



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2023 – 02:36 PM EDT

PDB ID : 6NXL
Title : Ubiquitin binding variants
Authors : Miller, D.J.; Watson, E.R.
Deposited on : 2019-02-08
Resolution : 2.80 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 2.80 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 is only 1 type of molecule in this entry. The entry contains 4490 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 Polyubiquitin-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	75	588	373	98	116	1	0	0	0
1	B	74	567	363	93	110	1	0	0	0
1	C	73	541	348	85	107	1	0	0	0
1	D	74	583	373	95	114	1	0	0	0
1	E	75	563	361	93	108	1	0	0	0
1	F	74	567	363	93	110	1	0	0	0
1	G	73	565	360	93	111	1	0	0	0
1	H	74	516	336	86	93	1	0	0	0

There are 104 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP B4DV12
A	-4	SER	-	expression tag	UNP B4DV12
A	-3	GLY	-	expression tag	UNP B4DV12
A	-2	GLY	-	expression tag	UNP B4DV12
A	-1	SER	-	expression tag	UNP B4DV12
A	6	ASP	LYS	conflict	UNP B4DV12
A	8	VAL	LEU	conflict	UNP B4DV12
A	9	GLN	THR	conflict	UNP B4DV12
A	10	TRP	GLY	conflict	UNP B4DV12
A	66	ALA	THR	conflict	UNP B4DV12
A	68	ILE	HIS	conflict	UNP B4DV12
A	70	LEU	VAL	conflict	UNP B4DV12
A	72	THR	ARG	conflict	UNP B4DV12

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	GLY	-	expression tag	UNP B4DV12
B	-4	SER	-	expression tag	UNP B4DV12
B	-3	GLY	-	expression tag	UNP B4DV12
B	-2	GLY	-	expression tag	UNP B4DV12
B	-1	SER	-	expression tag	UNP B4DV12
B	6	ASP	LYS	conflict	UNP B4DV12
B	8	VAL	LEU	conflict	UNP B4DV12
B	9	GLN	THR	conflict	UNP B4DV12
B	10	TRP	GLY	conflict	UNP B4DV12
B	66	ALA	THR	conflict	UNP B4DV12
B	68	ILE	HIS	conflict	UNP B4DV12
B	70	LEU	VAL	conflict	UNP B4DV12
B	72	THR	ARG	conflict	UNP B4DV12
C	-5	GLY	-	expression tag	UNP B4DV12
C	-4	SER	-	expression tag	UNP B4DV12
C	-3	GLY	-	expression tag	UNP B4DV12
C	-2	GLY	-	expression tag	UNP B4DV12
C	-1	SER	-	expression tag	UNP B4DV12
C	6	ASP	LYS	conflict	UNP B4DV12
C	8	VAL	LEU	conflict	UNP B4DV12
C	9	GLN	THR	conflict	UNP B4DV12
C	10	TRP	GLY	conflict	UNP B4DV12
C	66	ALA	THR	conflict	UNP B4DV12
C	68	ILE	HIS	conflict	UNP B4DV12
C	70	LEU	VAL	conflict	UNP B4DV12
C	72	THR	ARG	conflict	UNP B4DV12
D	-5	GLY	-	expression tag	UNP B4DV12
D	-4	SER	-	expression tag	UNP B4DV12
D	-3	GLY	-	expression tag	UNP B4DV12
D	-2	GLY	-	expression tag	UNP B4DV12
D	-1	SER	-	expression tag	UNP B4DV12
D	6	ASP	LYS	conflict	UNP B4DV12
D	8	VAL	LEU	conflict	UNP B4DV12
D	9	GLN	THR	conflict	UNP B4DV12
D	10	TRP	GLY	conflict	UNP B4DV12
D	66	ALA	THR	conflict	UNP B4DV12
D	68	ILE	HIS	conflict	UNP B4DV12
D	70	LEU	VAL	conflict	UNP B4DV12
D	72	THR	ARG	conflict	UNP B4DV12
E	-5	GLY	-	expression tag	UNP B4DV12
E	-4	SER	-	expression tag	UNP B4DV12
E	-3	GLY	-	expression tag	UNP B4DV12

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	GLY	-	expression tag	UNP B4DV12
E	-1	SER	-	expression tag	UNP B4DV12
E	6	ASP	LYS	conflict	UNP B4DV12
E	8	VAL	LEU	conflict	UNP B4DV12
E	9	GLN	THR	conflict	UNP B4DV12
E	10	TRP	GLY	conflict	UNP B4DV12
E	66	ALA	THR	conflict	UNP B4DV12
E	68	ILE	HIS	conflict	UNP B4DV12
E	70	LEU	VAL	conflict	UNP B4DV12
E	72	THR	ARG	conflict	UNP B4DV12
F	-5	GLY	-	expression tag	UNP B4DV12
F	-4	SER	-	expression tag	UNP B4DV12
F	-3	GLY	-	expression tag	UNP B4DV12
F	-2	GLY	-	expression tag	UNP B4DV12
F	-1	SER	-	expression tag	UNP B4DV12
F	6	ASP	LYS	conflict	UNP B4DV12
F	8	VAL	LEU	conflict	UNP B4DV12
F	9	GLN	THR	conflict	UNP B4DV12
F	10	TRP	GLY	conflict	UNP B4DV12
F	66	ALA	THR	conflict	UNP B4DV12
F	68	ILE	HIS	conflict	UNP B4DV12
F	70	LEU	VAL	conflict	UNP B4DV12
F	72	THR	ARG	conflict	UNP B4DV12
G	-5	GLY	-	expression tag	UNP B4DV12
G	-4	SER	-	expression tag	UNP B4DV12
G	-3	GLY	-	expression tag	UNP B4DV12
G	-2	GLY	-	expression tag	UNP B4DV12
G	-1	SER	-	expression tag	UNP B4DV12
G	6	ASP	LYS	conflict	UNP B4DV12
G	8	VAL	LEU	conflict	UNP B4DV12
G	9	GLN	THR	conflict	UNP B4DV12
G	10	TRP	GLY	conflict	UNP B4DV12
G	66	ALA	THR	conflict	UNP B4DV12
G	68	ILE	HIS	conflict	UNP B4DV12
G	70	LEU	VAL	conflict	UNP B4DV12
G	72	THR	ARG	conflict	UNP B4DV12
H	-5	GLY	-	expression tag	UNP B4DV12
H	-4	SER	-	expression tag	UNP B4DV12
H	-3	GLY	-	expression tag	UNP B4DV12
H	-2	GLY	-	expression tag	UNP B4DV12
H	-1	SER	-	expression tag	UNP B4DV12
H	6	ASP	LYS	conflict	UNP B4DV12

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Chain	Residue	Modelled	Actual	Comment	Reference
H	8	VAL	LEU	conflict	UNP B4DV12
H	9	GLN	THR	conflict	UNP B4DV12
H	10	TRP	GLY	conflict	UNP B4DV12
H	66	ALA	THR	conflict	UNP B4DV12
H	68	ILE	HIS	conflict	UNP B4DV12
H	70	LEU	VAL	conflict	UNP B4DV12
H	72	THR	ARG	conflict	UNP B4DV12

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 41	Depositor
Cell constants a, b, c, α , β , γ	62.36Å 62.36Å 168.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.60 – 2.80	Depositor
% Data completeness (in resolution range)	95.9 (29.60-2.80)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.12 (at 2.80Å)	Xtrriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.213 , 0.265	Depositor
Wilson B-factor (Å ²)	57.6	Xtrriage
Anisotropy	0.594	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.064 for h,-k,-l	Xtrriage
Total number of atoms	4490	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical 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](#)

There are no ligands in this entry.

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

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.