wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 06:33 PM GMT

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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

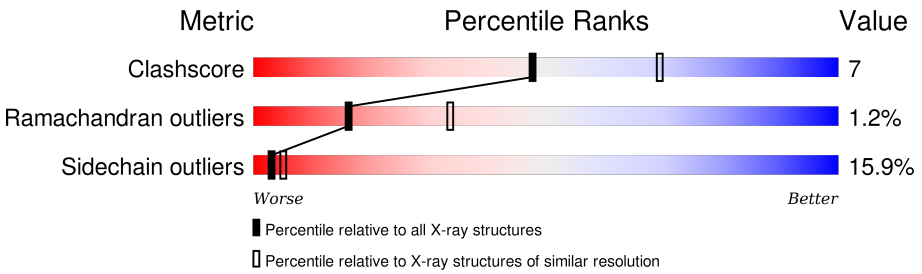
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (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 on the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	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

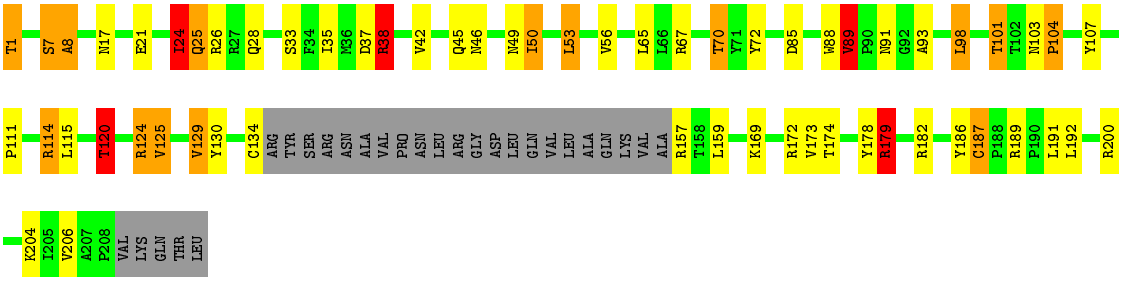
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

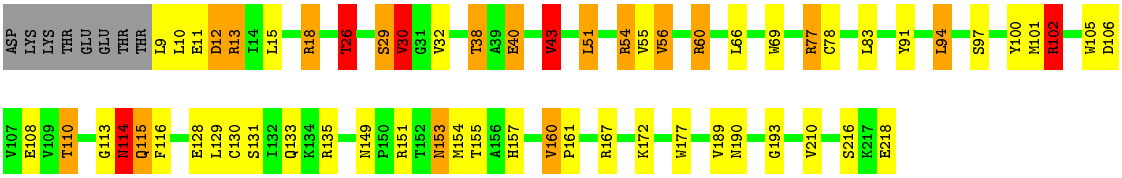
- Molecule 1: FOOT-AND-MOUTH DISEASE VIRUS (SUBUNIT VP1)

Chain 1:



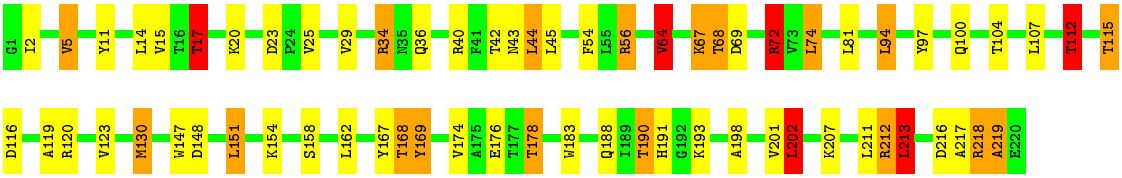
- Molecule 2: FOOT-AND-MOUTH DISEASE VIRUS (SUBUNIT VP2)

Chain 2:



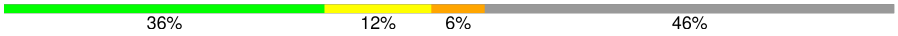
- Molecule 3: FOOT-AND-MOUTH DISEASE VIRUS (SUBUNIT VP3)

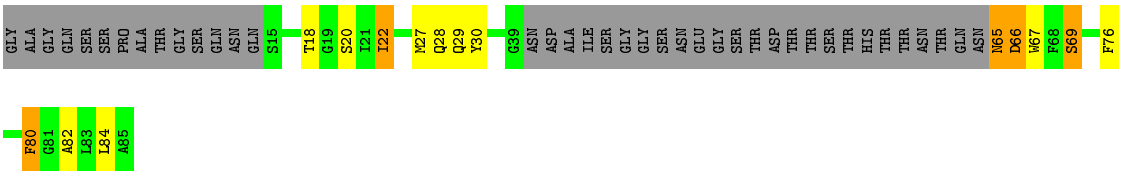
Chain 3:



- 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 I84 A85

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be 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:H	2:2:115:GLN:NE2	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%)	17	36
2	2	208/218 (95%)	195 (94%)	11 (5%)	2 (1%)	19	39
3	3	218/220 (99%)	211 (97%)	5 (2%)	2 (1%)	21	42
4	4	42/85 (49%)	35 (83%)	5 (12%)	2 (5%)	3	3
All	All	650/736 (88%)	617 (95%)	25 (4%)	8 (1%)	16	33

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	6
2	2	183/191 (96%)	157 (86%)	26 (14%)	4	7
3	3	176/176 (100%)	145 (82%)	31 (18%)	2	3
4	4	37/67 (55%)	30 (81%)	7 (19%)	2	3
All	All	555/617 (90%)	467 (84%)	88 (16%)	3	5

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

Mol	Chain	Res	Type
2	2	94	LEU
2	2	189	VAL
4	4	18	THR
2	2	102	ARG

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Mol	Chain	Res	Type
2	2	130	CYS

Some 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	149	ASN
2	2	153	ASN
3	3	100	GLN
2	2	115	GLN
3	3	43	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)

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates (i)

EDS was not executed - this section will therefore be empty.

6.4 Ligands (i)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers (i)

EDS was not executed - this section will therefore be empty.