



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2023 – 04:58 PM EDT

PDB ID : 6NOJ
Title : PD-L1 IgV domain V76T with fragment
Authors : Zhao, B.; Perry, E.
Deposited on : 2019-01-16
Resolution : 2.33 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**
Mogul : 1.8.5 (274361), CSD as541be (2020)
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 2.33 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 2042 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.

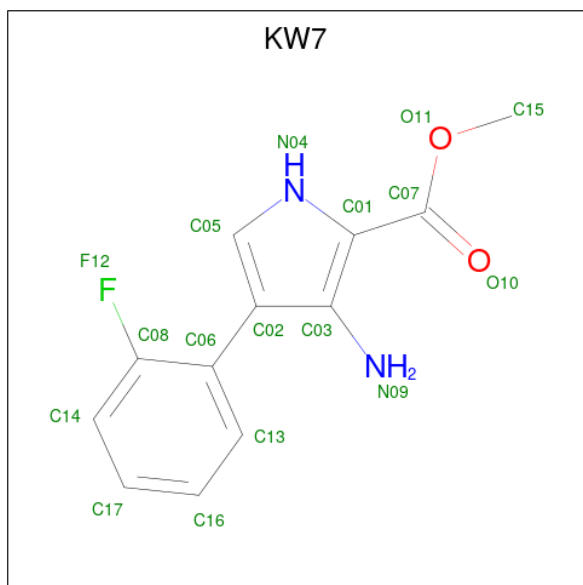
- Molecule 1 is a protein called Programmed cell death 1 ligand 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	125	972	622	166	179	5	0	0	0
1	B	126	981	624	169	183	5	0	0	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	76	THR	VAL	engineered mutation	UNP Q9NZQ7
A	135	ALA	-	expression tag	UNP Q9NZQ7
A	136	ALA	-	expression tag	UNP Q9NZQ7
A	137	ALA	-	expression tag	UNP Q9NZQ7
A	138	LEU	-	expression tag	UNP Q9NZQ7
A	139	HIS	-	expression tag	UNP Q9NZQ7
A	140	HIS	-	expression tag	UNP Q9NZQ7
A	141	HIS	-	expression tag	UNP Q9NZQ7
A	142	HIS	-	expression tag	UNP Q9NZQ7
A	143	HIS	-	expression tag	UNP Q9NZQ7
A	144	HIS	-	expression tag	UNP Q9NZQ7
B	76	THR	VAL	engineered mutation	UNP Q9NZQ7
B	135	ALA	-	expression tag	UNP Q9NZQ7
B	136	ALA	-	expression tag	UNP Q9NZQ7
B	137	ALA	-	expression tag	UNP Q9NZQ7
B	138	LEU	-	expression tag	UNP Q9NZQ7
B	139	HIS	-	expression tag	UNP Q9NZQ7
B	140	HIS	-	expression tag	UNP Q9NZQ7
B	141	HIS	-	expression tag	UNP Q9NZQ7
B	142	HIS	-	expression tag	UNP Q9NZQ7
B	143	HIS	-	expression tag	UNP Q9NZQ7
B	144	HIS	-	expression tag	UNP Q9NZQ7

- Molecule 2 is methyl 3-amino-4-(2-fluorophenyl)-1H-pyrrole-2-carboxylate (three-letter code: KW7) (formula: C₁₂H₁₁FN₂O₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
2	A	1	17	12	1	2	2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	38	Total	O	0	0
			38	38		
3	B	34	Total	O	0	0
			34	34		

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 2	Depositor
Cell constants a, b, c, α , β , γ	83.80Å 96.94Å 32.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.08 – 2.33	Depositor
% Data completeness (in resolution range)	99.6 (27.08-2.33)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 2.08Å)	Xtrriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.190 , 0.245	Depositor
Wilson B-factor (Å ²)	21.6	Xtrriage
Anisotropy	0.297	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	2042	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.45% 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](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	KW7	A	400	-	16,18,18	1.65	5 (31%)	16,25,25	1.98	3 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	KW7	A	400	-	-	0/9/10/10	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	400	KW7	O11-C07	3.50	1.41	1.33
2	A	400	KW7	C05-N04	-2.48	1.32	1.36
2	A	400	KW7	C03-N09	2.25	1.44	1.37
2	A	400	KW7	C02-C03	-2.24	1.39	1.41
2	A	400	KW7	C06-C02	2.06	1.53	1.49

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	400	KW7	O11-C07-C01	5.40	120.88	112.17
2	A	400	KW7	O11-C07-O10	-3.77	116.08	123.45
2	A	400	KW7	C07-C01-N04	2.73	125.57	120.42

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

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.