



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 7BII
Title : Crystal structure of Nematocida HUWE1
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Deposited on : 2021-01-12
Resolution : 3.04 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.26
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.26

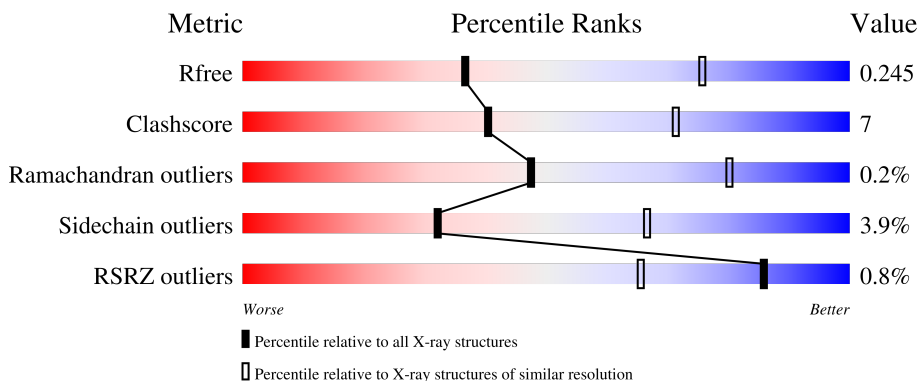
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


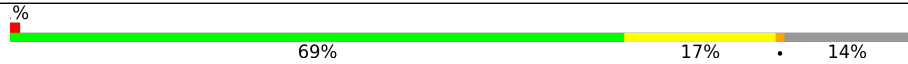
The reported resolution of this entry is 3.04 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2752 (3.08-3.00)
Clashscore	141614	3096 (3.08-3.00)
Ramachandran outliers	138981	2986 (3.08-3.00)
Sidechain outliers	138945	2988 (3.08-3.00)
RSRZ outliers	127900	2636 (3.08-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2492	 70% 15% 14%
1	B	2492	 69% 17% 14%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 34901 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 E3 ubiquitin-protein ligase HUWE1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	2143	17453	11280	2862	3213	98	0	0	0
1	B	2144	17448	11273	2861	3216	98	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP A0A177ELV2
A	0	PRO	-	expression tag	UNP A0A177ELV2
A	2457	ALA	CYS	engineered mutation	UNP A0A177ELV2
B	-1	GLY	-	expression tag	UNP A0A177ELV2
B	0	PRO	-	expression tag	UNP A0A177ELV2
B	2457	ALA	CYS	engineered mutation	UNP A0A177ELV2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	95.52Å 96.22Å 199.66Å 92.22° 100.45° 95.33°	Depositor
Resolution (Å)	196.03 – 3.04 196.03 – 3.04	Depositor EDS
% Data completeness (in resolution range)	56.3 (196.03-3.04) 56.3 (196.03-3.04)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.10 (at 3.01Å)	Xtriage
Refinement program	BUSTER 2.10.3 (6-FEB-2020)	Depositor
R, R_{free}	0.202 , 0.233 0.217 , 0.245	Depositor DCC
R_{free} test set	3733 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	75.9	Xtriage
Anisotropy	0.004	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	34901	wwPDB-VP
Average B, all atoms (Å ²)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.25% 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.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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 $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.33	0/17792	0.52	0/24002
1	B	0.32	0/17785	0.52	0/23989
All	All	0.32	0/35577	0.52	0/47991

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	17453	0	17745	251	0
1	B	17448	0	17737	252	0
All	All	34901	0	35482	503	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 503 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1059:ASP:HA	1:A:1063:LYS:HB3	1.29	1.15
1:B:1059:ASP:HA	1:B:1063:LYS:HB3	1.28	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2282:ILE:HG12	1:A:2286:LEU:HG	1.33	1.05
1:A:225:GLN:HE21	1:A:228:LYS:NZ	1.55	1.03
1:A:1987:HIS:CE1	1:A:1991:ILE:HD11	1.97	0.99

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	2129/2492 (85%)	2019 (95%)	106 (5%)	4 (0%)	47 80
1	B	2128/2492 (85%)	2011 (94%)	112 (5%)	5 (0%)	47 80
All	All	4257/4984 (85%)	4030 (95%)	218 (5%)	9 (0%)	47 80

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1064	THR
1	B	1064	THR
1	A	170	PRO
1	A	2481	GLU
1	B	170	PRO

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1955/2267 (86%)	1879 (96%)	76 (4%)	32	66
1	B	1955/2267 (86%)	1878 (96%)	77 (4%)	32	66
All	All	3910/4534 (86%)	3757 (96%)	153 (4%)	32	66

5 of 153 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1168	TYR
1	B	2331	LEU
1	B	1372	MET
1	B	1915	ASP
1	B	2433	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 84 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	755	ASN
1	B	1404	ASN
1	B	809	GLN
1	B	1024	HIS
1	B	1922	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9	
1	A	2143/2492 (85%)	-0.11	13 (0%)	89 72	45, 101, 157, 222	0
1	B	2144/2492 (86%)	-0.12	20 (0%)	84 62	44, 105, 152, 223	0
All	All	4287/4984 (86%)	-0.12	33 (0%)	86 65	44, 103, 155, 223	0

The worst 5 of 33 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1168	TYR	4.6
1	A	2064	ASN	4.2
1	A	1205	GLU	4.0
1	B	2286	LEU	3.4
1	B	1162	LEU	3.3

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.