



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 07:58 PM GMT

PDB ID : 4QL1
Title : Crystal structure of human WDR5 in complex with compound OICR-9429
Authors : Dong, A.; Dombrowski, L.; Walker, J.R.; Getlik, M.; Kuznetsova, E.; Smil, D.; Barsyte, D.; Li, F.; Poda, G.; Senisterra, G.; Marcellus, R.; Al-Awar, R.; Bountra, C.; Arrowsmith, C.H.; Edwards, A.M.; Brown, P.J.; Schapira, M.; Vedadi, M.; Wu, H.; Structural Genomics Consortium (SGC)
Deposited on : 2014-06-10
Resolution : 1.50 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
<http://wwpdb.org/validation/2016/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : **FAILED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

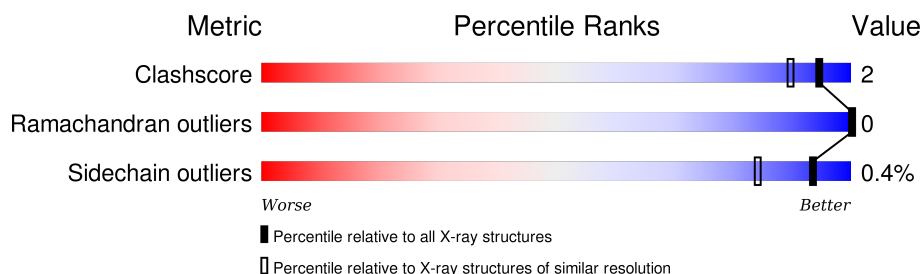
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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	102246	2274 (1.50-1.50)
Ramachandran outliers	100387	2218 (1.50-1.50)
Sidechain outliers	100360	2216 (1.50-1.50)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	312	 95%
1	B	312	 92%

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.

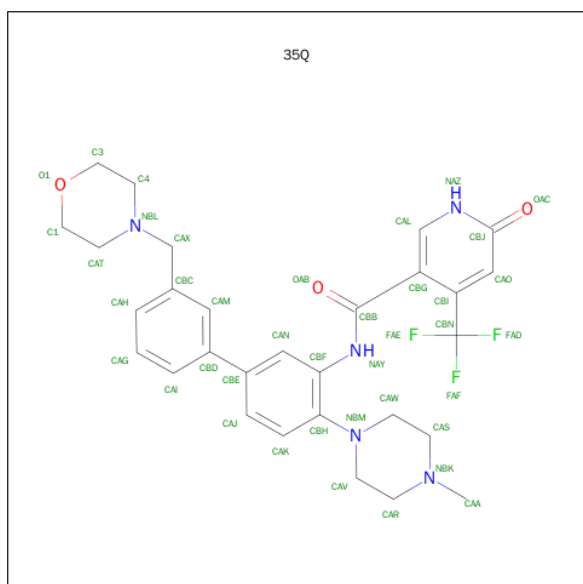
- Molecule 1 is a protein called WD repeat-containing protein 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	304	Total 2346	C 1501	N 387	O 448	S 10	0	6	0
1	B	302	Total 2353	C 1507	N 385	O 450	S 11	0	9	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	GLY	-	EXPRESSION TAG	UNP P61964
B	23	GLY	-	EXPRESSION TAG	UNP P61964

- Molecule 2 is N-(4-(4-METHYLPIPERAZIN-1-YL)-3'-(MORPHOLINOMETHYL)-[1,1'-BIPHENYL]-3-YL)-6-OXO-4-(TRIFLUOROMETHYL)-1,6-DIHYDROPYRIDINE-3-CARBOXYAMIDE (three-letter code: 35Q) (formula: $C_{29}H_{32}F_3N_5O_3$).

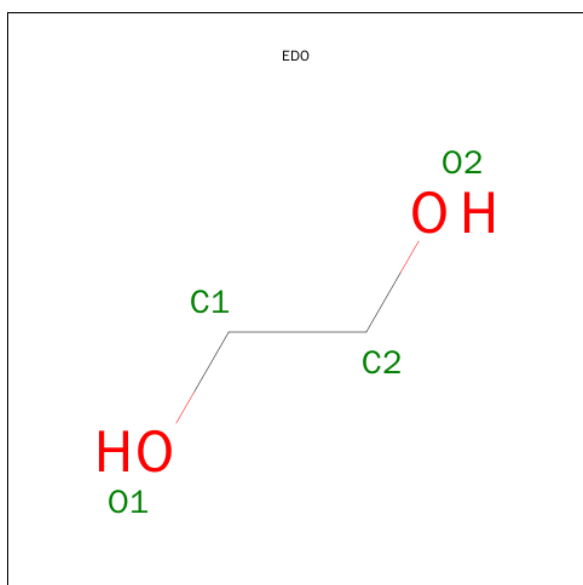


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			36	26	3	5	2		
2	B	1	Total	C	F	N	O	0	0
			36	26	3	5	2		

- Molecule 3 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	X	0	0
			1	1		
3	A	1	Total	X	0	0
			1	1		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	169	Total	O	0	4
			173	173		
6	B	157	Total	O	0	2
			159	159		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS failed to run properly.

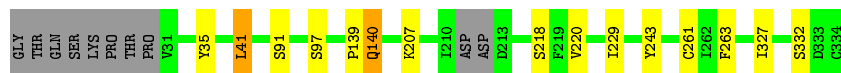
- Molecule 1: WD repeat-containing protein 5

Chain A:  95%



- Molecule 1: WD repeat-containing protein 5

Chain B:  92%



4 Data and refinement statistics

EDS failed to run properly - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	46.84Å 56.63Å 64.69Å 71.45° 88.94° 65.43°	Depositor
Resolution (Å)	50.00 – 1.50	Depositor
% Data completeness (in resolution range)	94.5 (50.00-1.50)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.61 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.8.0071, COOT 0.7.2	Depositor
R, R_{free}	0.195 , 0.227	Depositor
Wilson B-factor (Å ²)	13.2	Xtriage
Anisotropy	0.333	Xtriage
Estimated twinning fraction	0.118 for h,h-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 85825 reflections	Xtriage
Total number of atoms	5115	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.67% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UNX, GOL, EDO, 35Q

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	0.48	0/2414	0.65	0/3282
1	B	0.47	0/2435	0.66	0/3309
All	All	0.47	0/4849	0.65	0/6591

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

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	2346	0	2280	4	0
1	B	2353	0	2308	12	0
2	A	36	0	24	0	0
2	B	36	0	24	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	B	4	0	6	0	0
5	B	6	0	8	3	0
6	A	173	0	0	0	0
6	B	159	0	0	1	0
All	All	5115	0	4650	16	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 16 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:207:LYS:CD	1:B:243:TYR:O	2.48	0.62
1:B:263:PHE:CE1	5:B:403:GOL:H31	2.35	0.62
1:B:263:PHE:HE1	5:B:403:GOL:H31	1.66	0.60
1:A:209:LEU:HD12	1:A:229:ILE:HD11	1.88	0.55
1:B:91[A]:SER:HB2	6:B:569:HOH:O	2.11	0.50

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	308/312 (99%)	295 (96%)	13 (4%)	0	100	100
1	B	307/312 (98%)	297 (97%)	10 (3%)	0	100	100
All	All	615/624 (99%)	592 (96%)	23 (4%)	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	256/273 (94%)	256 (100%)	0	100	100
1	B	262/273 (96%)	259 (99%)	3 (1%)	80	58
All	All	518/546 (95%)	515 (99%)	3 (1%)	93	78

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	41	LEU
1	B	140[A]	GLN
1	B	140[B]	GLN

Some 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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are unknown - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	35Q	A	401	-	38,39,44	1.72	9 (23%)	50,56,63	1.47	6 (12%)
2	35Q	B	401	-	38,39,44	1.67	7 (18%)	50,56,63	1.48	8 (16%)
4	EDO	B	402	-	3,3,3	0.51	0	2,2,2	0.38	0
5	GOL	B	403	-	5,5,5	0.10	0	5,5,5	0.65	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	35Q	A	401	-	-	0/24/35/44	0/4/4/5
2	35Q	B	401	-	-	0/24/35/44	0/4/4/5
4	EDO	B	402	-	-	0/1/1/1	0/0/0/0
5	GOL	B	403	-	-	0/4/4/4	0/0/0/0

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	35Q	CAX-CBC	-5.29	1.39	1.51
2	B	401	35Q	CAX-CBC	-4.48	1.41	1.51
2	A	401	35Q	CBN-CBI	-4.39	1.40	1.50
2	B	401	35Q	CBG-CBB	-4.23	1.41	1.50
2	B	401	35Q	CBN-CBI	-4.21	1.41	1.50

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	35Q	CAO-CBJ-NAZ	-4.57	118.21	124.88
2	B	401	35Q	CAO-CBJ-NAZ	-3.97	119.09	124.88
2	B	401	35Q	CAW-CAS-NBK	-3.52	107.07	110.79
2	B	401	35Q	CAK-CBH-NBM	-3.11	117.09	122.23
2	A	401	35Q	CAK-CBH-NBM	-2.41	118.25	122.23

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	403	GOL	3	0

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS failed to run properly - this section will therefore be empty.

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

EDS failed to run properly - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS failed to run properly - this section will therefore be empty.

6.4 Ligands ⓘ

EDS failed to run properly - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS failed to run properly - this section will therefore be empty.