



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 9KZS / pdb_00009kzs
Title : PEDV 3CLpro mutant (C144A) in complex with nsp10/11 peptide substrate
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Deposited on : 2024-12-11
Resolution : 1.88 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	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
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)	:	2.47

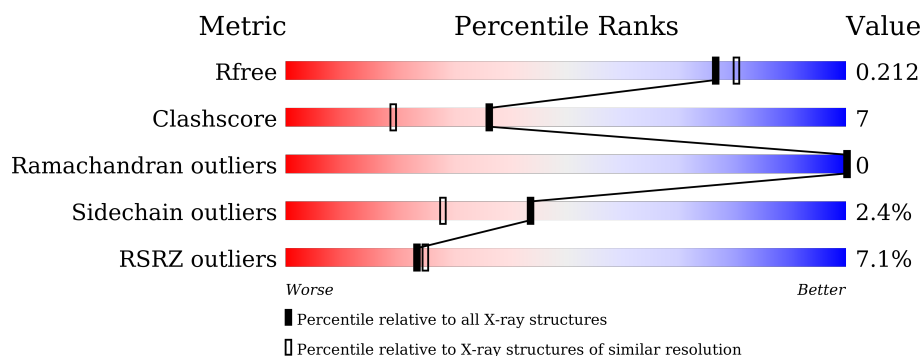
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.88 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	1090 (1.88-1.88)
Clashscore	180529	1144 (1.88-1.88)
Ramachandran outliers	177936	1135 (1.88-1.88)
Sidechain outliers	177891	1135 (1.88-1.88)
RSRZ outliers	164620	1090 (1.88-1.88)

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	<div> <div>7%</div> <div> <div></div> <div>85%</div> <div>11%</div> <div>.</div> </div> </div>
1	B	310	<div> <div>6%</div> <div> <div></div> <div>84%</div> <div>11%</div> <div>..</div> </div> </div>
2	C	6	<div> <div></div> <div> <div>83%</div> <div>17%</div> </div> </div>
2	D	6	<div> <div>50%</div> <div> <div>50%</div> <div>17%</div> <div>17%</div> <div>17%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5008 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	299	Total	C	N	O	S	0	0	0
			2279	1440	393	431	15			
1	B	298	Total	C	N	O	S	0	0	0
			2268	1432	392	429	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 polyprotein 1a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	5	Total	C	N	O	S	0	0	0
			42	25	9	7	1			
2	D	5	Total	C	N	O	S	0	0	0
			42	25	9	7	1			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	155	Total	O	0	0
			155	155		
3	B	215	Total	O	0	0
			215	215		
3	C	4	Total	O	0	0
			4	4		
3	D	3	Total	O	0	0
			3	3		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	57.03Å 92.07Å 58.18Å 90.00° 100.17° 90.00°	Depositor
Resolution (Å)	34.30 – 1.88 34.30 – 1.88	Depositor EDS
% Data completeness (in resolution range)	99.5 (34.30-1.88) 99.5 (34.30-1.88)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.94 (at 1.88Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.189 , 0.215 0.188 , 0.212	Depositor DCC
R_{free} test set	2009 reflections (4.17%)	wwPDB-VP
Wilson B-factor (Å ²)	20.0	Xtriage
Anisotropy	0.464	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 34.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.022 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5008	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.19% 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	0.42	0/2326	0.66	0/3159
1	B	0.45	1/2313 (0.0%)	0.68	1/3140 (0.0%)
2	C	0.34	0/41	0.73	0/52
2	D	0.91	0/41	1.25	0/52
All	All	0.44	1/4721 (0.0%)	0.67	1/6403 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	140	ILE	C-N	-6.50	1.24	1.33

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	169	GLY	N-CA-C	-6.38	106.87	115.36

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	2279	0	2230	28	0
1	B	2268	0	2219	35	0
2	C	42	0	45	0	0
2	D	42	0	45	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	155	0	0	9	0
3	B	215	0	0	10	0
3	C	4	0	0	0	0
3	D	3	0	0	0	0
All	All	5008	0	4539	65	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 7.

The worst 5 of 65 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:A:49:SER:HB3	3:A:404:HOH:O	1.68	0.92
2:D:145:ILE:HG22	2:D:147:GLN:HE21	1.50	0.77
1:A:249:ILE:HD11	1:A:293:ILE:HD11	1.67	0.76
1:B:19:ARG:HH12	1:B:21:CYS:HB2	1.52	0.74
1:B:27:LEU:HD23	2:D:147:GLN:HB3	1.70	0.73

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	297/310 (96%)	293 (99%)	4 (1%)	0	100	100
1	B	294/310 (95%)	284 (97%)	10 (3%)	0	100	100
2	C	3/6 (50%)	3 (100%)	0	0	100	100
2	D	3/6 (50%)	2 (67%)	1 (33%)	0	100	100
All	All	597/632 (94%)	582 (98%)	15 (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	245/256 (96%)	240 (98%)	5 (2%)	50	36
1	B	244/256 (95%)	238 (98%)	6 (2%)	42	26
2	C	5/6 (83%)	5 (100%)	0	100	100
2	D	5/6 (83%)	4 (80%)	1 (20%)	1	0
All	All	499/524 (95%)	487 (98%)	12 (2%)	44	28

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

Mol	Chain	Res	Type
1	B	168	SER
1	B	249	ILE
2	D	145	ILE
1	B	276	GLN
1	A	242	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	87	GLN
1	B	153	ASN
1	B	271	ASN
1	A	266	GLN
1	A	24	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	299/310 (96%)	0.32	21 (7%) 24 25	10, 24, 47, 64	0
1	B	298/310 (96%)	0.14	19 (6%) 27 28	10, 21, 40, 71	0
2	C	5/6 (83%)	0.81	0 100 100	21, 25, 33, 44	0
2	D	5/6 (83%)	2.19	3 (60%) 0 0	28, 29, 34, 43	0
All	All	607/632 (96%)	0.25	43 (7%) 23 25	10, 22, 43, 71	0

The worst 5 of 43 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	47	THR	4.9
1	A	299	VAL	4.8
1	B	47	THR	4.3
2	D	147	GLN	4.0
1	B	48	THR	4.0

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 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.