

Full wwPDB X-ray Structure Validation Report (i)

Nov 23, 2020 - 09:05 am GMT

PDB ID : 6ZAB

Title: Structure of the transcriptional repressor Atu1419 (VanR) from agrobacterium

fabrum in complex a palindromic DNA (P6422 space group)

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Deposited on : 2020-06-05

Resolution : 2.80 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
A user guide is available at

https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity : 4.02b-467

Mogul: 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : 2.14.6

 $buster\text{-}report \quad : \quad 1.1.7 \ (2018)$

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

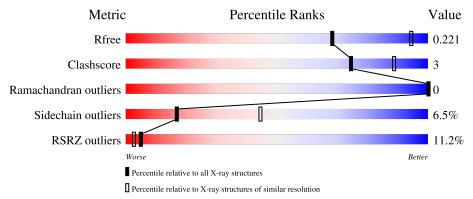
Validation Pipeline (wwPDB-VP) : 2.14.6

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	Similar resolution
Metric	$(\# { m Entries})$	$(\# ext{Entries}, ext{resolution range}(ext{Å}))$
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 respectively. 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 <=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	250	82%	12% • •				
2	В	10	90%	10%				



2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 2084 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 Transcriptional regulator, GntR family.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Λ	239	Total	С	N	О	S	0	9	0
1	Α	239	1834	1142	344	342	6	0	2	U

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	245	HIS	_	expression tag	UNP A9CJ36
A	246	HIS	-	expression tag	UNP A9CJ36
A	247	HIS	_	expression tag	UNP A9CJ36
A	248	HIS	_	expression tag	UNP A9CJ36
A	249	HIS	_	expression tag	UNP A9CJ36
A	250	HIS	-	expression tag	UNP A9CJ36

• Molecule 2 is a DNA chain called DNA (5'-D(*AP*TP*GP*TP*AP*TP*AP*CP*AP*T)-3').

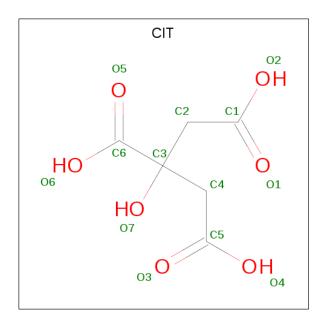
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
9	D	10	Total	С	N	О	Р	0	0	0
	D	10	202	99	36	58	9	U	0	U

• Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by author).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Zn 1 1	0	0

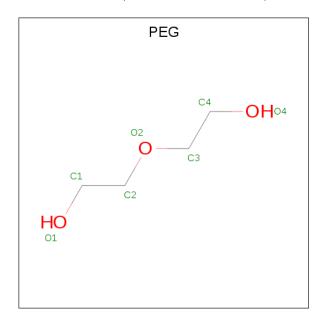
• Molecule 4 is CITRIC ACID (three-letter code: CIT) (formula: C₆H₈O₇).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 13	C 6	O 7	0	0

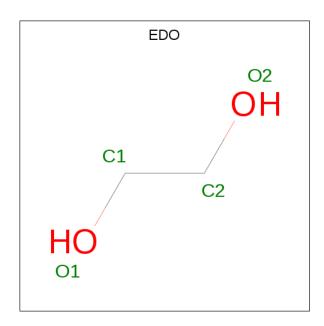
 $\bullet \ \ Molecule \ 5 \ is \ DI(HYDROXYETHYL)ETHER \ (three-letter \ code: \ PEG) \ (formula: \ C_4H_{10}O_3).$



Mol	Chain	Residues	Ato	Atoms		ZeroOcc	AltConf
5	A	1	Total 7	C 4	O 3	0	0

 \bullet Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $\mathrm{C_2H_6O_2}).$





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	Δ	1	Total	С	О	0	0
0	Λ	1	4	2	2	0	0

• Molecule 7 is water.

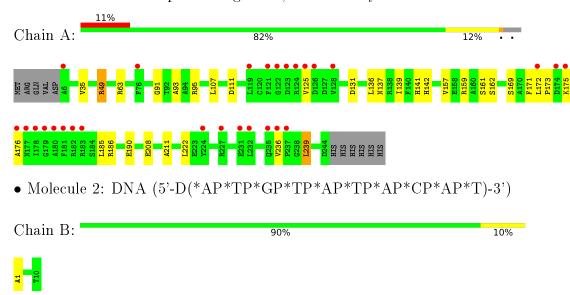
\mathbf{Mol}	Chain	Residues	${f Atoms}$	ZeroOcc	AltConf
7	A	18	Total O 18 18	0	0
7	В	5	Total O 5 5	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Transcriptional regulator, GntR family





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants	179.18Å 179.18Å 96.74Å	Danagitan
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.61 - 2.80	Depositor
Resolution (A)	46.18 - 2.80	EDS
% Data completeness	70.8 (45.61-2.80)	Depositor
(in resolution range)	70.8 (46.18-2.80)	EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.83 (at 2.81Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
D D.	0.188 , 0.199	Depositor
R, R_{free}	0.206 , 0.221	DCC
R_{free} test set	817 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	71.2	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.32,66.6	EDS
L-test for twinning ²	$ < L > = 0.48, < L^2> = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2084	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.38% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of <|L|>, $< L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

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: ZN, PEG, EDO, CIT

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		
MIOI		RMSZ	# Z >5	RMSZ	# Z > 5	
1	A	0.45	0/1864	0.64	0/2514	
2	В	0.99	0/226	0.93	0/347	
All	All	0.53	0/2090	0.68	0/2861	

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
2	В	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	В	1	DA	Sidechain

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	1834	0	1861	13	0
2	В	202	0	116	0	0
3	A	1	0	0	0	0
4	A	13	0	5	0	0
5	A	7	0	10	0	0
6	A	4	0	6	0	0
7	A	18	0	0	0	0
7	В	5	0	0	0	0
All	All	2084	0	1998	13	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 (13) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{array}{ll} ext{Interatomic} \ ext{distance} \ (ext{\AA}) \end{array}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$
1:A:137:ASN:HD22	1:A:169:SER:HB3	1.65	0.62
1:A:93:ALA:HB2	1:A:157:VAL:HG21	1.83	0.61
1:A:136:LEU:HA	1:A:139:ILE:HD12	1.86	0.57
1:A:159:ARG:O	1:A:162:SER:HB3	2.05	0.57
1:A:172:LEU:HD21	1:A:185:LEU:HD21	1.85	0.56
1:A:236:VAL:HB	1:A:239:LEU:HB2	1.92	0.52
1:A:49[A]:ARG:HH12	1:A:63:ARG:HH12	1.59	0.49
1:A:91:GLY:HA2	1:A:211:ALA:HB3	1.95	0.49
1:A:173:PRO:HD2	1:A:176:ALA:HB3	1.95	0.48
1:A:172:LEU:N	1:A:173:PRO:HD3	2.29	0.47
1:A:137:ASN:O	1:A:141:HIS:HD2	2.00	0.43
1:A:171:PHE:CE1	1:A:222:LEU:HB2	2.53	0.43
1:A:95:ARG:HB2	1:A:208:GLU:HB2	2.02	0.42

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	$239/250 \ (96\%)$	227 (95%)	12 (5%)	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	Analysed Rotameric		Percentiles	
1	A	186/195~(95%)	173 (93%)	13 (7%)	15 40	

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	VAL
1	A	49[A]	ARG
1	A	49[B]	ARG
1	A	107	LEU
1	A	111	ASP
1	A	125	VAL
1	A	131	ASP
1	A	142	HIS
1	A	161	SER
1	A	175	LYS
1	A	186	ARG
1	A	190	GLU
1	A	239	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	9	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 for Mogul analysis.

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	Tuna	Chain	Res	Link	B	ond leng	$_{ m gths}$	В	ond ang	gles
WIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	CIT	A	502	3	3,12,12	0.35	0	3,17,17	1.80	1 (33%)
5	PEG	A	503	-	6,6,6	0.16	0	5,5,5	0.02	0
6	EDO	A	504	-	3,3,3	0.86	0	2,2,2	0.27	0

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
4	CIT	A	502	3	_	1/6/16/16	-
5	PEG	A	503	_	-	1/4/4/4	-
6	EDO	A	504	-	-	0/1/1/1	=

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
4	A	502	CIT	C3-C4-C5	2.43	118.87	114.98

There are no chirality outliers.



All (2) torsion outliers are listed below:

	Mol	Chain	Res	Type	Atoms
ſ	5	Α	503	PEG	C4-C3-O2-C2
	4	A	502	CIT	O7-C3-C4-C5

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^{th} 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 $>$	$\#\mathrm{RSRZ}{>}2$	$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q < 0.9
1	A	$239/250 \ (95\%)$	0.10	28 (11%) 4 2	36, 70, 164, 197	0
2	В	10/10 (100%)	-0.47	0 100 100	52, 58, 82, 86	0
All	All	249/260 (95%)	0.08	28 (11%) 5 3	36, 70, 163, 197	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	6	ALA	5.6
1	A	125	VAL	4.5
1	A	181	PHE	4.5
1	A	179	GLY	4.4
1	A	124	ARG	4.1
1	A	172	LEU	4.1
1	A	122	GLY	4.1
1	A	180	ALA	4.1
1	A	175	LYS	3.9
1	A	231	GLU	3.8
1	A	178	ILE	3.7
1	A	183	ARG	3.6
1	A	236	VAL	3.4
1	A	174	ASP	3.3
1	A	123	ASP	3.3
1	A	182	ARG	3.2
1	A	227	ARG	3.1
1	A	224	TYR	2.9
1	A	237	PRO	2.8
1	A	121	PHE	2.7
1	A	232	LEU	2.7
1	A	128	VAL	2.7
1	A	126	ASP	2.7
1	A	177	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	235	GLN	2.5
1	A	119	LEU	2.5
1	A	76	PHE	2.3
1	A	176	ALA	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 monosaccharides in this entry.

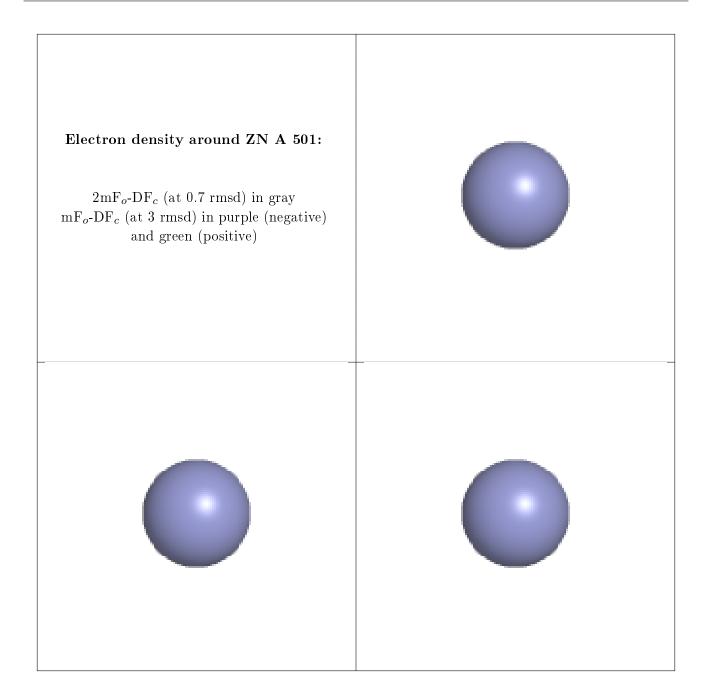
6.4 Ligands (i)

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. The B-factors column lists the minimum, median, 95^{th} 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	${f B-factors}({f A}^2)$	Q<0.9
5	PEG	A	503	7/7	0.84	0.16	98,104,106,106	0
6	EDO	A	504	4/4	0.93	0.18	68,68,69,69	0
4	CIT	A	502	13/13	0.97	0.25	124,127,132,134	0
3	ZN	A	501	1/1	0.98	0.08	107,107,107,107	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





6.5 Other polymers (i)

There are no such residues in this entry.

