



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 9Y76 / pdb_00009y76
Title : Crystal structure of the human DCAF1 WDR domain in complex with OICR-40120
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Deposited on : 2025-09-09
Resolution : 1.56 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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	FAILED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

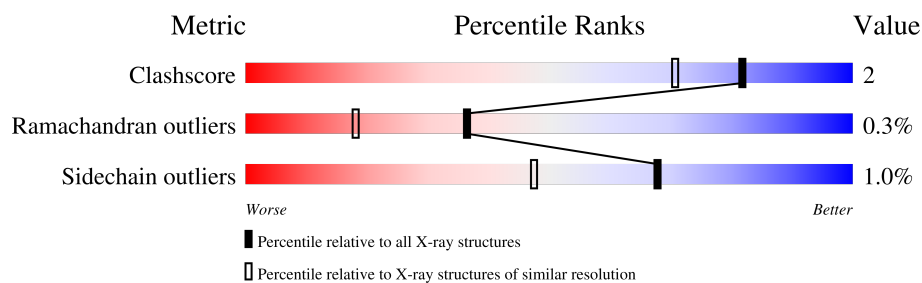
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.56 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))
Clashscore	190562	2189 (1.56-1.56)
Ramachandran outliers	187476	2153 (1.56-1.56)
Sidechain outliers	187428	2150 (1.56-1.56)

ENTRY-COMPOSITION INFOmissingINFO

SEQUENCE-PLOTS INFOmissingINFO

2 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	48.95Å 88.41Å 73.56Å 90.00° 97.86° 90.00°	Depositor
Resolution (Å)	38.83 – 1.56	Depositor
% Data completeness (in resolution range)	98.0 (38.83-1.56)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.49 (at 1.56Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.167 , 0.208	Depositor
Wilson B-factor (Å ²)	21.4	Xtriage
Anisotropy	0.494	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5236	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.58% 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.

3 Model quality

3.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UNX, A1CSX

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	0.62	0/2413	0.89	1/3279 (0.0%)
1	B	0.74	2/2422 (0.1%)	0.94	1/3291 (0.0%)
All	All	0.68	2/4835 (0.0%)	0.92	2/6570 (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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1239	ASN	C-O	10.20	1.35	1.23
1	B	1194	GLY	C-O	5.08	1.30	1.23

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1218	ASP	CA-CB-CG	7.68	120.28	112.60
1	A	1198	ASP	CA-CB-CG	6.59	119.19	112.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1335	ARG	Sidechain

3.2 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	2354	0	2207	13	0
1	B	2368	0	2222	10	0
2	A	42	0	0	1	0
2	B	42	0	0	1	0
3	A	1	0	0	0	0
4	A	208	0	0	1	0
4	B	221	0	0	0	0
All	All	5236	0	4429	23	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 2.

The worst 5 of 23 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:B:1083:ILE:HD11	1:B:1388:GLU:HG3	1.66	0.78
1:B:1227[A]:CYS:SG	2:B:1401:A1CSX:CL2	2.84	0.72
1:A:1181:TYR:CD2	1:A:1227[B]:CYS:SG	2.83	0.70
1:A:1227[B]:CYS:SG	2:A:1401:A1CSX:CL2	2.88	0.69
1:B:1181:TYR:CD2	1:B:1227[A]:CYS:SG	2.85	0.60

There are no symmetry-related clashes.

3.3 Torsion angles [i](#)

3.3.1 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	301/315 (96%)	292 (97%)	7 (2%)	2 (1%)	18	5
1	B	298/315 (95%)	292 (98%)	6 (2%)	0	100	100
All	All	599/630 (95%)	584 (98%)	13 (2%)	2 (0%)	36	18

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1177	THR
1	A	1168	SER

3.3.2 Protein sidechains ⓘ

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	253/276 (92%)	251 (99%)	2 (1%)	73	56
1	B	257/276 (93%)	254 (99%)	3 (1%)	63	40
All	All	510/552 (92%)	505 (99%)	5 (1%)	68	47

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1235	ASP
1	A	1259	ASN
1	B	1166	MET
1	B	1259	ASN
1	B	1357	LEU

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

3.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

3.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

3.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 could not be matched to an existing wwPDB Chemical Component Dictionary definition at this stage and 1 is 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.

3.7 Other polymers [i](#)

There are no such residues in this entry.

3.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

4 Fit of model and data

4.1 Protein, DNA and RNA chains

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

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

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

4.3 Carbohydrates

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

4.4 Ligands

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

4.5 Other polymers

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