



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2023 – 03:59 PM EDT

PDB ID : 6N31
Title : WD repeats of human WDR12
Authors : Halabelian, L.; Zeng, H.; Tempel, W.; Li, Y.; Seitova, A.; Hutchinson, A.; Bountra, C.; Edwards, A.M.; Arrowsmith, C.H.; Structural Genomics Consortium (SGC)
Deposited on : 2018-11-14
Resolution : 2.60 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 2.60 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 2 unique types of molecules in this entry. The entry contains 4743 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 Ribosome biogenesis protein WDR12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	308	2339	1485	395	444	15	0	3	1
1	B	312	2368	1506	400	446	16	0	2	0

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	72	MET	-	initiating methionine	UNP Q9GZL7
A	73	HIS	-	expression tag	UNP Q9GZL7
A	74	HIS	-	expression tag	UNP Q9GZL7
A	75	HIS	-	expression tag	UNP Q9GZL7
A	76	HIS	-	expression tag	UNP Q9GZL7
A	77	HIS	-	expression tag	UNP Q9GZL7
A	78	HIS	-	expression tag	UNP Q9GZL7
A	79	SER	-	expression tag	UNP Q9GZL7
A	80	SER	-	expression tag	UNP Q9GZL7
A	81	GLY	-	expression tag	UNP Q9GZL7
A	82	ARG	-	expression tag	UNP Q9GZL7
A	83	GLU	-	expression tag	UNP Q9GZL7
A	84	ASN	-	expression tag	UNP Q9GZL7
A	85	LEU	-	expression tag	UNP Q9GZL7
A	86	TYR	-	expression tag	UNP Q9GZL7
A	87	PHE	-	expression tag	UNP Q9GZL7
A	88	GLN	-	expression tag	UNP Q9GZL7
A	89	GLY	-	expression tag	UNP Q9GZL7
A	286	GLY	GLU	conflict	UNP Q9GZL7
B	72	MET	-	initiating methionine	UNP Q9GZL7
B	73	HIS	-	expression tag	UNP Q9GZL7
B	74	HIS	-	expression tag	UNP Q9GZL7
B	75	HIS	-	expression tag	UNP Q9GZL7
B	76	HIS	-	expression tag	UNP Q9GZL7
B	77	HIS	-	expression tag	UNP Q9GZL7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	78	HIS	-	expression tag	UNP Q9GZL7
B	79	SER	-	expression tag	UNP Q9GZL7
B	80	SER	-	expression tag	UNP Q9GZL7
B	81	GLY	-	expression tag	UNP Q9GZL7
B	82	ARG	-	expression tag	UNP Q9GZL7
B	83	GLU	-	expression tag	UNP Q9GZL7
B	84	ASN	-	expression tag	UNP Q9GZL7
B	85	LEU	-	expression tag	UNP Q9GZL7
B	86	TYR	-	expression tag	UNP Q9GZL7
B	87	PHE	-	expression tag	UNP Q9GZL7
B	88	GLN	-	expression tag	UNP Q9GZL7
B	89	GLY	-	expression tag	UNP Q9GZL7
B	286	GLY	GLU	conflict	UNP Q9GZL7

- Molecule 2 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	14	Total X 14 14	0	0
2	B	22	Total X 22 22	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	52.74Å 87.05Å 155.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	76.00 – 2.60	Depositor
% Data completeness (in resolution range)	95.9 (76.00-2.60)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.61Å)	Xtrriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.203 , 0.233	Depositor
Wilson B-factor (Å ²)	47.3	Xtrriage
Anisotropy	0.315	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	4743	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.06 % 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 7.6059e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 36 ligands modelled in this entry, 36 are unknown - 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 [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.