wwPDB X-ray Structure Validation Summary Report (i)

Oct 2, 2023 – 12:51 PM EDT

PDB ID	:	6NJG
Title	:	Ubiquitin Variant in Complex with Ubiquitin Interacting Motif
Authors	:	Manczyk, N.; Sicheri, F.
Deposited on	:	2019-01-03
Resolution	:	2.35 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 2.35 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 726 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 Vacuolar protein sorting-associated protein 27.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
1	B	17	139	89	21	29	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	TYR	-	expression tag	UNP P40343

- Molecule 2 is a protein called Polyubiquitin-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	76	579	366	98	112	3	0	0	0

There are 29 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	GLY	-	expression tag	UNP J3QS39
C	-5	GLY	-	expression tag	UNP J3QS39
C	-4	ALA	-	expression tag	UNP J3QS39
C	-3	ALA	-	expression tag	UNP J3QS39
C	-2	GLN	-	expression tag	UNP J3QS39
C	-1	PRO	-	expression tag	UNP J3QS39
C	0	ALA	-	expression tag	UNP J3QS39
C	6	GLN	LYS	engineered mutation	UNP J3QS39
C	8	ILE	LEU	engineered mutation	UNP J3QS39
C	10	VAL	GLY	engineered mutation	UNP J3QS39
C	11	MET	LYS	engineered mutation	UNP J3QS39
C	12	ARG	THR	engineered mutation	UNP J3QS39
C	14	ALA	THR	engineered mutation	UNP J3QS39
C	48	MET	LYS	engineered mutation	UNP J3QS39
C	62	LYS	GLN	engineered mutation	UNP J3QS39

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Chain	Residue	Modelled	Actual	Comment	Reference
C	63	ARG	LYS	engineered mutation	UNP J3QS39
C	64	ASP	GLU	engineered mutation	UNP J3QS39
C	66	ASN	THR	engineered mutation	UNP J3QS39
C	68	TYR	HIS	engineered mutation	UNP J3QS39
C	71	SER	LEU	engineered mutation	UNP J3QS39
C	72	SER	ARG	engineered mutation	UNP J3QS39
C	75	SER	GLY	engineered mutation	UNP J3QS39
C	76	LEU	GLY	engineered mutation	UNP J3QS39
C	77	ARG	MET	engineered mutation	UNP J3QS39
C	78	ALA	GLN	engineered mutation	UNP J3QS39
C	79	GLY	-	expression tag	UNP J3QS39
C	80	ALA	-	expression tag	UNP J3QS39
C	81	ALA	-	expression tag	UNP J3QS39
C	82	ALA	-	expression tag	UNP J3QS39

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total O 1 1	0	0
3	C	7	Total O 7 7	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 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	44.61Å 44.61Å 104.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.43 – 2.35	Depositor
% Data completeness (in resolution range)	98.4 (27.43-2.35)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.48 (at 2.34Å)	Xtriage
Refinement program	PHENIX (1.14_3211:000), REFMAC 5.8.0103	Depositor
R, R_{free}	0.206 , 0.244	Depositor
Wilson B-factor (Å^2)	54.5	Xtriage
Anisotropy	0.592	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	726	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.08% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

4.1 Standard geometry

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

4.2 Too-close contacts

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

4.3 Torsion angles

4.3.1 Protein backbone

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

4.3.2 Protein sidechains

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

4.3.3 RNA

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

4.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

4.5 Carbohydrates

There are no monosaccharides in this entry.

4.6 Ligand geometry

There are no ligands in this entry.

4.7 Other polymers

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.