



wwPDB EM Validation Summary Report ⓘ

Apr 28, 2024 – 10:18 am BST

PDB ID : 2YKR
EMDB ID : EMD-1884
Title : 30S ribosomal subunit with RsgA bound in the presence of GMPPNP
Authors : Guo, Q.; Yuan, Y.; Xu, Y.; Feng, B.; Liu, L.; Chen, K.; Lei, J.; Gao, N.
Deposited on : 2011-05-30
Resolution : 9.80 Å(reported)
Based on initial models : 3OFA, 2RCN

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.dev92
MolProbity : 4.02b-467
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

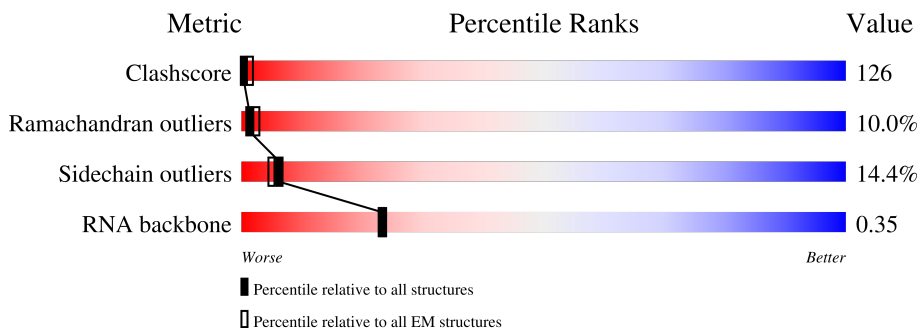
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 9.80 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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1533	14% (red), 86% (grey)
2	B	218	26% (green), 44% (yellow), 24% (orange), 6% (red)
3	C	206	27% (green), 43% (yellow), 25% (orange), 5% (red)
4	D	205	29% (green), 48% (yellow), 16% (orange), 7% (red)
5	E	150	21% (green), 51% (yellow), 19% (orange), 9% (red)
6	F	100	31% (green), 40% (yellow), 21% (orange), 8% (red)
7	G	151	9% (red), 52% (green), 32% (yellow), 11% (orange), 5% (red)

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Mol	Chain	Length	Quality of chain
8	H	129	26% 39% 26% 9%
9	I	127	31% 41% 17% 12%
10	J	98	21% 50% 18% 10%
11	K	117	30% 37% 28% 5%
12	L	123	33% 41% 18% 9%
13	M	114	25% 35% 26% 13%
14	N	100	29% 40% 20% 8% .
15	O	88	25% 47% 20% 8%
16	P	82	28% 43% 23% 6%
17	Q	80	18% 32% 36% 14%
18	R	55	29% 49% 16% 5%
19	S	79	32% 43% 16% 9%
20	T	85	31% 44% 21% 5%
21	U	51	37% 57% 33% 6% .
22	W	350	38% 30% 11% . 19%

2 Entry composition [i](#)

There are 22 unique types of molecules in this entry. The entry contains 53633 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S RRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	1533	32892	14671	6036	10653	1532	0	0

- Molecule 2 is a protein called 30S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	218	1705	1081	305	312	7	0	0

- Molecule 3 is a protein called 30S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	206	1625	1028	305	289	3	0	0

- Molecule 4 is a protein called 30S RIBOSOMAL PROTEIN S4.

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

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	150	1106	687	211	202	6	0	0

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	100	818	515	148	149	6	0	0

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	151	1182	735	227	216	4	0	0

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S8.

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

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S9.

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

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	98	787	493	150	143	1	0	0

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	117	877	540	174	160	3	0	0

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S12.

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

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	M	114	884	546	178	157	3	0	0

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	N	97	775	483	161	128	3	0	1

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	39	ASP	GLU	conflict	UNP B7M1M1

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S15.

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

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S16.

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

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	Q	80	649	411	121	114	3	0	0

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
18	R	55	456	288	86	82	0	0

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	S	79	638	408	120	108	2	0	0

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S20.

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

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	U	51	426	265	86	74	1	0	0

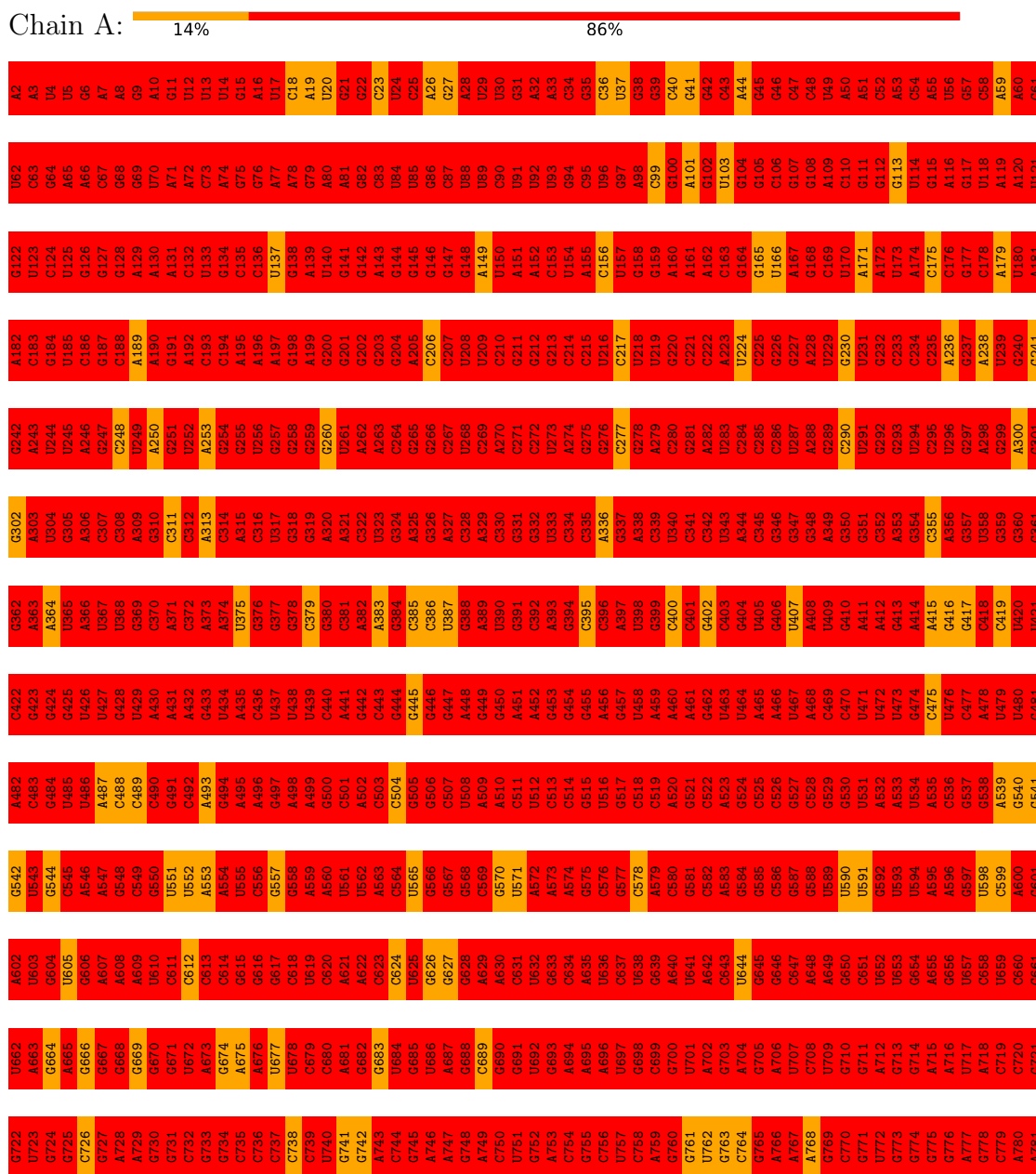
- Molecule 22 is a protein called PUTATIVE RIBOSOME BIOGENESIS GTPASE RSGA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	W	282	2186	1378	388	410	10	0	4

3 Residue-property plots i

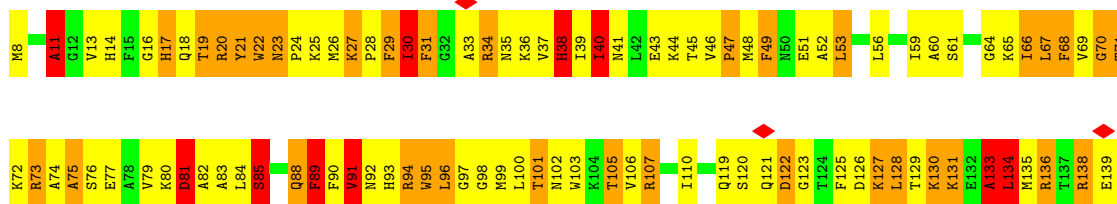
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

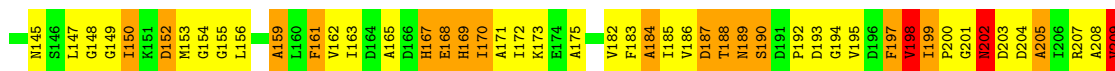
• Molecule 1: 16S rRNA



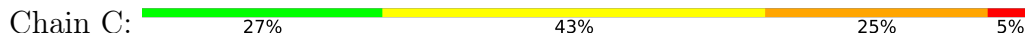
A782	A783	A784	A785	A786	A787	A788	A789	A790	A791	A792	A793	A794	A795	A796	A797	A798	A799	A800	A801	A802	A803	A804	A805	A806	A807	A808	A809	A810	A811	A812	A813	A814	A815	A816	A817	A818	A819	A820	A821	A822	A823	A824	A825	A826	A827	A828	A829	A830	A831	A832	A833	A834	A835	A836	A837	A838	A839	A840	A841	A842	A843	A844	A845	A846	A847	A848	A849	A850	A851	A852	A853	A854	A855	A856	A857	A858	A859	A860	A861	A862	A863	A864	A865	A866	A867	A868	A869	A870	A871	A872	A873	A874	A875	A876	A877	A878	A879	A880	A881	A882	A883	A884	A885	A886	A887	A888	A889	A890	A891	A892	A893	A894	A895	A896	A897	A898	A899	A900	A901
A902	A903	A904	A905	A906	A907	A908	A909	A910	A911	A912	A913	A914	A915	A916	A917	A918	A919	A920	A921	A922	A923	A924	A925	A926	A927	A928	A929	A930	A931	A932	A933	A934	A935	A936	A937	A938	A939	A940	A941	A942	A943	A944	A945	A946	A947	A948	A949	A950	A951	A952	A953	A954	A955	A956	A957	A958	A959	A960	A961	A962	A963	A964	A965	A966	A967	A968	A969	A970	A971	A972	A973	A974	A975	A976	A977	A978	A979	A980	A981	A982	A983	A984	A985	A986	A987	A988	A989	A990	A991	A992	A993	A994	A995	A996	A997	A998	A999	A1000	A1001	A1002	A1003	A1004	A1005	A1006	A1007	A1008	A1009	A1010	A1011	A1012	A1013	A1014	A1015	A1016	A1017	A1018	A1019	A1020	A1021
A1022	A1023	A1024	A1025	A1026	A1027	A1028	A1029	A1030	A1031	A1032	A1033	A1034	A1035	A1036	A1037	A1038	A1039	A1040	A1041	A1042	A1043	A1044	A1045	A1046	A1047	A1048	A1049	A1050	A1051	A1052	A1053	A1054	A1055	A1056	A1057	A1058	A1059	A1060	A1061	A1062	A1063	A1064	A1065	A1066	A1067	A1068	A1069	A1070	A1071	A1072	A1073	A1074	A1075	A1076	A1077	A1078	A1079	A1080	A1081																																																												
A1082	A1083	A1084	A1085	A1086	A1087	A1088	A1089	A1090	A1091	A1092	A1093	A1094	A1095	A1096	A1097	A1098	A1099	A1100	A1101	A1102	A1103	A1104	A1105	A1106	A1107	A1108	A1109	A1110	A1111	A1112	A1113	A1114	A1115	A1116	A1117	A1118	A1119	A1120	A1121	A1122	A1123	A1124	A1125	A1126	A1127	A1128	A1129	A1130	A1131	A1132	A1133	A1134	A1135	A1136	A1137	A1138	A1139	A1140	A1141																																																												
A1142	A1143	A1144	A1145	A1146	A1147	A1148	A1149	A1150	A1151	A1152	A1153	A1154	A1155	A1156	A1157	A1158	A1159	A1160	A1161	A1162	A1163	A1164	A1165	A1166	A1167	A1168	A1169	A1170	A1171	A1172	A1173	A1174	A1175	A1176	A1177	A1178	A1179	A1180	A1181	A1182	A1183	A1184	A1185	A1186	A1187	A1188	A1189	A1190	A1191	A1192	A1193	A1194	A1195	A1196	A1197	A1198	A1199	A1200	A1201																																																												
A1202	A1203	A1204	A1205	A1206	A1207	A1208	A1209	A1210	A1211	A1212	A1213	A1214	A1215	A1216	A1217	A1218	A1219	A1220	A1221	A1222	A1223	A1224	A1225	A1226	A1227	A1228	A1229	A1230	A1231	A1232	A1233	A1234	A1235	A1236	A1237	A1238	A1239	A1240	A1241	A1242	A1243	A1244	A1245	A1246	A1247	A1248	A1249	A1250	A1251	A1252	A1253	A1254	A1255	A1256	A1257	A1258	A1259	A1260	A1261																																																												
A1262	A1263	A1264	A1265	A1266	A1267	A1268	A1269	A1270	A1271	A1272	A1273	A1274	A1275	A1276	A1277	A1278	A1279	A1280	A1281	A1282	A1283	A1284	A1285	A1286	A1287	A1288	A1289	A1290	A1291	A1292	A1293	A1294	A1295	A1296	A1297	A1298	A1299	A1300	A1301	A1302	A1303	A1304	A1305	A1306	A1307	A1308	A1309	A1310	A1311	A1312	A1313	A1314	A1315	A1316	A1317	A1318	A1319	A1320	A1321																																																												
A1322	A1323	A1324	A1325	A1326	A1327	A1328	A1329	A1330	A1331	A1332	A1333	A1334	A1335	A1336	A1337	A1338	A1339	A1340	A1341	A1342	A1343	A1344	A1345	A1346	A1347	A1348	A1349	A1350	A1351	A1352	A1353	A1354	A1355	A1356	A1357	A1358	A1359	A1360	A1361	A1362	A1363	A1364	A1365	A1366	A1367	A1368	A1369	A1370	A1371	A1372	A1373	A1374	A1375	A1376	A1377	A1378	A1379	A1380	A1381																																																												
A1382	A1383	A1384	A1385	A1386	A1387	A1388	A1389	A1390	A1391	A1392	A1393	A1394	A1395	A1396	A1397	A1398	A1399	A1400	A1401	A1402	A1403	A1404	A1405	A1406	A1407	A1408	A1409	A1410	A1411	A1412	A1413	A1414	A1415	A1416	A1417	A1418	A1419	A1420	A1421	A1422	A1423	A1424	A1425	A1426	A1427	A1428	A1429	A1430	A1431	A1432	A1433	A1434	A1435	A1436	A1437	A1438	A1439	A1440	A1441																																																												
A1442	A1443	A1444	A1445	A1446	A1447	A1448	A1449	A1450	A1451	A1452	A1453	A1454	A1455	A1456	A1457	A1458	A1459	A1460	A1461	A1462	A1463	A1464	A1465	A1466	A1467	A1468	A1469	A1470	A1471	A1472	A1473	A1474	A1475	A1476	A1477	A1478	A1479	A1480	A1481	A1482	A1483	A1484	A1485	A1486	A1487	A1488	A1489	A1490	A1491	A1492	A1493	A1494	A1495	A1496	A1497	A1498	A1499	A1500	A1501																																																												
A1502	A1503	A1504	A1505	A1506	A1507	A1508	A1509	A1510	A1511	A1512	A1513	A1514	A1515	A1516	A1517	A1518	A1519	A1520	A1521	A1522	A1523	A1524	A1525	A1526	A1527	A1528	A1529	A1530	A1531	A1532	A1533	A1534	A1535	A1536	A1537	A1538	A1539	A1540	A1541	A1542	A1543	A1544	A1545	A1546	A1547	A1548	A1549	A1550	A1551	A1552	A1553	A1554	A1555	A1556	A1557	A1558	A1559	A1560	A1561	A1562	A1563	A1564	A1565	A1566	A1567	A1568	A1569	A1570	A1571	A1572	A1573	A1574	A1575	A1576	A1577	A1578	A1579	A1580	A1581	A1582	A1583	A1584	A1585	A1586	A1587	A1588	A1589	A1590	A1591	A1592	A1593	A1594	A1595	A1596	A1597	A1598	A1599	A1600	A1601																				

Molecule 2: 30S RIBOSOMAL PROTEIN S2

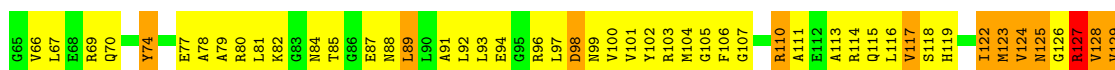
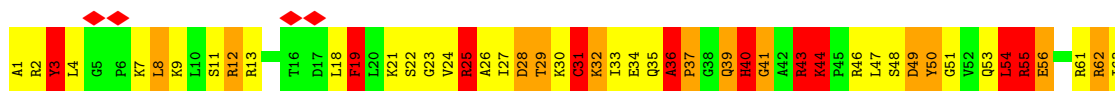
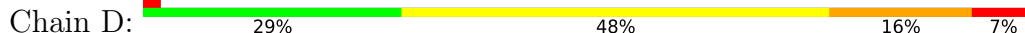




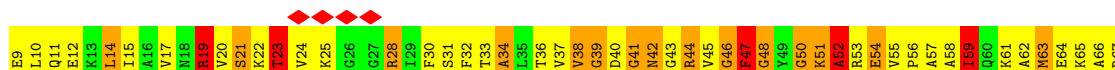
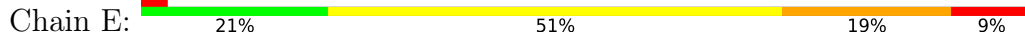
• Molecule 3: 30S RIBOSOMAL PROTEIN S3



• Molecule 4: 30S RIBOSOMAL PROTEIN S4

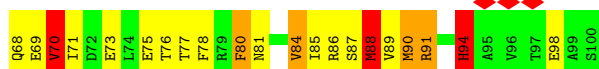
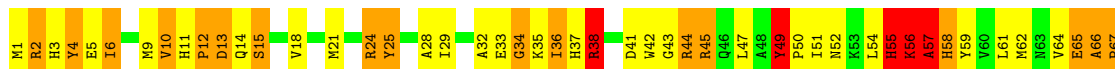


• Molecule 5: 30S RIBOSOMAL PROTEIN S5

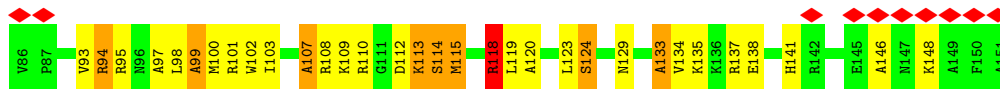
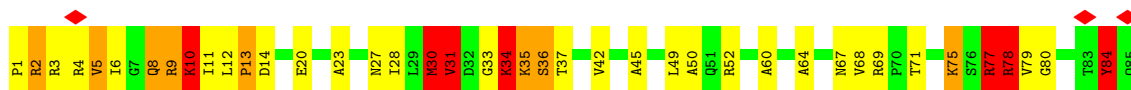




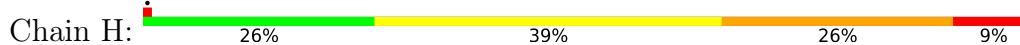
• Molecule 6: 30S RIBOSOMAL PROTEIN S6



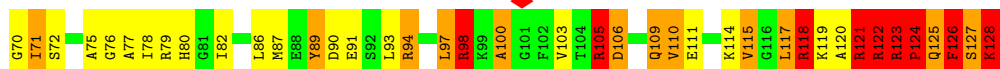
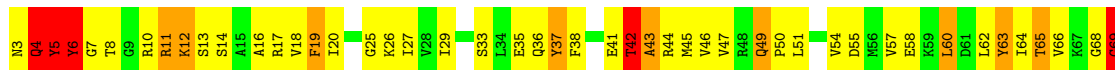
• Molecule 7: 30S RIBOSOMAL PROTEIN S7



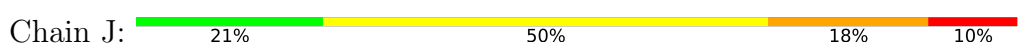
• Molecule 8: 30S RIBOSOMAL PROTEIN S8



• Molecule 9: 30S RIBOSOMAL PROTEIN S9

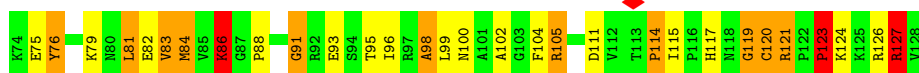
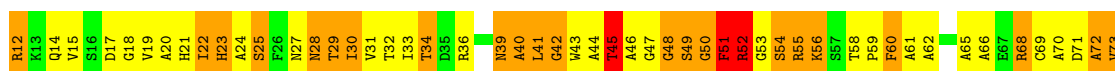
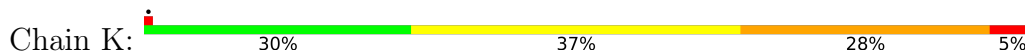


• Molecule 10: 30S RIBOSOMAL PROTEIN S10

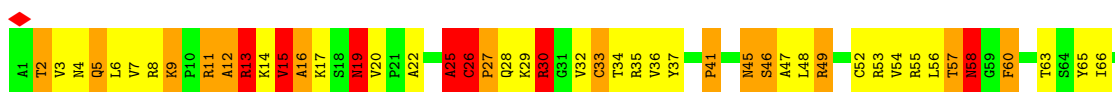
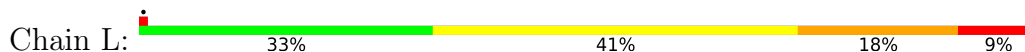




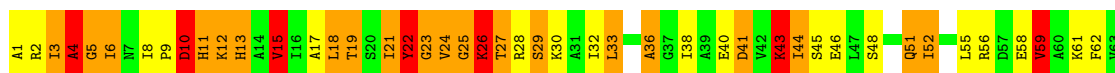
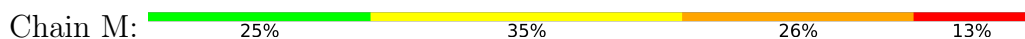
- Molecule 11: 30S RIBOSOMAL PROTEIN S11



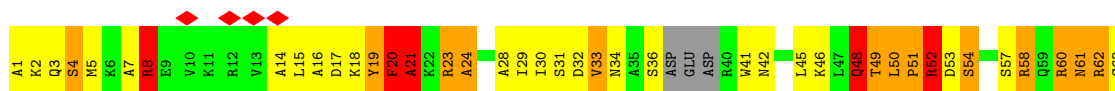
- Molecule 12: 30S RIBOSOMAL PROTEIN S12



- Molecule 13: 30S RIBOSOMAL PROTEIN S13



- Molecule 14: 30S RIBOSOMAL PROTEIN S14

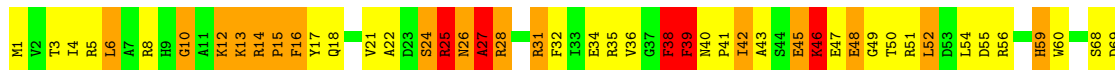


- Molecule 15: 30S RIBOSOMAL PROTEIN S15





• Molecule 16: 30S RIBOSOMAL PROTEIN S16



• Molecule 17: 30S RIBOSOMAL PROTEIN S17



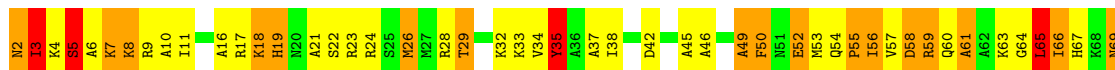
• Molecule 18: 30S RIBOSOMAL PROTEIN S18

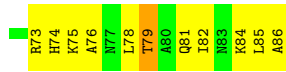


• Molecule 19: 30S RIBOSOMAL PROTEIN S19

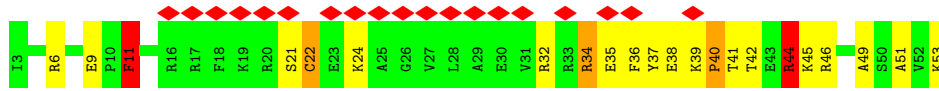


• Molecule 20: 30S RIBOSOMAL PROTEIN S20

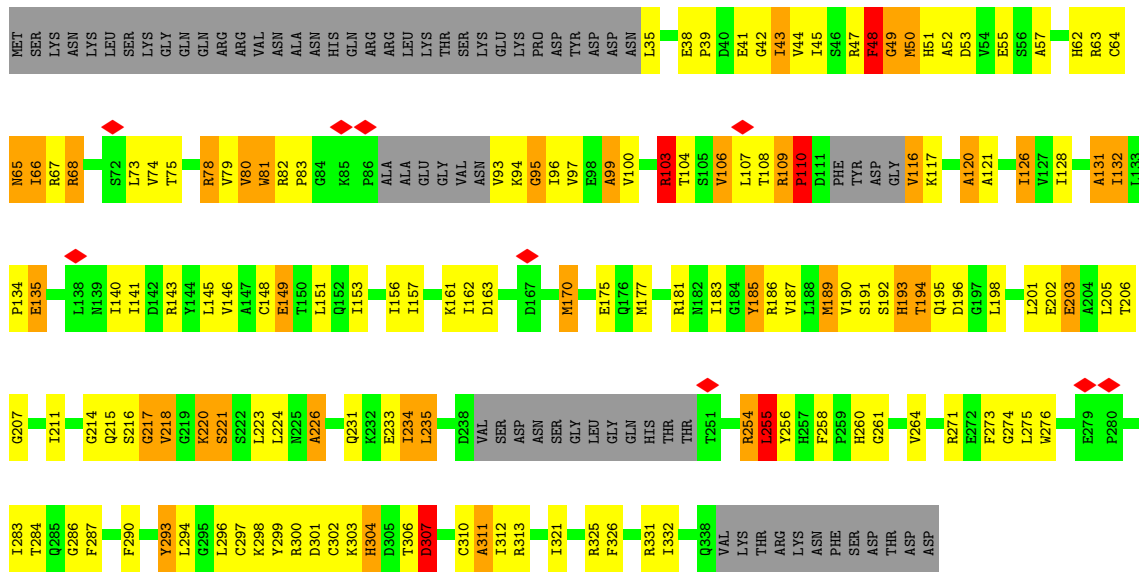




• Molecule 21: 30S RIBOSOMAL PROTEIN S21



• Molecule 22: PUTATIVE RIBOSOME BIOGENESIS GTPASE RSGA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	77483	Depositor
Resolution determination method	Not provided	
CTF correction method	MAPS FROM EACH DEFOCUS GROUP	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	3850	Depositor
Magnification	59000	Depositor
Image detector	FEI EAGLE (4k x 4k)	Depositor
Maximum map value	19.771	Depositor
Minimum map value	-6.451	Depositor
Average map value	0.106	Depositor
Map value standard deviation	1.371	Depositor
Recommended contour level	3.16	Depositor
Map size (\AA)	362.5, 362.5, 362.5	wwPDB
Map dimensions	125, 125, 125	wwPDB
Map angles ($^\circ$)	90, 90, 90	wwPDB
Pixel spacing (\AA)	2.9, 2.9, 2.9	Depositor

5 Model quality i

5.1 Standard geometry i

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	3.88	6344/36831 (17.2%)	4.27	11020/57458 (19.2%)
2	B	1.35	2/1736 (0.1%)	1.90	59/2338 (2.5%)
3	C	1.48	2/1652 (0.1%)	1.88	48/2225 (2.2%)
4	D	1.45	4/1665 (0.2%)	1.82	40/2227 (1.8%)
5	E	1.57	8/1119 (0.7%)	1.93	38/1504 (2.5%)
6	F	1.37	1/836 (0.1%)	1.96	29/1128 (2.6%)
7	G	1.27	2/1196 (0.2%)	1.59	18/1602 (1.1%)
8	H	1.42	2/989 (0.2%)	1.96	36/1326 (2.7%)
9	I	1.45	1/1034 (0.1%)	1.93	36/1375 (2.6%)
10	J	1.41	0/797	2.00	23/1077 (2.1%)
11	K	1.61	4/893 (0.4%)	1.82	24/1205 (2.0%)
12	L	1.42	1/969 (0.1%)	1.88	27/1300 (2.1%)
13	M	1.60	5/893 (0.6%)	1.97	30/1193 (2.5%)
14	N	1.33	0/786	1.93	19/1045 (1.8%)
15	O	1.42	2/722 (0.3%)	1.99	26/964 (2.7%)
16	P	1.42	0/659	2.00	27/884 (3.1%)
17	Q	1.69	4/658 (0.6%)	2.31	40/881 (4.5%)
18	R	1.35	0/463	1.99	14/621 (2.3%)
19	S	1.20	1/653 (0.2%)	1.69	14/877 (1.6%)
20	T	1.37	1/671 (0.1%)	1.96	18/888 (2.0%)
21	U	1.28	0/431	1.60	2/570 (0.4%)
22	W	1.30	3/2223 (0.1%)	1.58	40/3008 (1.3%)
All	All	3.21	6387/57876 (11.0%)	3.66	11628/85696 (13.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1238
2	B	0	14
3	C	0	16

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Mol	Chain	#Chirality outliers	#Planarity outliers
4	D	0	15
5	E	0	6
6	F	0	7
7	G	0	4
8	H	0	12
9	I	0	15
10	J	0	6
11	K	0	10
12	L	0	7
13	M	0	13
14	N	0	9
15	O	0	9
16	P	0	5
17	Q	0	7
18	R	0	4
19	S	0	8
20	T	0	5
21	U	0	2
22	W	0	7
All	All	0	1419

The worst 5 of 6387 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1306	A	N7-C5	-22.89	1.25	1.39
1	A	466	A	N7-C5	-22.87	1.25	1.39
1	A	627	G	N7-C5	-22.74	1.25	1.39
1	A	373	A	N9-C4	-22.28	1.24	1.37
1	A	78	A	N9-C4	22.19	1.51	1.37

The worst 5 of 11628 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1399	C	P-O3'-C3'	47.06	176.18	119.70
1	A	1139	G	P-O3'-C3'	47.02	176.13	119.70
1	A	556	C	C6-N1-C2	-44.83	102.37	120.30
1	A	306	A	P-O3'-C3'	39.05	166.56	119.70
1	A	73	C	C6-N1-C2	-38.49	104.91	120.30

There are no chirality outliers.

5 of 1419 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2	A	Sidechain
1	A	3	A	Sidechain
1	A	4	U	Sidechain
1	A	5	U	Sidechain
1	A	6	G	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32892	0	16464	9848	0
2	B	1705	0	1732	204	0
3	C	1625	0	1699	204	0
4	D	1643	0	1710	176	0
5	E	1106	0	1148	142	0
6	F	818	0	808	110	0
7	G	1182	0	1239	124	0
8	H	979	0	1034	139	0
9	I	1022	0	1070	132	0
10	J	787	0	828	130	0
11	K	877	0	887	165	0
12	L	955	0	1019	106	0
13	M	884	0	944	126	0
14	N	775	0	827	111	0
15	O	714	0	737	111	0
16	P	649	0	666	67	0
17	Q	649	0	690	143	0
18	R	456	0	478	57	0
19	S	638	0	665	75	0
20	T	665	0	714	109	0
21	U	426	0	449	19	0
22	W	2186	0	2180	107	0
All	All	53633	0	37988	11504	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 126.

The worst 5 of 11504 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)
1:A:429:U:H5'	4:D:8:LEU:HD13	1.45	0.99
1:A:688:G:H5''	1:A:688:G:C8	1.99	0.98
1:A:82:G:H22	1:A:84:U:H3	1.11	0.95
1:A:450:G:H1	1:A:483:C:H42	1.13	0.95
1:A:1469:C:H5'	1:A:1469:C:C6	2.02	0.94

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	
2	B	216/218 (99%)	149 (69%)	41 (19%)	26 (12%)	0	6
3	C	204/206 (99%)	158 (78%)	28 (14%)	18 (9%)	1	11
4	D	203/205 (99%)	139 (68%)	41 (20%)	23 (11%)	0	7
5	E	148/150 (99%)	104 (70%)	25 (17%)	19 (13%)	0	5
6	F	98/100 (98%)	75 (76%)	16 (16%)	7 (7%)	1	14
7	G	149/151 (99%)	118 (79%)	20 (13%)	11 (7%)	1	14
8	H	127/129 (98%)	90 (71%)	26 (20%)	11 (9%)	1	11
9	I	125/127 (98%)	83 (66%)	25 (20%)	17 (14%)	0	4
10	J	96/98 (98%)	74 (77%)	10 (10%)	12 (12%)	0	5
11	K	115/117 (98%)	81 (70%)	20 (17%)	14 (12%)	0	6
12	L	121/123 (98%)	85 (70%)	22 (18%)	14 (12%)	0	6
13	M	112/114 (98%)	82 (73%)	16 (14%)	14 (12%)	0	5
14	N	93/100 (93%)	61 (66%)	21 (23%)	11 (12%)	0	6
15	O	86/88 (98%)	65 (76%)	16 (19%)	5 (6%)	1	18
16	P	80/82 (98%)	58 (72%)	13 (16%)	9 (11%)	0	7
17	Q	78/80 (98%)	55 (70%)	16 (20%)	7 (9%)	1	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	R	53/55 (96%)	33 (62%)	12 (23%)	8 (15%)	0	3
19	S	77/79 (98%)	61 (79%)	12 (16%)	4 (5%)	2	19
20	T	83/85 (98%)	64 (77%)	14 (17%)	5 (6%)	1	17
21	U	49/51 (96%)	28 (57%)	11 (22%)	10 (20%)	0	2
22	W	274/350 (78%)	236 (86%)	25 (9%)	13 (5%)	2	21
All	All	2587/2708 (96%)	1899 (73%)	430 (17%)	258 (10%)	1	9

5 of 258 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	11	ALA
2	B	18	GLN
2	B	23	ASN
2	B	27	LYS
2	B	30	ILE

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	
2	B	180/180 (100%)	156 (87%)	24 (13%)	4	18
3	C	170/170 (100%)	146 (86%)	24 (14%)	3	16
4	D	172/172 (100%)	147 (86%)	25 (14%)	3	15
5	E	113/113 (100%)	94 (83%)	19 (17%)	2	12
6	F	87/87 (100%)	74 (85%)	13 (15%)	3	15
7	G	124/124 (100%)	113 (91%)	11 (9%)	9	30
8	H	104/104 (100%)	84 (81%)	20 (19%)	1	8
9	I	105/105 (100%)	91 (87%)	14 (13%)	4	18
10	J	86/86 (100%)	71 (83%)	15 (17%)	2	11
11	K	90/90 (100%)	75 (83%)	15 (17%)	2	12
12	L	103/103 (100%)	88 (85%)	15 (15%)	3	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	M	92/92 (100%)	74 (80%)	18 (20%)	1	8
14	N	79/83 (95%)	67 (85%)	12 (15%)	3	14
15	O	76/76 (100%)	68 (90%)	8 (10%)	7	24
16	P	65/65 (100%)	57 (88%)	8 (12%)	4	19
17	Q	74/74 (100%)	52 (70%)	22 (30%)	0	2
18	R	48/48 (100%)	44 (92%)	4 (8%)	11	34
19	S	70/70 (100%)	58 (83%)	12 (17%)	2	11
20	T	65/65 (100%)	56 (86%)	9 (14%)	3	17
21	U	44/44 (100%)	40 (91%)	4 (9%)	9	29
22	W	238/302 (79%)	215 (90%)	23 (10%)	8	27
All	All	2185/2253 (97%)	1870 (86%)	315 (14%)	6	16

5 of 315 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
15	O	79	GLN
20	T	69	ASN
16	P	59	HIS
17	Q	70	LYS
22	W	116	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 53 such sidechains are listed below:

Mol	Chain	Res	Type
11	K	28	ASN
15	O	49	HIS
22	W	215	GLN
11	K	117	HIS
14	N	70	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1532/1533 (99%)	479 (31%)	200 (13%)

5 of 479 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	3	A
1	A	4	U
1	A	5	U
1	A	6	G
1	A	7	A

5 of 200 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	817	C
1	A	1087	G
1	A	1533	C
1	A	845	A
1	A	974	A

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	70:U	O3'	71:A	P	1.39

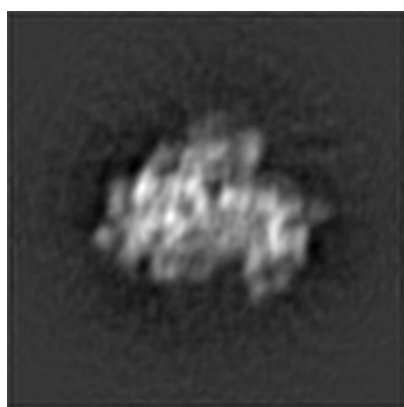
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-1884. These allow visual inspection of the internal detail of the map and identification of artifacts.

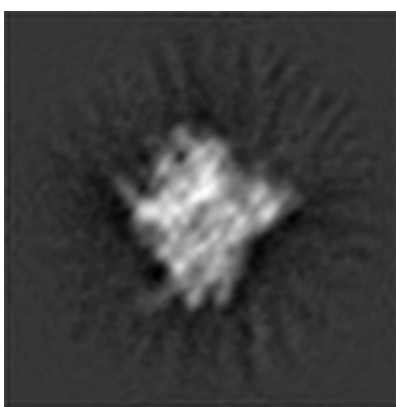
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

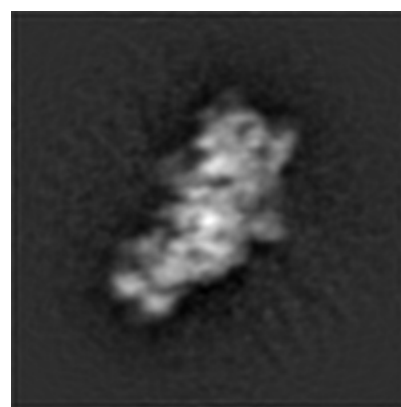
6.1.1 Primary map



X



Y

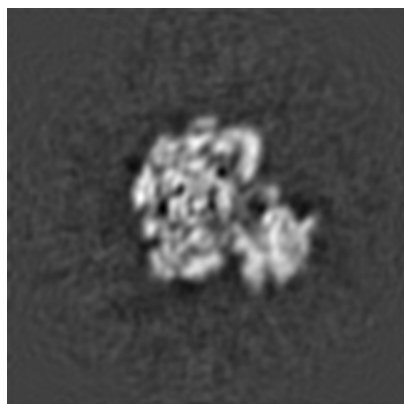


Z

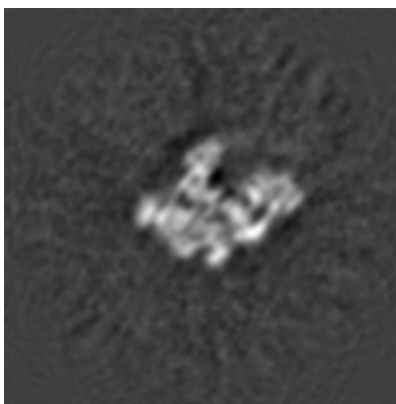
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

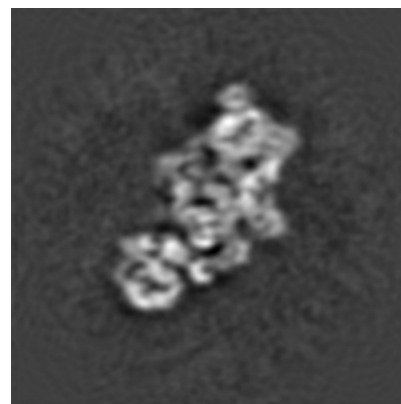
6.2.1 Primary map



X Index: 62



Y Index: 62

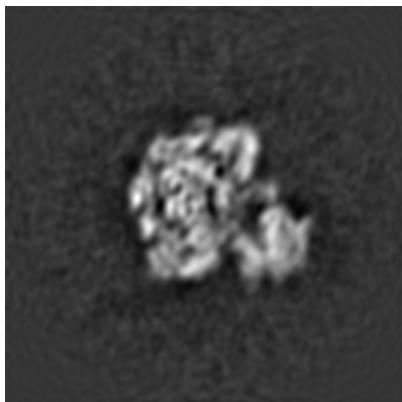


Z Index: 62

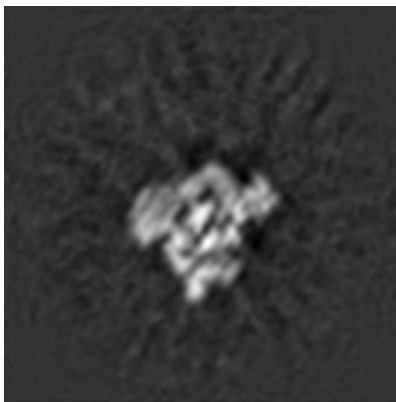
The images above show central slices of the map in three orthogonal directions.

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

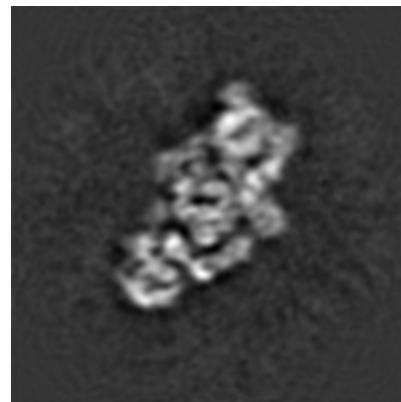
6.3.1 Primary map



X Index: 61



Y Index: 51

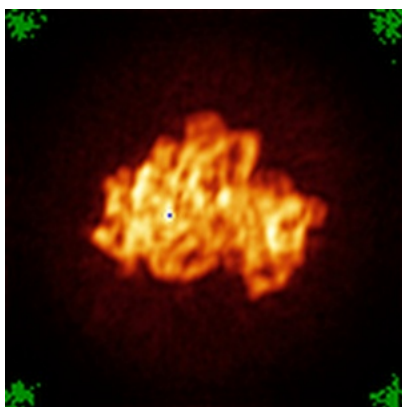


Z Index: 63

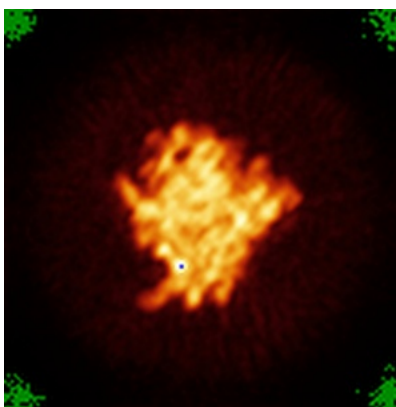
The images above show the largest variance slices of the map in three orthogonal directions.

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

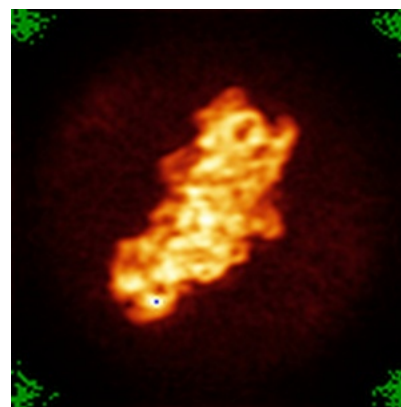
6.4.1 Primary map



X



Y

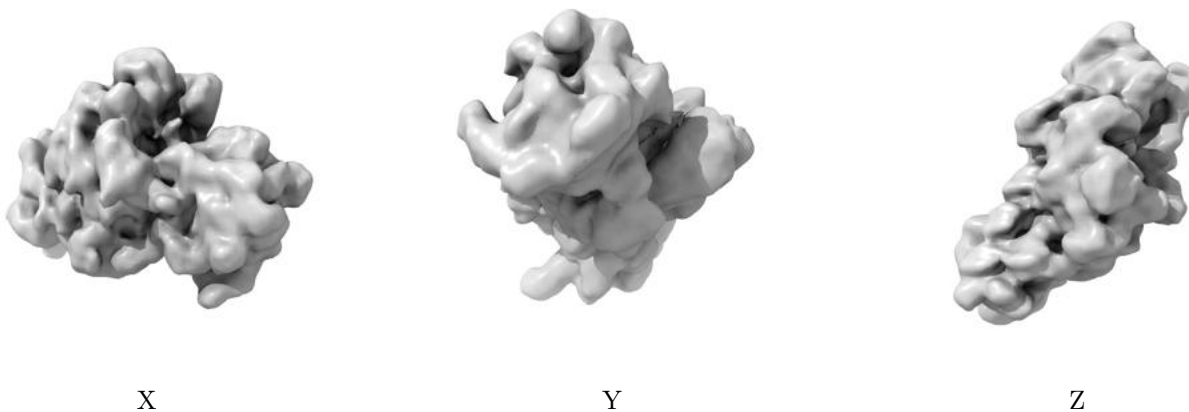


Z

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 3.16. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

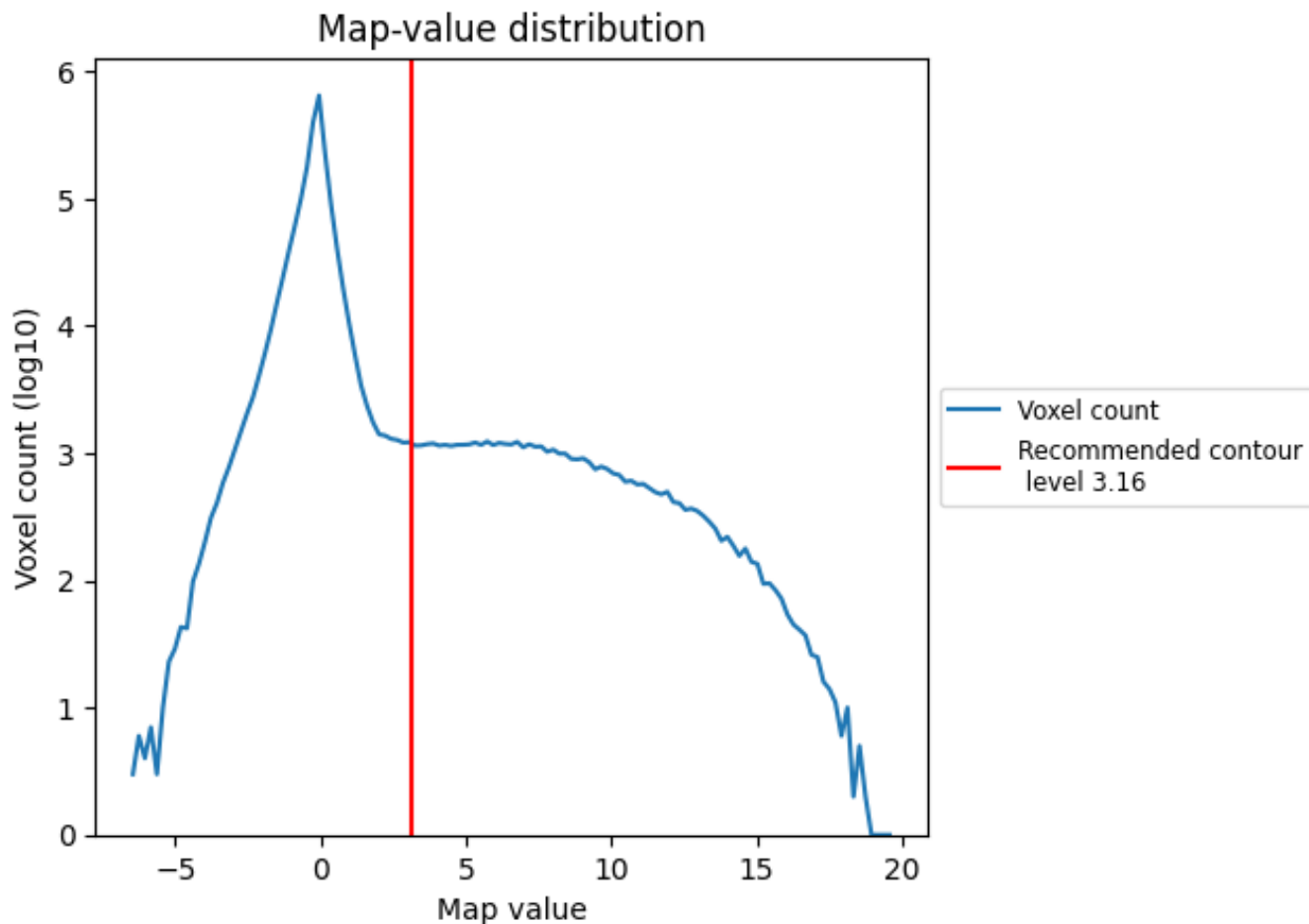
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

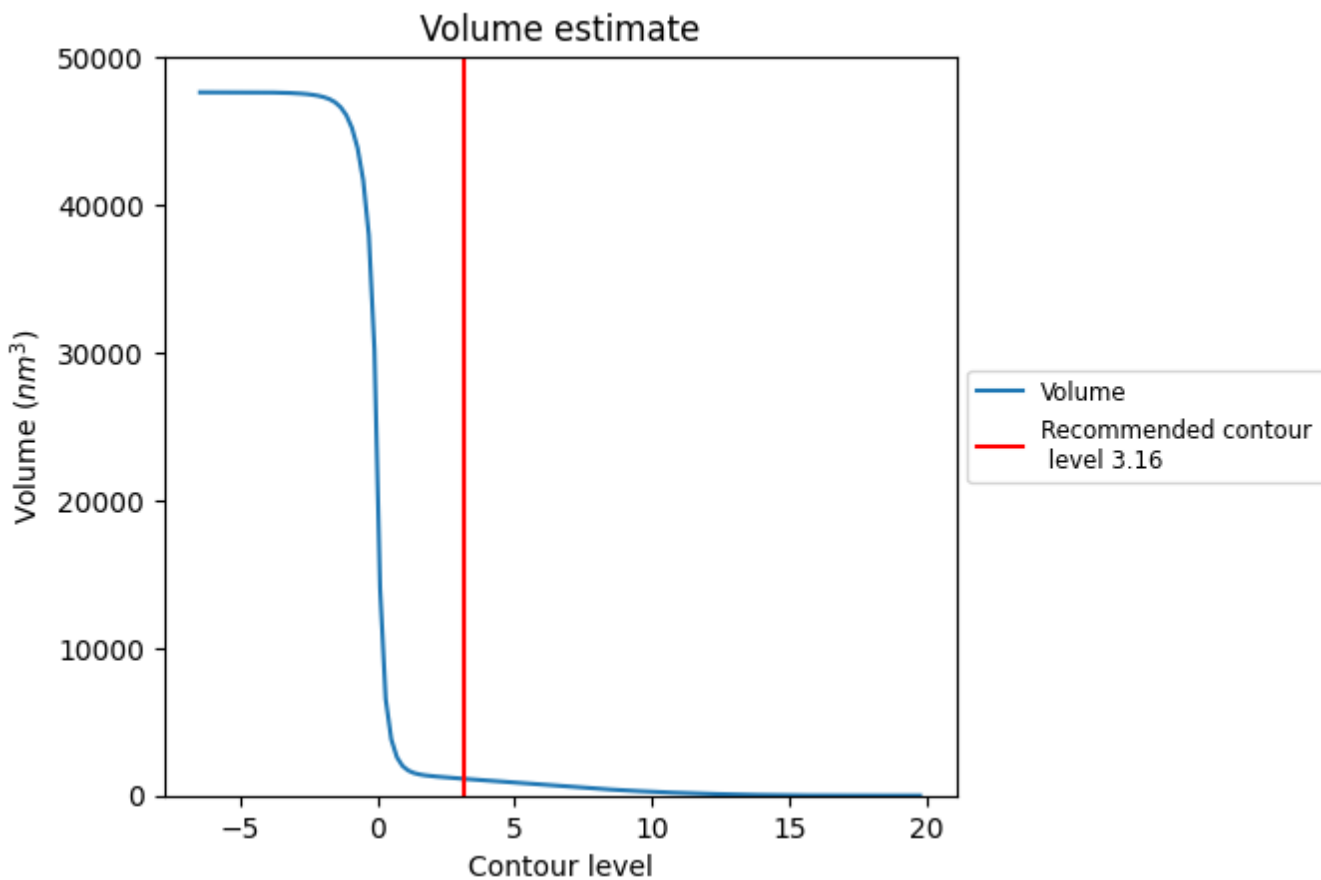
This section contains the results of statistical analysis of the map.

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.

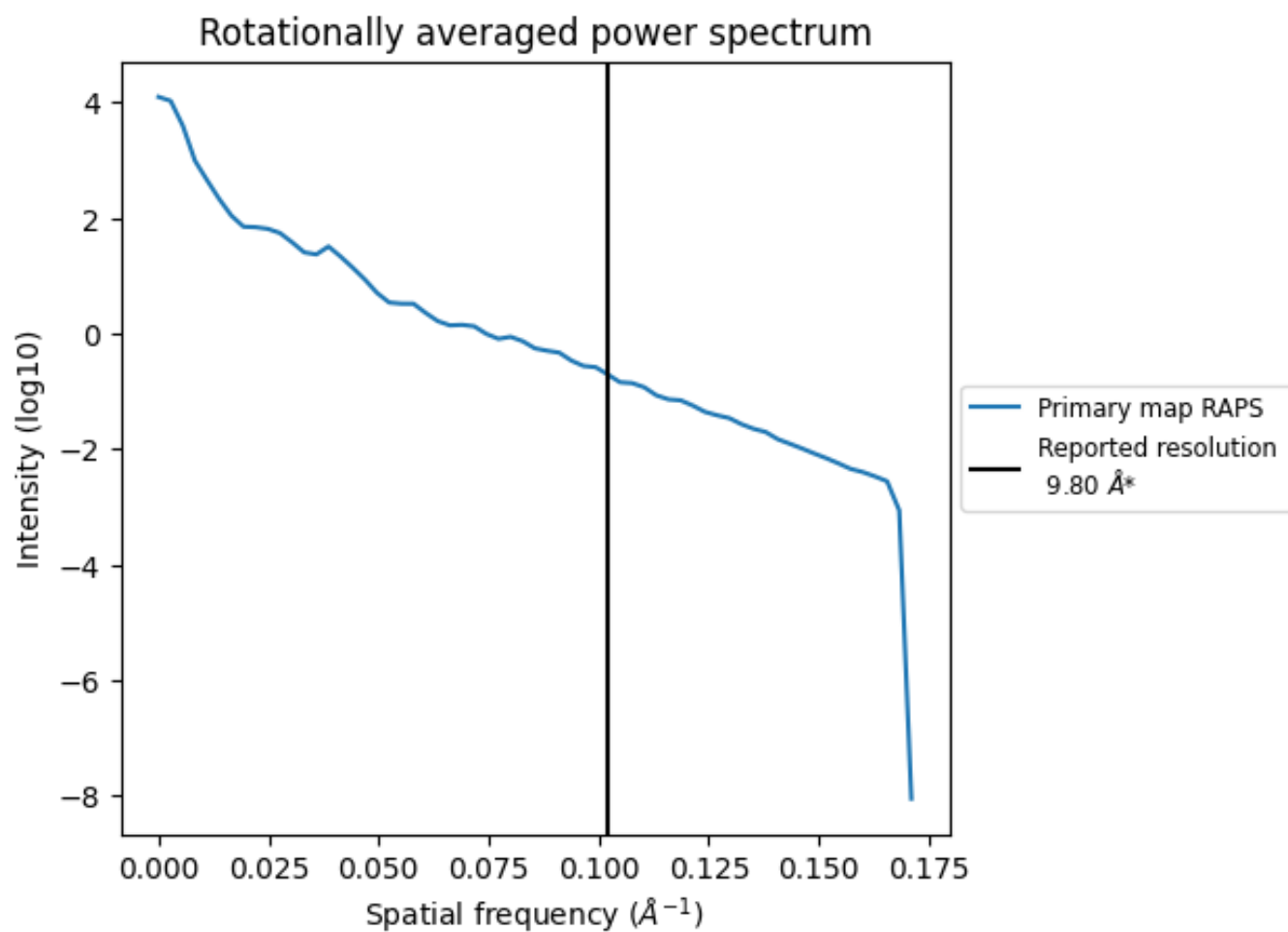
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1134 nm³; this corresponds to an approximate mass of 1025 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 0.102 Å⁻¹

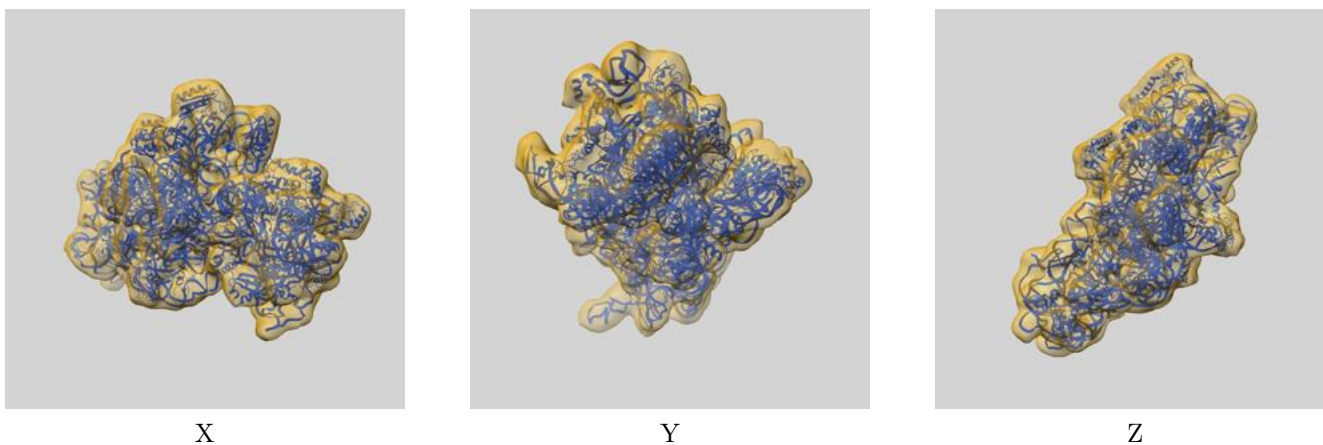
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

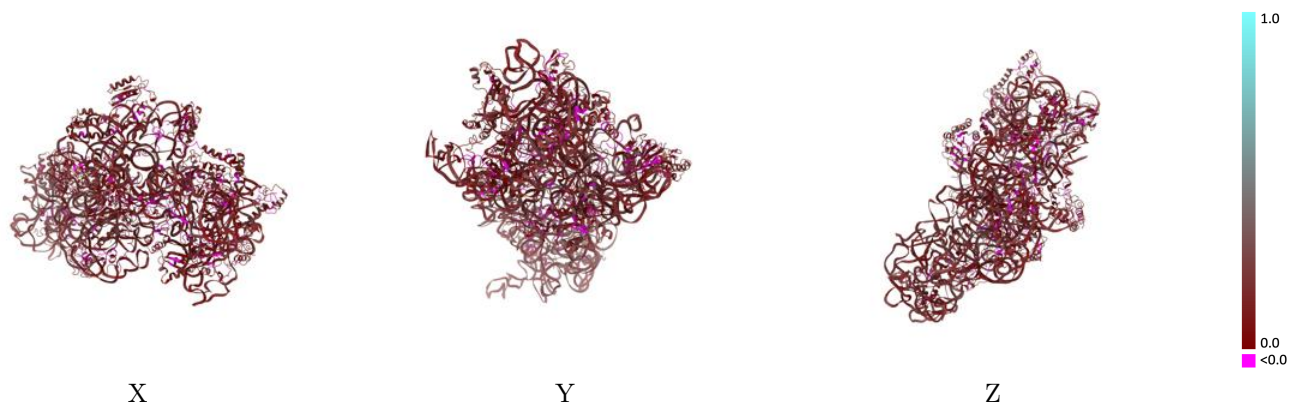
This section contains information regarding the fit between EMDB map EMD-1884 and PDB model 2YKR. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



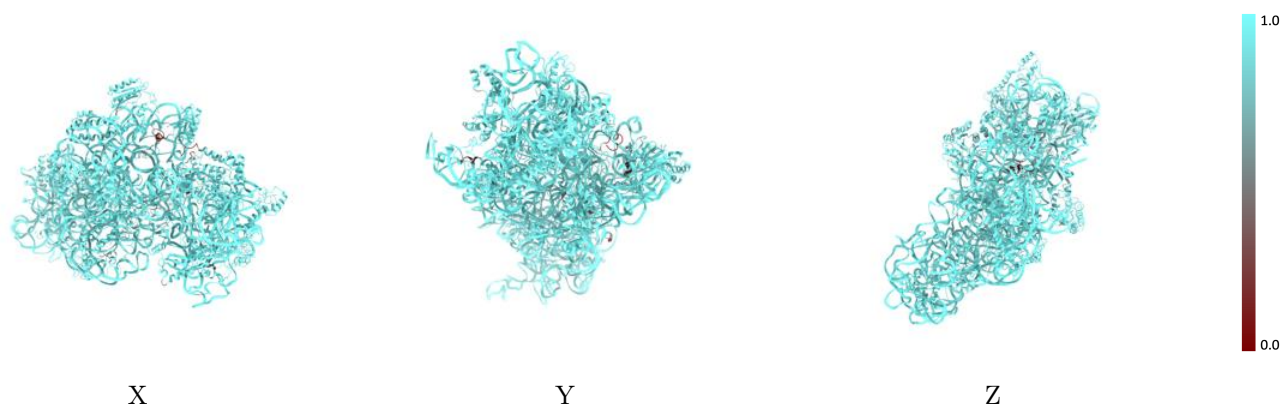
The images above show the 3D surface view of the map at the recommended contour level 3.16 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



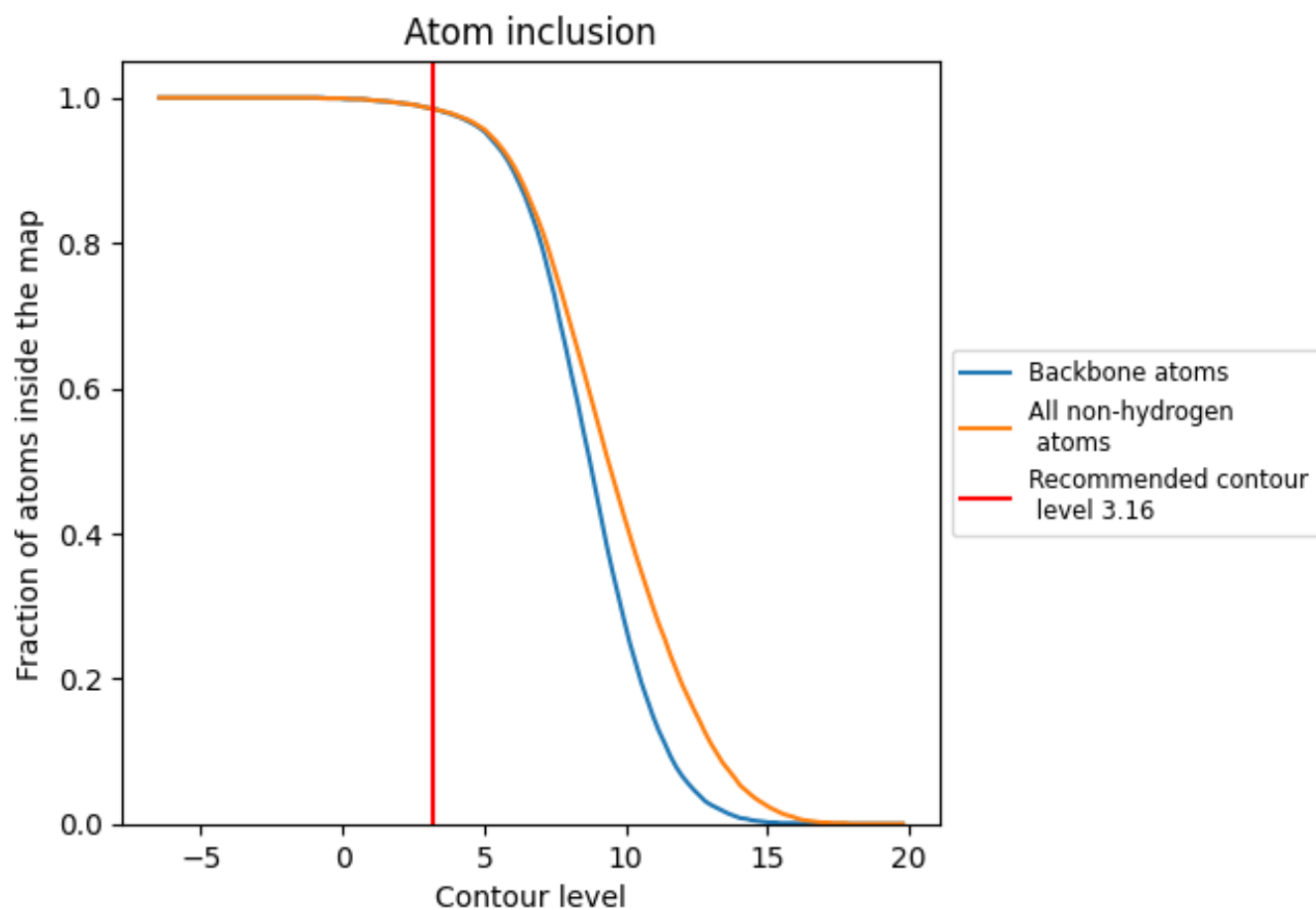
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3.16).















































9.4 Atom inclusion [i](#)



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

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (3.16) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9850	 0.1530
A	 0.9990	 0.1730
B	 0.9700	 0.1270
C	 0.9850	 0.1370
D	 0.9760	 0.1140
E	 0.9800	 0.1420
F	 0.9650	 0.1330
G	 0.8990	 0.1010
H	 0.9830	 0.1310
I	 0.9910	 0.1110
J	 0.9650	 0.0940
K	 0.9800	 0.1120
L	 0.9870	 0.1060
M	 0.9950	 0.1390
N	 0.9560	 0.0920
O	 0.9940	 0.1460
P	 0.9950	 0.1050
Q	 0.9730	 0.1290
R	 1.0000	 0.1060
S	 0.9970	 0.1010
T	 0.9990	 0.1300
U	 0.5600	 0.0310
W	 0.9350	 0.1390

