



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 07:24 PM GMT

PDB ID : 4OTO  
Title : Crystal structure of the S505W mutant of TAL effector dHax3  
Authors : Deng, D.; Wu, J.P.; Yan, C.Y.; Pan, X.J.; Yan, N.  
Deposited on : 2014-02-14  
Resolution : 2.59 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  
<http://wwpdb.org/validation/2016/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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

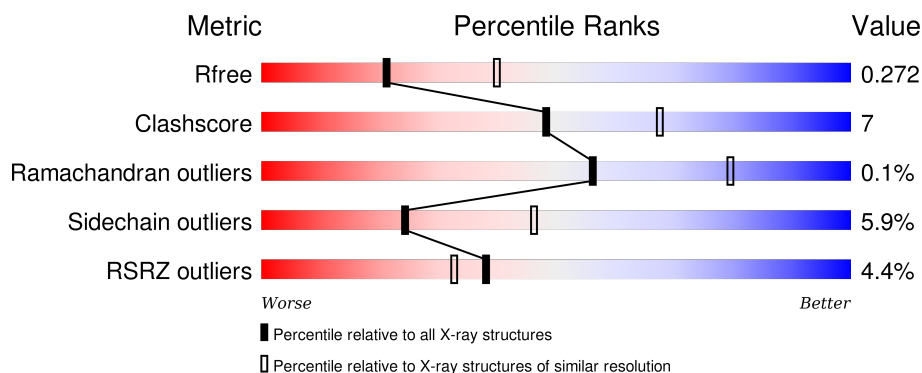
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.59 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))
$R_{free}$	91344	2636 (2.60-2.56)
Clashscore	102246	3003 (2.60-2.56)
Ramachandran outliers	100387	2956 (2.60-2.56)
Sidechain outliers	100360	2956 (2.60-2.56)
RSRZ outliers	91569	2642 (2.60-2.56)

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  $\geq 3$ , 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	499	<div> <div>3%</div> <div>75%</div> <div>21%</div> <div>• •</div> </div>
1	B	499	<div> <div>4%</div> <div>83%</div> <div>13%</div> <div>• •</div> </div>
2	G	17	<div> <div>12%</div> <div>65%</div> <div>29%</div> <div>6%</div> </div>
2	I	17	<div> <div>12%</div> <div>71%</div> <div>18%</div> <div>12%</div> </div>
3	H	17	<div> <div>18%</div> <div>47%</div> <div>29%</div> <div>24%</div> </div>

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Mol	Chain	Length	Quality of chain
3	J	17	 A horizontal bar chart showing the quality of chain J. The bar is divided into four segments: red (24%), green (65%), yellow (24%), and orange (12%). The percentages are labeled above each segment.

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8598 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 Hax3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	491	Total	C	N	O	S	1	5	0
			3597	2250	670	665	12			
1	B	486	Total	C	N	O	S	11	8	0
			3581	2239	665	664	13			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	230	MET	-	EXPRESSION TAG	UNP Q3ZD72
A	300	HIS	ASN	ENGINEERED MUTATION	UNP Q3ZD72
A	301	ASP	ILE	ENGINEERED MUTATION	UNP Q3ZD72
A	368	HIS	ASN	ENGINEERED MUTATION	UNP Q3ZD72
A	369	ASP	ILE	ENGINEERED MUTATION	UNP Q3ZD72
A	402	ASN	HIS	ENGINEERED MUTATION	UNP Q3ZD72
A	403	GLY	ASP	ENGINEERED MUTATION	UNP Q3ZD72
A	436	ASN	HIS	ENGINEERED MUTATION	UNP Q3ZD72
A	437	GLY	ASP	ENGINEERED MUTATION	UNP Q3ZD72
A	470	ASN	HIS	ENGINEERED MUTATION	UNP Q3ZD72
A	471	GLY	ASP	ENGINEERED MUTATION	UNP Q3ZD72
A	505	TRP	SER	ENGINEERED MUTATION	UNP Q3ZD72
A	539	GLY	SER	ENGINEERED MUTATION	UNP Q3ZD72
A	572	HIS	ASN	ENGINEERED MUTATION	UNP Q3ZD72
A	573	ASP	SER	ENGINEERED MUTATION	UNP Q3ZD72
A	606	ASN	HIS	ENGINEERED MUTATION	UNP Q3ZD72
A	607	GLY	ASP	ENGINEERED MUTATION	UNP Q3ZD72
A	640	HIS	ASN	ENGINEERED MUTATION	UNP Q3ZD72
A	641	ASP	ILE	ENGINEERED MUTATION	UNP Q3ZD72
A	721	LEU	-	EXPRESSION TAG	UNP Q3ZD72
A	722	GLU	-	EXPRESSION TAG	UNP Q3ZD72
A	723	HIS	-	EXPRESSION TAG	UNP Q3ZD72
A	724	HIS	-	EXPRESSION TAG	UNP Q3ZD72
A	725	HIS	-	EXPRESSION TAG	UNP Q3ZD72
A	726	HIS	-	EXPRESSION TAG	UNP Q3ZD72

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Chain	Residue	Modelled	Actual	Comment	Reference
A	727	HIS	-	EXPRESSION TAG	UNP Q3ZD72
A	728	HIS	-	EXPRESSION TAG	UNP Q3ZD72
B	230	MET	-	EXPRESSION TAG	UNP Q3ZD72
B	300	HIS	ASN	ENGINEERED MUTATION	UNP Q3ZD72
B	301	ASP	ILE	ENGINEERED MUTATION	UNP Q3ZD72
B	368	HIS	ASN	ENGINEERED MUTATION	UNP Q3ZD72
B	369	ASP	ILE	ENGINEERED MUTATION	UNP Q3ZD72
B	402	ASN	HIS	ENGINEERED MUTATION	UNP Q3ZD72
B	403	GLY	ASP	ENGINEERED MUTATION	UNP Q3ZD72
B	436	ASN	HIS	ENGINEERED MUTATION	UNP Q3ZD72
B	437	GLY	ASP	ENGINEERED MUTATION	UNP Q3ZD72
B	470	ASN	HIS	ENGINEERED MUTATION	UNP Q3ZD72
B	471	GLY	ASP	ENGINEERED MUTATION	UNP Q3ZD72
B	505	TRP	SER	ENGINEERED MUTATION	UNP Q3ZD72
B	539	GLY	SER	ENGINEERED MUTATION	UNP Q3ZD72
B	572	HIS	ASN	ENGINEERED MUTATION	UNP Q3ZD72
B	573	ASP	SER	ENGINEERED MUTATION	UNP Q3ZD72
B	606	ASN	HIS	ENGINEERED MUTATION	UNP Q3ZD72
B	607	GLY	ASP	ENGINEERED MUTATION	UNP Q3ZD72
B	640	HIS	ASN	ENGINEERED MUTATION	UNP Q3ZD72
B	641	ASP	ILE	ENGINEERED MUTATION	UNP Q3ZD72
B	721	LEU	-	EXPRESSION TAG	UNP Q3ZD72
B	722	GLU	-	EXPRESSION TAG	UNP Q3ZD72
B	723	HIS	-	EXPRESSION TAG	UNP Q3ZD72
B	724	HIS	-	EXPRESSION TAG	UNP Q3ZD72
B	725	HIS	-	EXPRESSION TAG	UNP Q3ZD72
B	726	HIS	-	EXPRESSION TAG	UNP Q3ZD72
B	727	HIS	-	EXPRESSION TAG	UNP Q3ZD72
B	728	HIS	-	EXPRESSION TAG	UNP Q3ZD72

- Molecule 2 is a DNA chain called DNA (5'-D(\*TP\*GP\*TP\*CP\*CP\*CP\*TP\*TP\*TP\*AP\*TP\*CP\*TP\*CP\*TP\*CP\*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	17	Total	C	N	O	P	0	0	0
			333	163	46	108	16			
2	I	17	Total	C	N	O	P	0	0	0
			334	164	46	108	16			

- Molecule 3 is a DNA chain called DNA (5'-D(\*AP\*GP\*AP\*GP\*AP\*GP\*AP\*TP\*AP\*AP\*AP\*GP\*GP\*GP\*AP\*CP\*A)-3').

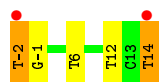
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	17	Total 357	C 169	N 80	O 92	P 16	0	0	0
3	J	17	Total 357	C 169	N 80	O 92	P 16	0	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	10	Total 10	O 10	0	0
4	B	13	Total 13	O 13	0	0
4	G	4	Total 4	O 4	0	0
4	I	9	Total 9	O 9	0	0
4	H	1	Total 1	O 1	0	0
4	J	2	Total 2	O 2	0	0



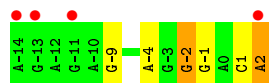
- Molecule 2: DNA (5'-D(\*TP\*GP\*TP\*CP\*CP\*CP\*TP\*TP\*TP\*AP\*TP\*CP\*TP\*CP\*TP\*CP\*T)-3')



- Molecule 3: DNA (5'-D(\*AP\*GP\*AP\*GP\*AP\*GP\*AP\*TP\*AP\*AP\*AP\*GP\*GP\*GP\*AP\*CP\*A)-3')



- Molecule 3: DNA (5'-D(\*AP\*GP\*AP\*GP\*AP\*GP\*AP\*TP\*AP\*AP\*AP\*GP\*GP\*GP\*AP\*CP\*A)-3')





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.44Å 87.07Å 87.97Å 90.00° 103.24° 90.00°	Depositor
Resolution (Å)	38.42 – 2.59 39.64 – 2.59	Depositor EDS
% Data completeness (in resolution range)	99.4 (38.42-2.59) 99.4 (39.64-2.59)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.17 (at 2.58Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, $R_{free}$	0.219 , 0.274 0.215 , 0.272	Depositor DCC
$R_{free}$ test set	1858 reflections (4.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	44.4	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 39.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 37250 reflections (0.005%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	8598	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.88% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.43	1/3650 (0.0%)	0.58	1/4986 (0.0%)
1	B	0.43	0/3633	0.58	0/4960
2	G	0.86	0/368	1.49	7/564 (1.2%)
2	I	0.90	0/369	1.59	7/566 (1.2%)
3	H	0.83	0/405	1.47	8/625 (1.3%)
3	J	0.79	1/405 (0.2%)	1.36	4/625 (0.6%)
All	All	0.53	2/8830 (0.0%)	0.83	27/12326 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	-9	DG	C3'-O3'	-6.14	1.35	1.44
1	A	291	PRO	N-CD	5.27	1.55	1.47

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	-4	DA	O4'-C1'-N9	8.34	113.84	108.00
3	J	-2	DG	O4'-C1'-N9	7.94	113.56	108.00
2	I	6	DT	C4-C5-C7	7.71	123.62	119.00
2	I	-2	DT	O4'-C1'-N1	6.95	112.86	108.00
3	J	-9	DG	C3'-C2'-C1'	-6.30	94.94	102.50

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	3597	0	3744	71	0
1	B	3581	0	3714	43	1
2	G	333	0	195	1	1
2	I	334	0	198	4	0
3	H	357	0	190	5	0
3	J	357	0	190	2	0
4	A	10	0	0	1	0
4	B	13	0	0	4	0
4	G	4	0	0	0	0
4	H	1	0	0	0	0
4	I	9	0	0	0	0
4	J	2	0	0	0	0
All	All	8598	0	8231	121	1

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 7.

The worst 5 of 121 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:253:LEU:O	1:A:254:GLN:HG2	1.54	1.07
1:B:321:HIS:O	4:B:808:HOH:O	1.85	0.93
1:A:255:LEU:HD12	1:A:260:LEU:CD2	2.03	0.89
1:A:632:GLU:O	4:A:810:HOH:O	1.96	0.82
1:A:255:LEU:HD12	1:A:260:LEU:HD23	1.67	0.77

All (1) 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)
1:B:524:ALA:O	2:G:-2:DT:O5'[2_344]	2.07	0.13

## 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	494/499 (99%)	469 (95%)	24 (5%)	1 (0%)	52	75
1	B	490/499 (98%)	465 (95%)	25 (5%)	0	100	100
All	All	984/998 (99%)	934 (95%)	49 (5%)	1 (0%)	56	79

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	383	PRO

### 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	379/383 (99%)	349 (92%)	30 (8%)	15	29
1	B	377/383 (98%)	360 (96%)	17 (4%)	34	60
All	All	756/766 (99%)	709 (94%)	47 (6%)	24	43

5 of 47 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	623	LEU
1	A	690	ARG
1	B	585	LEU
1	A	656	VAL
1	A	693	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	702	HIS

### 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 [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	491/499 (98%)	0.17	14 (2%) 55 51	17, 39, 76, 172	12 (2%)
1	B	486/499 (97%)	0.20	21 (4%) 39 33	22, 43, 79, 110	11 (2%)
2	G	17/17 (100%)	0.16	2 (11%) 6 4	27, 29, 92, 150	0
2	I	17/17 (100%)	0.36	2 (11%) 6 4	23, 25, 106, 119	0
3	H	17/17 (100%)	0.55	3 (17%) 2 1	37, 48, 114, 116	0
3	J	17/17 (100%)	0.90	4 (23%) 1 0	37, 47, 107, 128	0
All	All	1045/1066 (98%)	0.21	46 (4%) 38 33	17, 41, 79, 172	23 (2%)

The worst 5 of 46 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	232	TRP	5.8
1	A	524	ALA	5.8
2	G	14	DT	5.6
1	B	255	LEU	5.2
3	J	2	DA	5.0

### 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.