

wwPDB X-ray Structure Validation Summary Report (i)

Oct 1, 2023 – 11:34 PM EDT

PDB ID	:	6MRQ
Title	:	Structure of ToPI1 inhibitor from Tityus obscurus scorpion venom in complex
		with trypsin
Authors	:	Fernandes, J.C.; Mourao, C.B.F.; Schwartz, E.F.; Barbosa, J.A.R.G.
Deposited on		
Resolution	:	1.29 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 (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
Mogul	:	1.8.5 (274361), CSD as541be (2020)
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: $X\hbox{-}RAY\,DIFFRACTION$

The reported resolution of this entry is 1.29 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.



6MRQ

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4086 atoms, of which 1877 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 Cationic trypsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
1	А	223	Total 3250	C 1022	H 1607	N 279	O 328	S 14	0	5	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	246	CYS	-	expression tag	UNP P00760
A	247	ASN	-	expression tag	UNP P00760
A	248	TYR	-	expression tag	UNP P00760
А	249	VAL	-	expression tag	UNP P00760
A	250	SER	-	expression tag	UNP P00760
А	251	TRP	-	expression tag	UNP P00760
А	252	ILE	-	expression tag	UNP P00760
A	253	LYS	-	expression tag	UNP P00760
А	254	GLN	-	expression tag	UNP P00760
A	255	THR	-	expression tag	UNP P00760
А	256	ILE	-	expression tag	UNP P00760
А	257	ALA	-	expression tag	UNP P00760
А	258	SER	-	expression tag	UNP P00760
А	259	ASN	-	expression tag	UNP P00760

• Molecule 2 is a protein called inhibitor from Tityus obscurus scorpion venom (TopI1).

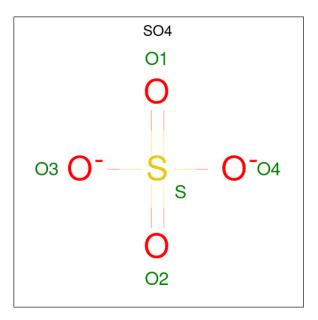
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
2	Ι	32	Total 523	C 158	Н 270	N 46	0 42	${ m S} 7$	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	Total Ca 1 1	0	0



• Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
4	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
4	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	260	Total O 260 260	0	0
5	Ι	37	Total O 37 37	0	0

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



3 Data and refinement statistics (i)

Property	Value	Source	
Space group	P 21 21 21	Depositor	
Cell constants	46.82Å 59.02Å 79.08Å	Depositor	
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor	
Resolution (Å)	27.65 - 1.29	Depositor	
% Data completeness	99.2 (27.65-1.29)	Depositor	
(in resolution range)		-	
R _{merge}	0.05	Depositor	
R _{sym}	(Not available)	Depositor	
$< I/\sigma(I) > 1$	$0.84 (at 1.29 \text{\AA})$	Xtriage	
Refinement program	PHENIX (1.13_2998: ???)	Depositor	
R, R_{free}	0.165 , 0.180	Depositor	
Wilson B-factor $(Å^2)$	13.2	Xtriage	
Anisotropy	0.289	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	4086	wwPDB-VP	
Average B, all atoms $(Å^2)$	23.0	wwPDB-VP	

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

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 7.01% of the height of the origin peak. No significant pseudotranslation is detected.

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.



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 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol Type Chair		Chain	Dec	Link	B	ond leng	gths	Bond angles		
	Type	Chain	Res		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
4	SO4	А	303	-	4,4,4	0.15	0	$6,\!6,\!6$	0.10	0
4	SO4	А	304	-	4,4,4	0.15	0	$6,\!6,\!6$	0.19	0
4	SO4	А	302	-	4,4,4	0.15	0	$6,\!6,\!6$	0.22	0

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.

