Full wwPDB X-ray Structure Validation Report ⓘ

Oct 3, 2023 – 04:48 AM EDT

PDB ID	:	6UGK
Title	:	CRYSTAL STRUCTURE OF CIRCULARLY PERMUTED HUMAN TASPASE-1
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Deposited on	:	2019-09-26
Resolution	:	2.15 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)	:	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 2.15 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 4 unique types of molecules in this entry. The entry contains 4556 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 Threonine aspartase 1,Threonine aspartase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	316	Total	C	N	O	S	0	1	0
			2235	1390	397	430	18			
1	B	304	Total	C	N	O	S	0	2	0
			2132	1324	379	411	18			

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
A	186	SER	-	linker	UNP Q9H6P5
A	187	GLY	-	linker	UNP Q9H6P5
A	188	SER	-	linker	UNP Q9H6P5
A	332	LEU	-	expression tag	UNP Q9H6P5
A	333	GLU	-	expression tag	UNP Q9H6P5
A	334	HIS	-	expression tag	UNP Q9H6P5
A	335	HIS	-	expression tag	UNP Q9H6P5
A	336	HIS	-	expression tag	UNP Q9H6P5
A	337	HIS	-	expression tag	UNP Q9H6P5
A	338	HIS	-	expression tag	UNP Q9H6P5
A	339	HIS	-	expression tag	UNP Q9H6P5
B	1	MET	-	initiating methionine	UNP Q9H6P5
B	185	GLY	-	linker	UNP Q9H6P5
B	186	SER	-	linker	UNP Q9H6P5
B	187	GLY	-	linker	UNP Q9H6P5
B	188	SER	-	linker	UNP Q9H6P5
B	332	LEU	-	expression tag	UNP Q9H6P5
B	333	GLU	-	expression tag	UNP Q9H6P5
B	334	HIS	-	expression tag	UNP Q9H6P5
B	335	HIS	-	expression tag	UNP Q9H6P5
B	336	HIS	-	expression tag	UNP Q9H6P5
B	337	HIS	-	expression tag	UNP Q9H6P5
B	338	HIS	-	expression tag	UNP Q9H6P5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	339	HIS	-	expression tag	UNP Q9H6P5

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Na 1 1	0	0
2	B	1	Total Na 1 1	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Cl 2 2	0	0
3	B	2	Total Cl 2 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	97	Total O 97 97	0	0
4	B	86	Total O 86 86	0	0

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	P 65	Depositor
Cell constants a, b, c, α, β, γ	60.30Å 60.30Å 319.01Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.41 – 2.15	Depositor
% Data completeness (in resolution range)	100.0 (40.41-2.15)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.39 (at 2.16Å)	Xtriage
Refinement program	PHENIX DEV_2328	Depositor
R, R_{free}	0.159 , 0.197	Depositor
Wilson B-factor (Å^2)	32.1	Xtriage
Anisotropy	0.222	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.097 for h,-h-k,-l	Xtriage
Total number of atoms	4556	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical 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.

4 Model quality

4.1 Standard geometry

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

4.2 Too-close contacts

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

4.3 Torsion angles

4.3.1 Protein backbone

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

4.3.2 Protein sidechains

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

4.3.3 RNA

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

4.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

4.5 Carbohydrates

There are no monosaccharides in this entry.

4.6 Ligand geometry

Of 6 ligands modelled in this entry, 6 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

5.1 Protein, DNA and RNA chains

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

5.2 Non-standard residues in protein, DNA, RNA chains

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

5.3 Carbohydrates

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

5.4 Ligands

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

5.5 Other polymers

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