



Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 12:43 AM GMT

PDB ID : 3V6T
Title : Crystal structure of the DNA-bound dHax3, a TAL effector, at 1.85 angstrom
Authors : Deng, D.; Yan, C.Y.; Pan, X.J.; Wang, J.W.; Yan, N.; Shi, Y.G.
Deposited on : 2011-12-20
Resolution : 1.85 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

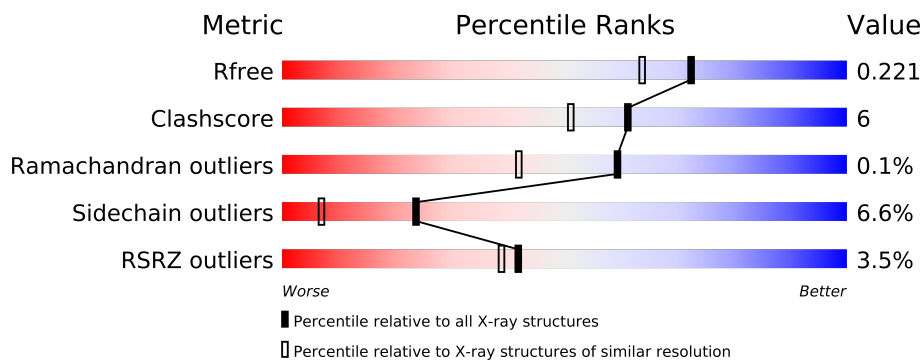
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.85 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}	66092	1269 (1.86-1.86)
Clashscore	79885	1470 (1.86-1.86)
Ramachandran outliers	78287	1451 (1.86-1.86)
Sidechain outliers	78261	1451 (1.86-1.86)
RSRZ outliers	66119	1269 (1.86-1.86)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	499	
1	B	499	
2	G	17	
2	I	17	
3	H	17	
3	J	17	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9608 atoms, of which 0 are hydrogen and 0 are deuterium.

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 dHax3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	491	Total	C	N	O	S	0	6	0
			3599	2251	671	665	12			
1	B	487	Total	C	N	O	S	0	8	0
			3582	2236	666	667	13			

- 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	C	N	O	P	0	0	0
			357	169	80	92	16			
3	J	17	Total	C	N	O	P	0	0	0
			357	169	80	92	16			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	406	Total	O	0	0
			406	406		
4	B	368	Total	O	0	0
			368	368		
4	G	75	Total	O	0	0
			75	75		

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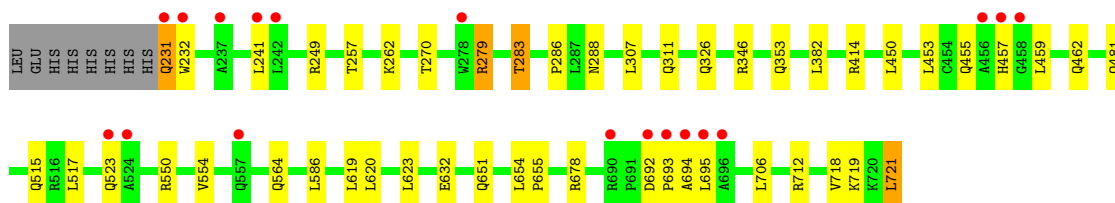
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	62	Total 62	O 62	0	0
4	I	69	Total 69	O 69	0	0
4	J	66	Total 66	O 66	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

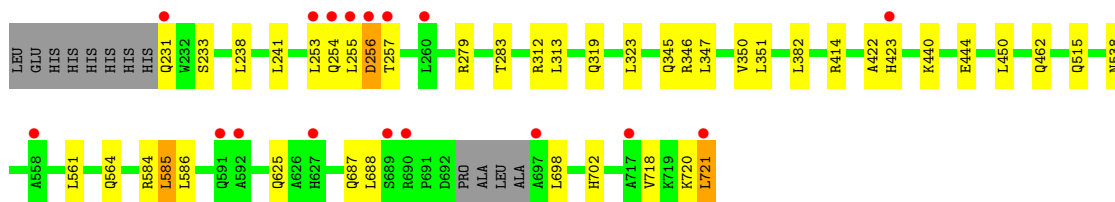
- Molecule 1: dHax3

Chain A: 



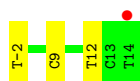
- Molecule 1: dHax3

Chain B: 



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

Chain G: 



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

Chain I: 



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

Chain H: 



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

Chain J: 

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.72Å 87.68Å 88.49Å 90.00° 103.04° 90.00°	Depositor
Resolution (Å)	32.32 – 1.85 32.32 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.5 (32.32-1.85) 99.5 (32.32-1.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.66 (at 1.85Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.205 , 0.222 0.204 , 0.221	Depositor DCC
R_{free} test set	5160 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	25.1	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 44.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 103205 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9608	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	0.39	0/3652	0.51	0/4989
1	B	0.34	0/3632	0.48	0/4957
2	G	0.71	0/368	1.44	2/564 (0.4%)
2	I	0.79	0/369	1.40	3/566 (0.5%)
3	H	0.64	0/405	1.16	2/625 (0.3%)
3	J	0.55	0/405	1.00	0/625
All	All	0.44	0/8831	0.71	7/12326 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	12	DT	O4'-C1'-N1	-6.80	103.24	108.00
2	I	12	DT	O4'-C1'-N1	-6.54	103.42	108.00
3	H	-4	DA	P-O3'-C3'	6.24	127.18	119.70
2	G	9	DC	O4'-C1'-N1	-6.00	103.80	108.00
2	I	5	DT	O4'-C1'-N1	-6.00	103.80	108.00
3	H	-5	DA	O4'-C1'-N9	-5.09	104.44	108.00
2	I	0	DT	O4'-C1'-N1	-5.00	104.50	108.00

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3599	0	0	23	0
1	B	3582	0	0	19	0
2	G	333	0	0	1	0
2	I	334	0	0	1	0
3	H	357	0	0	2	0
3	J	357	0	0	0	0
4	A	406	0	0	11	0
4	B	368	0	0	11	0
4	G	75	0	0	0	0
4	H	62	0	0	0	0
4	I	69	0	0	0	0
4	J	66	0	0	0	0
All	All	9608	0	0	44	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

All (44) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:423[B]:HIS:O	1:B:450:LEU:CD2	2.08	1.01
1:B:312:ARG:NH2	4:B:816:HOH:O	2.03	0.91
1:A:695:LEU:CD1	1:A:718:VAL:CG1	2.49	0.90
1:A:262:LYS:NZ	4:A:1026:HOH:O	2.08	0.85
1:B:233:SER:OG	4:B:911:HOH:O	1.96	0.81
2:G:-2:DT:N3	3:H:2:DA:C2	2.57	0.72
1:A:632:GLU:OE1	4:A:81:HOH:O	2.11	0.69
1:B:253:LEU:CD1	1:B:283:THR:CG2	2.71	0.69
1:A:692:ASP:OD1	1:A:693:PRO:CD	2.42	0.67
1:B:256:ASP:OD1	1:B:256:ASP:N	2.30	0.65
1:A:270[A]:THR:CG2	4:A:1037:HOH:O	2.45	0.65
1:B:687:GLN:NE2	4:B:832:HOH:O	2.30	0.63
1:B:422[A]:ALA:O	1:B:423[A]:HIS:CB	2.48	0.62
1:B:414:ARG:NE	4:B:773:HOH:O	2.33	0.61
1:A:414:ARG:NH1	4:A:796:HOH:O	2.32	0.61
3:H:-4:DA:C2'	3:H:-3:DG:O5'	2.49	0.61
1:A:678:ARG:NH2	4:A:823:HOH:O	2.33	0.60
1:A:718:VAL:CA	1:A:721:LEU:CD1	2.79	0.59
1:B:414:ARG:NH1	4:B:900:HOH:O	2.36	0.59
1:A:249:ARG:NH1	1:A:257:THR:OG1	2.36	0.58
1:A:457:HIS:CE1	1:A:481:GLN:O	2.57	0.57
1:B:538:ASN:ND2	4:B:728:HOH:O	2.38	0.56
1:A:692:ASP:OD1	1:A:692:ASP:C	2.44	0.55
1:A:564:GLN:CG	4:A:902:HOH:O	2.58	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:721:LEU:CD1	2:I:14:DT:C7	2.89	0.51
1:B:345:GLN:NE2	4:B:774:HOH:O	2.44	0.49
1:B:698:LEU:CG	1:B:702:HIS:CD2	2.95	0.49
1:B:515:GLN:NE2	4:B:999:HOH:O	2.46	0.48
1:B:346:ARG:NH2	4:B:940:HOH:O	2.47	0.48
1:A:692:ASP:OD1	1:A:693:PRO:N	2.46	0.47
1:A:346:ARG:NE	4:A:772:HOH:O	2.48	0.46
1:A:654:LEU:N	1:A:655:PRO:CD	2.80	0.45
1:A:712:ARG:NH2	4:A:999:HOH:O	2.49	0.44
1:B:584:ARG:NH2	1:B:585:LEU:CD1	2.81	0.44
1:A:279[B]:ARG:O	1:A:283:THR:OG1	2.36	0.44
1:B:462:GLN:NE2	4:B:812:HOH:O	2.52	0.43
1:A:231:GLN:O	1:A:232:TRP:C	2.57	0.43
1:A:692:ASP:OD1	1:A:694:ALA:N	2.51	0.43
1:A:279[A]:ARG:O	1:A:283:THR:OG1	2.36	0.43
1:B:440:LYS:NZ	1:B:444:GLU:OE2	2.52	0.42
1:A:311:GLN:NE2	4:A:189:HOH:O	2.52	0.42
1:B:319:GLN:NE2	4:B:797:HOH:O	2.53	0.41
1:A:550:ARG:NH1	4:A:1008:HOH:O	2.53	0.41
1:A:564:GLN:NE2	4:A:902:HOH:O	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	495/499 (99%)	472 (95%)	22 (4%)	1 (0%)	56	38
1	B	491/499 (98%)	473 (96%)	18 (4%)	0	100	100
All	All	986/998 (99%)	945 (96%)	40 (4%)	1 (0%)	59	42

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	286	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%)	352 (93%)	27 (7%)	21	5
1	B	378/383 (99%)	355 (94%)	23 (6%)	26	8
All	All	757/766 (99%)	707 (93%)	50 (7%)	24	7

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	231	GLN
1	A	241	LEU
1	A	279[A]	ARG
1	A	279[B]	ARG
1	A	283	THR
1	A	288	ASN
1	A	307	LEU
1	A	326	GLN
1	A	353	GLN
1	A	382	LEU
1	A	450	LEU
1	A	453	LEU
1	A	455	GLN
1	A	459	LEU
1	A	462	GLN
1	A	515	GLN
1	A	517	LEU
1	A	523	GLN
1	A	554	VAL
1	A	586	LEU
1	A	619	LEU
1	A	620	LEU
1	A	623	LEU
1	A	651	GLN
1	A	706	LEU

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Mol	Chain	Res	Type
1	A	719	LYS
1	A	721	LEU
1	B	231	GLN
1	B	238	LEU
1	B	241	LEU
1	B	254	GLN
1	B	255	LEU
1	B	256	ASP
1	B	257	THR
1	B	279	ARG
1	B	313	LEU
1	B	323	LEU
1	B	347	LEU
1	B	350	VAL
1	B	351	LEU
1	B	382	LEU
1	B	561	LEU
1	B	564	GLN
1	B	585	LEU
1	B	586	LEU
1	B	625	GLN
1	B	688	LEU
1	B	718	VAL
1	B	720	LYS
1	B	721	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains 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	491/499 (98%)	0.01	18 (3%) 39 36	13, 26, 60, 89	15 (3%)
1	B	487/499 (97%)	0.07	17 (3%) 42 39	13, 27, 59, 94	9 (1%)
2	G	17/17 (100%)	-0.27	1 (5%) 22 20	15, 19, 45, 90	0
2	I	17/17 (100%)	-0.39	0 100 100	15, 17, 67, 92	0
3	H	17/17 (100%)	0.35	1 (5%) 22 20	27, 34, 62, 72	0
3	J	17/17 (100%)	0.06	0 100 100	23, 35, 66, 69	0
All	All	1046/1066 (98%)	0.03	37 (3%) 42 39	13, 27, 61, 94	24 (2%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	721	LEU	6.3
1	A	456	ALA	5.0
1	B	255	LEU	4.4
1	B	591	GLN	3.9
1	B	697	ALA	3.9
1	B	423[A]	HIS	3.8
1	A	231	GLN	3.7
1	A	557	GLN	3.7
1	B	257	THR	3.5
1	B	253	LEU	3.5
1	A	278[A]	TRP	3.5
1	A	457	HIS	3.4
1	B	558	ALA	3.1
1	A	694	ALA	3.1
1	B	690	ARG	3.0
1	B	231	GLN	3.0
1	A	237	ALA	2.8
2	G	14	DT	2.7
1	A	695	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	232	TRP	2.7
3	H	-14	DA	2.6
1	B	260	LEU	2.6
1	B	254	GLN	2.5
1	A	693	PRO	2.4
1	A	524	ALA	2.4
1	A	523	GLN	2.4
1	B	689	SER	2.4
1	B	717	ALA	2.4
1	A	690	ARG	2.3
1	A	458	GLY	2.3
1	A	241	LEU	2.3
1	B	592	ALA	2.2
1	A	692	ASP	2.2
1	B	256	ASP	2.1
1	A	242	LEU	2.1
1	B	627	HIS	2.1
1	A	696	ALA	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.