



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 4, 2017 – 06:40 PM EDT

PDB ID : 1Z1C  
Title : Structural Determinants of Tissue Tropism and In Vivo Pathogenicity for the Parvovirus Minute virus of Mice  
Authors : Kontou, M.; Govindasamy, L.; Nam, H.J.; Bryant, N.; Llamas-Saiz, A.L.; Foces-Foces, C.; Hernando, E.; Rubio, M.P.; McKenna, R.; Almendral, J.M.; Agbandje-McKenna, M.  
Deposited on : unknown  
Resolution : 3.50 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](mailto: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.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

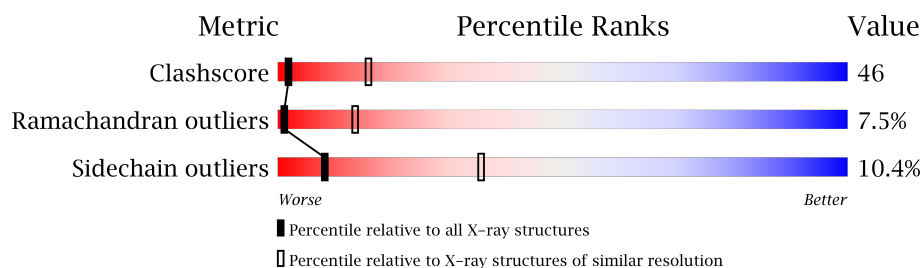
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 Å.

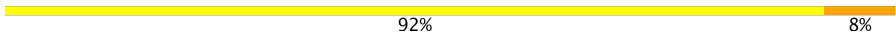
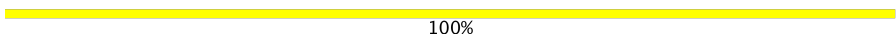

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	1322 (3.60-3.40)
Ramachandran outliers	110173	1283 (3.60-3.40)
Sidechain outliers	110143	1284 (3.60-3.40)

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  $\geq 3$ , 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	B	12	
2	C	9	
3	A	587	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4864 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 DNA chain called 5'-D(\*AP\*TP\*CP\*CP\*TP\*CP\*TP\*AP\*TP\*CP\*AP\*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	12	Total	C	N	O	P	0	0	0
			235	115	38	71	11			

- Molecule 2 is a DNA chain called 5'-D(\*AP\*CP\*AP\*CP\*CP\*AP\*AP\*AP\*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	9	Total	C	N	O	P	0	0	0
			180	87	39	46	8			

- Molecule 3 is a protein called Coat protein VP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	549	Total	C	N	O	S	0	0	0
			4328	2727	751	830	20			

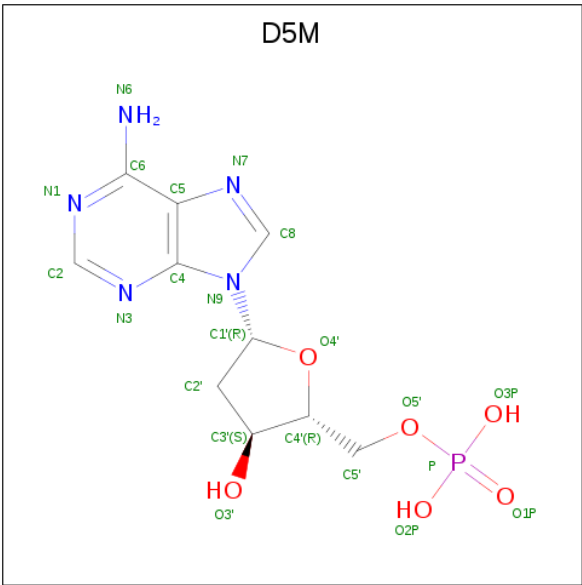
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	366	MET	VAL	SEE REMARK 999	UNP P07302
A	455	THR	ALA	SEE REMARK 999	UNP P07302

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Ca	0	0
			2	2		

- Molecule 5 is 2'-DEOXYADENOSINE-5'-MONOPHOSPHATE (three-letter code: D5M) (formula: C<sub>10</sub>H<sub>14</sub>N<sub>5</sub>O<sub>6</sub>P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			18	10	5	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	5	Total	O	0	0
			5	5		
6	C	11	Total	O	0	0
			11	11		
6	A	85	Total	O	0	0
			85	85		



K523	K524	K528	K529	K530	L531	T532	K533	L537	K540	T541	T542	K543	K544	P545	V546	T547	V551	E552	D553	K554	G555	S560	V561	T562	K563	K564	L565	P566	T567	K571	K572	Q573	P576	L577	T578	T579	K580	P581	V582	K583	K584	K585	T586	Y587
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## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	448.70 Å 416.70 Å 305.30 Å 90.00° 95.80° 90.00°	Depositor
Resolution (Å)	20.00 – 3.50	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-3.50)	Depositor
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.325 , 0.329	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4864	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, D5M

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	B	0.74	0/261	0.84	0/399
2	C	0.74	0/203	0.90	0/310
3	A	1.14	8/4452 (0.2%)	1.08	31/6088 (0.5%)
All	All	1.11	8/4916 (0.2%)	1.06	31/6797 (0.5%)

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
3	A	0	3
All	All	0	4

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	586	THR	N-CA	41.38	2.29	1.46
3	A	418	PRO	N-CD	37.60	2.00	1.47
3	A	234	HIS	N-CA	26.69	1.99	1.46
3	A	227	ASN	N-CA	13.98	1.74	1.46
3	A	581	PRO	N-CD	11.41	1.63	1.47

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	585	ASN	C-N-CA	-21.02	69.14	121.70
3	A	418	PRO	N-CA-CB	18.13	125.05	103.30
3	A	418	PRO	CA-N-CD	-17.05	87.63	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	233	GLU	C-N-CA	-14.67	85.02	121.70
3	A	586	THR	N-CA-CB	-14.06	83.58	110.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	194	SER	Mainchain
3	A	363	THR	Peptide
3	A	417	ALA	Peptide
1	B	7	DT	Sidechain

## 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	B	235	0	138	30	0
2	C	180	0	101	19	0
3	A	4328	0	4124	384	0
4	B	2	0	0	0	0
5	B	18	0	12	3	0
6	A	85	0	0	0	0
6	B	5	0	0	0	0
6	C	11	0	0	0	0
All	All	4864	0	4375	421	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 46.

The worst 5 of 421 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)
3:A:227:ASN:CA	3:A:227:ASN:N	1.74	1.51
3:A:380:LYS:NZ	3:A:386:TRP:O	1.56	1.34
3:A:385:ASN:OD1	3:A:386:TRP:N	1.67	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:234:HIS:CA	3:A:234:HIS:N	1.99	1.25
3:A:418:PRO:CD	3:A:418:PRO:N	2.00	1.23

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	
3	A	547/587 (93%)	432 (79%)	74 (14%)	41 (8%)	1	13

5 of 41 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	218	ASP
3	A	226	GLU
3	A	233	GLU
3	A	380	LYS
3	A	381	GLN

### 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	
3	A	472/492 (96%)	423 (90%)	49 (10%)	8	36

5 of 49 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	320	MET
3	A	377	SER
3	A	562	THR
3	A	359	PRO
3	A	385	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
3	A	286	ASN
3	A	381	GLN
3	A	573	GLN
3	A	335	GLN
3	A	371	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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
5	D5M	B	231	-	17,20,24	0.54	0	18,29,36	0.59	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
5	D5M	B	231	-	-	0/2/18/22	0/3/3/3

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 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	231	D5M	3	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

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.