



wwPDB/EMDatabank EM Map/Model Validation Summary Report

Feb 21, 2018 – 07:28 PM EST

PDB ID : 6C4H
EMDB ID: : EMD-7340
Title : Conformation of methylated GGQ in the peptidyl transferase center during translation termination (PTC region)
Authors : Zeng, F.; Jin, H.
Deposited on : 2018-01-12
Resolution : 3.10 Å(reported)

This is a wwPDB/EMDatabank EM Map/Model Validation Summary Report for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the  symbol.

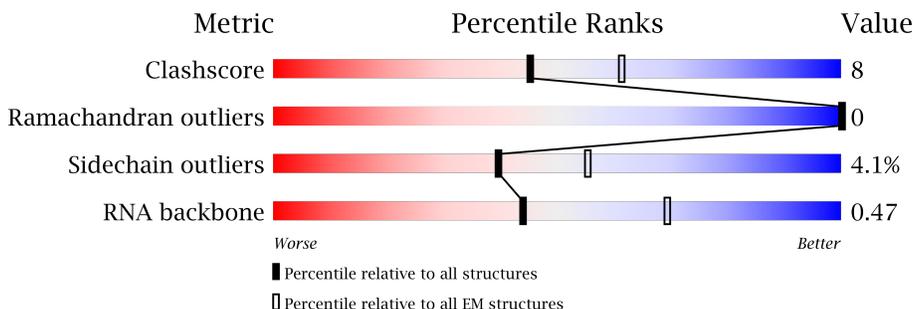
MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030736

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 3.10 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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026
RNA backbone	3398	335

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	A	2904	13% 8% 78%
2	C	273	14% 83%
3	D	209	15% 7% 78%
4	N	136	12% 88%
5	X	85	9% 88%
6	x	77	13% 84%
7	v	384	16% 84%

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
1	G7M	A	2069	-	-	X	-

2 Entry composition i

There are 8 unique types of molecules in this entry. The entry contains 15326 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 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	636	13622	6086	2470	4430	636	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	887	A	U	conflict	GB 687670942

- Molecule 2 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	47	361	224	77	59	1	0	0

- Molecule 3 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	47	361	224	73	63	1	0	0

- Molecule 4 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	N	17	125	77	24	23	1	0	0

- Molecule 5 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	X	10	75	40	17	18	0	0

- Molecule 6 is a RNA chain called P-site tRNA fMet.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	x	12	252	114	48	79	11	0	0

- Molecule 7 is a protein called Peptide chain release factor RF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	v	63	496	301	99	93	3	0	0

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
v	-18	ALA	-	expression tag	UNP P07012
v	-17	HIS	-	expression tag	UNP P07012
v	-16	HIS	-	expression tag	UNP P07012
v	-15	HIS	-	expression tag	UNP P07012
v	-14	HIS	-	expression tag	UNP P07012
v	-13	HIS	-	expression tag	UNP P07012
v	-12	HIS	-	expression tag	UNP P07012
v	-11	SER	-	expression tag	UNP P07012
v	-10	ALA	-	expression tag	UNP P07012
v	-9	ALA	-	expression tag	UNP P07012
v	-8	LEU	-	expression tag	UNP P07012
v	-7	GLU	-	expression tag	UNP P07012
v	-6	VAL	-	expression tag	UNP P07012
v	-5	LEU	-	expression tag	UNP P07012
v	-4	PHE	-	expression tag	UNP P07012
v	-3	GLN	-	expression tag	UNP P07012
v	-2	GLY	-	expression tag	UNP P07012
v	-1	PRO	-	expression tag	UNP P07012
v	0	GLY	-	expression tag	UNP P07012

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
8	A	34	34	34	0

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	143372	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL 3200FS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	83822	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, OMC, MG, OMG, OMU, G7M, 2MA, MEQ, 2MG, 5MC, 1MG, PSU

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	A	0.25	0/14827	0.65	0/23099
2	C	0.37	0/373	0.68	0/504
3	D	0.38	0/369	0.61	0/493
4	N	0.43	0/125	0.78	0/164
5	X	0.45	0/74	0.76	0/97
6	x	0.21	0/280	0.64	0/432
7	v	0.37	0/491	0.64	0/658
All	All	0.26	0/16539	0.65	0/25447

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	13622	0	6888	159	0
2	C	361	0	357	11	0
3	D	361	0	359	12	0
4	N	125	0	135	0	0
5	X	75	0	66	0	0
6	x	252	0	135	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	v	496	0	501	0	0
8	A	34	0	0	0	0
All	All	15326	0	8441	167	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 8.

The worst 5 of 167 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:2074:U:H2'	1:A:2075:U:C6	1.88	1.08
1:A:742:A:H2'	1:A:743:A:C8	1.97	1.00
1:A:2244:U:H2'	1:A:2245:U:C6	1.97	0.99
1:A:754:U:H2'	1:A:755:U:C6	2.05	0.92
1:A:2069:G7M:O6	1:A:2070:A:N6	2.13	0.81

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	C	45/273 (16%)	44 (98%)	1 (2%)	0	100	100
3	D	45/209 (22%)	40 (89%)	5 (11%)	0	100	100
4	N	15/136 (11%)	13 (87%)	2 (13%)	0	100	100
5	X	8/85 (9%)	7 (88%)	1 (12%)	0	100	100
7	v	60/384 (16%)	60 (100%)	0	0	100	100
All	All	173/1087 (16%)	164 (95%)	9 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	C	36/218 (16%)	36 (100%)	0	100	100
3	D	37/164 (23%)	37 (100%)	0	100	100
4	N	13/109 (12%)	12 (92%)	1 (8%)	15	48
5	X	8/63 (13%)	6 (75%)	2 (25%)	1	2
7	v	53/324 (16%)	50 (94%)	3 (6%)	24	60
All	All	147/878 (17%)	141 (96%)	6 (4%)	40	72

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	X	17	GLU
7	v	278	ARG
7	v	256	ARG
5	X	14	ARG
7	v	262	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
7	v	253	HIS
7	v	290	GLN
7	v	283	ASN
3	D	150	GLN
7	v	273	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	625/2904 (21%)	128 (20%)	11 (1%)
6	x	10/77 (12%)	2 (20%)	0
All	All	635/2981 (21%)	130 (20%)	11 (1%)

5 of 130 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	738	G
1	A	747	5MU
1	A	748	G
1	A	749	A
1	A	752	A

5 of 11 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	791	C
1	A	1128	G
1	A	2468	A
1	A	784	G
1	A	1900	A

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

18 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	2MG	A	1835	1	19,26,27	1.37	2 (10%)	20,38,41	2.34	7 (35%)
1	5MU	A	1939	1	14,22,23	0.84	0	16,32,35	2.34	4 (25%)
1	5MC	A	1962	1	15,22,23	1.59	1 (6%)	17,32,35	1.00	0
1	G7M	A	2069	1	19,26,27	1.65	2 (10%)	19,39,42	3.62	8 (42%)
1	OMG	A	2251	1,6	18,26,27	1.33	2 (11%)	22,38,41	2.16	6 (27%)
1	2MG	A	2445	1	19,26,27	1.36	2 (10%)	20,38,41	2.50	8 (40%)
1	PSU	A	2457	1	16,21,22	1.39	1 (6%)	20,30,33	3.61	6 (30%)
1	OMC	A	2498	1,8	15,22,23	0.89	1 (6%)	19,31,34	1.07	1 (5%)
1	2MA	A	2503	1	18,25,26	1.77	3 (16%)	17,37,40	2.15	2 (11%)
1	PSU	A	2504	1	16,21,22	1.09	1 (6%)	20,30,33	3.63	8 (40%)
1	OMU	A	2552	1,8	14,22,23	0.91	1 (7%)	18,31,34	2.07	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	A	2580	1	16,21,22	1.28	1 (6%)	20,30,33	3.56	8 (40%)
1	PSU	A	2605	1	16,21,22	1.17	1 (6%)	20,30,33	3.49	7 (35%)
1	1MG	A	745	1	18,26,27	1.51	3 (16%)	18,39,42	1.88	3 (16%)
1	PSU	A	746	1	16,21,22	1.11	1 (6%)	20,30,33	3.68	5 (25%)
1	5MU	A	747	1	14,22,23	0.91	0	16,32,35	2.55	3 (18%)
1	PSU	A	955	1	16,21,22	1.24	1 (6%)	20,30,33	3.35	7 (35%)
7	MEQ	v	252	7	9,9,10	0.50	0	7,10,12	0.99	0

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
1	2MG	A	1835	1	-	0/5/27/28	0/3/3/3
1	5MU	A	1939	1	-	0/3/25/26	0/2/2/2
1	5MC	A	1962	1	-	0/3/25/26	0/2/2/2
1	G7M	A	2069	1	-	0/3/25/26	0/3/3/3
1	OMG	A	2251	1,6	-	0/5/27/28	0/3/3/3
1	2MG	A	2445	1	-	0/5/27/28	0/3/3/3
1	PSU	A	2457	1	-	0/7/25/26	0/2/2/2
1	OMC	A	2498	1,8	-	0/5/27/28	0/2/2/2
1	2MA	A	2503	1	-	0/3/25/26	0/3/3/3
1	PSU	A	2504	1	-	0/7/25/26	0/2/2/2
1	OMU	A	2552	1,8	-	0/5/27/28	0/2/2/2
1	PSU	A	2580	1	-	0/7/25/26	0/2/2/2
1	PSU	A	2605	1	-	0/7/25/26	0/2/2/2
1	1MG	A	745	1	-	0/3/25/26	0/3/3/3
1	PSU	A	746	1	-	0/7/25/26	0/2/2/2
1	5MU	A	747	1	-	0/3/25/26	0/2/2/2
1	PSU	A	955	1	-	0/7/25/26	0/2/2/2
7	MEQ	v	252	7	-	0/7/9/11	0/0/0/0

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2069	G7M	C2'-C1'	-5.16	1.45	1.53
1	A	2457	PSU	C5-C1'	-3.99	1.48	1.52
1	A	2580	PSU	C5-C1'	-3.53	1.49	1.52
1	A	955	PSU	C5-C1'	-3.20	1.49	1.52
1	A	746	PSU	C5-C1'	-3.02	1.49	1.52

The worst 5 of 85 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	746	PSU	N1-C2-N3	-10.70	120.70	128.40
1	A	2069	G7M	C4'-O4'-C1'	-9.52	99.64	109.77
1	A	2605	PSU	N1-C2-N3	-9.39	121.64	128.40
1	A	2580	PSU	N1-C2-N3	-9.11	121.85	128.40
1	A	2457	PSU	N1-C2-N3	-9.07	121.88	128.40

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1939	5MU	1	0
1	A	2069	G7M	12	0
1	A	2445	2MG	1	0
1	A	2503	2MA	1	0
1	A	2605	PSU	1	0
1	A	747	5MU	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 34 ligands modelled in this entry, 34 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.