



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 25, 2014 – 12:53 AM EDT

PDB ID : 4C03
Title : Crystal structure of M. musculus protein arginine methyltransferase PRMT6 reduced
Authors : Bonnefond, L.; Cura, V.; Troffer-Charlier, N.; Mailliot, J.; Wurtz, J.M.; Cavarelli, J.
Deposited on : 2013-07-31
Resolution : 1.58 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

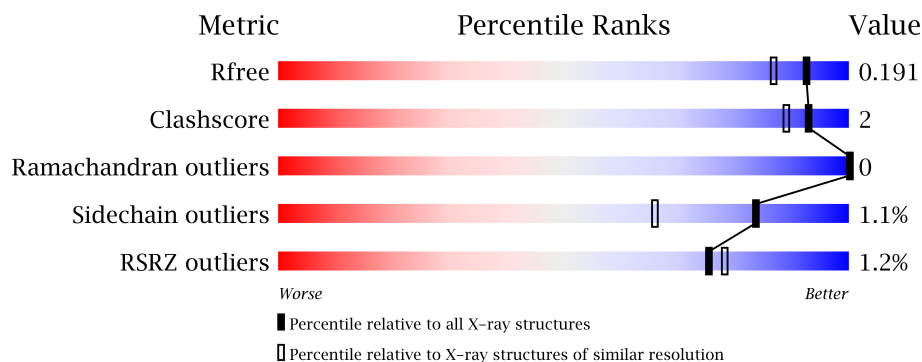
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable23489
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23489

1 Overall quality at a glance

The reported resolution of this entry is 1.58 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}	66092	2778 (1.60-1.56)
Clashscore	79885	3207 (1.60-1.56)
Ramachandran outliers	78287	3107 (1.60-1.56)
Sidechain outliers	78261	3104 (1.60-1.56)
RSRZ outliers	66119	2778 (1.60-1.56)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	382	
1	B	382	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11339 atoms, of which 5368 are hydrogens and 0 are deuterium.

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.

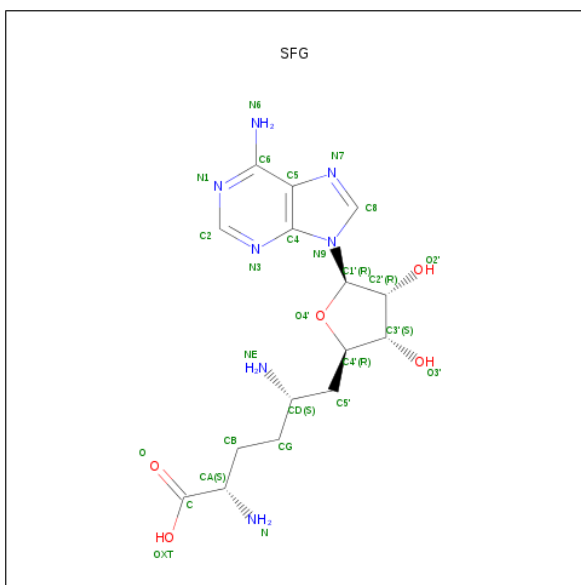
- Molecule 1 is a protein called PROTEIN ARGININE N-METHYLTRANSFERASE 6.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	337	Total	C	H	N	O	S	0	13	0
			5391	1712	2691	467	507	14			
1	B	328	Total	C	H	N	O	S	0	11	0
			5261	1675	2635	453	484	14			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	ARG	-	EXPRESSION TAG	UNP Q6NZB1
A	-2	GLY	-	EXPRESSION TAG	UNP Q6NZB1
A	-1	SER	-	EXPRESSION TAG	UNP Q6NZB1
A	0	HIS	-	EXPRESSION TAG	UNP Q6NZB1
A	315	LEU	PHE	VARIANT	UNP Q6NZB1
B	-3	ARG	-	EXPRESSION TAG	UNP Q6NZB1
B	-2	GLY	-	EXPRESSION TAG	UNP Q6NZB1
B	-1	SER	-	EXPRESSION TAG	UNP Q6NZB1
B	0	HIS	-	EXPRESSION TAG	UNP Q6NZB1
B	315	LEU	PHE	VARIANT	UNP Q6NZB1

- Molecule 2 is SINEFUNGIN (three-letter code: SFG) (formula: C₁₅H₂₃N₇O₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 48	C 15	H 21	N 7	O 5	0	0
2	B	1	Total 48	C 15	H 21	N 7	O 5	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	309	Total O 309 309	0	0
3	B	282	Total O 282 282	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	118.72Å 143.34Å 41.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.56 – 1.58 45.72 – 1.58	Depositor EDS
% Data completeness (in resolution range)	99.0 (39.56-1.58) 99.0 (45.72-1.58)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 1.58Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.160 , 0.191 0.160 , 0.191	Depositor DCC
R_{free} test set	4908 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	20.8	Xtriage
Anisotropy	0.619	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 41.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 98190 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	11339	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.56% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SFG

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	0.49	0/2802	0.64	1/3803 (0.0%)
1	B	0.48	0/2719	0.63	1/3689 (0.0%)
All	All	0.49	0/5521	0.64	2/7492 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	347	LEU	CA-CB-CG	6.01	129.11	115.30
1	A	347	LEU	CA-CB-CG	5.46	127.85	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2700	2691	0	10	0
1	B	2626	2635	0	8	0
2	A	27	21	1	0	0
2	B	27	21	1	0	0
3	A	309	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	282	0	0	1	0
All	All	5971	5368	2	18	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 2.

All (18) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:127:VAL:HG23	1:B:136:VAL:HG13	1.91	0.51
1:A:124:ARG:NE	3:A:2091:HOH:O	2.45	0.49
1:B:57:VAL:HG11	1:B:58:SER:N	2.29	0.47
1:A:90:LEU:CD1	1:A:114:VAL:HG22	2.45	0.47
1:A:122:GLN:OE1	3:A:2080:HOH:O	2.21	0.47
1:A:273:GLY:HA2	1:A:347:LEU:HD11	1.98	0.45
1:A:127:VAL:HG23	1:A:136:VAL:HG13	1.99	0.44
1:B:273:GLY:CA	1:B:347:LEU:HD11	2.47	0.44
1:A:127:VAL:HG12	1:A:136:VAL:HB	1.99	0.43
1:B:259:LEU:HD22	1:B:274[A]:VAL:HG12	2.00	0.43
1:A:243:ASP:OD1	1:A:243:ASP:N	2.49	0.43
1:B:127:VAL:HG12	1:B:136:VAL:HB	1.99	0.43
1:A:57:VAL:HG11	1:A:58:SER:N	2.35	0.42
1:B:270:LEU:HD21	1:B:274[A]:VAL:HG22	2.02	0.42
1:B:47:ASP:N	3:B:2001:HOH:O	2.52	0.42
1:A:259:LEU:N	1:A:259:LEU:HD13	2.35	0.41
1:A:243:ASP:OD1	3:A:2218:HOH:O	2.21	0.41
1:B:188:LEU:CD2	1:B:300:PRO:HD2	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	348/382 (91%)	343 (99%)	5 (1%)	0	100	100
1	B	335/382 (88%)	331 (99%)	4 (1%)	0	100	100
All	All	683/764 (89%)	674 (99%)	9 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	295/313 (94%)	291 (99%)	4 (1%)	78	55
1	B	285/313 (91%)	283 (99%)	2 (1%)	91	80
All	All	580/626 (93%)	574 (99%)	6 (1%)	84	69

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	85	ARG
1	A	147	GLU
1	A	158	GLU
1	A	285	SER
1	B	158	GLU
1	B	351	ASP

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 chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

2 ligands 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	SFG	A	1378	-	29,29,29	0.94	2 (6%)	42,42,42	2.11	7 (16%)
2	SFG	B	1378	-	29,29,29	1.03	1 (3%)	42,42,42	2.11	8 (19%)

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	SFG	A	1378	-	-	0/17/33/33	0/3/3/3
2	SFG	B	1378	-	-	0/17/33/33	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1378	SFG	O4'-C1'	3.36	1.45	1.41
2	A	1378	SFG	O4'-C1'	2.33	1.44	1.41
2	A	1378	SFG	CG-CD	2.07	1.55	1.53

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1378	SFG	N3-C2-N1	-8.62	121.30	128.89
2	A	1378	SFG	N3-C2-N1	-7.93	121.91	128.89
2	A	1378	SFG	C5-C4-N3	-6.05	120.08	125.98
2	A	1378	SFG	N3-C4-N9	5.29	134.46	125.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1378	SFG	C5-C4-N3	-5.04	121.07	125.98
2	B	1378	SFG	N3-C4-N9	4.28	132.73	125.39
2	A	1378	SFG	O4'-C4'-C5'	-3.30	104.48	109.44
2	B	1378	SFG	O4'-C1'-C2'	-2.56	102.97	106.69
2	A	1378	SFG	O4'-C1'-C2'	-2.48	103.08	106.69
2	B	1378	SFG	C2-N3-C4	2.43	120.27	113.27
2	A	1378	SFG	C2-N3-C4	2.35	120.05	113.27
2	B	1378	SFG	C5'-CD-NE	-2.34	102.46	109.13
2	B	1378	SFG	C4-C5-N7	-2.27	107.22	109.41
2	A	1378	SFG	C-CA-N	-2.15	105.75	109.31
2	B	1378	SFG	C5'-C4'-C3'	-2.03	112.91	115.19

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	337/382 (88%)	-0.22	3 (0%) 81 84	15, 26, 49, 96	0
1	B	328/382 (85%)	-0.21	5 (1%) 70 73	17, 27, 54, 91	0
All	All	665/764 (87%)	-0.21	8 (1%) 75 78	15, 26, 51, 96	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	41	ARG	4.8
1	B	351	ASP	2.8
1	A	49	LEU	2.6
1	B	206	TRP	2.6
1	B	48	GLN	2.4
1	A	42	THR	2.3
1	B	50	TYR	2.3
1	B	49	LEU	2.2

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	SFG	A	1378	27/27	0.07	-0.39	16,18,22,22	0
2	SFG	B	1378	27/27	0.06	-0.58	23,25,29,31	0

6.5 Other polymers ⓘ

There are no such residues in this entry.