



wwPDB EM Validation Summary Report ⓘ

Oct 6, 2024 – 09:42 am BST

PDB ID : 5APO
EMDB ID : EMD-3151
Title : Structure of the yeast 60S ribosomal subunit in complex with Arx1, Alb1 and C-terminally tagged Rei1
Authors : Greber, B.J.; Gerhardy, S.; Leitner, A.; Leibundgut, M.; Salem, M.; Boehringer, D.; Leulliot, N.; Aebersold, R.; Panse, V.G.; Ban, N.
Deposited on : 2015-09-17
Resolution : 3.41 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

The types of validation reports are described at

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

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

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

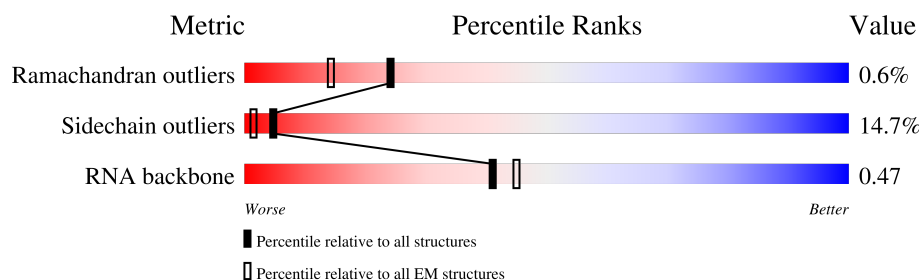
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.41 Å.

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









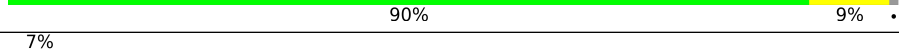
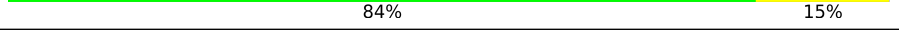
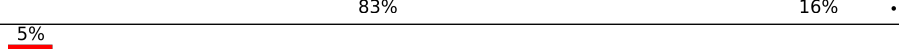
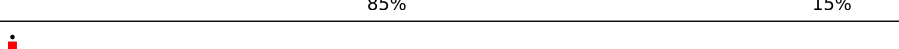
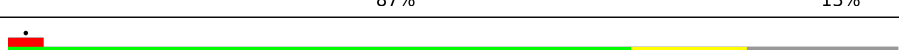

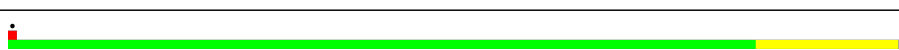

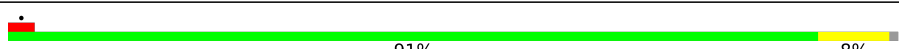





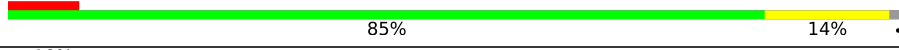
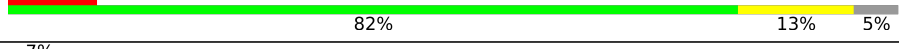



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	5	3396	
2	7	121	
3	8	158	
4	A	254	
5	B	387	
6	C	362	
7	D	297	
8	E	176	

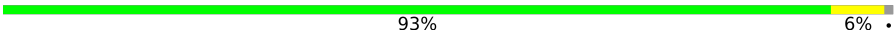











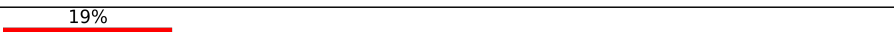

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	F	244	
10	G	256	
11	H	191	
12	I	221	
13	J	174	
14	L	199	
15	M	138	
16	N	204	
17	O	199	
18	P	184	
19	Q	186	
20	R	189	
21	S	172	
22	T	160	
23	U	121	
24	V	137	
25	W	155	
26	X	142	
27	Y	127	
28	Z	136	
29	a	149	
30	b	59	
31	c	105	
32	d	113	
33	e	130	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	f	107	
35	g	121	
36	h	120	
37	i	100	
38	j	88	
39	k	78	
40	l	51	
41	m	128	
42	o	106	
43	p	92	
44	q	312	
45	x	616	
46	y	401	
47	z	95	

2 Entry composition

There are 49 unique types of molecules in this entry. The entry contains 129386 atoms, of which 3 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 ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	5	3112	Total	C	N	O	P	0	0
			66537	29736	11996	21694	3111		

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	7	121	Total	C	N	O	P	0	0
			2579	1152	461	845	121		

- Molecule 3 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	8	158	Total	C	N	O	P	0	0
			3353	1500	586	1109	158		

- Molecule 4 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	212	Total	C	N	O	S	0	0
			1630	1021	325	283	1		

- Molecule 5 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	386	Total	C	N	O	S	0	0
			3075	1950	584	533	8		

- Molecule 6 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	361	Total	C	N	O	S	0	0
			2748	1729	522	494	3		

- Molecule 7 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	294	Total	C	N	O	S	0	0
			2359	1489	412	456	2		

- Molecule 8 is a protein called 60S RIBOSOMAL PROTEIN EL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	175	Total	C	N	O	S	0	0
			1356	878	242	235	1		

- Molecule 9 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	223	Total	C	N	O	S	0	0
			1791	1155	325	310	1		

- Molecule 10 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	231	Total	C	N	O	S	0	0
			1763	1130	316	314	3		

- Molecule 11 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	H	191	Total	C	N	O	S	0	0
			1518	963	274	277	4		

- Molecule 12 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	I	213	Total	C	N	O	S	0	0
			1722	1094	325	297	6		

- Molecule 13 is a protein called 60S ribosomal protein L11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	J	169	Total	C	N	O	S	0	0
			1353	847	253	249	4		

- Molecule 14 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	L	194	Total	C	N	O	0	0
			1548	965	316	267		

- Molecule 15 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	M	137	Total	C	N	O	S	0
			1059	678	200	179	2	0

- Molecule 16 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	N	203	Total	C	N	O	S	0
			1720	1077	361	281	1	0

- Molecule 17 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	O	197	Total	C	N	O	S	0
			1555	1003	289	262	1	0

- Molecule 18 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	P	183	Total	C	N	O		0
			1442	896	287	259		0

- Molecule 19 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	Q	185	Total	C	N	O	S	0
			1441	908	290	241	2	0

- Molecule 20 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	R	156	Total	C	N	O		0
			1258	781	265	212		0

- Molecule 21 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	S	171	Total	C	N	O	S	0	0
			1437	925	266	243	3		

- Molecule 22 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	T	159	Total	C	N	O	S	0	0
			1276	805	246	221	4		

- Molecule 23 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	U	102	Total	C	N	O		0	0
			808	524	132	152			

- Molecule 24 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	V	136	Total	C	N	O	S	0	0
			1003	628	189	179	7		

- Molecule 25 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	W	63	Total	C	N	O	S	0	0
			521	336	102	82	1		

- Molecule 26 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	X	120	Total	C	N	O	S	0	0
			959	617	168	172	2		

- Molecule 27 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Y	126	Total	C	N	O		0	0
			993	625	192	176			

- Molecule 28 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	Z	135	Total	C	N	O	0	0
			1092	710	202	180		

- Molecule 29 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	a	148	Total	C	N	O	S	0	0
			1173	749	231	190	3		

- Molecule 30 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	b	58	Total	C	N	O	0	0
			462	289	100	73		

- Molecule 31 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	c	100	Total	C	N	O	S	0	0
			767	492	128	146	1		

- Molecule 32 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	d	109	Total	C	N	O	S	0	0
			883	559	167	156	1		

- Molecule 33 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	e	129	Total	C	N	O	S	0	0
			1034	655	207	171	1		

- Molecule 34 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	f	106	Total	C	N	O	S	0	0
			850	540	165	144	1		

- Molecule 35 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	g	112	Total	C	N	O	S	0	0
			880	545	179	152	4		

- Molecule 36 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	h	119	Total	C	N	O	S	0	0
			965	612	185	167	1		

- Molecule 37 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	i	99	Total	C	N	O	S	0	0
			770	481	156	131	2		

- Molecule 38 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	j	87	Total	C	N	O	S	0	0
			681	414	148	114	5		

- Molecule 39 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	k	77	Total	C	N	O	0	0
			608	388	114	106		

- Molecule 40 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	l	50	Total	C	N	O	S	0	0
			436	272	97	65	2		

- Molecule 41 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	m	52	Total	C	N	O	S	0	0
			417	259	86	67	5		

- Molecule 42 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	o	105	Total	C	N	O	S	0	0
			847	534	170	138	5		

- Molecule 43 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	p	91	Total	C	N	O	S	0	0
			694	429	138	121	6		

- Molecule 44 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	q	120	Total	C	N	O	S	0	0
			962	618	169	172	3		

- Molecule 45 is a protein called Probable metalloprotease ARX1.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	x	579	Total	C	N	O	S	0	0
			4477	2823	772	867	15		

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
x	-22	MET	-	initiating methionine	UNP Q03862
x	-21	GLY	-	expression tag	UNP Q03862
x	-20	SER	-	expression tag	UNP Q03862
x	-19	SER	-	expression tag	UNP Q03862
x	-18	HIS	-	expression tag	UNP Q03862
x	-17	HIS	-	expression tag	UNP Q03862
x	-16	HIS	-	expression tag	UNP Q03862
x	-15	HIS	-	expression tag	UNP Q03862
x	-14	HIS	-	expression tag	UNP Q03862
x	-13	HIS	-	expression tag	UNP Q03862
x	-12	SER	-	expression tag	UNP Q03862
x	-11	SER	-	expression tag	UNP Q03862
x	-10	GLY	-	expression tag	UNP Q03862
x	-9	LEU	-	expression tag	UNP Q03862
x	-8	VAL	-	expression tag	UNP Q03862
x	-7	PRO	-	expression tag	UNP Q03862
x	-6	ARG	-	expression tag	UNP Q03862
x	-5	GLY	-	expression tag	UNP Q03862
x	-4	SER	-	expression tag	UNP Q03862

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
x	-3	HIS	-	expression tag	UNP Q03862
x	-2	MET	-	expression tag	UNP Q03862
x	-1	LEU	-	expression tag	UNP Q03862
x	0	GLU	-	expression tag	UNP Q03862

- Molecule 46 is a protein called CYTOPLASMIC 60S SUBUNIT BIOGENESIS FACTOR REI1.

Mol	Chain	Residues	Atoms						AltConf	Trace
46	y	217	Total	C	H	N	O	S	0	0
			1788	1131	3	324	322	8		

- Molecule 47 is a protein called ALB1.

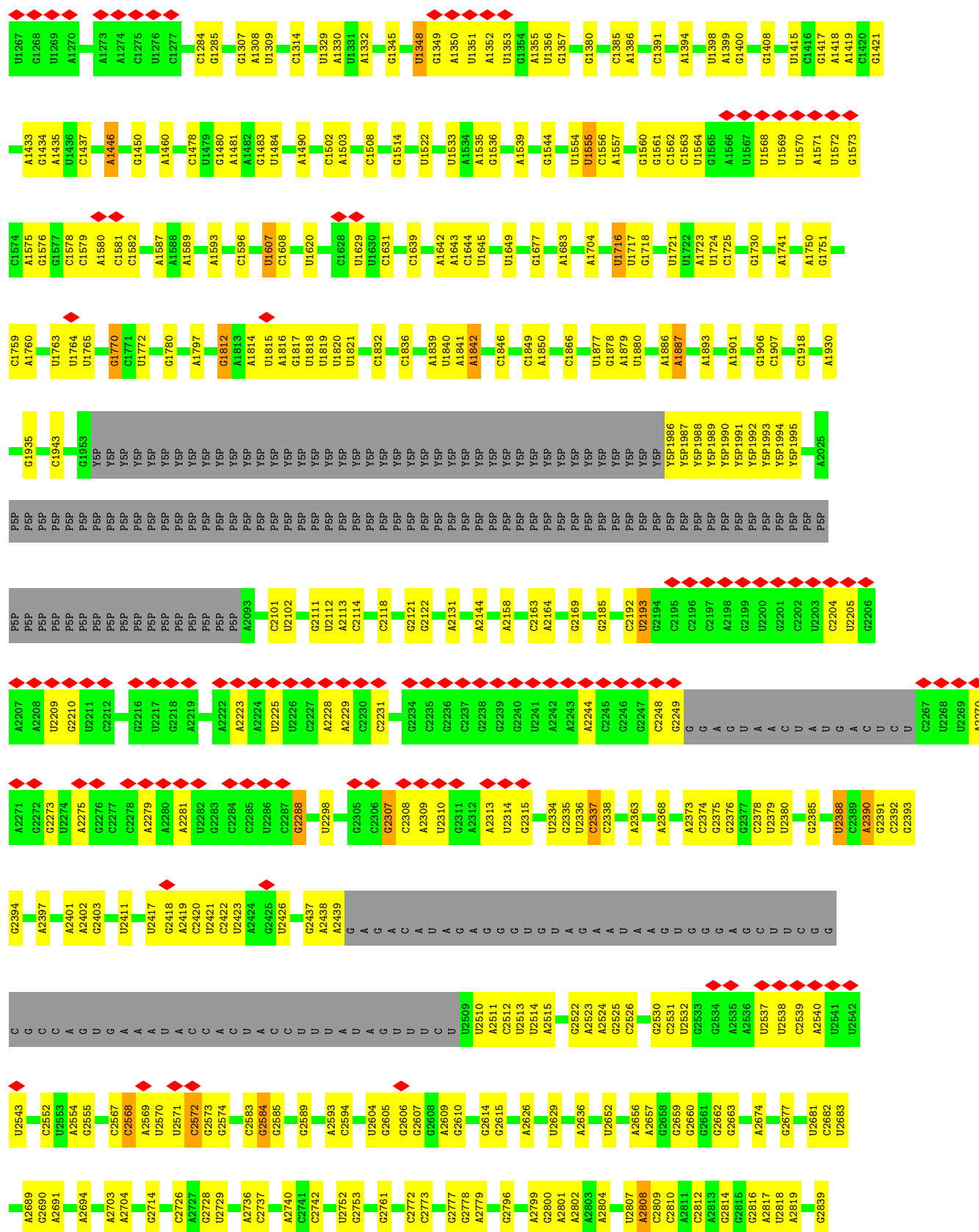
Mol	Chain	Residues	Atoms				AltConf	Trace
47	z	85	Total	C	N	O	0	0
			510	340	85	85		

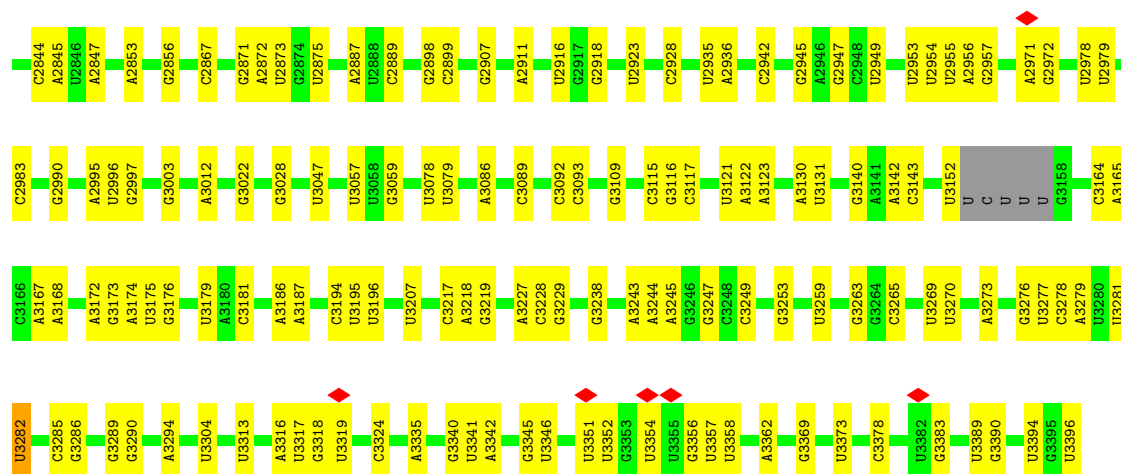
- Molecule 48 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
48	5	259	Total	Mg	0
			259	259	
48	7	6	Total	Mg	0
			6	6	
48	8	7	Total	Mg	0
			7	7	
48	B	2	Total	Mg	0
			2	2	
48	C	1	Total	Mg	0
			1	1	
48	N	1	Total	Mg	0
			1	1	
48	P	1	Total	Mg	0
			1	1	
48	R	1	Total	Mg	0
			1	1	
48	V	1	Total	Mg	0
			1	1	
48	y	1	Total	Mg	0
			1	1	

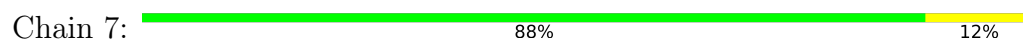
- Molecule 49 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
49	j	1	Total 1	Zn 1	0
49	m	1	Total 1	Zn 1	0
49	o	1	Total 1	Zn 1	0
49	p	1	Total 1	Zn 1	0
49	y	2	Total 2	Zn 2	0

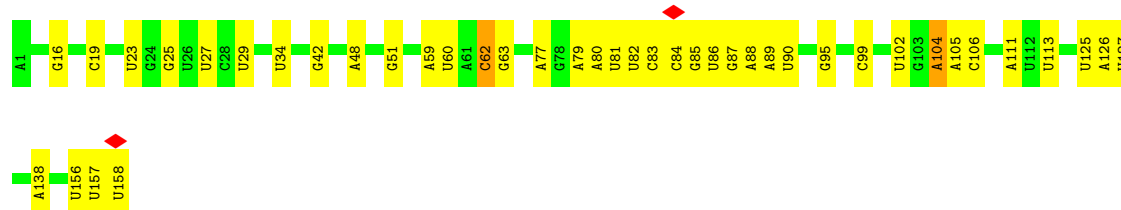




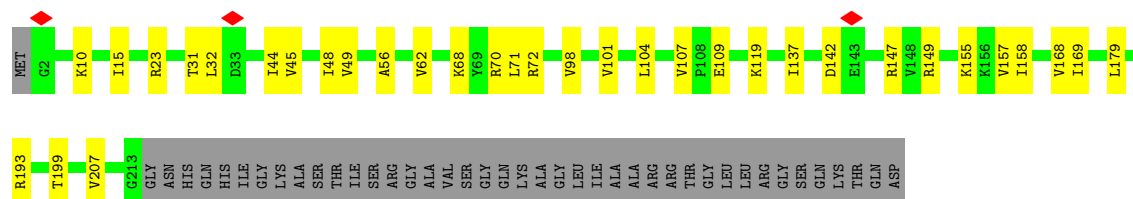
- Molecule 2: 5S ribosomal RNA



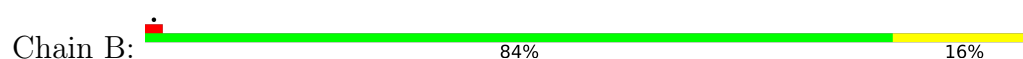
- Molecule 3: 5.8S ribosomal RNA

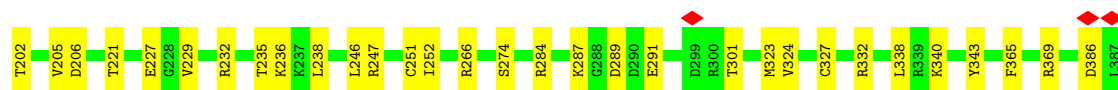


- Molecule 4: 60S ribosomal protein L2-A

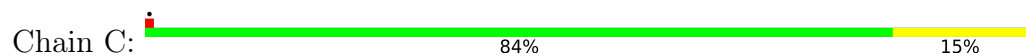


- Molecule 5: 60S ribosomal protein L3

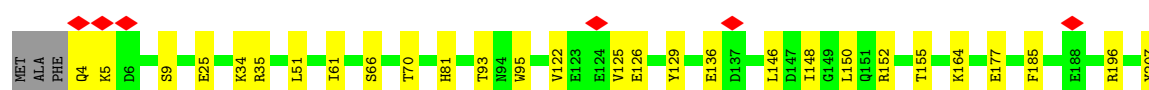
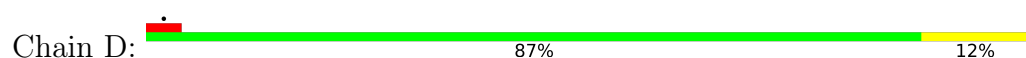




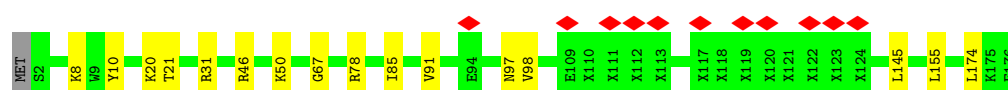
- Molecule 6: 60S ribosomal protein L4-A



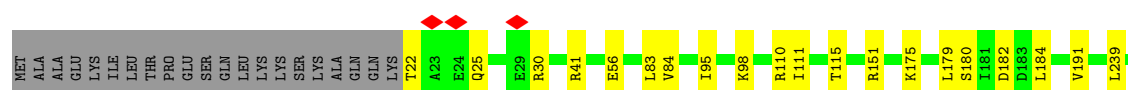
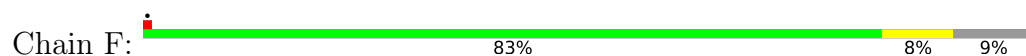
- Molecule 7: 60S ribosomal protein L5



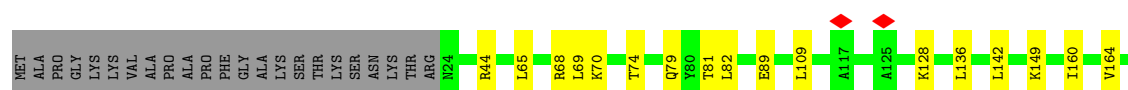
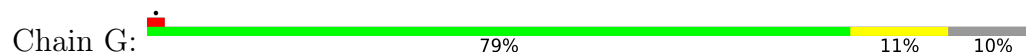
- Molecule 8: 60S RIBOSOMAL PROTEIN EL6

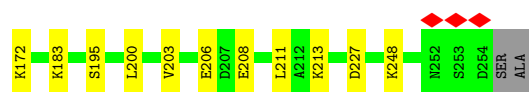


- Molecule 9: 60S ribosomal protein L7-A

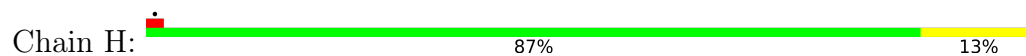


- Molecule 10: 60S ribosomal protein L8-A

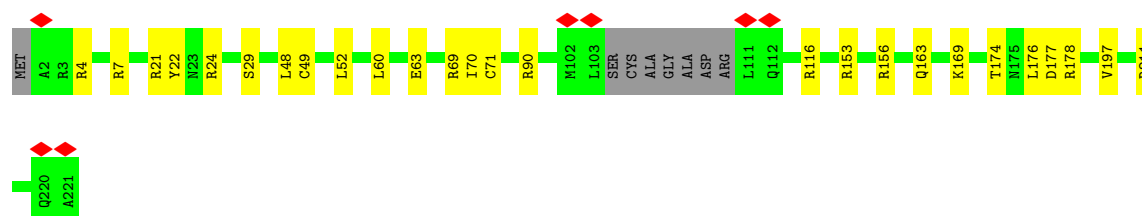
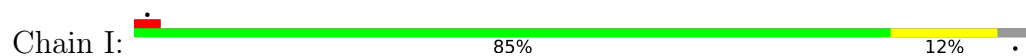




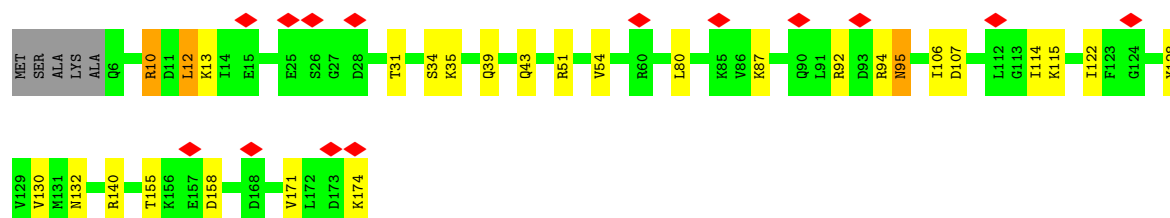
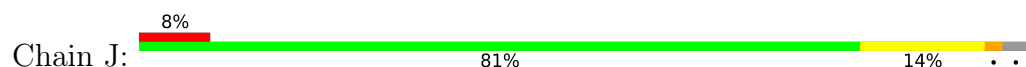
- Molecule 11: 60S ribosomal protein L9-A



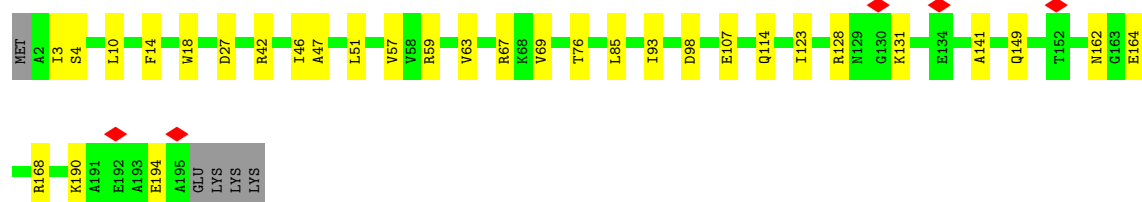
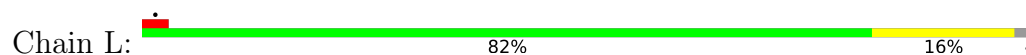
- Molecule 12: 60S ribosomal protein L10



- Molecule 13: 60S ribosomal protein L11-A



- Molecule 14: 60S ribosomal protein L13-A

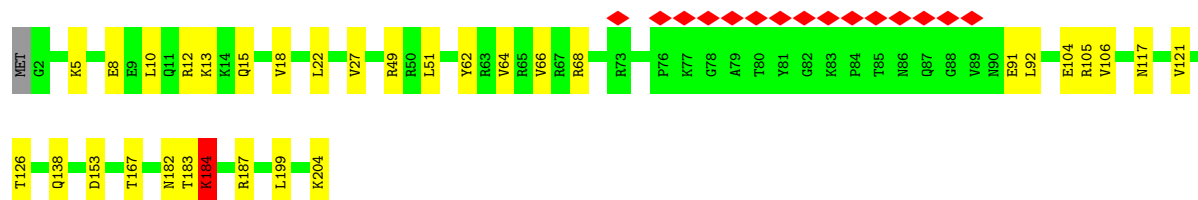
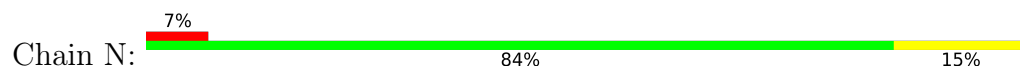


- Molecule 15: 60S ribosomal protein L14-A

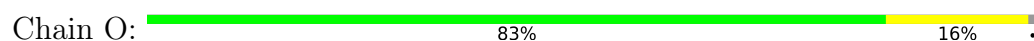




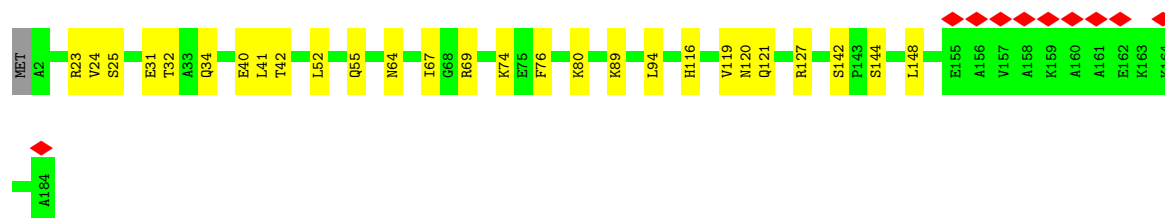
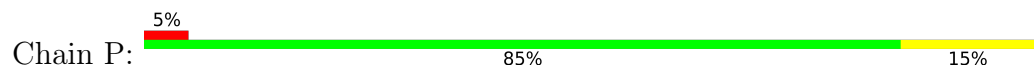
- Molecule 16: 60S ribosomal protein L15-A



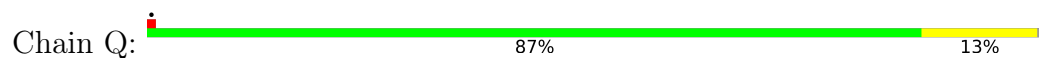
- Molecule 17: 60S ribosomal protein L16-A



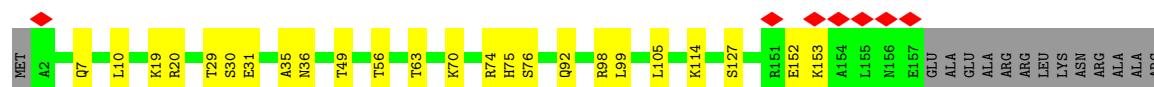
- Molecule 18: 60S ribosomal protein L17-A



- Molecule 19: 60S ribosomal protein L18-A



- Molecule 20: 60S ribosomal protein L19-A





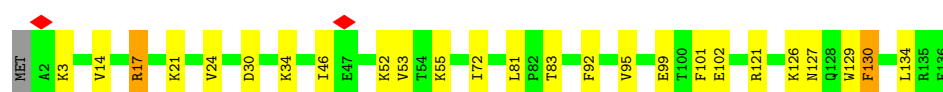
- Molecule 27: 60S ribosomal protein L26-A

Chain Y: 88% 10% ..



- Molecule 28: 60S ribosomal protein L27-A

Chain Z: 81% 17% ..



- Molecule 29: 60S ribosomal protein L28

Chain a: 91% 9% .



- Molecule 30: 60S ribosomal protein L29

Chain b: 8% 85% 14% .



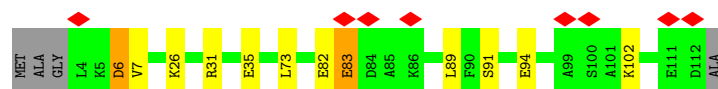
- Molecule 31: 60S ribosomal protein L30

Chain c: 10% 82% 13% 5%




- Molecule 32: 60S ribosomal protein L31-A

Chain d: 7% 86% 9% . .



- Molecule 33: 60S ribosomal protein L32

Chain e:  87% 12%




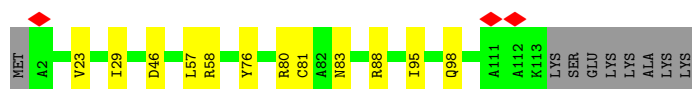
- Molecule 34: 60S ribosomal protein L33-A

Chain f:  93% 6%




- Molecule 35: 60S ribosomal protein L34-A

Chain g:  83% 10% 7%




- Molecule 36: 60S ribosomal protein L35-A

Chain h:  83% 16%




- Molecule 37: 60S ribosomal protein L36-A

Chain i:  6% 76% 23%




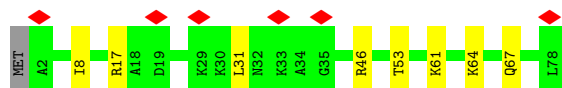
- Molecule 38: 60S ribosomal protein L37-A

Chain j:  86% 13%




- Molecule 39: 60S ribosomal protein L38

Chain k:  8% 88% 10%




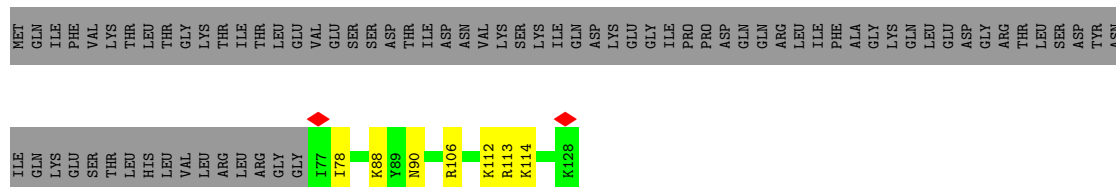
• Molecule 40: 60S ribosomal protein L39

Chain l:  78% 20%




• Molecule 41: Ubiquitin-60S ribosomal protein L40

Chain m:  35% 5% 59%




• Molecule 42: 60S ribosomal protein L42-A

Chain o:  20% 82% 17%




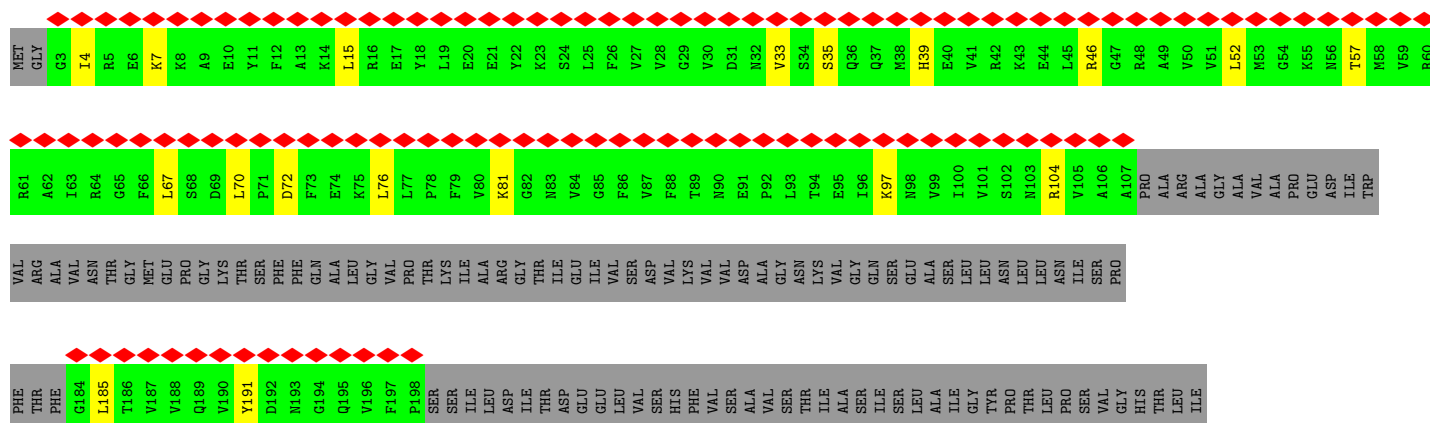
• Molecule 43: 60S ribosomal protein L43-A

Chain p:  80% 18%

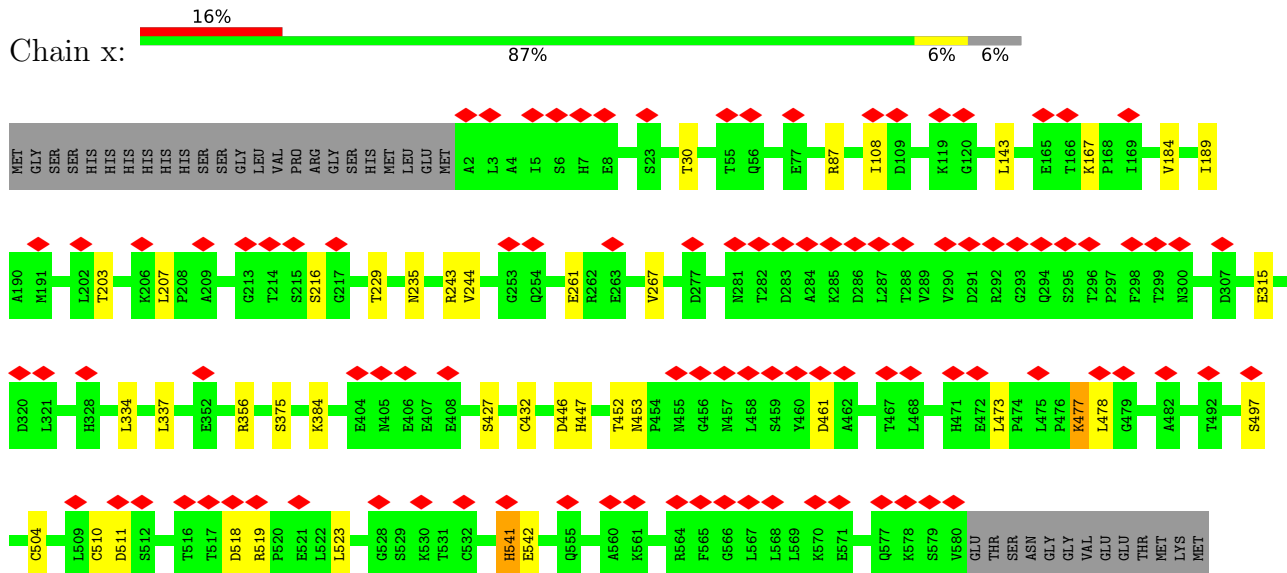


• Molecule 44: 60S acidic ribosomal protein P0

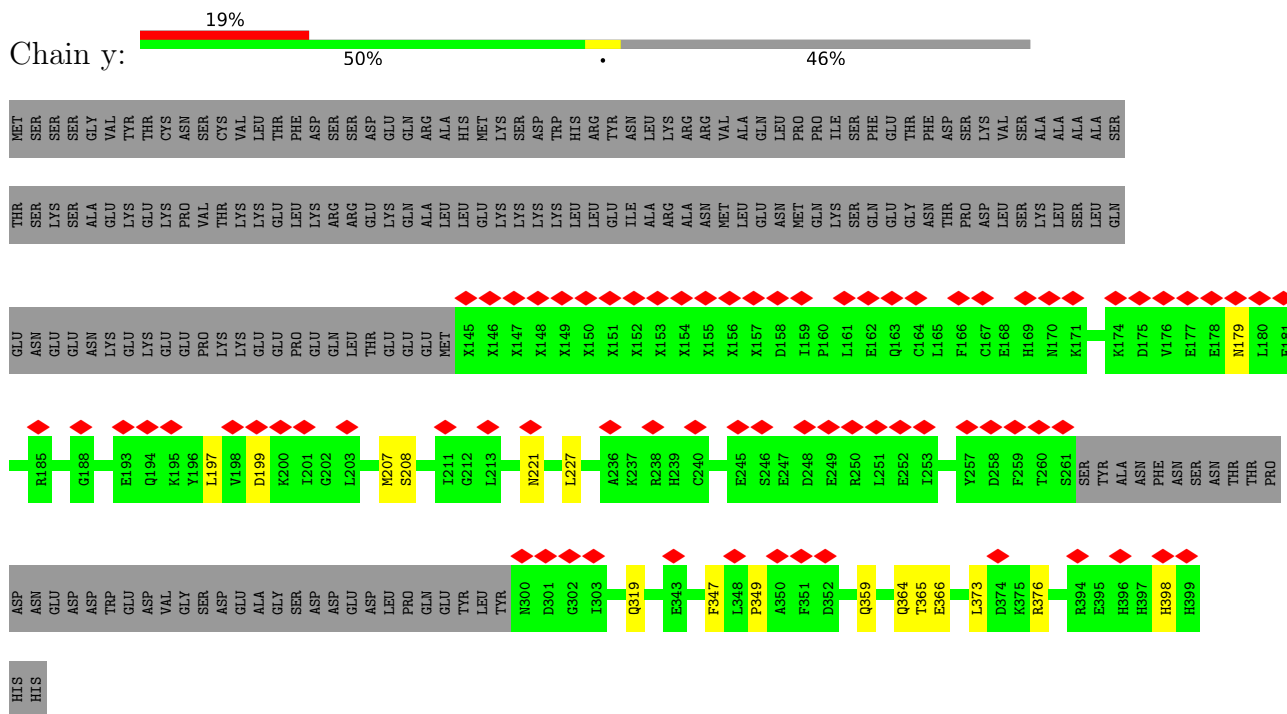
Chain q:  38% 33% 6% 62%



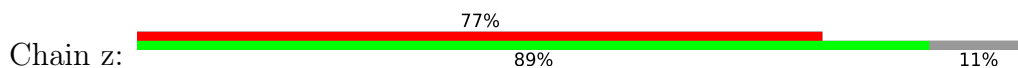
- Molecule 45: Probable metalloprotease ARX1



- Molecule 46: CYTOPLASMIC 60S SUBUNIT BIOGENESIS FACTOR REI1



- Molecule 47: ALB1



X141	X65
X142	X70
X143	X71
X144	
X145	X76
X146	X77
X147	X78
X148	X79
X149	X80
X150	X81
X151	X82
X152	X83
X153	X84
X154	X85
X155	X86
X156	X87
X157	X88
X158	X89
X159	X90
UNK	X91
UNK	X92
UNK	X93
UNK	X94
UNK	X95
UNK	X96
UNK	X97
UNK	X98
UNK	X99
	X100
	X101
	X102
	X103
	X104
	X105
	X106
	X107
	X115
	X116
	X117
	X118
	X119
	X120
	X121
	X122
	X123
	X124
	X125
	X126
	X127
	X131
	X132
	X133
	X134
	X135
	X136
	X137
	X138
	X139
	X140

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	134701	Depositor
Resolution determination method	Not provided	
CTF correction method	PER DETECTOR FRAME	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	800.00	Depositor
Maximum defocus (nm)	3000.00	Depositor
Magnification	100720	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	1.020	Depositor
Minimum map value	-0.642	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.055	Depositor
Recommended contour level	0.1	Depositor
Map size (\AA)	300.24, 300.24, 300.24	wwPDB
Map dimensions	216, 216, 216	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.39, 1.39, 1.39	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, Y5P, P5P, 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	5	0.66	12/74039 (0.0%)	1.09	121/115426 (0.1%)
2	7	0.41	0/2883	0.90	1/4491 (0.0%)
3	8	0.69	0/3746	1.12	8/5832 (0.1%)
4	A	0.41	0/1662	0.60	0/2236
5	B	0.46	0/3146	0.59	0/4228
6	C	0.47	0/2800	0.67	1/3790 (0.0%)
7	D	0.34	0/2408	0.50	0/3248
8	E	0.39	0/1269	0.58	0/1705
9	F	0.46	0/1828	0.58	0/2461
10	G	0.38	0/1795	0.58	0/2429
11	H	0.40	0/1539	0.54	0/2073
12	I	0.36	0/1758	0.57	0/2358
13	J	0.34	0/1374	0.55	0/1842
14	L	0.46	0/1573	0.61	0/2113
15	M	0.38	0/1074	0.55	0/1446
16	N	0.52	0/1757	0.65	0/2354
17	O	0.48	0/1585	0.63	1/2128 (0.0%)
18	P	0.50	0/1465	0.60	0/1968
19	Q	0.42	0/1465	0.61	0/1965
20	R	0.39	0/1275	0.52	0/1702
21	S	0.45	0/1473	0.59	0/1980
22	T	0.42	0/1300	0.56	0/1743
23	U	0.36	0/825	0.56	0/1120
24	V	0.43	0/1018	0.60	0/1369
25	W	0.40	0/533	0.53	0/707
26	X	0.42	0/974	0.62	0/1314
27	Y	0.43	0/1004	0.62	0/1341
28	Z	0.38	0/1118	0.62	0/1497
29	a	0.47	0/1204	0.64	0/1612
30	b	0.39	0/473	0.53	0/629
31	c	0.35	0/775	0.52	0/1040
32	d	0.46	0/897	0.62	0/1205

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	e	0.52	0/1055	0.63	0/1413
34	f	0.52	0/868	0.67	0/1168
35	g	0.43	0/890	0.63	0/1189
36	h	0.42	0/974	0.58	0/1297
37	i	0.35	0/777	0.55	0/1033
38	j	0.51	0/696	0.65	0/923
39	k	0.34	0/614	0.53	0/822
40	l	0.46	0/443	0.57	0/588
41	m	0.40	0/423	0.55	0/562
42	o	0.41	0/860	0.56	0/1136
43	p	0.46	0/701	0.62	0/934
44	q	0.58	0/977	0.61	0/1313
45	x	0.37	0/4557	0.57	0/6189
46	y	0.39	0/1746	0.54	0/2346
All	All	0.57	12/137616 (0.0%)	0.93	132/202265 (0.1%)

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
6	C	0	3
8	E	0	1
14	L	0	1
16	N	0	1
27	Y	0	1
28	Z	0	1
32	d	0	3
37	i	0	1
45	x	0	3
46	y	0	1
All	All	0	16

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	1152	G	N9-C4	-7.14	1.32	1.38
1	5	2368	A	N9-C4	-6.55	1.33	1.37
1	5	336	A	N9-C4	-6.44	1.33	1.37
1	5	2392	C	N1-C6	-6.25	1.33	1.37
1	5	1446	A	N9-C4	-6.19	1.34	1.37

The worst 5 of 132 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	1152	G	N3-C4-C5	10.03	133.61	128.60
1	5	408	A	N1-C6-N6	-8.94	113.24	118.60
1	5	1232	C	O4'-C1'-N1	8.59	115.07	108.20
1	5	2193	U	N1-C2-N3	8.32	119.89	114.90
3	8	62	C	C6-N1-C2	8.32	123.63	120.30

There are no chirality outliers.

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	C	145	ILE	Peptide
6	C	148	ILE	Peptide
6	C	300	ARG	Peptide
8	E	67	GLY	Peptide
14	L	141	ALA	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	
4	A	210/254 (83%)	195 (93%)	14 (7%)	1 (0%)	25	55
5	B	384/387 (99%)	367 (96%)	17 (4%)	0	100	100
6	C	359/362 (99%)	329 (92%)	28 (8%)	2 (1%)	22	51
7	D	292/297 (98%)	282 (97%)	8 (3%)	2 (1%)	19	48
8	E	155/176 (88%)	143 (92%)	9 (6%)	3 (2%)	6	26
9	F	221/244 (91%)	210 (95%)	10 (4%)	1 (0%)	25	55

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	G	229/256 (90%)	200 (87%)	28 (12%)	1 (0%)	30	61
11	H	189/191 (99%)	178 (94%)	10 (5%)	1 (0%)	25	55
12	I	209/221 (95%)	193 (92%)	16 (8%)	0	100	100
13	J	167/174 (96%)	143 (86%)	18 (11%)	6 (4%)	3	17
14	L	192/199 (96%)	170 (88%)	20 (10%)	2 (1%)	13	40
15	M	135/138 (98%)	133 (98%)	2 (2%)	0	100	100
16	N	201/204 (98%)	187 (93%)	13 (6%)	1 (0%)	25	55
17	O	195/199 (98%)	193 (99%)	2 (1%)	0	100	100
18	P	181/184 (98%)	176 (97%)	5 (3%)	0	100	100
19	Q	183/186 (98%)	174 (95%)	8 (4%)	1 (0%)	25	55
20	R	154/189 (82%)	148 (96%)	5 (3%)	1 (1%)	22	51
21	S	169/172 (98%)	163 (96%)	6 (4%)	0	100	100
22	T	157/160 (98%)	151 (96%)	4 (2%)	2 (1%)	10	34
23	U	100/121 (83%)	95 (95%)	5 (5%)	0	100	100
24	V	134/137 (98%)	130 (97%)	4 (3%)	0	100	100
25	W	61/155 (39%)	57 (93%)	3 (5%)	1 (2%)	8	29
26	X	118/142 (83%)	109 (92%)	9 (8%)	0	100	100
27	Y	124/127 (98%)	118 (95%)	5 (4%)	1 (1%)	16	45
28	Z	133/136 (98%)	112 (84%)	18 (14%)	3 (2%)	5	24
29	a	146/149 (98%)	132 (90%)	13 (9%)	1 (1%)	19	48
30	b	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
31	c	98/105 (93%)	92 (94%)	6 (6%)	0	100	100
32	d	107/113 (95%)	97 (91%)	8 (8%)	2 (2%)	6	26
33	e	127/130 (98%)	120 (94%)	7 (6%)	0	100	100
34	f	104/107 (97%)	100 (96%)	4 (4%)	0	100	100
35	g	110/121 (91%)	104 (94%)	5 (4%)	1 (1%)	14	43
36	h	117/120 (98%)	109 (93%)	8 (7%)	0	100	100
37	i	97/100 (97%)	86 (89%)	8 (8%)	3 (3%)	3	19
38	j	85/88 (97%)	77 (91%)	8 (9%)	0	100	100
39	k	75/78 (96%)	70 (93%)	4 (5%)	1 (1%)	10	34
40	l	48/51 (94%)	47 (98%)	1 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	m	50/128 (39%)	46 (92%)	3 (6%)	1 (2%)	6	25
42	o	103/106 (97%)	94 (91%)	9 (9%)	0	100	100
43	p	89/92 (97%)	82 (92%)	7 (8%)	0	100	100
44	q	116/312 (37%)	111 (96%)	4 (3%)	1 (1%)	14	43
45	x	577/616 (94%)	544 (94%)	32 (6%)	1 (0%)	44	73
46	y	201/401 (50%)	191 (95%)	10 (5%)	0	100	100
All	All	6958/7887 (88%)	6511 (94%)	407 (6%)	40 (1%)	24	51

5 of 40 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	E	98	VAL
13	J	10	ARG
13	J	95	ASN
16	N	184	LYS
25	W	25	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A	166/196 (85%)	133 (80%)	33 (20%)	1	3
5	B	321/323 (99%)	260 (81%)	61 (19%)	1	4
6	C	288/289 (100%)	234 (81%)	54 (19%)	1	4
7	D	243/245 (99%)	209 (86%)	34 (14%)	3	11
8	E	135/136 (99%)	123 (91%)	12 (9%)	8	27
9	F	187/205 (91%)	168 (90%)	19 (10%)	6	22
10	G	177/208 (85%)	150 (85%)	27 (15%)	2	9
11	H	171/171 (100%)	148 (86%)	23 (14%)	3	12
12	I	179/187 (96%)	153 (86%)	26 (14%)	2	10
13	J	147/150 (98%)	122 (83%)	25 (17%)	1	7

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	L	154/159 (97%)	126 (82%)	28 (18%)	1	5
15	M	108/109 (99%)	95 (88%)	13 (12%)	4	16
16	N	175/176 (99%)	143 (82%)	32 (18%)	1	5
17	O	160/162 (99%)	129 (81%)	31 (19%)	1	3
18	P	145/146 (99%)	118 (81%)	27 (19%)	1	4
19	Q	150/151 (99%)	127 (85%)	23 (15%)	2	9
20	R	129/154 (84%)	106 (82%)	23 (18%)	1	5
21	S	155/156 (99%)	131 (84%)	24 (16%)	2	9
22	T	136/137 (99%)	113 (83%)	23 (17%)	1	7
23	U	89/107 (83%)	80 (90%)	9 (10%)	6	22
24	V	104/105 (99%)	93 (89%)	11 (11%)	5	20
25	W	55/129 (43%)	52 (94%)	3 (6%)	18	43
26	X	104/118 (88%)	86 (83%)	18 (17%)	1	6
27	Y	109/110 (99%)	96 (88%)	13 (12%)	4	16
28	Z	115/116 (99%)	92 (80%)	23 (20%)	1	3
29	a	118/119 (99%)	106 (90%)	12 (10%)	6	22
30	b	46/47 (98%)	38 (83%)	8 (17%)	1	6
31	c	84/88 (96%)	70 (83%)	14 (17%)	2	7
32	d	94/97 (97%)	85 (90%)	9 (10%)	7	24
33	e	110/111 (99%)	94 (86%)	16 (14%)	2	10
34	f	90/91 (99%)	84 (93%)	6 (7%)	13	38
35	g	95/103 (92%)	84 (88%)	11 (12%)	4	17
36	h	103/105 (98%)	84 (82%)	19 (18%)	1	5
37	i	80/82 (98%)	61 (76%)	19 (24%)	0	1
38	j	70/71 (99%)	59 (84%)	11 (16%)	2	8
39	k	67/69 (97%)	60 (90%)	7 (10%)	5	21
40	l	45/46 (98%)	35 (78%)	10 (22%)	1	2
41	m	47/116 (40%)	41 (87%)	6 (13%)	3	14
42	o	90/91 (99%)	72 (80%)	18 (20%)	1	3
43	p	71/72 (99%)	54 (76%)	17 (24%)	0	1
44	q	105/254 (41%)	88 (84%)	17 (16%)	2	8

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	x	508/540 (94%)	469 (92%)	39 (8%)	10	33
46	y	187/355 (53%)	171 (91%)	16 (9%)	8	28
All	All	5912/6602 (90%)	5042 (85%)	870 (15%)	5	10

5 of 870 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
19	Q	161	LYS
26	X	117	ASN
44	q	7	LYS
20	R	49	THR
19	Q	150	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 107 such sidechains are listed below:

Mol	Chain	Res	Type
22	T	16	GLN
30	b	6	ASN
45	x	405	ASN
22	T	77	ASN
26	X	65	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	5	3084/3396 (90%)	669 (21%)	73 (2%)
2	7	120/121 (99%)	14 (11%)	0
3	8	157/158 (99%)	36 (22%)	5 (3%)
All	All	3361/3675 (91%)	719 (21%)	78 (2%)

5 of 719 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	5	14	U
1	5	15	C
1	5	22	G
1	5	26	A
1	5	40	A

5 of 78 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	5	2872	A
1	5	3341	U
1	5	2971	A
1	5	3195	U
3	8	88	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	Y5P	5	1993	1	14,19,20	2.34	1 (7%)	18,26,29	1.01	1 (5%)
1	P5P	5	2017	1	16,23,24	0.78	0	14,33,36	0.77	0
1	P5P	5	2021	1	16,23,24	0.78	0	14,33,36	0.75	0
1	Y5P	5	1987	1	14,19,20	2.32	1 (7%)	18,26,29	1.03	1 (5%)
1	Y5P	5	1992	1	14,19,20	2.22	1 (7%)	18,26,29	1.04	1 (5%)
1	Y5P	5	1989	1	14,19,20	2.31	1 (7%)	18,26,29	0.98	1 (5%)
1	Y5P	5	1991	1	14,19,20	2.35	1 (7%)	18,26,29	1.01	1 (5%)
1	Y5P	5	1988	1	14,19,20	2.28	1 (7%)	18,26,29	1.03	1 (5%)
1	P5P	5	2025	1	16,23,24	0.77	0	14,33,36	0.75	0
1	P5P	5	2016	1	16,23,24	0.77	0	14,33,36	0.76	0
1	P5P	5	2020	1	16,23,24	0.77	0	14,33,36	0.78	0
1	P5P	5	2022	1	16,23,24	0.78	0	14,33,36	0.79	0
1	P5P	5	2018	1	16,23,24	0.79	0	14,33,36	0.77	0
1	Y5P	5	1995	1	14,19,20	2.31	1 (7%)	18,26,29	0.97	1 (5%)
1	Y5P	5	1986	1	14,19,20	2.27	1 (7%)	18,26,29	1.02	1 (5%)
1	P5P	5	2023	1	16,23,24	0.81	0	14,33,36	0.83	0
1	Y5P	5	1990	1	14,19,20	2.28	1 (7%)	18,26,29	1.06	1 (5%)
1	P5P	5	2019	1	16,23,24	0.79	0	14,33,36	0.80	0
1	Y5P	5	1994	1	14,19,20	2.30	1 (7%)	18,26,29	1.06	1 (5%)
1	P5P	5	2024	1	16,23,24	0.77	0	14,33,36	0.77	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
1	Y5P	5	1993	1	-	1/7/33/34	0/2/2/2
1	P5P	5	2017	1	-	0/3/25/26	0/3/3/3
1	P5P	5	2021	1	-	0/3/25/26	0/3/3/3
1	Y5P	5	1987	1	-	1/7/33/34	0/2/2/2
1	Y5P	5	1992	1	-	1/7/33/34	0/2/2/2
1	Y5P	5	1989	1	-	1/7/33/34	0/2/2/2
1	Y5P	5	1991	1	-	1/7/33/34	0/2/2/2
1	Y5P	5	1988	1	-	1/7/33/34	0/2/2/2
1	P5P	5	2025	1	-	0/3/25/26	0/3/3/3
1	P5P	5	2016	1	-	0/3/25/26	0/3/3/3
1	P5P	5	2020	1	-	0/3/25/26	0/3/3/3
1	P5P	5	2022	1	-	0/3/25/26	0/3/3/3
1	P5P	5	2018	1	-	0/3/25/26	0/3/3/3
1	Y5P	5	1995	1	-	1/7/33/34	0/2/2/2
1	Y5P	5	1986	1	-	1/7/33/34	0/2/2/2
1	P5P	5	2023	1	-	0/3/25/26	0/3/3/3
1	Y5P	5	1990	1	-	1/7/33/34	0/2/2/2
1	P5P	5	2019	1	-	0/3/25/26	0/3/3/3
1	Y5P	5	1994	1	-	1/7/33/34	0/2/2/2
1	P5P	5	2024	1	-	0/3/25/26	0/3/3/3

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	1991	Y5P	C4-N3	-8.62	1.38	1.46
1	5	1993	Y5P	C4-N3	-8.54	1.38	1.46
1	5	1987	Y5P	C4-N3	-8.51	1.38	1.46
1	5	1995	Y5P	C4-N3	-8.46	1.38	1.46
1	5	1989	Y5P	C4-N3	-8.45	1.38	1.46

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	1986	Y5P	N1-C2-N3	-3.75	114.34	125.33
1	5	1994	Y5P	N1-C2-N3	-3.74	114.37	125.33
1	5	1992	Y5P	N1-C2-N3	-3.69	114.50	125.33
1	5	1990	Y5P	N1-C2-N3	-3.68	114.53	125.33
1	5	1988	Y5P	N1-C2-N3	-3.66	114.61	125.33

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	5	1987	Y5P	O4'-C1'-N1-C2
1	5	1989	Y5P	O4'-C1'-N1-C2
1	5	1990	Y5P	O4'-C1'-N1-C2
1	5	1991	Y5P	O4'-C1'-N1-C2
1	5	1993	Y5P	O4'-C1'-N1-C2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 286 ligands modelled in this entry, 286 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
47	z	2
1	5	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	z	107:UNK	C	115:UNK	N	20.22
1	5	1995:Y5P	O3'	2016:P5P	P	17.42
1	z	127:UNK	C	131:UNK	N	9.67

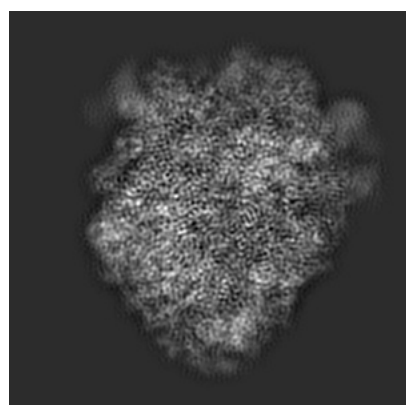
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3151. These allow visual inspection of the internal detail of the map and identification of artifacts.

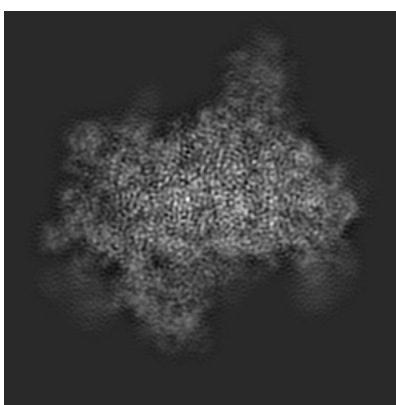
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

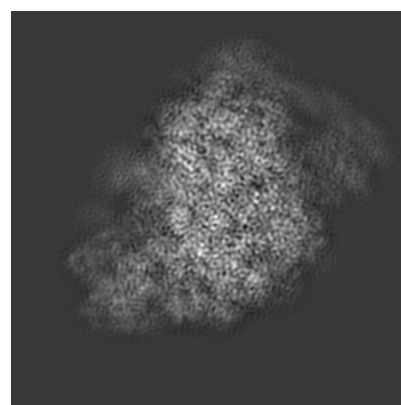
6.1.1 Primary map



X



Y

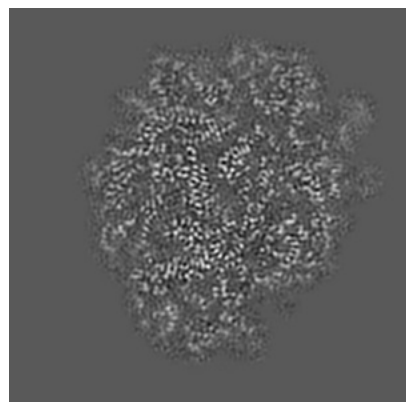


Z

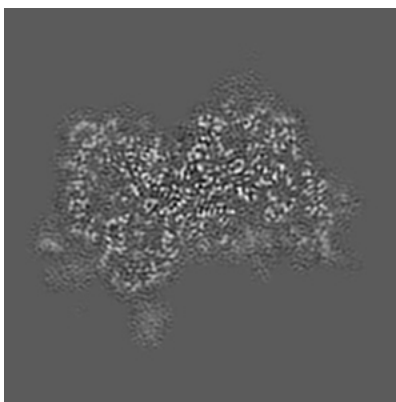
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

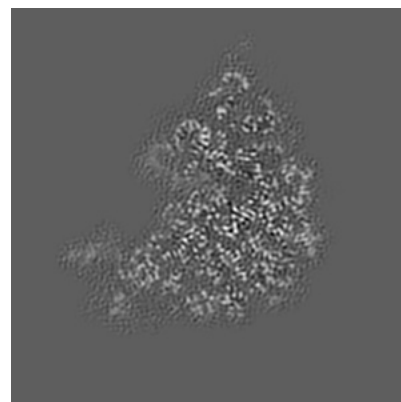
6.2.1 Primary map



X Index: 108



Y Index: 108

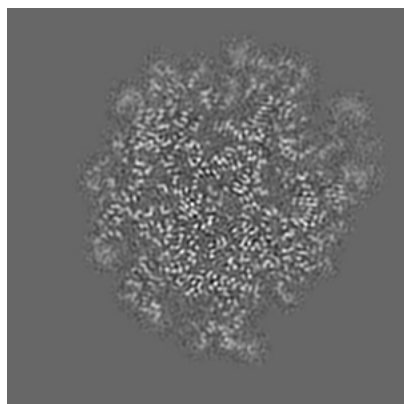


Z Index: 108

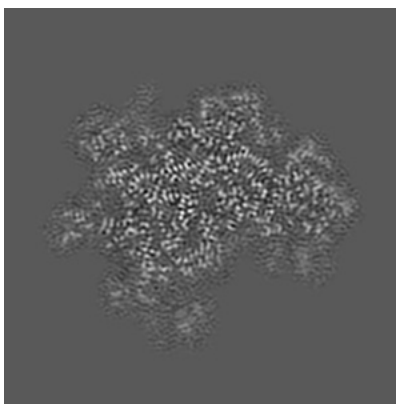
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 116



Y Index: 91

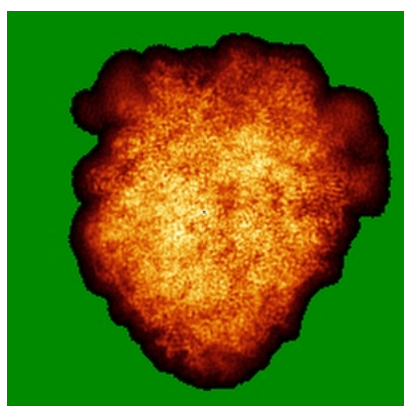


Z Index: 94

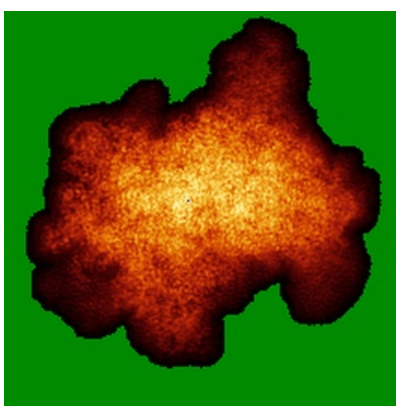
The images above show the largest variance slices of the map in three orthogonal directions.

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

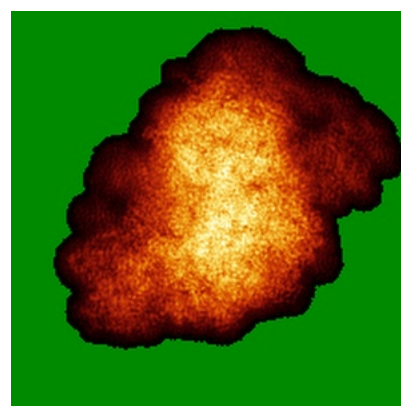
6.4.1 Primary map



X



Y

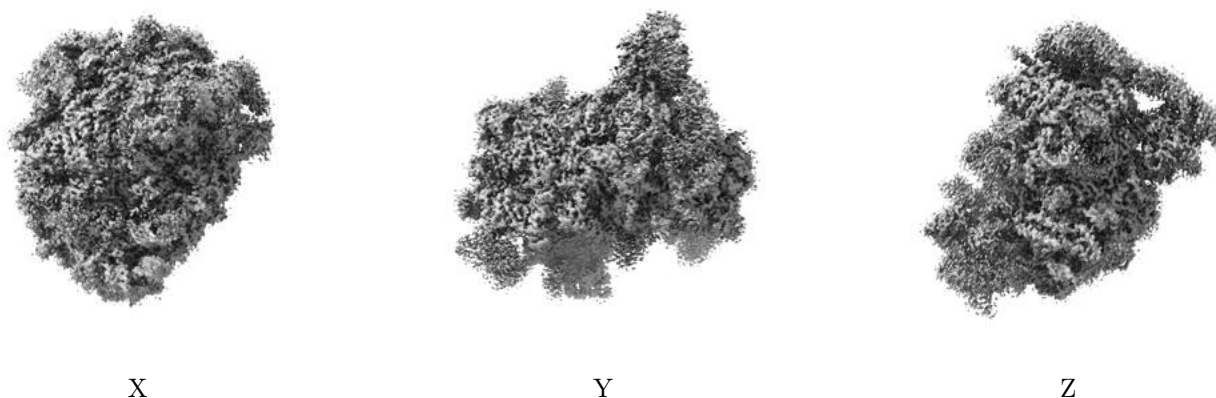


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

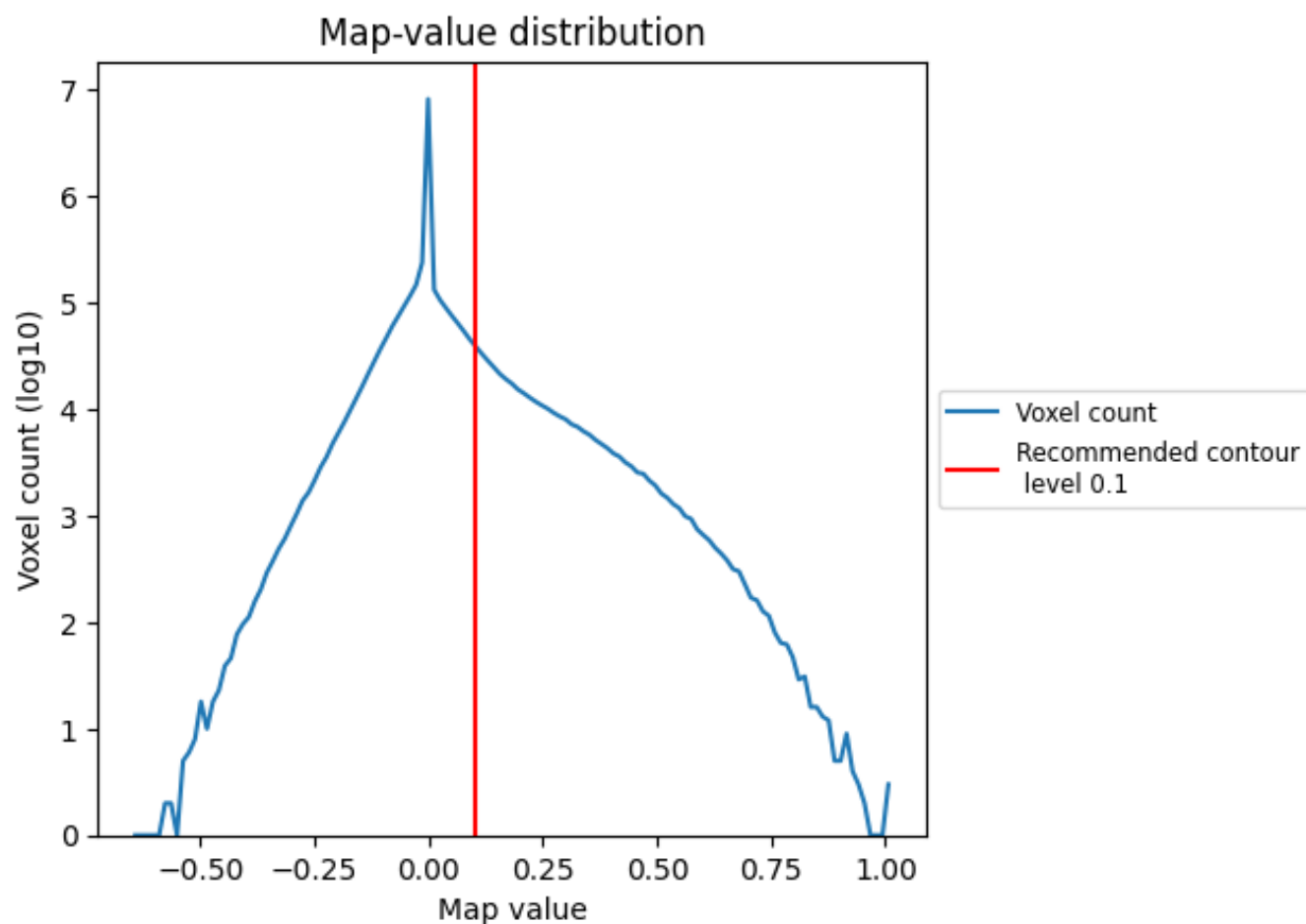
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

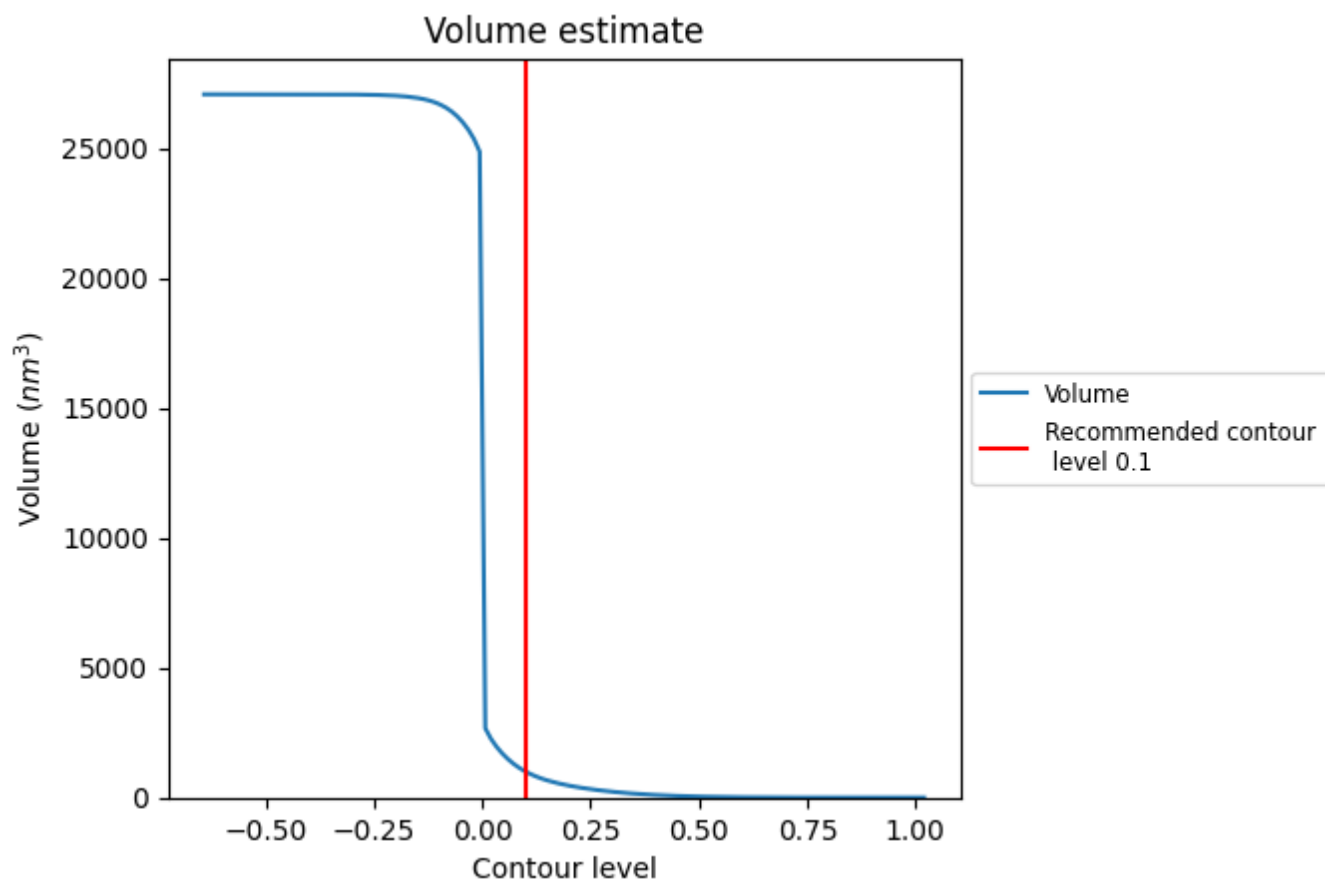
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

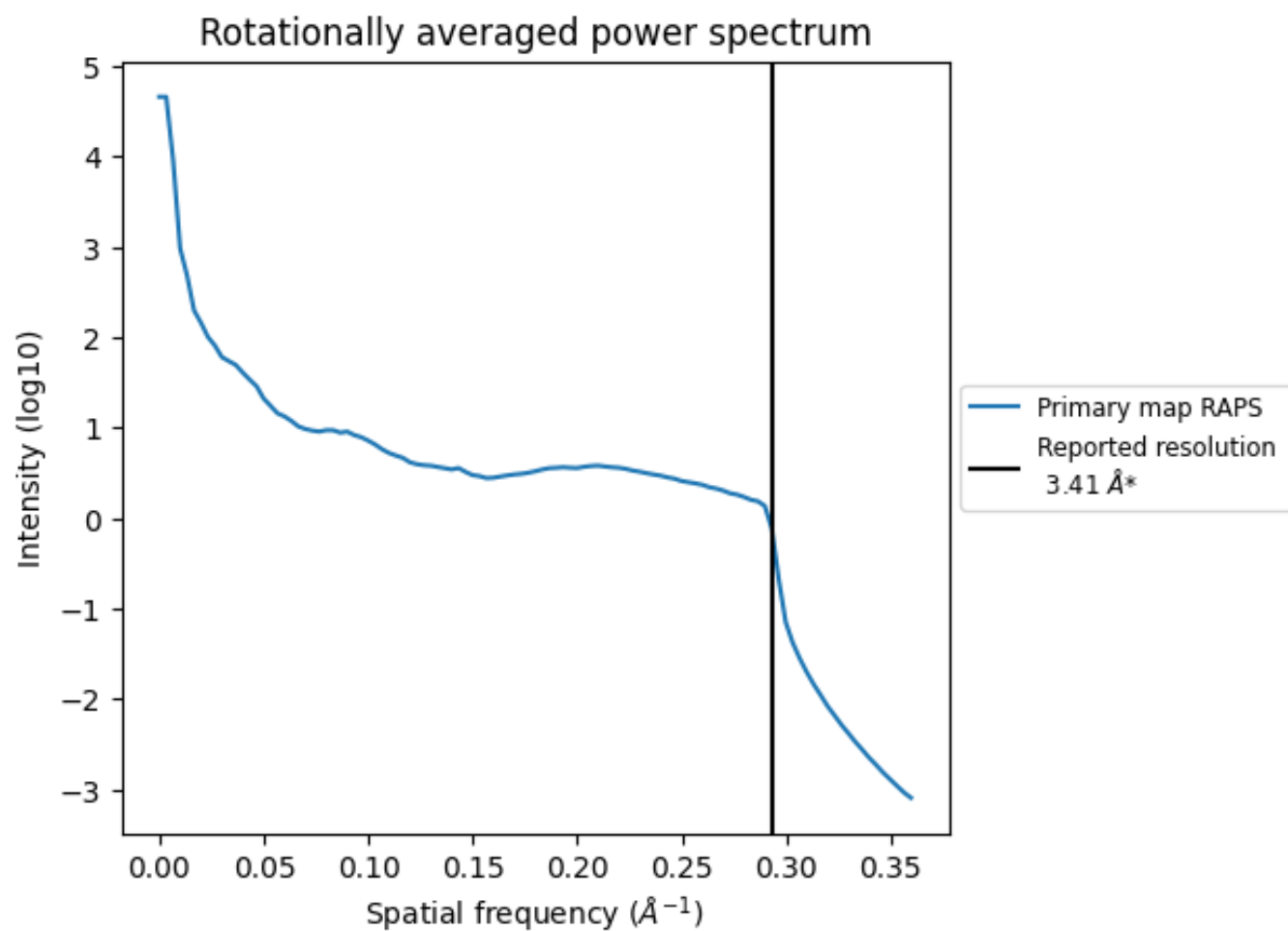
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1001 nm³; this corresponds to an approximate mass of 904 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 0.293 Å⁻¹

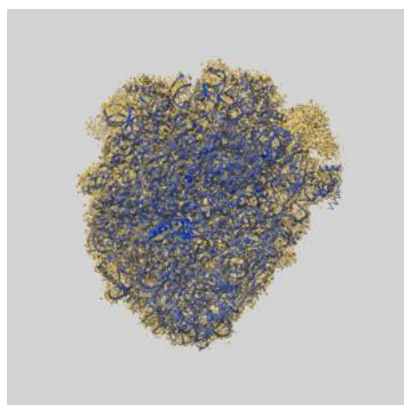
8 Fourier-Shell correlation

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

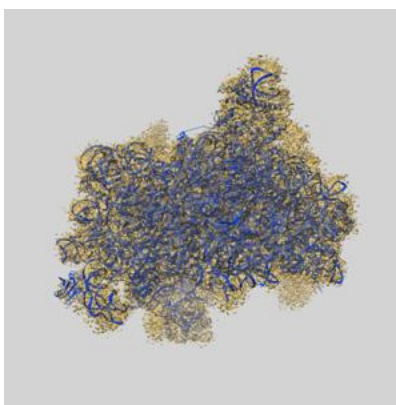
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3151 and PDB model 5APO. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

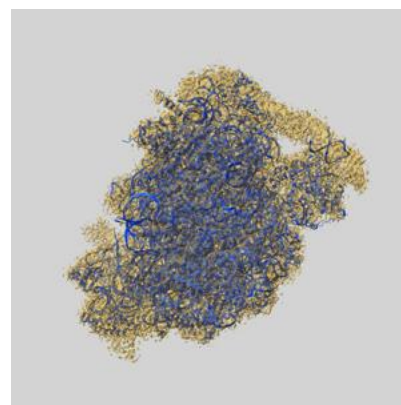
9.1 Map-model overlay [i](#)



X



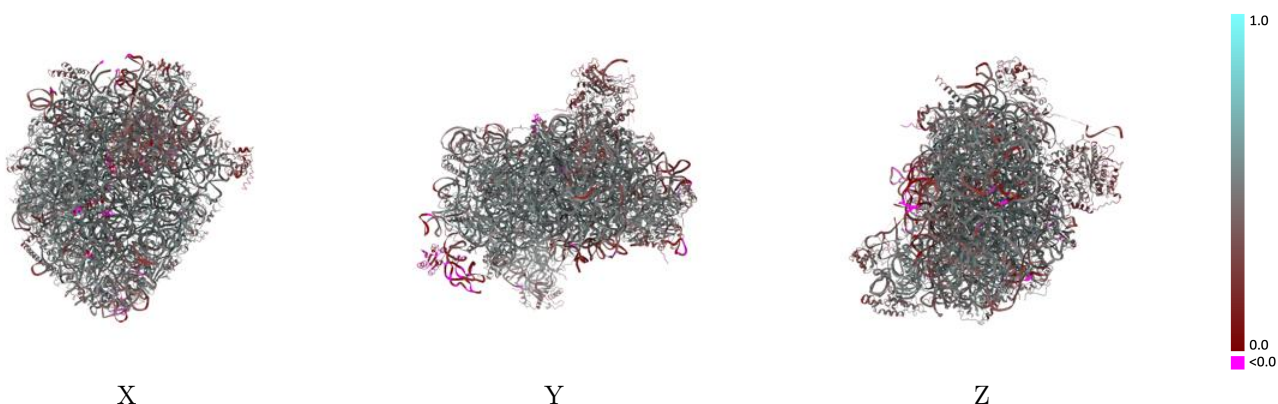
Y



Z

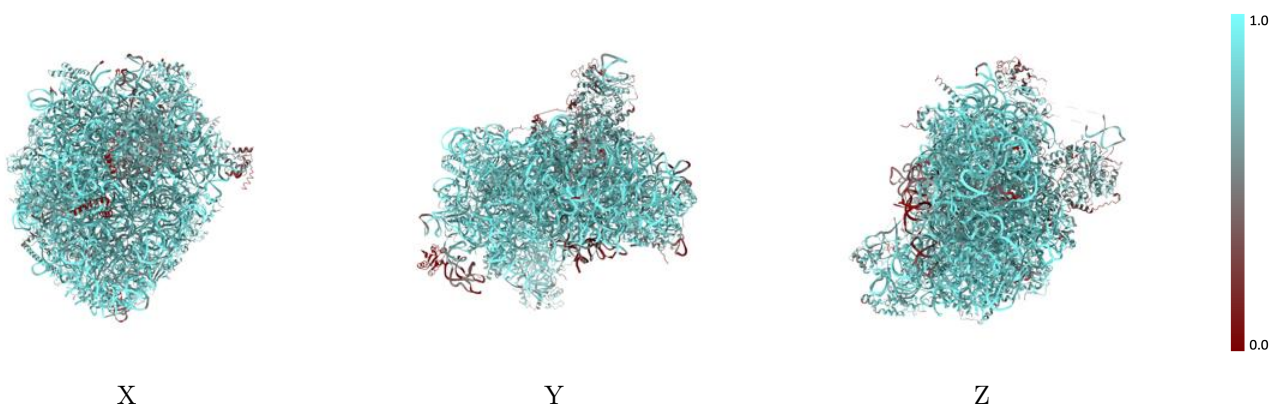
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



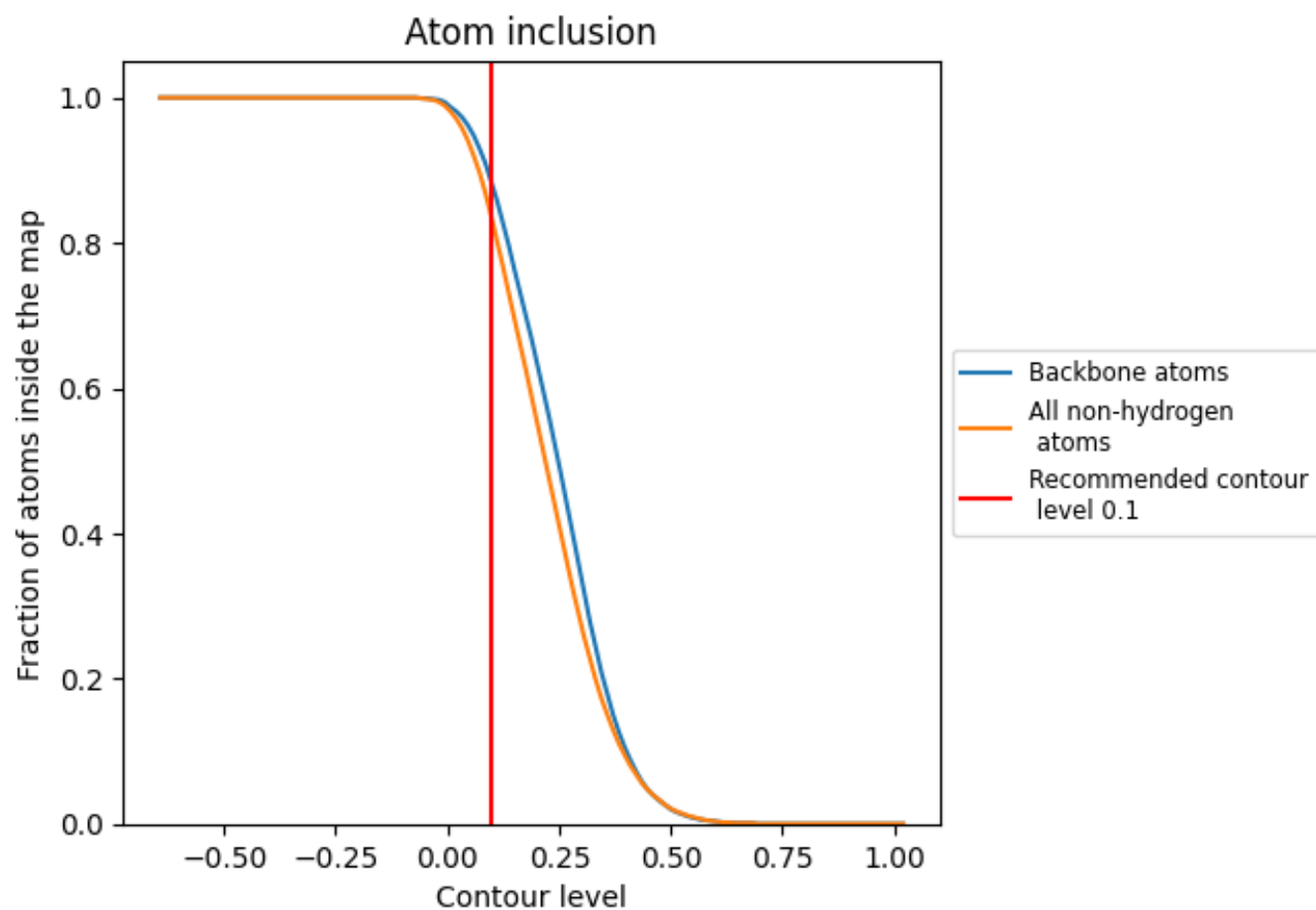
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 83% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ



























The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8320	 0.4600
5	 0.8790	 0.4610
7	 0.9300	 0.4640
8	 0.9160	 0.4870
A	 0.8160	 0.5030
B	 0.8610	 0.5040
C	 0.8540	 0.5080
D	 0.7770	 0.4220
E	 0.7700	 0.4440
F	 0.8600	 0.5080
G	 0.7920	 0.4370
H	 0.8090	 0.4780
I	 0.7880	 0.4720
J	 0.7020	 0.3630
L	 0.8340	 0.4890
M	 0.8430	 0.4840
N	 0.8130	 0.5010
O	 0.8650	 0.5110
P	 0.8180	 0.5010
Q	 0.8520	 0.5180
R	 0.8170	 0.4810
S	 0.8480	 0.5050
T	 0.8160	 0.4920
U	 0.7240	 0.4450
V	 0.8220	 0.4870
W	 0.8260	 0.4880
X	 0.8120	 0.4890
Y	 0.8170	 0.4890
Z	 0.7700	 0.4300
a	 0.8570	 0.5030
b	 0.7630	 0.4570
c	 0.7300	 0.4050
d	 0.7670	 0.4720
e	 0.8480	 0.5200
f	 0.8760	 0.5270



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
g	 0.7980	 0.4900
h	 0.8130	 0.4970
i	 0.7450	 0.4320
j	 0.8830	 0.5260
k	 0.6920	 0.4240
l	 0.8360	 0.5070
m	 0.7850	 0.4820
o	 0.6490	 0.4210
p	 0.8010	 0.4720
q	 0.0520	 0.0480
x	 0.6010	 0.3600
y	 0.5160	 0.3680
z	 0.1490	 0.1330