

wwPDB X-ray Structure Validation Summary Report (i)

Feb 18, 2024 – 10:42 PM EST

PDB ID : 4GH4

Title: Crystal Structure of Foot and Mouth Disease Virus A22 Serotype

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Deposited on : 2012-08-07

Resolution : 3.00 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 (1)) were used in the production of this report:

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

EDS : 2.36

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

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)
oteins) : Engh & Huber (200)

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

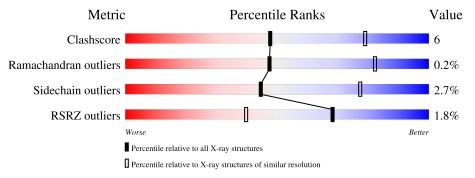
Validation Pipeline (wwPDB-VP) : 2.36

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 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	Similar resolution		
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{resolution range}(ext{Å}))$		
Clashscore	141614	2416 (3.00-3.00)		
Ramachandran outliers	138981	2333 (3.00-3.00)		
Sidechain outliers	138945	2336 (3.00-3.00)		
RSRZ outliers	127900	1990 (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 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% 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	74%	16% • 9%
2	В	207	86%	14%
3	С	221	88%	10% •
4	D	45	78%	22%



2 Entry composition (i)

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.

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

• Molecule 2 is a protein called capsid protein VP2.

\mathbf{Mol}	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	207	Total	С	N	О	S	0	0	0
4	В	201	1649	1053	286	305	5	0	0	

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	13	ARG	ALA	$\operatorname{conflict}$	UNP Q9Q2N8
В	14	LEU	ILE	conflict	UNP Q9Q2N8
В	135	ARG	ALA	conflict	UNP Q9Q2N8

• Molecule 3 is a protein called capsid protein VP3.

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

• Molecule 4 is a protein called capsid protein VP4.

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

• Molecule 5 is water.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	
5	5 A	84	Total O	0	0	
	11	04	84 84		U	
5	В	84	Total O	0	0	
	D	04	84 84		U	
5	С	75	Total O	0	0	
5	C	10	75 75		U	
5	D	15	Total O	0	0	
	D	10	15 15	0	U	



Chain D:

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 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.

• Molecule 1: capsid protein VP1

Chain A:

74%

16%

9%

Nolecule 2: capsid protein VP2

Chain B:

86%

14%

• Molecule 3: capsid protein VP3

Chain C:

88%

10%

• Molecule 4: capsid protein VP4

78%



22%

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants	328.20Å 341.80Å 363.75Å	Danagitan
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 - 3.00	Depositor
Resolution (A)	249.09 - 3.00	EDS
% Data completeness	61.7 (25.00-3.00)	Depositor
(in resolution range)	98.7 (249.09-3.00)	EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.26 (at 3.01Å)	Xtriage
Refinement program	CNS, X-PLOR	Depositor
D.D.	0.167 , (Not available)	Depositor
R, R_{free}	0.178 , (Not available)	DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	22.5	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.36,65.6	EDS
L-test for twinning ²	$< L > = 0.49, < L^2> = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5457	wwPDB-VP
Average B, all atoms (\mathring{A}^2)	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.

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	Bo	nd lengths	Bond angles		
		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.48	1/1528 (0.1%)	0.72	1/2084 (0.0%)	
2	В	0.47	0/1697	0.73	1/2312 (0.0%)	
3	С	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	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}(\text{\AA})$
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	$\mathbf{Observed}(^{o})$	$\operatorname{Ideal}({}^{o})$
3	С	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	В	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	В	1649	0	1608	16	0

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Continued	trom	mmoninonic	maaa
COHABABACA		DIEUIUU	DUIUE
0 0 1000100000			

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	С	1707	0	1635	20	0
4	D	349	0	321	11	0
5	A	84	0	0	3	0
5	В	84	0	0	4	0
5	С	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.

The worst 5 of 62 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$
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

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	Perce	ntiles
1	A	187/210 (89%)	180 (96%)	7 (4%)	0	100	100
2	В	205/207 (99%)	196 (96%)	8 (4%)	1 (0%)	29	68
3	С	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%)	47	82



All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	В	41	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	Rotameric Outliers		Percentiles		
1	A	161/171~(94%)	156 (97%)	5 (3%)	40	75	
2	В	182/182 (100%)	177 (97%)	5 (3%)	44	77	
3	С	185/185~(100%)	181 (98%)	4 (2%)	52	81	
4	D	37/37 (100%)	36 (97%)	1 (3%)	44	77	
All	All	565/575~(98%)	550 (97%)	15 (3%)	44	77	

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	В	140	LEU
3	С	194	LYS
2	В	163	LEU
4	D	79	LEU
3	С	147	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
4	D	24	ASN
4	D	31	GLN
3	С	71	GLN
3	С	153	ASN
3	С	180	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:

Mol	Chain	Number of breaks
4	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	38:LEU	С	65:ASN	N	14.86



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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^{th} 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>	$\# \mathrm{RSRZ}{>}2$	$OWAB(Å^2)$	Q<0.9
1	A	191/210 (90%)	-0.15	2 (1%) 82 59	4, 11, 67, 101	0
2	В	207/207 (100%)	-0.25	4 (1%) 66 37	5, 11, 39, 95	0
3	С	221/221 (100%)	-0.21	4 (1%) 68 40	4, 11, 53, 96	0
4	D	45/45 (100%)	0.46	2 (4%) 34 13	10, 36, 75, 85	0
All	All	664/683 (97%)	-0.16	12 (1%) 68 40	4, 12, 63, 101	0

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	198	GLN	4.8
2	В	41	ASP	4.0
3	С	178	THR	3.5
4	D	15	SER	3.4
2	В	39	GLN	3.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides 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.

