



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 01:06 am GMT

PDB ID : 4LDX  
Title : Crystal structure of the DNA binding domain of arabidopsis thaliana auxin response factor 1 (ARF1) in complex with protomor-like sequence ER7  
Authors : Boer, D.R.; Freire-Rios, A.; van den Berg, W.M.A.; Weijers, D.; Coll, M.  
Deposited on : 2013-06-25  
Resolution : 2.90 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  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

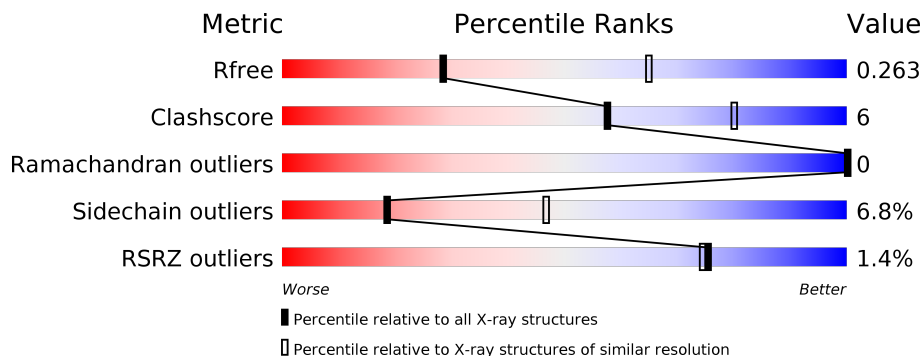
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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))
$R_{free}$	100719	1586 (2.90-2.90)
Clashscore	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)
RSRZ outliers	101464	1596 (2.90-2.90)

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	363	<div> <div>0%</div> <div> <div></div> <div>74%</div> <div>15%</div> <div>9%</div> </div> </div>
1	B	363	<div> <div>2%</div> <div> <div></div> <div>75%</div> <div>18%</div> <div>7%</div> </div> </div>
2	C	21	<div> <div></div> <div> <div></div> <div>67%</div> <div>33%</div> </div> </div>
3	D	21	<div> <div>5%</div> <div> <div></div> <div>71%</div> <div>29%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6274 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 Auxin response factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	332	Total	C	N	O	S	0	0	0
			2671	1684	481	492	14			
1	B	337	Total	C	N	O	S	0	0	0
			2715	1713	487	501	14			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	356	ASN	-	EXPRESSION TAG	UNP Q8L7G0
A	357	SER	-	EXPRESSION TAG	UNP Q8L7G0
A	358	TYR	-	EXPRESSION TAG	UNP Q8L7G0
A	359	SER	-	EXPRESSION TAG	UNP Q8L7G0
A	360	GLN	-	EXPRESSION TAG	UNP Q8L7G0
A	361	SER	-	EXPRESSION TAG	UNP Q8L7G0
A	362	MET	-	EXPRESSION TAG	UNP Q8L7G0
A	363	CYS	-	EXPRESSION TAG	UNP Q8L7G0
B	356	ASN	-	EXPRESSION TAG	UNP Q8L7G0
B	357	SER	-	EXPRESSION TAG	UNP Q8L7G0
B	358	TYR	-	EXPRESSION TAG	UNP Q8L7G0
B	359	SER	-	EXPRESSION TAG	UNP Q8L7G0
B	360	GLN	-	EXPRESSION TAG	UNP Q8L7G0
B	361	SER	-	EXPRESSION TAG	UNP Q8L7G0
B	362	MET	-	EXPRESSION TAG	UNP Q8L7G0
B	363	CYS	-	EXPRESSION TAG	UNP Q8L7G0

- Molecule 2 is a DNA chain called ER7, forward sequence.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	21	Total	C	N	O	P	0	0	0
			426	205	74	127	20			

- Molecule 3 is a DNA chain called ER7, reverse sequence.

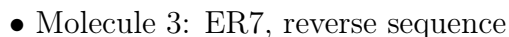
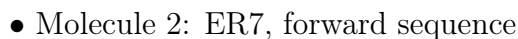
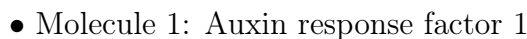
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	21	Total 429	C 205	N 83	O 121	P 20	0	0	0

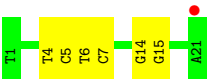
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	16	Total 16	O 16	0	0
4	B	15	Total 15	O 15	0	0
4	D	2	Total 2	O 2	0	0



- Molecule 1: Auxin response factor 1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	43.52Å 105.19Å 127.91Å 90.00° 98.14° 90.00°	Depositor
Resolution (Å)	33.81 – 2.90 33.79 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.4 (33.81-2.90) 98.6 (33.79-2.90)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.80 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.214 , 0.259 0.218 , 0.263	Depositor DCC
$R_{free}$ test set	1203 reflections (5.05%)	DCC
Wilson B-factor (Å <sup>2</sup> )	42.2	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 41.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.047 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	6274	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.62% 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	0.64	0/2742	0.79	3/3715 (0.1%)
1	B	0.58	0/2788	0.78	1/3781 (0.0%)
2	C	0.45	0/476	0.85	0/733
3	D	0.46	0/482	0.83	0/742
All	All	0.59	0/6488	0.79	4/8971 (0.0%)

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	B	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	219	ARG	NE-CZ-NH1	-6.68	116.96	120.30
1	A	219	ARG	NE-CZ-NH2	5.62	123.11	120.30
1	A	89	ASP	CB-CG-OD1	5.53	123.27	118.30
1	B	329	ARG	NE-CZ-NH1	5.04	122.82	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	116	PRO	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	2671	0	2607	31	0
1	B	2715	0	2655	31	0
2	C	426	0	240	5	0
3	D	429	0	237	4	0
4	A	16	0	0	4	0
4	B	15	0	0	3	0
4	D	2	0	0	0	0
All	All	6274	0	5739	67	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 6.

All (67) 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:245:GLY:O	1:A:249:THR:HB	1.92	0.69
1:A:186:ARG:HB2	1:A:186:ARG:HH11	1.58	0.68
1:B:200:LYS:O	1:B:224:ARG:NH2	2.29	0.66
1:B:296:MET:HE2	1:B:352:LEU:HD23	1.77	0.66
1:A:297:ARG:HD3	1:A:307:ARG:NH2	2.11	0.65
1:A:287:LYS:N	4:A:414:HOH:O	2.28	0.64
1:B:296:MET:CE	1:B:352:LEU:HD23	2.28	0.64
1:B:23:LEU:HD22	1:B:219:ARG:HB3	1.84	0.60
1:A:23:LEU:HD22	1:A:219:ARG:HB3	1.84	0.60
1:A:241:SER:HB3	1:B:249:THR:OG1	2.02	0.60
1:B:296:MET:CE	1:B:352:LEU:CD2	2.81	0.59
1:B:227:ARG:O	1:B:229:GLN:HG2	2.04	0.57
3:D:14:DG:H4'	3:D:15:DG:OP1	2.05	0.57
1:A:170:HIS:O	1:A:171:ASN:HB2	2.04	0.55
1:A:200:LYS:O	1:A:224:ARG:NH1	2.41	0.54
1:B:53:GLU:HG2	1:B:59:GLY:HA3	1.89	0.54
1:B:170:HIS:O	1:B:171:ASN:HB2	2.09	0.53
1:B:272:GLU:HG2	4:B:403:HOH:O	2.07	0.53
1:A:41:VAL:HG12	1:A:276:SER:HA	1.93	0.51
1:B:128:LEU:HD11	1:B:208:PHE:HB2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:SER:OG	3:D:4:DT:OP2	2.28	0.51
1:A:128:LEU:HD11	1:A:208:PHE:HB2	1.93	0.51
1:A:61:GLU:O	1:A:62:GLN:C	2.50	0.50
1:A:286:GLN:CA	4:A:414:HOH:O	2.59	0.50
1:A:280:TYR:OH	1:A:327:GLU:OE1	2.29	0.50
1:B:295:LYS:HD3	4:B:409:HOH:O	2.12	0.50
1:B:41:VAL:HG12	1:B:276:SER:HA	1.95	0.49
1:A:286:GLN:HB3	4:A:414:HOH:O	2.13	0.49
1:A:280:TYR:CE2	1:A:327:GLU:OE1	2.65	0.49
1:B:16:SER:HB2	1:B:217:GLU:OE1	2.14	0.48
1:B:16:SER:CB	1:B:217:GLU:OE1	2.61	0.47
1:B:237:ILE:HD11	1:B:242:MET:HG2	1.97	0.47
1:B:124:PHE:CE2	1:B:210:PHE:HB3	2.51	0.46
1:B:204:ALA:O	1:B:226:MET:HG3	2.15	0.46
1:B:79:ASN:ND2	1:B:80:ILE:H	2.14	0.46
1:B:276:SER:HB3	4:B:404:HOH:O	2.16	0.45
1:A:227:ARG:O	1:A:228:GLN:HB2	2.15	0.45
1:A:124:PHE:CE2	1:A:210:PHE:HB3	2.52	0.45
1:A:36:ARG:NE	1:A:115:GLU:OE1	2.50	0.45
1:A:249:THR:CG2	1:A:250:ALA:N	2.80	0.45
2:C:6:DT:H2''	2:C:7:DC:OP2	2.16	0.44
3:D:6:DT:H2''	3:D:7:DC:OP2	2.16	0.44
1:A:214:GLU:N	4:A:408:HOH:O	2.49	0.44
1:B:167:THR:HA	1:B:172:SER:O	2.17	0.44
1:B:56:MET:HA	1:B:233:PRO:HB3	2.00	0.44
1:A:225:HIS:O	1:A:227:ARG:HG2	2.17	0.44
1:B:277:VAL:HG23	1:B:278:ASN:N	2.32	0.44
1:B:123:SER:HA	1:B:210:PHE:O	2.18	0.44
1:A:237:ILE:HD11	1:A:242:MET:HG2	1.99	0.44
1:A:280:TYR:HE2	1:A:327:GLU:OE1	2.01	0.43
3:D:5:DC:H2''	3:D:6:DT:OP2	2.17	0.43
1:B:139:PHE:HB3	1:B:189:LEU:HB2	2.01	0.43
2:C:5:DC:H2''	2:C:6:DT:OP2	2.20	0.42
1:A:123:SER:HA	1:A:210:PHE:O	2.19	0.42
1:B:81:GLN:OE1	1:B:94:GLN:NE2	2.53	0.42
1:B:82:ARG:O	1:B:83:ARG:HG3	2.19	0.42
1:A:167:THR:HA	1:A:172:SER:O	2.20	0.41
1:A:139:PHE:HB3	1:A:189:LEU:HB2	2.01	0.41
1:A:272:GLU:CD	1:A:279:ARG:HH22	2.22	0.41
1:B:86:PRO:HA	1:B:170:HIS:CE1	2.56	0.41
1:B:184:PRO:HG2	2:C:1:DT:H71	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:PHE:CE1	1:A:72:LYS:HB3	2.56	0.41
1:A:315:VAL:O	1:A:316:GLN:C	2.59	0.41
1:A:58:GLN:HG2	1:A:59:GLY:N	2.36	0.40
2:C:13:DG:H1'	2:C:14:DG:C8	2.57	0.40
1:B:131:SER:OG	2:C:4:DT:OP2	2.37	0.40
1:B:225:HIS:O	1:B:226:MET:C	2.59	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	326/363 (90%)	313 (96%)	13 (4%)	0	100	100
1	B	333/363 (92%)	318 (96%)	15 (4%)	0	100	100
All	All	659/726 (91%)	631 (96%)	28 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	298/323 (92%)	277 (93%)	21 (7%)	18	45
1	B	304/323 (94%)	284 (93%)	20 (7%)	19	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	602/646 (93%)	561 (93%)	41 (7%)	18	47

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	SER
1	A	33	THR
1	A	52	LEU
1	A	61	GLU
1	A	76	LYS
1	A	114	GLN
1	A	131	SER
1	A	172	SER
1	A	177	ARG
1	A	186	ARG
1	A	203	VAL
1	A	234	SER
1	A	239	SER
1	A	241	SER
1	A	249	THR
1	A	261	SER
1	A	271	SER
1	A	277	VAL
1	A	285	THR
1	A	289	SER
1	A	337	GLU
1	B	15	LEU
1	B	17	ASP
1	B	52	LEU
1	B	60	LEU
1	B	62	GLN
1	B	76	LYS
1	B	118	LYS
1	B	121	VAL
1	B	131	SER
1	B	135	THR
1	B	142	LEU
1	B	172	SER
1	B	203	VAL
1	B	232	ILE
1	B	239	SER
1	B	261	SER

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Mol	Chain	Res	Type
1	B	271	SER
1	B	289	SER
1	B	327	GLU
1	B	332	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	GLN
1	B	79	ASN
1	B	229	GLN

### 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	332/363 (91%)	-0.43	2 (0%) 89 88	19, 30, 76, 120	0
1	B	337/363 (92%)	-0.26	7 (2%) 64 60	21, 46, 91, 123	0
2	C	21/21 (100%)	-0.36	0 100 100	35, 77, 88, 102	0
3	D	21/21 (100%)	-0.14	1 (4%) 31 27	28, 68, 88, 122	0
All	All	711/768 (92%)	-0.34	10 (1%) 75 74	19, 38, 88, 123	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	225	HIS	3.0
1	B	340	SER	2.7
1	B	15	LEU	2.5
1	B	58	GLN	2.4
3	D	21	DA	2.3
1	B	227	ARG	2.2
1	A	321	SER	2.1
1	B	63	GLN	2.1
1	B	226	MET	2.1
1	A	355	LEU	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.