Full wwPDB EM Validation Report (i)

Nov 7, 2022 – 04:55 PM JST

PDB ID	:	5XY3
EMDB ID	:	EMD-6784
Title	:	Large subunit of Trichomonas vaginalis ribosome
Authors	:	Li, Z.; Guo, Q.; Zheng, L.; Ji, Y.; Xie, Y.; Lai, D.; Lun, Z.; Suo, X.; Gao, N.
Deposited on	:	2017-07-06
Resolution	:	3.20 Å(reported)

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

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

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

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

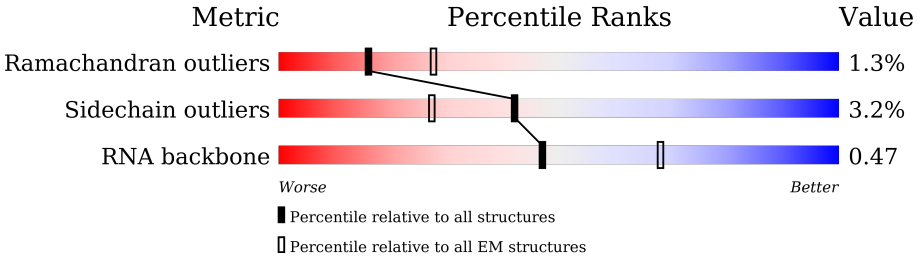
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	1	2765	• 72% 20% 8%
2	3	118	76% 23% •
3	4	162	7% 69% 26% 5%
4	A	251	7% 90% • 6%
5	B	415	8% 92% • •
6	C	370	8% 93% 5% •
7	D	308	11% 87% • 12%
8	E	151	26% 81% 8% 11%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	F	239	6% 95%
10	G	244	16% 68% 29%
11	H	197	22% 92% 5%
12	I	209	10% 90% 7%
13	J	169	34% 93%
14	L	189	17% 95%
15	M	128	14% 91% 5%
16	N	204	92% 7%
17	O	200	8% 94%
18	P	164	5% 93% 5%
19	Q	186	5% 96%
20	R	178	13% 89% 9%
21	S	176	5% 94% 5%
22	T	159	9% 97%
23	U	106	18% 89% 8%
24	V	140	13% 90% 6%
25	W	113	25% 51% 48%
26	X	140	6% 71% 28%
27	Y	138	17% 95%
28	Z	139	45% 93%
29	a	151	7% 94% 5%
30	b	58	7% 83% 14%
31	c	112	52% 83% 14%
32	d	110	7% 87% 10%
33	e	132	7% 89% 5% 7%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	f	102	6% 86% 9% 5%
35	g	116	29% 97%
36	h	124	17% 97%
37	i	91	15% 79% 20%
38	j	81	88% 7% 5%
39	k	74	19% 91% 8%
40	l	51	14% 94%
41	m	132	7% 37% 61%
42	o	104	89% 11%
43	p	92	7% 96%

2 Entry composition (i)

There are 43 unique types of molecules in this entry. The entry contains 107145 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 25S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	1	2544	54325	24285	9748	17748	2544	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	3	117	2493	1112	449	815	117	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	4	154	3289	1472	595	1068	154	0	0

- Molecule 4 is a protein called Ribosomal protein L8, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	A	237	1785	1105	365	306	9	0	0

- Molecule 5 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	B	400	3175	2002	608	554	11	0	0

- Molecule 6 is a protein called Ribosomal protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	C	362	2772	1751	513	501	7	0	0

- Molecule 7 is a protein called Ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	D	272	2167	1384	394	384	5	0	0

- Molecule 8 is a protein called 60S ribosomal protein L6, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	E	135	1014	651	180	181	2	0	0

- Molecule 9 is a protein called Ribosomal protein L30p/L7e, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	F	231	1832	1174	330	324	4	0	0

- Molecule 10 is a protein called Ribosomal protein L7Ae, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	G	174	1384	892	245	239	8	0	0

- Molecule 11 is a protein called Ribosomal protein L6, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	H	192	1556	994	274	281	7	0	0

- Molecule 12 is a protein called Ribosomal protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	I	195	1569	989	304	264	12	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	J	164	1320	827	258	230	5	0	0

- Molecule 14 is a protein called Ribosomal protein L13e, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	L	185	1498	947	296	252	3	0	0

- Molecule 15 is a protein called Ribosomal protein L14, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	M	124	1004	650	176	177	1	0	0

- Molecule 16 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	N	202	1696	1076	343	271	6	0	0

- Molecule 17 is a protein called Ribosomal protein L13, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	O	196	1559	988	295	271	5	0	0

- Molecule 18 is a protein called Ribosomal protein L22, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	P	155	1230	781	231	211	7	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	Q	185	1465	907	295	255	8	0	0

- Molecule 20 is a protein called 60S ribosomal protein L19-3, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	R	162	1299	805	277	213	4	0	0

- Molecule 21 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	S	175	1384	882	252	247	3	0	0

- Molecule 22 is a protein called Ribosomal protein L21e, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	T	158	1255	797	249	207	2	0	0

- Molecule 23 is a protein called 60S ribosomal protein L22-1, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	U	97	794	511	140	141	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	V	134	986	622	185	172	7	0	0

- Molecule 25 is a protein called Ribosomal protein L24e, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	W	59	513	323	108	79	3	0	0

- Molecule 26 is a protein called Ribosomal protein L23, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	X	101	803	518	141	141	3	0	0

- Molecule 27 is a protein called Ribosomal protein L24, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	Y	134	1068	671	204	188	5	0	0

- Molecule 28 is a protein called Ribosomal protein L27e, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	Z	135	1042	682	184	172	4	0	0

- Molecule 29 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	a	149	1179	749	229	196	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	b	50	415	256	92	65	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	c	96	727	462	121	140	4	0	0

- Molecule 32 is a protein called Ribosomal protein L31e, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	d	99	783	497	149	134	3	0	0

- Molecule 33 is a protein called Ribosomal protein L32, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	e	123	1003	633	198	169	3	0	0

- Molecule 34 is a protein called Ribosomal protein L35Ae, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	f	97	781	511	137	131	2	0	0

- Molecule 35 is a protein called Ribosomal protein L34e, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	g	115	921	565	191	158	7	0	0

- Molecule 36 is a protein called Ribosomal protein L29, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	h	122	984	623	190	169	2	0	0

- Molecule 37 is a protein called Ribosomal protein L36e, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	i	73	616	385	128	101	2	0	0

- Molecule 38 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	j	77	616	380	128	101	7	0	0

- Molecule 39 is a protein called Ribosomal protein L38e, putative.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
39	k	68	547	358	90	99	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	l	50	428	267	97	59	5	0	0

- Molecule 41 is a protein called Ubiquitin, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	m	52	417	254	89	69	5	0	0

- Molecule 42 is a protein called 60S ribosomal protein L44, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	o	93	773	486	158	121	8	0	0

- Molecule 43 is a protein called Uncharacterized protein.

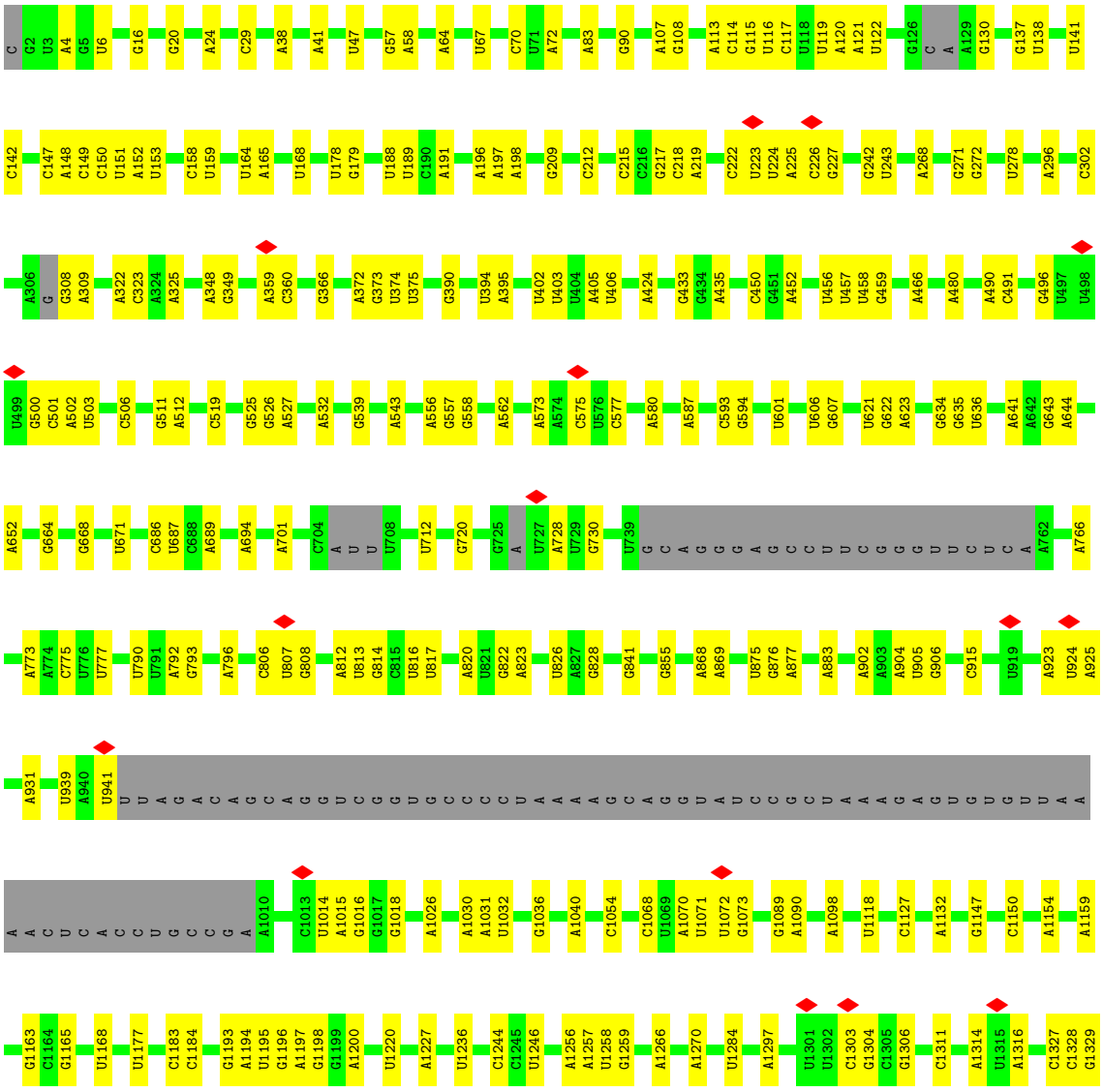
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	p	89	678	426	133	114	5	0	0

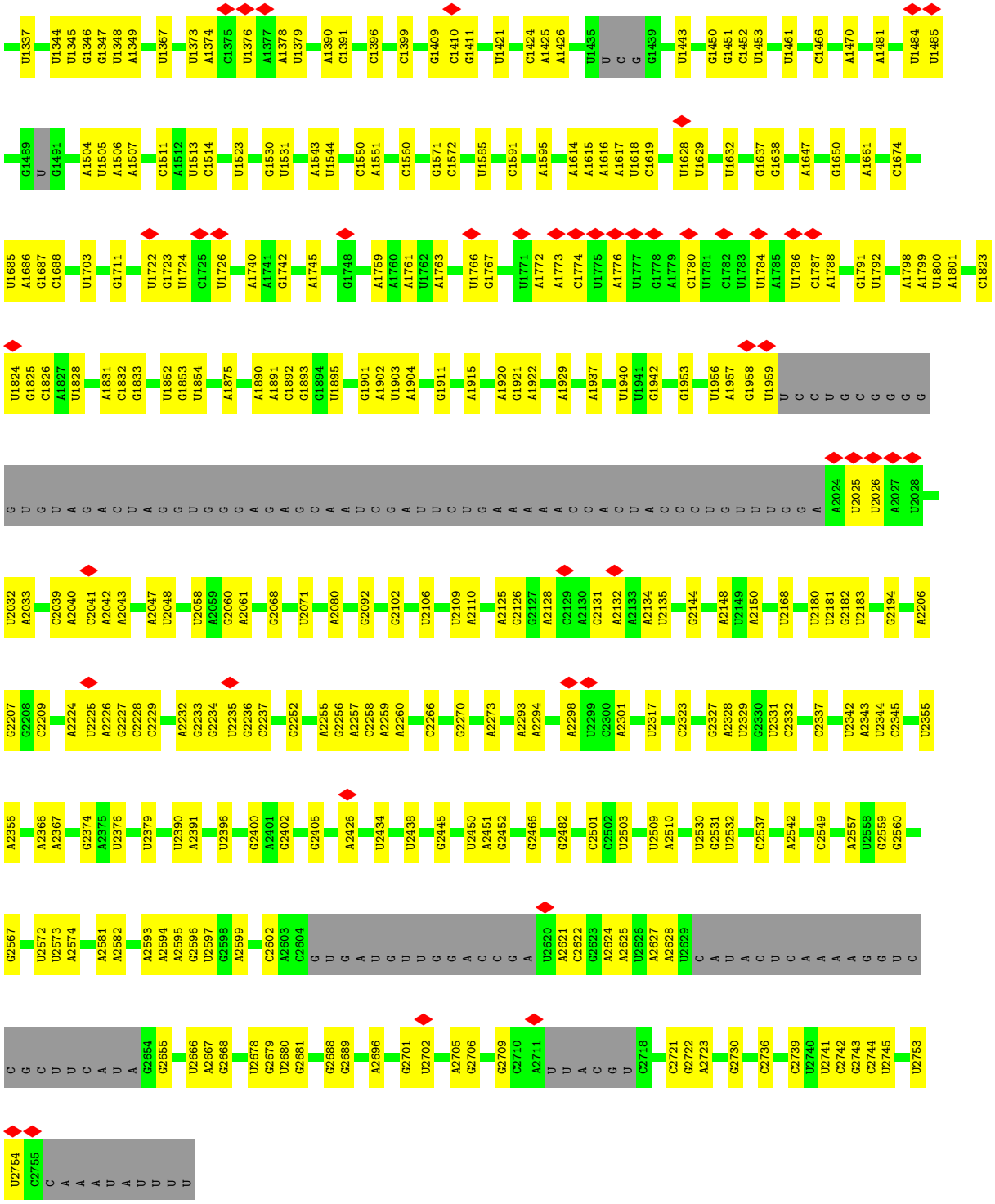
3 Residue-property plots (i)

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

- Molecule 1: 25S ribosomal RNA

Chain 1:



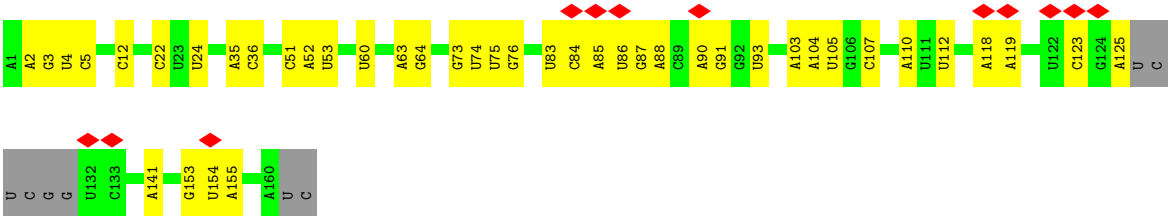


- Molecule 2: 5S ribosomal RNA

Chain 3:

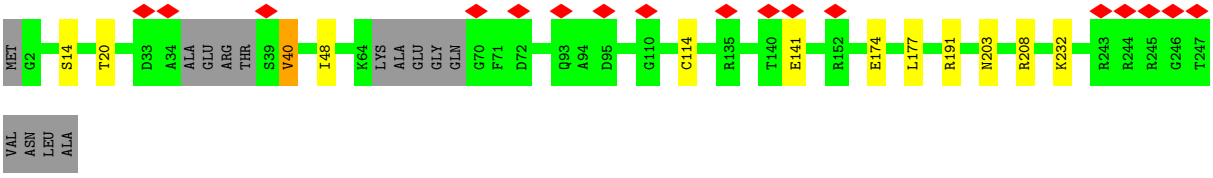
- Molecule 3: 5.8S ribosomal RNA

Chain 4: 7% 69% 26% 5%



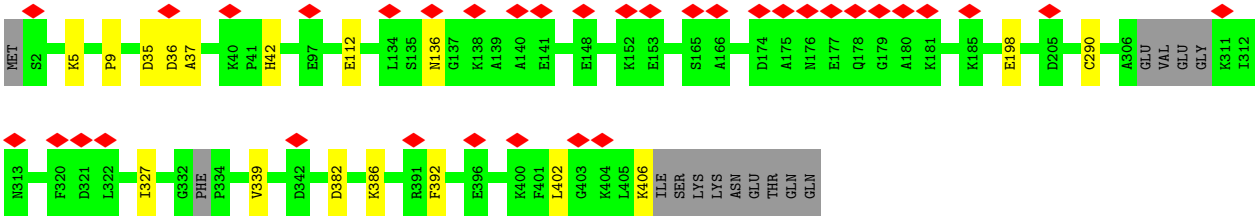
- Molecule 4: Ribosomal protein L8, putative

Chain A: 7% 90% 6%



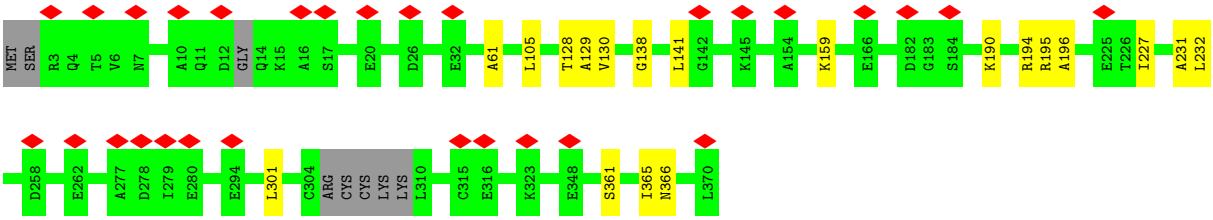
- Molecule 5: Uncharacterized protein

Chain B: 8% 92%



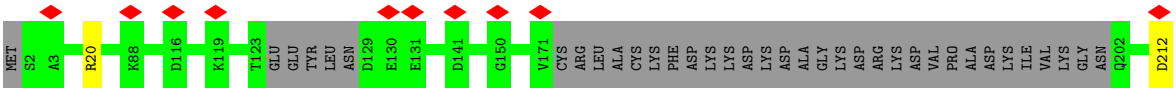
- Molecule 6: Ribosomal protein, putative

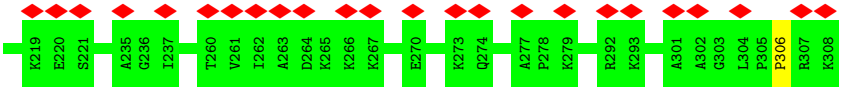
Chain C: 8% 93% 5%



- Molecule 7: Ribosomal protein L5

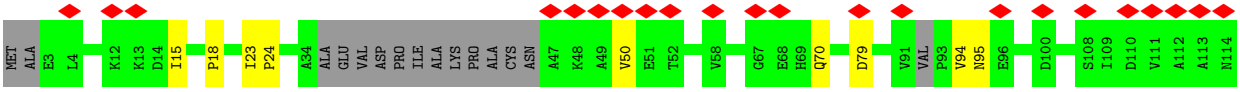
Chain D: 11% 87% 12%

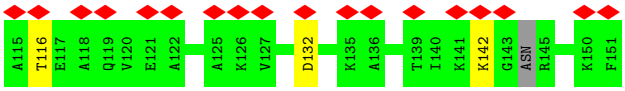




- Molecule 8: 60S ribosomal protein L6, putative

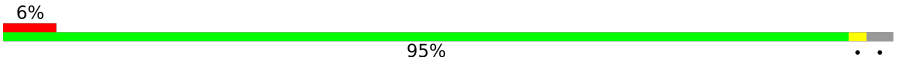
Chain E:

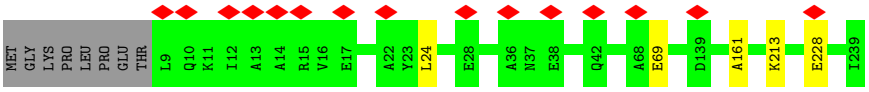




- Molecule 9: Ribosomal protein L30p/L7e, putative

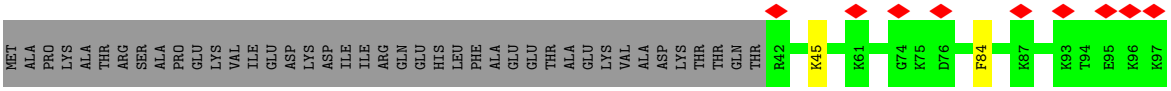
Chain F:

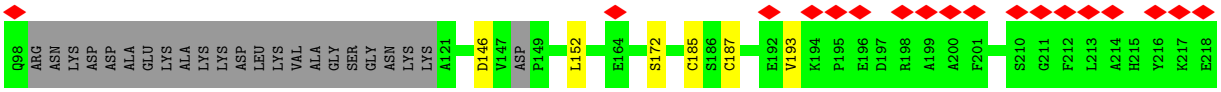


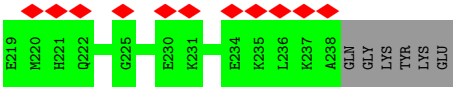


- Molecule 10: Ribosomal protein L7Ae, putative

Chain G:

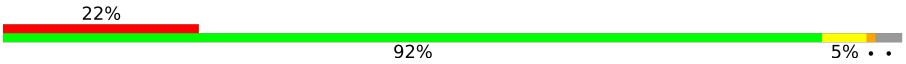


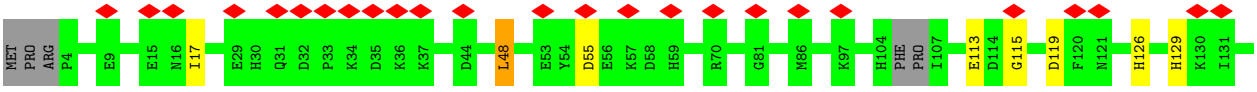


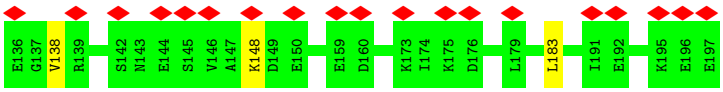


- Molecule 11: Ribosomal protein L6, putative

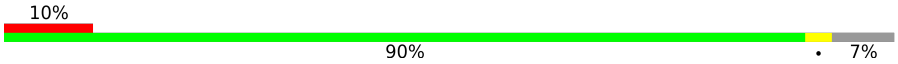
Chain H:

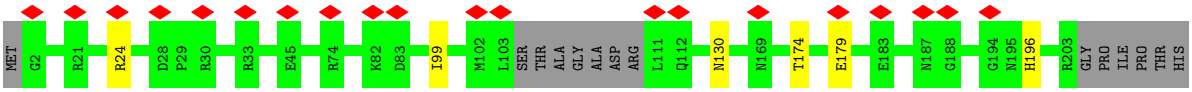




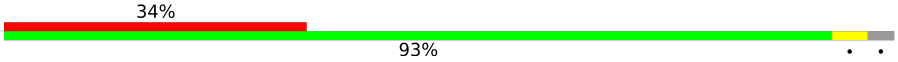


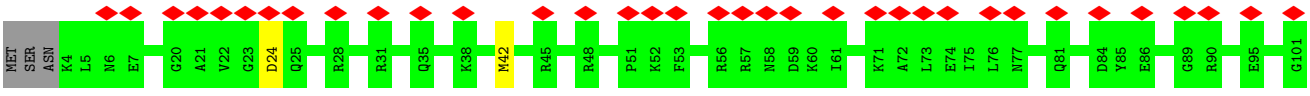
- Molecule 12: Ribosomal protein, putative

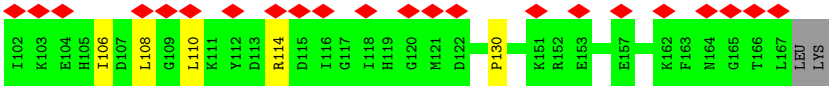
Chain I: 



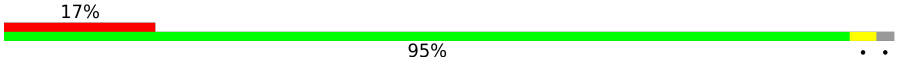
- Molecule 13: 60S ribosomal protein L11, putative

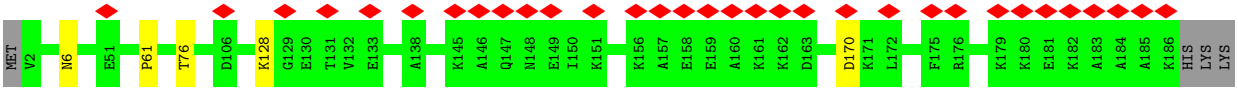
Chain J: 



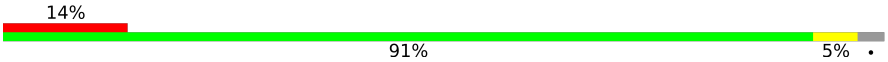


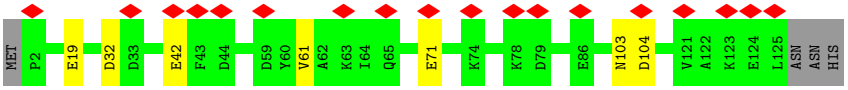
- Molecule 14: Ribosomal protein L13e, putative

Chain L: 



- Molecule 15: Ribosomal protein L14, putative

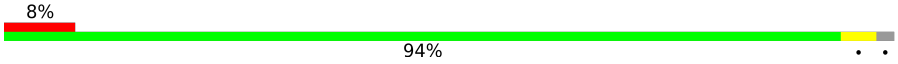
Chain M: 

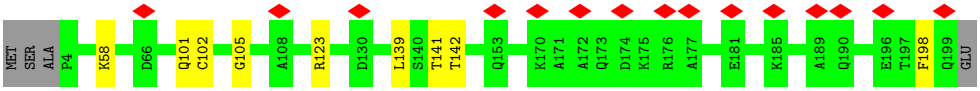


- Molecule 16: Ribosomal protein L15

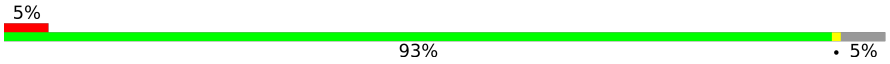
Chain N:

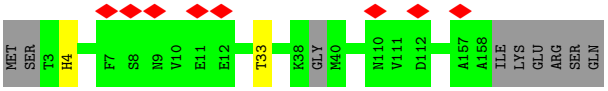
- Molecule 17: Ribosomal protein L13, putative

Chain O: 



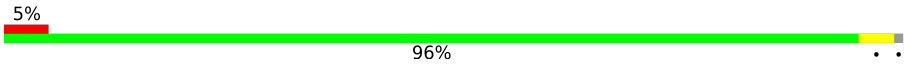
- Molecule 18: Ribosomal protein L22, putative

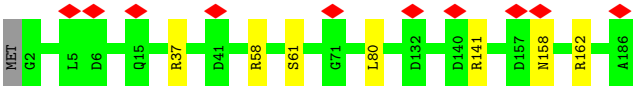
Chain P: 



• Molecule 19: 60S ribosomal protein L18, putative

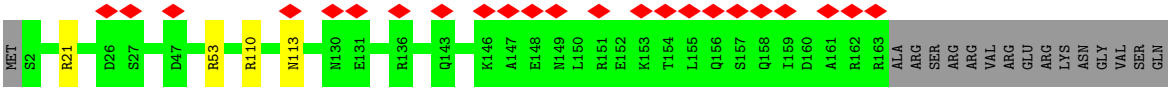
Chain Q:





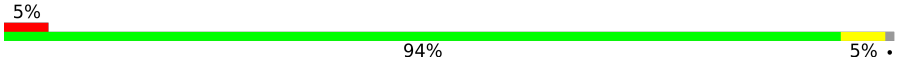
• Molecule 20: 60S ribosomal protein L19-3, putative

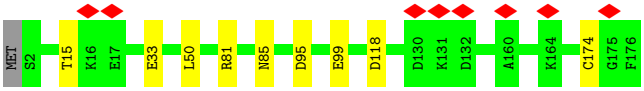
Chain R:



• Molecule 21: 60S ribosomal protein L18a

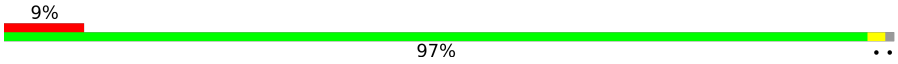
Chain S:

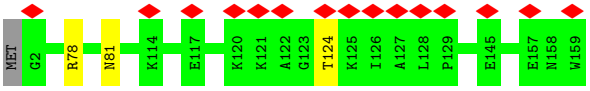




• Molecule 22: Ribosomal protein L21e, putative

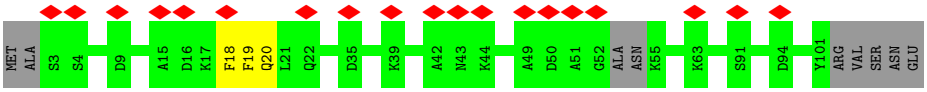
Chain T:





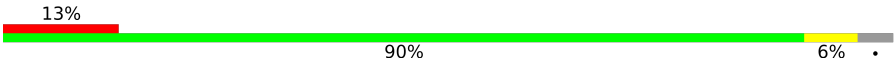
• Molecule 23: 60S ribosomal protein L22-1, putative

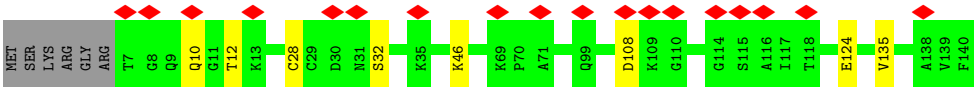
Chain U:



• Molecule 24: 60S ribosomal protein L23, putative

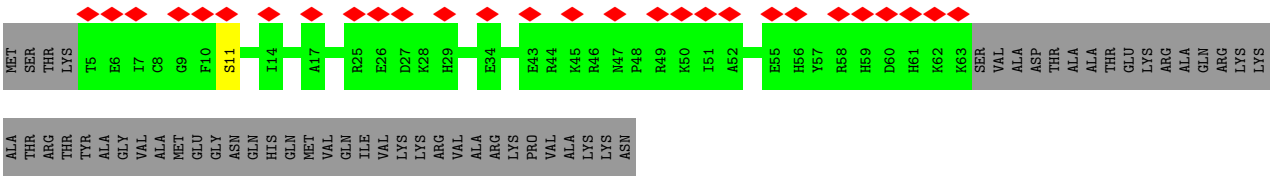
Chain V:





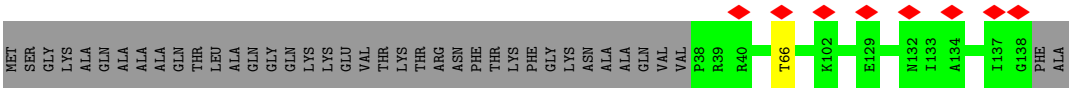
• Molecule 25: Ribosomal protein L24e, putative

Chain W:



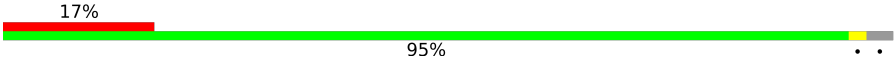
- Molecule 26: Ribosomal protein L23, putative

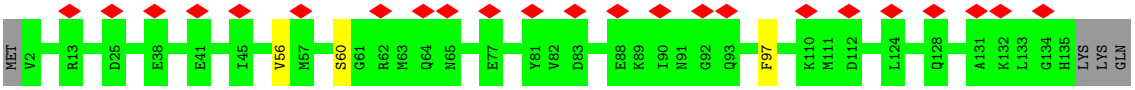
Chain X:



- Molecule 27: Ribosomal protein L24, putative

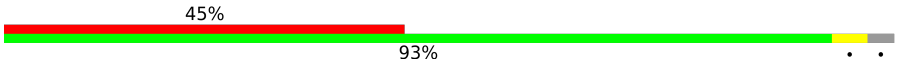
Chain Y:

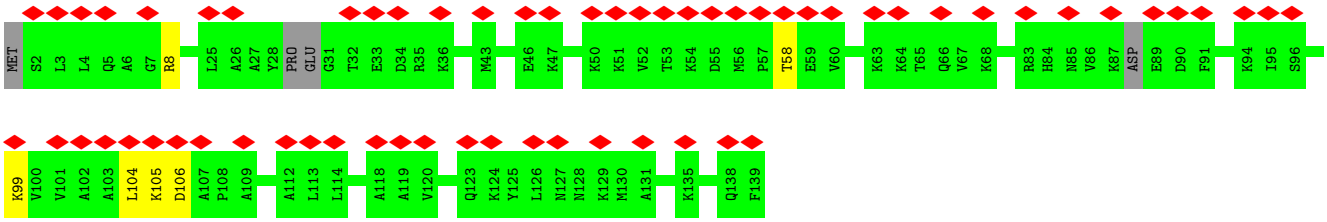




- Molecule 28: Ribosomal protein L27e, putative

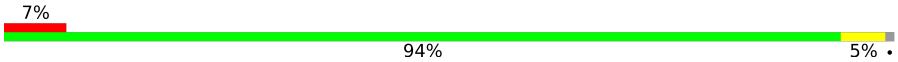
Chain Z:

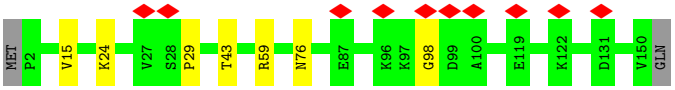




- Molecule 29: Uncharacterized protein

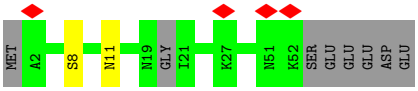
Chain a:





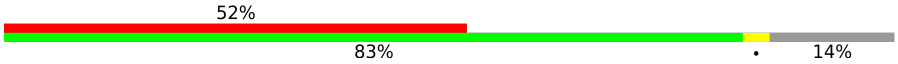
- Molecule 30: 60S ribosomal protein L29

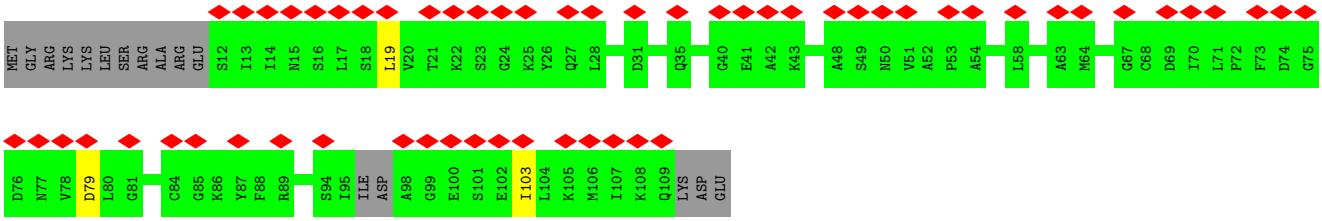
Chain b:



- Molecule 31: 60S ribosomal protein L30, putative

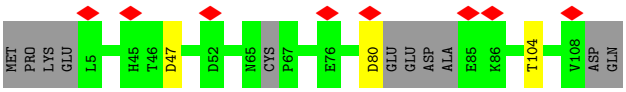
Chain c:





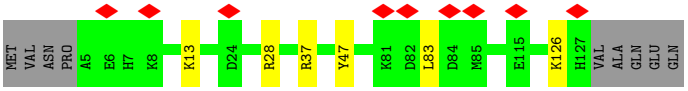
- Molecule 32: Ribosomal protein L31e, putative

Chain d:



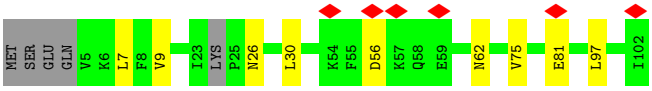
- Molecule 33: Ribosomal protein L32, putative

Chain e:



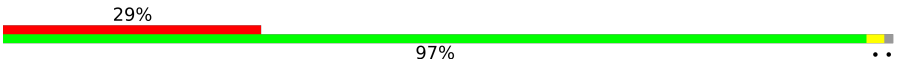
- Molecule 34: Ribosomal protein L35Ae, putative

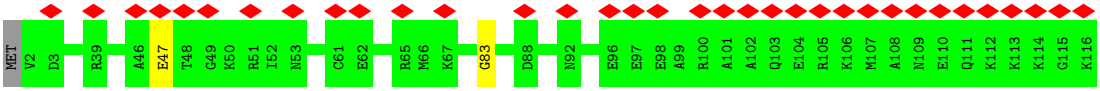
Chain f:



- Molecule 35: Ribosomal protein L34e, putative

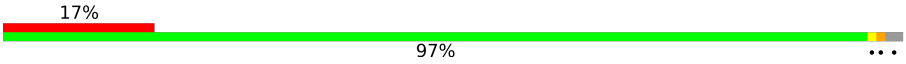
Chain g:

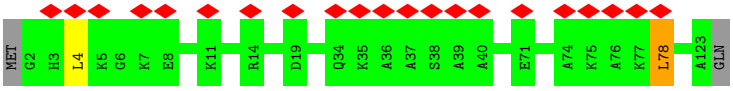




- Molecule 36: Ribosomal protein L29, putative

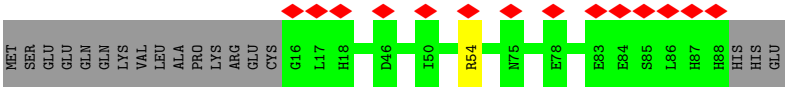
Chain h:





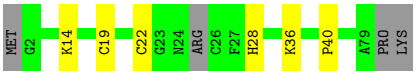
- Molecule 37: Ribosomal protein L36e, putative

Chain i:



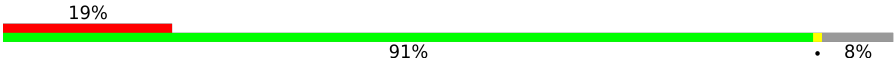
• Molecule 38: Ribosomal protein L37

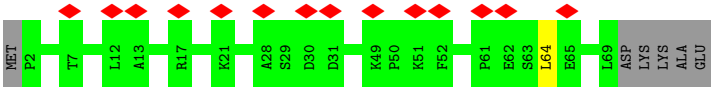
Chain j:



• Molecule 39: Ribosomal protein L38e, putative

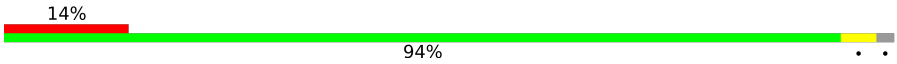
Chain k:

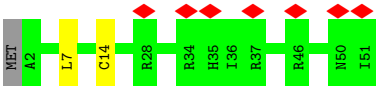




• Molecule 40: 60S ribosomal protein L39, putative

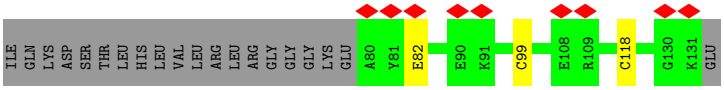
Chain l:





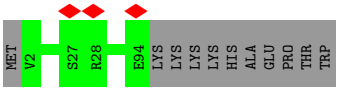
• Molecule 41: Ubiquitin, putative

Chain m:



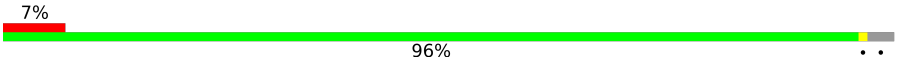
• Molecule 42: 60S ribosomal protein L44, putative

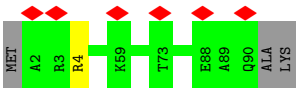
Chain o:



• Molecule 43: Uncharacterized protein

Chain p:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	57162	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	2	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.399	Depositor
Minimum map value	-0.231	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.044	Depositor
Map size (Å)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.32, 1.32, 1.32	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	1	0.20	0/60789	0.68	0/94723
2	3	0.20	0/2785	0.67	0/4339
3	4	0.20	0/3681	0.67	0/5732
4	A	0.38	0/1822	0.61	0/2450
5	B	0.36	0/3237	0.60	0/4340
6	C	0.38	0/2819	0.59	0/3816
7	D	0.37	0/2201	0.57	0/2950
8	E	0.42	0/1028	0.63	0/1388
9	F	0.36	0/1864	0.51	0/2507
10	G	0.46	0/1409	0.62	0/1892
11	H	0.34	0/1589	0.51	0/2136
12	I	0.37	0/1603	0.59	0/2151
13	J	0.35	0/1341	0.55	0/1797
14	L	0.35	0/1525	0.57	0/2042
15	M	0.34	0/1020	0.54	0/1371
16	N	0.38	0/1739	0.63	0/2332
17	O	0.39	0/1591	0.58	0/2141
18	P	0.33	0/1260	0.52	0/1701
19	Q	0.37	0/1488	0.63	0/1996
20	R	0.35	0/1314	0.59	0/1754
21	S	0.37	0/1416	0.55	0/1922
22	T	0.34	0/1288	0.55	0/1743
23	U	0.39	0/809	0.56	0/1085
24	V	0.34	0/1000	0.53	0/1346
25	W	0.37	0/530	0.56	0/705
26	X	0.34	0/819	0.46	0/1106
27	Y	0.35	0/1082	0.54	0/1447
28	Z	0.38	0/1061	0.51	0/1428
29	a	0.36	0/1209	0.55	0/1619
30	b	0.37	0/423	0.57	0/559
31	c	0.37	0/735	0.47	0/987
32	d	0.40	0/794	0.58	0/1065
33	e	0.34	0/1027	0.56	0/1381
34	f	0.41	0/799	0.60	0/1075

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
35	g	0.35	0/933	0.56	0/1243
36	h	0.37	0/993	0.57	0/1316
37	i	0.36	0/627	0.56	0/835
38	j	0.45	0/631	0.69	0/839
39	k	0.39	0/557	0.52	0/752
40	l	0.35	0/436	0.66	0/580
41	m	0.35	0/422	0.63	0/558
42	o	0.35	0/788	0.55	0/1038
43	p	0.35	0/688	0.58	0/919
All	All	0.28	0/115172	0.64	0/169106

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	231/251 (92%)	210 (91%)	18 (8%)	3 (1%)	12 47
5	B	394/415 (95%)	357 (91%)	32 (8%)	5 (1%)	12 47
6	C	356/370 (96%)	329 (92%)	16 (4%)	11 (3%)	4 26
7	D	266/308 (86%)	238 (90%)	26 (10%)	2 (1%)	19 58
8	E	127/151 (84%)	113 (89%)	8 (6%)	6 (5%)	2 17
9	F	229/239 (96%)	215 (94%)	11 (5%)	3 (1%)	12 47

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	G	168/244 (69%)	151 (90%)	14 (8%)	3 (2%)	8	41
11	H	188/197 (95%)	175 (93%)	8 (4%)	5 (3%)	5	30
12	I	191/209 (91%)	175 (92%)	15 (8%)	1 (0%)	29	67
13	J	162/169 (96%)	155 (96%)	5 (3%)	2 (1%)	13	49
14	L	183/189 (97%)	167 (91%)	14 (8%)	2 (1%)	14	51
15	M	122/128 (95%)	118 (97%)	3 (2%)	1 (1%)	19	58
16	N	198/204 (97%)	189 (96%)	9 (4%)	0	100	100
17	O	194/200 (97%)	188 (97%)	3 (2%)	3 (2%)	10	44
18	P	151/164 (92%)	138 (91%)	12 (8%)	1 (1%)	22	61
19	Q	183/186 (98%)	168 (92%)	14 (8%)	1 (0%)	29	67
20	R	160/178 (90%)	150 (94%)	9 (6%)	1 (1%)	25	64
21	S	173/176 (98%)	166 (96%)	7 (4%)	0	100	100
22	T	156/159 (98%)	145 (93%)	10 (6%)	1 (1%)	25	64
23	U	93/106 (88%)	83 (89%)	9 (10%)	1 (1%)	14	51
24	V	132/140 (94%)	124 (94%)	7 (5%)	1 (1%)	19	58
25	W	57/113 (50%)	54 (95%)	2 (4%)	1 (2%)	8	41
26	X	99/140 (71%)	92 (93%)	7 (7%)	0	100	100
27	Y	132/138 (96%)	124 (94%)	7 (5%)	1 (1%)	19	58
28	Z	129/139 (93%)	117 (91%)	8 (6%)	4 (3%)	4	26
29	a	147/151 (97%)	135 (92%)	8 (5%)	4 (3%)	5	30
30	b	46/58 (79%)	44 (96%)	2 (4%)	0	100	100
31	c	92/112 (82%)	86 (94%)	5 (5%)	1 (1%)	14	51
32	d	93/110 (84%)	91 (98%)	2 (2%)	0	100	100
33	e	121/132 (92%)	113 (93%)	5 (4%)	3 (2%)	5	32
34	f	93/102 (91%)	83 (89%)	8 (9%)	2 (2%)	6	35
35	g	113/116 (97%)	105 (93%)	6 (5%)	2 (2%)	8	41
36	h	120/124 (97%)	112 (93%)	7 (6%)	1 (1%)	19	58
37	i	71/91 (78%)	64 (90%)	7 (10%)	0	100	100
38	j	73/81 (90%)	69 (94%)	4 (6%)	0	100	100
39	k	66/74 (89%)	64 (97%)	2 (3%)	0	100	100
40	l	48/51 (94%)	43 (90%)	5 (10%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	m	50/132 (38%)	46 (92%)	3 (6%)	1 (2%)	7	38
42	o	91/104 (88%)	87 (96%)	4 (4%)	0	100	100
43	p	87/92 (95%)	82 (94%)	5 (6%)	0	100	100
All	All	5785/6443 (90%)	5365 (93%)	347 (6%)	73 (1%)	16	47

All (73) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	B	42	HIS
7	D	306	PRO
8	E	15	ILE
8	E	94	VAL
10	G	193	VAL
13	J	106	ILE
15	M	104	ASP
22	T	81	ASN
28	Z	58	THR
4	A	40	VAL
4	A	232	LYS
5	B	339	VAL
7	D	20	ARG
8	E	116	THR
9	F	161	ALA
10	G	172	SER
11	H	48	LEU
11	H	148	LYS
23	U	20	GLN
34	f	56	ASP
4	A	141	GLU
6	C	105	LEU
6	C	129	ALA
6	C	195	ARG
6	C	232	LEU
8	E	18	PRO
9	F	213	LYS
11	H	115	GLY
14	L	61	PRO
17	O	198	PHE
18	P	4	HIS
24	V	10	GLN
28	Z	106	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
31	c	103	ILE
33	e	126	LYS
34	f	7	LEU
6	C	138	GLY
6	C	196	ALA
6	C	361	SER
9	F	228	GLU
12	I	24	ARG
14	L	128	LYS
17	O	58	LYS
17	O	105	GLY
19	Q	162	ARG
28	Z	99	LYS
28	Z	105	LYS
33	e	47	TYR
35	g	47	GLU
41	m	82	GLU
6	C	61	ALA
6	C	130	VAL
6	C	231	ALA
6	C	365	ILE
8	E	24	PRO
10	G	45	LYS
13	J	130	PRO
25	W	11	SER
27	Y	60	SER
29	a	24	LYS
33	e	13	LYS
35	g	83	GLY
36	h	78	LEU
5	B	5	LYS
5	B	37	ALA
29	a	15	VAL
29	a	29	PRO
29	a	98	GLY
8	E	50	VAL
5	B	9	PRO
11	H	17	ILE
11	H	138	VAL
20	R	53	ARG

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A	181/191 (95%)	171 (94%)	10 (6%)	21	57
5	B	333/347 (96%)	321 (96%)	12 (4%)	35	69
6	C	294/301 (98%)	286 (97%)	8 (3%)	44	75
7	D	225/256 (88%)	224 (100%)	1 (0%)	91	95
8	E	106/118 (90%)	100 (94%)	6 (6%)	20	56
9	F	185/192 (96%)	183 (99%)	2 (1%)	73	88
10	G	151/209 (72%)	146 (97%)	5 (3%)	38	71
11	H	171/179 (96%)	164 (96%)	7 (4%)	30	66
12	I	167/177 (94%)	162 (97%)	5 (3%)	41	73
13	J	139/144 (96%)	134 (96%)	5 (4%)	35	69
14	L	150/155 (97%)	147 (98%)	3 (2%)	55	80
15	M	103/107 (96%)	97 (94%)	6 (6%)	20	55
16	N	175/177 (99%)	161 (92%)	14 (8%)	12	42
17	O	160/163 (98%)	154 (96%)	6 (4%)	33	67
18	P	127/135 (94%)	126 (99%)	1 (1%)	81	93
19	Q	151/153 (99%)	145 (96%)	6 (4%)	31	66
20	R	130/156 (83%)	127 (98%)	3 (2%)	50	78
21	S	149/151 (99%)	140 (94%)	9 (6%)	19	54
22	T	131/132 (99%)	129 (98%)	2 (2%)	65	85
23	U	85/92 (92%)	83 (98%)	2 (2%)	49	77
24	V	103/108 (95%)	96 (93%)	7 (7%)	16	49
25	W	51/94 (54%)	51 (100%)	0	100	100
26	X	89/117 (76%)	88 (99%)	1 (1%)	73	88
27	Y	118/122 (97%)	116 (98%)	2 (2%)	60	83
28	Z	102/119 (86%)	100 (98%)	2 (2%)	55	80
29	a	120/122 (98%)	117 (98%)	3 (2%)	47	77

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	b	42/49 (86%)	40 (95%)	2 (5%)	25	61
31	c	81/95 (85%)	79 (98%)	2 (2%)	47	77
32	d	84/94 (89%)	81 (96%)	3 (4%)	35	69
33	e	108/116 (93%)	105 (97%)	3 (3%)	43	74
34	f	85/90 (94%)	78 (92%)	7 (8%)	11	41
35	g	97/98 (99%)	97 (100%)	0	100	100
36	h	103/105 (98%)	101 (98%)	2 (2%)	57	81
37	i	65/82 (79%)	64 (98%)	1 (2%)	65	85
38	j	62/66 (94%)	56 (90%)	6 (10%)	8	31
39	k	63/68 (93%)	62 (98%)	1 (2%)	62	84
40	l	46/47 (98%)	44 (96%)	2 (4%)	29	64
41	m	45/116 (39%)	43 (96%)	2 (4%)	28	64
42	o	84/94 (89%)	84 (100%)	0	100	100
43	p	67/69 (97%)	66 (98%)	1 (2%)	65	85
All	All	4928/5406 (91%)	4768 (97%)	160 (3%)	42	71

All (160) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	14	SER
4	A	20	THR
4	A	40	VAL
4	A	48	ILE
4	A	114	CYS
4	A	174	GLU
4	A	177	LEU
4	A	191	ARG
4	A	203	ASN
4	A	208	ARG
5	B	35	ASP
5	B	36	ASP
5	B	112	GLU
5	B	136	ASN
5	B	198	GLU
5	B	290	CYS
5	B	327	ILE
5	B	382	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	B	386	LYS
5	B	392	PHE
5	B	402	LEU
5	B	406	LYS
6	C	128	THR
6	C	141	LEU
6	C	159	LYS
6	C	190	LYS
6	C	194	ARG
6	C	227	ILE
6	C	301	LEU
6	C	366	ASN
7	D	212	ASP
8	E	23	ILE
8	E	70	GLN
8	E	79	ASP
8	E	95	ASN
8	E	132	ASP
8	E	142	LYS
9	F	24	LEU
9	F	69	GLU
10	G	84	PHE
10	G	146	ASP
10	G	152	LEU
10	G	185	CYS
10	G	187	CYS
11	H	48	LEU
11	H	55	ASP
11	H	113	GLU
11	H	119	ASP
11	H	126	HIS
11	H	129	HIS
11	H	183	LEU
12	I	99	ILE
12	I	130	ASN
12	I	174	THR
12	I	179	GLU
12	I	196	HIS
13	J	24	ASP
13	J	42	MET
13	J	108	LEU
13	J	110	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	J	114	ARG
14	L	6	ASN
14	L	76	THR
14	L	170	ASP
15	M	19	GLU
15	M	32	ASP
15	M	42	GLU
15	M	61	VAL
15	M	71	GLU
15	M	103	ASN
16	N	5	THR
16	N	17	GLU
16	N	26	ARG
16	N	76	SER
16	N	87	HIS
16	N	92	LEU
16	N	115	LEU
16	N	143	GLN
16	N	159	ARG
16	N	174	LEU
16	N	179	HIS
16	N	182	ARG
16	N	184	LEU
16	N	187	SER
17	O	101	GLN
17	O	102	CYS
17	O	123	ARG
17	O	139	LEU
17	O	141	THR
17	O	142	THR
18	P	33	THR
19	Q	37	ARG
19	Q	58	ARG
19	Q	61	SER
19	Q	80	LEU
19	Q	141	ARG
19	Q	158	ASN
20	R	21	ARG
20	R	110	ARG
20	R	113	ASN
21	S	15	THR
21	S	33	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
21	S	50	LEU
21	S	81	ARG
21	S	85	ASN
21	S	95	ASP
21	S	99	GLU
21	S	118	ASP
21	S	174	CYS
22	T	78	ARG
22	T	124	THR
23	U	18	PHE
23	U	19	PHE
24	V	12	THR
24	V	28	CYS
24	V	32	SER
24	V	46	LYS
24	V	108	ASP
24	V	124	GLU
24	V	135	VAL
26	X	66	THR
27	Y	56	VAL
27	Y	97	PHE
28	Z	8	ARG
28	Z	104	LEU
29	a	43	THR
29	a	59	ARG
29	a	76	ASN
30	b	8	SER
30	b	11	ASN
31	c	19	LEU
31	c	79	ASP
32	d	47	ASP
32	d	80	ASP
32	d	104	THR
33	e	28	ARG
33	e	37	ARG
33	e	83	LEU
34	f	9	VAL
34	f	26	ASN
34	f	30	LEU
34	f	62	ASN
34	f	75	VAL
34	f	81	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	f	97	LEU
36	h	4	LEU
36	h	78	LEU
37	i	54	ARG
38	j	14	LYS
38	j	19	CYS
38	j	22	CYS
38	j	28	HIS
38	j	36	LYS
38	j	40	PRO
39	k	64	LEU
40	l	7	LEU
40	l	14	CYS
41	m	99	CYS
41	m	118	CYS
43	p	4	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	50	HIS
4	A	207	HIS
4	A	216	HIS
5	B	136	ASN
5	B	195	HIS
5	B	287	GLN
5	B	292	HIS
5	B	297	ASN
5	B	328	ASN
5	B	367	ASN
5	B	393	GLN
6	C	82	ASN
6	C	84	ASN
6	C	186	HIS
6	C	220	ASN
6	C	363	GLN
6	C	366	ASN
7	D	282	GLN
8	E	70	GLN
8	E	99	GLN
9	F	152	ASN
10	G	67	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	G	71	HIS
10	G	145	HIS
10	G	178	GLN
11	H	30	HIS
11	H	109	HIS
11	H	121	ASN
11	H	129	HIS
12	I	73	ASN
12	I	185	GLN
12	I	187	ASN
12	I	196	HIS
16	N	80	GLN
16	N	88	HIS
17	O	24	GLN
18	P	110	ASN
19	Q	158	ASN
20	R	63	HIS
21	S	5	GLN
21	S	62	HIS
21	S	85	ASN
21	S	87	HIS
24	V	36	ASN
29	a	76	ASN
30	b	11	ASN
30	b	36	ASN
31	c	55	HIS
32	d	56	ASN
34	f	26	ASN
34	f	62	ASN
34	f	72	ASN
35	g	29	ASN
35	g	103	GLN
36	h	87	GLN
38	j	16	HIS
38	j	24	ASN
38	j	28	HIS
42	o	18	HIS
42	o	33	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	2532/2765 (91%)	523 (20%)	97 (3%)
2	3	116/118 (98%)	25 (21%)	3 (2%)
3	4	152/162 (93%)	40 (26%)	6 (3%)
All	All	2800/3045 (91%)	588 (21%)	106 (3%)

All (588) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	4	A
1	1	6	U
1	1	16	G
1	1	20	G
1	1	24	A
1	1	29	C
1	1	38	A
1	1	41	A
1	1	47	U
1	1	57	G
1	1	58	A
1	1	64	A
1	1	67	U
1	1	70	C
1	1	72	A
1	1	83	A
1	1	90	G
1	1	107	A
1	1	108	G
1	1	114	C
1	1	115	G
1	1	116	U
1	1	117	C
1	1	119	U
1	1	120	A
1	1	121	A
1	1	122	U
1	1	130	G
1	1	137	G
1	1	138	U
1	1	141	U
1	1	142	C
1	1	148	A
1	1	150	C
1	1	151	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	152	A
1	1	153	U
1	1	158	C
1	1	159	U
1	1	164	U
1	1	165	A
1	1	168	U
1	1	178	U
1	1	179	G
1	1	188	U
1	1	189	U
1	1	191	A
1	1	196	A
1	1	197	A
1	1	198	A
1	1	209	G
1	1	212	C
1	1	215	C
1	1	217	G
1	1	218	C
1	1	219	A
1	1	222	C
1	1	223	U
1	1	224	U
1	1	225	A
1	1	226	C
1	1	227	G
1	1	242	G
1	1	243	U
1	1	268	A
1	1	271	G
1	1	272	G
1	1	278	U
1	1	296	A
1	1	302	C
1	1	309	A
1	1	322	A
1	1	323	C
1	1	325	A
1	1	348	A
1	1	349	G
1	1	359	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	360	C
1	1	366	G
1	1	372	A
1	1	373	G
1	1	375	U
1	1	390	G
1	1	394	U
1	1	395	A
1	1	402	U
1	1	403	U
1	1	405	A
1	1	406	U
1	1	424	A
1	1	433	G
1	1	435	A
1	1	450	C
1	1	452	A
1	1	456	U
1	1	457	U
1	1	458	U
1	1	459	G
1	1	466	A
1	1	480	A
1	1	490	A
1	1	491	C
1	1	496	G
1	1	500	G
1	1	501	C
1	1	502	A
1	1	503	U
1	1	506	C
1	1	511	G
1	1	512	A
1	1	519	C
1	1	526	G
1	1	527	A
1	1	532	A
1	1	539	G
1	1	543	A
1	1	556	A
1	1	557	G
1	1	558	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	562	A
1	1	573	A
1	1	575	C
1	1	577	C
1	1	580	A
1	1	587	A
1	1	593	C
1	1	594	G
1	1	601	U
1	1	606	U
1	1	607	G
1	1	621	U
1	1	622	G
1	1	623	A
1	1	634	G
1	1	635	G
1	1	636	U
1	1	641	A
1	1	643	G
1	1	644	A
1	1	652	A
1	1	664	G
1	1	668	G
1	1	671	U
1	1	686	C
1	1	687	U
1	1	689	A
1	1	694	A
1	1	701	A
1	1	712	U
1	1	720	G
1	1	728	A
1	1	730	G
1	1	766	A
1	1	773	A
1	1	775	C
1	1	777	U
1	1	790	U
1	1	792	A
1	1	793	G
1	1	796	A
1	1	807	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	808	G
1	1	813	U
1	1	814	G
1	1	816	U
1	1	817	U
1	1	820	A
1	1	823	A
1	1	826	U
1	1	828	G
1	1	841	G
1	1	855	G
1	1	869	A
1	1	875	U
1	1	876	G
1	1	877	A
1	1	883	A
1	1	902	A
1	1	904	A
1	1	905	U
1	1	906	G
1	1	915	C
1	1	923	A
1	1	924	U
1	1	925	A
1	1	931	A
1	1	939	U
1	1	941	U
1	1	1014	U
1	1	1015	A
1	1	1016	G
1	1	1018	G
1	1	1026	A
1	1	1030	A
1	1	1031	A
1	1	1032	U
1	1	1036	G
1	1	1040	A
1	1	1054	C
1	1	1068	C
1	1	1070	A
1	1	1071	U
1	1	1072	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	1073	G
1	1	1089	G
1	1	1090	A
1	1	1098	A
1	1	1118	U
1	1	1127	C
1	1	1132	A
1	1	1147	G
1	1	1150	C
1	1	1154	A
1	1	1159	A
1	1	1163	G
1	1	1165	G
1	1	1168	U
1	1	1177	U
1	1	1183	C
1	1	1184	C
1	1	1194	A
1	1	1195	U
1	1	1197	A
1	1	1198	G
1	1	1200	A
1	1	1220	U
1	1	1227	A
1	1	1236	U
1	1	1244	C
1	1	1246	U
1	1	1256	A
1	1	1257	A
1	1	1259	G
1	1	1266	A
1	1	1270	A
1	1	1284	U
1	1	1297	A
1	1	1303	C
1	1	1304	G
1	1	1306	G
1	1	1311	C
1	1	1314	A
1	1	1316	A
1	1	1328	C
1	1	1329	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	1337	U
1	1	1344	U
1	1	1345	U
1	1	1346	G
1	1	1348	U
1	1	1349	A
1	1	1373	U
1	1	1374	A
1	1	1376	U
1	1	1379	U
1	1	1390	A
1	1	1391	C
1	1	1396	C
1	1	1399	C
1	1	1409	G
1	1	1410	C
1	1	1411	G
1	1	1421	U
1	1	1424	C
1	1	1425	A
1	1	1426	A
1	1	1443	U
1	1	1450	G
1	1	1451	G
1	1	1452	C
1	1	1453	U
1	1	1461	U
1	1	1470	A
1	1	1481	A
1	1	1484	U
1	1	1485	U
1	1	1504	A
1	1	1505	U
1	1	1506	A
1	1	1507	A
1	1	1511	C
1	1	1513	U
1	1	1514	C
1	1	1530	G
1	1	1531	U
1	1	1543	A
1	1	1544	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	1551	A
1	1	1560	C
1	1	1571	G
1	1	1572	C
1	1	1585	U
1	1	1591	C
1	1	1595	A
1	1	1614	A
1	1	1615	A
1	1	1616	A
1	1	1618	U
1	1	1619	C
1	1	1628	U
1	1	1629	U
1	1	1632	U
1	1	1637	G
1	1	1638	G
1	1	1647	A
1	1	1650	G
1	1	1661	A
1	1	1674	C
1	1	1685	U
1	1	1686	A
1	1	1688	C
1	1	1703	U
1	1	1711	G
1	1	1722	U
1	1	1723	G
1	1	1724	U
1	1	1726	U
1	1	1740	A
1	1	1742	G
1	1	1745	A
1	1	1759	A
1	1	1761	A
1	1	1763	A
1	1	1766	U
1	1	1767	G
1	1	1772	A
1	1	1773	A
1	1	1774	C
1	1	1776	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	1780	C
1	1	1784	U
1	1	1786	U
1	1	1787	C
1	1	1788	A
1	1	1791	G
1	1	1792	U
1	1	1798	A
1	1	1799	A
1	1	1800	U
1	1	1801	A
1	1	1824	U
1	1	1825	G
1	1	1826	C
1	1	1828	U
1	1	1831	A
1	1	1832	C
1	1	1833	G
1	1	1852	U
1	1	1853	G
1	1	1854	U
1	1	1875	A
1	1	1890	A
1	1	1891	A
1	1	1892	C
1	1	1893	G
1	1	1901	G
1	1	1903	U
1	1	1904	A
1	1	1911	G
1	1	1915	A
1	1	1920	A
1	1	1921	G
1	1	1922	A
1	1	1929	A
1	1	1937	A
1	1	1940	U
1	1	1942	G
1	1	1953	G
1	1	1956	U
1	1	1957	A
1	1	1959	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	2025	U
1	1	2026	U
1	1	2032	U
1	1	2033	A
1	1	2039	C
1	1	2040	A
1	1	2041	C
1	1	2043	A
1	1	2047	A
1	1	2048	U
1	1	2058	U
1	1	2060	G
1	1	2061	A
1	1	2068	G
1	1	2080	A
1	1	2092	G
1	1	2102	G
1	1	2106	U
1	1	2109	U
1	1	2110	A
1	1	2125	A
1	1	2126	G
1	1	2128	A
1	1	2131	G
1	1	2132	A
1	1	2135	U
1	1	2144	G
1	1	2148	A
1	1	2150	A
1	1	2168	U
1	1	2180	U
1	1	2182	G
1	1	2183	U
1	1	2194	G
1	1	2206	A
1	1	2207	G
1	1	2209	C
1	1	2225	U
1	1	2226	A
1	1	2227	G
1	1	2228	C
1	1	2229	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	2232	A
1	1	2233	G
1	1	2234	G
1	1	2235	U
1	1	2236	G
1	1	2237	C
1	1	2252	G
1	1	2255	A
1	1	2256	G
1	1	2257	A
1	1	2258	C
1	1	2259	A
1	1	2260	A
1	1	2266	C
1	1	2270	G
1	1	2273	A
1	1	2293	A
1	1	2294	A
1	1	2298	A
1	1	2301	A
1	1	2317	U
1	1	2323	C
1	1	2327	G
1	1	2328	A
1	1	2329	U
1	1	2331	U
1	1	2332	C
1	1	2337	C
1	1	2343	A
1	1	2344	U
1	1	2345	C
1	1	2355	U
1	1	2356	A
1	1	2366	A
1	1	2367	A
1	1	2374	G
1	1	2376	U
1	1	2379	U
1	1	2390	U
1	1	2391	A
1	1	2396	U
1	1	2400	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	2402	G
1	1	2426	A
1	1	2438	U
1	1	2445	G
1	1	2450	U
1	1	2451	A
1	1	2452	G
1	1	2466	G
1	1	2482	G
1	1	2501	C
1	1	2503	U
1	1	2509	U
1	1	2510	A
1	1	2530	U
1	1	2531	G
1	1	2532	U
1	1	2537	C
1	1	2542	A
1	1	2549	C
1	1	2557	A
1	1	2559	G
1	1	2560	G
1	1	2567	G
1	1	2573	U
1	1	2574	A
1	1	2581	A
1	1	2582	A
1	1	2593	A
1	1	2594	A
1	1	2595	A
1	1	2596	G
1	1	2597	U
1	1	2599	A
1	1	2602	C
1	1	2621	A
1	1	2622	C
1	1	2624	A
1	1	2625	A
1	1	2627	A
1	1	2628	A
1	1	2655	G
1	1	2666	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	2667	A
1	1	2668	G
1	1	2678	U
1	1	2679	G
1	1	2680	U
1	1	2681	G
1	1	2688	G
1	1	2689	G
1	1	2696	A
1	1	2702	U
1	1	2705	A
1	1	2706	G
1	1	2709	G
1	1	2721	C
1	1	2722	G
1	1	2723	A
1	1	2730	G
1	1	2736	C
1	1	2739	C
1	1	2741	U
1	1	2742	C
1	1	2743	G
1	1	2744	C
1	1	2745	U
1	1	2753	U
1	1	2754	U
2	3	8	C
2	3	21	G
2	3	26	A
2	3	32	C
2	3	33	U
2	3	36	A
2	3	38	U
2	3	42	A
2	3	48	G
2	3	49	A
2	3	52	U
2	3	53	U
2	3	54	A
2	3	64	G
2	3	88	C
2	3	89	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	3	93	U
2	3	100	A
2	3	103	G
2	3	106	C
2	3	107	G
2	3	110	G
2	3	113	U
2	3	114	G
2	3	115	C
3	4	2	A
3	4	3	G
3	4	4	U
3	4	5	C
3	4	12	C
3	4	22	C
3	4	24	U
3	4	35	A
3	4	36	C
3	4	51	C
3	4	52	A
3	4	53	U
3	4	60	U
3	4	63	A
3	4	64	G
3	4	73	G
3	4	74	U
3	4	75	U
3	4	76	G
3	4	83	U
3	4	84	C
3	4	85	A
3	4	86	U
3	4	87	G
3	4	88	A
3	4	91	G
3	4	93	U
3	4	103	A
3	4	104	A
3	4	105	U
3	4	107	C
3	4	112	U
3	4	118	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	4	119	A
3	4	123	C
3	4	125	A
3	4	141	A
3	4	153	G
3	4	154	U
3	4	155	A

All (106) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	38	A
1	1	113	A
1	1	137	G
1	1	147	C
1	1	149	C
1	1	151	U
1	1	152	A
1	1	164	U
1	1	222	C
1	1	225	A
1	1	271	G
1	1	308	G
1	1	374	U
1	1	394	U
1	1	456	U
1	1	457	U
1	1	525	G
1	1	526	G
1	1	621	U
1	1	623	A
1	1	643	G
1	1	686	C
1	1	806	C
1	1	807	U
1	1	812	A
1	1	822	G
1	1	868	A
1	1	876	G
1	1	1014	U
1	1	1030	A
1	1	1070	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	1071	U
1	1	1072	U
1	1	1193	G
1	1	1196	G
1	1	1258	U
1	1	1327	C
1	1	1328	C
1	1	1347	G
1	1	1348	U
1	1	1367	U
1	1	1373	U
1	1	1378	A
1	1	1466	C
1	1	1505	U
1	1	1507	A
1	1	1523	U
1	1	1530	G
1	1	1543	A
1	1	1550	C
1	1	1614	A
1	1	1615	A
1	1	1617	A
1	1	1618	U
1	1	1619	C
1	1	1628	U
1	1	1685	U
1	1	1687	G
1	1	1766	U
1	1	1787	C
1	1	1823	C
1	1	1824	U
1	1	1895	U
1	1	1902	A
1	1	1903	U
1	1	1958	G
1	1	2039	C
1	1	2040	A
1	1	2042	A
1	1	2047	A
1	1	2071	U
1	1	2131	G
1	1	2134	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	2181	U
1	1	2224	A
1	1	2225	U
1	1	2226	A
1	1	2232	A
1	1	2331	U
1	1	2342	U
1	1	2367	A
1	1	2405	G
1	1	2434	U
1	1	2450	U
1	1	2451	A
1	1	2509	U
1	1	2567	G
1	1	2572	U
1	1	2596	G
1	1	2621	A
1	1	2627	A
1	1	2678	U
1	1	2701	G
1	1	2705	A
1	1	2721	C
1	1	2722	G
1	1	2743	G
2	3	53	U
2	3	109	U
2	3	112	U
3	4	4	U
3	4	74	U
3	4	87	G
3	4	90	A
3	4	110	A
3	4	153	G

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

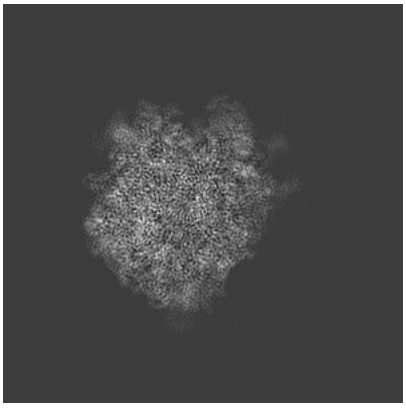
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-6784. These allow visual inspection of the internal detail of the map and identification of artifacts.

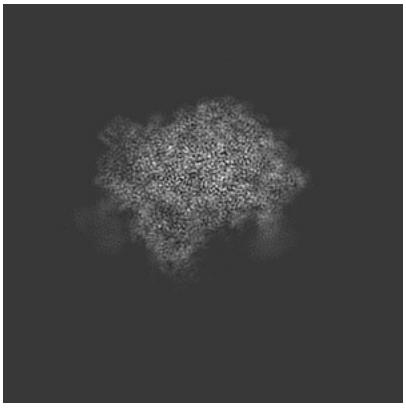
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

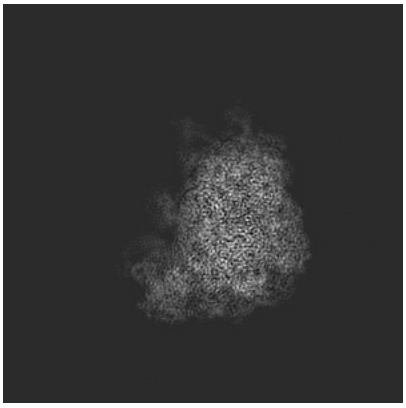
6.1.1 Primary map



X



Y

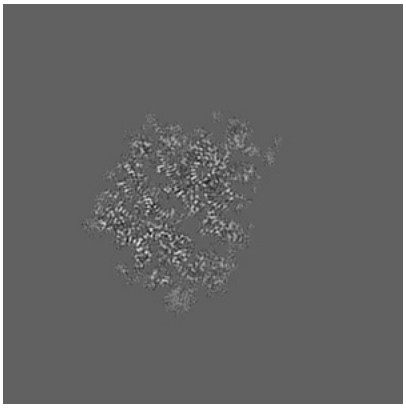


Z

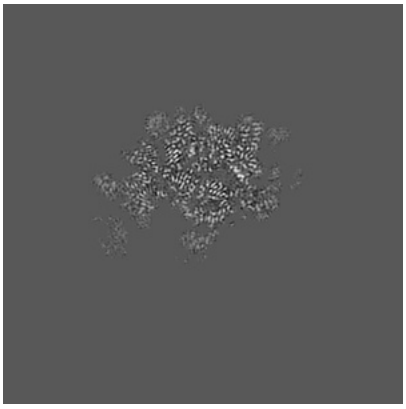
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

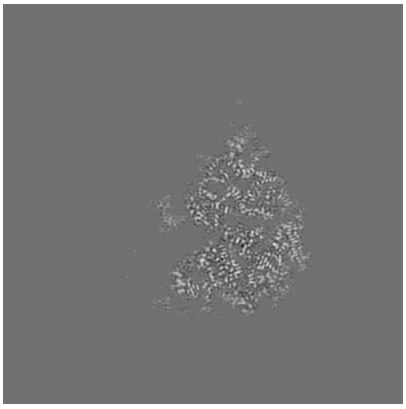
6.2.1 Primary map



X Index: 160



Y Index: 160

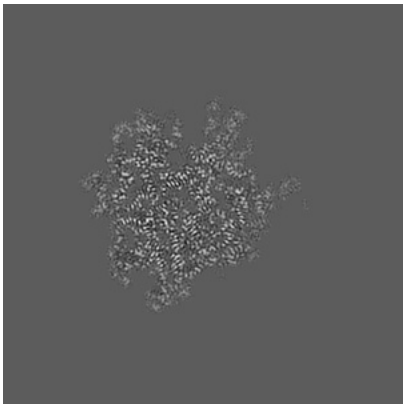


Z Index: 160

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: 189

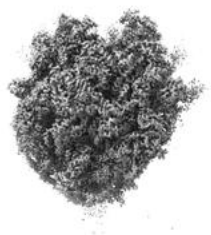
Y Index: 120

Z Index: 174

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.044. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

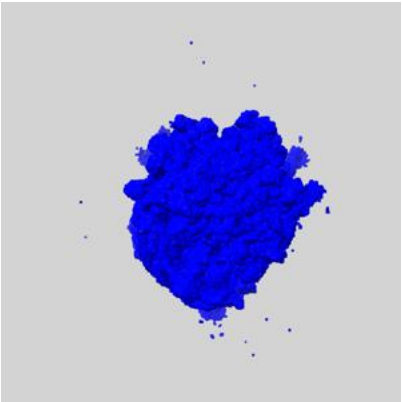
6.5 Mask visualisation (i)

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

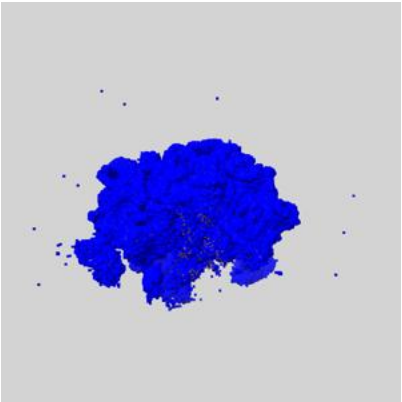
A mask typically either:

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

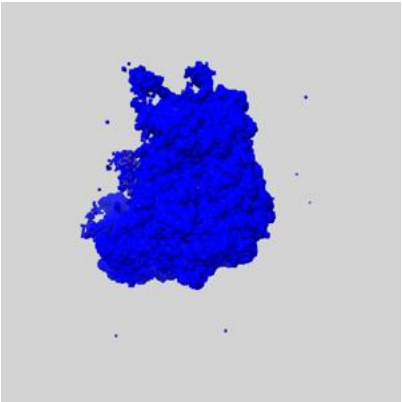
6.5.1 emd_6784_msk_1.map (i)



X



Y

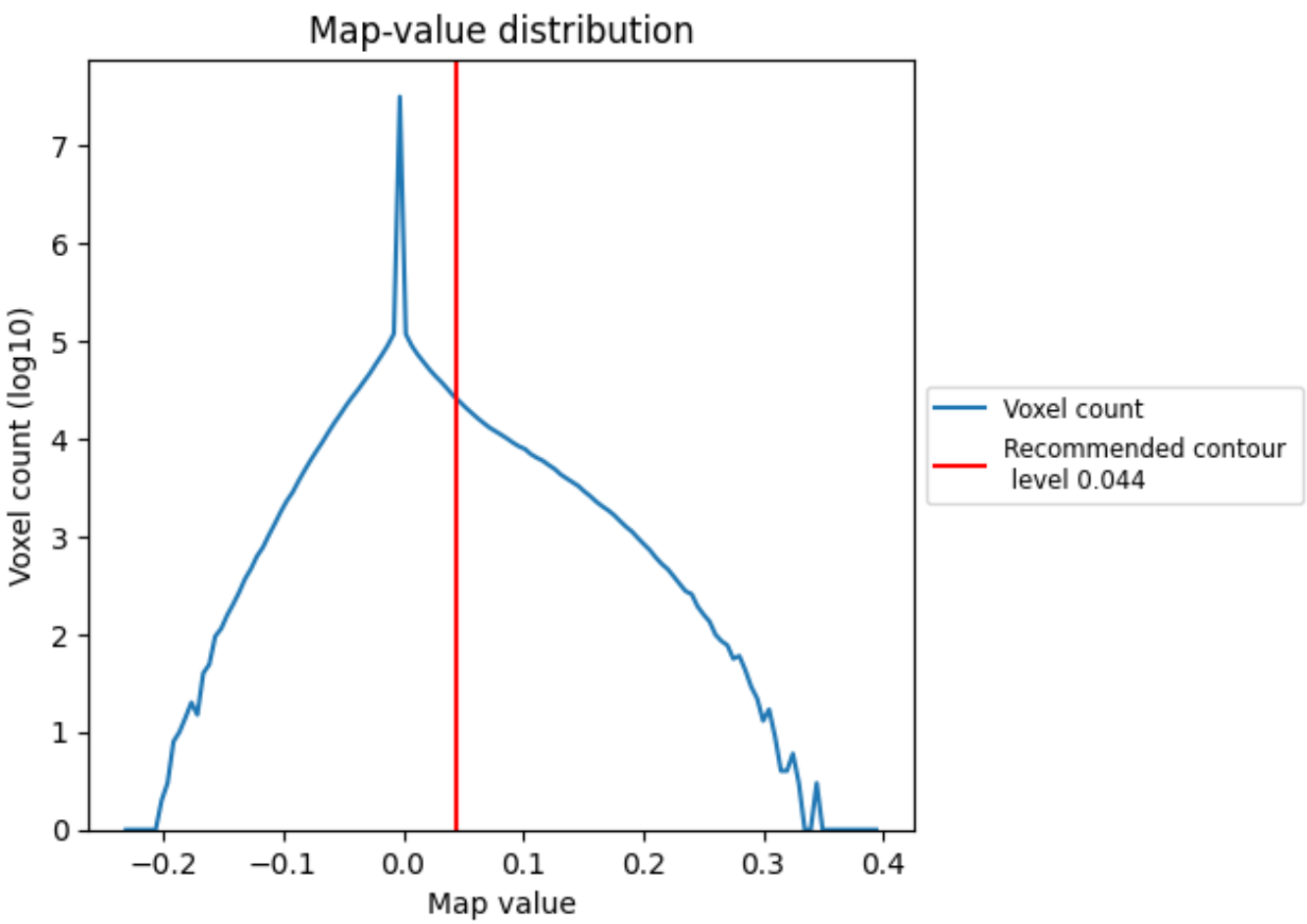


Z

7 Map analysis (i)

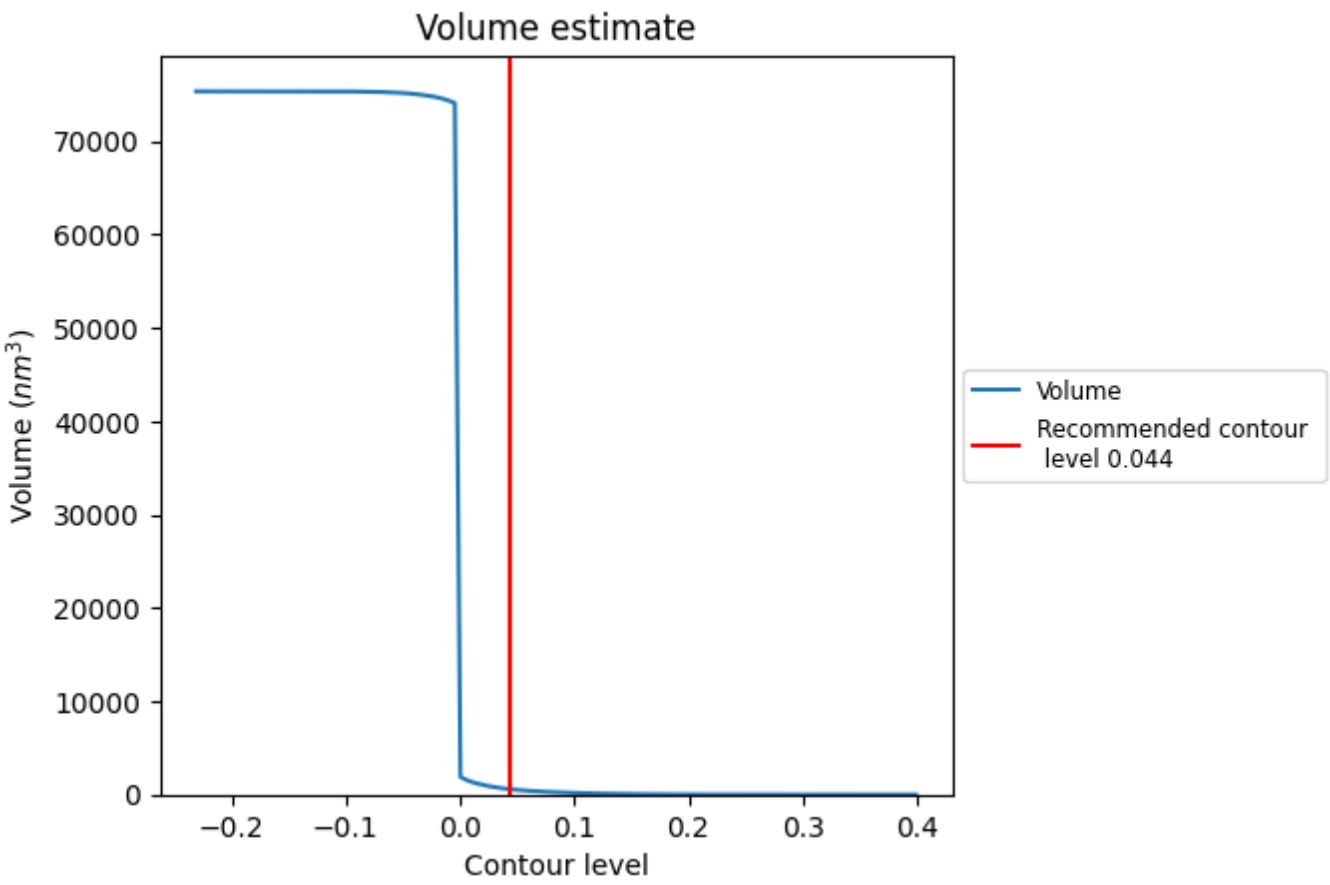
This section contains the results of statistical analysis of the map.

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.

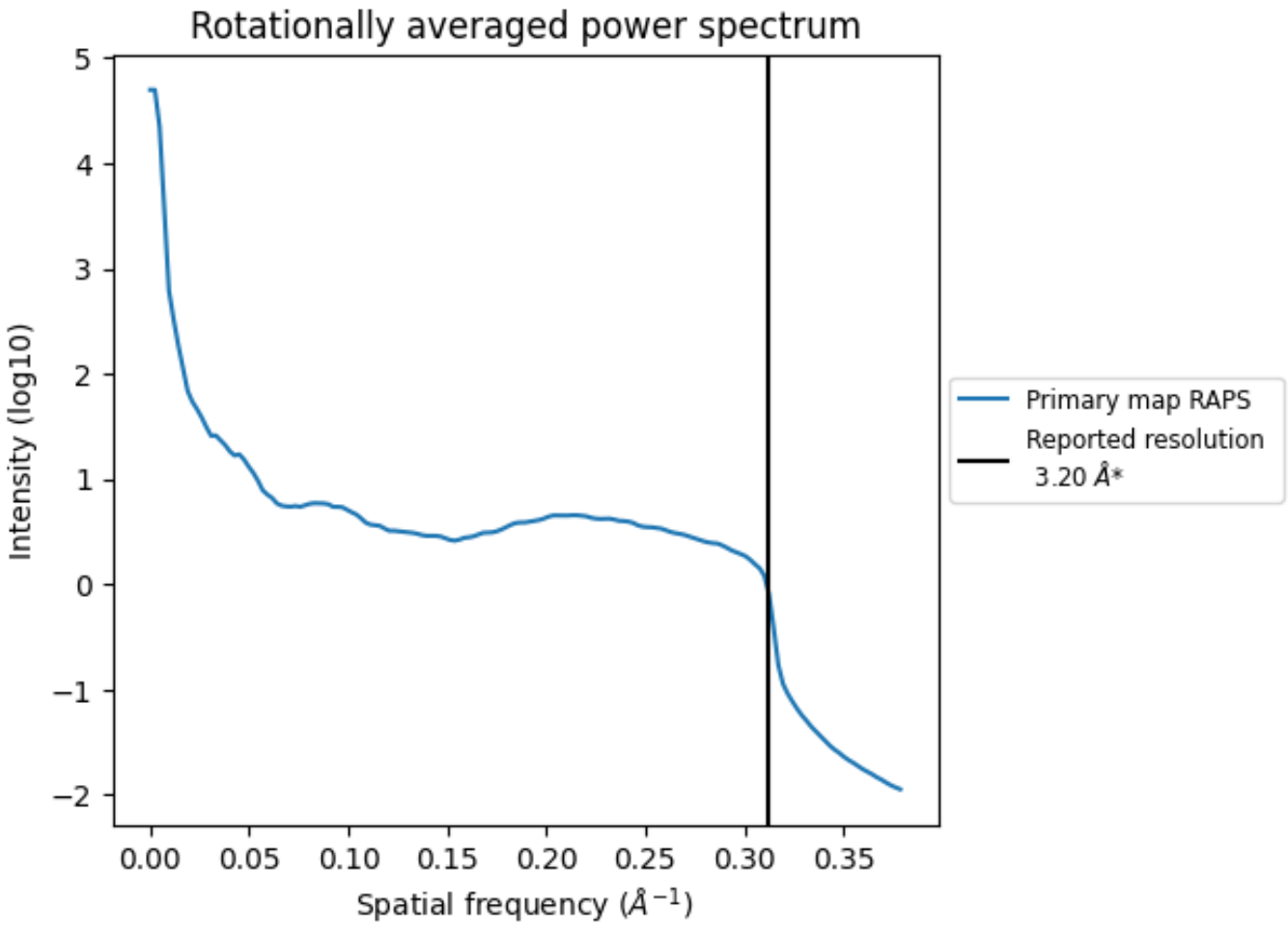
7.2 Volume estimate (i)



The volume at the recommended contour level is 572 nm^3; this corresponds to an approximate mass of 517 kDa.

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

7.3 Rotationally averaged power spectrum (i)

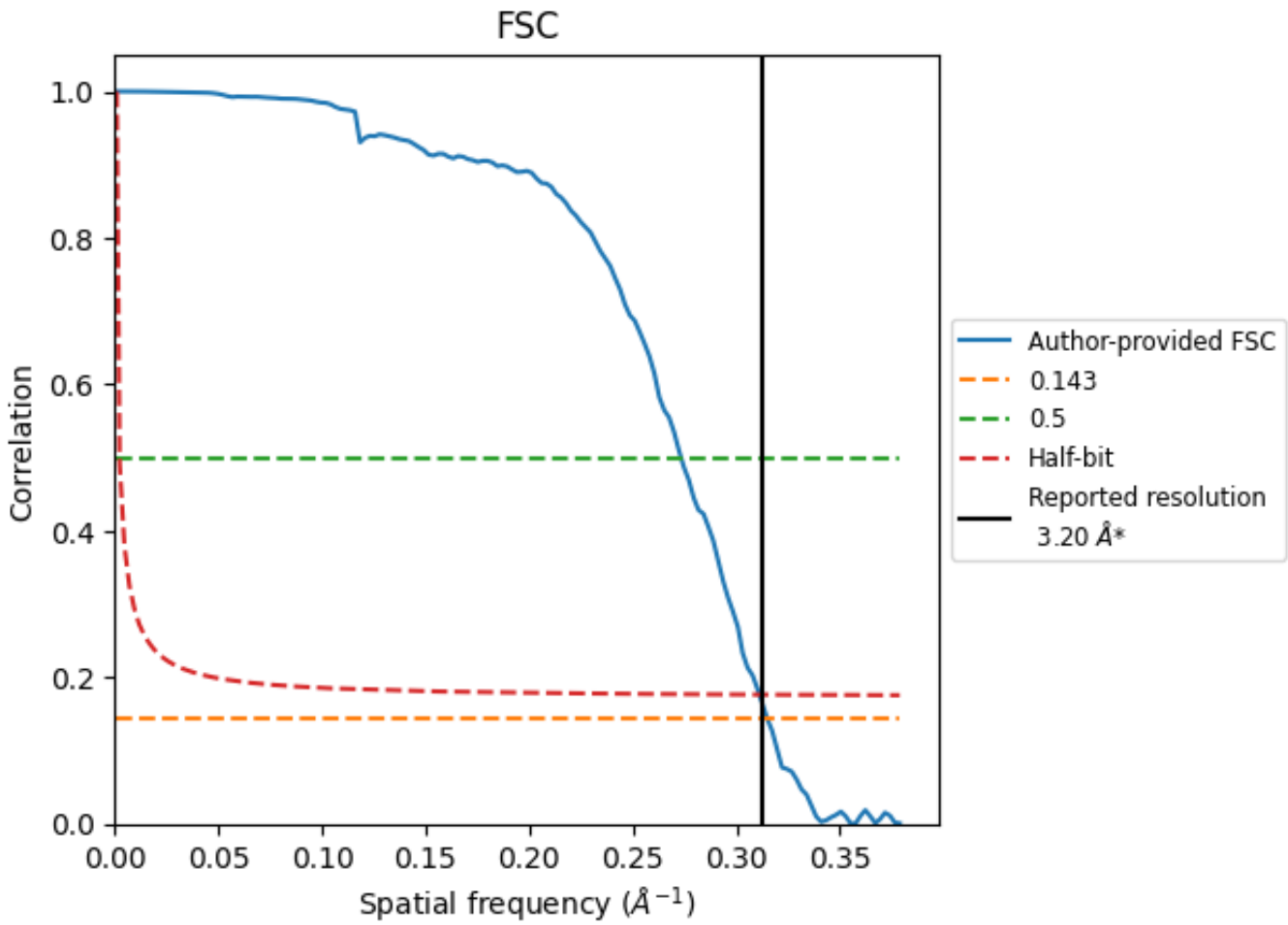


*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8.2 Resolution estimates (i)

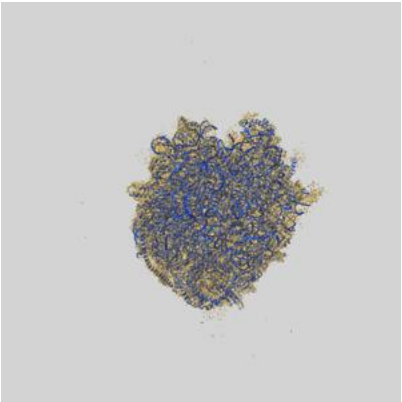
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.18	3.66	3.21
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

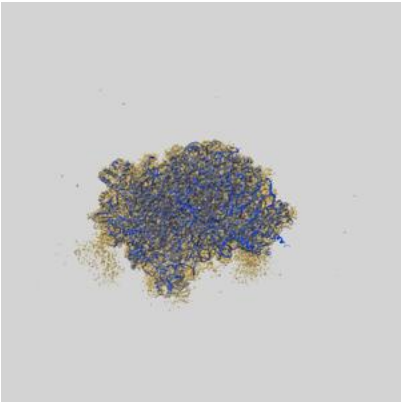
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-6784 and PDB model 5XY3. Per-residue inclusion information can be found in section 3 on page 12.

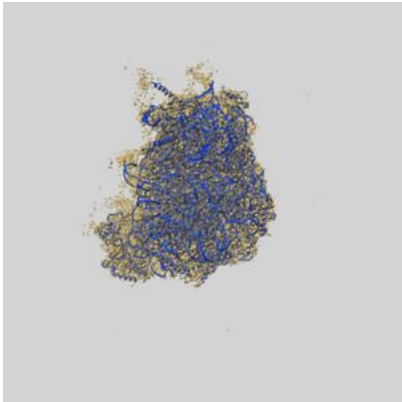
9.1 Map-model overlay (i)



X



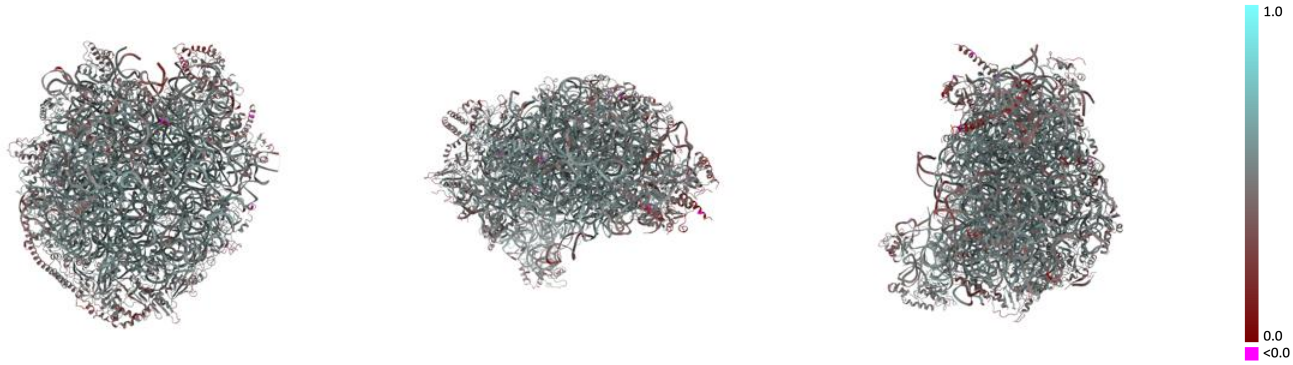
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.044 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

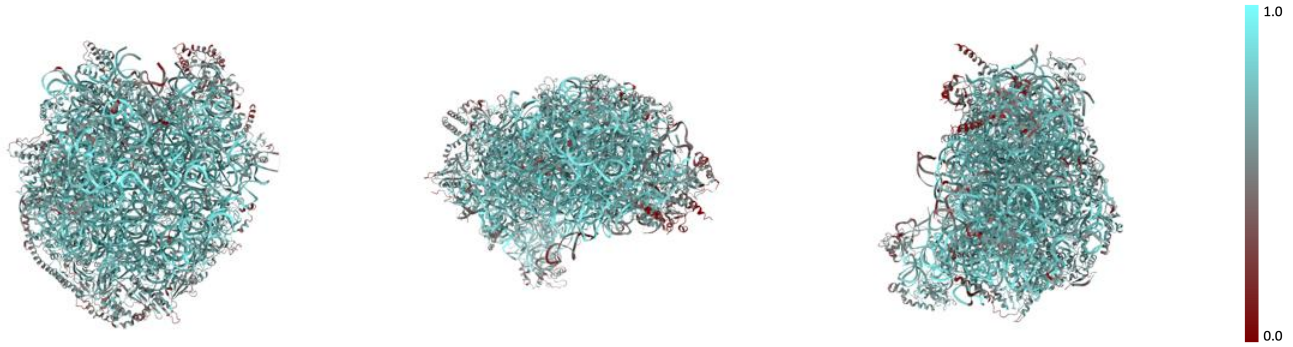
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

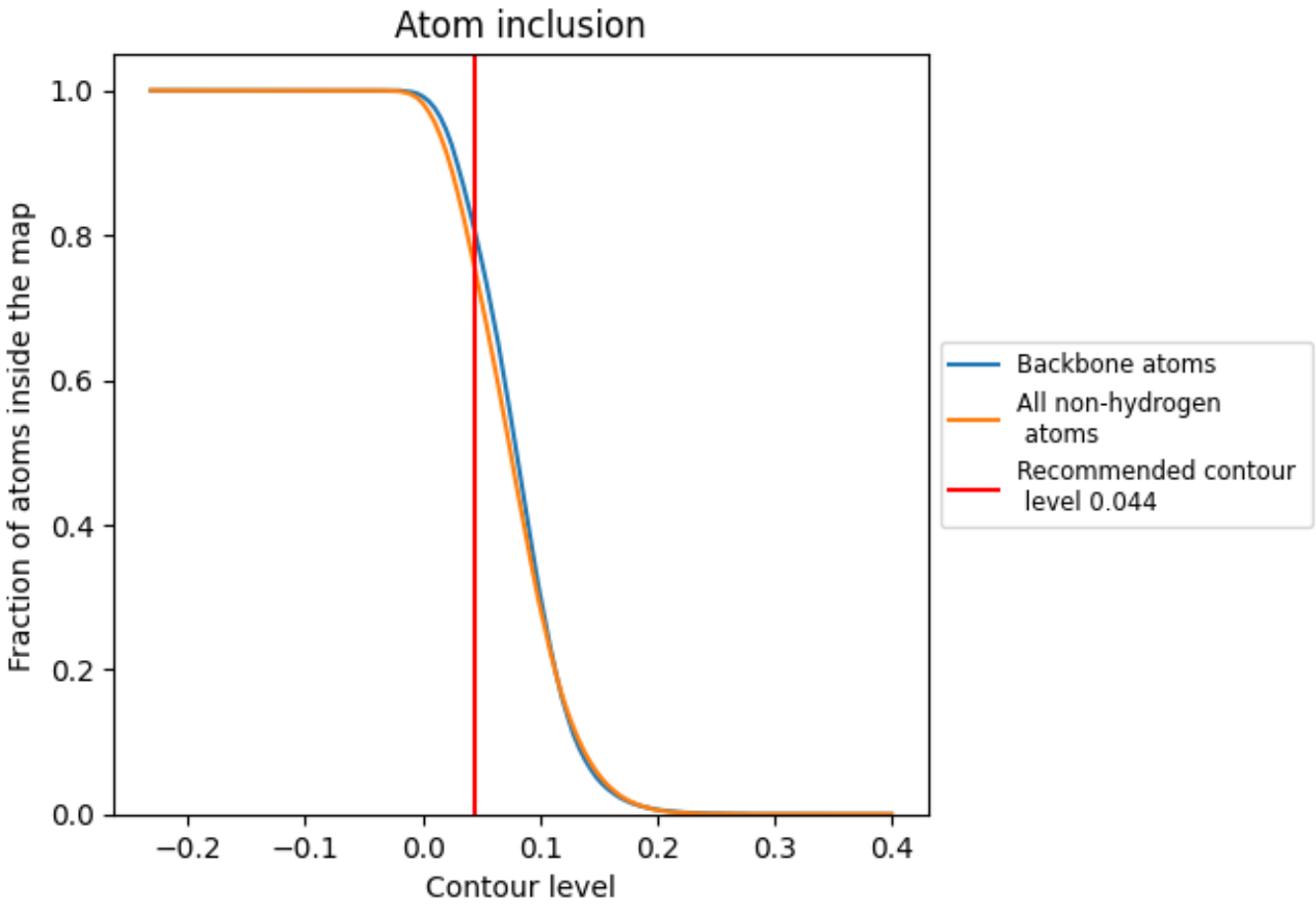
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.044).

9.4 Atom inclusion (i)



At the recommended contour level, 81% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.044) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7586	0.5100
1	0.8444	0.5360
3	0.8456	0.5180
4	0.7780	0.5050
A	0.7017	0.5180
B	0.6949	0.5050
C	0.6866	0.4940
D	0.6426	0.4700
E	0.5507	0.4410
F	0.7010	0.4880
G	0.5749	0.4470
H	0.5681	0.4500
I	0.6858	0.5060
J	0.4965	0.4080
L	0.6444	0.4690
M	0.6037	0.4480
N	0.7837	0.5430
O	0.6870	0.4990
P	0.7314	0.5160
Q	0.7237	0.5130
R	0.6508	0.4680
S	0.7068	0.5060
T	0.7107	0.5000
U	0.5718	0.4450
V	0.6488	0.4880
W	0.4271	0.3950
X	0.6527	0.4860
Y	0.6190	0.4540
Z	0.4444	0.3740
a	0.7398	0.5220
b	0.7270	0.5050
c	0.3696	0.3400
d	0.6802	0.5040
e	0.7008	0.5090
f	0.7132	0.5210

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
g	0.5445	0.4090
h	0.5863	0.4390
i	0.6111	0.4600
j	0.7869	0.5490
k	0.5593	0.4370
l	0.7101	0.5130
m	0.6135	0.4650
o	0.6823	0.5070
p	0.6453	0.4780