wwPDB X-ray Structure Validation Summary Report (i)

Jan 27, 2024 – 10:29 AM EST

PDB ID	:	1BBT
Title	:	METHODS USED IN THE STRUCTURE DETERMINATION OF FOOT AND MOUTH DISEASE VIRUS
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Deposited on	:	1992-05-18
Resolution	:	2.60 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

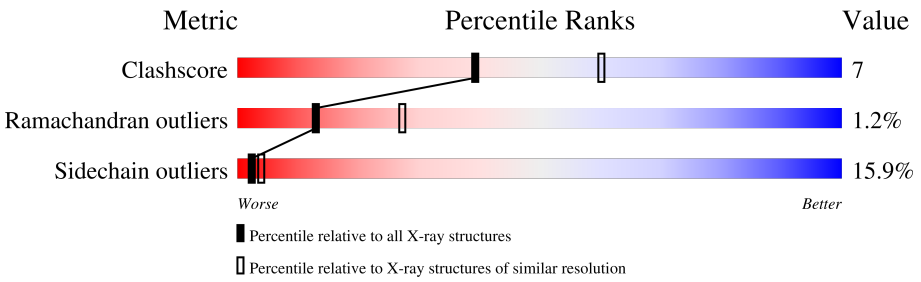
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.60 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	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)

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	1	213	59% 19% 7% • 13%
2	2	218	68% 18% 7% • •
3	3	220	70% 19% 8% •
4	4	85	36% 12% 6% 46%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5142 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 (SUBUNIT VP1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	1	186	1456	920	257	274	5	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	56	VAL	ILE	conflict	UNP Q84771
1	64	GLY	ALA	conflict	UNP Q84771
1	137	SER	ASN	conflict	UNP Q84771

- Molecule 2 is a protein called FOOT-AND-MOUTH DISEASE VIRUS (SUBUNIT VP2).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	2	210	1652	1052	282	311	7	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	130	CYS	TYR	conflict	UNP Q84771

- Molecule 3 is a protein called FOOT-AND-MOUTH DISEASE VIRUS (SUBUNIT VP3).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	3	220	1681	1075	275	322	9	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	85	HIS	GLN	conflict	UNP Q84771

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Chain	Residue	Modelled	Actual	Comment	Reference
3	168	THR	ALA	conflict	UNP Q84771
3	173	ASP	GLY	conflict	UNP Q84771

- Molecule 4 is a protein called FOOT-AND-MOUTH DISEASE VIRUS (SUBUNIT VP4).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	4	46	353	222	57	72	2	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	40	ASN	ASP	conflict	UNP O90754
4	41	ASP	ASN	conflict	UNP O90754

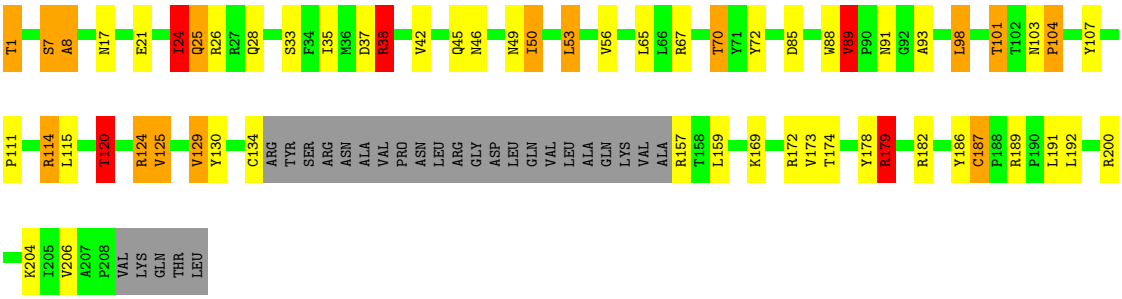
3 Residue-property plots (i)

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.

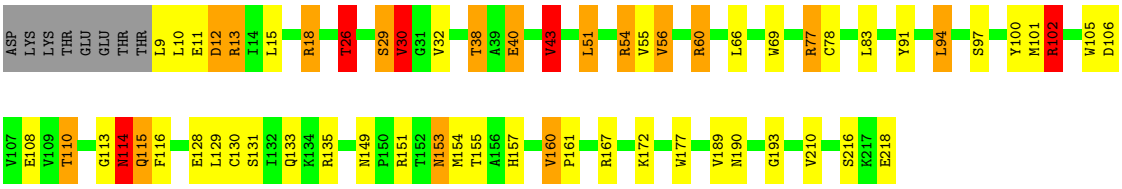
• Molecule 1: FOOT-AND-MOUTH DISEASE VIRUS (SUBUNIT VP1)

Chain 1:



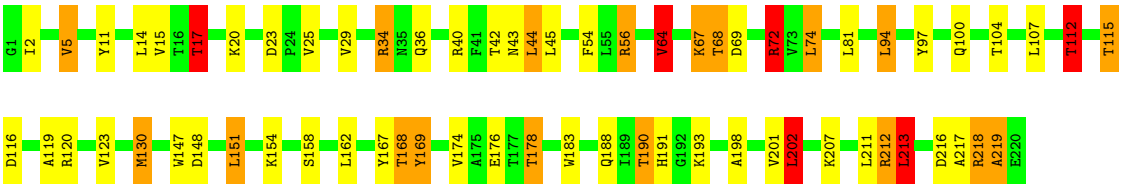
• Molecule 2: FOOT-AND-MOUTH DISEASE VIRUS (SUBUNIT VP2)

Chain 2:



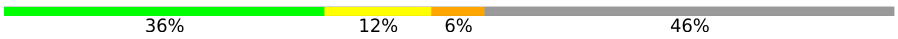
• Molecule 3: FOOT-AND-MOUTH DISEASE VIRUS (SUBUNIT VP3)

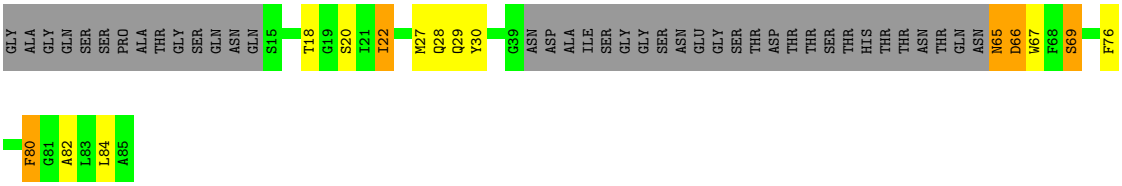
Chain 3:



• Molecule 4: FOOT-AND-MOUTH DISEASE VIRUS (SUBUNIT VP4)

Chain 4:




GLY
ALA
GLY
GLN
SER
SER
PRO
ALA
THR
GLY
SER
GLN
ASN
GLN
S15
T18
G19
S20
I21
I22
M27
Q28
Q29
Y30
G39
ASN
ASP
ALA
ILE
SER
GLY
GLY
SER
ASN
GLU
GLY
SER
THR
ASP
THR
THR
SER
THR
HIS
THR
THR
ASN
THR
GLN
ASN
N65
D66
W67
F68
S69
F76
F80
G81
A82
L83
L84
A85

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α, β, γ	345.00Å 345.00Å 345.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.169 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5142	wwPDB-VP
Average B, all atoms ($Å^2$)	13.0	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	1	1.08	1/1490 (0.1%)	2.04	44/2035 (2.2%)
2	2	1.15	3/1695 (0.2%)	1.98	55/2314 (2.4%)
3	3	1.08	0/1729	1.93	63/2361 (2.7%)
4	4	1.17	2/359 (0.6%)	2.04	10/481 (2.1%)
All	All	1.11	6/5273 (0.1%)	1.99	172/7191 (2.4%)

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

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	4	69	SER	CA-CB	-8.85	1.39	1.52
2	2	167	ARG	CZ-NH2	5.29	1.40	1.33
2	2	97	SER	CA-CB	-5.29	1.45	1.52
2	2	108	GLU	CD-OE2	-5.18	1.20	1.25
1	1	21	GLU	CA-CB	-5.11	1.42	1.53

The worst 5 of 172 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	135	ARG	NE-CZ-NH1	18.03	129.31	120.30
1	1	179	ARG	NE-CZ-NH1	17.84	129.22	120.30
2	2	135	ARG	NE-CZ-NH2	-17.26	111.67	120.30
1	1	182	ARG	NE-CZ-NH1	15.53	128.06	120.30
1	1	38	ARG	NE-CZ-NH2	-15.06	112.77	120.30

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	1456	0	1453	27	0
2	2	1652	0	1610	22	0
3	3	1681	0	1616	24	0
4	4	353	0	324	7	0
All	All	5142	0	5003	75	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 7.

The worst 5 of 75 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)
2:2:11:GLU:HG2	2:2:13:ARG:HD3	1.39	1.04
1:1:70:THR:HG23	1:1:187:CYS:HB2	1.47	0.95
3:3:100:GLN:HE22	3:3:212:ARG:HH21	1.15	0.92
1:1:103:ASN:HD21	3:3:216:ASP:H	1.25	0.85
2:2:115:GLN:NE2	2:2:115:GLN:H	1.82	0.77

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	182/213 (85%)	176 (97%)	4 (2%)	2 (1%)	14	30
2	2	208/218 (95%)	195 (94%)	11 (5%)	2 (1%)	15	32
3	3	218/220 (99%)	211 (97%)	5 (2%)	2 (1%)	17	35
4	4	42/85 (49%)	35 (83%)	5 (12%)	2 (5%)	2	2
All	All	650/736 (88%)	617 (95%)	25 (4%)	8 (1%)	13	27

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	2	30	VAL
2	2	131	SER
4	4	80	PHE
1	1	104	PRO
3	3	219	ALA

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	159/183 (87%)	135 (85%)	24 (15%)	3	4
2	2	183/191 (96%)	157 (86%)	26 (14%)	3	5
3	3	176/176 (100%)	145 (82%)	31 (18%)	2	3
4	4	37/67 (55%)	30 (81%)	7 (19%)	1	2
All	All	555/617 (90%)	467 (84%)	88 (16%)	2	4

5 of 88 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	3	64	VAL
3	3	168	THR
3	3	68	THR
3	3	107	LEU

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Mol	Chain	Res	Type
3	3	201	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
2	2	153	ASN
2	2	157	HIS
4	4	17	ASN
3	3	100	GLN
3	3	152	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)

There are no chain breaks in this entry.

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.