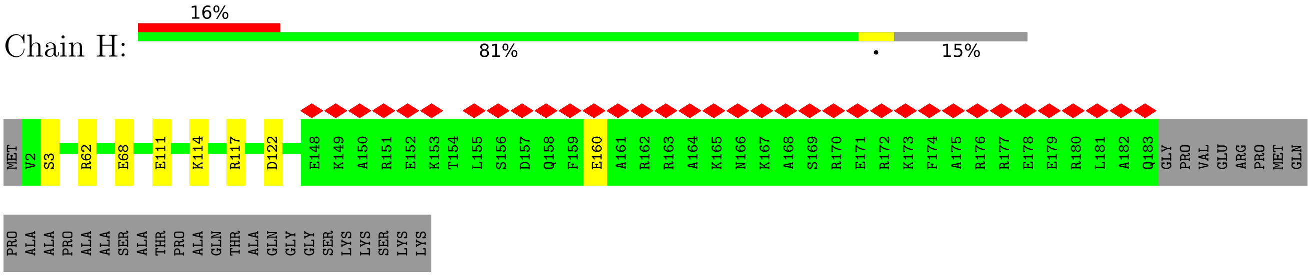


- Molecule 5: eL18 (60S ribosomal protein L18)



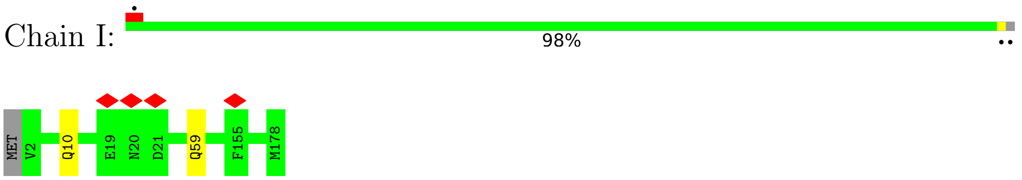
- Molecule 6: eL19 (60S ribosomal protein L19)

Chain H:



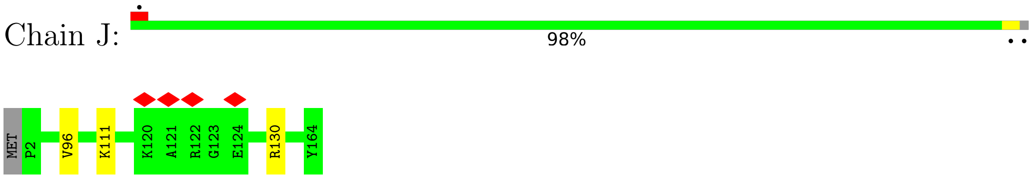
- Molecule 7: eL20 (60S ribosomal protein L18a)

Chain I:



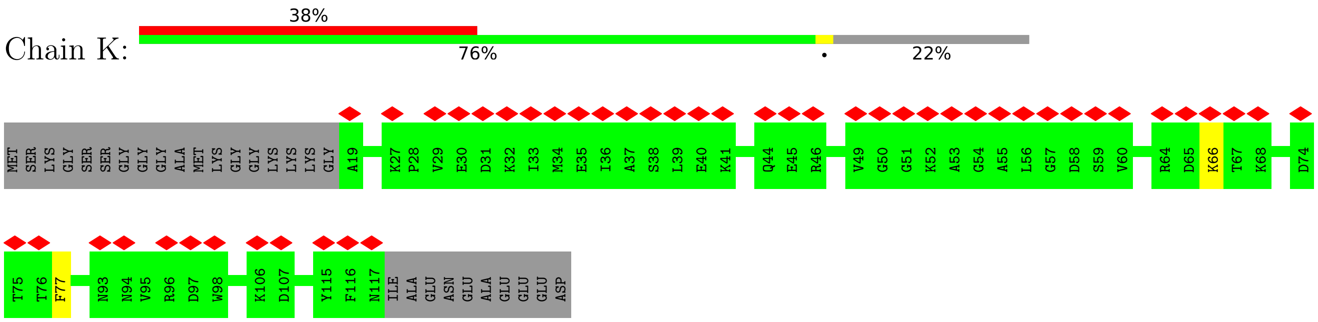
- Molecule 8: eL21 (60S ribosomal protein L21)

Chain J:



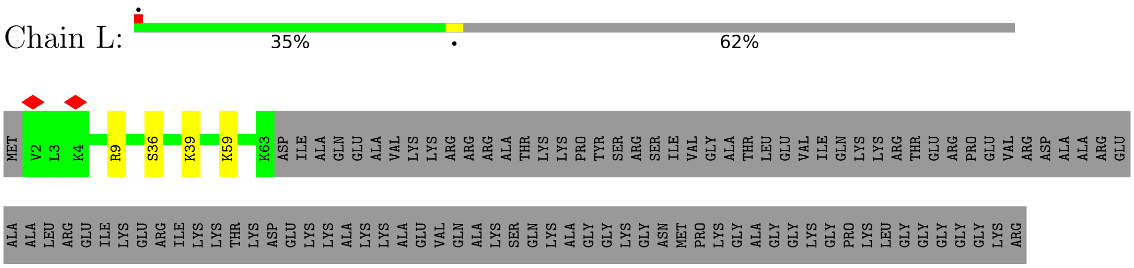
- Molecule 9: eL22 (60S ribosomal protein L22)

Chain K:



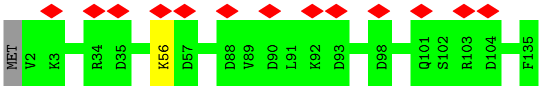
- Molecule 10: eL24 (60S ribosomal protein L24)

Chain L:



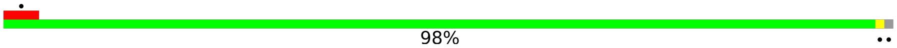
- Molecule 11: eL27 (60S ribosomal protein L27)

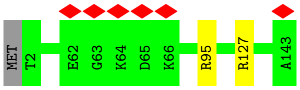
Chain M:



- Molecule 12: eL28 (60S ribosomal protein L28)

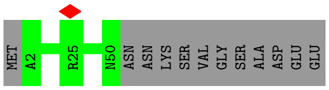
Chain N:





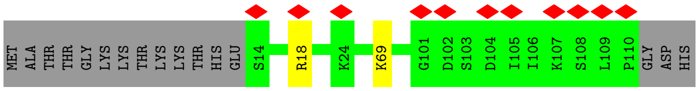
- Molecule 13: eL29 (60S ribosomal protein L29)

Chain O:



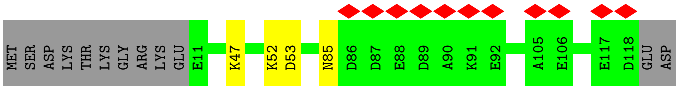
- Molecule 14: eL30 (60S ribosomal protein L30)

Chain P:



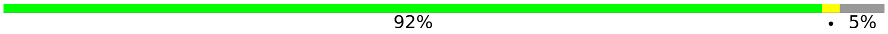
- Molecule 15: eL31 (60S ribosomal protein L31)

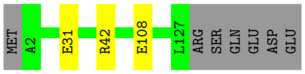
Chain Q:



- Molecule 16: eL32 (60S ribosomal protein L32)

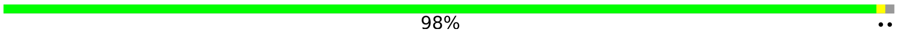
Chain R:

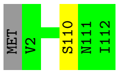




- Molecule 17: eL33 (60S ribosomal protein L35a)

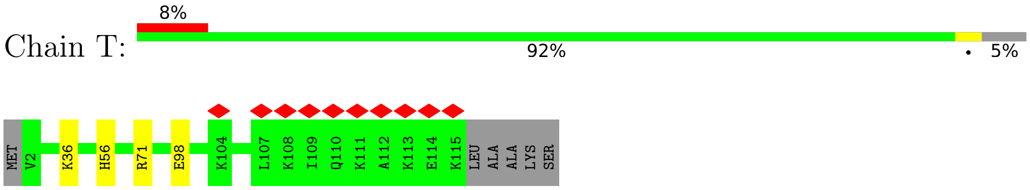
Chain S:





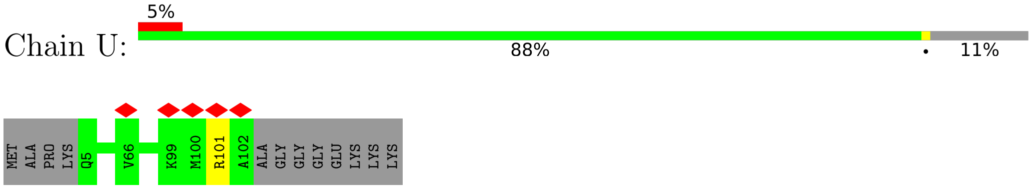
- Molecule 18: eL34 (60S ribosomal protein L34)

Chain T:



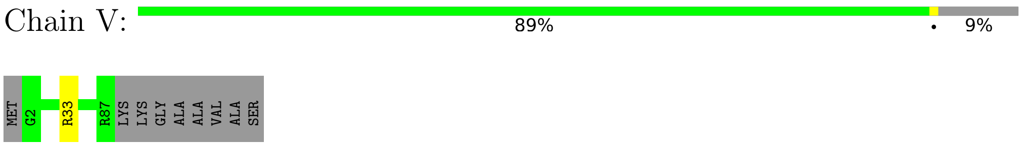
- Molecule 19: eL36 (60S ribosomal protein L36)

Chain U:



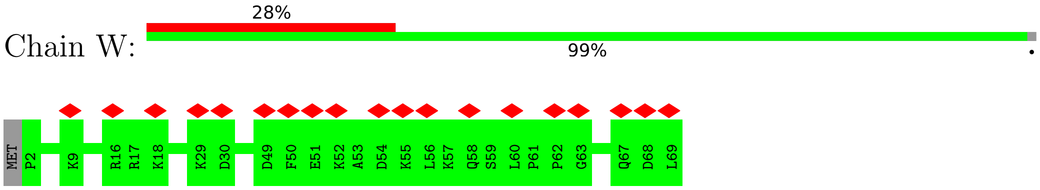
- Molecule 20: eL37 (60S ribosomal protein L37)

Chain V:



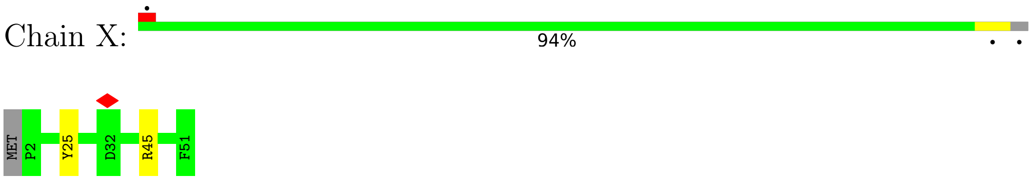
- Molecule 21: eL38 (60S ribosomal protein L38)

Chain W:



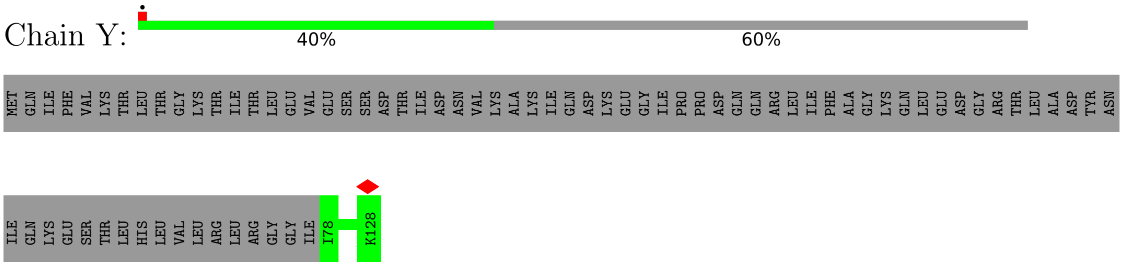
- Molecule 22: eL39 (60S ribosomal protein L39)

Chain X:



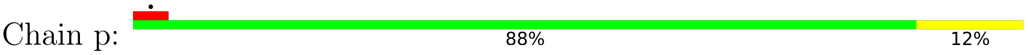
- Molecule 23: eL40 (60S ribosomal protein L40)

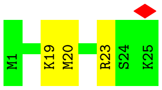
Chain Y:



- Molecule 24: eL41 (60S ribosomal protein L41)

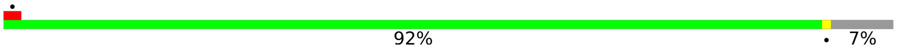
Chain p:

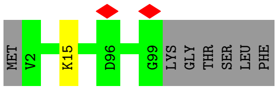




- Molecule 25: eL42 (60S ribosomal protein L42)

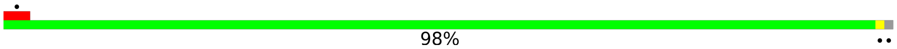
Chain Z:

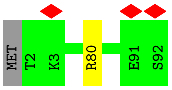




- Molecule 26: eL43 (60S ribosomal protein L37a)

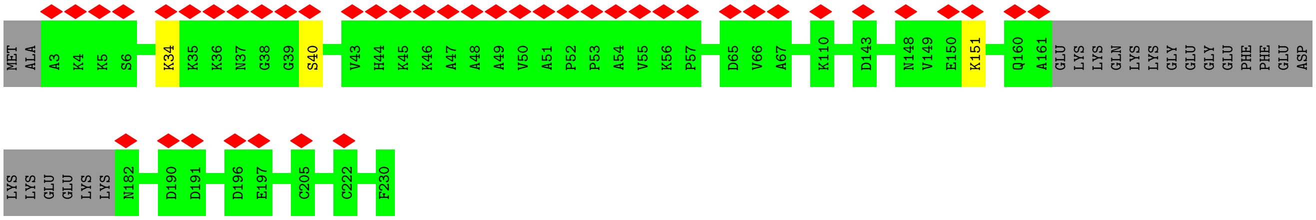
Chain a:





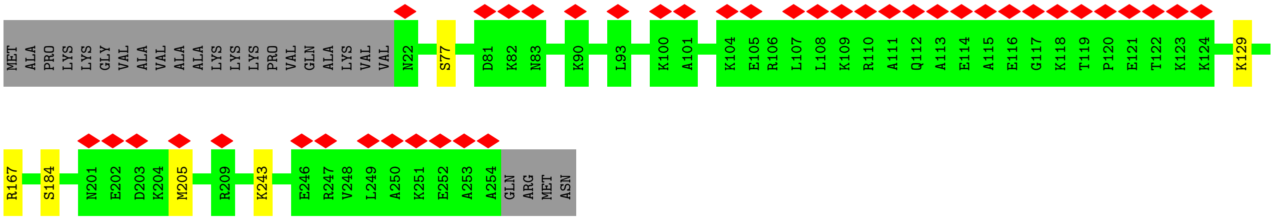
- Molecule 27: eL6 (60S ribosomal protein L6)

Chain b:



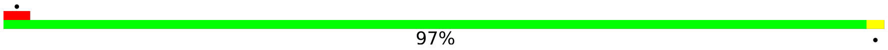
- Molecule 28: eL8 (60S ribosomal protein L7a)

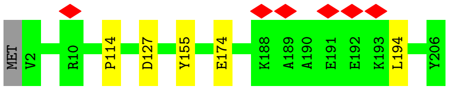
Chain c:



- Molecule 29: uL13 (60S ribosomal protein L13a)

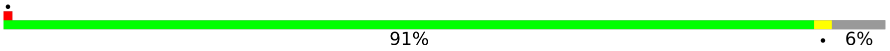
Chain d:

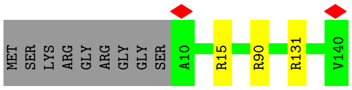




- Molecule 30: uL14 (60S ribosomal protein L23)

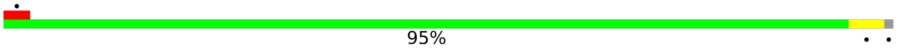
Chain e:

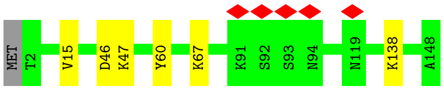




- Molecule 31: uL15 (60S ribosomal protein L27a)

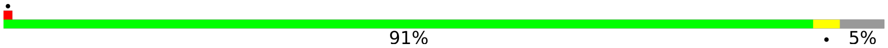
Chain f:

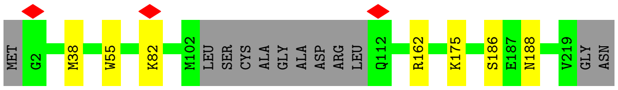




- Molecule 32: uL16 (60S ribosomal protein L10)

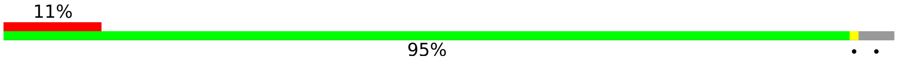
Chain g:

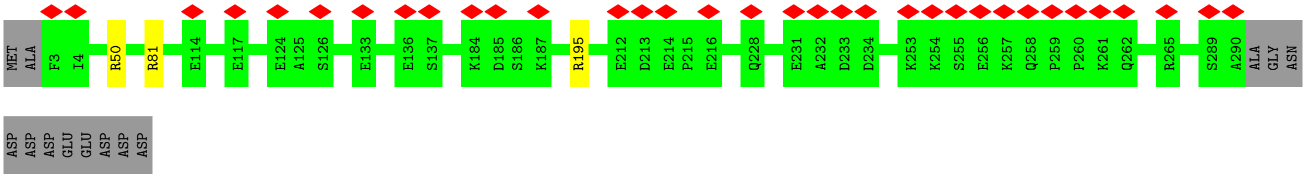




- Molecule 33: uL18 (60S ribosomal protein L5)

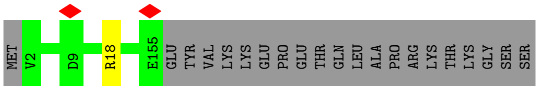
Chain h:





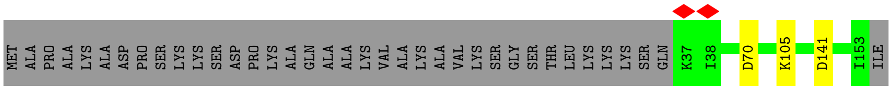
- Molecule 34: uL22 (60S ribosomal protein L17)

Chain j:



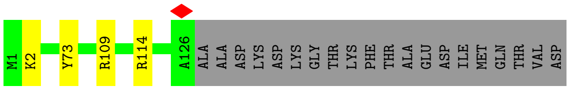
- Molecule 35: uL23 (60S ribosomal protein L23a)

Chain k:



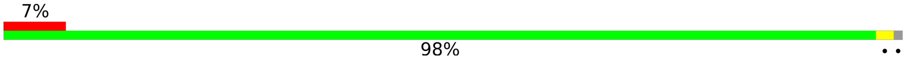
- Molecule 36: uL24 (60S ribosomal protein L26)

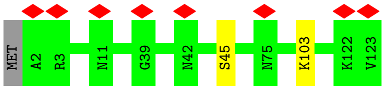
Chain m:



- Molecule 37: uL29 (60S ribosomal protein L35)

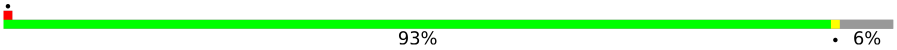
Chain n:

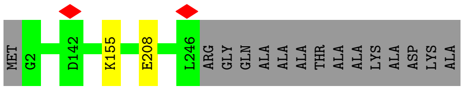




- Molecule 38: uL2 (60S ribosomal protein L8)

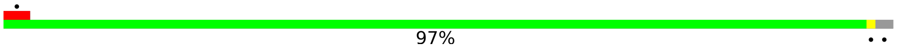
Chain o:

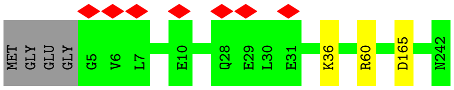




- Molecule 39: uL30 (60S ribosomal protein L7)

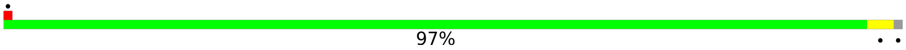
Chain q:

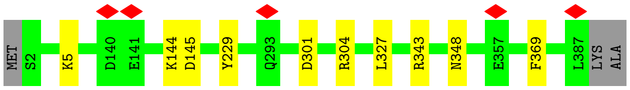




- Molecule 40: uL3 (60S ribosomal protein L3)

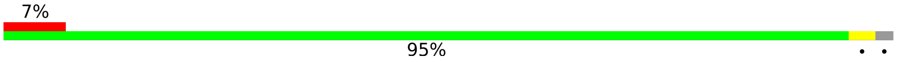
Chain r:

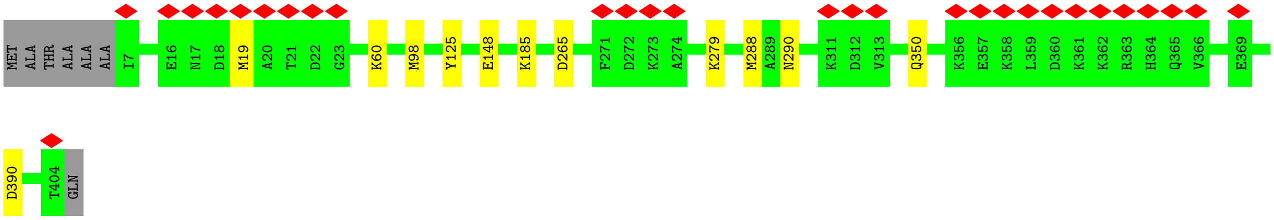




- Molecule 41: uL4 (60S ribosomal protein L4)

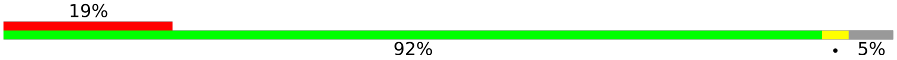
Chain s:

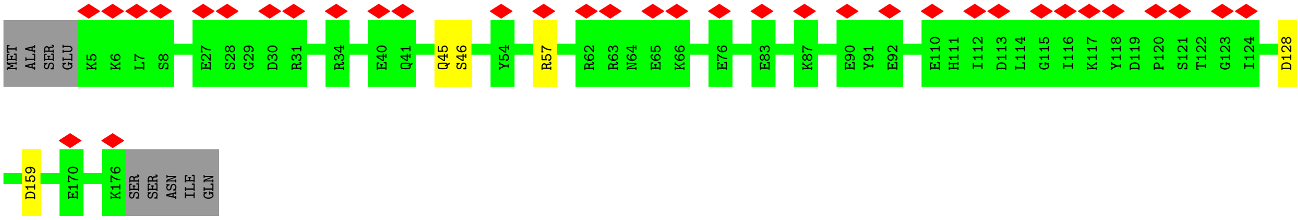




- Molecule 42: uL5 (60S ribosomal protein L11)

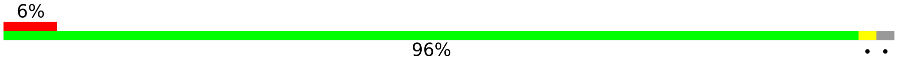
Chain t:

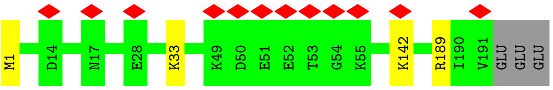




- Molecule 43: uL6 (60S ribosomal protein L9)

Chain u:



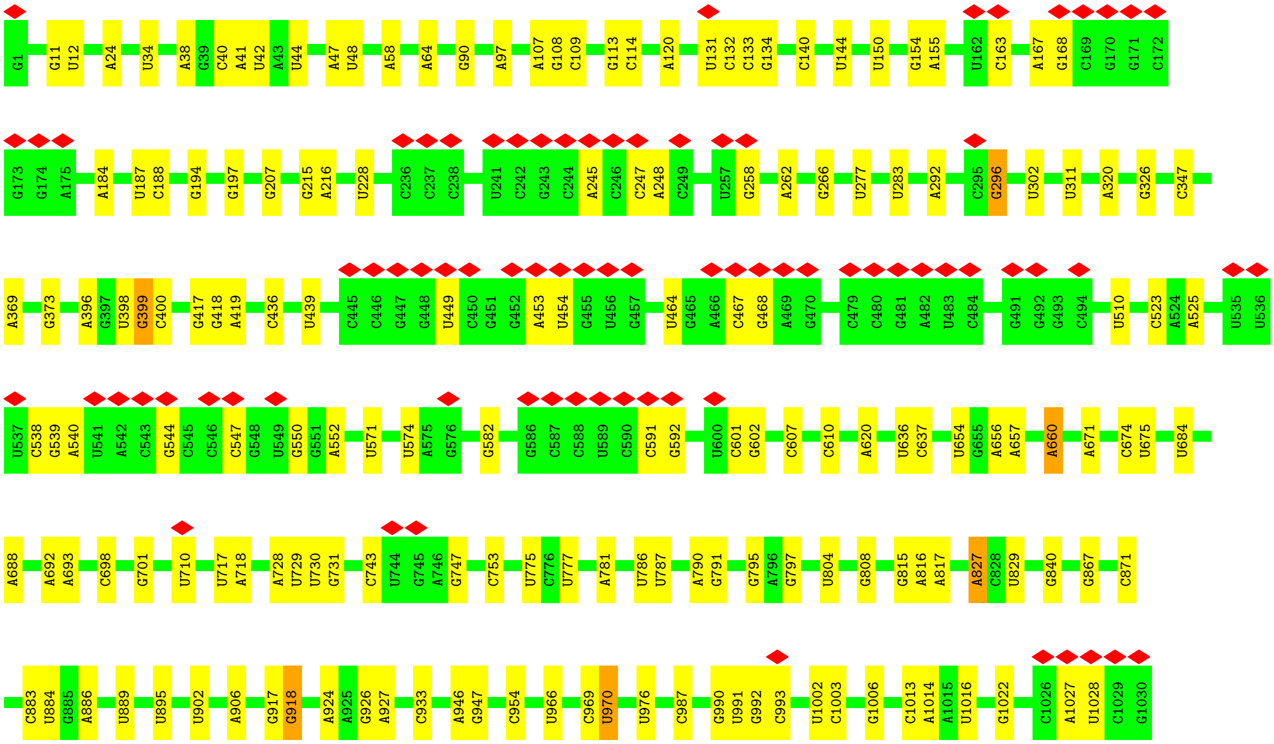


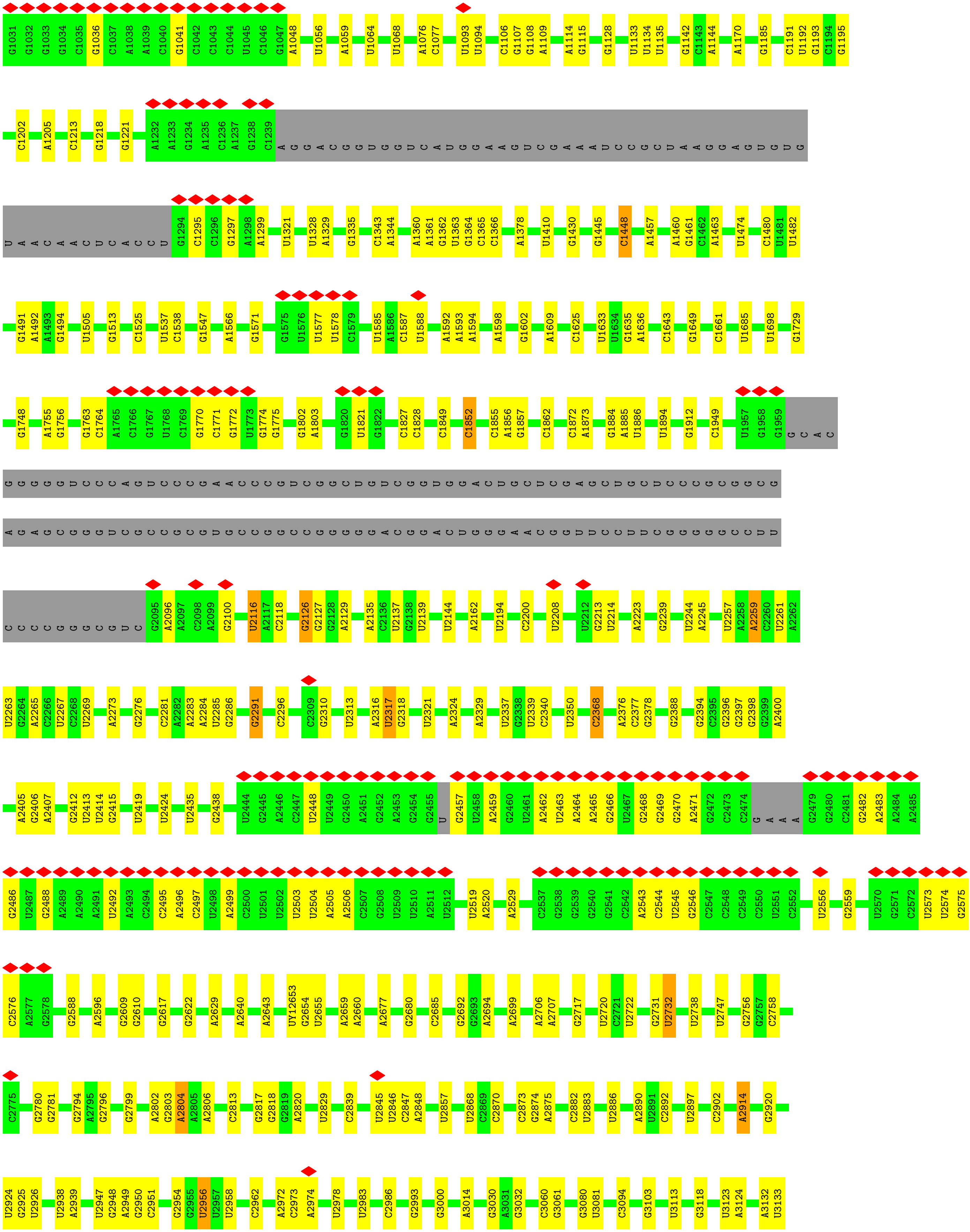
- Molecule 44: nascent chain

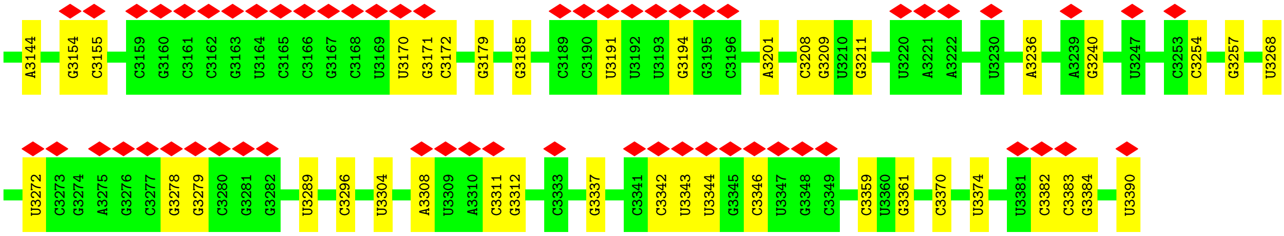
Chain l:

- Molecule 45: 25S rRNA

Chain A:

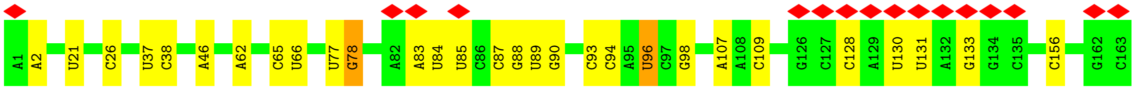



G1031 G1032 G1033 G1034 C1035 G1036 C1037 A1038 A1039 C1040 G1041 C1042 G1043 C1044 U1045 C1046 G1047 A1048 U1056 A1059 U1064 U1068 A1076 C1077 U1093 U1094 C1106 G1107 G1108 A1109 A1114 G1115 G1128 U1133 U1134 U1135 G1142 C1143 A1144 A1170 G1185 C1191 U1192 G1193 C1194 G1195
C1202 A1205 C1213 G1218 G1221 A1232 A1233 G1234 A1235 C1236 A1237 G1238 C1239 A G G A C G G U G G U C A U G G A A G U C G A A A U C C G C U A A G G A G U G U G
U A A C A A C U C A C C U G1294 C1295 C1296 G1297 A1298 A1299 U1321 U1328 A1329 G1335 C1343 A1344 A1360 A1361 G1362 U1363 G1364 C1365 C1366 A1378 U1410 G1430 G1445 C1448 A1457 A1460 G1461 C1462 A1463 U1474 C1480 U1481 U1482
G1491 A1492 A1493 G1494 U1505 G1513 C1525 U1537 C1538 G1547 A1566 G1571 G1575 U1576 U1577 U1578 C1579 U1585 A1586 C1587 U1588 A1592 A1593 A1594 A1598 G1602 A1609 C1625 U1633 U1634 G1635 A1636 C1643 G1649 C1661 U1685 U1698 G1729
G1748 A1755 G1756 G1763 C1764 A1765 C1766 G1767 U1768 C1769 G1770 C1771 G1772 U1773 G1774 G1775 G1802 A1803 G1820 U1821 G1822 C1827 C1828 C1849 C1852 C1855 A1856 G1857 C1862 C1872 A1873 G1884 A1885 U1886 U1894 G1912 C1949 U1957 G1958 G1959 G C A C
G G G G G U C C C A G U C C C G A A C C C G U C G G C U G U C G G U G G A C U G C U C G A G C U G C U C C C G C G G C G
A G A G C G G G U C G C C G C G U G C C G G C C G G G G G A C G G A C U G G G A A C G G U U C C U U C G G G G G C C U U
C C C C G G G C G U C G2095 A2096 A2097 C2098 A2099 G2100 U2116 A2117 C2118 G2126 G2127 G2128 A2129 A2135 C2136 U2137 G2138 U2139 U2144 A2162 U2194 C2200 U2208 U2212 G2213 U2214 A2223 G2239 U2244 A2245 U2257 A2258 A2259 C2260 U2261 A2262
U2263 G2264 A2265 C2266 U2267 C2268 U2269 A2273 G2276 C2281 A2282 A2283 A2284 U2285 G2286 G2291 C2296 C2309 G2310 U2313 A2316 U2317 G2318 U2321 A2324 A2329 U2337 G2338 U2339 C2340 U2350 C2368 A2376 C2377 G2378 G2388 G2394 C2395 G2396 G2397 G2398 G2399 A2400
A2405 G2406 A2407 G2412 U2413 U2414 G2415 U2419 U2424 U2435 G2438 U2444 G2445 A2446 C2447 U2448 U2449 G2450 A2451 G2452 A2453 G2454 G2455 U G2457 U2458 A2459 G2460 U2461 A2462 U2463 A2464 A2465 G2466 U2467 G2468 G2469 G2470 A2471 G2472 C2473 C2474 G A A A G2479 G2480 C2481 G2482 A2483 A2484 A2485
G2486 U2487 G2488 A2489 A2490 A2491 U2492 A2493 C2494 C2495 A2496 C2497 U2498 A2499 C2500 U2501 U2502 U2503 U2504 A2505 A2506 C2507 G2508 U2509 U2510 A2511 U2512 U2519 A2520 A2529 C2537 G2538 G2539 G2540 G2541 C2542 A2543 C2544 U2545 G2546 C2547 C2548 C2549 C2550 U2551 C2552 U2556 G2559 U2570 G2571 C2572 U2573 U2574 G2575
C2576 A2577 G2578 G2588 A2596 G2609 G2610 G2617 G2622 A2629 A2640 A2643 UY12653 G2654 U2655 A2659 A2660 A2677 G2680 C2685 G2692 G2693 A2694 A2699 A2706 A2707 G2717 U2720 C2721 U2722 G2731 U2732 U2738 U2747 G2756 G2757 C2758
C2775 G2780 G2781 G2794 A2795 G2796 G2799 A2802 G2803 A2804 A2805 A2806 C2813 G2817 G2818 G2819 A2820 U2829 C2839 U2845 U2846 C2847 A2848 U2857 U2868 C2869 C2870 C2873 G2874 A2875 G2882 U2883 U2886 A2890 U2891 C2892 U2897 C2902 A2914 G2920
U2924 G2925 U2926 U2938 A2939 U2947 G2948 A2949 G2950 C2951 G2954 G2955 U2956 U2957 U2958 C2962 A2972 C2973 A2974 U2978 U2983 C2986 G2993 G3000 A3014 G3030 A3031 G3032 C3060 G3061 G3080 U3081 C3094 G3103 U3113 G3118 U3123 A3124 A3132 U3133



- Molecule 46: 5.8S rRNA

Chain B:



4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	335291	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	27	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	15.519	Depositor
Minimum map value	-7.827	Depositor
Average map value	0.020	Depositor
Map value standard deviation	0.314	Depositor
Recommended contour level	1.05	Depositor
Map size (Å)	381.6, 381.6, 381.6	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.848, 0.848, 0.848	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 1MA, MG, UY1, K, OMU, OMC, 5MC, A2M, SPM, OMG, UR3, SPD, PSU

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	C	0.18	0/2837	0.71	0/4420
2	D	0.25	0/1635	0.55	0/2194
3	E	0.24	0/1069	0.52	0/1427
4	F	0.24	0/1740	0.59	0/2333
5	G	0.25	0/1487	0.55	0/1989
6	H	0.24	0/1548	0.57	0/2042
7	I	0.25	0/1544	0.51	0/2071
8	J	0.24	0/1331	0.54	0/1784
9	K	0.24	0/819	0.51	0/1098
10	L	0.26	0/539	0.52	0/716
11	M	0.25	0/1118	0.52	0/1492
12	N	0.24	0/1126	0.47	0/1508
13	O	0.26	0/422	0.54	0/558
14	P	0.25	0/757	0.47	0/1018
15	Q	0.25	0/885	0.55	0/1184
16	R	0.24	0/1053	0.56	0/1408
17	S	0.26	0/920	0.52	0/1232
18	T	0.25	0/939	0.58	0/1251
19	U	0.25	0/791	0.56	0/1047
20	V	0.27	0/714	0.64	0/949
21	W	0.25	0/566	0.49	0/752
22	X	0.22	0/460	0.58	0/611
23	Y	0.25	0/427	0.54	0/562
24	p	0.25	0/239	0.68	0/302
25	Z	0.25	0/801	0.48	0/1058
26	a	0.24	0/717	0.55	0/952
27	b	0.26	0/1645	0.45	0/2210
28	c	0.25	0/1912	0.49	0/2562
29	d	0.25	0/1669	0.52	0/2235
30	e	0.25	0/1001	0.54	0/1345
31	f	0.25	0/1190	0.49	0/1591
32	g	0.25	0/1707	0.54	0/2283

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	h	0.25	0/2386	0.51	0/3200
34	j	0.25	0/1270	0.56	0/1704
35	k	0.25	0/965	0.48	0/1295
36	m	0.24	0/1035	0.57	0/1383
37	n	0.24	0/1009	0.50	0/1343
38	o	0.25	0/1924	0.56	0/2585
39	q	0.27	0/1992	0.49	0/2670
40	r	0.24	0/3172	0.51	0/4249
41	s	0.24	0/3159	0.51	0/4259
42	t	0.25	0/1414	0.54	0/1890
43	u	0.25	0/1539	0.50	0/2059
45	A	0.21	5/73586 (0.0%)	0.74	9/114785 (0.0%)
46	B	0.20	0/3772	0.74	0/5878
All	All	0.23	5/132831 (0.0%)	0.67	9/195484 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	A	2972	A	O3'-P	9.05	1.72	1.61
45	A	654	U	O3'-P	7.35	1.70	1.61
45	A	1491	G	O3'-P	5.98	1.68	1.61
45	A	2973	C	O3'-P	5.31	1.67	1.61
45	A	2116	U	O3'-P	5.02	1.67	1.61

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	A	654	U	P-O3'-C3'	10.41	132.19	119.70
45	A	2972	A	P-O3'-C3'	10.05	131.76	119.70
45	A	657	A	O5'-P-OP1	-9.56	97.09	105.70
45	A	808	G	P-O3'-C3'	8.50	129.90	119.70
45	A	1491	G	P-O3'-C3'	7.67	128.91	119.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	198/206 (96%)	195 (98%)	3 (2%)	0	100	100
3	E	128/134 (96%)	127 (99%)	1 (1%)	0	100	100
4	F	201/204 (98%)	197 (98%)	4 (2%)	0	100	100
5	G	184/187 (98%)	182 (99%)	2 (1%)	0	100	100
6	H	180/214 (84%)	180 (100%)	0	0	100	100
7	I	175/178 (98%)	174 (99%)	1 (1%)	0	100	100
8	J	161/164 (98%)	158 (98%)	3 (2%)	0	100	100
9	K	97/127 (76%)	96 (99%)	1 (1%)	0	100	100
10	L	60/164 (37%)	60 (100%)	0	0	100	100
11	M	132/135 (98%)	131 (99%)	1 (1%)	0	100	100
12	N	140/143 (98%)	137 (98%)	3 (2%)	0	100	100
13	O	47/61 (77%)	44 (94%)	3 (6%)	0	100	100
14	P	95/113 (84%)	94 (99%)	1 (1%)	0	100	100
15	Q	106/120 (88%)	106 (100%)	0	0	100	100
16	R	124/133 (93%)	124 (100%)	0	0	100	100
17	S	109/112 (97%)	108 (99%)	1 (1%)	0	100	100
18	T	112/120 (93%)	112 (100%)	0	0	100	100
19	U	96/110 (87%)	96 (100%)	0	0	100	100
20	V	84/95 (88%)	83 (99%)	1 (1%)	0	100	100
21	W	66/69 (96%)	66 (100%)	0	0	100	100
22	X	48/51 (94%)	48 (100%)	0	0	100	100
23	Y	49/128 (38%)	49 (100%)	0	0	100	100
24	p	23/25 (92%)	23 (100%)	0	0	100	100
25	Z	96/105 (91%)	95 (99%)	1 (1%)	0	100	100
26	a	89/92 (97%)	85 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	b	204/230 (89%)	200 (98%)	4 (2%)	0	100	100
28	c	231/258 (90%)	229 (99%)	2 (1%)	0	100	100
29	d	203/206 (98%)	203 (100%)	0	0	100	100
30	e	129/140 (92%)	126 (98%)	3 (2%)	0	100	100
31	f	145/148 (98%)	138 (95%)	6 (4%)	1 (1%)	22	14
32	g	205/221 (93%)	202 (98%)	3 (2%)	0	100	100
33	h	286/301 (95%)	281 (98%)	5 (2%)	0	100	100
34	j	152/175 (87%)	150 (99%)	2 (1%)	0	100	100
35	k	115/154 (75%)	115 (100%)	0	0	100	100
36	m	124/146 (85%)	122 (98%)	2 (2%)	0	100	100
37	n	120/123 (98%)	117 (98%)	3 (2%)	0	100	100
38	o	243/260 (94%)	234 (96%)	9 (4%)	0	100	100
39	q	236/242 (98%)	231 (98%)	5 (2%)	0	100	100
40	r	384/389 (99%)	379 (99%)	5 (1%)	0	100	100
41	s	396/405 (98%)	391 (99%)	5 (1%)	0	100	100
42	t	170/181 (94%)	168 (99%)	2 (1%)	0	100	100
43	u	189/194 (97%)	188 (100%)	1 (0%)	0	100	100
All	All	6332/6963 (91%)	6244 (99%)	87 (1%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
31	f	15	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	165/171 (96%)	161 (98%)	4 (2%)	49	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	E	114/117 (97%)	113 (99%)	1 (1%)	78	81
4	F	176/177 (99%)	172 (98%)	4 (2%)	50	51
5	G	154/155 (99%)	150 (97%)	4 (3%)	46	45
6	H	160/182 (88%)	152 (95%)	8 (5%)	24	20
7	I	163/164 (99%)	161 (99%)	2 (1%)	71	74
8	J	140/141 (99%)	137 (98%)	3 (2%)	53	54
9	K	91/109 (84%)	89 (98%)	2 (2%)	52	53
10	L	57/133 (43%)	53 (93%)	4 (7%)	15	9
11	M	117/118 (99%)	116 (99%)	1 (1%)	78	81
12	N	123/124 (99%)	121 (98%)	2 (2%)	62	65
13	O	43/53 (81%)	43 (100%)	0	100	100
14	P	85/98 (87%)	83 (98%)	2 (2%)	49	49
15	Q	95/106 (90%)	91 (96%)	4 (4%)	30	26
16	R	114/121 (94%)	111 (97%)	3 (3%)	46	45
17	S	98/99 (99%)	97 (99%)	1 (1%)	76	79
18	T	100/104 (96%)	96 (96%)	4 (4%)	31	28
19	U	83/90 (92%)	82 (99%)	1 (1%)	71	74
20	V	72/77 (94%)	71 (99%)	1 (1%)	67	70
21	W	64/65 (98%)	64 (100%)	0	100	100
22	X	47/48 (98%)	45 (96%)	2 (4%)	29	25
23	Y	46/114 (40%)	46 (100%)	0	100	100
24	p	24/24 (100%)	21 (88%)	3 (12%)	4	1
25	Z	86/92 (94%)	85 (99%)	1 (1%)	71	74
26	a	73/74 (99%)	72 (99%)	1 (1%)	67	70
27	b	175/194 (90%)	172 (98%)	3 (2%)	60	63
28	c	202/221 (91%)	196 (97%)	6 (3%)	41	39
29	d	173/174 (99%)	168 (97%)	5 (3%)	42	40
30	e	103/109 (94%)	100 (97%)	3 (3%)	42	40
31	f	119/120 (99%)	114 (96%)	5 (4%)	30	26
32	g	173/181 (96%)	166 (96%)	7 (4%)	31	28
33	h	244/254 (96%)	241 (99%)	3 (1%)	71	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	j	135/154 (88%)	134 (99%)	1 (1%)	84	87
35	k	106/134 (79%)	103 (97%)	3 (3%)	43	42
36	m	115/131 (88%)	111 (96%)	4 (4%)	36	33
37	n	109/110 (99%)	107 (98%)	2 (2%)	59	60
38	o	190/197 (96%)	188 (99%)	2 (1%)	73	76
39	q	207/209 (99%)	204 (99%)	3 (1%)	67	70
40	r	330/332 (99%)	320 (97%)	10 (3%)	41	39
41	s	326/329 (99%)	314 (96%)	12 (4%)	34	31
42	t	149/157 (95%)	144 (97%)	5 (3%)	37	34
43	u	167/170 (98%)	163 (98%)	4 (2%)	49	49
All	All	5513/5932 (93%)	5377 (98%)	136 (2%)	50	47

5 of 136 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
41	s	19	MET
41	s	148	GLU
42	t	128	ASP
18	T	98	GLU
18	T	71	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
15	Q	85	ASN
33	h	122	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C	118/119 (99%)	8 (6%)	0
45	A	3191/3390 (94%)	415 (13%)	16 (0%)
46	B	162/163 (99%)	26 (16%)	0
All	All	3471/3672 (94%)	449 (12%)	16 (0%)

5 of 449 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C	2	G
1	C	25	G
1	C	33	U
1	C	38	U
1	C	53	U

5 of 16 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
45	A	2543	A
45	A	2503	U
45	A	1027	A
45	A	2496	A
45	A	990	G

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

135 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
45	OMU	A	2738	45	19,22,23	3.21	8 (42%)	26,31,34	1.69	5 (19%)
45	OMC	A	2951	45	19,22,23	3.24	8 (42%)	26,31,34	0.77	0
46	A2M	B	46	46	18,25,26	4.14	7 (38%)	18,36,39	3.84	4 (22%)
45	OMC	A	1849	45	19,22,23	3.26	8 (42%)	26,31,34	0.72	0
45	PSU	A	1482	45	18,21,22	4.65	8 (44%)	22,30,33	1.81	5 (22%)
45	OMG	A	296	45	18,26,27	2.84	8 (44%)	19,38,41	1.55	5 (26%)
45	A2M	A	2329	45	18,25,26	4.13	7 (38%)	18,36,39	3.78	5 (27%)
45	PSU	A	1134	45	18,21,22	4.61	8 (44%)	22,30,33	1.86	5 (22%)
45	5MC	A	2281	45	18,22,23	4.00	7 (38%)	26,32,35	1.00	2 (7%)
45	OMG	A	918	48,45	18,26,27	2.81	8 (44%)	19,38,41	1.49	4 (21%)
45	1MA	A	656	45	16,25,26	1.51	2 (12%)	18,37,40	1.09	2 (11%)
45	PSU	A	786	45	18,21,22	4.65	8 (44%)	22,30,33	1.75	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
45	OMU	A	1537	45	19,22,23	3.21	8 (42%)	26,31,34	1.61	4 (15%)
45	OMU	A	1894	45	19,22,23	3.21	8 (42%)	26,31,34	1.72	5 (19%)
45	PSU	A	829	45	18,21,22	4.63	8 (44%)	22,30,33	1.86	5 (22%)
45	PSU	A	34	45	18,21,22	4.63	8 (44%)	22,30,33	1.91	5 (22%)
45	PSU	A	2857	45	18,21,22	4.63	8 (44%)	22,30,33	1.88	5 (22%)
45	PSU	A	2978	45	18,21,22	4.64	8 (44%)	22,30,33	1.78	5 (22%)
45	OMU	A	787	45	19,22,23	3.21	8 (42%)	26,31,34	1.64	5 (19%)
45	PSU	A	277	45	18,21,22	4.61	8 (44%)	22,30,33	1.83	5 (22%)
45	PSU	A	2321	45,47	18,21,22	4.63	8 (44%)	22,30,33	1.87	5 (22%)
45	OMC	A	1852	45	19,22,23	3.30	8 (42%)	26,31,34	0.75	0
45	PSU	A	2267	45	18,21,22	4.64	8 (44%)	22,30,33	1.83	5 (22%)
45	OMG	A	2291	45	18,26,27	2.83	8 (44%)	19,38,41	1.52	4 (21%)
45	A2M	A	817	45	18,25,26	4.13	7 (38%)	18,36,39	3.79	5 (27%)
45	A2M	A	2914	45	18,25,26	4.15	7 (38%)	18,36,39	3.90	4 (22%)
45	OMU	A	2424	45	19,22,23	3.22	8 (42%)	26,31,34	1.68	5 (19%)
45	PSU	A	2137	48,45	18,21,22	4.64	8 (44%)	22,30,33	1.93	5 (22%)
45	OMC	A	2685	45	19,22,23	3.29	8 (42%)	26,31,34	0.71	0
45	OMC	A	2962	45	19,22,23	3.26	8 (42%)	26,31,34	0.74	0
45	OMU	A	3289	45	19,22,23	3.21	8 (42%)	26,31,34	1.68	4 (15%)
45	PSU	A	2435	45	18,21,22	4.64	8 (44%)	22,30,33	1.90	6 (27%)
45	OMG	A	399	45	18,26,27	2.87	8 (44%)	19,38,41	1.53	4 (21%)
45	PSU	A	1064	48,45	18,21,22	4.64	8 (44%)	22,30,33	1.85	5 (22%)
45	OMC	A	2296	45	19,22,23	3.29	8 (42%)	26,31,34	0.74	0
45	OMU	A	44	48,45	19,22,23	3.23	8 (42%)	26,31,34	1.63	4 (15%)
45	OMU	A	675	45	19,22,23	3.22	8 (42%)	26,31,34	1.68	5 (19%)
45	A2M	A	1460	45	18,25,26	4.13	7 (38%)	18,36,39	3.81	5 (27%)
45	A2M	A	827	48,45,47	18,25,26	4.18	7 (38%)	18,36,39	3.86	4 (22%)
45	PSU	A	2747	45	18,21,22	4.63	8 (44%)	22,30,33	1.78	5 (22%)
45	PSU	A	970	45	18,21,22	4.66	8 (44%)	22,30,33	1.87	6 (27%)
45	OMU	A	2413	48,45	19,22,23	3.19	8 (42%)	26,31,34	1.58	4 (15%)
45	UR3	A	2956	45	19,22,23	2.80	8 (42%)	26,32,35	1.31	2 (7%)
45	PSU	A	2257	45	18,21,22	4.66	8 (44%)	22,30,33	1.85	5 (22%)
45	A2M	A	1144	45	18,25,26	4.11	7 (38%)	18,36,39	3.87	4 (22%)
45	PSU	A	2269	45	18,21,22	4.69	8 (44%)	22,30,33	1.77	5 (22%)
45	OMU	A	2350	45	19,22,23	3.23	8 (42%)	26,31,34	1.66	5 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
45	OMC	A	40	45	19,22,23	3.26	8 (42%)	26,31,34	0.88	1 (3%)
45	PSU	A	966	45	18,21,22	4.61	8 (44%)	22,30,33	1.73	5 (22%)
45	PSU	A	510	45	18,21,22	4.65	8 (44%)	22,30,33	1.84	5 (22%)
45	OMU	A	48	45	19,22,23	3.18	8 (42%)	26,31,34	1.61	4 (15%)
45	OMG	A	2394	45	18,26,27	2.83	8 (44%)	19,38,41	1.58	5 (26%)
45	PSU	A	2883	45	18,21,22	4.64	8 (44%)	22,30,33	1.85	6 (27%)
45	PSU	A	1056	45	18,21,22	4.65	8 (44%)	22,30,33	1.84	5 (22%)
45	OMU	A	1068	45	19,22,23	3.22	8 (42%)	26,31,34	1.71	5 (19%)
45	OMC	A	1448	45	19,22,23	3.29	8 (42%)	26,31,34	0.73	0
45	OMG	A	2398	45	18,26,27	2.80	8 (44%)	19,38,41	1.60	5 (26%)
45	OMU	A	144	45	19,22,23	3.21	8 (42%)	26,31,34	1.65	4 (15%)
45	A2M	A	2129	45	18,25,26	4.16	7 (38%)	18,36,39	3.83	4 (22%)
45	UY1	A	2653	45	19,22,23	4.18	7 (36%)	22,31,34	1.84	5 (22%)
46	PSU	B	96	48,46	18,21,22	4.66	8 (44%)	22,30,33	1.76	5 (22%)
45	A2M	A	2284	45	18,25,26	4.05	7 (38%)	18,36,39	4.00	4 (22%)
45	PSU	A	2139	45	18,21,22	4.63	8 (44%)	22,30,33	1.82	5 (22%)
45	PSU	A	2947	48,45	18,21,22	4.63	9 (50%)	22,30,33	1.86	6 (27%)
45	OMC	A	674	45	19,22,23	3.24	8 (42%)	26,31,34	0.68	0
45	PSU	A	1016	48,45	18,21,22	4.66	8 (44%)	22,30,33	1.85	5 (22%)
45	OMU	A	3304	45	19,22,23	3.21	8 (42%)	26,31,34	1.65	4 (15%)
45	PSU	A	902	48,45,47	18,21,22	4.64	8 (44%)	22,30,33	1.82	5 (22%)
46	PSU	B	77	46	18,21,22	4.64	8 (44%)	22,30,33	1.86	5 (22%)
45	PSU	A	464	45	18,21,22	4.66	8 (44%)	22,30,33	1.80	6 (27%)
45	5MC	A	2873	48,45	18,22,23	4.02	7 (38%)	26,32,35	1.11	1 (3%)
45	OMG	A	2796	45	18,26,27	2.80	8 (44%)	19,38,41	1.53	5 (26%)
45	A2M	A	2804	45	18,25,26	4.10	7 (38%)	18,36,39	4.13	6 (33%)
45	OMG	A	2127	45	18,26,27	2.82	8 (44%)	19,38,41	1.64	5 (26%)
45	OMG	A	1857	45	18,26,27	2.80	8 (44%)	19,38,41	1.50	5 (26%)
45	PSU	A	2419	45	18,21,22	4.63	8 (44%)	22,30,33	1.79	5 (22%)
45	OMC	A	1862	45	19,22,23	3.25	8 (42%)	26,31,34	0.66	0
45	OMC	A	2368	45	19,22,23	3.26	8 (42%)	26,31,34	0.69	0
45	PSU	A	2868	45	18,21,22	4.64	8 (44%)	22,30,33	1.87	6 (27%)
45	PSU	A	2194	48,45	18,21,22	4.64	8 (44%)	22,30,33	1.81	5 (22%)
45	PSU	A	42	48,45	18,21,22	4.63	8 (44%)	22,30,33	1.82	5 (22%)
45	A2M	A	2643	45	18,25,26	4.12	7 (38%)	18,36,39	3.74	4 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
45	PSU	A	150	48,45	18,21,22	4.64	8 (44%)	22,30,33	1.87	5 (22%)
45	PSU	A	895	45	18,21,22	4.61	8 (44%)	22,30,33	1.79	5 (22%)
45	OMG	A	1461	45	18,26,27	2.80	8 (44%)	19,38,41	1.53	4 (21%)
45	PSU	A	2261	45	18,21,22	4.66	8 (44%)	22,30,33	1.81	5 (22%)
45	OMU	A	2886	45	19,22,23	3.22	8 (42%)	26,31,34	1.64	4 (15%)
45	PSU	A	2958	45	18,21,22	4.66	8 (44%)	22,30,33	1.83	5 (22%)
45	PSU	A	2926	48,45	18,21,22	4.64	8 (44%)	22,30,33	1.88	5 (22%)
45	A2M	A	2324	45	18,25,26	4.09	7 (38%)	18,36,39	3.82	4 (22%)
45	PSU	A	228	45	18,21,22	4.66	8 (44%)	22,30,33	1.84	5 (22%)
45	PSU	A	684	45	18,21,22	4.63	8 (44%)	22,30,33	1.80	5 (22%)
45	PSU	A	1135	45	18,21,22	4.65	8 (44%)	22,30,33	1.86	5 (22%)
45	PSU	A	976	48,45	18,21,22	4.66	8 (44%)	22,30,33	1.82	5 (22%)
46	PSU	B	21	45,46	18,21,22	4.60	8 (44%)	22,30,33	1.83	5 (22%)
45	A2M	A	2259	45	18,25,26	4.17	7 (38%)	18,36,39	3.89	4 (22%)
45	OMG	A	2920	45	18,26,27	2.81	8 (44%)	19,38,41	1.54	5 (26%)
45	OMC	A	1480	45	19,22,23	3.30	8 (42%)	26,31,34	0.71	0
45	PSU	A	3113	45	18,21,22	4.62	8 (44%)	22,30,33	1.75	5 (22%)
45	PSU	A	1685	45	18,21,22	4.66	8 (44%)	22,30,33	1.88	6 (27%)
45	PSU	A	2829	45	18,21,22	4.62	8 (44%)	22,30,33	1.86	6 (27%)
45	OMG	A	2794	45	18,26,27	2.79	8 (44%)	19,38,41	1.47	4 (21%)
45	A2M	A	886	45	18,25,26	4.14	7 (38%)	18,36,39	3.75	6 (33%)
45	OMG	A	2126	45	18,26,27	2.81	8 (44%)	19,38,41	1.56	5 (26%)
45	PSU	A	1133	45	18,21,22	4.66	8 (44%)	22,30,33	1.82	5 (22%)
45	PSU	A	717	45	18,21,22	4.65	8 (44%)	22,30,33	1.83	5 (22%)
45	PSU	A	2317	48,45	18,21,22	4.66	8 (44%)	22,30,33	1.90	5 (22%)
45	OMC	A	2200	48,45	19,22,23	3.29	8 (42%)	26,31,34	0.79	0
45	PSU	A	2214	45	18,21,22	4.64	8 (44%)	22,30,33	1.84	6 (27%)
45	A2M	A	946	45	18,25,26	4.12	8 (44%)	18,36,39	4.01	7 (38%)
45	OMU	A	2720	45	19,22,23	3.21	8 (42%)	26,31,34	1.67	5 (19%)
45	A2M	A	660	45	18,25,26	4.13	7 (38%)	18,36,39	3.99	6 (33%)
45	A2M	A	1378	45	18,25,26	4.13	7 (38%)	18,36,39	3.72	4 (22%)
45	OMG	A	2239	45	18,26,27	2.84	8 (44%)	19,38,41	1.52	4 (21%)
45	OMG	A	815	45	18,26,27	2.83	8 (44%)	19,38,41	1.54	5 (26%)
45	PSU	A	1002	45	18,21,22	4.67	8 (44%)	22,30,33	1.85	6 (27%)
45	A2M	A	2949	45	18,25,26	4.14	7 (38%)	18,36,39	3.78	4 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
45	A2M	A	369	45	18,25,26	4.12	7 (38%)	18,36,39	3.84	5 (27%)
45	OMU	A	2732	45	19,22,23	3.19	8 (42%)	26,31,34	1.62	4 (15%)
45	OMG	A	2412	48,45	18,26,27	2.83	8 (44%)	19,38,41	1.58	5 (26%)
45	PSU	A	2263	45	18,21,22	4.66	8 (44%)	22,30,33	1.84	6 (27%)
45	OMG	A	2622	45	18,26,27	2.83	8 (44%)	19,38,41	1.52	4 (21%)
46	OMG	B	78	46	18,26,27	2.81	8 (44%)	19,38,41	1.52	5 (26%)
45	OMC	A	2340	45	19,22,23	3.26	8 (42%)	26,31,34	0.68	0
45	OMG	A	2925	45	18,26,27	2.81	8 (44%)	19,38,41	1.51	4 (21%)
45	OMG	A	2654	45	18,26,27	2.79	8 (44%)	19,38,41	1.67	6 (31%)
45	OMC	A	2882	45	19,22,23	3.27	8 (42%)	26,31,34	0.75	0
45	OMU	A	2924	48,45	19,22,23	3.21	8 (42%)	26,31,34	1.68	5 (19%)
45	A2M	A	2223	45	18,25,26	4.16	7 (38%)	18,36,39	3.78	4 (22%)
45	PSU	A	2897	45	18,21,22	4.65	8 (44%)	22,30,33	1.79	5 (22%)
45	PSU	A	311	48,45	18,21,22	4.66	8 (44%)	22,30,33	1.76	5 (22%)
45	OMG	A	2818	45	18,26,27	2.79	8 (44%)	19,38,41	1.57	5 (26%)
45	OMU	A	804	45	19,22,23	3.20	8 (42%)	26,31,34	1.67	5 (19%)
45	OMC	A	2839	45	19,22,23	3.29	8 (42%)	26,31,34	0.76	0
45	PSU	A	1474	45	18,21,22	4.63	8 (44%)	22,30,33	1.81	6 (27%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	OMU	A	2738	45	-	0/9/27/28	0/2/2/2
45	OMC	A	2951	45	-	0/9/27/28	0/2/2/2
46	A2M	B	46	46	-	0/5/27/28	0/3/3/3
45	OMC	A	1849	45	-	0/9/27/28	0/2/2/2
45	PSU	A	1482	45	-	0/7/25/26	0/2/2/2
45	OMG	A	296	45	-	2/5/27/28	0/3/3/3
45	A2M	A	2329	45	-	0/5/27/28	0/3/3/3
45	PSU	A	1134	45	-	0/7/25/26	0/2/2/2
45	5MC	A	2281	45	-	0/7/25/26	0/2/2/2
45	OMG	A	918	48,45	-	2/5/27/28	0/3/3/3
45	1MA	A	656	45	-	0/3/25/26	0/3/3/3
45	PSU	A	786	45	-	1/7/25/26	0/2/2/2
45	OMU	A	1537	45	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	OMU	A	1894	45	-	0/9/27/28	0/2/2/2
45	PSU	A	829	45	-	0/7/25/26	0/2/2/2
45	PSU	A	34	45	-	0/7/25/26	0/2/2/2
45	PSU	A	2857	45	-	0/7/25/26	0/2/2/2
45	PSU	A	2978	45	-	0/7/25/26	0/2/2/2
45	OMU	A	787	45	-	0/9/27/28	0/2/2/2
45	PSU	A	277	45	-	0/7/25/26	0/2/2/2
45	PSU	A	2321	45,47	-	2/7/25/26	0/2/2/2
45	OMC	A	1852	45	-	0/9/27/28	0/2/2/2
45	PSU	A	2267	45	-	0/7/25/26	0/2/2/2
45	OMG	A	2291	45	-	2/5/27/28	0/3/3/3
45	A2M	A	817	45	-	0/5/27/28	0/3/3/3
45	A2M	A	2914	45	-	2/5/27/28	0/3/3/3
45	OMU	A	2424	45	-	0/9/27/28	0/2/2/2
45	PSU	A	2137	48,45	-	0/7/25/26	0/2/2/2
45	OMC	A	2685	45	-	0/9/27/28	0/2/2/2
45	OMC	A	2962	45	-	0/9/27/28	0/2/2/2
45	OMU	A	3289	45	-	0/9/27/28	0/2/2/2
45	PSU	A	2435	45	-	0/7/25/26	0/2/2/2
45	OMG	A	399	45	-	2/5/27/28	0/3/3/3
45	PSU	A	1064	48,45	-	0/7/25/26	0/2/2/2
45	OMC	A	2296	45	-	0/9/27/28	0/2/2/2
45	OMU	A	44	48,45	-	0/9/27/28	0/2/2/2
45	OMU	A	675	45	-	0/9/27/28	0/2/2/2
45	A2M	A	1460	45	-	0/5/27/28	0/3/3/3
45	A2M	A	827	48,45,47	-	3/5/27/28	0/3/3/3
45	PSU	A	2747	45	-	0/7/25/26	0/2/2/2
45	PSU	A	970	45	-	1/7/25/26	0/2/2/2
45	OMU	A	2413	48,45	-	2/9/27/28	0/2/2/2
45	UR3	A	2956	45	-	2/7/25/26	0/2/2/2
45	PSU	A	2257	45	-	0/7/25/26	0/2/2/2
45	A2M	A	1144	45	-	0/5/27/28	0/3/3/3
45	PSU	A	2269	45	-	2/7/25/26	0/2/2/2
45	OMU	A	2350	45	-	0/9/27/28	0/2/2/2
45	OMC	A	40	45	-	1/9/27/28	0/2/2/2
45	PSU	A	966	45	-	0/7/25/26	0/2/2/2
45	PSU	A	510	45	-	0/7/25/26	0/2/2/2
45	OMU	A	48	45	-	0/9/27/28	0/2/2/2
45	OMG	A	2394	45	-	0/5/27/28	0/3/3/3
45	PSU	A	2883	45	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	PSU	A	1056	45	-	0/7/25/26	0/2/2/2
45	OMU	A	1068	45	-	0/9/27/28	0/2/2/2
45	OMC	A	1448	45	-	3/9/27/28	0/2/2/2
45	OMG	A	2398	45	-	0/5/27/28	0/3/3/3
45	OMU	A	144	45	-	1/9/27/28	0/2/2/2
45	A2M	A	2129	45	-	0/5/27/28	0/3/3/3
45	UY1	A	2653	45	-	0/9/27/28	0/2/2/2
46	PSU	B	96	48,46	-	2/7/25/26	0/2/2/2
45	A2M	A	2284	45	-	2/5/27/28	0/3/3/3
45	PSU	A	2139	45	-	0/7/25/26	0/2/2/2
45	PSU	A	2947	48,45	-	2/7/25/26	0/2/2/2
45	OMC	A	674	45	-	0/9/27/28	0/2/2/2
45	PSU	A	1016	48,45	-	0/7/25/26	0/2/2/2
45	OMU	A	3304	45	-	0/9/27/28	0/2/2/2
45	PSU	A	902	48,45,47	-	0/7/25/26	0/2/2/2
46	PSU	B	77	46	-	0/7/25/26	0/2/2/2
45	PSU	A	464	45	-	0/7/25/26	0/2/2/2
45	5MC	A	2873	48,45	-	4/7/25/26	0/2/2/2
45	OMG	A	2796	45	-	0/5/27/28	0/3/3/3
45	A2M	A	2804	45	-	2/5/27/28	0/3/3/3
45	OMG	A	2127	45	-	0/5/27/28	0/3/3/3
45	OMG	A	1857	45	-	0/5/27/28	0/3/3/3
45	PSU	A	2419	45	-	0/7/25/26	0/2/2/2
45	OMC	A	1862	45	-	0/9/27/28	0/2/2/2
45	OMC	A	2368	45	-	2/9/27/28	0/2/2/2
45	PSU	A	2868	45	-	0/7/25/26	0/2/2/2
45	PSU	A	2194	48,45	-	0/7/25/26	0/2/2/2
45	PSU	A	42	48,45	-	0/7/25/26	0/2/2/2
45	A2M	A	2643	45	-	0/5/27/28	0/3/3/3
45	PSU	A	150	48,45	-	0/7/25/26	0/2/2/2
45	PSU	A	895	45	-	0/7/25/26	0/2/2/2
45	OMG	A	1461	45	-	1/5/27/28	0/3/3/3
45	PSU	A	2261	45	-	1/7/25/26	0/2/2/2
45	OMU	A	2886	45	-	0/9/27/28	0/2/2/2
45	PSU	A	2958	45	-	0/7/25/26	0/2/2/2
45	PSU	A	2926	48,45	-	3/7/25/26	0/2/2/2
45	A2M	A	2324	45	-	0/5/27/28	0/3/3/3
45	PSU	A	228	45	-	2/7/25/26	0/2/2/2
45	PSU	A	684	45	-	0/7/25/26	0/2/2/2
45	PSU	A	1135	45	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	PSU	A	976	48,45	-	0/7/25/26	0/2/2/2
46	PSU	B	21	45,46	-	0/7/25/26	0/2/2/2
45	A2M	A	2259	45	-	2/5/27/28	0/3/3/3
45	OMG	A	2920	45	-	0/5/27/28	0/3/3/3
45	OMC	A	1480	45	-	0/9/27/28	0/2/2/2
45	PSU	A	3113	45	-	0/7/25/26	0/2/2/2
45	PSU	A	1685	45	-	0/7/25/26	0/2/2/2
45	PSU	A	2829	45	-	0/7/25/26	0/2/2/2
45	OMG	A	2794	45	-	0/5/27/28	0/3/3/3
45	A2M	A	886	45	-	0/5/27/28	0/3/3/3
45	OMG	A	2126	45	-	0/5/27/28	0/3/3/3
45	PSU	A	1133	45	-	0/7/25/26	0/2/2/2
45	PSU	A	717	45	-	0/7/25/26	0/2/2/2
45	PSU	A	2317	48,45	-	3/7/25/26	0/2/2/2
45	OMC	A	2200	48,45	-	4/9/27/28	0/2/2/2
45	PSU	A	2214	45	-	0/7/25/26	0/2/2/2
45	A2M	A	946	45	-	0/5/27/28	0/3/3/3
45	OMU	A	2720	45	-	0/9/27/28	0/2/2/2
45	A2M	A	660	45	-	2/5/27/28	0/3/3/3
45	A2M	A	1378	45	-	2/5/27/28	0/3/3/3
45	OMG	A	2239	45	-	0/5/27/28	0/3/3/3
45	OMG	A	815	45	-	0/5/27/28	0/3/3/3
45	PSU	A	1002	45	-	2/7/25/26	0/2/2/2
45	A2M	A	2949	45	-	0/5/27/28	0/3/3/3
45	A2M	A	369	45	-	1/5/27/28	0/3/3/3
45	OMU	A	2732	45	-	0/9/27/28	0/2/2/2
45	OMG	A	2412	48,45	-	1/5/27/28	0/3/3/3
45	PSU	A	2263	45	-	0/7/25/26	0/2/2/2
45	OMG	A	2622	45	-	0/5/27/28	0/3/3/3
46	OMG	B	78	46	-	2/5/27/28	0/3/3/3
45	OMC	A	2340	45	-	0/9/27/28	0/2/2/2
45	OMG	A	2925	45	-	0/5/27/28	0/3/3/3
45	OMG	A	2654	45	-	0/5/27/28	0/3/3/3
45	OMC	A	2882	45	-	0/9/27/28	0/2/2/2
45	OMU	A	2924	48,45	-	0/9/27/28	0/2/2/2
45	A2M	A	2223	45	-	0/5/27/28	0/3/3/3
45	PSU	A	2897	45	-	0/7/25/26	0/2/2/2
45	PSU	A	311	48,45	-	0/7/25/26	0/2/2/2
45	OMG	A	2818	45	-	0/5/27/28	0/3/3/3
45	OMU	A	804	45	-	0/9/27/28	0/2/2/2
45	OMC	A	2839	45	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	PSU	A	1474	45	-	0/7/25/26	0/2/2/2

The worst 5 of 1053 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	A	2269	PSU	C6-C5	12.27	1.49	1.35
45	A	1002	PSU	C6-C5	12.24	1.49	1.35
45	A	2317	PSU	C6-C5	12.23	1.49	1.35
45	A	311	PSU	C6-C5	12.21	1.49	1.35
45	A	2137	PSU	C6-C5	12.21	1.49	1.35

The worst 5 of 572 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	A	946	A2M	C5-C6-N6	10.90	136.92	120.35
45	A	2284	A2M	C5-C6-N6	10.82	136.80	120.35
45	A	2804	A2M	C5-C6-N6	10.80	136.77	120.35
45	A	817	A2M	C5-C6-N6	10.72	136.65	120.35
45	A	2914	A2M	C5-C6-N6	10.71	136.62	120.35

There are no chirality outliers.

5 of 68 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	B	78	OMG	O4'-C4'-C5'-O5'
46	B	78	OMG	C3'-C4'-C5'-O5'
46	B	96	PSU	C3'-C4'-C5'-O5'
46	B	96	PSU	O4'-C4'-C5'-O5'
45	A	40	OMC	C3'-C2'-O2'-CM2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 161 ligands modelled in this entry, 158 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z|>2$	Counts	RMSZ	$\#|Z|>2$
51	SPM	A	3453	-	13,13,13	0.38	0	12,12,12	1.01	0
51	SPM	A	3452	-	13,13,13	0.37	0	12,12,12	1.02	0
50	SPD	A	3451	-	9,9,9	0.32	0	8,8,8	0.51	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
51	SPM	A	3453	-	-	7/11/11/11	-
51	SPM	A	3452	-	-	5/11/11/11	-
50	SPD	A	3451	-	-	2/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
51	A	3453	SPM	N10-C11-C12-C13
51	A	3453	SPM	C7-C8-C9-N10
51	A	3453	SPM	C2-C3-C4-N5
51	A	3453	SPM	N5-C6-C7-C8
50	A	3451	SPD	C2-C3-C4-C5

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

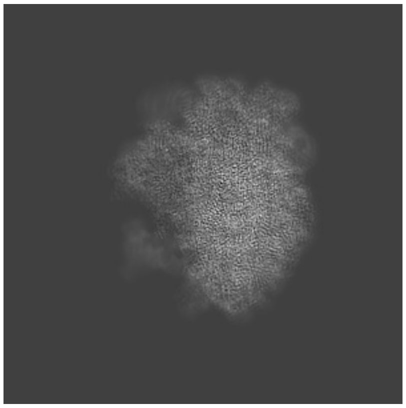
6 Map visualisation

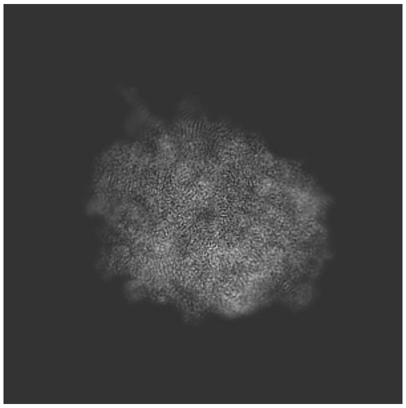
This section contains visualisations of the EMDB entry EMD-15773. These allow visual inspection of the internal detail of the map and identification of artifacts.

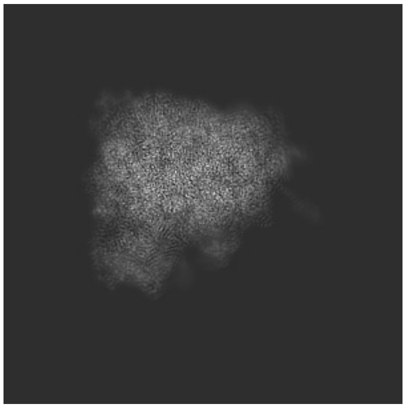
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

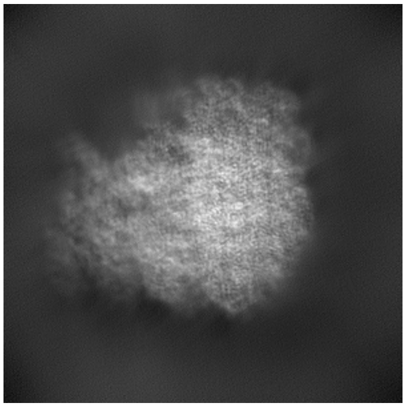
6.1.1 Primary map

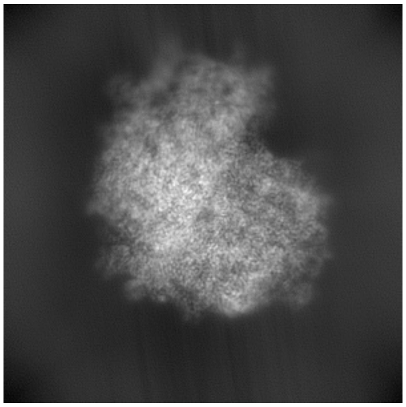

X

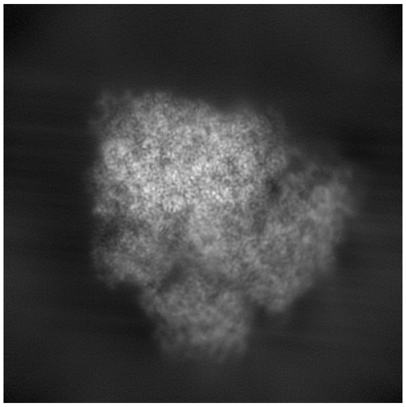

Y


Z

6.1.2 Raw map


X

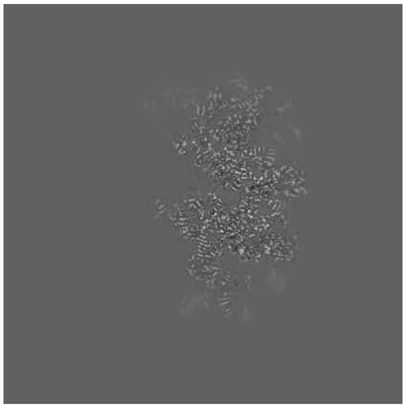

Y

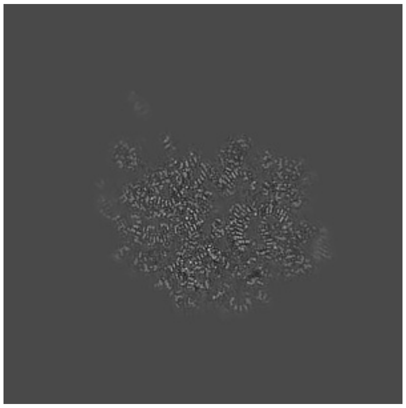

Z

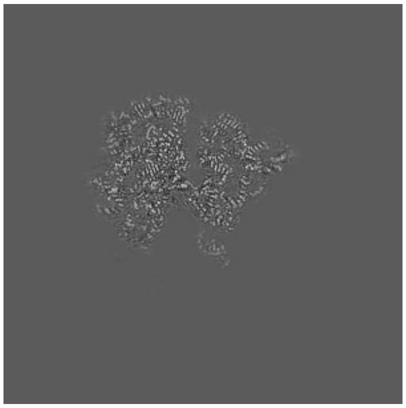
The images above show the map projected in three orthogonal directions.

6.2 Central slices

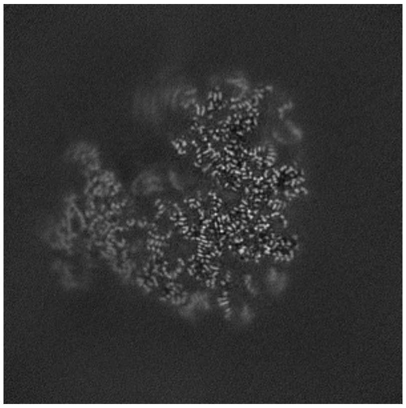
6.2.1 Primary map

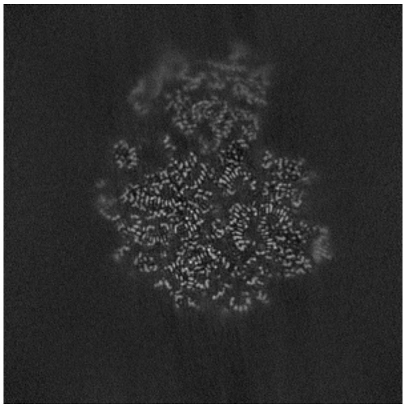

X Index: 225

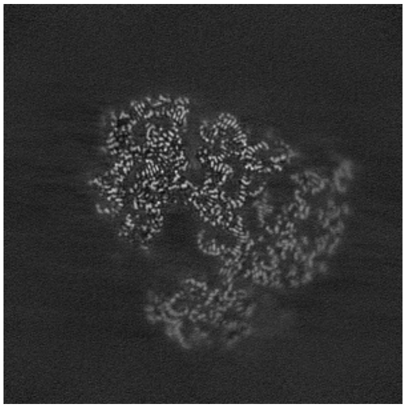

Y Index: 225


Z Index: 225

6.2.2 Raw map


X Index: 225

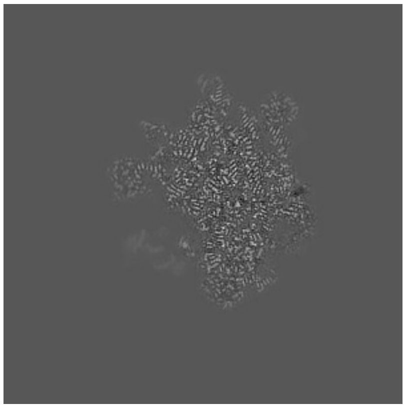

Y Index: 225


Z Index: 225

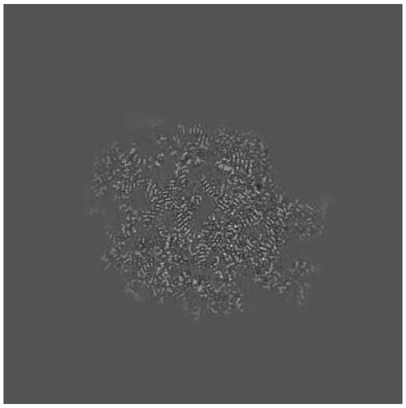
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices

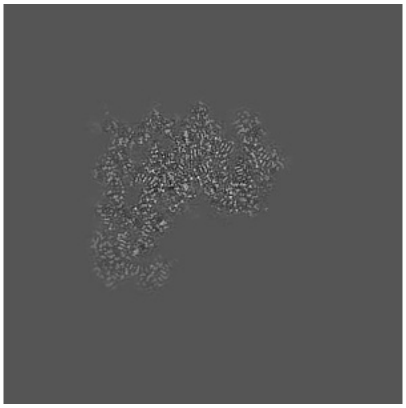
6.3.1 Primary map



X Index: 169

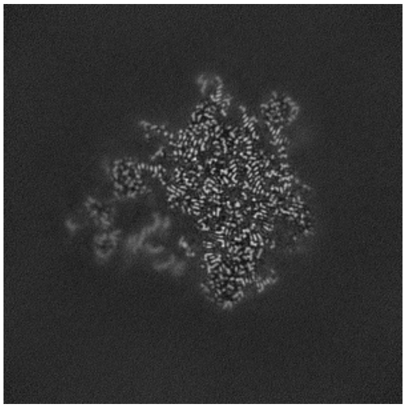


Y Index: 262

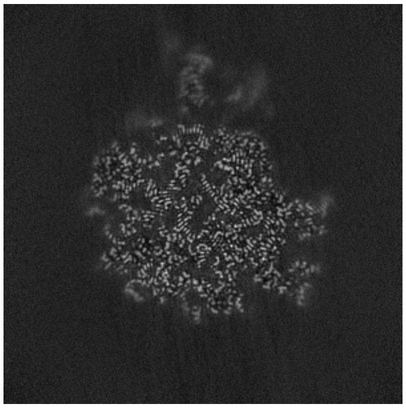


Z Index: 250

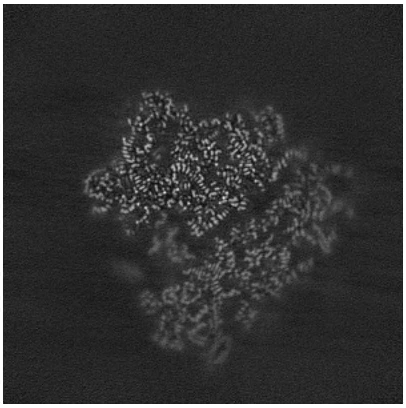
6.3.2 Raw map



X Index: 169



Y Index: 262

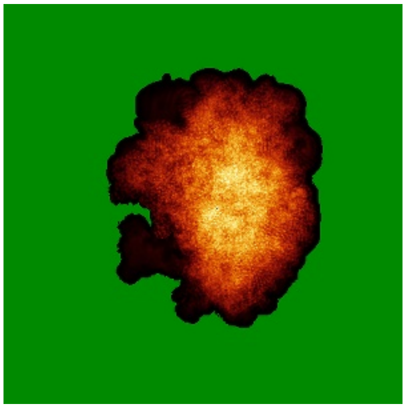


Z Index: 206

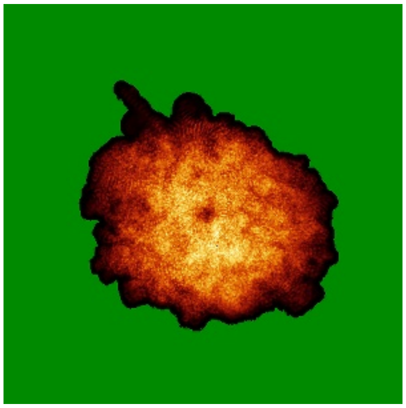
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color)

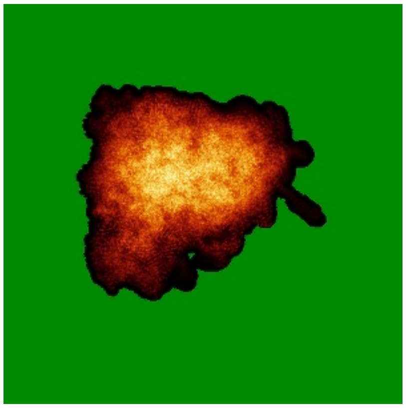
6.4.1 Primary map



X

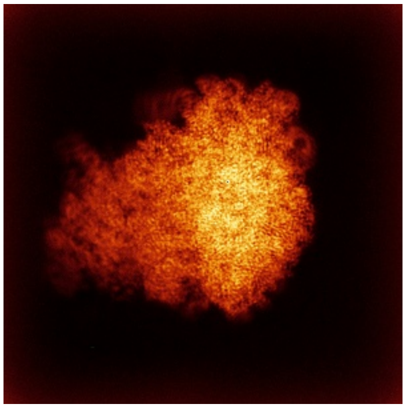


Y

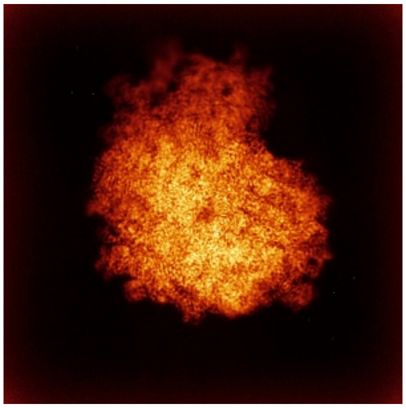


Z

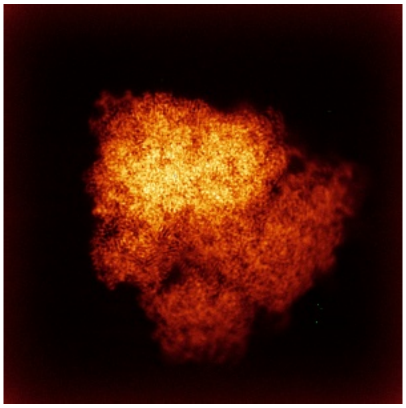
6.4.2 Raw map



X



Y

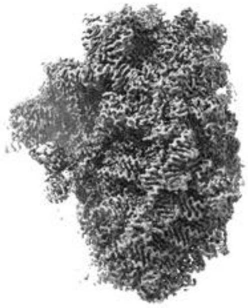


Z

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 ⓘ

6.5.1 Primary map



X

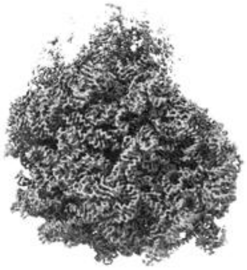
Y

Z

The images above show the 3D surface view of the map at the recommended contour level 1.05. 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.

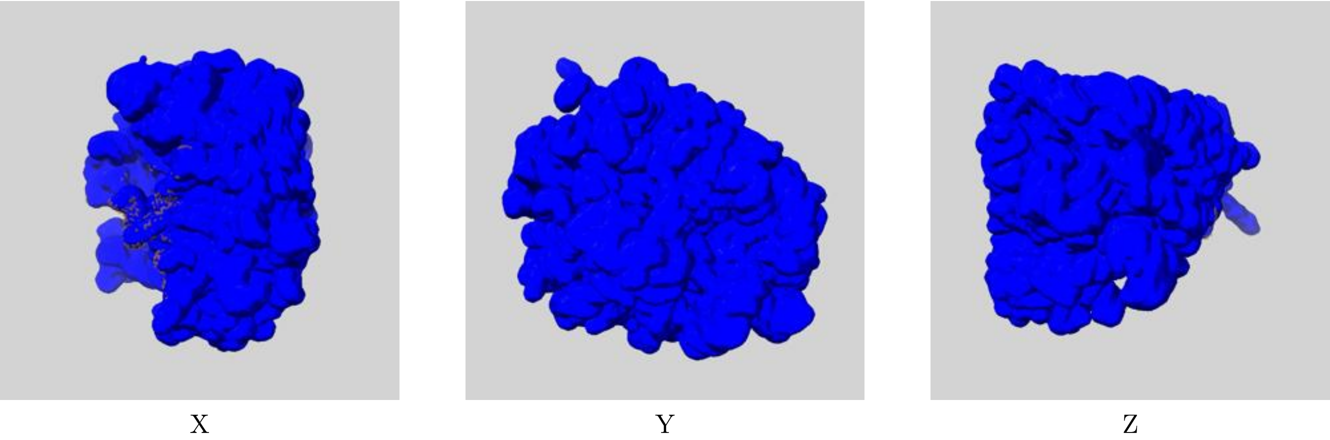
6.6 Mask visualisation ⓘ

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

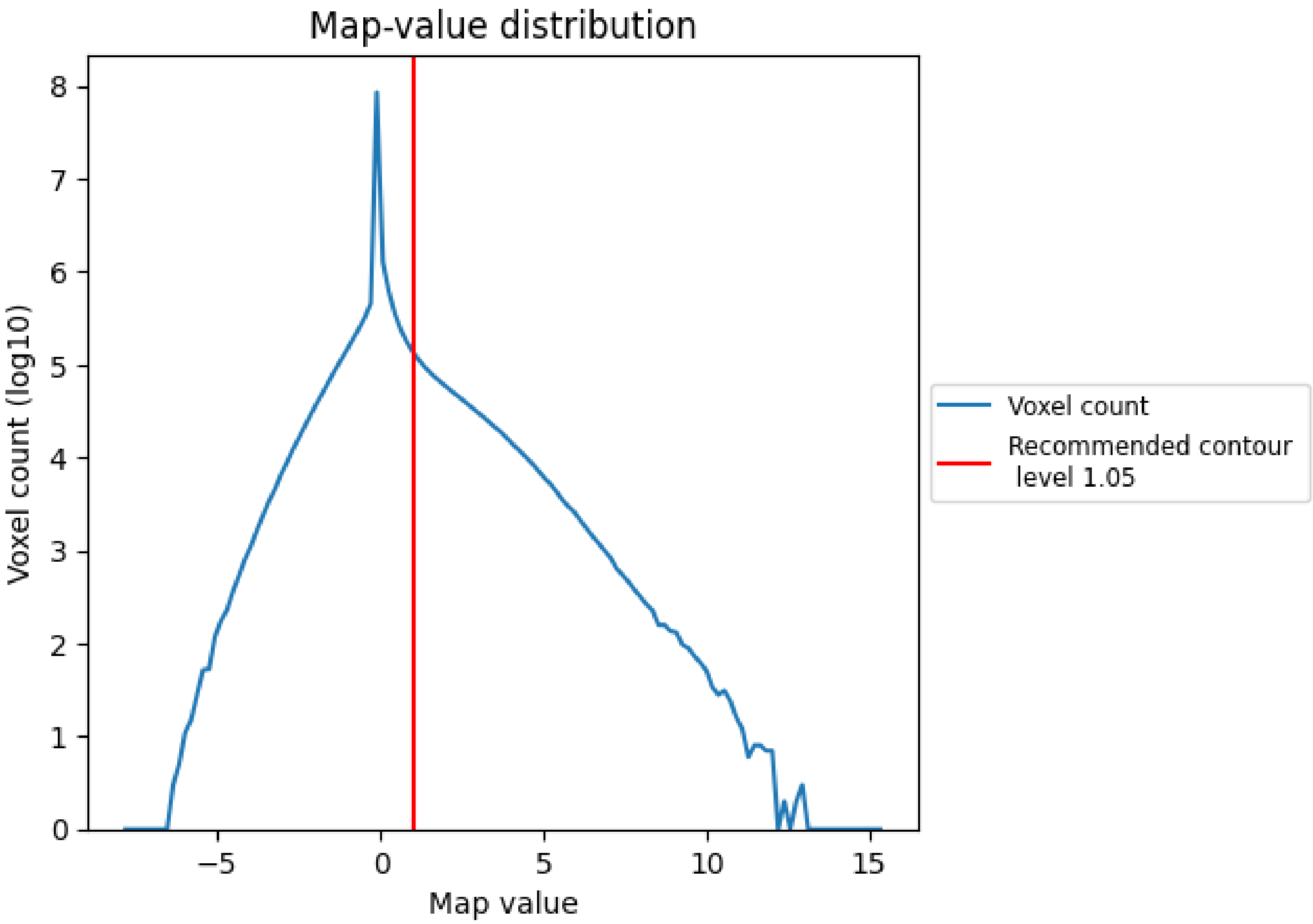
6.6.1 emd_15773_msk_1.map ⓘ



7 Map analysis ⓘ

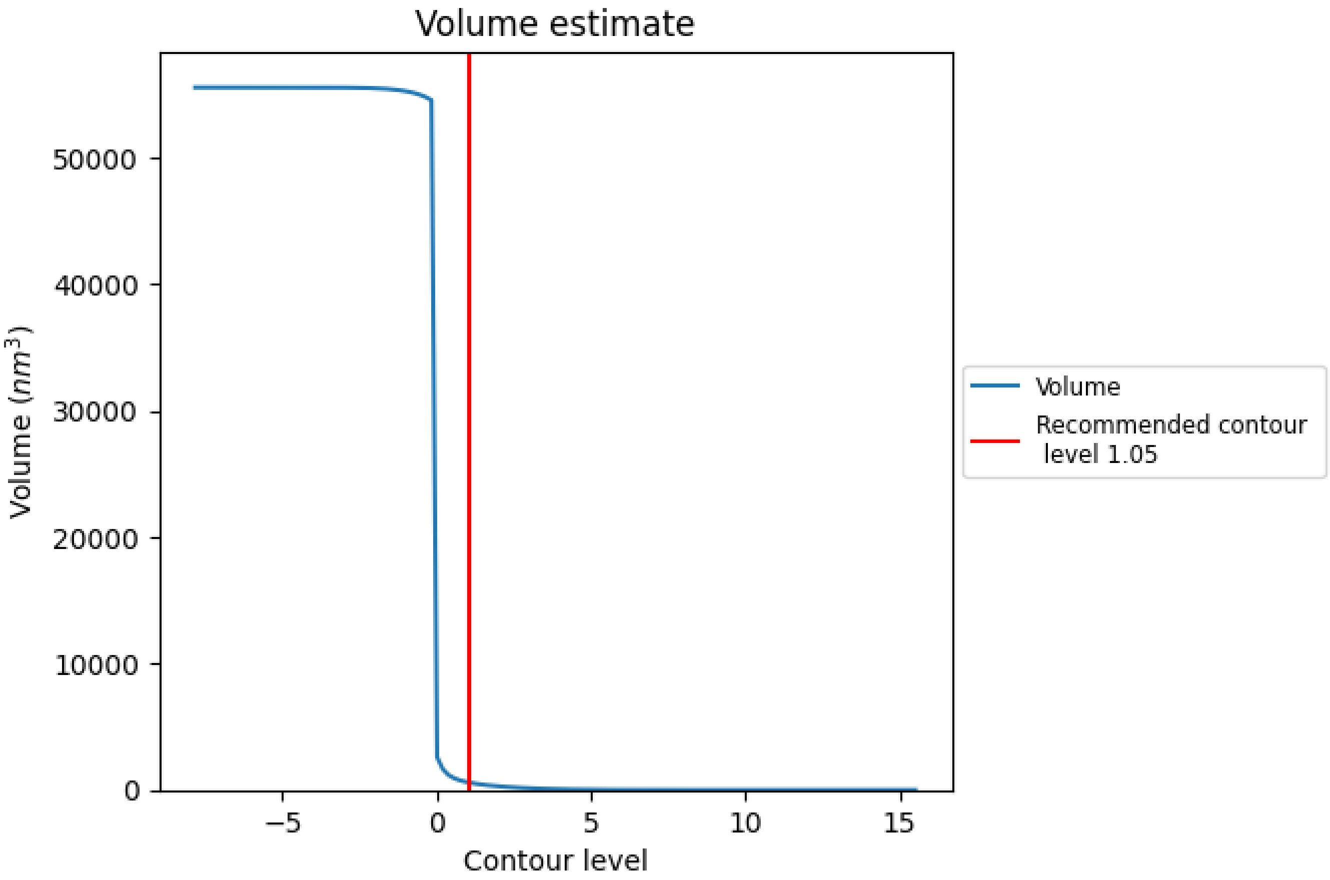
This section contains the results of statistical analysis of the map.

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.

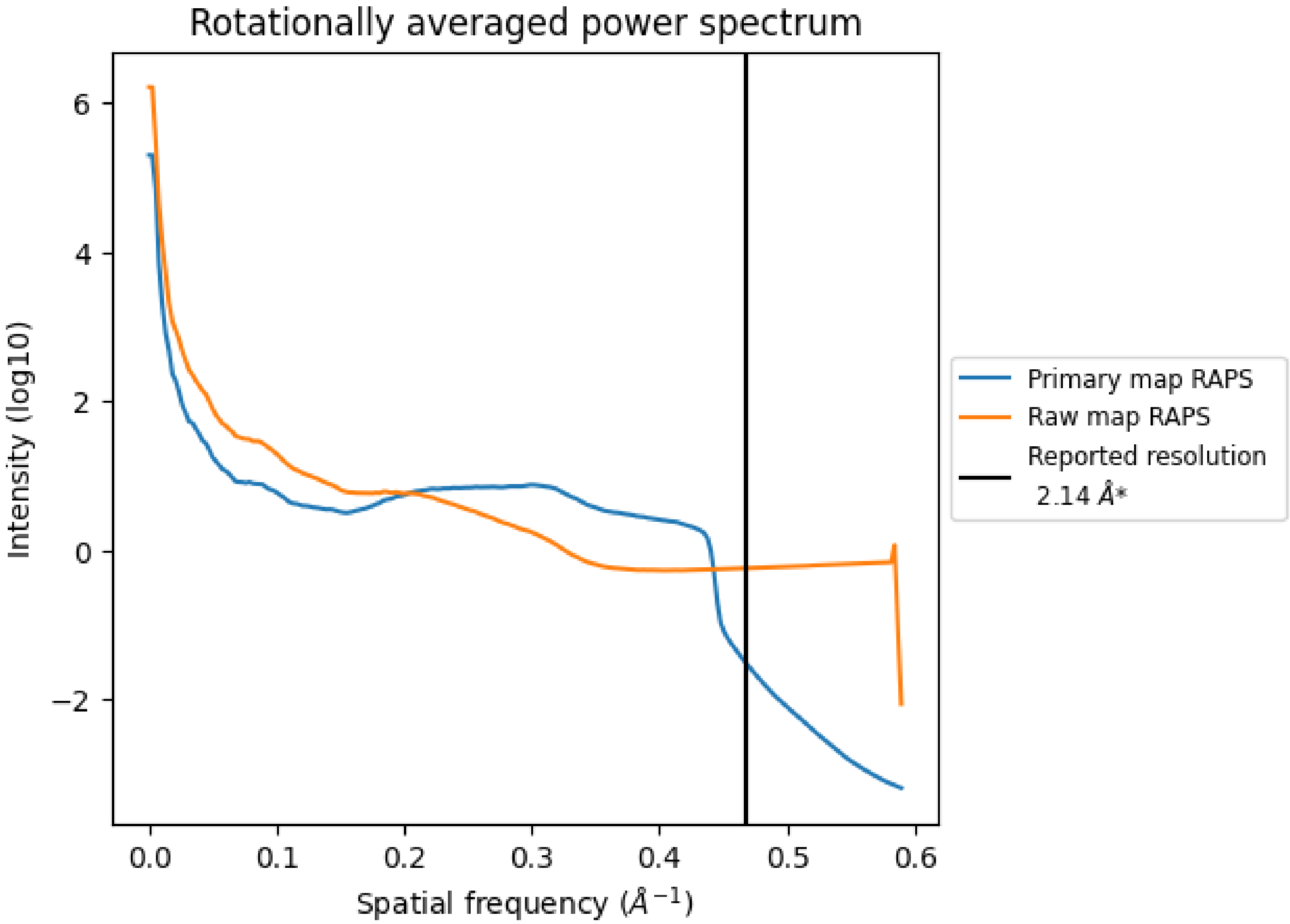
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 586 nm^3; this corresponds to an approximate mass of 530 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

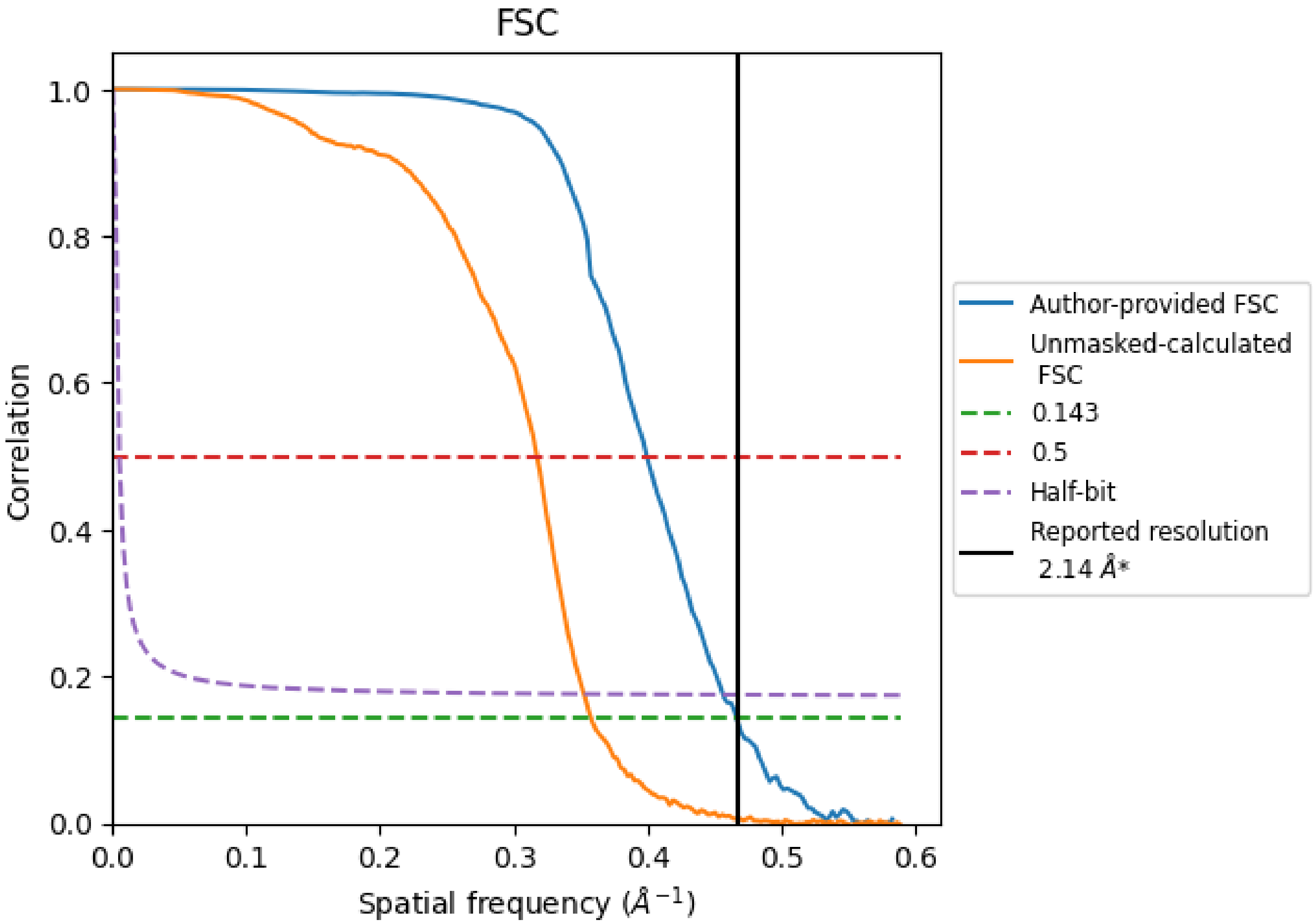


*Reported resolution corresponds to spatial frequency of 0.467 $Å^{-1}$

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 0.467 Å^{-1}

8.2 Resolution estimates ⓘ

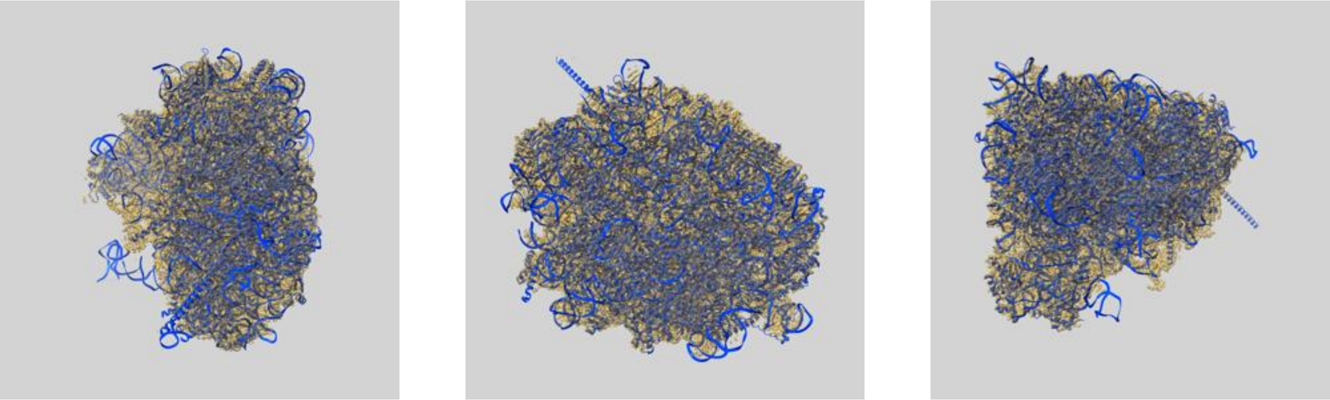
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	2.14	-	-
Author-provided FSC curve	2.14	2.50	2.19
Unmasked-calculated*	2.79	3.15	2.84

*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 2.79 differs from the reported value 2.14 by more than 10 %

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-15773 and PDB model 8AZW. Per-residue inclusion information can be found in section 3 on page 16.

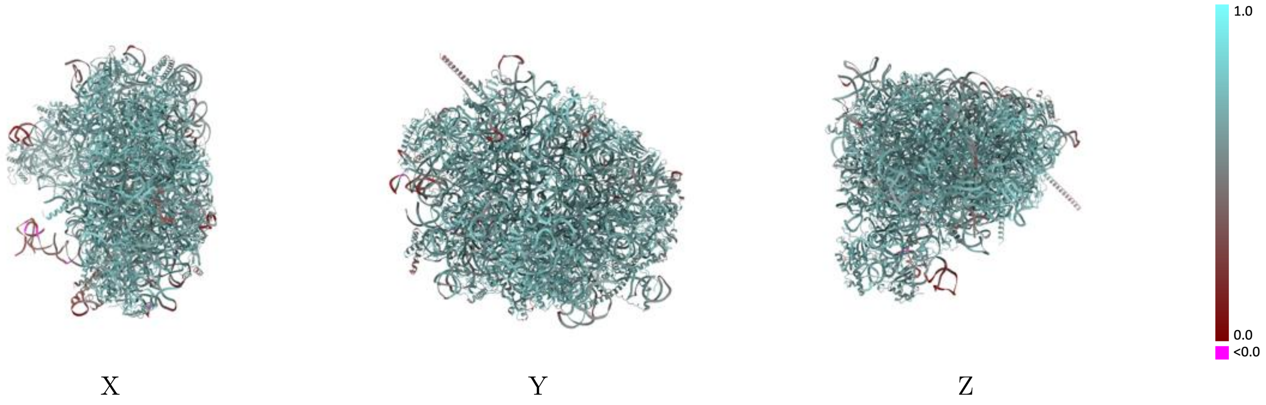
9.1 Map-model overlay ⓘ



X Y Z

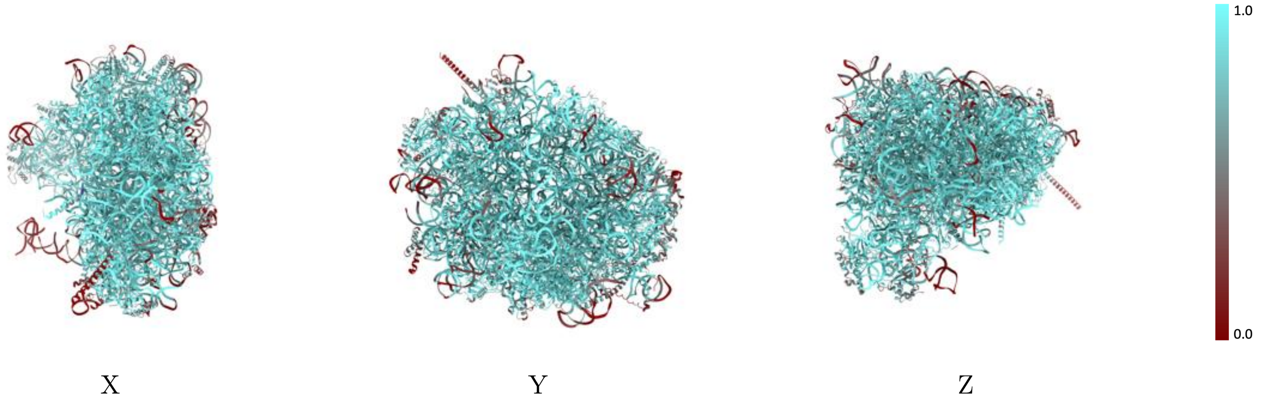
The images above show the 3D surface view of the map at the recommended contour level 1.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model ⓘ



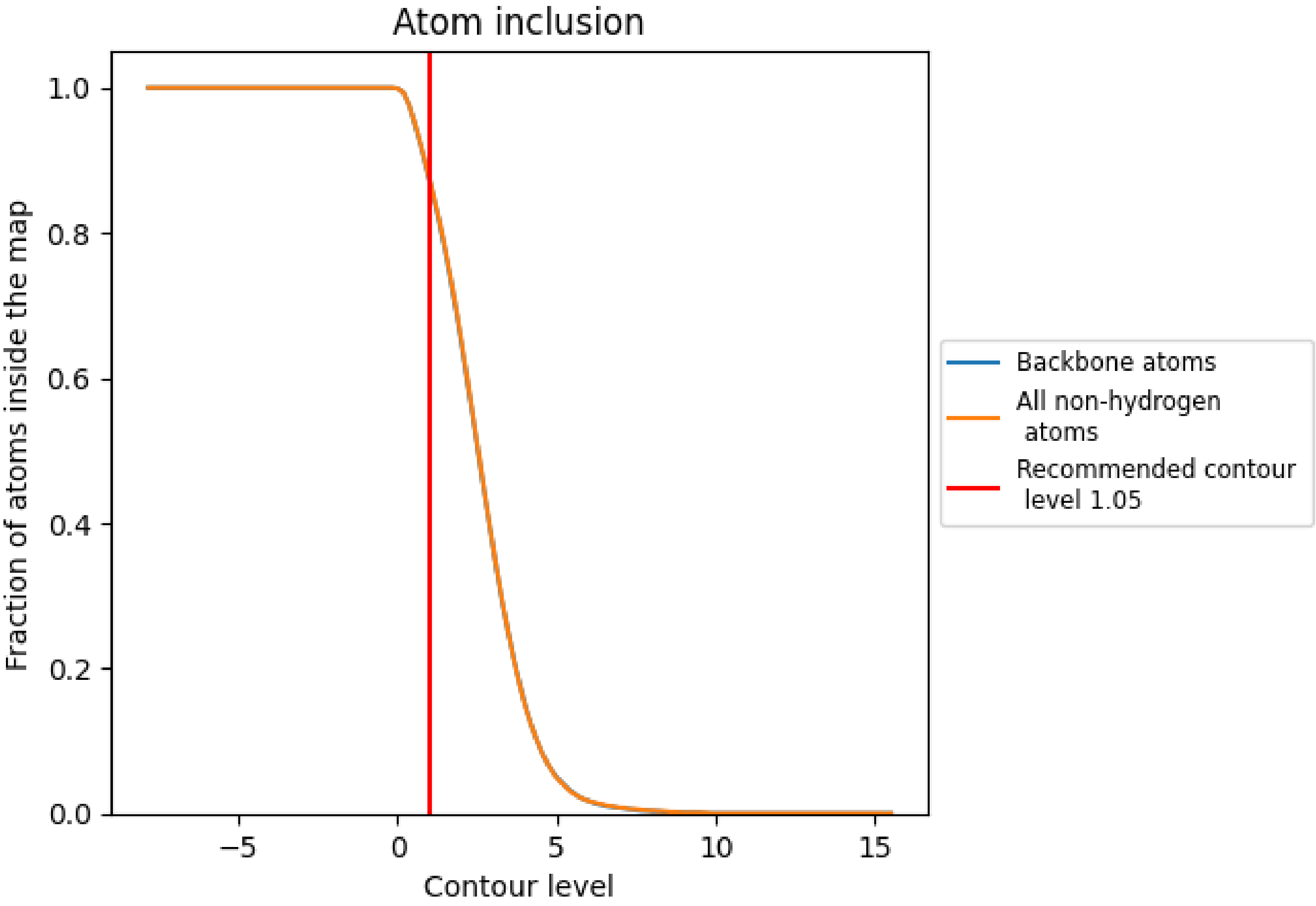
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 (1.05).

9.4 Atom inclusion ⓘ



At the recommended contour level, 87% of all backbone atoms, 87% 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 (1.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8680	0.6750
A	0.8750	0.6650
B	0.8640	0.6600
C	0.9510	0.6770
D	0.8720	0.6980
E	0.8390	0.6830
F	0.9900	0.7400
G	0.9570	0.7290
H	0.7360	0.6410
I	0.9230	0.7090
J	0.9000	0.7040
K	0.4530	0.5630
L	0.9020	0.7060
M	0.8090	0.6660
N	0.8800	0.6960
O	0.9370	0.7180
P	0.8020	0.6560
Q	0.8100	0.6730
R	0.9530	0.7270
S	0.9520	0.7200
T	0.8750	0.6860
U	0.8550	0.6790
V	0.9760	0.7370
W	0.6570	0.6140
X	0.9530	0.7270
Y	0.9170	0.7030
Z	0.9240	0.7210
a	0.8980	0.7110
b	0.6980	0.6420
c	0.7390	0.6490
d	0.9140	0.7150
e	0.9160	0.7120
f	0.9170	0.7130
g	0.8950	0.6980
h	0.7670	0.6560

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Chain	Atom inclusion	Q-score
j	0.9210	0.7100
k	0.8620	0.6920
l	0.3000	0.3230
m	0.9060	0.6940
n	0.8290	0.6700
o	0.9710	0.7300
p	0.7670	0.6500
q	0.8870	0.7030
r	0.9320	0.7210
s	0.8690	0.6930
t	0.6530	0.6230
u	0.8140	0.6700