



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 8OK1 / pdb_00008ok1
Title : WD repeat containing protein 5 (WDR5)- N225A mutant
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Deposited on : 2023-03-26
Resolution : 1.38 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

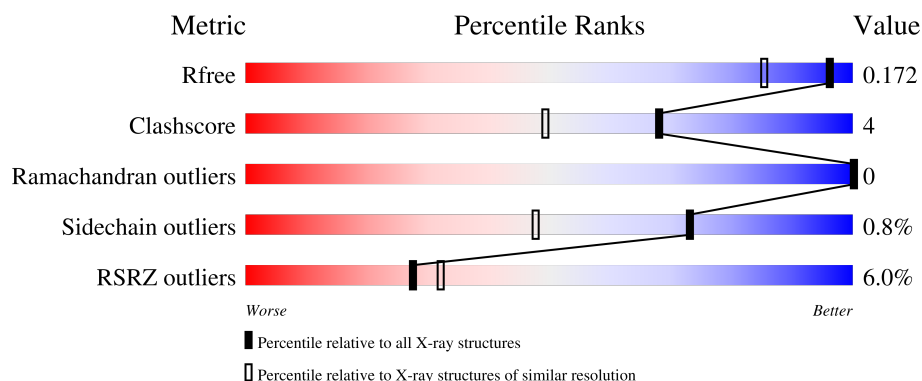
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.38 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}	180053	4403 (1.40-1.36)
Clashscore	190562	4528 (1.40-1.36)
Ramachandran outliers	187476	4459 (1.40-1.36)
Sidechain outliers	187428	4458 (1.40-1.36)
RSRZ outliers	180081	4399 (1.40-1.36)

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	555	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2594 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 Glutathione S-transferase class-mu 26 kDa isozyme, WD repeat-containing protein 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	302	Total	C	N	O	S	0	2	0
			2349	1505	388	447	9			

There are 35 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-220	MET	-	initiating methionine	UNP P08515
A	-219	LYS	-	expression tag	UNP P08515
A	-218	HIS	-	expression tag	UNP P08515
A	-217	HIS	-	expression tag	UNP P08515
A	-216	HIS	-	expression tag	UNP P08515
A	-215	HIS	-	expression tag	UNP P08515
A	-214	HIS	-	expression tag	UNP P08515
A	-213	HIS	-	expression tag	UNP P08515
A	-212	ASN	-	expression tag	UNP P08515
A	-211	THR	-	expression tag	UNP P08515
A	-210	SER	-	expression tag	UNP P08515
A	-209	SER	-	expression tag	UNP P08515
A	-208	ASN	-	expression tag	UNP P08515
A	-207	SER	-	expression tag	UNP P08515
A	12	SER	-	linker	UNP P08515
A	13	ASP	-	linker	UNP P08515
A	14	LEU	-	linker	UNP P08515
A	15	GLU	-	linker	UNP P08515
A	16	VAL	-	linker	UNP P08515
A	17	LEU	-	linker	UNP P08515
A	18	PHE	-	linker	UNP P08515
A	19	GLN	-	linker	UNP P08515
A	20	GLY	-	linker	UNP P08515
A	21	PRO	-	linker	UNP P08515
A	22	SER	-	linker	UNP P08515
A	23	ALA	-	linker	UNP P08515

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Chain	Residue	Modelled	Actual	Comment	Reference
A	24	THR	-	linker	UNP P08515
A	25	GLN	-	linker	UNP P08515
A	26	SER	-	linker	UNP P08515
A	27	LYS	-	linker	UNP P08515
A	28	PRO	-	linker	UNP P08515
A	29	THR	-	linker	UNP P08515
A	30	PRO	-	linker	UNP P08515
A	31	VAL	-	linker	UNP P08515
A	225	ALA	ASN	conflict	UNP P61965

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	245	Total O 245 245	0	0

i

● Molecule 1: Glutathione S-transferase class-mu 26 kDa isozyme, WD repeat-containing protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	78.50Å 98.13Å 80.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.67 – 1.38 48.67 – 1.38	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.67-1.38) 99.1 (48.67-1.38)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.66 (at 1.38Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.194 , 0.218 0.148 , 0.172	Depositor DCC
R_{free} test set	3068 reflections (4.65%)	wwPDB-VP
Wilson B-factor (Å ²)	20.8	Xtriage
Anisotropy	0.163	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 28.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	2594	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.88% 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	1.03	1/2407 (0.0%)	1.10	2/3267 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	140	GLN	C-O	5.50	1.31	1.24

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	141	SER	CB-CA-C	6.16	121.32	111.66
1	A	116	VAL	CA-C-O	-5.31	115.43	120.95

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	2349	0	2316	17	1
2	A	245	0	0	7	1
All	All	2594	0	2316	17	2

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 4.

The worst 5 of 17 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:140:GLN:O	2:A:401:HOH:O	1.82	0.97
1:A:236:ASN:HD22	1:A:257:ASN:H	1.20	0.88
1:A:178:HIS:HD2	1:A:222:PHE:H	1.23	0.86
1:A:157:ASP:OD2	1:A:159:LYS:HD3	1.79	0.82
1:A:263:PHE:HZ	2:A:599:HOH:O	1.63	0.81

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:401:HOH:O	2:A:401:HOH:O[4_555]	1.57	0.63
1:A:87:LYS:NZ	1:A:212:ASP:OD1[8_545]	2.07	0.13

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	302/555 (54%)	285 (94%)	17 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	262/490 (54%)	260 (99%)	2 (1%)	73	48

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	159	LYS
1	A	263	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	ASN
1	A	136	ASN
1	A	178	HIS
1	A	236	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	302/555 (54%)	0.42	18 (5%)	27 32	8, 16, 27, 44	2 (0%)

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	263	PHE	7.6
1	A	333	ASP	5.1
1	A	225	ALA	4.7
1	A	226	GLY	3.7
1	A	140	GLN	2.8

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 oligosaccharides 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.