

Full wwPDB X-ray Structure Validation Report (i)

Oct 5, 2023 – 01:43 AM EDT

PDB ID : 6UMV

Title : Human apo PD-1 double mutant

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Deposited on : 2019-10-10

Resolution : 1.42 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: $X\text{-}RAY\ DIFFRACTION$

The reported resolution of this entry is 1.42 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 3 unique types of molecules in this entry. The entry contains 1135 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		At	oms			ZeroOcc	AltConf	Trace
1	Λ	116	Total	С	N	О	S	0	30	0
1	Λ	110	1048	664	183	192	9	0	30	U

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	32	MET	-	initiating methionine	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 3 3	1	1

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	82	Total O 84 84	0	2



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	46.20Å 46.20Å 89.41Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	36.52 - 1.42	Depositor
% Data completeness	99.7 (36.52-1.42)	Depositor
(in resolution range)	,	-
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.18 (at 1.42Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.161 , 0.189	Depositor
Wilson B-factor (A^2)	21.1	Xtriage
Anisotropy	0.237	Xtriage
L-test for twinning ²	$< L > = 0.50, < L^2> = 0.33$	Xtriage
Estimated twinning fraction	0.038 for -h,-k,l	Xtriage
Total number of atoms	1135	wwPDB-VP
Average B, all atoms (\mathring{A}^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 11.14% 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.



 $^{^1 {\}rm Intensities}$ 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 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 (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.

