



## wwPDB EM Validation Summary Report ⓘ

Nov 20, 2022 – 09:06 AM EST

PDB ID : 4V6K  
EMDB ID : EMD-1849  
Title : Structural insights into cognate vs. near-cognate discrimination during decoding.  
Authors : Agirrezabala, X.; Schreiner, E.; Trabuco, L.G.; Lei, J.; Ortiz-Meoz, R.F.; Schulten, K.; Green, R.; Frank, J.  
Deposited on : 2011-01-07  
Resolution : 8.25 Å(reported)  
Based on initial model : 2I2V

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

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

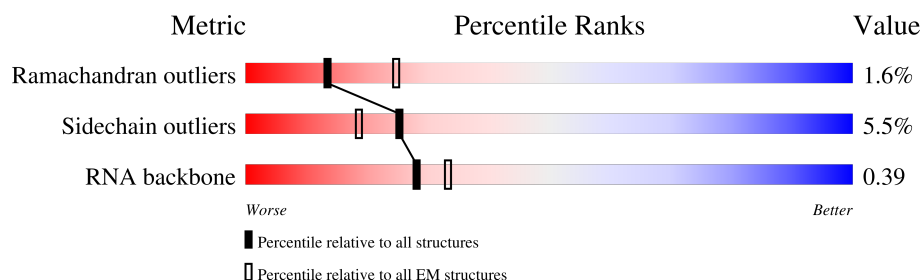
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 8.25 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	AA	120	<div> <div>33%</div> <div>45%</div> <div>18%</div> <div>.</div> </div>
2	AB	2904	<div> <div>25%</div> <div>49%</div> <div>23%</div> <div>.</div> </div>
3	AC	234	<div> <div>17%</div> <div>93%</div> <div>7%</div> </div>
4	AD	273	<div> <div>92%</div> <div>7%</div> </div>
5	AE	209	<div> <div>92%</div> <div>8%</div> </div>
6	AF	201	<div> <div>95%</div> <div>5%</div> </div>
7	AG	179	<div> <div>92%</div> <div>7%</div> <div>..</div> </div>
8	AH	177	<div> <div>90%</div> <div>10%</div> <div>.</div> </div>

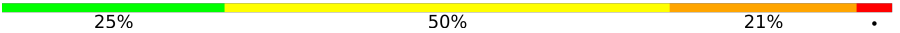
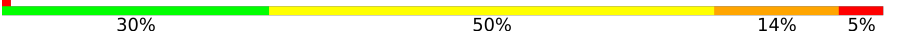
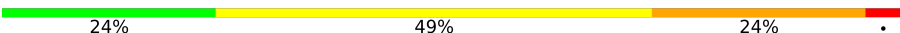
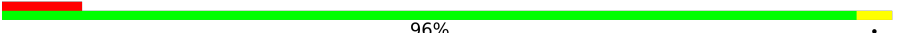











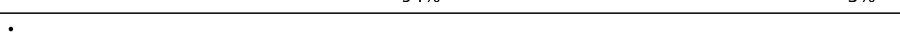

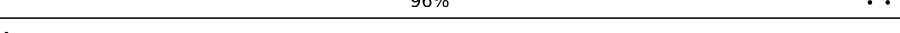

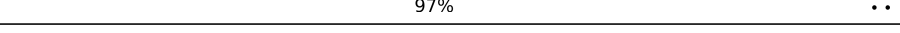
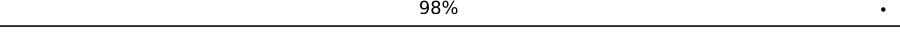
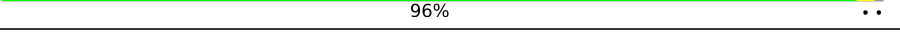


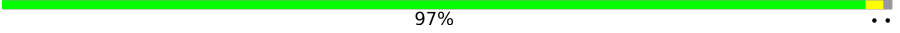
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Mol	Chain	Length	Quality of chain
9	AI	149	
10	AJ	142	
11	AK	142	
12	AL	123	
13	AM	144	
14	AN	136	
15	AO	127	
16	AP	117	
17	AQ	115	
18	AR	118	
19	AS	103	
20	AT	110	
21	AU	100	
22	AV	104	
23	AW	94	
24	AX	85	
25	AY	78	
26	AZ	63	
27	Aa	59	
28	Ab	70	
29	Ac	57	
30	Ad	55	
31	Ae	46	
32	Af	65	
33	Ag	38	

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Mol	Chain	Length	Quality of chain
34	BA	1542	
35	BB	76	
35	BE	76	
36	BC	393	
37	BD	24	
38	BF	241	
39	BG	233	
40	BH	206	
41	BI	167	
42	BJ	135	
43	BK	179	
44	BL	130	
45	BM	130	
46	BN	103	
47	BO	129	
48	BP	124	
49	BQ	118	
50	BR	101	
51	BS	89	
52	BT	82	
53	BU	84	
54	BV	75	
55	BW	92	
56	BX	87	
57	BY	71	

## 2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 153634 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 RNA chain called ribosomal RNA 5S.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	120	Total	C	N	O	P	0	0
			2566	1144	468	835	119		

- Molecule 2 is a RNA chain called ribosomal RNA 23S.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AB	2904	Total	C	N	O	P	0	0
			62351	27824	11469	20155	2903		

- Molecule 3 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AC	234	Total	C	N	O	S	0	0
			1733	1081	315	330	7		

- Molecule 4 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AD	272	Total	C	N	O	S	0	0
			2092	1294	425	366	7		

- Molecule 5 is a protein called 50S ribosomal protein L3.

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

- Molecule 6 is a protein called 50S ribosomal protein L4.

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

- Molecule 7 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AG	178	Total	C	N	O	S	0	0
			1420	905	251	258	6		

- Molecule 8 is a protein called 50S ribosomal protein L6.

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

- Molecule 9 is a protein called 50S ribosomal protein L9.

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

- Molecule 10 is a protein called 50S ribosomal protein L11.

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

- Molecule 11 is a protein called 50S ribosomal protein L13.

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

- Molecule 12 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AL	123	Total	C	N	O	S	0	0
			947	593	181	167	6		

- Molecule 13 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AM	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 14 is a protein called 50S ribosomal protein L16.

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

- Molecule 15 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AO	127	Total	C	N	O	S	0	0
			1008	621	204	178	5		

- Molecule 16 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AP	117	Total	C	N	O	S	0	0
			900	557	179	163	1		

- Molecule 17 is a protein called 50S ribosomal protein L19.

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

- Molecule 18 is a protein called 50S ribosomal protein L20.

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

- Molecule 19 is a protein called 50S ribosomal protein L21.

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

- Molecule 20 is a protein called 50S ribosomal protein L22.

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

- Molecule 21 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AU	100	Total	C	N	O	S	0	0
			787	496	146	143	2		

- Molecule 22 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AV	103	Total	C	N	O	S	0	0
			789	498	148	143			

- Molecule 23 is a protein called 50S ribosomal protein L25.

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

- Molecule 24 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	AX	84	Total	C	N	O	S	0	0
			634	391	129	113	1		

- Molecule 25 is a protein called 50S ribosomal protein L28.

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

- Molecule 26 is a protein called 50S ribosomal protein L29.

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

- Molecule 27 is a protein called 50S ribosomal protein L30.

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

- Molecule 28 is a protein called 50S ribosomal protein L31.



Mol	Chain	Residues	Atoms					AltConf	Trace
28	Ab	70	Total	C	N	O	S	0	0
			549	339	104	100	6		

- Molecule 29 is a protein called 50S ribosomal protein L32.

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

- Molecule 30 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Ad	54	Total	C	N	O	S	0	0
			441	284	81	76			

- Molecule 31 is a protein called 50S ribosomal protein L34.

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

- Molecule 32 is a protein called 50S ribosomal protein L35.

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

- Molecule 33 is a protein called 50S ribosomal protein L36.

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

- Molecule 34 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	BA	1542	Total	C	N	O	P	0	0
			33089	14767	6064	10717	1541		

- Molecule 35 is a RNA chain called A/T-site tRNA Phe.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	BB	76	Total	C	N	O	P	S	0	0
			1635	735	291	532	75	2		
35	BE	76	Total	C	N	O	P	S	0	0
			1635	735	291	532	75	2		

- Molecule 36 is a protein called Elongation factor Tu 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	BC	393	Total	C	N	O	S	0	0
			3036	1918	523	582	13		

- Molecule 37 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	BD	24	Total	C	N	O	P	0	0
			495	222	68	181	24		

- Molecule 38 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	BF	240	Total	C	N	O	S	0	0
			1872	1180	332	352	8		

- Molecule 39 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	BG	232	Total	C	N	O	S	0	0
			1822	1149	346	323	4		

- Molecule 40 is a protein called 30S ribosomal protein S4.

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

- Molecule 41 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	BI	166	Total	C	N	O	S	0	0
			1225	761	232	226	6		

- Molecule 42 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	BJ	135	Total	C	N	O	S	0	0
			1101	677	198	219	7		

- Molecule 43 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	BK	178	Total	C	N	O	S	0	0
			1400	874	269	253	4		

- Molecule 44 is a protein called 30S ribosomal protein S8.

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

- Molecule 45 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	BM	129	Total	C	N	O	S	0	0
			1036	642	208	183	3		

- Molecule 46 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BN	103	Total	C	N	O	S	0	0
			825	514	158	151	2		

- Molecule 47 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	BO	128	Total	C	N	O	S	0	0
			965	595	196	171	3		

- Molecule 48 is a protein called 30S ribosomal protein S12.

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

- Molecule 49 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	BQ	117	Total	C	N	O	S	0	0
			910	564	183	160	3		

- Molecule 50 is a protein called 30S ribosomal protein S14.

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

- Molecule 51 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	BS	88	Total	C	N	O	S	0	0
			716	440	146	129	1		

- Molecule 52 is a protein called 30S ribosomal protein S16.

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

- Molecule 53 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	BU	83	Total	C	N	O	S	0	0
			672	425	124	120	3		

- Molecule 54 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	BV	74	Total	C	N	O	S	0	0
			626	395	123	107	1		

- Molecule 55 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	BW	91	Total	C	N	O	S	0	0
			727	464	139	122	2		

- Molecule 56 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	BX	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

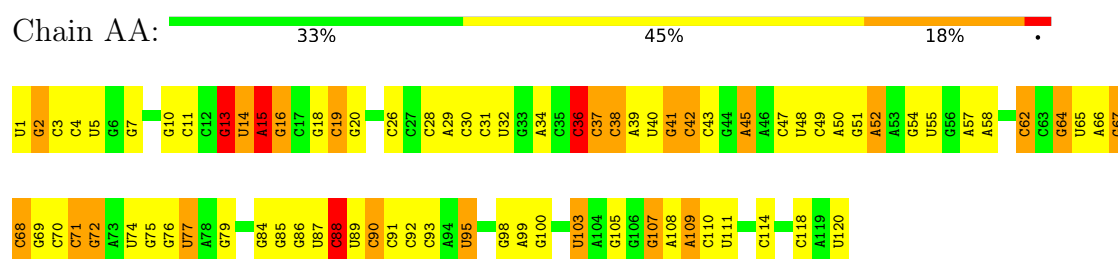
- Molecule 57 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	BY	70	Total	C	N	O	S	0	0
			590	366	125	98	1		

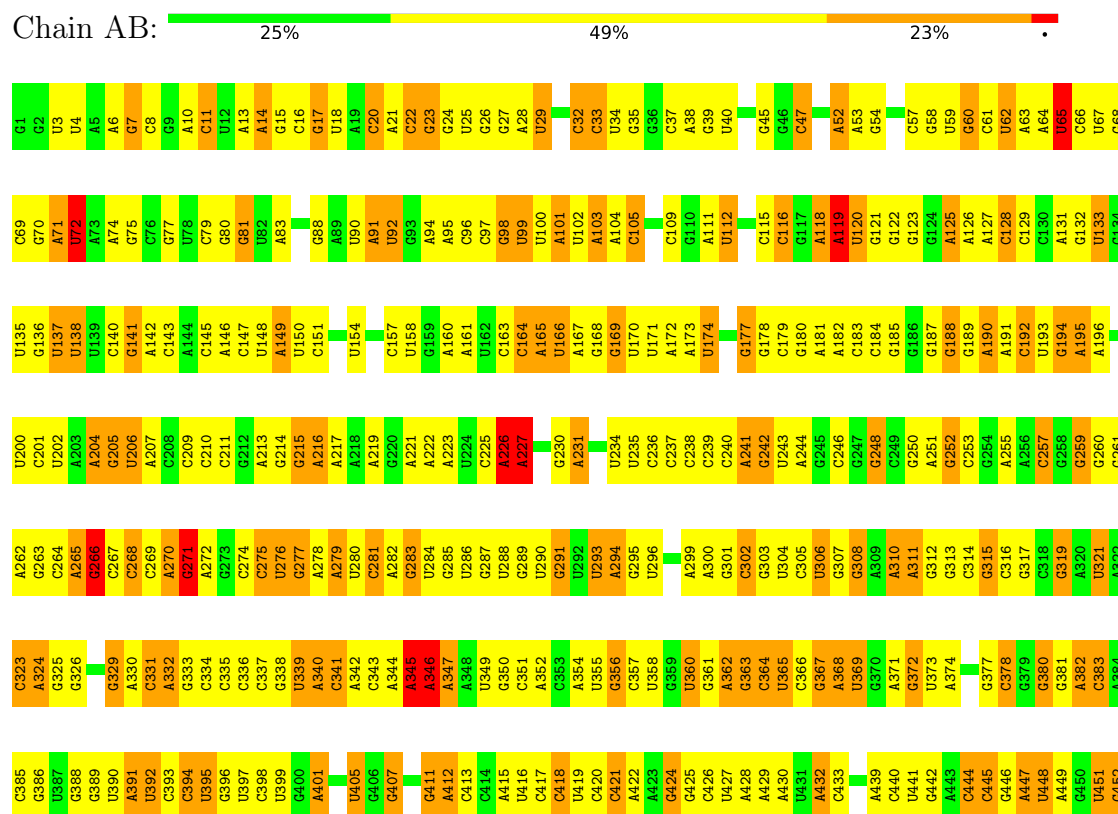
### 3 Residue-property plots

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: ribosomal RNA 5S



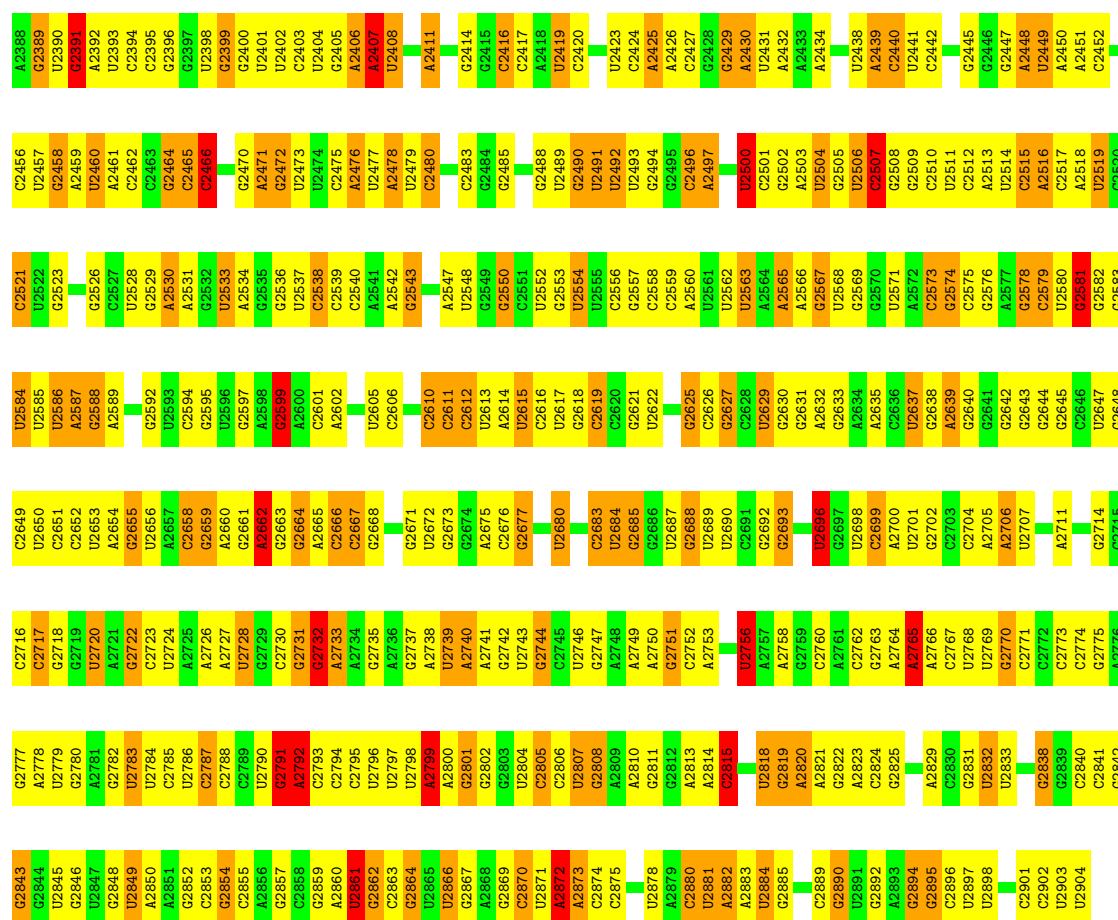
#### • Molecule 2: ribosomal RNA 23S



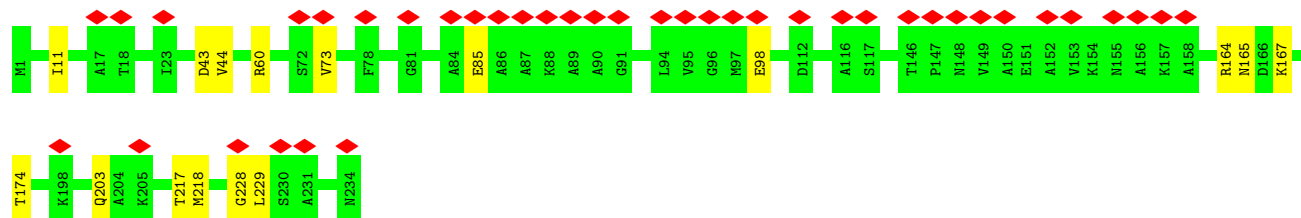
C1351	A1284	U1217	C1153	G1091	C964	C901	U839	G776	U714	G648	G579	C516	C456
U1352	A1285	G1218	G1154	C1092	C965	G902	C840	G777	A715	G649	U580	C517	C457
A1363	A1286	U1219	G1093	G1094	G966	C903	G841	G778	A716	C650	C581	U519	G458
G1355	A1287	G1220	U1159	U1094	U967	U906	U842	G779	C717	G651	A582	U518	G459
G1356	G1288	C1221	G1161	A1096	G968	G907	G843	G780	A718	G652	C584	U521	A460
C1357	G1289	U1222	G1162	A1097	G969	C908	A844	G781	C719	A654	G585	A522	C461
G1358	C1290	G1293	G1163	A1098	U970	G909	A845	A782	U720	G655	G586	C523	C462
A1359	C1291	U1224	C1164	A1099	G971	A909	U846	A783	A721	G656	C587	G524	G463
G1360	G1292	G1225	C1165	G1037	A972	A910	C848	G784	A722	U657	C588	U525	U464
G1361	U1294	A1227	G1166	U1101	G973	C912	G786	G785	U724	G658	U588	A526	G465
C1362	G1295	G1228	C1167	G1038	A974	C913	G787	C787	U725	C660	A590	G527	A466
G1363	G1296	U1229	G1167	A1039	A975	U913	U852	A788	G726	A661	U591	A528	G467
G1364	C1297	A1230	G1170	A1040	G976	C914	C853	A789	G727	G662	A592	A529	G468
A1365	C1298	U1231	G1171	G1041	G977	C915	C854	G790	A728	G663	U593	G530	G469
G1366	G1299	G1232	C1172	G1106	A978	G916	G855	U790	G729	G664	U594	C531	A470
A1367	G1300	C1233	U1173	U1107	A979	A917	G856	G791	G730	U665	C595	A532	A471
G1368	A1301	U1234	U1174	U1108	A980	U918	G857	A792	A730	A666	U596	G533	A472
G1369	G1302	G1235	A1175	C1109	A981	U919	G858	A793	C731	U667	G597	U534	G473
G1370	G1303	A1236	U1176	G1110	C982	A920	G859	A794	G732	U668	U598	G535	G474
C1371	A1304	G1237	G1177	A1048	A983	C921	U860	G795	G733	G669	A599	G536	C475
A1372	C1305	G1238	G1178	C1049	A984	C922	A861	G796	A734	G670	G600	G537	A476
G1373	G1306	U1239	U1179	G1112	C987	G923	G862	G797	C735	C671	C601	A538	A477
G1374	A1307	A1241	U1180	U1113	A988	G924	G863	G798	A736	G672	A602	G539	A478
U1375	U1308	U1242	U1181	G1114	G989	A925	G864	G801	G737	C673	A603	C540	A479
C1376	G1309	C1243	G1182	G1116	A990	G926	C865	A892	G738	G674	A604	A541	A480
C1377	G1310	A1244	U1183	C1117	C991	A927	A866	U803	A739	A675	G604	C542	G481
A1378	U1311	G1245	U1184	U1118	C992	G930	U868	A804	U741	A676	G543	C544	C482
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G1381	U1316	U1248	G1187	C1121	C995	A933	U871	U807	U744	C611	G612	A547	C485
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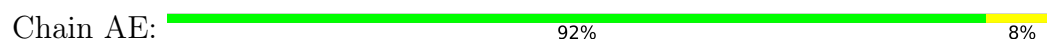
• Molecule 3: 50S ribosomal protein L1

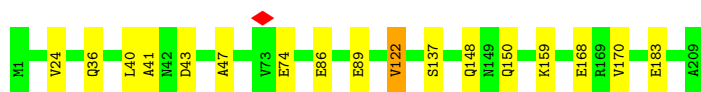


• Molecule 4: 50S ribosomal protein L2



• Molecule 5: 50S ribosomal protein L3





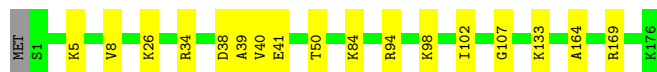
- Molecule 6: 50S ribosomal protein L4



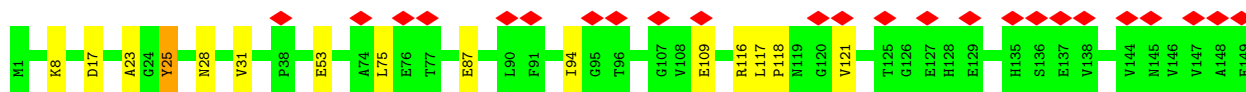
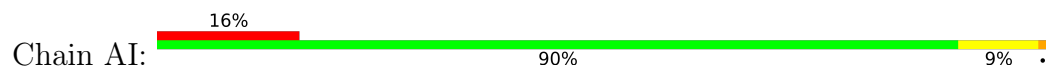
- Molecule 7: 50S ribosomal protein L5



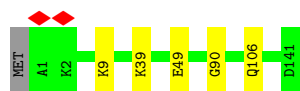
- Molecule 8: 50S ribosomal protein L6



- Molecule 9: 50S ribosomal protein L9



- Molecule 10: 50S ribosomal protein L11

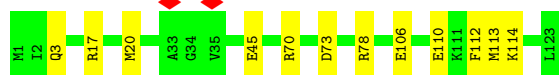


- Molecule 11: 50S ribosomal protein L13



- Molecule 12: 50S ribosomal protein L14

Chain AL:  90% 10%



- Molecule 13: 50S ribosomal protein L15

Chain AM:  96% .



- Molecule 14: 50S ribosomal protein L16

Chain AN:  93% 6% .



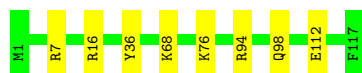
- Molecule 15: 50S ribosomal protein L17

Chain AO:  97% .




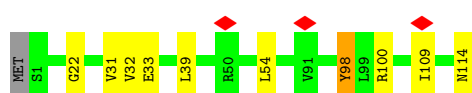
- Molecule 16: 50S ribosomal protein L18

Chain AP:  93% 7%



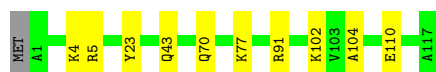
- Molecule 17: 50S ribosomal protein L19

Chain AQ:  90% 8% ..



- Molecule 18: 50S ribosomal protein L20

Chain AR:  91% 8% .



- Molecule 19: 50S ribosomal protein L21

Chain AS:  90% 10%



- Molecule 20: 50S ribosomal protein L22

Chain AT:  95% 5%



- Molecule 21: 50S ribosomal protein L23

Chain AU:  93% 7%



- Molecule 22: 50S ribosomal protein L24

Chain AV:  95% 5%



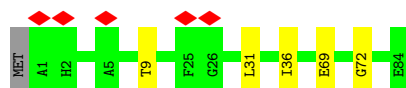
- Molecule 23: 50S ribosomal protein L25

Chain AW:  91% 9%



- Molecule 24: 50S ribosomal protein L27

Chain AX:  6% 93% 6%




- Molecule 25: 50S ribosomal protein L28

Chain AY:  96% 4%



- Molecule 26: 50S ribosomal protein L29

Chain AZ:  86% 13%




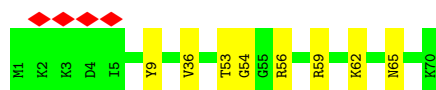
- Molecule 27: 50S ribosomal protein L30

Chain Aa:  92% 7%




- Molecule 28: 50S ribosomal protein L31

Chain Ab:  6% 89% 11%



- Molecule 29: 50S ribosomal protein L32

Chain Ac:  88% 11%




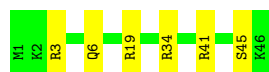
- Molecule 30: 50S ribosomal protein L33

Chain Ad:  93% 5%



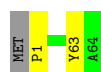
- Molecule 31: 50S ribosomal protein L34

Chain Ae:  87% 13%



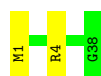
- Molecule 32: 50S ribosomal protein L35

Chain Af:  95%



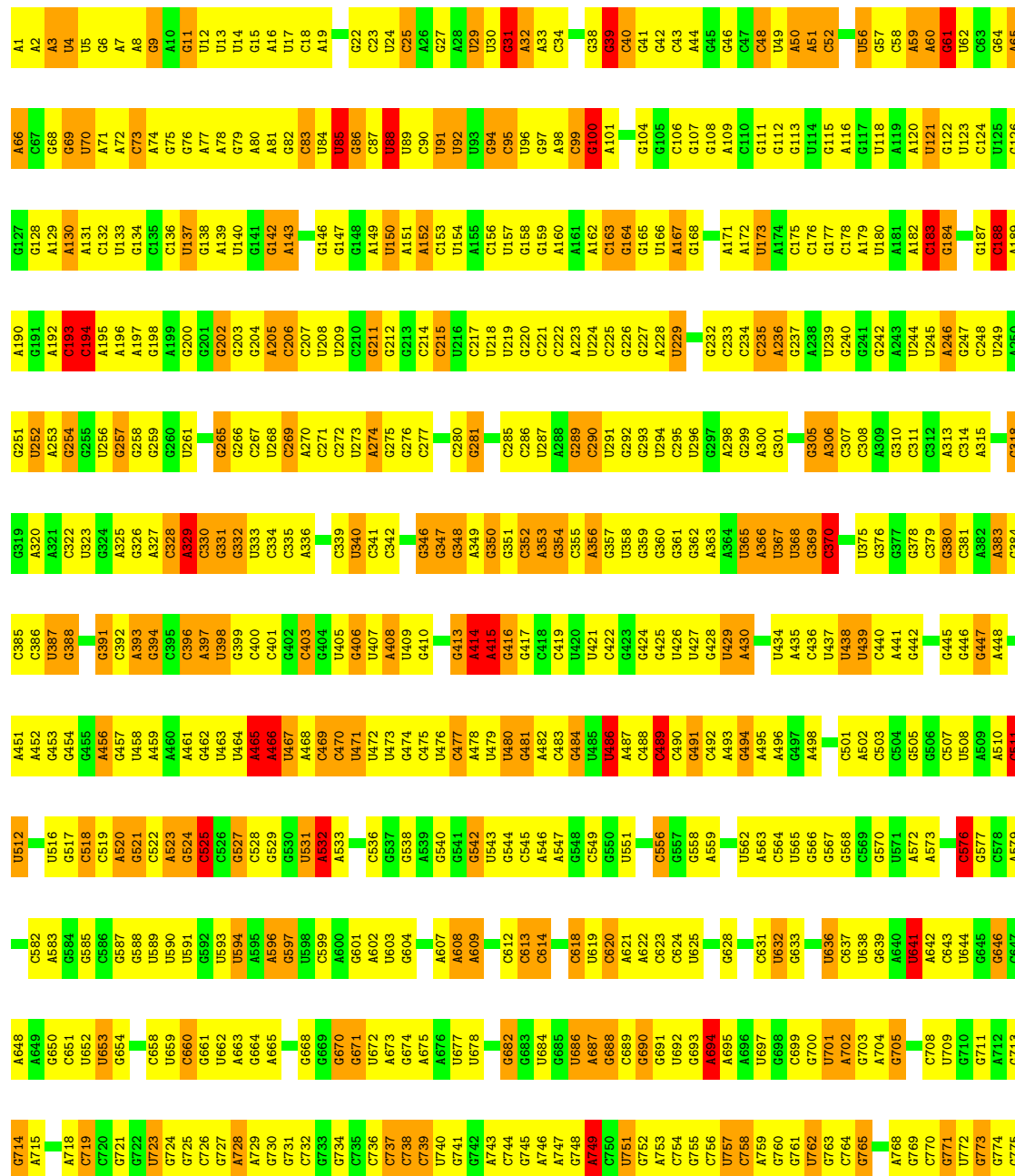
● Molecule 33: 50S ribosomal protein L36

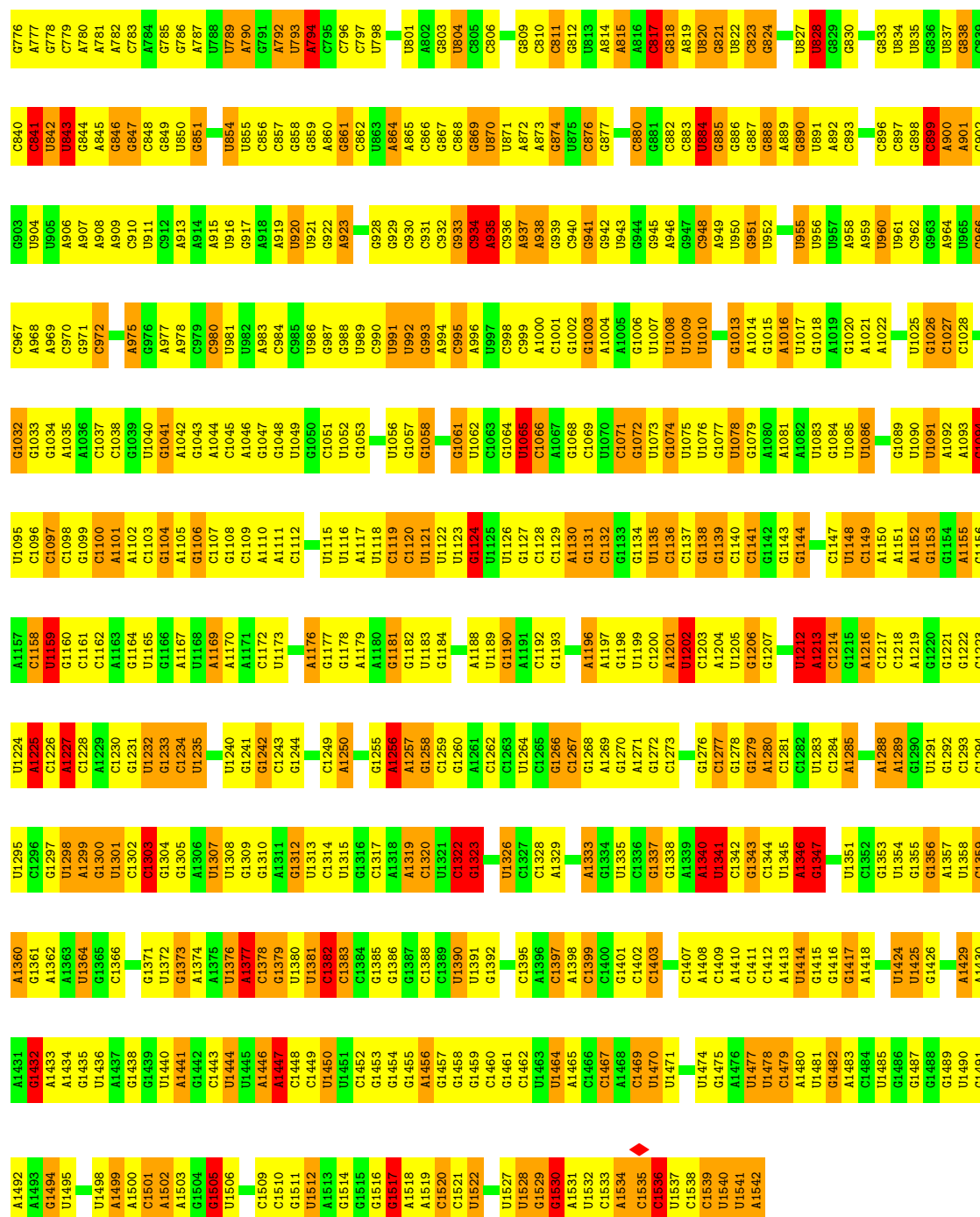
Chain Ag:  95% 5%



● Molecule 34: 16S ribosomal RNA

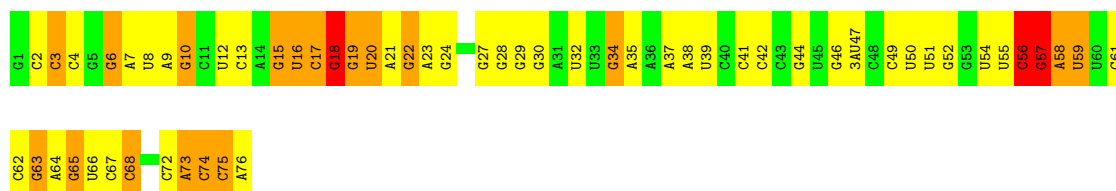
Chain BA:  25% 50% 21% .





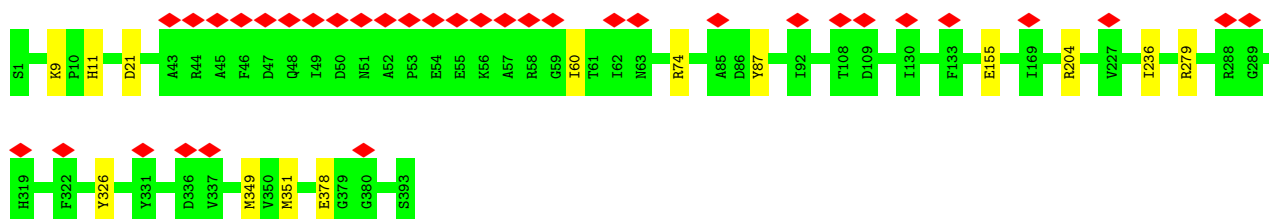
- Molecule 35: A/T-site tRNA Phe

Chain BE: 



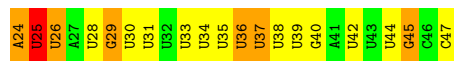
- Molecule 36: Elongation factor Tu 2

Chain BC: 



- Molecule 37: mRNA

Chain BD: 



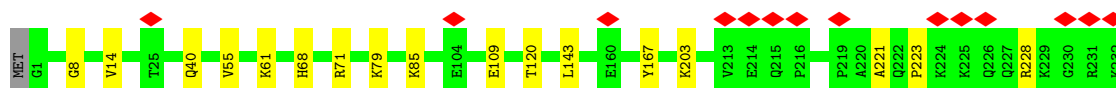
- Molecule 38: 30S ribosomal protein S2

Chain BF: 



- Molecule 39: 30S ribosomal protein S3

Chain BG: 



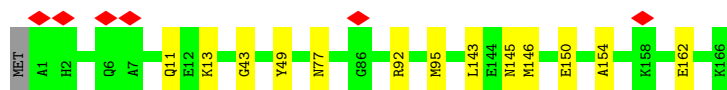
- Molecule 40: 30S ribosomal protein S4

Chain BH: 

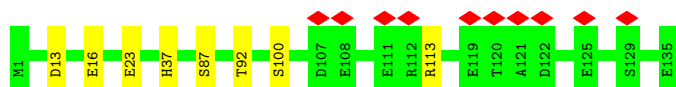




## • Molecule 41: 30S ribosomal protein S5

Chain BI:  92% 8%

## • Molecule 42: 30S ribosomal protein S6

Chain BJ:  7% 94% 6%

## • Molecule 43: 30S ribosomal protein S7

Chain BK:  93% 7%

## • Molecule 44: 30S ribosomal protein S8

Chain BL:  93% 6%

## • Molecule 45: 30S ribosomal protein S9

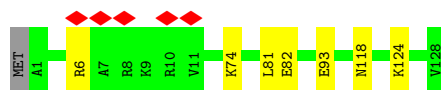
Chain BM:  90% 9%

## • Molecule 46: 30S ribosomal protein S10

Chain BN:  86% 14%

## • Molecule 47: 30S ribosomal protein S11

Chain BO:  94% 5%



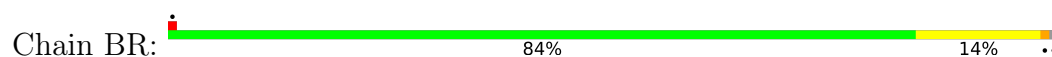
- Molecule 48: 30S ribosomal protein S12



- Molecule 49: 30S ribosomal protein S13



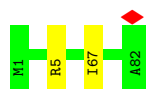
- Molecule 50: 30S ribosomal protein S14



- Molecule 51: 30S ribosomal protein S15




- Molecule 52: 30S ribosomal protein S16



- Molecule 53: 30S ribosomal protein S17



- Molecule 54: 30S ribosomal protein S18

Chain BV:  87% 9% ..



- Molecule 55: 30S ribosomal protein S19

Chain BW:  5% 92% 5% ..




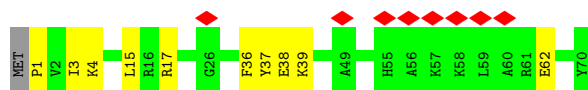
- Molecule 56: 30S ribosomal protein S20

Chain BX:  97% ..



- Molecule 57: 30S ribosomal protein S21

Chain BY:  11% 85% 14% ..



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	359223	Depositor
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	20	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	59000	Depositor
Image detector	TVIPS TEMCAM-F415 (4k x 4k)	Depositor
Maximum map value	299.406	Depositor
Minimum map value	-102.404	Depositor
Average map value	5.380	Depositor
Map value standard deviation	28.487	Depositor
Recommended contour level	32.4	Depositor
Map size ( $\text{\AA}$ )	375, 375, 375	wwPDB
Map dimensions	250, 250, 250	wwPDB
Map angles ( $^\circ$ )	90, 90, 90	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.5, 1.5, 1.5	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: H2U, 7MG, 1MG, 3TD, 6MZ, 2MG, 5MC, 2MA, CH, 3AU, 5MU, OMG, MIA, OMC, OMU, 4OC, 4SU, MA6, PSU, UR3

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	AA	1.18	0/2869	2.04	104/4474 (2.3%)
2	AB	1.17	0/69257	1.96	2261/108040 (2.1%)
3	AC	0.56	0/1748	0.96	1/2355 (0.0%)
4	AD	0.60	0/2131	1.07	1/2863 (0.0%)
5	AE	0.58	0/1586	1.02	0/2134
6	AF	0.57	0/1571	0.99	0/2113
7	AG	0.65	0/1444	1.10	4/1937 (0.2%)
8	AH	0.59	0/1343	1.02	0/1816
9	AI	0.57	0/1122	1.01	1/1515 (0.1%)
10	AJ	0.57	0/1046	0.92	0/1410
11	AK	0.63	0/1152	0.99	0/1551
12	AL	0.57	0/956	1.00	0/1279
13	AM	0.60	0/1062	1.01	0/1413
14	AN	0.63	0/1093	1.05	1/1460 (0.1%)
15	AO	0.61	0/1021	1.03	0/1364
16	AP	0.60	0/910	1.00	0/1219
17	AQ	0.61	0/929	1.06	0/1242
18	AR	0.67	0/960	1.02	1/1278 (0.1%)
19	AS	0.62	0/829	1.01	0/1107
20	AT	0.52	0/864	0.96	0/1156
21	AU	0.55	0/794	0.99	0/1060
22	AV	0.56	0/797	1.03	0/1062
23	AW	0.60	0/766	0.97	0/1025
24	AX	0.64	0/642	1.09	0/848
25	AY	0.64	0/635	1.06	0/848
26	AZ	0.56	0/510	1.10	1/677 (0.1%)
27	Aa	0.54	0/453	0.98	0/605
28	Ab	0.63	0/559	1.17	2/745 (0.3%)
29	Ac	0.59	0/450	1.05	0/599
30	Ad	0.61	0/448	1.00	0/594
31	Ae	0.63	0/380	1.11	1/498 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	Af	0.58	0/513	1.01	1/676 (0.1%)
33	Ag	0.53	0/303	1.00	0/397
34	BA	1.17	1/36769 (0.0%)	1.96	1171/57354 (2.0%)
35	BB	1.23	0/1580	1.96	45/2459 (1.8%)
35	BE	1.20	0/1580	2.05	59/2459 (2.4%)
36	BC	0.61	0/3092	0.96	1/4183 (0.0%)
37	BD	1.30	0/548	1.88	16/848 (1.9%)
38	BF	0.60	0/1904	1.00	0/2565
39	BG	0.60	0/1852	1.04	0/2490
40	BH	0.63	0/1665	1.02	0/2227
41	BI	0.56	0/1239	1.00	1/1664 (0.1%)
42	BJ	0.61	0/1121	1.05	0/1509
43	BK	0.62	0/1422	1.04	1/1908 (0.1%)
44	BL	0.58	0/989	0.97	0/1326
45	BM	0.65	0/1048	1.03	0/1394
46	BN	0.59	0/835	1.08	0/1127
47	BO	0.61	0/982	1.00	0/1323
48	BP	0.61	0/969	1.09	0/1300
49	BQ	0.57	0/919	1.01	0/1226
50	BR	0.63	0/817	1.14	1/1088 (0.1%)
51	BS	0.58	0/724	1.00	1/966 (0.1%)
52	BT	0.63	0/659	1.04	0/884
53	BU	0.58	0/681	0.99	0/913
54	BV	0.71	0/637	1.06	0/851
55	BW	0.60	0/744	1.02	3/995 (0.3%)
56	BX	0.55	0/676	0.91	0/895
57	BY	0.69	0/598	1.17	1/792 (0.1%)
All	All	1.03	1/165193 (0.0%)	1.75	3679/246106 (1.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	0	27
2	AB	0	821
3	AC	0	2
5	AE	0	3
6	AF	0	1
8	AH	0	2
9	AI	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
11	AK	0	2
15	AO	0	1
17	AQ	0	1
18	AR	0	1
28	Ab	0	1
30	Ad	0	1
31	Ae	0	2
34	BA	0	473
35	BB	0	12
35	BE	0	15
37	BD	0	4
38	BF	0	1
39	BG	0	2
40	BH	0	2
41	BI	0	3
42	BJ	0	1
43	BK	0	2
45	BM	0	2
47	BO	0	1
48	BP	0	1
50	BR	0	1
54	BV	0	1
55	BW	0	1
57	BY	0	3
All	All	0	1392

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	BA	1535	C	P-O5'	5.14	1.64	1.59

The worst 5 of 3679 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	13	G	O4'-C1'-N9	15.20	120.36	108.20
2	AB	736	C	O4'-C1'-N1	14.43	119.74	108.20
34	BA	465	A	O4'-C1'-N9	13.60	119.08	108.20
2	AB	2832	U	O4'-C1'-N1	12.97	118.58	108.20
34	BA	1152	A	O4'-C1'-N9	12.96	118.57	108.20

There are no chirality outliers.

5 of 1392 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	13	G	Sidechain
1	AA	14	U	Sidechain
1	AA	15	A	Sidechain
1	AA	2	G	Sidechain
1	AA	7	G	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	AA	2566	0	1302	0	0
2	AB	62351	0	31387	0	0
3	AC	1733	0	1824	0	0
4	AD	2092	0	2170	0	0
5	AE	1565	0	1616	0	0
6	AF	1552	0	1619	0	0
7	AG	1420	0	1460	0	0
8	AH	1323	0	1374	0	0
9	AI	1111	0	1148	0	0
10	AJ	1032	0	1088	0	0
11	AK	1129	0	1162	0	0
12	AL	947	0	1023	0	0
13	AM	1053	0	1129	0	0
14	AN	1074	0	1157	0	0
15	AO	1008	0	1045	0	0
16	AP	900	0	935	0	0
17	AQ	917	0	965	0	0
18	AR	947	0	1022	0	0
19	AS	816	0	839	0	0
20	AT	857	0	922	0	0
21	AU	787	0	846	0	0
22	AV	789	0	847	0	0
23	AW	753	0	780	0	0
24	AX	634	0	656	0	0
25	AY	625	0	655	0	0
26	AZ	509	0	543	0	0
27	Aa	449	0	491	0	0
28	Ab	549	0	552	0	0
29	Ac	444	0	461	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	Ad	441	0	485	0	0
31	Ae	377	0	418	0	0
32	Af	504	0	574	0	0
33	Ag	302	0	343	0	0
34	BA	33089	0	16678	0	0
35	BB	1635	0	849	0	0
35	BE	1635	0	849	0	0
36	BC	3036	0	3052	0	0
37	BD	495	0	249	0	0
38	BF	1872	0	1885	0	0
39	BG	1822	0	1913	0	0
40	BH	1643	0	1710	0	0
41	BI	1225	0	1273	0	0
42	BJ	1101	0	1050	0	0
43	BK	1400	0	1449	0	0
44	BL	979	0	1034	0	0
45	BM	1036	0	1084	0	0
46	BN	825	0	865	0	0
47	BO	965	0	997	0	0
48	BP	955	0	1019	0	0
49	BQ	910	0	981	0	0
50	BR	805	0	847	0	0
51	BS	716	0	742	0	0
52	BT	649	0	666	0	0
53	BU	672	0	716	0	0
54	BV	626	0	651	0	0
55	BW	727	0	769	0	0
56	BX	670	0	722	0	0
57	BY	590	0	631	0	0
All	All	153634	0	105519	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	AC	232/234 (99%)	204 (88%)	25 (11%)	3 (1%)	12	48
4	AD	270/273 (99%)	239 (88%)	23 (8%)	8 (3%)	4	28
5	AE	207/209 (99%)	186 (90%)	15 (7%)	6 (3%)	4	29
6	AF	199/201 (99%)	182 (92%)	14 (7%)	3 (2%)	10	46
7	AG	176/179 (98%)	147 (84%)	27 (15%)	2 (1%)	14	52
8	AH	174/177 (98%)	163 (94%)	8 (5%)	3 (2%)	9	42
9	AI	147/149 (99%)	126 (86%)	16 (11%)	5 (3%)	3	26
10	AJ	139/142 (98%)	123 (88%)	15 (11%)	1 (1%)	22	63
11	AK	140/142 (99%)	132 (94%)	8 (6%)	0	100	100
12	AL	121/123 (98%)	106 (88%)	13 (11%)	2 (2%)	9	42
13	AM	142/144 (99%)	125 (88%)	15 (11%)	2 (1%)	11	46
14	AN	134/136 (98%)	122 (91%)	9 (7%)	3 (2%)	6	35
15	AO	125/127 (98%)	117 (94%)	7 (6%)	1 (1%)	19	60
16	AP	115/117 (98%)	104 (90%)	10 (9%)	1 (1%)	17	57
17	AQ	112/115 (97%)	100 (89%)	10 (9%)	2 (2%)	8	40
18	AR	115/118 (98%)	110 (96%)	4 (4%)	1 (1%)	17	57
19	AS	101/103 (98%)	91 (90%)	6 (6%)	4 (4%)	3	23
20	AT	108/110 (98%)	98 (91%)	9 (8%)	1 (1%)	17	57
21	AU	98/100 (98%)	85 (87%)	11 (11%)	2 (2%)	7	38
22	AV	101/104 (97%)	89 (88%)	11 (11%)	1 (1%)	15	55
23	AW	92/94 (98%)	85 (92%)	5 (5%)	2 (2%)	6	35
24	AX	82/85 (96%)	67 (82%)	12 (15%)	3 (4%)	3	24
25	AY	75/78 (96%)	64 (85%)	9 (12%)	2 (3%)	5	31
26	AZ	61/63 (97%)	49 (80%)	9 (15%)	3 (5%)	2	20
27	Aa	56/59 (95%)	54 (96%)	1 (2%)	1 (2%)	8	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	Ab	68/70 (97%)	57 (84%)	10 (15%)	1 (2%)	10	46
29	Ac	54/57 (95%)	47 (87%)	5 (9%)	2 (4%)	3	24
30	Ad	52/55 (94%)	45 (86%)	7 (14%)	0	100	100
31	Ae	44/46 (96%)	40 (91%)	4 (9%)	0	100	100
32	Af	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
33	Ag	36/38 (95%)	32 (89%)	3 (8%)	1 (3%)	5	30
36	BC	391/393 (100%)	368 (94%)	20 (5%)	3 (1%)	19	60
38	BF	238/241 (99%)	215 (90%)	20 (8%)	3 (1%)	12	48
39	BG	230/233 (99%)	211 (92%)	17 (7%)	2 (1%)	17	57
40	BH	203/206 (98%)	191 (94%)	10 (5%)	2 (1%)	15	55
41	BI	164/167 (98%)	144 (88%)	17 (10%)	3 (2%)	8	40
42	BJ	133/135 (98%)	128 (96%)	3 (2%)	2 (2%)	10	46
43	BK	176/179 (98%)	160 (91%)	14 (8%)	2 (1%)	14	52
44	BL	127/130 (98%)	117 (92%)	8 (6%)	2 (2%)	9	44
45	BM	127/130 (98%)	111 (87%)	14 (11%)	2 (2%)	9	44
46	BN	101/103 (98%)	86 (85%)	11 (11%)	4 (4%)	3	23
47	BO	126/129 (98%)	113 (90%)	11 (9%)	2 (2%)	9	44
48	BP	121/124 (98%)	104 (86%)	12 (10%)	5 (4%)	3	23
49	BQ	115/118 (98%)	108 (94%)	7 (6%)	0	100	100
50	BR	98/101 (97%)	83 (85%)	8 (8%)	7 (7%)	1	14
51	BS	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
52	BT	80/82 (98%)	79 (99%)	1 (1%)	0	100	100
53	BU	81/84 (96%)	73 (90%)	8 (10%)	0	100	100
54	BV	72/75 (96%)	65 (90%)	5 (7%)	2 (3%)	5	30
55	BW	89/92 (97%)	80 (90%)	9 (10%)	0	100	100
56	BX	84/87 (97%)	78 (93%)	6 (7%)	0	100	100
57	BY	68/71 (96%)	60 (88%)	7 (10%)	1 (2%)	10	46
All	All	6548/6682 (98%)	5904 (90%)	536 (8%)	108 (2%)	13	44

5 of 108 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	AD	260	LYS

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Mol	Chain	Res	Type
5	AE	122	VAL
5	AE	150	GLN
5	AE	170	VAL
9	AI	23	ALA

### 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	
3	AC	181/181 (100%)	171 (94%)	10 (6%)	21	47
4	AD	217/218 (100%)	204 (94%)	13 (6%)	19	44
5	AE	164/164 (100%)	154 (94%)	10 (6%)	18	44
6	AF	165/165 (100%)	158 (96%)	7 (4%)	30	54
7	AG	149/150 (99%)	138 (93%)	11 (7%)	13	38
8	AH	137/138 (99%)	125 (91%)	12 (9%)	10	31
9	AI	114/114 (100%)	106 (93%)	8 (7%)	15	40
10	AJ	109/110 (99%)	105 (96%)	4 (4%)	34	58
11	AK	116/116 (100%)	113 (97%)	3 (3%)	46	66
12	AL	104/104 (100%)	94 (90%)	10 (10%)	8	27
13	AM	103/103 (100%)	99 (96%)	4 (4%)	32	56
14	AN	109/109 (100%)	103 (94%)	6 (6%)	21	47
15	AO	103/103 (100%)	101 (98%)	2 (2%)	57	75
16	AP	87/87 (100%)	80 (92%)	7 (8%)	12	35
17	AQ	99/100 (99%)	91 (92%)	8 (8%)	11	35
18	AR	89/90 (99%)	82 (92%)	7 (8%)	12	35
19	AS	84/84 (100%)	78 (93%)	6 (7%)	14	39
20	AT	93/93 (100%)	89 (96%)	4 (4%)	29	53
21	AU	84/84 (100%)	79 (94%)	5 (6%)	19	44
22	AV	84/85 (99%)	81 (96%)	3 (4%)	35	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	AW	78/78 (100%)	72 (92%)	6 (8%)	13	37
24	AX	62/63 (98%)	60 (97%)	2 (3%)	39	61
25	AY	67/68 (98%)	67 (100%)	0	100	100
26	AZ	55/55 (100%)	49 (89%)	6 (11%)	6	23
27	Aa	48/49 (98%)	45 (94%)	3 (6%)	18	43
28	Ab	62/62 (100%)	58 (94%)	4 (6%)	17	42
29	Ac	47/48 (98%)	43 (92%)	4 (8%)	10	33
30	Ad	48/49 (98%)	46 (96%)	2 (4%)	30	54
31	Ae	38/38 (100%)	35 (92%)	3 (8%)	12	35
32	Af	51/52 (98%)	50 (98%)	1 (2%)	55	74
33	Ag	34/34 (100%)	33 (97%)	1 (3%)	42	64
36	BC	326/326 (100%)	316 (97%)	10 (3%)	40	62
38	BF	198/199 (100%)	188 (95%)	10 (5%)	24	48
39	BG	189/190 (100%)	176 (93%)	13 (7%)	15	40
40	BH	172/173 (99%)	164 (95%)	8 (5%)	26	51
41	BI	125/126 (99%)	118 (94%)	7 (6%)	21	46
42	BJ	116/116 (100%)	111 (96%)	5 (4%)	29	53
43	BK	146/147 (99%)	139 (95%)	7 (5%)	25	51
44	BL	104/105 (99%)	98 (94%)	6 (6%)	20	45
45	BM	106/107 (99%)	98 (92%)	8 (8%)	13	38
46	BN	90/90 (100%)	80 (89%)	10 (11%)	6	22
47	BO	98/99 (99%)	94 (96%)	4 (4%)	30	55
48	BP	103/104 (99%)	100 (97%)	3 (3%)	42	64
49	BQ	95/96 (99%)	91 (96%)	4 (4%)	30	54
50	BR	83/84 (99%)	76 (92%)	7 (8%)	11	33
51	BS	76/77 (99%)	75 (99%)	1 (1%)	69	81
52	BT	65/65 (100%)	63 (97%)	2 (3%)	40	62
53	BU	77/78 (99%)	75 (97%)	2 (3%)	46	66
54	BV	64/65 (98%)	56 (88%)	8 (12%)	4	19
55	BW	78/79 (99%)	74 (95%)	4 (5%)	24	48
56	BX	65/66 (98%)	63 (97%)	2 (3%)	40	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
57	BY	60/61 (98%)	55 (92%)	5 (8%)	11	34
All	All	5417/5447 (99%)	5119 (94%)	298 (6%)	25	47

5 of 298 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
43	BK	164	GLN
54	BV	69	TYR
45	BM	12	LYS
48	BP	81	ILE
14	AN	100	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	119/120 (99%)	15 (12%)	3 (2%)
2	AB	2898/2904 (99%)	396 (13%)	130 (4%)
34	BA	1538/1542 (99%)	192 (12%)	77 (5%)
35	BB	73/76 (96%)	12 (16%)	2 (2%)
35	BE	73/76 (96%)	12 (16%)	6 (8%)
37	BD	24/24 (100%)	4 (16%)	5 (20%)
All	All	4725/4742 (99%)	631 (13%)	223 (4%)

5 of 631 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	10	G
1	AA	13	G
1	AA	15	A
1	AA	16	G
1	AA	36	C

5 of 223 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	AB	2602	A
35	BE	56	C

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Mol	Chain	Res	Type
34	BA	193	C
35	BE	18	G
34	BA	1302	C

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

55 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	1MG	AB	745	2	18,26,27	1.16	2 (11%)	19,39,42	1.34	2 (10%)
2	PSU	AB	2605	2	18,21,22	0.91	0	22,30,33	0.94	1 (4%)
35	7MG	BB	46	35	22,26,27	4.67	2 (9%)	29,39,42	1.34	2 (6%)
2	PSU	AB	2457	2	18,21,22	0.98	1 (5%)	22,30,33	1.37	3 (13%)
35	PSU	BE	55	35	18,21,22	1.00	1 (5%)	22,30,33	0.94	1 (4%)
2	PSU	AB	1917	2	18,21,22	0.92	0	22,30,33	0.72	1 (4%)
2	7MG	AB	2069	2	22,26,27	4.64	1 (4%)	29,39,42	1.34	1 (3%)
2	OMG	AB	2251	2	18,26,27	1.11	2 (11%)	19,38,41	0.90	0
2	3TD	AB	1915	2	18,22,23	0.80	0	22,32,35	0.93	1 (4%)
2	PSU	AB	746	2	18,21,22	1.00	1 (5%)	22,30,33	1.31	2 (9%)
34	7MG	BA	527	34	22,26,27	4.60	1 (4%)	29,39,42	1.40	3 (10%)
35	5MU	BE	54	35	19,22,23	0.67	0	28,32,35	1.15	3 (10%)
35	4SU	BB	8	35	18,21,22	1.41	1 (5%)	26,30,33	1.15	3 (11%)
2	5MU	AB	1939	2	19,22,23	0.66	0	28,32,35	1.25	3 (10%)
2	6MZ	AB	2030	2	18,25,26	0.97	1 (5%)	16,36,39	1.39	3 (18%)
2	OMC	AB	2498	2	19,22,23	0.56	0	26,31,34	0.87	0
34	MA6	BA	1519	34	19,26,27	1.05	1 (5%)	18,38,41	1.21	2 (11%)
34	5MC	BA	967	34	18,22,23	0.65	0	26,32,35	0.84	1 (3%)
35	H2U	BE	16	35	18,21,22	0.84	0	21,30,33	1.07	1 (4%)
35	7MG	BE	46	35	22,26,27	4.63	2 (9%)	29,39,42	1.40	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
34	PSU	BA	516	34	18,21,22	0.93	1 (5%)	22,30,33	1.11	1 (4%)
2	2MG	AB	2445	2	18,26,27	1.21	2 (11%)	16,38,41	0.77	0
35	5MU	BB	54	35	19,22,23	0.66	0	28,32,35	1.23	3 (10%)
34	UR3	BA	1498	34	19,22,23	0.72	0	26,32,35	0.92	1 (3%)
35	H2U	BB	16	35	18,21,22	0.82	0	21,30,33	1.08	1 (4%)
2	PSU	AB	1911	2	18,21,22	0.90	0	22,30,33	0.81	1 (4%)
35	3AU	BB	47	-	25,28,29	0.88	1 (4%)	32,40,43	0.90	1 (3%)
35	PSU	BB	32	35	18,21,22	0.95	1 (5%)	22,30,33	1.09	2 (9%)
2	6MZ	AB	1618	2	18,25,26	0.98	1 (5%)	16,36,39	1.32	2 (12%)
35	PSU	BB	39	35	18,21,22	0.86	0	22,30,33	0.94	1 (4%)
35	H2U	BE	20	35	18,21,22	0.81	0	21,30,33	1.26	2 (9%)
35	MIA	BE	37	35	24,31,32	1.10	3 (12%)	26,44,47	1.56	4 (15%)
2	5MC	AB	1962	2	18,22,23	0.56	0	26,32,35	1.17	3 (11%)
2	PSU	AB	955	2	18,21,22	0.88	0	22,30,33	1.08	1 (4%)
2	CH	AB	2575	2	16,21,22	1.03	1 (6%)	20,30,33	1.26	2 (10%)
35	PSU	BE	32	35	18,21,22	0.96	1 (5%)	22,30,33	1.08	2 (9%)
35	MIA	BB	37	35	24,31,32	1.09	3 (12%)	26,44,47	1.72	5 (19%)
2	OMU	AB	2552	2	19,22,23	0.71	0	26,31,34	0.95	2 (7%)
35	4SU	BE	8	35	18,21,22	1.40	1 (5%)	26,30,33	1.64	6 (23%)
34	2MG	BA	966	34	18,26,27	1.17	1 (5%)	16,38,41	1.31	3 (18%)
34	2MG	BA	1516	34	18,26,27	1.21	3 (16%)	16,38,41	0.83	1 (6%)
35	3AU	BE	47	-	25,28,29	0.90	1 (4%)	32,40,43	1.22	4 (12%)
2	2MA	AB	2503	2	17,25,26	1.17	2 (11%)	17,37,40	1.33	2 (11%)
2	PSU	AB	2580	2	18,21,22	0.96	0	22,30,33	1.24	2 (9%)
34	5MC	BA	1407	34	18,22,23	0.65	0	26,32,35	0.93	1 (3%)
2	H2U	AB	2449	2	18,21,22	0.81	0	21,30,33	0.91	1 (4%)
34	2MG	BA	1207	34	18,26,27	1.20	1 (5%)	16,38,41	0.95	0
34	4OC	BA	1402	34	20,23,24	0.71	0	26,32,35	1.08	2 (7%)
2	PSU	AB	2504	2	18,21,22	1.09	2 (11%)	22,30,33	1.30	2 (9%)
35	PSU	BE	39	35	18,21,22	0.93	1 (5%)	22,30,33	1.00	1 (4%)
35	H2U	BB	20	35	18,21,22	0.81	0	21,30,33	1.00	1 (4%)
2	5MU	AB	747	2	19,22,23	0.71	0	28,32,35	1.39	3 (10%)
34	MA6	BA	1518	34	19,26,27	1.06	2 (10%)	18,38,41	0.74	0
35	PSU	BB	55	35	18,21,22	0.93	1 (5%)	22,30,33	1.04	1 (4%)
2	2MG	AB	1835	2	18,26,27	1.16	2 (11%)	16,38,41	1.00	1 (6%)



In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	1MG	AB	745	2	-	0/3/25/26	0/3/3/3
2	PSU	AB	2605	2	-	0/7/25/26	0/2/2/2
35	7MG	BB	46	35	-	1/7/37/38	0/3/3/3
2	PSU	AB	2457	2	-	0/7/25/26	0/2/2/2
35	PSU	BE	55	35	-	1/7/25/26	0/2/2/2
2	PSU	AB	1917	2	-	0/7/25/26	0/2/2/2
2	7MG	AB	2069	2	-	0/7/37/38	0/3/3/3
2	OMG	AB	2251	2	-	0/5/27/28	0/3/3/3
2	3TD	AB	1915	2	-	0/7/25/26	0/2/2/2
2	PSU	AB	746	2	-	2/7/25/26	0/2/2/2
34	7MG	BA	527	34	-	1/7/37/38	0/3/3/3
35	5MU	BE	54	35	-	0/7/25/26	0/2/2/2
35	4SU	BB	8	35	-	0/7/25/26	0/2/2/2
2	5MU	AB	1939	2	-	0/7/25/26	0/2/2/2
2	6MZ	AB	2030	2	-	1/5/27/28	0/3/3/3
2	OMC	AB	2498	2	-	1/9/27/28	0/2/2/2
34	MA6	BA	1519	34	-	0/7/29/30	0/3/3/3
34	5MC	BA	967	34	-	0/7/25/26	0/2/2/2
35	H2U	BE	16	35	-	0/7/38/39	0/2/2/2
35	7MG	BE	46	35	-	0/7/37/38	0/3/3/3
34	PSU	BA	516	34	-	0/7/25/26	0/2/2/2
2	2MG	AB	2445	2	-	0/5/27/28	0/3/3/3
35	5MU	BB	54	35	-	0/7/25/26	0/2/2/2
34	UR3	BA	1498	34	-	0/7/25/26	0/2/2/2
35	H2U	BB	16	35	-	1/7/38/39	0/2/2/2
2	PSU	AB	1911	2	-	0/7/25/26	0/2/2/2
35	3AU	BB	47	-	-	2/16/34/35	0/2/2/2
35	PSU	BB	32	35	-	2/7/25/26	0/2/2/2
2	6MZ	AB	1618	2	-	0/5/27/28	0/3/3/3
35	PSU	BB	39	35	-	0/7/25/26	0/2/2/2
35	H2U	BE	20	35	-	0/7/38/39	0/2/2/2
35	MIA	BE	37	35	-	0/11/33/34	0/3/3/3
2	5MC	AB	1962	2	-	5/7/25/26	0/2/2/2
2	PSU	AB	955	2	-	0/7/25/26	0/2/2/2
2	CH	AB	2575	2	-	1/5/25/26	0/2/2/2
35	PSU	BE	32	35	-	0/7/25/26	0/2/2/2
35	MIA	BB	37	35	-	1/11/33/34	0/3/3/3
2	OMU	AB	2552	2	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	4SU	BE	8	35	-	0/7/25/26	0/2/2/2
34	2MG	BA	966	34	-	0/5/27/28	0/3/3/3
34	2MG	BA	1516	34	-	0/5/27/28	0/3/3/3
35	3AU	BE	47	-	-	5/16/34/35	0/2/2/2
2	2MA	AB	2503	2	-	0/3/25/26	0/3/3/3
2	PSU	AB	2580	2	-	0/7/25/26	0/2/2/2
34	5MC	BA	1407	34	-	0/7/25/26	0/2/2/2
2	H2U	AB	2449	2	-	0/7/38/39	0/2/2/2
34	2MG	BA	1207	34	-	0/5/27/28	0/3/3/3
34	4OC	BA	1402	34	-	0/9/29/30	0/2/2/2
2	PSU	AB	2504	2	-	2/7/25/26	0/2/2/2
35	PSU	BE	39	35	-	0/7/25/26	0/2/2/2
35	H2U	BB	20	35	-	1/7/38/39	0/2/2/2
2	5MU	AB	747	2	-	4/7/25/26	0/2/2/2
34	MA6	BA	1518	34	-	0/7/29/30	0/3/3/3
35	PSU	BB	55	35	-	1/7/25/26	0/2/2/2
2	2MG	AB	1835	2	-	0/5/27/28	0/3/3/3

The worst 5 of 47 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	BB	46	7MG	C8-N9	-21.59	1.33	1.46
2	AB	2069	7MG	C8-N9	-21.49	1.34	1.46
35	BE	46	7MG	C8-N9	-21.44	1.34	1.46
34	BA	527	7MG	C8-N9	-21.30	1.34	1.46
35	BB	8	4SU	C5-C4	-5.01	1.36	1.42

The worst 5 of 100 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	BB	37	MIA	C11-S10-C2	5.98	106.73	102.27
35	BE	46	7MG	N9-C8-N7	5.91	111.82	103.38
2	AB	2069	7MG	N9-C8-N7	5.82	111.70	103.38
34	BA	527	7MG	N9-C8-N7	5.72	111.56	103.38
35	BB	46	7MG	N9-C8-N7	5.60	111.39	103.38

There are no chirality outliers.

5 of 32 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	AB	747	5MU	C2'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
34	BA	527	7MG	C4'-C5'-O5'-P
35	BB	37	MIA	N6-C12-C13-C14
35	BB	46	7MG	C4'-C5'-O5'-P
2	AB	1962	5MC	C2'-C1'-N1-C6

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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.

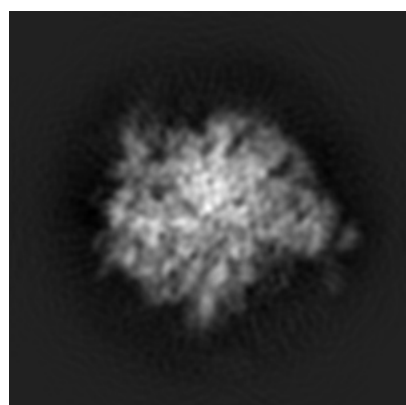
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-1849. These allow visual inspection of the internal detail of the map and identification of artifacts.

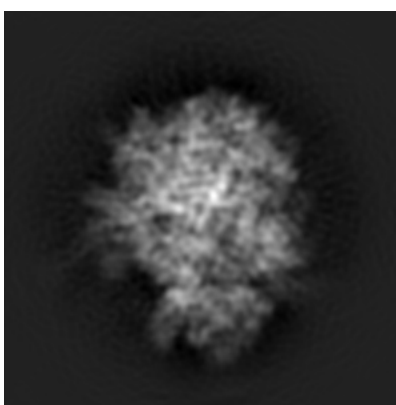
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

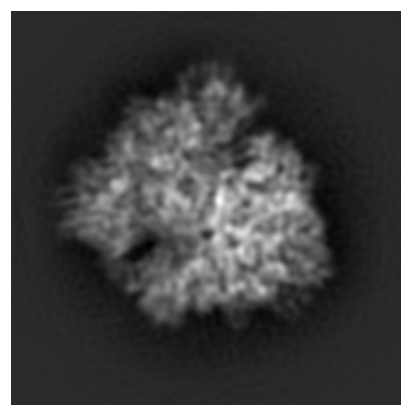
#### 6.1.1 Primary map



X



Y

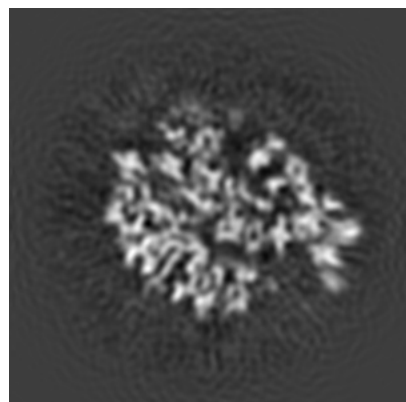


Z

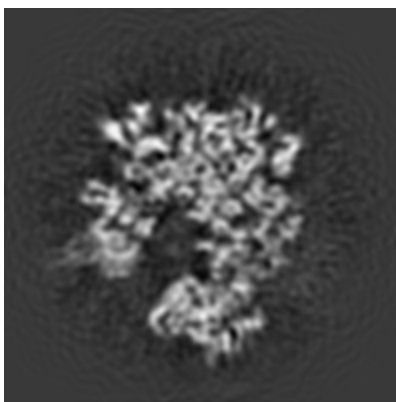
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

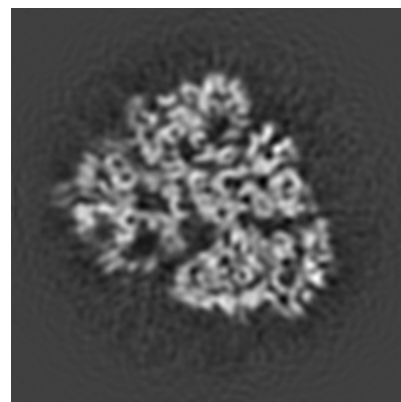
#### 6.2.1 Primary map



X Index: 125



Y Index: 125

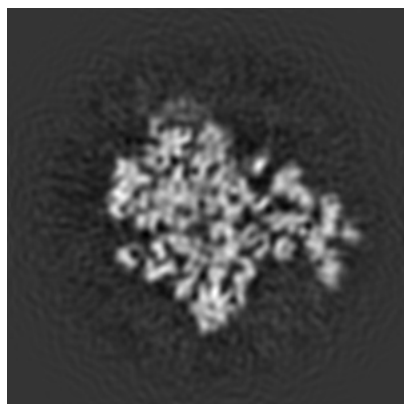


Z Index: 125

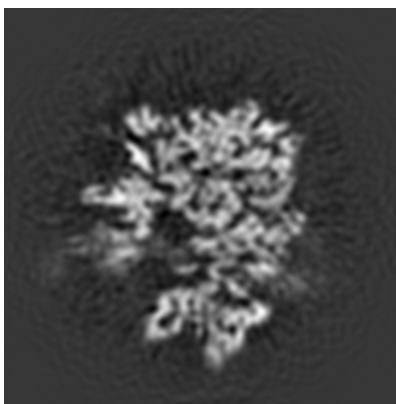
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

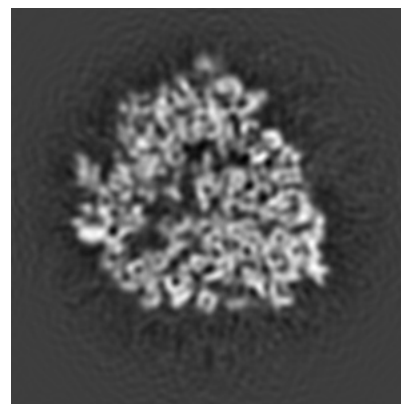
### 6.3.1 Primary map



X Index: 130



Y Index: 130

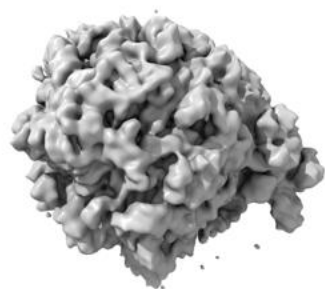


Z Index: 117

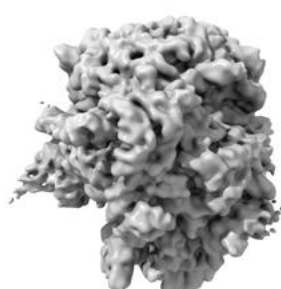
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

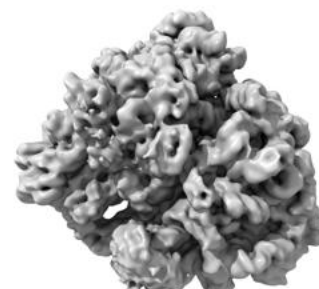
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 32.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

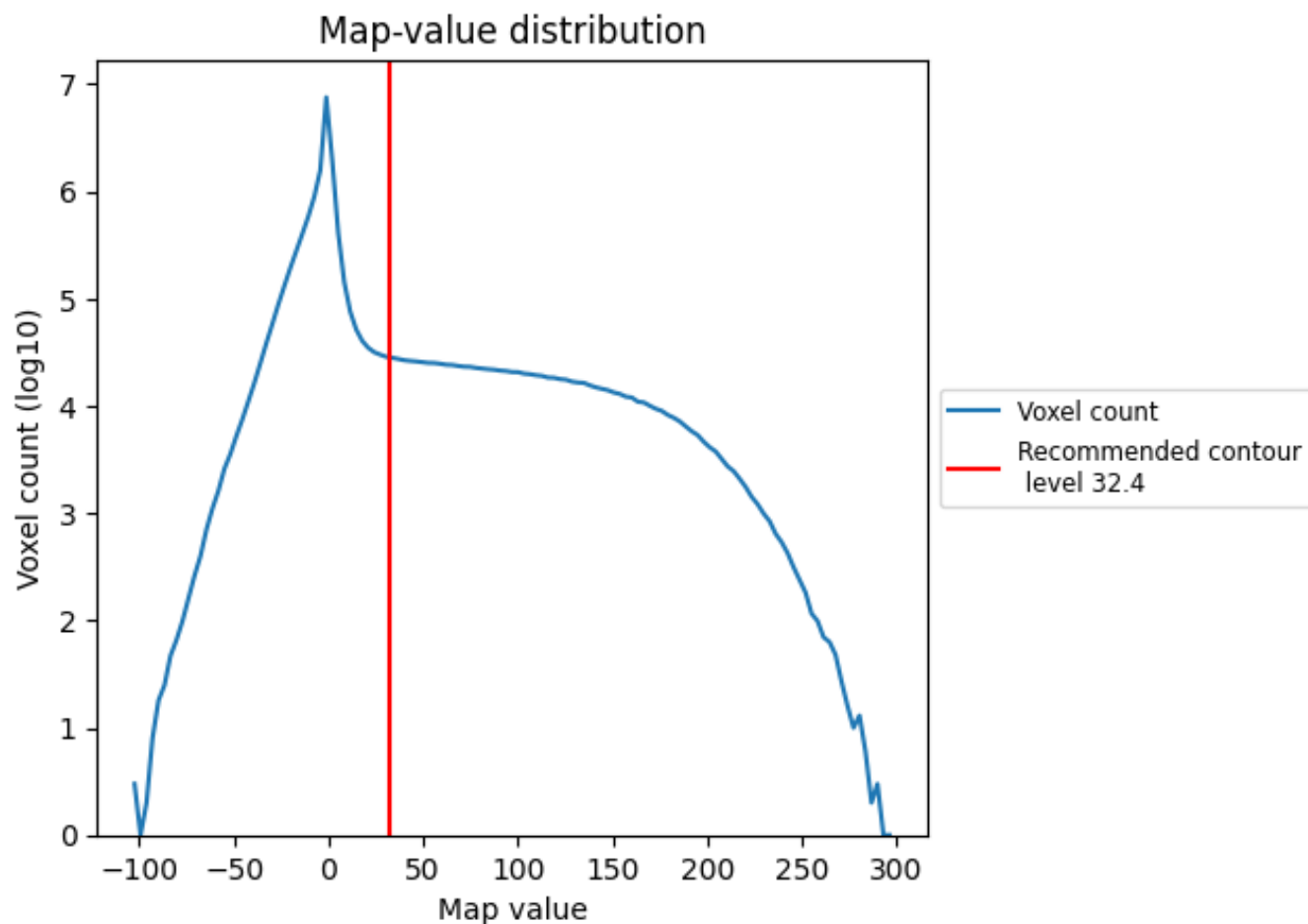
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

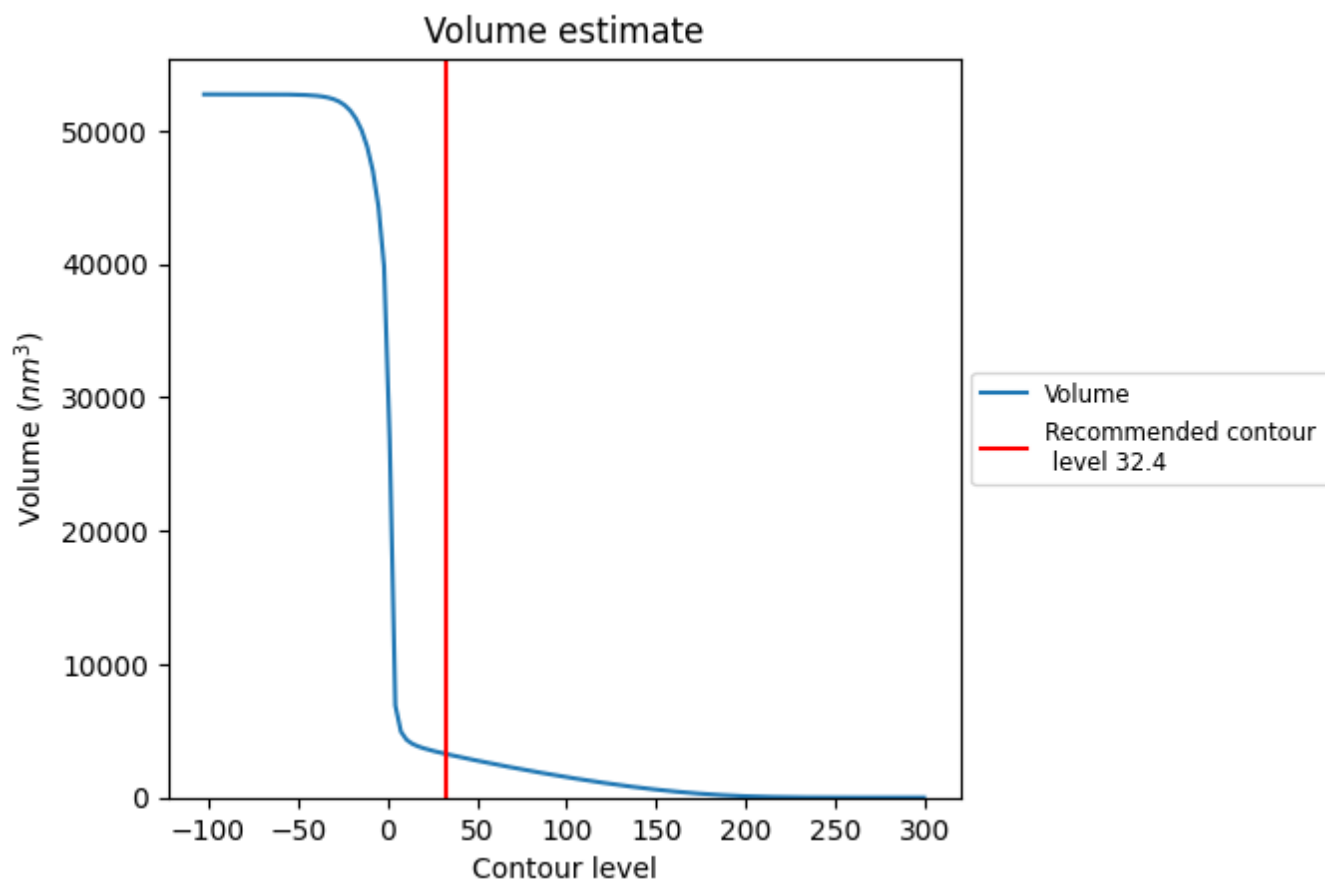
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

## 7.2 Volume estimate [i](#)

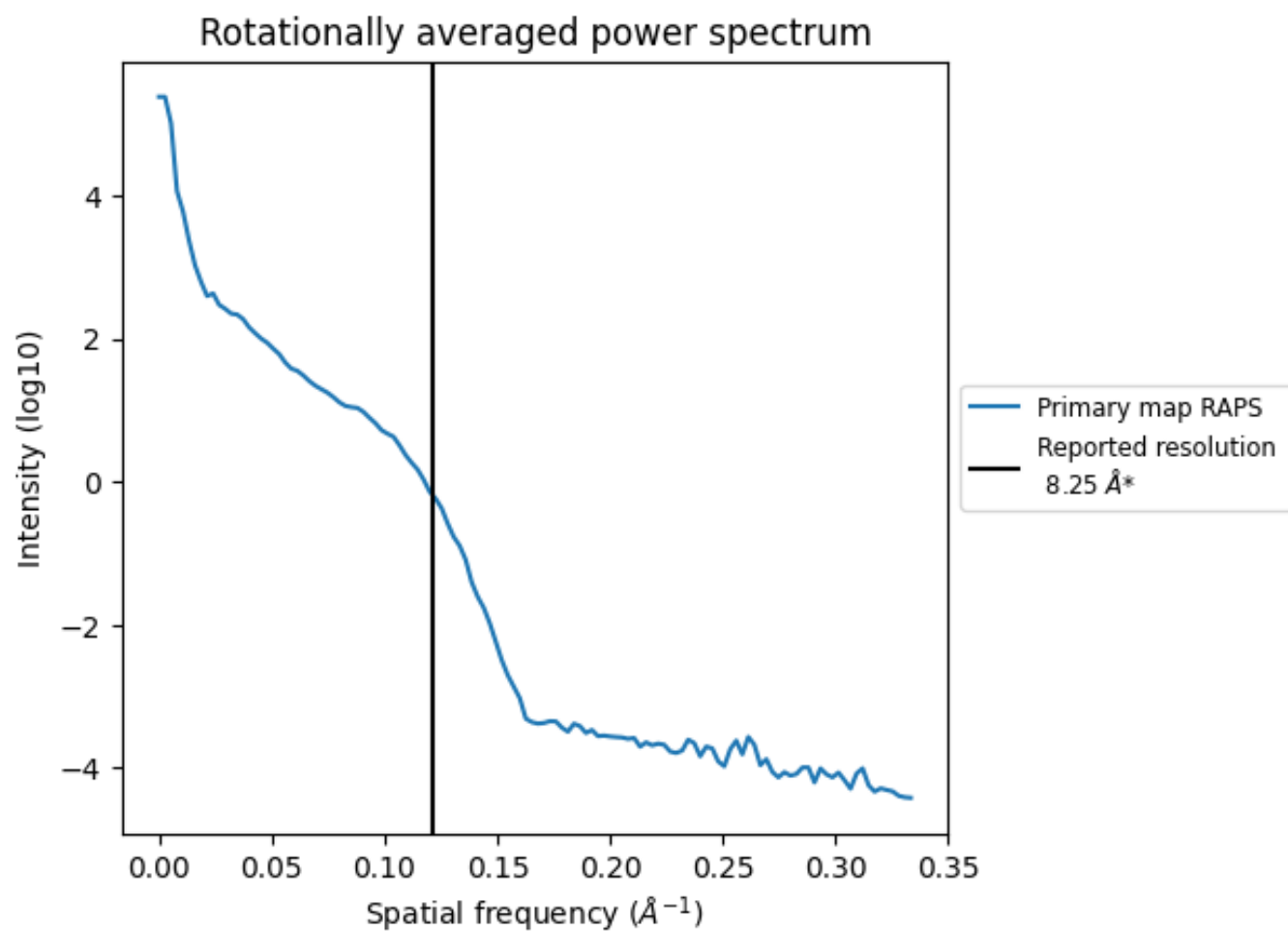


The volume at the recommended contour level is 3278 nm<sup>3</sup>; this corresponds to an approximate mass of 2961 kDa.

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 0.121 Å<sup>-1</sup>

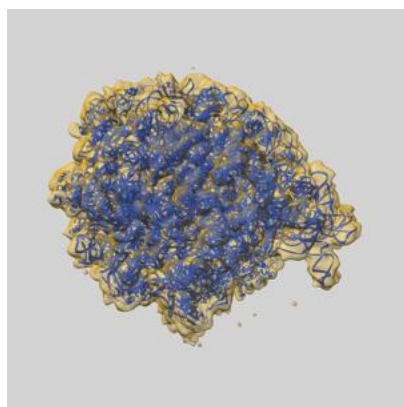
## 8 Fourier-Shell correlation

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

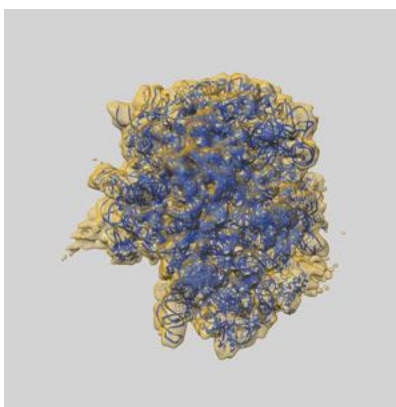
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-1849 and PDB model 4V6K. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

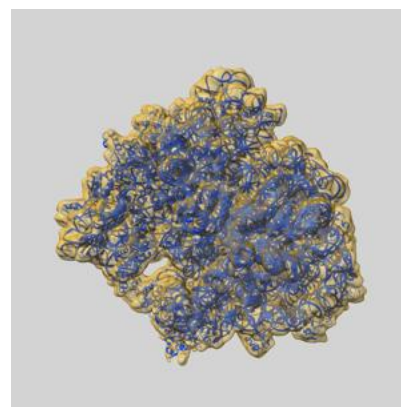
### 9.1 Map-model overlay [i](#)



X



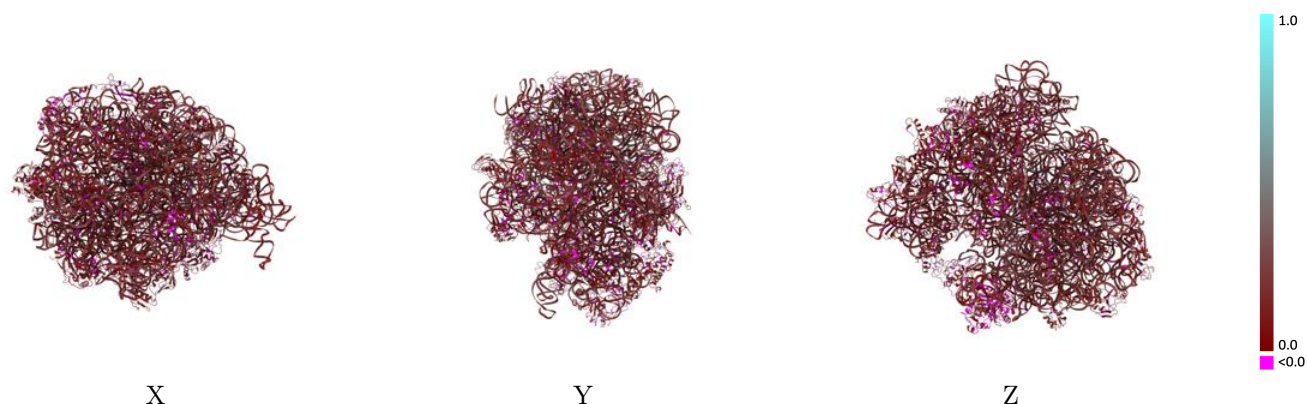
Y



Z

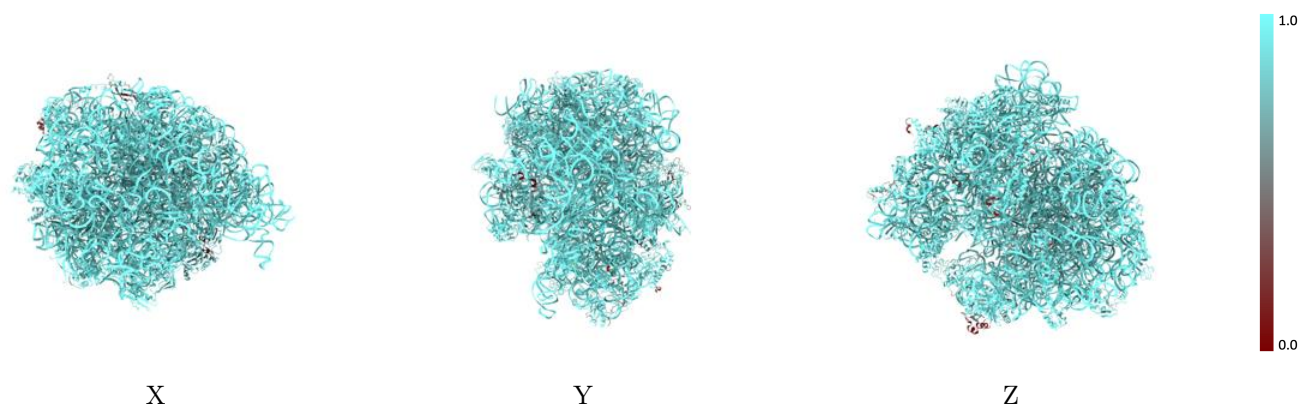
The images above show the 3D surface view of the map at the recommended contour level 32.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



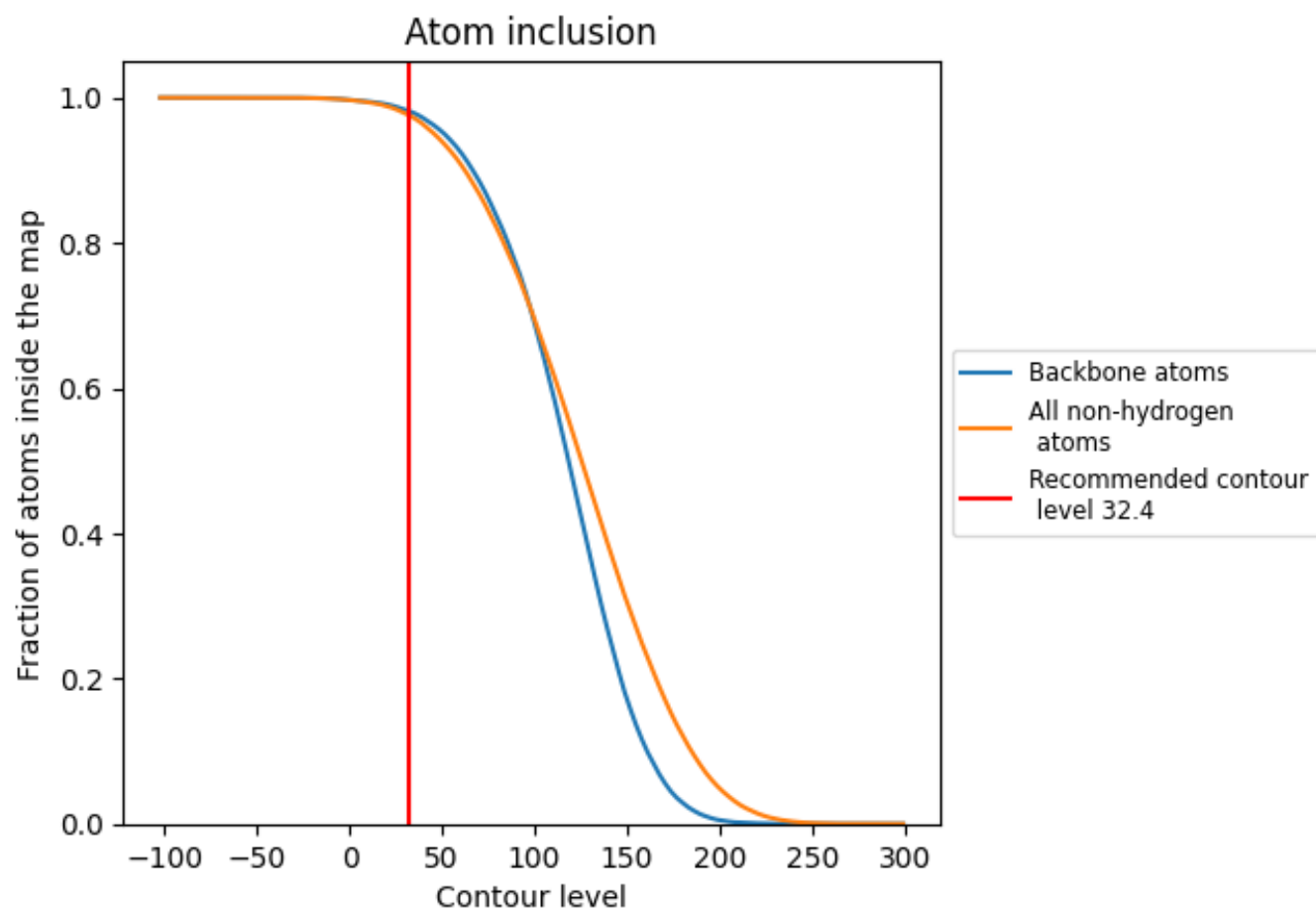
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (32.4).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 98% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ

















































The table lists the average atom inclusion at the recommended contour level (32.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9754	 0.1600
AA	 0.9981	 0.1930
AB	 0.9959	 0.1830
AC	 0.7851	 0.0430
AD	 0.9684	 0.1080
AE	 0.9694	 0.1100
AF	 0.9618	 0.1180
AG	 0.9740	 0.1250
AH	 0.9830	 0.1540
AI	 0.7901	 0.1140
AJ	 0.9599	 0.0990
AK	 0.9327	 0.1130
AL	 0.9501	 0.1230
AM	 0.9668	 0.1220
AN	 0.9607	 0.1210
AO	 0.9804	 0.1190
AP	 0.9897	 0.1380
AQ	 0.9414	 0.1510
AR	 0.9570	 0.1030
AS	 0.9435	 0.1270
AT	 0.9701	 0.1360
AU	 0.9702	 0.1300
AV	 0.9820	 0.1410
AW	 0.9851	 0.1560
AX	 0.8981	 0.0680
AY	 0.9517	 0.1110
AZ	 0.9517	 0.1250
Aa	 0.9794	 0.1460
Ab	 0.8829	 0.0890
Ac	 0.9860	 0.0910
Ad	 0.9607	 0.1000
Ae	 0.9746	 0.0930
Af	 0.9796	 0.1240
Ag	 0.9658	 0.0680
BA	 0.9963	 0.1780



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Chain	Atom inclusion	Q-score
BB	 0.9315	 0.1780
BC	 0.8140	 0.1240
BD	 0.9778	 0.1760
BE	 0.9804	 0.1800
BF	 0.9337	 0.1320
BG	 0.9012	 0.1260
BH	 0.9428	 0.1040
BI	 0.9244	 0.1220
BJ	 0.8731	 0.1110
BK	 0.9653	 0.1270
BL	 0.9812	 0.1450
BM	 0.9688	 0.1090
BN	 0.9250	 0.0960
BO	 0.9390	 0.1190
BP	 0.9501	 0.1150
BQ	 0.9784	 0.1320
BR	 0.9793	 0.1030
BS	 0.9855	 0.1310
BT	 0.9697	 0.1100
BU	 0.9787	 0.1210
BV	 0.9883	 0.1210
BW	 0.9058	 0.0800
BX	 0.9847	 0.1370
BY	 0.8661	 0.0860