



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 29, 2025 – 02:42 AM EDT

PDB ID : 4IV3 / pdb_00004iv3
Title : Crystal structure of recombinant foot-and-mouth-disease virus A22-H2093C empty capsid
Authors : Porta, C.; Kotecha, A.; Burman, A.; Jackson, T.; Ren, J.; Loureiro, S.; Jones, I.M.; Fry, E.E.; Stuart, D.I.; Charleston, B.
Deposited on : 2013-01-22
Resolution : 2.90 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0rc1
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

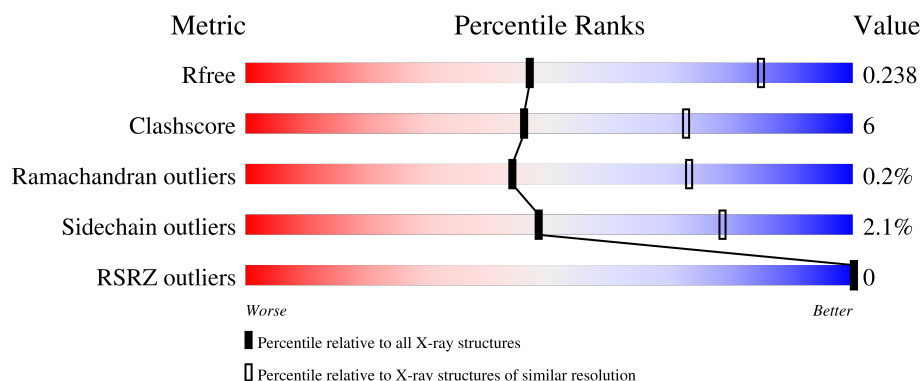
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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))
R_{free}	164625	2335 (2.90-2.90)
Clashscore	180529	2564 (2.90-2.90)
Ramachandran outliers	177936	2514 (2.90-2.90)
Sidechain outliers	177891	2516 (2.90-2.90)
RSRZ outliers	164620	2337 (2.90-2.90)

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 $\leq 5\%$. 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	211	 71% 13% 16%
2	B	218	 81% 14% 5%
3	C	221	 84% 15%
4	D	85	 6% 93%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4848 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	178	Total	C	N	O	S	0	0	0
			1398	887	253	254	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
			1645	1050	284	305	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	93	CYS	HIS	engineered mutation	UNP Q6PN23

- 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	6	Total	C	N	O	0	0	0
			42	29	6	7			

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	19	Total	O	0	0
			19	19		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	16	Total	O	0	0
			16	16		
5	C	21	Total	O	0	0
			21	21		

ASN	THR	GLN	ASN	ASN	ASP	TRP	PHE	SER	LYS	LEU	ALA	SER	SER	ALA	PHE	SER	GLY	LEU	F80	L84	A85
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	328.02Å 341.49Å 363.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.56 – 2.90 49.56 – 2.90	Depositor EDS
% Data completeness (in resolution range)	79.3 (49.56-2.90) 58.6 (49.56-2.90)	Depositor EDS
R_{merge}	0.41	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 2.91Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.235 , 0.239 0.234 , 0.238	Depositor DCC
R_{free} test set	17689 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	36.2	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 0.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.014 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.36	EDS
Total number of atoms	4848	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.84% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	0.39	0/1430	0.92	4/1950 (0.2%)
2	B	0.40	0/1692	0.92	2/2305 (0.1%)
3	C	0.41	0/1755	0.94	5/2400 (0.2%)
4	D	0.57	0/42	0.54	0/54
All	All	0.40	0/4919	0.93	11/6709 (0.2%)

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	191	THR	N-CA-C	-7.54	104.08	113.28
1	A	42	ILE	N-CA-C	-6.32	98.42	107.77
2	B	126	VAL	N-CA-C	6.11	114.88	107.61
3	C	54	PHE	N-CA-C	6.02	119.71	110.20
1	A	191	LEU	N-CA-C	5.80	118.93	109.59

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1398	0	1401	18	0
2	B	1645	0	1606	14	1
3	C	1707	0	1635	24	1
4	D	42	0	43	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	19	0	0	0	0
5	B	16	0	0	0	0
5	C	21	0	0	0	0
All	All	4848	0	4685	54	1

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 54 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:B:214:LEU:HD23	3:C:127:PRO:HG2	1.69	0.74
1:A:40:VAL:HG21	1:A:62:VAL:HB	1.71	0.71
3:C:76:LYS:HE3	3:C:133:PRO:HG2	1.75	0.68
3:C:68:THR:HG22	3:C:70:GLU:HG3	1.74	0.68
2:B:81:LEU:HD11	2:B:85:THR:HG21	1.76	0.66

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:27:GLN:OE1	3:C:151:GLY:N[2_555]	2.14	0.06

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	A	174/211 (82%)	166 (95%)	8 (5%)	0	100	100
2	B	205/218 (94%)	191 (93%)	14 (7%)	0	100	100
3	C	219/221 (99%)	201 (92%)	17 (8%)	1 (0%)	25	56

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	4/85 (5%)	3 (75%)	1 (25%)	0	100	100
All	All	602/735 (82%)	561 (93%)	40 (7%)	1 (0%)	44	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	58	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	150/172 (87%)	146 (97%)	4 (3%)	40	73
2	B	182/193 (94%)	179 (98%)	3 (2%)	58	84
3	C	185/185 (100%)	181 (98%)	4 (2%)	47	78
4	D	3/67 (4%)	3 (100%)	0	100	100
All	All	520/617 (84%)	509 (98%)	11 (2%)	48	78

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	58	ASP
3	C	65	VAL
3	C	179	THR
3	C	84	LYS
2	B	40	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
3	C	71	GLN
3	C	192	HIS
1	A	201	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	103	ASN
2	B	114	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 oligosaccharides 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](#)

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, 95th 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 ²)	Q<0.9
1	A	178/211 (84%)	-1.43	0 100 100	15, 25, 88, 153	0
2	B	207/218 (94%)	-1.40	0 100 100	12, 25, 79, 159	0
3	C	221/221 (100%)	-1.40	0 100 100	14, 26, 77, 111	0
4	D	6/85 (7%)	0.08	0 100 100	96, 118, 135, 154	0
All	All	612/735 (83%)	-1.39	0 100 100	12, 26, 88, 159	0

There are no RSRZ outliers to report.

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.