



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 12, 2017 – 09:48 pm GMT

PDB ID : 4XXE  
Title : Structure of AgrA LytTR domain in complex with promoters  
Authors : Gopal, B.; Rajasree, K.  
Deposited on : 2015-01-30  
Resolution : 3.20 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

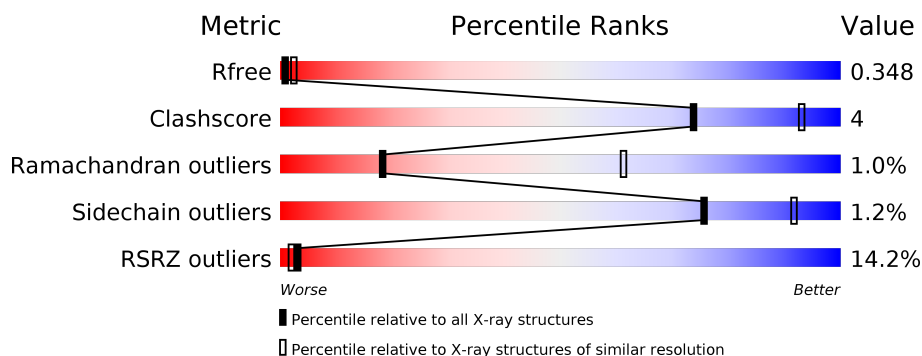
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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	1015 (3.22-3.18)
Clashscore	112137	1009 (3.20-3.20)
Ramachandran outliers	110173	1118 (3.22-3.18)
Sidechain outliers	110143	1117 (3.22-3.18)
RSRZ outliers	101464	1020 (3.22-3.18)

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	99	<div> <div>16%</div> <div> <div></div> <div>91%</div> <div>8%</div> </div> </div>
1	D	99	<div> <div>16%</div> <div> <div></div> <div>93%</div> <div>7%</div> </div> </div>
2	B	13	<div> <div>8%</div> <div> <div></div> <div>77%</div> <div>15%</div> <div>8%</div> </div> </div>
3	C	15	<div> <div>7%</div> <div> <div></div> <div>73%</div> <div>13%</div> <div>13%</div> </div> </div>
3	F	15	<div> <div>13%</div> <div> <div></div> <div>87%</div> <div>7%</div> <div>7%</div> </div> </div>
4	E	13	<div> <div></div> <div> <div></div> <div>77%</div> <div>23%</div> </div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2726 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 Accessory gene regulator A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	99	Total	C	N	O	S	0	0	0
			794	500	140	151	3			
1	D	99	Total	C	N	O	S	0	0	0
			787	494	139	151	3			

- Molecule 2 is a DNA chain called DNA (5'-D(P\*TP\*AP\*CP\*AP\*GP\*TP\*TP\*AP\*GP\*GP\*CP\*AP\*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	13	Total	C	N	O	P	0	0	0
			269	128	52	76	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	15	Total	C	N	O	P	0	0	0
			304	147	54	89	14			
3	F	15	Total	C	N	O	P	0	0	0
			304	147	54	89	14			

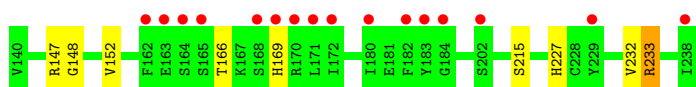
- Molecule 4 is a DNA chain called DNA (5'-D(P\*TP\*AP\*CP\*AP\*GP\*TP\*TP\*AP\*GP\*GP\*CP\*AP\*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	13	Total	C	N	O	P	0	0	0
			268	128	49	78	13			

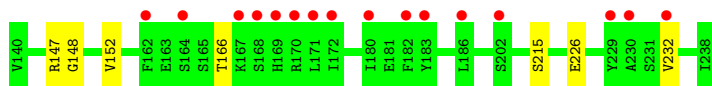
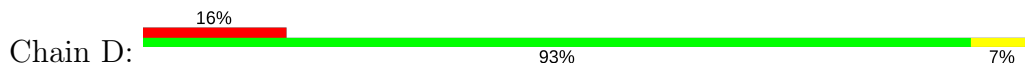
### 3 Residue-property plots [i](#)

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

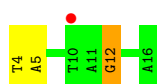
- Molecule 1: Accessory gene regulator A



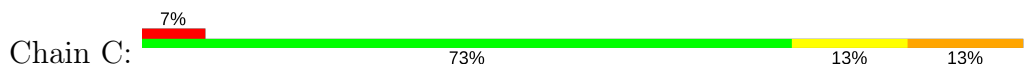
- Molecule 1: Accessory gene regulator A



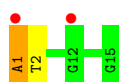
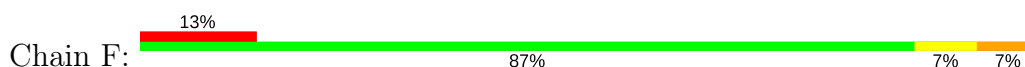
- Molecule 2: DNA (5'-D(P\*TP\*AP\*CP\*AP\*GP\*TP\*TP\*AP\*GP\*GP\*CP\*AP\*A)-3')




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



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



- Molecule 4: DNA (5'-D(P\*TP\*AP\*CP\*AP\*GP\*TP\*TP\*AP\*GP\*GP\*CP\*AP\*T)-3')

Chain E:  77% 23%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 42	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.76Å 96.76Å 51.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	96.76 – 3.20 68.42 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (96.76-3.20) 99.9 (68.42-3.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.13	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.08 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, $R_{free}$	0.315 , 0.355 0.318 , 0.348	Depositor DCC
$R_{free}$ test set	759 reflections (10.50%)	DCC
Wilson B-factor (Å <sup>2</sup> )	101.0	Xtriage
Anisotropy	0.449	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 474.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.448 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	2726	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	138.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% 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	0.59	0/809	0.79	1/1089 (0.1%)
1	D	0.59	0/802	0.76	0/1080
2	B	0.51	0/302	0.87	1/464 (0.2%)
3	C	0.52	0/340	0.96	4/523 (0.8%)
3	F	0.48	0/340	0.96	2/523 (0.4%)
4	E	0.53	0/300	0.87	1/461 (0.2%)
All	All	0.56	0/2893	0.85	9/4140 (0.2%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	DA	C5'-C4'-C3'	6.08	125.05	114.10
3	F	1	DA	C5'-C4'-C3'	6.02	124.94	114.10
3	C	1	DA	C5'-C4'-O4'	5.60	119.94	109.30
3	F	1	DA	C5'-C4'-O4'	5.57	119.89	109.30
1	A	233	ARG	CA-CB-CG	5.46	125.40	113.40
2	B	12	DG	O5'-P-OP1	5.37	117.14	110.70
4	E	12	DG	O5'-P-OP1	5.34	117.10	110.70
3	C	2	DT	O5'-P-OP1	-5.26	100.96	105.70
3	C	3	DT	C1'-O4'-C4'	-5.02	105.08	110.10

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	794	0	731	6	0
1	D	787	0	708	4	0
2	B	269	0	147	6	0
3	C	304	0	172	3	0
3	F	304	0	172	2	0
4	E	268	0	148	3	0
All	All	2726	0	2078	18	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 4.

All (18) 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)
2:B:4:DT:H2''	2:B:5:DA:O5'	2.04	0.57
1:D:147:ARG:HD3	1:D:152:VAL:HG23	1.88	0.56
1:A:147:ARG:HD3	1:A:152:VAL:HG23	1.89	0.54
3:C:1:DA:H1'	3:C:2:DT:H5''	1.90	0.52
1:D:148:GLY:HA3	3:F:1:DA:H3'	1.92	0.52
1:A:148:GLY:HA3	3:C:1:DA:H3'	1.92	0.52
3:F:1:DA:H1'	3:F:2:DT:H5''	1.91	0.52
2:B:4:DT:C2'	2:B:5:DA:C8	2.93	0.52
4:E:4:DT:H2''	4:E:5:DA:O5'	2.11	0.51
2:B:4:DT:H6	2:B:4:DT:O5'	1.95	0.50
2:B:4:DT:H2'	2:B:5:DA:C8	2.48	0.48
2:B:4:DT:H2''	2:B:5:DA:C8	2.48	0.48
1:A:227:HIS:CE1	1:D:166:THR:HB	2.49	0.47
4:E:4:DT:H2'	4:E:5:DA:C8	2.53	0.43
1:A:169:HIS:CE1	2:B:12:DG:C8	3.07	0.43
1:A:166:THR:OG1	1:D:226:GLU:HA	2.20	0.41
4:E:4:DT:C2'	4:E:5:DA:C8	3.04	0.41
1:A:233:ARG:HD2	3:C:11:DT:OP2	2.21	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	97/99 (98%)	93 (96%)	3 (3%)	1 (1%)	18	61
1	D	97/99 (98%)	93 (96%)	3 (3%)	1 (1%)	18	61
All	All	194/198 (98%)	186 (96%)	6 (3%)	2 (1%)	18	61

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	232	VAL
1	A	232	VAL

### 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	84/95 (88%)	83 (99%)	1 (1%)	75	91
1	D	81/95 (85%)	80 (99%)	1 (1%)	75	91
All	All	165/190 (87%)	163 (99%)	2 (1%)	75	91

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	215	SER
1	D	215	SER

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	169	HIS
1	A	179	GLN
1	D	179	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 ⓘ

### 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, 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	99/99 (100%)	0.51	16 (16%) 2 1	77, 128, 175, 192	0
1	D	99/99 (100%)	0.50	16 (16%) 2 1	71, 128, 171, 182	0
2	B	13/13 (100%)	0.12	1 (7%) 14 8	103, 146, 179, 200	0
3	C	15/15 (100%)	0.71	1 (6%) 19 10	107, 153, 213, 242	0
3	F	15/15 (100%)	0.68	2 (13%) 4 2	115, 145, 214, 214	0
4	E	13/13 (100%)	0.01	0 100 100	92, 140, 167, 178	0
All	All	254/254 (100%)	0.48	36 (14%) 3 2	71, 133, 179, 242	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	169	HIS	7.8
1	D	168	SER	6.5
1	D	169	HIS	5.0
1	A	171	LEU	4.9
1	A	170	ARG	4.5
1	A	168	SER	4.4
1	D	180	ILE	4.4
1	D	171	LEU	3.8
1	A	183	TYR	3.8
1	D	186	LEU	3.7
1	A	164	SER	3.6
3	C	14	DA	3.5
1	D	229	TYR	3.5
1	A	162	PHE	3.4
1	D	182	PHE	3.4
1	D	183	TYR	3.3
1	D	170	ARG	3.3
1	D	162	PHE	3.3
1	D	232	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	182	PHE	3.1
3	F	1	DA	3.1
1	A	180	ILE	3.0
1	D	164	SER	3.0
1	D	167	LYS	2.7
1	D	230	ALA	2.6
1	A	163	GLU	2.5
1	A	184	GLY	2.5
1	A	165	SER	2.5
1	A	202	SER	2.4
1	A	238	ILE	2.2
1	A	172	ILE	2.2
1	D	172	ILE	2.2
1	A	229	TYR	2.2
1	D	202	SER	2.2
2	B	10	DT	2.2
3	F	12	DG	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.