



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2018 – 08:41 pm GMT

PDB ID : 3D45
Title : Crystal structure of mouse PARN in complex with m7GpppG
Authors : Wu, M.; Song, H.
Deposited on : 2008-05-13
Resolution : 3.00 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

<https://www.wwpdb.org/validation/2017/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 : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

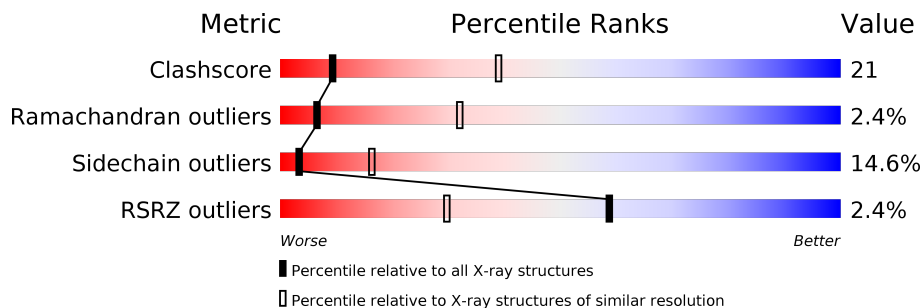
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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))
Clashscore	122126	2167 (3.00-3.00)
Ramachandran outliers	120053	2101 (3.00-3.00)
Sidechain outliers	120020	2104 (3.00-3.00)
RSRZ outliers	108989	1751 (3.00-3.00)

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	507	<div> <div>2%</div> <div>45%</div> <div>25%</div> <div>5%</div> <div>24%</div> </div>
1	B	507	<div> <div>2%</div> <div>39%</div> <div>27%</div> <div>7%</div> <div>26%</div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6307 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.

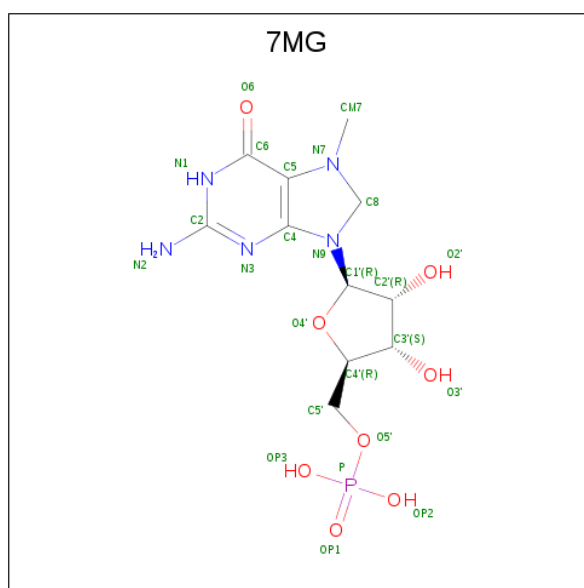
- Molecule 1 is a protein called Poly(A)-specific ribonuclease PARN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	383	Total	C	N	O	S	0	0	0
			3109	2005	503	586	15			
1	B	373	Total	C	N	O	S	0	0	0
			3016	1947	488	567	14			

There are 4 discrepancies between the modelled and reference sequences:

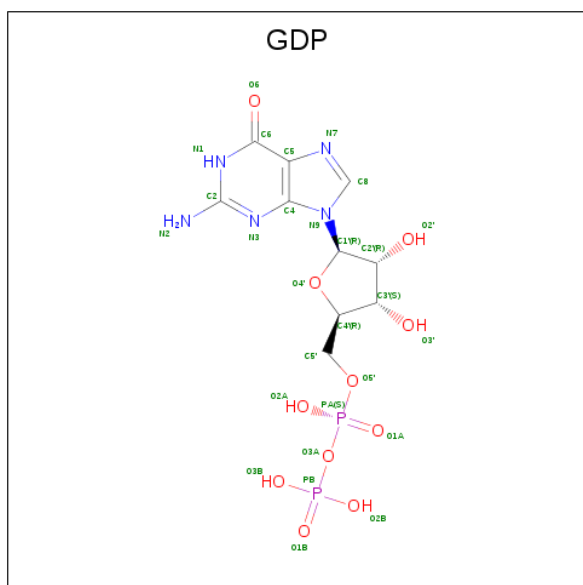
Chain	Residue	Modelled	Actual	Comment	Reference
A	901	GLY	-	EXPRESSION TAG	UNP Q8VDG3
A	900	PRO	-	EXPRESSION TAG	UNP Q8VDG3
B	901	GLY	-	EXPRESSION TAG	UNP Q8VDG3
B	900	PRO	-	EXPRESSION TAG	UNP Q8VDG3

- Molecule 2 is 7N-METHYL-8-HYDROGUANOSINE-5'-MONOPHOSPHATE (three-letter code: 7MG) (formula: $C_{11}H_{18}N_5O_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			24	11	5	7	1		
2	B	1	Total	C	N	O	P	0	0
			24	11	5	7	1		

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



D470	D471	A474	F475	V476	S477	Q480	Q483	V484	Q485	I486	A487	N488	N489	T490	S491	K492	Y493	A494	E495	S496	Y497	R498	I499	Q500	T501	Y502	A503	E504	Y505																										
PRO	LYS	MET	CYS	VAL	SER	ALA	ARG	S405	K406	L407	I408	E409	F410	F411	F412	N413	K414	L415	F416	L417	M418	R419	VAL	MET	ASP	I423	P424	Y425	L426	M427	L428	E429	G430	P431	D432	L433	Q434	F435	K436	R437	D438	H439	V440	L441	H442	V443	P446	W449	F461	G462	M463	I464	Q465	I466	I469
HIS	ILE	VAL	ILE	SER	LYS	VAL	ASP	GLU	GLU	GLU	ARG	LYS	ARG	ARG	GLU	GLN	GLU	LYS	TYR	T251	E252	E253	Q254	E255	E256	L257	N258	D259	A260	V261	Q262	A271	V278	G279	M282	L283	L284	D285	H288	T289	I290	H291	Q292	F293	Y294	C295	P296	L297	V311	F312	P313	R314	L315	L316	
D317	T318	K319	T324	Q325	P326	F327	K328	I331	N332	N333	T334	S335	E340	K341	R342	L343	K344	E345	T346	P347	F348	D349	P350	P351	K352	E357	GLY	PHE	PRO	TYR	SER	ASP	THR	ALA	SER	GLU	GLN	LEU	H370	E371	A372	G373	Y374	L381	S385	L390	G391	SER	LEU	LEU	SER	PRO			

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.01Å 128.35Å 176.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	103.69 – 3.00 72.82 – 2.92	Depositor EDS
% Data completeness (in resolution range)	94.7 (103.69-3.00) 94.0 (72.82-2.92)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.299 , 0.334 0.294 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	78.7	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 70.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	6307	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.61% 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: GDP, 7MG

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	0.65	2/3189 (0.1%)	0.73	0/4306
1	B	0.67	0/3093	0.74	0/4179
All	All	0.66	2/6282 (0.0%)	0.74	0/8485

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	108	CYS	CB-SG	-5.96	1.72	1.81
1	A	310	CYS	CB-SG	-5.18	1.73	1.81

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	430	GLY	Peptide

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	3109	0	2999	112	0
1	B	3016	0	2926	138	0
2	A	24	0	16	4	0
2	B	24	0	16	6	0
3	A	28	0	12	4	0
3	B	28	0	12	4	0
4	A	34	0	0	6	0
4	B	44	0	0	9	0
All	All	6307	0	5981	257	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 21.

The worst 5 of 257 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:325:GLN:HE21	1:B:325:GLN:HA	1.07	1.09
1:B:484:VAL:O	1:B:488:VAL:HG23	1.71	0.90
1:A:470:ASP:HB2	1:A:473:SER:OG	1.70	0.90
1:B:66:LEU:H	1:B:292:GLN:HE22	1.03	0.90
1:B:325:GLN:CA	1:B:325:GLN:HE21	1.86	0.89

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	373/507 (74%)	322 (86%)	43 (12%)	8 (2%)	8 36
1	B	363/507 (72%)	316 (87%)	37 (10%)	10 (3%)	5 28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	736/1014 (73%)	638 (87%)	80 (11%)	18 (2%)	6	32

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	405	SER
1	A	438	ASP
1	B	433	LEU
1	B	491	SER
1	A	252	LYS

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	345/458 (75%)	303 (88%)	42 (12%)	5	23
1	B	335/458 (73%)	278 (83%)	57 (17%)	2	11
All	All	680/916 (74%)	581 (85%)	99 (15%)	3	16

5 of 99 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	25	PHE
1	B	104	VAL
1	B	471	ASP
1	B	39	SER
1	B	66	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	463	ASN
1	B	17	GLN
1	B	427	ASN

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Mol	Chain	Res	Type
1	A	485	GLN
1	B	89	ASN

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 ⓘ

4 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	7MG	A	651	-	20,26,27	1.80	3 (15%)	23,39,42	2.68	6 (26%)
3	GDP	A	652	-	25,30,30	1.15	2 (8%)	27,47,47	1.98	8 (29%)
3	GDP	B	1151	-	25,30,30	1.37	2 (8%)	27,47,47	2.20	8 (29%)
2	7MG	B	1152	-	20,26,27	1.41	3 (15%)	23,39,42	2.31	6 (26%)

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	7MG	A	651	-	-	0/7/37/38	0/3/3/3
3	GDP	A	652	-	-	0/12/32/32	0/3/3/3
3	GDP	B	1151	-	-	0/12/32/32	0/3/3/3
2	7MG	B	1152	-	-	0/7/37/38	0/3/3/3

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	651	7MG	O5'-C5'	-5.08	1.37	1.44
2	A	651	7MG	C8-N9	-3.32	1.37	1.45
2	B	1152	7MG	C8-N9	-2.55	1.39	1.45
2	B	1152	7MG	C2-N3	-2.44	1.31	1.35
3	A	652	GDP	C5-C4	2.94	1.47	1.40

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	651	7MG	C5-C6-N1	-7.51	111.59	123.34
2	B	1152	7MG	C5-C6-N1	-6.80	112.70	123.34
3	A	652	GDP	C6-C5-C4	-4.30	116.63	120.85
3	B	1151	GDP	PA-O3A-PB	-4.17	118.62	132.63
3	B	1151	GDP	C6-C5-C4	-4.06	116.86	120.85

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	651	7MG	4	0
3	A	652	GDP	4	0
3	B	1151	GDP	4	0
2	B	1152	7MG	6	0

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 [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	383/507 (75%)	0.41	8 (2%) 63 34	58, 75, 95, 110	0
1	B	373/507 (73%)	0.35	10 (2%) 54 26	57, 76, 95, 107	0
All	All	756/1014 (74%)	0.38	18 (2%) 59 30	57, 75, 95, 110	0

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	494	ALA	3.6
1	B	385	SER	3.4
1	B	465	GLN	3.0
1	A	497	TYR	2.9
1	A	495	GLU	2.9

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. 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	B-factors(\AA^2)	Q<0.9
3	GDP	B	1151	28/28	0.81	0.23	114,118,121,122	0
2	7MG	B	1152	24/25	0.91	0.19	61,68,75,76	0
2	7MG	A	651	24/25	0.93	0.21	54,64,65,68	0
3	GDP	A	652	28/28	0.96	0.20	57,60,64,65	0

6.5 Other polymers [i](#)

There are no such residues in this entry.