Full wwPDB NMR Structure Validation Report (i)

Apr 20, 2024 – 09:01 PM EDT

PDB ID	:	2KIM
Title	:	1.7-mm microcryoprobe solution NMR structure of an O6-methylguanine DNA methyltransferase family protein from Vibrio parahaemolyticus. Northeast Structural Genomics Consortium target VpR247.
Authors	:	Aramini, J.M.; Belote, R.L.; Ciccosanti, C.T.; Jiang, M.; Rost, B.; Nair, R.; Swapna, G.V.T.; Acton, T.B.; Xiao, R.; Everett, J.K.; Montelione, G.T.; Northeast Structural Genomics Consortium (NESG)
Deposited on	:	2009-05-07

This is a Full wwPDB NMR Structure Validation 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/NMRValidationReportHelp
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 (i)) were used in the production of this report:

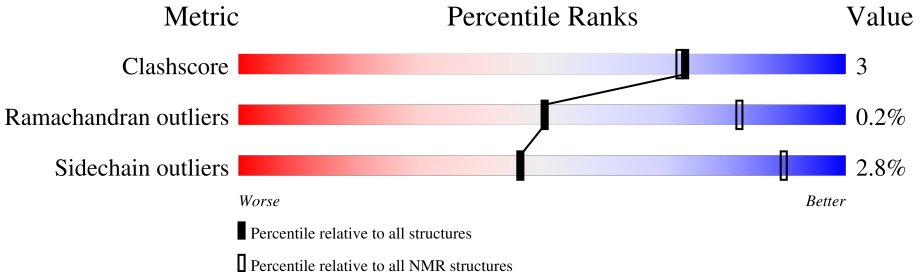
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson 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:
SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	108	

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 15 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:2-A:100 (99)	0.79	15

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 3 clusters and 5 single-model clusters were found.

Cluster number	Models
1	2, 3, 4, 6, 7, 10, 15, 16, 20
2	1, 9, 13, 14
3	11, 19
Single-model clusters	5; 8; 12; 17; 18

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1658 atoms, of which 847 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called O6-methylguanine-DNA methyltransferase.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	102	1658	524	847	144	141	2	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	101	LEU	-	expression tag	UNP A6B4U8
A	102	GLU	-	expression tag	UNP A6B4U8
A	103	HIS	-	expression tag	UNP A6B4U8
A	104	HIS	-	expression tag	UNP A6B4U8
A	105	HIS	-	expression tag	UNP A6B4U8
A	106	HIS	-	expression tag	UNP A6B4U8
A	107	HIS	-	expression tag	UNP A6B4U8
A	108	HIS	-	expression tag	UNP A6B4U8

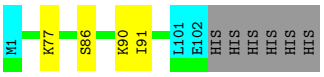
4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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 outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: O6-methylguanine-DNA methyltransferase

Chain A:



4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: O6-methylguanine-DNA methyltransferase

Chain A:

4.2.2 Score per residue for model 2

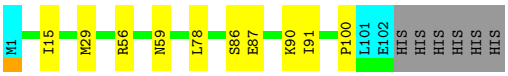
• Molecule 1: O6-methylguanine-DNA methyltransferase

Chain A:

4.2.3 Score per residue for model 3

- Molecule 1: O6-methylguanine-DNA methyltransferase

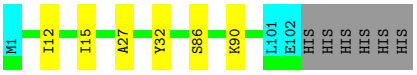
Chain A: 82% 9% • 6%



4.2.4 Score per residue for model 4

- Molecule 1: O6-methylguanine-DNA methyltransferase

Chain A: 86% 6% • 6%



4.2.5 Score per residue for model 5

- Molecule 1: O6-methylguanine-DNA methyltransferase

Chain A: 81% 10% • 6%

4.2.6 Score per residue for model 6

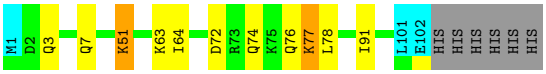
- Molecule 1: O6-methylguanine-DNA methyltransferase

Chain A: 79% 10% • • 6%

4.2.7 Score per residue for model 7

- Molecule 1: O6-methylguanine-DNA methyltransferase

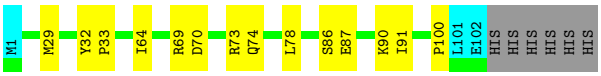
Chain A: 81% 8% • • 6%



4.2.8 Score per residue for model 8

- Molecule 1: O6-methylguanine-DNA methyltransferase

Chain A: 79% 13% • 6%



4.2.9 Score per residue for model 9

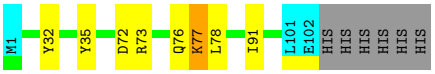
- Molecule 1: O6-methylguanine-DNA methyltransferase

Chain A: 81% 9% • • 6%

4.2.10 Score per residue for model 10

- Molecule 1: O6-methylguanine-DNA methyltransferase

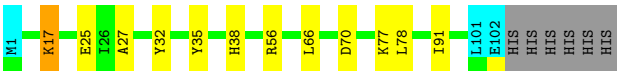
Chain A: 84% 6% • • 6%



4.2.11 Score per residue for model 11

- Molecule 1: O6-methylguanine-DNA methyltransferase

Chain A: 81% 10% • • 6%



4.2.12 Score per residue for model 12

- Molecule 1: O6-methylguanine-DNA methyltransferase

Chain A: 79% 12% • • 6%

4.2.13 Score per residue for model 13

- Molecule 1: O6-methylguanine-DNA methyltransferase

Chain A: 82% 9% • 6%

M1 I15 T22 R56 V57 I58 N59 K63 S86 E87 K90 L93 L101 E102 HIS HIS HIS HIS HIS HIS

4.2.14 Score per residue for model 14

- Molecule 1: O6-methylguanine-DNA methyltransferase

Chain A: 81% 10% • 6%

M1 K17 M29 E48 I58 R73 Q76 I88 G89 K90 L93 R94 K95 P100 L101 E102 HIS HIS HIS HIS HIS HIS

4.2.15 Score per residue for model 15 (medoid)

- Molecule 1: O6-methylguanine-DNA methyltransferase

Chain A: 79% 12% • • 6%

M1 N45 I58 K63 I64 K67 D72 R73 Q74 K75 Q76 K77 V85 K90 L93 K97 L101 E102 HIS HIS HIS HIS HIS HIS

4.2.16 Score per residue for model 16

- Molecule 1: O6-methylguanine-DNA methyltransferase

Chain A: 81% 8% • • 6%

M1 K17 K41 N45 K63 D72 Q76 K77 L78 S86 G89 K90 I91 L101 E102 HIS HIS HIS HIS HIS HIS

4.2.17 Score per residue for model 17

- Molecule 1: O6-methylguanine-DNA methyltransferase

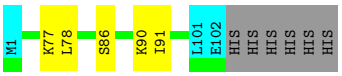
Chain A: 79% 12% • • 6%

M1 K17 E25 E48 K51 R56 V57 I58 N59 K67 L71 D72 R73 K77 E87 I91 A92 L93 L101 E102 HIS HIS HIS HIS HIS HIS

4.2.18 Score per residue for model 18

- Molecule 1: O6-methylguanine-DNA methyltransferase

Chain A: 87% 5% • 6%



4.2.19 Score per residue for model 19

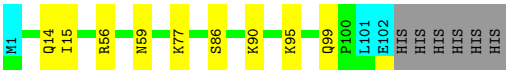
- Molecule 1: O6-methylguanine-DNA methyltransferase

Chain A: 79% 13% • 6%

4.2.20 Score per residue for model 20

- Molecule 1: O6-methylguanine-DNA methyltransferase

Chain A: 83% 8% • 6%



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *simulated annealing*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
CYANA	structure solution	3.0
CNS	refinement	1.2

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 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 each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	786	819	819	5±2
All	All	15720	16380	16380	105

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 3.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:86:SER:HB3	1:A:90:LYS:HB3	0.71	1.63	16	7
1:A:17:LYS:HA	1:A:56:ARG:HH22	0.69	1.48	11	2
1:A:77:LYS:HE2	1:A:77:LYS:HA	0.60	1.72	5	6
1:A:29:MET:SD	1:A:100:PRO:HG3	0.60	2.35	14	2
1:A:29:MET:SD	1:A:100:PRO:HG2	0.60	2.37	3	2
1:A:86:SER:HB2	1:A:90:LYS:HB3	0.60	1.73	1	3
1:A:77:LYS:HA	1:A:77:LYS:HE3	0.56	1.78	7	4
1:A:78:LEU:HD13	1:A:91:ILE:HD11	0.56	1.76	8	7
1:A:73:ARG:O	1:A:77:LYS:HG2	0.56	2.01	17	1
1:A:15:ILE:HB	1:A:56:ARG:HH11	0.55	1.61	3	3
1:A:58:ILE:HD11	1:A:93:LEU:HD21	0.55	1.78	1	9
1:A:69:ARG:H	1:A:69:ARG:HD3	0.53	1.63	6	1
1:A:69:ARG:HA	1:A:69:ARG:HE	0.53	1.64	9	1
1:A:41:LYS:HE2	1:A:41:LYS:HA	0.51	1.81	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:51:LYS:HD2	1:A:51:LYS:H	0.51	1.65	17	1
1:A:73:ARG:O	1:A:76:GLN:HG2	0.51	2.06	12	2
1:A:86:SER:HB2	1:A:90:LYS:HB2	0.50	1.84	8	1
1:A:69:ARG:HD3	1:A:69:ARG:N	0.50	2.22	6	1
1:A:67:LYS:HD2	1:A:71:LEU:HD12	0.50	1.83	17	1
1:A:72:ASP:O	1:A:76:GLN:HG2	0.48	2.08	16	3
1:A:86:SER:OG	1:A:90:LYS:HB3	0.47	2.09	13	1
1:A:17:LYS:HA	1:A:56:ARG:NH2	0.47	2.22	6	3
1:A:41:LYS:HA	1:A:41:LYS:HE3	0.47	1.85	12	1
1:A:64:ILE:HG23	1:A:74:GLN:OE1	0.47	2.10	8	1
1:A:90:LYS:NZ	1:A:90:LYS:HB3	0.46	2.25	15	1
1:A:32:TYR:N	1:A:33:PRO:HD3	0.46	2.26	8	1
1:A:22:THR:HA	1:A:58:ILE:O	0.46	2.10	13	1
1:A:27:ALA:HB1	1:A:32:TYR:O	0.46	2.10	4	3
1:A:97:LYS:HD3	1:A:99:GLN:HE21	0.45	1.71	19	1
1:A:72:ASP:HB3	1:A:76:GLN:NE2	0.45	2.27	15	1
1:A:48:GLU:HG3	1:A:73:ARG:HD2	0.44	1.88	1	1
1:A:22:THR:OG1	1:A:25:GLU:HG2	0.44	2.12	5	1
1:A:66:LEU:HB3	1:A:70:ASP:HB2	0.44	1.88	11	1
1:A:64:ILE:O	1:A:67:LYS:NZ	0.44	2.46	15	1
1:A:63:LYS:HG2	1:A:64:ILE:N	0.44	2.28	7	1
1:A:38:HIS:ND1	1:A:41:LYS:NZ	0.44	2.64	6	1
1:A:59:ASN:ND2	1:A:61:GLN:HB2	0.43	2.28	12	1
1:A:12:ILE:O	1:A:15:ILE:HG12	0.43	2.13	4	2
1:A:58:ILE:HD13	1:A:91:ILE:HD12	0.43	1.89	19	3
1:A:75:LYS:O	1:A:79:GLU:HG2	0.43	2.14	2	1
1:A:35:TYR:HA	1:A:38:HIS:ND1	0.43	2.27	11	1
1:A:88:ILE:HG13	1:A:90:LYS:HB2	0.43	1.90	14	1
1:A:63:LYS:HA	1:A:89:GLY:O	0.42	2.13	16	1
1:A:3:GLN:O	1:A:7:GLN:HG2	0.42	2.15	12	3
1:A:24:GLY:O	1:A:28:LYS:HG3	0.42	2.14	2	1
1:A:51:LYS:N	1:A:51:LYS:HD2	0.42	2.30	7	1
1:A:41:LYS:NZ	1:A:45:ASN:OD1	0.42	2.52	16	1
1:A:15:ILE:HG22	1:A:56:ARG:NH1	0.42	2.29	6	1
1:A:48:GLU:HB2	1:A:73:ARG:HD2	0.42	1.90	6	1
1:A:7:GLN:O	1:A:11:VAL:HG23	0.42	2.15	12	1
1:A:32:TYR:HB3	1:A:35:TYR:CD2	0.41	2.51	10	1
1:A:58:ILE:HG21	1:A:91:ILE:HD12	0.41	1.92	12	1
1:A:72:ASP:HA	1:A:75:LYS:HB3	0.41	1.93	19	1
1:A:8:ILE:O	1:A:12:ILE:HG13	0.41	2.16	1	1
1:A:63:LYS:HB2	1:A:63:LYS:NZ	0.41	2.31	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:15:ILE:HG21	1:A:56:ARG:HB3	0.40	1.91	13	1
1:A:75:LYS:HG3	1:A:85:VAL:HB	0.40	1.93	15	1
1:A:58:ILE:HB	1:A:63:LYS:O	0.40	2.15	15	1

6.3 Torsion angles (i)

6.3.1 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 NMR 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	
1	A	99/108 (92%)	92±2 (93±2%)	7±2 (7±2%)	0±1 (0±1%)	50	82
All	All	1980/2160 (92%)	1834 (93%)	142 (7%)	4 (0%)	50	82

All 3 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	17	LYS	2
1	A	47	PRO	1
1	A	100	PRO	1

6.3.2 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 NMR 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	
1	A	81/90 (90%)	79±1 (97±2%)	2±1 (3±2%)	46	90
All	All	1620/1800 (90%)	1575 (97%)	45 (3%)	46	90

All 18 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	87	GLU	6
1	A	48	GLU	5
1	A	59	ASN	5
1	A	69	ARG	4
1	A	77	LYS	4
1	A	73	ARG	4
1	A	51	LYS	2
1	A	17	LYS	2
1	A	25	GLU	2
1	A	41	LYS	2
1	A	95	LYS	2
1	A	37	ARG	1
1	A	74	GLN	1
1	A	70	ASP	1
1	A	45	ASN	1
1	A	97	LYS	1
1	A	90	LYS	1
1	A	14	GLN	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

No chemical shift data were provided