



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 9KZ3 / pdb_00009kz3
Title : PEDV 3CLpro mutant (C144A) in complex with nsp8|9 peptide substrate
Authors : Zhang, Y.; Zhang, D.; Zhang, Z.T.; Shi, Y.J.; Peng, G.Q.
Deposited on : 2024-12-09
Resolution : 1.93 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

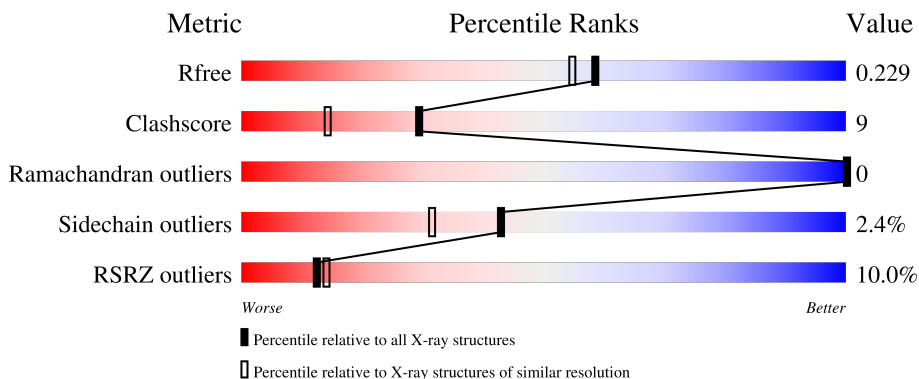
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.93 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	1452 (1.94-1.94)
Clashscore	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)
RSRZ outliers	180081	1453 (1.94-1.94)

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	310	10% 79% 17% .
1	B	310	8% 82% 12% 5%
2	C	6	17% 50% 17% 17% 17%
3	D	6	67% 17% 50% 17% 17%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4859 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 ORF1ab polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	297	Total	C	N	O	S	0	0	0
			2265	1431	391	428	15			
1	B	295	Total	C	N	O	S	0	0	0
			2248	1420	389	424	15			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP A0A023J7B5
A	144	ALA	CYS	engineered mutation	UNP A0A023J7B5
A	300	LEU	-	expression tag	UNP A0A023J7B5
A	301	GLU	-	expression tag	UNP A0A023J7B5
A	302	HIS	-	expression tag	UNP A0A023J7B5
A	303	HIS	-	expression tag	UNP A0A023J7B5
A	304	HIS	-	expression tag	UNP A0A023J7B5
A	305	HIS	-	expression tag	UNP A0A023J7B5
A	306	HIS	-	expression tag	UNP A0A023J7B5
A	307	HIS	-	expression tag	UNP A0A023J7B5
A	308	HIS	-	expression tag	UNP A0A023J7B5
A	309	HIS	-	expression tag	UNP A0A023J7B5
B	0	MET	-	initiating methionine	UNP A0A023J7B5
B	144	ALA	CYS	engineered mutation	UNP A0A023J7B5
B	300	LEU	-	expression tag	UNP A0A023J7B5
B	301	GLU	-	expression tag	UNP A0A023J7B5
B	302	HIS	-	expression tag	UNP A0A023J7B5
B	303	HIS	-	expression tag	UNP A0A023J7B5
B	304	HIS	-	expression tag	UNP A0A023J7B5
B	305	HIS	-	expression tag	UNP A0A023J7B5
B	306	HIS	-	expression tag	UNP A0A023J7B5
B	307	HIS	-	expression tag	UNP A0A023J7B5
B	308	HIS	-	expression tag	UNP A0A023J7B5
B	309	HIS	-	expression tag	UNP A0A023J7B5

- Molecule 2 is a protein called Replicase polypeptide 1a.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	5	Total	C	N	O	0	0	0
			41	28	7	6			

- Molecule 3 is a protein called Replicase polypeptide 1a.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	5	Total	C	N	O	0	0	0
			41	28	7	6			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	123	Total	O	0	0
			123	123		
4	B	134	Total	O	0	0
			134	134		
4	C	3	Total	O	0	0
			3	3		
4	D	4	Total	O	0	0
			4	4		

Q188				
L189				
K190				
V191				
I192				
ARG				

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	56.87Å 92.38Å 58.09Å 90.00° 100.07° 90.00°	Depositor
Resolution (Å)	35.94 – 1.93 35.94 – 1.93	Depositor EDS
% Data completeness (in resolution range)	97.3 (35.94-1.93) 97.6 (35.94-1.93)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 1.92Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.214 , 0.226 0.216 , 0.229	Depositor DCC
R_{free} test set	2103 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	26.1	Xtriage
Anisotropy	0.366	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 35.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.029 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4859	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.04% 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 [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	0.38	0/2311	0.61	0/3136
1	B	0.39	0/2292	0.61	0/3109
2	C	0.80	0/40	1.21	0/52
3	D	0.80	0/40	1.55	0/52
All	All	0.39	0/4683	0.63	0/6349

There are no bond length outliers.

There are no bond angle outliers.

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	2265	0	2213	40	0
1	B	2248	0	2200	37	0
2	C	41	0	51	3	0
3	D	41	0	51	7	0
4	A	123	0	0	5	0
4	B	134	0	0	13	0
4	C	3	0	0	1	0
4	D	4	0	0	0	0
All	All	4859	0	4515	78	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 9.

The worst 5 of 78 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)
1:B:196:SER:HA	4:B:403:HOH:O	1.67	0.94
1:B:61:ARG:HD3	4:B:401:HOH:O	1.70	0.90
1:A:61:ARG:HB2	1:A:64:ASN:HD22	1.40	0.86
1:B:35:THR:HG23	4:B:471:HOH:O	1.87	0.74
1:B:281:THR:O	1:B:284:THR:HG22	1.90	0.72

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	A	293/310 (94%)	286 (98%)	7 (2%)	0	100	100
1	B	289/310 (93%)	286 (99%)	3 (1%)	0	100	100
2	C	3/6 (50%)	3 (100%)	0	0	100	100
3	D	3/6 (50%)	2 (67%)	1 (33%)	0	100	100
All	All	588/632 (93%)	577 (98%)	11 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	243/256 (95%)	239 (98%)	4 (2%)	55	46
1	B	241/256 (94%)	236 (98%)	5 (2%)	47	37
2	C	5/6 (83%)	4 (80%)	1 (20%)	1	0
3	D	5/6 (83%)	3 (60%)	2 (40%)	0	0
All	All	494/524 (94%)	482 (98%)	12 (2%)	43	31

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	271	ASN
1	B	284	THR
3	D	192	ILE
2	C	143	ILE
1	A	242	VAL

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

Mol	Chain	Res	Type
1	B	276	GLN
1	B	243	ASN
1	A	266	GLN
1	A	243	ASN
1	B	236	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

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	297/310 (95%)	0.76	31 (10%)	11 13	15, 30, 51, 68	0
1	B	295/310 (95%)	0.60	24 (8%)	18 20	16, 28, 45, 62	0
2	C	5/6 (83%)	1.17	1 (20%)	3 3	26, 28, 34, 42	0
3	D	5/6 (83%)	3.30	4 (80%)	0 0	35, 36, 45, 51	0
All	All	602/632 (95%)	0.70	60 (9%)	12 14	15, 30, 49, 68	0

The worst 5 of 60 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	241	VAL	4.9
2	C	143	ILE	4.6
3	D	191	VAL	4.5
1	A	48	THR	4.4
3	D	189	LEU	4.2

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 oligosaccharides 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.