Full wwPDB X-ray Structure Validation Report (i)

Oct 3, 2023 – 02:18 AM EDT

PDB ID	:	6UMU
Title	:	Human apo PD-1 triple mutant
Authors	:	Tang, S.; Kim, P.S.
Deposited on	:	2019-10-10
Resolution	:	1.18 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 (i)) 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 1.18 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 are 3 unique types of molecules in this entry. The entry contains 1156 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 Programmed cell death protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	112	Total	C	N	O	S	0	31	0
			1001	645	167	179	10			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	32	MET	-	initiating methionine	UNP Q15116
A	74	GLY	ASN	engineered mutation	UNP Q15116
A	76	PRO	THR	engineered mutation	UNP Q15116
A	93	SER	CYS	conflict	UNP Q15116
A	132	VAL	ALA	engineered mutation	UNP Q15116
A	151	GLY	-	expression tag	UNP Q15116
A	152	SER	-	expression tag	UNP Q15116
A	153	TRP	-	expression tag	UNP Q15116
A	154	SER	-	expression tag	UNP Q15116
A	155	HIS	-	expression tag	UNP Q15116
A	156	PRO	-	expression tag	UNP Q15116
A	157	GLN	-	expression tag	UNP Q15116
A	158	PHE	-	expression tag	UNP Q15116
A	159	GLU	-	expression tag	UNP Q15116
A	160	LYS	-	expression tag	UNP Q15116

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Cl	0	1
			3	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	144	Total O 152 152	0	8

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 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	46.17Å 46.17Å 89.27Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	36.49 – 1.18	Depositor
% Data completeness (in resolution range)	99.7 (36.49-1.18)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.61 (at 1.18Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.154 , 0.164	Depositor
Wilson B-factor (Å^2)	16.4	Xtriage
Anisotropy	0.020	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.036 for -h,-k,l	Xtriage
Total number of atoms	1156	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.72% 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 3 ligands modelled in this entry, 3 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.