



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:52 PM GMT

PDB ID : 4GH4  
Title : Crystal Structure of Foot and Mouth Disease Virus A22 Serotype  
Authors : Kotecha, A.; Jinshan, R.; Curry, S.; Fry, E.; Stuart, D.  
Deposited on : 2012-08-07  
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

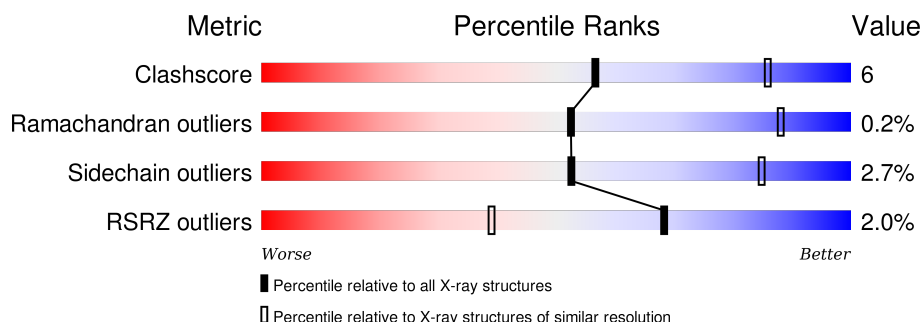
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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  $\geq 3$ , 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  $\leq 5\%$ . 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.

Mol	Chain	Length	Quality of chain
1	A	210	<div> <div>74%</div> <div>16%</div> <div>9%</div> </div>
2	B	207	<div> <div>86%</div> <div>14%</div> </div>
3	C	221	<div> <div>88%</div> <div>10%</div> </div>
4	D	45	<div> <div>78%</div> <div>22%</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5457 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 capsid protein VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	191	Total	C	N	O	S	0	0	0
			1494	945	267	278	4			

- Molecule 2 is a protein called capsid protein VP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	207	Total	C	N	O	S	0	0	0
			1649	1053	286	305	5			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	13	ARG	ALA	CONFLICT	UNP Q9Q2N8
B	14	LEU	ILE	CONFLICT	UNP Q9Q2N8
B	135	ARG	ALA	CONFLICT	UNP Q9Q2N8

- Molecule 3 is a protein called capsid protein VP3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	221	Total	C	N	O	S	0	0	0
			1707	1087	277	334	9			

- Molecule 4 is a protein called capsid protein VP4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	45	Total	C	N	O	S	0	0	0
			349	220	56	71	2			

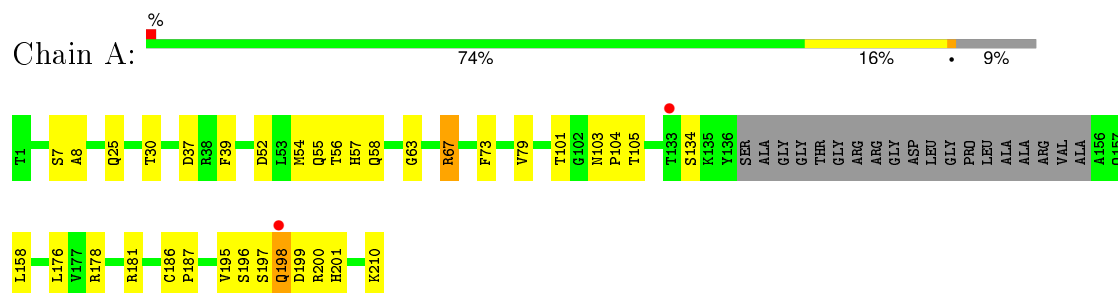
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	84	Total 84	O 84	0	0
5	B	84	Total 84	O 84	0	0
5	C	75	Total 75	O 75	0	0
5	D	15	Total 15	O 15	0	0

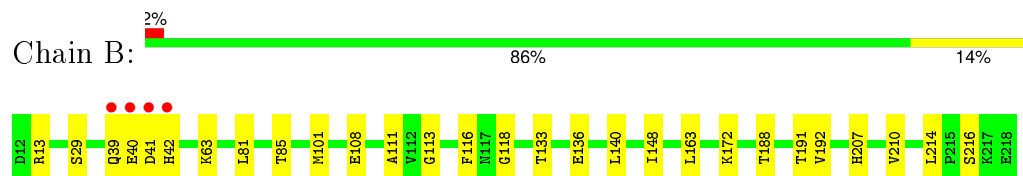
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 ( $\text{RSRZ} > 2$ ). 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.

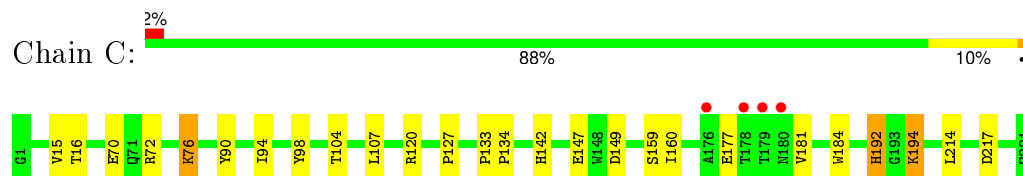
#### • Molecule 1: capsid protein VP1



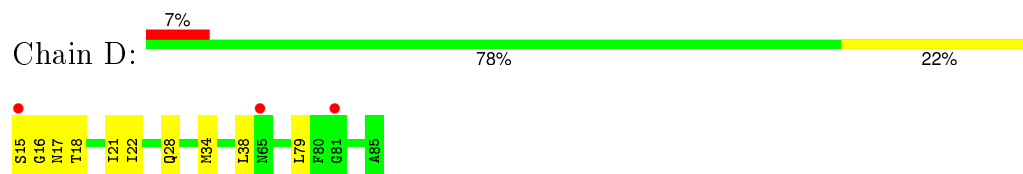
#### • Molecule 2: capsid protein VP2



#### • Molecule 3: capsid protein VP3



#### • Molecule 4: capsid protein VP4



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	328.20Å 341.80Å 363.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 3.00 249.09 – 3.00	Depositor EDS
% Data completeness (in resolution range)	61.7 (25.00-3.00) 98.7 (249.09-3.00)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.26 (at 3.01Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.167 , (Not available) 0.175 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	22.5	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 65.6	EDS
Estimated twinning fraction	0.000 for -k,-h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 398369 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	5457	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.75% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 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	0.48	1/1528 (0.1%)	0.72	1/2084 (0.0%)
2	B	0.47	0/1697	0.73	1/2312 (0.0%)
3	C	0.52	0/1755	0.77	1/2400 (0.0%)
4	D	0.51	0/355	0.65	0/476
All	All	0.49	1/5335 (0.0%)	0.74	3/7272 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	187	PRO	N-CD	5.34	1.55	1.47

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	217	ASP	C-N-CD	5.99	140.98	128.40
1	A	186	CYS	C-N-CD	5.46	139.86	128.40
2	B	113	GLY	N-CA-C	-5.22	100.05	113.10

There are no chirality outliers.

There are no planarity outliers.

### 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	1494	0	1493	24	0
2	B	1649	0	1608	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1707	0	1635	20	0
4	D	349	0	321	11	0
5	A	84	0	0	3	0
5	B	84	0	0	4	0
5	C	75	0	0	1	0
5	D	15	0	0	0	0
All	All	5457	0	5057	62	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 6.

All (62) 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)
4:D:28:GLN:HG2	4:D:34:MET:HE3	1.51	0.91
2:B:81:LEU:HD11	2:B:85:THR:HG21	1.60	0.82
4:D:28:GLN:HG2	4:D:34:MET:CE	2.09	0.81
1:A:198:GLN:HG2	5:A:384:HOH:O	1.81	0.79
1:A:37:ASP:O	4:D:17:ASN:ND2	2.16	0.75
1:A:56:THR:O	1:A:67:ARG:NH2	2.20	0.73
1:A:195:VAL:HG22	1:A:201:HIS:HB2	1.74	0.69
2:B:172:LYS:HG3	5:B:329:HOH:O	1.96	0.66
1:A:197:SER:O	1:A:198:GLN:HB2	1.94	0.66
4:D:21:ILE:HG22	4:D:22:ILE:HD12	1.79	0.64
3:C:90:TYR:CE1	3:C:94:ILE:HD11	2.35	0.61
3:C:120:ARG:NH1	3:C:149:ASP:OD2	2.34	0.61
1:A:134:SER:O	3:C:177:GLU:HG3	2.01	0.60
4:D:22:ILE:HD12	4:D:22:ILE:N	2.16	0.59
1:A:37:ASP:OD2	4:D:16:GLY:O	2.20	0.59
1:A:58:GLN:HG2	5:A:332:HOH:O	2.03	0.58
2:B:101:MET:HG2	2:B:210:VAL:HG12	1.86	0.58
2:B:85:THR:HG22	5:B:371:HOH:O	2.05	0.57
1:A:101:THR:HG23	3:C:16:THR:HG21	1.87	0.56
1:A:7:SER:O	1:A:8:ALA:HB3	2.06	0.56
2:B:172:LYS:CG	5:B:329:HOH:O	2.51	0.55
2:B:13:ARG:O	2:B:29:SER:HB3	2.08	0.54
3:C:72:ARG:HD2	5:C:352:HOH:O	2.10	0.52
3:C:104:THR:CG2	3:C:159:SER:HB3	2.41	0.51
1:A:73:PHE:CD1	1:A:73:PHE:C	2.85	0.50
1:A:57:HIS:O	1:A:63:GLY:HA3	2.11	0.49
2:B:118:GLY:HA3	2:B:188:THR:OG1	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:116:PHE:CD2	2:B:192:VAL:HG12	2.48	0.48
4:D:22:ILE:CD1	4:D:22:ILE:N	2.76	0.48
3:C:133:PRO:HG3	3:C:184:TRP:CD2	2.49	0.47
2:B:214:LEU:HD23	3:C:127:PRO:HG2	1.97	0.47
4:D:15:SER:O	4:D:18:THR:OG1	2.29	0.46
2:B:42:HIS:CG	4:D:38:LEU:CD1	3.00	0.45
2:B:40:GLU:HG3	2:B:207:HIS:CD2	2.52	0.45
3:C:194:LYS:HA	3:C:194:LYS:HD2	1.80	0.45
1:A:198:GLN:CG	5:A:384:HOH:O	2.53	0.44
1:A:105:THR:O	3:C:15:VAL:HA	2.16	0.44
1:A:79:VAL:HB	1:A:176:LEU:HB2	1.98	0.44
4:D:28:GLN:CG	4:D:34:MET:CE	2.89	0.44
1:A:52:ASP:O	1:A:55:GLN:HB2	2.19	0.43
3:C:76:LYS:CD	3:C:133:PRO:HG2	2.49	0.43
3:C:181:VAL:HG13	3:C:181:VAL:O	2.19	0.43
1:A:199:ASP:OD1	1:A:200:ARG:N	2.51	0.43
2:B:133:THR:OG1	2:B:136:GLU:HG3	2.18	0.42
2:B:81:LEU:CD1	2:B:85:THR:HG21	2.40	0.42
2:B:216:SER:HB3	3:C:142:HIS:CD2	2.55	0.42
3:C:98:TYR:HA	3:C:214:LEU:O	2.20	0.42
1:A:39:PHE:CD1	1:A:178:ARG:HB2	2.54	0.42
2:B:39:GLN:HA	5:B:376:HOH:O	2.18	0.42
3:C:107:LEU:HG	3:C:160:ILE:HD11	2.01	0.42
2:B:111:ALA:HB3	2:B:148:ILE:HG21	2.02	0.41
3:C:70:GLU:OE1	3:C:72:ARG:NH1	2.49	0.41
1:A:103:ASN:O	1:A:104:PRO:C	2.59	0.41
1:A:198:GLN:HB3	1:A:198:GLN:HE21	1.68	0.41
1:A:54:MET:HG3	1:A:158:LEU:HD11	2.03	0.41
3:C:133:PRO:HA	3:C:134:PRO:HD3	1.94	0.41
3:C:192:HIS:ND1	3:C:192:HIS:C	2.73	0.41
1:A:37:ASP:HB3	4:D:17:ASN:HB3	2.03	0.41
3:C:76:LYS:HE2	3:C:76:LYS:HB3	1.65	0.41
3:C:76:LYS:HD2	3:C:133:PRO:HG2	2.03	0.40
1:A:210:LYS:HG2	1:A:210:LYS:OXT	2.21	0.40
1:A:181:ARG:HH11	1:A:181:ARG:HD2	1.78	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	187/210 (89%)	180 (96%)	7 (4%)	0	100	100
2	B	205/207 (99%)	196 (96%)	8 (4%)	1 (0%)	34	76
3	C	219/221 (99%)	204 (93%)	15 (7%)	0	100	100
4	D	41/45 (91%)	38 (93%)	3 (7%)	0	100	100
All	All	652/683 (96%)	618 (95%)	33 (5%)	1 (0%)	52	88

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	41	ASP

### 5.3.2 Protein sidechains

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	161/171 (94%)	156 (97%)	5 (3%)	47	83
2	B	182/182 (100%)	177 (97%)	5 (3%)	52	85
3	C	185/185 (100%)	181 (98%)	4 (2%)	60	88
4	D	37/37 (100%)	36 (97%)	1 (3%)	52	85
All	All	565/575 (98%)	550 (97%)	15 (3%)	52	85

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	30	THR
1	A	67	ARG
1	A	196	SER
1	A	198	GLN
2	B	63	LYS
2	B	108	GLU
2	B	140	LEU
2	B	163	LEU
2	B	191	THR
3	C	76	LYS
3	C	147	GLU
3	C	192	HIS
3	C	194	LYS
4	D	79	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
1	A	198	GLN
2	B	103	ASN
3	C	71	GLN
3	C	153	ASN
3	C	180	ASN
3	C	197	GLN
4	D	24	ASN
4	D	31	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 carbohydrates in this entry.

## 5.6 Ligand geometry

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	191/210 (90%)	-0.13	2 (1%) 84 60	4, 11, 67, 101	0
2	B	207/207 (100%)	-0.24	4 (1%) 70 41	5, 11, 39, 95	0
3	C	221/221 (100%)	-0.19	4 (1%) 71 43	4, 11, 53, 96	0
4	D	45/45 (100%)	0.50	3 (6%) 21 7	10, 36, 75, 85	0
All	All	664/683 (97%)	-0.14	13 (1%) 68 39	4, 12, 63, 101	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	198	GLN	4.9
2	B	41	ASP	4.1
3	C	178	THR	3.6
4	D	15	SER	3.5
2	B	39	GLN	3.1
3	C	179	THR	2.7
4	D	65	ASN	2.7
1	A	133	THR	2.5
2	B	42	HIS	2.4
3	C	180	ASN	2.2
3	C	176	ALA	2.2
2	B	40	GLU	2.1
4	D	81	GLY	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.