



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 21, 2017 – 12:45 PM EST

PDB ID : 5FWA
Title : Crystal Structure of Mus musculus Protein Arginine Methyltransferase 2 with CP1
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Deposited on : 2016-02-16
Resolution : 1.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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-20028442
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-20028442

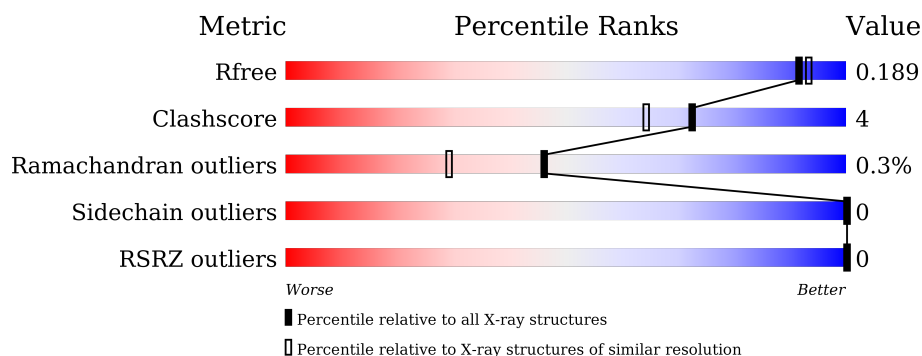
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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	446	

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
3	PG4	A	1447	-	-	X	X
5	EDO	A	1450	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	EDO	A	1451	-	-	-	X

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 3078 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.

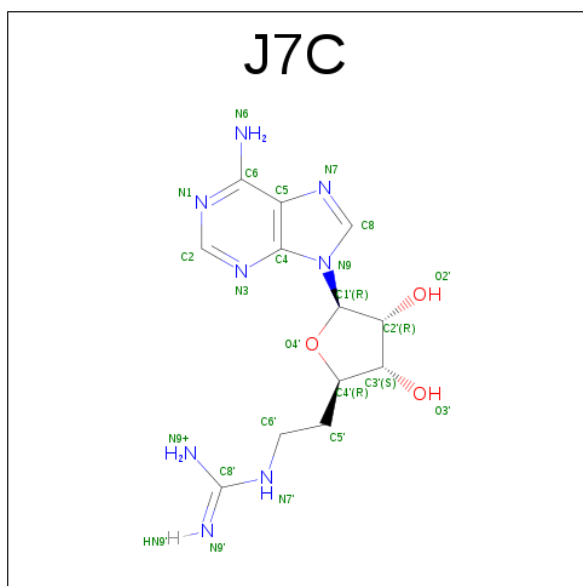
- Molecule 1 is a protein called PROTEIN ARGININE N-METHYLTRANSFERASE 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	339	Total	C	N	O	S	0	0	0
			2723	1752	451	505	15			

There are 2 discrepancies between the modelled and reference sequences:

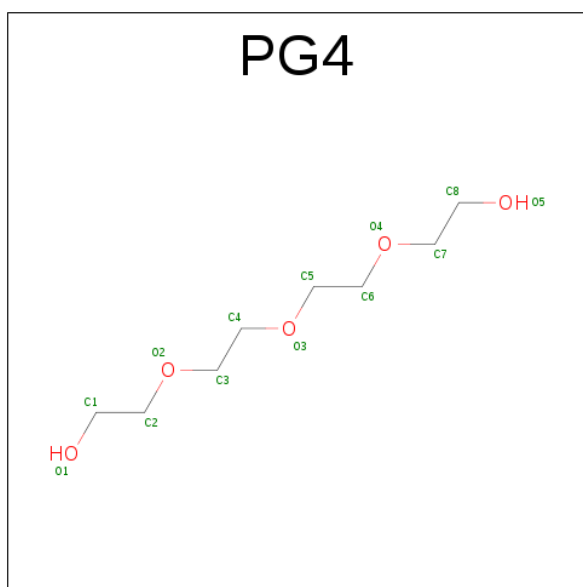
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	EXPRESSION TAG	UNP Q3UKX1
A	445	TRP	ARG	ENGINEERED	UNP Q3UKX1

- Molecule 2 is 9-(6-carbamimidamido-5,6-dideoxy-beta-D-ribo-hexofuranosyl)-9H-purin-6-amine (three-letter code: J7C) (formula: C₁₂H₁₈N₈O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			23	12	8	3		

- Molecule 3 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).

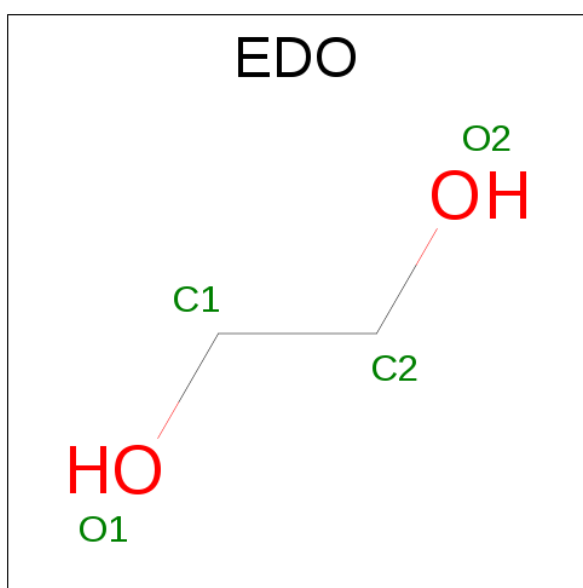


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	8	5		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	2	Total Ca 2 2	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	304	Total O 304 304	0	0

● Molecule 1: PROTEIN ARGININE N-METHYLTRANSFERASE 2

E245	GLN	GLY
E232	LEU	MET
F233	SER	GLU
	PHE	ALA
I251	LEU	PRO
	ARG	GLY
H271	GLY	GLU
	GLY	GLY
L275	LYS	PRO
	ILE	CYS
A280	LEU	SER
	ILE	GLU
L285	LEU	SER
	ARG	GLN
F300	GLN	VAL
	THR	ILE
I319	THR	PRO
	ALA	VAL
M334	ASP	LEU
	TRP	GLU
L362	TRP	GLU
	GLY	ASP
Q369	GLU	PRO
V370	ARG	VAL
L371	ALA	ASP
	GLY	TYR
Q408	CYS	GLY
R409	CYS	CYS
	GLY	GLU
V412	TYR	MET
R414	ILE	LEU
	PRO	GLN
F441	ALA	GLN
F442	ASN	ASP
I443	HIS	GLY
W444	LEU	ALA
W445	GLY	GLN
	LYS	LEU
	GLN	GLN
	LEU	LEU
	GLU	GLU
	TYR	LEU
	ASP	PRO
	PRO	GLU
	GLU	GLU
	DI107	PHE
	T108	VAL
	K136	ALA
	Q143	ALA
	K151	ASP
	H170	THR
	D199	THR
		GLU

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	66.18Å 114.68Å 132.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.37 – 1.80 43.37 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (43.37-1.80) 99.9 (43.37-1.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 1.79Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.172 , 0.191 0.167 , 0.189	Depositor DCC
R_{free} test set	2343 reflections (4.98%)	DCC
Wilson B-factor (Å ²)	29.9	Xtriage
Anisotropy	0.358	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.024 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.029 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	3078	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.48% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PG4, CA, J7C, EDO, CL

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	0.26	0/2798	0.43	0/3811

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

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	2723	0	2673	23	0
2	A	23	0	0	0	0
3	A	13	0	18	7	0
4	A	1	0	0	0	0
5	A	12	0	18	0	0
6	A	2	0	0	0	0
7	A	304	0	0	4	1
All	All	3078	0	2709	23	1

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 4.

The worst 5 of 23 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:362:LEU:HD22	3:A:1447:PG4:H21	1.64	0.79
1:A:170:HIS:NE2	7:A:2032:HOH:O	2.24	0.70
1:A:319:LEU:HD11	1:A:334:MET:HE2	1.78	0.66
1:A:151:LYS:HE2	3:A:1447:PG4:H62	1.79	0.64
1:A:107:ASP:OD2	7:A:2002:HOH:O	2.16	0.62

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:2125:HOH:O	7:A:2210:HOH:O[3_454]	2.19	0.01

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	337/446 (76%)	331 (98%)	5 (2%)	1 (0%)	46 29

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	232	GLU

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	305/394 (77%)	305 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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 ⓘ

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 ⓘ

Of 8 ligands modelled in this entry, 3 are monoatomic - leaving 5 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	$\# Z > 2$
2	J7C	A	1446	-	19,25,25	0.54	0	16,36,36	0.44	0
3	PG4	A	1447	-	12,12,12	0.51	0	11,11,11	0.32	0
5	EDO	A	1449	-	3,3,3	0.44	0	2,2,2	0.43	0
5	EDO	A	1450	-	3,3,3	0.45	0	2,2,2	0.40	0
5	EDO	A	1451	-	3,3,3	0.47	0	2,2,2	0.35	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
2	J7C	A	1446	-	-	0/4/26/26	0/3/3/3
3	PG4	A	1447	-	-	0/10/10/10	0/0/0/0
5	EDO	A	1449	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1450	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1451	-	-	0/1/1/1	0/0/0/0

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.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1447	PG4	7	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	339/446 (76%)	-0.38	0 100 100	23, 32, 48, 67	0

There are no RSRZ outliers to report.

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

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

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(Å ²)	Q<0.9
5	EDO	A	1451	4/4	0.61	0.26	16.44	61,61,61,63	0
5	EDO	A	1450	4/4	0.82	0.20	7.86	58,58,59,60	0
3	PG4	A	1447	13/13	0.84	0.15	3.71	43,48,59,63	0
2	J7C	A	1446	23/23	0.97	0.12	0.49	20,24,29,30	0
4	CL	A	1448	1/1	0.99	0.05	-1.63	40,40,40,40	0
6	CA	A	1453	1/1	0.95	0.06	-	78,78,78,78	1
5	EDO	A	1449	4/4	0.76	0.14	-	62,63,63,63	0
6	CA	A	1452	1/1	0.63	0.16	-	91,91,91,91	0

6.5 Other polymers [i](#)

There are no such residues in this entry.