



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 10:21 am BST

PDB ID : 5V89
Title : Structure of DCN4 PONY domain bound to CUL1 WHB
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Deposited on : 2017-03-21
Resolution : 1.55 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 : 2.11
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) : 2.11

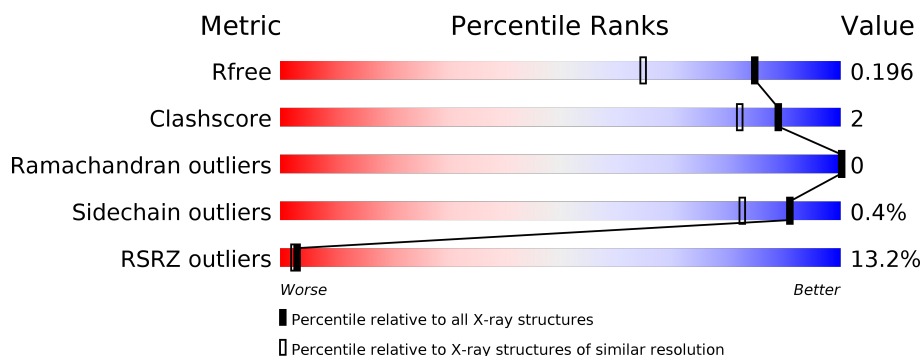
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.55 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	1483 (1.56-1.56)
Clashscore	141614	1529 (1.56-1.56)
Ramachandran outliers	138981	1498 (1.56-1.56)
Sidechain outliers	138945	1495 (1.56-1.56)
RSRZ outliers	127900	1465 (1.56-1.56)

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 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	193	
2	C	77	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4520 atoms, of which 2088 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 DCN1-like protein 4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	190	Total	C	H	N	O	S	0	5	0
			3176	1042	1569	253	300	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	GLY	-	expression tag	UNP Q92564
A	101	SER	-	expression tag	UNP Q92564

- Molecule 2 is a protein called Cullin-1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	67	Total	C	H	N	O	S	0	0	0
			1032	334	519	82	95	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	700	GLY	-	expression tag	UNP Q13616
C	701	SER	-	expression tag	UNP Q13616

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	279	Total	O	0	0
			279	279		
3	C	33	Total	O	0	0
			33	33		

3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA and DNA 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.

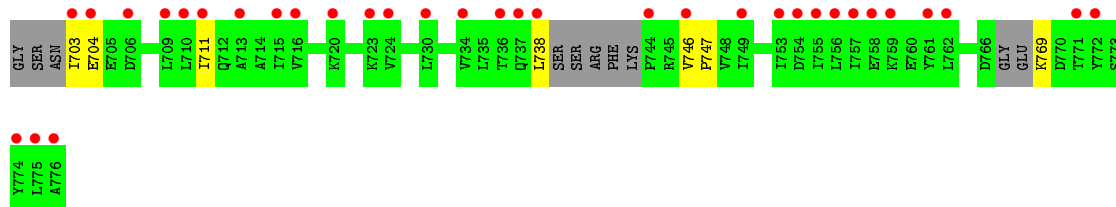
- Molecule 1: DCN1-like protein 4

Chain A:  95%



- Molecule 2: Cullin-1

Chain C:  44% 78% 9% 13%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	118.93Å 62.48Å 38.58Å 90.00° 105.48° 90.00°	Depositor
Resolution (Å)	23.92 – 1.55 37.18 – 1.55	Depositor EDS
% Data completeness (in resolution range)	93.4 (23.92-1.55) 93.4 (37.18-1.55)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 1.55Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.151 , 0.194 0.153 , 0.196	Depositor DCC
R_{free} test set	1869 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	14.7	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 56.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4520	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.79% 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 ⓘ

5.1 Standard geometry ⓘ

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	0.50	0/1662	0.59	0/2247
2	C	0.34	0/516	0.49	0/696
All	All	0.47	0/2178	0.57	0/2943

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	1607	1569	1569	4	0
2	C	513	519	519	4	0
3	A	279	0	0	1	2
3	C	33	0	0	1	0
All	All	2432	2088	2088	8	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 2.

All (8) 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)
2:C:769:LYS:N	3:C:801:HOH:O	1.94	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:ILE:HG21	1:A:176[A]:LEU:HD23	1.88	0.55
1:A:159:GLN:OE1	3:A:301:HOH:O	2.18	0.50
2:C:711:ILE:HA	2:C:738:LEU:HD11	1.96	0.46
2:C:746:VAL:CG2	2:C:747:PRO:HD3	2.46	0.46
1:A:153:MET:HA	1:A:203:PHE:CE1	2.53	0.42
1:A:285:TRP:NE1	1:A:289:LYS:HE2	2.35	0.42
2:C:703:ILE:HD12	2:C:704:GLU:HG3	2.02	0.42

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)
3:A:489:HOH:O	3:A:504:HOH:O[4_545]	2.02	0.18
3:A:498:HOH:O	3:A:562:HOH:O[2_554]	2.15	0.05

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	193/193 (100%)	192 (100%)	1 (0%)	0	100	100
2	C	61/77 (79%)	59 (97%)	2 (3%)	0	100	100
All	All	254/270 (94%)	251 (99%)	3 (1%)	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	179/176 (102%)	178 (99%)	1 (1%)	86	73
2	C	53/71 (75%)	53 (100%)	0	100	100
All	All	232/247 (94%)	231 (100%)	1 (0%)	91	82

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	289	LYS

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](#)

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

6.1 Protein, DNA and RNA chains

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	190/193 (98%)	-0.15	0	100 100	9, 15, 31, 45	0
2	C	67/77 (87%)	2.70	34 (50%)	0 0	29, 45, 68, 93	0
All	All	257/270 (95%)	0.60	34 (13%)	3 2	9, 18, 59, 93	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	775	LEU	8.8
2	C	776	ALA	8.7
2	C	744	PRO	7.6
2	C	703	ILE	7.5
2	C	746	VAL	5.7
2	C	774	TYR	5.7
2	C	709	LEU	5.5
2	C	761	TYR	5.4
2	C	716	VAL	5.1
2	C	713	ALA	4.9
2	C	753	ILE	4.9
2	C	734	VAL	4.5
2	C	738	LEU	4.5
2	C	710	LEU	4.3
2	C	724	VAL	4.1
2	C	755	ILE	3.9
2	C	757	ILE	3.9
2	C	736	THR	3.5
2	C	730	LEU	3.4
2	C	704	GLU	3.4
2	C	762	LEU	2.9
2	C	771	THR	2.8
2	C	737	GLN	2.7
2	C	706	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
2	C	749	ILE	2.6
2	C	756	LEU	2.5
2	C	772	TYR	2.4
2	C	723	LYS	2.3
2	C	715	ILE	2.3
2	C	711	ILE	2.2
2	C	759	LYS	2.2
2	C	754	ASP	2.2
2	C	720	LYS	2.1
2	C	758	GLU	2.1

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 carbohydrates 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.