



wwPDB EM Validation Summary Report ⓘ

Mar 25, 2026 – 10:56 AM UTC

PDB ID : 5KPS / pdb_00005kps
EMDB ID : EMD-8279
Title : Structure of RelA bound to ribosome in absence of A/R tRNA (Structure I)
Authors : Loveland, A.B.; Bah, E.; Madireddy, R.; Zhang, Y.; Brilot, A.F.; Grigorieff, N.; Korostelev, A.A.
Deposited on : 2016-07-05
Resolution : 3.90 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:

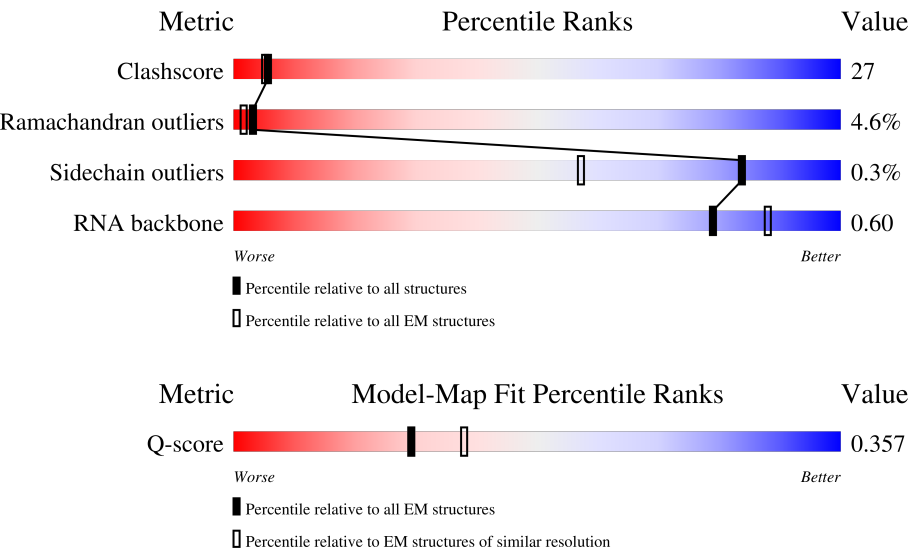
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.90 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.



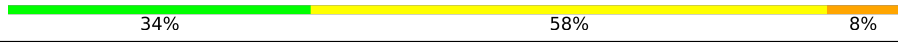
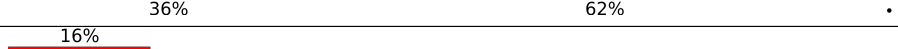
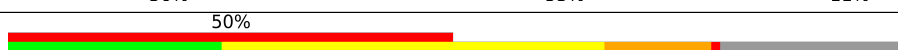
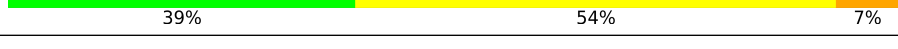
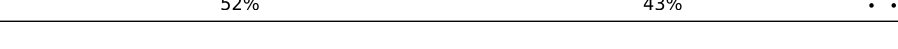
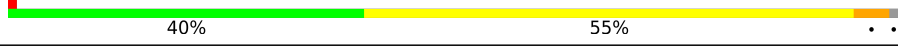
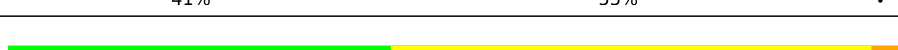
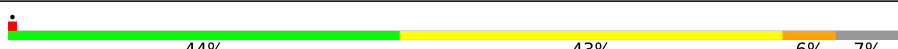
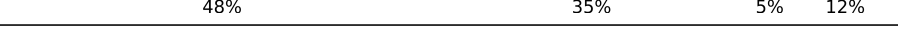
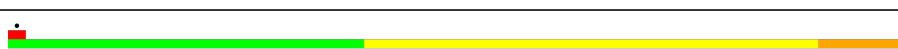
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	8855 (3.40 - 4.40)

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	A	750	
2	B	273	
3	C	209	

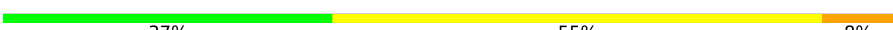
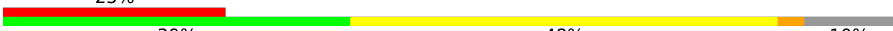
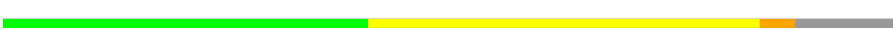
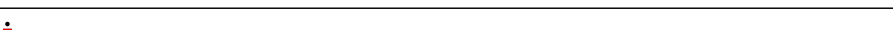
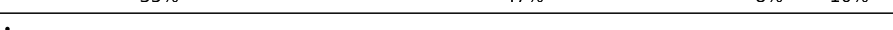
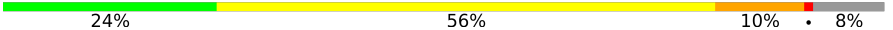
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Mol	Chain	Length	Quality of chain
4	D	201	
5	E	179	
6	F	177	
7	G	149	
8	H	165	
9	I	142	
10	J	142	
11	K	123	
12	L	144	
13	M	136	
14	N	127	
15	O	117	
16	P	115	
17	Q	118	
18	R	103	
19	S	110	
20	T	100	
21	U	104	
22	V	94	
23	W	85	
24	X	78	
25	Y	63	
26	Z	59	
27	1	70	
28	2	57	

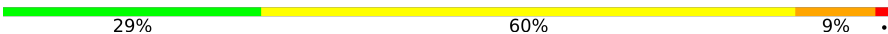
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Mol	Chain	Length	Quality of chain
29	3	55	
30	4	46	
31	5	65	
32	6	38	
33	7	241	
34	8	233	
35	9	206	
36	10	167	
37	11	135	
38	12	179	
39	13	130	
40	14	130	
41	15	103	
42	16	129	
43	17	124	
44	18	118	
45	19	101	
46	20	89	
47	21	82	
48	22	84	
49	23	75	
50	24	92	
51	25	87	
52	26	71	
53	27	1539	

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Mol	Chain	Length	Quality of chain
54	28	2903	 26% 63% 10%
55	29	120	 29% 60% 9% •
56	30	18	 11% 44% 44% 1%
57	31	77	 45% 55%
58	32	77	 26% 55% 19%

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 149128 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 GTP pyrophosphokinase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	143	Total	C	N	O	S	0	0
			1103	685	209	204	5		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	expression tag	UNP P0AG20
A	-4	HIS	-	expression tag	UNP P0AG20
A	-3	HIS	-	expression tag	UNP P0AG20
A	-2	HIS	-	expression tag	UNP P0AG20
A	-1	HIS	-	expression tag	UNP P0AG20
A	0	HIS	-	expression tag	UNP P0AG20
A	1	HIS	-	expression tag	UNP P0AG20

- Molecule 2 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 3 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 4 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 5 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 6 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 7 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 8 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	131	Total	C	N	O	S	0	0
			988	625	175	183	5		

- Molecule 9 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 10 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 11 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 12 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 13 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 14 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 15 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	O	116	Total	C	N	O	0	0
			892	552	178	162		

- Molecule 16 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 17 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	Q	117	Total	C	N	O	0	0
			947	604	192	151		

- Molecule 18 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 19 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 20 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 21 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	102	Total	C	N	O		0	0
			779	492	146	141			

- Molecule 22 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 23 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	75	Total	C	N	O	S	0	0
			575	356	116	102	1		

- Molecule 24 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 25 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 26 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 27 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	1	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

- Molecule 28 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	2	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 29 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	3	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 30 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	4	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 31 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	5	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 32 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	6	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 33 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	7	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- Molecule 34 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	8	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 35 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	9	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 36 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	10	157	Total	C	N	O	S	0	0
			1156	719	218	213	6		

- Molecule 37 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	11	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

- Molecule 38 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	12	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 39 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	13	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 40 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	14	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 41 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	15	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 42 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	16	116	Total	C	N	O	S	0	0
			869	535	173	158	3		

- Molecule 43 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	17	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 44 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	18	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

- Molecule 45 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	19	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 46 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	20	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 47 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	21	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 48 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	22	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 49 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	23	65	Total	C	N	O	S	0	0
			535	339	100	95	1		

- Molecule 50 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	24	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

- Molecule 51 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	25	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 52 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	26	65	Total	C	N	O	S	0	0
			544	335	117	91	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
53	27	1539	Total	C	N	O	P	0	0
			33016	14725	6052	10700	1539		

- Molecule 54 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	28	2903	Total	C	N	O	P	0	0
			62322	27801	11468	20150	2903		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
28	747	C	U	conflict	GB 802133627
28	1847	G	A	conflict	GB 802133627

- Molecule 55 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	29	120	Total	C	N	O	P	0	0
			2572	1145	471	836	120		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
29	120	A	-	conflict	GB 1028475309

- Molecule 56 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	30	18	Total	C	N	O	P	0	0
			388	175	76	120	17		

- Molecule 57 is a RNA chain called P site tRNA^fmet.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	31	77	Total	C	N	O	P	0	0
			1644	732	297	538	77		

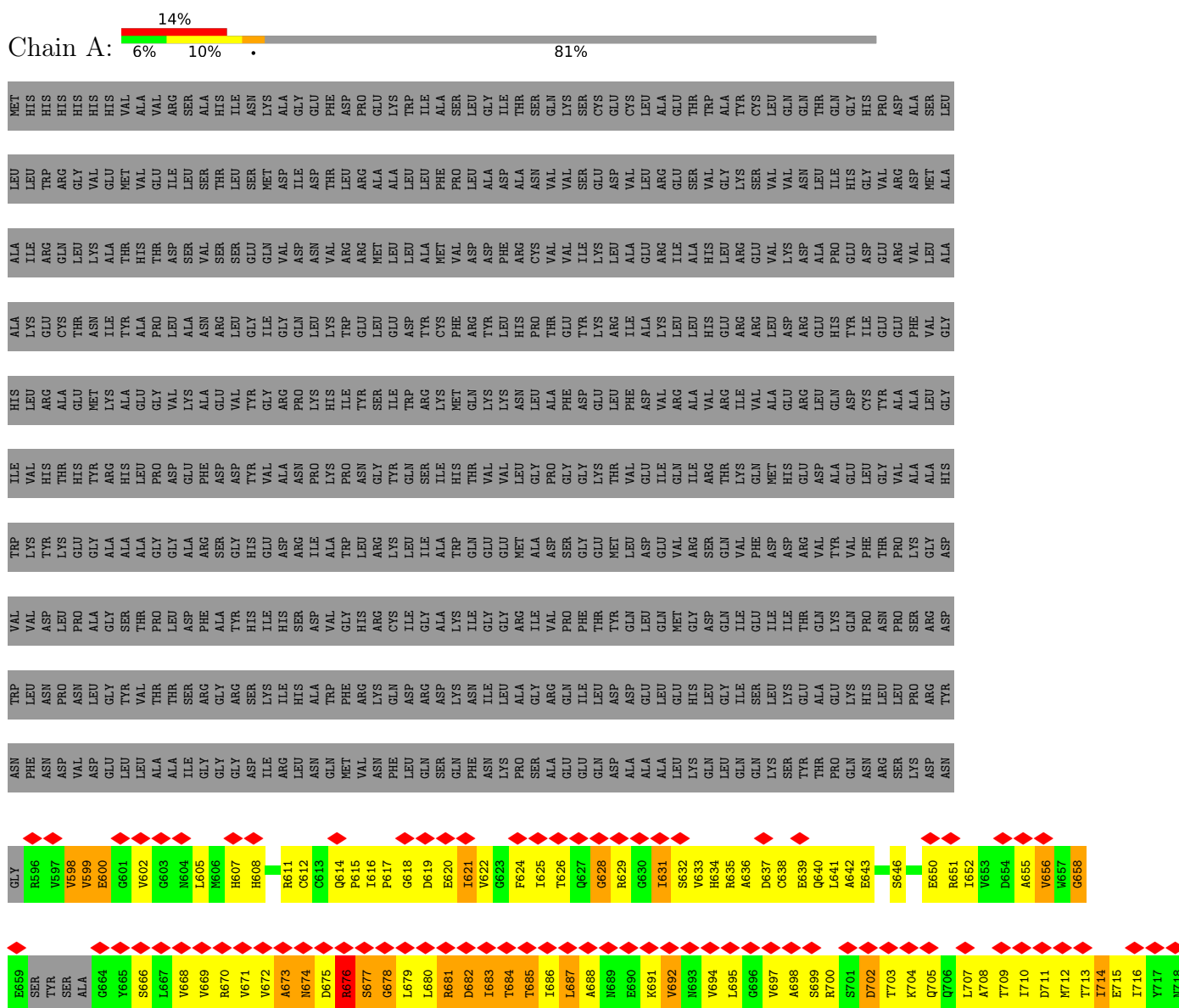
- Molecule 58 is a RNA chain called E-site tRNA^fMet.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	32	77	Total	C	N	O	P	0	0
			1643	732	297	537	77		

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.

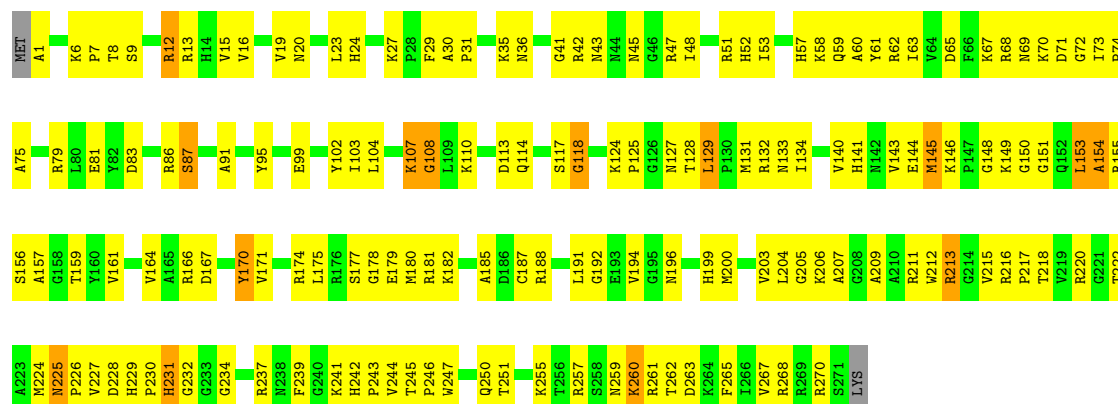
• Molecule 1: GTP pyrophosphokinase





• Molecule 2: 50S ribosomal protein L2

Chain B: 41% 53% 5%



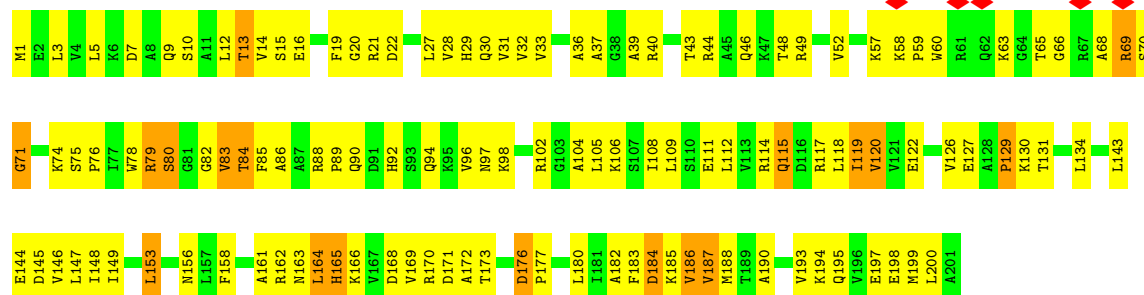
• Molecule 3: 50S ribosomal protein L3

Chain C: 49% 45% 5%



• Molecule 4: 50S ribosomal protein L4

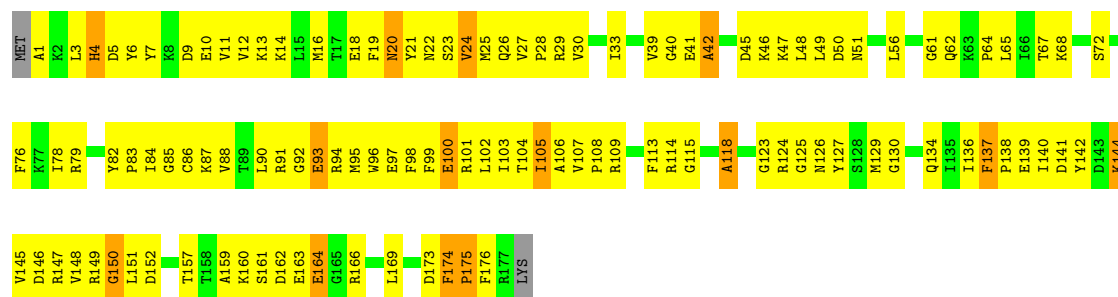
Chain D: 39% 52% 9%



• Molecule 5: 50S ribosomal protein L5

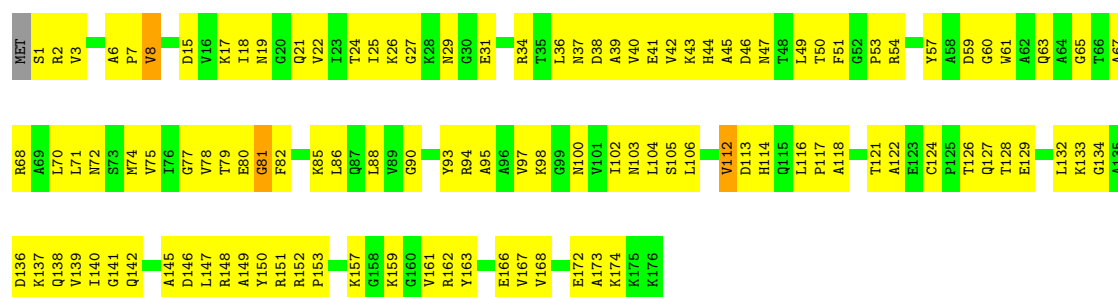
Chain E: 34% 58% 8%





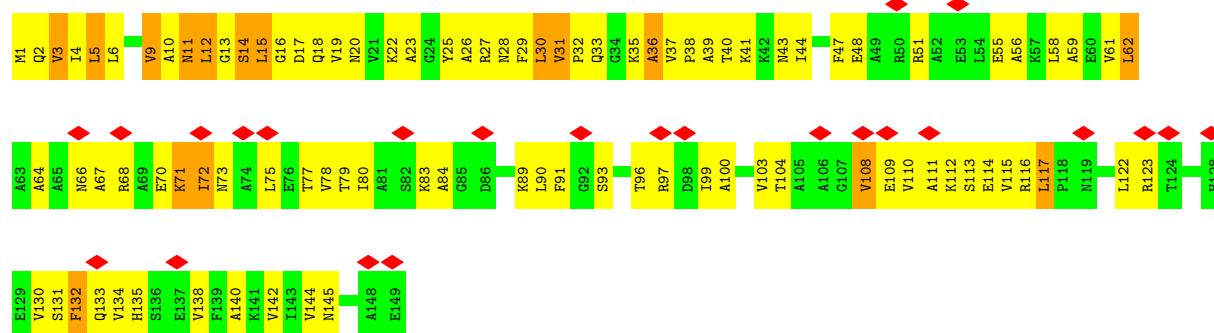
• Molecule 6: 50S ribosomal protein L6

Chain F: 36% 62% ..



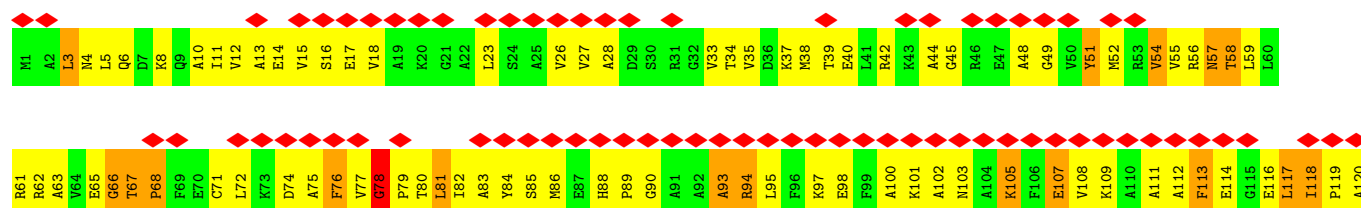
• Molecule 7: 50S ribosomal protein L9

Chain G: 16% 36% 53% 11%



• Molecule 8: 50S ribosomal protein L10

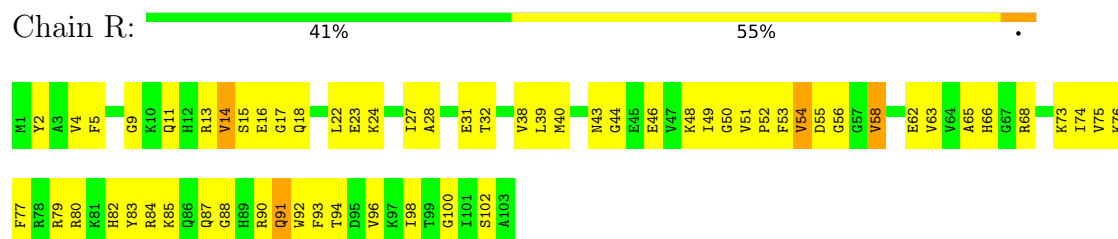
Chain H: 24% 50% 43% 12% 21%



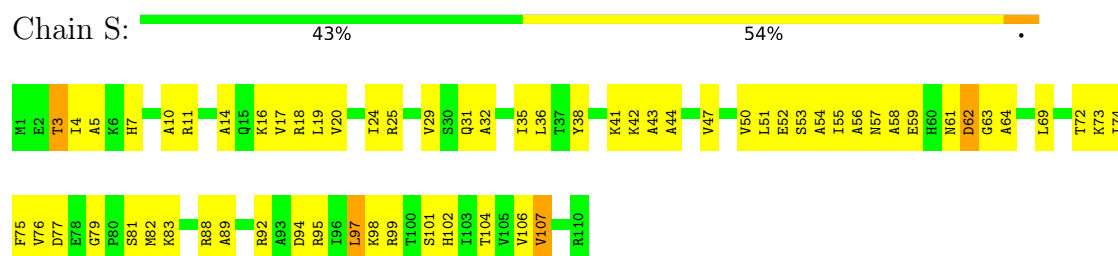
Chain M:  57% 40%



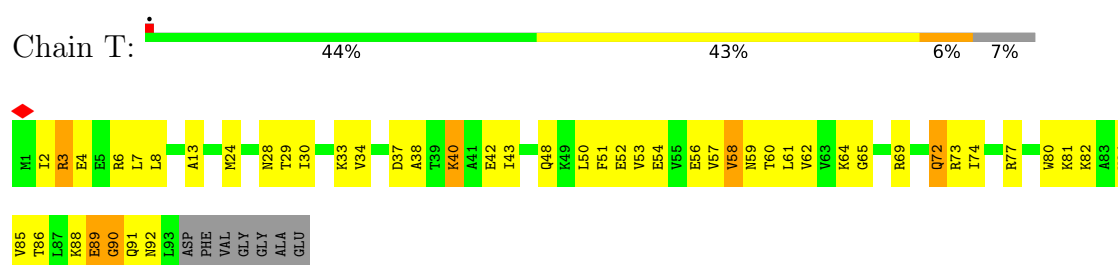
- Molecule 18: 50S ribosomal protein L21



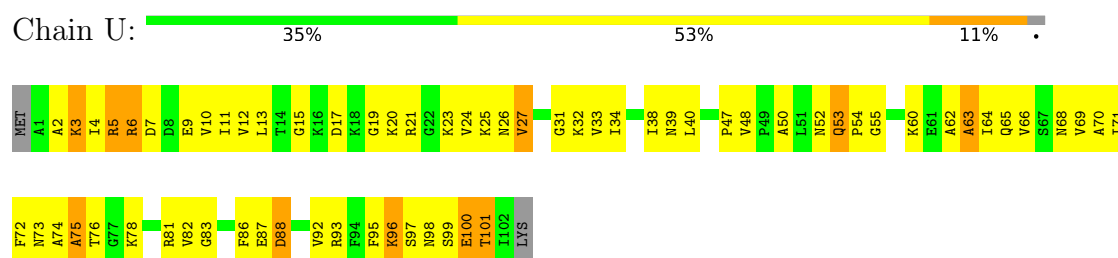
- Molecule 19: 50S ribosomal protein L22



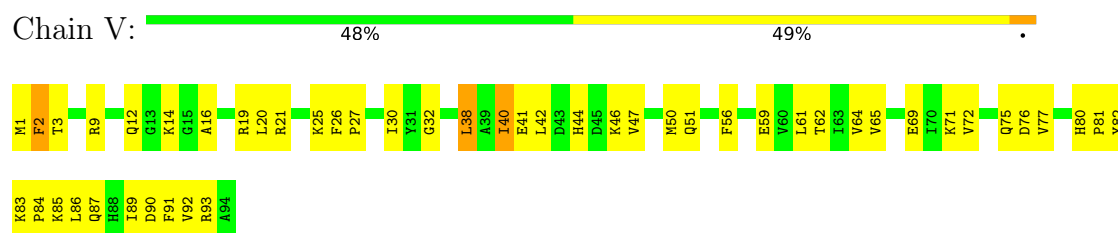
- Molecule 20: 50S ribosomal protein L23



- Molecule 21: 50S ribosomal protein L24

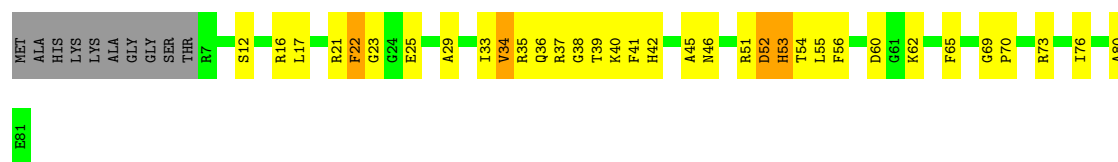


- Molecule 22: 50S ribosomal protein L25

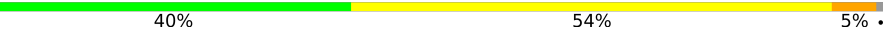


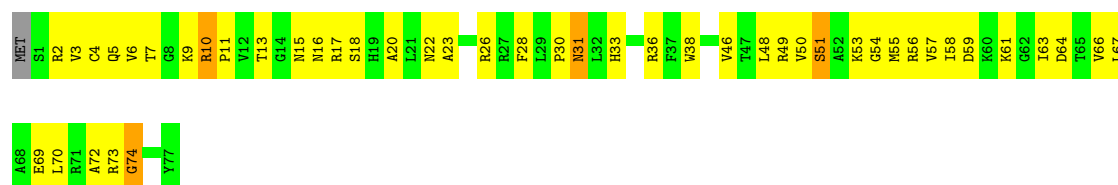
- Molecule 23: 50S ribosomal protein L27

Chain W: 

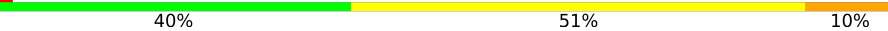


- Molecule 24: 50S ribosomal protein L28

Chain X: 



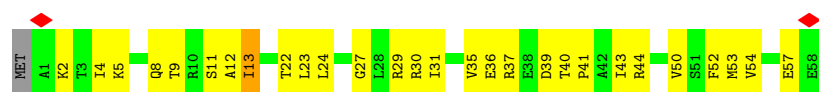
- Molecule 25: 50S ribosomal protein L29

Chain Y: 

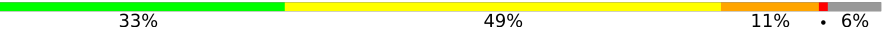


- Molecule 26: 50S ribosomal protein L30

Chain Z: 



- Molecule 27: 50S ribosomal protein L31

Chain 1: 



- Molecule 28: 50S ribosomal protein L32

Chain 2: 



- Molecule 29: 50S ribosomal protein L33

Chain 3:  51% 36% 9%



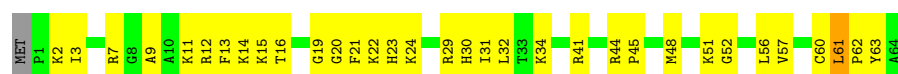
- Molecule 30: 50S ribosomal protein L34

Chain 4:  50% 41% 7%



- Molecule 31: 50S ribosomal protein L35

Chain 5:  48% 49%



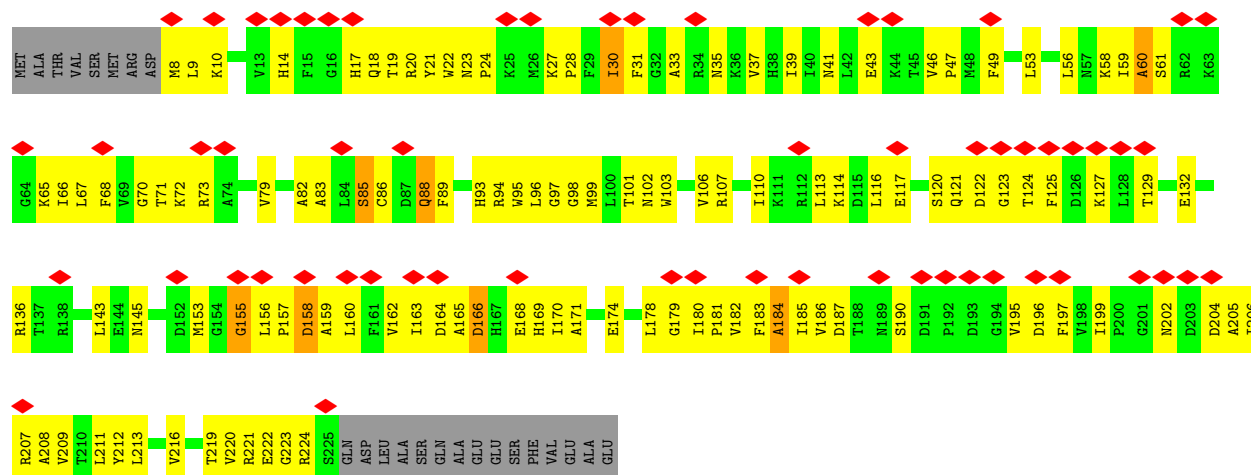
- Molecule 32: 50S ribosomal protein L36

Chain 6:  37% 55% 8%



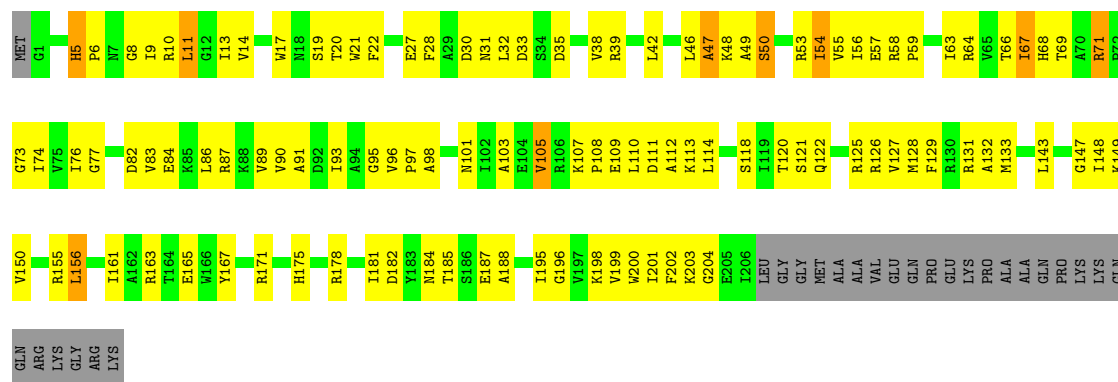
- Molecule 33: 30S ribosomal protein S2

Chain 7:  25% 39% 48% 10%

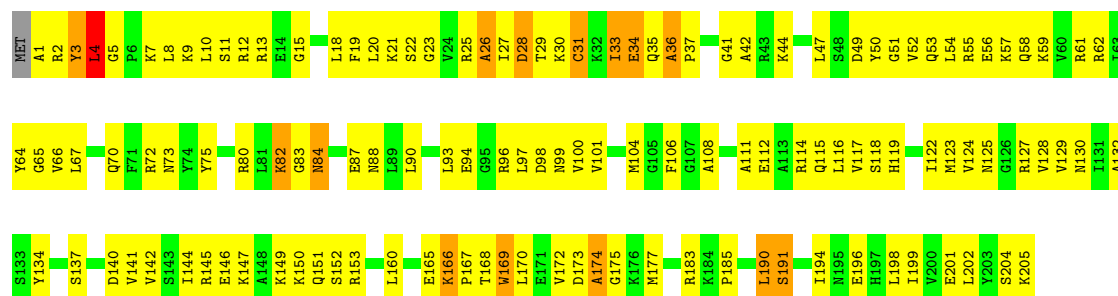


- Molecule 34: 30S ribosomal protein S3

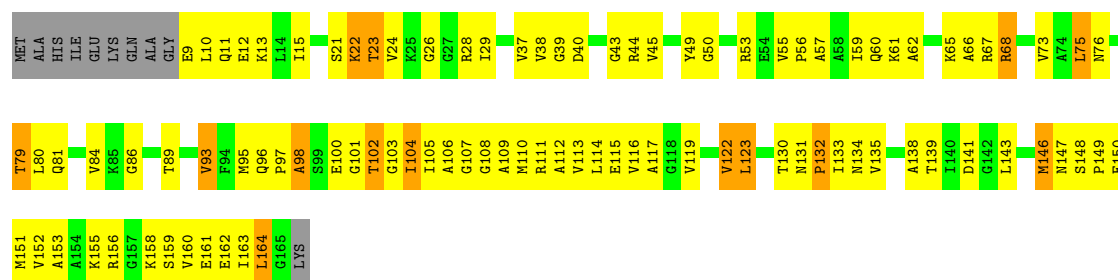
Chain 8:  41% 44% 12%



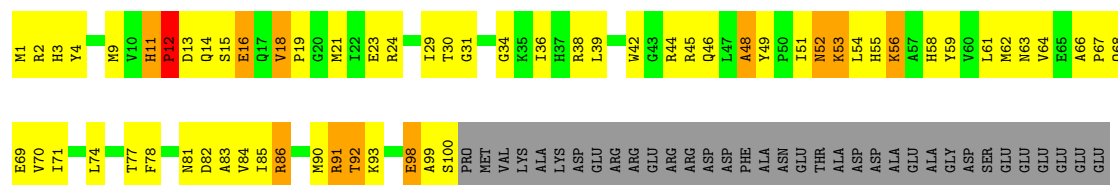
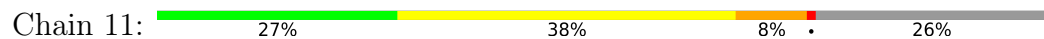
• Molecule 35: 30S ribosomal protein S4



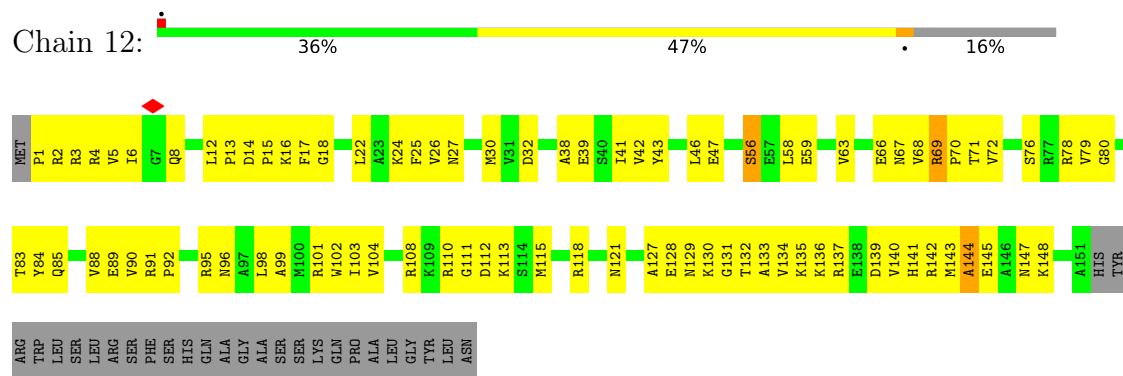
• Molecule 36: 30S ribosomal protein S5



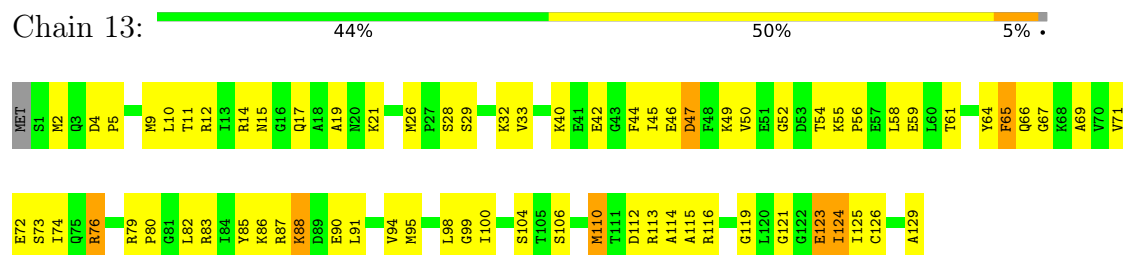
• Molecule 37: 30S ribosomal protein S6



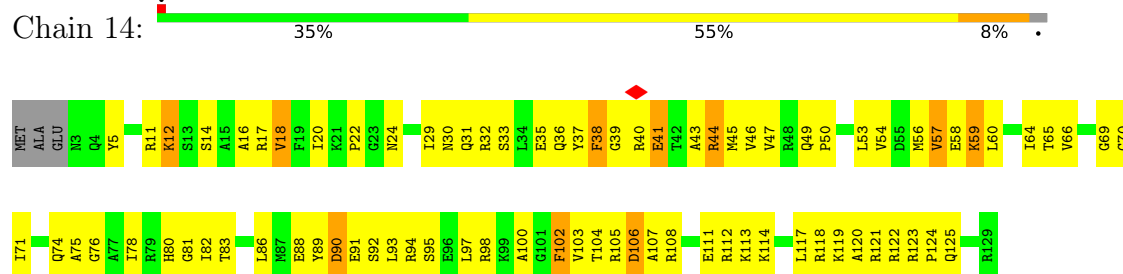
• Molecule 38: 30S ribosomal protein S7



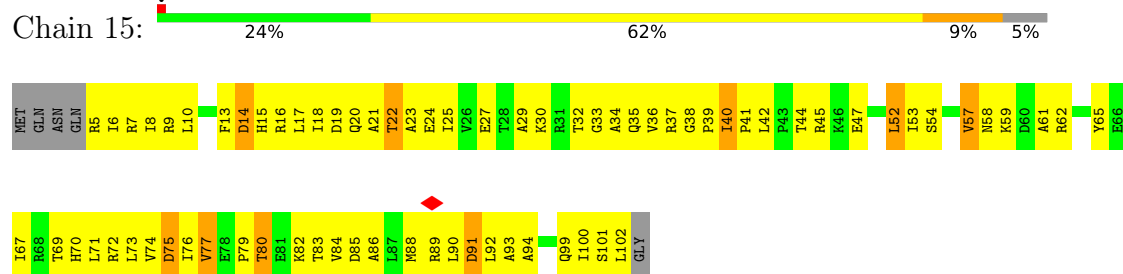
• Molecule 39: 30S ribosomal protein S8



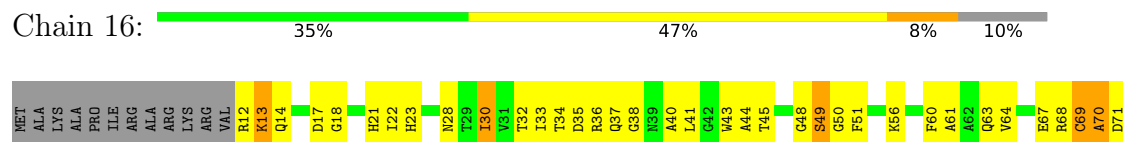
• Molecule 40: 30S ribosomal protein S9

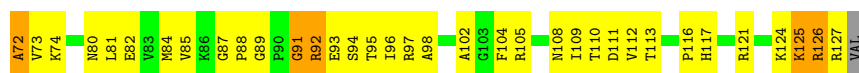


• Molecule 41: 30S ribosomal protein S10



• Molecule 42: 30S ribosomal protein S11

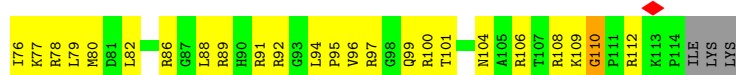
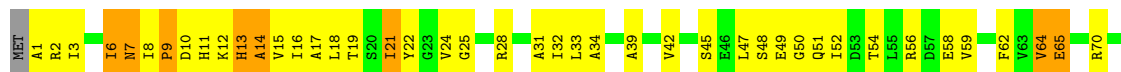




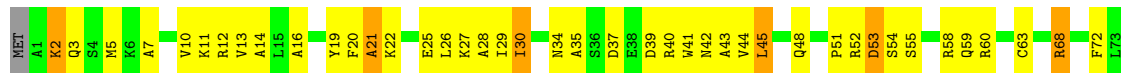
• Molecule 43: 30S ribosomal protein S12



• Molecule 44: 30S ribosomal protein S13



• Molecule 45: 30S ribosomal protein S14

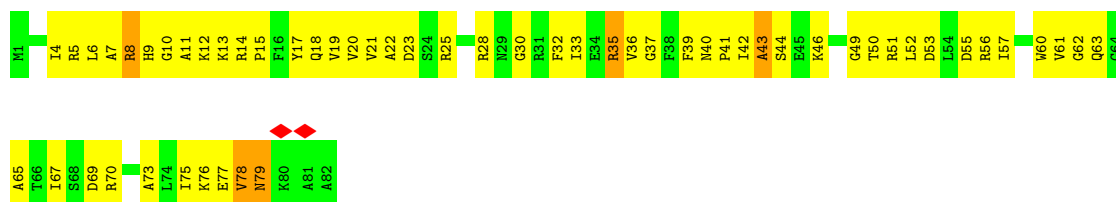


• Molecule 46: 30S ribosomal protein S15



• Molecule 47: 30S ribosomal protein S16





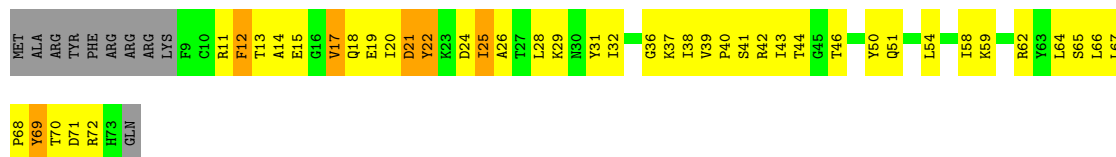
• Molecule 48: 30S ribosomal protein S17

Chain 22: 35% 55% 6% 5%



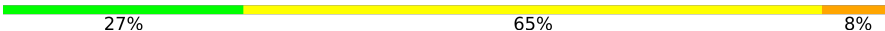
• Molecule 49: 30S ribosomal protein S18

Chain 23: 29% 49% 8% 13%

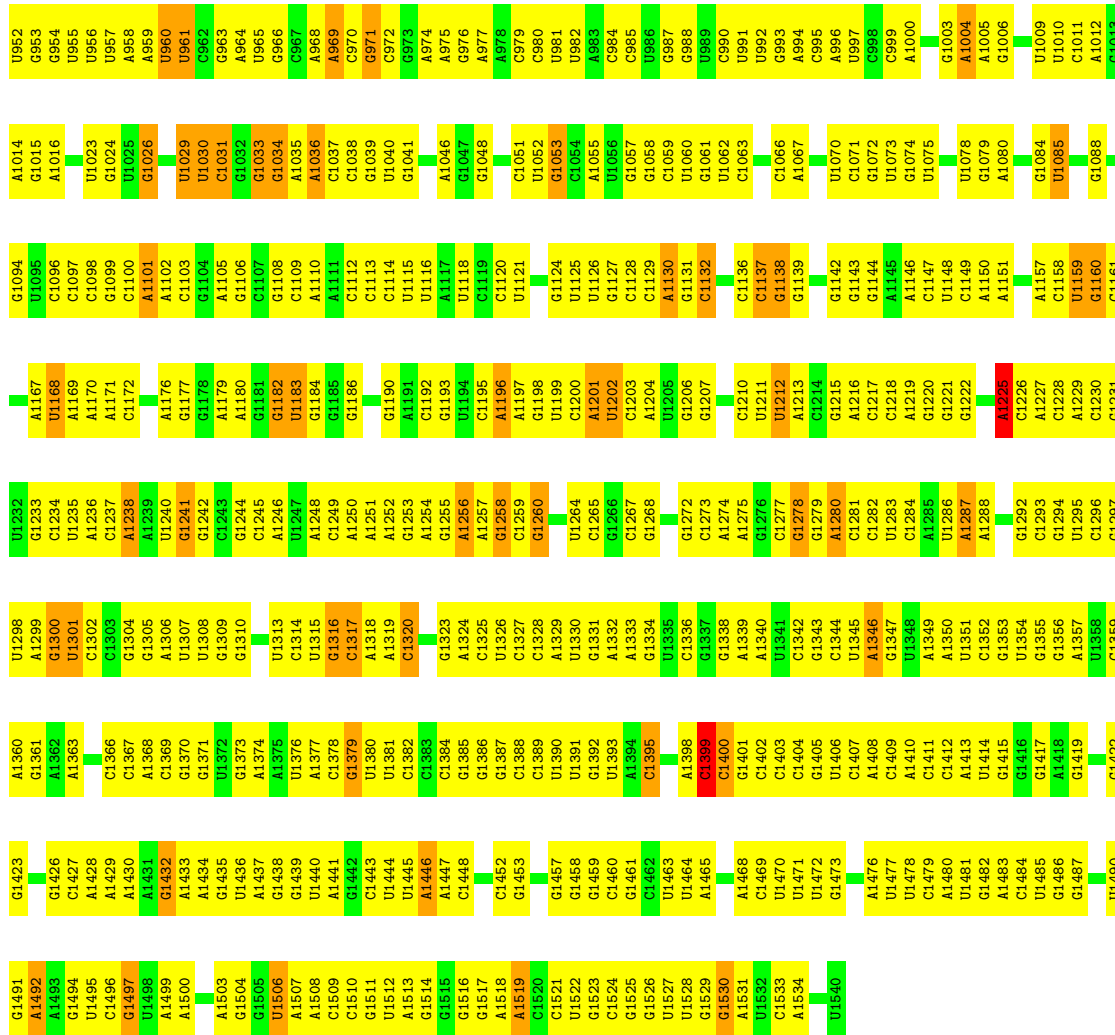


T67
ARG
LEU
TYR

• Molecule 53: 16S ribosomal RNA

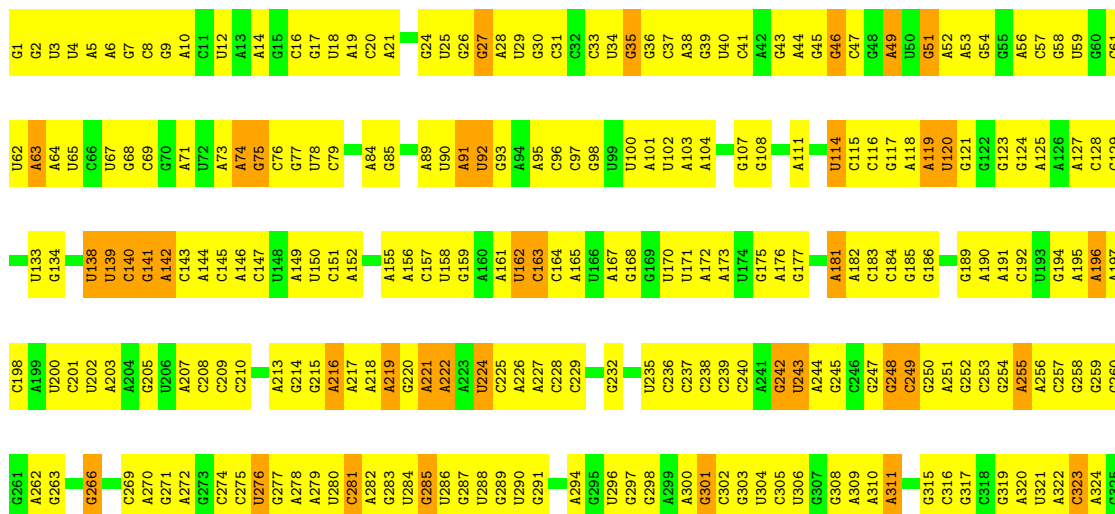
Chain 27:  27% 65% 8%

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A815	A816	A817	A818	U820	U821	U822	G824	G825	G826	U827			G833	U834	U835	U836	U837	G838	C839	C840	C841	U842	U843	U844	A845	G846	G847	C848		C856	C857	G858	C859	A860	G861	C862	U863	A864	A865	C866		C867	U868	U869	U870	U871	A872	A873	C874	U875	C876	G877	A878	C879	C880	G881	C882	A883	U884																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
G752	G753	G754	G755	C756	U757	C758	U759	G760	G761	U762	G763	G764	G765	A766	A767	U768	G769	C770	G771	C772	G773	G774	G775	G776	A777	G778	C779	A780	G781	A782	C783	U784	G785	G786	A787	U788	U789		U793	A794			C797	U798	G799	G800	U801	A802	G803	U804	C805	C806	A807	C808	G809	C810	C811	G812	U813	A814																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
U884	G885	U886	A887	G888	C889	G890	G891	U892	G893	A894	A895	A896	U901	A902	A903	G904	U905	A906	A907	C908	C909	G910	A911	U912		A915	U916	G917	A918	A919	U920	U921	G922	A923	C924	G925	G926	G927	G928	G929	C932	G933	C934	A935	C936	A937	A938	G939	C940	G941	G945	A946	G947	C948	A949	U950																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
C545	A546	A547	G548	C549	G550	U551	U552	A553	A554	U555	C556		G494	A495	A496	U497	A498	A499	G500	C501	A502	C503	C504		U434	A435	C436	U437	U438	A448	G449	C450	A451	A452	G453	G454	G455	A456	G457	U458	A459	A460	A461	G462	U463	U464	A465	A466	U467	A468		U471	U472	U473	G474	C475	U476	C477	U478	U479																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
U409	C410	A411	A412	G413	A414	A415		C418	C419	U420	U421	A422	G423	G424	A425	U426	U427	G428	U429	A430				U434	A435	C436	U437	U438	A448	G449	C450	A451	A452	G453	G454	G455	A456	G457	U458	A459	A460	A461	G462	U463	U464	A465	A466	U467	A468		U471	U472	U473	G474	C475	U476	C477	U478	U479																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
C334	C335	A336	G337	A338	C339	U340		C345	C346		C352	A353	G354	C355	A356	G357	U358	G359	G360	G361	G362	A363			U367	U368	G369	C370	A371	C372	A373	A374	U375	G376	G377		C381	A382	A383	G384		U387		U390	G391	C392	A393	G394		U398	G399	C400	C401	G402	A403	C404	U405	A406	U407	A408																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
G289	C290	A291	C292	G293	U294	C295	U296	G297	A298	G299	A300	G301		U304	C305	A306	C307	C308	A309	G310	C311	C312	A313	C314	A315	C316	U317	G318	G319	A320	A321	C322	U323	C324	G325			C328	A329	G330	C331	C332	U333		G337	A338	C339	A340	G341	C342	A343	G344	C345	A346	G347	C348	U349	A350	A351	C352	U353	A354	G355	U356	G357	C358	A359	A360	G361	U362	C363	A364	G365	U366	C367	G368	A369	A370	G371	C372	A373	A374	U375	G376	G377	C378	A379	U380	A381	A382	C383	G384	U385	A386	U387	A388	C389	U390	G391	C392	A393	G394		U398	G399	C400	C401	G402	A403	C404	U405	A406	U407	A408	C409	U410	G411	C412	A413	U414	G415	A416	U417	A418	C419	A420	G421	C422	U423	U424	A425	U426	C427	A428	U429	C430	A431	C432	U433	A434	U435	C436	U437	U438	A439	A440	C441	A442	U443	G444	C445	A446	U447	A448	C449	U450	G451	C452	A453	U454	G455	A456	U457	C458	A459	A460	U461	C462	A463	U464	G465	C466	A467	U468	C469	U470	A471	C472	A473	U474	G475	A476	C477	A478	U479	C480	A481	C482	U483	A484	C485	U486	A487	C488	U489	A490	C491	U492	A493	C494	U495	A496	C497	U498	A499	C500	U501	A502	C503	U504	A505	C506	U507	A508	C509	U510	A511	C512	U513	A514	C515	U516	A517	C518	U519	A520	C521	U522	A523	U524	C525	U526	A527	C528	A529	A530	U531	C532	A533	U534	G535	A536	C537	U538	A539	U540	C541	A542	U543	G544	C545	A546	U547	A548	C549	U550	A551	C552	U553	A554	C555	U556	A557	C558	U559	A560	C561	U562	A563	C564	U565	A566	C567	U568	A569	C570	U571	A572	C573	U574	A575	C576	U577	A578	C579	U580	A581	C582	U583	A584	C585	U586	A587	C588	U589	A590	C591	U592	A593	C594	U595	A596	C597	U598	A599	C600	U601	A602	C603	U604	A605	C606	U607	A608	C609	U610	A611	C612	U613	A614	C615	U616	A617	C618	U619	A620	C621	U622	A623	U624	C625	U626	A627	C628	U629	A630	C631	U632	A633	C634	U635	A636	C637	U638	A639	C640	U641	A642	C643	U644	A645	C646	U647	A648	C649	U650	A651	C652	U653	A654	C655	U656	A657	C658	U659	A660	C661	U662	A663	C664	U665	A666	C667	U668	A669	C670	U671	A672	C673	U674	A675	C676	U677	A678	C679	U680	A681	C682	U683	A684	C685	U686	A687	C688	U689	A690	C691	U692	A693	C694	U695	A696	C697	U698	A699	C700	U701	A702	C703	U704	A705	C706	U707	A708	C709	U710	A711	C712	U713	A714	C715	U716	A717	C718	U719	A720	C721	U722	A723	C724	U725	A726	C727	U728	A729	C730	U731	A732	C733	U734	A735	C736	U737	A738	C739	U740	A741	C742	U743	A744	C745	U746	A747	C748	U749	A750	C751	U752	A753	C754	U755	A756	C757	U758	A759	C760	U761	A762	C763	U764	A765	C766	U767	A768	C769	U770	A771	C772	U773	A774	C775	U776	A777	C778	U779	A780	C781	U782	A783	C784	U785	A786	C787	U788	A789	C790	U791	A792	C793	U794	A795	C796	U797	A798	C799	U800	A801	C802	U803	A804	C805	U806	A807	C808	U809	A810	C811	U812	A813	C814	U815	A816	C817	U818	A819	C820	U821	A822	C823	U824	A825	C826	U827	A828	C829	U830	A831	C832	U833	A834	C835	U836	U837	A838	C839	U840	A841	C842	U843	A844	C845	U846	A847	C848	U849	A850	C851	U852	A853	C854	U855	A856	C857	U858	A859	C860	U861	A862	C863	U864	A865	C866	U867	A868	C869	U870	A871	C872	U873	A874	C875	U876	A877	C878	U879	A880	C881	U882	A883	C884	U885	A886	C887	U888	A889	C890	U891	A892	C893	U894	A895	C896	U897	A898	C899	U900	A901	C902	U903	A904	C905	U906	A907	C908	U909	A910	C911	U912	A913	C914	U915	A916	C917	U918	A919	C920	U921	A922	C923	U924	A925	C926	U927	A928	C929	U930	A931	C932	U933	A934	C935	U936	A937	C938	U939	A940	C941	U942	A943	C944	U945	A946	C947	U948	A949	C950	U951	A952	C953	U954	A955	C956	U957	A958	C959	U960	A961	C962	U963	A964	C965	U966	A967	C968	U969	A970	C971	U972	A973	C974	U975	A976	C977	U978	A979	C980	U981	A982	C983	U984	A985	C986	U987	A988	C989	U990	A991	C992	U993	A994	C995	U996	A997	C998	U999	A1000



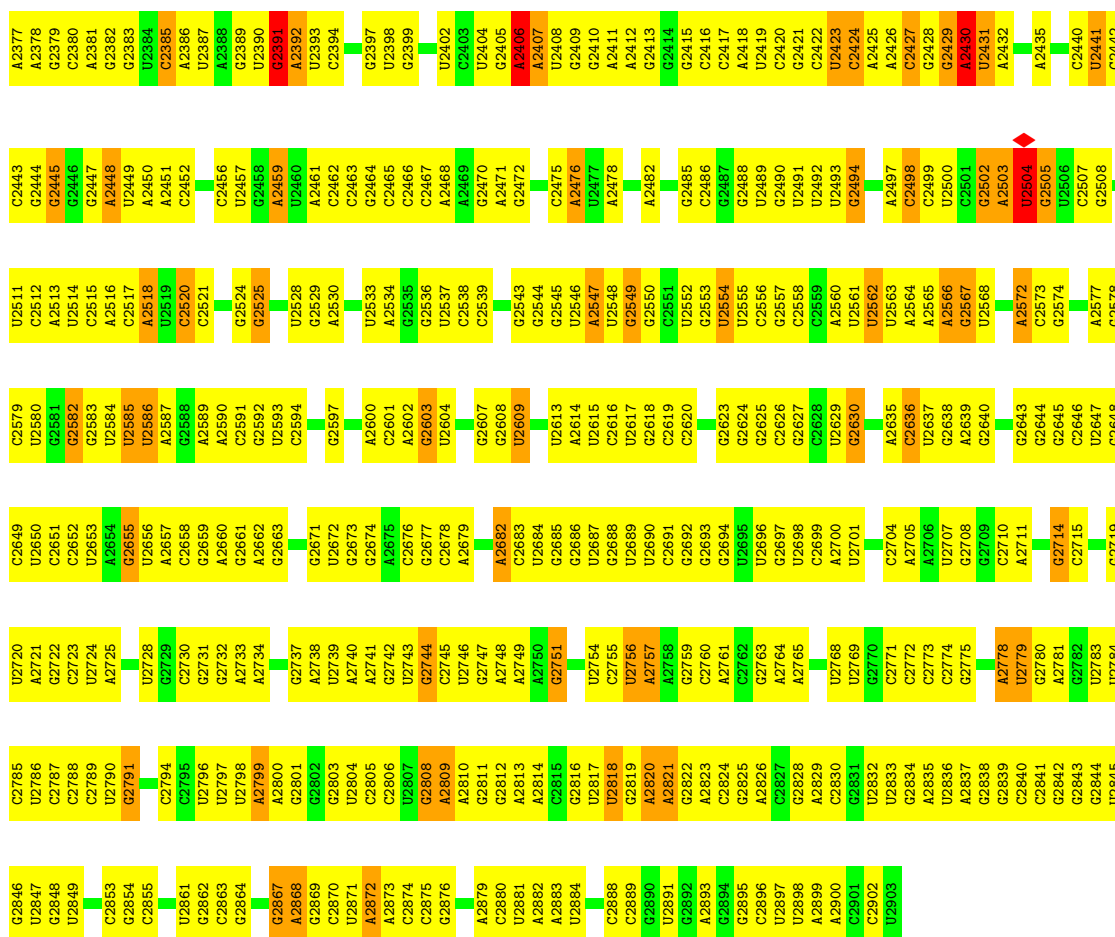
● Molecule 54: 23S ribosomal RNA

Chain 28: 26% 63% 10%



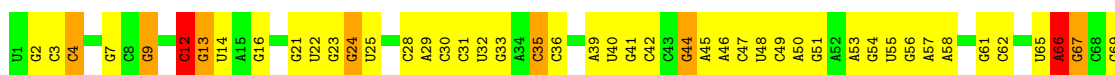


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G2318	A2247	A2183	C2044	C1973	C1907	C1833		G1703	A1632	C1564	U1487	A1420	
G2319	G2248	A2184	C2045	C1974	C1908		G1770	C1704	G1633	C1565		G1421	C1351
U2320	U2249	U2185	G2046	U1982	G1910	C1837	G1771	U1709	A1635	G1567	A1490	G1424	U1352
G2250	G2250	G2112	G2047	G1983	U1911	C1839	A1772	G1710	G1636	G1568	G1491	G1425	A1353
A2322	U2187	U2113	G2048		U1912	G1840	G1773	A1711	U1637	A1569	G1492	G1426	A1354
G2323	U2188	G2114	C2049	G1989	A1913	U1841	C1774	U1712	A1638	A1570		A1427	G1356
G2324	U2189	G2115	C2050	U1990	G1914	G1842	U1776	U1713	A1640	A1571	C1499	G1428	C1357
G2325	A2190		A2051	U1991	U1915	C1843	G1777	A1713	G1640	G1572	G1500	G1429	G1358
C2326	C2191	A2052	A2052	G1992	U1916	C1844	U1778	U1714	A1641	G1573	A1504	G1430	A1359
A2327	U2189		C2055	U1993	U1917		U1779	G1715	G1642	C1574	A1505	A1431	G1360
G2328	G2193	G2119	G2056	C1994	A1918	G1847	A1780	U1716	G1643		U1506	A1432	G1361
U2329	G2057	U1996	G2057	U1995	A1919	A1948		A1717	C1644	U1577	U1507	A1433	G1362
G2330	A2058	C1996		U1996		A1948	A1784	G1718	G1645	U1578	A1508	A1434	C1363
C2331	U2195	C1997	A2059	U1997	G1922	U1851	A1785	U1719	C1646	A1579	A1509	G1435	G1364
C2332	G2203	A1998	G2060	A1998	U1923	U1852	G1786	G1720	U1647	A1580		G1436	A1365
U2334	G2061	C1999	G2061	C1999	G1924	A1853	A1787	G1721	U1648	G1581	A1515	A1437	A1366
A2335	A2062	C2000	C2062	C2000	C1925	A1854	C1788	A1722	G1649		G1516	U1438	A1367
A2336	C2063	C2001	U2063	C2001	U1926	U1855	G1789		U1650	U1584	G1517	A1439	G1368
	U2064	A2003	G2064	A2003	A1927	G1856	A1791	C1726	G1651	C1585	U1520	U1440	G1369
C2339	G2065	G2002	C2065	G2002	A1928	U1857	C1790	C1728	A1652		G1521	G1441	C1370
A2340	G2066	G2004	G2066	G2004	G1929	A1858	A1794	U1729	G1653	U1588		U1442	G1371
G2341	G2067	A2005	G2067	A2005	G1930		C1795	C1730	A1654	A1590	G1524	U1443	U1372
C2342	U2068	C2006	U2068	C2006	U1931	U1864	C1796	G1731	A1655	A1591	A1525	G1444	A1373
U2343	G2069	U2007	G2069	U2007	A1932	U1865	U1796	G1732	U1656	C1592	A1526	G1445	
G2344	A2070	C2008	A2070	C2008	G1933	A1866	G1797	G1733	U1657	C1593	G1527	G1446	C1376
G2345	U2071	A2009	A2071	A2009	U1934	G1867	U1798		C1658	A1593	G1527	G1447	G1377
A2346	C2072	G2010	C2072	G2010	G1935		G1799	G1741	G1659	U1594	A1528	G1448	A1378
C2347	G2073	U2011	G2073	U2011	A1936	A1871	C1800	U1736	G1660	C1595	G1529	G1449	U1379
U2348	U2074	C2012	U2074	C2012	U1937	A1872	A1801	G1737	G1661	A1596	G1530	G1450	
U2349	U2075	A2013	U2075	A2013	A1938	G1873	A1802	G1738	U1662	A1597	C1531	C1451	A1383
U2350	C2078	A2014	C2078	A2014	U1939	C1874	A1803	A1739	G1663	A1598	A1532	G1452	A1384
G2351	G2217	A2015	G2217	A2015	U1940	G1875	C1804	A1746	A1664	C1599	C1533	A1453	A1385
A2352	A2147	U2016	A2147	U2016	U1943	A1876	A1805	U1747	A1665	C1600	U1534	C1454	C1386
G2353	G2148	U2017	G2148	U2017	U1943	A1877	C1806	C1748	G1666	G1601	A1535	G1455	A1387
U2354	U2149	G2018	U2149	G2018		C1878	G1807	G1743		U1602	C1536	G1463	G1388
G2355	C2150	A2019	C2150	A2019	U1946	C1879	A1808	A1744	A1669	U1603	G1537	U1458	
U2356	G2221	A2020	G2221	A2020	C1947	U1880	A1809	A1745	C1670	C1604	U1538	G1459	U1394
G2357	G2223	C2021	G2223	C2021	G1948	C1881	A1810	A1746	U1671	C1605	U1539	U1460	A1395
A2358	G2087	U2022	G2087	U2022		U1882	G1811	U1747		C1606	G1540	C1461	U1396
G2359	C2088	C2023	C2088	C2023	U1951	G1883		C1748	G1674	C1607	C1541	G1462	U1397
C2360	C2089	G2024	C2089	G2024	A1952	U1884	G1814	A1749	C1675	A1608	U1542	C1463	C1398
G2361	A2090	C2025	A2090	C2025	A1953	A1885	A1815	G1750	A1676	A1609	G1543	G1464	
C2362	C2091	U2026	C2091	U2026	G1954		G1816	C1751	A1677	A1610	A1544	G1465	U1401
G2363	U2092	G2027	U2092	G2027	U1955	A1889	G1817	C1752	A1678	C1611	A1545		U1402
C2364	G2093	U2028	G2093	U2028	U1956	A1890	G1817	C1753	A1679	C1612	A1548	A1463	A1403
G2365	A2094	G2029	A2094	G2029	C1957	G1891	A1819	A1754	U1680	G1613	A1549	A1470	C1404
U2366	U2095	A2030	U2095	A2030	C1958	C1892	A1820	A1755	G1681	A1614	C1550	U1471	U1405
G2367	C2096	A2031	C2096	A2031	G1959		A1821	G1756	G1682	C1615		G1475	U1406
C2368	A2097	U2034	A2097	U2034		G1896	C1822	A1757	U1683	A1616	A1551		
A2369	U2098	G2035	U2098	G2035	C1962	G1897	G1823	U1758	G1694	C1617		G1476	
G2370		C2036		C2036	U1963	U1898	G1824	A1759	C1685	A1618	G1555	A1477	G1410
U2371	A2101	A2037	A2101	A2037	G1964	A1899	G1825	C1760	C1686	G1619		G1478	U1411
G2372	G2102	G2037	G2102	G2037		A1900	G1826	C1761	G1687		C1556	U1412	U1413
C2373	C2103	G2038	C2103	G2038	C1967	A1901	U1827	A1762	U1688	A1626	C1558	G1414	
G2374	C2104	U2039	C2104	U2039	G1968	A1902	G1828	G1763	U1689	G1627	U1559	U1482	U1415
U2375	A2314	G2040	U2314	G2040	A1969	G1903	A1829	C1764	A1690	C1628		G1483	G1416
A2376	U2106	U2041	U2106	U2041	A1970	G1904	C1830	U1765		U1629	C1561	U1484	C1417



• Molecule 55: 5S ribosomal RNA

Chain 29: 29% 60% 9%



• Molecule 56: mRNA

Chain 30: 11% 44% 44% 11%



• Molecule 57: P site tRNA^{fmet}

Chain 31: 45% 55%



● Molecule 58: E-site tRNAfMet



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	76158	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 ($e^-/\text{\AA}^2$)	1.6	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	30488	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.465	Depositor
Minimum map value	-0.124	Depositor
Average map value	-0.006	Depositor
Map value standard deviation	0.041	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	393.6, 393.6, 393.6	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82, 0.82, 0.82	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.88	1/1115 (0.1%)	1.33	18/1510 (1.2%)
2	B	0.46	0/2121	1.17	21/2852 (0.7%)
3	C	0.44	0/1586	1.12	14/2134 (0.7%)
4	D	0.51	0/1571	1.20	18/2113 (0.9%)
5	E	0.43	0/1434	1.12	16/1926 (0.8%)
6	F	0.46	0/1343	1.06	9/1816 (0.5%)
7	G	0.58	0/1122	1.21	15/1515 (1.0%)
8	H	0.73	0/1001	1.32	18/1350 (1.3%)
9	I	0.82	0/1046	1.51	32/1410 (2.3%)
10	J	0.46	0/1152	1.07	4/1551 (0.3%)
11	K	0.41	0/947	1.06	6/1268 (0.5%)
12	L	0.41	0/1054	1.09	5/1403 (0.4%)
13	M	0.44	0/1093	1.02	4/1460 (0.3%)
14	N	0.38	0/973	0.98	4/1301 (0.3%)
15	O	0.40	0/902	0.96	3/1209 (0.2%)
16	P	0.39	0/929	1.02	4/1242 (0.3%)
17	Q	0.42	0/960	1.00	5/1278 (0.4%)
18	R	0.42	0/829	1.08	6/1107 (0.5%)
19	S	0.40	0/864	0.96	3/1156 (0.3%)
20	T	0.40	0/744	1.01	5/994 (0.5%)
21	U	0.39	0/787	1.09	5/1051 (0.5%)
22	V	0.42	0/766	0.99	2/1025 (0.2%)
23	W	0.39	0/582	1.09	6/769 (0.8%)
24	X	0.41	0/635	0.96	2/848 (0.2%)
25	Y	0.47	0/510	1.09	5/677 (0.7%)
26	Z	0.40	0/453	0.95	0/605
27	1	0.59	0/531	1.26	5/709 (0.7%)
28	2	0.39	0/450	0.98	2/599 (0.3%)
29	3	0.47	0/416	1.00	5/554 (0.9%)
30	4	0.45	0/380	1.17	5/498 (1.0%)
31	5	0.41	0/513	0.94	3/676 (0.4%)
32	6	0.68	0/303	1.27	4/397 (1.0%)
33	7	0.53	0/1735	1.04	7/2338 (0.3%)
34	8	0.47	0/1651	1.03	9/2225 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
35	9	0.41	0/1665	1.08	10/2227 (0.4%)
36	10	0.42	0/1169	1.08	7/1573 (0.4%)
37	11	0.47	0/835	1.09	9/1128 (0.8%)
38	12	0.39	0/1195	1.02	6/1602 (0.4%)
39	13	0.41	0/989	1.11	11/1326 (0.8%)
40	14	0.40	0/1034	1.03	5/1375 (0.4%)
41	15	0.47	0/796	1.04	8/1077 (0.7%)
42	16	0.44	0/885	1.26	12/1195 (1.0%)
43	17	0.46	0/969	1.12	10/1300 (0.8%)
44	18	0.48	0/892	1.10	7/1193 (0.6%)
45	19	0.42	0/817	1.01	7/1088 (0.6%)
46	20	0.40	0/722	1.02	7/964 (0.7%)
47	21	0.41	0/659	0.99	4/884 (0.5%)
48	22	0.39	0/657	1.01	4/881 (0.5%)
49	23	0.47	0/544	1.11	3/731 (0.4%)
50	24	0.60	0/652	1.13	5/877 (0.6%)
51	25	0.40	0/671	1.02	4/888 (0.5%)
52	26	0.48	0/550	1.06	4/728 (0.5%)
53	27	0.45	0/36967	0.55	7/57666 (0.0%)
54	28	0.46	0/69801	0.55	18/108894 (0.0%)
55	29	0.44	0/2876	0.54	1/4483 (0.0%)
56	30	0.55	0/436	0.62	1/679 (0.1%)
57	31	0.46	0/1836	0.49	0/2859
58	32	0.57	0/1835	0.56	0/2857
All	All	0.46	1/161950 (0.0%)	0.74	420/242041 (0.2%)

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
53	27	0	6
54	28	0	9
55	29	0	1
All	All	0	16

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	684	THR	C-O	8.87	1.34	1.24

The worst 5 of 420 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	10	101	GLY	N-CA-C	-13.65	99.65	114.67
1	A	678	GLY	N-CA-C	11.64	127.41	113.79
1	A	681	ARG	N-CA-C	-11.64	98.67	111.36
4	D	120	VAL	N-CA-C	10.91	124.76	107.73
33	7	85	SER	N-CA-C	-10.85	99.24	111.82

There are no chirality outliers.

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
53	27	80	A	Sidechain
53	27	82	G	Sidechain
53	27	820	U	Sidechain
53	27	898	G	Sidechain
53	27	938	A	Sidechain

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	A	1103	0	1130	106	0
2	B	2082	0	2157	143	0
3	C	1565	0	1616	97	0
4	D	1552	0	1619	127	0
5	E	1410	0	1447	130	0
6	F	1323	0	1374	96	0
7	G	1111	0	1148	88	0
8	H	988	0	1025	130	0
9	I	1032	0	1088	133	0
10	J	1129	0	1162	74	0
11	K	938	0	1012	72	0
12	L	1045	0	1117	76	0
13	M	1074	0	1157	48	0
14	N	960	0	1000	54	0
15	O	892	0	923	59	0
16	P	917	0	965	81	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	Q	947	0	1022	72	0
18	R	816	0	839	61	0
19	S	857	0	922	54	0
20	T	738	0	807	40	0
21	U	779	0	834	64	0
22	V	753	0	780	41	0
23	W	575	0	592	33	0
24	X	625	0	655	45	0
25	Y	509	0	543	39	0
26	Z	449	0	491	26	0
27	1	522	0	521	50	0
28	2	444	0	461	40	0
29	3	409	0	440	15	0
30	4	377	0	418	29	0
31	5	504	0	574	28	0
32	6	302	0	343	25	0
33	7	1704	0	1732	107	0
34	8	1624	0	1699	103	0
35	9	1643	0	1710	129	0
36	10	1156	0	1199	97	0
37	11	817	0	808	74	0
38	12	1181	0	1240	86	0
39	13	979	0	1034	70	0
40	14	1022	0	1070	103	0
41	15	786	0	828	83	0
42	16	869	0	878	70	0
43	17	955	0	1019	104	0
44	18	883	0	944	78	0
45	19	805	0	847	59	0
46	20	714	0	737	48	0
47	21	649	0	666	59	0
48	22	648	0	691	58	0
49	23	535	0	552	45	0
50	24	637	0	665	76	0
51	25	665	0	714	46	0
52	26	544	0	579	58	0
53	27	33016	0	16617	1319	0
54	28	62322	0	31345	2456	0
55	29	2572	0	1302	114	0
56	30	388	0	196	10	0
57	31	1644	0	836	32	0
58	32	1643	0	836	66	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	149128	0	100926	6808	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 27.

The worst 5 of 6808 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)
9:I:7:TYR:HA	9:I:58:ILE:O	1.26	1.26
22:V:75:GLN:HB3	22:V:90:ASP:O	1.47	1.13
9:I:90:GLY:HA2	54:28:1064:C:H1'	1.26	1.13
9:I:133:ARG:NH1	54:28:1079:C:H4'	1.63	1.12
53:27:1259:C:H3'	53:27:1260:G:H5''	1.31	1.11

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	A	139/750 (18%)	106 (76%)	21 (15%)	12 (9%)	0	10
2	B	269/273 (98%)	227 (84%)	31 (12%)	11 (4%)	2	20
3	C	207/209 (99%)	183 (88%)	17 (8%)	7 (3%)	3	24
4	D	199/201 (99%)	162 (81%)	28 (14%)	9 (4%)	2	19
5	E	175/179 (98%)	140 (80%)	31 (18%)	4 (2%)	5	30
6	F	174/177 (98%)	145 (83%)	27 (16%)	2 (1%)	11	43
7	G	147/149 (99%)	115 (78%)	23 (16%)	9 (6%)	1	15
8	H	129/165 (78%)	85 (66%)	29 (22%)	15 (12%)	0	5
9	I	139/142 (98%)	112 (81%)	21 (15%)	6 (4%)	2	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	J	140/142 (99%)	123 (88%)	13 (9%)	4 (3%)	3	26
11	K	120/123 (98%)	102 (85%)	12 (10%)	6 (5%)	1	18
12	L	141/144 (98%)	110 (78%)	25 (18%)	6 (4%)	2	20
13	M	134/136 (98%)	115 (86%)	16 (12%)	3 (2%)	5	31
14	N	118/127 (93%)	96 (81%)	18 (15%)	4 (3%)	3	24
15	O	114/117 (97%)	100 (88%)	10 (9%)	4 (4%)	3	23
16	P	112/115 (97%)	99 (88%)	11 (10%)	2 (2%)	6	34
17	Q	115/118 (98%)	105 (91%)	10 (9%)	0	100	100
18	R	101/103 (98%)	84 (83%)	13 (13%)	4 (4%)	2	21
19	S	108/110 (98%)	95 (88%)	8 (7%)	5 (5%)	2	19
20	T	91/100 (91%)	77 (85%)	8 (9%)	6 (7%)	1	14
21	U	100/104 (96%)	83 (83%)	8 (8%)	9 (9%)	0	10
22	V	92/94 (98%)	79 (86%)	12 (13%)	1 (1%)	11	43
23	W	73/85 (86%)	66 (90%)	6 (8%)	1 (1%)	9	38
24	X	75/78 (96%)	67 (89%)	5 (7%)	3 (4%)	2	21
25	Y	61/63 (97%)	53 (87%)	5 (8%)	3 (5%)	1	18
26	Z	56/59 (95%)	52 (93%)	3 (5%)	1 (2%)	6	34
27	1	64/70 (91%)	48 (75%)	10 (16%)	6 (9%)	0	9
28	2	54/57 (95%)	46 (85%)	7 (13%)	1 (2%)	6	33
29	3	48/55 (87%)	45 (94%)	2 (4%)	1 (2%)	5	31
30	4	44/46 (96%)	40 (91%)	4 (9%)	0	100	100
31	5	62/65 (95%)	54 (87%)	6 (10%)	2 (3%)	3	25
32	6	36/38 (95%)	29 (81%)	6 (17%)	1 (3%)	4	27
33	7	216/241 (90%)	170 (79%)	36 (17%)	10 (5%)	2	19
34	8	204/233 (88%)	179 (88%)	20 (10%)	5 (2%)	4	29
35	9	203/206 (98%)	167 (82%)	22 (11%)	14 (7%)	1	13
36	10	155/167 (93%)	117 (76%)	26 (17%)	12 (8%)	1	12
37	11	98/135 (73%)	77 (79%)	13 (13%)	8 (8%)	0	11
38	12	149/179 (83%)	127 (85%)	18 (12%)	4 (3%)	4	28
39	13	127/130 (98%)	116 (91%)	8 (6%)	3 (2%)	4	29
40	14	125/130 (96%)	105 (84%)	10 (8%)	10 (8%)	1	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	15	96/103 (93%)	75 (78%)	16 (17%)	5 (5%)	1	17
42	16	114/129 (88%)	95 (83%)	13 (11%)	6 (5%)	1	17
43	17	121/124 (98%)	91 (75%)	24 (20%)	6 (5%)	1	18
44	18	112/118 (95%)	98 (88%)	8 (7%)	6 (5%)	1	17
45	19	98/101 (97%)	80 (82%)	13 (13%)	5 (5%)	1	17
46	20	86/89 (97%)	62 (72%)	14 (16%)	10 (12%)	0	5
47	21	80/82 (98%)	64 (80%)	11 (14%)	5 (6%)	1	15
48	22	78/84 (93%)	60 (77%)	13 (17%)	5 (6%)	1	15
49	23	63/75 (84%)	52 (82%)	6 (10%)	5 (8%)	1	11
50	24	77/92 (84%)	64 (83%)	11 (14%)	2 (3%)	4	28
51	25	83/87 (95%)	77 (93%)	6 (7%)	0	100	100
52	26	63/71 (89%)	39 (62%)	15 (24%)	9 (14%)	0	3
All	All	5985/6970 (86%)	4958 (83%)	749 (12%)	278 (5%)	3	19

5 of 278 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	599	VAL
1	A	666	SER
1	A	677	SER
1	A	702	ASP
2	B	107	LYS

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	A	121/635 (19%)	120 (99%)	1 (1%)	73	77
2	B	216/218 (99%)	216 (100%)	0	100	100
3	C	164/164 (100%)	164 (100%)	0	100	100
4	D	165/165 (100%)	165 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	148/150 (99%)	147 (99%)	1 (1%)	76	78
6	F	137/138 (99%)	136 (99%)	1 (1%)	76	78
7	G	114/114 (100%)	114 (100%)	0	100	100
8	H	100/123 (81%)	99 (99%)	1 (1%)	68	75
9	I	109/110 (99%)	108 (99%)	1 (1%)	70	75
10	J	116/116 (100%)	116 (100%)	0	100	100
11	K	103/104 (99%)	101 (98%)	2 (2%)	50	66
12	L	102/103 (99%)	101 (99%)	1 (1%)	68	75
13	M	109/109 (100%)	109 (100%)	0	100	100
14	N	100/103 (97%)	100 (100%)	0	100	100
15	O	86/87 (99%)	86 (100%)	0	100	100
16	P	99/100 (99%)	98 (99%)	1 (1%)	68	75
17	Q	89/90 (99%)	89 (100%)	0	100	100
18	R	84/84 (100%)	84 (100%)	0	100	100
19	S	93/93 (100%)	93 (100%)	0	100	100
20	T	80/84 (95%)	80 (100%)	0	100	100
21	U	83/85 (98%)	82 (99%)	1 (1%)	63	72
22	V	78/78 (100%)	78 (100%)	0	100	100
23	W	57/63 (90%)	57 (100%)	0	100	100
24	X	67/68 (98%)	67 (100%)	0	100	100
25	Y	55/55 (100%)	55 (100%)	0	100	100
26	Z	48/49 (98%)	48 (100%)	0	100	100
27	1	59/62 (95%)	58 (98%)	1 (2%)	53	68
28	2	47/48 (98%)	47 (100%)	0	100	100
29	3	45/49 (92%)	45 (100%)	0	100	100
30	4	38/38 (100%)	37 (97%)	1 (3%)	40	60
31	5	51/52 (98%)	51 (100%)	0	100	100
32	6	34/34 (100%)	34 (100%)	0	100	100
33	7	180/199 (90%)	180 (100%)	0	100	100
34	8	170/190 (90%)	170 (100%)	0	100	100
35	9	172/173 (99%)	170 (99%)	2 (1%)	63	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	10	119/126 (94%)	119 (100%)	0	100	100
37	11	87/116 (75%)	86 (99%)	1 (1%)	65	74
38	12	124/147 (84%)	124 (100%)	0	100	100
39	13	104/105 (99%)	104 (100%)	0	100	100
40	14	105/107 (98%)	105 (100%)	0	100	100
41	15	86/90 (96%)	86 (100%)	0	100	100
42	16	89/99 (90%)	88 (99%)	1 (1%)	65	74
43	17	103/104 (99%)	103 (100%)	0	100	100
44	18	92/96 (96%)	92 (100%)	0	100	100
45	19	83/84 (99%)	83 (100%)	0	100	100
46	20	76/77 (99%)	76 (100%)	0	100	100
47	21	65/65 (100%)	65 (100%)	0	100	100
48	22	74/78 (95%)	74 (100%)	0	100	100
49	23	56/65 (86%)	56 (100%)	0	100	100
50	24	70/79 (89%)	70 (100%)	0	100	100
51	25	65/66 (98%)	65 (100%)	0	100	100
52	26	55/61 (90%)	55 (100%)	0	100	100
All	All	4972/5698 (87%)	4956 (100%)	16 (0%)	84	85

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
37	11	12	PRO
35	9	190	LEU
16	P	113	LEU
35	9	4	LEU
12	L	89	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 116 such sidechains are listed below:

Mol	Chain	Res	Type
23	W	72	ASN
49	23	18	GLN
33	7	14	HIS
48	22	30	HIS

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Mol	Chain	Res	Type
45	19	3	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
53	27	1538/1539 (99%)	171 (11%)	7 (0%)
54	28	2902/2903 (99%)	387 (13%)	20 (0%)
55	29	119/120 (99%)	12 (10%)	3 (2%)
56	30	17/18 (94%)	3 (17%)	0
57	31	76/77 (98%)	5 (6%)	0
58	32	76/77 (98%)	17 (22%)	0
All	All	4728/4734 (99%)	595 (12%)	30 (0%)

5 of 595 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
53	27	4	U
53	27	6	G
53	27	9	G
53	27	13	U
53	27	22	G

5 of 30 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
54	28	1378	A
55	29	44	G
54	28	1730	C
55	29	88	C
54	28	2566	A

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

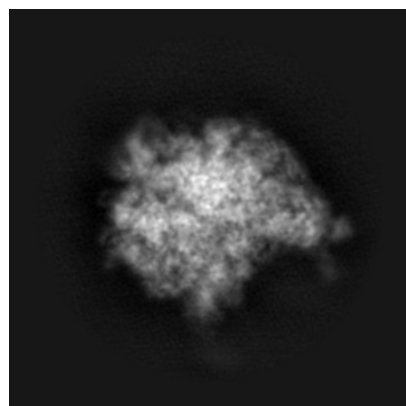
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8279. These allow visual inspection of the internal detail of the map and identification of artifacts.

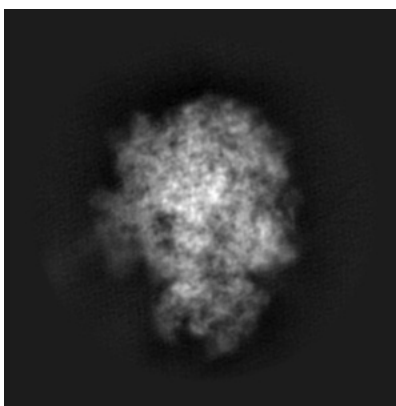
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

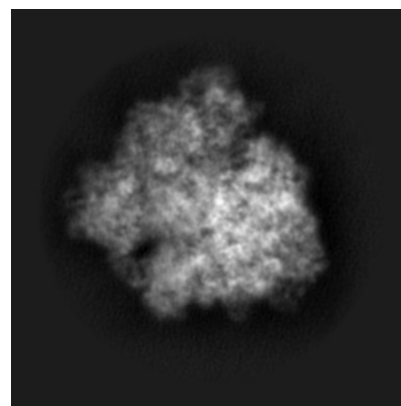
6.1.1 Primary map



X

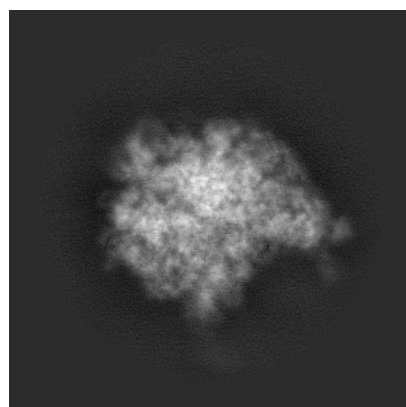


Y

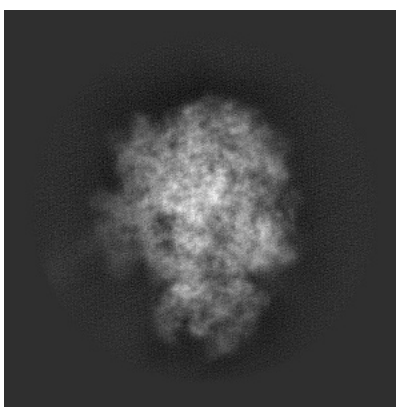


Z

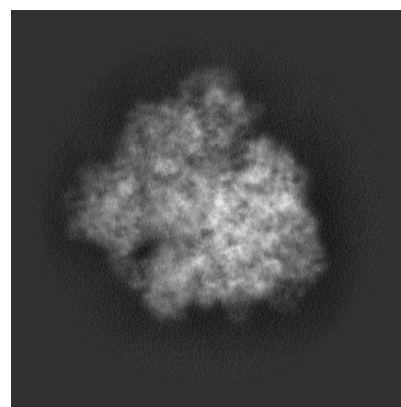
6.1.2 Raw map



X



Y

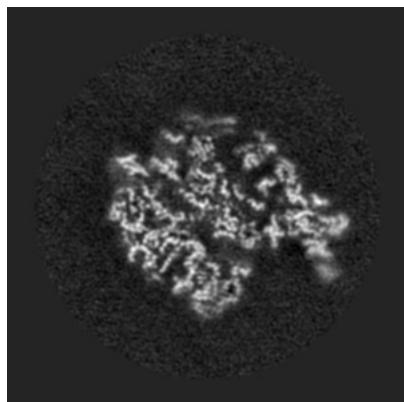


Z

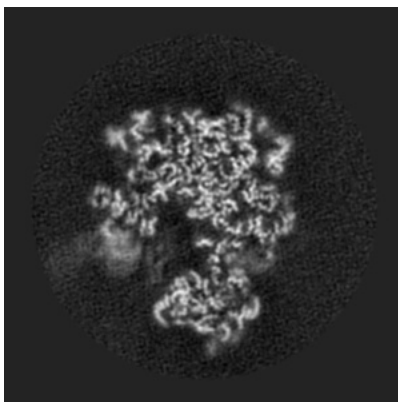
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

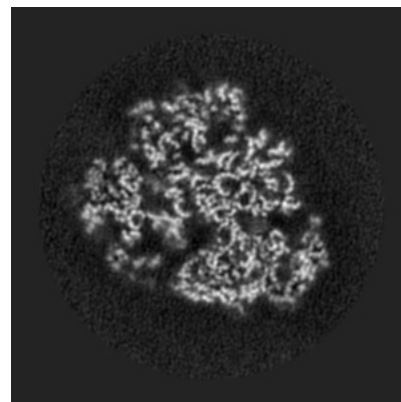
6.2.1 Primary map



X Index: 240

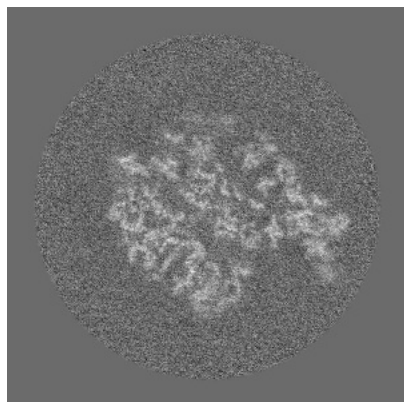


Y Index: 240

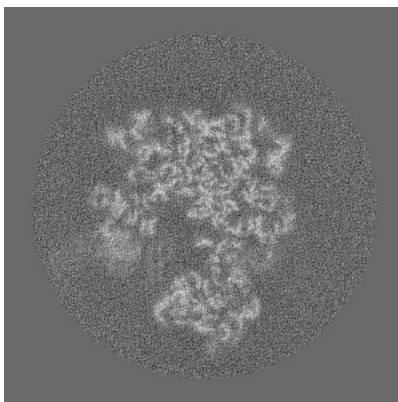


Z Index: 240

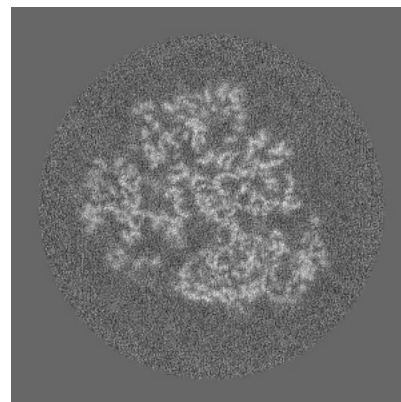
6.2.2 Raw map



X Index: 240



Y Index: 240

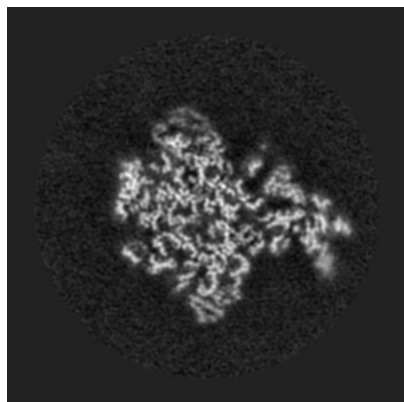


Z Index: 240

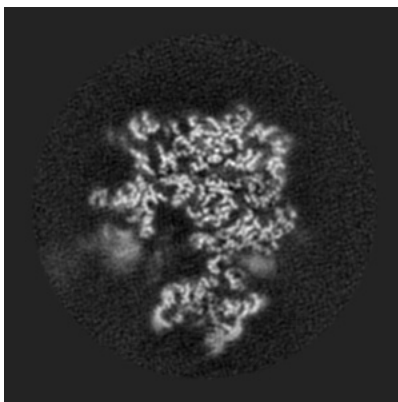
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

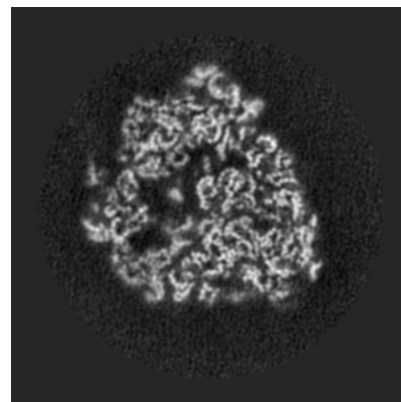
6.3.1 Primary map



X Index: 249

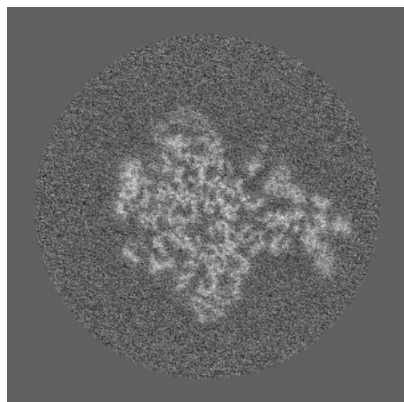


Y Index: 247

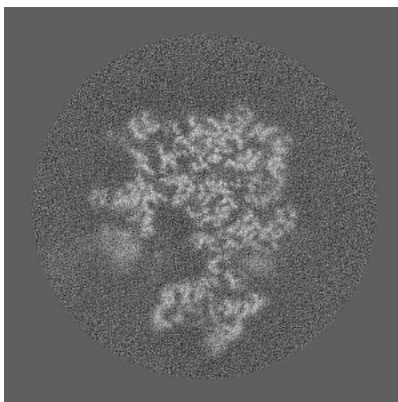


Z Index: 225

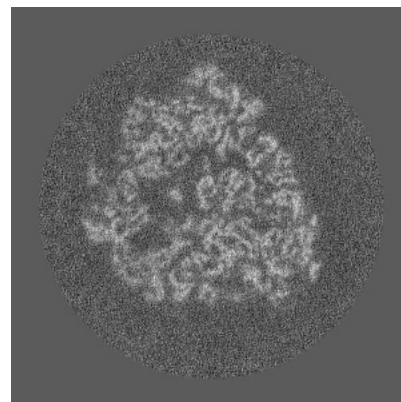
6.3.2 Raw map



X Index: 249



Y Index: 247

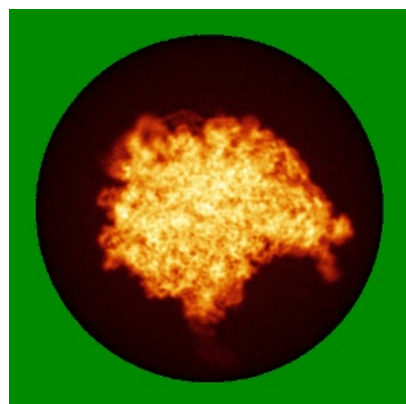


Z Index: 225

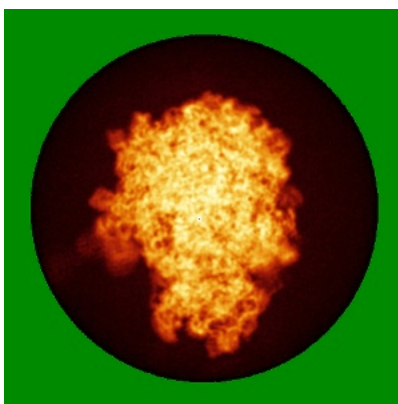
The images above show the largest variance slices of the map in three orthogonal directions.

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

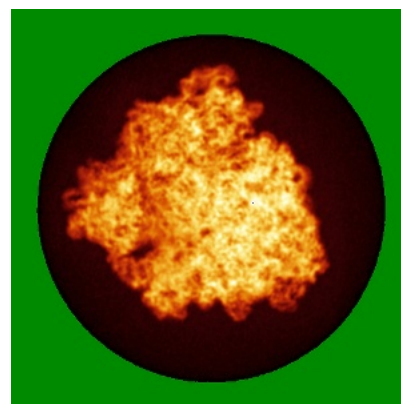
6.4.1 Primary map



X

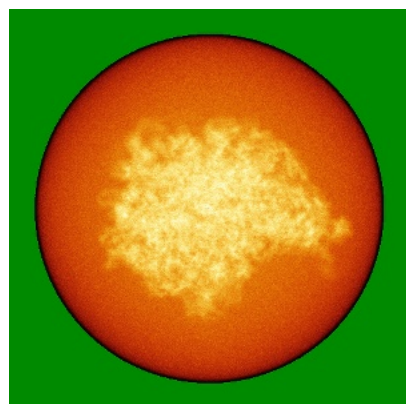


Y

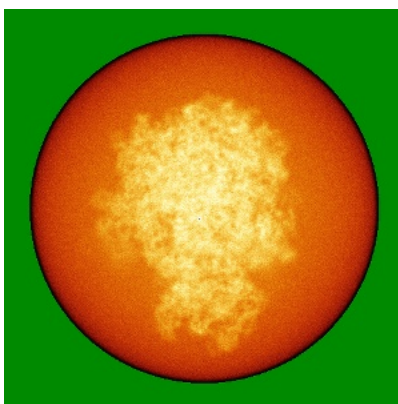


Z

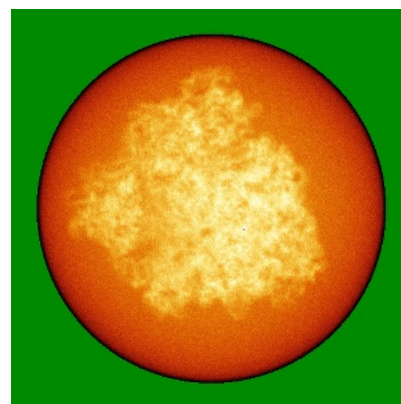
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

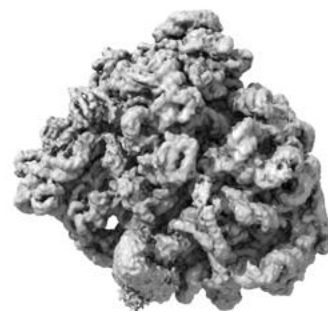
6.5.1 Primary map



X



Y



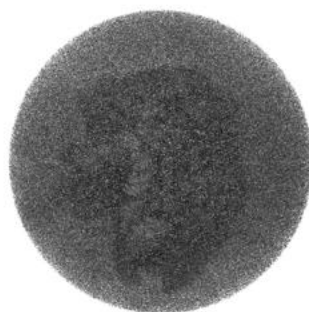
Z

The images above show the 3D surface view of the map at the recommended contour level 0.08. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

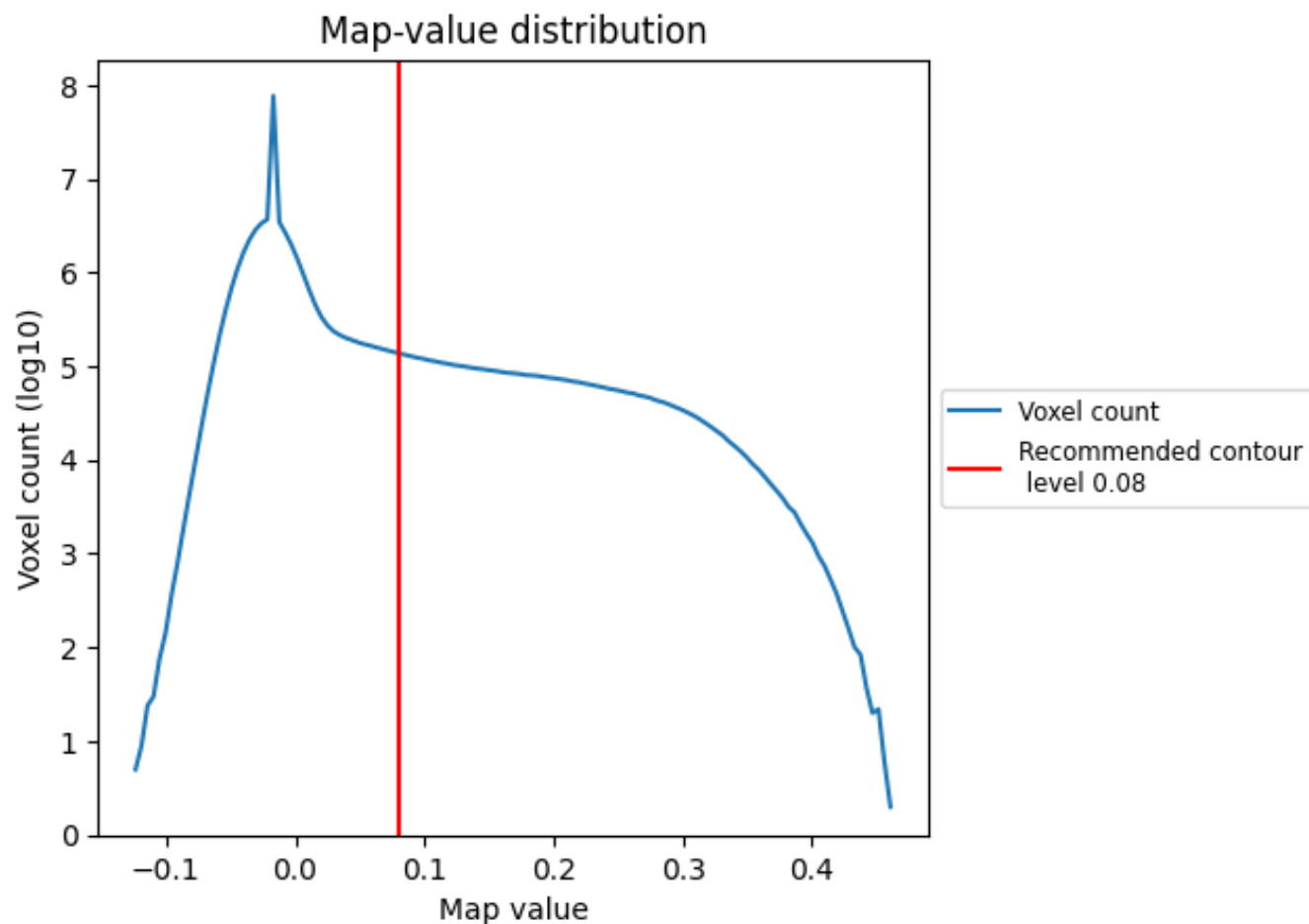
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

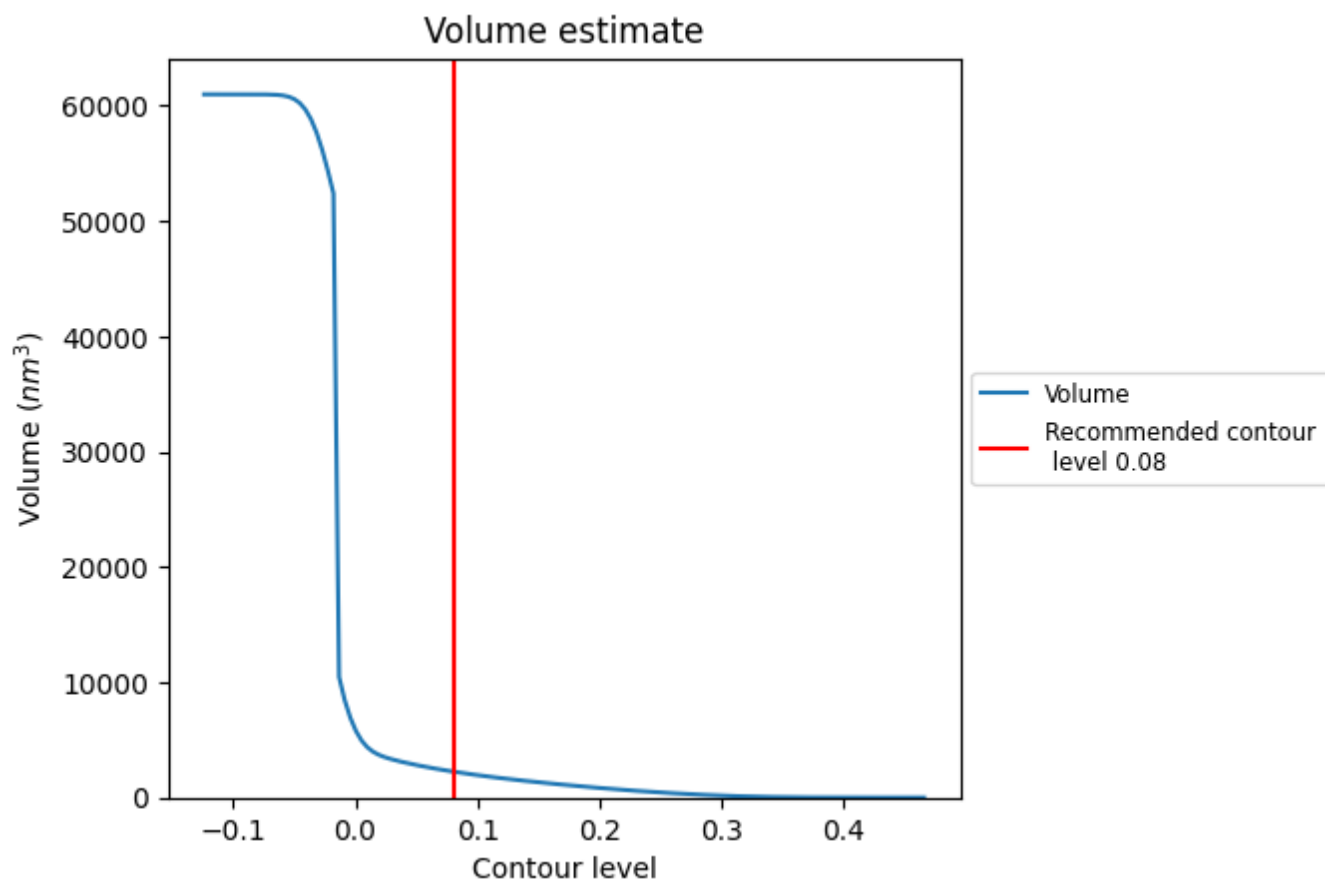
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

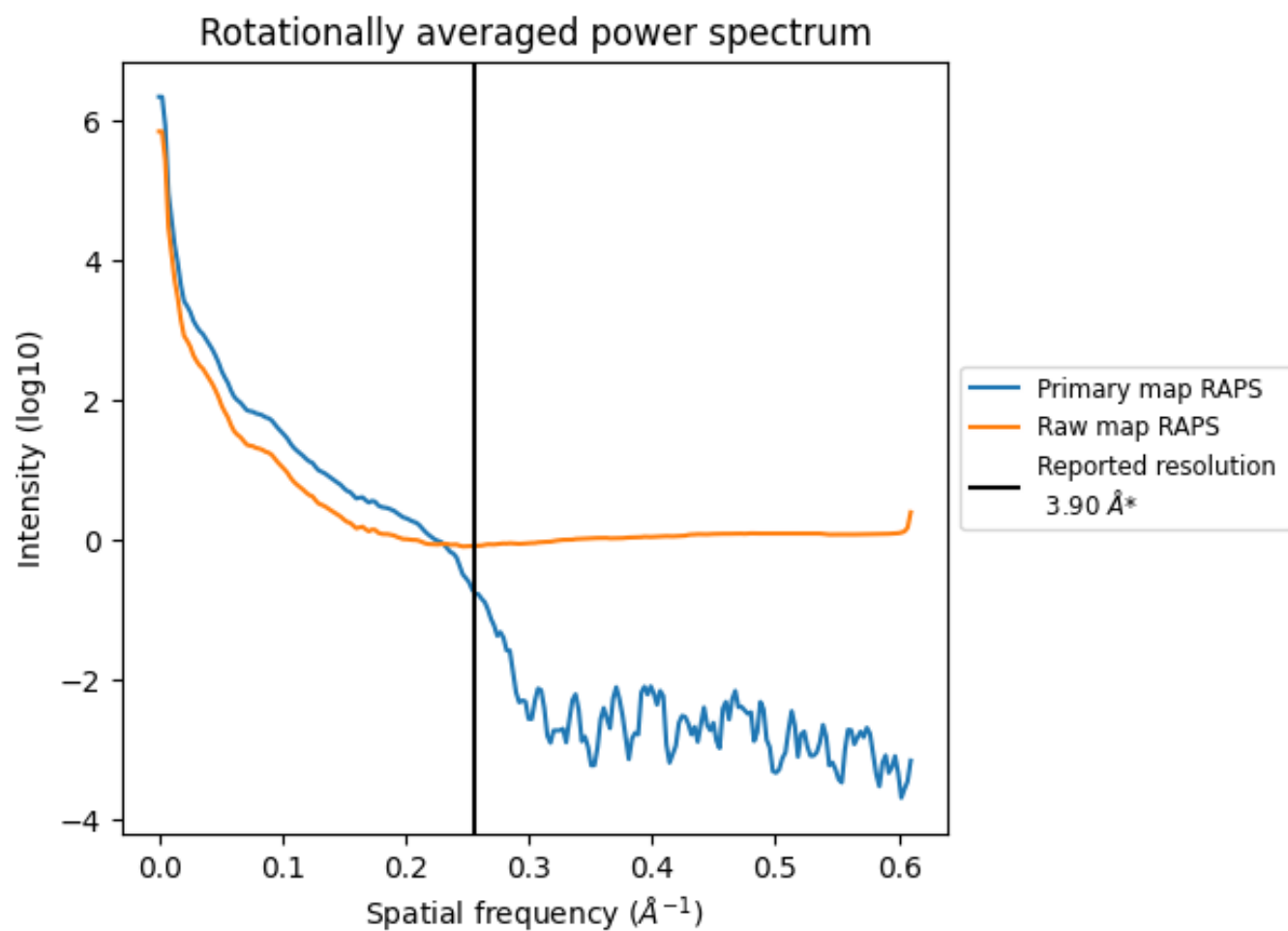
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2253 nm³; this corresponds to an approximate mass of 2035 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 ⓘ

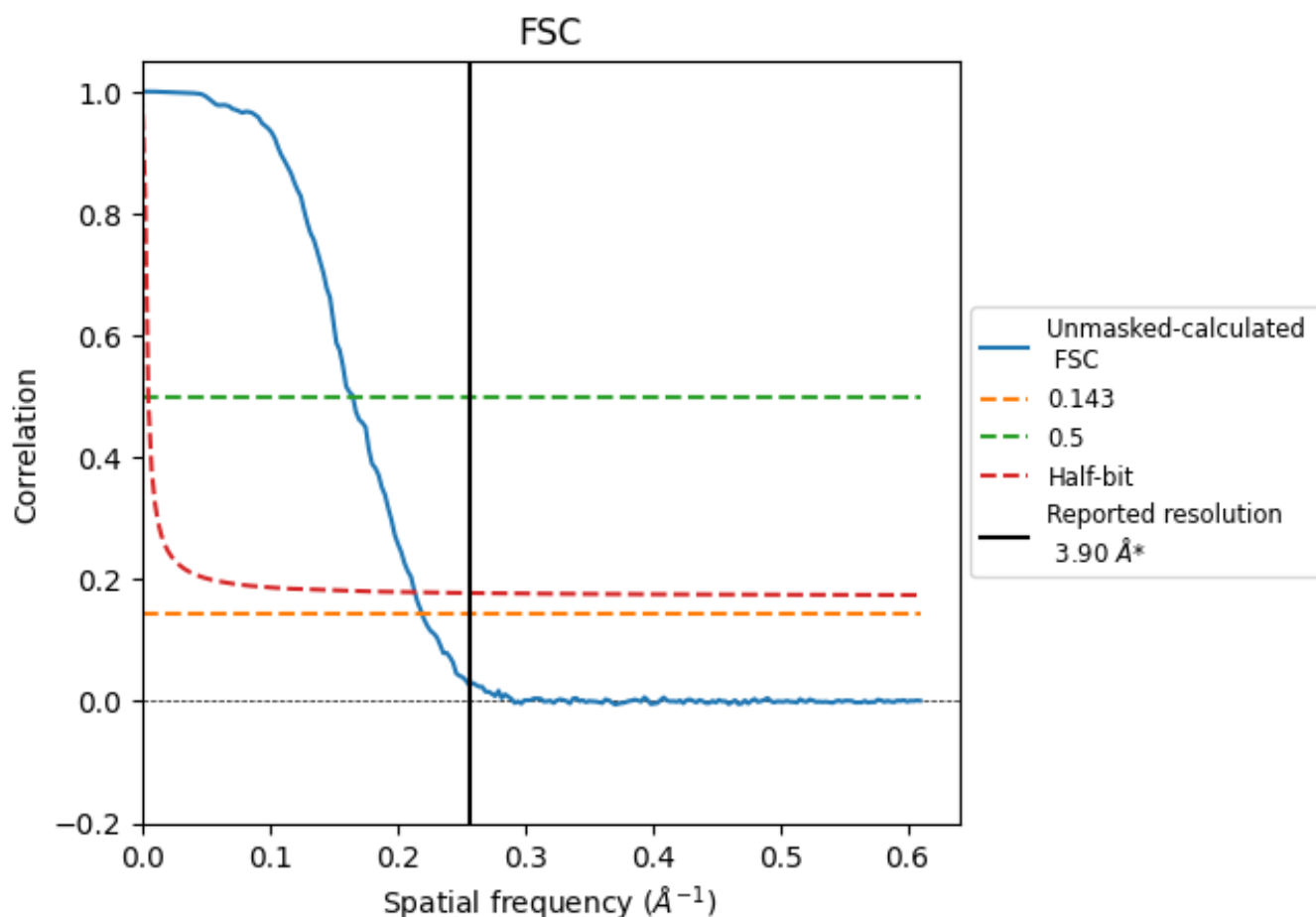


*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

8.2 Resolution estimates [i](#)

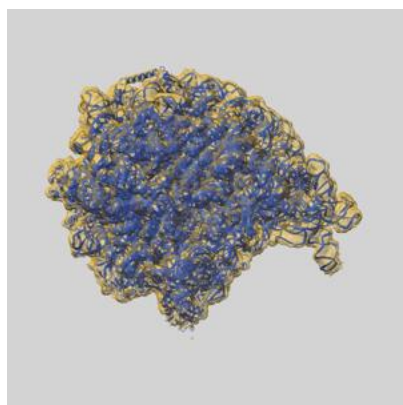
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.55	6.05	4.68

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.55 differs from the reported value 3.9 by more than 10 %

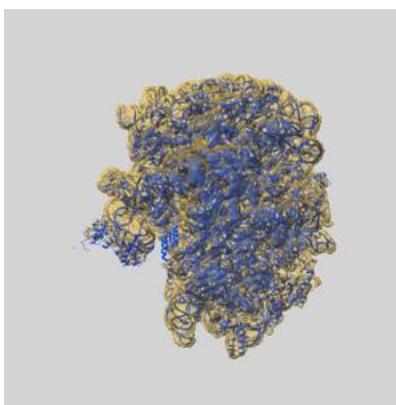
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8279 and PDB model 5KPS. Per-residue inclusion information can be found in section [3](#) on page [15](#).

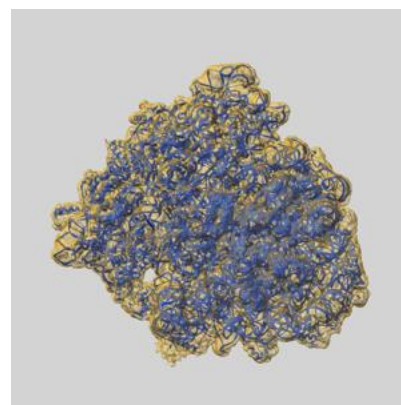
9.1 Map-model overlay [i](#)



X



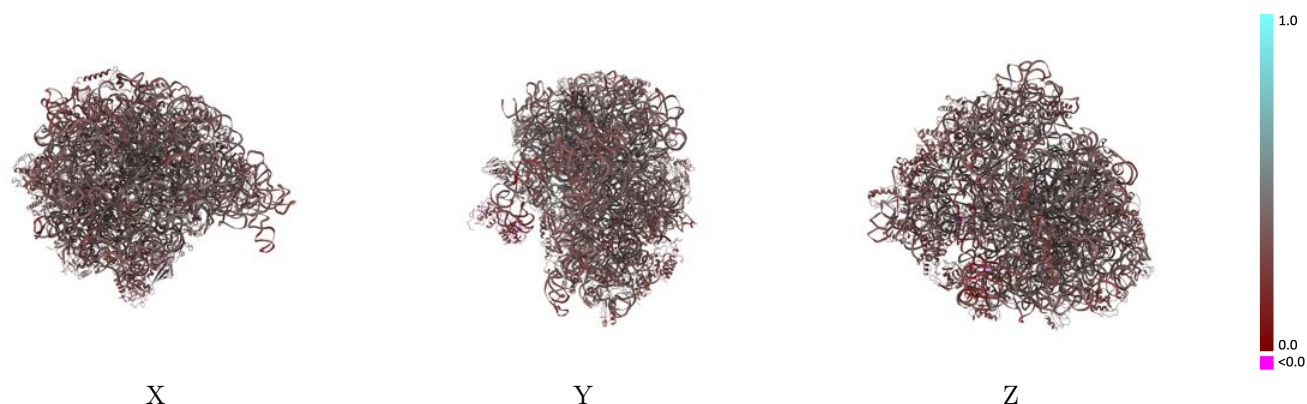
Y



Z

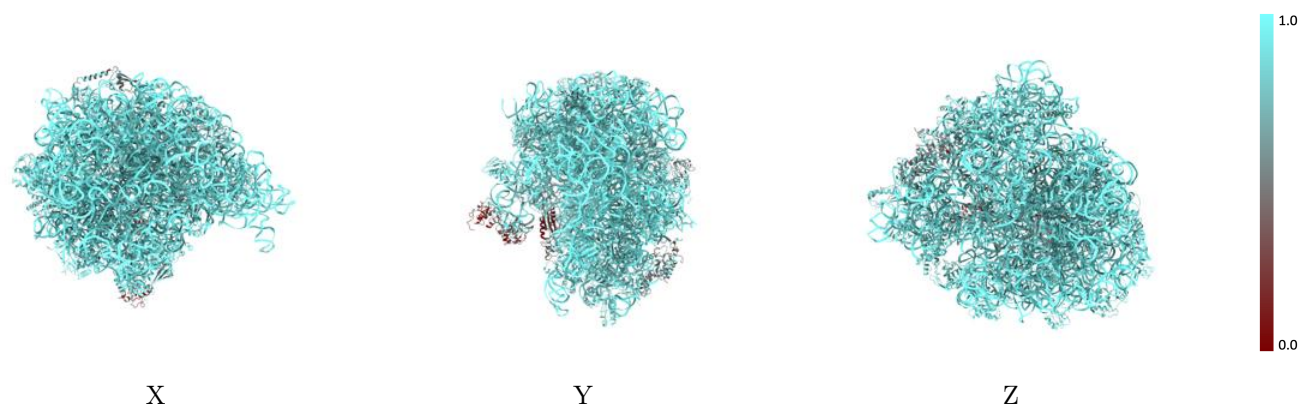
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



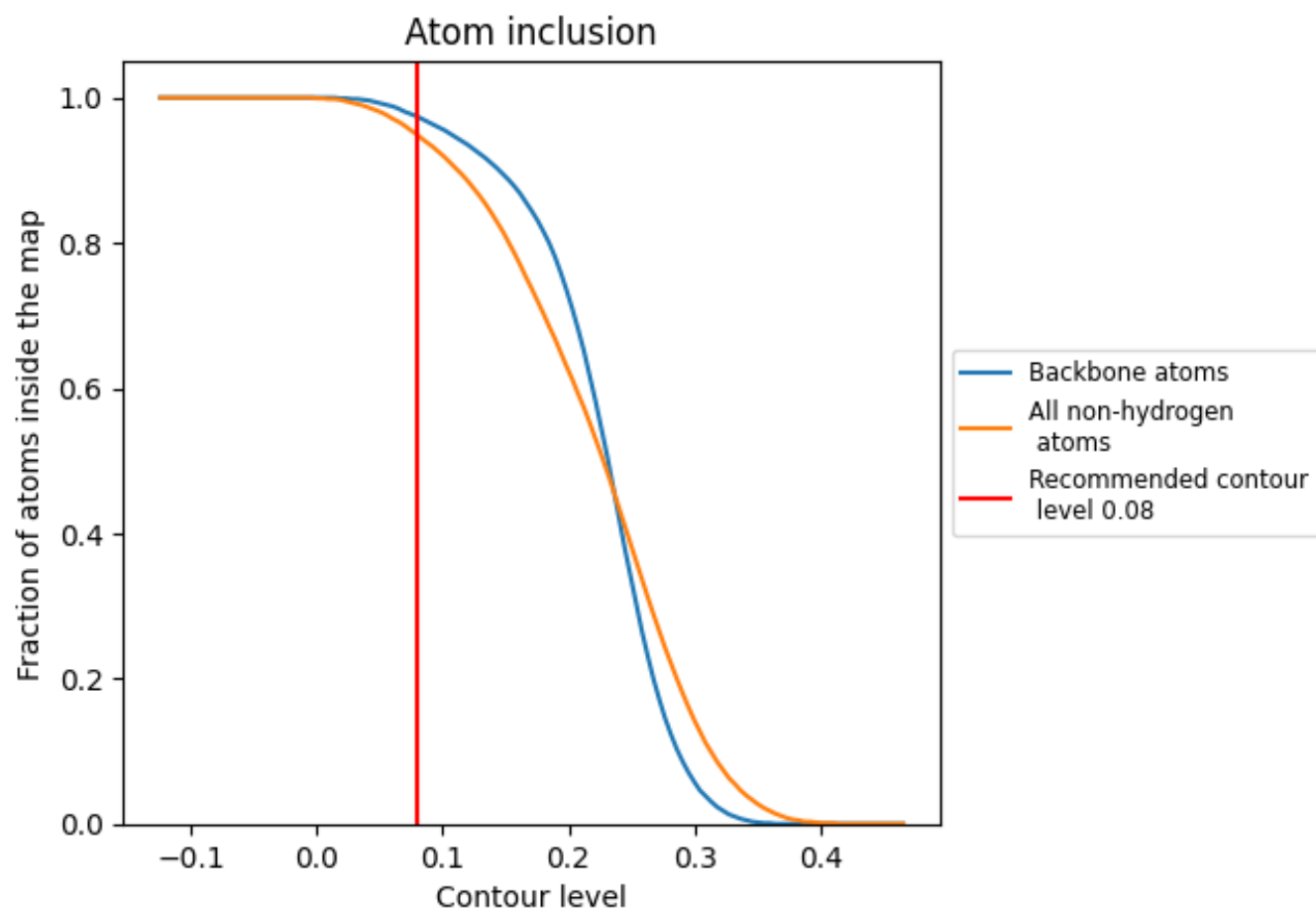
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.08).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 95% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9490	 0.3570
1	 0.9200	 0.3200
10	 0.9010	 0.3680
11	 0.9200	 0.3430
12	 0.8990	 0.3220
13	 0.9060	 0.3600
14	 0.9260	 0.3390
15	 0.8370	 0.3340
16	 0.9290	 0.3590
17	 0.8690	 0.3670
18	 0.9200	 0.3290
19	 0.8990	 0.3330
2	 0.9210	 0.3770
20	 0.9290	 0.3340
21	 0.9310	 0.3600
22	 0.9210	 0.3640
23	 0.9510	 0.3520
24	 0.9110	 0.3380
25	 0.9170	 0.3250
26	 0.8120	 0.2830
27	 0.9960	 0.3650
28	 0.9950	 0.3670
29	 0.9990	 0.3590
3	 0.8900	 0.3700
30	 0.8810	 0.2920
31	 0.9850	 0.3510
32	 0.9410	 0.2110
4	 0.9270	 0.3570
5	 0.9180	 0.3880
6	 0.9280	 0.3710
7	 0.5330	 0.3050
8	 0.8520	 0.3600
9	 0.8910	 0.3310
A	 0.2630	 0.2840
B	 0.9170	 0.3940



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Chain	Atom inclusion	Q-score
C	 0.9230	 0.3900
D	 0.8760	 0.3400
E	 0.9200	 0.3370
F	 0.9340	 0.3620
G	 0.6670	 0.2960
H	 0.3170	 0.2070
I	 0.4130	 0.1980
J	 0.9080	 0.3640
K	 0.8890	 0.3910
L	 0.9230	 0.3730
M	 0.8910	 0.3850
N	 0.9250	 0.3650
O	 0.9430	 0.3470
P	 0.9130	 0.3900
Q	 0.9330	 0.3400
R	 0.9220	 0.3770
S	 0.8680	 0.3690
T	 0.9070	 0.3700
U	 0.9170	 0.3600
V	 0.9250	 0.3560
W	 0.9190	 0.3920
X	 0.9150	 0.3690
Y	 0.9010	 0.2940
Z	 0.8970	 0.3590