

Full wwPDB X-ray Structure Validation Report (i)

Oct 1, 2023 – 10:11 PM EDT

PDB ID : 6N9D

Title: Complex of tissue inhibitor of metalloproteinases-1 (TIMP-1) mutant (L34G

/L133P/L151C/G154A) with matrix metalloproteinase-3 catalytic domain

(MMP-3cd)

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Deposited on : 2018-12-03

Resolution : 2.67 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 (i) 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 (1)) were used in the production of this report:

MolProbity : FAILED Xtriage (Phenix) : 1.13 EDS : FAILED

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

Validation Pipeline (wwPDB-VP) : 2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 2.67 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 (i)

There are 5 unique types of molecules in this entry. The entry contains 2675 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 Stromelysin-1.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	A	161	Total 1272	C 816	N 210	O 244	S 2	0	0	0

• Molecule 2 is a protein called Metalloproteinase inhibitor 1.

\mathbf{Mol}	Chain	Residues		\mathbf{A}^{1}	toms			ZeroOcc	AltConf	Trace
2	В	175	Total 1352	C 858	N 228	O 250	S 16	12	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	34	GLY	LEU	engineered mutation	UNP P01033
В	133	PRO	LEU	engineered mutation	UNP P01033
В	151	CYS	LEU	engineered mutation	UNP P01033
В	154	ALA	GLY	engineered mutation	UNP P01033

• Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	3	Total Ca 3 3	0	0

• Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	$\begin{array}{cc} \text{Total} & \text{Zn} \\ 2 & 2 \end{array}$	0	0

• Molecule 5 is water.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	21	Total O 21 21	0	0
5	В	25	Total O 25 25	0	0

Mol Probity and EDS failed to run properly - this section is therefore empty.



3 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source	
Space group	P 65 2 2	Depositor	
Cell constants	70.03Å 70.03Å 319.51Å	Depositor	
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor	
Resolution (Å)	43.99 - 2.67	Depositor	
% Data completeness	99.8 (43.99-2.67)	Depositor	
(in resolution range)	33.0 (43.33-2.01)	Dehogicor	
R_{merge}	0.25	Depositor	
R_{sym}	(Not available)	Depositor	
$< I/\sigma(I) > 1$	1.75 (at 2.69Å)	Xtriage	
Refinement program	PHENIX 1.9_1692	Depositor	
R, R_{free}	0.184 , 0.258	Depositor	
Wilson B-factor (A^2)	50.9	Xtriage	
Anisotropy	0.243	Xtriage	
L-test for twinning ²	$ < L > = 0.45, < L^2> = 0.28$	Xtriage	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	2675	wwPDB-VP	
Average B, all atoms (Å ²)	55.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.98% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of <|L|>, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

4 Model quality (i)

4.1 Standard geometry (i)

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

4.2 Too-close contacts (i)

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

4.3 Torsion angles (i)

4.3.1 Protein backbone (i)

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

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 monosaccharides in this entry.

4.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.



There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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)

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

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

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

5.3 Carbohydrates (i)

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

5.4 Ligands (i)

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

5.5 Other polymers (i)

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

