



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:46 PM BST

PDB ID : 3J2C
EMDB ID: : EMD-5504
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 : 13.20 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

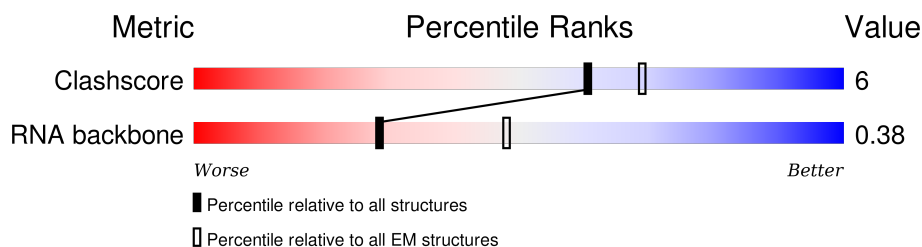
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

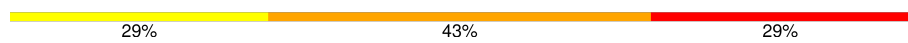


The reported resolution of this entry is 13.20 Å.

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	M	462	 29% 43% 29%
2	N	927	 23% 44% 32%
3	O	144	 31% 48% 21%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 49444 atoms, of which 16558 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 head domain.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	M	462	Total	C	H	N	O	P	0	0
			14865	4410	4987	1793	3214	461		

- Molecule 2 is a RNA chain called 16S rRNA body domain.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	N	927	Total	C	H	N	O	P	0	0
			29941	8884	10017	3681	6433	926		

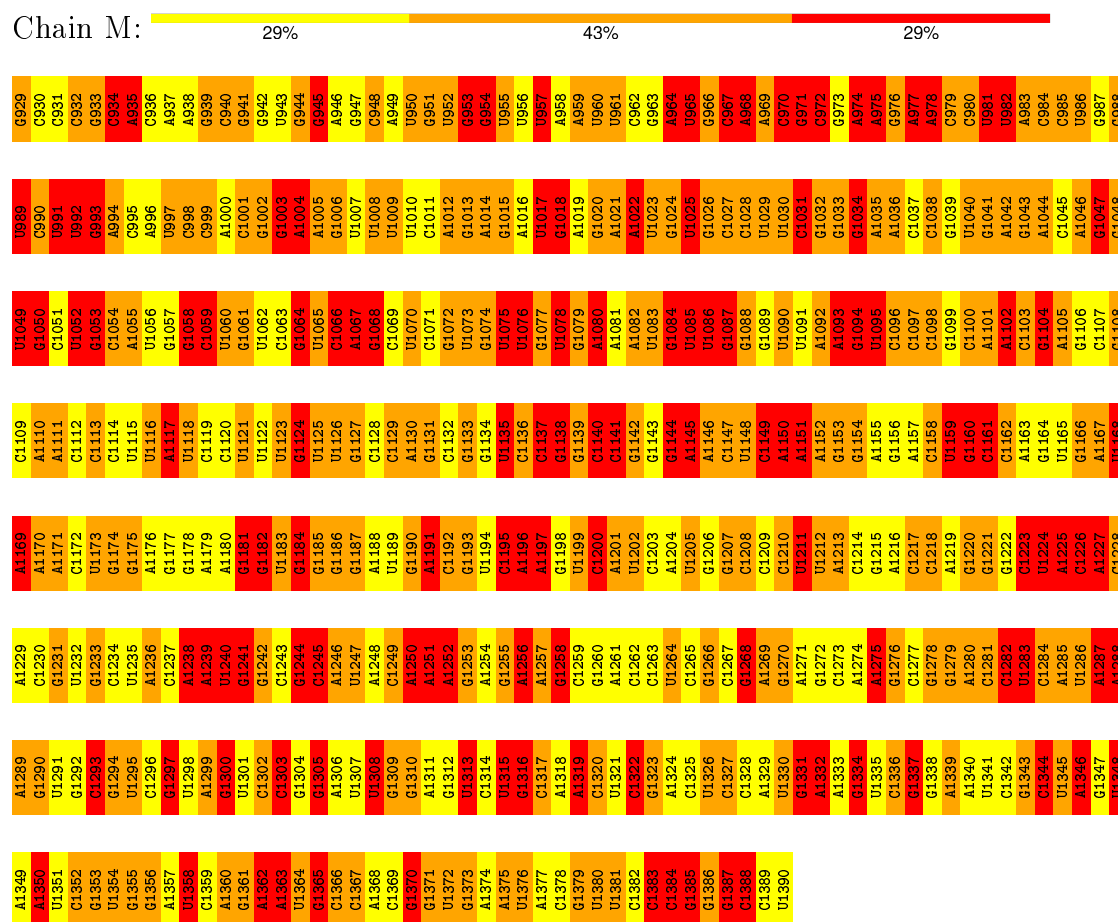
- Molecule 3 is a RNA chain called 16S rRNA body domain.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	O	144	Total	C	H	N	O	P	0	0
			4638	1377	1554	562	1002	143		

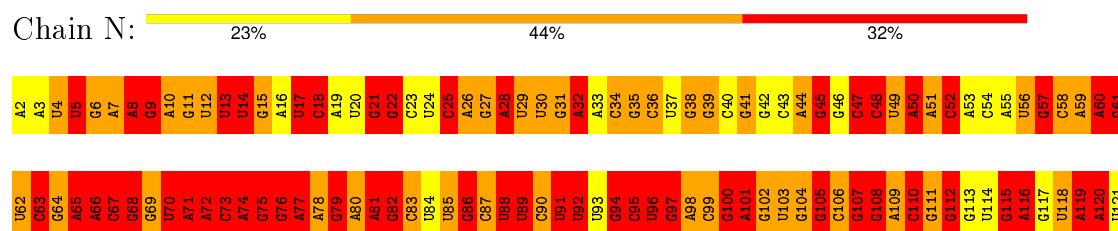
3 Residue-property plots

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 head domain



- Molecule 2: 16S rRNA body domain



G122	G123	G182	G183	G242	G302	G362	G422	G482	G542	G602	G662	G722	G782	G842	G902
U123	U124	C183	C184	A243	A303	A363	G423	C483	U543	U603	U663	U723	U783	U843	G903
U125	U185	U185	U185	U244	G304	G364	G424	G484	G544	G604	G664	G724	G784	G844	U904
G126	G126	C186	C186	A246	A306	A366	G426	U486	G546	G606	G666	G726	G786	G846	U906
G127	G127	G187	G187	G247	G307	G367	U427	A487	A547	A607	G667	G727	G787	G847	A907
G128	G128	C188	C188	C248	G308	G368	G428	C488	G548	A608	G668	A728	U788	C848	A908
A129	A129	A189	A189	U249	A309	G369	U429	C489	C549	A609	G669	A729	U789	G849	A909
A130	A130	A190	A190	A250	G310	C370	A430	C490	G550	U610	G670	A730	U790	U850	C910
A131	A131	G191	G191	G251	C311	A371	A431	G491	U611	C611	G671	G731	G791	G851	U911
C132	C132	A192	A192	U252	C312	C372	A432	C492	U612	C612	G672	G732	G792	G852	C912
C133	C133	A193	A193	A253	A313	A373	G433	A493	A553	C613	G673	G733	G793	C853	A913
C134	C134	C194	C194	G254	C314	A374	U434	G494	A554	C614	G674	G734	G794	U854	A914
C136	C136	A196	A196	G255	A316	U375	A435	A495	U555	G615	G675	C735	C795	U855	A915
C136	C136	A196	A196	U256	C316	G376	A436	A496	G556	G616	A676	C736	C796	C856	U916
U137	U137	G197	G197	G257	U317	G377	U437	G497	G557	G617	U677	C737	C797	C857	U917
G138	G138	G198	G198	G258	G318	G378	U438	A498	G558	U618	U678	C738	C798	G858	A918
A139	A139	A199	A199	G259	G319	C379	U439	A499	G559	U619	U679	C739	C799	G859	A919
U140	U140	G200	G200	G260	A320	G380	C440	G500	A560	C620	G680	U740	U800	A860	U920
U141	U141	G201	G201	U261	A321	C381	A441	C501	U561	A621	A681	G741	U801	G861	U921
G142	G142	G202	G202	A262	C322	A382	G442	A502	U562	A622	G682	G742	U802	G862	U922
G143	G143	G203	G203	A263	U323	A383	C443	C503	A563	C623	U683	A743	G803	U863	A923
G144	G144	G204	G204	C264	G324	G384	G444	C504	C564	C624	U684	C744	U804	A864	C924
G145	G145	A205	A205	G265	A325	C385	G445	G505	U565	U625	U685	G745	C805	A865	G925
G146	G146	G206	G206	G266	G326	C386	G446	G506	G566	G626	U686	A746	C806	C866	G926
G147	G147	C207	C207	G267	A327	U387	G447	C507	G567	G627	A687	A747	A807	G867	G927
G148	G148	U208	U208	U268	C328	G388	A448	U508	G568	G628	G688	G748	C808	G868	U928
A149	A149	U209	U209	C269	A329	A389	G449	A509	C569	A629	G689	A749	G809	G869	U929
U150	U150	C210	C210	A270	G330	U390	G450	A510	U570	A630	G690	C750	C810	U870	U930
A151	A151	G211	G211	C271	G331	U391	A461	C511	U571	C631	G691	U751	C811	U871	A931
C152	C152	G212	G212	C272	G332	C392	A462	U512	A572	U632	U692	G752	C812	A872	G932
C153	C153	G213	G213	U273	U333	A393	G463	C513	A573	G633	G693	A753	U813	A873	G933
U154	U154	C214	C214	A274	C334	G394	G464	C514	A574	C634	A694	C754	A814	G874	G934
C156	C156	C215	C215	G275	C335	C395	G465	G515	G575	A635	A695	G755	A815	U875	U935
C157	C157	C217	C217	C277	G337	G397	A467	U517	G577	U637	G697	U757	C817	G877	U937
G158	G158	U218	U218	G278	A338	U398	U468	C518	G578	U638	G698	C758	G818	A878	U938
G159	G159	U219	U219	A279	C339	G399	A469	C519	A579	G639	C699	A759	A819	C879	U939
A160	A160	G220	G220	C280	U340	C400	A460	A520	G580	A640	G700	G760	U820	C880	U940
A161	A161	C221	C221	G281	C341	C401	A461	G521	G581	U641	G701	G761	U821	G881	U941
A162	A162	C222	C222	A282	C342	A402	G462	C522	C582	A642	A702	G762	U822	C882	U942
C163	C163	A223	A223	U283	U343	C403	U463	A523	A583	C643	G703	G763	C823	C883	U943
G164	G164	U224	U224	C284	A344	G404	U464	G524	G584	U644	A704	C764	G824	U884	U944
G165	G165	C225	C225	G285	G345	U405	A465	C525	G585	G645	A705	C765	A825	G885	U945
U166	U166	G226	G226	C286	G346	G406	A466	C526	G586	G646	A706	C766	A826	G886	U946
A167	A167	G227	G227	U287	G347	U407	U467	C527	G587	C647	U707	A767	U827	G887	U947
G168	G168	A228	A228	G288	G348	A408	A468	C528	G588	A648	C708	A768	U828	G888	U948
C169	C169	U229	U229	C289	A349	U409	C469	G529	U589	A649	U709	G769	C829	A889	U949
U170	U170	G230	G230	C290	G350	G410	C470	G530	U590	G650	G710	G770	A831	G890	U950
A171	A171	U231	U231	U291	G351	A411	U471	U531	U591	C651	G711	G771	A831	U891	U951
A172	A172	G232	G232	G292	C352	A412	U472	A532	G592	U652	A712	U772	C832	A892	U952
U173	U173	C233	C233	G293	A353	G413	U473	A533	U593	U653	G713	G773	C833	C893	U953
A174	A174	C234	C234	U294	G354	A414	G474	U534	U594	G654	G714	G774	U834	G894	U954
C175	C175	C235	C235	G295	C355	A415	C475	A535	A595	A655	A715	G775	U835	G895	U955
C176	C176	A236	A236	U296	A356	G416	U476	C536	A596	G656	A716	G776	G836	C896	U956
G177	G177	G237	G237	G297	G357	G417	C477	G537	G597	U657	U717	A777	U837	C897	U957
C178	C178	A238	A238	A298	U358	G418	A478	G538	U598	C658	A718	G778	G838	G898	U958
U179	U179	G239	G239	G299	G359	C419	U479	A539	C599	U659	C719	G779	C839	C899	U959
A180	A180	G240	G240	A300	A360	U420	U480	G540	C600	G660	C720	A780	C840	A900	U960
A181	A181	G241	G241	G301	G361	U421	G481	G541	G601	G661	G721	A781	C841	U901	U961

● Molecule 3: 16S rRNA body domain

Chain O:  31% 48% 21%

U1451	U1391
C1452	G1392
G1453	U1393
G1454	A1394
G1455	C1395
A1456	A906
G1457	A907
G1458	A908
G1459	A909
C1460	C910
G1461	G911
C1462	C912
U1463	A913
U1464	A914
A1465	A915
C1466	C916
C1467	G917
A1468	A918
C1469	A919
U1470	U920
U1471	U921
U1472	G922
G1473	A923
U1474	C924
G1475	G925
A1476	C926
U1477	G927
U1478	G928
C1479	U929
A1480	U930
G1481	G931
G1482	C932
A1483	A933
C1484	C934
U1485	U935
G1486	G936
G1487	C937
G1488	A938
U1489	U939
G1490	C940
G1491	G941
A1492	C942
A1493	A943
C1494	C944
U1495	U945
C1496	G946
U1497	A947
U1498	C948
A1499	G949
U1500	U950
C1501	A951
A1502	C952
A1503	G953
G1504	U954
U1505	C955
U1506	A956
A1507	G957
A1508	U958
C1509	C959
C1510	U960
U1510	A961

G1511	U1512	A1513	G1514	G1515	G1516	G1517	A1518	A1519	C1520	C1521	U1522	G1523	C1524	G1525	G1526	U1527	U1528	G1529	G1530	A1531	U1532	C1533	A1534
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4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	44392	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	4K*4K CCD 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	M	3.43	1534/11053 (13.9%)	3.80	2624/17234 (15.2%)
2	N	3.44	3141/22318 (14.1%)	3.88	5510/34825 (15.8%)
3	O	3.32	455/3452 (13.2%)	3.95	849/5383 (15.8%)
All	All	3.43	5130/36823 (13.9%)	3.86	8983/57442 (15.6%)

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	M	0	236
2	N	0	522
3	O	0	78
All	All	0	836

The worst 5 of 5130 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	1502	A	N7-C5	-20.70	1.26	1.39
1	M	1251	A	N9-C4	18.33	1.48	1.37
2	N	124	C	N1-C6	-18.06	1.26	1.37
2	N	533	A	N7-C5	-17.64	1.28	1.39
2	N	350	G	C6-N1	17.60	1.51	1.39

The worst 5 of 8983 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	1253	G	N1-C6-O6	26.96	136.07	119.90
3	O	1455	G	N1-C6-O6	26.35	135.71	119.90
3	O	1458	G	N1-C6-O6	25.20	135.02	119.90
1	M	1362	A	P-O3'-C3'	24.79	149.44	119.70
3	O	1405	G	C5-C6-O6	-24.61	113.83	128.60

There are no chirality outliers.

5 of 836 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	M	929	G	Sidechain
1	M	933	G	Sidechain
1	M	934	C	Sidechain
1	M	935	A	Sidechain
1	M	939	G	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	M	9878	4987	4986	67	0
2	N	19924	10017	10006	206	0
3	O	3084	1554	1553	14	0
All	All	32886	16558	16545	281	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 6.

The worst 5 of 281 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:M:998:C:H42	1:M:1042:A:H61	1.38	0.71
2:N:50:A:H1'	2:N:52:C:C6	2.25	0.71
2:N:664:G:H22	2:N:741:G:H1	1.38	0.70
2:N:858:G:H1	2:N:869:G:H2'	1.55	0.70
2:N:411:A:H61	2:N:428:G:H1'	1.57	0.70

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 [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	M	461/462 (99%)	152 (32%)	41 (8%)
2	N	926/927 (99%)	255 (27%)	84 (9%)
3	O	143/144 (99%)	31 (21%)	9 (6%)
All	All	1530/1533 (99%)	438 (28%)	134 (8%)

5 of 438 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	M	932	C
1	M	934	C
1	M	935	A
1	M	944	G
1	M	953	G

5 of 134 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	N	119	A
2	N	250	A
2	N	884	U
2	N	129	A
2	N	181	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.