



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:36 PM GMT

PDB ID : 4FL0  
Title : Crystal structure of ALD1 from Arabidopsis thaliana  
Authors : Sobolev, V.; Edelman, M.; Dym, O.; Unger, T.; Albeck, S.; Kirma, M.; Galili, G.; Israel Structural Proteomics Center (ISPC)  
Deposited on : 2012-06-14  
Resolution : 2.30 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](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

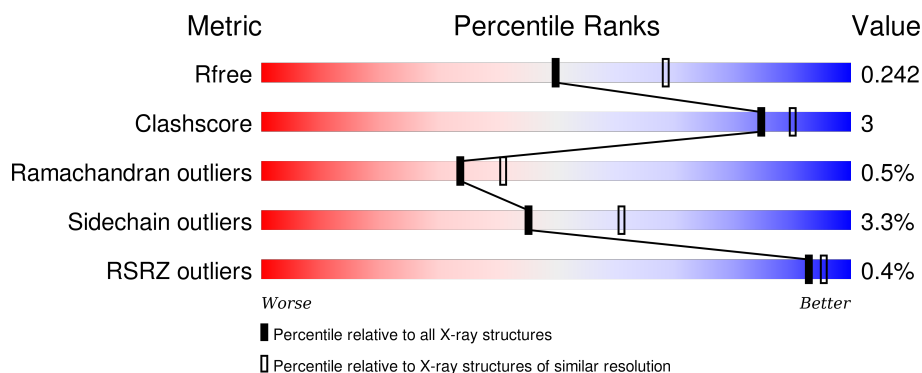
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*



The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	456	 81% 7% • 11%
1	B	456	 80% 8% • 10%

## 2 Entry composition [i](#)

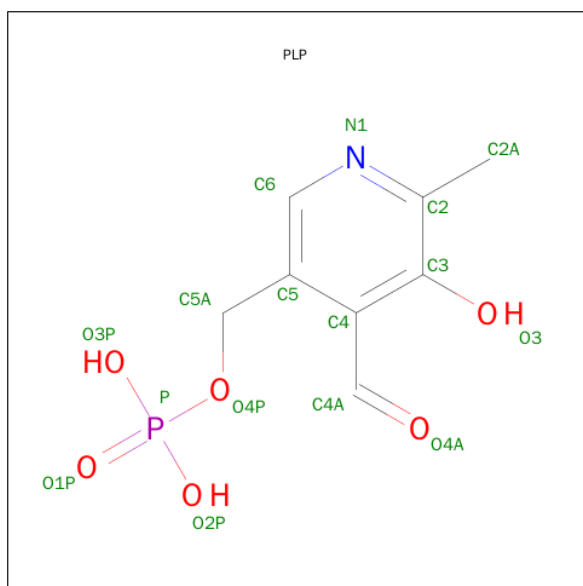
There are 3 unique types of molecules in this entry. The entry contains 6368 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Aminotransferase ALD1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	406	Total	C	N	O	S	0	0	0
			3154	2015	541	591	7			
1	B	409	Total	C	N	O	S	0	0	0
			3169	2023	539	600	7			

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula:  $C_8H_{10}NO_6P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
2	B	1	Total	C	N	O	P	0	0
			16	8	1	6	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	7	Total 7	O 7	0	0
3	B	6	Total 6	O 6	0	0



- Molecule 1: Aminotransferase ALD1

ASN	R231	R234	T258	E259	D260	R264	F282	F285	R292	L293	D300	E301	L302	L303	R315	T345	N355	R356	L363	L368	P377	R378	R379	K384	H400	R425	H440	THR	ARG	THR	LYS	HIS	PRO	THR	THR	LEU	SER	SER	THR	SER	THR	ASN	THR	
MET	VAL	SER	LEU	MET	PRO	ALA	SER	PRO	LEU	CYS	SER	SER	PRO	SER	LYS	ILE	PRO	LYS	ALA	SER	LEU	ASP	GLU	MET	LYS	LYS	LEU	GLY	GLY	S35	T36	R37	L38	L47	F53	N57	L61	V70	T89	S147	I175	M195	P205	P212

- Molecule 1: Aminotransferase ALD1

THR	SER	ASN	THR	ASN	Q190	M196	P205	R212	L234	A241	I248	I258	D259	D260	R264	F282	R292	L293	D300	E301	L302	L303	N355	R356	L366	P377	P405	G408	E414	E415	R425	Q436	T441	R442	THR	LYS	HIS	PRO	THR	TYR	LEU	SER	ASP							
MET	VAL	SER	LEU	MET	PHE	PHE	SER	SER	ALA	SER	PRO	LEU	CYS	SER	SER	PRO	SER	LYS	ILE	PRO	LYS	ALA	SER	LEU	ASP	PHE	GLU	MET	LYS	LYS	LEU	GLY	G34	S35	T36	P37	L38	L47	L52	P53	P54	E55	L56	L61	N69	T77	T89	S147	I175	H182

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.28 Å 89.87 Å 180.70 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.42 – 2.30 48.38 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.42-2.30) 99.9 (48.38-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.59 (at 2.29 Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.205 , 0.241 0.209 , 0.242	Depositor DCC
$R_{free}$ test set	2138 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	38.0	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 24.9	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	0 of 42289 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6368	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.96% 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PLP

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	0.84	0/3230	0.84	2/4381 (0.0%)
1	B	0.81	2/3246 (0.1%)	0.86	3/4408 (0.1%)
All	All	0.83	2/6476 (0.0%)	0.85	5/8789 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	61	LEU	C-N	-5.75	1.20	1.34
1	B	147	SER	CB-OG	5.62	1.49	1.42

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	292	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	B	260	ASP	CB-CA-C	-6.25	97.90	110.40
1	A	292	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	A	231	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	B	292	ARG	NE-CZ-NH1	5.05	122.82	120.30

There are no chirality outliers.

There are no planarity outliers.

### 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	3154	0	3074	18	0
1	B	3169	0	3051	20	0
2	A	16	0	7	0	0
2	B	16	0	7	0	0
3	A	7	0	0	0	0
3	B	6	0	0	0	0
All	All	6368	0	6139	36	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 (36) 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:303:LEU:O	1:B:36:THR:HB	1.83	0.78
1:B:356:ARG:HD3	1:B:377:PRO:HA	1.73	0.71
1:B:355:ASN:OD1	1:B:425:ARG:NH1	2.23	0.69
1:A:356:ARG:HD3	1:A:377:PRO:HA	1.73	0.69
1:A:355:ASN:OD1	1:A:425:ARG:NH1	2.21	0.68
1:B:36:THR:HG22	1:B:38:LEU:H	1.59	0.67
1:A:36:THR:HG22	1:A:38:LEU:H	1.63	0.63
1:B:241:ALA:HB2	1:B:248:ILE:HD11	1.80	0.62
1:A:36:THR:HB	1:B:303:LEU:O	2.02	0.59
1:B:47:LEU:HD22	1:B:175:ILE:HD11	1.87	0.56
1:A:47:LEU:HD22	1:A:175:ILE:HD11	1.89	0.54
1:B:56:ILE:HD11	1:B:405:PRO:HD2	1.91	0.53
1:B:282:PHE:CE1	1:B:293:LEU:HD13	2.46	0.51
1:A:282:PHE:CE1	1:A:293:LEU:HD13	2.46	0.50
1:B:195:MET:HB3	1:B:205:PRO:HB3	1.93	0.50
1:A:363:LEU:HD22	1:A:368:LEU:HD12	1.95	0.49
1:A:379:LEU:HD23	1:A:379:LEU:N	2.28	0.48
1:B:441:THR:HB	1:B:442:ARG:HA	1.95	0.48
1:B:441:THR:HB	1:B:442:ARG:CA	2.43	0.47
1:B:366:LEU:HD21	1:B:436:GLN:OE1	2.15	0.47
1:B:52:LEU:HD22	1:B:408:GLY:HA3	1.96	0.47
1:A:195:MET:HB3	1:A:205:PRO:HB3	1.97	0.45
1:A:70:VAL:HG11	1:A:400:HIS:CD2	2.51	0.45
1:B:36:THR:CG2	1:B:38:LEU:H	2.28	0.45
1:B:258:ILE:O	1:B:264:ARG:NH2	2.50	0.45
1:A:258:ILE:O	1:A:264:ARG:NH2	2.51	0.44
1:A:53:PHE:O	1:A:57:ASN:HB2	2.17	0.43
1:A:36:THR:CG2	1:A:38:LEU:H	2.29	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:HIS:ND1	1:B:190:GLN:OE1	2.52	0.42
1:B:414:GLU:O	1:B:415:GLU:HB2	2.19	0.42
1:A:175:ILE:HD13	1:A:175:ILE:HA	1.88	0.42
1:A:282:PHE:CD1	1:A:293:LEU:HD13	2.55	0.41
1:A:285:PHE:CE1	1:A:345:ILE:HG21	2.55	0.41
1:B:175:ILE:HD13	1:B:175:ILE:HA	1.91	0.41
1:A:70:VAL:HG11	1:A:400:HIS:CG	2.56	0.40
1:B:53:PHE:N	1:B:54:PRO:CD	2.84	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	404/456 (89%)	391 (97%)	11 (3%)	2 (0%)	34	41
1	B	407/456 (89%)	392 (96%)	13 (3%)	2 (0%)	34	41
All	All	811/912 (89%)	783 (96%)	24 (3%)	4 (0%)	34	41

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	260	ASP
1	B	300	ASP
1	A	300	ASP
1	B	441	THR

### 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	339/395 (86%)	327 (96%)	12 (4%)	43	58
1	B	337/395 (85%)	327 (97%)	10 (3%)	48	65
All	All	676/790 (86%)	654 (97%)	22 (3%)	45	61

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	THR
1	A	57	ASN
1	A	61	LEU
1	A	89	THR
1	A	147	SER
1	A	212	ARG
1	A	234	LEU
1	A	293	LEU
1	A	302	LEU
1	A	315	HIS
1	A	379	LEU
1	A	384	LYS
1	B	36	THR
1	B	61	LEU
1	B	69	ASN
1	B	77	THR
1	B	89	THR
1	B	147	SER
1	B	212	ARG
1	B	234	LEU
1	B	293	LEU
1	B	302	LEU

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

Mol	Chain	Res	Type
1	A	382	HIS

### 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 ⓘ

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	PLP	A	501	-	16,16,16	1.32	3 (18%)	21,23,23	2.07	4 (19%)
2	PLP	B	501	-	16,16,16	2.35	3 (18%)	21,23,23	1.76	4 (19%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PLP	A	501	-	-	0/8/8/8	0/1/1/1
2	PLP	B	501	-	-	0/8/8/8	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	PLP	O3-C3	-2.29	1.31	1.37
2	A	501	PLP	C4-C3	2.08	1.43	1.40
2	B	501	PLP	C4-C5	2.84	1.45	1.42
2	A	501	PLP	C3-C2	2.94	1.42	1.40
2	B	501	PLP	C4-C3	5.08	1.47	1.40
2	B	501	PLP	C3-C2	6.61	1.45	1.40

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	PLP	O4A-C4A-C4	-6.43	112.12	125.11
2	B	501	PLP	C2A-C2-C3	-3.38	116.96	121.04
2	B	501	PLP	C3-C4-C5	-3.37	115.58	118.11
2	B	501	PLP	O4A-C4A-C4	-3.26	118.53	125.11
2	A	501	PLP	O3P-P-O1P	2.21	117.70	110.58
2	A	501	PLP	O2P-P-O1P	2.26	117.85	110.58
2	B	501	PLP	O2P-P-O1P	2.80	119.61	110.58
2	A	501	PLP	O4P-C5A-C5	4.24	116.01	108.99

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	406/456 (89%)	-0.39	1 (0%) 95 97	20, 33, 54, 78	0
1	B	409/456 (89%)	-0.24	2 (0%) 91 94	25, 41, 58, 112	0
All	All	815/912 (89%)	-0.31	3 (0%) 93 95	20, 37, 57, 112	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	35	SER	2.3
1	A	35	SER	2.2
1	B	442	ARG	2.0

### 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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	PLP	B	501	16/16	0.98	0.13	0.91	26,31,48,65	0
2	PLP	A	501	16/16	0.98	0.11	0.77	22,26,36,45	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.