



wwPDB EM Validation Summary Report ⓘ

Nov 9, 2024 – 09:12 AM EST

PDB ID : 5KPS
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:

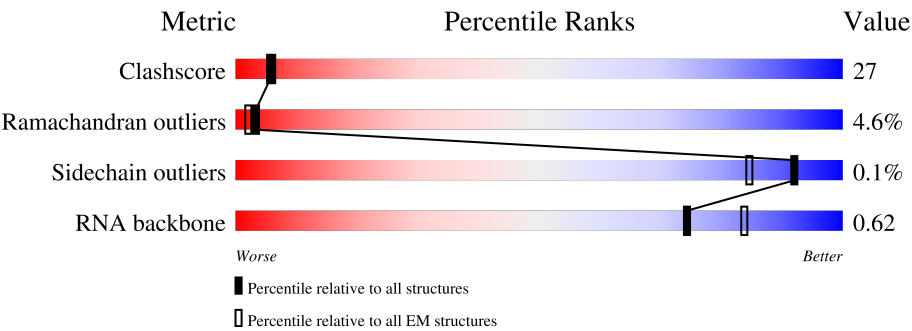
EMDB validation analysis : 0.0.1.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

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.



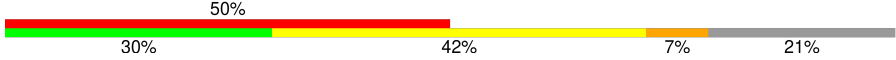



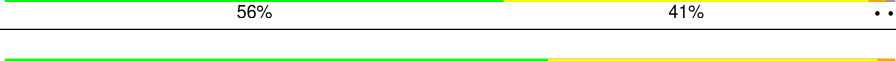


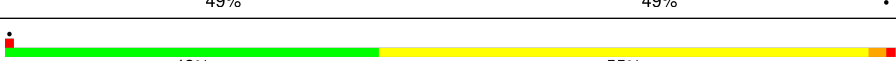

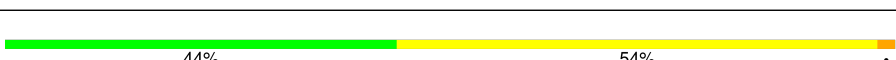
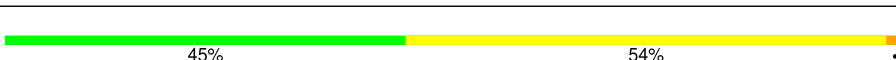
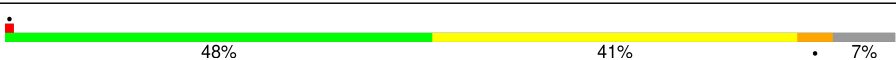



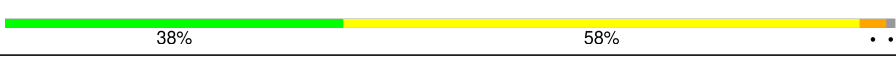

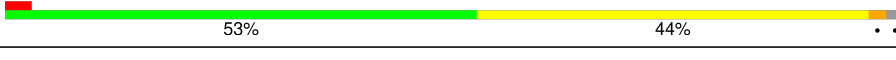

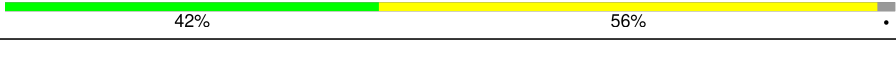


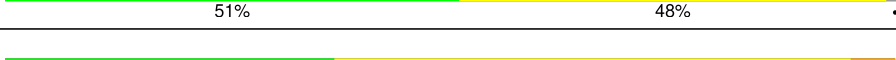


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	<div><div>14% 7% 11% .</div><div>81%</div></div>
2	B	273	<div><div>47% 51% ..</div></div>
3	C	209	<div><div>54% 43% .</div></div>
4	D	201	<div><div>43% 52% .</div></div>
5	E	179	<div><div>40% 56% ..</div></div>
6	F	177	<div><div>41% 58% ..</div></div>
7	G	149	<div><div>16% 38% 58% .</div></div>

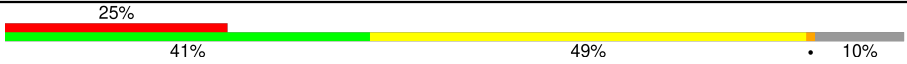
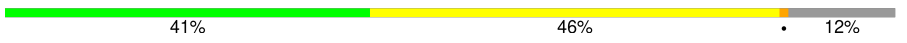


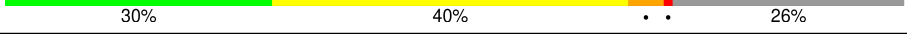
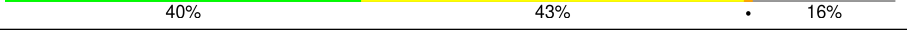
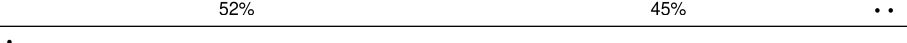
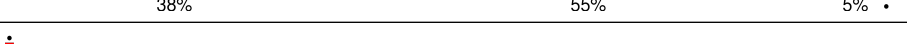
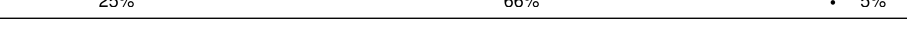
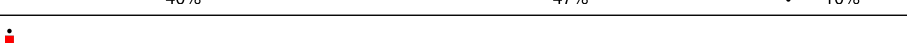
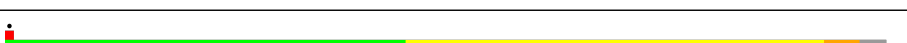
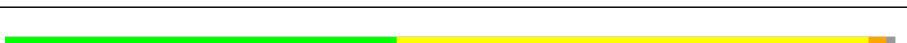
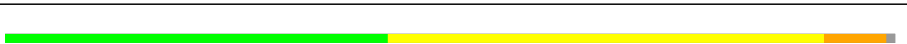


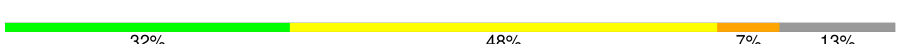
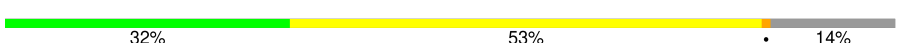


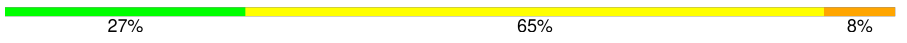





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Mol	Chain	Length	Quality of chain
8	H	165	
9	I	142	
10	J	142	
11	K	123	
12	L	144	
13	M	136	
14	N	127	
15	O	117	
16	P	115	
17	Q	118	
18	R	103	
19	S	110	
20	T	100	
21	U	104	
22	V	94	
23	W	85	
24	X	78	
25	Y	63	
26	Z	59	
27	1	70	
28	2	57	
29	3	55	
30	4	46	
31	5	65	
32	6	38	

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Mol	Chain	Length	Quality of chain
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	
54	28	2903	
55	29	120	
56	30	18	
57	31	77	

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Mol	Chain	Length	Quality of chain
58	32	77	 A horizontal bar chart showing the quality of the chain. The bar is divided into three segments: green (26%), yellow (53%), and orange (21%). A small red dot is at the beginning of the green segment.

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 tRNAfmet.

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

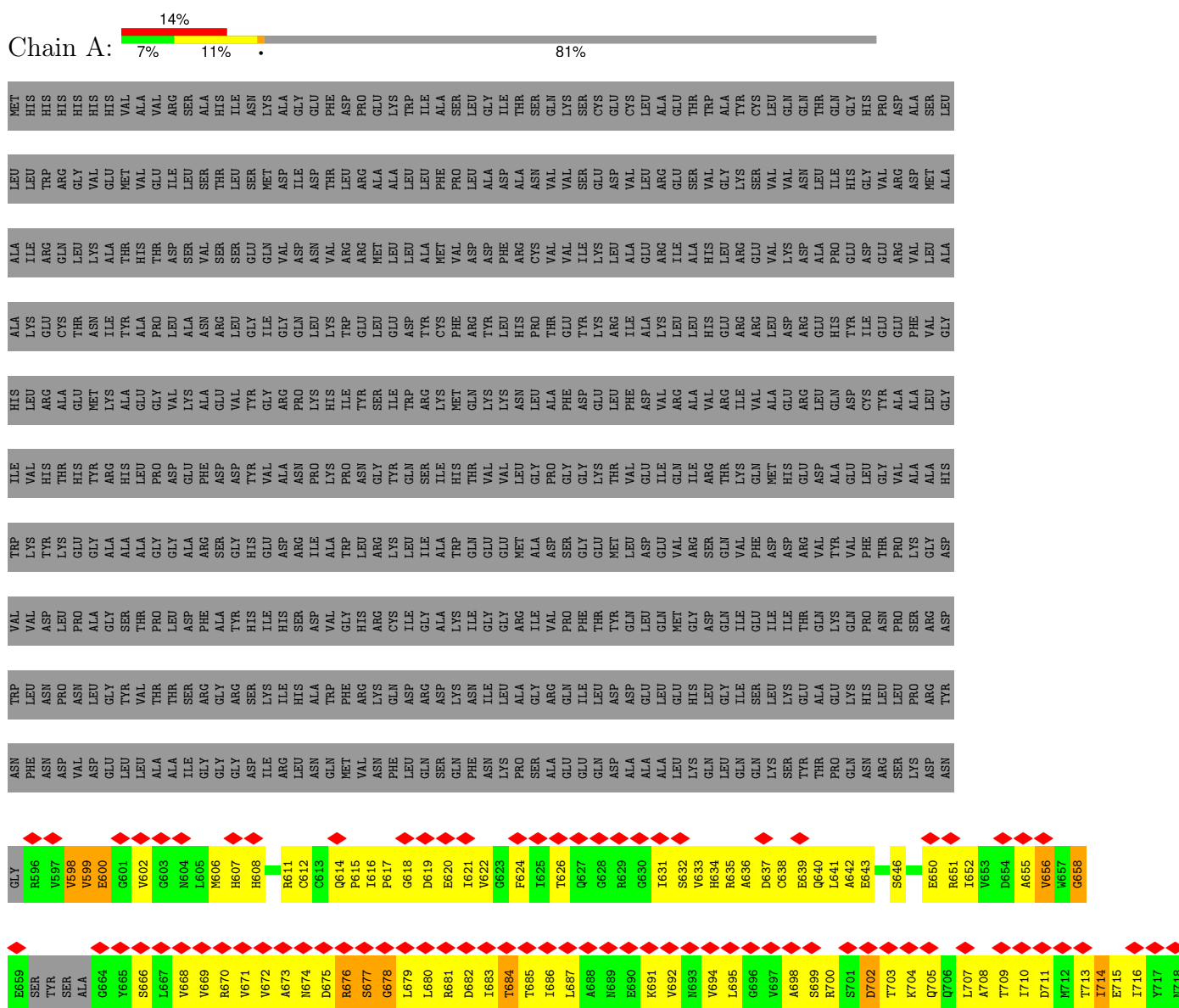
- Molecule 58 is a RNA chain called E-site tRNAfMet.

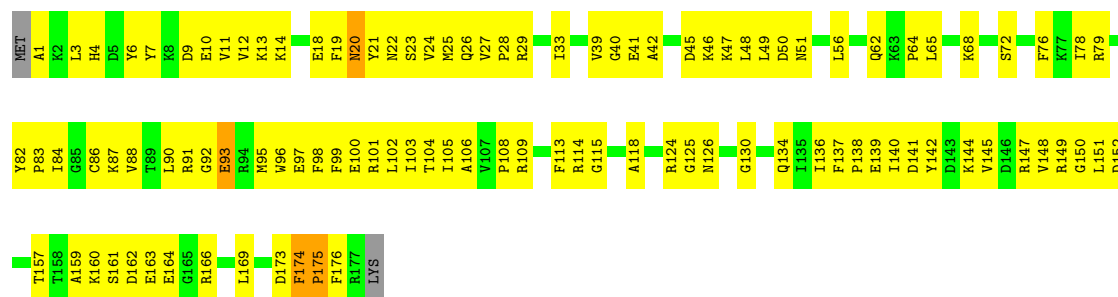
Mol	Chain	Residues	Atoms					AltConf	Trace
58	32	77	Total	C	N	O	P	0	0
			1643	732	297	537	77		

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.

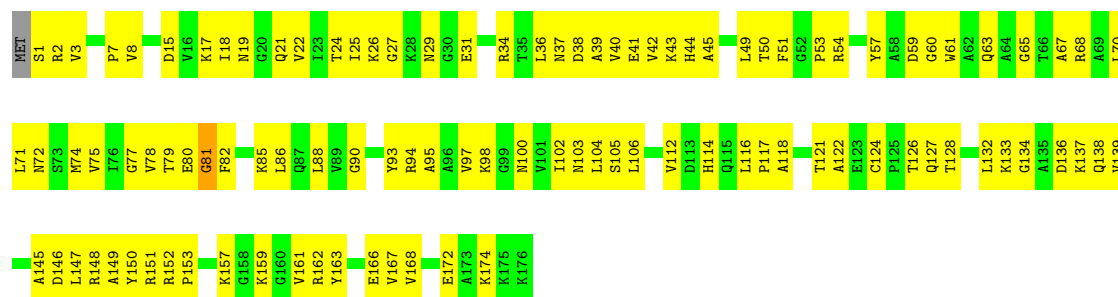
• Molecule 1: GTP pyrophosphokinase





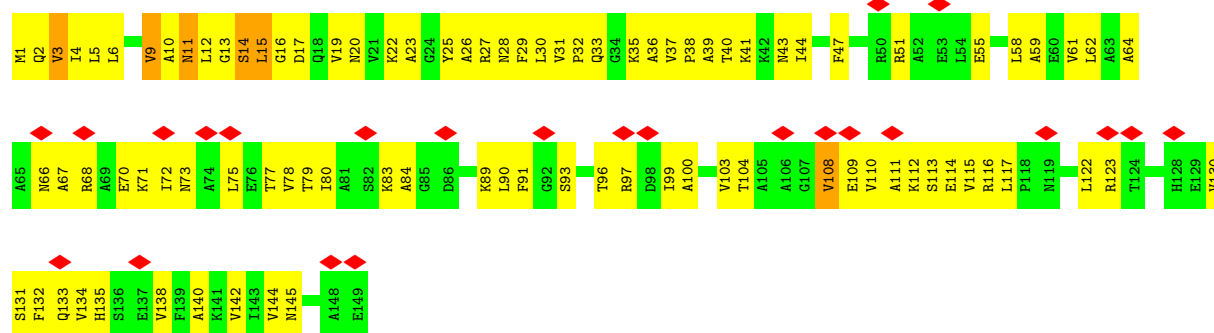
• Molecule 6: 50S ribosomal protein L6

Chain F: 41% 58%



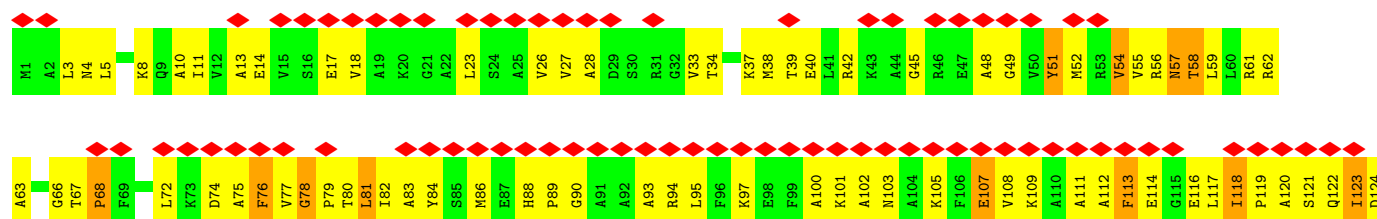
• Molecule 7: 50S ribosomal protein L9

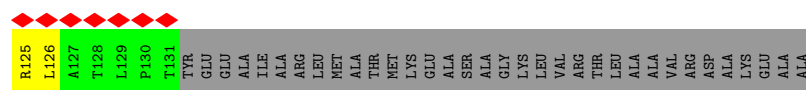
Chain G: 16% 38% 58%



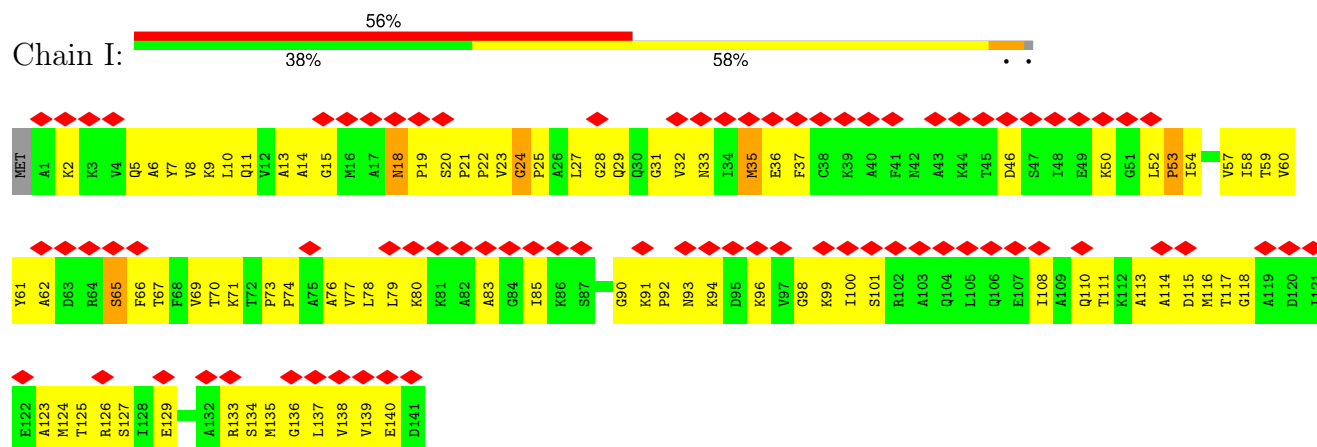
• Molecule 8: 50S ribosomal protein L10

Chain H: 50% 30% 42% 7% 21%

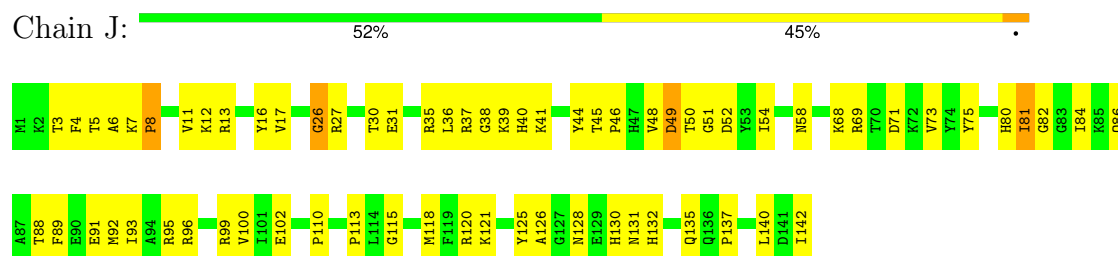




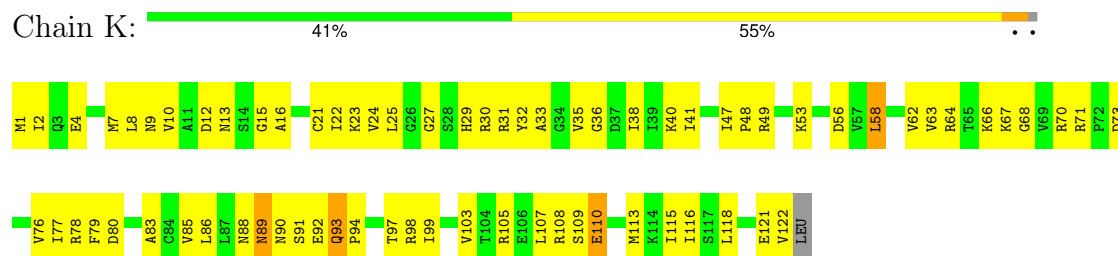
• Molecule 9: 50S ribosomal protein L11



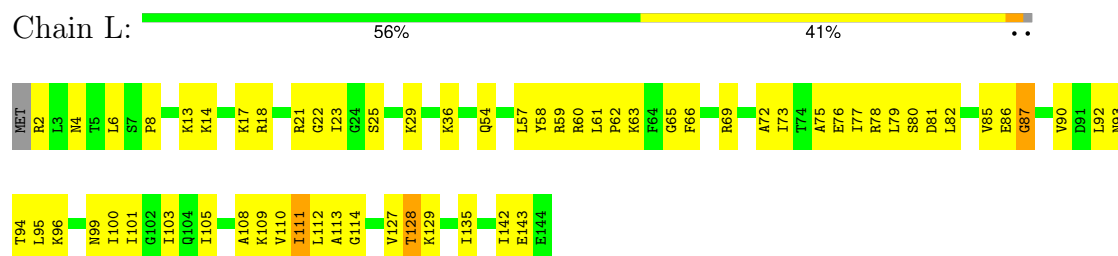
• Molecule 10: 50S ribosomal protein L13



• Molecule 11: 50S ribosomal protein L14

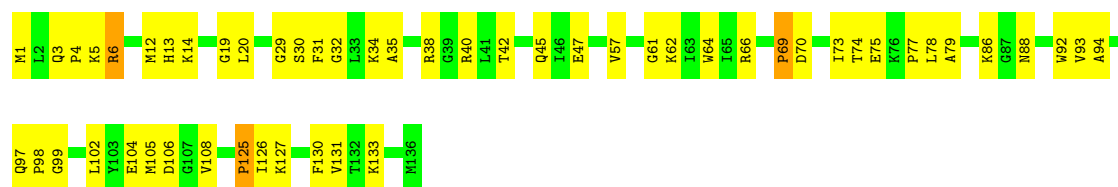


• Molecule 12: 50S ribosomal protein L15



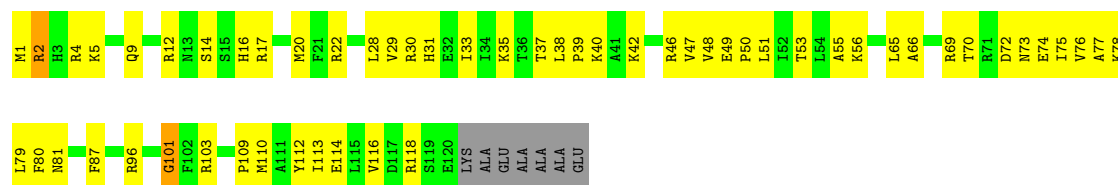
• Molecule 13: 50S ribosomal protein L16

Chain M:  61% 37%



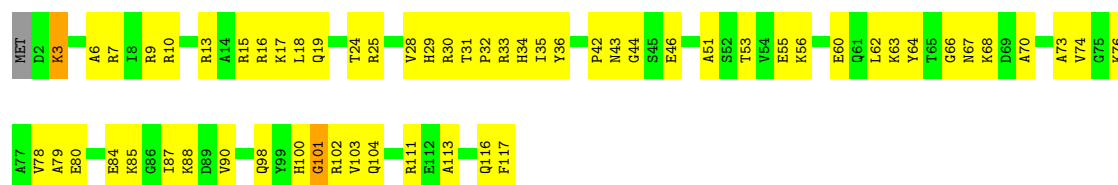
• Molecule 14: 50S ribosomal protein L17

Chain N:  50% 43% 6%



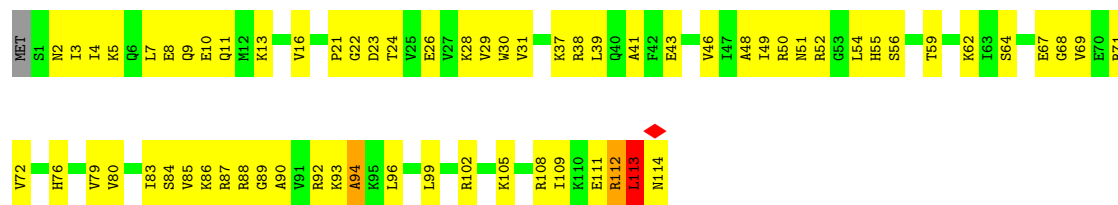
• Molecule 15: 50S ribosomal protein L18

Chain O:  49% 49%



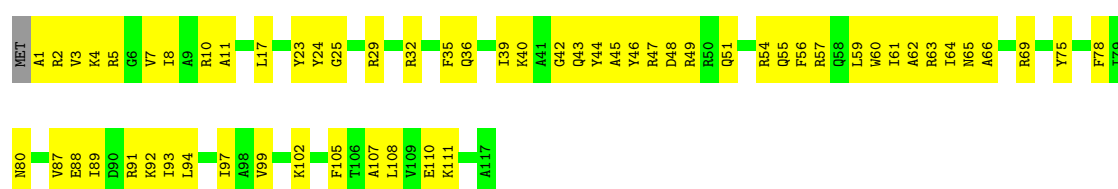
• Molecule 16: 50S ribosomal protein L19

Chain P:  42% 55%

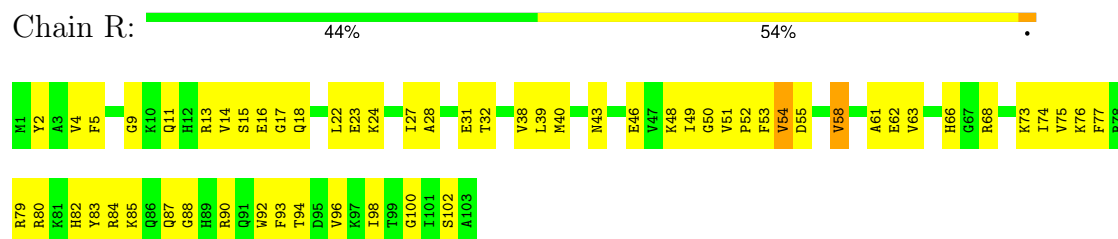


• Molecule 17: 50S ribosomal protein L20

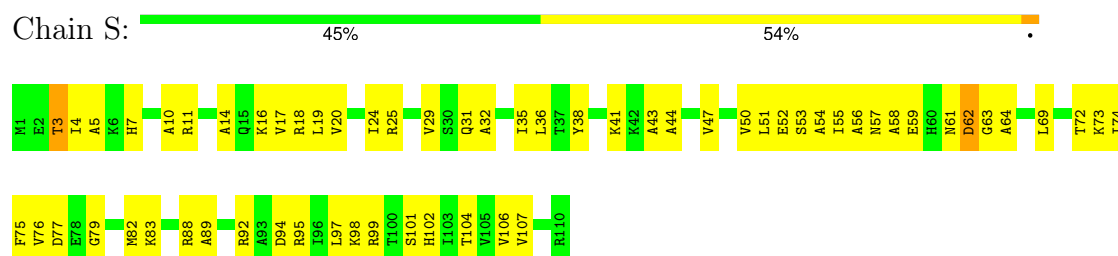
Chain Q:  49% 50%



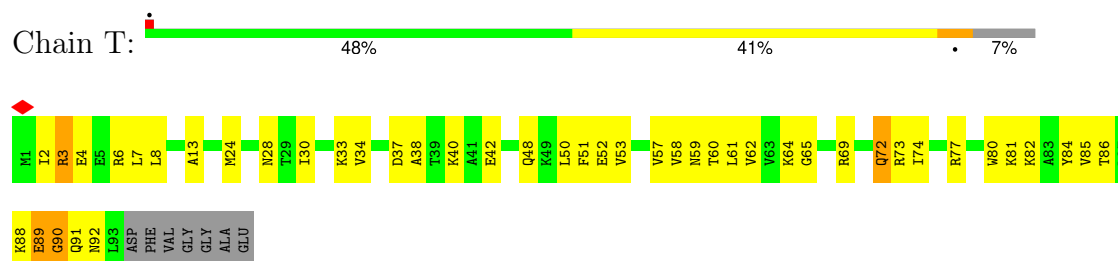
- Molecule 18: 50S ribosomal protein L21



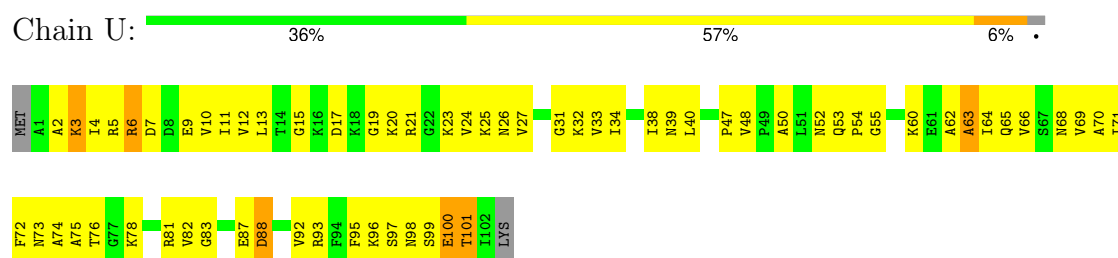
- Molecule 19: 50S ribosomal protein L22



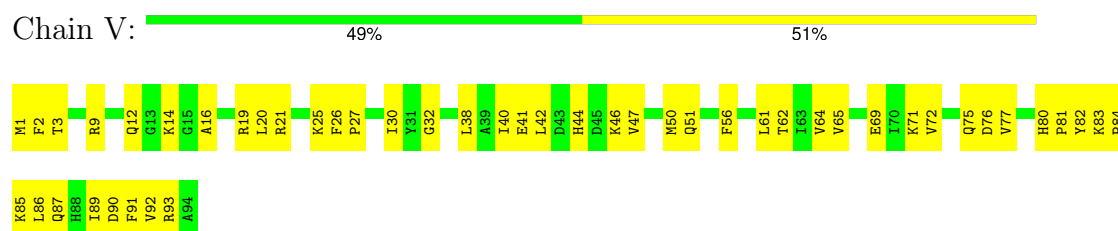
- Molecule 20: 50S ribosomal protein L23



- Molecule 21: 50S ribosomal protein L24

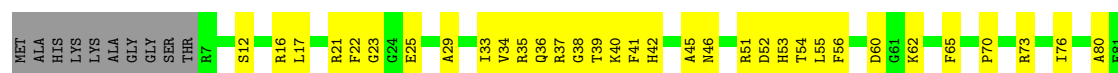


- Molecule 22: 50S ribosomal protein L25



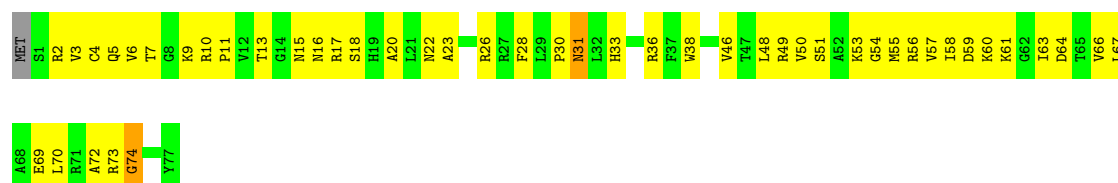
- Molecule 23: 50S ribosomal protein L27

Chain W: 



- Molecule 24: 50S ribosomal protein L28

Chain X: 



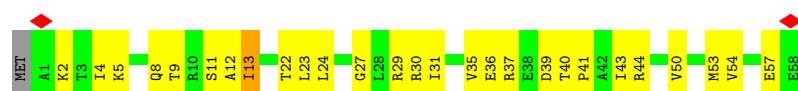
- Molecule 25: 50S ribosomal protein L29

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

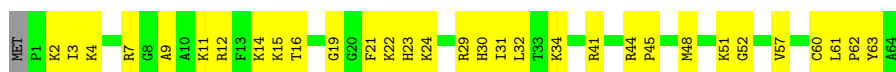
Chain 3: 



- Molecule 30: 50S ribosomal protein L34



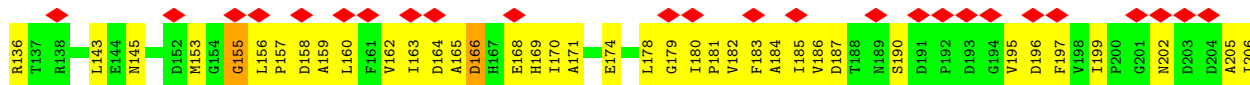
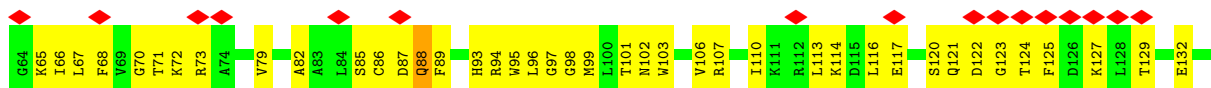
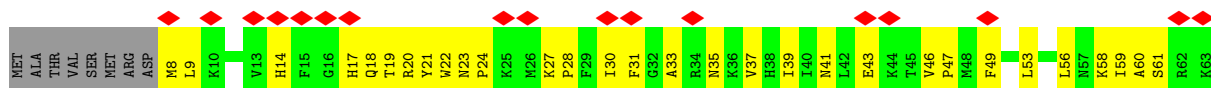
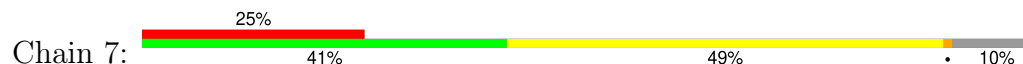
- Molecule 31: 50S ribosomal protein L35



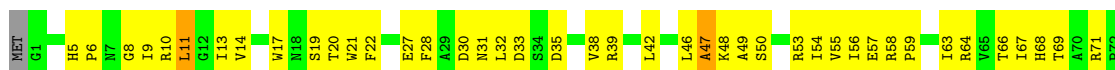
- Molecule 32: 50S ribosomal protein L36



- Molecule 33: 30S ribosomal protein S2



- Molecule 34: 30S ribosomal protein S3

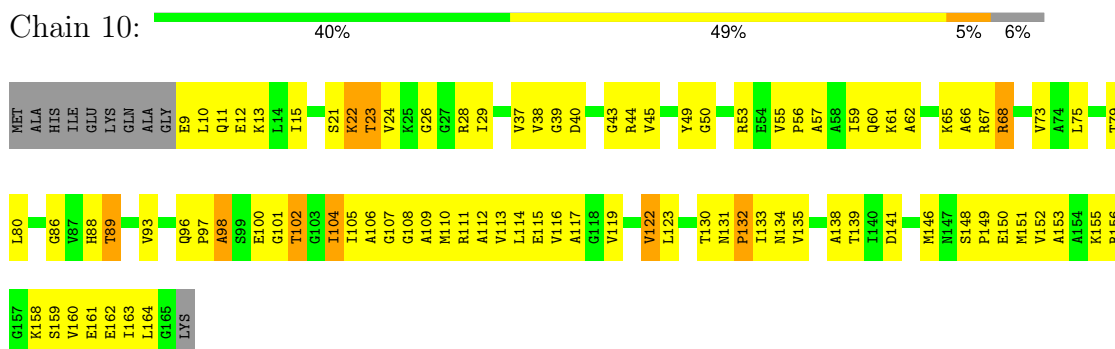




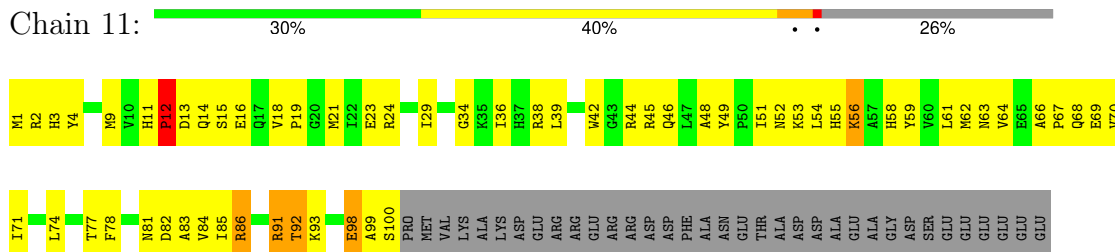
- Molecule 35: 30S ribosomal protein S4



- Molecule 36: 30S ribosomal protein S5



- Molecule 37: 30S ribosomal protein S6



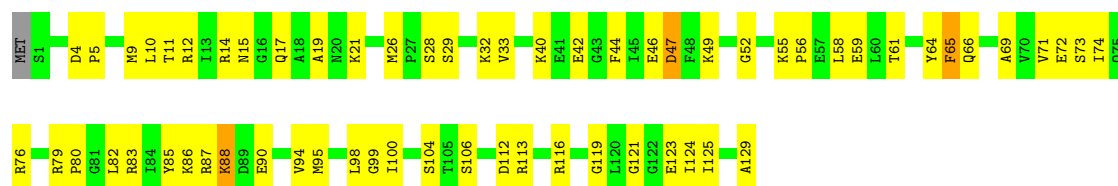
- Molecule 38: 30S ribosomal protein S7





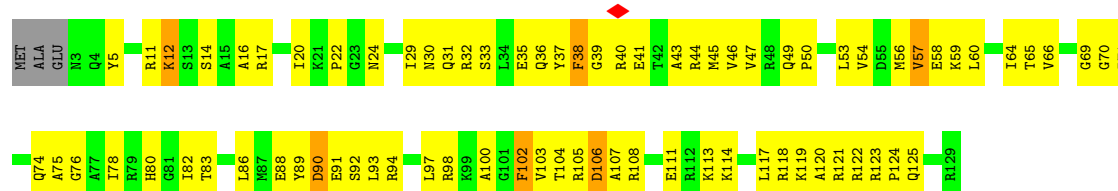
- Molecule 39: 30S ribosomal protein S8

Chain 13: 52% 45%



- Molecule 40: 30S ribosomal protein S9

Chain 14: 38% 55% 5%



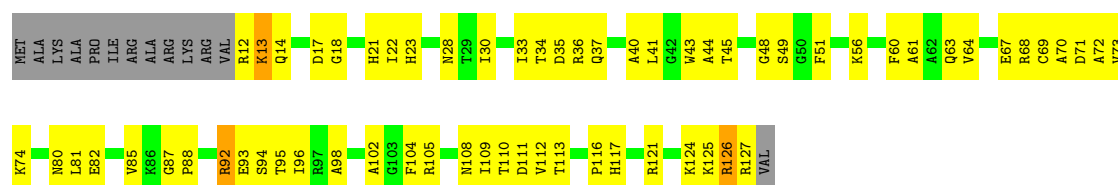
- Molecule 41: 30S ribosomal protein S10

Chain 15: 25% 66% 5%

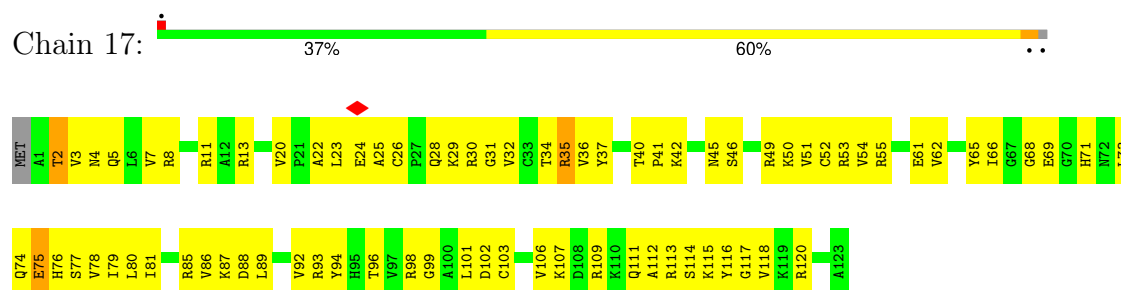


- Molecule 42: 30S ribosomal protein S11

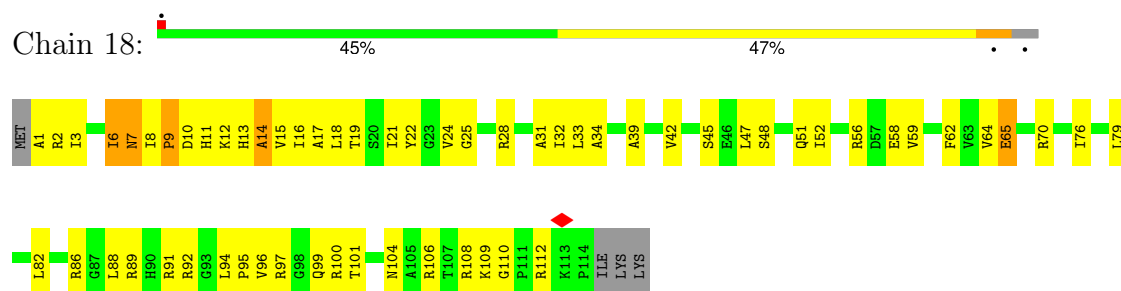
Chain 16: 40% 47% 10%



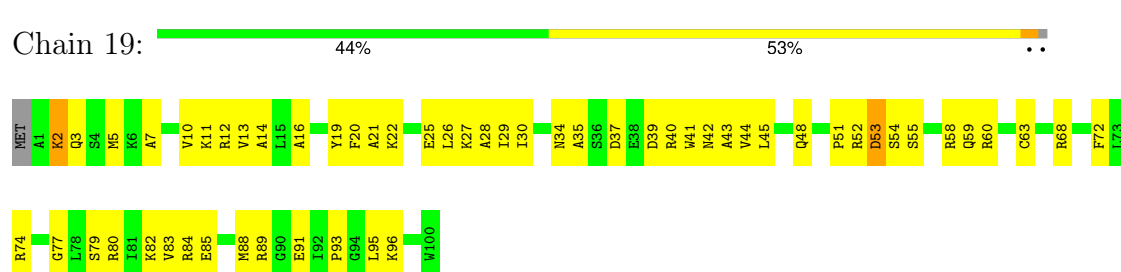
- Molecule 43: 30S ribosomal protein S12



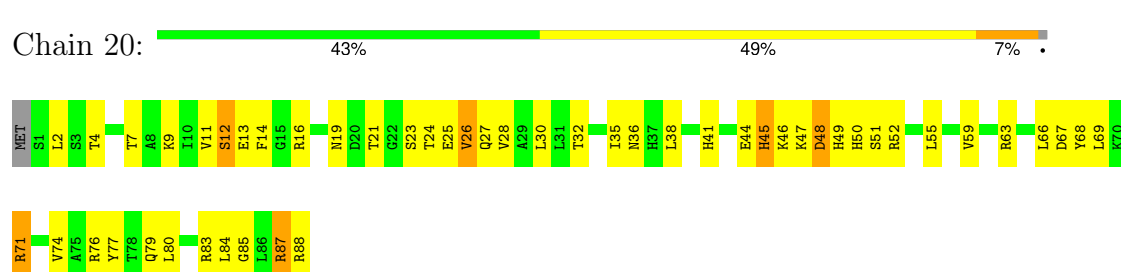
- Molecule 44: 30S ribosomal protein S13



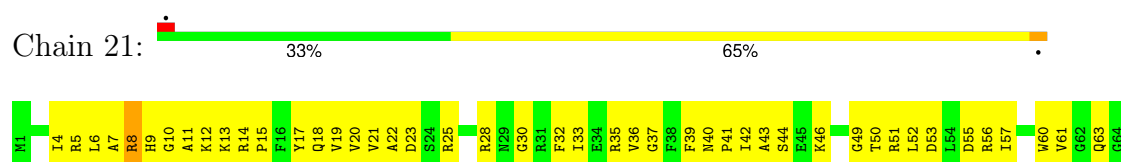
- Molecule 45: 30S ribosomal protein S14

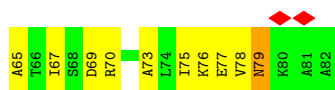


- Molecule 46: 30S ribosomal protein S15



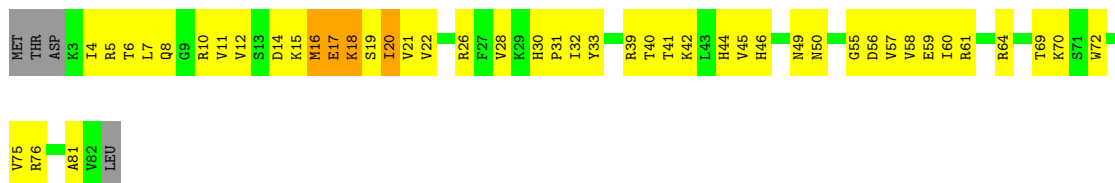
- Molecule 47: 30S ribosomal protein S16





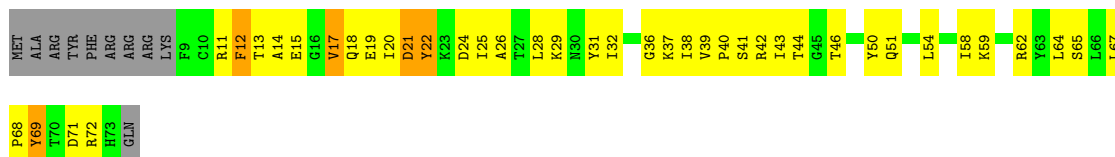
- Molecule 48: 30S ribosomal protein S17

Chain 22: 40% 50% 5% 5%



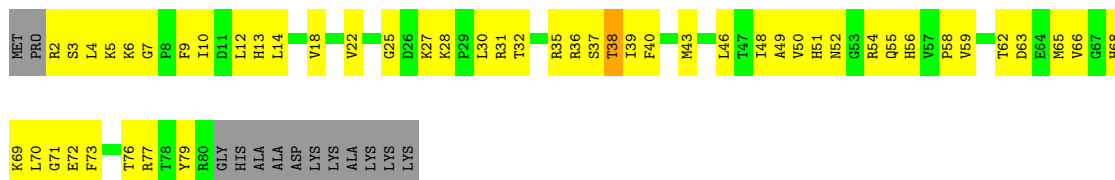
- Molecule 49: 30S ribosomal protein S18

Chain 23: 32% 48% 7% 13%



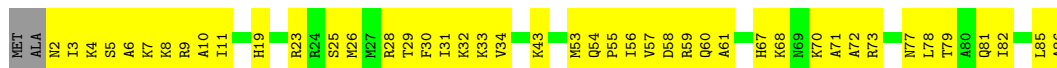
- Molecule 50: 30S ribosomal protein S19

Chain 24: 32% 53% 14%



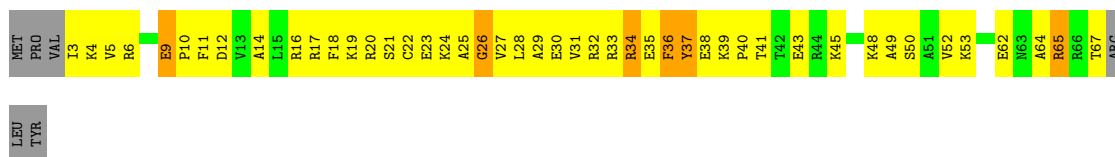
- Molecule 51: 30S ribosomal protein S20

Chain 25: 47% 51%



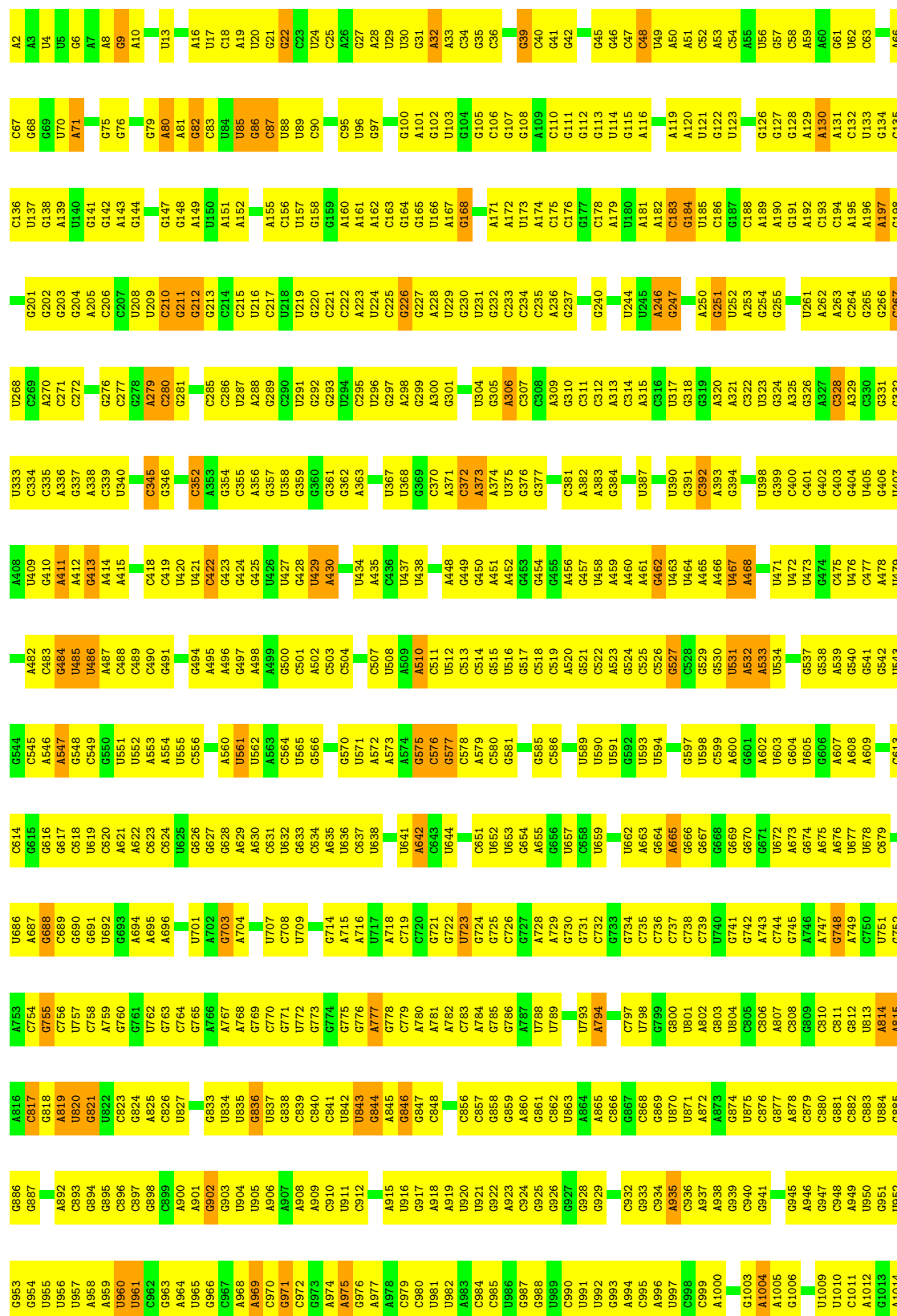
- Molecule 52: 30S ribosomal protein S21

Chain 26: 27% 56% 8% 8%



● Molecule 53: 16S ribosomal RNA

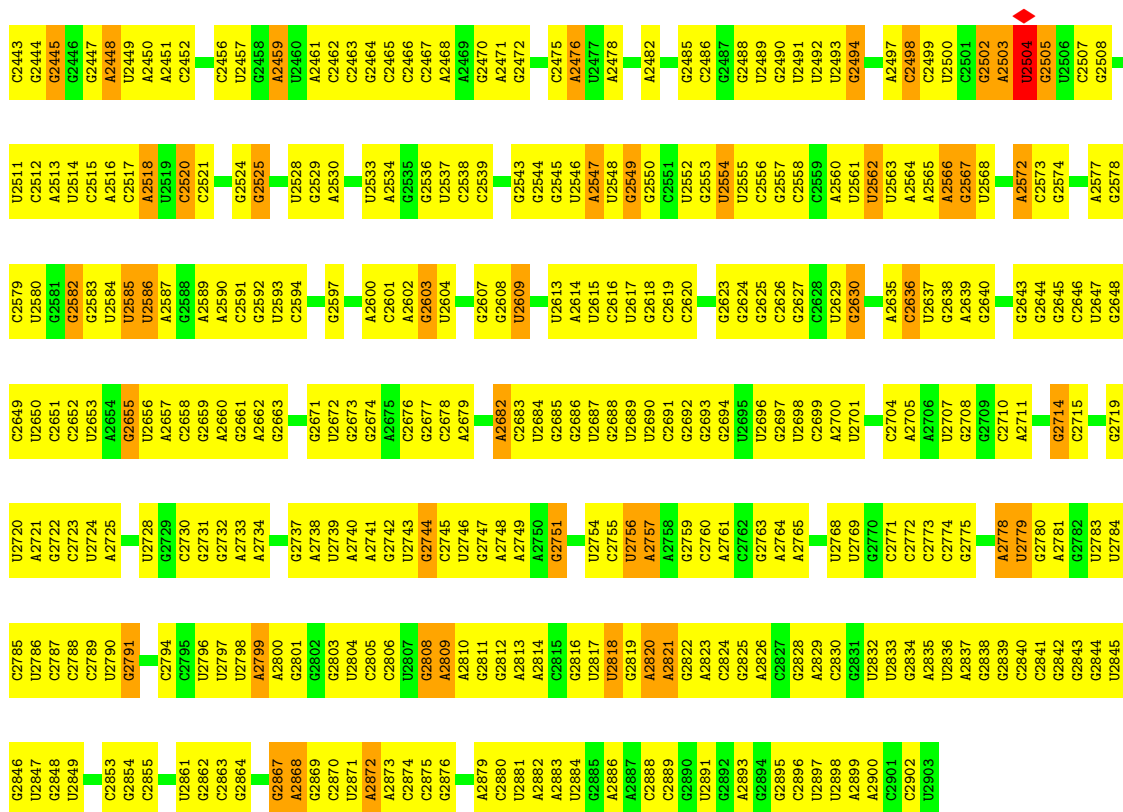
Chain 27:  27% 65% 8%





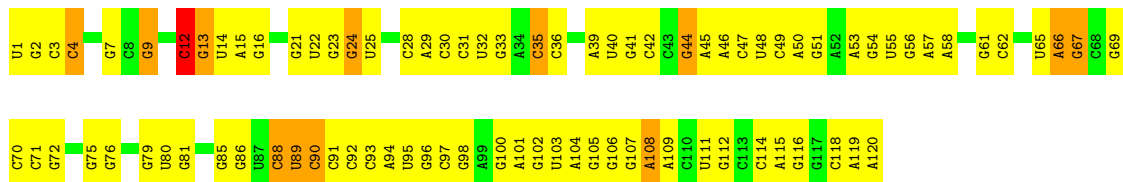
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G1345	C1270	G1202	C1140	C1077	C998	A933	C865	G799	C732	A670	A599	A538	U397
	A1272	A1205	U1141	U1078	U999	U934	A866	A800	G733	C671	G469	G468	U398
			A1142	C1079	A1000	C935	C867			C672	A470	G470	U399
			A1144	U1080	A1001	A936	U868	U803	C737	C673	A541	A441	G400
			C1145	A1081	C937	G938	U871	G805	G738	G674	C542	A401	A402
			C1146	U1082	G939	U872	U806	C806	A739		G543	U403	U404
			U1147	U1083	G940	C873	U807	U807	C740		C544	A405	A406
			U1148	U1084	A941	C876	G808	G808	A742		U546	G406	G407
			U1149	A1085	G942	C877	U810	G809	A743		A547	A477	A478
			C1150	A1086	A943	A877	U811	G811	A744		G548	A479	A480
			A1151	U1087		C879	U812	C812	G745		G549	A481	G409
			C1152	U1088	C946			U813	G746		C550	G410	G411
			C1153	A1089	A947			U814	C747		G551		
			G1154	A1090	C948			C815	G748		U552		
			A1155		G949			C816	A749		G553		
			A1156	U1094	G950			C817			U554		
			G1157	A1095	C951			C818	A752		U555		
			C1158	U1096	G952			G819	A753		A556		
			U1159	U1097	G953			A819	U754		C557		
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			C1161	U1099	U955			A821	A756		G559		
			G1162	G1099	U956			C822	A757		C560		
			U1163	C1100	C957			G823	G758		G561		
			C1164	U1101	C958			U824	C759		U562		
			A1165	C1102	U959			A825	G760		A563		
			G1166	A1103	A960			U826			C564		
			C1167	U1105	C961			C827	G763		C565		
			U1168	G1106	A896			U828	C698		A503		
			A1169	U1107	C898			U829	G765		A505		
			C1170	C1109	A899			G830	A764		A506		
			G1171	G1110	C901			C831	A699		G507		
			U1172	A1111	U967			U832	C634		A507		
			C1173	G1112	C968			A833	U703		C508		
			U1174	U1113	U969			C834	A705		C509		
			A1175		G969			G835	A637		U573		
			U1176		U970				A706		U574		
			G1177	C1117	G971			C838	G707		A575		
			C1178	C1118	A972			U839	G708		A576		
			U1179	G1119	A973			C840	U709		A514		
			A1180	U1120	C974				G710		A515		
			U1181	C1121	A975			A845	G711		C516		
			G1182	G1122	C915			U846			C517		
			U1183	C1123	G916			U847	U714		U448		
			C1184	G1124	A917			C848	A715		C518		
			U1185	G1125	A918			A849	A716		U519		
			G1186	A1126	C982			U850	C717		G520		
			U1187	A1127	A983			C851	A718		U521		
			C1188	A1127	U984			U852	G784		A522		
			U1189	G1128	C985			C853	G785		C523		
			G1190	U1129	C986				U720		C587		
			C1191	G1130	U987			C856	A721		U588		
			U1192	G1131	C987			A857	A722		C527		
			A1193	U1132	A988			C858	C723		A457		
			C1194	C1064	C989			G859	U724		A529		
			G1195	A1133	A990			U860	G725		C531		
			C1196	A1264	C991			A861	G726		A460		
			U1197	A1265				U862	A727		A532		
			C1198	G1135	C995			C863	G728		U594		
			U1199	G1136	U999			G864	A729		C533		
			G1200	G1137	C995			A863	G729		U595		
				U1138	A996				G797		C534		
											U464		
											G465		
											G466		

A2377	G2316	U2245	G2107	A2042	U1971	C1905	G1831	G1766	A1698	A1630	U1562	U1485	G1418
A2378	A2317	G2246	A2108	C2043	G1972	G1906	C1832	G1767	G1702	G1631	U1563	U1486	A1419
G2379	G2318	A2247	U2109	C2044	G1973	C1907	C1833	G1770	G1703	A1632	U1564	U1487	A1420
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A2381	U2249	G2186	G2112	C2046		G1910	C1838	A1772	A1634	A1635	G1566	G1490	G1424
G2382	U2321	G2260	U2113	G2047	U1982	U1911	C1839	A1773	U1709	G1636	G1567	G1491	G1425
G2383	A2322	U2187	U2113	G2048	G1983	A1912	G1840	C1774	G1710	U1637	U1568	G1492	G1426
A2384	G2323	U2188	A2114	G2049	G1989	A1913	U1841	C1775	G1711	C1638	A1569		
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A2386	G2325	G2190		A2051	U1991	U1915	C1843	U1777	G1713	A1640	A1572	G1500	G1429
U2387	C2326	C2380	A2191	A2052	U1992	A1916	C1844	U1778	U1714	A1641	G1573		
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G2389	A2328	G2193	A2120	C2055	U1993	G1917	G1847	A1780	U1716	G1643	C1577	A1505	A1431
U2390	U2329	U2194	G2121	G2056	C1994	A1918	A1848		G1717	C1644	U1577	U1506	G1432
G2391	G2330	U2195		G2057	C1995	A1919	A1849	A1784	G1718	G1645	C1578	C1507	A1433
A2392	G2331	C2264	U2122	A2058				A1785	G1719	A1646	A1579	A1508	A1436
U2393	G2332	U2197	G2128	G2061	C1998	U1923	U1852	A1786	U1720	G1647	A1580	A1509	
G2394	A2333	U2198	A2129	A2062	C2000	C1925	A1854	A1787	U1721	U1648	G1581	A1515	C1437
	A2334	C2207	G2135	G2063	C2001	U1926	A1855	C1788	A1722	G1649	U1584	G1516	U1439
U2397	A2335	U2203	A2132	C2065	A2002	A1928	G1857	C1790	C1726	A1650	U1585	G1517	U1440
G2398	A2336	G2271	G2133	G2066	G2004	A1928	G1857	A1791	C1727	G1651	C1586	U1520	U1441
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U2400	G2339	A2275	A2136	U2668	C2006	G1930		A1794	U1729	G1654	U1589		U1443
G2401	A2340	A2277	G2137	G2069	C2007	U1931	U1864	C1795	G1730	A1655	A1590	G1524	G1444
U2402	G2341	A2278	U2137	A2070	C2008	A1932	U1865	U1796	G1731	C1656	A1591	A1525	G1445
G2403	C2342	G2277	U2137	A2071	A2009	G1933	G1867	U1798	C1732	C1657	C1592	C1526	C1446
U2404	U2343	G2278	G2141	A2072	G2010	C1935		U1799	G1733	C1658	U1593	G1527	C1447
A2406	A2344	G2279	G2142	C2073	G2011	A1936	A1871	C1800	U1736	G1660	C1595	A1528	U1448
G2407	G2345	G2280	A2143	U2074	U2012	A1937	A1872	A1801	G1737	C1661	U1596	G1529	G1449
A2408	A2346	A2281	C2143	C2075	G2013	A1938	G1873	A1802	U1738	U1662	A1597	G1530	G1450
G2409	C2347	A2282	G2144	U2075	A2014	U1938	C1874	A1803	G1739	C1663	A1598	C1532	C1451
G2410	U2348	C2283	C2145		A2015	U1940	G1875	C1804	G1740	A1664	U1599	A1533	A1452
A2411	G2349	G2284	G2146	U2079	U2016		A1876	A1805	U1742	A1665	C1600	U1534	C1454
U2412	C2350	G2285	A2147	U2080	U2017	U1943	A1877	C1806	G1743	G1666	G1601	A1535	G1455
G2413	G2351	A2286	G2148	U2081	G2018		G1878	G1807	G1743	U1602	U1602	C1536	
A2414	A2352	G2287	U2149	A2082	A2019	U1946	C1879	A1808	A1744	A1669	A1603	G1537	U1458
G2415	G2353	A2288	C2150		A2020	C1947	U1880	A1809	A1745	C1670	C1604	G1538	G1459
C2416	C2354	U2291	G2151	U2086	A2021	G1948	C1881	A1810	A1746	U1671	C1605	U1539	U1460
A2417	G2355	G2292	C2152	G2087	C2022		U1882	G1811	U1747	C1606	C1606	G1540	C1461
U2418	U2356	G2293	G2153	A2088	C2023	U1951	U1883	G1814	G1748	C1674	C1607	C1541	C1462
G2419	G2357	A2294	G2156	C2089	G2024	A1952	G1884	A1815	A1749	C1675	A1608	U1542	C1463
U2420	A2358	U2295	G2157	A2090	C2025	A1953	A1885	C1816	G1750	A1676	A1609	G1543	G1464
G2421	G2359	G2296	A2158	C2091	U2026	G1954		G1817	U1751	A1677	C1610	A1544	G1465
C2422	C2360	A2297	G2159	U2092	G2027	U1955	A1889	G1818	C1752	A1678	C1611		
U2423	G2361	U2298	C2160	G2093	U2028	U1956	A1890	U1818	G1753	A1679	C1612	A1548	A1469
A2425	G2362	U2299	C2161	A2094	G2029	C1957	G1891	A1819	A1754	U1680	G1613	A1470	A1471
G2426	A2363	U2300	G2162	A2095	A2030	C1958	C1892	U1820	A1755	G1681	C1614	A1549	
A2427	G2364	U2301	C2163	C2096	A2031	G1959	G1896	A1822	G1756	G1682	C1615	C1550	
G2428	A2366	G2302	C2165	A2097	U2034		G1897	G1822	U1757	U1683	A1616	A1551	G1475
U2429	G2367	U2303	U2166	U2098	G2035	C1962	U1898	G1823	U1758	G1684	C1617		U1476
A2430	A2368	G2307	U2167	A2101	C2036	U1963	G1899	G1824	A1759	C1685	C1618	G1565	A1477
U2431	G2369	U2240	G2168	G2102	G2037	G1964	U1899	U1825	C1760	C1686	G1619	C1566	G1478
A2432	U2371	U2241	A2169	C2103	A2037	A1900	A1900	G1826	C1761	G1687	C1557	C1557	G1479
A2435	G2372	U2240	G2169	C2103	G2038	C1967	A1901	U1827	A1762	U1688	A1626	C1558	
G2437	G2373	A2241	A2170	C2104	G2039	G1968	A1902	G1828	G1763	A1689	G1627	U1559	G1482
U2440	C2374	G2242	A2171	U2105	G2040	A1969	G1903	A1829	C1764	A1690	C1628	U1560	A1483
G2442	A2376	U2244	A2173	U2106	U2041	A1970	G1904	C1830	U1765		U1629	G1454	U1484



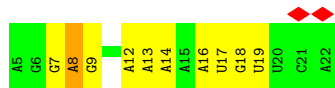
• Molecule 55: 5S ribosomal RNA

Chain 29: 28% 62% 10%



• Molecule 56: mRNA

Chain 30: 11% 44% 50% 6%

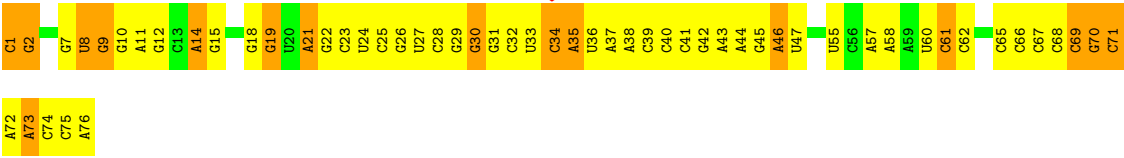
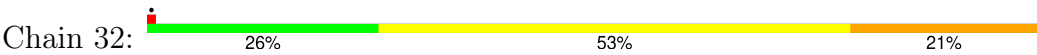


• Molecule 57: P site tRNA^{fmet}

Chain 31: 45% 53%



• Molecule 58: E-site tRNA^{fMet}



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 (\AA)	393.6, 393.6, 393.6	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	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	0.63	1/1115 (0.1%)	0.83	1/1510 (0.1%)
2	B	0.38	0/2121	0.71	0/2852
3	C	0.39	0/1586	0.69	1/2134 (0.0%)
4	D	0.44	0/1571	0.71	1/2113 (0.0%)
5	E	0.40	0/1434	0.64	0/1926
6	F	0.38	0/1343	0.67	1/1816 (0.1%)
7	G	0.49	0/1122	0.73	0/1515
8	H	0.60	0/1001	0.75	0/1350
9	I	0.60	0/1046	0.86	2/1410 (0.1%)
10	J	0.40	0/1152	0.64	0/1551
11	K	0.35	0/947	0.63	0/1268
12	L	0.36	0/1054	0.68	0/1403
13	M	0.39	0/1093	0.64	0/1460
14	N	0.37	0/973	0.62	0/1301
15	O	0.36	0/902	0.59	0/1209
16	P	0.37	0/929	0.67	1/1242 (0.1%)
17	Q	0.42	0/960	0.57	0/1278
18	R	0.41	0/829	0.70	1/1107 (0.1%)
19	S	0.34	0/864	0.60	0/1156
20	T	0.36	0/744	0.63	0/994
21	U	0.37	0/787	0.69	0/1051
22	V	0.40	0/766	0.61	0/1025
23	W	0.40	0/582	0.65	0/769
24	X	0.38	0/635	0.62	0/848
25	Y	0.40	0/510	0.60	0/677
26	Z	0.35	0/453	0.61	0/605
27	1	0.55	0/531	0.81	0/709
28	2	0.34	0/450	0.66	0/599
29	3	0.41	0/416	0.65	0/554
30	4	0.42	0/380	0.67	0/498
31	5	0.38	0/513	0.62	0/676
32	6	0.53	0/303	0.91	2/397 (0.5%)
33	7	0.46	0/1735	0.64	0/2338
34	8	0.39	0/1651	0.62	0/2225

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
35	9	0.37	0/1665	0.63	0/2227
36	10	0.36	0/1169	0.67	1/1573 (0.1%)
37	11	0.39	0/835	0.70	0/1128
38	12	0.35	0/1195	0.59	0/1602
39	13	0.35	0/989	0.66	0/1326
40	14	0.37	0/1034	0.64	0/1375
41	15	0.38	0/796	0.67	0/1077
42	16	0.38	0/885	0.71	0/1195
43	17	0.38	0/969	0.66	1/1300 (0.1%)
44	18	0.39	0/892	0.66	0/1193
45	19	0.38	0/817	0.57	0/1088
46	20	0.34	0/722	0.61	0/964
47	21	0.39	0/659	0.62	0/884
48	22	0.36	0/657	0.67	0/881
49	23	0.42	0/544	0.66	0/731
50	24	0.48	0/652	0.70	0/877
51	25	0.37	0/671	0.52	0/888
52	26	0.45	0/550	0.64	0/728
53	27	0.46	1/36967 (0.0%)	0.67	1/57666 (0.0%)
54	28	0.49	1/69801 (0.0%)	0.67	5/108894 (0.0%)
55	29	0.40	1/2876 (0.0%)	0.66	0/4483
56	30	0.62	0/436	0.69	0/679
57	31	0.45	1/1836 (0.1%)	0.66	0/2859
58	32	0.71	1/1835 (0.1%)	0.68	0/2857
All	All	0.46	6/161950 (0.0%)	0.67	18/242041 (0.0%)

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

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	29	1	U	OP3-P	-6.99	1.52	1.61
53	27	2	A	OP3-P	-6.92	1.52	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	31	1	C	OP3-P	-6.89	1.52	1.61
54	28	1	G	OP3-P	-6.88	1.52	1.61
58	32	1	C	OP3-P	-6.86	1.52	1.61

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	28	2504	U	N1-C1'-C2'	7.12	123.26	114.00
32	6	19	ARG	NE-CZ-NH1	-6.43	117.09	120.30
43	17	115	LYS	N-CA-C	-5.96	94.89	111.00
1	A	678	GLY	N-CA-C	5.72	127.41	113.10
16	P	113	LEU	CA-CB-CG	5.67	128.34	115.30

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

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	102	0
2	B	2082	0	2157	138	0
3	C	1565	0	1616	96	0
4	D	1552	0	1619	118	0
5	E	1410	0	1447	121	0
6	F	1323	0	1374	92	0
7	G	1111	0	1148	84	0
8	H	988	0	1025	127	0
9	I	1032	0	1088	128	0
10	J	1129	0	1162	70	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	K	938	0	1012	68	0
12	L	1045	0	1117	73	0
13	M	1074	0	1157	47	0
14	N	960	0	1000	52	0
15	O	892	0	923	57	0
16	P	917	0	965	80	0
17	Q	947	0	1022	71	0
18	R	816	0	839	60	0
19	S	857	0	922	53	0
20	T	738	0	807	39	0
21	U	779	0	834	64	0
22	V	753	0	780	37	0
23	W	575	0	592	33	0
24	X	625	0	655	44	0
25	Y	509	0	543	38	0
26	Z	449	0	491	25	0
27	1	522	0	521	47	0
28	2	444	0	461	40	0
29	3	409	0	440	14	0
30	4	377	0	418	29	0
31	5	504	0	574	27	0
32	6	302	0	343	26	0
33	7	1704	0	1732	104	0
34	8	1624	0	1699	99	0
35	9	1643	0	1710	121	0
36	10	1156	0	1199	90	0
37	11	817	0	808	71	0
38	12	1181	0	1240	79	0
39	13	979	0	1034	64	0
40	14	1022	0	1070	98	0
41	15	786	0	828	81	0
42	16	869	0	878	67	0
43	17	955	0	1019	100	0
44	18	883	0	944	73	0
45	19	805	0	847	58	0
46	20	714	0	737	46	0
47	21	649	0	666	59	0
48	22	648	0	691	55	0
49	23	535	0	552	44	0
50	24	637	0	665	72	0
51	25	665	0	714	46	0
52	26	544	0	579	59	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	27	33016	0	16617	1316	0
54	28	62322	0	31345	2457	0
55	29	2572	0	1302	116	0
56	30	388	0	196	10	0
57	31	1644	0	836	31	0
58	32	1643	0	836	66	0
All	All	149128	0	100926	6677	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 6677 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	22
3	C	207/209 (99%)	183 (88%)	17 (8%)	7 (3%)	3	25
4	D	199/201 (99%)	162 (81%)	28 (14%)	9 (4%)	2	20
5	E	175/179 (98%)	140 (80%)	31 (18%)	4 (2%)	5	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	174/177 (98%)	145 (83%)	27 (16%)	2 (1%)	12	45
7	G	147/149 (99%)	115 (78%)	23 (16%)	9 (6%)	1	16
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	21
10	J	140/142 (99%)	123 (88%)	13 (9%)	4 (3%)	3	27
11	K	120/123 (98%)	102 (85%)	12 (10%)	6 (5%)	1	19
12	L	141/144 (98%)	110 (78%)	25 (18%)	6 (4%)	2	21
13	M	134/136 (98%)	115 (86%)	16 (12%)	3 (2%)	5	32
14	N	118/127 (93%)	96 (81%)	18 (15%)	4 (3%)	3	25
15	O	114/117 (97%)	100 (88%)	10 (9%)	4 (4%)	3	24
16	P	112/115 (97%)	99 (88%)	11 (10%)	2 (2%)	7	35
17	Q	115/118 (98%)	105 (91%)	10 (9%)	0	100	100
18	R	101/103 (98%)	84 (83%)	13 (13%)	4 (4%)	2	22
19	S	108/110 (98%)	95 (88%)	8 (7%)	5 (5%)	2	20
20	T	91/100 (91%)	77 (85%)	8 (9%)	6 (7%)	1	15
21	U	100/104 (96%)	83 (83%)	8 (8%)	9 (9%)	0	10
22	V	92/94 (98%)	79 (86%)	12 (13%)	1 (1%)	12	45
23	W	73/85 (86%)	66 (90%)	6 (8%)	1 (1%)	9	39
24	X	75/78 (96%)	67 (89%)	5 (7%)	3 (4%)	2	22
25	Y	61/63 (97%)	53 (87%)	5 (8%)	3 (5%)	2	19
26	Z	56/59 (95%)	52 (93%)	3 (5%)	1 (2%)	7	35
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	34
29	3	48/55 (87%)	45 (94%)	2 (4%)	1 (2%)	5	33
30	4	44/46 (96%)	40 (91%)	4 (9%)	0	100	100
31	5	62/65 (95%)	54 (87%)	6 (10%)	2 (3%)	3	26
32	6	36/38 (95%)	29 (81%)	6 (17%)	1 (3%)	4	28
33	7	216/241 (90%)	170 (79%)	36 (17%)	10 (5%)	2	20
34	8	204/233 (88%)	179 (88%)	20 (10%)	5 (2%)	4	30
35	9	203/206 (98%)	167 (82%)	22 (11%)	14 (7%)	1	14
36	10	155/167 (93%)	117 (76%)	26 (17%)	12 (8%)	1	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	11	98/135 (73%)	77 (79%)	13 (13%)	8 (8%)	1	11
38	12	149/179 (83%)	127 (85%)	18 (12%)	4 (3%)	4	29
39	13	127/130 (98%)	116 (91%)	8 (6%)	3 (2%)	5	30
40	14	125/130 (96%)	105 (84%)	10 (8%)	10 (8%)	1	12
41	15	96/103 (93%)	75 (78%)	16 (17%)	5 (5%)	1	18
42	16	114/129 (88%)	95 (83%)	13 (11%)	6 (5%)	1	18
43	17	121/124 (98%)	91 (75%)	24 (20%)	6 (5%)	1	19
44	18	112/118 (95%)	98 (88%)	8 (7%)	6 (5%)	1	18
45	19	98/101 (97%)	80 (82%)	13 (13%)	5 (5%)	1	18
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	16
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	12
50	24	77/92 (84%)	64 (83%)	11 (14%)	2 (3%)	4	29
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	20

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%)	121 (100%)	0	100	100
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
5	E	148/150 (99%)	147 (99%)	1 (1%)	81	86
6	F	137/138 (99%)	136 (99%)	1 (1%)	81	86
7	G	114/114 (100%)	114 (100%)	0	100	100
8	H	100/123 (81%)	100 (100%)	0	100	100
9	I	109/110 (99%)	109 (100%)	0	100	100
10	J	116/116 (100%)	116 (100%)	0	100	100
11	K	103/104 (99%)	102 (99%)	1 (1%)	73	81
12	L	102/103 (99%)	102 (100%)	0	100	100
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%)	73	81
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%)	83 (100%)	0	100	100
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%)	56	72
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%)	38 (100%)	0	100	100
31	5	51/52 (98%)	51 (100%)	0	100	100
32	6	34/34 (100%)	34 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	172 (100%)	0	100	100
36	10	119/126 (94%)	119 (100%)	0	100	100
37	11	87/116 (75%)	86 (99%)	1 (1%)	70	79
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%)	89 (100%)	0	100	100
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%)	4966 (100%)	6 (0%)	92	95

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	P	113	LEU
27	1	37	CYS
37	11	12	PRO
6	F	117	PRO
5	E	174	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 94 such sidechains are listed below:

Mol	Chain	Res	Type
33	7	189	ASN
40	14	4	GLN
35	9	73	ASN
37	11	63	ASN
42	16	80	ASN

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%)	386 (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%)	594 (12%)	30 (0%)

5 of 594 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 [i](#)

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.

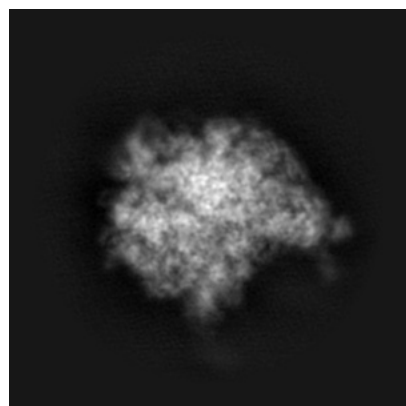
6 Map visualisation [i](#)

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.

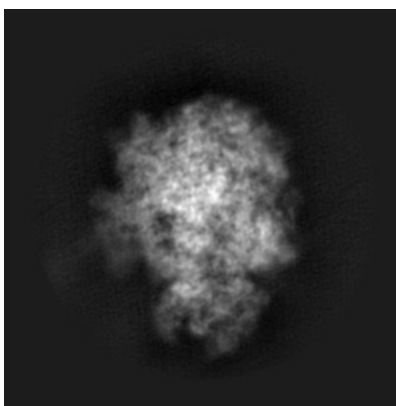
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

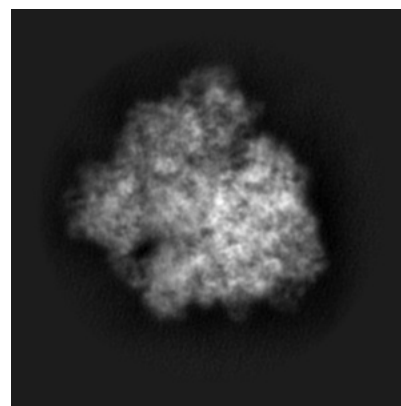
6.1.1 Primary map



X

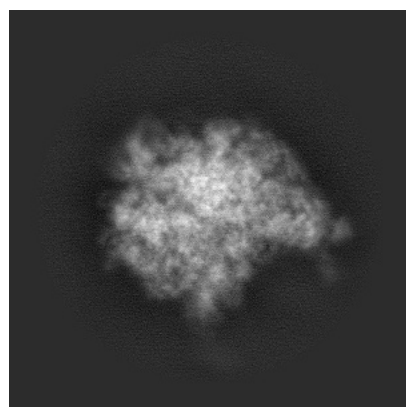


Y

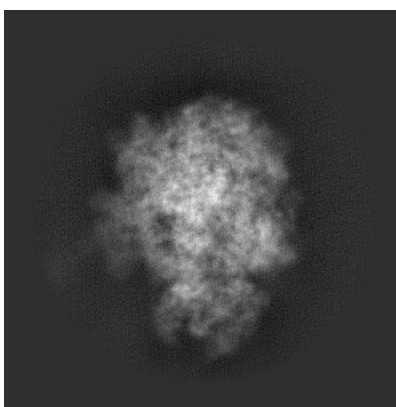


Z

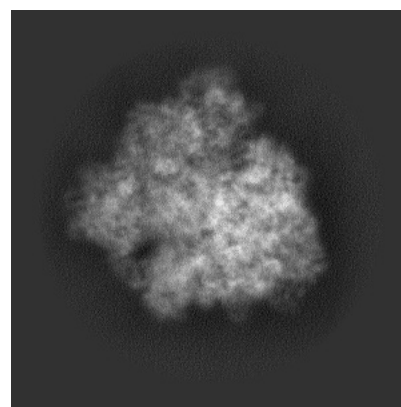
6.1.2 Raw map



X



Y

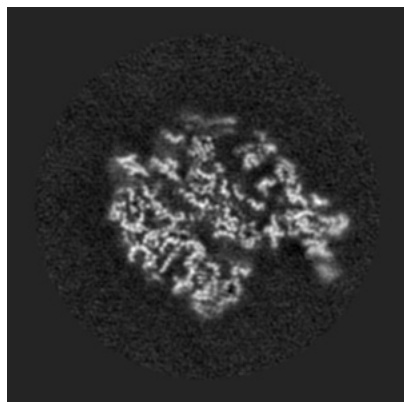


Z

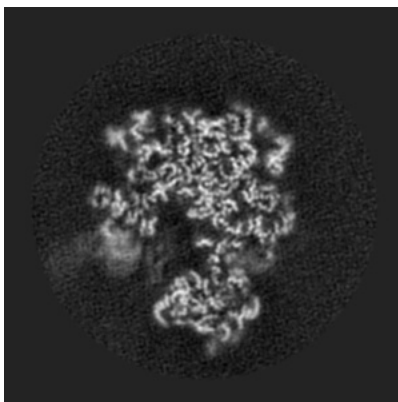
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

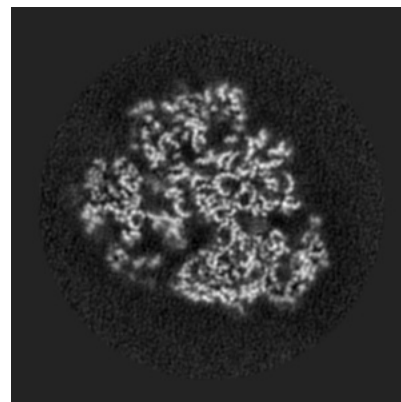
6.2.1 Primary map



X Index: 240

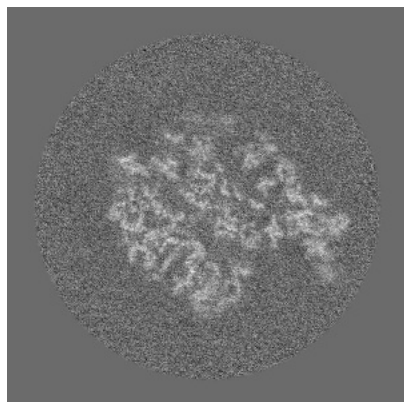


Y Index: 240

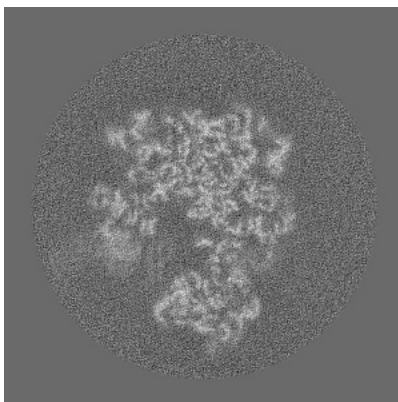


Z Index: 240

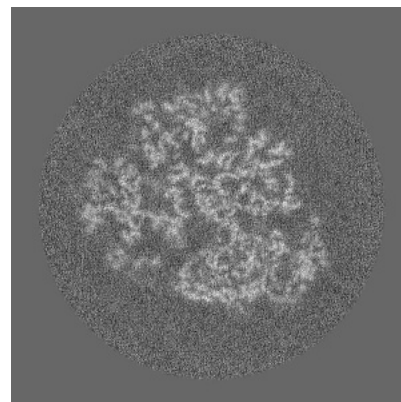
6.2.2 Raw map



X Index: 240



Y Index: 240

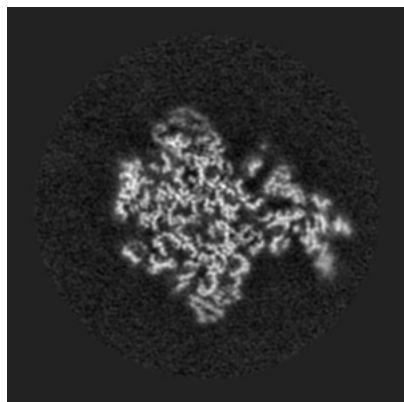


Z Index: 240

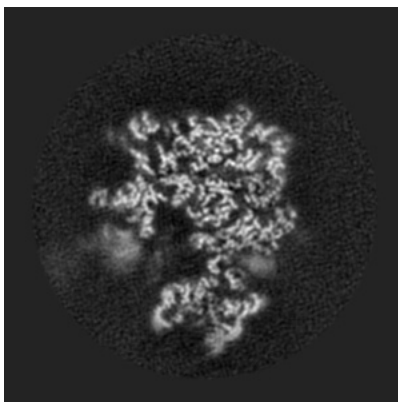
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

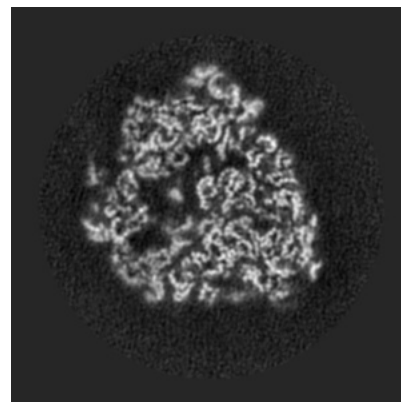
6.3.1 Primary map



X Index: 249

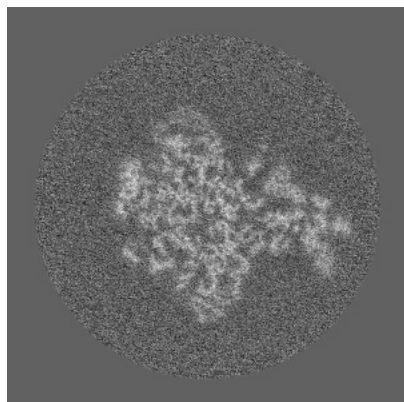


Y Index: 247

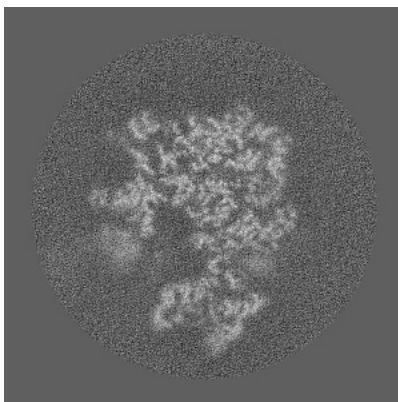


Z Index: 225

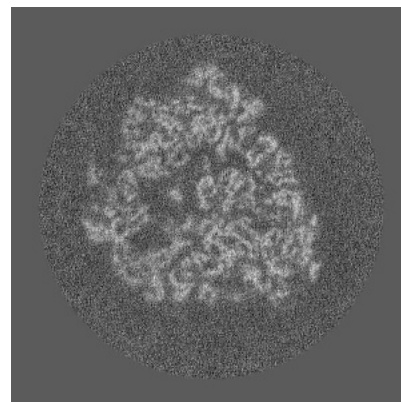
6.3.2 Raw map



X Index: 249



Y Index: 247

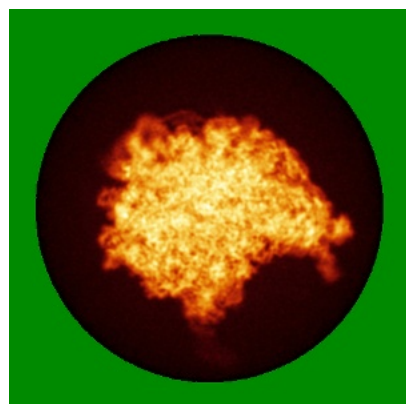


Z Index: 225

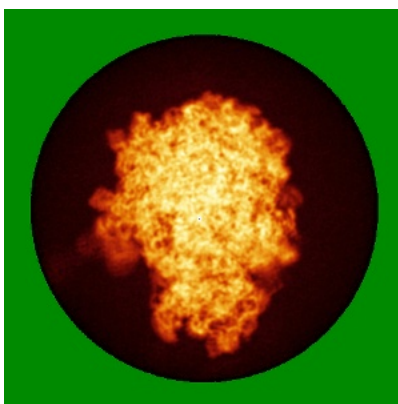
The images above show the largest variance slices of the map in three orthogonal directions.

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

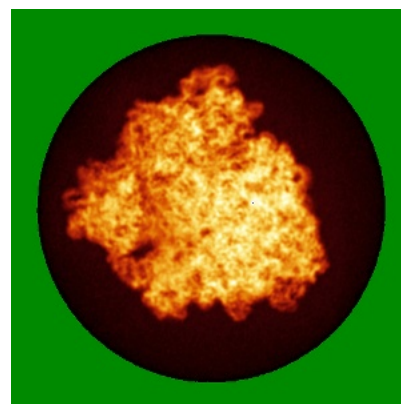
6.4.1 Primary map



X

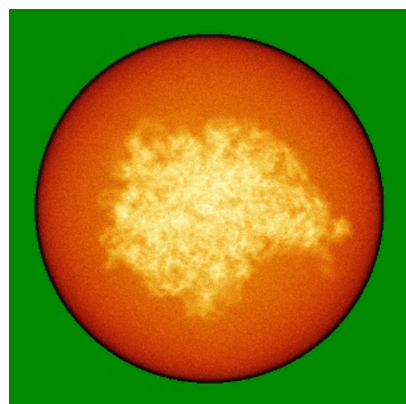


Y

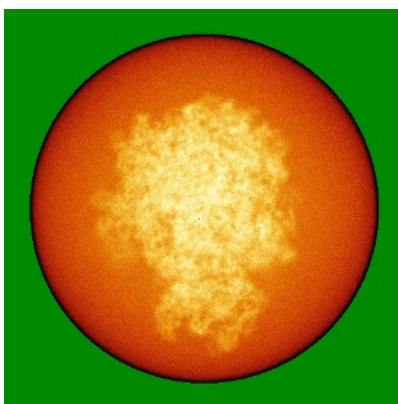


Z

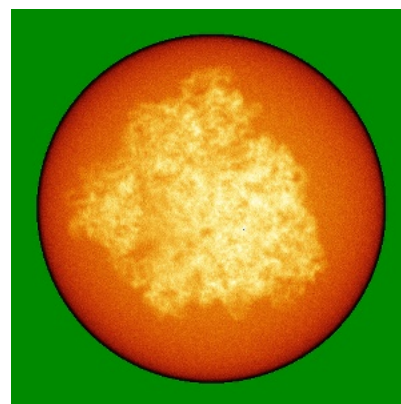
6.4.2 Raw map



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



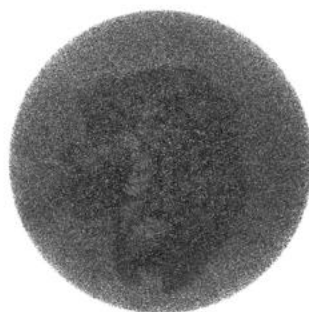
Z

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.

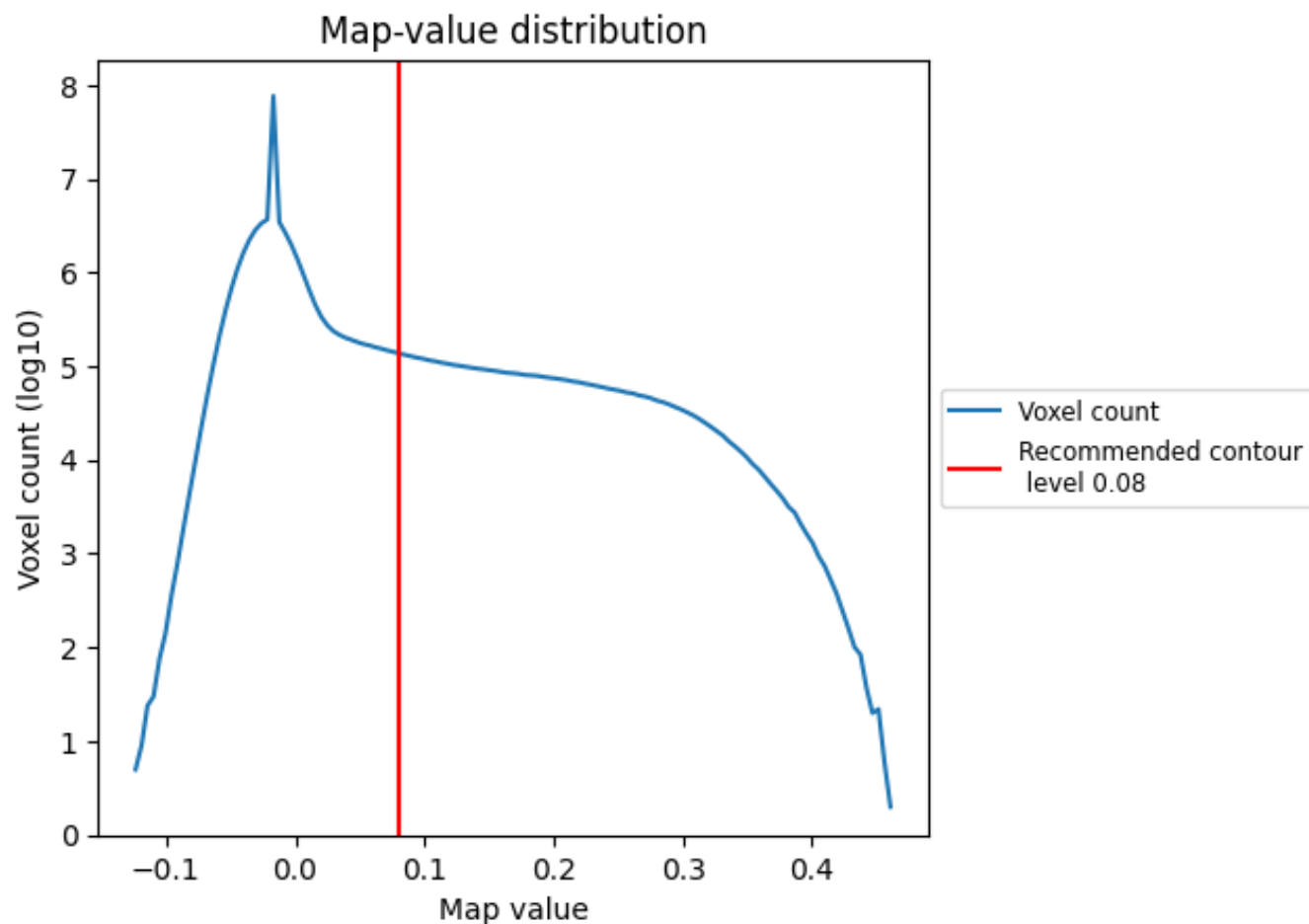
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

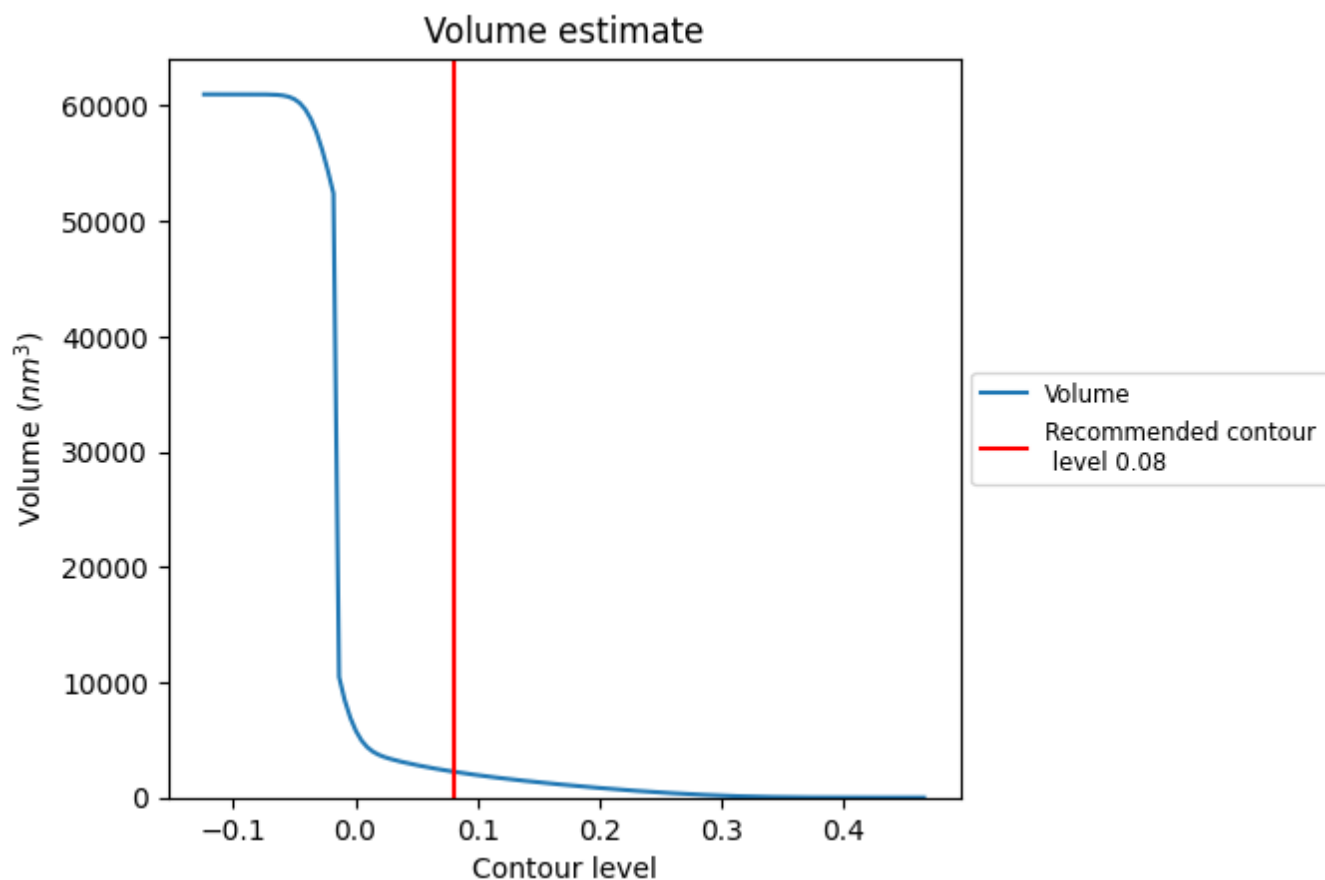
This section contains the results of statistical analysis of the map.

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.

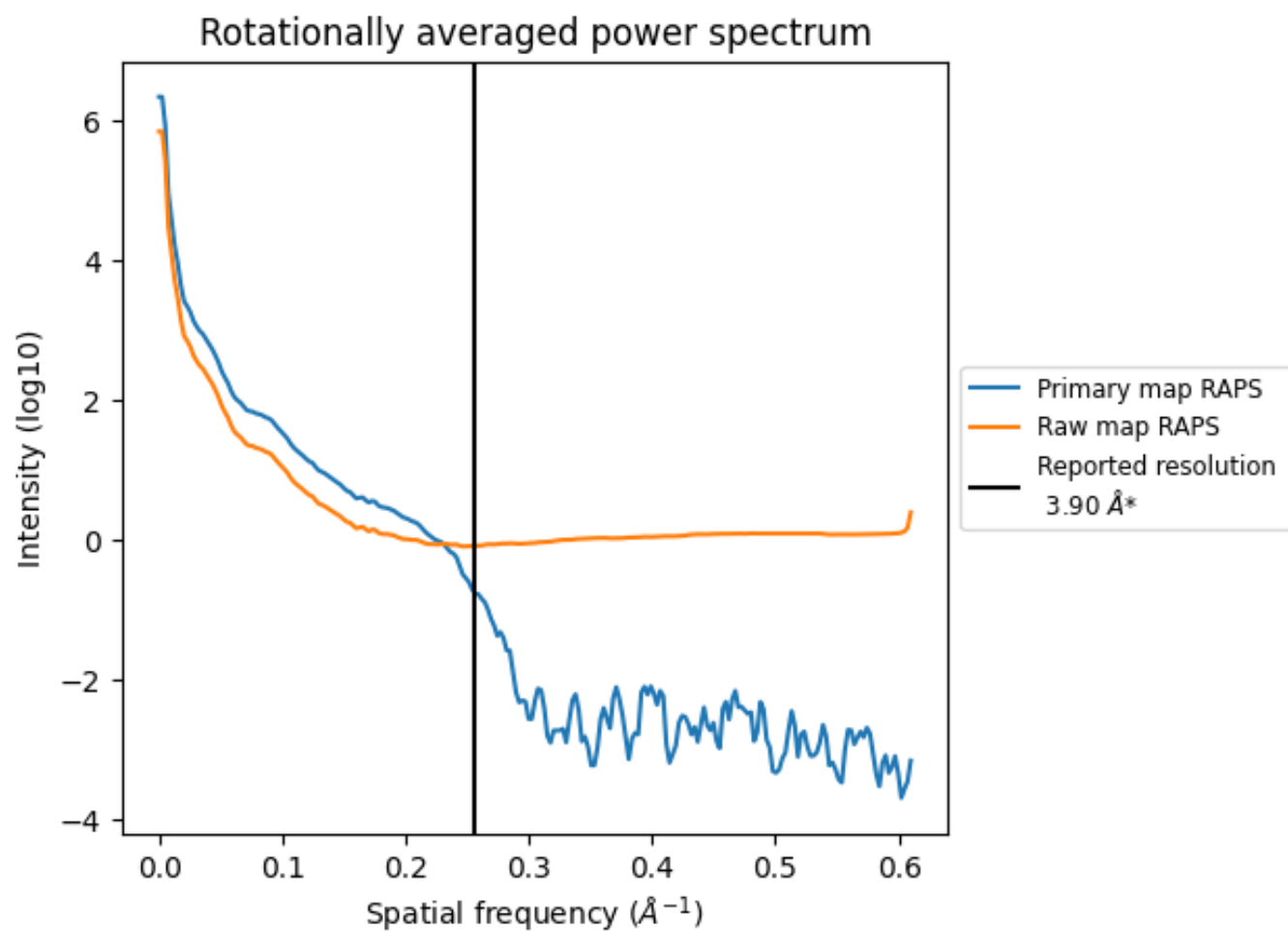
7.2 Volume estimate [i](#)



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 ⓘ

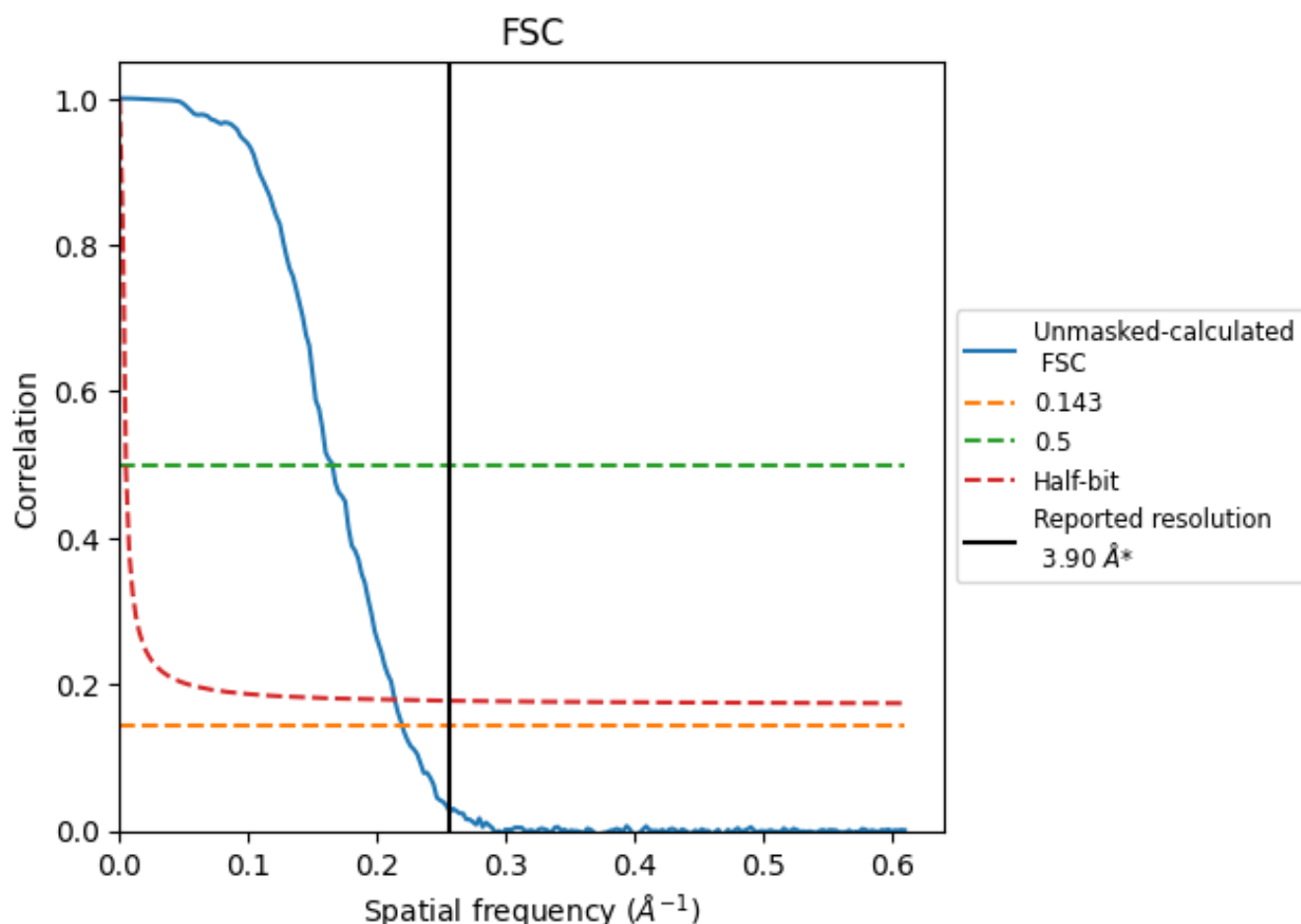


*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

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](#)

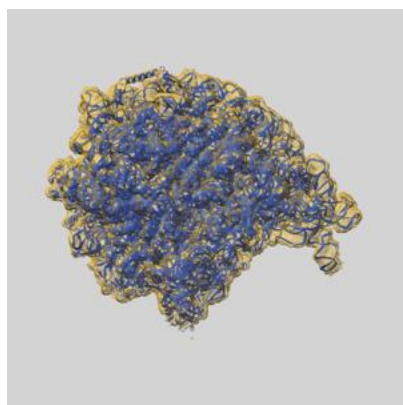
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.55	6.05	4.68

*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 %

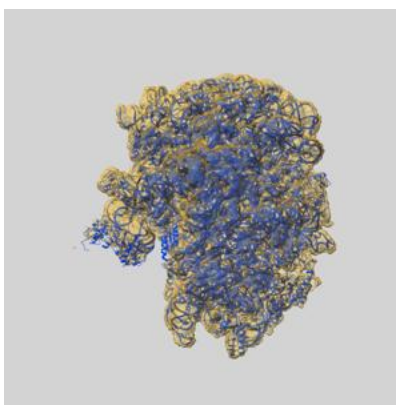
9 Map-model fit [i](#)

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](#).

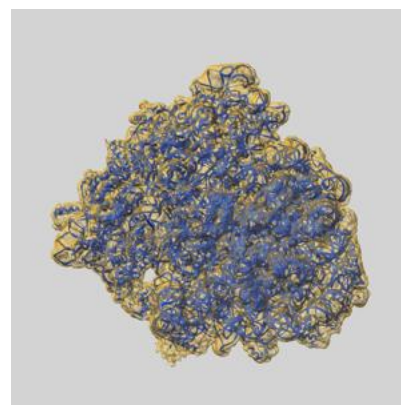
9.1 Map-model overlay [i](#)



X



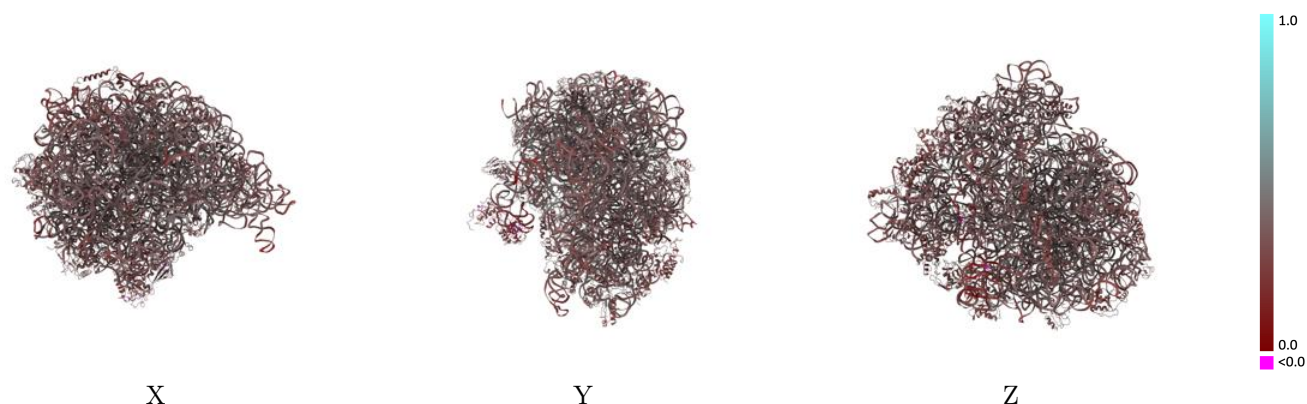
Y



Z

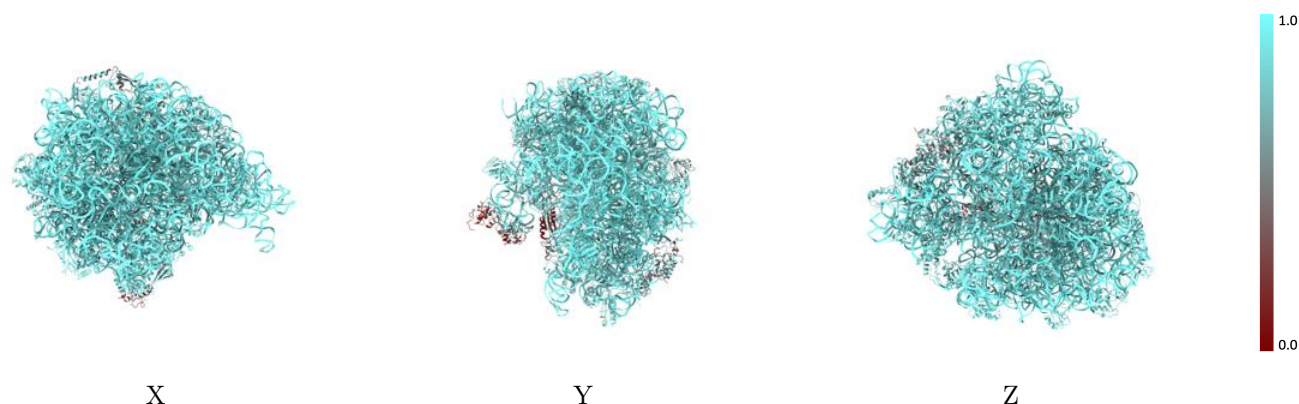
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



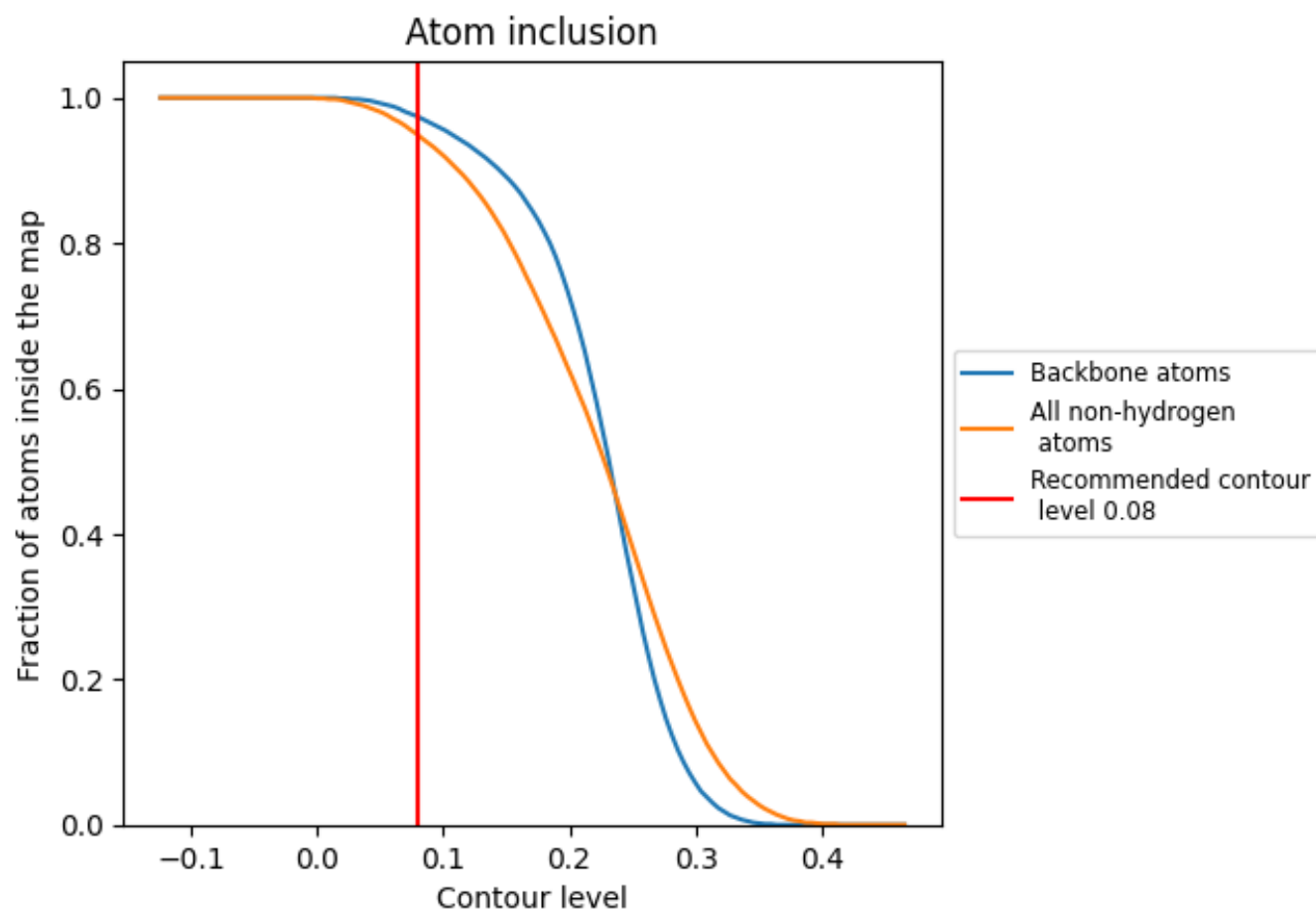
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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