



wwPDB EM Validation Summary Report ⓘ

Mar 28, 2026 – 05:47 PM UTC

PDB ID : 8VKI / pdb_00008vki
EMDB ID : EMD-43317
Title : Structure of Mycobacterium smegmatis 50S ribosomal subunit bound to HflX:50S-HflX-C
Authors : Majumdar, S.; Koripella, R.K.; Sharma, M.R.; Manjari, S.R.; Banavali, N.K.; Agrawal, R.K.
Deposited on : 2024-01-09
Resolution : 2.96 Å (reported)
Based on initial models : 5O61, 6DZI

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

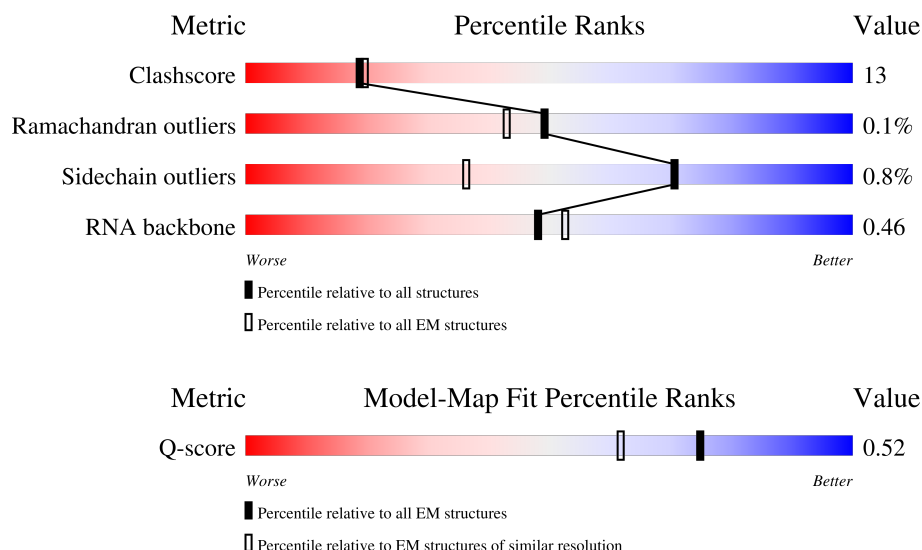
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.96 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13155 (2.46 - 3.46)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	2	61	
2	3	24	

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Mol	Chain	Length	Quality of chain
3	4	470	
4	B	118	
5	C	278	
6	D	217	
7	E	215	
8	F	187	
9	G	179	
10	H	151	
11	I	175	
12	J	142	
13	K	147	
14	L	122	
15	M	147	
16	N	138	
17	O	199	
18	P	127	
19	Q	113	
20	R	129	
21	S	103	
22	T	153	
23	U	100	
24	V	105	
25	W	215	
26	X	88	
27	Y	64	

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Mol	Chain	Length	Quality of chain
28	Z	77	
29	b	57	
30	c	55	
31	d	47	
32	e	64	
33	f	37	
34	A	3120	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
35	GCP	4	501	-	-	X	-

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 96565 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 L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	2	59	Total	C	N	O	0	0
			474	292	95	87		

- Molecule 2 is a protein called 50S Ribosomal Protein L37.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	3	23	Total	C	N	O	0	0
			189	111	50	28		

- Molecule 3 is a protein called GTPase HflX.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	466	Total	C	N	O	S	0	0
			3516	2171	649	689	7		

- Molecule 4 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	118	Total	C	N	O	P	0	0
			2522	1126	468	810	118		

- Molecule 5 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	275	Total	C	N	O	S	0	0
			2110	1298	438	370	4		

- Molecule 6 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	214	Total	C	N	O	S	0	0
			1587	982	310	290	5		

- Molecule 7 is a protein called 50S Ribosomal Protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	E	209	Total	C	N	O	S	0	0
			1569	969	295	303	2		

- Molecule 8 is a protein called 50S Ribosomal Protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	F	182	Total	C	N	O	S	0	0
			1445	907	271	261	6		

- Molecule 9 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	G	176	Total	C	N	O	S	0	0
			1348	845	249	253	1		

- Molecule 10 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	H	151	Total	C	N	O	S	0	0
			1018	635	188	194	1		

- Molecule 11 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	I	126	Total	C	N	O	S	0	0
			918	580	156	180	2		

- Molecule 12 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	J	132	Total	C	N	O	S	0	0
			958	602	172	181	3		

- Molecule 13 is a protein called 50S Ribosomal Protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	K	146	Total	C	N	O	S	0	0
			1130	722	207	200	1		

- Molecule 14 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	L	122	Total	C	N	O	S	0	0
			938	586	179	170	3		

- Molecule 15 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	M	145	Total	C	N	O	S	0	0
			1078	676	205	194	3		

- Molecule 16 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	N	136	Total	C	N	O	S	0	0
			1092	690	213	187	2		

- Molecule 17 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	O	118	Total	C	N	O	S	0	0
			928	583	180	163	2		

- Molecule 18 is a protein called 50S Ribosomal Protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	P	126	Total	C	N	O		0	0
			956	586	199	171			

- Molecule 19 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Q	113	Total	C	N	O	S	0	0
			907	570	171	165	1		

- Molecule 20 is a protein called 50S Ribosomal Protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	R	124	Total	C	N	O		0	0
			988	613	203	172			

- Molecule 21 is a protein called 50S Ribosomal Protein L21.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	S	100	Total	C	N	O	0	0
			754	478	137	139		

- Molecule 22 is a protein called 50S Ribosomal Protein L22.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	T	114	Total	C	N	O	0	0
			873	543	171	159		

- Molecule 23 is a protein called 50S Ribosomal Protein L23.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	U	97	Total	C	N	O	0	0
			756	479	138	139		

- Molecule 24 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	V	97	Total	C	N	O	S	0	0
			732	456	137	137	2		

- Molecule 25 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	W	95	Total	C	N	O	0	0
			735	452	149	134		

- Molecule 26 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	X	79	Total	C	N	O	0	0
			586	361	123	102		

- Molecule 27 is a protein called 50S Ribosomal Protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Y	63	Total	C	N	O	S	0	0
			470	283	103	80	4		

- Molecule 28 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Z	64	Total	C	N	O	S	0	0
			531	324	103	103	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	b	54	Total	C	N	O	S	0	0
			423	260	93	69	1		

- Molecule 30 is a protein called 50S Ribosomal Protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	c	49	Total	C	N	O	S	0	0
			405	248	82	71	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	d	46	Total	C	N	O	S	0	0
			377	225	97	54	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
32	e	63	Total	C	N	O	0	0
			502	302	115	85		

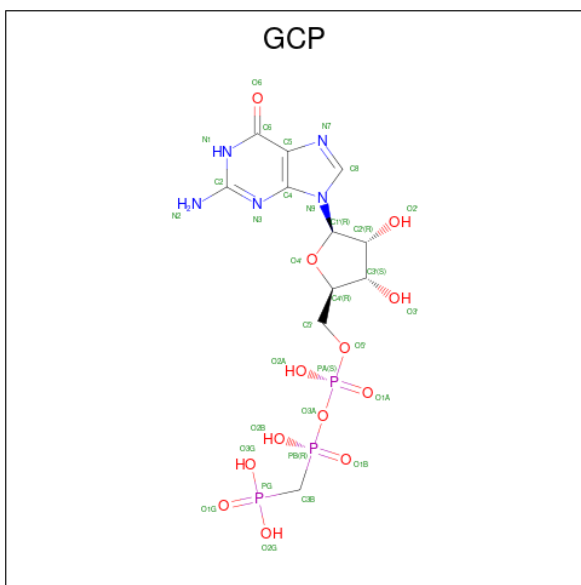
- Molecule 33 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	f	37	Total	C	N	O	0	0
			299	181	66	47	5	

- Molecule 34 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	A	2952	Total	C	N	O	P	0	0
			63419	28264	11675	20528	2952		

- Molecule 35 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (CCD ID: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).

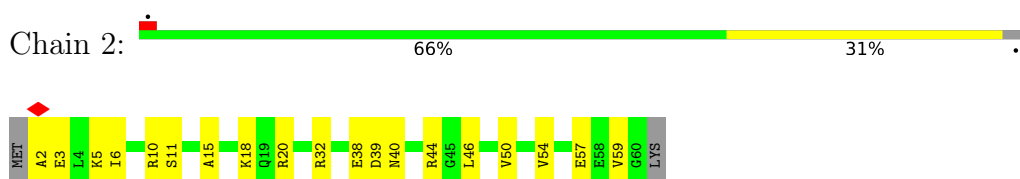


Mol	Chain	Residues	Atoms					AltConf
35	4	1	Total	C	N	O	P	0
			32	11	5	13	3	

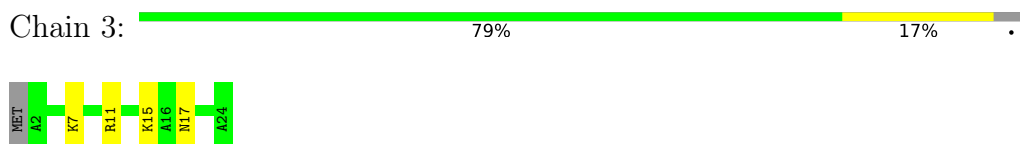
3 Residue-property plots

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.

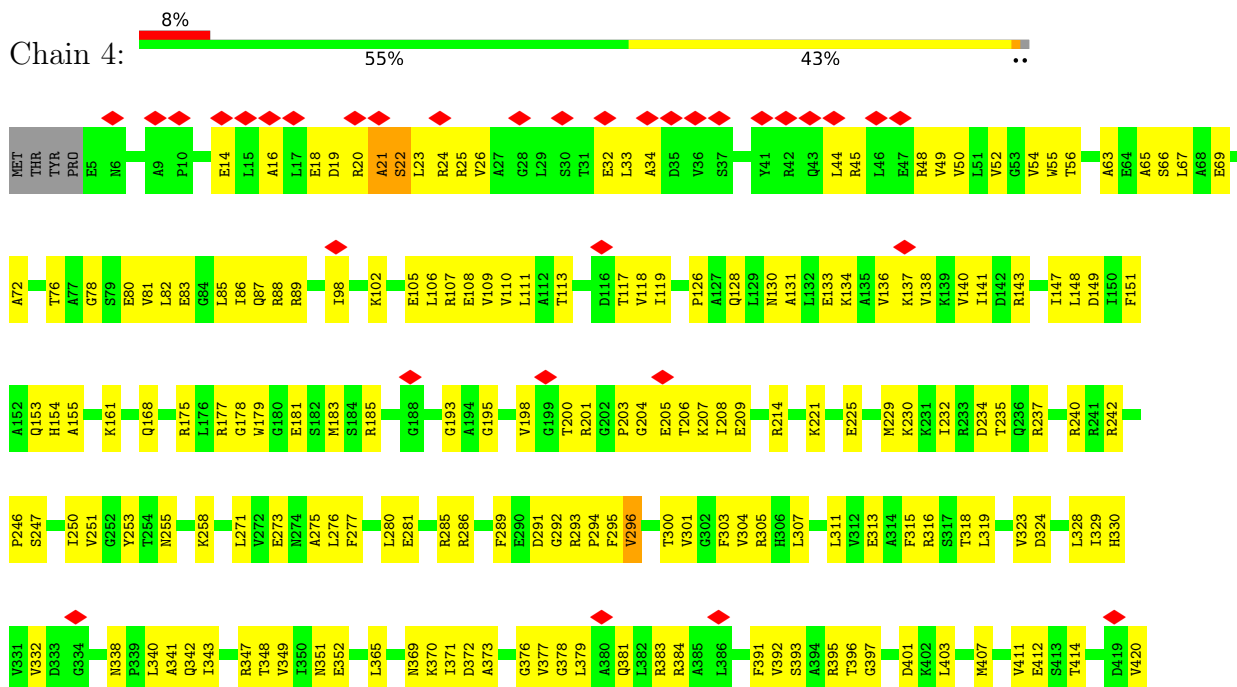
- Molecule 1: 50S ribosomal protein L30



- Molecule 2: 50S Ribosomal Protein L37

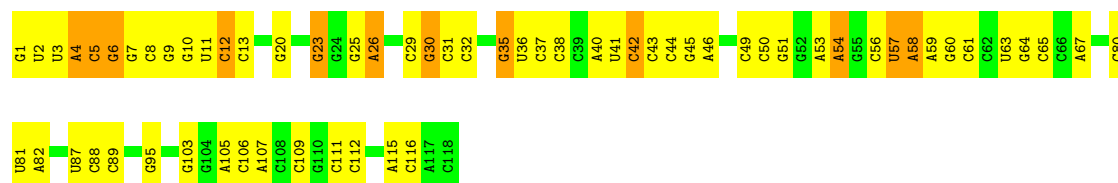


- Molecule 3: GTPase HflX

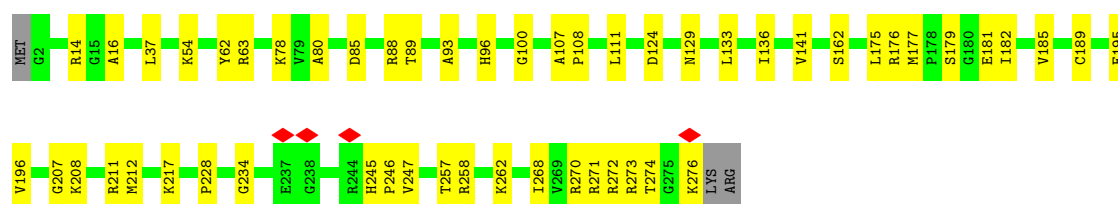
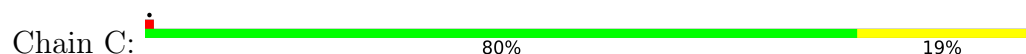




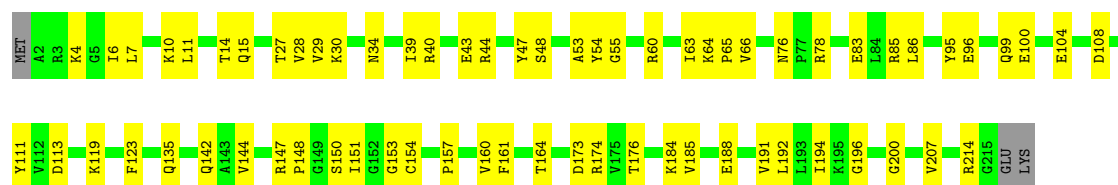
• Molecule 4: 5S ribosomal RNA



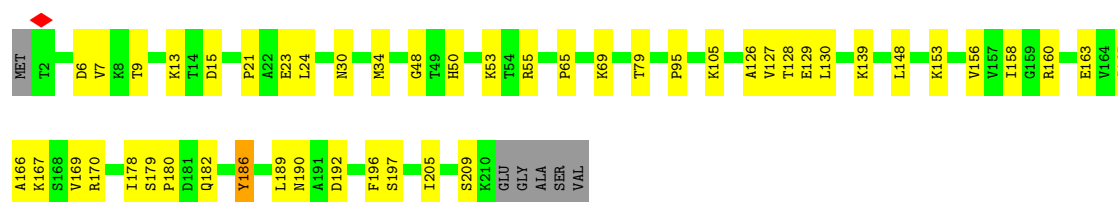
• Molecule 5: 50S ribosomal protein L2



• Molecule 6: 50S ribosomal protein L3

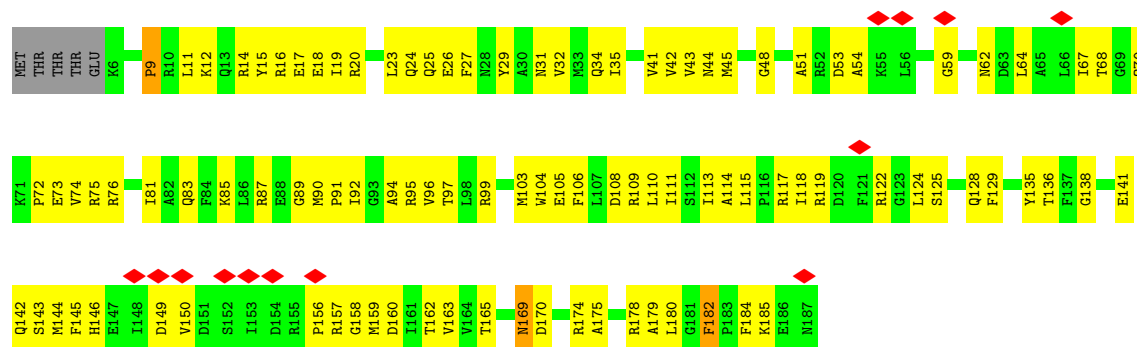


• Molecule 7: 50S Ribosomal Protein L4

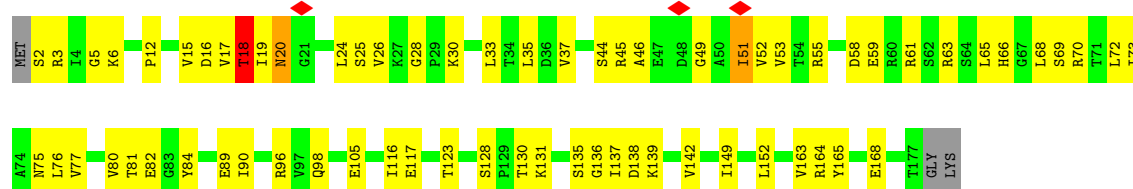


• Molecule 8: 50S Ribosomal Protein L5

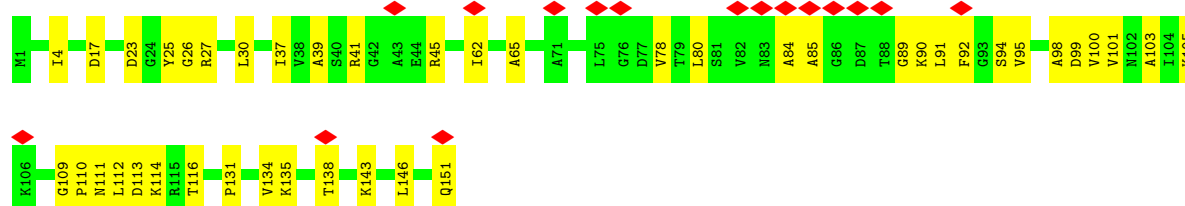




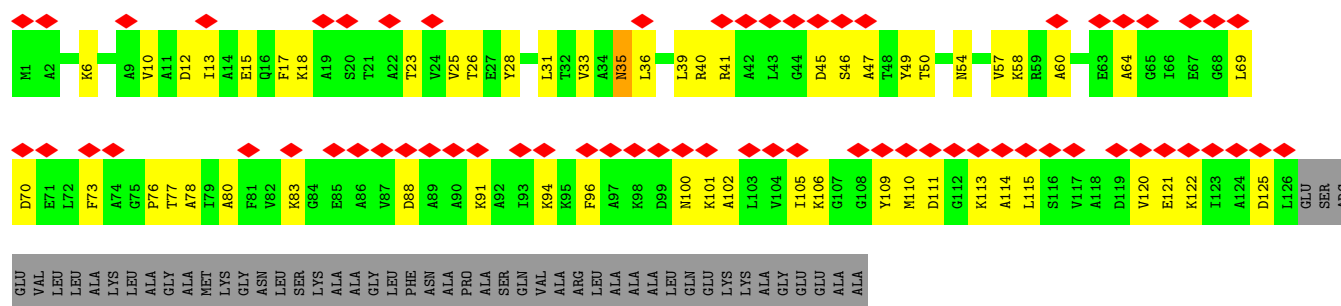
• Molecule 9: 50S ribosomal protein L6



• Molecule 10: 50S ribosomal protein L9

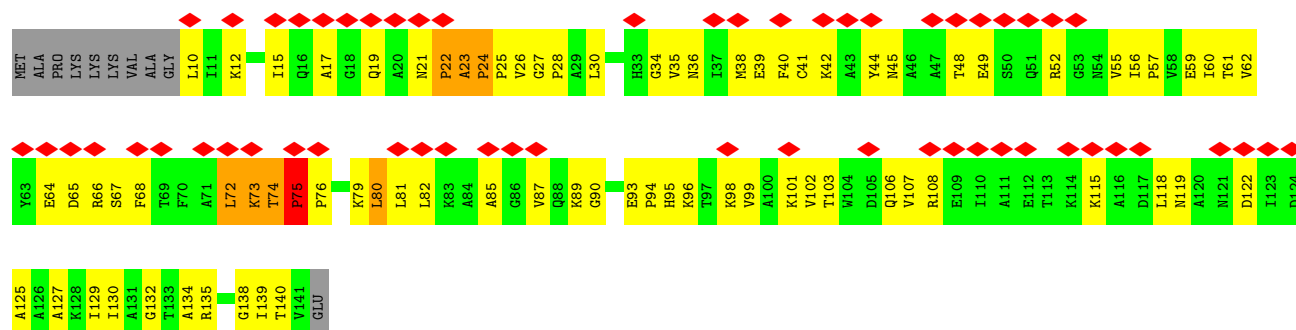


• Molecule 11: 50S ribosomal protein L10



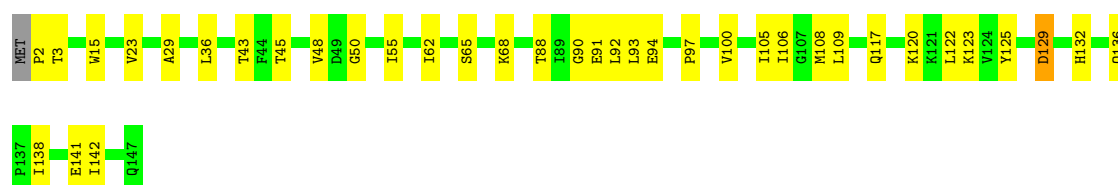
• Molecule 12: 50S ribosomal protein L11





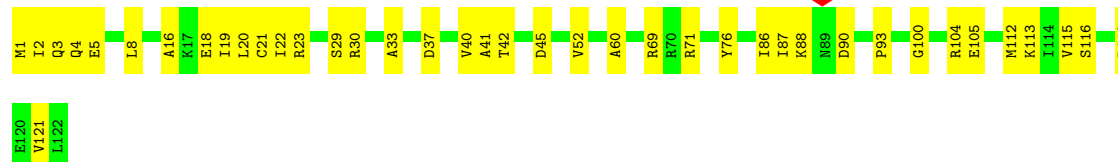
• Molecule 13: 50S Ribosomal Protein L13

Chain K: 74% 24%



• Molecule 14: 50S ribosomal protein L14

Chain L: 67% 33%



• Molecule 15: 50S ribosomal protein L15

Chain M: 63% 36%



• Molecule 16: Large ribosomal subunit protein uL16

Chain N: 77% 22%

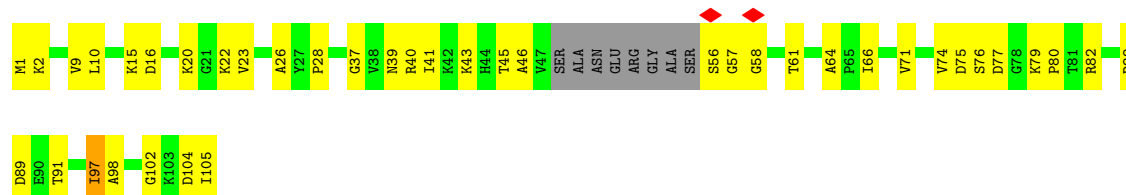


• Molecule 17: 50S ribosomal protein L17

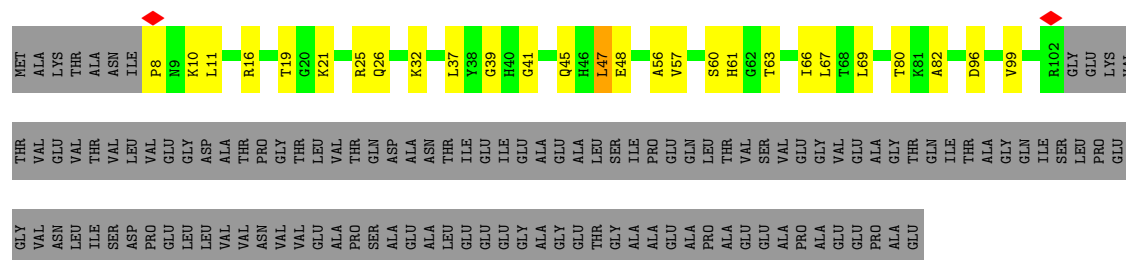
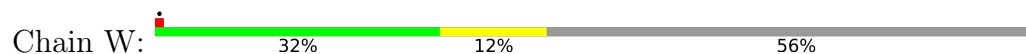
- Molecule 23: 50S Ribosomal Protein L23



- Molecule 24: 50S ribosomal protein L24



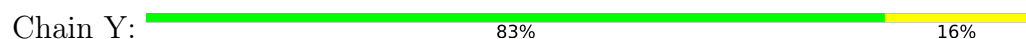
- Molecule 25: 50S ribosomal protein L25



- Molecule 26: 50S ribosomal protein L27



- Molecule 27: 50S Ribosomal Protein L28



- Molecule 28: 50S ribosomal protein L29





- Molecule 29: 50S ribosomal protein L32

Chain b: 68% 26% 5%



- Molecule 30: 50S Ribosomal Protein L33

Chain c: 60% 29% 11%



- Molecule 31: 50S ribosomal protein L34

Chain d: 64% 34% 2%



- Molecule 32: 50S ribosomal protein L35

Chain e: 69% 30% 1%



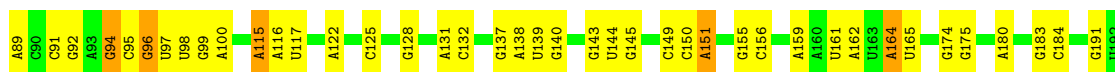
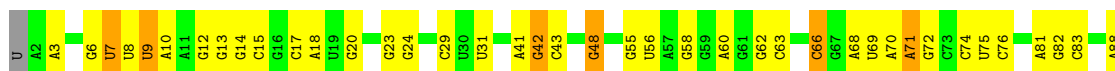
- Molecule 33: 50S ribosomal protein L36

Chain f: 78% 22% 0%



- Molecule 34: 23S ribosomal RNA

Chain A: 49% 36% 10% 5%



G1411	U1316	G1225	G1152	G1073	G853	U767	G695	U519	G437	C346	A282	G193
A1415	G1317	U1226	G1156	A1074	A854	G768	A696	U523	U438	U347	U283	A194
A1416	C1318	C1227	G1157	U1075	G872	U769	G697	C524	C139	G348	G284	A195
A1417	A1319	A1228	U1158	A1076	G877	A770	G698	A524	G349	G349	U285	A196
G1418	G1323	A1229	G1159	A1077	G878	U771	U699	A527	U440	A350	G286	C197
A1419	G1324	G1230	G1160	G1078	A879	G773	C704	G528	G441	G351	A287	A198
	U1325	U1231	C1161		G885		G705		U442	G352	U288	
G1424	G1326	U1234	G1162	G1085	G886	U782	G706	A531	U443	G353	U289	A206
G1425	U1235	G1235	G1165	C1086	G887	G783	G707	A535	U444	G356	C290	C207
G1426	G1236	U1236	A1166	U1087	G888	G789	G708	A535	U445	G357	G291	A212
U1427	U1237	U1237	A1166	U1088	G890		U709	A535	G446	G357	G292	G213
U1428	G1330		A1169	G1089	G891	U801	C718	G539	A447	A363	G293	G214
G1429	C1334	G1243		G1090	G897	C802	G719		U448	A364	G294	A215
C1430	G1335	A1244	G1174	A1091	A897		G720	U643	U449	A364	U295	
A1431	G1337		G1175	G1092	A898		C721	U643	G450	G366	A296	A216
G1434	A1340	U1250	A1176	A1098	G899	A808	A721	U644	U451	G367	G297	G217
C1435	G1343	G1251	U1177	C1100	G900		G722	A545	G452	U368	G298	A218
C1436		C1253	U1178	A1101		C813	G723	G555	U453	G369	G299	G219
	A1344	G1254	U1179	G1102	A904		G724	G556	U454	G370	A220	A220
G1443	G1345	U1255	G1180	C1103	A907	U818	A725	G556	C455	G371	U301	A221
U1444	U1346	G1256	G1181	C1104	U911	A821	G726	A558			U302	A222
C1445	G1347		C1182	A1105	C912	G822	A727	A559	G460	G376	G303	A227
	G1347	U1259	U1183	A1106	G920	G823	C728	U560	G468	G377	U304	A228
G1449	G1351	C1260	U1184	G1107	G924	G824	G730	G564	G469	G378	G305	U229
G1456	A1352	A1261		A1108	G925	G825	A731	A565		G379	G306	G230
	G1353		A1187	U1109	U926	G826	G732	A566	C473	A380	U307	U231
C1465	G1365	C1272	A1188	C1110	U927	G827	G733	A567	U475	A381	G232	A233
G1466	A1366	G1278	G1189	G1111	U928	G828	U734	A568	G476	U382	U234	U235
U1467	G1367	G1279	A1191	C1112	U929	G829	A737	U570	A479	G384	U315	
A1468	A1368		G1192	G1113	U930	U830	A738	A571		G385	U316	G242
	C1369		C1193	G1114	U931	U831	A739	C572	U482	U387	U318	U246
G1473	U1370	C1283	C1194	G1115	C930	G832	A740	G576	U483	G388	G319	
A1474	G1371	A1284	U1117	C1116	C931	A833	G741	G577	C484	G389		G247
G1475		G1285	A1195	U1118	C932	G834	G742	G578	A489	G390	G248	G249
G1476		C1286	C1196	A1119		G835	G743	G578	A490	A392	G250	
	U1378	C1287	C1197	A1119	A940	G836	C744	G582	U491	G394	G254	
C1477	G1379	A1287	U1198		U941	G837	G745	G587	C492	U327		G263
G1478	A1380	A1288	C1199		U942	G838	G746	G587	U493	C328	G264	A265
G1479		C1290	U1200	A1127	U943	U839	A747	G587	U494	U329	U266	
A1480	G1384	G1291	G1201	A1128	A944	G840	U748	A590	G495	U330	G268	
A1481	C1385	U1292	A1202	G1129	G945	A842		A591	G499	U331		A271
A1482	G1386	G1293	A1203	C1130	G946	G843	A751	G592	A500	A404	G332	A273
	A1387	A1294	A1204	G1131	G947	G844	C752	G593	G499	U410	G333	A274
U1487		U1295	G1205	G1135	G948	G845	A753	G594	A501	G411	G334	C275
A1488	G1398	G1296	A1206		G949	C846	C754	A595	C501	G412	U277	A278
	A1399	G1297	U1208	A1033	A950	C847	A755	C596	C502	A413	G335	U279
A1493	G1400			U1034	U954	G848	A756	C597	A503	G414	G336	G280
U1494	A1401	G1301	U1212	G1035	C955	A849	G757	U598	C504	U337	U337	G342
A1499	C1402	A1214	A1213	A1042	G956	U853	G759	A600	C505	G428	A340	A278
C1501	C1403	G1302	A1214	A1047	G957	U857	U760	G604	G508	A429	G341	U279
G1502	A1404	A1303	U1215	A1048	G960	A858	A762	G605	G512	A430	C342	G281
	U1405	G1305	C1220	G1049	U963		G763	G609	G516	A431	G343	
U1509	G1407	G1306	A1221	G1053	G964	U861	G764	G692	A517	C432	G344	
A1510	C1408	U1313	C1222	G1063	U965	U862	G765	G693	A518	G434	G345	
U1511	U1409	C1314	U1223	C1065	G966	U863	G766					
U1512	U1512	G1315	G1224		G967	U864						

G2581	G2495	C2397	A2337	G	U2044	G1936	A1828	G1736	G1642	C	G1513
G2585	U2496	C2398	G2338	A	G2045	U1937	A1832	A1737	G1645	C	C1514
G2586	A2497	A2399	G2339	A	A2046	G1938	C1832	G1746	U1646	U	A1518
G2587	A2498	C2400	A2340	U	U2051	C1944	C1834	C1752	G1647	U	G1524
G2588	G2503	C2401	U2341	U	G2052	U1945	G1835	C1753	A1648	C	U1525
G2589	C2507	U2402	A2342	A	C2053	U1946	G1840	G1754	C1649	G	G1528
A2590	G2508	U2403	G2343	A	C2054	U1947	G1840	G1755	G1650	G	U1529
A2593	C2509	G2404	A2344	G	C2055	G1951	C1843	A1756	C1651	G	G1530
A2597	A2510	A2405	U2345	C	C2056	G1952	A1844	U1757	G1652	U	C1531
C2598	U2406	G2278	G2346	C	G2057	A1955	A1852	A1758	G1654	G	G1532
G2599	G2280	C2279	G2347	U	U2058	A1956	A1853	G1759	C1658	U	U1533
A2600	G2348	A2281	G2347	U	G2059	G1959	U1854	G1760	C1658	G	C1534
G2603	C2408	A2282	G2348	C	G2060	U1960	C1855	G1761	U1671	C	C1535
U2604	U2410	A2283	A2349	G	U2061	G1961	U1864	A1764	A1672	G	A1536
U2604	A2411	G2284	G2350	G	U2062	U1962	A1865	U1767	A1673	U	U1537
C2605	U2412	G2285	A2351	A	G2063	G1963	A1866	C1768	U1674	G	G1538
G2607	G2413	A2286	C2352	C	A	U1964	G1867	G1769	G1676	U	A1541
G2608	G2414	C2287	U2353	U	U2063	U1964	A1868	G1770	A1680	U	A1542
G2610	G2415	C2288	G2354	G	A	C1977	U1870	U1778	U1681	G	U1544
A2609	C2416	C2289	U2355	C	A	U1981	G1869	A1779	U1681	G	C1545
G2613	C2417	A2294	U2356	A	A	A1985	U1871	U1780	A1691	C	A
U2614	U2418	C2295	G2356	C	G	A1990	A1872	G1780	G1692	U	C
G2615	C2419	U2298	A2357	G	A	U1996	U1877	C1784	G1696	C	C
G2618	A2421	C2299	G2358	U	A	U1999	A1883	C1785	U1703	G	G
A2623	G2427	G2300	C2360	A	A	A2000	G1884	G1786	U1704	U	G
C2624	C2431	U2301	U2361	G	A	A2001	G1885	A1787	C1705	C	G
G2625	A2436	U2302	G2362	G	A	C2007	U1889	A1788	A1789	U	G
U2626	G2436	U2303	A2363	G	A	A2008	G1891	A1789	A1791	C	U
G2627	U2447	G2310	C2364	C	A	G2014	U1898	U1798	U1709	C	A
U2628	G2448	U2311	A2365	C	A	U2015	G1899	A1799	A1710	C	C
G2629	A2449	U2312	G2366	U	A	G2016	C1900	A1803	G1711	C	C
A2630	U2450	U2313	U2367	A	U	C2017	C1901	A1804	G1712	U	A
U2635	G2462	U2314	C2368	A	U	A2018	G1904	G1805	U1620	C	C
A2636	U2463	U2315	G2369	A	U	A2019	C1904	A1806	U1621	C	C
G2637	G2466	U2316	A2370	C	U	A2020	A1907	C1807	U1622	C	C
U2641	U2467	U2317	G2371	C	U	A2021	A1908	A1808	U1623	C	C
G2644	U2468	U2318	U2372	C	U	C2025	U1911	G1809	U1624	C	C
U2649	U2469	U2319	G2373	C	U	A2026	G1917	C1811	G1625	C	C
A2650	A2471	U2320	U2374	C	U	A2027	G1917	A1812	U1626	C	C
A2651	G2472	U2321	G2375	C	U	G2028	G1917	A1815	U1627	C	C
G2652	U2473	U2322	U2376	C	U	G2031	G1917	C1816	A1628	C	C
U2653	G2474	U2323	A2377	C	U	A2032	C1928	U1728	G1629	C	C
G2654	U2475	U2324	G2378	C	U	U2033	A1931	A1729	U1630	C	C
A2655	G2476	U2325	U2379	C	U	A2038	U1932	U1730	G1631	C	C
U2656	U2477	U2326	G2380	C	U	G2039	G1933	U1731	A1632	C	C
A2657	U2478	U2327	A2381	C	U	G2040	C1934	C1822	G1633	C	C
G2658	G2479	U2328	G2382	C	U	G2041	C1935	A1827	U1735	C	C
U2659	U2480	U2329	U2383	C	U	G2042	C1935	A1827	A1640	C	C
A2660	U2481	U2330	G2384	C	U	G2043	C1935	A1827	U1641	C	C
A2661	U2482	U2331	U2385	C	U	G2044	C1935	A1827	U1641	C	C
G2662	U2483	U2332	G2386	C	U	G2045	C1935	A1827	U1641	C	C
U2663	U2484	U2333	U2387	C	U	G2046	C1935	A1827	U1641	C	C
A2664	U2485	U2334	G2388	C	U	G2047	C1935	A1827	U1641	C	C
G2665	U2486	U2335	U2389	C	U	G2048	C1935	A1827	U1641	C	C
A2666	U2487	U2336	U2390	C	U	G2049	C1935	A1827	U1641	C	C
U2667	U2488	U2337	G2391	C	U	G2050	C1935	A1827	U1641	C	C
G2668	U2489	U2338	A2392	C	U	G2051	C1935	A1827	U1641	C	C
A2669	U2490	U2339	U2393	C	U	G2052	C1935	A1827	U1641	C	C
U2670	U2491	U2340	A2394	C	U	G2053	C1935	A1827	U1641	C	C
G2671	U2492	U2341	U2395	C	U	G2054	C1935	A1827	U1641	C	C
A2672	U2493	U2342	A2396	C	U	G2055	C1935	A1827	U1641	C	C
U2673	U2494	U2343	U2397	C	U	G2056	C1935	A1827	U1641	C	C
G2674	U2495	U2344	A2398	C	U	G2057	C1935	A1827	U1641	C	C
A2675	U2496	U2345	U2399	C	U	G2058	C1935	A1827	U1641	C	C
U2676	U2497	U2346	G2400	C	U	G2059	C1935	A1827	U1641	C	C
G2677	U2498	U2347	A2401	C	U	G2060	C1935	A1827	U1641	C	C
A2678	U2499	U2348	U2402	C	U	G2061	C1935	A1827	U1641	C	C
U2679	U2500	U2349	G2403	C	U	G2062	C1935	A1827	U1641	C	C
G2680	U2501	U2350	A2404	C	U	G2063	C1935	A1827	U1641	C	C
A2681	U2502	U2351	U2405	C	U	G2064	C1935	A1827	U1641	C	C
U2682	U2503	U2352	G2406	C	U	G2065	C1935	A1827	U1641	C	C
G2683	U2504	U2353	A2407	C	U	G2066	C1935	A1827	U1641	C	C
A2684	U2505	U2354	G2408	C	U	G2067	C1935	A1827	U1641	C	C
U2685	U2506	U2355	U2409	C	U	G2068	C1935	A1827	U1641	C	C
G2686	U2507	U2356	A2410	C	U	G2069	C1935	A1827	U1641	C	C
A2687	U2508	U2357	U2411	C	U	G2070	C1935	A1827	U1641	C	C
U2688	U2509	U2358	U2412	C	U	G2071	C1935	A1827	U1641	C	C
G2689	U2510	U2359	G2413	C	U	G2072	C1935	A1827	U1641	C	C
A2690	U2511	U2360	A2414	C	U	G2073	C1935	A1827	U1641	C	C
U2691	U2512	U2361	G2415	C	U	G2074	C1935	A1827	U1641	C	C
G2692	U2513	U2362	U2416	C	U	G2075	C1935	A1827	U1641	C	C
A2693	U2514	U2363	A2417	C	U	G2076	C1935	A1827	U1641	C	C
U2694	U2515	U2364	G2418	C	U	G2077	C1935	A1827	U1641	C	C
G2695	U2516	U2365	U2419	C	U	G2078	C1935	A1827	U1641	C	C
A2696	U2517	U2366	A2420	C	U	G2079	C1935	A1827	U1641	C	C
U2697	U2518	U2367	G2421	C	U	G2080	C1935	A1827	U1641	C	C
G2698	U2519	U2368	U2422	C	U	G2081	C1935	A1827	U1641	C	C
A2699	U2520	U2369	A2423	C	U	G2082	C1935	A1827	U1641	C	C
U2700	U2521	U2370	G2424	C	U	G2083	C1935	A1827	U1641	C	C
G2701	U2522	U2371	U2425	C	U	G2084	C1935	A1827	U1641	C	C
A2702	U2523	U2372	A2426	C	U	G2085	C1935	A1827	U1641	C	C
U2703	U2524	U2373	G2427	C	U	G2086	C1935	A1827	U1641	C	C
G2704	U2525	U2374	U2428	C	U	G2087	C1935	A1827	U1641	C	C
A2705	U2526	U2375	A2429	C	U	G2088	C1935	A1827	U1641	C	C
U2706	U2527	U2376	G2430	C	U	G2089	C1935	A1827	U1641	C	C
G2707	U2528	U2377	U2431	C	U	G2090	C1935	A1827	U1641	C	C
A2708	U2529	U2378	A2432	C	U	G2091	C1935	A1827	U1641	C	C
U2709	U2530	U2379	G2433	C	U	G2092	C1935	A1827	U1641	C	C
G2710	U2531	U2380	U2434	C	U	G2093	C1935	A1827	U1641	C	C
A2711	U2532	U2381	A2435	C	U	G2094	C1935	A1827	U1641	C	C
U2712	U2533	U2382	G2436	C	U	G2095	C1935	A1827	U1641	C	C
G2713	U2534	U2383	U2437	C	U	G2096	C1935	A1827	U1641	C	C
A2714	U2535	U2384	A2438	C	U	G2097	C1935	A1827	U1641	C	C
U2715	U2536	U2385	G2439	C	U	G2098	C1935	A1827	U1641	C	C
G2716	U2537	U2386	U2440	C	U	G2099	C1935	A1827	U1641	C	C
A2717	U2538	U2387	A2441	C	U	G2100	C1935	A1827	U1641	C	C
U2718	U2539	U2388	G2442	C	U	G2101	C1935	A1827	U1641	C	C
G2719	U2540	U2389	U2443	C	U	G2102	C1935	A1827	U1641	C	C
A2720	U2541	U2390	A2444	C	U	G2103	C1935	A1827	U1641	C	C
U2721	U2542	U2391	G2445	C	U	G2104	C1935	A1827	U1641	C	C
G2722	U2543	U2392	U2446	C	U	G2105	C1935	A1827	U1641	C	C
A2723	U2544	U2393	A2447	C	U	G2106	C1935	A1827	U1641	C	C
U2724	U2545	U2394	G2448	C	U	G2107	C1935	A1827	U1641	C	C
G2725	U2546	U2395	U2449	C	U	G2108	C1935	A1827	U1641	C	C
A2726	U2547	U2396	A2450	C	U	G2109	C1935	A1827	U1641	C	C
U2727	U2548	U2397	G2451	C	U	G2110	C1935	A1827	U1641	C	C
G2728	U2549	U2398	U2452	C	U	G2111	C1935	A1827	U1641	C	C
A2729	U2550	U2399	A2453	C	U	G2112	C1935	A1827	U1641	C	C
U2730	U2551	U2400	G2454	C	U	G2113	C1935	A1827	U1641	C	C
G2731	A2552	U2401	U2455	C	U	G2114	C1935	A1827	U1641	C	C
A2732	U2553	U2402	A2456	C	U	G2115	C1935	A1827	U1641		

G3078	G3087	G3088	G3089	G3093	A3100	G3101	G3102	A3103	A3104	A3112	A3113	A3114	A3115	G3116	G3117	G3118	A3119	G3120	C2998	C2999	A3000	G3001	A3002	C3003	C3008	C3009	U3010	C3011	U3012	C3013	A3014	C3015	C3016	C3017	C3018	C3019	U3020	A3021	G3022	G3023	A3024	G3025	G3026	G3027	A3028	U3029	A3030	A3031	G3032	G3033	C3034	C3037	G3040	C3041	A3042	G3043	A3044	C3045	A3046	A3047	A3052	U3053	U3054	G3055	G3064	G3070	A3071	A3072	G3073	C3074	C3075
C2869	C2870	C2871	C2872	C2873	C2874	C2879	C2883	A2884	C2885	A2886	C2887	C2888	A2899	C3017	C3018	C3019	U3020	A3021	G3022	G3023	A3024	G3025	G3026	G3027	A3028	U3029	A3030	A3031	G3032	G3033	C3034	C3037	G3040	C3041	A3042	G3043	A3044	C3045	A3046	A3047	A3052	U3053	U3054	G3055	G3064	G3070	A3071	A3072	G3073	C3074	C3075																				
U2771	U2776	G2777	U2778	U2779	C2780	G2781	C7782	A2788	G2789	A2790	G2791	C7792	C7795	A2796	C7797	G2798	U2809	U2810	U2820	A2826	G2827	U2833	C2834	U2835	G2836	U2837	A2838	U2839	G2842	G2847	C2848	G2849	C2850	G2851	A2854	A2857	G2858	C2859	U2860	U2861	G2862	G2865	U2866	C2762																											
A2672	A2673	A2674	A2675	A2676	A2677	A2678	A2679	A2680	A2681	A2682	A2683	A2684	A2695	A2696	U2697	C2698	C2699	A2700	C2704	G2705	A2706	G2710	G2713	G2714	U2715	C2720	G2726	A2727	U2728	G2729	U2735	C2736	G2740	C2741	A2742	U2743	C2744	G2753	G2754	A2755	C2756	A2758	U2759	G2760	U2761	C2762																									

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	132147	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	51.85	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	64000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.399	Depositor
Minimum map value	-1.560	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.111	Depositor
Recommended contour level	0.35	Depositor
Map size (Å)	430.4, 430.4, 430.4	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.076, 1.076, 1.076	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GCP

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	2	0.36	0/477	0.45	0/640
2	3	0.37	0/191	0.40	0/247
3	4	0.36	2/3558 (0.1%)	0.69	7/4822 (0.1%)
4	B	0.32	0/2821	0.32	0/4396
5	C	0.36	0/2153	0.38	0/2895
6	D	0.38	0/1609	0.44	0/2165
7	E	0.35	0/1592	0.39	0/2153
8	F	0.36	2/1467 (0.1%)	0.68	2/1973 (0.1%)
9	G	0.29	0/1369	0.52	1/1848 (0.1%)
10	H	0.28	0/1027	0.48	0/1398
11	I	0.18	0/925	0.48	0/1246
12	J	0.43	1/971 (0.1%)	1.26	12/1315 (0.9%)
13	K	0.35	0/1157	0.40	0/1567
14	L	0.35	0/946	0.46	0/1268
15	M	0.34	0/1091	0.41	0/1457
16	N	0.35	0/1118	0.39	0/1506
17	O	0.36	0/945	0.38	0/1267
18	P	0.29	0/966	0.39	0/1298
19	Q	0.31	0/921	0.45	0/1236
20	R	0.41	0/1000	0.42	0/1341
21	S	0.39	1/764 (0.1%)	0.45	0/1030
22	T	0.36	0/887	0.41	0/1204
23	U	0.33	0/766	0.37	0/1030
24	V	0.27	0/738	0.47	0/987
25	W	0.25	0/745	0.39	0/1008
26	X	0.37	0/595	0.38	0/798
27	Y	0.44	0/478	0.38	0/641
28	Z	0.28	0/534	0.42	0/713
29	b	0.38	0/427	0.38	0/572
30	c	0.35	0/413	0.40	0/553
31	d	0.40	0/380	0.42	0/500
32	e	0.39	0/507	0.39	0/672

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	f	0.37	0/303	0.39	0/401
34	A	0.42	0/71013	0.36	2/110798 (0.0%)
All	All	0.40	6/104854 (0.0%)	0.41	24/156945 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
12	J	0	1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	4	458	PRO	CG-CD	-11.14	1.12	1.50
3	4	458	PRO	CB-CG	-6.34	1.18	1.49
21	S	29	SER	C-N	-5.71	1.21	1.33
8	F	9	PRO	CG-CD	-5.53	1.31	1.50
12	J	21	ASN	N-CA	5.52	1.53	1.46

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	4	458	PRO	N-CD-CG	-21.18	71.43	103.20
3	4	458	PRO	CA-CB-CG	-15.88	74.33	104.50
12	J	74	THR	CA-C-N	15.83	136.68	120.38
12	J	74	THR	C-N-CA	15.83	136.68	120.38
8	F	9	PRO	CA-N-CD	-12.70	94.22	112.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	J	72	LEU	Mainchain

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	2	474	0	500	16	0
2	3	189	0	205	4	0
3	4	3516	0	3564	205	0
4	B	2522	0	1285	45	0
5	C	2110	0	2165	40	0
6	D	1587	0	1630	60	0
7	E	1569	0	1607	37	0
8	F	1445	0	1476	97	0
9	G	1348	0	1399	59	0
10	H	1018	0	988	34	0
11	I	918	0	959	49	0
12	J	958	0	961	137	0
13	K	1130	0	1167	26	0
14	L	938	0	1000	27	0
15	M	1078	0	1151	40	0
16	N	1092	0	1128	23	0
17	O	928	0	972	26	0
18	P	956	0	991	39	0
19	Q	907	0	938	25	0
20	R	988	0	1038	24	0
21	S	754	0	802	24	0
22	T	873	0	909	22	0
23	U	756	0	802	22	0
24	V	732	0	782	33	0
25	W	735	0	756	18	0
26	X	586	0	601	14	0
27	Y	470	0	484	5	0
28	Z	531	0	541	15	0
29	b	423	0	463	12	0
30	c	405	0	411	13	0
31	d	377	0	411	12	0
32	e	502	0	541	13	0
33	f	299	0	324	7	0
34	A	63419	0	31905	1035	0
35	4	32	0	14	11	0
All	All	96565	0	64870	2038	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 13.

The worst 5 of 2038 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)
12:J:56:ILE:CD1	12:J:74:THR:HG22	1.48	1.39
12:J:56:ILE:HD13	12:J:74:THR:CG2	1.49	1.39
12:J:56:ILE:HD12	12:J:74:THR:CA	1.52	1.37
12:J:56:ILE:CD1	12:J:74:THR:HA	1.58	1.31
12:J:24:PRO:HG2	12:J:25:PRO:CD	1.58	1.30

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	2	57/61 (93%)	54 (95%)	3 (5%)	0	100	100
2	3	21/24 (88%)	21 (100%)	0	0	100	100
3	4	464/470 (99%)	396 (85%)	67 (14%)	1 (0%)	43	66
5	C	273/278 (98%)	256 (94%)	17 (6%)	0	100	100
6	D	212/217 (98%)	197 (93%)	15 (7%)	0	100	100
7	E	207/215 (96%)	192 (93%)	15 (7%)	0	100	100
8	F	180/187 (96%)	162 (90%)	18 (10%)	0	100	100
9	G	174/179 (97%)	153 (88%)	21 (12%)	0	100	100
10	H	149/151 (99%)	117 (78%)	32 (22%)	0	100	100
11	I	124/175 (71%)	103 (83%)	21 (17%)	0	100	100
12	J	130/142 (92%)	113 (87%)	16 (12%)	1 (1%)	16	37
13	K	144/147 (98%)	133 (92%)	11 (8%)	0	100	100
14	L	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
15	M	143/147 (97%)	128 (90%)	15 (10%)	0	100	100
16	N	134/138 (97%)	125 (93%)	9 (7%)	0	100	100
17	O	116/199 (58%)	111 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	P	124/127 (98%)	112 (90%)	12 (10%)	0	100	100
19	Q	111/113 (98%)	97 (87%)	14 (13%)	0	100	100
20	R	122/129 (95%)	119 (98%)	3 (2%)	0	100	100
21	S	98/103 (95%)	90 (92%)	8 (8%)	0	100	100
22	T	112/153 (73%)	101 (90%)	11 (10%)	0	100	100
23	U	95/100 (95%)	88 (93%)	7 (7%)	0	100	100
24	V	93/105 (89%)	80 (86%)	13 (14%)	0	100	100
25	W	93/215 (43%)	85 (91%)	8 (9%)	0	100	100
26	X	77/88 (88%)	75 (97%)	2 (3%)	0	100	100
27	Y	61/64 (95%)	59 (97%)	2 (3%)	0	100	100
28	Z	62/77 (80%)	60 (97%)	2 (3%)	0	100	100
29	b	52/57 (91%)	49 (94%)	3 (6%)	0	100	100
30	c	47/55 (86%)	45 (96%)	2 (4%)	0	100	100
31	d	44/47 (94%)	39 (89%)	5 (11%)	0	100	100
32	e	61/64 (95%)	59 (97%)	2 (3%)	0	100	100
33	f	35/37 (95%)	35 (100%)	0	0	100	100
All	All	3935/4386 (90%)	3566 (91%)	367 (9%)	2 (0%)	49	72

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	J	75	PRO
3	4	22	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	2	52/54 (96%)	52 (100%)	0	100	100
2	3	18/19 (95%)	18 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	4	367/372 (99%)	365 (100%)	2 (0%)	81	90
5	C	215/218 (99%)	215 (100%)	0	100	100
6	D	160/163 (98%)	160 (100%)	0	100	100
7	E	169/173 (98%)	167 (99%)	2 (1%)	63	79
8	F	151/156 (97%)	148 (98%)	3 (2%)	48	71
9	G	148/150 (99%)	145 (98%)	3 (2%)	48	71
10	H	90/116 (78%)	90 (100%)	0	100	100
11	I	89/120 (74%)	88 (99%)	1 (1%)	65	80
12	J	93/108 (86%)	93 (100%)	0	100	100
13	K	119/120 (99%)	118 (99%)	1 (1%)	73	85
14	L	100/100 (100%)	100 (100%)	0	100	100
15	M	112/114 (98%)	112 (100%)	0	100	100
16	N	114/116 (98%)	114 (100%)	0	100	100
17	O	97/158 (61%)	96 (99%)	1 (1%)	68	82
18	P	93/94 (99%)	92 (99%)	1 (1%)	65	80
19	Q	100/100 (100%)	98 (98%)	2 (2%)	48	71
20	R	97/99 (98%)	96 (99%)	1 (1%)	68	82
21	S	81/83 (98%)	81 (100%)	0	100	100
22	T	90/117 (77%)	89 (99%)	1 (1%)	65	80
23	U	83/85 (98%)	83 (100%)	0	100	100
24	V	81/86 (94%)	79 (98%)	2 (2%)	42	66
25	W	77/168 (46%)	75 (97%)	2 (3%)	40	65
26	X	58/63 (92%)	58 (100%)	0	100	100
27	Y	50/51 (98%)	49 (98%)	1 (2%)	48	71
28	Z	58/66 (88%)	58 (100%)	0	100	100
29	b	43/46 (94%)	42 (98%)	1 (2%)	44	67
30	c	47/52 (90%)	47 (100%)	0	100	100
31	d	35/36 (97%)	35 (100%)	0	100	100
32	e	53/54 (98%)	53 (100%)	0	100	100
33	f	35/35 (100%)	34 (97%)	1 (3%)	37	61
All	All	3175/3492 (91%)	3150 (99%)	25 (1%)	70	85

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
19	Q	8	ASP
22	T	92	ILE
33	f	17	ILE
20	R	36	LYS
24	V	61	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
15	M	69	ASN
18	P	3	HIS
30	c	31	ASN
17	O	77	HIS
18	P	50	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
34	A	2946/3120 (94%)	662 (22%)	23 (0%)
4	B	117/118 (99%)	29 (24%)	0
All	All	3063/3238 (94%)	691 (22%)	23 (0%)

5 of 691 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	B	4	A
4	B	5	C
4	B	6	G
4	B	8	C
4	B	9	G

5 of 23 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
34	A	2122	U
34	A	2125	A
34	A	2124	A
34	A	2336	U
34	A	1002	C

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	$\# Z > 2$
35	GCP	4	501	-	32,34,34	1.37	5 (15%)	49,54,54	1.85	6 (12%)

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	GCP	4	501	-	-	7/19/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	4	501	GCP	C5-C4	3.01	1.47	1.38
35	4	501	GCP	PG-O2G	2.82	1.61	1.55
35	4	501	GCP	PG-O3G	2.75	1.61	1.55
35	4	501	GCP	C6-N1	-2.59	1.34	1.38
35	4	501	GCP	C5-N7	-2.18	1.34	1.39

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	4	501	GCP	C5-C4-N3	-5.98	118.87	128.39
35	4	501	GCP	PB-O3A-PA	-5.08	115.78	132.37
35	4	501	GCP	C2-N3-C4	4.91	120.76	112.30
35	4	501	GCP	N9-C4-N3	4.30	134.54	125.95
35	4	501	GCP	C6-C5-N7	3.45	136.56	130.29

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

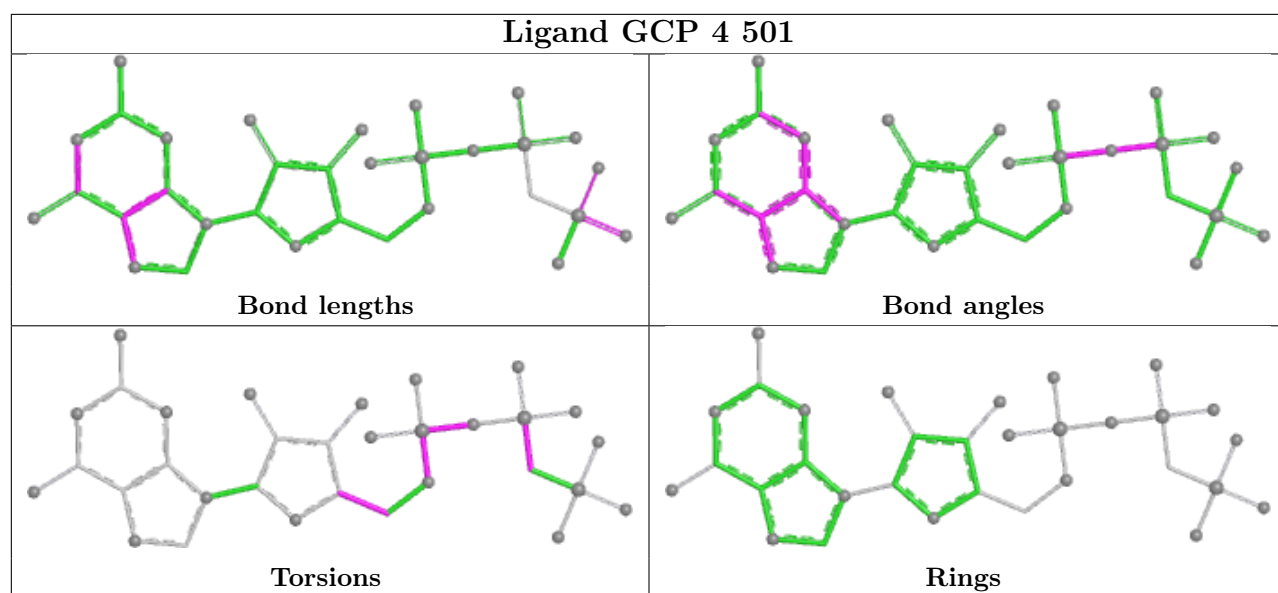
Mol	Chain	Res	Type	Atoms
35	4	501	GCP	C5'-O5'-PA-O3A
35	4	501	GCP	C5'-O5'-PA-O1A
35	4	501	GCP	C5'-O5'-PA-O2A
35	4	501	GCP	O4'-C4'-C5'-O5'
35	4	501	GCP	C3'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	4	501	GCP	11	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.

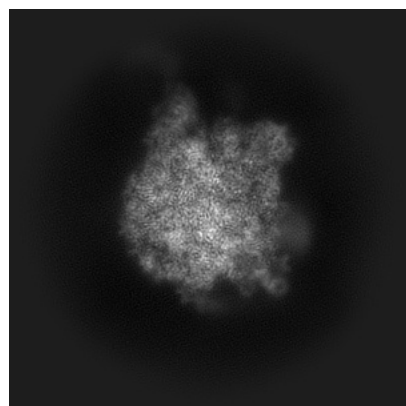
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43317. These allow visual inspection of the internal detail of the map and identification of artifacts.

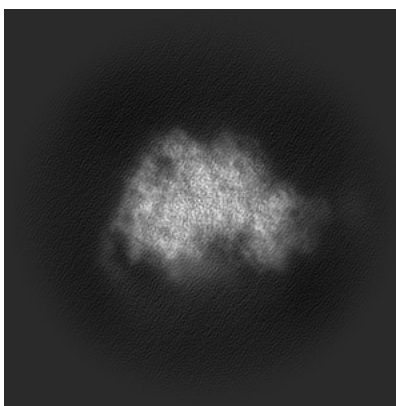
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

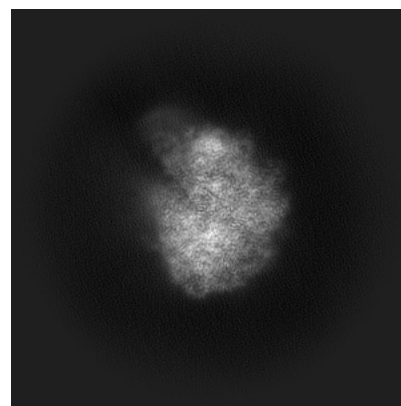
6.1.1 Primary map



X

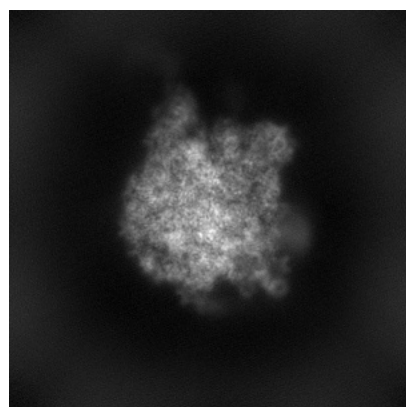


Y

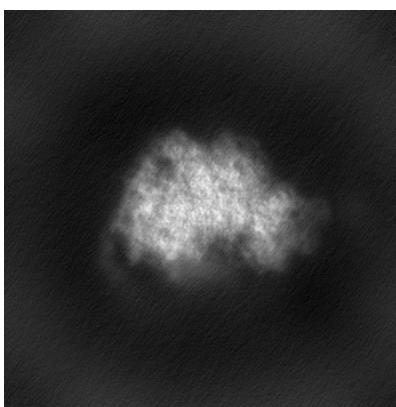


Z

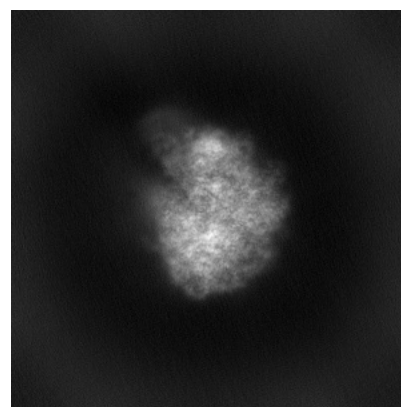
6.1.2 Raw map



X



Y

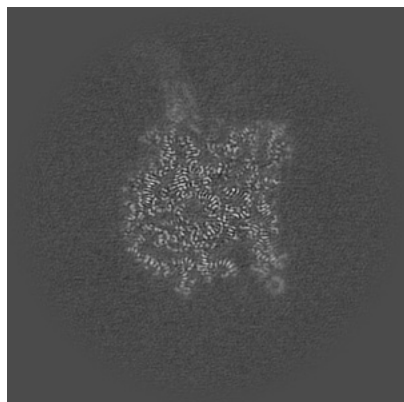


Z

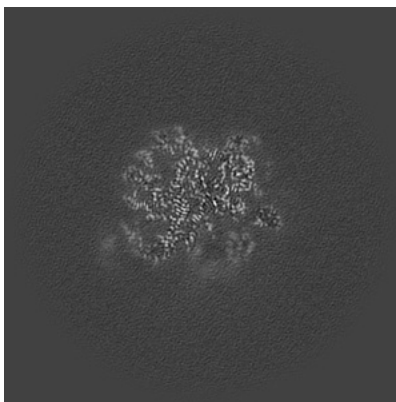
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

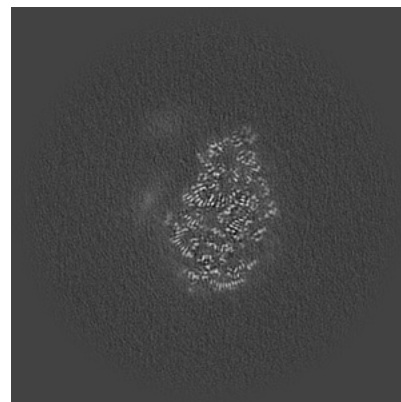
6.2.1 Primary map



X Index: 200

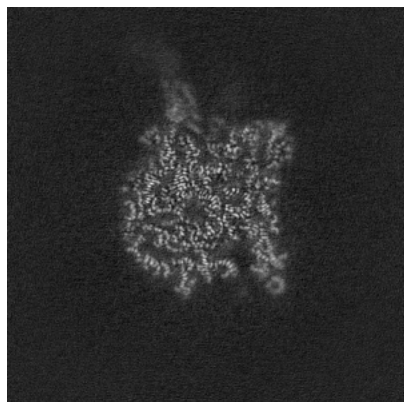


Y Index: 200

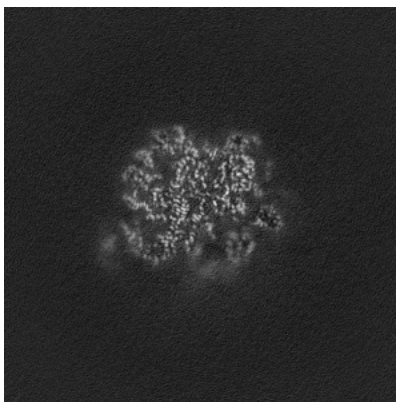


Z Index: 200

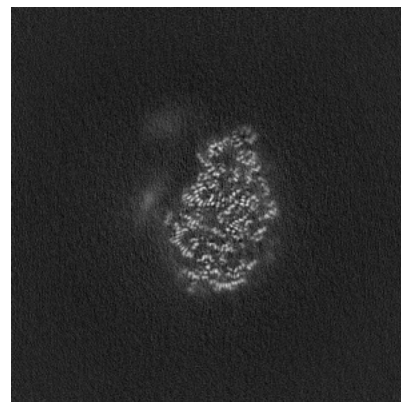
6.2.2 Raw map



X Index: 200



Y Index: 200

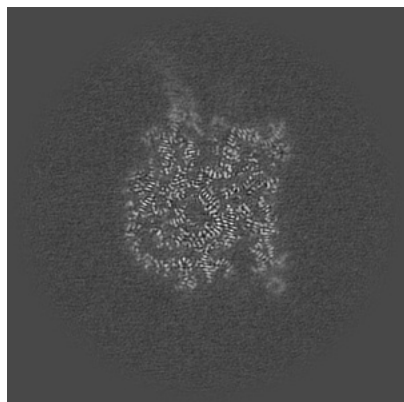


Z Index: 200

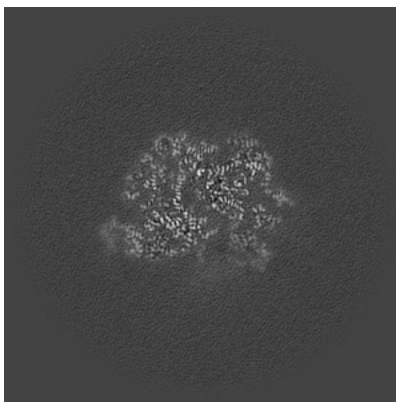
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

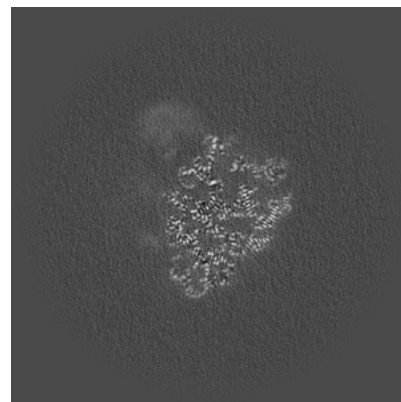
6.3.1 Primary map



X Index: 202

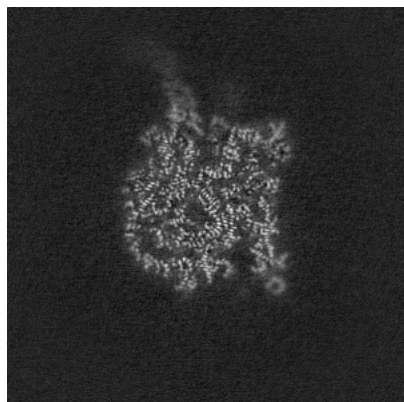


Y Index: 192

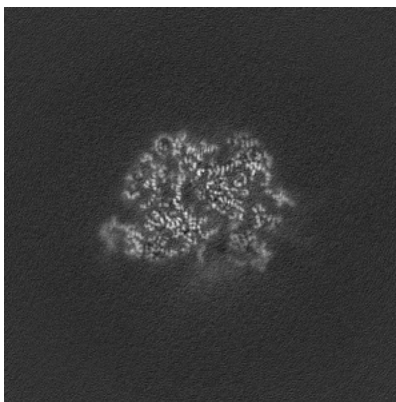


Z Index: 176

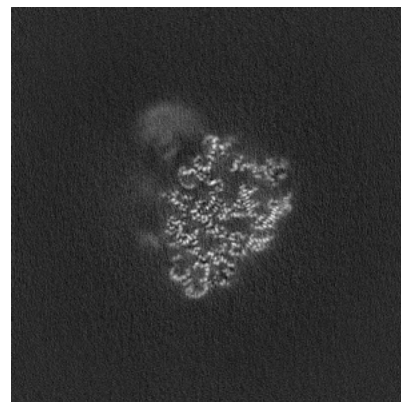
6.3.2 Raw map



X Index: 202



Y Index: 192

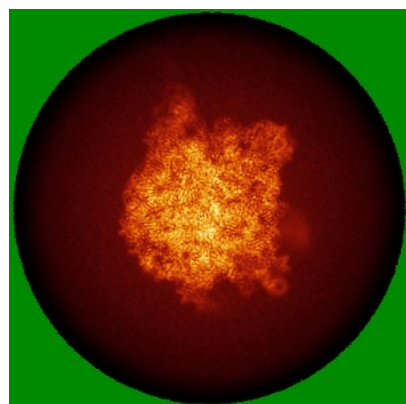


Z Index: 176

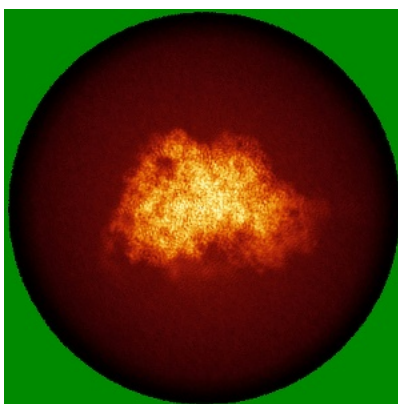
The images above show the largest variance slices of the map in three orthogonal directions.

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

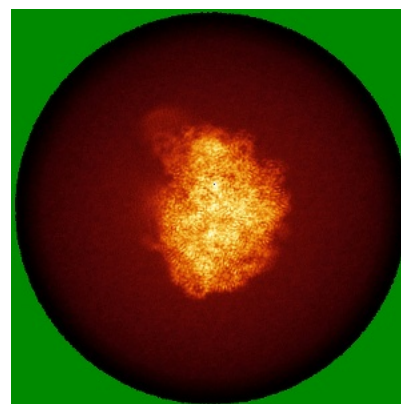
6.4.1 Primary map



X

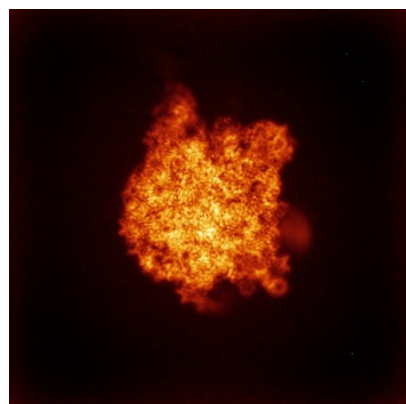


Y

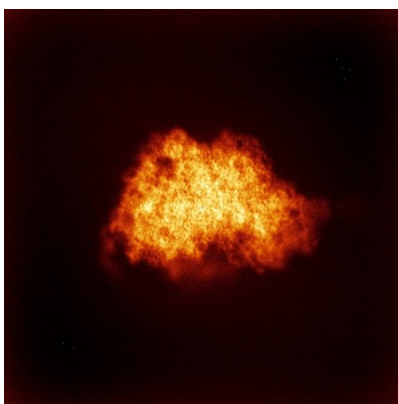


Z

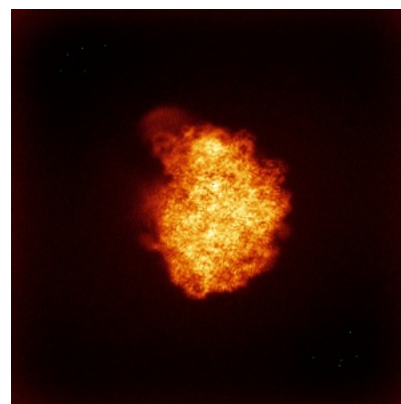
6.4.2 Raw map



X



Y



Z

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

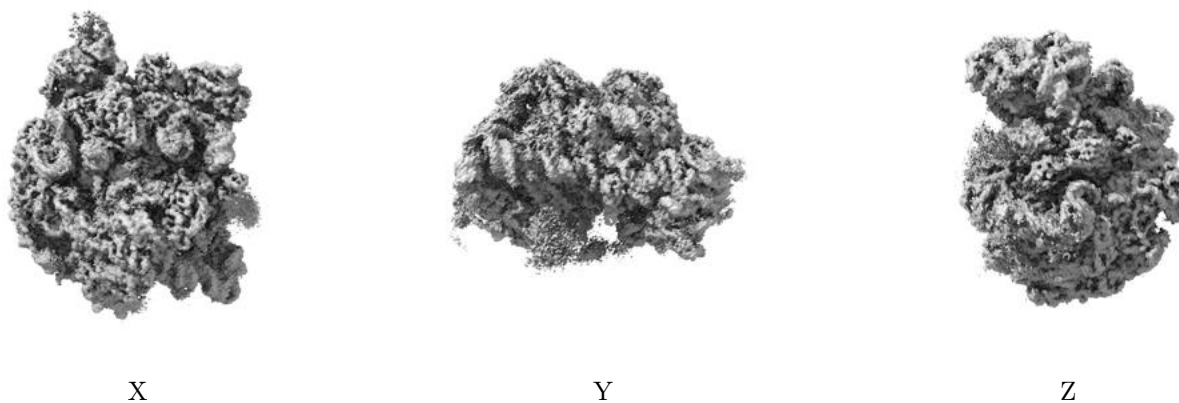
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.35. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

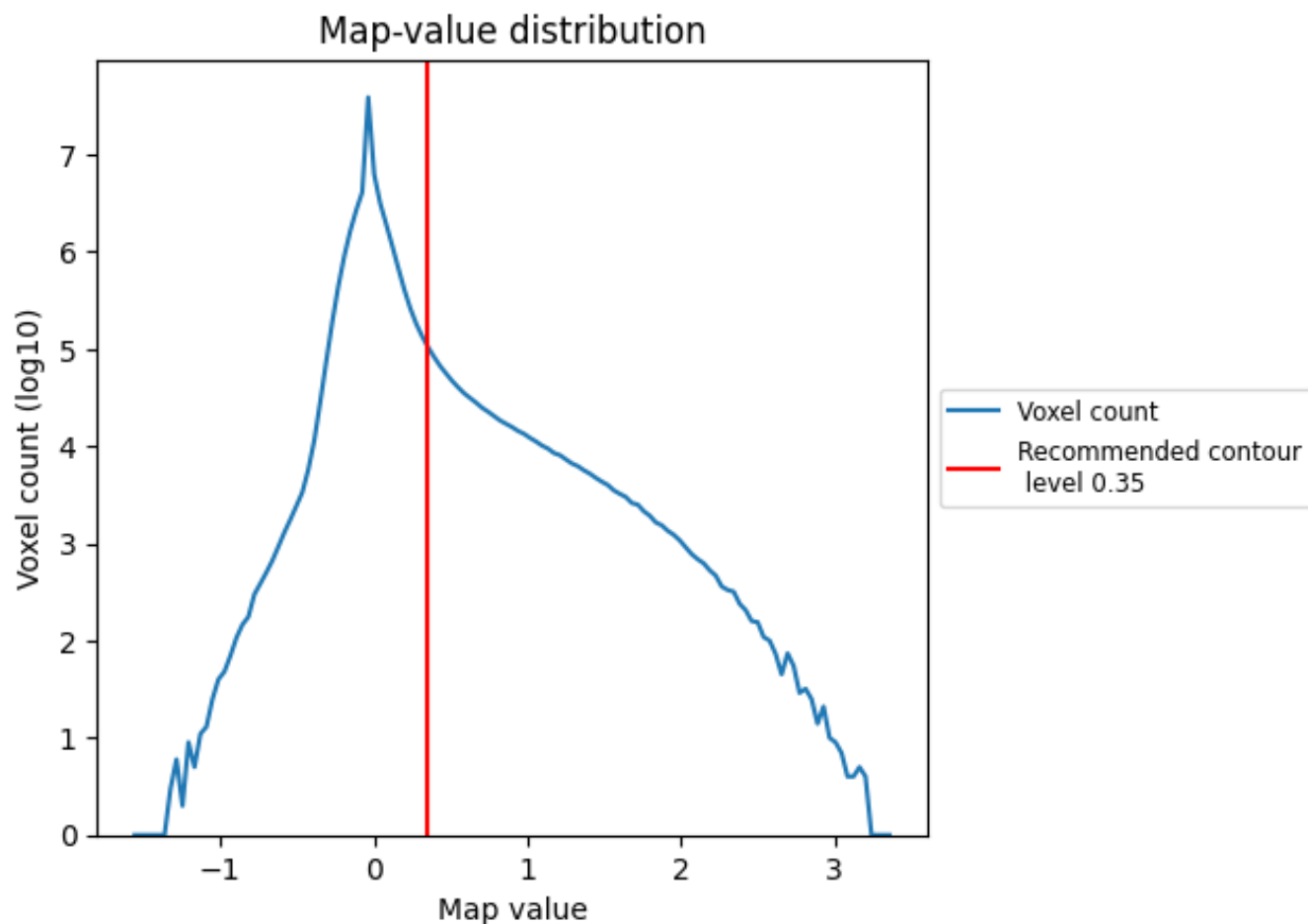
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

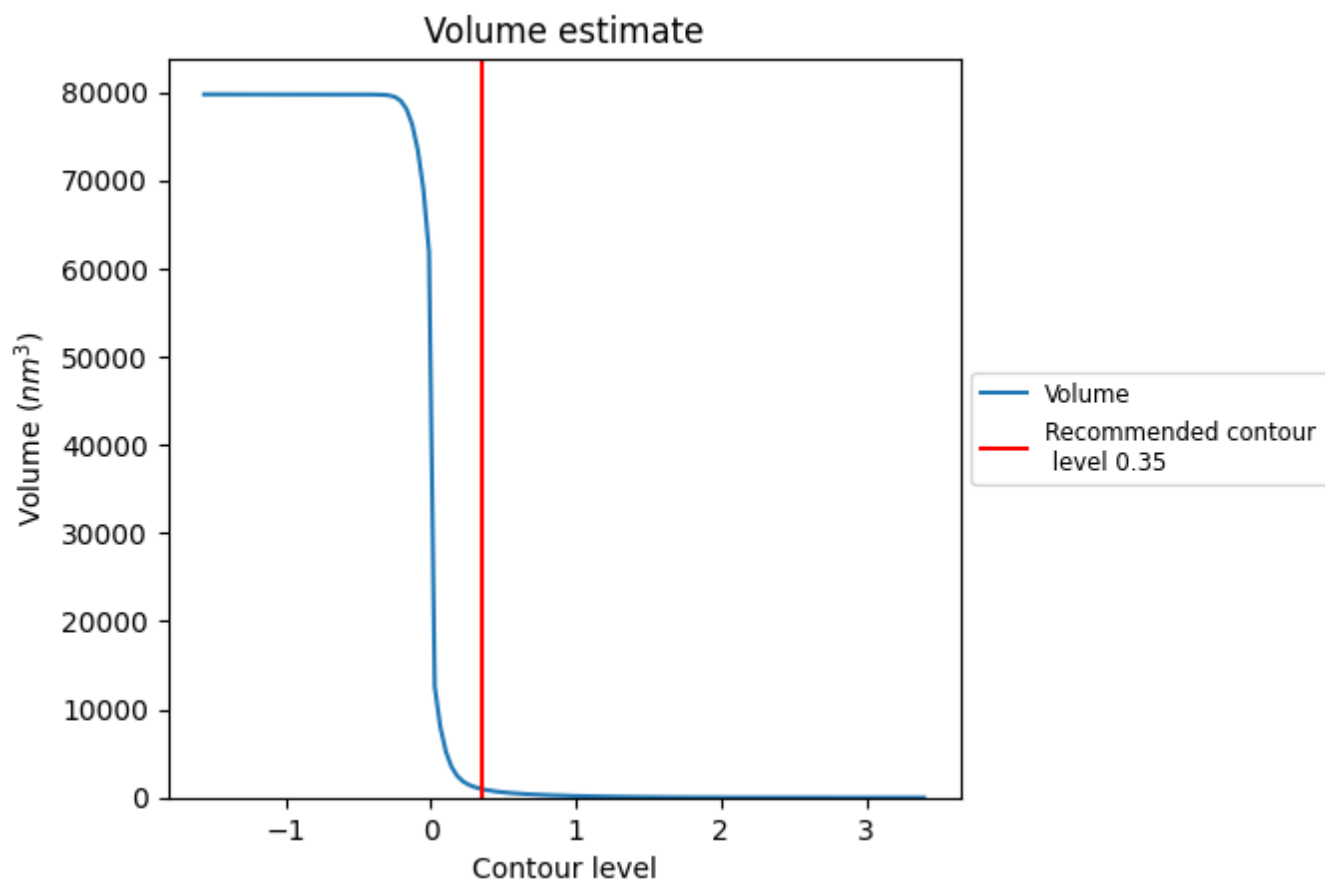
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

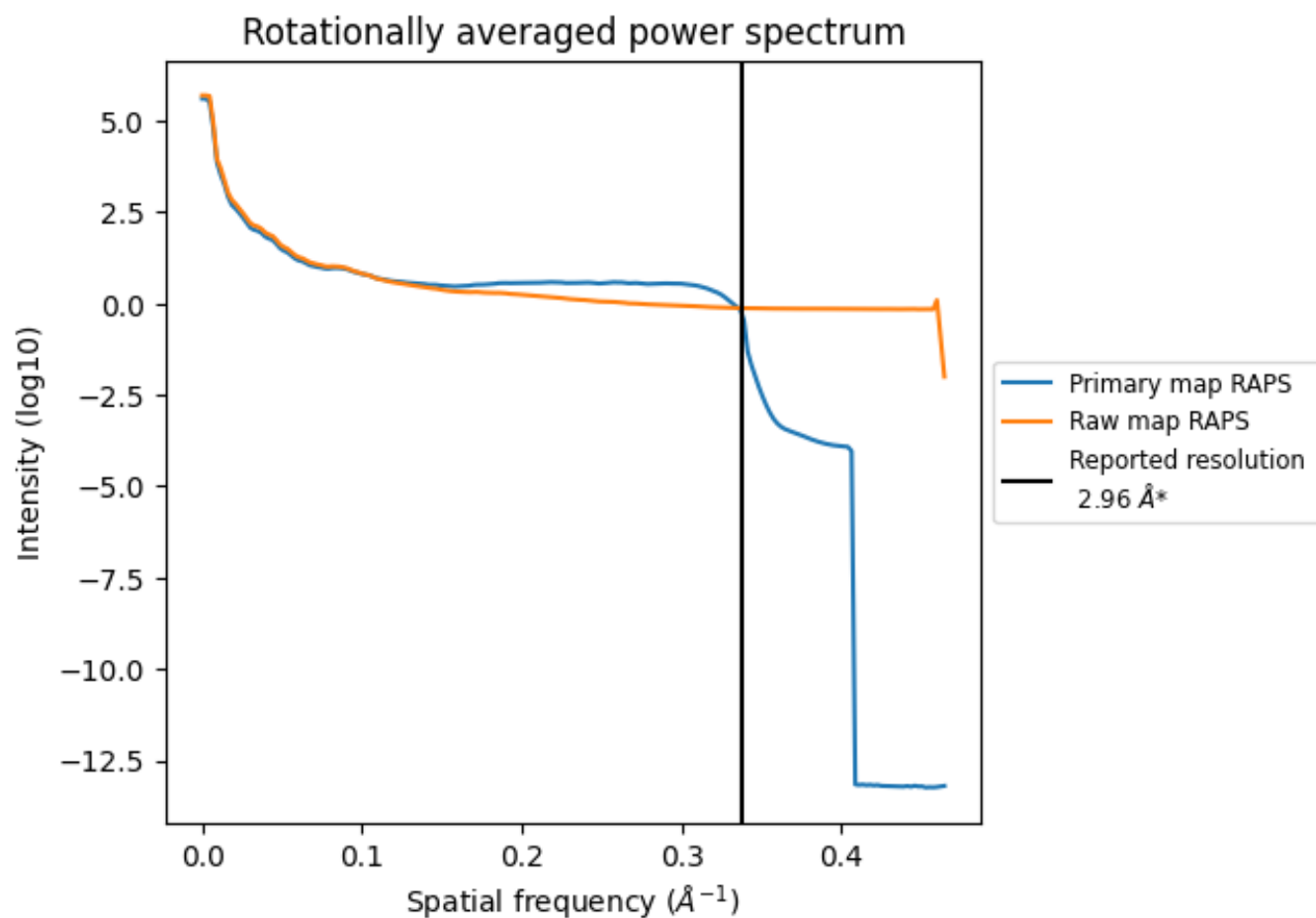
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 982 nm³; this corresponds to an approximate mass of 887 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 ⓘ

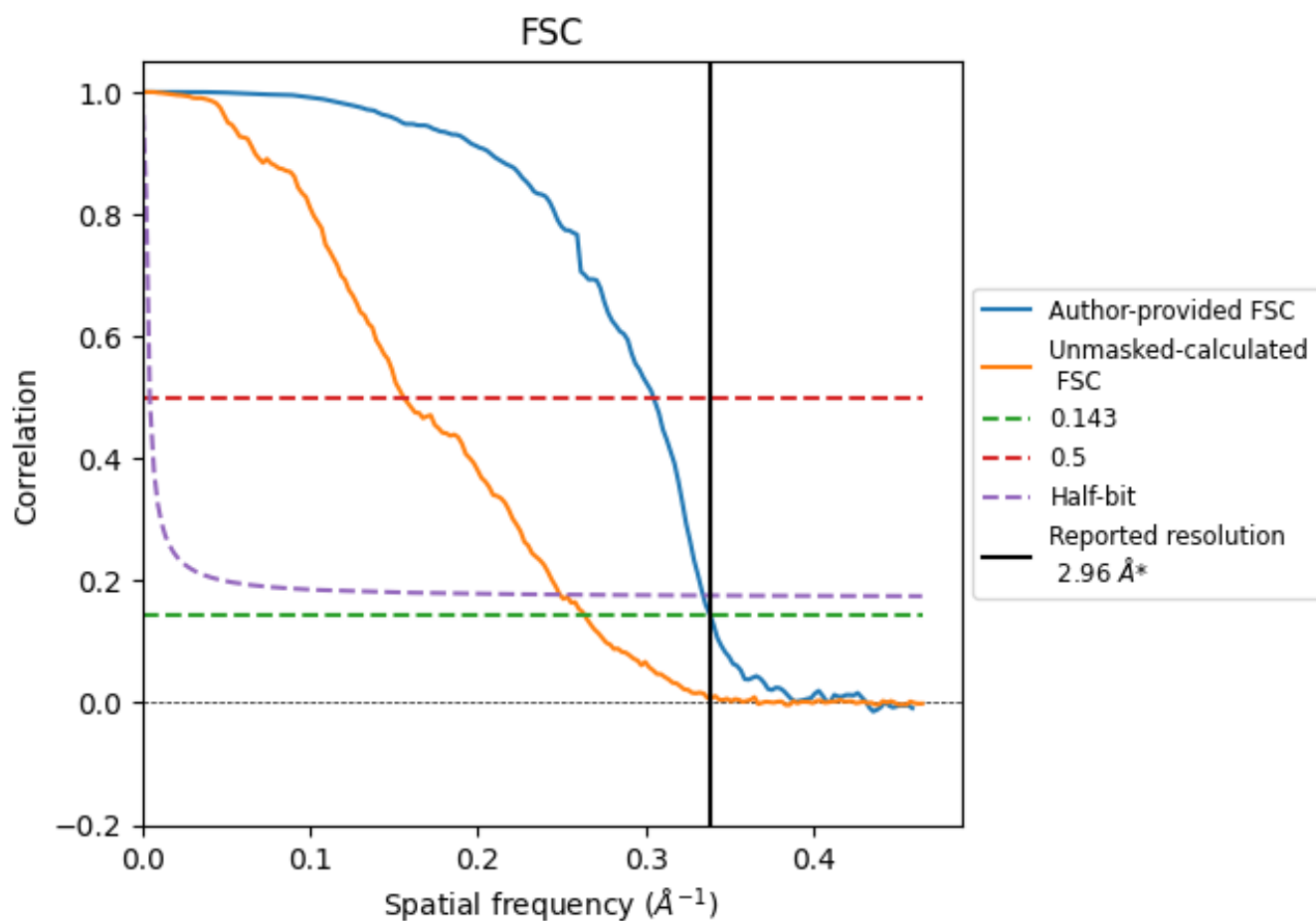


*Reported resolution corresponds to spatial frequency of 0.338 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.338 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

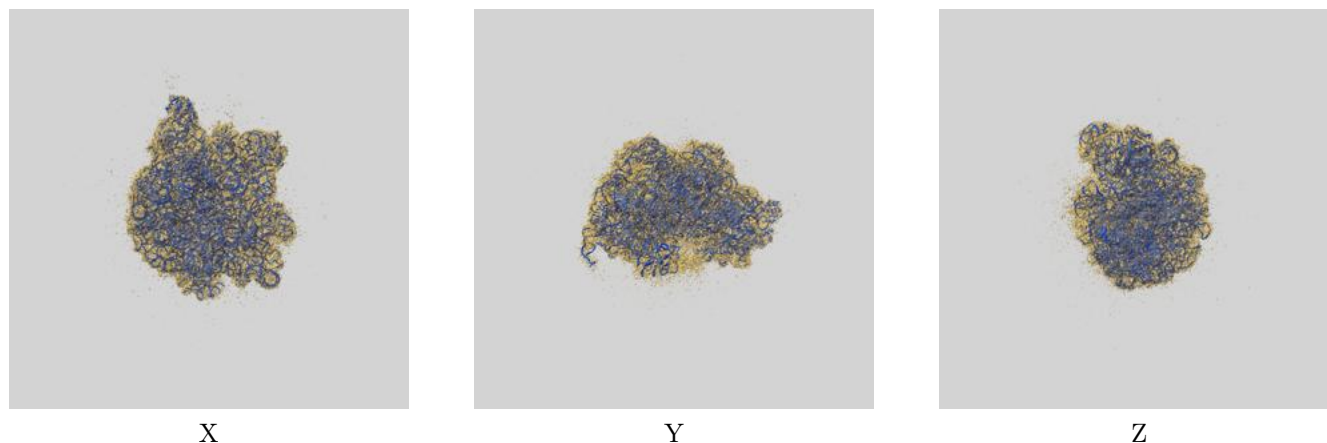
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.96	-	-
Author-provided FSC curve	2.96	3.28	2.99
Unmasked-calculated*	3.79	6.43	4.02

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.79 differs from the reported value 2.96 by more than 10 %

9 Map-model fit [i](#)

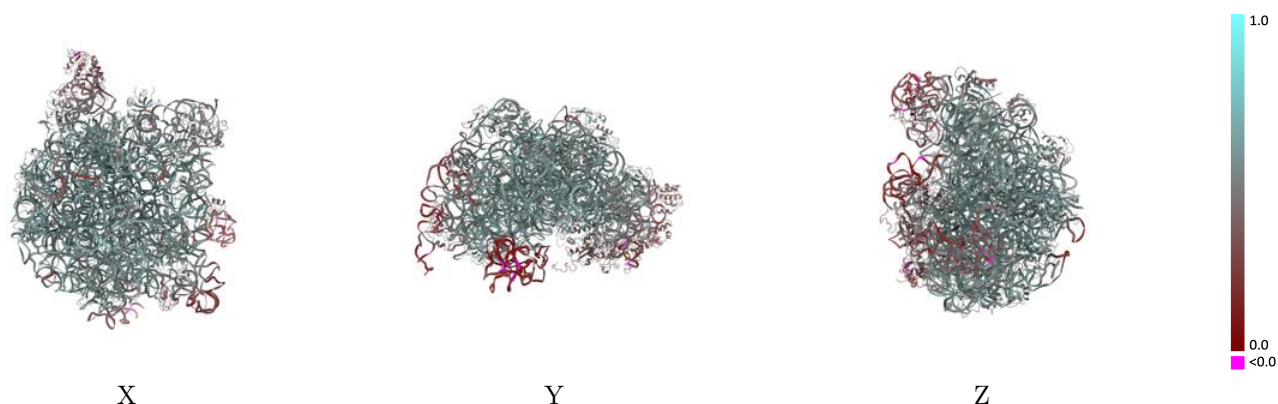
This section contains information regarding the fit between EMDB map EMD-43317 and PDB model 8VKI. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



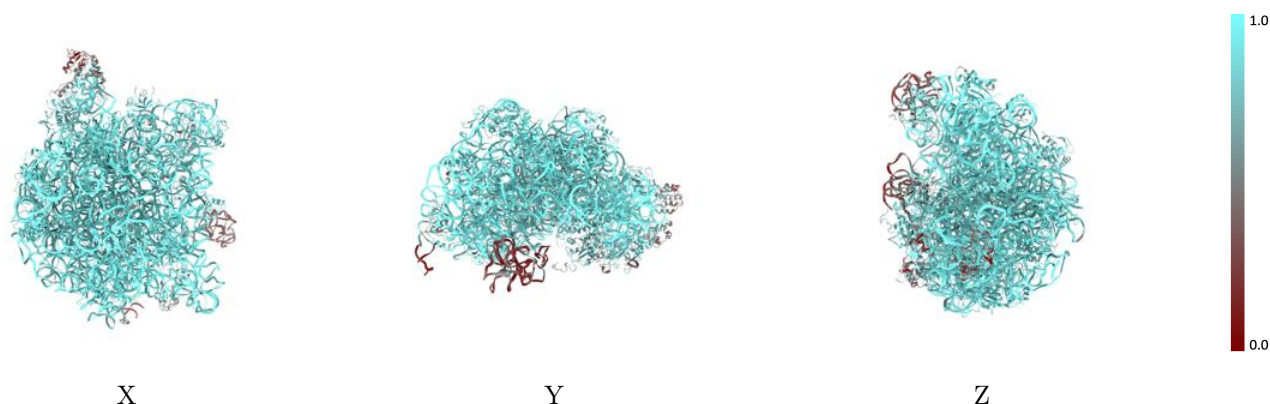
The images above show the 3D surface view of the map at the recommended contour level 0.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



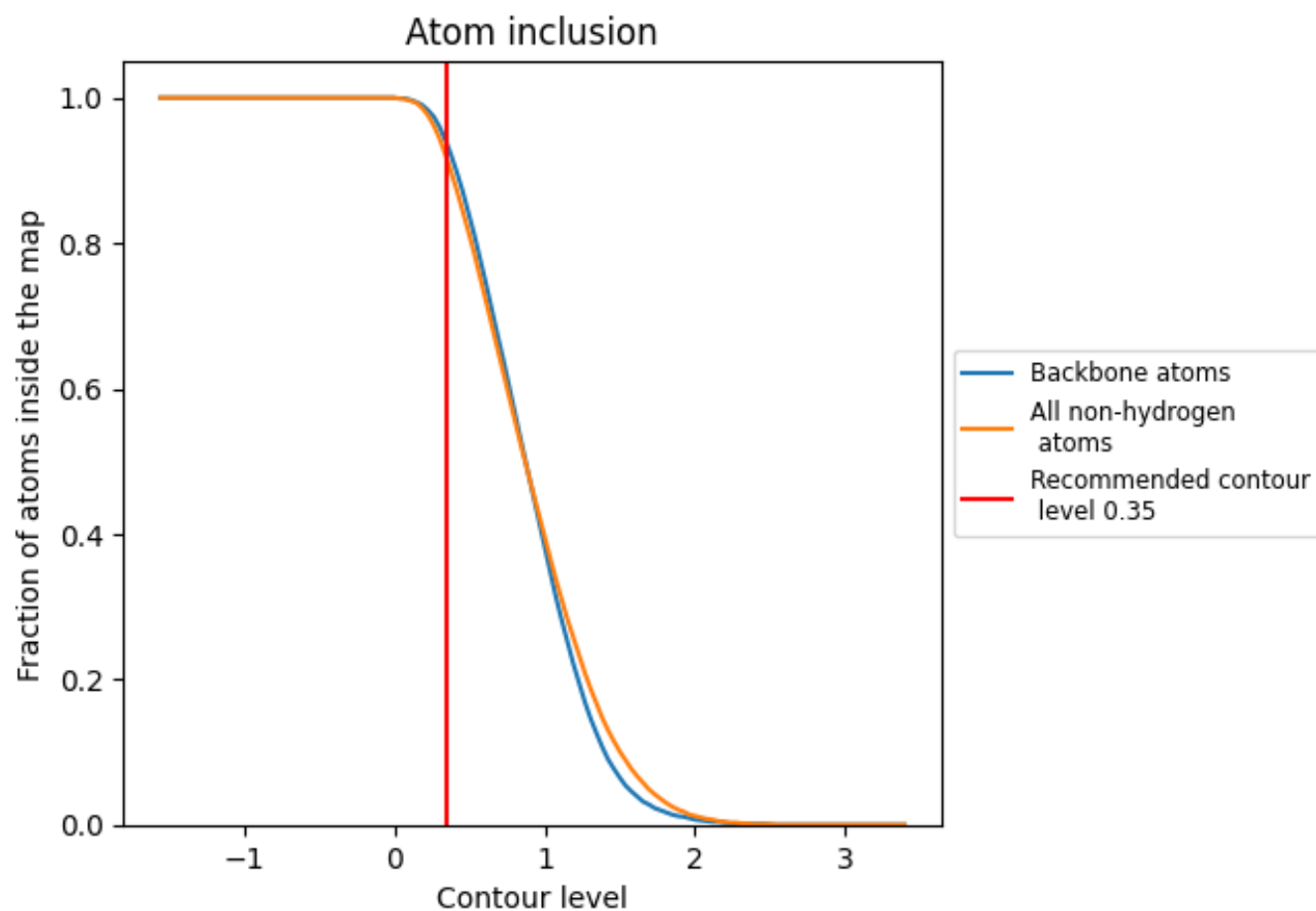
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.35).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 92% 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 (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9150	 0.5200
2	 0.9350	 0.5680
3	 0.9550	 0.6090
4	 0.7710	 0.4150
A	 0.9370	 0.5250
B	 0.9700	 0.5110
C	 0.9330	 0.5660
D	 0.9530	 0.5670
E	 0.9240	 0.5470
F	 0.7600	 0.3950
G	 0.8260	 0.4740
H	 0.7230	 0.4480
I	 0.4020	 0.3090
J	 0.4590	 0.3130
K	 0.9520	 0.5700
L	 0.9310	 0.5560
M	 0.9350	 0.5590
N	 0.9280	 0.5670
O	 0.9500	 0.5720
P	 0.9050	 0.4960
Q	 0.8870	 0.5250
R	 0.9570	 0.5700
S	 0.9100	 0.5550
T	 0.9490	 0.5720
U	 0.9430	 0.5490
V	 0.8940	 0.5020
W	 0.8450	 0.5210
X	 0.9400	 0.5810
Y	 0.9690	 0.5700
Z	 0.9250	 0.5290
b	 0.9680	 0.5820
c	 0.9570	 0.5620
d	 0.9600	 0.5930
e	 0.9750	 0.5890
f	 0.9650	 0.5780

