



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:45 PM BST

PDB ID : 3J28
EMDB ID: : EMD-5500
Title : Dissecting the in vivo assembly of the 30S ribosomal subunit reveals the role of RimM
Authors : Guo, Q.; Goto, S.; Chen, Y.; Muto, A.; Himeno, H.; Deng, H.; Lei, J.; Gao, N.
Deposited on : 2012-09-28
Resolution : 12.90 Å(reported)
Based on PDB ID : 3OFA

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

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

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

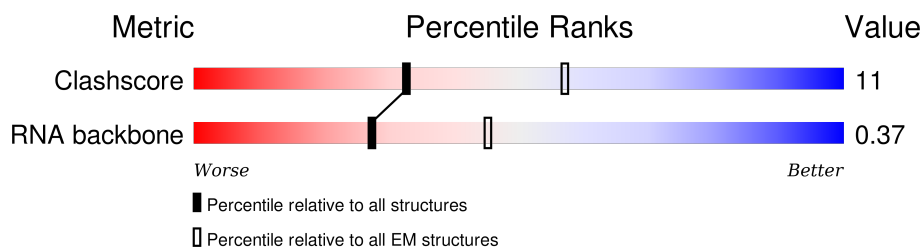
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY


The reported resolution of this entry is 12.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
RNA backbone	3027	244

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	N	1533	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 49446 atoms, of which 16554 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.

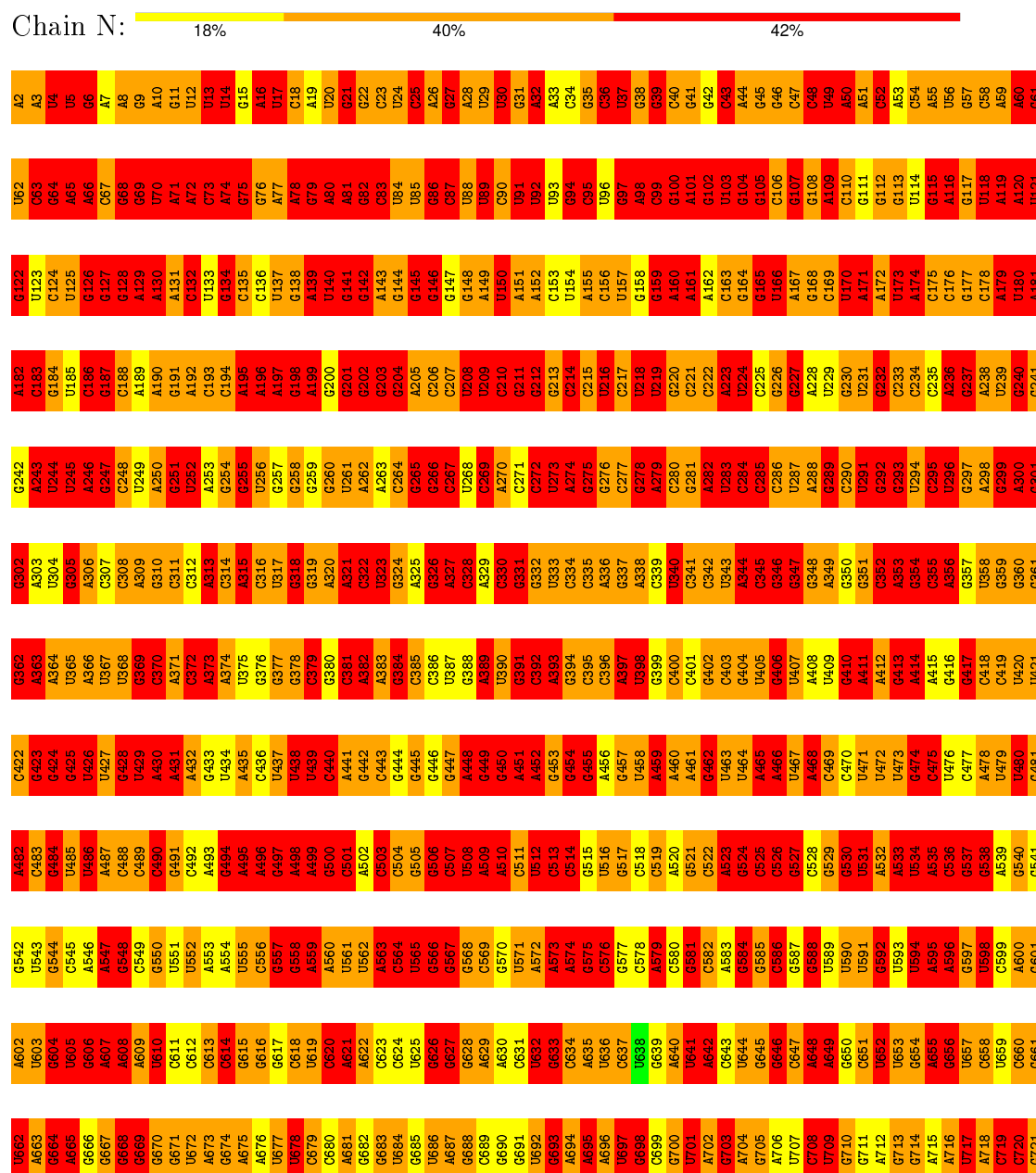
- Molecule 1 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	N	1533	Total	C	H	N	O	P	0	0
			49446	14671	16554	6036	10653	1532		

3 Residue-property plots

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



A1502	C1442	C1382	C1322	C1262	C1202	G1142	A1082	A1022	C962	G902	U842	A782	G722
A1503	C1443	C1383	G1323	C1263	C1203	G1143	U1083	U1023	G963	G903	U843	C783	G723
A1504	C1444	C1384	A1324	U1264	A1204	G1144	G1084	G1024	A964	U904	A844	A784	G724
G1505	U1445	G1385	C1325	C1265	A1205	A1145	U1085	U1025	U965	U905	A845	G785	G725
A1506	A1446	G1386	U1326	G1266	G1206	A1146	U1086	G1026	G966	A906	G846	G786	G726
A1507	A1447	G1387	C1327	C1267	G1207	C1147	G1087	G1027	G967	A907	G847	A787	G727
A1508	C1448	C1388	C1328	G1268	C1208	U1148	G1088	U1028	A968	A908	C848	U788	A728
C1509	C1449	C1389	A1329	A1269	C1209	C1149	G1089	U1029	A969	A909	G849	U789	A729
U1510	U1450	U1390	U1330	G1270	C1210	A1150	U1090	U1030	C970	C910	U850	A790	G730
U1511	U1451	U1391	G1331	A1271	U1211	A1151	U1091	C1031	G971	U911	G851	G791	G731
U1512	C1452	G1392	A1332	G1272	U1212	A1152	A1092	C1032	G972	C912	G852	A792	G732
A1513	G1453	U1393	A1333	C1273	A1213	G1153	A1093	G1033	G973	A913	C853	U793	G733
G1514	A1454	A1394	G1334	A1274	C1214	G1154	G1094	G1034	A974	A914	U854	G794	G734
G1515	G1455	U1395	U1335	A1275	G1215	A1155	U1095	A1035	A975	A915	U855	C795	G735
A1516	A1456	A1396	C1336	G1276	A1216	G1156	C1096	A1036	G976	U916	C856	C796	G736
G1517	C1457	G1397	G1337	C1277	C1217	A1157	G977	C1037	A977	G917	C857	C797	G737
A1518	G1458	A1398	G1338	G1278	A1218	C1158	C1098	C1038	A978	A918	C858	U798	G738
A1519	G1459	A1399	A1339	G1279	A1219	U1159	G1099	G1039	G979	A919	C859	G799	G739
C1520	C1460	G1400	A1340	A1280	G1220	C1160	C1100	U1040	C980	U920	A860	G800	U740
C1521	G1461	U1401	U1341	C1281	G1221	C1161	A1101	G1041	U981	U921	G861	U801	G741
U1522	C1462	C1402	G1342	C1282	G1222	C1162	A1102	U982	U982	G922	C862	A802	G742
G1523	U1463	C1403	G1343	C1283	C1223	C1163	C1103	G1043	A983	A923	U863	G803	G743
C1524	U1464	C1404	C1344	C1284	U1224	G1164	G1104	A1044	C984	A924	A864	U804	G744
G1525	A1465	G1405	U1345	A1285	A1225	U1165	A1105	C1045	C985	G925	A865	C805	G745
U1526	C1466	U1406	A1346	U1286	C1226	G1166	G1106	A1046	U986	G926	C866	C806	G746
U1527	C1467	C1407	G1347	A1287	A1227	A1167	C1107	G1047	G987	G927	G867	A807	A747
U1528	A1468	A1408	U1348	A1288	C1228	U1168	C1108	U1048	G988	G928	C868	C808	G748
G1529	C1469	C1409	A1349	A1289	A1229	U1169	C1109	U1049	U989	G929	C869	G809	A749
G1530	U1470	A1410	A1350	G1290	C1230	A1170	A1110	G1050	C990	C930	U870	C810	G750
A1531	U1471	C1411	U1351	U1291	G1231	A1171	A1111	C1051	U991	C931	U871	C811	G751
U1532	U1472	C1412	C1352	G1292	U1232	C1172	C1112	U1052	U992	C932	A872	G812	G752
C1533	G1473	A1413	G1353	C1293	G1233	U1173	C1113	G1053	C993	C933	A873	U813	A753
A1534	U1474	U1414	U1354	G1294	C1234	C1174	C1114	C1054	A994	A934	G874	A814	C754
	G1475	G1415	G1355	U1295	U1235	G1175	U1115	A1055	C995	A935	U875	A815	G755
	A1476	G1416	G1356	C1296	A1236	A1176	U1116	U1056	A996	C936	C876	A816	C756
	U1477	G1417	A1357	G1297	C1237	G1177	A1117	G1057	U997	A937	G877	C817	U757
	U1478	A1418	U1358	U1298	A1238	C1178	U1118	G1058	C998	A938	A878	G818	C758
	C1479	G1419	C1359	A1299	C1239	A1179	C1119	C1059	C999	G939	C879	A819	A759
	A1480	U1420	A1360	U1300	U1240	A1180	C1120	U1060	A1000	C940	C880	U820	G760
	U1481	G1421	G1361	U1301	G1241	C1181	U1121	G1061	C1001	G941	C881	G821	G761
	G1482	G1422	A1362	C1302	G1242	G1182	U1122	U1062	G1002	G942	C882	U822	U762
	A1483	G1423	A1363	C1303	C1243	U1183	U1123	C1063	G1003	U943	C883	C823	G763
	C1484	U1424	U1364	G1304	G1244	G1184	G1124	G1064	A1004	G944	U884	G824	C764
	U1485	U1425	G1365	G1305	C1245	G1185	U1125	U1065	A1005	G945	C885	A825	G765
	G1486	G1426	C1366	A1306	A1246	G1186	U1126	C1066	G1006	A946	G886	C826	A766
	G1487	C1427	C1367	U1307	U1247	G1187	G1127	A1067	U1007	G947	G887	U827	A767
	G1488	A1428	A1368	U1308	A1248	U1188	C1128	G1068	U1008	C948	G888	U828	A768
	G1489	A1429	C1369	G1309	C1249	U1189	C1129	C1069	U1009	A949	A889	G829	G769
	U1490	A1430	G1370	G1310	A1250	G1190	A1130	U1070	U1010	U950	G890	G830	C770
	G1491	A1431	G1371	A1311	A1251	A1191	G1131	C1071	C1011	G951	U891	A831	G771
	A1492	G1432	U1372	G1312	A1252	C1192	C1132	G1072	A1012	U952	A892	G832	U772
	A1493	G1433	G1373	U1313	G1253	G1193	C1133	U1073	G1013	G953	C893	G833	G773
	G1494	A1434	A1374	C1314	A1254	U1194	G1134	G1074	A1014	G954	A894	U834	G774
	U1495	G1435	A1375	G1315	G1255	C1195	U1135	U1075	G1015	U955	C895	U835	G775
	C1496	U1436	U1376	G1316	A1256	A1196	C1136	U1076	A1016	U956	C896	G836	G776
	G1497	A1437	G1377	C1317	A1257	A1197	G1137	G1077	U1017	U957	C897	U837	A777
	U1498	G1438	C1378	A1318	G1258	G1198	G1138	U1078	G1018	A958	G898	G838	G778
	A1499	G1439	G1379	A1319	C1259	U1199	G1139	G1079	A1019	A959	C899	C839	A779
	U1500	U1440	U1380	C1320	G1260	C1140	U1020	A1080	G1020	U960	A900	C840	A780
	C1501	A1441	U1381	U1321	A1261	A1201	C1141	A1081	A1021	U961	A901	C841	A781

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	32152	Depositor
Resolution determination method	FSC at 0.5 cut-off	Depositor
CTF correction method	Weiner filter	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	80000	Depositor
Image detector	GATAN 4000	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 2$	RMSZ	$\# Z > 2$
1	N	3.47	5260/36831 (14.3%)	3.94	9443/57458 (16.4%)

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	N	0	948

The worst 5 of 5260 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	16	A	N7-C5	-19.48	1.27	1.39
1	N	563	A	N7-C5	-18.95	1.27	1.39
1	N	1396	A	N3-C4	-18.85	1.23	1.34
1	N	28	A	N7-C5	-18.07	1.28	1.39
1	N	1243	C	N1-C6	17.88	1.47	1.37

The worst 5 of 9443 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	1362	A	P-O3'-C3'	29.77	155.43	119.70
1	N	1004	A	N1-C6-N6	26.64	134.59	118.60
1	N	766	A	N1-C6-N6	26.51	134.50	118.60
1	N	191	G	C5-C6-O6	-25.76	113.14	128.60
1	N	94	G	P-O3'-C3'	24.94	149.63	119.70

There are no chirality outliers.

5 of 948 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	N	10	A	Sidechain
1	N	2	A	Sidechain
1	N	4	U	Sidechain
1	N	5	U	Sidechain
1	N	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	N	32892	16554	16511	547	0
All	All	32892	16554	16511	547	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

The worst 5 of 547 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:N:664:G:H22	1:N:741:G:H1	1.31	0.76
1:N:596:A:H61	1:N:644:U:H3	1.37	0.73
1:N:116:A:H61	1:N:313:A:H1'	1.56	0.70
1:N:67:C:H2'	1:N:68:G:C8	2.26	0.70
1:N:381:C:C5	1:N:382:A:C5	2.81	0.69

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein molecules in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein molecules in this entry.

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	N	1532/1533 (99%)	451 (29%)	150 (9%)

5 of 451 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	N	3	A
1	N	4	U
1	N	5	U
1	N	6	G
1	N	8	A

5 of 150 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	N	535	A
1	N	774	G
1	N	1364	U
1	N	559	A
1	N	695	A

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.