



# wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 5GXU  
Title : Crystal structure of Arabidopsis ATR2  
Authors : Niu, G.; Liu, L.  
Deposited on : 2016-09-20  
Resolution : 2.30 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	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
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)	:	rb-20028442

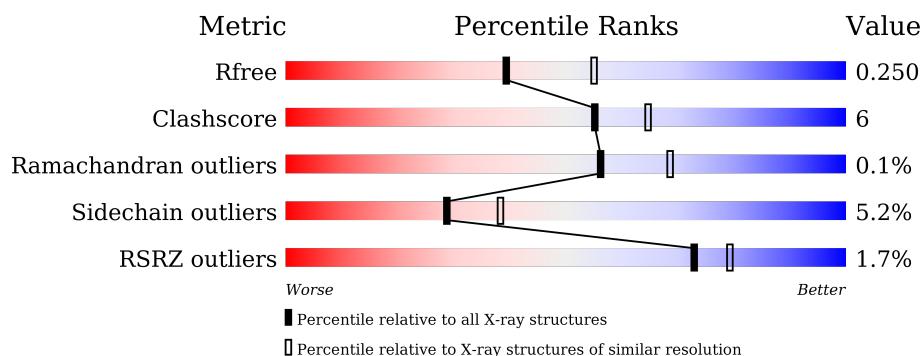
# 1 Overall quality at a glance

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	640	<div> <div>2%</div> <div> <div></div> <div>74%</div> <div>12%</div> <div>•</div> <div>14%</div> </div> </div>
1	B	640	<div> <div>%</div> <div> <div></div> <div>50%</div> <div>10%</div> <div>•</div> <div>38%</div> </div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7780 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.

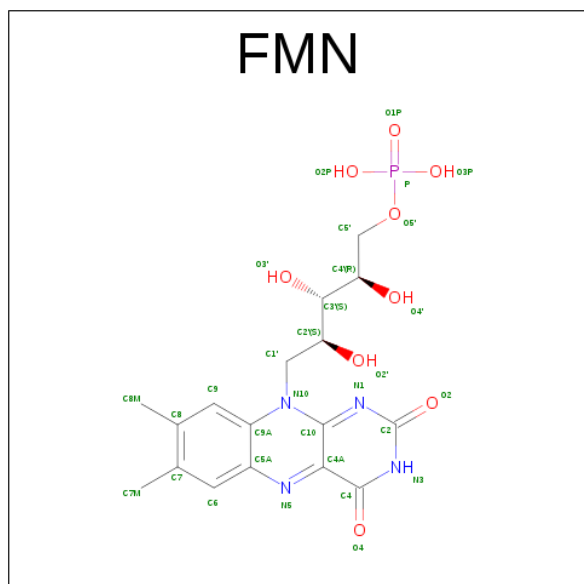
- Molecule 1 is a protein called NADPH–cytochrome P450 reductase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	552	Total	C	N	O	S	0	2	0
			4251	2715	725	790	21			
1	B	394	Total	C	N	O	S	0	3	0
			3017	1918	519	560	20			

There are 2 discrepancies between the modelled and reference sequences:

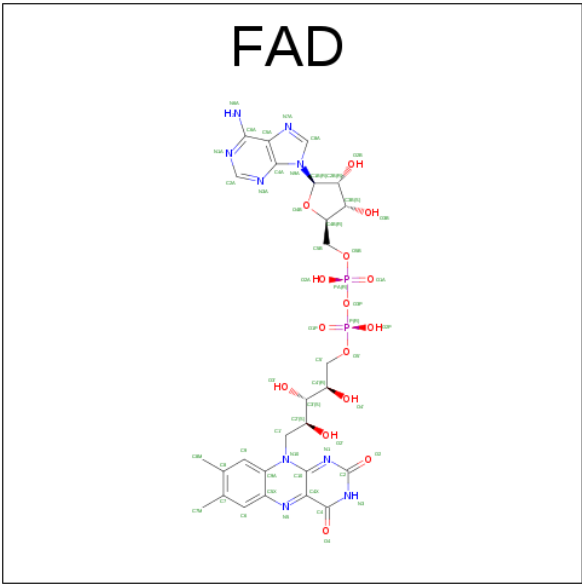
Chain	Residue	Modelled	Actual	Comment	Reference
A	72	GLY	-	expression tag	UNP Q9SUM3
B	72	GLY	-	expression tag	UNP Q9SUM3

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C<sub>17</sub>H<sub>21</sub>N<sub>4</sub>O<sub>9</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).

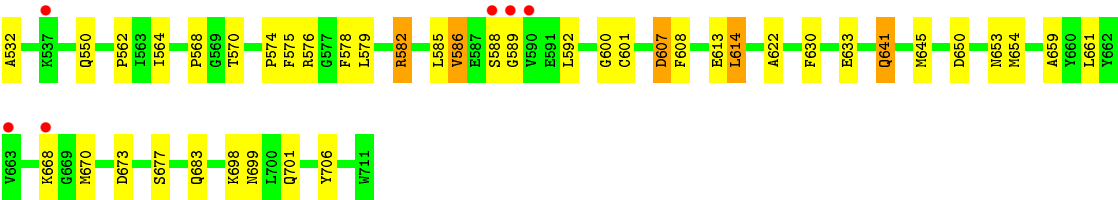


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	205	Total	O	0	0
			205	205		
4	B	170	Total	O	0	0
			170	170		





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	55.33Å 61.82Å 88.33Å 97.84° 100.51° 90.27°	Depositor
Resolution (Å)	30.61 – 2.30 30.61 – 2.30	Depositor EDS
% Data completeness (in resolution range)	90.8 (30.61-2.30) 86.7 (30.61-2.30)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.87 (at 2.31Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.200 , 0.248 0.200 , 0.250	Depositor DCC
$R_{free}$ test set	2311 reflections (5.12%)	DCC
Wilson B-factor (Å <sup>2</sup> )	31.0	Xtriage
Anisotropy	0.192	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 30.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7780	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.14% 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.31	0/4358	0.49	0/5909
1	B	0.33	0/3100	0.52	0/4208
All	All	0.32	0/7458	0.50	0/10117

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	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	538	SER	Peptide
1	A	606	MET	Peptide

### 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	4251	0	4088	40	0
1	B	3017	0	2934	50	0
2	A	31	0	19	1	0
3	A	53	0	31	4	0
3	B	53	0	31	3	0
4	A	205	0	0	6	0
4	B	170	0	0	10	0
All	All	7780	0	7103	91	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.

The worst 5 of 91 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:B:505:HIS:HD2	1:B:576:ARG:HH22	1.19	0.91
1:B:588:SER:H	1:B:589:GLY:HA2	1.35	0.90
1:B:505:HIS:CD2	1:B:576:ARG:HH22	2.03	0.76
1:B:582:ARG:HH11	1:B:582:ARG:HG3	1.54	0.71
1:A:121:LYS:HD3	1:A:138:ILE:HD13	1.75	0.67

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	548/640 (86%)	531 (97%)	16 (3%)	1 (0%)	52	64
1	B	393/640 (61%)	379 (96%)	14 (4%)	0	100	100
All	All	941/1280 (74%)	910 (97%)	30 (3%)	1 (0%)	56	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	169	GLY

### 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	434/538 (81%)	412 (95%)	22 (5%)	29	39
1	B	320/538 (60%)	302 (94%)	18 (6%)	26	35
All	All	754/1076 (70%)	714 (95%)	40 (5%)	29	37

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	608	PHE
1	B	321	ARG
1	B	614	LEU
1	A	619	GLU
1	B	485[A]	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	505	HIS
1	B	683	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

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

3 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	FMN	A	801	-	32,33,33	1.12	3 (9%)	34,50,50	1.85	5 (14%)
3	FAD	A	802	-	52,58,58	2.37	17 (32%)	52,89,89	2.26	8 (15%)
3	FAD	B	801	-	52,58,58	2.40	17 (32%)	52,89,89	2.33	9 (17%)

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	FMN	A	801	-	-	0/18/18/18	0/3/3/3
3	FAD	A	802	-	-	0/30/50/50	0/6/6/6
3	FAD	B	801	-	-	0/30/50/50	0/6/6/6

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	802	FAD	C2B-C1B	-5.17	1.45	1.53
3	B	801	FAD	C2B-C1B	-5.01	1.45	1.53
3	B	801	FAD	C2B-C3B	-3.61	1.43	1.53
3	A	802	FAD	C2B-C3B	-3.53	1.43	1.53
3	A	802	FAD	O3'-C3'	-2.60	1.36	1.43

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	801	FAD	N3A-C2A-N1A	-10.80	120.39	128.87
3	A	802	FAD	N3A-C2A-N1A	-10.57	120.57	128.87
3	B	801	FAD	N3-C2-N1	-4.36	120.35	127.69
3	B	801	FAD	C4B-O4B-C1B	-4.28	105.10	109.64
2	A	801	FMN	N3-C2-N1	-4.27	120.50	127.69

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	FMN	1	0
3	A	802	FAD	4	0
3	B	801	FAD	3	0

## 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	552/640 (86%)	0.05	10 (1%) 71 78	8, 23, 43, 51	5 (0%)
1	B	394/640 (61%)	-0.04	6 (1%) 76 81	8, 18, 32, 39	2 (0%)
All	All	946/1280 (73%)	0.01	16 (1%) 73 79	8, 20, 40, 51	7 (0%)

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	156	LYS	3.4
1	B	589	GLY	3.4
1	A	129	ALA	3.0
1	A	195	LYS	2.8
1	A	262	LEU	2.7

### 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
3	FAD	A	802	53/53	0.95	0.15	0.47	8,11,21,21	0
3	FAD	B	801	53/53	0.95	0.14	0.24	7,10,18,20	0
2	FMN	A	801	31/31	0.96	0.11	-0.71	27,34,36,36	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.