



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2018 – 11:25 am GMT

PDB ID : 2A90  
Title : Crystal Structure of the tandem WWE domain of Drosophila Deltex  
Authors : Zweifel, M.E.; Leahy, D.J.; Barrick, D.  
Deposited on : 2005-07-10  
Resolution : 2.15 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](mailto: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.

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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 : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

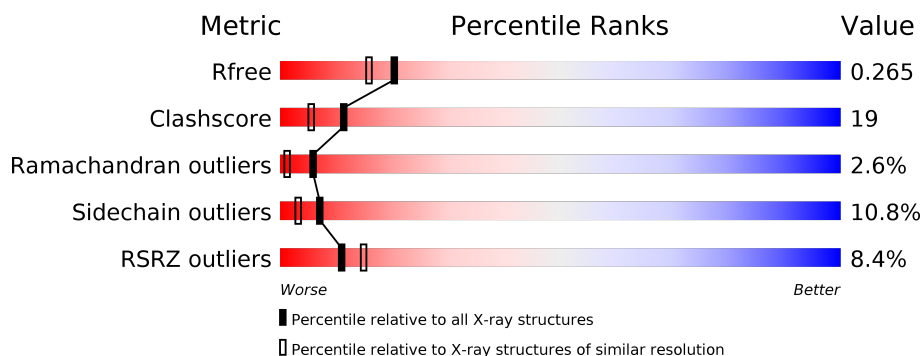
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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))
$R_{free}$	111664	1287 (2.16-2.16)
Clashscore	122126	1390 (2.16-2.16)
Ramachandran outliers	120053	1368 (2.16-2.16)
Sidechain outliers	120020	1367 (2.16-2.16)
RSRZ outliers	108989	1262 (2.16-2.16)

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  $\geq 3$ , 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	240	<div> <div>5%</div> <div>48%</div> <div>13%</div> <div>• •</div> <div>33%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1340 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 Deltex protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	160	Total	C	N	O	Se	0	0	0
			1286	809	234	238	5			

There are 13 discrepancies between the modelled and reference sequences:

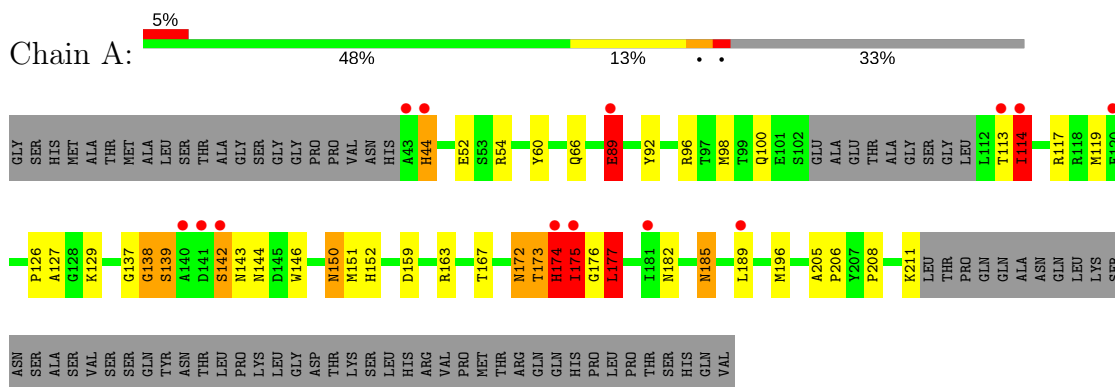
Chain	Residue	Modelled	Actual	Comment	Reference
A	22	GLY	-	CLONING ARTIFACT	UNP Q23985
A	23	SER	-	CLONING ARTIFACT	UNP Q23985
A	24	HIS	-	CLONING ARTIFACT	UNP Q23985
A	25	MET	-	CLONING ARTIFACT	UNP Q23985
A	47	SER	CYS	SEE REMARK 999	UNP Q23985
A	80	MSE	MET	MODIFIED RESIDUE	UNP Q23985
A	98	MSE	MET	MODIFIED RESIDUE	UNP Q23985
A	119	MSE	MET	MODIFIED RESIDUE	UNP Q23985
A	151	MSE	MET	MODIFIED RESIDUE	UNP Q23985
A	155	SER	CYS	SEE REMARK 999	UNP Q23985
A	171	SER	CYS	SEE REMARK 999	UNP Q23985
A	184	SER	CYS	SEE REMARK 999	UNP Q23985
A	196	MSE	MET	MODIFIED RESIDUE	UNP Q23985

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	54	Total	O	0	0
			54	54		

**i**

- Molecule 1: Deltex protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.76Å 57.76Å 80.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.80 – 2.15 46.83 – 2.15	Depositor EDS
% Data completeness (in resolution range)	95.8 (40.80-2.15) 98.2 (46.83-2.15)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.29 (at 2.14Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.230 , 0.247 0.246 , 0.265	Depositor DCC
$R_{free}$ test set	1345 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.6	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 52.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.044 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	1340	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.09% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.77	0/1317	1.29	15/1782 (0.8%)

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

There are no bond length outliers.

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	175	ILE	N-CA-C	15.01	151.52	111.00
1	A	175	ILE	N-CA-CB	-9.65	88.60	110.80
1	A	175	ILE	CG1-CB-CG2	8.74	130.64	111.40
1	A	174	HIS	N-CA-C	8.00	132.61	111.00
1	A	129	LYS	CB-CG-CD	-7.29	92.64	111.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	174	HIS	Peptide

### 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	1286	0	1246	48	0
2	A	54	0	0	4	0
All	All	1340	0	1246	48	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 19.

The worst 5 of 48 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:174:HIS:HB2	1:A:175:ILE:HB	1.18	1.14
1:A:175:ILE:HG23	1:A:176:GLY:N	1.71	1.05
1:A:126:PRO:HB2	1:A:151:MSE:HE1	1.45	0.96
1:A:175:ILE:HG23	1:A:177:LEU:H	1.27	0.95
1:A:119:MSE:HE3	2:A:277:HOH:O	1.70	0.92

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	156/240 (65%)	147 (94%)	5 (3%)	4 (3%)	<b>6</b> <b>1</b>

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	173	THR
1	A	89	GLU
1	A	138	GLY
1	A	175	ILE

### 5.3.2 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	139/200 (70%)	124 (89%)	15 (11%)	<b>7</b> <b>3</b>

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	114	ILE
1	A	139	SER
1	A	177	LEU
1	A	113	THR
1	A	175	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	154	GLN
1	A	188	GLN
1	A	174	HIS
1	A	100	GLN
1	A	185	ASN

### 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 [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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	155/240 (64%)	0.94	13 (8%) <b>11</b> <b>15</b>	36, 51, 83, 93	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	175	ILE	3.9
1	A	43	ALA	3.9
1	A	113	THR	3.5
1	A	140	ALA	3.2
1	A	142	SER	3.2

### 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.