wwPDB EM Validation Summary Report ⓘ

Nov 22, 2022 – 11:48 PM JST

PDB ID	:	7F5S
EMDB ID	:	EMD-31465
Title	:	human delta-METTL18 60S ribosome
Authors	:	Takahashi, M.; Kashiwagi, K.; Ito, T.
Deposited on	:	2021-06-22
Resolution	:	2.72 Å(reported)

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

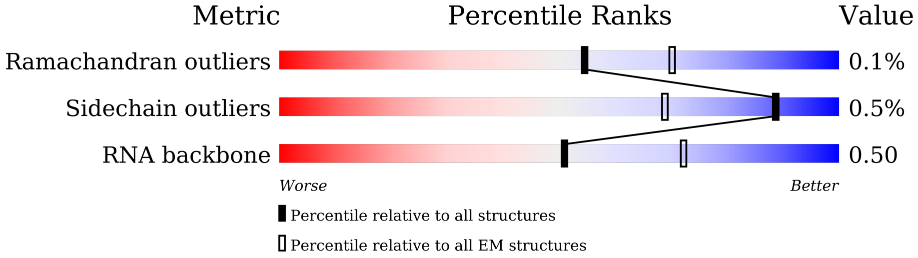
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance

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

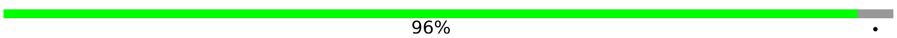
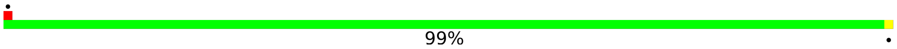
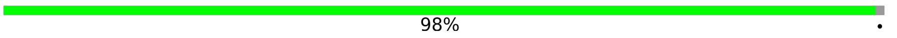
The reported resolution of this entry is 2.72 Å.

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	LA	257	 96%
2	LB	403	 99%
3	L5	5070	 53% 19% 27%
4	L7	120	 89% 11%
5	L8	156	 79% 21%
6	LC	427	 86% 14%
7	LD	297	 98%
8	LE	288	 76% 23%

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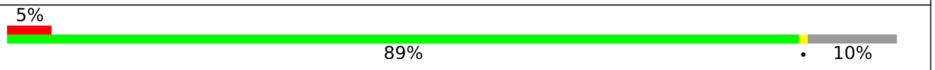
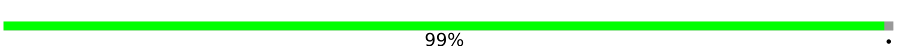
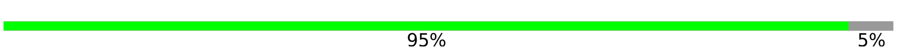
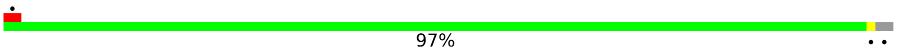
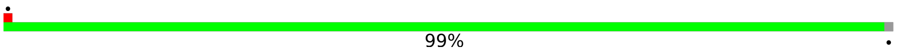
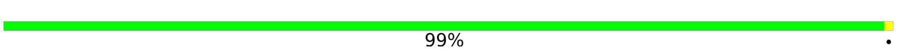
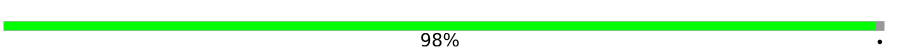
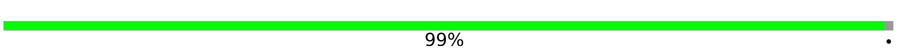
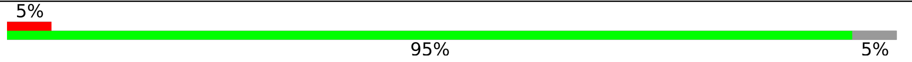
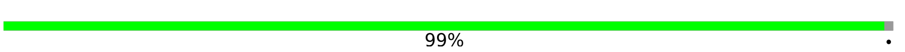
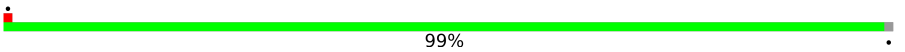
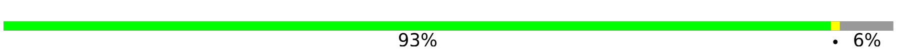
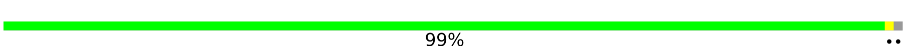
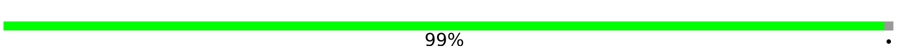
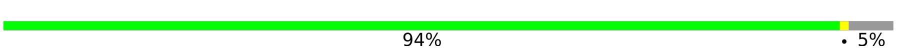
Mol	Chain	Length	Quality of chain
9	LF	248	
10	LG	266	
11	LH	192	
12	LI	214	
13	LJ	178	
14	LL	211	
15	LM	215	
16	LN	204	
17	LO	203	
18	LP	184	
19	LQ	188	
20	LR	196	
21	LS	176	
22	LT	160	
23	LU	128	
24	LV	140	
25	LW	157	
26	LX	156	
27	LY	145	
28	LZ	136	
29	La	148	
30	Lb	159	
31	Lc	115	
32	Ld	125	
33	Le	135	

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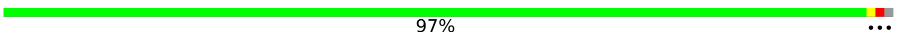
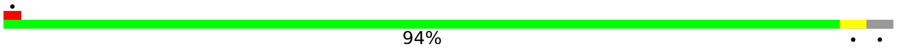
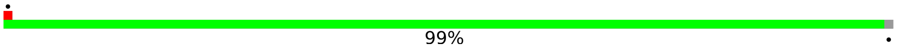
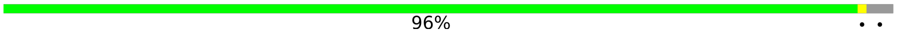
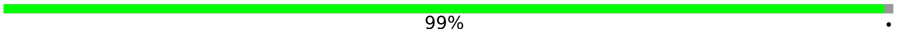
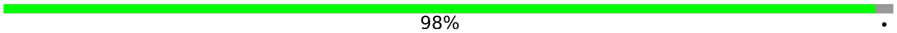
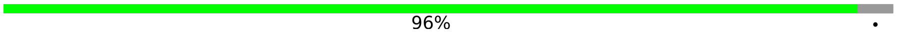
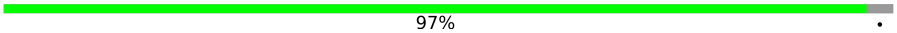
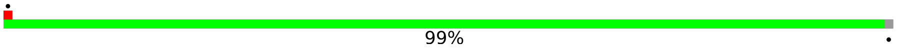
Mol	Chain	Length	Quality of chain
34	Lf	110	
35	Lg	117	
36	Lh	123	
37	Li	105	
38	Lj	97	
39	Lk	70	
40	Ll	51	
41	Lm	128	
42	Ln	25	
43	Lo	106	
44	Lp	92	
45	Lr	137	

2 Entry composition ⓘ

There are 48 unique types of molecules in this entry. The entry contains 138619 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 protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	LA	248	1898	1189	389	314	6	0	0

- Molecule 2 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	LB	402	3238	2060	608	556	14	0	0

- Molecule 3 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	L5	3715	79671	35522	14563	25871	3715	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L5	3818	UY1	U	conflict	GB NR_003287

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	L7	120	2558	1141	456	842	119	0	0

- Molecule 5 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	L8	156	3315	1481	585	1094	155	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	LC	368	Total	C	N	O	S	0	0
			2928	1841	583	489	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	LD	293	Total	C	N	O	S	0	0
			2382	1507	434	427	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	LE	223	Total	C	N	O	S	0	0
			1791	1153	338	296	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	LF	225	Total	C	N	O	S	0	0
			1870	1202	358	301	9		

- Molecule 10 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	LG	240	Total	C	N	O	S	0	0
			1922	1226	370	322	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	LH	190	Total	C	N	O	S	0	0
			1518	956	284	272	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	LI	204	Total	C	N	O	S	0	0
			1656	1052	319	272	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	LJ	175	1401	882	261	252	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	LL	208	1682	1052	348	278	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	LM	139	1138	730	218	183	7	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	LN	203	1701	1072	359	266	4	0	0

- Molecule 17 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	LO	200	1641	1058	320	258	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	LP	153	1242	776	241	216	9	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	LQ	187	1513	944	314	250	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	LR	187	1566	971	336	250	9	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	LS	175	1453	925	283	235	10	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	LT	159	1298	823	252	217	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	LU	101	825	529	144	150	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	LV	131	979	618	184	172	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	LW	76	639	403	128	105	3	0	0

- Molecule 26 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	LX	119	976	624	183	168	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	LY	134	1115	700	226	186	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	LZ	135	1107	714	208	182	3	0	0

- Molecule 29 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	La	147	1162	736	237	186	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	Lb	108	877	546	191	136	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	Lc	98	764	485	135	138	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	Ld	107	888	560	171	155	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	Le	128	1053	667	216	165	5	0	0

- Molecule 34 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	Lf	109	876	555	174	144	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	Lg	113	897	560	185	146	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	Lh	122	1015	641	205	168	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	Li	102	832	521	177	129	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	Lj	86	705	434	155	111	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	Lk	69	569	366	103	99	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	Ll	50	444	281	98	64	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	Lm	52	430	267	90	67	6	0	0

- Molecule 42 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	Ln	24	230	139	62	26	3	0	0

- Molecule 43 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	Lo	103	842	528	172	136	6	0	0

- Molecule 44 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	Lp	91	708	445	136	120	7	0	0

- Molecule 45 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	Lr	125	1002	622	207	168	5	0	0

- Molecule 46 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
46	LA	1	1	1	0
46	L5	260	260	260	0
46	L7	3	3	3	0
46	L8	5	5	5	0
46	LI	2	2	2	0
46	LN	1	1	1	0

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Mol	Chain	Residues	Atoms	AltConf
46	LP	1	Total Mg 1 1	0
46	LR	1	Total Mg 1 1	0
46	LS	1	Total Mg 1 1	0
46	LV	1	Total Mg 1 1	0
46	Le	1	Total Mg 1 1	0
46	Lf	1	Total Mg 1 1	0
46	Lg	1	Total Mg 1 1	0

- Molecule 47 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
47	Lg	1	Total Zn 1 1	0
47	Lj	1	Total Zn 1 1	0
47	Lm	1	Total Zn 1 1	0
47	Lo	1	Total Zn 1 1	0
47	Lp	1	Total Zn 1 1	0

- Molecule 48 is water.

Mol	Chain	Residues	Atoms	AltConf
48	L5	11	Total O 11 11	0
48	LH	1	Total O 1 1	0
48	La	2	Total O 2 2	0
48	Lb	1	Total O 1 1	0
48	Le	1	Total O 1 1	0

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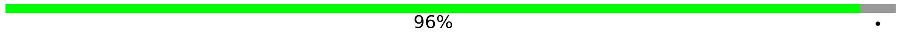
Mol	Chain	Residues	Atoms	AltConf
48	Lf	1	Total O 1 1	0
48	Lm	1	Total O 1 1	0

3 Residue-property plots ⓘ

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

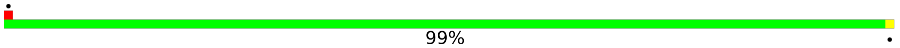
- Molecule 1: 60S ribosomal protein L8

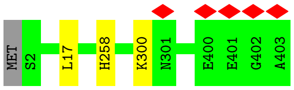
Chain LA:



- Molecule 2: 60S ribosomal protein L3

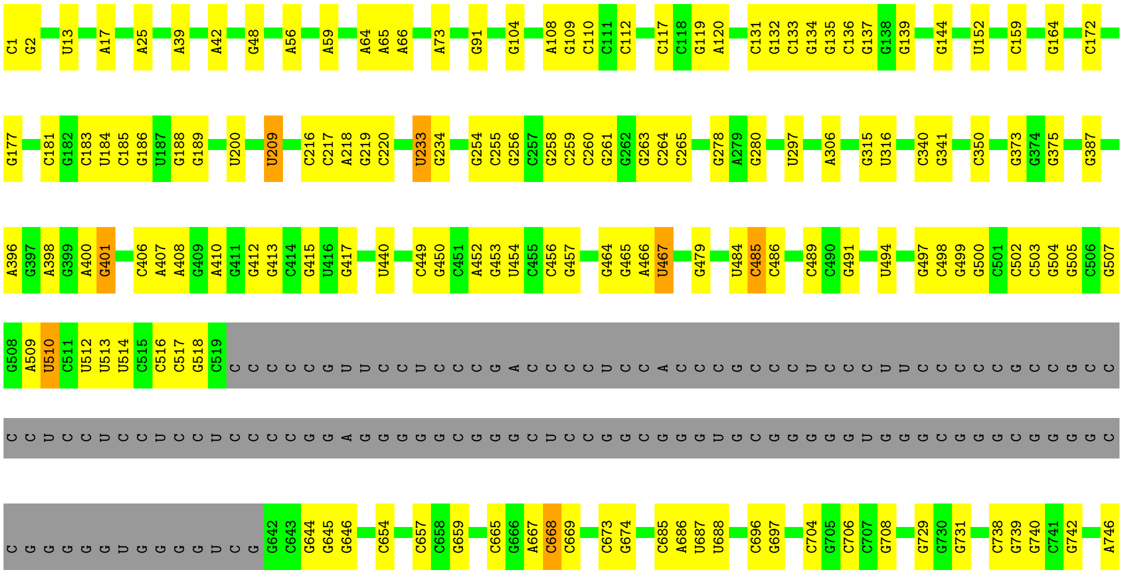
Chain LB:

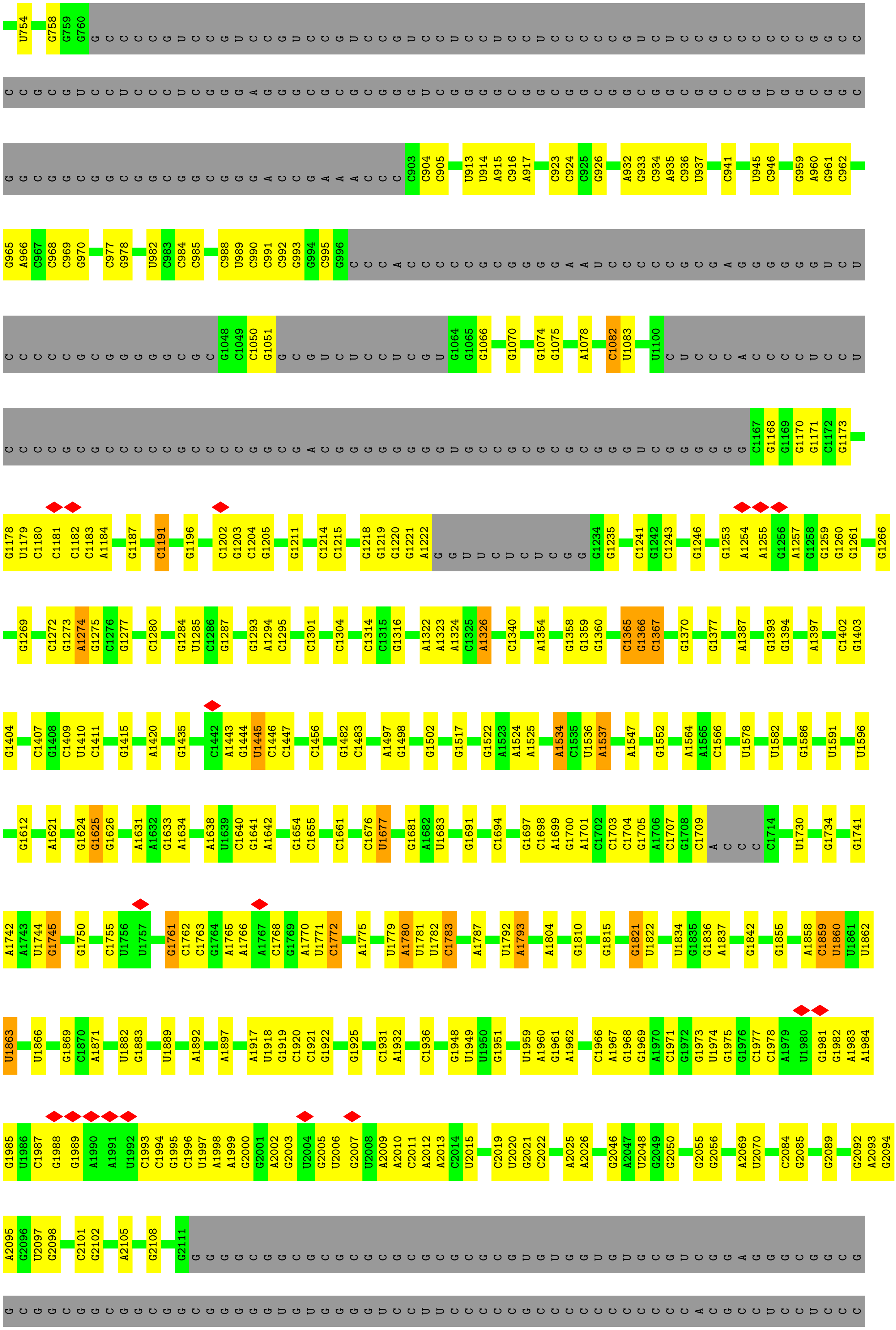




- Molecule 3: 28S rRNA

Chain L5:

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C C G C G U C C U C C C U C G G G A G G G C G C G C G G G U C G G G G C G G C G G C G G C G G C G G C G G U G G C G G C
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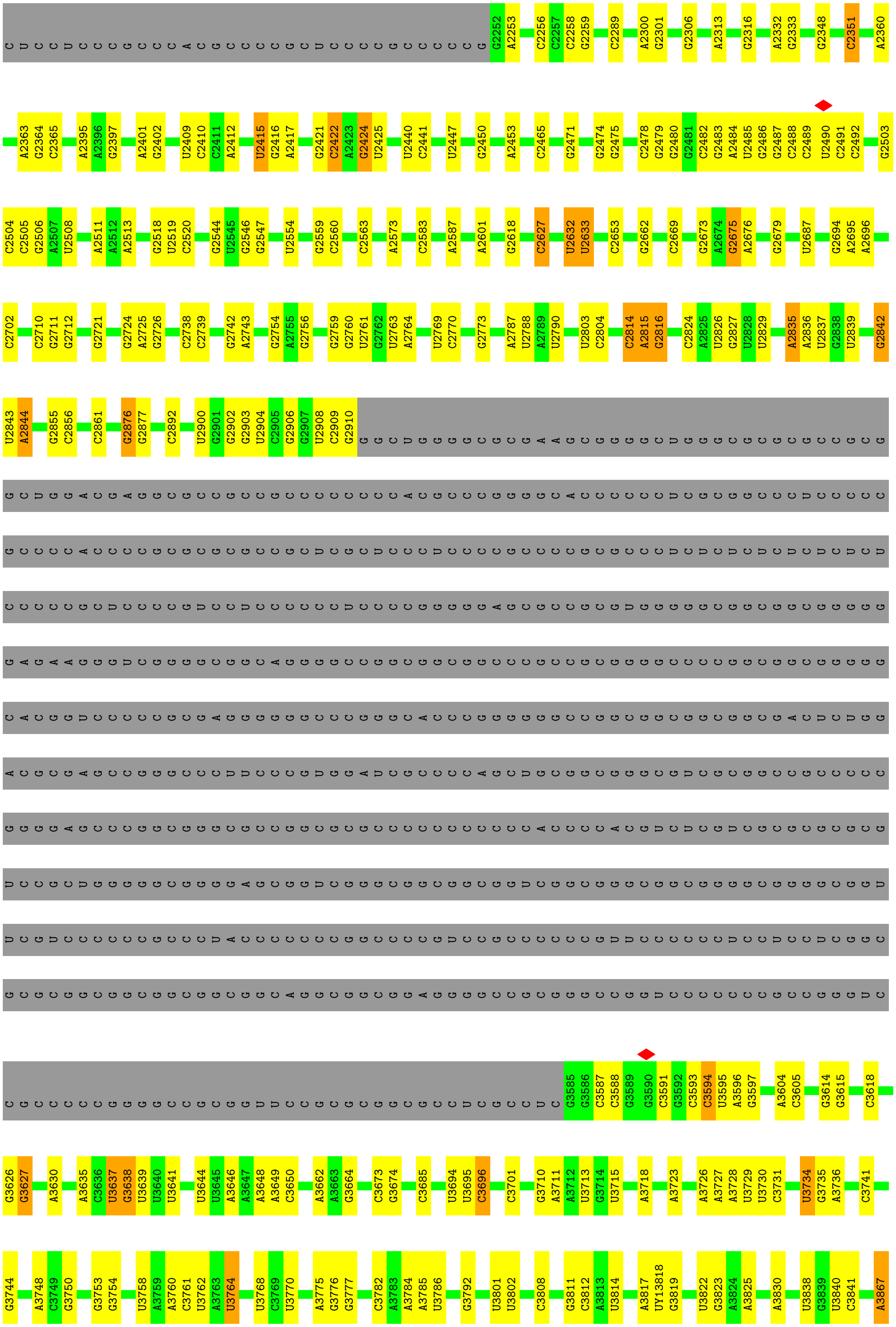
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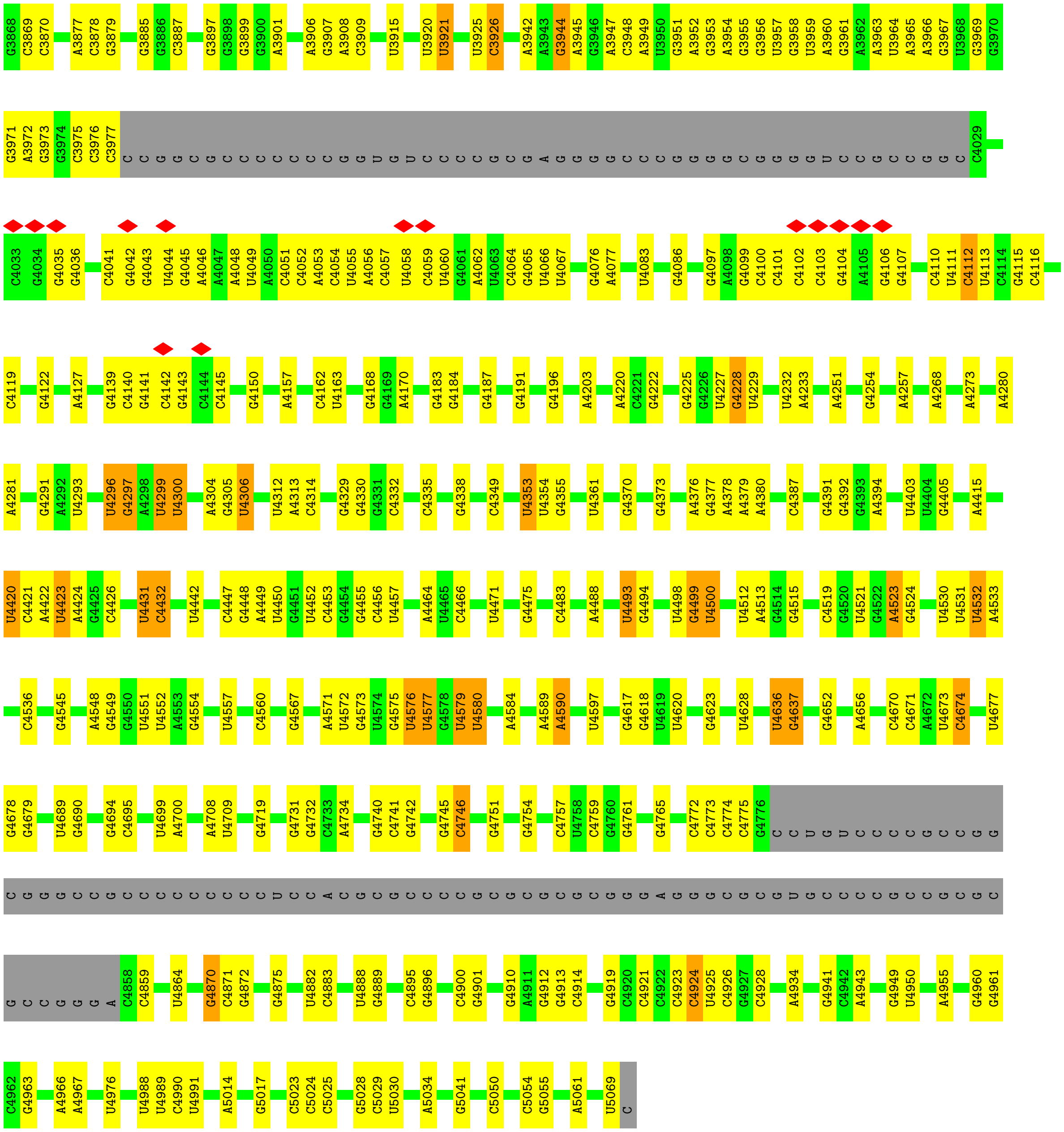
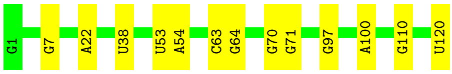


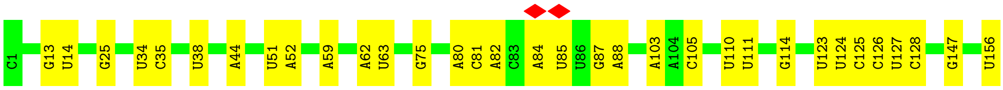
- Molecule 4: 5S rRNA

Chain L7:

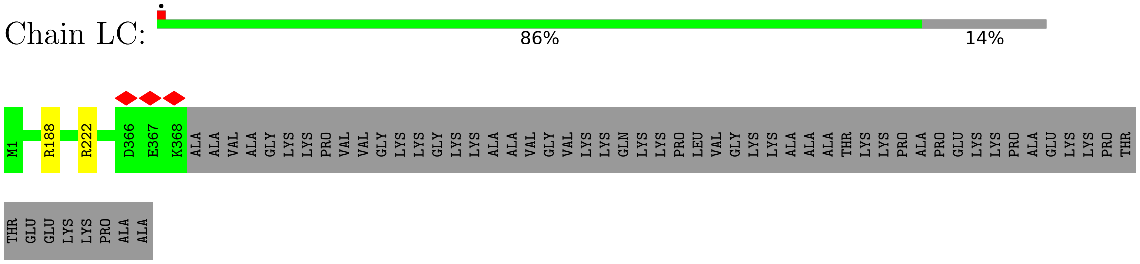


- Molecule 5: 5.8S rRNA

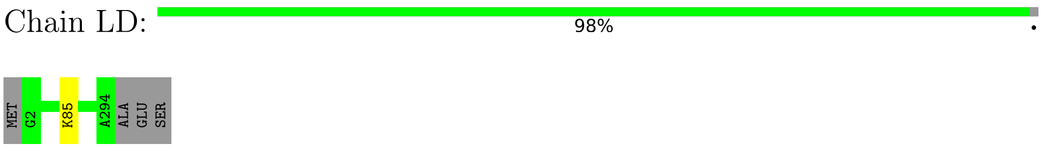
Chain L8:



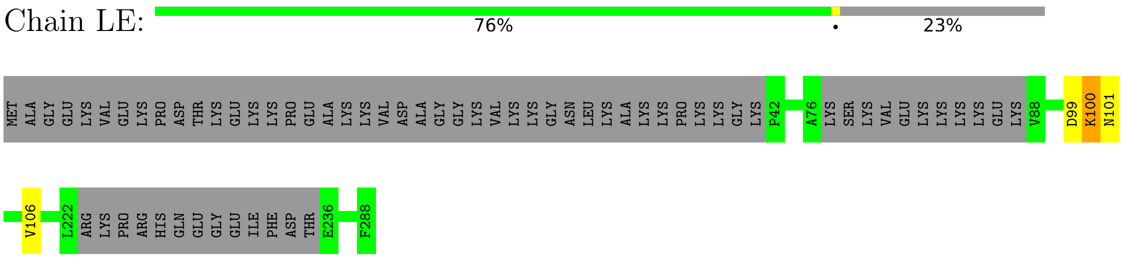
- Molecule 6: 60S ribosomal protein L4



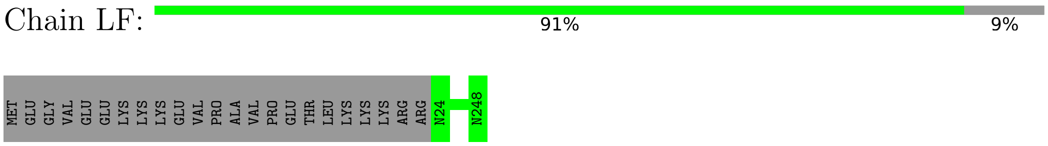
- Molecule 7: 60S ribosomal protein L5



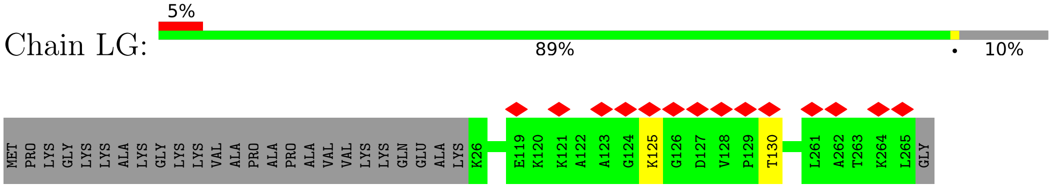
- Molecule 8: 60S ribosomal protein L6



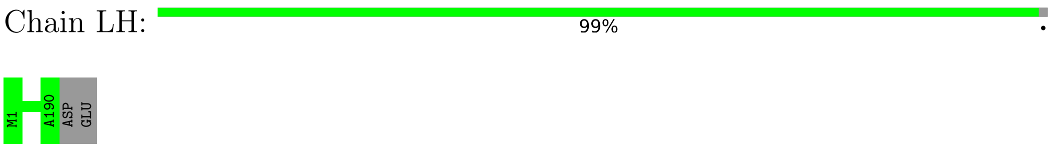
- Molecule 9: 60S ribosomal protein L7



- Molecule 10: 60S ribosomal protein L7a

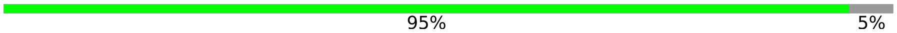


- Molecule 11: 60S ribosomal protein L9



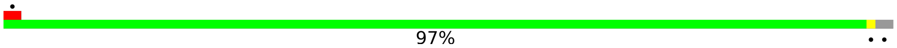
- Molecule 12: 60S ribosomal protein L10

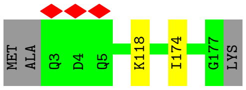
Chain LI:



- Molecule 13: 60S ribosomal protein L11

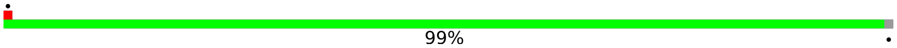
Chain LJ:

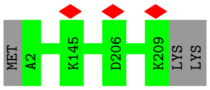




- Molecule 14: 60S ribosomal protein L13

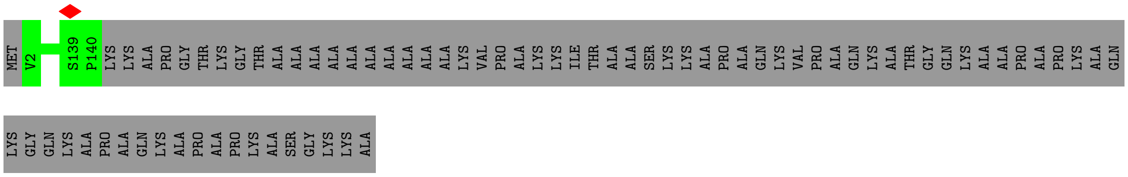
Chain LL:





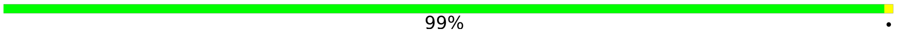
- Molecule 15: 60S ribosomal protein L14

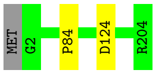
Chain LM:



- Molecule 16: 60S ribosomal protein L15

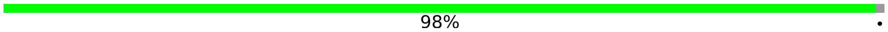
Chain LN:

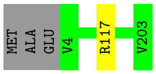




- Molecule 17: 60S ribosomal protein L13a

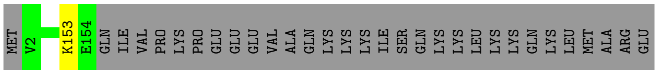
Chain LO:





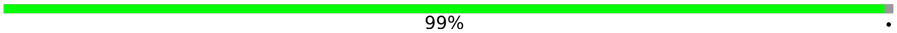
- Molecule 18: 60S ribosomal protein L17

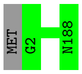
Chain LP:



- Molecule 19: 60S ribosomal protein L18

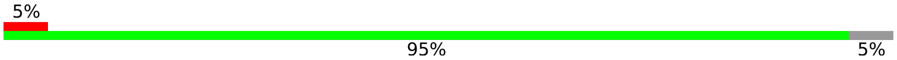
Chain LQ:

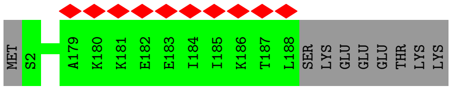




- Molecule 20: 60S ribosomal protein L19

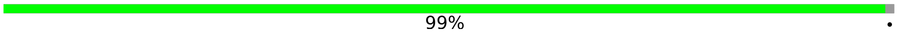
Chain LR:

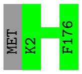




- Molecule 21: 60S ribosomal protein L18a

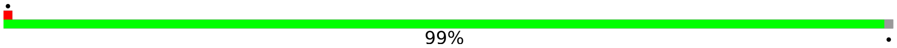
Chain LS:

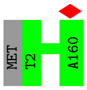




- Molecule 22: 60S ribosomal protein L21

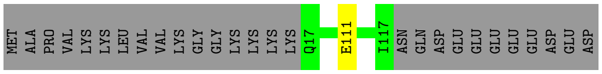
Chain LT:





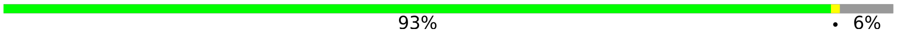
- Molecule 23: 60S ribosomal protein L22

Chain LU:



- Molecule 24: 60S ribosomal protein L23

Chain LV:

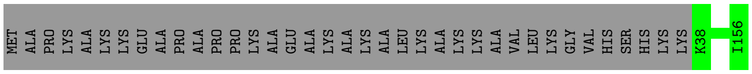


- Molecule 25: 60S ribosomal protein L24

Chain LW:

- Molecule 26: 60S ribosomal protein L23a

Chain LX:

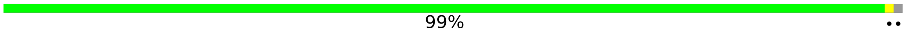


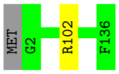
- Molecule 27: 60S ribosomal protein L26

Chain LY:

- Molecule 28: 60S ribosomal protein L27

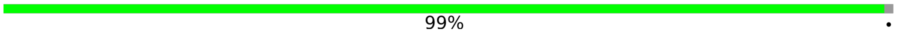
Chain LZ:

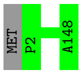




- Molecule 29: 60S ribosomal protein L27a

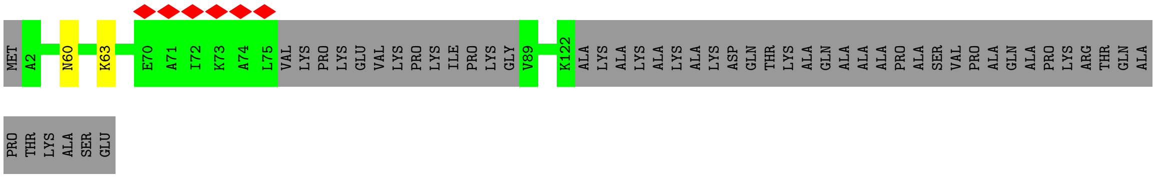
Chain La:





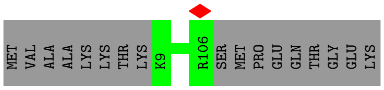
- Molecule 30: 60S ribosomal protein L29

Chain Lb:



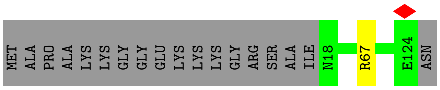
- Molecule 31: 60S ribosomal protein L30

Chain Lc:



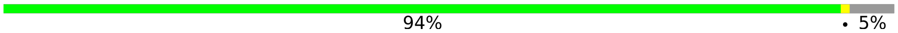
- Molecule 32: 60S ribosomal protein L31

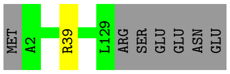
Chain Ld:



- Molecule 33: 60S ribosomal protein L32

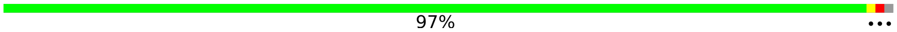
Chain Le:

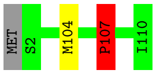




- Molecule 34: 60S ribosomal protein L35a

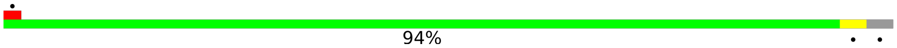
Chain Lf:

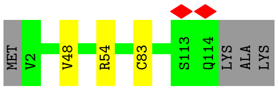




- Molecule 35: 60S ribosomal protein L34

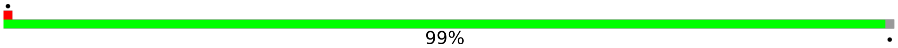
Chain Lg:

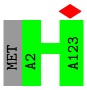




- Molecule 36: 60S ribosomal protein L35

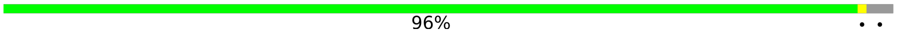
Chain Lh:

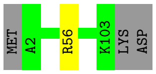




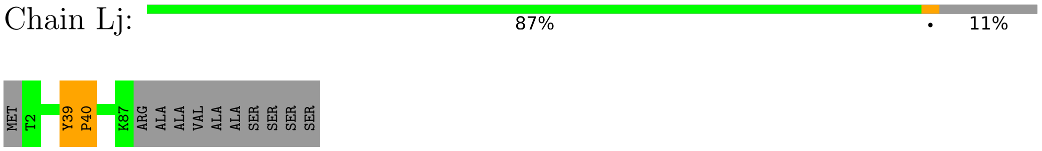
- Molecule 37: 60S ribosomal protein L36

Chain Li:

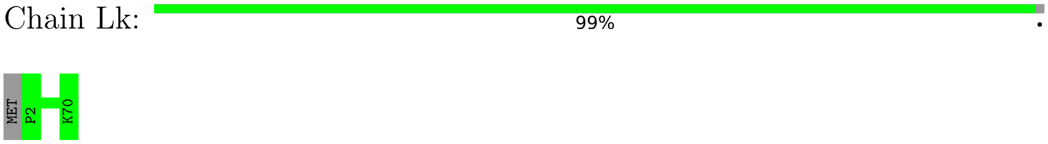




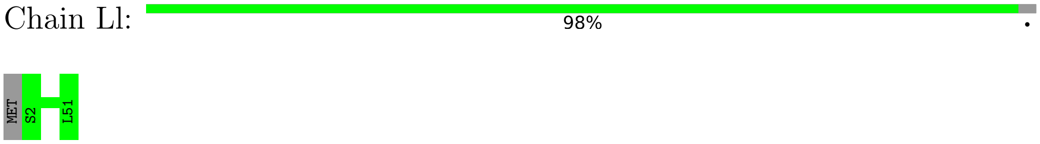
- Molecule 38: 60S ribosomal protein L37



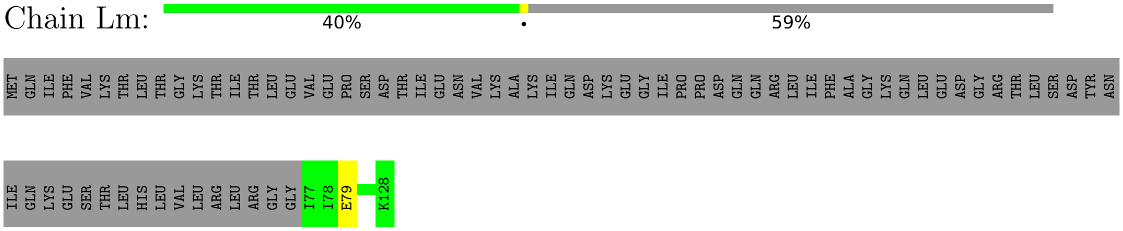
- Molecule 39: 60S ribosomal protein L38



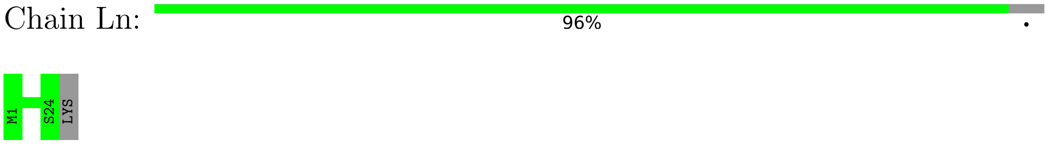
- Molecule 40: 60S ribosomal protein L39



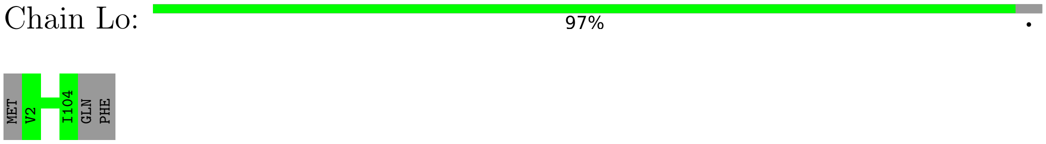
- Molecule 41: Ubiquitin-60S ribosomal protein L40



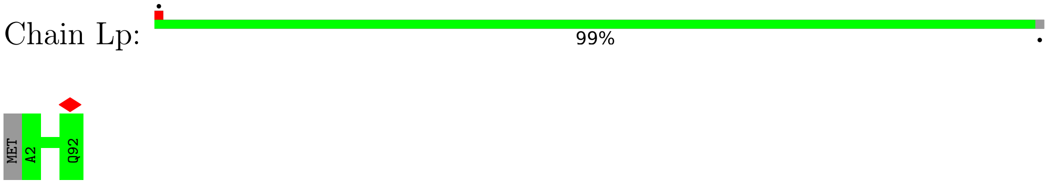
- Molecule 42: 60S ribosomal protein L41



- Molecule 43: 60S ribosomal protein L36a



- Molecule 44: 60S ribosomal protein L37a



- Molecule 45: 60S ribosomal protein L28

Chain Lr:

4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	118470	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose $(e^-/\text{Å}^2)$	50	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	32.789	Depositor
Minimum map value	-7.797	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	2.5	Depositor
Map size (Å)	485.0, 485.0, 485.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.97, 0.97, 0.97	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MLZ, OMG, 5MU, ZN, A2M, UR3, 2MG, B8T, MG, UY1, 1MA, OMC, PSU, 6MZ, OMU, 5MC, JMH

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	LA	0.56	0/1936	0.55	0/2596
2	LB	0.54	0/3306	0.56	2/4424 (0.0%)
3	L5	1.00	3/85750 (0.0%)	0.87	126/133763 (0.1%)
4	L7	1.03	0/2858	0.81	0/4455
5	L8	1.02	0/3679	0.81	2/5732 (0.0%)
6	LC	0.51	0/2971	0.51	0/3988
7	LD	0.49	0/2428	0.49	0/3252
8	LE	0.44	0/1825	0.55	1/2448 (0.0%)
9	LF	0.54	0/1905	0.49	0/2539
10	LG	0.44	0/1955	0.53	0/2632
11	LH	0.45	0/1537	0.51	0/2066
12	LI	0.50	0/1694	0.51	0/2261
13	LJ	0.42	0/1424	0.54	0/1904
14	LL	0.47	0/1713	0.50	0/2293
15	LM	0.48	0/1161	0.48	0/1554
16	LN	0.58	0/1746	0.52	0/2338
17	LO	0.52	0/1673	0.48	0/2238
18	LP	0.53	0/1268	0.50	0/1701
19	LQ	0.53	0/1537	0.50	0/2052
20	LR	0.42	0/1582	0.45	0/2091
21	LS	0.55	0/1493	0.47	0/2003
22	LT	0.52	0/1326	0.50	0/1770
23	LU	0.42	0/839	0.54	0/1126
24	LV	0.52	0/993	0.56	0/1332
25	LW	0.45	0/652	0.48	0/866
26	LX	0.45	0/993	0.47	0/1334
27	LY	0.51	0/1132	0.50	0/1504
28	LZ	0.51	0/1130	0.48	0/1507
29	La	0.56	0/1191	0.50	0/1591
30	Lb	0.38	0/890	0.49	0/1175
31	Lc	0.49	0/774	0.50	0/1038

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	Ld	0.50	0/903	0.50	0/1216
33	Le	0.55	0/1071	0.54	1/1429 (0.1%)
34	Lf	0.57	0/895	0.64	2/1198 (0.2%)
35	Lg	0.49	0/907	0.55	0/1209
36	Lh	0.43	0/1023	0.45	0/1351
37	Li	0.40	0/843	0.45	0/1115
38	Lj	0.56	0/720	0.61	2/952 (0.2%)
39	Lk	0.43	0/575	0.49	0/761
40	Ll	0.49	0/454	0.46	0/599
41	Lm	0.47	0/425	0.50	0/561
42	Ln	0.38	0/231	0.47	0/294
43	Lo	0.50	0/855	0.52	0/1128
44	Lp	0.55	0/718	0.52	0/953
45	Lr	0.51	0/1017	0.49	0/1364
All	All	0.85	3/145998 (0.0%)	0.77	136/215703 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	4533	A	O3'-P	-5.24	1.54	1.61
3	L5	1677	PSU	O3'-P	-5.21	1.54	1.61
3	L5	1858	A	O3'-P	-5.07	1.55	1.61

The worst 5 of 136 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L5	1772	C	N3-C4-N4	-15.13	107.41	118.00
3	L5	1761	G	N1-C6-O6	-13.24	111.96	119.90
3	L5	1761	G	C5-C6-O6	12.39	136.04	128.60
3	L5	485	C	C2-N1-C1'	10.46	130.30	118.80
3	L5	3728	A	OP1-P-O3'	10.06	127.34	105.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	LA	246/257 (96%)	220 (89%)	26 (11%)	0	100	100
2	LB	400/403 (99%)	375 (94%)	25 (6%)	0	100	100
6	LC	365/427 (86%)	336 (92%)	28 (8%)	1 (0%)	41	65
7	LD	291/297 (98%)	276 (95%)	15 (5%)	0	100	100
8	LE	217/288 (75%)	197 (91%)	19 (9%)	1 (0%)	29	53
9	LF	223/248 (90%)	211 (95%)	12 (5%)	0	100	100
10	LG	238/266 (90%)	220 (92%)	17 (7%)	1 (0%)	34	58
11	LH	188/192 (98%)	175 (93%)	13 (7%)	0	100	100
12	LI	200/214 (94%)	187 (94%)	13 (6%)	0	100	100
13	LJ	173/178 (97%)	161 (93%)	12 (7%)	0	100	100
14	LL	206/211 (98%)	188 (91%)	18 (9%)	0	100	100
15	LM	137/215 (64%)	131 (96%)	6 (4%)	0	100	100
16	LN	201/204 (98%)	188 (94%)	11 (6%)	2 (1%)	15	35
17	LO	198/203 (98%)	193 (98%)	5 (2%)	0	100	100
18	LP	151/184 (82%)	142 (94%)	9 (6%)	0	100	100
19	LQ	185/188 (98%)	178 (96%)	7 (4%)	0	100	100
20	LR	185/196 (94%)	181 (98%)	4 (2%)	0	100	100
21	LS	173/176 (98%)	162 (94%)	11 (6%)	0	100	100
22	LT	157/160 (98%)	148 (94%)	9 (6%)	0	100	100
23	LU	99/128 (77%)	84 (85%)	15 (15%)	0	100	100
24	LV	129/140 (92%)	122 (95%)	7 (5%)	0	100	100
25	LW	74/157 (47%)	67 (90%)	7 (10%)	0	100	100
26	LX	117/156 (75%)	116 (99%)	1 (1%)	0	100	100
27	LY	132/145 (91%)	124 (94%)	8 (6%)	0	100	100
28	LZ	133/136 (98%)	123 (92%)	10 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	La	145/148 (98%)	137 (94%)	8 (6%)	0	100	100
30	Lb	104/159 (65%)	97 (93%)	7 (7%)	0	100	100
31	Lc	96/115 (84%)	91 (95%)	5 (5%)	0	100	100
32	Ld	105/125 (84%)	95 (90%)	10 (10%)	0	100	100
33	Le	126/135 (93%)	119 (94%)	7 (6%)	0	100	100
34	Lf	107/110 (97%)	101 (94%)	5 (5%)	1 (1%)	17	38
35	Lg	111/117 (95%)	111 (100%)	0	0	100	100
36	Lh	120/123 (98%)	117 (98%)	3 (2%)	0	100	100
37	Li	100/105 (95%)	94 (94%)	6 (6%)	0	100	100
38	Lj	84/97 (87%)	78 (93%)	4 (5%)	2 (2%)	6	13
39	Lk	67/70 (96%)	66 (98%)	1 (2%)	0	100	100
40	Ll	48/51 (94%)	45 (94%)	3 (6%)	0	100	100
41	Lm	49/128 (38%)	47 (96%)	2 (4%)	0	100	100
42	Ln	22/25 (88%)	21 (96%)	1 (4%)	0	100	100
43	Lo	101/106 (95%)	97 (96%)	4 (4%)	0	100	100
44	Lp	89/92 (97%)	85 (96%)	4 (4%)	0	100	100
45	Lr	123/137 (90%)	112 (91%)	11 (9%)	0	100	100
All	All	6415/7212 (89%)	6018 (94%)	389 (6%)	8 (0%)	54	77

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	LC	222	ARG
8	LE	100	LYS
16	LN	124	ASP
34	Lf	107	PRO
38	Lj	39	TYR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	LA	190/199 (96%)	189 (100%)	1 (0%)	88	95
2	LB	348/349 (100%)	347 (100%)	1 (0%)	92	97
6	LC	305/347 (88%)	304 (100%)	1 (0%)	92	97
7	LD	246/250 (98%)	245 (100%)	1 (0%)	91	96
8	LE	197/252 (78%)	194 (98%)	3 (2%)	65	85
9	LF	194/215 (90%)	194 (100%)	0	100	100
10	LG	203/223 (91%)	202 (100%)	1 (0%)	88	95
11	LH	169/171 (99%)	169 (100%)	0	100	100
12	LI	174/181 (96%)	173 (99%)	1 (1%)	86	94
13	LJ	147/149 (99%)	145 (99%)	2 (1%)	67	85
14	LL	174/177 (98%)	174 (100%)	0	100	100
15	LM	118/161 (73%)	118 (100%)	0	100	100
16	LN	171/172 (99%)	171 (100%)	0	100	100
17	LO	172/174 (99%)	171 (99%)	1 (1%)	86	94
18	LP	134/163 (82%)	133 (99%)	1 (1%)	84	93
19	LQ	164/165 (99%)	164 (100%)	0	100	100
20	LR	166/175 (95%)	166 (100%)	0	100	100
21	LS	156/157 (99%)	156 (100%)	0	100	100
22	LT	139/140 (99%)	139 (100%)	0	100	100
23	LU	91/115 (79%)	90 (99%)	1 (1%)	73	89
24	LV	101/107 (94%)	100 (99%)	1 (1%)	76	90
25	LW	67/126 (53%)	67 (100%)	0	100	100
26	LX	107/133 (80%)	107 (100%)	0	100	100
27	LY	124/135 (92%)	122 (98%)	2 (2%)	62	83
28	LZ	117/118 (99%)	116 (99%)	1 (1%)	78	91
29	La	120/121 (99%)	120 (100%)	0	100	100
30	Lb	89/126 (71%)	87 (98%)	2 (2%)	52	78
31	Lc	83/97 (86%)	83 (100%)	0	100	100
32	Ld	98/110 (89%)	97 (99%)	1 (1%)	76	90
33	Le	114/121 (94%)	114 (100%)	0	100	100
34	Lf	88/89 (99%)	87 (99%)	1 (1%)	73	89
35	Lg	97/100 (97%)	94 (97%)	3 (3%)	40	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	Lh	109/110 (99%)	109 (100%)	0	100	100
37	Li	86/89 (97%)	85 (99%)	1 (1%)	71	88
38	Lj	73/80 (91%)	73 (100%)	0	100	100
39	Lk	64/65 (98%)	64 (100%)	0	100	100
40	Ll	47/48 (98%)	47 (100%)	0	100	100
41	Lm	47/115 (41%)	46 (98%)	1 (2%)	53	79
42	Ln	23/24 (96%)	23 (100%)	0	100	100
43	Lo	91/94 (97%)	91 (100%)	0	100	100
44	Lp	74/75 (99%)	74 (100%)	0	100	100
45	Lr	109/121 (90%)	109 (100%)	0	100	100
All	All	5586/6139 (91%)	5559 (100%)	27 (0%)	89	95

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
24	LV	48	ARG
28	LZ	102	ARG
35	Lg	83	CYS
27	LY	84	ARG
30	Lb	60	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
9	LF	119	ASN
13	LJ	168	GLN
24	LV	135	ASN
39	Lk	28	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	L5	3693/5070 (72%)	890 (24%)	39 (1%)
4	L7	119/120 (99%)	13 (10%)	0
5	L8	155/156 (99%)	30 (19%)	1 (0%)
All	All	3967/5346 (74%)	933 (23%)	40 (1%)

5 of 933 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	L5	2	G
3	L5	13	U
3	L5	17	A
3	L5	25	A
3	L5	39	A

5 of 40 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	L5	4354	U
3	L5	4699	U
3	L5	4378	A
3	L5	4576	PSU
3	L5	4913	G

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

143 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	$\#\|Z\| > 2$
3	A2M	L5	3723	3	18,25,26	0.94	1 (5%)	18,36,39	1.17	2 (11%)
3	PSU	L5	1781	3	18,21,22	1.88	5 (27%)	22,30,33	2.26	5 (22%)
3	OMC	L5	4456	3	19,22,23	1.20	2 (10%)	26,31,34	1.16	3 (11%)
3	OMG	L5	4618	3	18,26,27	1.02	1 (5%)	19,38,41	1.19	2 (10%)
3	PSU	L5	3768	3	18,21,22	1.44	3 (16%)	22,30,33	2.03	4 (18%)
3	PSU	L5	4673	3	18,21,22	2.00	6 (33%)	22,30,33	2.46	7 (31%)
3	OMG	L5	4637	3	18,26,27	1.06	1 (5%)	19,38,41	1.15	2 (10%)
3	PSU	L5	3639	3	18,21,22	1.55	4 (22%)	22,30,33	1.98	4 (18%)
3	OMG	L5	3627	3	18,26,27	1.12	1 (5%)	19,38,41	1.21	2 (10%)
3	OMG	L5	3944	3	18,26,27	1.08	1 (5%)	19,38,41	1.23	2 (10%)
3	OMU	L5	2415	3	19,22,23	1.51	4 (21%)	26,31,34	2.09	7 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	A2M	L5	4571	3	18,25,26	0.97	1 (5%)	18,36,39	1.25	2 (11%)
3	6MZ	L5	4220	3	18,25,26	0.82	0	16,36,39	2.24	4 (25%)
3	OMC	L5	1340	3	19,22,23	0.94	2 (10%)	26,31,34	0.81	0
3	PSU	L5	4293	3	18,21,22	1.57	4 (22%)	22,30,33	1.88	3 (13%)
3	OMG	L5	1883	3	18,26,27	1.04	1 (5%)	19,38,41	1.31	2 (10%)
3	OMG	L5	4392	3	18,26,27	1.06	1 (5%)	19,38,41	1.19	2 (10%)
3	A2M	L5	2363	46,3	18,25,26	0.95	0	18,36,39	1.23	2 (11%)
3	UR3	L5	1866	3	19,22,23	0.95	2 (10%)	26,32,35	1.37	2 (7%)
3	PSU	L5	2839	3	18,21,22	1.83	5 (27%)	22,30,33	2.20	5 (22%)
6	MLZ	LC	333	6	8,9,10	0.89	0	4,9,11	0.72	0
3	2MG	L5	1517	3	18,26,27	1.02	1 (5%)	16,38,41	1.36	3 (18%)
3	PSU	L5	1782	3	18,21,22	1.92	6 (33%)	22,30,33	2.44	7 (31%)
3	A2M	L5	3718	3	18,25,26	0.94	1 (5%)	18,36,39	1.15	2 (11%)
3	PSU	L5	4423	3	18,21,22	1.73	4 (22%)	22,30,33	2.04	4 (18%)
3	OMC	L5	2804	3	19,22,23	0.93	2 (10%)	26,31,34	0.89	1 (3%)
3	OMC	L5	3909	3	19,22,23	0.92	2 (10%)	26,31,34	0.98	2 (7%)
3	5MC	L5	3782	46,3	18,22,23	0.99	2 (11%)	26,32,35	1.17	3 (11%)
3	PSU	L5	4532	3	18,21,22	1.93	4 (22%)	22,30,33	2.23	9 (40%)
3	PSU	L5	1860	3	18,21,22	1.88	6 (33%)	22,30,33	2.26	5 (22%)
3	OMC	L5	2422	46,3	19,22,23	0.90	2 (10%)	26,31,34	0.90	0
3	5MC	L5	4447	46,3	18,22,23	1.06	2 (11%)	26,32,35	1.38	3 (11%)
3	PSU	L5	4500	3	18,21,22	1.49	5 (27%)	22,30,33	2.07	4 (18%)
3	OMC	L5	3808	3	19,22,23	0.93	2 (10%)	26,31,34	0.87	1 (3%)
3	OMG	L5	4196	46,3	18,26,27	1.00	1 (5%)	19,38,41	1.13	2 (10%)
3	JMH	L5	1456	3	18,22,23	1.24	2 (11%)	21,32,35	0.84	0
3	PSU	L5	1792	3	18,21,22	1.97	4 (22%)	22,30,33	2.27	5 (22%)
5	OMU	L8	14	3,5	19,22,23	1.39	4 (21%)	26,31,34	1.85	5 (19%)
3	PSU	L5	3730	3	18,21,22	1.66	4 (22%)	22,30,33	2.17	5 (22%)
3	OMC	L5	3701	46,3	19,22,23	0.87	1 (5%)	26,31,34	0.78	0
3	OMG	L5	2364	3	18,26,27	1.03	1 (5%)	19,38,41	1.16	2 (10%)
3	OMC	L5	3869	3	19,22,23	0.91	2 (10%)	26,31,34	0.78	0
3	PSU	L5	1582	3	18,21,22	1.49	4 (22%)	22,30,33	1.89	3 (13%)
3	PSU	L5	3764	3	18,21,22	1.41	4 (22%)	22,30,33	1.88	4 (18%)
3	PSU	L5	4361	3	18,21,22	1.98	5 (27%)	22,30,33	2.24	5 (22%)
3	OMC	L5	3841	3	19,22,23	0.94	2 (10%)	26,31,34	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
3	PSU	L5	1779	3	18,21,22	1.73	4 (22%)	22,30,33	2.20	5 (22%)
3	PSU	L5	4521	46,3	18,21,22	1.54	5 (27%)	22,30,33	2.02	4 (18%)
3	A2M	L5	3830	3	18,25,26	0.94	0	18,36,39	1.27	3 (16%)
41	MLZ	Lm	98	41	8,9,10	0.82	0	4,9,11	0.68	0
3	PSU	L5	4296	3	18,21,22	1.83	4 (22%)	22,30,33	2.28	6 (27%)
3	UR3	L5	4530	3	19,22,23	0.91	1 (5%)	26,32,35	1.41	1 (3%)
3	OMU	L5	4498	46,3	19,22,23	1.37	4 (21%)	26,31,34	1.79	6 (23%)
3	PSU	L5	1536	3	18,21,22	2.14	5 (27%)	22,30,33	2.48	6 (27%)
3	OMG	L5	2876	3	18,26,27	1.12	1 (5%)	19,38,41	1.21	3 (15%)
3	OMG	L5	3899	3	18,26,27	1.04	1 (5%)	19,38,41	1.18	1 (5%)
3	OMU	L5	4227	3	19,22,23	1.40	4 (21%)	26,31,34	1.87	5 (19%)
3	1MA	L5	4415	3	16,25,26	1.47	2 (12%)	18,37,40	0.98	2 (11%)
3	OMG	L5	4623	3	18,26,27	1.05	1 (5%)	19,38,41	1.27	2 (10%)
3	PSU	L5	4403	3	18,21,22	2.12	7 (38%)	22,30,33	2.77	7 (31%)
3	PSU	L5	4628	3	18,21,22	1.49	3 (16%)	22,30,33	1.96	3 (13%)
3	PSU	L5	4312	3	18,21,22	1.91	5 (27%)	22,30,33	2.42	5 (22%)
3	PSU	L5	3822	3	18,21,22	1.49	5 (27%)	22,30,33	1.93	3 (13%)
3	OMU	L5	4306	3	19,22,23	1.37	4 (21%)	26,31,34	1.73	4 (15%)
3	PSU	L5	4493	46,3	18,21,22	1.91	4 (22%)	22,30,33	2.20	5 (22%)
3	OMG	L5	4870	3	18,26,27	1.00	1 (5%)	19,38,41	1.10	2 (10%)
3	OMU	L5	2837	3	19,22,23	1.68	4 (21%)	26,31,34	2.23	8 (30%)
3	PSU	L5	2508	3	18,21,22	1.49	4 (22%)	22,30,33	1.94	4 (18%)
3	OMG	L5	4187	3	18,26,27	1.40	2 (11%)	19,38,41	1.80	6 (31%)
3	A2M	L5	1871	46,3	18,25,26	0.93	0	18,36,39	1.28	2 (11%)
3	5MU	L5	4083	3	19,22,23	1.40	3 (15%)	28,32,35	2.21	6 (21%)
3	PSU	L5	4636	3	18,21,22	1.48	3 (16%)	22,30,33	2.05	5 (22%)
3	OMU	L5	3925	3	19,22,23	1.93	5 (26%)	26,31,34	2.37	9 (34%)
3	PSU	L5	4442	3	18,21,22	1.52	5 (27%)	22,30,33	2.05	5 (22%)
3	PSU	L5	4576	3	18,21,22	1.98	4 (22%)	22,30,33	2.45	9 (40%)
3	PSU	L5	4457	3	18,21,22	1.55	4 (22%)	22,30,33	2.06	6 (27%)
3	A2M	L5	1326	3	18,25,26	0.96	1 (5%)	18,36,39	1.30	2 (11%)
3	1MA	L5	1322	46,3	16,25,26	1.40	2 (12%)	18,37,40	1.12	3 (16%)
3	OMC	L5	2861	3	19,22,23	0.88	2 (10%)	26,31,34	0.85	1 (3%)
3	A2M	L5	4523	46,3	18,25,26	0.95	0	18,36,39	1.29	2 (11%)
3	PSU	L5	1683	3	18,21,22	1.58	3 (16%)	22,30,33	2.01	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
3	OMG	L5	4499	3	18,26,27	1.09	1 (5%)	19,38,41	1.07	2 (10%)
3	A2M	L5	3867	3	18,25,26	0.93	0	18,36,39	1.30	2 (11%)
3	OMG	L5	4370	3	18,26,27	0.99	1 (5%)	19,38,41	1.15	3 (15%)
3	OMG	L5	1316	3	18,26,27	1.08	1 (5%)	19,38,41	1.30	3 (15%)
3	OMC	L5	2351	46,3	19,22,23	1.05	2 (10%)	26,31,34	1.22	3 (11%)
3	2MG	L5	978	3	18,26,27	1.00	1 (5%)	16,38,41	1.18	3 (18%)
3	A2M	L5	2815	3	18,25,26	1.03	0	18,36,39	1.62	4 (22%)
3	B8T	L5	4671	3	19,22,23	1.04	2 (10%)	26,31,34	0.95	1 (3%)
3	PSU	L5	2632	3	18,21,22	1.79	5 (27%)	22,30,33	2.24	5 (22%)
3	PSU	L5	4689	3	18,21,22	2.15	5 (27%)	22,30,33	2.44	8 (36%)
3	OMG	L5	373	3	18,26,27	1.03	1 (5%)	19,38,41	1.25	3 (15%)
3	A2M	L5	2401	3	18,25,26	0.90	0	18,36,39	1.19	2 (11%)
3	OMC	L5	4536	3	19,22,23	0.94	2 (10%)	26,31,34	0.84	0
3	PSU	L5	3762	3	18,21,22	1.39	2 (11%)	22,30,33	1.89	3 (13%)
3	A2M	L5	4590	3	18,25,26	0.96	1 (5%)	18,36,39	1.42	1 (5%)
3	A2M	L5	400	3	18,25,26	0.97	0	18,36,39	1.34	2 (11%)
3	OMG	L5	4228	3	18,26,27	0.98	1 (5%)	19,38,41	1.21	3 (15%)
3	A2M	L5	1524	3	18,25,26	0.92	0	18,36,39	1.21	2 (11%)
3	A2M	L5	1534	46,3	18,25,26	0.95	0	18,36,39	1.38	3 (16%)
3	PSU	L5	4299	3	18,21,22	2.08	7 (38%)	22,30,33	2.24	9 (40%)
3	PSU	L5	4471	3	18,21,22	1.99	5 (27%)	22,30,33	2.19	6 (27%)
3	PSU	L5	4531	3	18,21,22	1.43	2 (11%)	22,30,33	1.95	4 (18%)
3	5MC	L5	4335	3	18,22,23	1.02	2 (11%)	26,32,35	1.23	2 (7%)
3	OMU	L5	4620	3	19,22,23	1.40	4 (21%)	26,31,34	1.86	5 (19%)
3	OMG	L5	1625	3	18,26,27	1.01	1 (5%)	19,38,41	1.18	3 (15%)
3	OMC	L5	3887	3	19,22,23	0.88	2 (10%)	26,31,34	0.88	0
3	OMC	L5	2365	46,3	19,22,23	0.91	2 (10%)	26,31,34	0.81	0
3	A2M	L5	3785	3	18,25,26	0.83	0	18,36,39	1.32	2 (11%)
3	OMG	L5	1522	3	18,26,27	1.04	1 (5%)	19,38,41	1.21	2 (10%)
3	OMG	L5	2050	3	18,26,27	1.07	1 (5%)	19,38,41	1.11	3 (15%)
3	PSU	L5	1744	46,3	18,21,22	1.79	5 (27%)	22,30,33	2.22	7 (31%)
3	PSU	L5	4552	3	18,21,22	1.98	5 (27%)	22,30,33	2.17	5 (22%)
3	A2M	L5	398	3	18,25,26	0.96	1 (5%)	18,36,39	1.28	2 (11%)
3	OMC	L5	2824	3	19,22,23	0.87	0	26,31,34	0.92	1 (3%)
3	PSU	L5	1677	3	18,21,22	2.02	6 (33%)	22,30,33	2.32	7 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
3	OMG	L5	2424	3	18,26,27	1.02	1 (5%)	19,38,41	1.09	1 (5%)
3	OMG	L5	2773	3	18,26,27	0.94	1 (5%)	19,38,41	1.15	3 (15%)
3	PSU	L5	4353	3	18,21,22	1.97	5 (27%)	22,30,33	2.21	6 (27%)
3	UY1	L5	3818	46,3	19,22,23	2.56	9 (47%)	22,31,34	1.90	4 (18%)
3	PSU	L5	4450	46,3	18,21,22	1.47	3 (16%)	22,30,33	2.01	4 (18%)
3	PSU	L5	2843	3	18,21,22	2.01	6 (33%)	22,30,33	2.19	5 (22%)
3	A2M	L5	1323	3	18,25,26	0.97	0	18,36,39	1.25	3 (16%)
3	PSU	L5	3920	46,3	18,21,22	2.20	6 (33%)	22,30,33	2.26	7 (31%)
3	PSU	L5	4431	3	18,21,22	1.95	5 (27%)	22,30,33	2.29	6 (27%)
3	2MG	L5	4872	3	18,26,27	1.10	1 (5%)	16,38,41	1.48	3 (18%)
3	2MG	L5	729	46,3	18,26,27	1.08	1 (5%)	16,38,41	1.22	3 (18%)
3	PSU	L5	3715	3	18,21,22	1.42	4 (22%)	22,30,33	1.97	5 (22%)
3	OMG	L5	3744	3	18,26,27	1.14	1 (5%)	19,38,41	1.13	2 (10%)
3	PSU	L5	1862	3	18,21,22	2.08	6 (33%)	22,30,33	2.43	7 (31%)
3	PSU	L5	3734	3	18,21,22	1.43	4 (22%)	22,30,33	2.05	4 (18%)
3	PSU	L5	4579	3	18,21,22	1.96	6 (33%)	22,30,33	2.43	5 (22%)
3	PSU	L5	3770	3	18,21,22	1.41	3 (16%)	22,30,33	1.97	4 (18%)
3	A2M	L5	2787	46,3	18,25,26	0.88	0	18,36,39	1.36	2 (11%)
3	OMG	L5	4494	3	18,26,27	1.41	2 (11%)	19,38,41	1.34	3 (15%)
3	B8T	L5	4483	3	19,22,23	1.05	2 (10%)	26,31,34	0.86	0
3	PSU	L5	3695	3	18,21,22	1.87	5 (27%)	22,30,33	2.38	5 (22%)
3	PSU	L5	3758	3	18,21,22	1.39	3 (16%)	22,30,33	2.03	6 (27%)
3	OMG	L5	3792	3	18,26,27	1.01	1 (5%)	19,38,41	1.11	2 (10%)
3	A2M	L5	3825	3	18,25,26	0.92	0	18,36,39	1.17	2 (11%)
3	PSU	L5	3637	3	18,21,22	2.21	7 (38%)	22,30,33	2.45	7 (31%)
3	UR3	L5	4597	3	19,22,23	0.91	1 (5%)	26,32,35	1.32	2 (7%)
3	PSU	L5	4420	3	18,21,22	1.45	3 (16%)	22,30,33	2.25	4 (18%)

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
3	A2M	L5	3723	3	-	0/5/27/28	0/3/3/3
3	PSU	L5	1781	3	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMC	L5	4456	3	-	1/9/27/28	0/2/2/2
3	OMG	L5	4618	3	-	1/5/27/28	0/3/3/3
3	PSU	L5	3768	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4673	3	-	1/7/25/26	0/2/2/2
3	OMG	L5	4637	3	-	0/5/27/28	0/3/3/3
3	PSU	L5	3639	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	3627	3	-	2/5/27/28	0/3/3/3
3	OMG	L5	3944	3	-	2/5/27/28	0/3/3/3
3	OMU	L5	2415	3	-	2/9/27/28	0/2/2/2
3	A2M	L5	4571	3	-	0/5/27/28	0/3/3/3
3	6MZ	L5	4220	3	-	0/5/27/28	0/3/3/3
3	OMC	L5	1340	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	4293	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	1883	3	-	1/5/27/28	0/3/3/3
3	OMG	L5	4392	3	-	0/5/27/28	0/3/3/3
3	A2M	L5	2363	46,3	-	1/5/27/28	0/3/3/3
3	UR3	L5	1866	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	2839	3	-	0/7/25/26	0/2/2/2
6	MLZ	LC	333	6	-	2/7/8/10	-
3	2MG	L5	1517	3	-	0/5/27/28	0/3/3/3
3	PSU	L5	1782	3	-	1/7/25/26	0/2/2/2
3	A2M	L5	3718	3	-	0/5/27/28	0/3/3/3
3	PSU	L5	4423	3	-	2/7/25/26	0/2/2/2
3	OMC	L5	2804	3	-	0/9/27/28	0/2/2/2
3	OMC	L5	3909	3	-	2/9/27/28	0/2/2/2
3	5MC	L5	3782	46,3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4532	3	-	1/7/25/26	0/2/2/2
3	PSU	L5	1860	3	-	2/7/25/26	0/2/2/2
3	OMC	L5	2422	46,3	-	1/9/27/28	0/2/2/2
3	5MC	L5	4447	46,3	-	4/7/25/26	0/2/2/2
3	PSU	L5	4500	3	-	5/7/25/26	0/2/2/2
3	OMC	L5	3808	3	-	0/9/27/28	0/2/2/2
3	OMG	L5	4196	46,3	-	0/5/27/28	0/3/3/3
3	JMH	L5	1456	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	1792	3	-	0/7/25/26	0/2/2/2
5	OMU	L8	14	3,5	-	1/9/27/28	0/2/2/2
3	PSU	L5	3730	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	3701	46,3	-	4/9/27/28	0/2/2/2
3	OMG	L5	2364	3	-	2/5/27/28	0/3/3/3
3	OMC	L5	3869	3	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PSU	L5	1582	3	-	1/7/25/26	0/2/2/2
3	PSU	L5	3764	3	-	3/7/25/26	0/2/2/2
3	PSU	L5	4361	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	3841	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	1779	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4521	46,3	-	0/7/25/26	0/2/2/2
3	A2M	L5	3830	3	-	1/5/27/28	0/3/3/3
41	MLZ	Lm	98	41	-	1/7/8/10	-
3	PSU	L5	4296	3	-	2/7/25/26	0/2/2/2
3	UR3	L5	4530	3	-	0/7/25/26	0/2/2/2
3	OMU	L5	4498	46,3	-	0/9/27/28	0/2/2/2
3	PSU	L5	1536	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	2876	3	-	3/5/27/28	0/3/3/3
3	OMG	L5	3899	3	-	0/5/27/28	0/3/3/3
3	OMU	L5	4227	3	-	3/9/27/28	0/2/2/2
3	1MA	L5	4415	3	-	0/3/25/26	0/3/3/3
3	OMG	L5	4623	3	-	1/5/27/28	0/3/3/3
3	PSU	L5	4403	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4628	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4312	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3822	3	-	0/7/25/26	0/2/2/2
3	OMU	L5	4306	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	4493	46,3	-	2/7/25/26	0/2/2/2
3	OMG	L5	4870	3	-	3/5/27/28	0/3/3/3
3	OMU	L5	2837	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	2508	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	4187	3	-	0/5/27/28	0/3/3/3
3	A2M	L5	1871	46,3	-	0/5/27/28	0/3/3/3
3	5MU	L5	4083	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4636	3	-	4/7/25/26	0/2/2/2
3	OMU	L5	3925	3	-	2/9/27/28	0/2/2/2
3	PSU	L5	4442	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4576	3	-	1/7/25/26	0/2/2/2
3	PSU	L5	4457	3	-	2/7/25/26	0/2/2/2
3	A2M	L5	1326	3	-	3/5/27/28	0/3/3/3
3	1MA	L5	1322	46,3	-	0/3/25/26	0/3/3/3
3	OMC	L5	2861	3	-	0/9/27/28	0/2/2/2
3	A2M	L5	4523	46,3	-	0/5/27/28	0/3/3/3
3	PSU	L5	1683	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	4499	3	-	2/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A2M	L5	3867	3	-	2/5/27/28	0/3/3/3
3	OMG	L5	4370	3	-	0/5/27/28	0/3/3/3
3	OMG	L5	1316	3	-	0/5/27/28	0/3/3/3
3	OMC	L5	2351	46,3	-	4/9/27/28	0/2/2/2
3	2MG	L5	978	3	-	0/5/27/28	0/3/3/3
3	A2M	L5	2815	3	-	2/5/27/28	0/3/3/3
3	B8T	L5	4671	3	-	1/7/27/28	0/2/2/2
3	PSU	L5	2632	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4689	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	373	3	-	1/5/27/28	0/3/3/3
3	A2M	L5	2401	3	-	0/5/27/28	0/3/3/3
3	OMC	L5	4536	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	3762	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	4590	3	-	3/5/27/28	0/3/3/3
3	A2M	L5	400	3	-	0/5/27/28	0/3/3/3
3	OMG	L5	4228	3	-	0/5/27/28	0/3/3/3
3	A2M	L5	1524	3	-	0/5/27/28	0/3/3/3
3	A2M	L5	1534	46,3	-	1/5/27/28	0/3/3/3
3	PSU	L5	4299	3	-	2/7/25/26	0/2/2/2
3	PSU	L5	4471	3	-	2/7/25/26	0/2/2/2
3	PSU	L5	4531	3	-	0/7/25/26	0/2/2/2
3	5MC	L5	4335	3	-	0/7/25/26	0/2/2/2
3	OMU	L5	4620	3	-	0/9/27/28	0/2/2/2
3	OMG	L5	1625	3	-	2/5/27/28	0/3/3/3
3	OMC	L5	3887	3	-	1/9/27/28	0/2/2/2
3	OMC	L5	2365	46,3	-	0/9/27/28	0/2/2/2
3	A2M	L5	3785	3	-	2/5/27/28	0/3/3/3
3	OMG	L5	1522	3	-	0/5/27/28	0/3/3/3
3	OMG	L5	2050	3	-	0/5/27/28	0/3/3/3
3	PSU	L5	1744	46,3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4552	3	-	1/7/25/26	0/2/2/2
3	A2M	L5	398	3	-	1/5/27/28	0/3/3/3
3	OMC	L5	2824	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	1677	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	2424	3	-	2/5/27/28	0/3/3/3
3	OMG	L5	2773	3	-	0/5/27/28	0/3/3/3
3	PSU	L5	4353	3	-	0/7/25/26	0/2/2/2
3	UY1	L5	3818	46,3	-	4/9/27/28	0/2/2/2
3	PSU	L5	4450	46,3	-	3/7/25/26	0/2/2/2
3	PSU	L5	2843	3	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A2M	L5	1323	3	-	3/5/27/28	0/3/3/3
3	PSU	L5	3920	46,3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4431	3	-	1/7/25/26	0/2/2/2
3	2MG	L5	4872	3	-	0/5/27/28	0/3/3/3
3	2MG	L5	729	46,3	-	3/5/27/28	0/3/3/3
3	PSU	L5	3715	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	3744	3	-	0/5/27/28	0/3/3/3
3	PSU	L5	1862	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3734	3	-	2/7/25/26	0/2/2/2
3	PSU	L5	4579	3	-	2/7/25/26	0/2/2/2
3	PSU	L5	3770	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	2787	46,3	-	0/5/27/28	0/3/3/3
3	OMG	L5	4494	3	-	0/5/27/28	0/3/3/3
3	B8T	L5	4483	3	-	0/7/27/28	0/2/2/2
3	PSU	L5	3695	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3758	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	3792	3	-	0/5/27/28	0/3/3/3
3	A2M	L5	3825	3	-	0/5/27/28	0/3/3/3
3	PSU	L5	3637	3	-	3/7/25/26	0/2/2/2
3	UR3	L5	4597	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4420	3	-	2/7/25/26	0/2/2/2

The worst 5 of 376 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	3818	UY1	C3'-C4'	-5.54	1.38	1.53
3	L5	4403	PSU	C4-N3	-4.67	1.30	1.38
3	L5	3637	PSU	C4-N3	-4.52	1.30	1.38
3	L5	4689	PSU	C2'-C1'	-4.49	1.47	1.53
3	L5	3920	PSU	C4-N3	-4.37	1.30	1.38

The worst 5 of 498 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L5	4403	PSU	N1-C2-N3	8.22	124.45	115.13
3	L5	3695	PSU	N1-C2-N3	7.43	123.55	115.13
3	L5	1536	PSU	N1-C2-N3	7.29	123.39	115.13
3	L5	1860	PSU	N1-C2-N3	7.17	123.25	115.13
3	L5	4296	PSU	N1-C2-N3	7.16	123.24	115.13

There are no chirality outliers.

5 of 122 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	L5	729	2MG	N1-C2-N2-CM2
3	L5	729	2MG	N3-C2-N2-CM2
3	L5	1860	PSU	C3'-C4'-C5'-O5'
3	L5	2351	OMC	C3'-C4'-C5'-O5'
3	L5	2351	OMC	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 284 ligands modelled in this entry, 284 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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

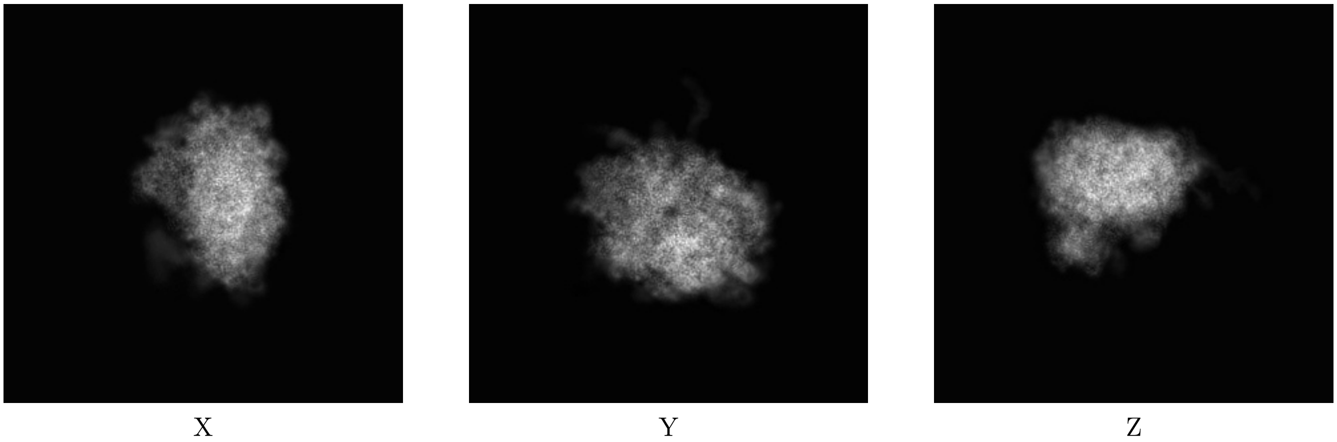
6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-31465. 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 ⓘ

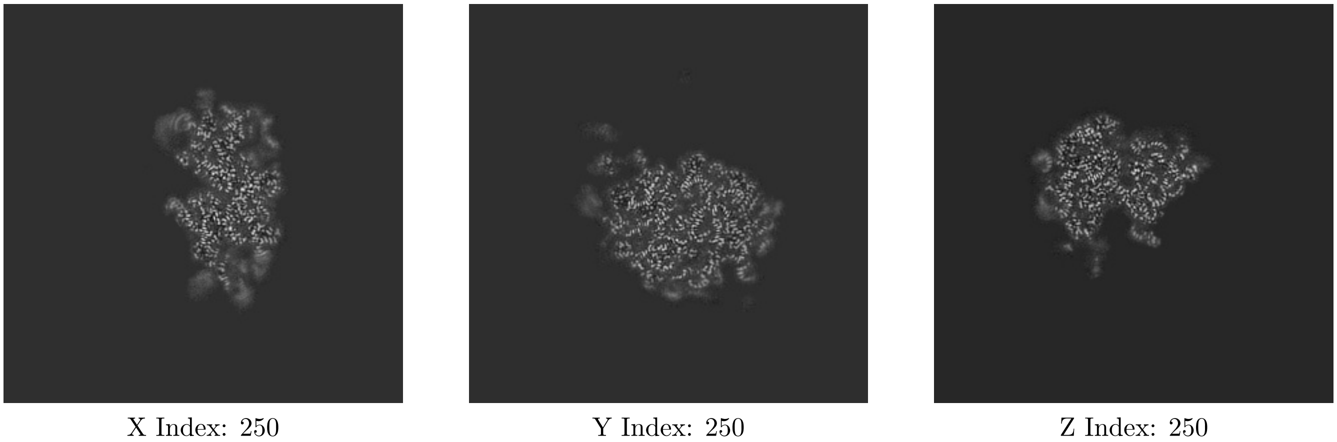
6.1.1 Primary map



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

6.2 Central slices ⓘ

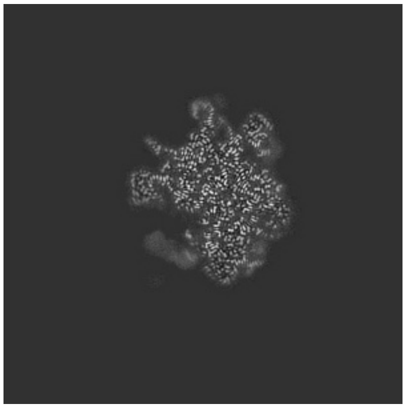
6.2.1 Primary map

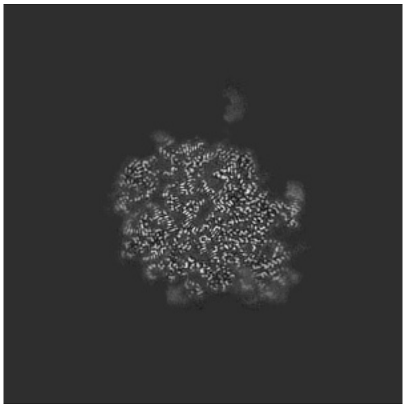


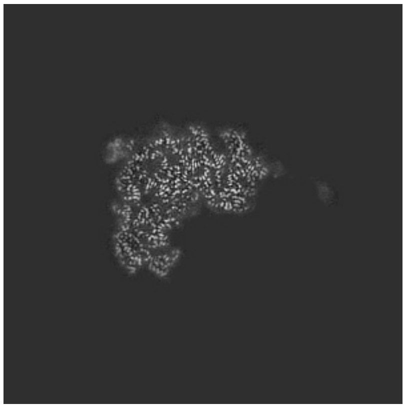
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices ⓘ

6.3.1 Primary map


X Index: 201


Y Index: 281

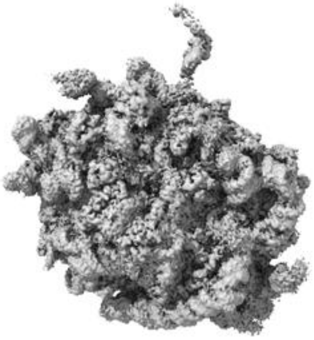

Z Index: 274

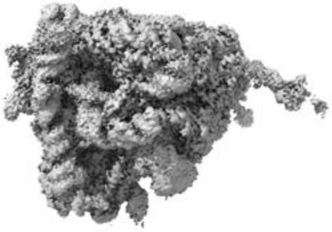
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views ⓘ

6.4.1 Primary map


X


Y


Z

The images above show the 3D surface view of the map at the recommended contour level 2.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

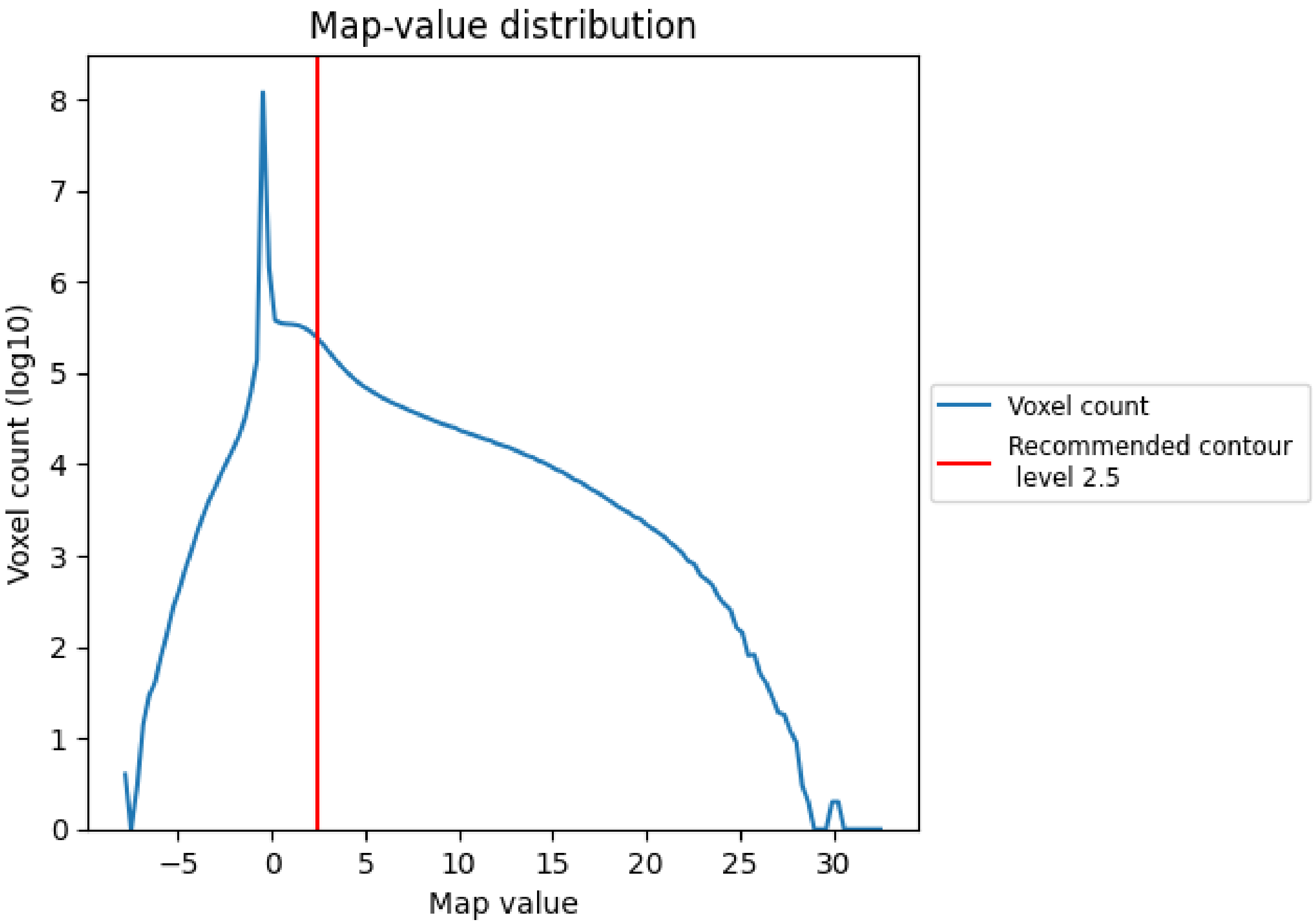
6.5 Mask visualisation ⓘ

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

7 Map analysis ⓘ

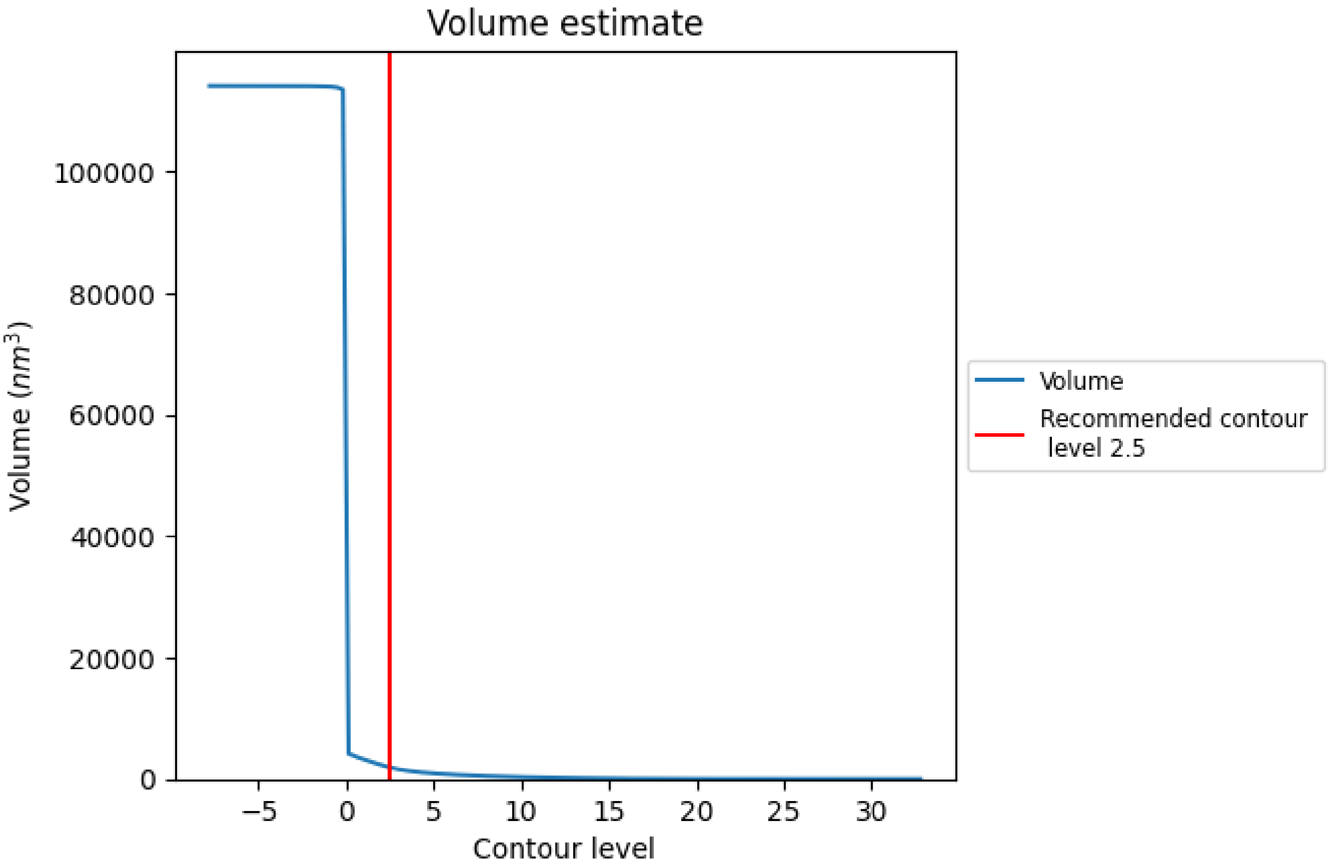
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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

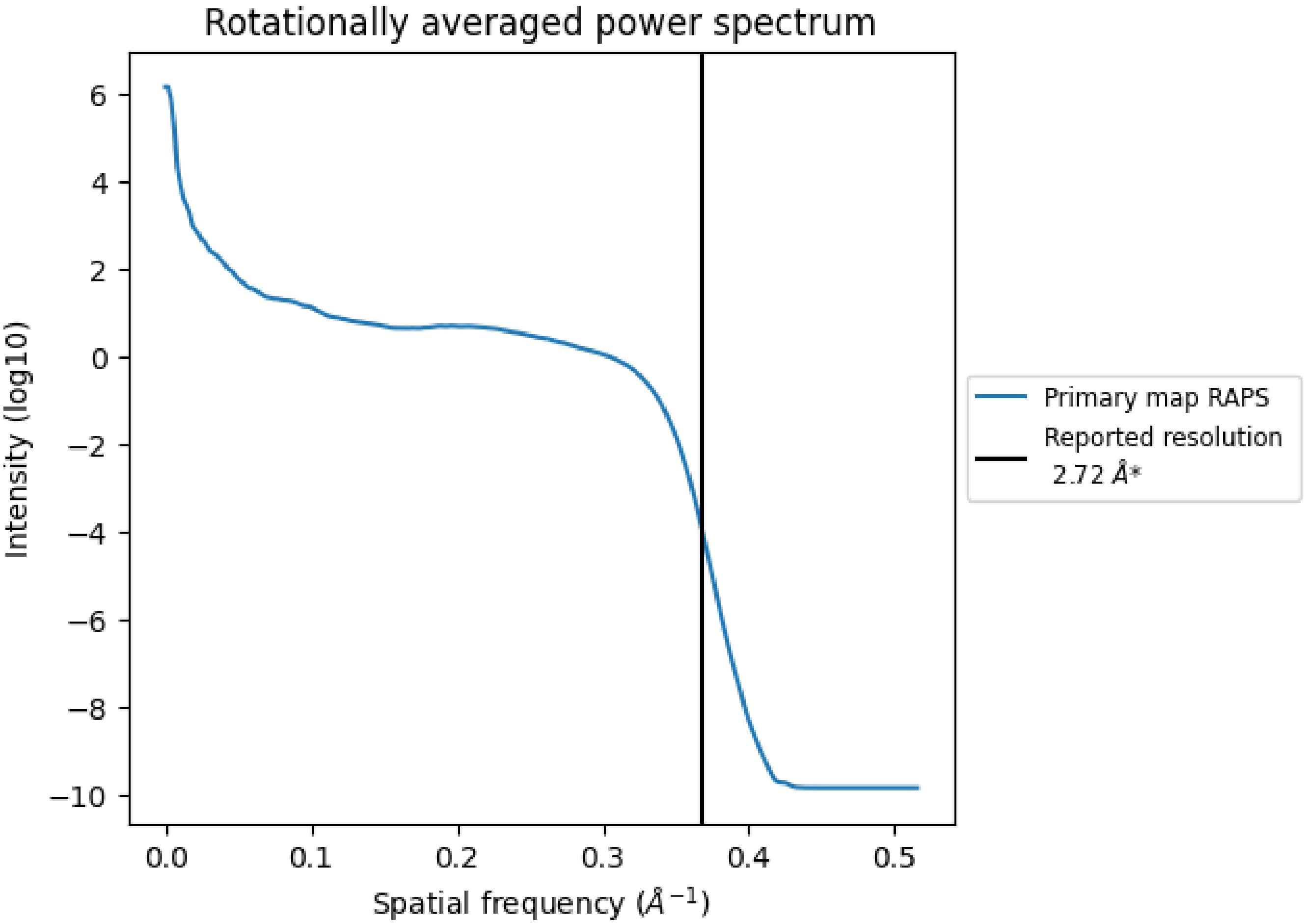
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 1927 nm^3; this corresponds to an approximate mass of 1741 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.368 Å^{-1}

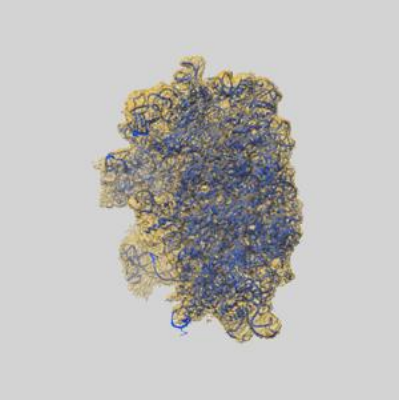
8 Fourier-Shell correlation

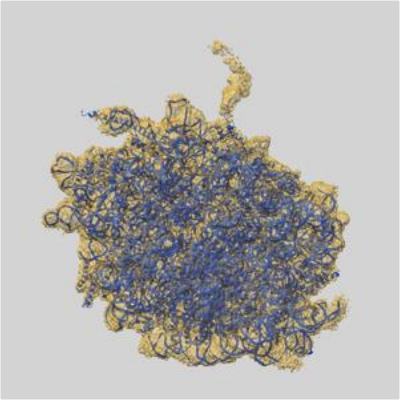
This section was not generated. No FSC curve or half-maps provided.

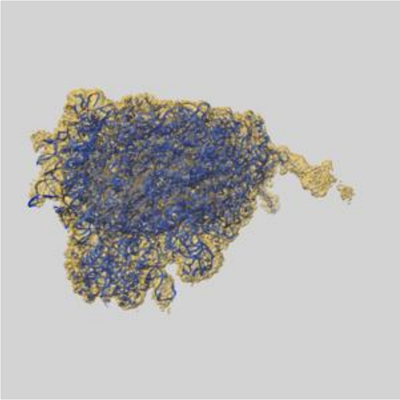
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-31465 and PDB model 7F5S. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay

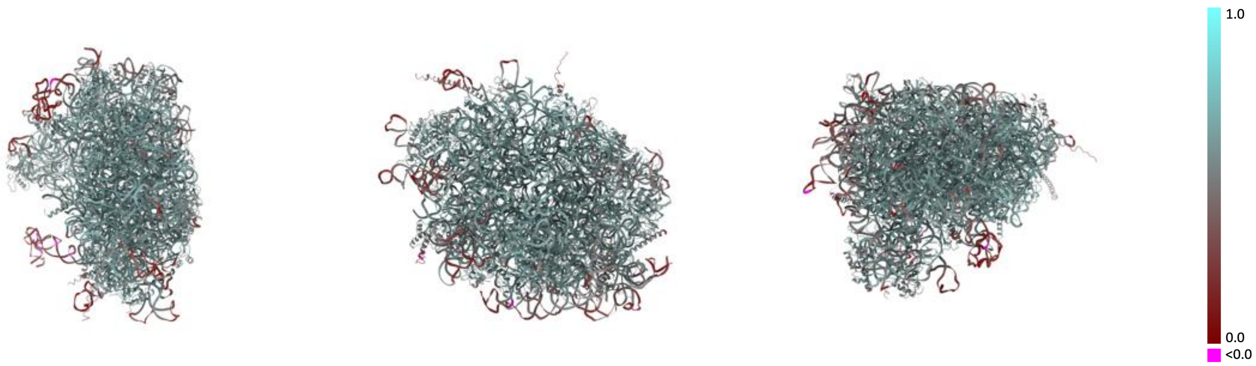

X


Y


Z

The images above show the 3D surface view of the map at the recommended contour level 2.5 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.

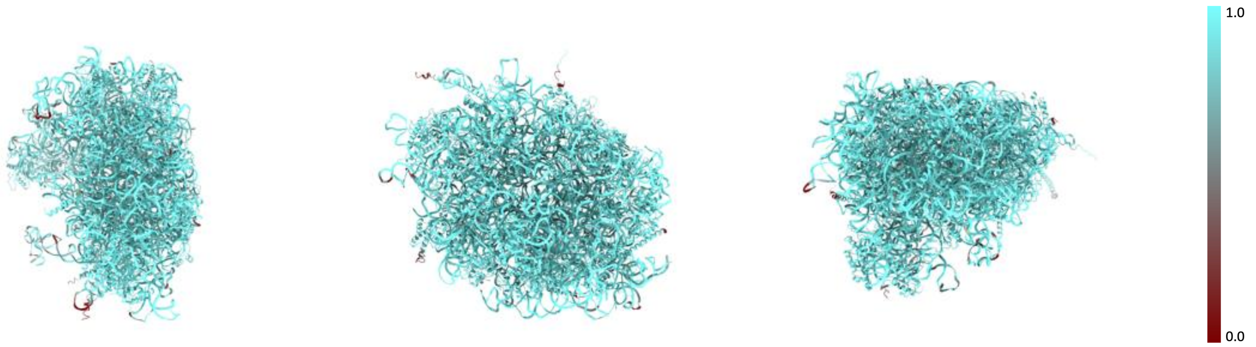
9.2 Q-score mapped to coordinate model ⓘ



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.

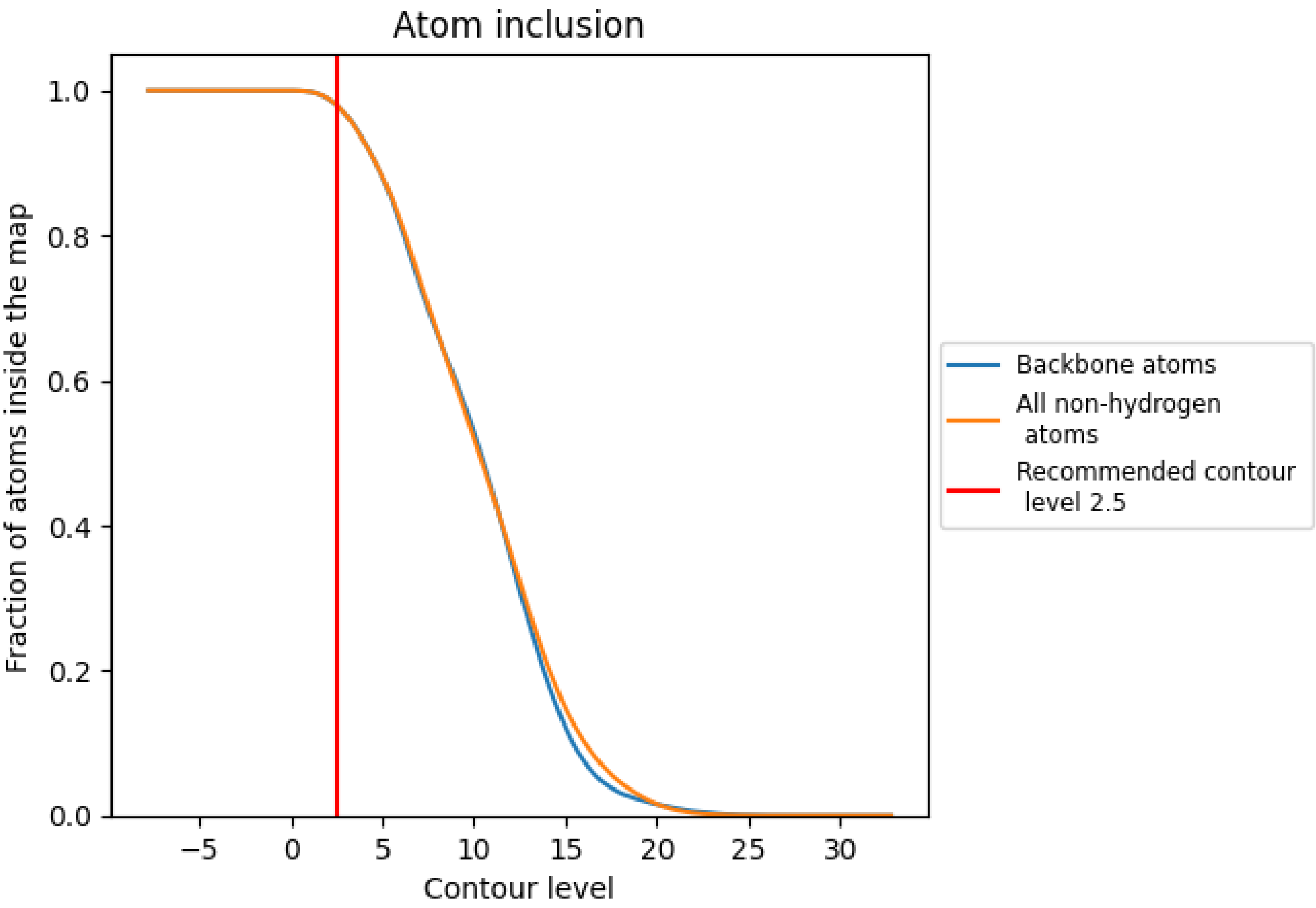
9.3 Atom inclusion mapped to coordinate model ⓘ



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 (2.5).

9.4 Atom inclusion ⓘ



At the recommended contour level, 98% of all backbone atoms, 98% 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 (2.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9800	0.5610
L5	0.9828	0.5480
L7	0.9984	0.5990
L8	0.9846	0.5760
LA	0.9951	0.6110
LB	0.9766	0.5930
LC	0.9816	0.5890
LD	0.9749	0.5620
LE	0.9822	0.5540
LF	0.9928	0.5900
LG	0.9251	0.5330
LH	0.9811	0.5810
LI	0.9726	0.5810
LJ	0.9294	0.5170
LL	0.9604	0.5700
LM	0.9819	0.5730
LN	0.9963	0.6120
LO	0.9887	0.5960
LP	0.9909	0.6020
LQ	0.9938	0.6100
LR	0.9167	0.5480
LS	0.9936	0.6060
LT	0.9770	0.5750
LU	0.9529	0.5120
LV	0.9843	0.5950
LW	0.9121	0.5180
LX	0.9831	0.5790
LY	0.9833	0.5820
LZ	0.9897	0.5760
La	0.9938	0.6120
Lb	0.9208	0.5280
Lc	0.9598	0.5590
Ld	0.9720	0.5850
Le	0.9951	0.6040
Lf	0.9905	0.6140

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Chain	**Atom inclusion**	**Q-score**
Lg	0.9780	0.5850
Lh	0.9766	0.5750
Li	0.9799	0.5670
Lj	0.9985	0.6060
Lk	0.9443	0.5470
Ll	0.9905	0.5840
Lm	0.9784	0.5880
Ln	0.9761	0.5480
Lo	0.9816	0.5850
Lp	0.9811	0.5870
Lr	0.9907	0.5940