



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 28, 2026 – 03:55 AM EDT

PDB ID : 9MYK / pdb_00009myk
Title : A domain-swapped structure of QEVKG mutant of Monellin
Authors : Manjula, R.; Subramanian, R.; Gosavi, S.
Deposited on : 2025-01-21
Resolution : 2.87 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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	:	FAILED
Xtriage (Phenix)	:	2.0
EDS	:	FAILED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
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 2.87 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3442 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 Single-chain Monellin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	90	Total	C	N	O	S	2	0	0
			723	469	119	133	2			
1	B	89	Total	C	N	O	S	7	0	0
			715	460	119	134	2			
1	C	90	Total	C	N	O	S	6	0	0
			719	465	120	132	2			
1	D	90	Total	C	N	O	S	13	0	0
			734	473	124	135	2			
1	E	75	Total	C	N	O	S	4	0	0
			551	350	93	106	2			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP P02882
A	48	GLN	-	linker	UNP P02882
A	49	GLU	-	linker	UNP P02882
A	50	VAL	-	linker	UNP P02882
B	1	MET	-	initiating methionine	UNP P02882
B	48	GLN	-	linker	UNP P02882
B	49	GLU	-	linker	UNP P02882
B	50	VAL	-	linker	UNP P02882
C	1	MET	-	initiating methionine	UNP P02882
C	48	GLN	-	linker	UNP P02882
C	49	GLU	-	linker	UNP P02882
C	50	VAL	-	linker	UNP P02882
D	1	MET	-	initiating methionine	UNP P02882
D	48	GLN	-	linker	UNP P02882
D	49	GLU	-	linker	UNP P02882
D	50	VAL	-	linker	UNP P02882
E	1	MET	-	initiating methionine	UNP P02882
E	48	GLN	-	linker	UNP P02882
E	49	GLU	-	linker	UNP P02882

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Chain	Residue	Modelled	Actual	Comment	Reference
E	50	VAL	-	linker	UNP P02882

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3 Data and refinement statistics

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Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	87.48Å 87.26Å 88.87Å 90.00° 103.41° 90.00°	Depositor
Resolution (Å)	60.92 – 2.87	Depositor
% Data completeness (in resolution range)	93.9 (60.92-2.87)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.18_3845	Depositor
R, R_{free}	0.245 , 0.315	Depositor
Wilson B-factor (Å ²)	77.8	Xtriage
Anisotropy	0.326	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.014 for l,-k,h	Xtriage
Total number of atoms	3442	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.48% 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 [i](#)

4.1 Standard geometry [i](#)

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4.2 Too-close contacts [i](#)

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4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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 ⓘ

There are no chain breaks in this entry.

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

5.1 Protein, DNA and RNA chains [i](#)

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

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5.3 Carbohydrates [i](#)

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