



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 5, 2023 – 05:20 AM EDT

PDB ID : 6UMT
Title : High-affinity human PD-1 PD-L2 complex
Authors : Tang, S.; Kim, P.S.
Deposited on : 2019-10-10
Resolution : 1.99 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**
Xtrriage (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

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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 1769 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
			Total	C	N	O	S			
1	A	109	874	548	152	167	7	0	6	0

There are 29 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	14	MET	-	expression tag	UNP Q15116
A	15	GLY	-	expression tag	UNP Q15116
A	16	TRP	-	expression tag	UNP Q15116
A	17	SER	-	expression tag	UNP Q15116
A	18	CYS	-	expression tag	UNP Q15116
A	19	ILE	-	expression tag	UNP Q15116
A	20	ILE	-	expression tag	UNP Q15116
A	21	LEU	-	expression tag	UNP Q15116
A	22	PHE	-	expression tag	UNP Q15116
A	23	LEU	-	expression tag	UNP Q15116
A	24	VAL	-	expression tag	UNP Q15116
A	25	ALA	-	expression tag	UNP Q15116
A	26	THR	-	expression tag	UNP Q15116
A	27	ALA	-	expression tag	UNP Q15116
A	28	THR	-	expression tag	UNP Q15116
A	29	GLY	-	expression tag	UNP Q15116
A	30	VAL	-	expression tag	UNP Q15116
A	31	HIS	-	expression tag	UNP Q15116
A	32	SER	-	expression tag	UNP Q15116
A	49	SER	ASN	conflict	UNP Q15116
A	58	SER	ASN	conflict	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	116	ASP	ASN	conflict	UNP Q15116
A	132	VAL	ALA	engineered mutation	UNP Q15116
A	151	PRO	-	expression tag	UNP Q15116

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Chain	Residue	Modelled	Actual	Comment	Reference
A	152	GLU	-	expression tag	UNP Q15116
A	153	ALA	-	expression tag	UNP Q15116

- Molecule 2 is a protein called Programmed cell death 1 ligand 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	99	769	497	126	144	2	0	2	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	37	ASP	ASN	conflict	UNP Q9BQ51
B	64	ASP	ASN	conflict	UNP Q9BQ51

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	A	1	1	1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	73	73	73	0	0
4	B	52	52	52	0	0

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

3 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	41.29Å 67.80Å 89.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.51 – 1.99	Depositor
% Data completeness (in resolution range)	98.5 (37.51-1.99)	Depositor
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 1.98Å)	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.198 , 0.226	Depositor
Wilson B-factor (Å ²)	34.1	Xtrriage
Anisotropy	0.452	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	1769	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.15% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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.

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 1 ligands modelled in this entry, 1 is 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.