



## wwPDB EM Validation Summary Report

Apr 22, 2024 – 06:55 pm BST

PDB ID : 7BL6  
EMDB ID : EMD-12219  
Title : 50S-ObgE-GMPPNP particle  
Authors : Hilal, T.; Nikolay, R.; Schmidt, S.; Spahn, C.M.T.  
Deposited on : 2021-01-18  
Resolution : 4.00 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](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:

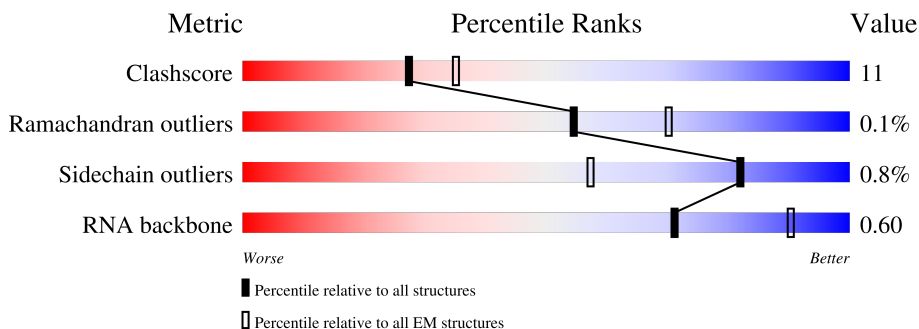
EMDB validation analysis : 0.0.1.dev92  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36.2

# 1 Overall quality at a glance

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

The reported resolution of this entry is 4.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	g	38	
2	C	273	
3	D	209	
4	E	201	
5	F	179	
6	G	177	
7	J	142	

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Mol	Chain	Length	Quality of chain
8	L	144	80% 20%
9	N	120	78% 22%
10	O	117	72% 27%
11	Q	118	81% 18%
12	R	103	76% 24%
13	S	110	71% 29%
14	T	100	64% 29% 7%
15	U	104	82% 16%
16	V	94	74% 24%
17	W	85	72% 18% 11%
18	X	78	71% 28%
19	Y	63	5% 62% 38%
20	Z	59	76% 22%
21	0	57	70% 28%
22	1	55	65% 24% 9%
23	2	46	70% 28%
24	K	123	70% 29%
25	P	115	81% 17%
26	M	136	76% 23%
27	H	149	40% 72% 26%
28	d	70	17% 66% 33%
29	A	2904	48% 47% 6%
30	B	119	48% 49%
31	9	390	7% 71% 16% 13%
32	3	65	71% 26%

## 2 Entry composition [i](#)

There are 36 unique types of molecules in this entry. The entry contains 92769 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 50S ribosomal protein L36.

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	193	1483	932	266	280	5	0	0

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

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

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

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

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

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

- Molecule 8 is a protein called 50S ribosomal protein L15.

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

- Molecule 9 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	N	120	961	593	196	167	5	0	0

- Molecule 10 is a protein called 50S ribosomal protein L18.

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

- Molecule 11 is a protein called 50S ribosomal protein L20.

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

- Molecule 12 is a protein called 50S ribosomal protein L21.

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

- Molecule 13 is a protein called 50S ribosomal protein L22.

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

- Molecule 14 is a protein called 50S ribosomal protein L23.

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

- Molecule 15 is a protein called 50S ribosomal protein L24.

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

- Molecule 16 is a protein called 50S ribosomal protein L25.

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

- Molecule 17 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	W	76	577	357	117	102	1	0	0

- Molecule 18 is a protein called 50S ribosomal protein L28.

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

- Molecule 19 is a protein called 50S ribosomal protein L29.

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

- Molecule 20 is a protein called 50S ribosomal protein L30.

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

- Molecule 21 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	0	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 22 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	1	50	Total	C	N	O	S	0	0
			409	263	75	71			

- Molecule 23 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 24 is a protein called 50S ribosomal protein L14.

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

- Molecule 25 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	P	113	Total	C	N	O	S	0	0
			911	571	178	161	1		

- Molecule 26 is a protein called 50S ribosomal protein L16.

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

- Molecule 27 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	H	149	Total	C	N	O	S	0	0
			1110	699	197	213	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	d	47	Total	C	N	O	S	0	0
			364	227	64	67	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	A	2897	Total	C	N	O	P	0	0
			62195	27745	11446	20107	2897		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	B	119	Total	C	N	O	P	0	0
			2548	1135	466	829	118		

- Molecule 31 is a protein called GTPase ObgE/CgtA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	9	338	Total	C	N	O	S	0	0
			2582	1626	453	490	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 33 is ZINC ION (three-letter code: ZN) (formula: Zn).

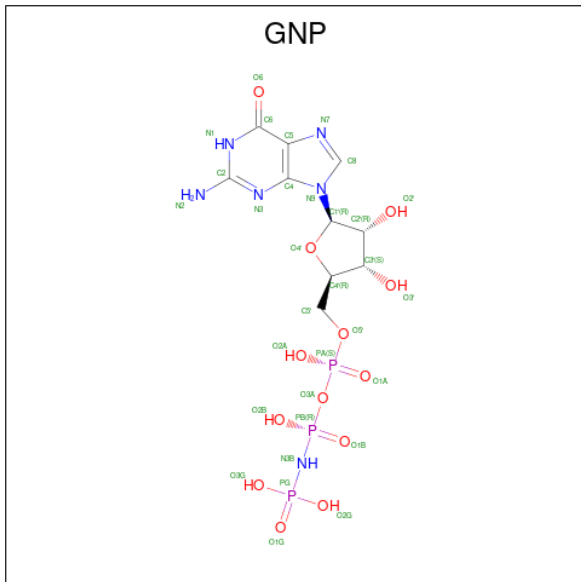
Mol	Chain	Residues	Atoms		AltConf
33	g	1	Total	Zn	0
			1	1	
33	d	1	Total	Zn	0
			1	1	

- Molecule 34 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
34	A	1	Total	Mg	0
			1	1	
34	9	1	Total	Mg	0
			1	1	



- Molecule 35 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula:  $C_{10}H_{17}N_6O_{13}P_3$ ).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
35	9	1	32	10	6	13	3	0

- Molecule 36 is water.

Mol	Chain	Residues	Atoms		AltConf
36	C	1	Total	O	0
			1	1	
36	F	1	Total	O	0
			1	1	
36	N	3	Total	O	0
			3	3	
36	S	1	Total	O	0
			1	1	
36	A	20	Total	O	0
			20	20	
36	B	1	Total	O	0
			1	1	

### 3 Residue-property plots [i](#)

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

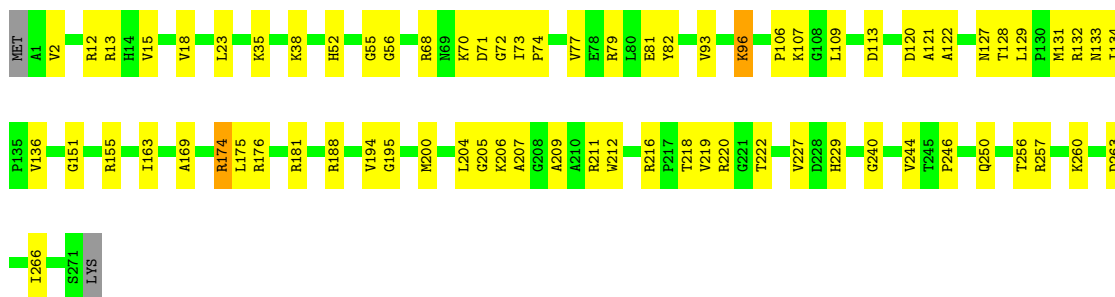
- Molecule 1: 50S ribosomal protein L36

Chain g:  100%

There are no outlier residues recorded for this chain.

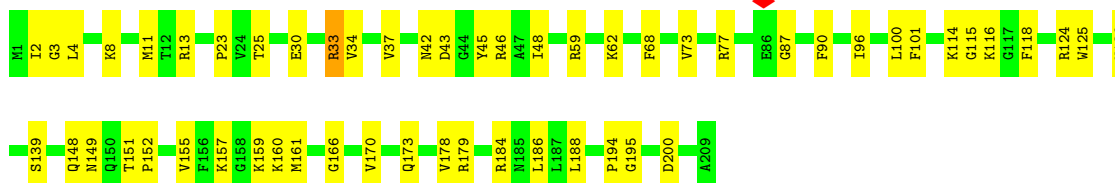
- Molecule 2: 50S ribosomal protein L2

Chain C:  73% 26% ..



- Molecule 3: 50S ribosomal protein L3

Chain D:  74% 26%



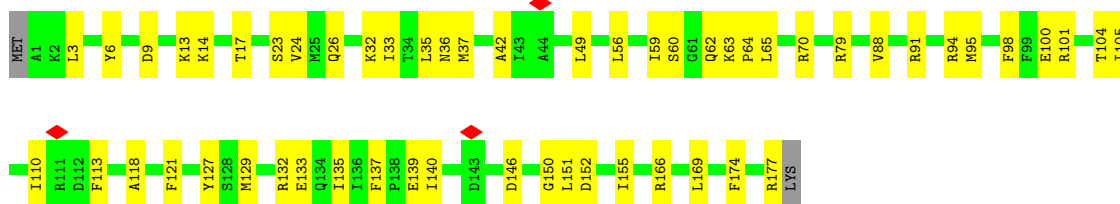
- Molecule 4: 50S ribosomal protein L4

Chain E:  76% 20%

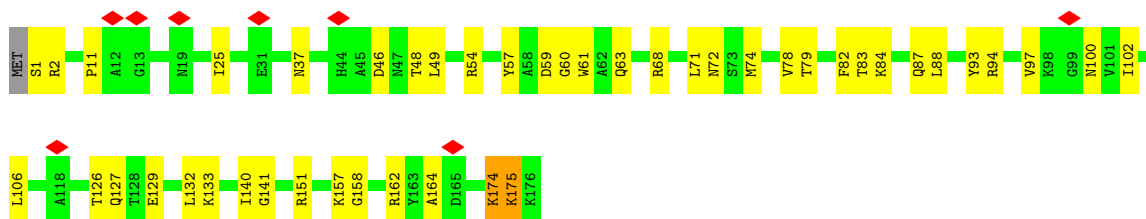
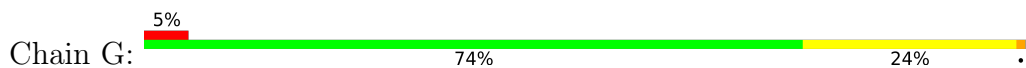




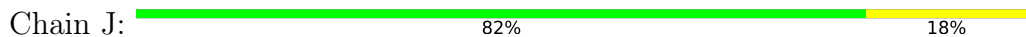
- Molecule 5: 50S ribosomal protein L5



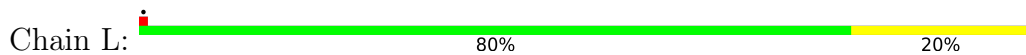
- Molecule 6: 50S ribosomal protein L6



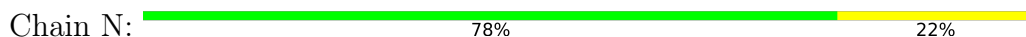
- Molecule 7: 50S ribosomal protein L13



- Molecule 8: 50S ribosomal protein L15

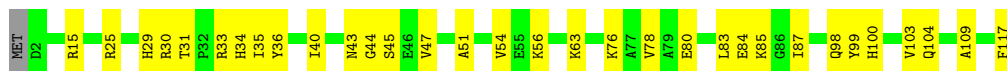


- Molecule 9: 50S ribosomal protein L17

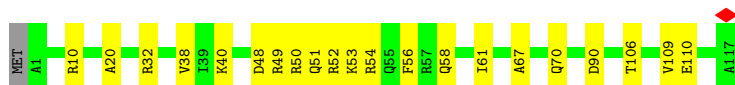
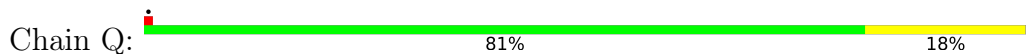


- Molecule 10: 50S ribosomal protein L18

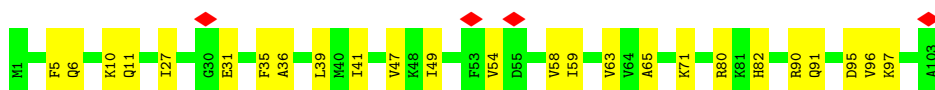
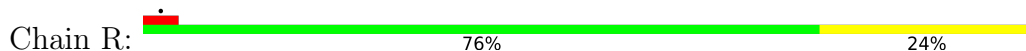




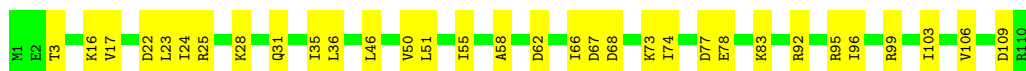
- Molecule 11: 50S ribosomal protein L20



- Molecule 12: 50S ribosomal protein L21



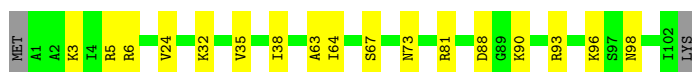
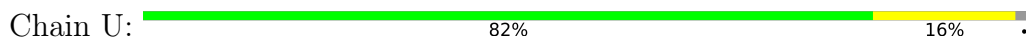
- Molecule 13: 50S ribosomal protein L22



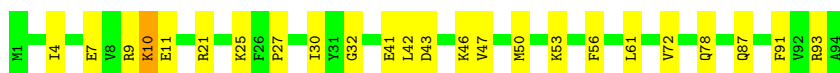
- Molecule 14: 50S ribosomal protein L23



- Molecule 15: 50S ribosomal protein L24



- Molecule 16: 50S ribosomal protein L25



- Molecule 17: 50S ribosomal protein L27

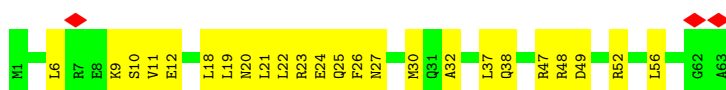




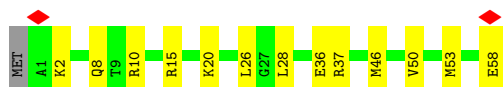
- Molecule 18: 50S ribosomal protein L28



- Molecule 19: 50S ribosomal protein L29



- Molecule 20: 50S ribosomal protein L30



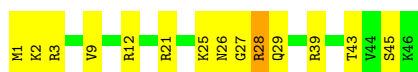
- Molecule 21: 50S ribosomal protein L32



- Molecule 22: 50S ribosomal protein L33



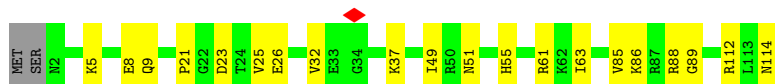
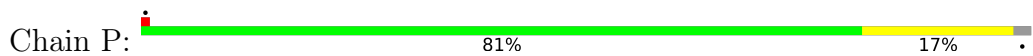
- Molecule 23: 50S ribosomal protein L34



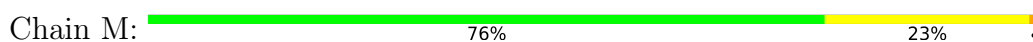
- Molecule 24: 50S ribosomal protein L14



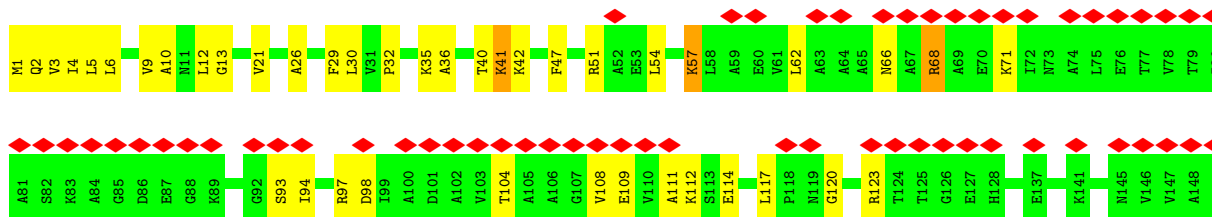
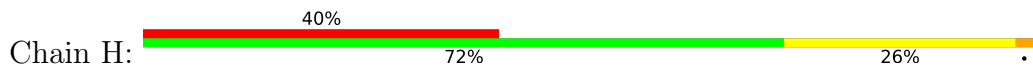
• Molecule 25: 50S ribosomal protein L19



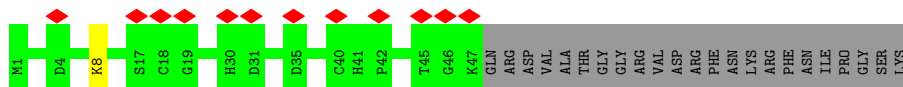
• Molecule 26: 50S ribosomal protein L16



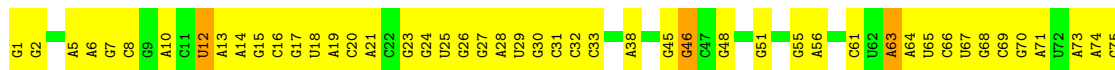
• Molecule 27: 50S ribosomal protein L9



• Molecule 28: 50S ribosomal protein L31



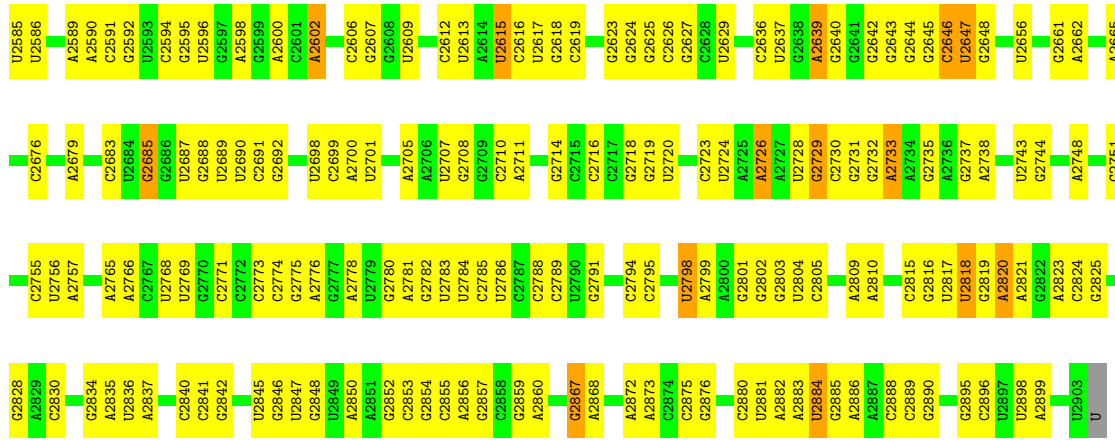
• Molecule 29: 23S ribosomal RNA



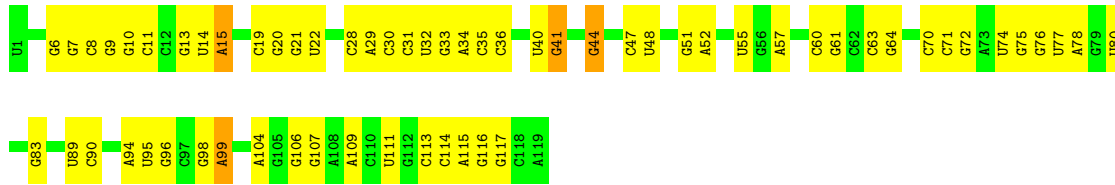
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G1291	G1220	G1136	G1056	G971	A892	U810	A739	C660	A507	C420	C331	A244	A160
G1292	C1221	G1137	G1057	A972	A896	U811	C740	G661	A508	G424	U339	G245	A161
G1293	G1222	G1138	A1057	A973	G900	C812	U741	G662	C510	G248	C341	U162	U162
C1294	G1223	G1139	G1058	G974	A900	C813	A742	A654	A513	C249	C340	G249	C163
C1295	U1224	C1140	U1059	A975	A901	C814	A743	A655	A514	U430	C341	G168	G168
	G1225	U1141	U1060	G976	U826	C815	U744	A656	A515	U431	A342	G169	G169
	A1226	A1142	U1061	G977	U827	C816	G745	A657	A516	C432	A343	U170	U170
	C1229	A1147	U1066	G978	U828	C817	U746	A658	A517	C433	A344	G253	G253
G1299	A1230	A1148	U1067	A979	U829	C818	U747	A659	A518	C434	A345	G254	U171
A1301	G1300	C1153	G1068	C982	U830	C819	U748	G663	C516	U435	A346	A255	A172
A1302	U1231	G1154	A1069	A983	G914	C820	U749	G664	C517	C436	A347	A173	A173
A1308	C1232	A1155	A1070	G987	U831	C821	A750	A668	C518	C437	A348	U174	U174
G1309	U1233	G1156	U1071	C988	U832	C822	A751	G669	G520	U437	C351	G175	G175
G1310	G1234	A1157	C1072	A988	U833	C823	A752	A670	A521	C438	A352	A265	A265
	C1235	G1158	U1073	G989	G914	C824	U753	A671	A522	A439	A353	G266	G266
	A1236	C1161	G1074	C990	G915	C825	C758	A672	A523	G442	U355	G267	G178
	G1238	G1162	G915	C991	A918	C826	G759	C678	A524	U451	G356	G271	G271
	U1242	G1163	A918	C992	G922	C827	A764	C679	A525	G452	U357	A272	A181
	C1243	A1165	G922	A925	G923	C828	C765	C680	A526	G453	U358	G273	A182
	A1244	G1166	G923	A926	G924	C829	U766	G681	A527	A457	C364	A278	C183
	G1250	C1167	A925	G927	A926	U839	U767	G682	A528	G458	U365	G283	C184
	G1251	G1168	A926	G928	G927	C845	C768	A685	A529	A460	C367	U284	G185
	G1252	A1169	G927	G929	A926	U846	G769	A686	A530	A461	U368	G285	A196
	U1253	C1170	G928	G930	G927	C846	A770	U687	A531	G462	U369	G286	A197
	A1254	G1171	A927	G931	G928	U847	U771	G688	A532	G463	U370	U287	C198
A1327	U1255	C1172	G928	G932	U931	C847	G772	A689	A533	U464	G371	G287	A199
A1328	C1256	G1173	A928	G933	U932	U848	G773	G690	A534	C465	A371	U288	U288
U1329	U1257	U1174	U932	G934	A933	C849	G774	A691	A535	A466	G372	G289	U290
	C1257	A1175	U933	G935	G933	U850	G775	G692	A536	G467	U373	U290	C201
	U1258	G1176	U934	G936	A934	C851	G776	C693	A537	G468	A374	U296	U296
	U1259	C1177	U935	G937	G935	C852	G777	A694	A538	G469	U375	G297	A203
	A1260	G1178	A935	G938	G936	U853	G778	U695	A539	A472	G377	U298	U298
	C1261	U1179	U936	G939	G937	C854	G779	G696	A540	C475	U376	A299	U206
	A1262	G1180	U937	G940	A934	U855	G780	G697	A541	G476	U377	A300	A207
	U1263	U1181	U938	G941	G938	C856	A781	A698	A542	C477	U378	G301	C210
	A1264	A1182	U939	G942	G939	U857	A782	G699	A543	A477	C383	G302	C211
	U1265	C1183	U940	G943	G940	U858	G783	U699	A544	G478	U384	G303	G212
	A1266	G1184	U941	G944	G941	C859	G784	G700	A545	A479	U385	U304	A213
	G1267	A1185	U942	G945	A941	U860	G785	G701	A546	A480	U386	G305	A214
	U1268	C1186	U943	G946	G942	C864	G786	G702	A547	A481	U387	C306	G215
	A1269	G1187	U944	G947	G943	U865	G787	U703	A548	A482	U388	U306	G216
	C1270	U1188	U945	G948	G944	U866	G788	G704	A549	A483	U389	G307	A216
	U1271	A1189	U946	G949	G945	U867	G789	G705	A550	C487	U402	G308	A221
	A1272	C1189	U947	G950	G946	C868	G790	G706	A551	G488	U403	A309	A222
	U1273	G1190	U948	G951	G947	U869	G791	G707	A552	A489	U404	A310	A223
	A1274	U1191	C948	G952	G948	C870	G792	G708	A553	G490	U405	A311	C225
	U1275	C1192	G949	G953	G949	C871	G793	G709	A554	A491	U406	A312	A226
	A1276	G1193	U949	G954	G950	U874	G794	U710	A555	A492	U407	G319	G319
	G1277	U1194	U950	G955	G951	C872	G795	G711	A556	A493	U408	A320	A320
	C1278	A1204	U951	G956	G952	U875	G796	G712	A557	G494	U409	U321	G230
	U1279	G1206	U952	G957	G953	C873	G797	G713	A558	A495	U410	U322	A231
	G1280	C1208	U953	G958	G954	U876	G798	G714	A559	A496	U411	G323	G232
A1365	U1281	U1130	C964	G959	G955	C874	G799	U715	A560	A497	U412	C324	A233
	U1282	G1212	C965	G960	G956	U877	G800	G729	A561	G498	U413	A324	A233
	G1283	A1213	G961	G961	G957	C875	G801	U730	A562	U499	C414	C414	A233
	A1286	U1217	U962	G962	G958	U878	G802	G731	A563	G500	A415	A415	C239
	A1287	G1218	U963	G963	G959	U879	G803	G732	A564	A503	U416	U416	C239
			U964	G964	G960	C880	G804	G733	A565	A504	U417	U328	U328
			U965	G965	G961	C881	G805	G734	A566	A505	U418	G329	G329
			U966	G966	G962	U882	G806						
			U967	G967	G963	C883	G807						
			U968	G968	G964	U884	G808						
			U969	G969	G965	C885	G809						
			A		G966	C886	G810						
			U		G967								
			C		U968								
			C		G969								



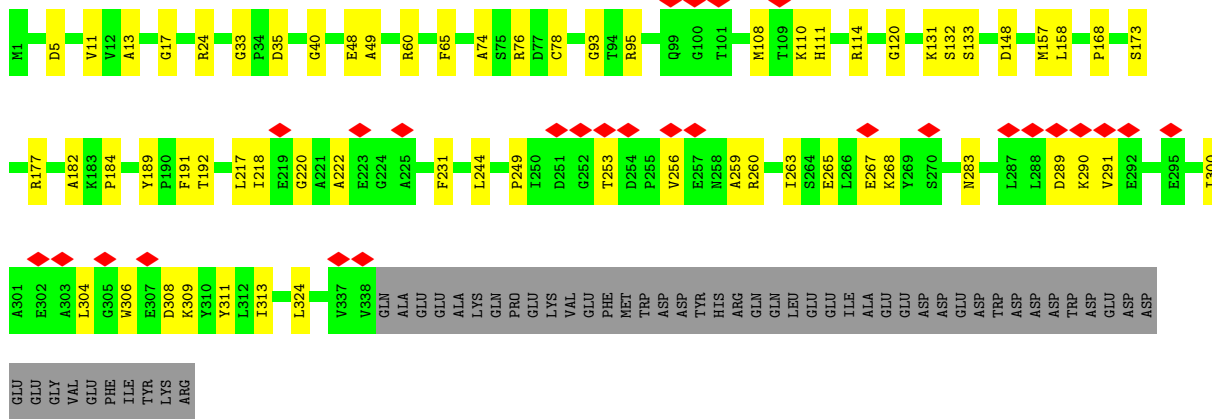




• Molecule 30: 5S ribosomal RNA



• Molecule 31: GTPase ObgE/CgtA



• Molecule 32: 50S ribosomal protein L35



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	45746	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	120000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	2.195	Depositor
Minimum map value	-0.000	Depositor
Average map value	0.034	Depositor
Map value standard deviation	0.170	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	417.6, 417.6, 417.6	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.74, 1.74, 1.74	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GNP, ZN, MG

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	g	0.23	0/303	0.44	0/397
2	C	0.23	0/2121	0.43	0/2852
3	D	0.24	0/1586	0.45	0/2134
4	E	0.23	0/1499	0.41	0/2016
5	F	0.24	0/1434	0.44	0/1926
6	G	0.24	0/1343	0.45	0/1816
7	J	0.23	0/1152	0.40	0/1551
8	L	0.25	0/1062	0.48	0/1413
9	N	0.24	0/974	0.42	0/1301
10	O	0.25	0/902	0.47	0/1209
11	Q	0.28	0/960	0.40	0/1278
12	R	0.25	0/829	0.46	0/1107
13	S	0.23	0/864	0.41	0/1156
14	T	0.23	0/744	0.44	0/994
15	U	0.24	0/787	0.46	0/1051
16	V	0.25	0/766	0.48	0/1025
17	W	0.25	0/584	0.42	0/772
18	X	0.22	0/635	0.41	0/848
19	Y	0.26	0/510	0.63	0/677
20	Z	0.23	0/453	0.44	0/605
21	0	0.21	0/450	0.48	0/599
22	1	0.24	0/416	0.44	0/554
23	2	0.22	0/380	0.39	0/498
24	K	0.24	0/947	0.47	0/1268
25	P	0.24	0/923	0.42	0/1234
26	M	0.24	0/1093	0.44	0/1460
27	H	0.24	0/1121	0.47	0/1515
28	d	0.24	0/371	0.48	0/496
29	A	0.16	0/69659	0.73	7/108672 (0.0%)
30	B	0.14	0/2847	0.70	0/4440
31	9	0.24	0/2626	0.45	0/3542
32	3	0.23	0/513	0.47	0/676

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
All	All	0.18	0/100854	0.67	7/151082 (0.0%)

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A	1313	U	C2-N1-C1'	6.94	126.03	117.70
29	A	1893	C	N3-C2-O2	-6.47	117.37	121.90
29	A	1313	U	N1-C2-O2	5.97	126.98	122.80
29	A	1313	U	N3-C2-O2	-5.66	118.24	122.20
29	A	1893	C	N1-C2-O2	5.39	122.13	118.90

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	g	302	0	340	0	0
2	C	2082	0	2157	58	0
3	D	1565	0	1616	40	0
4	E	1483	0	1548	25	0
5	F	1410	0	1447	39	0
6	G	1323	0	1374	28	0
7	J	1129	0	1162	19	0
8	L	1053	0	1129	24	0
9	N	961	0	1000	20	0
10	O	892	0	923	22	0
11	Q	947	0	1022	17	0
12	R	816	0	839	18	0
13	S	857	0	922	22	0
14	T	738	0	807	23	0
15	U	779	0	834	14	0
16	V	753	0	780	19	0
17	W	577	0	594	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	X	625	0	655	15	0
19	Y	509	0	543	20	0
20	Z	449	0	491	9	0
21	0	444	0	461	12	0
22	1	409	0	440	12	0
23	2	377	0	418	11	0
24	K	938	0	1012	24	0
25	P	911	0	957	13	0
26	M	1074	0	1157	20	0
27	H	1110	0	1148	30	0
28	d	364	0	364	0	0
29	A	62195	0	31280	1102	0
30	B	2548	0	1292	55	0
31	9	2582	0	2606	40	0
32	3	504	0	574	14	0
33	d	1	0	0	0	0
33	g	1	0	0	0	0
34	9	1	0	0	0	0
34	A	1	0	0	0	0
35	9	32	0	13	2	0
36	A	20	0	0	0	0
36	B	1	0	0	0	0
36	C	1	0	0	0	0
36	F	1	0	0	0	0
36	N	3	0	0	0	0
36	S	1	0	0	0	0
All	All	92769	0	61905	1601	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 11.

The worst 5 of 1601 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)
29:A:1433:A:N6	29:A:1560:G:H1	1.63	0.96
29:A:408:G:H1	29:A:419:U:H3	1.08	0.95
29:A:2102:G:H1	29:A:2187:U:H3	1.17	0.92
29:A:2475:C:H42	29:A:2529:G:H22	1.13	0.91
29:A:377:G:H1	29:A:397:U:H3	0.93	0.90

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	g	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
2	C	269/273 (98%)	258 (96%)	11 (4%)	0	100	100
3	D	207/209 (99%)	195 (94%)	12 (6%)	0	100	100
4	E	189/201 (94%)	180 (95%)	9 (5%)	0	100	100
5	F	175/179 (98%)	163 (93%)	12 (7%)	0	100	100
6	G	174/177 (98%)	165 (95%)	9 (5%)	0	100	100
7	J	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
8	L	142/144 (99%)	129 (91%)	13 (9%)	0	100	100
9	N	118/120 (98%)	112 (95%)	6 (5%)	0	100	100
10	O	114/117 (97%)	109 (96%)	5 (4%)	0	100	100
11	Q	115/118 (98%)	111 (96%)	4 (4%)	0	100	100
12	R	101/103 (98%)	100 (99%)	1 (1%)	0	100	100
13	S	108/110 (98%)	105 (97%)	3 (3%)	0	100	100
14	T	91/100 (91%)	85 (93%)	6 (7%)	0	100	100
15	U	100/104 (96%)	91 (91%)	9 (9%)	0	100	100
16	V	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
17	W	74/85 (87%)	71 (96%)	3 (4%)	0	100	100
18	X	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
19	Y	61/63 (97%)	54 (88%)	7 (12%)	0	100	100
20	Z	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
21	0	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
22	1	48/55 (87%)	48 (100%)	0	0	100	100
23	2	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
24	K	120/123 (98%)	114 (95%)	6 (5%)	0	100	100
25	P	111/115 (96%)	108 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	M	134/136 (98%)	131 (98%)	3 (2%)	0	100	100
27	H	147/149 (99%)	131 (89%)	16 (11%)	0	100	100
28	d	45/70 (64%)	44 (98%)	1 (2%)	0	100	100
31	9	336/390 (86%)	321 (96%)	15 (4%)	0	100	100
32	3	62/65 (95%)	59 (95%)	1 (2%)	2 (3%)	4	31
All	All	3538/3720 (95%)	3370 (95%)	166 (5%)	2 (0%)	54	84

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
32	3	31	ILE
32	3	32	LEU

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	g	34/34 (100%)	34 (100%)	0	100	100
2	C	216/218 (99%)	214 (99%)	2 (1%)	78	88
3	D	164/164 (100%)	163 (99%)	1 (1%)	86	92
4	E	159/165 (96%)	159 (100%)	0	100	100
5	F	148/150 (99%)	147 (99%)	1 (1%)	84	90
6	G	137/138 (99%)	133 (97%)	4 (3%)	42	65
7	J	116/116 (100%)	114 (98%)	2 (2%)	60	78
8	L	103/103 (100%)	103 (100%)	0	100	100
9	N	100/100 (100%)	100 (100%)	0	100	100
10	O	86/87 (99%)	86 (100%)	0	100	100
11	Q	89/90 (99%)	89 (100%)	0	100	100
12	R	84/84 (100%)	84 (100%)	0	100	100
13	S	93/93 (100%)	93 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	T	80/84 (95%)	80 (100%)	0	100	100
15	U	83/85 (98%)	83 (100%)	0	100	100
16	V	78/78 (100%)	77 (99%)	1 (1%)	69	82
17	W	57/63 (90%)	57 (100%)	0	100	100
18	X	67/68 (98%)	67 (100%)	0	100	100
19	Y	55/55 (100%)	54 (98%)	1 (2%)	59	77
20	Z	48/49 (98%)	48 (100%)	0	100	100
21	0	47/48 (98%)	47 (100%)	0	100	100
22	1	45/49 (92%)	44 (98%)	1 (2%)	52	71
23	2	38/38 (100%)	37 (97%)	1 (3%)	46	67
24	K	103/104 (99%)	103 (100%)	0	100	100
25	P	98/100 (98%)	98 (100%)	0	100	100
26	M	109/109 (100%)	108 (99%)	1 (1%)	78	88
27	H	114/114 (100%)	110 (96%)	4 (4%)	36	61
28	d	43/62 (69%)	42 (98%)	1 (2%)	50	70
31	9	273/321 (85%)	271 (99%)	2 (1%)	84	90
32	3	51/52 (98%)	51 (100%)	0	100	100
All	All	2918/3021 (97%)	2896 (99%)	22 (1%)	82	89

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
26	M	60	GLN
27	H	57	LYS
27	H	42	LYS
27	H	68	ARG
6	G	174	LYS

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

Mol	Chain	Res	Type
1	g	37	GLN
5	F	126	ASN
15	U	73	ASN
16	V	87	GLN



### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
29	A	2895/2904 (99%)	390 (13%)	9 (0%)
30	B	118/119 (99%)	9 (7%)	0
All	All	3013/3023 (99%)	399 (13%)	9 (0%)

5 of 399 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
29	A	10	A
29	A	12	U
29	A	14	A
29	A	27	G
29	A	46	G

5 of 9 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
29	A	2505	G
29	A	2756	U
29	A	1328	A
29	A	1378	A
29	A	2127	G

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 for Mogul analysis.

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	$\# Z  > 2$
35	GNP	9	402	34	29,34,34	1.63	7 (24%)	33,54,54	2.11	6 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	GNP	9	402	34	-	4/14/38/38	0/3/3/3

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	9	402	GNP	PB-O3A	4.53	1.64	1.59
35	9	402	GNP	C6-N1	3.14	1.38	1.33
35	9	402	GNP	PB-O1B	3.12	1.51	1.46
35	9	402	GNP	PG-N3B	3.04	1.71	1.63
35	9	402	GNP	PG-O1G	2.73	1.50	1.46

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	9	402	GNP	C5-C6-N1	-8.42	111.91	123.43
35	9	402	GNP	C2-N1-C6	5.82	125.18	115.93
35	9	402	GNP	N3-C2-N1	-2.71	123.60	127.22
35	9	402	GNP	PB-O3A-PA	-2.59	123.49	132.62
35	9	402	GNP	C4-C5-C6	-2.59	118.33	120.80

There are no chirality outliers.

All (4) torsion outliers are listed below:

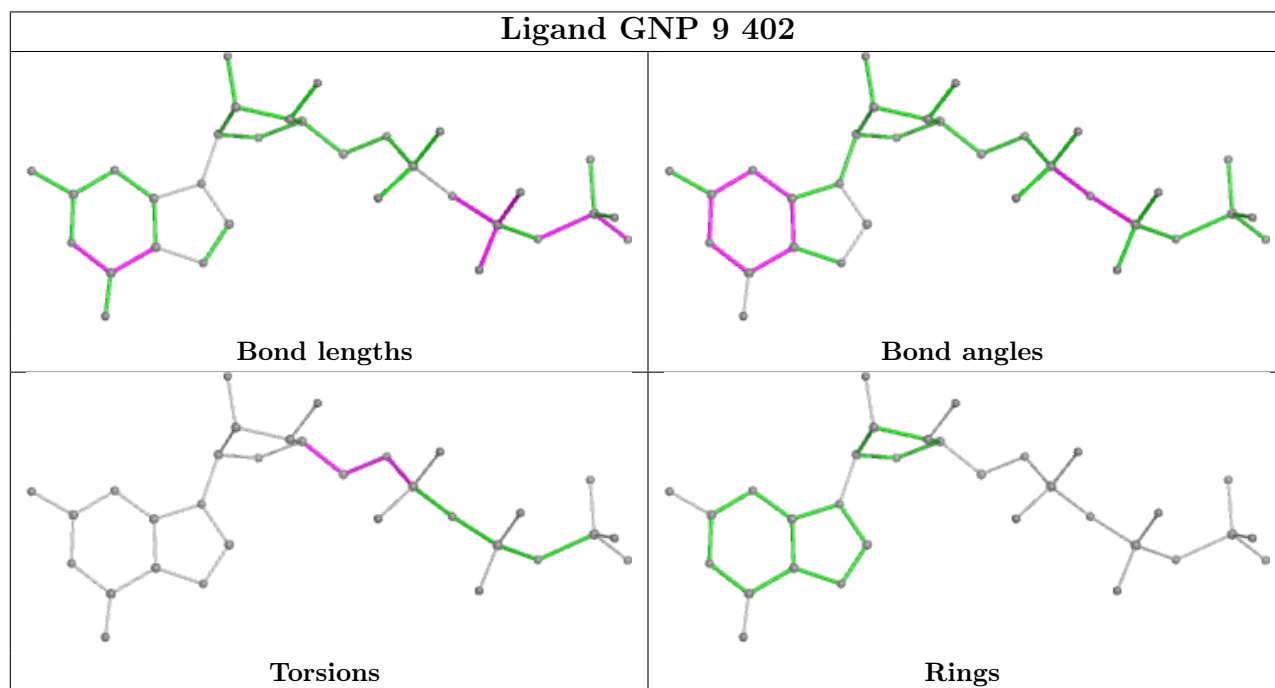
Mol	Chain	Res	Type	Atoms
35	9	402	GNP	C4'-C5'-O5'-PA
35	9	402	GNP	O4'-C4'-C5'-O5'
35	9	402	GNP	C5'-O5'-PA-O3A
35	9	402	GNP	C5'-O5'-PA-O1A

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	9	402	GNP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 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.

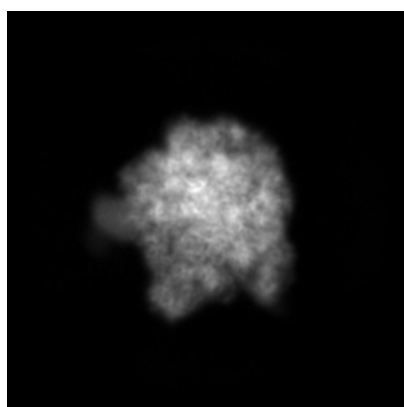
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12219. These allow visual inspection of the internal detail of the map and identification of artifacts.

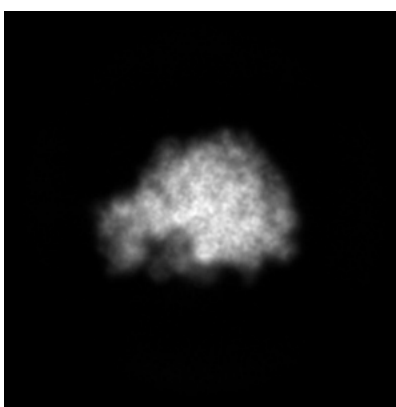
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

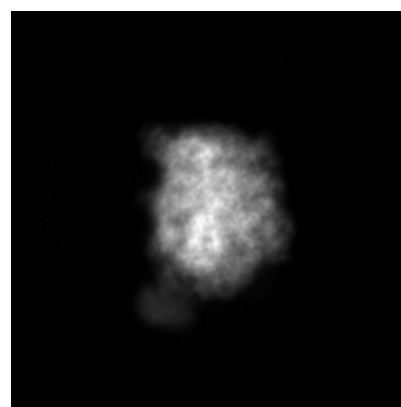
#### 6.1.1 Primary map



X



Y

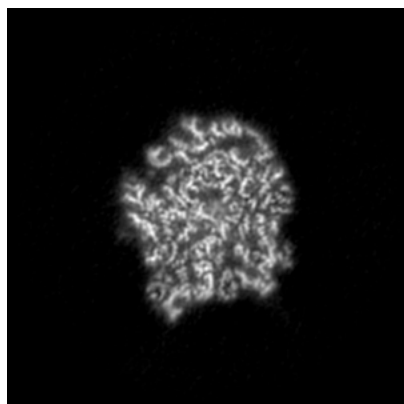


Z

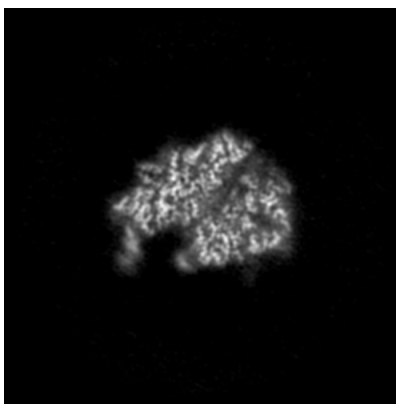
The images above show the map projected in three orthogonal directions.

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

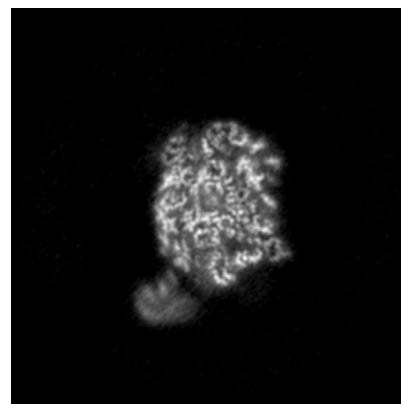
#### 6.2.1 Primary map



X Index: 120



Y Index: 120

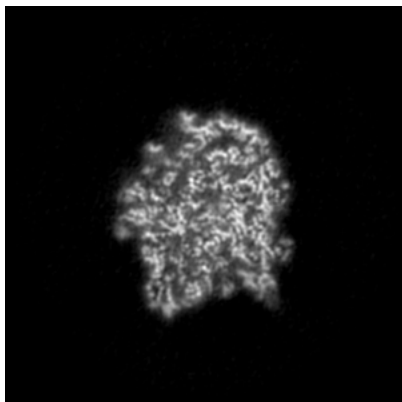


Z Index: 120

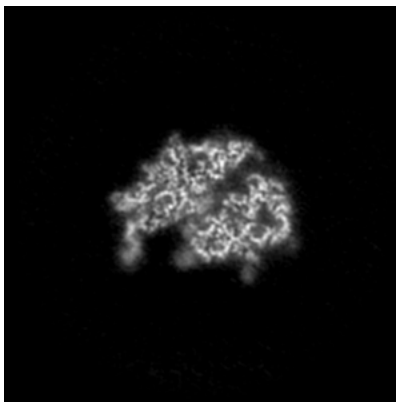
The images above show central slices of the map in three orthogonal directions.

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

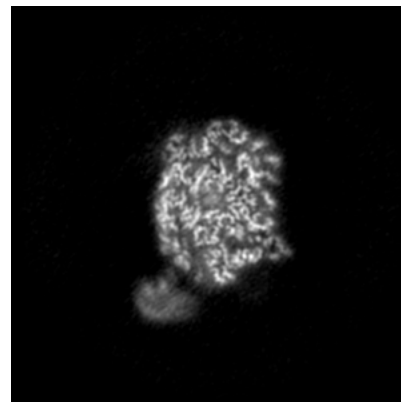
### 6.3.1 Primary map



X Index: 117



Y Index: 123

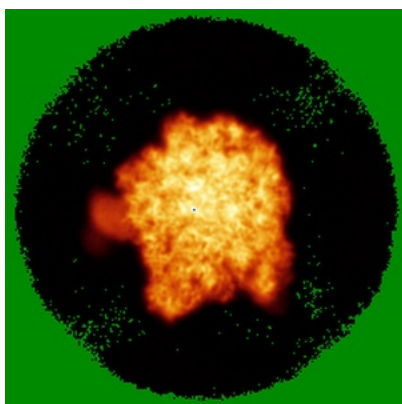


Z Index: 119

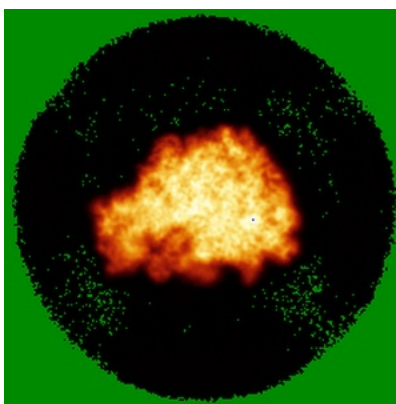
The images above show the largest variance slices of the map in three orthogonal directions.

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

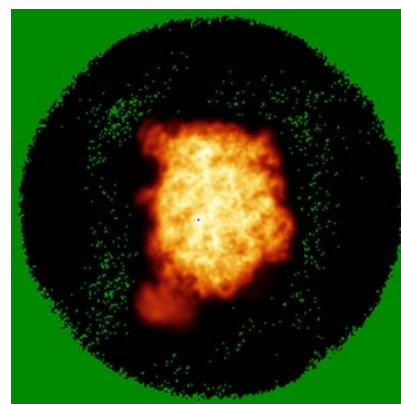
### 6.4.1 Primary map



X



Y

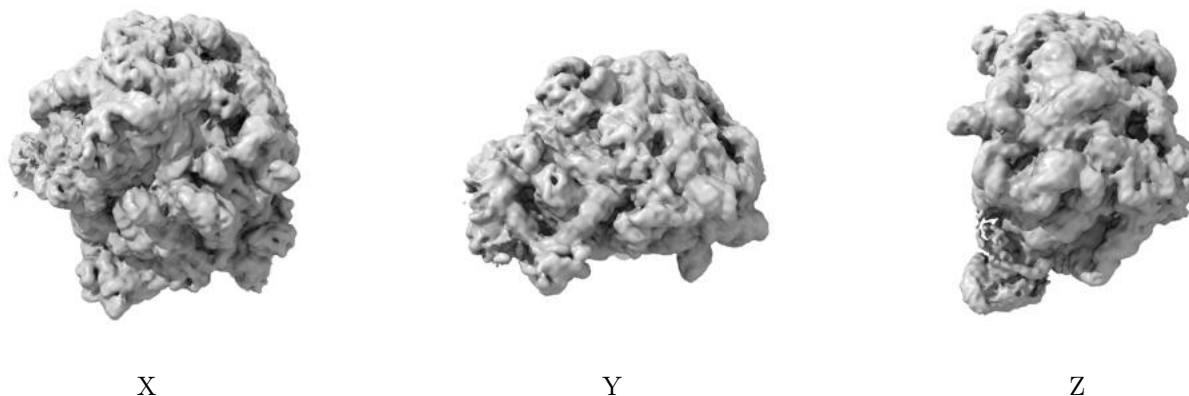


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

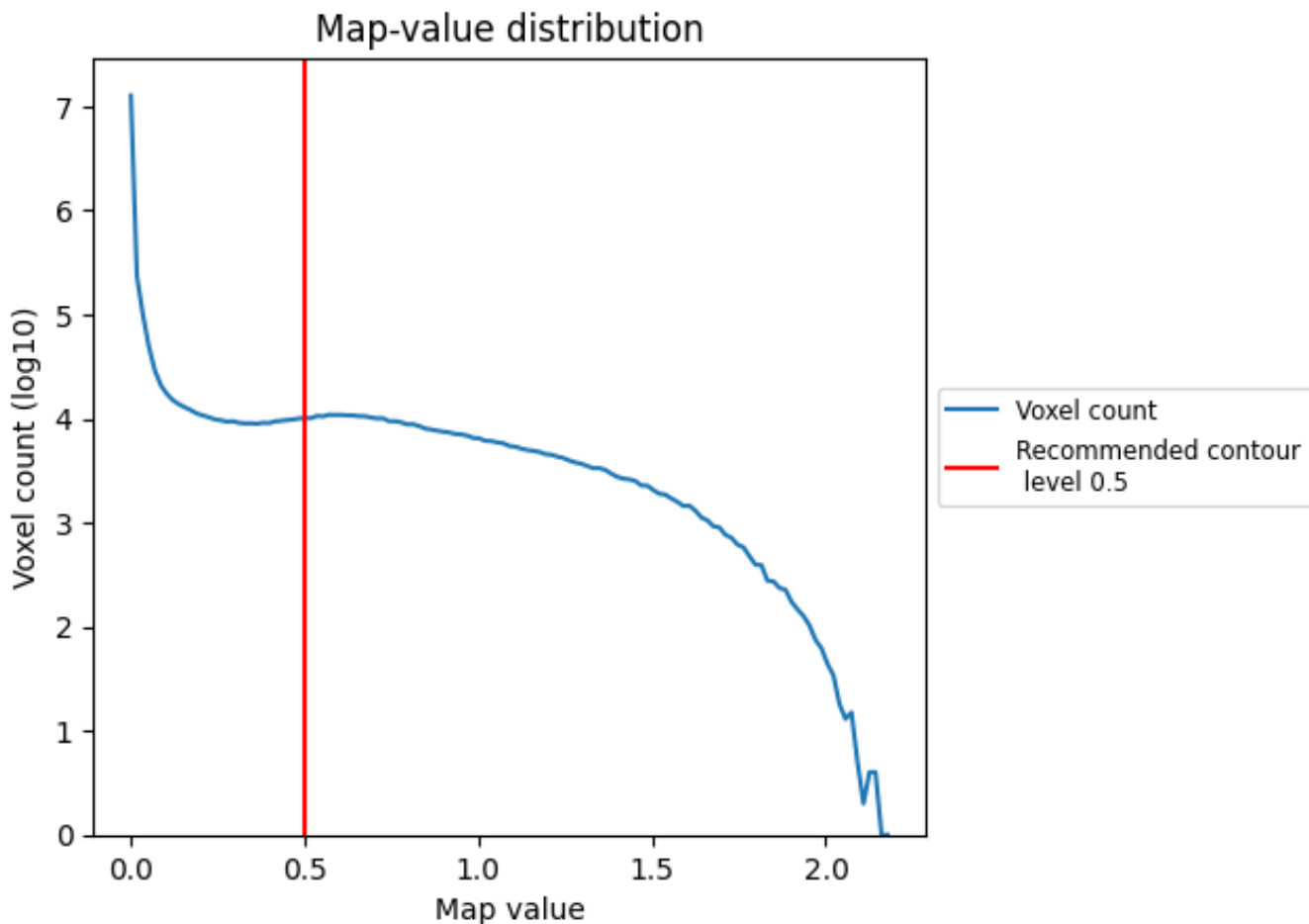
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

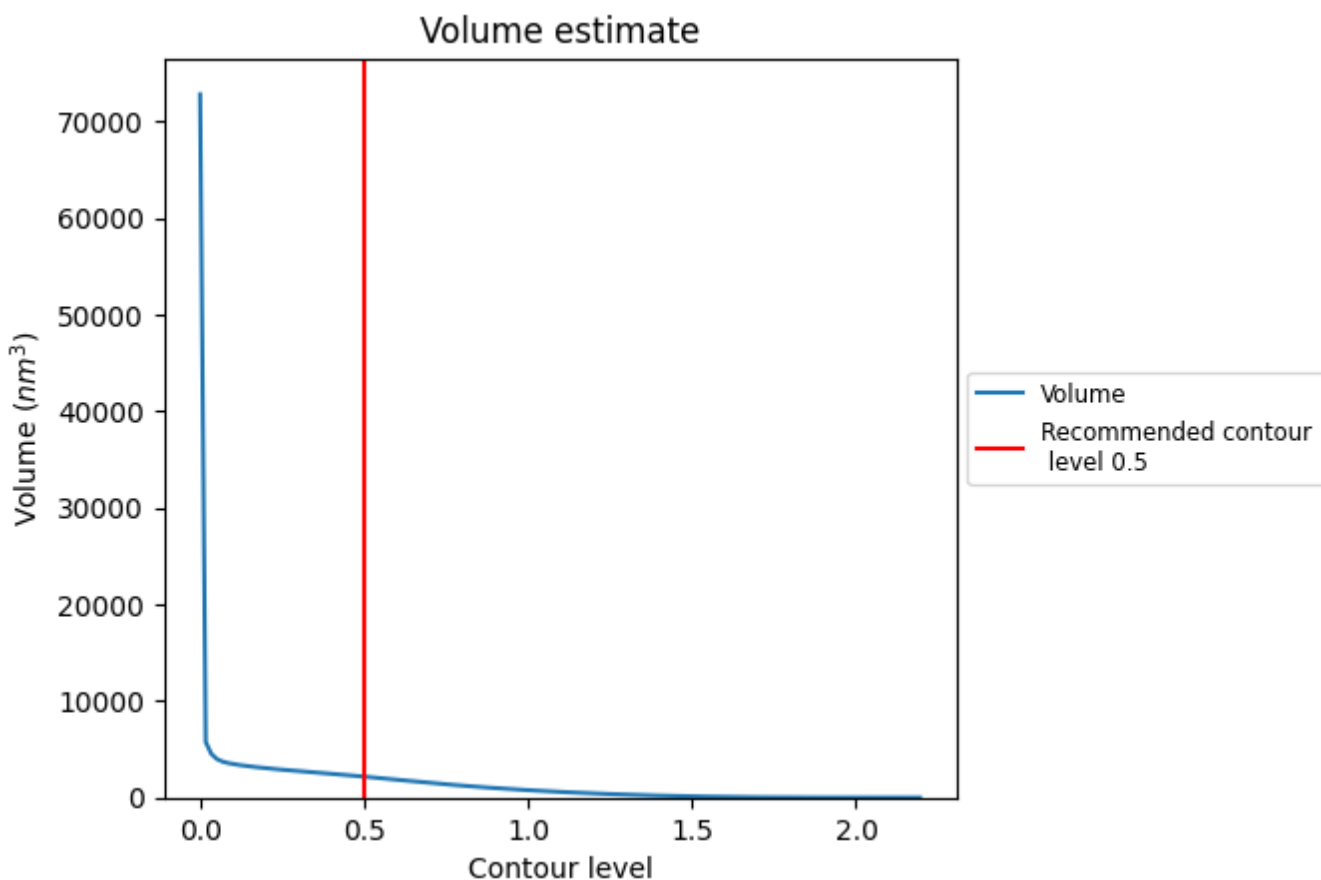
This section contains the results of statistical analysis of the map.

### 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](#)

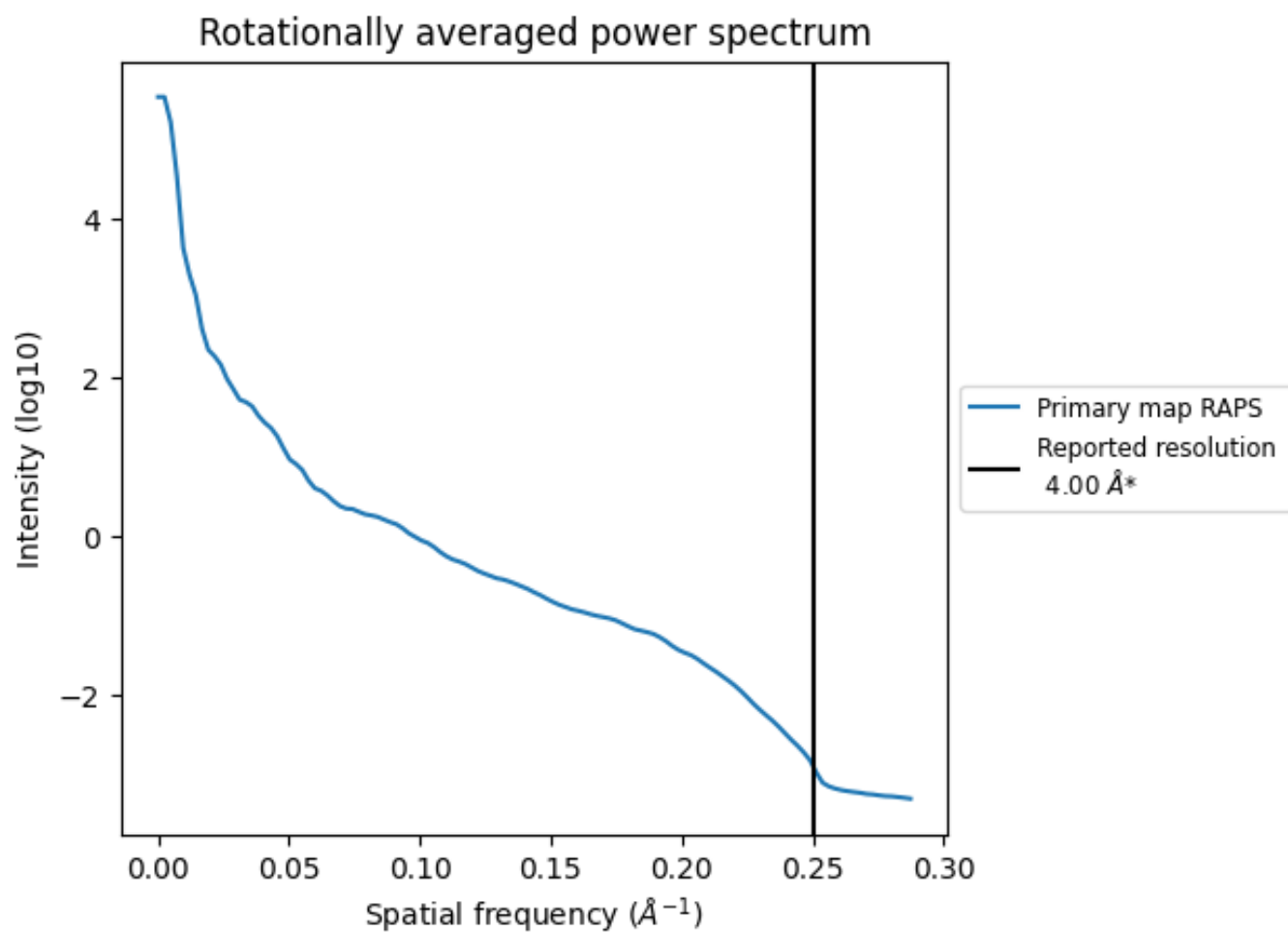


The volume at the recommended contour level is 2171  $\text{nm}^3$ ; this corresponds to an approximate mass of 1962 kDa.

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



### 7.3 Rotationally averaged power spectrum [i](#)

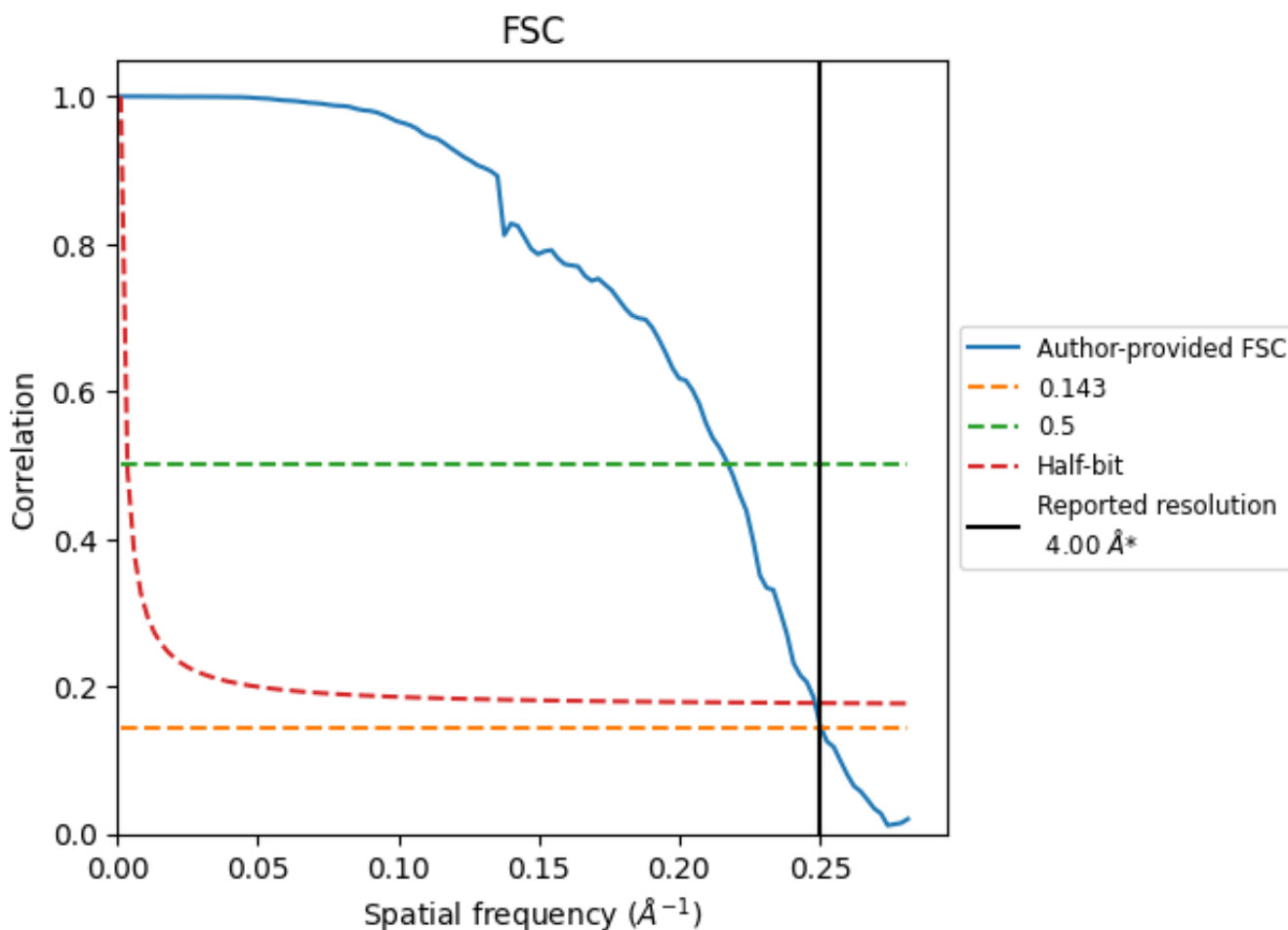


\*Reported resolution corresponds to spatial frequency of 0.250 Å<sup>-1</sup>

## 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 0.250 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

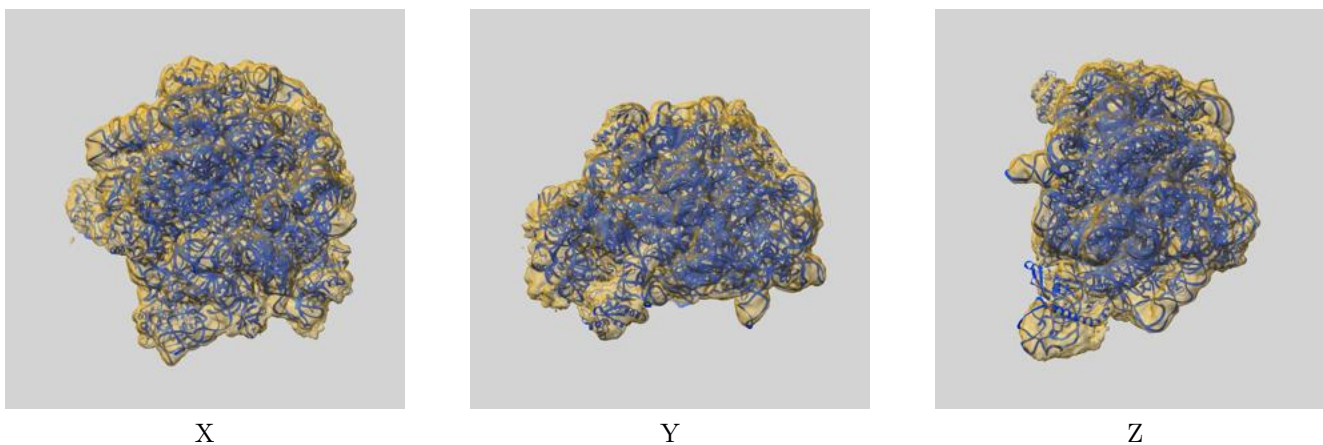
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	3.99	4.60	4.03
Unmasked-calculated*	-	-	-

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

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

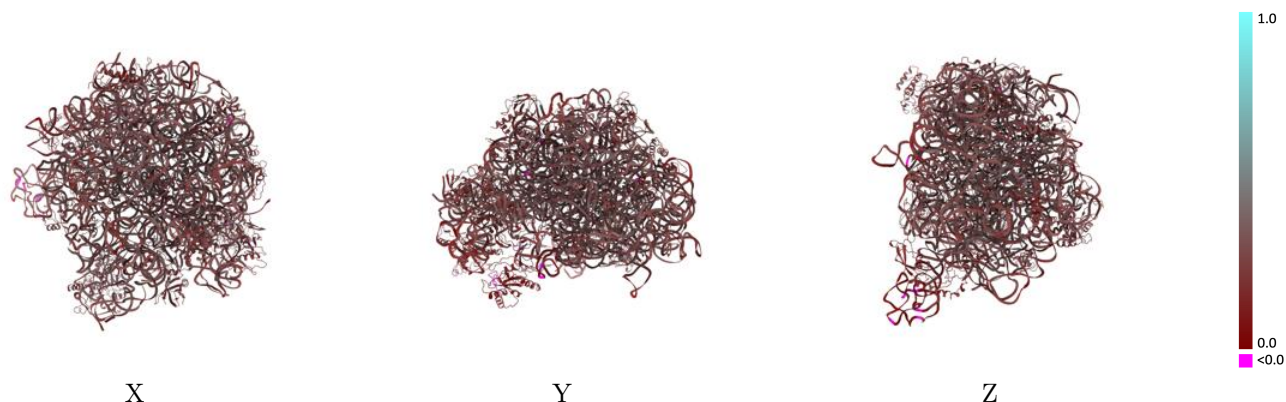
This section contains information regarding the fit between EMDB map EMD-12219 and PDB model 7BL6. Per-residue inclusion information can be found in section 3 on page 10.

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



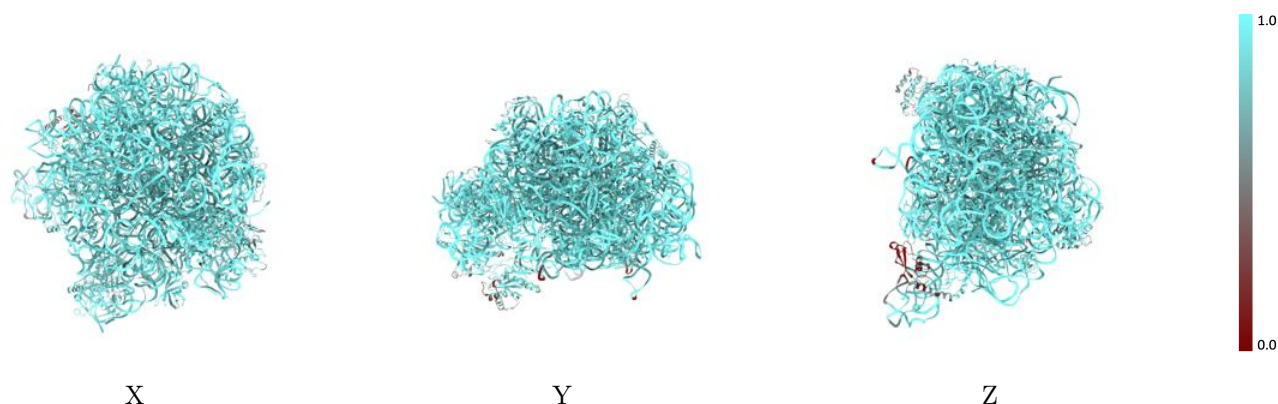
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



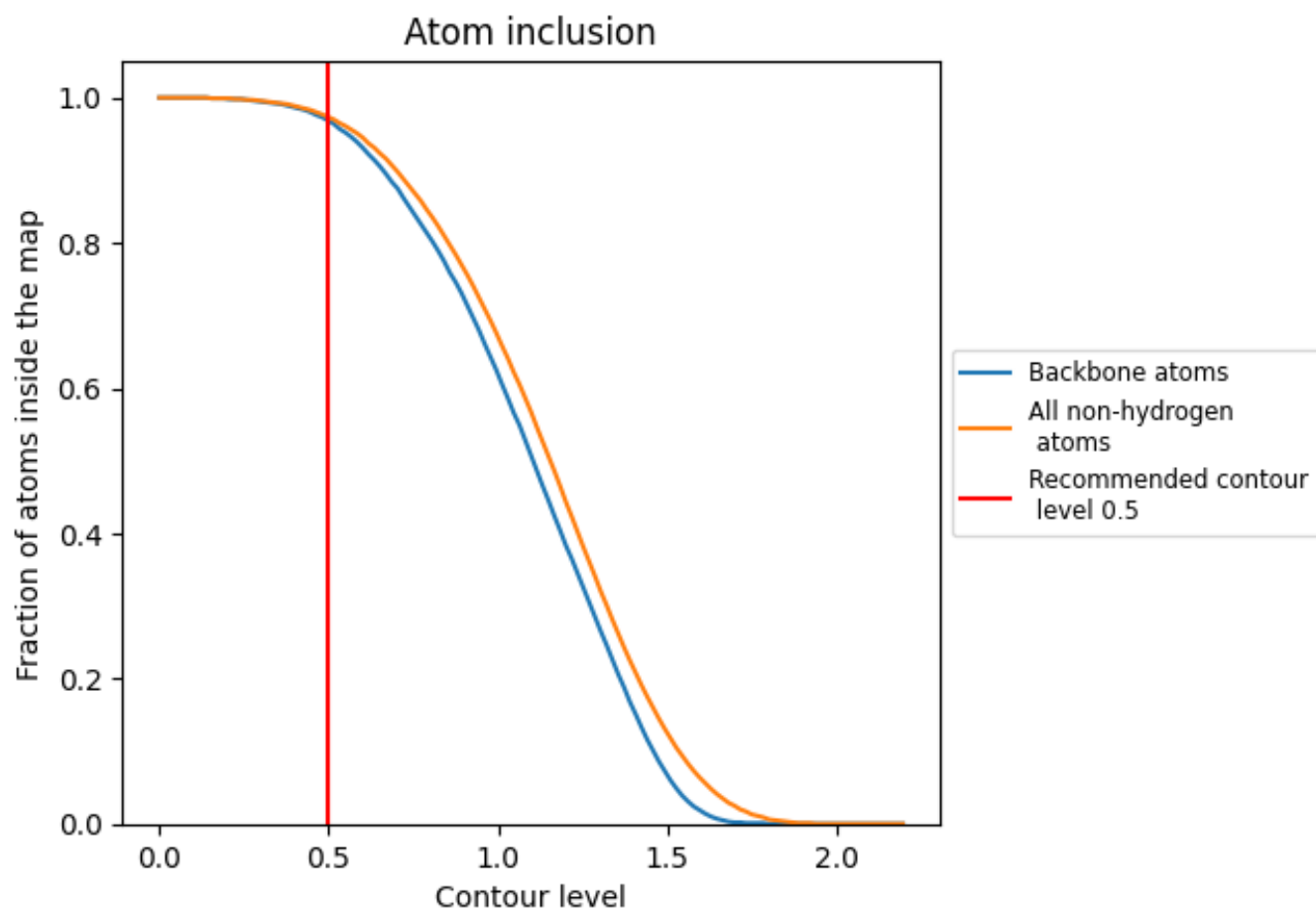
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.5).


































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 97% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9730	 0.2890
0	 0.9810	 0.2670
1	 0.9950	 0.2680
2	 0.9970	 0.2870
3	 1.0000	 0.2860
9	 0.8530	 0.1990
A	 0.9900	 0.3010
B	 0.9970	 0.2850
C	 0.9910	 0.3020
D	 0.9700	 0.3000
E	 0.9160	 0.2710
F	 0.8990	 0.2090
G	 0.9000	 0.2490
H	 0.5700	 0.2020
J	 0.9850	 0.2910
K	 0.9770	 0.2810
L	 0.9560	 0.2820
M	 0.9810	 0.2930
N	 0.9920	 0.2700
O	 0.9710	 0.2530
P	 0.9600	 0.2810
Q	 0.9850	 0.2690
R	 0.9270	 0.2820
S	 0.9820	 0.2780
T	 0.9830	 0.2920
U	 0.9620	 0.2600
V	 0.9510	 0.2710
W	 0.9930	 0.2860
X	 0.9900	 0.2870
Y	 0.9500	 0.2140
Z	 0.9410	 0.2580
d	 0.6740	 0.1790
g	 0.9930	 0.2860

