



wwPDB X-ray Structure Validation Summary Report

Mar 19, 2024 – 12:03 PM EDT

PDB ID : 8W3V
Title : Crystal structure of human WDR41
Authors : Hutchinson, A.; Dong, A.; Li, Y.; Seitova, A.; Bountra, C.; Arrowsmith, C.H.;
Edwards, A.M.; Halabelian, L.; Structural Genomics Consortium (SGC)
Deposited on : 2024-02-22
Resolution : 2.20 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 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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

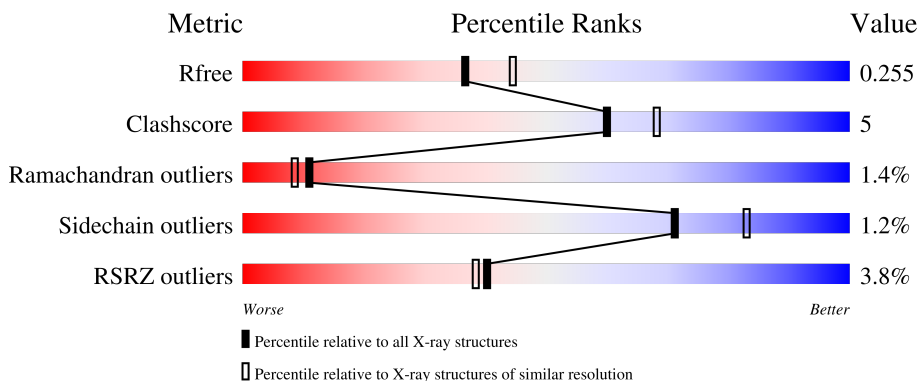
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	373	 3% 79% 10% 11%
1	B	373	 4% 76% 13% 11%

2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 4960 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 WD repeat-containing protein 41.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	333	2531	1630	423	466	12	0	0	0
1	B	332	2390	1527	408	445	10	0	0	0

There are 82 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	184	ALA	LYS	conflict	UNP Q9HAD4
A	209	ALA	GLU	conflict	UNP Q9HAD4
A	211	ALA	ASP	conflict	UNP Q9HAD4
A	?	-	LEU	deletion	UNP Q9HAD4
A	?	-	ALA	deletion	UNP Q9HAD4
A	?	-	ALA	deletion	UNP Q9HAD4
A	?	-	GLU	deletion	UNP Q9HAD4
A	?	-	PRO	deletion	UNP Q9HAD4
A	?	-	VAL	deletion	UNP Q9HAD4
A	?	-	PRO	deletion	UNP Q9HAD4
A	?	-	THR	deletion	UNP Q9HAD4
A	?	-	GLY	deletion	UNP Q9HAD4
A	?	-	PHE	deletion	UNP Q9HAD4
A	?	-	PHE	deletion	UNP Q9HAD4
A	?	-	ASN	deletion	UNP Q9HAD4
A	?	-	MET	deletion	UNP Q9HAD4
A	?	-	TRP	deletion	UNP Q9HAD4
A	?	-	GLY	deletion	UNP Q9HAD4
A	?	-	PHE	deletion	UNP Q9HAD4
A	?	-	GLY	deletion	UNP Q9HAD4
A	?	-	ARG	deletion	UNP Q9HAD4
A	?	-	VAL	deletion	UNP Q9HAD4
A	?	-	SER	deletion	UNP Q9HAD4
A	?	-	LYS	deletion	UNP Q9HAD4
A	?	-	GLN	deletion	UNP Q9HAD4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ALA	deletion	UNP Q9HAD4
A	?	-	SER	deletion	UNP Q9HAD4
A	?	-	GLN	deletion	UNP Q9HAD4
A	?	-	PRO	deletion	UNP Q9HAD4
A	?	-	VAL	deletion	UNP Q9HAD4
A	?	-	LYS	deletion	UNP Q9HAD4
A	?	-	LYS	deletion	UNP Q9HAD4
A	?	-	GLN	deletion	UNP Q9HAD4
A	?	-	GLN	deletion	UNP Q9HAD4
A	?	-	GLU	deletion	UNP Q9HAD4
A	?	-	ASN	deletion	UNP Q9HAD4
A	?	-	ALA	deletion	UNP Q9HAD4
A	?	-	THR	deletion	UNP Q9HAD4
A	?	-	SER	deletion	UNP Q9HAD4
A	?	-	CYS	deletion	UNP Q9HAD4
A	?	-	SER	deletion	UNP Q9HAD4
B	184	ALA	LYS	conflict	UNP Q9HAD4
B	209	ALA	GLU	conflict	UNP Q9HAD4
B	211	ALA	ASP	conflict	UNP Q9HAD4
B	?	-	LEU	deletion	UNP Q9HAD4
B	?	-	ALA	deletion	UNP Q9HAD4
B	?	-	ALA	deletion	UNP Q9HAD4
B	?	-	GLU	deletion	UNP Q9HAD4
B	?	-	PRO	deletion	UNP Q9HAD4
B	?	-	VAL	deletion	UNP Q9HAD4
B	?	-	PRO	deletion	UNP Q9HAD4
B	?	-	THR	deletion	UNP Q9HAD4
B	?	-	GLY	deletion	UNP Q9HAD4
B	?	-	PHE	deletion	UNP Q9HAD4
B	?	-	PHE	deletion	UNP Q9HAD4
B	?	-	ASN	deletion	UNP Q9HAD4
B	?	-	MET	deletion	UNP Q9HAD4
B	?	-	TRP	deletion	UNP Q9HAD4
B	?	-	GLY	deletion	UNP Q9HAD4
B	?	-	PHE	deletion	UNP Q9HAD4
B	?	-	GLY	deletion	UNP Q9HAD4
B	?	-	ARG	deletion	UNP Q9HAD4
B	?	-	VAL	deletion	UNP Q9HAD4
B	?	-	SER	deletion	UNP Q9HAD4
B	?	-	LYS	deletion	UNP Q9HAD4
B	?	-	GLN	deletion	UNP Q9HAD4
B	?	-	ALA	deletion	UNP Q9HAD4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	SER	deletion	UNP Q9HAD4
B	?	-	GLN	deletion	UNP Q9HAD4
B	?	-	PRO	deletion	UNP Q9HAD4
B	?	-	VAL	deletion	UNP Q9HAD4
B	?	-	LYS	deletion	UNP Q9HAD4
B	?	-	LYS	deletion	UNP Q9HAD4
B	?	-	GLN	deletion	UNP Q9HAD4
B	?	-	GLN	deletion	UNP Q9HAD4
B	?	-	GLU	deletion	UNP Q9HAD4
B	?	-	ASN	deletion	UNP Q9HAD4
B	?	-	ALA	deletion	UNP Q9HAD4
B	?	-	THR	deletion	UNP Q9HAD4
B	?	-	SER	deletion	UNP Q9HAD4
B	?	-	CYS	deletion	UNP Q9HAD4
B	?	-	SER	deletion	UNP Q9HAD4

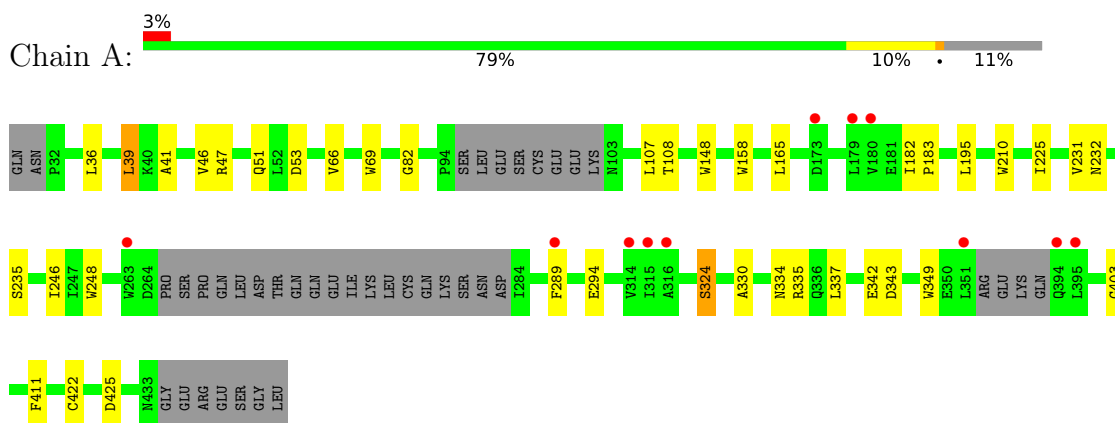
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	28	Total O 28 28	0	0
2	B	11	Total O 11 11	0	0

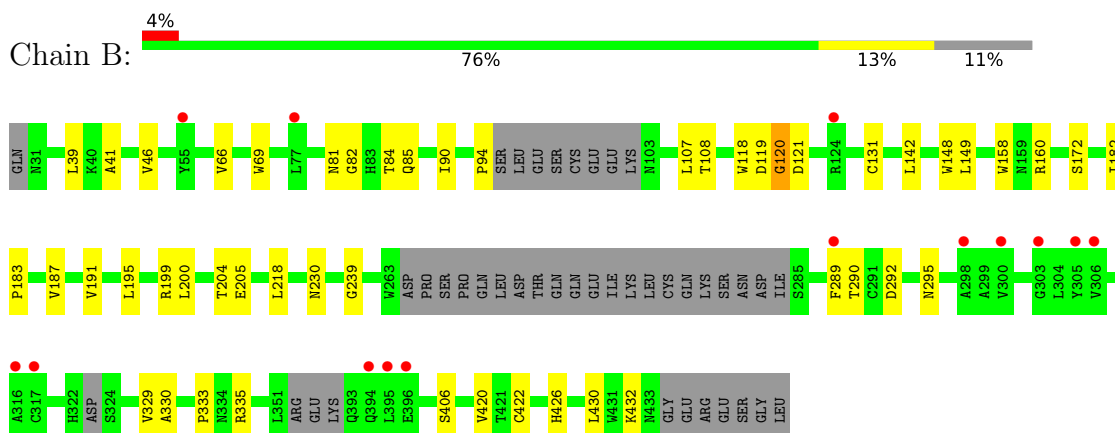
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: WD repeat-containing protein 41



- Molecule 1: WD repeat-containing protein 41



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	229.12Å 86.01Å 52.62Å 90.00° 94.06° 90.00°	Depositor
Resolution (Å)	34.36 – 2.20 34.36 – 2.20	Depositor EDS
% Data completeness (in resolution range)	95.2 (34.36-2.20) 95.2 (34.36-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.05 (at 2.20Å)	Xtrriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.214 , 0.253 0.218 , 0.255	Depositor DCC
R_{free} test set	2466 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	52.0	Xtrriage
Anisotropy	0.728	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 59.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4960	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.80% 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	0.43	0/2580	0.60	1/3521 (0.0%)
1	B	0.40	0/2431	0.56	0/3327
All	All	0.42	0/5011	0.58	1/6848 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	289	PHE	CB-CA-C	-6.04	98.33	110.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	47	ARG	Sidechain
1	B	199	ARG	Sidechain

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	2531	0	2433	21	0
1	B	2390	0	2183	24	0
2	A	28	0	0	0	0
2	B	11	0	0	1	0
All	All	4960	0	4616	44	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 5.

The worst 5 of 44 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:231:VAL:O	1:A:232:ASN:OD1	1.92	0.86
1:A:324:SER:OG	1:A:343:ASP:OD2	2.17	0.61
1:A:425:ASP:HA	1:B:204:THR:HG21	1.82	0.59
1:A:195:LEU:HD21	1:A:225:ILE:HD13	1.85	0.57
1:B:39:LEU:HB3	1:B:69:TRP:CZ3	2.41	0.55

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	325/373 (87%)	306 (94%)	15 (5%)	4 (1%)	13 10
1	B	322/373 (86%)	300 (93%)	17 (5%)	5 (2%)	9 7
All	All	647/746 (87%)	606 (94%)	32 (5%)	9 (1%)	11 8

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	329	VAL
1	B	120	GLY
1	B	205	GLU
1	A	41	ALA
1	B	41	ALA

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	261/331 (79%)	259 (99%)	2 (1%)	81	90
1	B	224/331 (68%)	220 (98%)	4 (2%)	59	72
All	All	485/662 (73%)	479 (99%)	6 (1%)	71	83

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	118	TRP
1	B	406	SER
1	B	426	HIS
1	A	324	SER
1	A	39	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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	333/373 (89%)	0.13	11 (3%) 46 44	46, 61, 89, 101	0
1	B	332/373 (89%)	0.23	14 (4%) 36 34	47, 74, 110, 129	0
All	All	665/746 (89%)	0.18	25 (3%) 40 38	46, 66, 102, 129	0

The worst 5 of 25 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	124	ARG	5.7
1	A	316	ALA	4.0
1	A	173	ASP	3.9
1	A	351	LEU	3.8
1	B	55	TYR	3.7

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.