Full wwPDB X-ray Structure Validation Report (i)

Oct 4, 2023 – 07:29 PM EDT

PDB ID	:	6NNV
Title	:	PD-L1 IgV domain complex with macro-cyclic peptide
Authors	:	Zhao, B.; Perry, E.
Deposited on	:	2019-01-15
Resolution	:	1.92 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 1.92 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 4561 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	119	925	594	150	176	5	0	0	0
1	B	121	935	599	151	180	5	0	0	0
1	C	123	959	614	159	181	5	0	0	0
1	D	121	928	594	152	177	5	0	0	0

There are 44 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	GLU	-	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	GLU	-	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

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

- Molecule 2 is a protein called macrocyclic peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	I	16	134	97	17	19	1	0	0	1
2	J	16	134	97	17	19	1	0	0	1
2	K	16	134	97	17	19	1	0	0	1
2	L	16	134	97	17	19	1	0	0	1

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	58	58	58	0	0
3	B	62	62	62	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	C	63	63	63	0	0
			Total	O		
3	D	72	72	72	0	0
			Total	O		
3	I	7	7	7	0	0
			Total	O		
3	J	7	7	7	0	0
			Total	O		
3	K	5	5	5	0	0
			Total	O		
3	L	4	4	4	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 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	56.84Å 61.68Å 80.89Å 90.00° 90.17° 90.00°	Depositor
Resolution (Å)	29.10 – 1.92	Depositor
% Data completeness (in resolution range)	97.0 (29.10-1.92)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.56 (at 1.92Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.215 , 0.253	Depositor
Wilson B-factor (Å^2)	17.6	Xtriage
Anisotropy	0.855	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.139 for h,-k,-l	Xtriage
Total number of atoms	4561	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.78 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.0147e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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 (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)

validation-pack failed to run properly - this section is therefore empty.

4.5 Carbohydrates (i)

validation-pack failed to run properly - this section is therefore empty.

4.6 Ligand geometry (i)

validation-pack failed to run properly - this section is therefore empty.

4.7 Other polymers (i)

validation-pack failed to run properly - this section is therefore empty.

4.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	44:VAL	C	47:GLU	N	6.24

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.