

wwPDB X-ray Structure Validation Summary Report (i)

Oct 5, 2023 – 02:39 AM EDT

PDB ID : 6VIN

Title : Crystallographic structure of the circularly permuted human Taspase1 protein

Authors: Martin-Garcia, J.M.; Fromme, P.

Deposited on : 2020-01-13

Resolution : 3.04 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 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 3.04 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 is only 1 type of molecule in this entry. The entry contains 10500 atoms, of which 5151 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 Threonine aspartase 1.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace			
1	A	364	Total 5257	C 1659	H 2582	N 484	O 511	S 21	129	0	0
1	В	364	Total 5243	C 1659	H 2569	N 483	O 511	S 21	129	0	0

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q9H6P5
A	185	GLY	-	linker	UNP Q9H6P5
	186		-	linker	•
A		SER	-		UNP Q9H6P5
A	187	GLY	-	linker	UNP Q9H6P5
A	188	SER	-	linker	UNP Q9H6P5
A	382	LEU	-	expression tag	UNP Q9H6P5
A	383	GLU	-	expression tag	UNP Q9H6P5
A	384	HIS	-	expression tag	UNP Q9H6P5
A	385	HIS	-	expression tag	UNP Q9H6P5
A	386	HIS	_	expression tag	UNP Q9H6P5
A	387	HIS	-	expression tag	UNP Q9H6P5
A	388	HIS	_	expression tag	UNP Q9H6P5
A	389	HIS	-	expression tag	UNP Q9H6P5
В	1	MET	_	initiating methionine	UNP Q9H6P5
В	185	GLY	-	linker	UNP Q9H6P5
В	186	SER	_	linker	UNP Q9H6P5
В	187	GLY	-	linker	UNP Q9H6P5
В	188	SER	-	linker	UNP Q9H6P5
В	382	LEU	-	expression tag	UNP Q9H6P5
В	383	GLU	-	expression tag	UNP Q9H6P5
В	384	HIS	_	expression tag	UNP Q9H6P5
В	385	HIS	_	expression tag	UNP Q9H6P5
В	386	HIS	-	expression tag	UNP Q9H6P5
В	387	HIS	_	expression tag	UNP Q9H6P5
В	388	HIS	-	expression tag	UNP Q9H6P5
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Chain	Residue	Modelled	Actual	Comment	Reference
В	389	HIS	-	expression tag	UNP Q9H6P5

MolProbity 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	H 3 2	Depositor	
Cell constants	196.00Å 196.00Å 196.91Å	Depositor	
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor	
Resolution (Å)	49.05 - 3.04	Depositor	
% Data completeness	54.4 (49.05-3.04)	Depositor	
(in resolution range)	04.4 (43.00-3.04)	Depositor	
R_{merge}	0.07	Depositor	
R_{sym}	(Not available)	Depositor	
$< I/\sigma(I) > 1$	1.37 (at 3.07Å)	Xtriage	
Refinement program	REFMAC 5.8.0253	Depositor	
R, R_{free}	0.237 , 0.307	Depositor	
Wilson B-factor (Å ²)	140.2	Xtriage	
Anisotropy	0.261	Xtriage	
L-test for twinning ²	$ < L > = 0.48, < L^2> = 0.31$	Xtriage	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	10500	wwPDB-VP	
Average B, all atoms (Å ²)	165.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.48% 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)

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 (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.

