

wwPDB X-ray Structure Validation Summary Report (i)

May 21, 2020 – 01:29 pm BST

PDB ID : 5DDJ

Title: Crystal structure of recombinant foot-and-mouth-disease virus O1M-S2093Y

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Deposited on : 2015-08-25

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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity : 4.02b-467 Xtriage (Phenix) : 1.13

EDS : 2.11

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

Refmac: 5.8.0158

CCP4 : 7.0.044 (Gargrove)

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

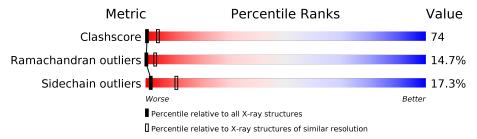
Validation Pipeline (wwPDB-VP) : 2.11

1 Overall quality at a glance (i)

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	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 on 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%

Mol	Chain	Length		Qu	ality of chair	1		
1	1	211	16%	48%		21%	•	13%
2	2	218	21%		52%	2	2%	
3	3	220	29%		52%	_	18%	•
4	4	85	16%	32%	6%	46%		



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5131 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 Foot and mouth disease virus, VP1.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	1	184	Total 1437	C 910	N 258	O 266	S 3	0	0	0

• Molecule 2 is a protein called Foot and mouth disease virus, VP2.

\mathbf{Mol}	Chain	Residues		\mathbf{At}	oms			ZeroOcc	${f AltConf}$	Trace
2	2	210	Total 1656	C 1057	N 282	O 310	S 7	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	93	TYR	SER	engineered mutation	UNP Q6PMW3

• Molecule 3 is a protein called Foot and mouth disease virus, VP3.

Mol	Chain	Residues		\mathbf{At}	oms			ZeroOcc	${f AltConf}$	Trace
3	3	220	Total 1685	C 1079	N 274	O 323	S 9	0	0	0

• Molecule 4 is a protein called Genome polyprotein.

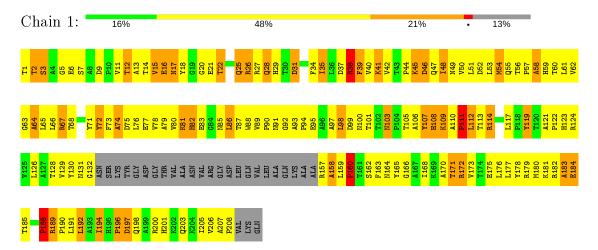
Mol	Chain	Residues		\mathbf{Atc}	$\mathbf{m}\mathbf{s}$			ZeroOcc	AltConf	Trace
4	4	46	Total 353	C 222	N 57	O 72	S 2	0	0	0



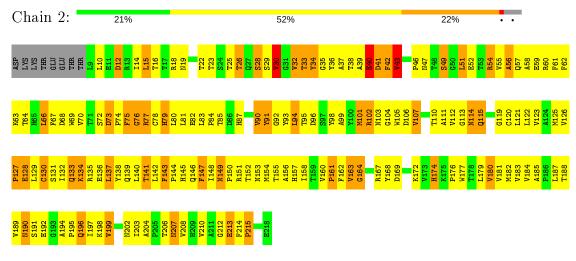
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

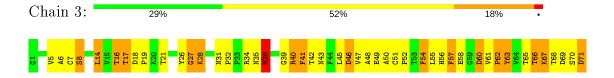
• Molecule 1: Foot and mouth disease virus, VP1



• Molecule 2: Foot and mouth disease virus, VP2



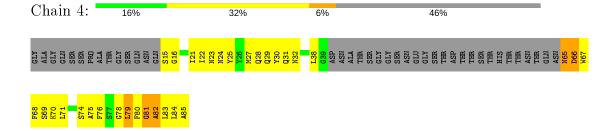
• Molecule 3: Foot and mouth disease virus, VP3







• Molecule 4: Genome polyprotein





4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants	344.08Å 344.08Å 344.08Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.66 - 3.50	Depositor
rtesolution (A)	45.98 - 3.50	EDS
% Data completeness	77.8 (49.66-3.50)	Depositor
(in resolution range)	77.8 (45.98-3.50)	EDS
R_{merge}	0.43	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.28 (at 3.48Å)	Xtriage
Refinement program	CNS 1.3	Depositor
D D.	0.361 , (Not available)	Depositor
R, R_{free}	0.361 , (Not available)	DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	65.1	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.30 , 87.1	EDS
L-test for twinning ²	$< L >=0.38, < L^2>=0.21$	Xtriage
Estimated twinning fraction	0.499 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.70	EDS
Total number of atoms	5131	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 1.90% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of <|L|>, $< L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

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		
MIOI	Chain	RMSZ # Z > 5		RMSZ	# Z > 5	
1	1	0.49	0/1471	0.82	$1/2012 \ (0.0\%)$	
2	2	0.52	0/1701	0.83	1/2323 (0.0%)	
3	3	0.56	0/1735	0.83	$2/2370 \ (0.1\%)$	
4	4	0.59	0/359	0.73	0/481	
All	All	0.53	0/5266	0.82	4/7186 (0.1%)	

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	1	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^o)$
2	2	28	SER	N-CA-C	-5.67	95.70	111.00
3	3	213	LEU	CA-CB-CG	5.58	128.14	115.30
1	1	81	LYS	N-CA-C	-5.21	96.94	111.00
3	3	79	LEU	CA-CB-CG	5.06	126.95	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	107	TYR	Sidechain



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	1	1437	0	1443	268	0
2	2	1656	0	1610	295	0
3	3	1685	0	1610	217	0
4	4	353	0	324	35	0
All	All	5131	0	4987	746	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 74.

The worst 5 of 746 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{aligned} ext{Interatomic} \ ext{distance} \ (ext{Å}) \end{aligned}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$
2:2:32:VAL:HG22	2:2:33:THR:H	1.02	1.11
2:2:91:TYR:HA	2:2:94:LEU:HD22	1.12	1.10
2:2:78:CYS:HB2	2:2:180:VAL:HG23	1.26	1.07
1:1:94:PRO:HG2	1:1:97:ALA:HB2	1.37	1.04
1:1:34:PHE:HA	4:4:16:GLY:HA2	1.35	1.04

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	1	180/211 (85%)	108 (60%)	42 (23%)	30 (17%)	0 2
2	2	$208/218 \; (95\%)$	124 (60%)	56 (27%)	28 (14%)	0 4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	3	218/220 (99%)	139 (64%)	50 (23%)	29 (13%)	0 4
4	4	42/85 (49%)	24 (57%)	10 (24%)	8 (19%)	0 2
All	All	648/734 (88%)	395 (61%)	158 (24%)	95 (15%)	0 3

5 of 95 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	15	VAL
1	1	16	GLU
1	1	38	ARG
1	1	39	PHE
1	1	45	LYS

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	1	153/173 (88%)	124 (81%)	29 (19%)	1 8
2	2	182/190 (96%)	149 (82%)	33 (18%)	1 9
3	3	176/176 (100%)	145 (82%)	31 (18%)	2 10
4	4	37/67 (55%)	35 (95%)	2 (5%)	22 55
All	All	548/606 (90%)	453 (83%)	95 (17%)	2 11

5 of 95 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	2	79	HIS
2	2	143	PHE
3	3	154	LYS
2	2	94	LEU
2	2	110	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:



Mol	Chain	Res	Type
2	2	19	ASN
2	2	103	ASN
3	3	141	HIS
1	1	108	HIS
3	3	191	HIS

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)

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)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

