



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 14, 2017 – 10:39 PM EDT

PDB ID : 3ODN
Title : The crystal structure of Drosophila Dally-Like Protein core domain
Authors : Kim, M.-S.; Leahy, D.J.
Deposited on : unknown
Resolution : 2.40 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

<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
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029824
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

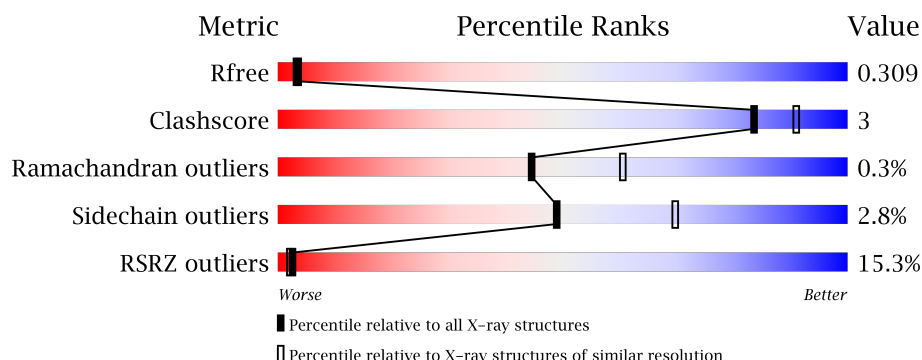
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	100719	3166 (2.40-2.40)
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (2.40-2.40)

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.

Mol	Chain	Length	Quality of chain
1	A	506	<div> <div>11%</div> <div>66%</div> <div>6%</div> <div>28%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3003 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 Dally-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	366	Total	C	N	O	S	0	0	0
			2934	1846	507	554	27			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	79	GLU	ASN	ENGINEERED MUTATION	UNP Q9GPL5
A	502	GLU	ASN	ENGINEERED MUTATION	UNP Q9GPL5

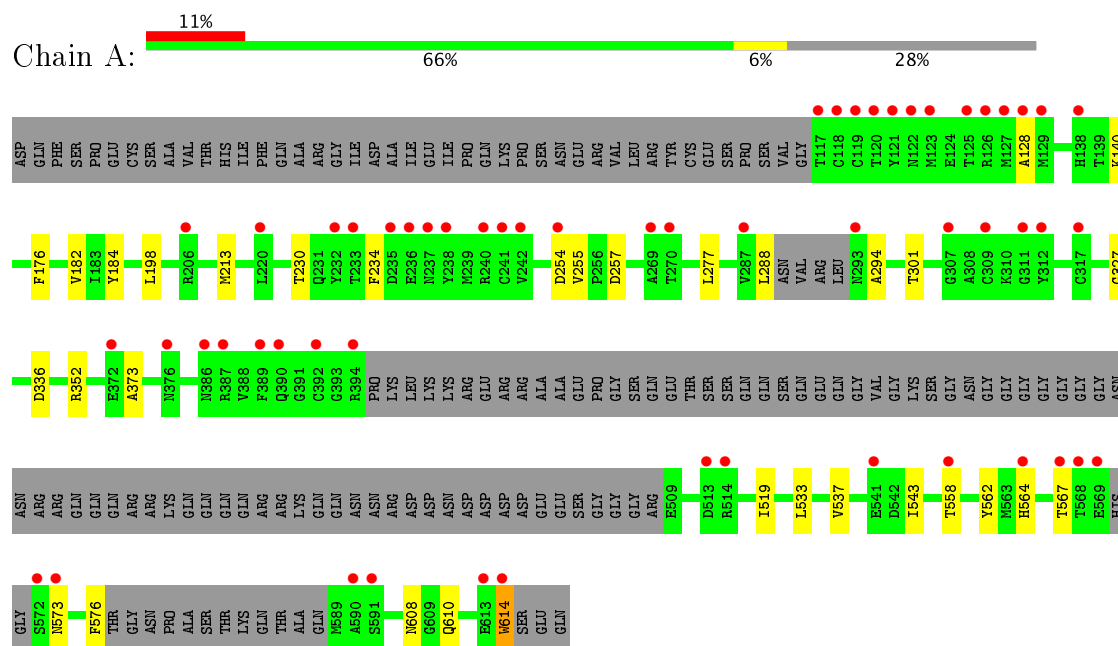
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	69	Total	O	0	0
			69	69		

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: Dally-like protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	97.02Å 66.42Å 85.72Å 90.00° 104.85° 90.00°	Depositor
Resolution (Å)	28.28 – 2.40 28.28 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (28.28-2.40) 98.8 (28.28-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.56 (at 2.39Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.247 , 0.298 0.257 , 0.309	Depositor DCC
R_{free} test set	1054 reflections (5.40%)	DCC
Wilson B-factor (Å ²)	50.0	Xtriage
Anisotropy	0.542	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 72.2	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	0.92	EDS
Total number of atoms	3003	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.89% 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	0.51	0/2989	0.71	0/4022

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 [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	2934	0	2836	16	0
2	A	69	0	0	0	0
All	All	3003	0	2836	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 3.

All (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:A:128:ALA:HA	1:A:301:THR:CG2	2.40	0.52
1:A:608:ASN:HB2	1:A:610:GLN:HE21	1.75	0.51
1:A:198:LEU:HD21	1:A:213:MET:HE3	1.94	0.50
1:A:562:TYR:CE2	1:A:564:HIS:HB2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:LEU:HD11	1:A:519:ILE:HG21	1.96	0.47
1:A:327:GLY:HA3	1:A:576:PHE:CE1	2.49	0.47
1:A:176:PHE:HB3	1:A:184:TYR:CD1	2.50	0.46
1:A:140:LYS:HG3	1:A:288:LEU:HD22	1.98	0.46
1:A:562:TYR:CZ	1:A:564:HIS:HB2	2.53	0.43
1:A:614:TRP:CE3	1:A:614:TRP:HA	2.53	0.43
1:A:533:LEU:O	1:A:537:VAL:HG23	2.18	0.43
1:A:614:TRP:HA	1:A:614:TRP:HE3	1.85	0.42
1:A:567:THR:HG21	1:A:573:ASN:HA	2.02	0.42
1:A:128:ALA:HA	1:A:301:THR:HG21	2.03	0.41
1:A:537:VAL:O	1:A:543:ILE:HD13	2.20	0.40
1:A:255:VAL:HG11	1:A:373:ALA:HB2	2.04	0.40

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	356/506 (70%)	344 (97%)	11 (3%)	1 (0%)	44 60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	294	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	323/444 (73%)	314 (97%)	9 (3%)	49 70

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	182	VAL
1	A	230	THR
1	A	234	PHE
1	A	254	ASP
1	A	257	ASP
1	A	336	ASP
1	A	352	ARG
1	A	558	THR
1	A	614	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	173	ASN
1	A	222	GLN
1	A	341	ASN
1	A	521	GLN
1	A	610	GLN

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 carbohydrates 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 ⓘ

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	366/506 (72%)	0.99	56 (15%) 2 2	41, 76, 120, 158	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	121	TYR	8.6
1	A	129	MET	8.4
1	A	614	TRP	6.3
1	A	117	THR	5.5
1	A	572	SER	5.5
1	A	118	CYS	5.2
1	A	307	GLY	5.0
1	A	241	CYS	4.7
1	A	392	CYS	4.7
1	A	389	PHE	4.5
1	A	390	GLN	4.1
1	A	126	ARG	4.0
1	A	119	CYS	3.7
1	A	569	GLU	3.5
1	A	254	ASP	3.5
1	A	568	THR	3.5
1	A	312	TYR	3.5
1	A	564	HIS	3.4
1	A	206	ARG	3.4
1	A	236	GLU	3.3
1	A	123	MET	3.3
1	A	238	TYR	3.2
1	A	235	ASP	3.1
1	A	237	ASN	3.1
1	A	309	CYS	3.1
1	A	387	ARG	3.1
1	A	128	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	120	THR	3.0
1	A	293	ASN	3.0
1	A	240	ARG	3.0
1	A	386	ASN	2.9
1	A	591	SER	2.9
1	A	232	TYR	2.9
1	A	567	THR	2.9
1	A	394	ARG	2.9
1	A	558	THR	2.8
1	A	317	CYS	2.7
1	A	122	ASN	2.7
1	A	138	HIS	2.7
1	A	233	THR	2.6
1	A	127	MET	2.5
1	A	270	THR	2.5
1	A	514	ARG	2.5
1	A	242	VAL	2.5
1	A	311	GLY	2.5
1	A	269	ALA	2.4
1	A	541	GLU	2.4
1	A	372	GLU	2.4
1	A	287	VAL	2.3
1	A	513	ASP	2.2
1	A	613	GLU	2.2
1	A	125	THR	2.2
1	A	376	ASN	2.1
1	A	590	ALA	2.1
1	A	220	LEU	2.1
1	A	573	ASN	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.