



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 7, 2016 – 05:41 PM EDT

PDB ID : 5JIY
Title : Structure of G9a SET-domain with Histone H3K9norLeucine mutant peptide and bound S-adenosylmethionine
Authors : Jayaram, H.; Bellon, S.F.; Poy, F.
Deposited on : 2016-04-22
Resolution : 1.48 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

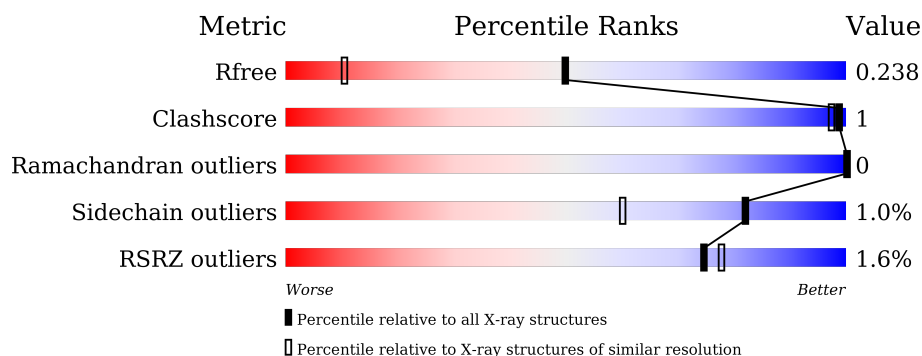
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.48 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3129 (1.50-1.46)
Clashscore	102246	3380 (1.50-1.46)
Ramachandran outliers	100387	3310 (1.50-1.46)
Sidechain outliers	100360	3308 (1.50-1.46)
RSRZ outliers	91569	3133 (1.50-1.46)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	274	<div> <div style="width: 94%;"></div> <div style="width: 5%;"></div> </div> <div>94% 5%</div>
1	B	274	<div> <div style="width: 93%;"></div> <div style="width: 5%;"></div> <div style="width: 2%;"></div> </div> <div>93% . .</div>
2	F	11	<div> <div style="width: 73%;"></div> <div style="width: 27%;"></div> </div> <div>73% 27%</div>
2	G	11	<div> <div style="width: 9%;"></div> <div style="width: 82%;"></div> <div style="width: 18%;"></div> </div> <div>9% 82% 18%</div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4704 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 protein called Histone-lysine N-methyltransferase EHMT2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	0	2	0
			2214	1379	389	422	24			
1	B	267	Total	C	N	O	S	0	1	0
			2160	1350	376	411	23			

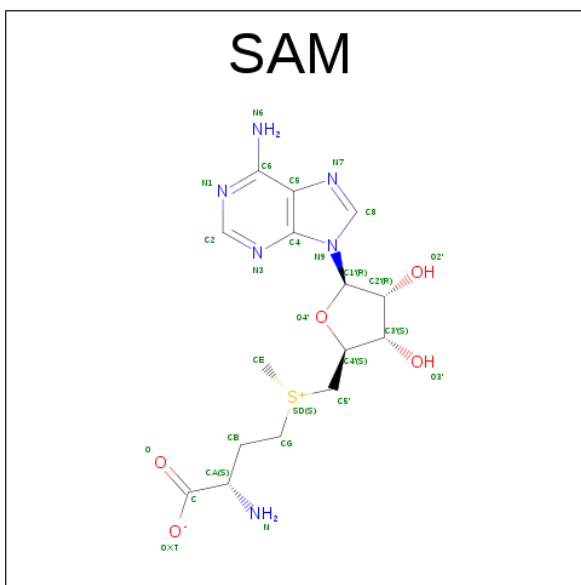
- Molecule 2 is a protein called Histone H3.1 mutant peptide with H3K9nor-leucine.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	F	8	Total	C	N	O	0	0	0
			62	37	13	12			
2	G	9	Total	C	N	O	0	0	0
			69	41	14	14			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	4	Total	Zn	0	0
			4	4		
3	A	4	Total	Zn	0	0
			4	4		

- Molecule 4 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula: C₁₅H₂₂N₆O₅S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 27	C 15	N 6	O 5	S 1	0	0
4	B	1	Total 27	C 15	N 6	O 5	S 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	77	Total O 77 77	0	0
5	F	1	Total O 1 1	0	0
5	B	59	Total O 59 59	0	0

- Molecule 1: Histone-lysine N-methyltransferase EHMT2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	56.61Å 78.46Å 73.08Å 90.00° 90.28° 90.00°	Depositor
Resolution (Å)	38.95 – 1.48 38.94 – 1.48	Depositor EDS
% Data completeness (in resolution range)	99.3 (38.95-1.48) 99.3 (38.94-1.48)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 1.48Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.209 , 0.233 0.216 , 0.238	Depositor DCC
R_{free} test set	5287 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	21.1	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 24.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.054 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4704	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.86% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: ZN, NLE, SAM

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	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.99	0/2260	1.10	10/3053 (0.3%)
1	B	1.02	1/2208 (0.0%)	1.04	8/2983 (0.3%)
2	F	1.09	0/52	1.05	0/66
2	G	0.74	0/59	0.91	0/76
All	All	1.00	1/4579 (0.0%)	1.07	18/6178 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1043	TYR	CD1-CE1	-5.61	1.30	1.39

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	962	MET	CG-SD-CE	-12.86	79.63	100.20
1	A	1142	ARG	NE-CZ-NH1	10.39	125.50	120.30
1	A	1039	ARG	NE-CZ-NH2	-8.49	116.05	120.30
1	B	1142	ARG	NE-CZ-NH1	8.10	124.35	120.30
1	B	1053	ARG	NE-CZ-NH2	-7.99	116.31	120.30
1	A	1143	ASP	CB-CG-OD1	7.79	125.31	118.30
1	A	1142	ARG	NE-CZ-NH2	-7.12	116.74	120.30
1	B	1102	ARG	NE-CZ-NH2	-6.45	117.07	120.30
1	A	962	MET	CA-CB-CG	6.02	123.54	113.30
1	A	993	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	B	1044	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	B	962	MET	CA-CB-CG	5.57	122.76	113.30
1	B	1025	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	B	1142	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	A	1153	ASP	CB-CG-OD2	-5.33	113.51	118.30
1	A	1132	ARG	NE-CZ-NH1	5.12	122.86	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1013	LEU	CA-CB-CG	5.06	126.94	115.30
1	B	1102	ARG	NE-CZ-NH1	5.05	122.82	120.30

There are no chirality outliers.

There are no planarity outliers.

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	A	2214	0	2109	4	0
1	B	2160	0	2058	3	0
2	F	62	0	67	0	0
2	G	69	0	74	0	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
4	A	27	0	22	0	0
4	B	27	0	22	0	0
5	A	77	0	0	0	0
5	B	59	0	0	0	0
5	F	1	0	0	0	0
All	All	4704	0	4352	7	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 1.

All (7) 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:B:1089:LEU:O	1:B:1090:ASP:HB2	2.03	0.59
1:A:978:ASP:HB3	1:A:980:CYS:H	1.75	0.51
1:A:917:ARG:HB3	1:A:917:ARG:NH1	2.29	0.47
1:B:960:SER:OG	1:B:962:MET:CE	2.64	0.45
1:A:1161:ILE:N	1:A:1161:ILE:HD12	2.33	0.43
1:B:960:SER:OG	1:B:962:MET:HE2	2.21	0.41
1:A:917:ARG:CZ	1:A:917:ARG:HB3	2.51	0.40

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 X-ray entries followed by that with respect to entries of similar resolution.

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	273/274 (100%)	266 (97%)	7 (3%)	0	100	100
1	B	264/274 (96%)	251 (95%)	13 (5%)	0	100	100
2	F	5/11 (46%)	5 (100%)	0	0	100	100
2	G	6/11 (54%)	6 (100%)	0	0	100	100
All	All	548/570 (96%)	528 (96%)	20 (4%)	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 X-ray entries followed by that with respect to entries of similar resolution.

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	248/247 (100%)	244 (98%)	4 (2%)	70	39
1	B	242/247 (98%)	241 (100%)	1 (0%)	93	84
2	F	6/7 (86%)	6 (100%)	0	100	100
2	G	7/7 (100%)	7 (100%)	0	100	100
All	All	503/508 (99%)	498 (99%)	5 (1%)	82	60

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	977	VAL
1	A	978	ASP
1	A	982	SER
1	A	1093	ASP
1	B	1176	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	$\# Z > 2$
2	NLE	F	9	2	5,7,8	1.01	0	5,7,9	1.15	1 (20%)
2	NLE	G	9	2	5,7,8	0.47	0	5,7,9	1.06	1 (20%)

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
2	NLE	F	9	2	-	0/4/6/8	0/0/0/0
2	NLE	G	9	2	-	0/4/6/8	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	9	NLE	O-C-CA	-2.25	119.70	125.72
2	G	9	NLE	O-C-CA	-2.08	120.15	125.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 10 ligands modelled in this entry, 8 are monoatomic - leaving 2 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	SAM	A	1205	-	23,29,29	1.19	2 (8%)	15,42,42	2.65	4 (26%)
4	SAM	B	1205	-	23,29,29	1.30	3 (13%)	15,42,42	1.90	2 (13%)

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
4	SAM	A	1205	-	-	0/8/33/33	0/3/3/3
4	SAM	B	1205	-	-	0/8/33/33	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1205	SAM	CG-SD	-3.84	1.72	1.80
4	A	1205	SAM	C2'-C1'	-2.64	1.49	1.53
4	B	1205	SAM	CG-CB	-2.10	1.49	1.52
4	B	1205	SAM	O4'-C1'	2.91	1.45	1.41
4	A	1205	SAM	O4'-C1'	3.34	1.46	1.41

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1205	SAM	N3-C2-N1	-7.30	123.14	128.87
4	A	1205	SAM	C1'-N9-C4	-2.39	124.14	126.81
4	B	1205	SAM	C4'-O4'-C1'	2.70	112.51	109.64
4	A	1205	SAM	C2-N1-C6	3.85	125.63	118.77
4	A	1205	SAM	N6-C6-N1	4.84	126.64	118.52
4	B	1205	SAM	N6-C6-N1	5.50	127.75	118.52

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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	273/274 (99%)	-0.34	4 (1%) 76 79	16, 25, 45, 62	0
1	B	267/274 (97%)	-0.30	4 (1%) 76 79	17, 25, 47, 85	0
2	F	7/11 (63%)	-0.14	0 100 100	24, 26, 34, 38	0
2	G	8/11 (72%)	0.56	1 (12%) 5 5	26, 28, 52, 63	0
All	All	555/570 (97%)	-0.31	9 (1%) 74 78	16, 25, 47, 85	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1189	LEU	9.3
2	G	3	THR	6.1
1	B	920	LYS	5.7
1	B	1095	GLU	4.1
1	A	1186	GLN	3.2
1	B	921	ILE	3.2
1	A	992	ILE	2.6
1	A	978	ASP	2.4
1	A	1187	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	NLE	F	9	8/9	0.96	0.07	-	19,22,25,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	NLE	G	9	8/9	0.94	0.08	-	22,23,33,33	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	SAM	B	1205	27/27	0.96	0.06	-0.06	21,24,28,33	0
3	ZN	B	1203	1/1	0.99	0.06	-0.11	19,19,19,19	0
3	ZN	B	1201	1/1	1.00	0.06	-0.18	19,19,19,19	0
3	ZN	A	1204	1/1	0.99	0.06	-0.36	24,24,24,24	0
3	ZN	B	1204	1/1	0.99	0.05	-0.73	26,26,26,26	0
3	ZN	A	1201	1/1	1.00	0.05	-0.76	24,24,24,24	0
3	ZN	B	1202	1/1	1.00	0.05	-0.78	18,18,18,18	0
3	ZN	A	1203	1/1	0.99	0.06	-0.98	23,23,23,23	0
4	SAM	A	1205	27/27	0.98	0.05	-1.27	17,20,24,26	0
3	ZN	A	1202	1/1	0.98	0.05	-1.29	25,25,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.