

wwPDB X-ray Structure Validation Summary Report (i)

Apr 10, 2023 – 05:29 PM EDT

PDB ID : 1MVM

Title: MVM(STRAIN I), COMPLEX(VIRAL COAT/DNA), VP2, PH=7.5, T=4

DEGREES C

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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.orgA user guide is available at

https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

MolProbity: 4.02b-467

Xtriage (Phenix) : NOT EXECUTED EDS : NOT EXECUTED

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

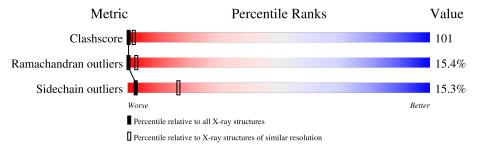
Validation Pipeline (wwPDB-VP) : 2.32.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY\ DIFFRACTION$

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	Similar resolution		
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$		
Clashscore	141614	1036 (3.58-3.42)		
Ramachandran outliers	138981	1005 (3.58-3.42)		
Sidechain outliers	138945	1006 (3.58-3.42)		

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain							
1	A	587	20%	46%	22%	5% 6%				
2	В	11	9%	73%		18%				
3	С	4	5	50%	50%					
4	D	1		100%						



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
1	A	549	Total 4328	C 2727	N 751	O 830	S 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*AP*AP*CP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	В	11	Total 218	C 103	N 41	O 63	P 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
3	С	4	Total 82	C 39	N 18	O 21	P 4	0	0	0

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

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

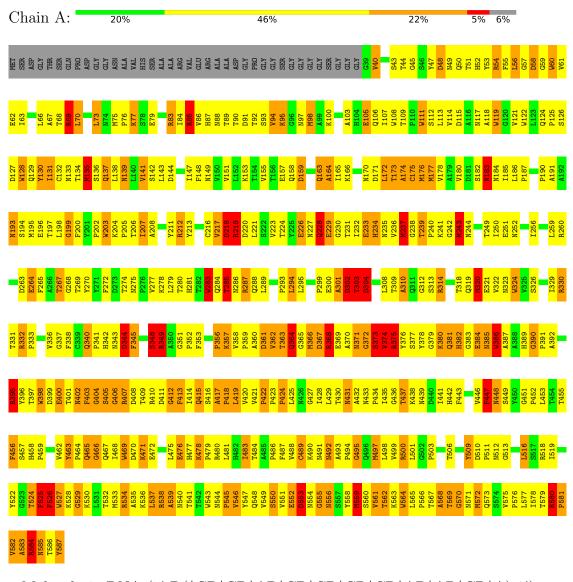


3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: PROTEIN (MURINE MINUTE VIRUS COAT PROTEIN)



• Molecule 2: DNA (5'-D(*CP*CP*AP*CP*CP*CP*CP*AP*AP*CP*A)-3')

Chain B: 9% 73% 18%



C1 C2 C4 C5 C6 C7 C7 A8 A9 A9

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

Chain C: 50% 50%

C14 A15 A16 A17

• Molecule 4: DNA (5'-D(P*A)-3')

Chain D: 100%

A20



4 Data and refinement statistics (i)

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

Property	Value	Source	
Space group	C 1 2 1	Depositor	
Cell constants	448.70Å 416.70Å 305.30Å	Depositor	
a, b, c, α , β , γ	90.00° 95.80° 90.00°	Depositor	
Resolution (Å)	(Not available) - 3.50	Depositor	
% Data completeness	(Not available) ((Not available)-3.50)	Depositor	
(in resolution range)	(110t available) ((110t available) 9.90)	1	
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.	Xtriage	
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	Bo	nd lengths	Bond angles		
WIOI		RMSZ	# Z > 5	RMSZ	# Z >5	
1	A	1.49	$25/4451 \ (0.6\%)$	1.38	61/6085 (1.0%)	
2	В	1.43	3/242 (1.2%)	1.15	0/364	
3	С	1.49	0/92	2.31	2/139 (1.4%)	
4	D	1.28	0/23	1.16	0/33	
All	All	1.48	$28/4808 \; (0.6\%)$	1.39	63/6621 (1.0%)	

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 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	Ideal(A)
1	A	587	TYR	C-OXT	-48.72	0.30	1.23
1	A	344	ASP	C-N	-25.89	0.74	1.34
1	A	373	SER	C-N	-24.52	0.77	1.34
1	A	555	GLY	CA-C	-24.12	1.13	1.51
1	A	174	ALA	C-N	22.05	1.84	1.34

The worst 5 of 63 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	373	SER	O-C-N	-20.05	90.62	122.70
3	С	14	DC	OP1-P-OP2	-20.02	89.57	119.60
1	A	374	VAL	O-C-N	14.52	145.94	122.70
1	A	525	PHE	O-C-N	-13.22	101.55	122.70
1	A	373	SER	CA-C-N	13.19	146.21	117.20

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	Peptide, Mainchain
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	4108	874	0
2	В	218	0	123	26	0
3	С	82	0	45	12	0
4	D	21	0	12	2	0
All	All	4649	0	4288	904	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 101.

The worst 5 of 904 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	1.45	1.48
1:A:558:TYR:CA	1:A:563:LYS:HZ1	1.26	1.48
1:A:344:ASP:C	1:A:345:PHE:CA	1.80	1.45
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 3

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	Analysed Rotameric Outliers		Percentiles	
1	A	472/492 (96%)	400 (85%)	72 (15%)	2 17	

5 of 72 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	415	GLN
1	A	559	MET
1	A	447	PHE
1	A	516	LEU
1	A	193	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	433	ASN
1	A	492	ASN

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Mol	Chain	Res	Type
1	A	458	HIS
1	A	540	ASN
1	A	133	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 monosaccharides 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:

N	/Iol	Chain	Number of breaks
	1	A	10
	2	В	1

The worst 5 of 11 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	В	10:DC	O3'	11:DA	Р	2.98
1	A	352:PRO	С	353:PHE	N	2.03
1	A	174:ALA	С	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	С	484:THR	N	1.84
1	A	526:PHE	С	527:TRP	N	1.78



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

