



wwPDB EM Validation Summary Report ⓘ

Nov 20, 2022 – 05:56 am GMT

PDB ID : 6GZQ
EMDB ID : EMD-0101
Title : T. thermophilus hibernating 70S ribosome
Authors : Flygaard, R.K.; Jenner, L.B.
Deposited on : 2018-07-04
Resolution : 3.28 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:

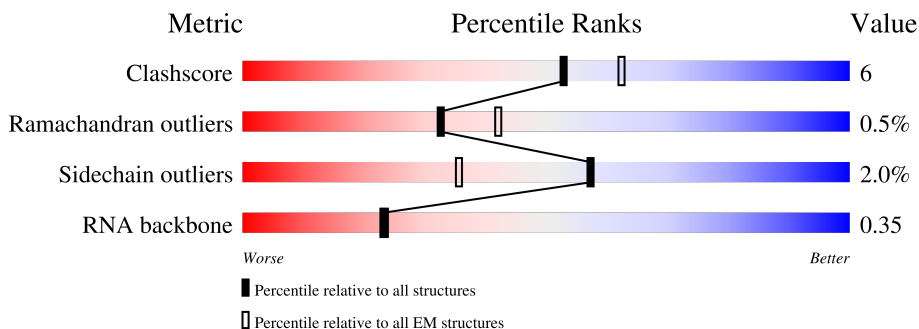
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance

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

The reported resolution of this entry is 3.28 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)
Clashscore	158937	4297
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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	C1	272	
2	D1	205	
3	E1	208	
4	F1	181	
5	G1	170	
6	H1	50	
7	I1	138	


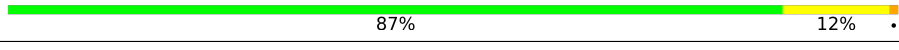
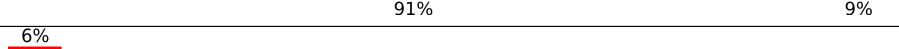




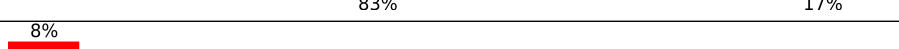


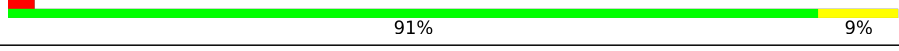
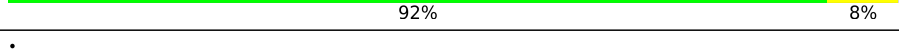
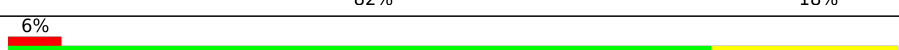
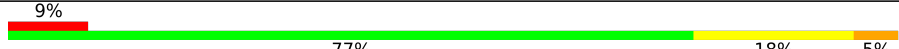


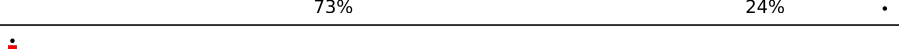
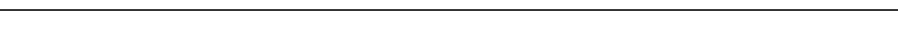



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Mol	Chain	Length	Quality of chain
8	J1	122	84% 16%
9	K1	150	81% 17%
10	L1	141	85% 13%
11	M1	117	83% 17%
12	N1	111	77% 23%
13	O1	137	78% 20%
14	P1	117	89% 9%
15	Q1	101	93% 6%
16	R1	113	82% 17%
17	S1	92	92% 8%
18	T1	102	77% 20%
19	U1	179	83% 15%
20	V1	77	88% 12%
21	W1	97	88% 12%
22	X1	69	88% 12%
23	Y1	59	92% 8%
24	Z1	63	65% 32%
25	a1	59	97%
26	b1	45	84% 13%
27	c1	49	96%
28	d1	61	89% 11%
29	A1	2912	48% 37% 14%
30	B1	122	55% 36% 9%
31	e1	36	94% 6%
32	B2	237	81% 17%

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Mol	Chain	Length	Quality of chain
33	C2	206	 86% 13%
34	D2	208	 87% 12%
35	E2	151	 91% 9%
36	F2	101	 6% 83% 17%
37	G2	155	 8% 77% 23%
38	H2	138	 89% 11%
39	I2	127	 8% 76% 24%
40	J2	99	 77% 22%
41	K2	118	 5% 83% 17%
42	L2	125	 8% 84% 15%
43	M2	117	 13% 74% 24%
44	N2	60	 88% 12%
45	O2	88	 91% 9%
46	P2	84	 92% 8%
47	Q2	100	 82% 18%
48	R2	62	 6% 79% 21%
49	S2	78	 9% 77% 18% 5%
50	T2	99	 89% 10%
51	U2	25	 72% 28%
52	V2	121	 12% 73% 24%
53	A2	1506	 42% 40% 15%

2 Entry composition [i](#)

There are 53 unique types of molecules in this entry. The entry contains 144138 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 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	C1	272	2116	1335	420	358	3	0	0

- Molecule 2 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D1	205	1569	991	300	272	6	0	0

- Molecule 3 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	E1	208	1628	1037	304	284	3	0	0

- Molecule 4 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	F1	181	1474	942	268	260	4	0	0

- Molecule 5 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	G1	170	1308	829	245	233	1	0	0

- Molecule 6 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	H1	50	383	245	66	71	1	0	0

- Molecule 7 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	I1	138	1105	712	206	183	4	0	0

- Molecule 8 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	J1	122	933	588	171	170	4	0	0

- Molecule 9 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	K1	150	1145	712	232	198	3	0	0

- Molecule 10 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	L1	141	1122	715	212	188	7	0	0

- Molecule 11 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
11	M1	117	960	599	202	159	0	0

- Molecule 12 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
12	N1	111	882	556	176	150	0	0

- Molecule 13 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	O1	137	1142	710	234	197	1	0	0

- Molecule 14 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	P1	117	Total	C	N	O	S	0	0
			964	610	202	151	1		

- Molecule 15 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Q1	101	Total	C	N	O	S	0	0
			779	501	142	135	1		

- Molecule 16 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	R1	113	Total	C	N	O	S	0	0
			900	566	177	155	2		

- Molecule 17 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	S1	92	Total	C	N	O	0	0
			726	471	131	124		

- Molecule 18 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T1	102	Total	C	N	O	S	0	0
			786	505	150	126	5		

- Molecule 19 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U1	179	Total	C	N	O	S	0	0
			1429	911	255	260	3		

- Molecule 20 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V1	77	Total	C	N	O	S	0	0
			613	379	129	104	1		

- Molecule 21 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W1	97	Total	C	N	O	S	0	0
			763	481	150	131	1		

- Molecule 22 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	X1	69	Total	C	N	O	S	0	0
			581	358	118	104	1		

- Molecule 23 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	Y1	59	Total	C	N	O	0	0
			469	298	90	81		

- Molecule 24 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Z1	63	Total	C	N	O	S	0	0
			516	326	93	92	5		

- Molecule 25 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	a1	59	Total	C	N	O	S	0	0
			459	288	90	76	5		

- Molecule 26 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	b1	45	Total	C	N	O	S	0	0
			390	241	79	66	4		

- Molecule 27 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	c1	49	Total	C	N	O	S	0	0
			430	263	108	57	2		

- Molecule 28 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	d1	61	Total	C	N	O	S	0	0
			489	312	99	76	2		

- Molecule 29 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	A1	2912	Total	C	N	O	P	0	0
			62707	27911	11722	20163	2911		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A1	156	U	UNK	conflict	GB 55771382
A1	682	A	G	conflict	GB 55771382
A1	686	C	G	conflict	GB 55771382
A1	697	G	C	conflict	GB 55771382
A1	701	A	C	conflict	GB 55771382
A1	1106	U	G	conflict	GB 55771382
A1	1128	A	C	conflict	GB 55771382

- Molecule 30 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	B1	122	Total	C	N	O	P	0	0
			2617	1166	486	844	121		

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	e1	36	Total	C	N	O	S	0	0
			299	183	67	46	3		

- Molecule 32 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	B2	237	Total	C	N	O	S	0	0
			1925	1228	344	348	5		

- Molecule 33 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	C2	206	Total	C	N	O	S	0	0
			1613	1016	314	282	1		

- Molecule 34 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	D2	208	1703	1066	339	291	7	0	0

- Molecule 35 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	E2	151	1156	729	218	205	4	0	0

- Molecule 36 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	F2	101	843	531	155	154	3	0	0

- Molecule 37 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	G2	155	1257	781	252	218	6	0	0

- Molecule 38 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	H2	138	1116	705	215	193	3	0	0

- Molecule 39 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
39	I2	127	1010	639	197	174	0	0

- Molecule 40 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	J2	99	802	504	157	140	1	0	0

- Molecule 41 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	K2	118	Total	C	N	O	S	0	0
			879	546	167	163	3		

- Molecule 42 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	L2	125	Total	C	N	O	S	0	0
			976	614	196	165	1		

- Molecule 43 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	M2	117	Total	C	N	O	S	0	0
			934	577	192	163	2		

- Molecule 44 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	N2	60	Total	C	N	O	S	0	0
			492	312	104	72	4		

- Molecule 45 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	O2	88	Total	C	N	O	S	0	0
			734	459	147	126	2		

- Molecule 46 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	P2	84	Total	C	N	O	S	0	0
			706	446	140	119	1		

- Molecule 47 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Q2	100	Total	C	N	O	S	0	0
			835	534	155	144	2		

- Molecule 48 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	R2	62	Total	C	N	O	0	0
			515	328	101	86		

- Molecule 49 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	S2	78	Total	C	N	O	S	0	0
			625	398	115	110	2		

- Molecule 50 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	T2	99	Total	C	N	O	S	0	0
			763	470	162	129	2		

- Molecule 51 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				AltConf	Trace
51	U2	25	Total	C	N	O	0	0
			218	134	52	32		

- Molecule 52 is a protein called Ribosome hibernation promoting factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	V2	121	Total	C	N	O	S	0	0
			983	615	185	182	1		

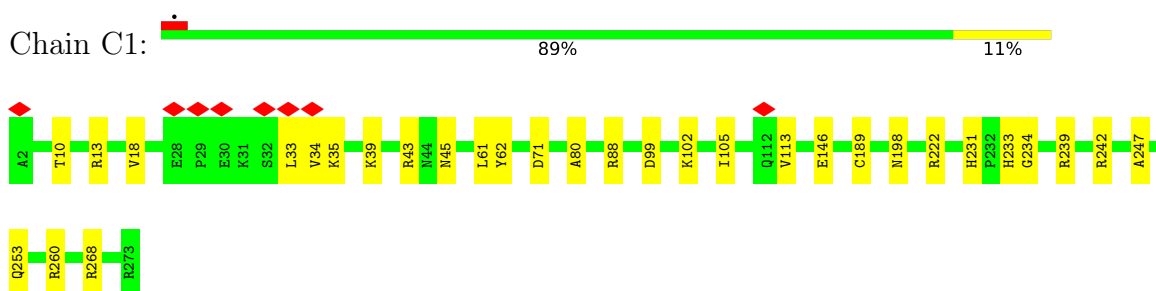
- Molecule 53 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	A2	1506	Total	C	N	O	P	0	0
			32369	14408	5997	10459	1505		

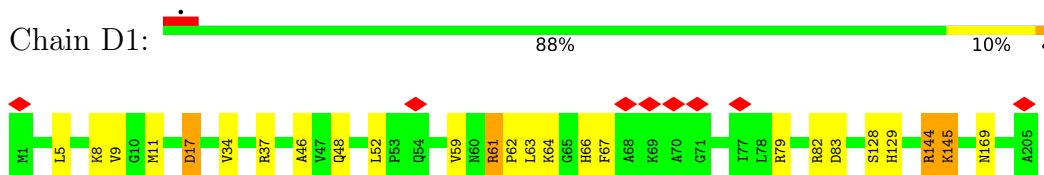
3 Residue-property plots [i](#)

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.

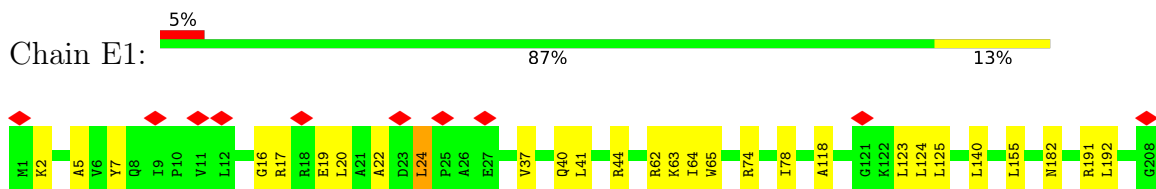
- Molecule 1: 50S ribosomal protein L2



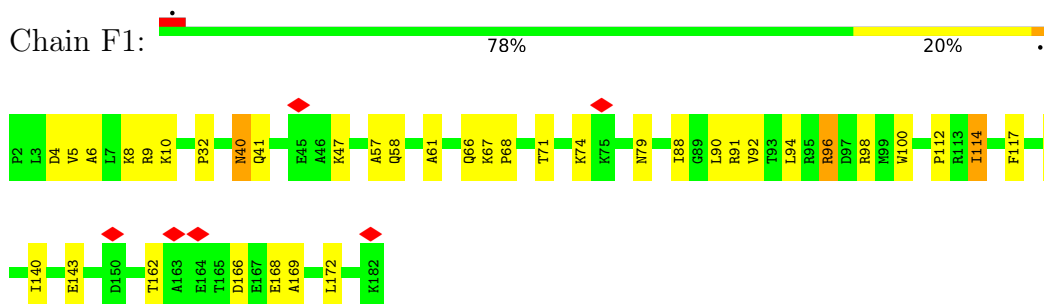
- Molecule 2: 50S ribosomal protein L3



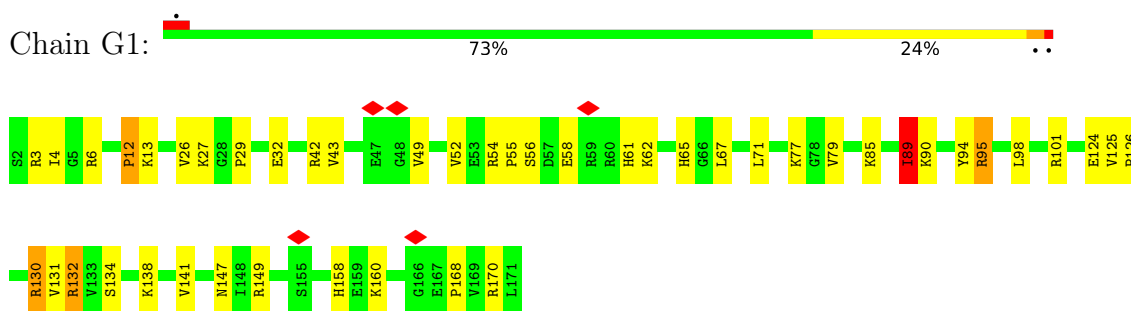
- Molecule 3: 50S ribosomal protein L4



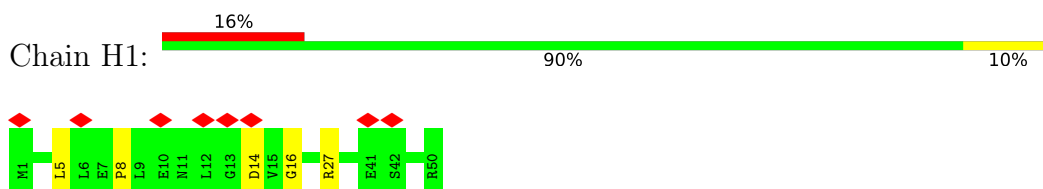
- Molecule 4: 50S ribosomal protein L5



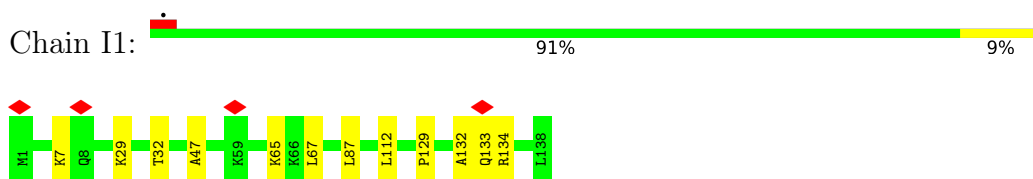
- Molecule 5: 50S ribosomal protein L6



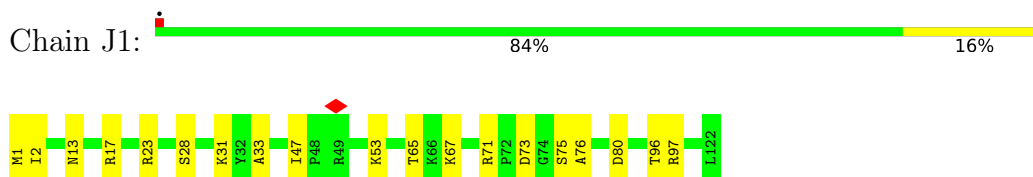
- Molecule 6: 50S ribosomal protein L9



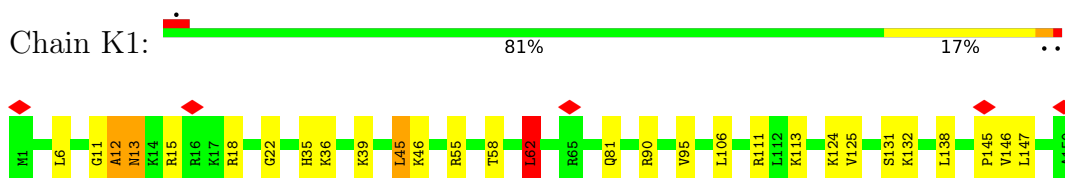
- Molecule 7: 50S ribosomal protein L13



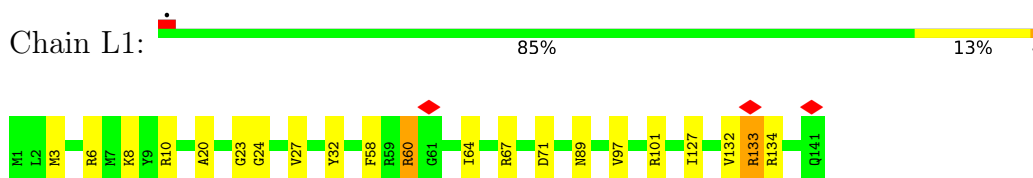
- Molecule 8: 50S ribosomal protein L14




- Molecule 9: 50S ribosomal protein L15



- Molecule 10: 50S ribosomal protein L16




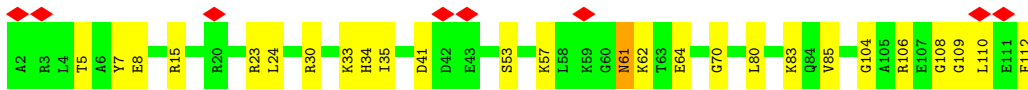
- Molecule 11: 50S ribosomal protein L17

Chain M1:  83% 17%




- Molecule 12: 50S ribosomal protein L18

Chain N1:  77% 23%




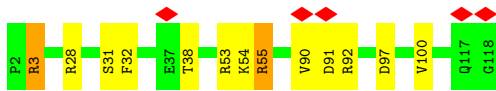
- Molecule 13: 50S ribosomal protein L19

Chain O1:  78% 20%



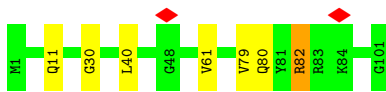
- Molecule 14: 50S ribosomal protein L20

Chain P1:  89% 9%




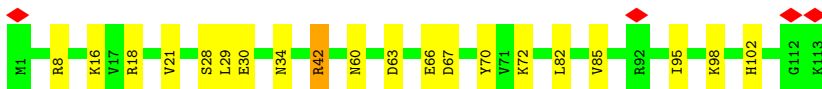
- Molecule 15: 50S ribosomal protein L21

Chain Q1:  93% 6%




- Molecule 16: 50S ribosomal protein L22

Chain R1:  82% 17%

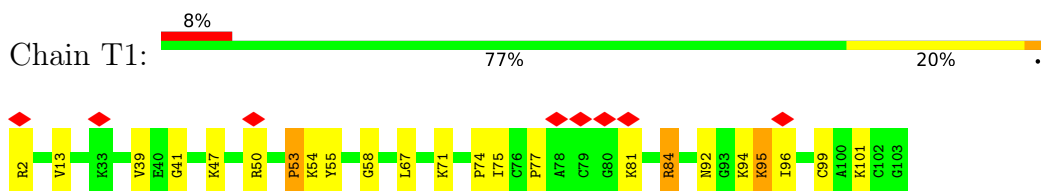


- Molecule 17: 50S ribosomal protein L23

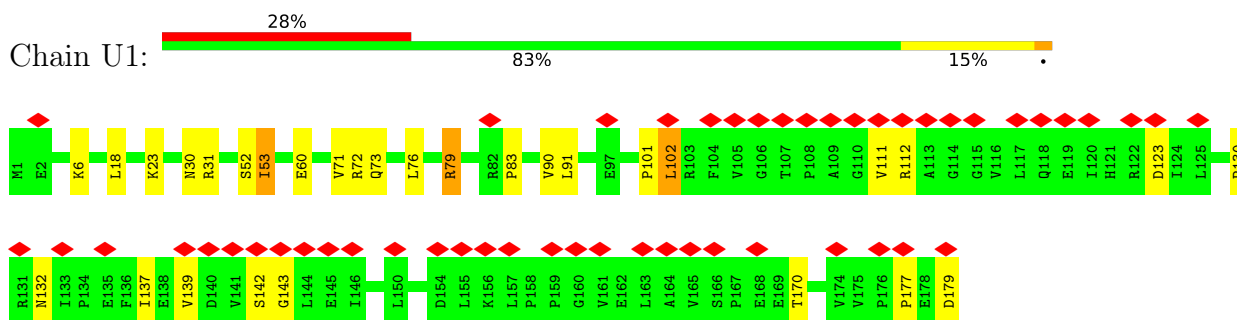
Chain S1:  92% 8%



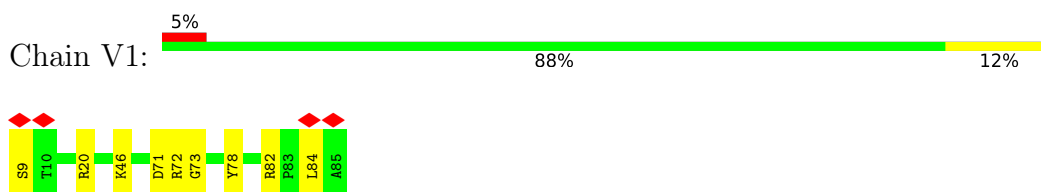
- Molecule 18: 50S ribosomal protein L24



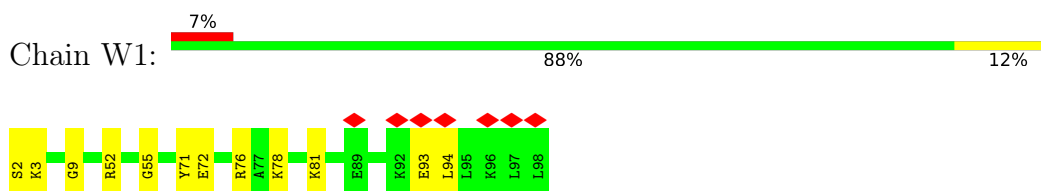
- Molecule 19: 50S ribosomal protein L25



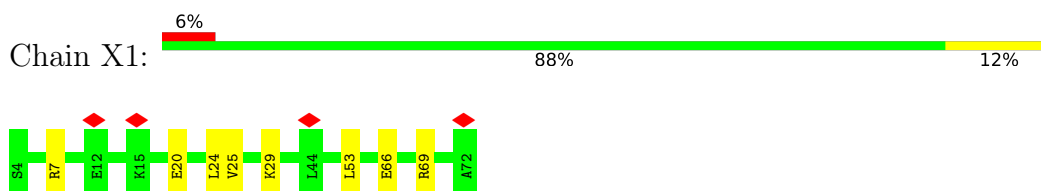
- Molecule 20: 50S ribosomal protein L27



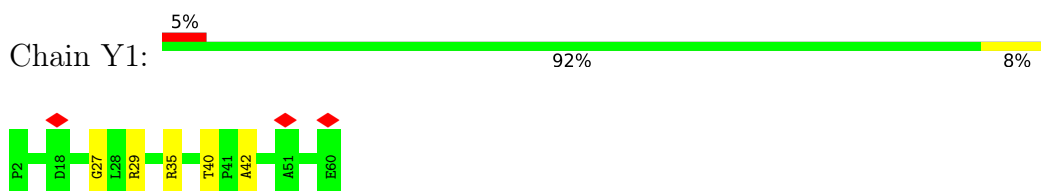
- Molecule 21: 50S ribosomal protein L28



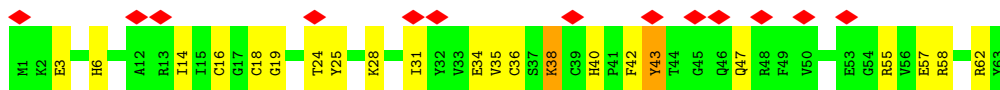
- Molecule 22: 50S ribosomal protein L29



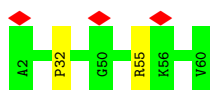
- Molecule 23: 50S ribosomal protein L30



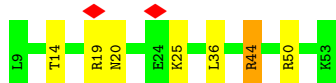
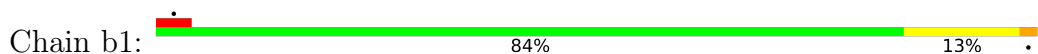
- Molecule 24: 50S ribosomal protein L31



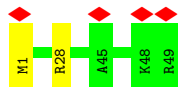
• Molecule 25: 50S ribosomal protein L32



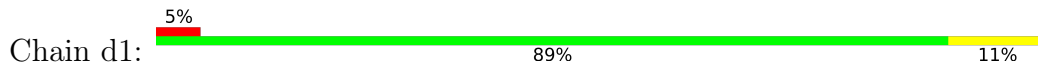
• Molecule 26: 50S ribosomal protein L33



• Molecule 27: 50S ribosomal protein L34

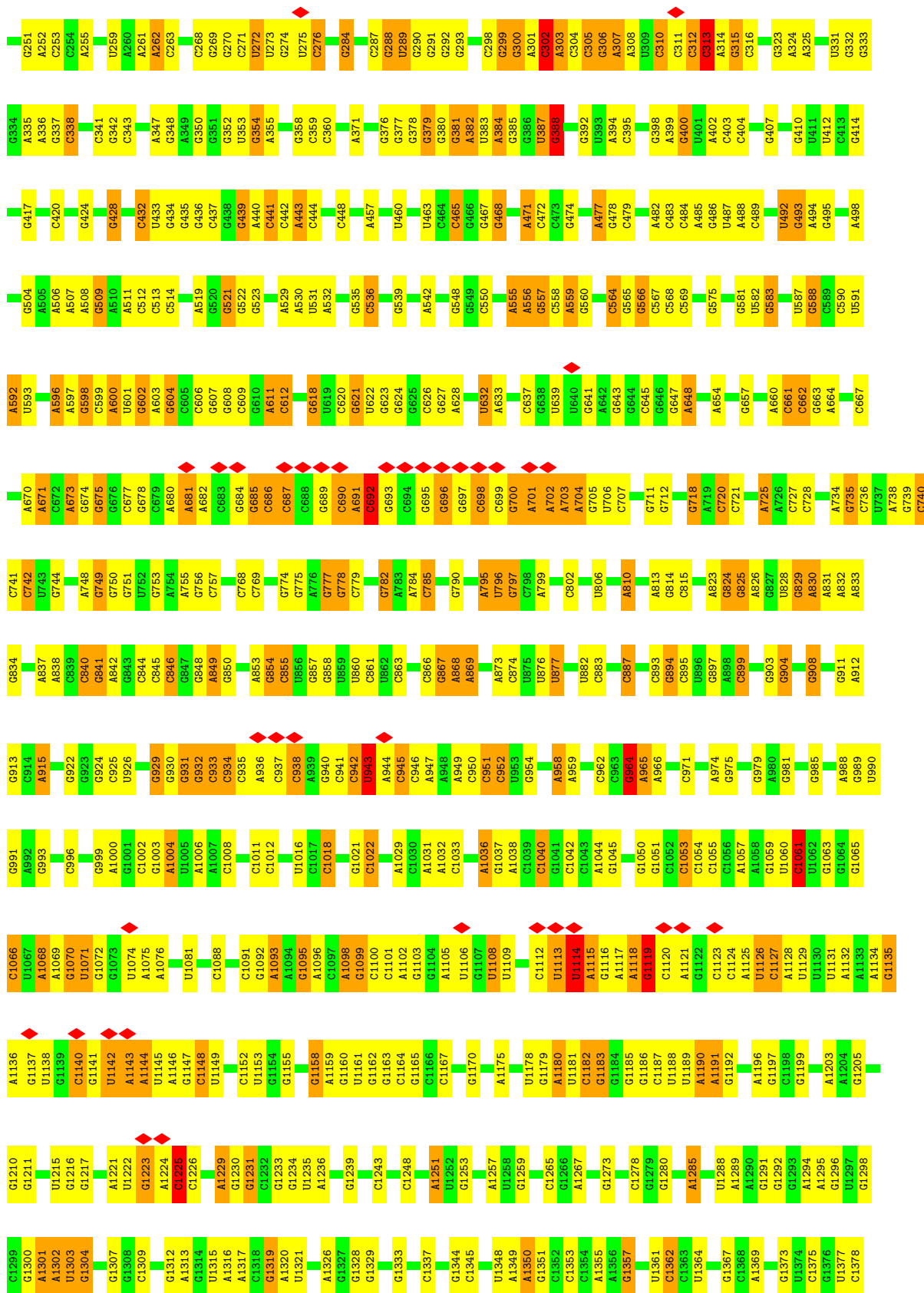


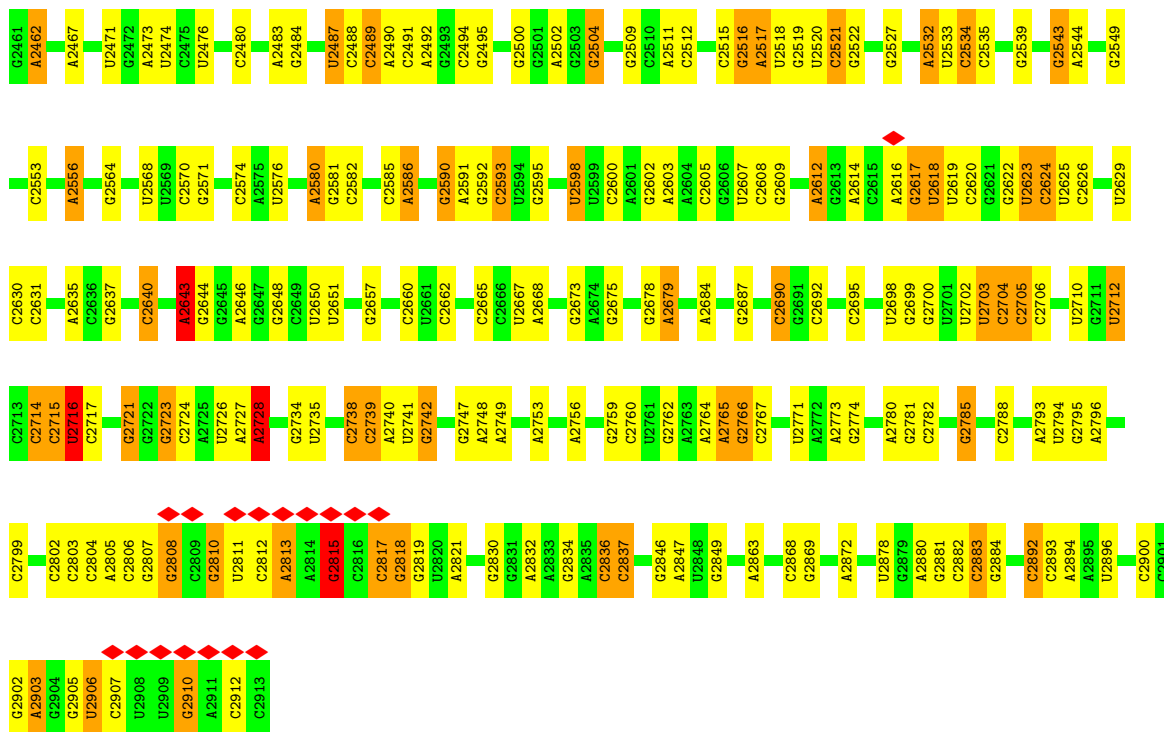
• Molecule 28: 50S ribosomal protein L35



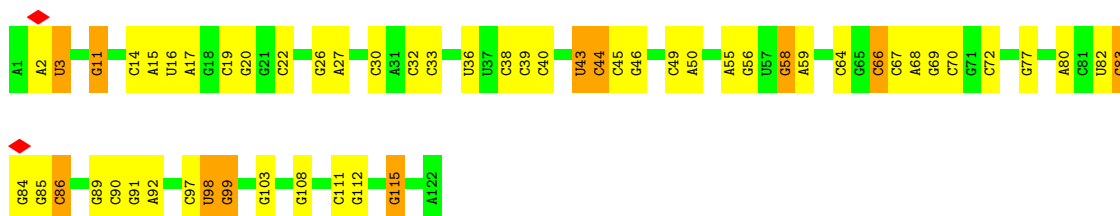
• Molecule 29: 23S ribosomal RNA



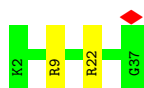




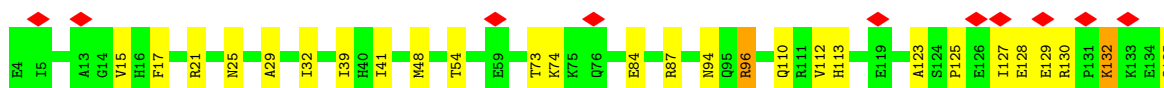
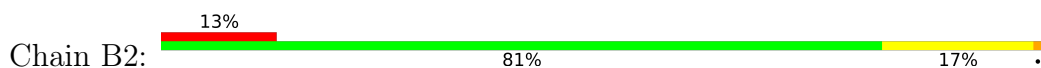
• Molecule 30: 5S ribosomal RNA

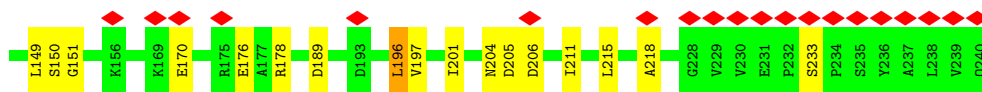


• Molecule 31: 50S ribosomal protein L36

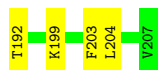
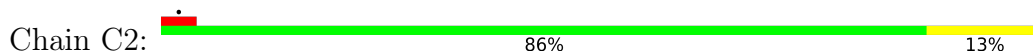


• Molecule 32: 30S ribosomal protein S2

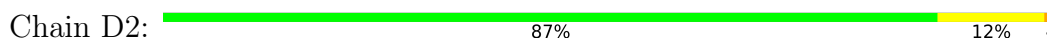




- Molecule 33: 30S ribosomal protein S3



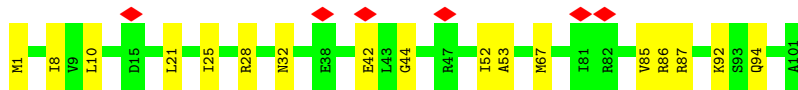
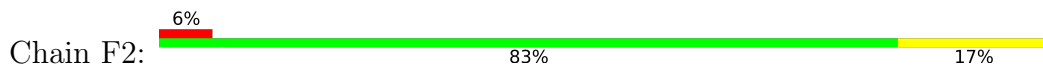
- Molecule 34: 30S ribosomal protein S4



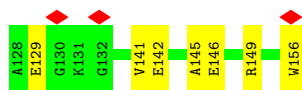
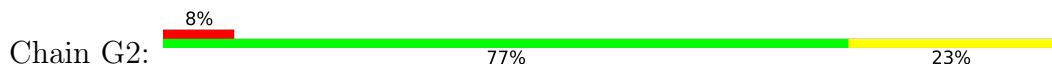
- Molecule 35: 30S ribosomal protein S5



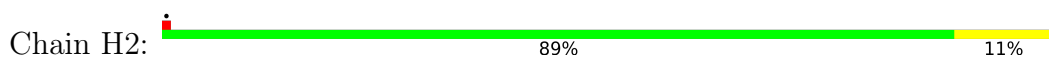
- Molecule 36: 30S ribosomal protein S6



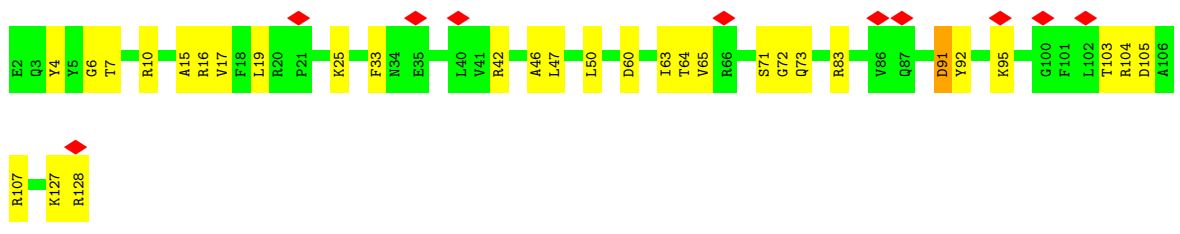
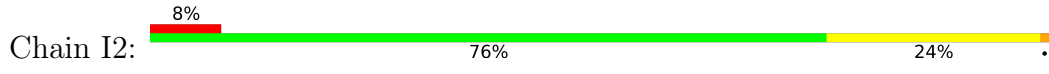
- Molecule 37: 30S ribosomal protein S7



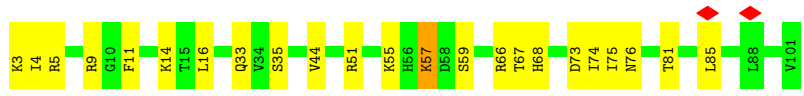
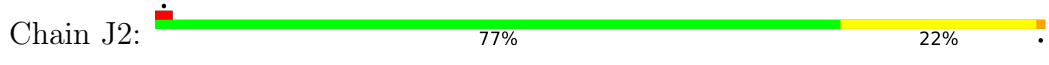
- Molecule 38: 30S ribosomal protein S8



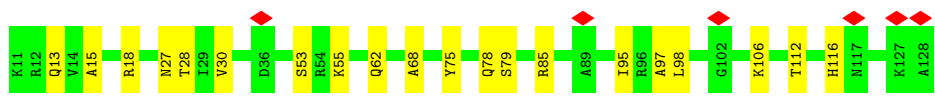
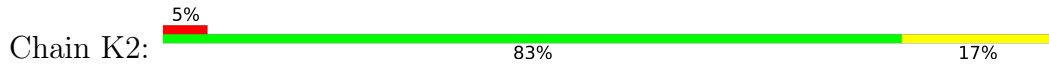
• Molecule 39: 30S ribosomal protein S9



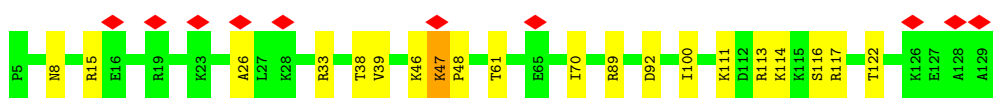
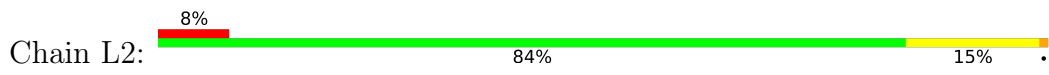
• Molecule 40: 30S ribosomal protein S10



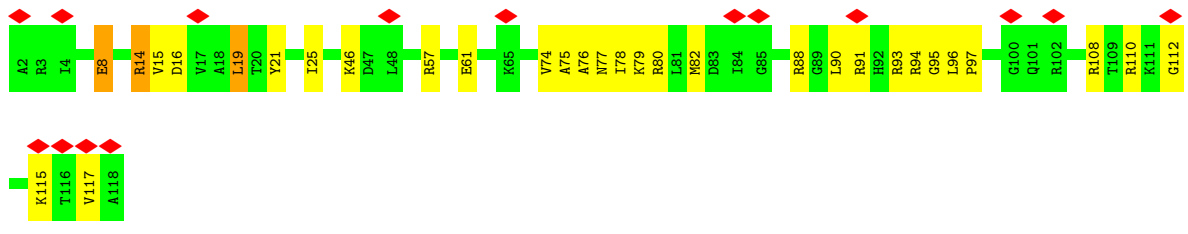
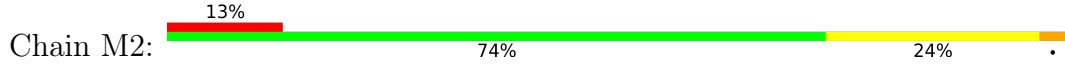
• Molecule 41: 30S ribosomal protein S11




• Molecule 42: 30S ribosomal protein S12

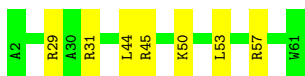


• Molecule 43: 30S ribosomal protein S13



- Molecule 44: 30S ribosomal protein S14 type Z

Chain N2:  88% 12%



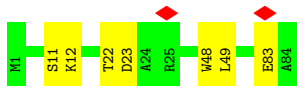
- Molecule 45: 30S ribosomal protein S15

Chain O2:  91% 9%




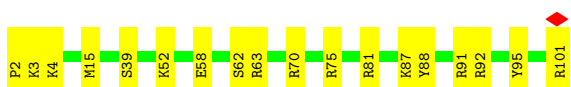
- Molecule 46: 30S ribosomal protein S16

Chain P2:  92% 8%




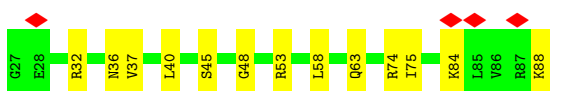
- Molecule 47: 30S ribosomal protein S17

Chain Q2:  82% 18%




- Molecule 48: 30S ribosomal protein S18

Chain R2:  6% 79% 21%



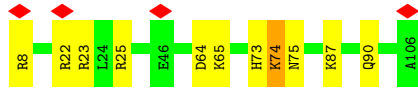
- Molecule 49: 30S ribosomal protein S19

Chain S2:  9% 77% 18% 5%

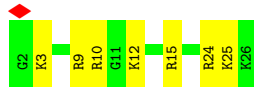
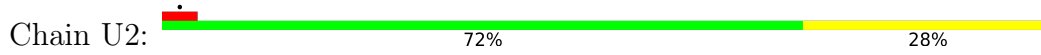


- Molecule 50: 30S ribosomal protein S20

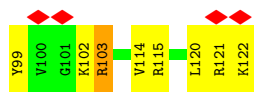
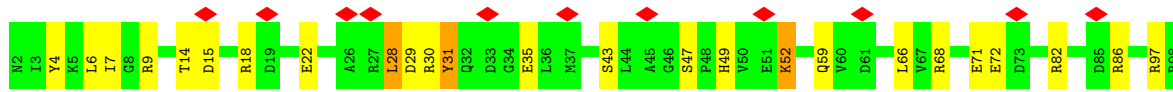
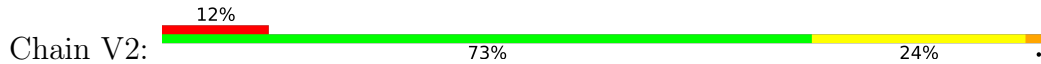
Chain T2:  89% 10%



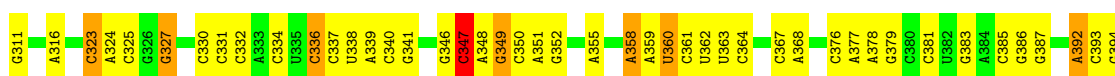
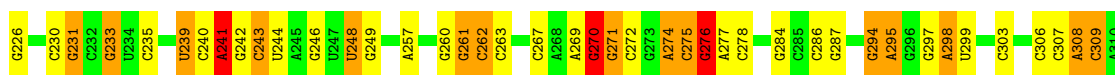
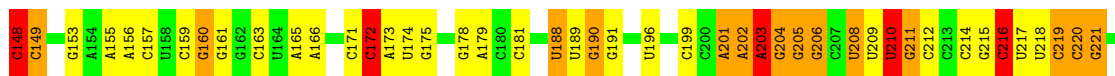
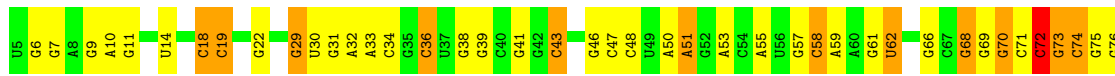
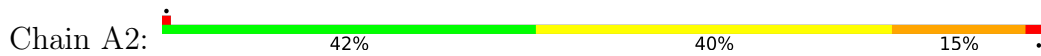
• Molecule 51: 30S ribosomal protein Thx

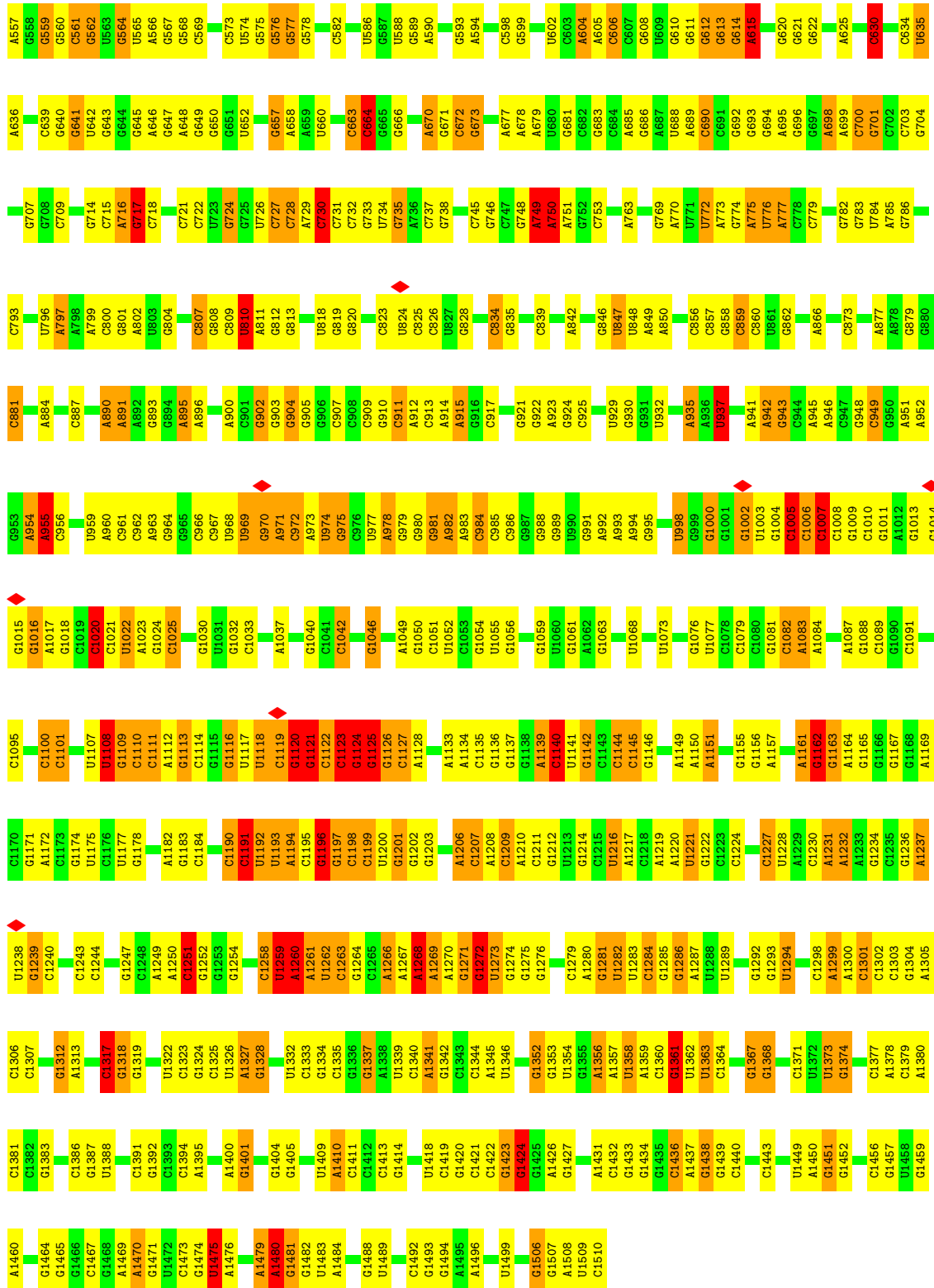


• Molecule 52: Ribosome hibernation promoting factor



• Molecule 53: 16S ribosomal RNA





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	45422	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 ($e^-/\text{\AA}^2$)	1.06	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	35.207	Depositor
Minimum map value	-15.042	Depositor
Average map value	0.016	Depositor
Map value standard deviation	0.439	Depositor
Recommended contour level	3.5	Depositor
Map size (Å)	770.0, 770.0, 770.0	wwPDB
Map dimensions	700, 700, 700	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality i

5.1 Standard geometry i

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	C1	0.77	1/2166 (0.0%)	0.76	0/2919
2	D1	0.71	0/1602	0.77	1/2160 (0.0%)
3	E1	0.72	0/1663	0.69	0/2249
4	F1	0.53	0/1499	0.66	0/2016
5	G1	0.52	0/1333	0.73	1/1802 (0.1%)
6	H1	0.49	0/387	0.71	0/523
7	I1	0.68	0/1132	0.68	0/1525
8	J1	0.70	0/943	0.69	0/1269
9	K1	0.61	0/1162	0.84	1/1544 (0.1%)
10	L1	0.65	0/1143	0.70	0/1527
11	M1	0.66	0/974	0.79	0/1302
12	N1	0.58	0/892	0.72	0/1187
13	O1	0.62	0/1156	0.67	0/1542
14	P1	0.77	0/982	0.68	0/1306
15	Q1	0.61	0/790	0.67	0/1057
16	R1	0.64	0/911	0.75	3/1220 (0.2%)
17	S1	0.68	0/740	0.72	0/993
18	T1	0.55	0/799	0.69	0/1064
19	U1	0.52	0/1461	0.66	1/1982 (0.1%)
20	V1	0.69	0/621	0.69	0/827
21	W1	0.66	0/770	0.74	0/1022
22	X1	0.52	0/583	0.69	0/771
23	Y1	0.65	0/474	0.68	0/635
24	Z1	0.48	0/528	0.78	0/709
25	a1	0.75	1/473 (0.2%)	0.71	0/639
26	b1	0.66	0/397	0.95	1/529 (0.2%)
27	c1	0.78	0/438	0.75	0/575
28	d1	0.74	0/495	0.99	3/649 (0.5%)
29	A1	1.64	325/70233 (0.5%)	1.41	861/109643 (0.8%)
30	B1	1.26	2/2928 (0.1%)	1.37	34/4568 (0.7%)
31	e1	0.71	0/302	0.69	0/397
32	B2	0.55	0/1960	0.68	0/2642
33	C2	0.61	0/1637	0.70	0/2205
34	D2	0.67	0/1733	0.76	0/2318

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
35	E2	0.66	0/1172	0.71	0/1576
36	F2	0.55	0/856	0.64	0/1154
37	G2	0.51	0/1276	0.66	1/1709 (0.1%)
38	H2	0.70	0/1136	0.68	0/1527
39	I2	0.54	0/1029	0.72	0/1379
40	J2	0.50	0/815	0.65	1/1095 (0.1%)
41	K2	0.58	0/894	0.68	0/1205
42	L2	0.68	0/992	0.72	0/1327
43	M2	0.43	0/944	0.71	0/1265
44	N2	0.62	0/501	0.69	0/664
45	O2	0.59	0/745	0.70	0/992
46	P2	0.71	0/722	0.69	0/970
47	Q2	0.66	0/848	0.66	0/1131
48	R2	0.55	0/520	0.73	0/690
49	S2	0.44	0/639	0.72	0/860
50	T2	0.49	0/765	0.69	0/1007
51	U2	0.54	0/222	0.67	0/288
52	V2	0.59	0/997	0.84	1/1341 (0.1%)
53	A2	3.30	114/36234 (0.3%)	1.91	551/56554 (1.0%)
All	All	1.97	443/156614 (0.3%)	1.41	1460/234050 (0.6%)

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
1	C1	0	1
2	D1	0	1
3	E1	0	1
4	F1	0	1
5	G1	0	1
9	K1	0	2
14	P1	0	1
15	Q1	0	1
17	S1	0	1
18	T1	0	2
19	U1	0	1
24	Z1	0	1
26	b1	0	2
28	d1	0	2
32	B2	0	2

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
33	C2	0	2
34	D2	0	3
37	G2	0	2
39	I2	0	1
40	J2	0	1
42	L2	0	2
43	M2	0	2
49	S2	0	1
51	U2	0	1
52	V2	0	2
All	All	0	37

The worst 5 of 443 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	A2	700	C	N1-C6	189.65	2.50	1.37
53	A2	717	G	C6-N1	170.78	2.59	1.39
53	A2	717	G	N3-C4	146.04	2.37	1.35
53	A2	136	G	C2-N2	143.97	2.78	1.34
53	A2	1121	G	C2-N2	142.36	2.77	1.34

The worst 5 of 1460 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	A2	700	C	C4-C5-C6	-192.11	21.34	117.40
53	A2	700	C	N1-C2-N3	-133.89	25.48	119.20
53	A2	700	C	C2-N3-C4	86.94	163.37	119.90
53	A2	700	C	C5-C6-N1	59.60	150.80	121.00
53	A2	700	C	C6-N1-C2	49.66	140.16	120.30

There are no chirality outliers.

5 of 37 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C1	33	LEU	Peptide
2	D1	61	ARG	Peptide
3	E1	24	LEU	Peptide
4	F1	114	ILE	Peptide
5	G1	89	ILE	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C1	2116	0	2194	20	0
2	D1	1569	0	1634	14	0
3	E1	1628	0	1680	17	0
4	F1	1474	0	1535	30	0
5	G1	1308	0	1382	29	0
6	H1	383	0	410	4	0
7	I1	1105	0	1180	8	0
8	J1	933	0	996	14	0
9	K1	1145	0	1228	17	0
10	L1	1122	0	1179	11	0
11	M1	960	0	1021	12	0
12	N1	882	0	943	17	0
13	O1	1142	0	1202	20	0
14	P1	964	0	1022	8	0
15	Q1	779	0	852	4	0
16	R1	900	0	964	10	0
17	S1	726	0	778	2	0
18	T1	786	0	878	15	0
19	U1	1429	0	1454	18	0
20	V1	613	0	633	6	0
21	W1	763	0	848	6	0
22	X1	581	0	629	5	0
23	Y1	469	0	518	2	0
24	Z1	516	0	514	15	0
25	a1	459	0	479	0	0
26	b1	390	0	404	0	0
27	c1	430	0	480	0	0
28	d1	489	0	560	0	0
29	A1	62707	0	31613	271	0
30	B1	2617	0	1328	12	0
31	e1	299	0	326	0	0
32	B2	1925	0	1975	27	0
33	C2	1613	0	1677	15	0
34	D2	1703	0	1765	19	0
35	E2	1156	0	1213	9	0
36	F2	843	0	857	12	0
37	G2	1257	0	1296	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	H2	1116	0	1177	10	0
39	I2	1010	0	1037	24	0
40	J2	802	0	849	13	0
41	K2	879	0	899	13	0
42	L2	976	0	1062	13	0
43	M2	934	0	992	25	0
44	N2	492	0	533	5	0
45	O2	734	0	771	6	0
46	P2	706	0	725	4	0
47	Q2	835	0	904	14	0
48	R2	515	0	568	8	0
49	S2	625	0	636	12	0
50	T2	763	0	861	7	0
51	U2	218	0	234	5	0
52	V2	983	0	1008	27	0
53	A2	32369	0	16339	365	0
All	All	144138	0	98242	1080	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 1080 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:A2:1110:C:C5	53:A2:1110:C:C6	1.92	1.57
53:A2:216:C:C6	53:A2:216:C:C5	1.89	1.55
53:A2:216:C:C5	53:A2:216:C:C4	2.03	1.47
53:A2:1110:C:C5	53:A2:1110:C:C4	2.06	1.41
53:A2:136:G:N2	53:A2:216:C:N3	1.78	1.32

There are no symmetry-related clashes.

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	
1	C1	270/272 (99%)	237 (88%)	32 (12%)	1 (0%)	34	67
2	D1	203/205 (99%)	164 (81%)	35 (17%)	4 (2%)	7	34
3	E1	206/208 (99%)	180 (87%)	26 (13%)	0	100	100
4	F1	179/181 (99%)	157 (88%)	22 (12%)	0	100	100
5	G1	168/170 (99%)	136 (81%)	28 (17%)	4 (2%)	6	29
6	H1	48/50 (96%)	38 (79%)	10 (21%)	0	100	100
7	I1	136/138 (99%)	121 (89%)	15 (11%)	0	100	100
8	J1	120/122 (98%)	97 (81%)	23 (19%)	0	100	100
9	K1	148/150 (99%)	107 (72%)	38 (26%)	3 (2%)	7	34
10	L1	139/141 (99%)	117 (84%)	20 (14%)	2 (1%)	11	40
11	M1	115/117 (98%)	106 (92%)	9 (8%)	0	100	100
12	N1	109/111 (98%)	94 (86%)	15 (14%)	0	100	100
13	O1	135/137 (98%)	114 (84%)	20 (15%)	1 (1%)	22	56
14	P1	115/117 (98%)	106 (92%)	9 (8%)	0	100	100
15	Q1	99/101 (98%)	83 (84%)	16 (16%)	0	100	100
16	R1	111/113 (98%)	101 (91%)	10 (9%)	0	100	100
17	S1	90/92 (98%)	77 (86%)	13 (14%)	0	100	100
18	T1	100/102 (98%)	77 (77%)	22 (22%)	1 (1%)	15	48
19	U1	177/179 (99%)	134 (76%)	42 (24%)	1 (1%)	25	58
20	V1	75/77 (97%)	68 (91%)	7 (9%)	0	100	100
21	W1	95/97 (98%)	81 (85%)	13 (14%)	1 (1%)	14	46
22	X1	67/69 (97%)	60 (90%)	7 (10%)	0	100	100
23	Y1	57/59 (97%)	50 (88%)	7 (12%)	0	100	100
24	Z1	61/63 (97%)	41 (67%)	17 (28%)	3 (5%)	2	14
25	a1	57/59 (97%)	47 (82%)	10 (18%)	0	100	100
26	b1	43/45 (96%)	29 (67%)	14 (33%)	0	100	100
27	c1	47/49 (96%)	42 (89%)	5 (11%)	0	100	100
28	d1	59/61 (97%)	48 (81%)	10 (17%)	1 (2%)	9	37
31	e1	34/36 (94%)	32 (94%)	2 (6%)	0	100	100
32	B2	235/237 (99%)	197 (84%)	38 (16%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	C2	204/206 (99%)	180 (88%)	24 (12%)	0	100	100
34	D2	206/208 (99%)	178 (86%)	27 (13%)	1 (0%)	29	62
35	E2	149/151 (99%)	134 (90%)	15 (10%)	0	100	100
36	F2	99/101 (98%)	86 (87%)	13 (13%)	0	100	100
37	G2	153/155 (99%)	126 (82%)	27 (18%)	0	100	100
38	H2	136/138 (99%)	123 (90%)	13 (10%)	0	100	100
39	I2	125/127 (98%)	100 (80%)	25 (20%)	0	100	100
40	J2	97/99 (98%)	84 (87%)	13 (13%)	0	100	100
41	K2	116/118 (98%)	97 (84%)	19 (16%)	0	100	100
42	L2	123/125 (98%)	97 (79%)	25 (20%)	1 (1%)	19	52
43	M2	115/117 (98%)	96 (84%)	18 (16%)	1 (1%)	17	50
44	N2	58/60 (97%)	47 (81%)	11 (19%)	0	100	100
45	O2	86/88 (98%)	76 (88%)	10 (12%)	0	100	100
46	P2	82/84 (98%)	74 (90%)	8 (10%)	0	100	100
47	Q2	98/100 (98%)	84 (86%)	14 (14%)	0	100	100
48	R2	60/62 (97%)	55 (92%)	5 (8%)	0	100	100
49	S2	76/78 (97%)	53 (70%)	23 (30%)	0	100	100
50	T2	97/99 (98%)	84 (87%)	12 (12%)	1 (1%)	15	48
51	U2	23/25 (92%)	21 (91%)	2 (9%)	0	100	100
52	V2	119/121 (98%)	92 (77%)	26 (22%)	1 (1%)	19	52
All	All	5720/5820 (98%)	4828 (84%)	865 (15%)	27 (0%)	32	62

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	G1	90	LYS
50	T2	74	LYS
9	K1	58	THR
19	U1	53	ILE
24	Z1	25	TYR

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	
1	C1	214/214 (100%)	210 (98%)	4 (2%)	57	77
2	D1	165/165 (100%)	164 (99%)	1 (1%)	86	91
3	E1	165/165 (100%)	163 (99%)	2 (1%)	71	83
4	F1	155/155 (100%)	152 (98%)	3 (2%)	57	77
5	G1	142/142 (100%)	135 (95%)	7 (5%)	25	56
6	H1	41/41 (100%)	41 (100%)	0	100	100
7	I1	117/117 (100%)	117 (100%)	0	100	100
8	J1	100/100 (100%)	99 (99%)	1 (1%)	76	85
9	K1	116/116 (100%)	111 (96%)	5 (4%)	29	59
10	L1	111/111 (100%)	106 (96%)	5 (4%)	27	58
11	M1	100/100 (100%)	98 (98%)	2 (2%)	55	76
12	N1	87/87 (100%)	84 (97%)	3 (3%)	37	65
13	O1	120/120 (100%)	115 (96%)	5 (4%)	30	60
14	P1	93/93 (100%)	90 (97%)	3 (3%)	39	67
15	Q1	82/82 (100%)	81 (99%)	1 (1%)	71	83
16	R1	92/92 (100%)	91 (99%)	1 (1%)	73	85
17	S1	74/74 (100%)	72 (97%)	2 (3%)	44	71
18	T1	85/85 (100%)	84 (99%)	1 (1%)	71	83
19	U1	158/158 (100%)	156 (99%)	2 (1%)	69	82
20	V1	62/62 (100%)	62 (100%)	0	100	100
21	W1	82/82 (100%)	81 (99%)	1 (1%)	71	83
22	X1	64/64 (100%)	63 (98%)	1 (2%)	62	79
23	Y1	51/51 (100%)	50 (98%)	1 (2%)	55	76
24	Z1	57/57 (100%)	55 (96%)	2 (4%)	36	64
25	a1	51/51 (100%)	50 (98%)	1 (2%)	55	76
26	b1	44/44 (100%)	39 (89%)	5 (11%)	5	23
27	c1	42/42 (100%)	40 (95%)	2 (5%)	25	56
28	d1	51/51 (100%)	49 (96%)	2 (4%)	32	62
31	e1	33/33 (100%)	31 (94%)	2 (6%)	18	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	B2	205/205 (100%)	201 (98%)	4 (2%)	55	76
33	C2	160/160 (100%)	158 (99%)	2 (1%)	69	82
34	D2	180/180 (100%)	179 (99%)	1 (1%)	86	91
35	E2	116/116 (100%)	115 (99%)	1 (1%)	78	87
36	F2	90/90 (100%)	90 (100%)	0	100	100
37	G2	126/126 (100%)	125 (99%)	1 (1%)	81	89
38	H2	119/119 (100%)	119 (100%)	0	100	100
39	I2	98/98 (100%)	98 (100%)	0	100	100
40	J2	89/89 (100%)	88 (99%)	1 (1%)	73	85
41	K2	89/89 (100%)	88 (99%)	1 (1%)	73	85
42	L2	104/104 (100%)	102 (98%)	2 (2%)	57	77
43	M2	94/94 (100%)	91 (97%)	3 (3%)	39	67
44	N2	49/49 (100%)	47 (96%)	2 (4%)	30	61
45	O2	79/79 (100%)	79 (100%)	0	100	100
46	P2	72/72 (100%)	72 (100%)	0	100	100
47	Q2	95/95 (100%)	94 (99%)	1 (1%)	73	85
48	R2	55/55 (100%)	53 (96%)	2 (4%)	35	63
49	S2	67/67 (100%)	63 (94%)	4 (6%)	19	49
50	T2	76/76 (100%)	75 (99%)	1 (1%)	69	82
51	U2	20/20 (100%)	19 (95%)	1 (5%)	24	55
52	V2	103/103 (100%)	98 (95%)	5 (5%)	25	56
All	All	4840/4840 (100%)	4743 (98%)	97 (2%)	57	76

5 of 97 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
26	b1	44	ARG
34	D2	49	ARG
27	c1	1	MET
32	B2	25	ASN
41	K2	18	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

Mol	Chain	Res	Type
22	X1	47	ASN
52	V2	107	GLN
32	B2	113	HIS
52	V2	2	ASN
48	R2	36	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
29	A1	2911/2912 (99%)	950 (32%)	25 (0%)
30	B1	121/122 (99%)	29 (23%)	0
53	A2	1505/1506 (99%)	522 (34%)	23 (1%)
All	All	4537/4540 (99%)	1501 (33%)	48 (1%)

5 of 1501 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
29	A1	2	G
29	A1	3	U
29	A1	4	C
29	A1	10	G
29	A1	15	G

5 of 48 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
53	A2	241	A
53	A2	890	A
53	A2	261	G
53	A2	562	G
53	A2	959	U

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C1	1
25	a1	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C1	239:ARG	C	240:ALA	N	1.18
1	a1	32:PRO	C	33:CYS	N	1.17

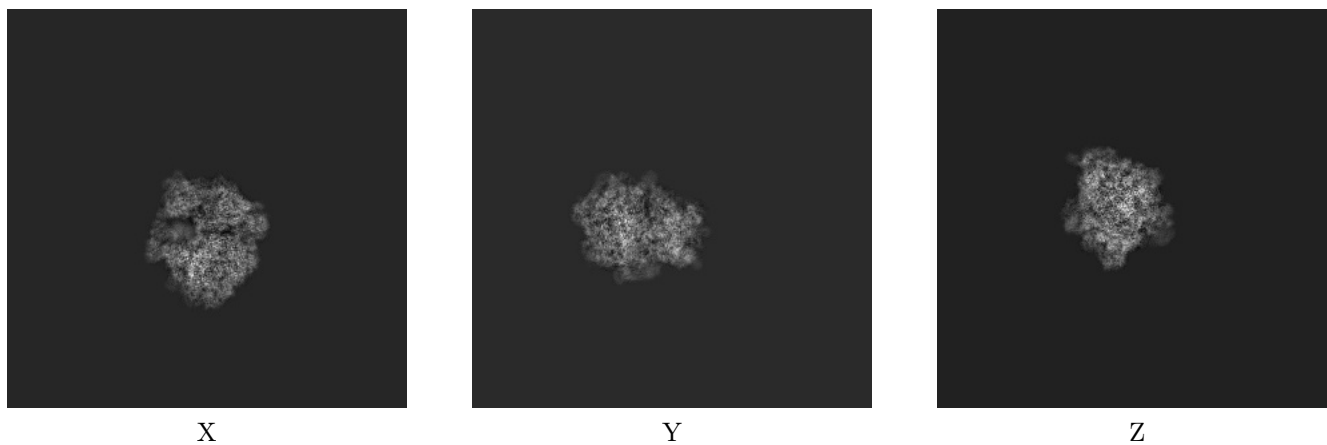
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0101. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections [i](#)

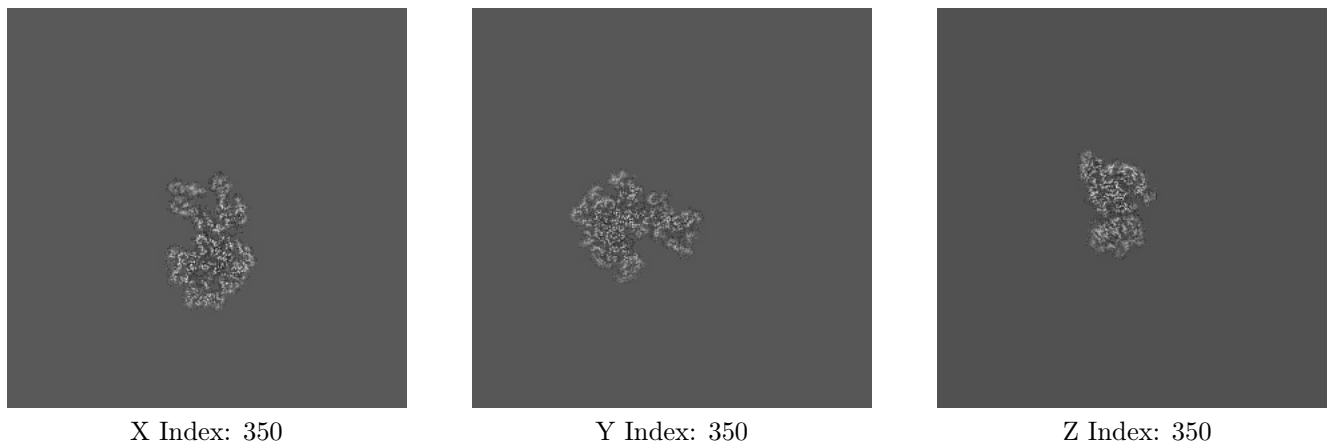
6.1.1 Primary map



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

6.2 Central slices [i](#)

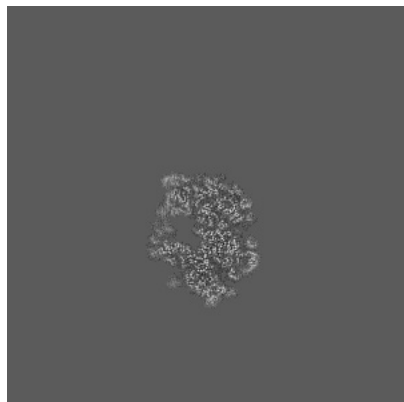
6.2.1 Primary map



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

6.3 Largest variance slices [i](#)

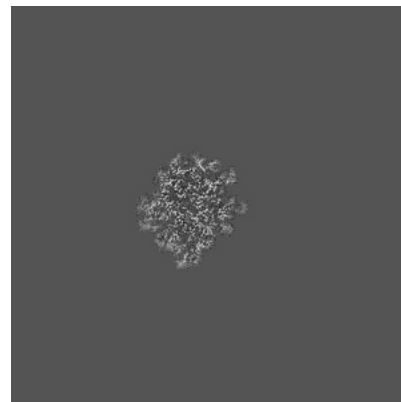
6.3.1 Primary map



X Index: 328



Y Index: 372



Z Index: 268

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 3.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

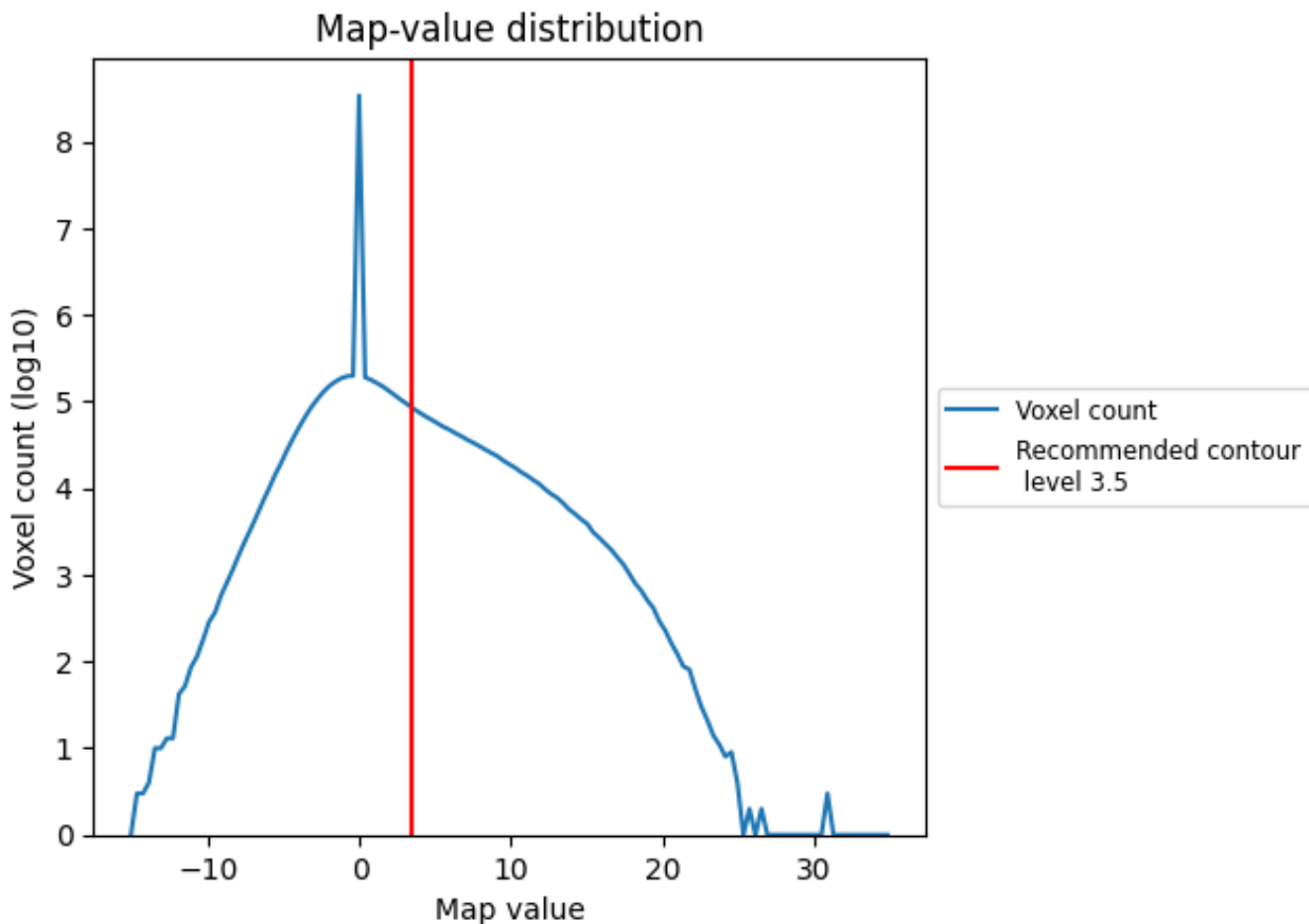
6.5 Mask visualisation

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

7 Map analysis [i](#)

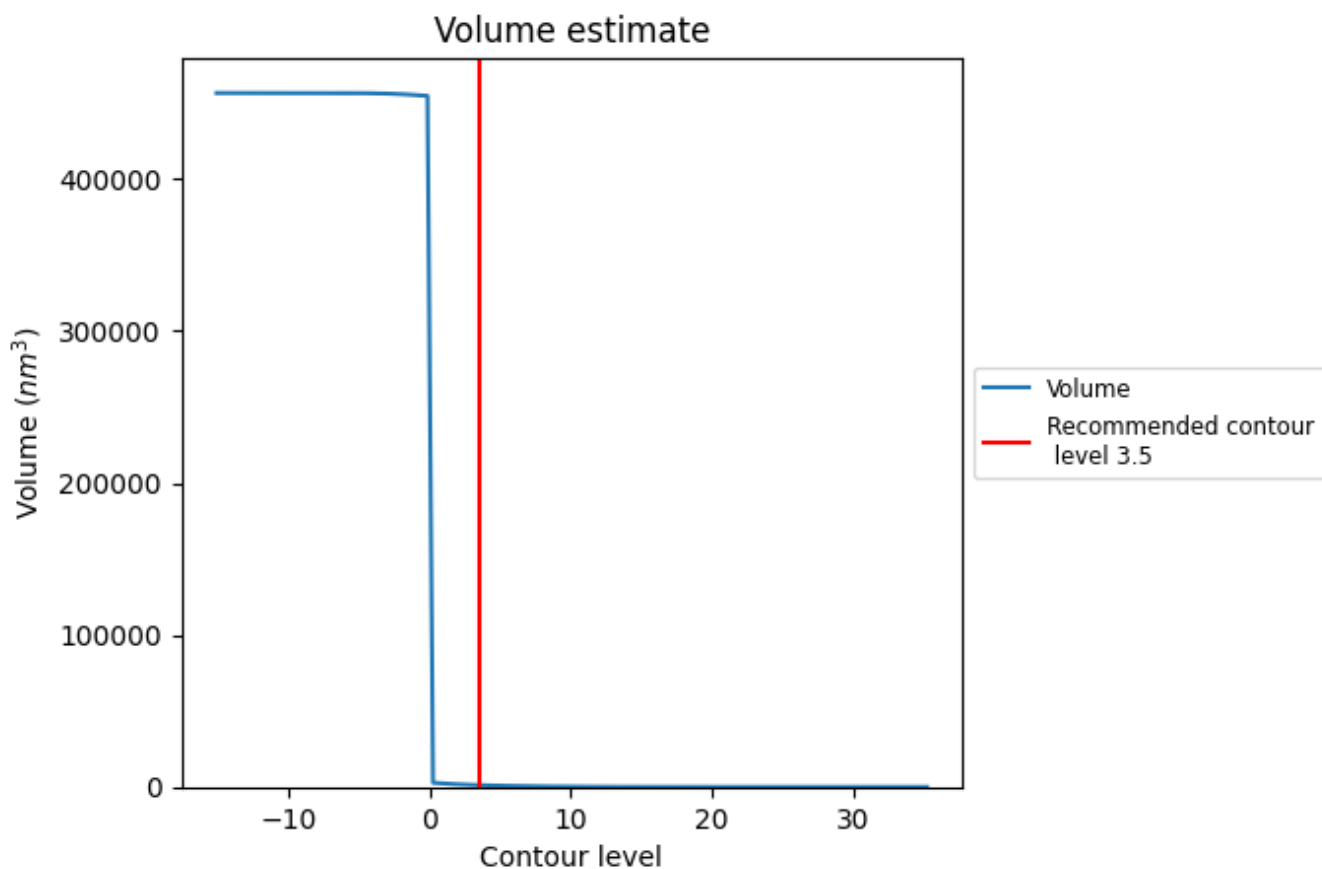
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

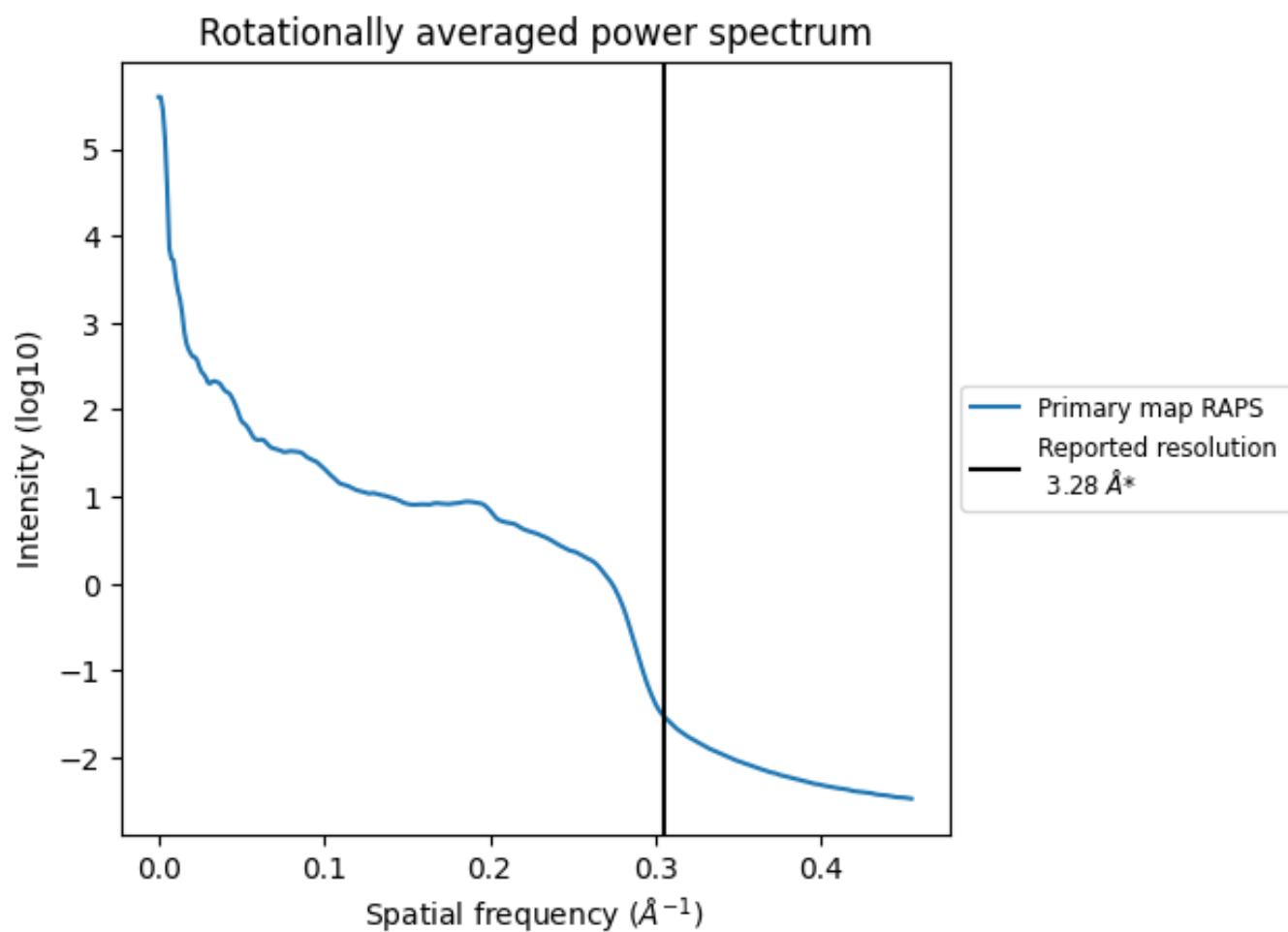
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1192 nm³; this corresponds to an approximate mass of 1077 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 0.305 Å⁻¹

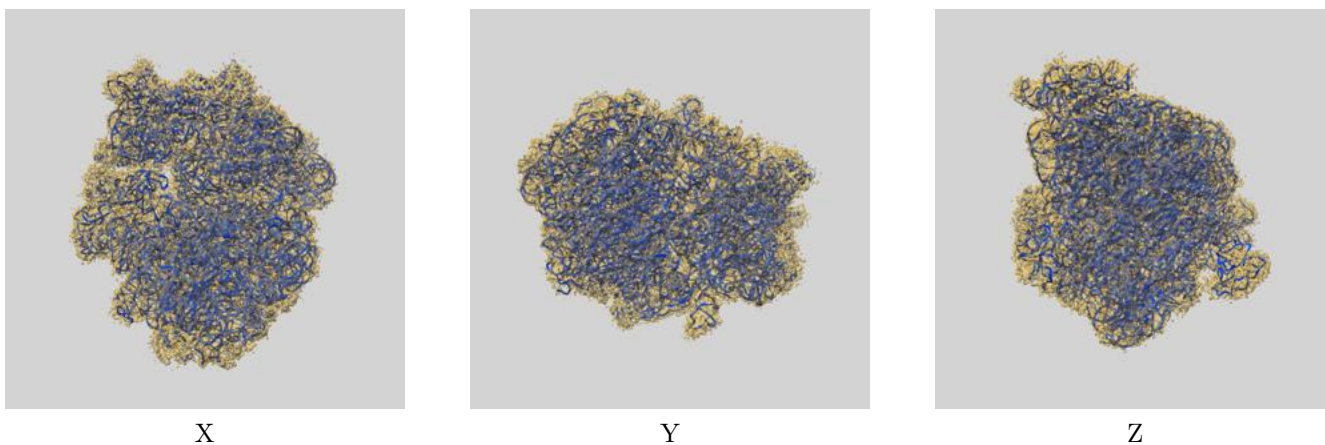
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

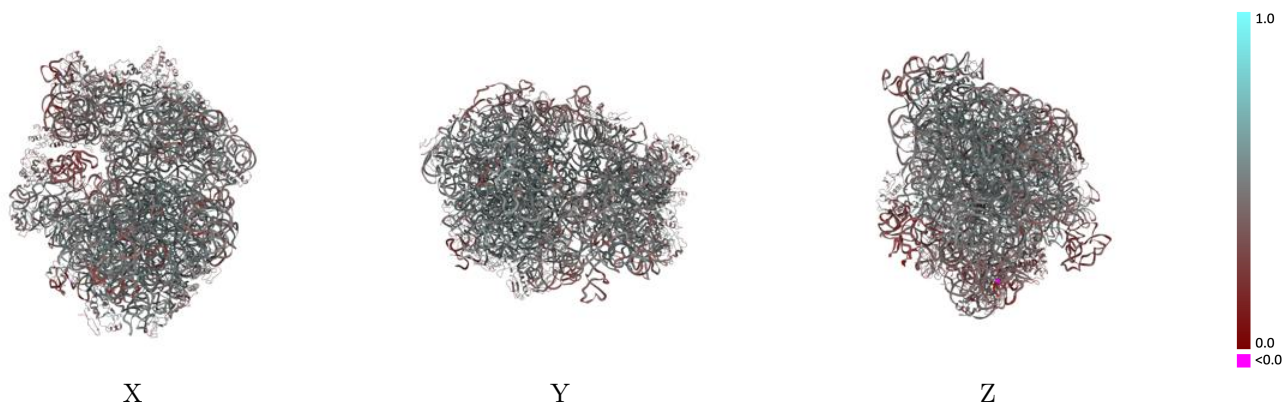
This section contains information regarding the fit between EMDB map EMD-0101 and PDB model 6GZQ. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay [i](#)



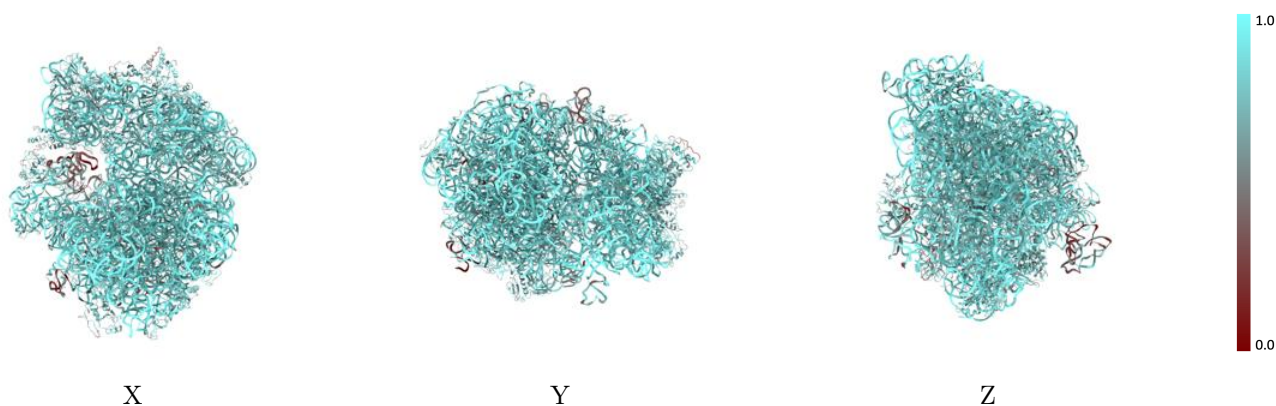
The images above show the 3D surface view of the map at the recommended contour level 3.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



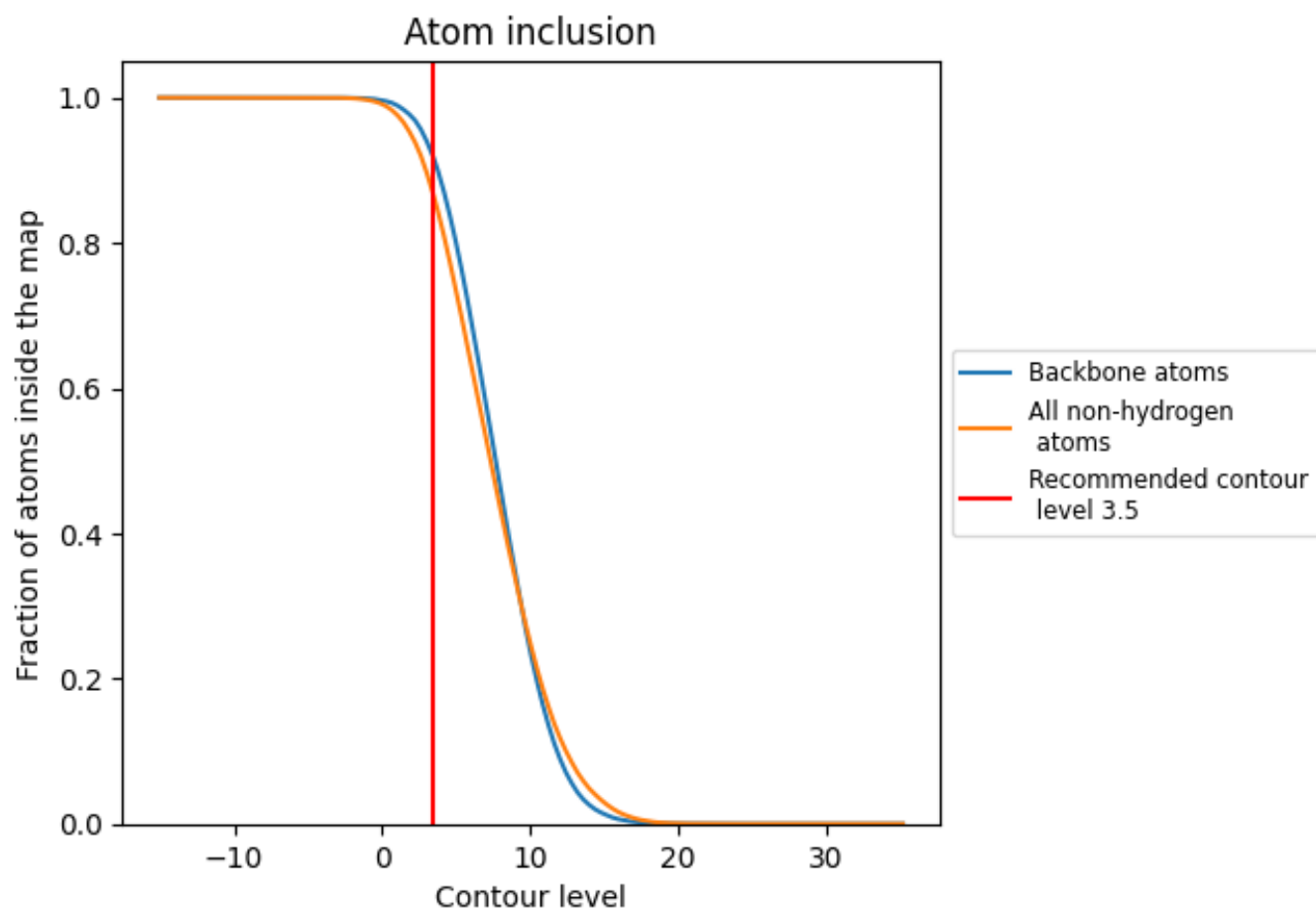
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3.5).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 86% 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 (3.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8646	 0.4640
A1	 0.9052	 0.4790
A2	 0.9268	 0.4550
B1	 0.9297	 0.4520
B2	 0.6967	 0.4040
C1	 0.8137	 0.5040
C2	 0.7503	 0.4450
D1	 0.8051	 0.4980
D2	 0.8103	 0.4570
E1	 0.7647	 0.4720
E2	 0.7788	 0.4800
F1	 0.7491	 0.4030
F2	 0.7380	 0.4110
G1	 0.7463	 0.4010
G2	 0.7119	 0.3950
H1	 0.6587	 0.4060
H2	 0.8223	 0.4730
I1	 0.7816	 0.4870
I2	 0.6852	 0.3770
J1	 0.7684	 0.4970
J2	 0.7198	 0.4080
K1	 0.7656	 0.4600
K2	 0.7970	 0.4540
L1	 0.7770	 0.4840
L2	 0.7709	 0.4770
M1	 0.8107	 0.5090
M2	 0.6891	 0.3530
N1	 0.8208	 0.4530
N2	 0.7773	 0.4590
O1	 0.7546	 0.4570
O2	 0.7952	 0.4560
P1	 0.8308	 0.4940
P2	 0.8321	 0.4910
Q1	 0.7795	 0.4640
Q2	 0.7908	 0.4740



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Chain	Atom inclusion	Q-score
R1	 0.7820	 0.4920
R2	 0.7389	 0.4300
S1	 0.8073	 0.4910
S2	 0.7234	 0.3600
T1	 0.7464	 0.4220
T2	 0.7591	 0.4450
U1	 0.5794	 0.4000
U2	 0.7463	 0.3720
V1	 0.8256	 0.5000
V2	 0.6811	 0.4230
W1	 0.7368	 0.4740
X1	 0.7629	 0.4220
Y1	 0.7675	 0.4790
Z1	 0.6420	 0.3110
a1	 0.7852	 0.4540
b1	 0.7520	 0.3760
c1	 0.7789	 0.5200
d1	 0.7552	 0.4690
e1	 0.8182	 0.5080