



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:28 AM UTC

PDB ID : 3ODN / pdb_00003odn
Title : The crystal structure of Drosophila Dally-Like Protein core domain
Authors : Kim, M.-S.; Leahy, D.J.
Deposited on : 2010-08-11
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

<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

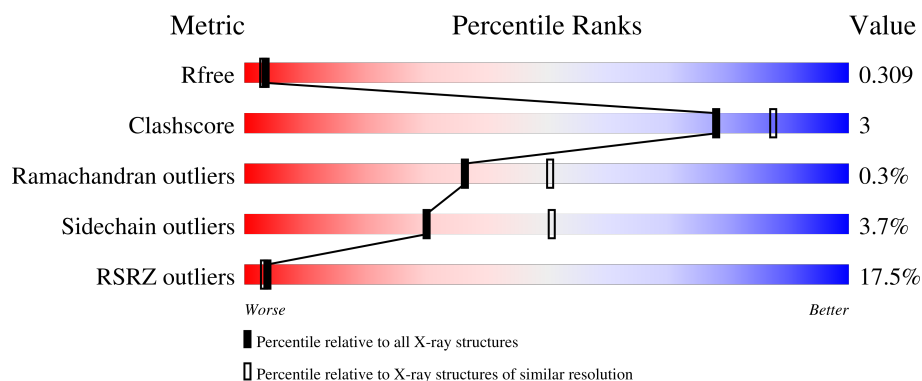
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 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	506	13% 62% 10% 28%

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
			Total	C	N	O	S			
1	A	366	2934	1846	507	554	27	0	0	0

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		

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) 98.9 (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	1058 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	50.0	Xtriage
Anisotropy	0.542	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 87.6	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	0.92	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

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	0.87	1/2989 (0.0%)	1.58	36/4022 (0.9%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	213	MET	SD-CE	-5.03	1.67	1.79

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	159	ASP	CA-CB-CG	6.99	119.59	112.60
1	A	357	PHE	CA-CB-CG	6.79	120.59	113.80
1	A	356	SER	N-CA-C	6.49	119.17	111.71
1	A	154	ALA	CA-C-N	6.42	128.89	120.28
1	A	154	ALA	C-N-CA	6.42	128.89	120.28
1	A	320	TYR	CA-C-N	6.34	129.06	120.38
1	A	320	TYR	C-N-CA	6.34	129.06	120.38
1	A	334	GLU	CA-C-N	6.18	128.56	120.28
1	A	334	GLU	C-N-CA	6.18	128.56	120.28
1	A	230	THR	CA-C-N	6.14	128.50	120.28
1	A	230	THR	C-N-CA	6.14	128.50	120.28
1	A	525	ASP	CA-CB-CG	6.02	118.62	112.60
1	A	123	MET	CA-C-N	5.94	128.73	120.29
1	A	123	MET	C-N-CA	5.94	128.73	120.29
1	A	541	GLU	CA-C-N	5.87	128.40	120.65
1	A	541	GLU	C-N-CA	5.87	128.40	120.65
1	A	542	ASP	CA-CB-CG	5.77	118.37	112.60
1	A	307	GLY	CA-C-N	5.71	128.51	120.28
1	A	307	GLY	C-N-CA	5.71	128.51	120.28
1	A	293	ASN	CA-C-N	5.59	132.22	121.54
1	A	293	ASN	C-N-CA	5.59	132.22	121.54
1	A	563	MET	N-CA-C	5.55	118.86	112.97
1	A	294	ALA	N-CA-C	5.42	122.34	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	211	GLU	CA-C-N	5.37	127.53	120.60
1	A	211	GLU	C-N-CA	5.37	127.53	120.60
1	A	293	ASN	CA-CB-CG	5.36	117.96	112.60
1	A	295	ASP	CA-C-N	5.29	127.37	120.28
1	A	295	ASP	C-N-CA	5.29	127.37	120.28
1	A	123	MET	N-CA-C	-5.26	105.63	111.36
1	A	306	CYS	N-CA-C	5.24	119.66	113.16
1	A	280	ALA	CA-C-N	5.17	127.21	120.28
1	A	280	ALA	C-N-CA	5.17	127.21	120.28
1	A	547	SER	CA-C-N	5.09	127.52	120.29
1	A	547	SER	C-N-CA	5.09	127.52	120.29
1	A	229	ASN	CA-C-N	5.09	127.11	120.28
1	A	229	ASN	C-N-CA	5.09	127.11	120.28

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:213:MET:HE3	1:A:263:ILE:HG21	1.89	0.55
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:562:TYR:CE2	1:A:564:HIS:HB2	2.48	0.48
1:A:277:LEU:HD11	1:A:519:ILE:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	36 50

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%)	311 (96%)	12 (4%)	30	51

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	166	LYS
1	A	182	VAL
1	A	230	THR
1	A	234	PHE
1	A	254	ASP
1	A	257	ASP
1	A	264	LYS
1	A	277	LEU
1	A	336	ASP
1	A	514	ARG
1	A	558	THR
1	A	614	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) 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	592	GLN
1	A	605	ASN
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 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 ⓘ

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%)	1.14	64 (17%) ⓘ ⓘ	41, 76, 120, 158	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	307	GLY	5.6
1	A	130	GLN	5.2
1	A	614	TRP	4.6
1	A	513	ASP	4.6
1	A	121	TYR	4.3
1	A	119	CYS	4.2
1	A	129	MET	3.9
1	A	205	GLY	3.9
1	A	138	HIS	3.9
1	A	294	ALA	3.8
1	A	380	SER	3.8
1	A	118	CYS	3.8
1	A	128	ALA	3.6
1	A	287	VAL	3.5
1	A	117	THR	3.4
1	A	394	ARG	3.4
1	A	317	CYS	3.1
1	A	389	PHE	3.0
1	A	594	SER	3.0
1	A	392	CYS	3.0
1	A	376	ASN	3.0
1	A	296	CYS	3.0
1	A	564	HIS	2.9
1	A	381	GLY	2.9
1	A	253	GLY	2.9
1	A	241	CYS	2.8
1	A	288	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	568	THR	2.7
1	A	306	CYS	2.7
1	A	254	ASP	2.6
1	A	559	ILE	2.6
1	A	572	SER	2.6
1	A	592	GLN	2.6
1	A	293	ASN	2.5
1	A	382	GLN	2.5
1	A	137	GLY	2.5
1	A	542	ASP	2.5
1	A	554	TRP	2.5
1	A	131	SER	2.5
1	A	144	SER	2.4
1	A	548	ASP	2.4
1	A	373	ALA	2.4
1	A	162	THR	2.3
1	A	282	GLU	2.3
1	A	133	GLN	2.3
1	A	377	PHE	2.3
1	A	561	ARG	2.2
1	A	140	LYS	2.2
1	A	249	LEU	2.2
1	A	174	SER	2.2
1	A	590	ALA	2.2
1	A	369	LYS	2.2
1	A	327	GLY	2.2
1	A	543	ILE	2.2
1	A	546	SER	2.2
1	A	598	ASN	2.1
1	A	591	SER	2.1
1	A	159	ASP	2.1
1	A	375	MET	2.1
1	A	233	THR	2.1
1	A	555	ASN	2.0
1	A	125	THR	2.0
1	A	352	ARG	2.0
1	A	302	LYS	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 [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.