



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 21, 2026 – 12:30 PM JST

PDB ID : 9UM4 / pdb_00009um4
Title : CaPETaseM9 SEC loop of 9CL variant
Authors : Kim, K.; Ki, D.; Park, J.
Deposited on : 2025-04-21
Resolution : 1.63 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

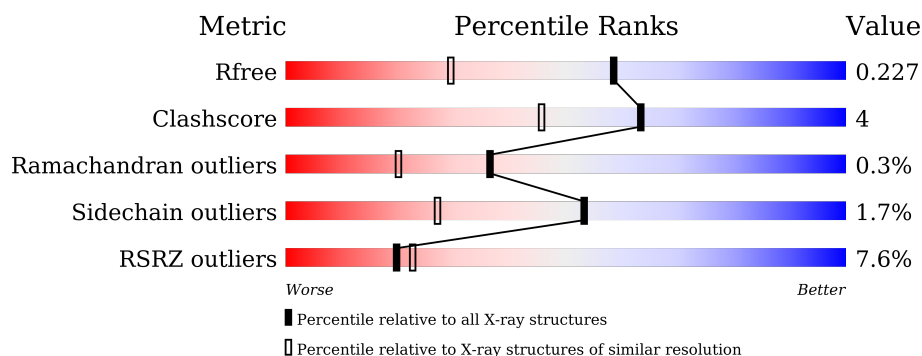
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.63 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	1141 (1.64-1.64)
Clashscore	190562	1171 (1.64-1.64)
Ramachandran outliers	187476	1151 (1.64-1.64)
Sidechain outliers	187428	1150 (1.64-1.64)
RSRZ outliers	180081	1141 (1.64-1.64)

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	264	<div> <div>2%</div> <div>89%</div> <div>8%</div> <div>•</div> </div>
1	B	264	<div> <div>4%</div> <div>85%</div> <div>11%</div> <div>••</div> </div>
1	C	264	<div> <div>2%</div> <div>89%</div> <div>7%</div> <div>••</div> </div>
1	D	264	<div> <div>21%</div> <div>78%</div> <div>15%</div> <div>• 5%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8110 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 Cutinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	0	0
			1956	1237	340	369	10			
1	B	257	Total	C	N	O	S	0	0	0
			1956	1237	340	369	10			
1	C	256	Total	C	N	O	S	0	0	0
			1954	1237	340	367	10			
1	D	250	Total	C	N	O	S	0	0	0
			1902	1205	330	357	10			

There are 100 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	41	ALA	-	expression tag	UNP A0A1M7II12
A	42	ALA	-	expression tag	UNP A0A1M7II12
A	109	ALA	ASN	engineered mutation	UNP A0A1M7II12
A	129	THR	VAL	engineered mutation	UNP A0A1M7II12
A	155	ARG	ALA	engineered mutation	UNP A0A1M7II12
A	180	CYS	LEU	engineered mutation	UNP A0A1M7II12
A	196	THR	GLY	engineered mutation	UNP A0A1M7II12
A	198	LYS	ARG	engineered mutation	UNP A0A1M7II12
A	202	CYS	ALA	engineered mutation	UNP A0A1M7II12
A	242	CYS	ARG	engineered mutation	UNP A0A1M7II12
A	?	-	PRO	deletion	UNP A0A1M7II12
A	282	ASN	SER	engineered mutation	UNP A0A1M7II12
A	283	HIS	THR	engineered mutation	UNP A0A1M7II12
A	284	THR	GLY	engineered mutation	UNP A0A1M7II12
A	285	SER	LEU	engineered mutation	UNP A0A1M7II12
A	286	ASP	PHE	engineered mutation	UNP A0A1M7II12
A	287	SER	ALA	engineered mutation	UNP A0A1M7II12
A	288	GLN	PRO	engineered mutation	UNP A0A1M7II12
A	290	CYS	SER	engineered mutation	UNP A0A1M7II12
A	299	LEU	-	expression tag	UNP A0A1M7II12
A	300	GLU	-	expression tag	UNP A0A1M7II12

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Chain	Residue	Modelled	Actual	Comment	Reference
A	301	HIS	-	expression tag	UNP A0A1M7II12
A	302	HIS	-	expression tag	UNP A0A1M7II12
A	303	HIS	-	expression tag	UNP A0A1M7II12
A	304	HIS	-	expression tag	UNP A0A1M7II12
B	41	ALA	-	expression tag	UNP A0A1M7II12
B	42	ALA	-	expression tag	UNP A0A1M7II12
B	109	ALA	ASN	engineered mutation	UNP A0A1M7II12
B	129	THR	VAL	engineered mutation	UNP A0A1M7II12
B	155	ARG	ALA	engineered mutation	UNP A0A1M7II12
B	180	CYS	LEU	engineered mutation	UNP A0A1M7II12
B	196	THR	GLY	engineered mutation	UNP A0A1M7II12
B	198	LYS	ARG	engineered mutation	UNP A0A1M7II12
B	202	CYS	ALA	engineered mutation	UNP A0A1M7II12
B	242	CYS	ARG	engineered mutation	UNP A0A1M7II12
B	?	-	PRO	deletion	UNP A0A1M7II12
B	282	ASN	SER	engineered mutation	UNP A0A1M7II12
B	283	HIS	THR	engineered mutation	UNP A0A1M7II12
B	284	THR	GLY	engineered mutation	UNP A0A1M7II12
B	285	SER	LEU	engineered mutation	UNP A0A1M7II12
B	286	ASP	PHE	engineered mutation	UNP A0A1M7II12
B	287	SER	ALA	engineered mutation	UNP A0A1M7II12
B	288	GLN	PRO	engineered mutation	UNP A0A1M7II12
B	290	CYS	SER	engineered mutation	UNP A0A1M7II12
B	299	LEU	-	expression tag	UNP A0A1M7II12
B	300	GLU	-	expression tag	UNP A0A1M7II12
B	301	HIS	-	expression tag	UNP A0A1M7II12
B	302	HIS	-	expression tag	UNP A0A1M7II12
B	303	HIS	-	expression tag	UNP A0A1M7II12
B	304	HIS	-	expression tag	UNP A0A1M7II12
C	41	ALA	-	expression tag	UNP A0A1M7II12
C	42	ALA	-	expression tag	UNP A0A1M7II12
C	109	ALA	ASN	engineered mutation	UNP A0A1M7II12
C	129	THR	VAL	engineered mutation	UNP A0A1M7II12
C	155	ARG	ALA	engineered mutation	UNP A0A1M7II12
C	180	CYS	LEU	engineered mutation	UNP A0A1M7II12
C	196	THR	GLY	engineered mutation	UNP A0A1M7II12
C	198	LYS	ARG	engineered mutation	UNP A0A1M7II12
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C	282	ASN	SER	engineered mutation	UNP A0A1M7II12
C	283	HIS	THR	engineered mutation	UNP A0A1M7II12

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Chain	Residue	Modelled	Actual	Comment	Reference
C	284	THR	GLY	engineered mutation	UNP A0A1M7II12
C	285	SER	LEU	engineered mutation	UNP A0A1M7II12
C	286	ASP	PHE	engineered mutation	UNP A0A1M7II12
C	287	SER	ALA	engineered mutation	UNP A0A1M7II12
C	288	GLN	PRO	engineered mutation	UNP A0A1M7II12
C	290	CYS	SER	engineered mutation	UNP A0A1M7II12
C	299	LEU	-	expression tag	UNP A0A1M7II12
C	300	GLU	-	expression tag	UNP A0A1M7II12
C	301	HIS	-	expression tag	UNP A0A1M7II12
C	302	HIS	-	expression tag	UNP A0A1M7II12
C	303	HIS	-	expression tag	UNP A0A1M7II12
C	304	HIS	-	expression tag	UNP A0A1M7II12
D	41	ALA	-	expression tag	UNP A0A1M7II12
D	42	ALA	-	expression tag	UNP A0A1M7II12
D	109	ALA	ASN	engineered mutation	UNP A0A1M7II12
D	129	THR	VAL	engineered mutation	UNP A0A1M7II12
D	155	ARG	ALA	engineered mutation	UNP A0A1M7II12
D	180	CYS	LEU	engineered mutation	UNP A0A1M7II12
D	196	THR	GLY	engineered mutation	UNP A0A1M7II12
D	198	LYS	ARG	engineered mutation	UNP A0A1M7II12
D	202	CYS	ALA	engineered mutation	UNP A0A1M7II12
D	242	CYS	ARG	engineered mutation	UNP A0A1M7II12
D	?	-	PRO	deletion	UNP A0A1M7II12
D	282	ASN	SER	engineered mutation	UNP A0A1M7II12
D	283	HIS	THR	engineered mutation	UNP A0A1M7II12
D	284	THR	GLY	engineered mutation	UNP A0A1M7II12
D	285	SER	LEU	engineered mutation	UNP A0A1M7II12
D	286	ASP	PHE	engineered mutation	UNP A0A1M7II12
D	287	SER	ALA	engineered mutation	UNP A0A1M7II12
D	288	GLN	PRO	engineered mutation	UNP A0A1M7II12
D	290	CYS	SER	engineered mutation	UNP A0A1M7II12
D	299	LEU	-	expression tag	UNP A0A1M7II12
D	300	GLU	-	expression tag	UNP A0A1M7II12
D	301	HIS	-	expression tag	UNP A0A1M7II12
D	302	HIS	-	expression tag	UNP A0A1M7II12
D	303	HIS	-	expression tag	UNP A0A1M7II12
D	304	HIS	-	expression tag	UNP A0A1M7II12

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	128	Total O 128 128	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	110	Total 110	O 110	0	0
2	C	79	Total 79	O 79	0	0
2	D	25	Total 25	O 25	0	0

- Molecule 1: Cutinase



L278	R162	ALA
C279	L163	ALA
G280	A164	ASP
PRO	A165	N44
ASN		P45
HIS	L168	Y46
THR		
D286	R176	G49
V289	R177	P50
C290	A178	D51
A291	A179	P52
S292	C180	T53
M293		N54
N294	I188	A55
T295	W200	S56
C296	S201	I57
F297	C202	E58
F298	T203	A59
LEU	T204	A60
GLU	V205	F64
HIS	P206	A65
HIS	A216	P85
HIS	D222	
HIS	P226	T91
HIS	F227	Y92
HIS	Y228	G93
		A94
		V95
	R233	I102
	A234	
	Y238	L115
	C242	F120
	N243	V121
	A244	
		G124
	F248	I130
	P249	
	T250	L133
	S251	P134
	A252	
		R137
	T261	
	S262	A143
	W263	
	W267	A148
	V268	R151
	D269	S152
		F153
	T272	V154
	R273	R155
	Y274	
	T275	I158
	D276	
	G277	T161

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	42.10Å 74.50Å 80.19Å 62.98° 87.75° 80.06°	Depositor
Resolution (Å)	28.14 – 1.63 28.14 – 1.63	Depositor EDS
% Data completeness (in resolution range)	95.1 (28.14-1.63) 95.1 (28.14-1.63)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 1.63Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.183 , 0.219 0.194 , 0.227	Depositor DCC
R_{free} test set	5047 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	19.4	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 31.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,-k+l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8110	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 14.95% 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	0.71	0/2013	1.16	5/2754 (0.2%)
1	B	0.72	0/2013	1.17	10/2754 (0.4%)
1	C	0.67	0/2011	1.09	4/2749 (0.1%)
1	D	0.58	0/1956	1.05	1/2673 (0.0%)
All	All	0.67	0/7993	1.12	20/10930 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
1	C	0	1
1	D	0	2
All	All	0	6

There are no bond length outliers.

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	151	ARG	NE-CZ-NH1	-7.93	113.57	121.50
1	B	151	ARG	CD-NE-CZ	6.72	133.81	124.40
1	C	269	ASP	CA-CB-CG	6.31	118.91	112.60
1	B	247	PHE	CA-CB-CG	-6.18	107.62	113.80
1	A	237	ASP	CA-CB-CG	6.05	118.65	112.60

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	182	ARG	Sidechain
1	B	137	ARG	Sidechain
1	B	182	ARG	Sidechain
1	C	160	ARG	Sidechain
1	D	137	ARG	Sidechain

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	1956	0	1871	7	1
1	B	1956	0	1871	16	1
1	C	1954	0	1865	12	0
1	D	1902	0	1829	31	0
2	A	128	0	0	0	0
2	B	110	0	0	0	0
2	C	79	0	0	0	0
2	D	25	0	0	0	0
All	All	8110	0	7436	60	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 4.

The worst 5 of 60 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:D:242:CYS:HG	1:D:290:CYS:HG	1.10	0.93
1:B:102:ILE:HA	1:B:130:ILE:HG12	1.58	0.85
1:B:102:ILE:HG21	1:C:170:MET:CE	2.10	0.81
1:D:102:ILE:HA	1:D:130:ILE:HG12	1.70	0.73
1:D:180:CYS:SG	1:D:202:CYS:SG	2.53	0.71

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)
1:A:151:ARG:NH1	1:B:288:GLN:OE1[1_455]	2.10	0.10

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	255/264 (97%)	247 (97%)	8 (3%)	0	100	100
1	B	255/264 (97%)	240 (94%)	12 (5%)	3 (1%)	10	1
1	C	252/264 (96%)	244 (97%)	8 (3%)	0	100	100
1	D	246/264 (93%)	233 (95%)	13 (5%)	0	100	100
All	All	1008/1056 (96%)	964 (96%)	41 (4%)	3 (0%)	36	20

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	288	GLN
1	B	285	SER
1	B	287	SER

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	206/211 (98%)	202 (98%)	4 (2%)	50	23
1	B	206/211 (98%)	202 (98%)	4 (2%)	50	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	205/211 (97%)	201 (98%)	4 (2%)	48	21
1	D	199/211 (94%)	197 (99%)	2 (1%)	68	49
All	All	816/844 (97%)	802 (98%)	14 (2%)	53	27

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	290	CYS
1	C	54	ASN
1	D	290	CYS
1	C	286	ASP
1	D	228	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	288	GLN
1	C	301	HIS
1	D	81	GLN
1	D	54	ASN
1	B	69	GLN

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 ⓘ

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	257/264 (97%)	-0.11	5 (1%) 66 72	12, 18, 30, 58	0
1	B	257/264 (97%)	0.06	11 (4%) 40 44	11, 18, 30, 67	0
1	C	256/264 (96%)	0.11	6 (2%) 61 66	13, 22, 35, 67	0
1	D	250/264 (94%)	1.37	56 (22%) 2 2	21, 36, 62, 78	0
All	All	1020/1056 (96%)	0.35	78 (7%) 20 23	11, 21, 48, 78	0

The worst 5 of 78 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	281	PRO	6.9
1	B	284	THR	6.2
1	B	287	SER	6.0
1	B	286	ASP	5.8
1	B	280	GLY	4.9

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.