

wwPDB EM Validation Summary Report (i)

Apr 16, 2024 - 01:04 am BST

PDB ID	:	5NO3
EMDB ID	:	EMD-3662
Title	:	RsgA-GDPNP bound to the 30S ribosomal subunit (RsgA assembly interme-
		diate without uS3)
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		mole, N.; Schedlbauer, A.; Hase, Y.; Goto, S.; Kurita, D.; Muto, A.; Zhou, S.;
		Naoe, C.; Mills, D.J.; Gil-Carton, D.; Takemoto, C.; Himeno, H.; Fucini, P.;
		Connell, S.R.
Deposited on	:	2017-04-10
Resolution	:	5.16 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org* A user guide is available at https://www.wwpdb.org/validation/2017/EMValidationReportHelp with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

EMDB validation analysis	:	0.0.1. dev 92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 5.16 Å.

There are no overall percentile quality scores available for this entry.

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.



2 Entry composition (i)

There are 23 unique types of molecules in this entry. The entry contains 50979 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 ribosomal RNA.

Mol	Chain	Residues		1	AltConf	Trace			
1	А	1534	Total 32930	C 14694	N 6041	O 10661	Р 1534	0	0

• Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues		At		AltConf	Trace		
2	В	224	Total 1753	C 1109	N 315	0 321	S 8	0	0

• Molecule 3 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues		At		AltConf	Trace		
3	D	205	Total 1643	C 1026	N 315	0 298	$\frac{S}{4}$	0	0

• Molecule 4 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues		At	oms		AltConf	Trace	
4	Е	155	Total 1144	С 711	N 216	0 211	S 6	0	0

• Molecule 5 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues		At	oms	AltConf	Trace		
5	F	106	Total 862	C 545	N 156	0 154	${f S}{7}$	0	0

• Molecule 6 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues		At	\mathbf{oms}		AltConf	Trace	
6	G	107	Total 841	C 525	N 160	0 153	${ m S} { m 3}$	0	0



• Molecule 7 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues		At	oms		AltConf	Trace	
7	Н	129	Total 979	C 616	N 173	0 184	S 6	0	0

• Molecule 8 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues		At	oms	AltConf	Trace		
8	Ι	127	Total 1022	C 634	N 206	0 179	${ m S} { m 3}$	0	0

• Molecule 9 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues		At	oms		AltConf	Trace	
9	J	99	Total 796	C 498	N 152	0 145	S 1	0	0

• Molecule 10 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues		At	\mathbf{oms}	AltConf	Trace		
10	K	117	Total 877	C 540	N 174	O 160	${ m S} { m 3}$	0	0

• Molecule 11 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	L	14	Total 114	C 70	N 27	O 17	0	0

• Molecule 12 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms			AltConf	Trace		
12	М	114	Total 884	C 546	N 178	0 157	${ m S} { m 3}$	0	0

• Molecule 13 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms			AltConf	Trace		
13	Ν	100	Total 805	C 499	N 164	O 139	${ m S} { m 3}$	0	0

• Molecule 14 is a protein called 30S ribosomal protein S15.



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

• Molecule 15 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms				AltConf	Trace	
15	Р	82	Total 649	C 406	N 128	0 114	S 1	0	0

• Molecule 16 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms			AltConf	Trace		
16	Q	80	Total 649	C 411	N 121	0 114	${ m S} { m 3}$	0	0

• Molecule 17 is a protein called 30S ribosomal protein S18.

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

• Molecule 18 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms			AltConf	Trace		
18	S	79	Total 638	C 408	N 120	0 108	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0

• Molecule 19 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms			AltConf	Trace		
19	Т	86	Total 670	C 414	N 138	0 115	${ m S} { m 3}$	0	0

• Molecule 20 is a protein called Small ribosomal subunit biogenesis GTPase RsgA.

Mol	Chain	Residues	Atoms			AltConf	Trace		
20	Z	313	Total 2448	C 1538	N 432	0 468	S 10	0	0

• Molecule 21 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).



Mol	Chain	Residues	Atoms	AltConf
21	А	67	Total Mg 67 67	0
21	Ν	1	Total Mg 1 1	0
21	Р	1	Total Mg 1 1	0
21	Т	1	Total Mg 1 1	0
21	Ζ	1	Total Mg 1 1	0

• Molecule 22 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
22	В	1	Total Zn 1 1	0
22	Ζ	1	Total Zn 1 1	0

• Molecule 23 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



Mol	Chain	Residues		Atoms				
23	Z	1	Total 32	C 10	N 6	O 13	Р 3	0

MolProbity failed to run properly - this section is therefore empty.



3 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	61908	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	2.3	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	101000	Depositor
Image detector	FEI FALCON II $(4k \times 4k)$	Depositor
Maximum map value	0.333	Depositor
Minimum map value	-0.120	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	355.84, 355.84, 355.84	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.39, 1.39, 1.39	Depositor



4 Model quality (i)

4.1 Standard geometry (i)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts (i)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles (i)

4.3.1 Protein backbone (i)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains (i)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA (i)

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains (i)

11 non-standard protein/DNA/RNA residues are 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 Tv	Turne	uno Chain		Bog Link Bond lengths		$_{\rm ths}$	Bond angles			
	Moi Type Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
1	2MG	А	1516	1	18,26,27	0.90	1 (5%)	$16,\!38,\!41$	1.11	2 (12%)
1	5MC	А	967	1	18,22,23	0.95	2 (11%)	26,32,35	1.14	3 (11%)
1	UR3	А	1498	21,1	19,22,23	0.97	0	26,32,35	1.43	1 (3%)



Mal	Turne	Chain	Dec	Tink	Bo	ond leng	ths	В	ond ang	les
1VIOI	Type	Unam	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
1	2MG	А	966	1	18,26,27	0.89	1 (5%)	$16,\!38,\!41$	1.13	2 (12%)
1	G7M	А	527	1	20,26,27	1.10	2 (10%)	$17,\!39,\!42$	0.86	0
1	PSU	А	516	21,1	18,21,22	1.36	2 (11%)	22,30,33	1.83	3 (13%)
1	5MC	А	1407	1	18,22,23	0.93	2 (11%)	26,32,35	1.08	3 (11%)
1	2MG	А	1207	1	18,26,27	0.95	1 (5%)	16,38,41	1.12	2 (12%)
1	MA6	А	1518	1	18,26,27	1.01	1 (5%)	19,38,41	1.88	6 (31%)
1	4OC	А	1402	1	20,23,24	0.77	0	26,32,35	1.01	1 (3%)
1	MA6	А	1519	1	18,26,27	0.97	1 (5%)	19,38,41	1.86	6 (31%)

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	\mathbf{Res}	Link	Chirals	Torsions	Rings
1	2MG	А	1516	1	-	0/5/27/28	0/3/3/3
1	5MC	А	967	1	-	0/7/25/26	0/2/2/2
1	UR3	А	1498	21,1	-	0/7/25/26	0/2/2/2
1	2MG	А	966	1	-	0/5/27/28	0/3/3/3
1	G7M	А	527	1	-	3/3/25/26	0/3/3/3
1	PSU	А	516	21,1	-	0/7/25/26	0/2/2/2
1	5MC	А	1407	1	-	0/7/25/26	0/2/2/2
1	2MG	А	1207	1	-	2/5/27/28	0/3/3/3
1	MA6	А	1518	1	-	4/7/29/30	0/3/3/3
1	4OC	А	1402	1	-	0/9/29/30	0/2/2/2
1	MA6	А	1519	1	_	4/7/29/30	0/3/3/3

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	А	516	PSU	C6-C5	3.27	1.39	1.35
1	А	527	G7M	C5-C4	2.90	1.44	1.39
1	А	967	5MC	C6-C5	2.72	1.39	1.34
1	А	1407	5MC	C6-C5	2.68	1.39	1.34
1	А	1207	2MG	C6-N1	-2.63	1.34	1.37

The worst 5 of 29 bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	1498	UR3	C4-N3-C2	-5.97	118.94	124.56
1	А	516	PSU	N1-C2-N3	5.85	121.75	115.13
1	А	1518	MA6	N1-C6-N6	4.79	122.10	117.06
1	А	516	PSU	C4-N3-C2	-3.69	121.03	126.34
1	А	1519	MA6	C10-N6-C6	-3.63	108.52	119.51

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Atoms
1	А	527	G7M	O4'-C4'-C5'-O5'
1	А	527	G7M	C3'-C4'-C5'-O5'
1	А	1518	MA6	C5-C6-N6-C9
1	А	1518	MA6	C5-C6-N6-C10
1	А	1518	MA6	N1-C6-N6-C9

There are no ring outliers.

No monomer is involved in short contacts.

4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

4.6 Ligand geometry (i)

Of 74 ligands modelled in this entry, 73 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol 7	Tuno	Chain	Res	Bog	Bog	Ros	Ros	Ros	Bog	Tink	Bo	ond leng	ths	Bond angles		
	туре	Ullalli		LINK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2						
23	GNP	Ζ	402	21	29,34,34	1.70	7 (24%)	33,54,54	2.36	9 (27%)						

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
23	GNP	Ζ	402	21	-	7/14/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
23	Ζ	402	GNP	PB-O3A	-4.70	1.53	1.59
23	Ζ	402	GNP	C6-N1	3.82	1.39	1.33
23	Ζ	402	GNP	PG-01G	3.12	1.51	1.46
23	Ζ	402	GNP	PB-O2B	-3.08	1.48	1.56
23	Ζ	402	GNP	C8-N7	-2.24	1.30	1.34

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
23	Ζ	402	GNP	C5-C6-N1	-8.61	111.65	123.43
23	Ζ	402	GNP	C2-N1-C6	5.60	124.83	115.93
23	Ζ	402	GNP	O3G-PG-O1G	-3.80	103.90	113.45
23	Ζ	402	GNP	O2B-PB-O1B	3.70	117.67	109.92
23	Ζ	402	GNP	C2-N3-C4	-3.10	111.81	115.36

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	Ζ	402	GNP	PG-N3B-PB-O1B
23	Ζ	402	GNP	PG-N3B-PB-O3A
23	Ζ	402	GNP	PA-O3A-PB-O1B
23	Ζ	402	GNP	C5'-O5'-PA-O1A
23	Ζ	402	GNP	C5'-O5'-PA-O3A

There are no ring outliers.

No monomer is involved in short contacts.

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 then 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.



4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



5 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-3662. 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.

5.1 Orthogonal projections (i)

5.1.1 Primary map



5.1.2 Raw map



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



5.2 Central slices (i)

5.2.1 Primary map



X Index: 128



Y Index: 128



Z Index: 128

5.2.2 Raw map



X Index: 128

Y Index: 128

Z Index: 128

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



5.3 Largest variance slices (i)

5.3.1 Primary map



X Index: 140



Y Index: 111



Z Index: 132

5.3.2 Raw map



X Index: 138

Y Index: 100

Z Index: 132

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



5.4 Orthogonal standard-deviation projections (False-color) (i)

5.4.1 Primary map



5.4.2 Raw map



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.



5.5 Orthogonal surface views (i)

5.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

5.5.2 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.

5.6 Mask visualisation (i)

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



6 Map analysis (i)

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

6.1 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.



6.2 Volume estimate (i)



The volume at the recommended contour level is 666 nm^3 ; this corresponds to an approximate mass of 601 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.



6.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.194 $\rm \AA^{-1}$



7 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.

7.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.194 $\mathrm{\AA^{-1}}$



7.2 Resolution estimates (i)

$\mathbf{Bosolution} \text{ ostimato } (\mathbf{\hat{\lambda}})$	Estimation criterion (FSC cut-off)		
Resolution estimate (A)	0.143	0.5	Half-bit
Reported by author	5.16	-	-
Author-provided FSC curve	5.34	6.69	5.42
Unmasked-calculated*	6.87	9.53	7.12

*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 6.87 differs from the reported value 5.16 by more than 10 %



8 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-3662 and PDB model 5NO3. Per-residue inclusion information can be found in section ?? on page ??.

8.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.06 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.



8.2 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.

8.3 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 (0.06).



8.4 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.



1.0

0.0 <0.0

8.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8540	0.2280
А	0.9670	0.2590
В	0.1400	0.1150
D	0.7110	0.1630
Е	0.7710	0.2090
F	0.7430	0.1910
G	0.2690	0.1120
Н	0.7520	0.1940
Ι	0.6820	0.1530
J	0.5250	0.1360
K	0.7510	0.1940
L	0.3240	0.1310
М	0.7830	0.1810
Ν	0.4900	0.1220
0	0.7560	0.1840
Р	0.7750	0.2070
Q	0.7630	0.2140
R	0.7850	0.2120
S	0.8390	0.2020
Т	0.7870	0.1740
Z	0.7230	0.1870

