



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 27, 2026 – 06:33 PM EDT

PDB ID : 5NE4 / pdb_00005ne4
Title : Crystal Structure of Foot and Mouth Disease Virus O PanAsia
Authors : Kotecha, A.; StuarT, D.
Deposited on : 2017-03-09
Resolution : 2.30 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 Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

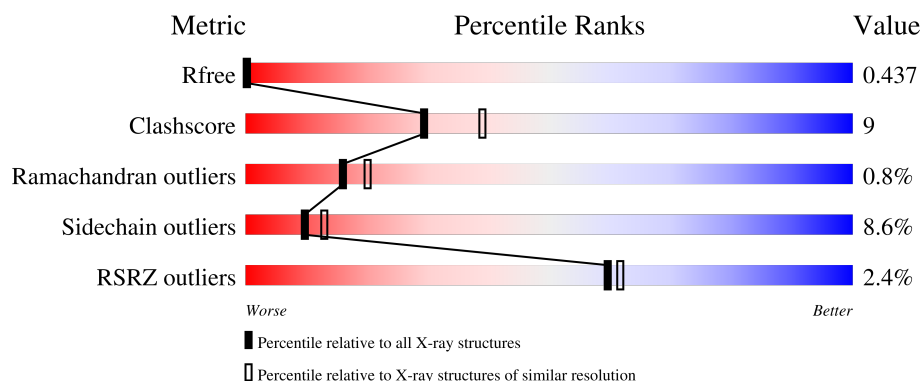
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5197 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 O PanAsia VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	184	Total	C	N	O	S	0	0	0
			1437	909	257	268	3			

- Molecule 2 is a protein called O PanAsia VP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	206	Total	C	N	O	S	0	0	0
			1620	1031	278	304	7			

- Molecule 3 is a protein called Polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	219	Total	C	N	O	S	0	0	0
			1677	1075	273	320	9			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	56	ARG	HIS	engineered mutation	UNP J3T9N5

- Molecule 4 is a protein called O PanAsia VP4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	4	46	Total	C	N	O	S	0	0	0
			353	222	56	73	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	65	ASP	ASN	conflict	UNP E6Y5R5

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	1	33	Total 33	O 33	0	0
5	2	25	Total 25	O 25	0	0
5	3	51	Total 51	O 51	0	0
5	4	1	Total 1	O 1	0	0

SEQUENCE-PLOTS INFOmissingINFO

3 Data and refinement statistics

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α , β , γ	345.01Å 345.01Å 345.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30 50.00 – 2.32	Depositor EDS
% Data completeness (in resolution range)	76.9 (50.00-2.30) 79.4 (50.00-2.32)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 2.32Å)	Xtriage
Refinement program	CNS v1.2	Depositor
R, R_{free}	0.210 , 0.220 0.435 , 0.437	Depositor DCC
R_{free} test set	11647 reflections (4.02%)	wwPDB-VP
Wilson B-factor (Å ²)	19.1	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 6.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.016 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.46	EDS
Total number of atoms	5197	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.57% 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.

4 Model quality

4.1 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	1	0.50	0/1471	1.05	11/2012 (0.5%)
2	2	0.53	0/1663	1.01	6/2271 (0.3%)
3	3	0.55	0/1726	1.07	15/2358 (0.6%)
4	4	0.50	0/359	0.91	2/481 (0.4%)
All	All	0.53	0/5219	1.03	34/7122 (0.5%)

There are no bond length outliers.

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	7	SER	N-CA-C	10.16	122.36	111.28
3	3	54	PHE	N-CA-C	7.52	121.41	110.28
4	4	67	TRP	N-CA-C	7.08	118.64	111.07
2	2	113	GLY	N-CA-C	-6.52	97.72	113.18
2	2	30	VAL	N-CA-C	-6.45	106.04	112.17

There are no chirality outliers.

There are no planarity outliers.

4.2 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	1	1437	0	1442	37	0
2	2	1620	0	1578	15	0
3	3	1677	0	1610	34	0
4	4	353	0	322	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	1	33	0	0	1	0
5	2	25	0	0	0	1
5	3	51	0	0	5	1
5	4	1	0	0	0	0
All	All	5197	0	4952	86	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 9.

The worst 5 of 86 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)
3:3:66:THR:HB	3:3:188:GLN:HE22	1.33	0.94
3:3:34:ARG:HD3	5:3:302:HOH:O	1.74	0.88
3:3:107:LEU:HD22	3:3:159:ILE:HD11	1.60	0.82
2:2:26:THR:HG22	2:2:28:SER:H	1.45	0.81
1:1:91:ASN:HB3	1:1:120:THR:HG23	1.68	0.76

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)
5:2:318:HOH:O	5:3:346:HOH:O[2_555]	1.38	0.82

4.3 Torsion angles [i](#)

4.3.1 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	180/211 (85%)	175 (97%)	4 (2%)	1 (1%)	21	27
2	2	204/218 (94%)	195 (96%)	7 (3%)	2 (1%)	12	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	3	217/220 (99%)	209 (96%)	7 (3%)	1 (0%)	24	31
4	4	42/85 (49%)	39 (93%)	2 (5%)	1 (2%)	4	4
All	All	643/734 (88%)	618 (96%)	20 (3%)	5 (1%)	16	20

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	3	218	ARG
2	2	131	SER
4	4	66	ASP
2	2	36	TYR
1	1	104	PRO

4.3.2 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	1	154/176 (88%)	140 (91%)	14 (9%)	9	11
2	2	180/192 (94%)	163 (91%)	17 (9%)	8	11
3	3	175/176 (99%)	159 (91%)	16 (9%)	9	11
4	4	37/67 (55%)	37 (100%)	0	100	100
All	All	546/611 (89%)	499 (91%)	47 (9%)	10	13

5 of 47 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	2	184	VAL
3	3	81	LEU
2	2	191	THR
3	3	29	VAL
3	3	107	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
3	3	188	GLN
3	3	181	GLN
2	2	157	HIS
2	2	79	HIS
3	3	152	ASN

4.3.3 RNA [i](#)

There are no RNA molecules in this entry.

4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

There are no ligands in this entry.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data [i](#)

5.1 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	1	184/211 (87%)	-0.46	2 (1%) 78 79	10, 16, 41, 95	0
2	2	206/218 (94%)	-0.52	2 (0%) 79 80	8, 15, 40, 86	0
3	3	219/220 (99%)	-0.51	6 (2%) 56 58	8, 15, 54, 80	0
4	4	46/85 (54%)	0.61	6 (13%) 7 8	12, 39, 79, 88	0
All	All	655/734 (89%)	-0.42	16 (2%) 59 62	8, 16, 52, 95	0

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	4	15	SER	3.8
4	4	23	ASN	3.7
2	2	131	SER	3.5
1	1	157	ARG	3.5
4	4	81	GLY	3.4

5.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.4 Ligands [i](#)

There are no ligands in this entry.

5.5 Other polymers [i](#)

There are no such residues in this entry.