



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 08:51 AM UTC

PDB ID : 1MVM / pdb_00001mvm
Title : MVM(STRAIN I), COMPLEX(VIRAL COAT/DNA), VP2, PH=7.5, T=4 DEGREES C
Authors : Llamas-Saiz, A.L.; Agbandje-McKenna, M.; Rossmann, M.G.
Deposited on : 1996-06-21
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

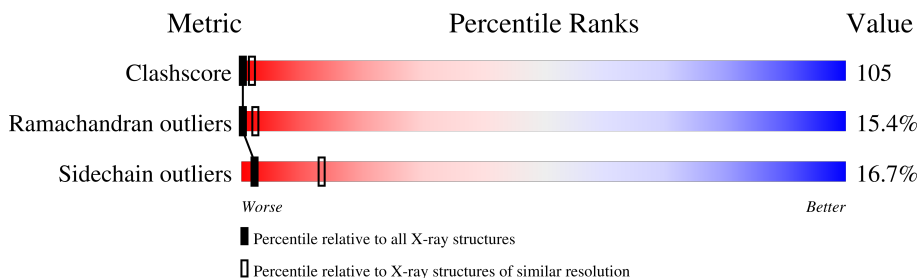
1 Overall quality at a glance

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	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	587	
2	B	11	
3	C	4	
4	D	1	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4649 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 (MURINE MINUTE VIRUS COAT PROTEIN).

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	366	MET	VAL	variant	UNP P07302
A	455	THR	ALA	variant	UNP P07302

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	B	11	218	103	41	63	11	0	0	0

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


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	C	4	82	39	18	21	4	0	0	0

- Molecule 4 is a DNA chain called DNA (5'-D(P*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
4	D	1	21	10	5	5	1	0	0	0

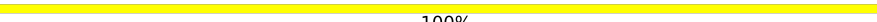
C1
C2
A3
C4
C5
C6
C7
A8
A9
C10
A11

- Molecule 3: DNA (5'-D(*CP*AP*AP*A)-3')

Chain C:  75% 25%

C14
A15
A16
A17

- Molecule 4: DNA (5'-D(P*A)-3')

Chain D:  100%

A20

4 Data and refinement statistics

Xtrriage (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, α , β , γ	448.70Å 416.70Å 305.30Å 90.00° 95.80° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.50	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.50)	Depositor
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	NONE	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	4649	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

5 Model quality i

5.1 Standard geometry i

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	1.97	45/4451 (1.0%)	1.62	79/6085 (1.3%)
2	B	0.88	2/242 (0.8%)	0.98	0/364
3	C	0.75	0/92	1.45	1/139 (0.7%)
4	D	0.61	0/23	0.90	0/33
All	All	1.91	47/4808 (1.0%)	1.59	80/6621 (1.2%)

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	A	0	5

The worst 5 of 47 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	587	TYR	C-OXT	-46.38	0.30	1.23
1	A	344	ASP	C-N	-42.27	0.74	1.33
1	A	373	SER	C-N	-41.17	0.77	1.33
1	A	174	ALA	C-N	36.89	1.84	1.33
1	A	526	PHE	C-N	34.51	1.78	1.33

The worst 5 of 80 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	373	SER	O-C-N	-26.45	90.62	122.89
1	A	539	ALA	CA-C-N	-19.54	90.91	122.76
1	A	539	ALA	C-N-CA	-19.54	90.91	122.76
1	A	374	VAL	O-C-N	18.70	145.94	122.57
1	A	373	SER	CA-C-N	17.20	152.93	121.97

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	373	SER	Mainchain
1	A	525	PHE	Mainchain,Peptide
1	A	537	LEU	Mainchain
1	A	539	ALA	Mainchain

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	4328	0	4109	908	0
2	B	218	0	123	26	0
3	C	82	0	45	12	0
4	D	21	0	12	2	0
All	All	4649	0	4289	938	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 105.

The worst 5 of 938 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:378:TYR:CE1	1:A:465:GLN:NE2	1.70	1.57
1:A:176:MET:HE1	1:A:525:PHE:CD1	1.38	1.56
1:A:344:ASP:C	1:A:345:PHE:CA	1.80	1.49
1:A:558:TYR:CA	1:A:563:LYS:HZ1	1.26	1.48
1:A:344:ASP:O	1:A:345:PHE:CD1	1.69	1.45

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	545/587 (93%)	374 (69%)	87 (16%)	84 (15%)	0 2

5 of 84 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	95	LYS
1	A	159	ASP
1	A	164	ALA
1	A	183	ASN
1	A	218	ASP

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	472/492 (96%)	393 (83%)	79 (17%)	2 13

5 of 79 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	389	HIS
1	A	516	LEU
1	A	405	SER
1	A	448	ASN
1	A	550	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	445	ASN
1	A	492	ASN

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Mol	Chain	Res	Type
1	A	573	GLN
1	A	458	HIS
1	A	496	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	10
2	B	1

The worst 5 of 11 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	10:DC	O3'	11:DA	P	2.98
1	A	352:PRO	C	353:PHE	N	2.03
1	A	174:ALA	C	175:CYS	N	1.84

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	483:ILE	C	484:THR	N	1.84
1	A	526:PHE	C	527:TRP	N	1.78

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.