wwPDB EM Validation Summary Report

Nov 2, 2022 – 12:50 AM EDT

PDB ID	:	5T5H
EMDB ID	:	EMD-8361
Title	:	Structure and assembly model for the Trypanosoma cruzi 60S ribosomal subunit
Authors	:	Liu, Z.; Gutierrez-Vargas, C.; Wei, J.; Grassucci, R.A.; Ramesh, M.; Espina, N.; Sun, M.; Tutuncuoglu, B.; Madison-Antenucci, S.; Woolford Jr., J.L.; Tong, L.; Frank, J.
Deposited on	:	2016-08-31
Resolution	:	2.54 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:

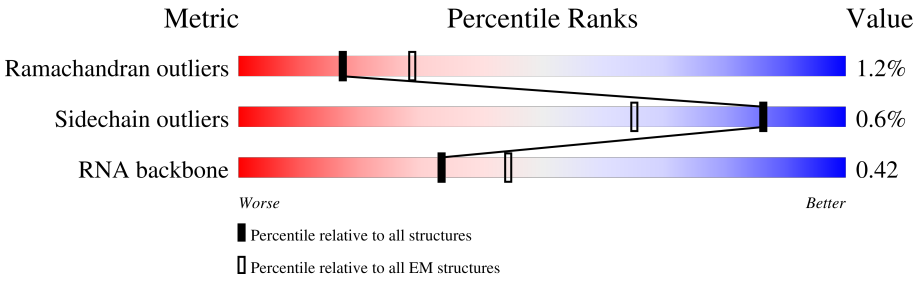
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 2.54 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	A	1278	69% 29%
2	B	941	5% 67% 31%
3	C	169	61% 22% 13%
4	D	118	75% 21%
5	E	146	77% 21%
6	F	46	50% 50%
7	G	123	73% 23%
8	H	91	75% 25%

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Mol	Chain	Length	Quality of chain
9	I	192	99%
10	L	65	26% 98%
11	N	205	81% 16%
12	O	203	99%
13	P	149	17% 95%
14	Q	203	99%
15	R	152	99%
16	S	177	10% 98%
17	T	150	7% 99%
18	U	146	84% 14%
19	V	99	9% 86% 14%
20	W	127	98%
21	X	116	93% 6%
22	Y	61	95% 5%
23	Z	113	99%
24	a	132	11% 77% 20%
25	b	144	97%
26	c	125	7% 94%
27	d	63	95% 5%
28	e	245	99%
29	f	397	96%
30	g	66	24% 95% 5%
31	h	169	18% 88% 11%
32	i	113	99%
33	j	104	100%

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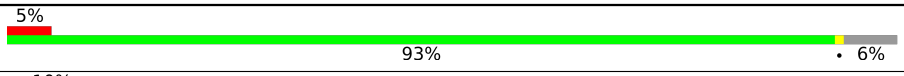
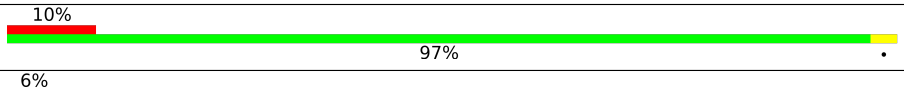
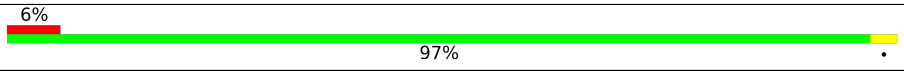
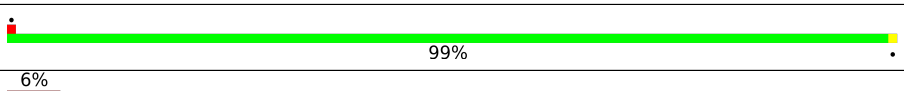
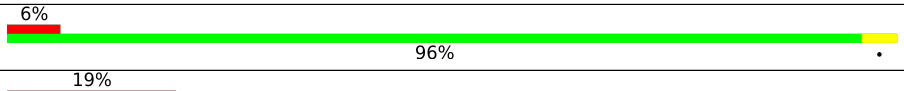
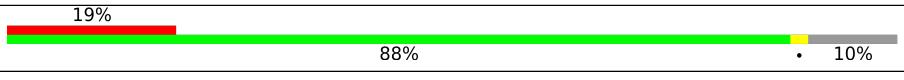
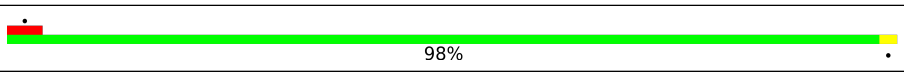
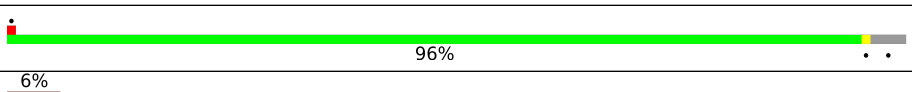
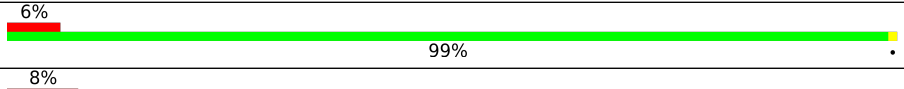
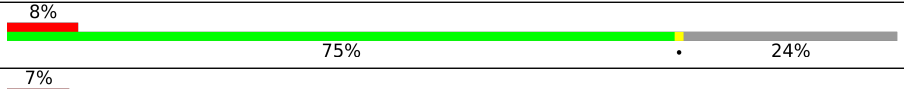
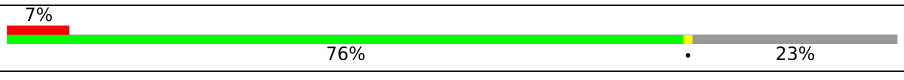
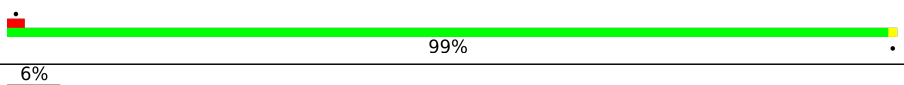
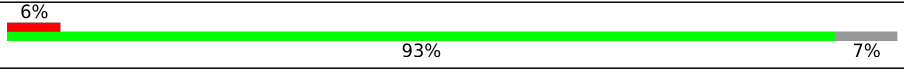
Mol	Chain	Length	Quality of chain
34	k	120	
35	l	136	
36	m	95	
37	n	81	
38	o	85	
39	p	58	
40	q	50	
41	r	337	
42	t	93	
43	u	254	
44	v	171	
45	w	215	
46	x	223	

2 Entry composition (i)

There are 49 unique types of molecules in this entry. The entry contains 105124 atoms, of which 12 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 RNA LARGE SUBUNIT ALPHA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
1	A	1278	27453	12272	12	5035	8856	1278	0	0

- Molecule 2 is a RNA chain called RNA LARGE SUBUNIT BETA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	941	20110	9007	3606	6556	941	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	C	147	3140	1408	557	1028	147	0	0

- Molecule 4 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	D	114	2432	1084	435	799	114	0	0

- Molecule 5 is a RNA chain called srRNA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	E	146	3110	1390	552	1022	146	0	0

- Molecule 6 is a RNA chain called srRNA3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	F	46	965	433	165	321	46	0	0

- Molecule 7 is a RNA chain called srRNA2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	121	Total	C	N	O	P	0	0
			2578	1150	455	852	121		

- Molecule 8 is a RNA chain called srRNA4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	91	Total	C	N	O	P	0	0
			1946	867	354	634	91		

- Molecule 9 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	192	Total	C	N	O	S	0	0
			1515	951	308	250	6		

- Molecule 10 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	65	Total	C	N	O	S	0	0
			535	333	112	85	5		

- Molecule 11 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	N	172	Total	C	N	O	S	0	0
			1413	892	291	224	6		

- Molecule 12 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	O	203	Total	C	N	O	S	0	1
			1642	1046	322	269	5		

- Molecule 13 is a protein called 40S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	P	149	Total	C	N	O	S	0	0
			1186	746	235	203	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	72	LYS	ARG	conflict	UNP Q4DQ35

- Molecule 14 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Q	203	Total	C	N	O	S	1	0
			1710	1076	365	263	6		

- Molecule 15 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	R	152	Total	C	N	O	S	0	0
			1226	768	243	205	10		

- Molecule 16 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	S	177	Total	C	N	O	S	0	0
			1449	919	282	242	6		

- Molecule 17 is a protein called Ribosomal protein L19-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	T	150	Total	C	N	O	S	0	0
			1273	789	273	205	6		

- Molecule 18 is a protein called Ribosomal protein L21E (60S).

Mol	Chain	Residues	Atoms					AltConf	Trace
18	U	126	Total	C	N	O	S	0	0
			1016	642	207	163	4		

- Molecule 19 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	V	85	Total	C	N	O	S	0	0
			730	481	127	120	2		

- Molecule 20 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	W	127	Total	C	N	O	S	0	0
			960	611	180	166	3		

- Molecule 21 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	X	109	Total	C	N	O	S	0	0
			890	565	164	157	4		

- Molecule 22 is a protein called Ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Y	61	Total	C	N	O	S	0	0
			519	340	98	77	4		

- Molecule 23 is a protein called 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Z	113	Total	C	N	O	S	0	0
			919	571	195	150	3		

- Molecule 24 is a protein called Ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	a	105	Total	C	N	O	S	0	0
			877	565	175	135	2		

- Molecule 25 is a protein called 60S ribosomal protein L27A/L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	b	144	Total	C	N	O	S	0	0
			1135	720	226	185	4		

- Molecule 26 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	c	120	Total	C	N	O	S	0	0
			935	583	187	161	4		

- Molecule 27 is a protein called Ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	d	63	Total	C	N	O	S	0	0
			518	314	122	81	1		

- Molecule 28 is a protein called 60S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	e	245	Total	C	N	O	S	0	0
			1874	1170	379	314	11		

- Molecule 29 is a protein called Ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	f	397	Total	C	N	O	S	0	0
			3189	2010	630	537	12		

- Molecule 30 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	g	66	Total	C	N	O	S	0	0
			523	335	91	93	4		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
g	91	VAL	ALA	conflict	UNP Q4DIC9
g	92	LEU	GLY	conflict	UNP Q4DIC9
g	93	SER	ASN	conflict	UNP Q4DIC9
g	94	ILE	ASN	conflict	UNP Q4DIC9
g	95	THR	LEU	conflict	UNP Q4DIC9
g	97	VAL	LEU	conflict	UNP Q4DIC9

- Molecule 31 is a protein called 60S ribosomal subunit protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	h	150	Total	C	N	O	S	0	0
			1064	671	208	183	2		

- Molecule 32 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	i	113	Total	C	N	O	S	0	0
			928	585	185	154	4		

- Molecule 33 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	j	104	Total	C	N	O	S	0	0
			863	532	191	137	3		

- Molecule 34 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	k	113	Total	C	N	O	S	0	0
			967	602	212	150	3		

- Molecule 35 is a protein called Ribosomal protein L35A.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	l	136	Total	C	N	O	S	0	0
			1057	662	217	174	4		

- Molecule 36 is a protein called Ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	m	95	Total	C	N	O	S	0	0
			757	474	159	121	3		

- Molecule 37 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	n	81	Total	C	N	O	S	0	0
			679	413	154	106	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	64	MET	CYS	conflict	UNP Q4DXW6

- Molecule 38 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	o	85	Total	C	N	O	S	0	0
			669	413	141	108	7		

- Molecule 39 is a protein called Ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	p	52	Total	C	N	O	S	0	0
			432	277	82	71	2		

- Molecule 40 is a protein called Ribosomal protein L39.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	q	50	Total	C	N	O	0	0
			456	297	98	61		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	r	325	Total	C	N	O	S	0	0
			2513	1575	489	434	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
42	t	93	Total	C	N	O	S	0	0
			763	486	149	123	5		

- Molecule 43 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	u	193	Total	C	N	O	S	0	0
			1541	982	292	262	5		

- Molecule 44 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	v	132	Total	C	N	O	S	0	0
			1037	661	194	179	3		

- Molecule 45 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	w	215	Total	C	N	O	S	0	0
			1749	1110	342	288	9		

- Molecule 46 is a protein called Ribosomal protein L7a-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	x	208	Total 1690	C 1062	N 338	O 284	S 6	0	0

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

Mol	Chain	Residues	Atoms		AltConf
47	A	66	Total 66	Mg 66	0
47	B	32	Total 32	Mg 32	0
47	C	2	Total 2	Mg 2	0
47	D	1	Total 1	Mg 1	0
47	E	1	Total 1	Mg 1	0
47	F	1	Total 1	Mg 1	0
47	G	1	Total 1	Mg 1	0
47	H	1	Total 1	Mg 1	0

- Molecule 48 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
48	n	1	Total 1	Zn 1	0
48	o	1	Total 1	Zn 1	0
48	t	1	Total 1	Zn 1	0

- Molecule 49 is water.

Mol	Chain	Residues	Atoms		AltConf
49	A	38	Total 38	O 38	0
49	B	26	Total 26	O 26	0
49	C	1	Total 1	O 1	0

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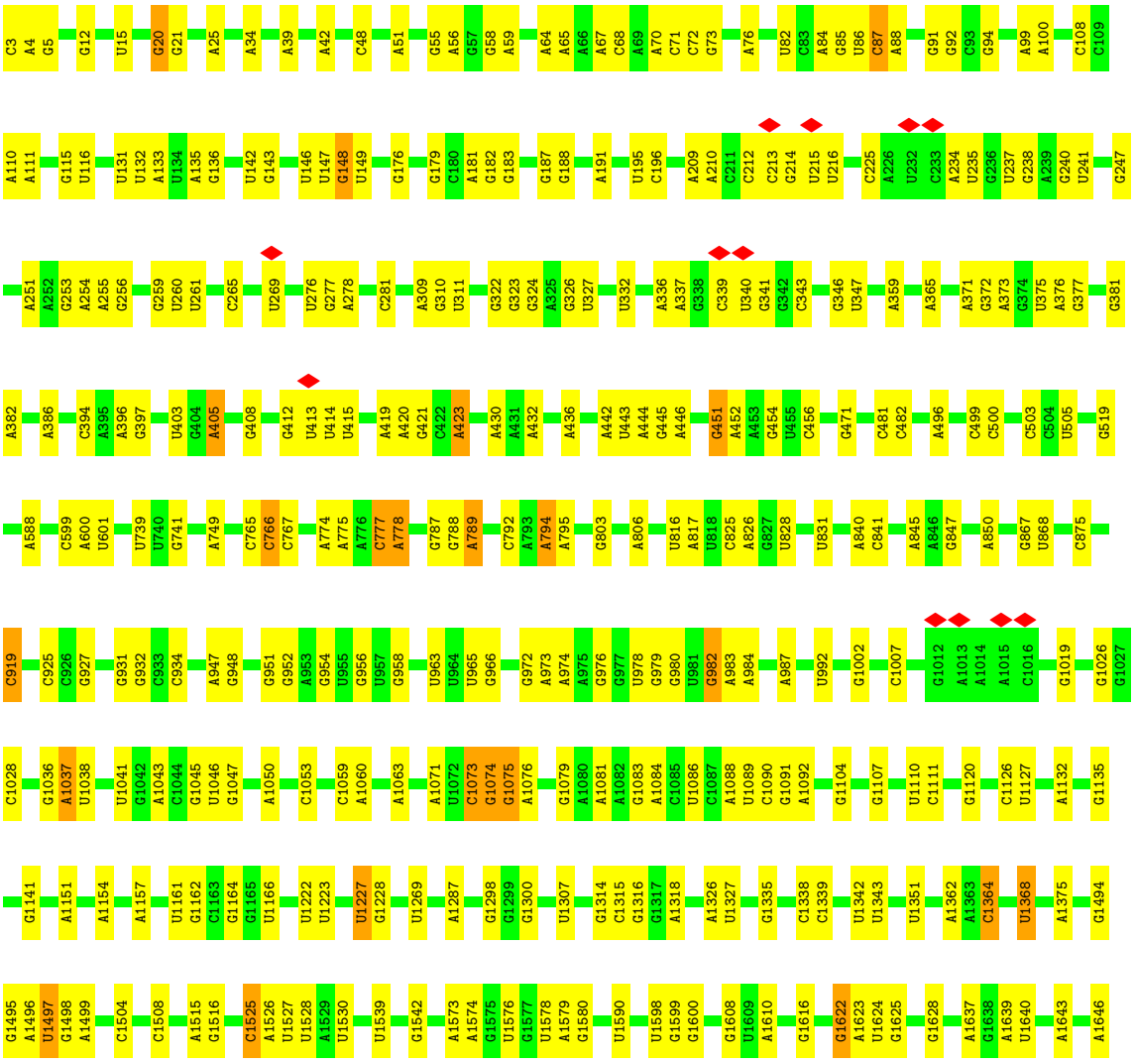
Mol	Chain	Residues	Atoms	AltConf
49	E	1	Total O 1 1	0
49	G	3	Total O 3 3	0
49	H	2	Total O 2 2	0
49	I	1	Total O 1 1	0
49	R	1	Total O 1 1	0
49	a	1	Total O 1 1	0
49	b	1	Total O 1 1	0
49	e	2	Total O 2 2	0
49	f	1	Total O 1 1	0
49	j	1	Total O 1 1	0
49	k	1	Total O 1 1	0
49	n	1	Total O 1 1	0
49	w	1	Total O 1 1	0
49	x	1	Total O 1 1	0

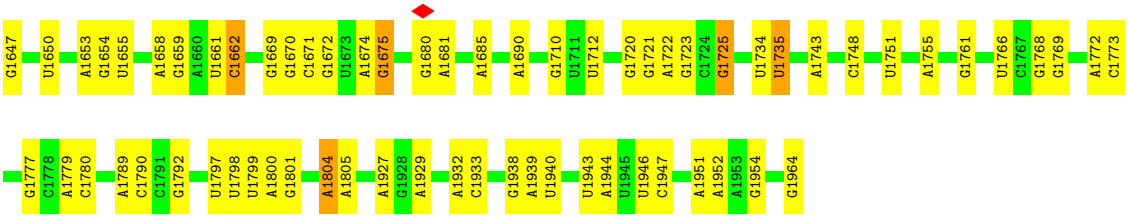
3 Residue-property plots (i)

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: RNA LARGE SUBUNIT ALPHA

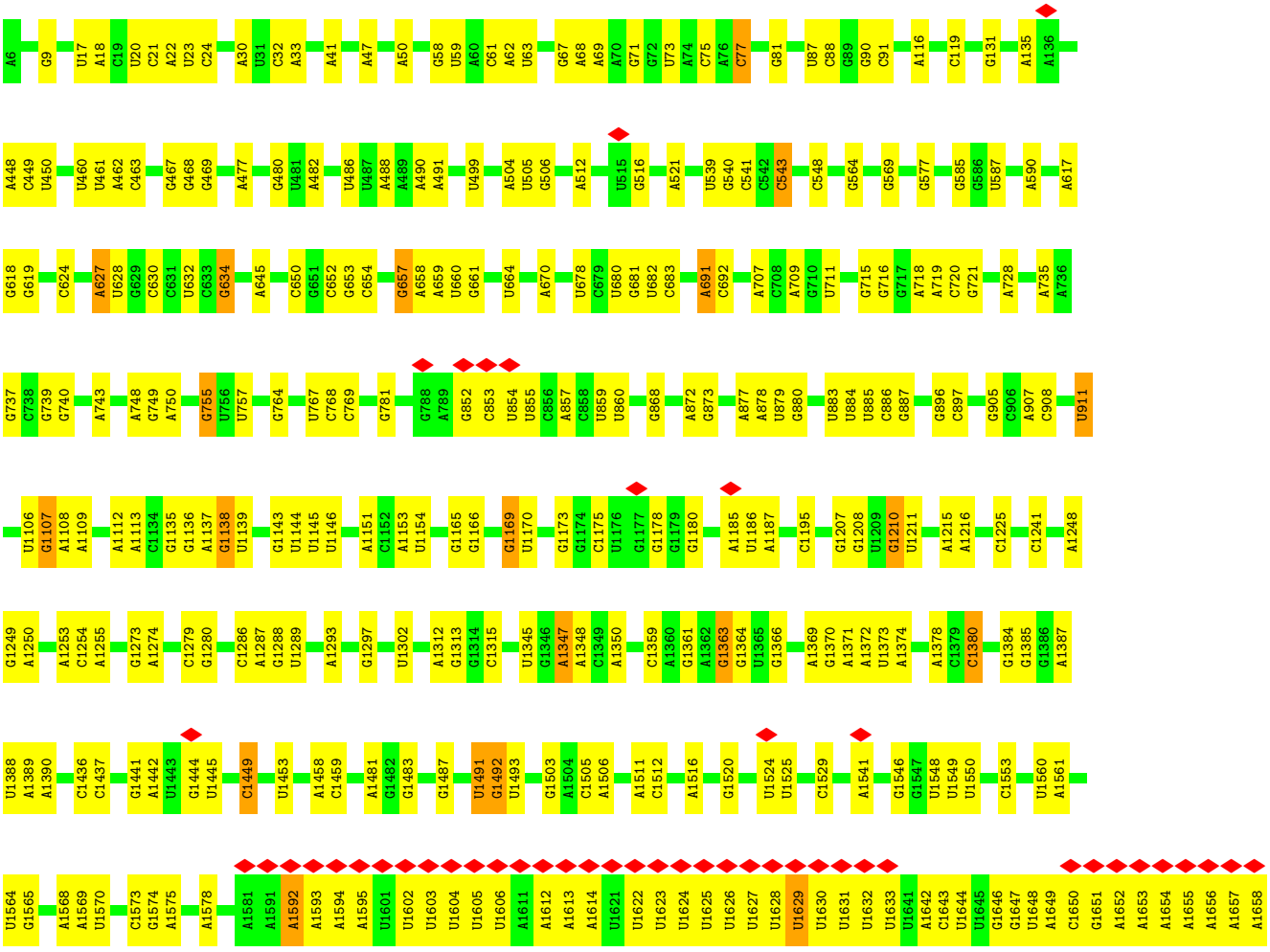
Chain A:





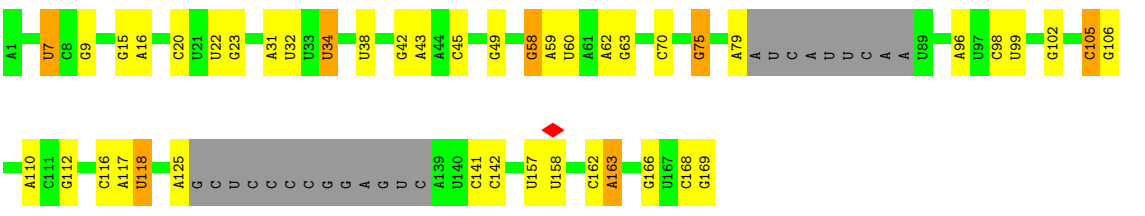
• Molecule 2: RNA LARGE SUBUNIT BETA

Chain B:



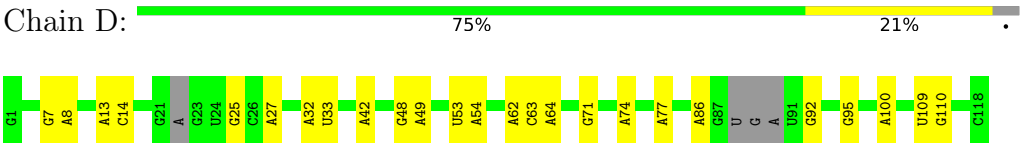
• Molecule 3: 5.8S rRNA

Chain C:



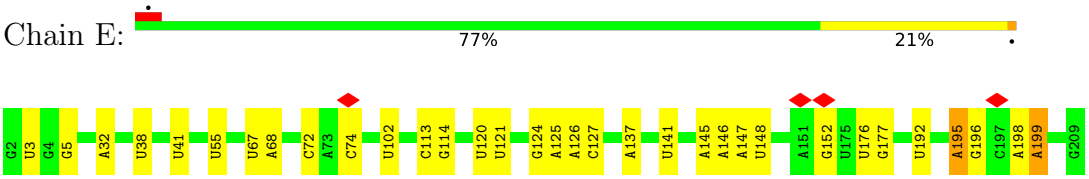
• Molecule 4: 5S rRNA

Chain D:



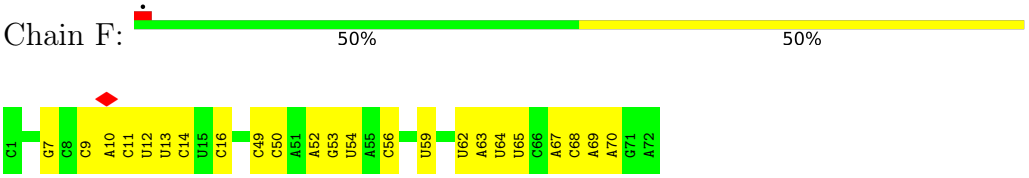
• Molecule 5: srRNA1

Chain E:



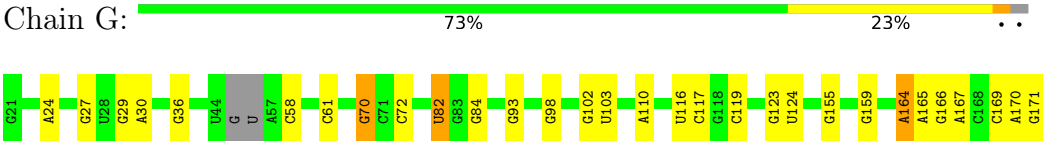
• Molecule 6: srRNA3

Chain F:



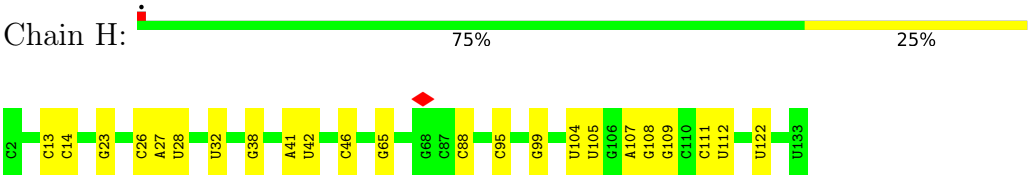
• Molecule 7: srRNA2

Chain G:



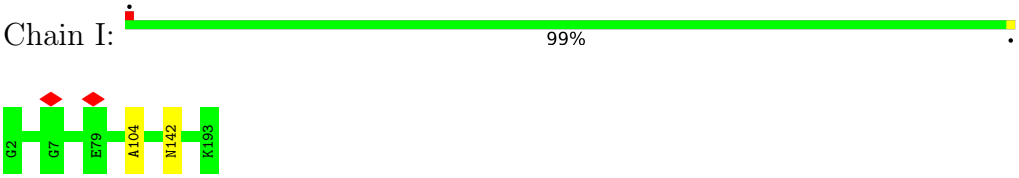
• Molecule 8: srRNA4

Chain H:



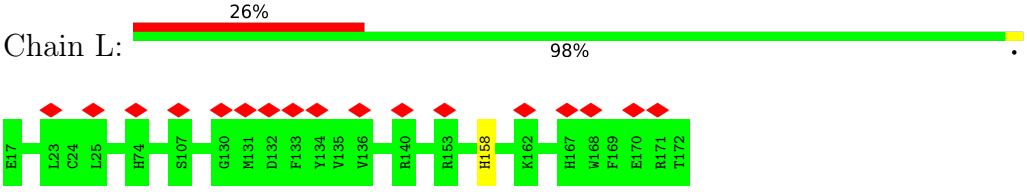
• Molecule 9: 60S ribosomal protein L18

Chain I:



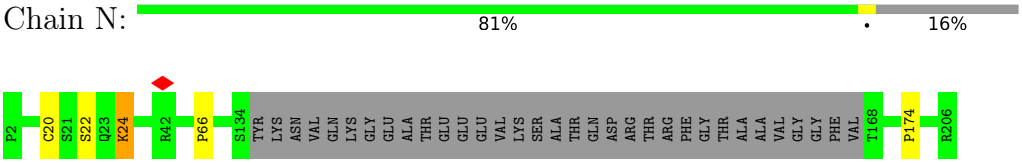
• Molecule 10: 60S ribosomal protein L11

Chain L:



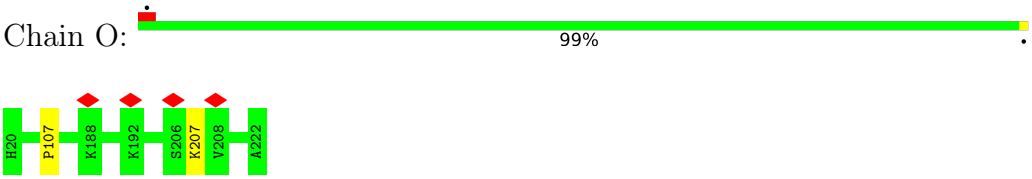
• Molecule 11: 60S ribosomal protein L13

Chain N:



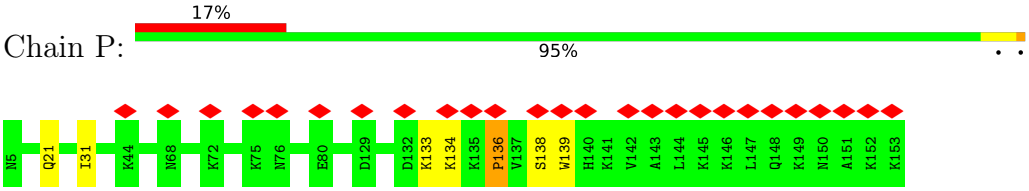
• Molecule 12: 60S ribosomal protein L13a

Chain O:



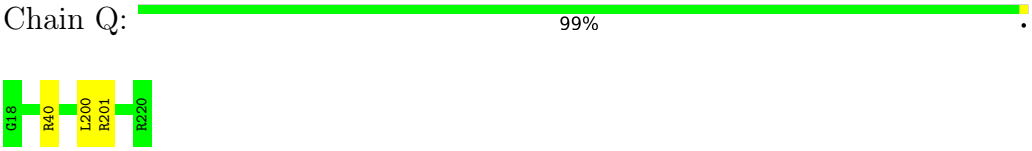
• Molecule 13: 40S ribosomal protein L14

Chain P:



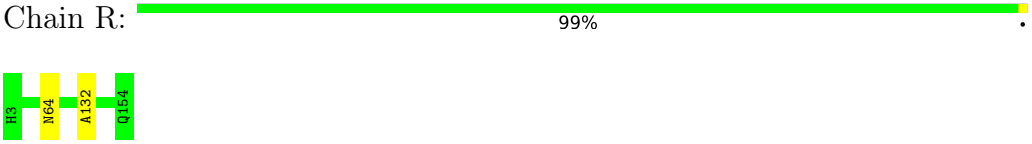
• Molecule 14: Ribosomal protein L15

Chain Q:



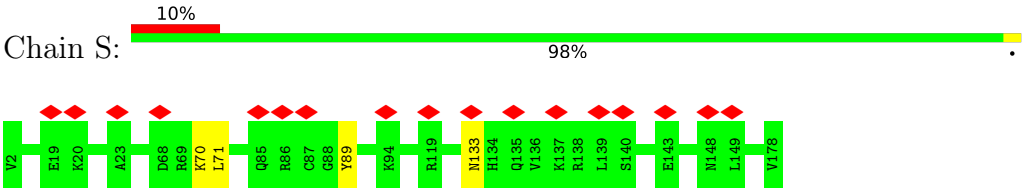
• Molecule 15: 60S ribosomal protein L17

Chain R:



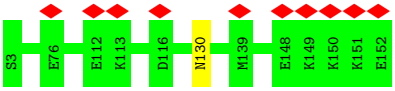
• Molecule 16: 60S ribosomal protein L18a

Chain S:



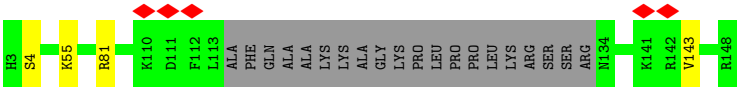
• Molecule 17: Ribosomal protein L19-like protein

Chain T:



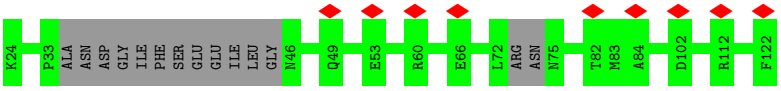
• Molecule 18: Ribosomal protein L21E (60S)

Chain U:



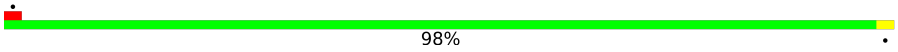
• Molecule 19: 60S ribosomal protein L22

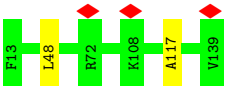
Chain V:



• Molecule 20: 60S ribosomal protein L23

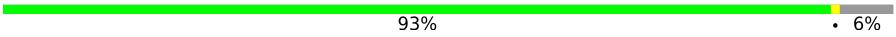
Chain W:

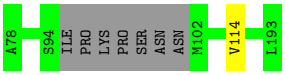




• Molecule 21: 60S ribosomal protein L23a

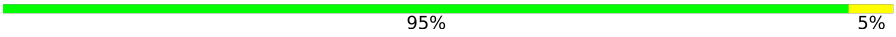
Chain X:

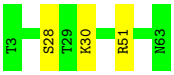




• Molecule 22: Ribosomal protein L24

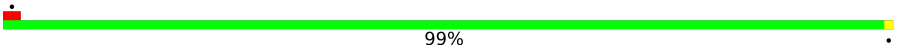
Chain Y:

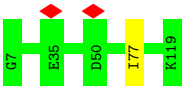




• Molecule 23: 60S ribosomal protein L26

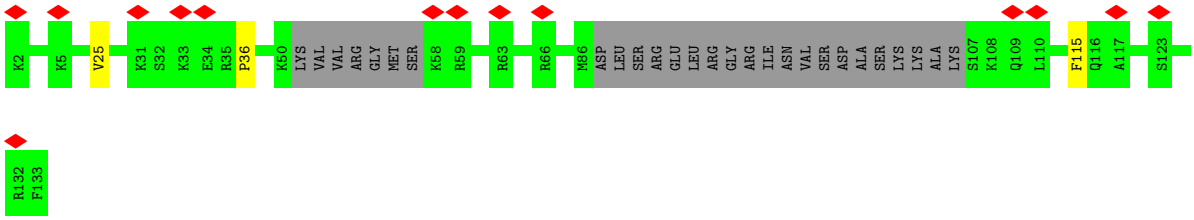
Chain Z:





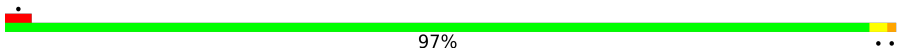
• Molecule 24: Ribosomal protein L27

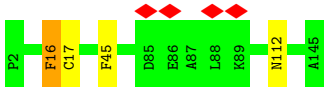
Chain a:



• Molecule 25: 60S ribosomal protein L27A/L29

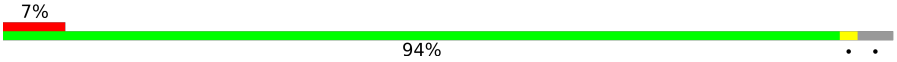
Chain b:

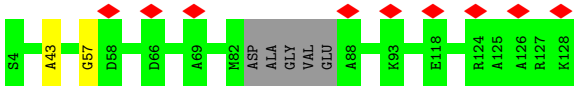




• Molecule 26: 60S ribosomal protein L28

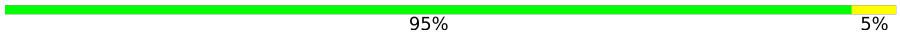
Chain c:





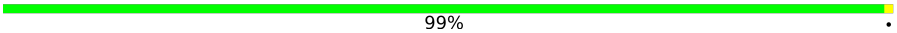
• Molecule 27: Ribosomal protein L29

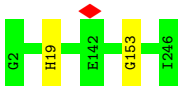
Chain d:



• Molecule 28: 60S ribosomal protein L2

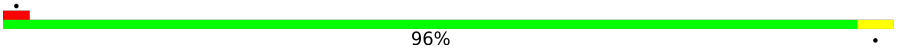
Chain e:

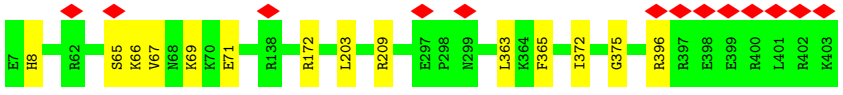




• Molecule 29: Ribosomal protein L13

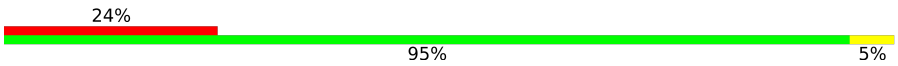
Chain f:

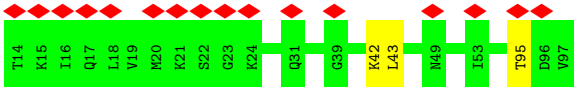




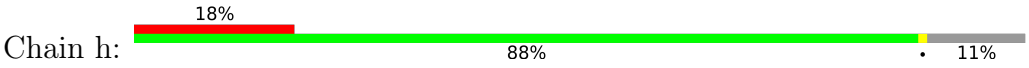
• Molecule 30: 60S ribosomal protein L30

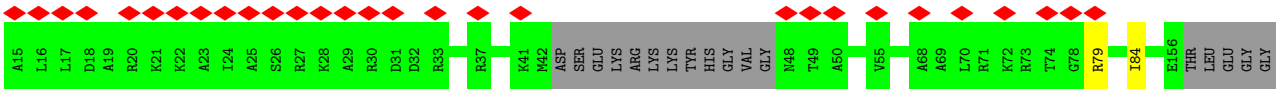
Chain g:

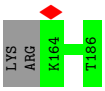




• Molecule 31: 60S ribosomal subunit protein L31

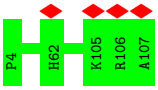




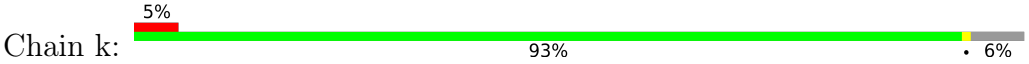


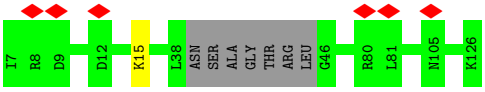
• Molecule 32: 60S ribosomal protein L32

• Molecule 33: 60S ribosomal protein L34

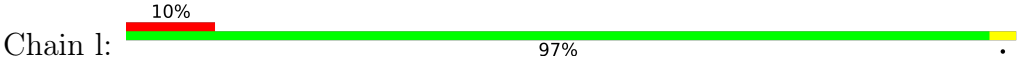


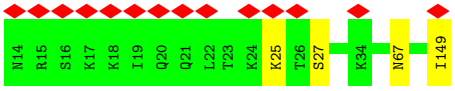
• Molecule 34: 60S ribosomal protein L35



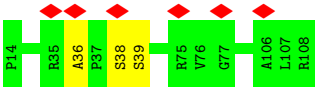


• Molecule 35: Ribosomal protein L35A

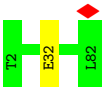




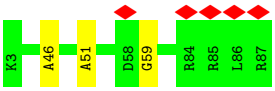
• Molecule 36: Ribosomal protein L36



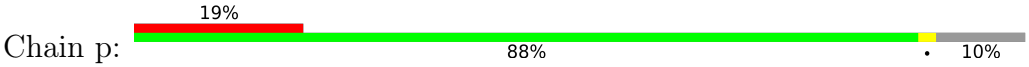
• Molecule 37: Ribosomal protein L37

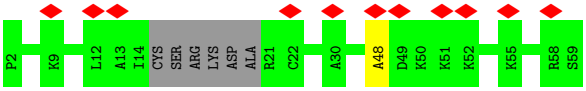


• Molecule 38: 60S ribosomal protein L37a

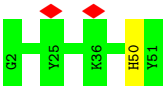


• Molecule 39: Ribosomal protein L38

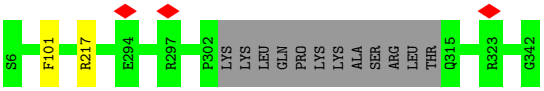




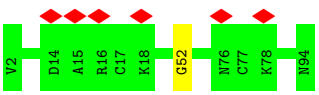
• Molecule 40: Ribosomal protein L39



• Molecule 41: 60S ribosomal protein L4

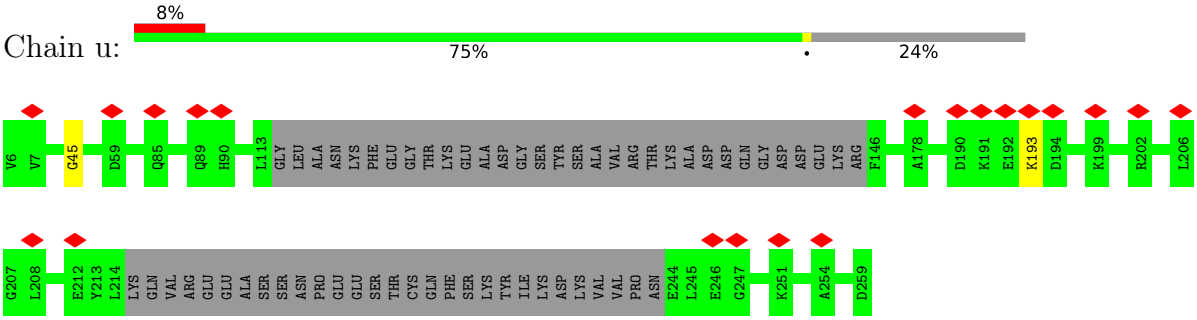


• Molecule 42: 60S ribosomal protein L44



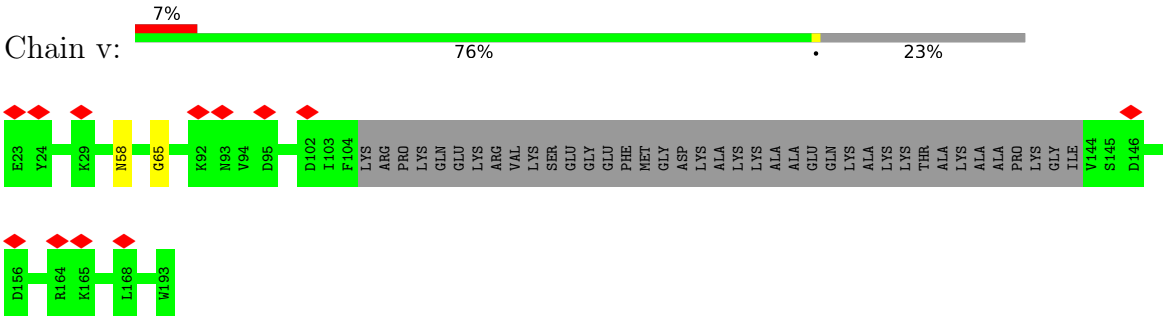
• Molecule 43: 60S ribosomal protein L5

Chain u:



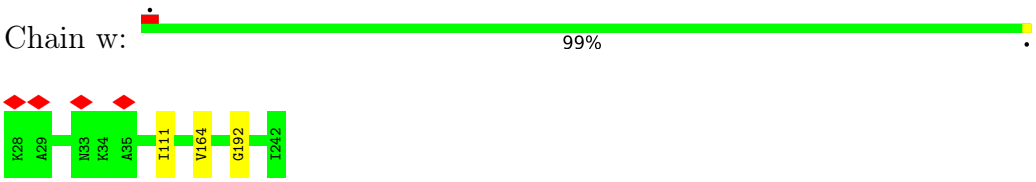
• Molecule 44: 60S ribosomal protein L6

Chain v:



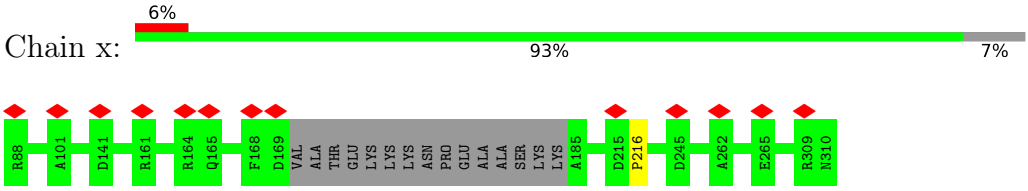
• Molecule 45: 60S ribosomal protein L7

Chain w:



• Molecule 46: Ribosomal protein L7a-like protein

Chain x:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	235000	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 ($e^-/Å^2$)	27	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.816	Depositor
Minimum map value	-0.455	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.053	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	240.34999, 240.34999, 240.34999	wwPDB
Map dimensions	230, 230, 230	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.045, 1.045, 1.045	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 7MG, OMC, MG, OMU, A2M, 5MC, OMG, 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	A	1.31	11/29897 (0.0%)	1.06	45/46554 (0.1%)
2	B	1.14	4/21699 (0.0%)	1.00	16/33776 (0.0%)
3	C	1.23	0/3306	1.04	3/5144 (0.1%)
4	D	0.83	0/2715	0.90	0/4226
5	E	0.95	2/3472 (0.1%)	0.92	1/5396 (0.0%)
6	F	0.88	0/1074	0.98	3/1665 (0.2%)
7	G	1.25	1/2849 (0.0%)	1.06	5/4431 (0.1%)
8	H	1.16	0/2171	1.01	1/3374 (0.0%)
9	I	0.67	0/1540	0.67	0/2058
10	L	0.38	0/542	0.52	0/718
11	N	0.66	0/1442	0.65	1/1926 (0.1%)
12	O	0.67	0/1673	0.62	0/2244
13	P	0.51	0/1204	0.60	1/1618 (0.1%)
14	Q	0.82	0/1752	0.80	7/2341 (0.3%)
15	R	0.74	0/1251	0.67	0/1678
16	S	0.62	0/1484	0.60	0/1997
17	T	0.57	0/1292	0.58	0/1711
18	U	0.67	0/1037	0.62	0/1389
19	V	0.49	0/742	0.57	0/986
20	W	0.64	0/977	0.61	0/1318
21	X	0.65	0/905	0.65	0/1215
22	Y	0.69	0/539	0.66	0/728
23	Z	0.56	0/934	0.59	0/1249
24	a	0.45	0/895	0.55	0/1190
25	b	0.73	0/1164	0.69	2/1558 (0.1%)
26	c	0.55	0/946	0.58	0/1263
27	d	0.57	0/527	0.67	0/703
28	e	0.72	0/1915	0.66	0/2576
29	f	0.72	0/3257	0.69	3/4376 (0.1%)
30	g	0.43	0/530	0.55	0/712
31	h	0.61	0/1076	0.60	0/1450
32	i	0.74	0/948	0.67	0/1265

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	j	0.62	0/879	0.62	0/1174
34	k	0.53	0/972	0.61	0/1283
35	l	0.77	0/1079	0.66	0/1451
36	m	0.53	0/767	0.62	0/1017
37	n	0.85	0/692	0.75	0/921
38	o	0.74	0/681	0.67	0/905
39	p	0.45	0/437	0.56	0/579
40	q	0.66	0/470	0.65	0/626
41	r	0.70	0/2560	0.63	0/3444
42	t	0.62	0/777	0.65	0/1030
43	u	0.52	0/1568	0.56	0/2104
44	v	0.51	0/1055	0.57	0/1420
45	w	0.68	0/1780	0.62	0/2384
46	x	0.60	0/1715	0.64	0/2306
All	All	1.02	18/111187 (0.0%)	0.90	88/163479 (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
14	Q	0	1
24	a	0	1
All	All	0	2

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1610	A	N9-C4	-6.70	1.33	1.37
1	A	1079	G	N9-C4	-6.39	1.32	1.38
2	B	1347	A	N9-C4	-6.00	1.34	1.37
1	A	20	G	N9-C4	-5.97	1.33	1.38
1	A	405	A	N9-C4	-5.83	1.34	1.37

The worst 5 of 88 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1578	U	OP2-P-O3'	-10.15	82.87	105.20
1	A	1578	U	OP1-P-O3'	-9.94	83.34	105.20
14	Q	40[A]	ARG	CA-C-O	9.91	140.91	120.10
14	Q	40[B]	ARG	CA-C-O	9.91	140.91	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	20	G	N3-C4-C5	9.68	133.44	128.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	Q	200	LEU	Peptide
24	a	115	PHE	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
9	I	190/192 (99%)	177 (93%)	11 (6%)	2 (1%)	14 19
10	L	57/65 (88%)	51 (90%)	5 (9%)	1 (2%)	8 10
11	N	168/205 (82%)	154 (92%)	12 (7%)	2 (1%)	13 17
12	O	201/203 (99%)	191 (95%)	8 (4%)	2 (1%)	15 22
13	P	147/149 (99%)	133 (90%)	11 (8%)	3 (2%)	7 8
14	Q	202/203 (100%)	188 (93%)	14 (7%)	0	100 100
15	R	150/152 (99%)	138 (92%)	10 (7%)	2 (1%)	12 16
16	S	175/177 (99%)	158 (90%)	13 (7%)	4 (2%)	6 6
17	T	148/150 (99%)	144 (97%)	3 (2%)	1 (1%)	22 30
18	U	122/146 (84%)	111 (91%)	7 (6%)	4 (3%)	4 2
19	V	79/99 (80%)	70 (89%)	9 (11%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
20	W	125/127 (98%)	120 (96%)	3 (2%)	2 (2%)	9 12
21	X	105/116 (90%)	101 (96%)	3 (3%)	1 (1%)	15 22
22	Y	59/61 (97%)	57 (97%)	2 (3%)	0	100 100
23	Z	111/113 (98%)	100 (90%)	10 (9%)	1 (1%)	17 24
24	a	99/132 (75%)	92 (93%)	5 (5%)	2 (2%)	7 8
25	b	142/144 (99%)	130 (92%)	11 (8%)	1 (1%)	22 30
26	c	116/125 (93%)	108 (93%)	6 (5%)	2 (2%)	9 11
27	d	61/63 (97%)	56 (92%)	2 (3%)	3 (5%)	2 1
28	e	243/245 (99%)	225 (93%)	16 (7%)	2 (1%)	19 27
29	f	395/397 (100%)	372 (94%)	19 (5%)	4 (1%)	15 22
30	g	62/66 (94%)	59 (95%)	2 (3%)	1 (2%)	9 12
31	h	140/169 (83%)	133 (95%)	7 (5%)	0	100 100
32	i	111/113 (98%)	108 (97%)	2 (2%)	1 (1%)	17 24
33	j	102/104 (98%)	98 (96%)	4 (4%)	0	100 100
34	k	109/120 (91%)	105 (96%)	3 (3%)	1 (1%)	17 24
35	l	134/136 (98%)	123 (92%)	9 (7%)	2 (2%)	10 14
36	m	93/95 (98%)	87 (94%)	3 (3%)	3 (3%)	4 3
37	n	79/81 (98%)	71 (90%)	7 (9%)	1 (1%)	12 16
38	o	83/85 (98%)	76 (92%)	4 (5%)	3 (4%)	3 2
39	p	48/58 (83%)	44 (92%)	3 (6%)	1 (2%)	7 7
40	q	48/50 (96%)	43 (90%)	4 (8%)	1 (2%)	7 7
41	r	321/337 (95%)	309 (96%)	10 (3%)	2 (1%)	25 34
42	t	91/93 (98%)	86 (94%)	4 (4%)	1 (1%)	14 19
43	u	187/254 (74%)	176 (94%)	9 (5%)	2 (1%)	14 19
44	v	128/171 (75%)	119 (93%)	7 (6%)	2 (2%)	9 12
45	w	213/215 (99%)	194 (91%)	16 (8%)	3 (1%)	11 15
46	x	204/223 (92%)	196 (96%)	7 (3%)	1 (0%)	29 40
All	All	5248/5634 (93%)	4903 (93%)	281 (5%)	64 (1%)	17 17

5 of 64 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	I	142	ASN

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Mol	Chain	Res	Type
11	N	66	PRO
11	N	174	PRO
13	P	21	GLN
15	R	132	ALA

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	
9	I	160/160 (100%)	160 (100%)	0	100	100
10	L	57/57 (100%)	57 (100%)	0	100	100
11	N	153/178 (86%)	150 (98%)	3 (2%)	55	70
12	O	175/175 (100%)	175 (100%)	0	100	100
13	P	119/131 (91%)	115 (97%)	4 (3%)	37	50
14	Q	177/176 (101%)	177 (100%)	0	100	100
15	R	131/131 (100%)	131 (100%)	0	100	100
16	S	158/158 (100%)	158 (100%)	0	100	100
17	T	134/134 (100%)	134 (100%)	0	100	100
18	U	108/123 (88%)	108 (100%)	0	100	100
19	V	79/90 (88%)	79 (100%)	0	100	100
20	W	99/99 (100%)	99 (100%)	0	100	100
21	X	96/103 (93%)	96 (100%)	0	100	100
22	Y	55/55 (100%)	52 (94%)	3 (6%)	21	29
23	Z	97/97 (100%)	97 (100%)	0	100	100
24	a	93/116 (80%)	93 (100%)	0	100	100
25	b	116/116 (100%)	114 (98%)	2 (2%)	60	75
26	c	99/102 (97%)	99 (100%)	0	100	100
27	d	52/52 (100%)	52 (100%)	0	100	100
28	e	194/194 (100%)	194 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
29	f	339/339 (100%)	332 (98%)	7 (2%)	53 68
30	g	62/62 (100%)	60 (97%)	2 (3%)	39 53
31	h	91/144 (63%)	89 (98%)	2 (2%)	52 66
32	i	100/100 (100%)	100 (100%)	0	100 100
33	j	90/90 (100%)	90 (100%)	0	100 100
34	k	103/108 (95%)	103 (100%)	0	100 100
35	l	102/112 (91%)	100 (98%)	2 (2%)	55 70
36	m	77/77 (100%)	77 (100%)	0	100 100
37	n	69/69 (100%)	69 (100%)	0	100 100
38	o	68/68 (100%)	68 (100%)	0	100 100
39	p	48/53 (91%)	48 (100%)	0	100 100
40	q	46/46 (100%)	46 (100%)	0	100 100
41	r	262/273 (96%)	262 (100%)	0	100 100
42	t	82/82 (100%)	82 (100%)	0	100 100
43	u	155/207 (75%)	155 (100%)	0	100 100
44	v	112/141 (79%)	112 (100%)	0	100 100
45	w	180/180 (100%)	180 (100%)	0	100 100
46	x	182/194 (94%)	182 (100%)	0	100 100
All	All	4520/4792 (94%)	4495 (99%)	25 (1%)	86 92

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
29	f	67	VAL
29	f	209	ARG
35	l	149	ILE
29	f	71	GLU
29	f	396	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 80 such sidechains are listed below:

Mol	Chain	Res	Type
29	f	248	HIS
41	r	42	ASN
29	f	289	GLN

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Mol	Chain	Res	Type
33	j	51	HIS
45	w	110	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1249/1278 (97%)	348 (27%)	33 (2%)
2	B	925/941 (98%)	275 (29%)	18 (1%)
3	C	144/169 (85%)	39 (27%)	2 (1%)
4	D	111/118 (94%)	23 (20%)	4 (3%)
5	E	141/146 (96%)	30 (21%)	4 (2%)
6	F	44/46 (95%)	21 (47%)	7 (15%)
7	G	117/123 (95%)	28 (23%)	2 (1%)
8	H	86/91 (94%)	20 (23%)	3 (3%)
All	All	2817/2912 (96%)	784 (27%)	73 (2%)

5 of 784 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	4	A
1	A	5	G
1	A	12	G
1	A	15	U
1	A	20	G

5 of 73 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	E	67	U
8	H	41	A
5	E	126	A
6	F	62	U
1	A	1083	G

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

72 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	$\#\|Z\| > 2$
2	OMC	B	77	2	19,22,23	2.40	6 (31%)	26,31,34	0.82	0
2	A2M	B	482	2	18,25,26	3.93	7 (38%)	18,36,39	2.64	3 (16%)
2	7MG	B	1138	2	22,26,27	2.49	9 (40%)	29,39,42	2.08	8 (27%)
2	OMU	B	1345	2	19,22,23	2.32	3 (15%)	26,31,34	1.82	5 (19%)
2	OMG	B	755	2	18,26,27	1.64	5 (27%)	19,38,41	1.83	5 (26%)
2	OMG	B	1363	2	18,26,27	1.78	5 (27%)	19,38,41	1.74	5 (26%)
2	OMG	B	1492	2	18,26,27	1.69	5 (27%)	19,38,41	1.48	5 (26%)
1	A2M	A	974	1	18,25,26	3.90	6 (33%)	18,36,39	2.74	5 (27%)
1	OMG	A	1316	1	18,26,27	1.71	5 (27%)	19,38,41	1.76	5 (26%)
2	OMG	B	1385	2	18,26,27	1.67	5 (27%)	19,38,41	1.59	6 (31%)
2	A2M	B	1516	2,47	18,25,26	4.07	7 (38%)	18,36,39	2.65	3 (16%)
1	OMG	A	1075	1	18,26,27	1.70	5 (27%)	19,38,41	1.78	4 (21%)
1	OMC	A	919	1	19,22,23	2.42	5 (26%)	26,31,34	1.23	3 (11%)
2	OMU	B	73	2	19,22,23	2.29	5 (26%)	26,31,34	1.70	4 (15%)
1	OMG	A	1675	2,1	18,26,27	1.58	4 (22%)	19,38,41	1.65	7 (36%)
1	OMG	A	972	1	18,26,27	1.67	4 (22%)	19,38,41	1.71	5 (26%)
1	7MG	A	931	1	22,26,27	2.01	8 (36%)	29,39,42	1.97	9 (31%)
1	OMC	A	1053	1	19,22,23	2.16	6 (31%)	26,31,34	1.55	5 (19%)
1	A2M	A	775	2,1	18,25,26	4.07	6 (33%)	18,36,39	2.55	4 (22%)
1	5MC	A	1525	1	18,22,23	2.51	5 (27%)	26,32,35	1.15	2 (7%)
1	A2M	A	1804	1	18,25,26	4.01	7 (38%)	18,36,39	2.79	6 (33%)
2	OMC	B	1529	2	19,22,23	2.20	5 (26%)	26,31,34	0.76	0
2	OMC	B	1449	2	19,22,23	2.25	6 (31%)	26,31,34	0.85	0
2	OMC	B	21	2,1	19,22,23	2.32	5 (26%)	26,31,34	0.82	0
2	OMG	B	634	2	18,26,27	1.58	5 (27%)	19,38,41	1.57	5 (26%)
2	A2M	B	691	2	18,25,26	4.08	7 (38%)	18,36,39	3.16	7 (38%)
1	OMU	A	1227	1	19,22,23	2.30	5 (26%)	26,31,34	1.82	4 (15%)
1	7MG	A	1725	2,1	22,26,27	2.15	8 (36%)	29,39,42	1.98	9 (31%)
2	OMG	B	564	2	18,26,27	1.76	5 (27%)	19,38,41	1.54	5 (26%)
1	OMU	A	1497	1	19,22,23	2.33	5 (26%)	26,31,34	2.18	7 (26%)
3	7MG	C	42	3	22,26,27	2.13	8 (36%)	29,39,42	2.16	9 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	A2M	C	43	3	18,25,26	3.97	7 (38%)	18,36,39	2.40	3 (16%)
3	OMG	C	75	3	18,26,27	1.68	5 (27%)	19,38,41	1.60	6 (31%)
1	OMC	A	792	1	19,22,23	2.29	5 (26%)	26,31,34	0.81	1 (3%)
2	A2M	B	50	2,47	18,25,26	3.95	7 (38%)	18,36,39	2.46	3 (16%)
2	A2M	B	728	2	18,25,26	3.93	7 (38%)	18,36,39	2.64	3 (16%)
1	A2M	A	1043	1	18,25,26	3.95	7 (38%)	18,36,39	2.89	3 (16%)
2	5MC	B	624	2	18,22,23	2.52	5 (27%)	26,32,35	1.30	4 (15%)
1	A2M	A	423	1	18,25,26	4.00	6 (33%)	18,36,39	2.63	4 (22%)
1	OMG	A	958	1	18,26,27	1.60	5 (27%)	19,38,41	1.71	4 (21%)
2	OMU	B	1491	2	19,22,23	2.17	4 (21%)	26,31,34	2.08	6 (23%)
1	A2M	A	1071	1	18,25,26	4.06	6 (33%)	18,36,39	2.54	3 (16%)
2	OMC	B	1380	2	19,22,23	2.29	5 (26%)	26,31,34	0.84	0
1	5MC	A	1073	1	18,22,23	2.46	6 (33%)	26,32,35	1.30	3 (11%)
2	7MG	B	1107	2	22,26,27	2.42	8 (36%)	29,39,42	2.10	8 (27%)
1	OMC	A	343	1	19,22,23	2.31	5 (26%)	26,31,34	0.88	0
3	OMU	C	118	3	19,22,23	2.30	4 (21%)	26,31,34	1.92	5 (19%)
2	OMC	B	543	2	19,22,23	2.23	5 (26%)	26,31,34	0.70	0
2	OMC	B	683	2	19,22,23	2.23	5 (26%)	26,31,34	0.83	0
1	OMU	A	963	1	19,22,23	2.38	5 (26%)	26,31,34	1.87	5 (19%)
2	OMG	B	1210	2	18,26,27	1.59	5 (27%)	19,38,41	1.92	7 (36%)
3	OMG	C	166	3,1	18,26,27	1.65	5 (27%)	19,38,41	1.69	5 (26%)
1	7MG	A	1045	1	22,26,27	2.20	7 (31%)	29,39,42	1.92	8 (27%)
2	OMU	B	767	2	19,22,23	2.28	4 (21%)	26,31,34	1.77	4 (15%)
2	OMG	B	1169	2	18,26,27	1.62	5 (27%)	19,38,41	1.63	5 (26%)
1	OMC	A	1662	1	19,22,23	2.20	6 (31%)	26,31,34	0.68	0
2	OMG	B	1361	2	18,26,27	1.64	5 (27%)	19,38,41	1.63	5 (26%)
2	OMG	B	71	2	18,26,27	1.77	5 (27%)	19,38,41	1.82	6 (31%)
3	A2M	C	163	3,1	18,25,26	3.92	7 (38%)	18,36,39	2.55	3 (16%)
2	A2M	B	627	2	18,25,26	3.83	7 (38%)	18,36,39	2.60	4 (22%)
2	7MG	B	657	2,47	22,26,27	2.18	8 (36%)	29,39,42	2.15	9 (31%)
7	OMG	G	70	7	18,26,27	1.58	4 (22%)	19,38,41	1.69	6 (31%)
1	OMC	A	777	1	19,22,23	2.36	6 (31%)	26,31,34	0.74	0
1	OMG	A	1659	1	18,26,27	1.57	5 (27%)	19,38,41	1.80	6 (31%)
1	A2M	A	1674	47,2,1	18,25,26	4.01	7 (38%)	18,36,39	2.46	3 (16%)
1	A2M	A	778	1	18,25,26	3.91	7 (38%)	18,36,39	2.27	3 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	A2M	A	794	1	18,25,26	4.04	7 (38%)	18,36,39	3.31	7 (38%)
1	OMG	A	1710	1	18,26,27	1.72	5 (27%)	19,38,41	1.64	5 (26%)
1	OMU	A	1127	1	19,22,23	2.36	5 (26%)	26,31,34	1.70	6 (23%)
1	OMG	A	927	1	18,26,27	1.71	5 (27%)	19,38,41	1.62	6 (31%)
3	OMU	C	7	3,1	19,22,23	2.45	6 (31%)	26,31,34	1.81	4 (15%)
3	OMC	C	105	3,47	19,22,23	2.28	7 (36%)	26,31,34	1.09	1 (3%)

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
2	OMC	B	77	2	-	2/9/27/28	0/2/2/2
2	A2M	B	482	2	-	0/5/27/28	0/3/3/3
2	7MG	B	1138	2	-	2/7/37/38	0/3/3/3
2	OMU	B	1345	2	-	0/9/27/28	0/2/2/2
2	OMG	B	755	2	-	4/5/27/28	0/3/3/3
2	OMG	B	1363	2	-	0/5/27/28	0/3/3/3
2	OMG	B	1492	2	-	2/5/27/28	0/3/3/3
1	A2M	A	974	1	-	0/5/27/28	0/3/3/3
1	OMG	A	1316	1	-	0/5/27/28	0/3/3/3
2	OMG	B	1385	2	-	0/5/27/28	0/3/3/3
2	A2M	B	1516	2,47	-	1/5/27/28	0/3/3/3
1	OMG	A	1075	1	-	0/5/27/28	0/3/3/3
1	OMC	A	919	1	-	5/9/27/28	0/2/2/2
2	OMU	B	73	2	-	3/9/27/28	0/2/2/2
1	OMG	A	1675	2,1	-	1/5/27/28	0/3/3/3
1	OMG	A	972	1	-	0/5/27/28	0/3/3/3
1	7MG	A	931	1	-	0/7/37/38	0/3/3/3
1	OMC	A	1053	1	-	3/9/27/28	0/2/2/2
1	A2M	A	775	2,1	-	0/5/27/28	0/3/3/3
1	5MC	A	1525	1	-	2/7/25/26	0/2/2/2
1	A2M	A	1804	1	-	4/5/27/28	0/3/3/3
2	OMC	B	1529	2	-	0/9/27/28	0/2/2/2
2	OMC	B	1449	2	-	0/9/27/28	0/2/2/2
2	OMC	B	21	2,1	-	0/9/27/28	0/2/2/2
2	OMG	B	634	2	-	1/5/27/28	0/3/3/3
2	A2M	B	691	2	-	3/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMU	A	1227	1	-	2/9/27/28	0/2/2/2
1	7MG	A	1725	2,1	-	2/7/37/38	0/3/3/3
2	OMG	B	564	2	-	2/5/27/28	0/3/3/3
1	OMU	A	1497	1	-	2/9/27/28	0/2/2/2
3	7MG	C	42	3	-	0/7/37/38	0/3/3/3
3	A2M	C	43	3	-	0/5/27/28	0/3/3/3
3	OMG	C	75	3	-	2/5/27/28	0/3/3/3
1	OMC	A	792	1	-	0/9/27/28	0/2/2/2
2	A2M	B	50	2,47	-	0/5/27/28	0/3/3/3
2	A2M	B	728	2	-	1/5/27/28	0/3/3/3
1	A2M	A	1043	1	-	0/5/27/28	0/3/3/3
2	5MC	B	624	2	-	2/7/25/26	0/2/2/2
1	A2M	A	423	1	-	2/5/27/28	0/3/3/3
1	OMG	A	958	1	-	0/5/27/28	0/3/3/3
2	OMU	B	1491	2	-	0/9/27/28	0/2/2/2
1	A2M	A	1071	1	-	1/5/27/28	0/3/3/3
2	OMC	B	1380	2	-	3/9/27/28	0/2/2/2
1	5MC	A	1073	1	-	2/7/25/26	0/2/2/2
2	7MG	B	1107	2	-	0/7/37/38	0/3/3/3
1	OMC	A	343	1	-	0/9/27/28	0/2/2/2
3	OMU	C	118	3	-	3/9/27/28	0/2/2/2
2	OMC	B	543	2	-	6/9/27/28	0/2/2/2
2	OMC	B	683	2	-	0/9/27/28	0/2/2/2
1	OMU	A	963	1	-	0/9/27/28	0/2/2/2
2	OMG	B	1210	2	-	2/5/27/28	0/3/3/3
3	OMG	C	166	3,1	-	0/5/27/28	0/3/3/3
1	7MG	A	1045	1	-	0/7/37/38	0/3/3/3
2	OMU	B	767	2	-	0/9/27/28	0/2/2/2
2	OMG	B	1169	2	-	2/5/27/28	0/3/3/3
1	OMC	A	1662	1	-	2/9/27/28	0/2/2/2
2	OMG	B	1361	2	-	2/5/27/28	0/3/3/3
2	OMG	B	71	2	-	0/5/27/28	0/3/3/3
3	A2M	C	163	3,1	-	2/5/27/28	0/3/3/3
2	A2M	B	627	2	-	3/5/27/28	0/3/3/3
2	7MG	B	657	2,47	-	2/7/37/38	0/3/3/3
7	OMG	G	70	7	-	2/5/27/28	0/3/3/3
1	OMC	A	777	1	-	2/9/27/28	0/2/2/2
1	OMG	A	1659	1	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	A2M	A	1674	47,2,1	-	0/5/27/28	0/3/3/3
1	A2M	A	778	1	-	3/5/27/28	0/3/3/3
1	A2M	A	794	1	-	2/5/27/28	0/3/3/3
1	OMG	A	1710	1	-	0/5/27/28	0/3/3/3
1	OMU	A	1127	1	-	3/9/27/28	0/2/2/2
1	OMG	A	927	1	-	0/5/27/28	0/3/3/3
3	OMU	C	7	3,1	-	2/9/27/28	0/2/2/2
3	OMC	C	105	3,47	-	3/9/27/28	0/2/2/2

The worst 5 of 412 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	794	A2M	O4'-C1'	14.68	1.61	1.41
2	B	691	A2M	O4'-C1'	14.56	1.61	1.41
2	B	1516	A2M	O4'-C1'	14.32	1.61	1.41
1	A	1804	A2M	O4'-C1'	14.21	1.60	1.41
1	A	775	A2M	O4'-C1'	14.10	1.60	1.41

The worst 5 of 309 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	794	A2M	C5-C6-N6	8.87	133.84	120.35
1	A	1043	A2M	C5-C6-N6	8.25	132.89	120.35
2	B	728	A2M	C5-C6-N6	7.88	132.32	120.35
1	A	974	A2M	C5-C6-N6	7.55	131.82	120.35
2	B	482	A2M	C5-C6-N6	7.53	131.79	120.35

There are no chirality outliers.

5 of 95 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	73	OMU	C1'-C2'-O2'-CM2
2	B	77	OMC	C3'-C4'-C5'-O5'
2	B	543	OMC	C2'-C1'-N1-C6
2	B	543	OMC	O4'-C4'-C5'-O5'
2	B	627	A2M	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 108 ligands modelled in this entry, 108 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
1	A	30
2	B	16
5	E	5
8	H	4
10	L	3
7	G	2
31	h	2
6	F	1
30	g	1

The worst 5 of 64 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	282:U	O3'	304:A	P	49.48
1	A	1269:U	O3'	1283:A	P	36.80
1	B	913:U	O3'	1105:C	P	35.79
1	A	1233:A	O3'	1245:C	P	34.48

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	154:A	O3'	175:U	P	29.48

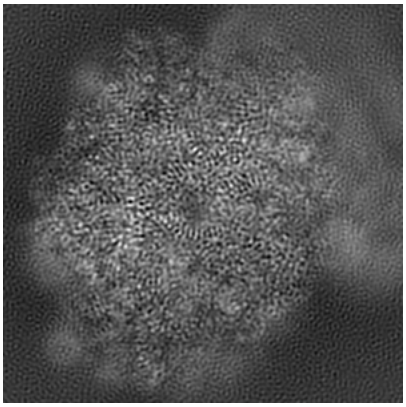
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-8361. These allow visual inspection of the internal detail of the map and identification of artifacts.

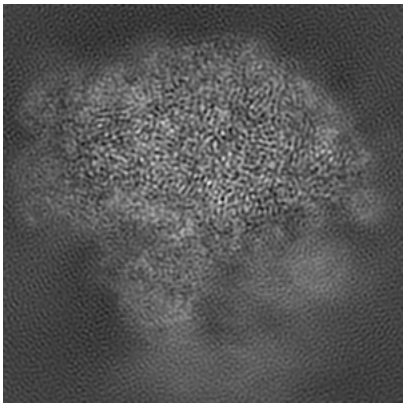
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

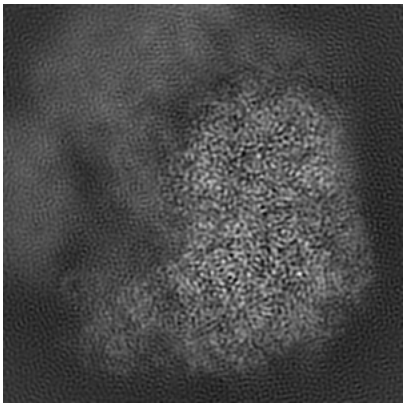
6.1.1 Primary map



X



Y

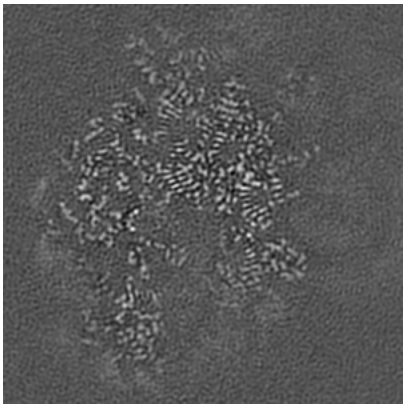


Z

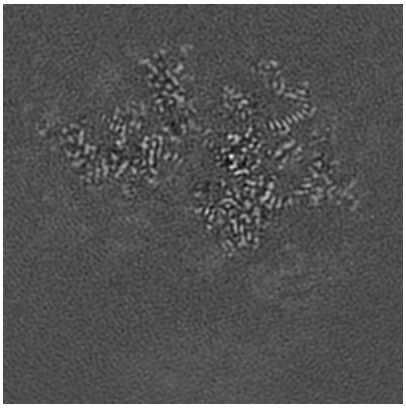
The images above show the map projected in three orthogonal directions.

6.2 Central slices

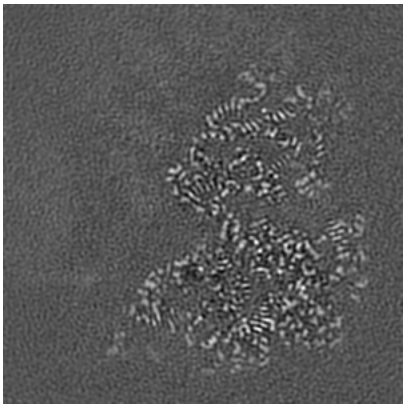
6.2.1 Primary map



X Index: 115



Y Index: 115

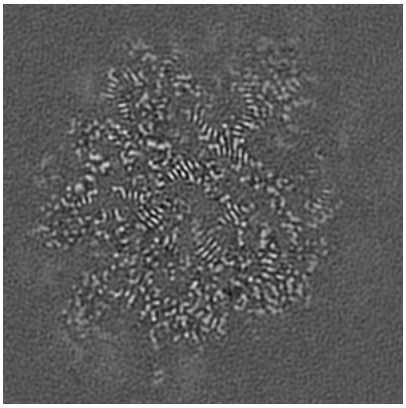


Z Index: 115

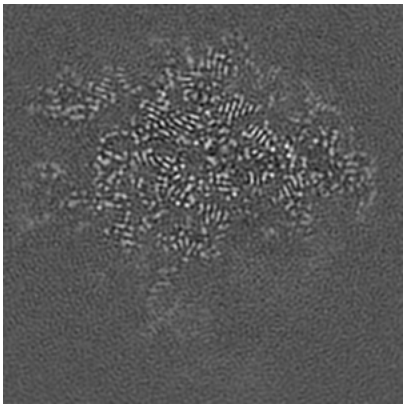
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

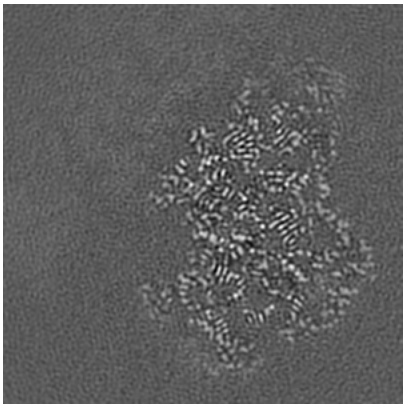
6.3.1 Primary map



X Index: 144



Y Index: 74

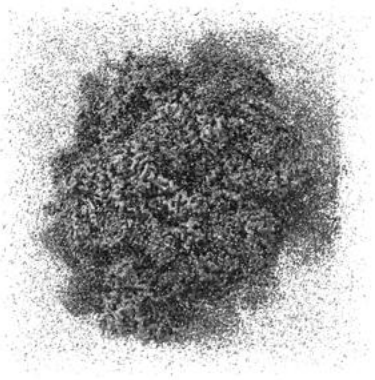


Z Index: 128

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

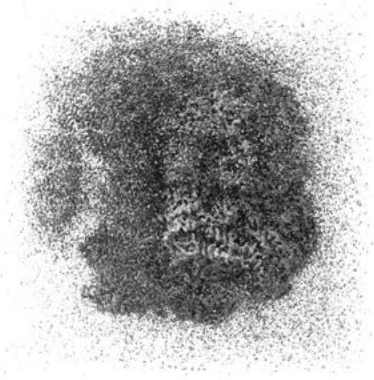
6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

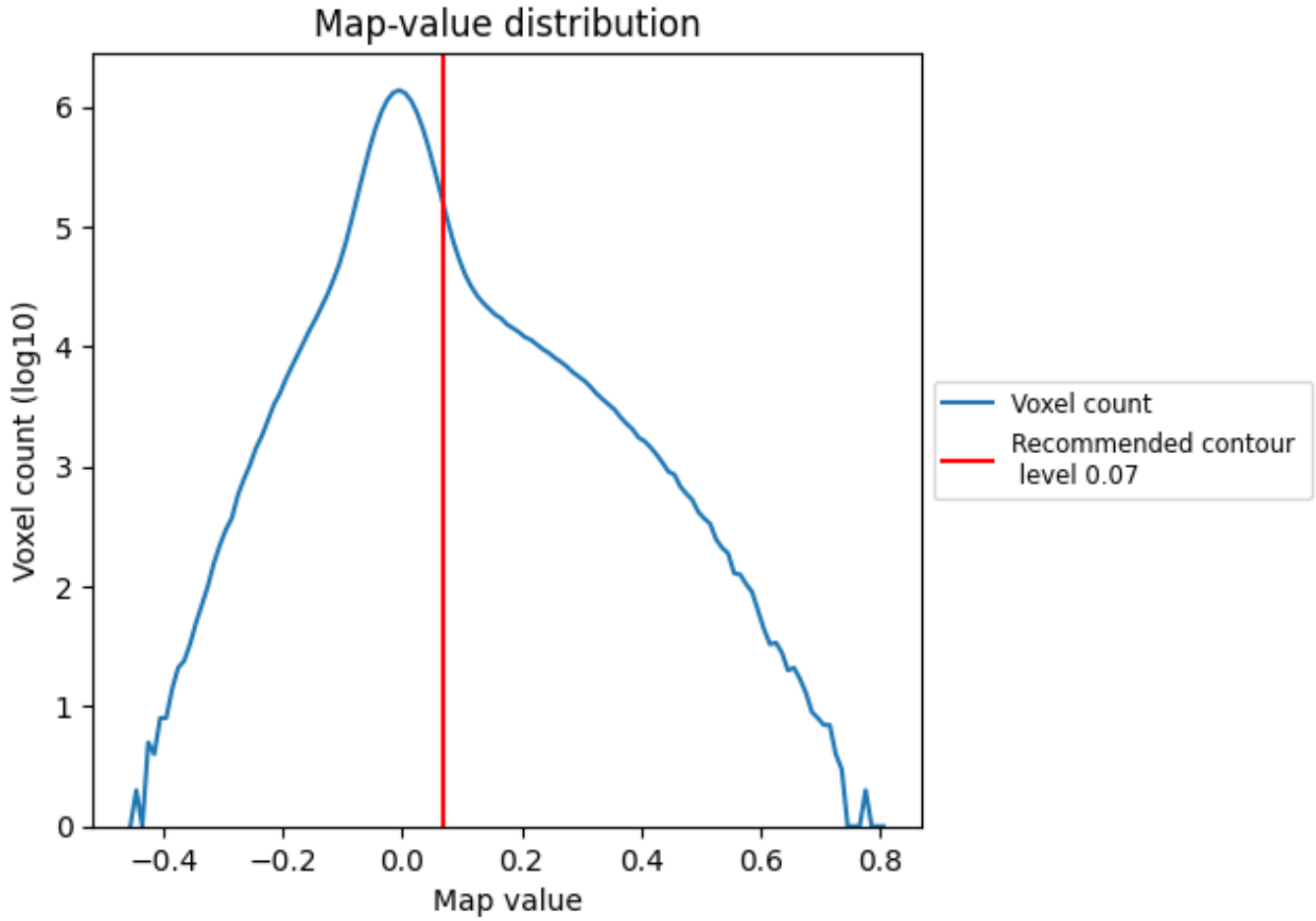
6.5 Mask visualisation (i)

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

7 Map analysis

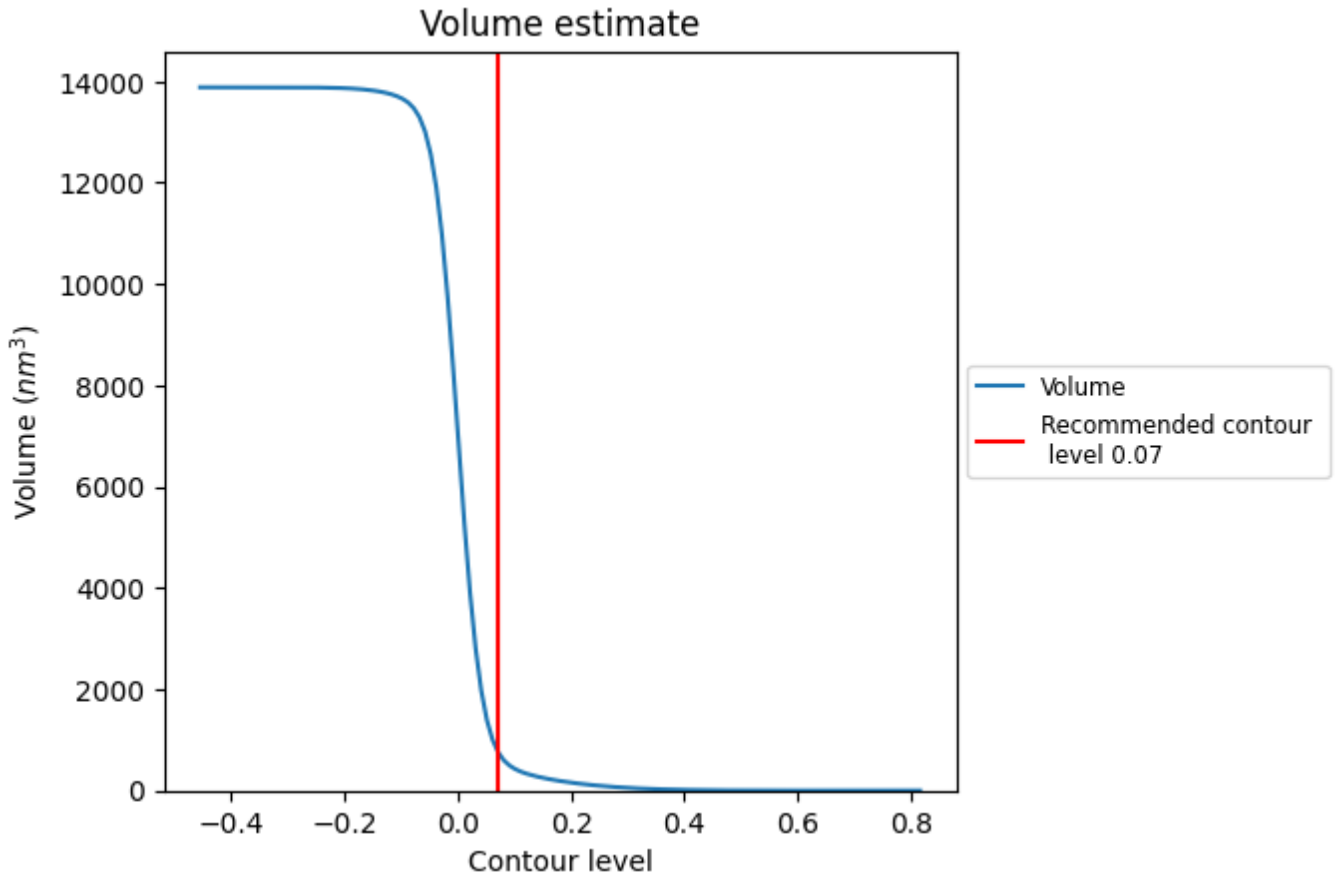
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

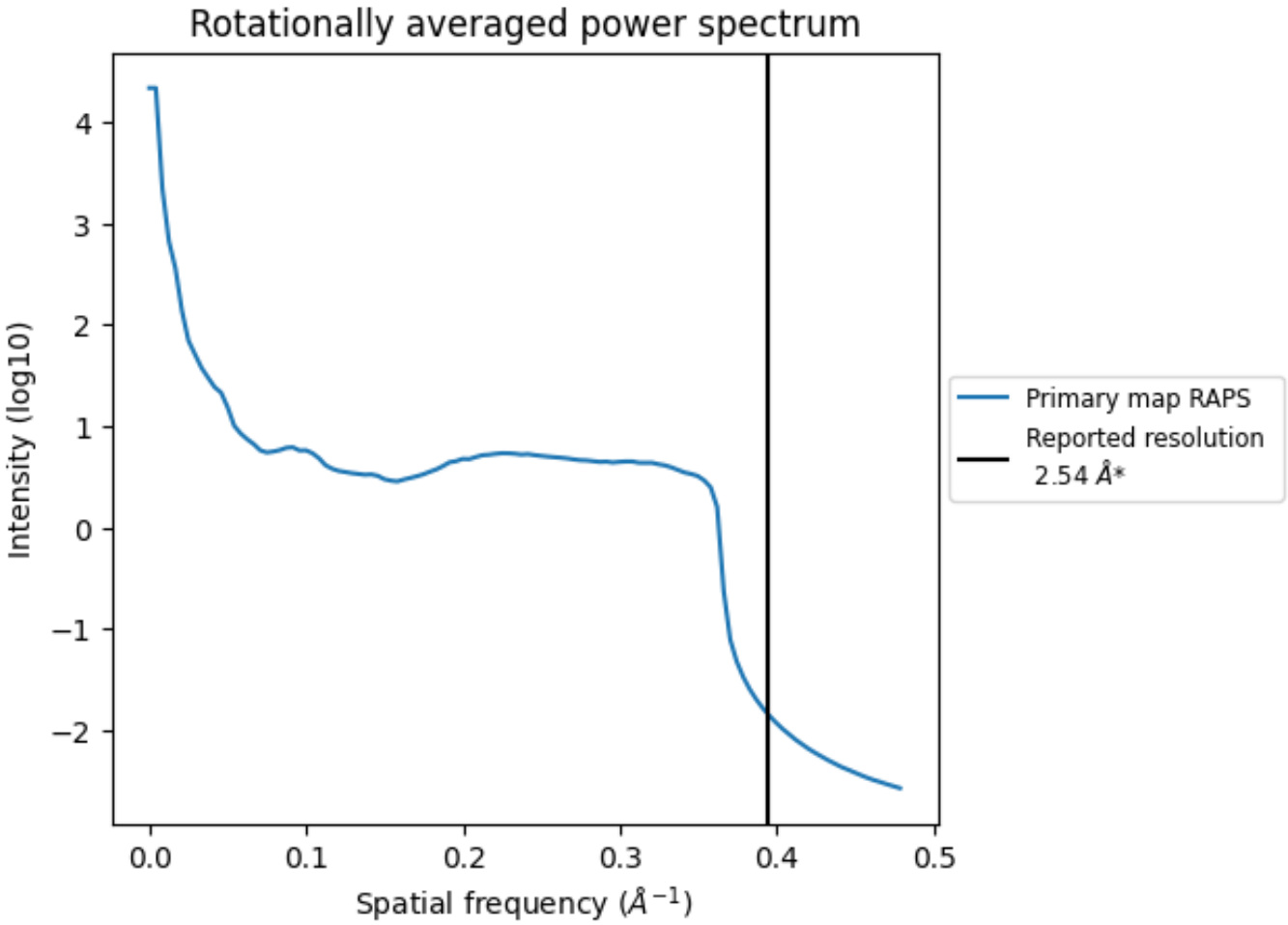
7.2 Volume estimate (i)



The volume at the recommended contour level is 791 nm^3; this corresponds to an approximate mass of 715 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 0.394 Å^{-1}

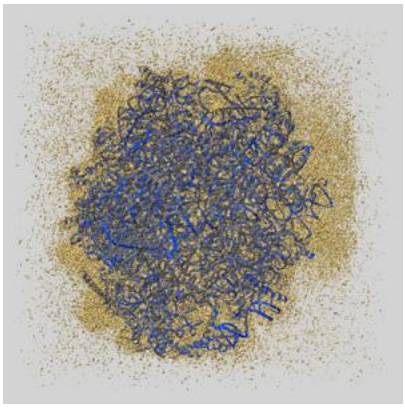
8 Fourier-Shell correlation

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

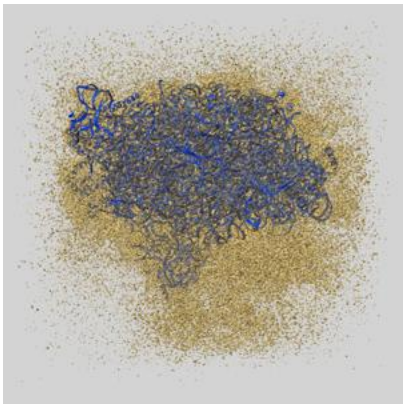
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-8361 and PDB model 5T5H. Per-residue inclusion information can be found in section 3 on page 14.

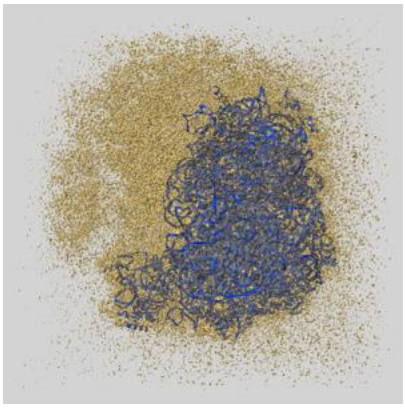
9.1 Map-model overlay



X



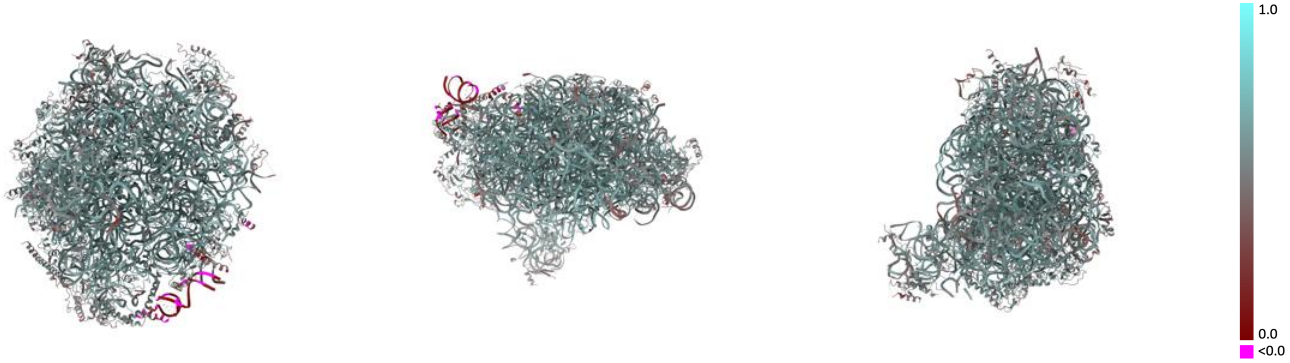
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.07 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.

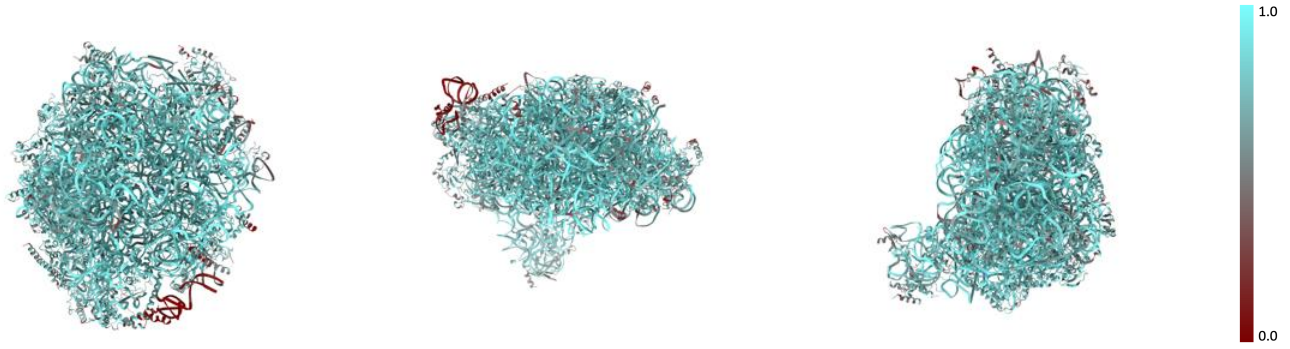
9.2 Q-score mapped to coordinate model



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.

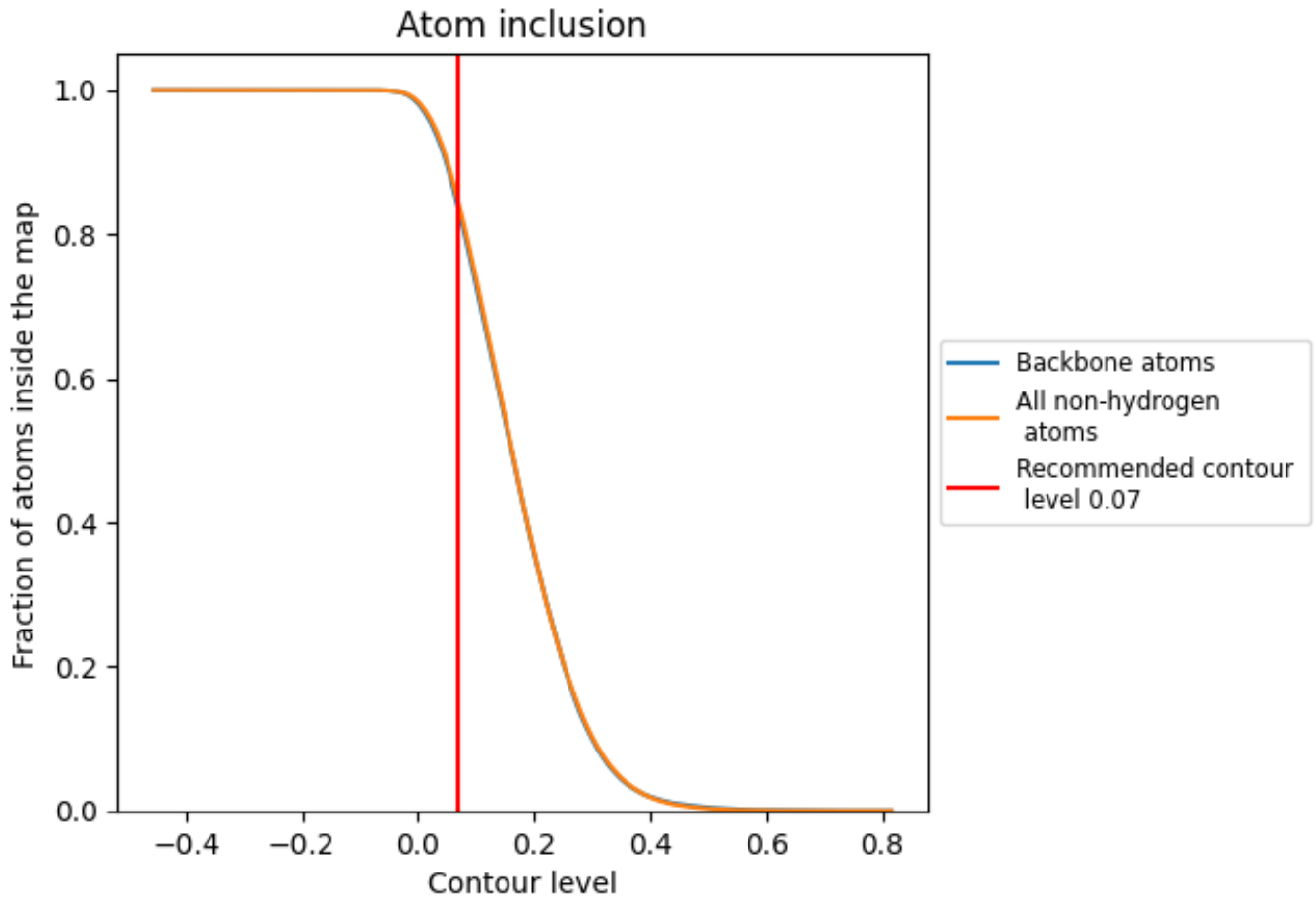
9.3 Atom inclusion mapped to coordinate model



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 (0.07).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 84% 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 (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8435	0.5690
A	0.9167	0.6020
B	0.8565	0.5680
C	0.9281	0.6040
D	0.8335	0.5320
E	0.8534	0.5690
F	0.8427	0.5310
G	0.9073	0.5890
H	0.8803	0.5810
I	0.8455	0.5800
L	0.5499	0.4390
N	0.8218	0.5520
O	0.8195	0.5570
P	0.6521	0.4780
Q	0.8977	0.6060
R	0.8587	0.5860
S	0.7320	0.5270
T	0.7399	0.5390
U	0.7961	0.5600
V	0.6442	0.4670
W	0.8090	0.5480
X	0.8181	0.5700
Y	0.7796	0.5520
Z	0.7662	0.5280
a	0.6639	0.4860
b	0.8541	0.5800
c	0.7231	0.5200
d	0.8185	0.5680
e	0.8795	0.5990
f	0.8162	0.5600
g	0.5302	0.4320
h	0.7162	0.5060
i	0.8672	0.5970
j	0.7888	0.5600
k	0.7563	0.5150

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Chain	Atom inclusion	Q-score
l	0.8192	0.5670
m	0.7610	0.5160
n	0.9016	0.6160
o	0.8031	0.5680
p	0.5952	0.4730
q	0.8449	0.5900
r	0.8328	0.5730
t	0.7513	0.5290
u	0.7019	0.4910
v	0.7326	0.5140
w	0.8274	0.5810
x	0.7629	0.5270