

Full wwPDB NMR Structure Validation Report (i)

May 28, 2020 – 10:54 pm BST

PDB ID : 2L19

Title: An arsenate reductase in the intermediate state

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Deposited on : 2010-07-26

This is a Full wwPDB NMR 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/NMRValidationReportHelp 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:

Cyrange : Kirchner and Güntert (2011)

NmrClust : Kelley et al. (1996)

MolProbity: 4.02b-467

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

RCI : v 1n 11 5 13 A (Berjanski et al., 2005)

PANAV : Wang et al. (2010)

ShiftChecker : 2.11

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

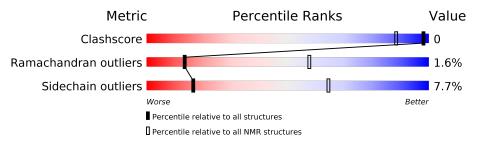
Validation Pipeline (wwPDB-VP) : 2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $SOLUTION\ NMR$

The overall completeness of chemical shifts assignment was not calculated.

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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$egin{array}{c} { m NMR \ archive} \ (\#{ m Entries}) \end{array}$	
Clashscore	158937	12864	
Ramachandran outliers	154571	11451	
Sidechain outliers	154315	11428	

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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%

Mol	Chain	Length	Quality of chain					
1	A	134	92%	6% •				



2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 2 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: lowest energy.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues					
Well-defined core Residue range (total) Backbone RMSD (Å) Medoid mode					
1	A:1-A:131 (131)	0.46	2		

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 3 clusters and 7 single-model clusters were found.

Cluster number	Models
1	1, 2, 14, 16, 19
2	7, 8, 11, 12
3	3, 10, 15, 20
Single-model clusters	4; 5; 6; 9; 13; 17; 18



3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1997 atoms, of which 990 are hydrogens and 0 are deuteriums.

• Molecule 1 is a protein called Arsenate reductase.

Mol	Chain	Residues		${f Atoms}$				Trace	
1	Λ	191	Total	С	Н	N	О	S	0
	A	131	1997	626	990	171	203	7	U

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP P74313
A	-1	SER	_	EXPRESSION TAG	UNP P74313
A	0	HIS	_	EXPRESSION TAG	UNP P74313
A	13	SER	CYS	ENGINEERED MUTATION	UNP P74313
A	35	SER	CYS	ENGINEERED MUTATION	UNP P74313
A	82	SER	CYS	ENGINEERED MUTATION	UNP P74313

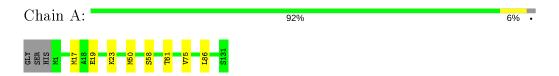


4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: Arsenate reductase

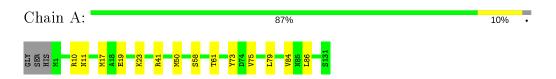


4.2 Scores per residue for each member of the ensemble

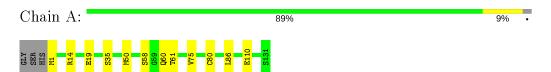
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Arsenate reductase



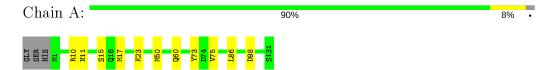
4.2.2 Score per residue for model 2 (medoid)





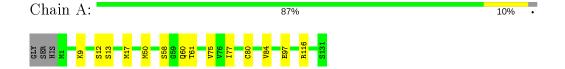
4.2.3 Score per residue for model 3

• Molecule 1: Arsenate reductase



4.2.4 Score per residue for model 4

• Molecule 1: Arsenate reductase



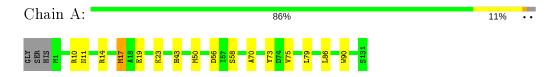
4.2.5 Score per residue for model 5

• Molecule 1: Arsenate reductase

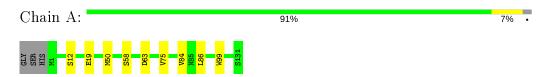


4.2.6 Score per residue for model 6

• Molecule 1: Arsenate reductase



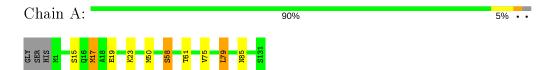
4.2.7 Score per residue for model 7





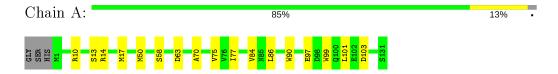
4.2.8 Score per residue for model 8

• Molecule 1: Arsenate reductase



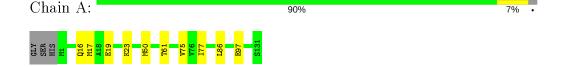
4.2.9 Score per residue for model 9

• Molecule 1: Arsenate reductase



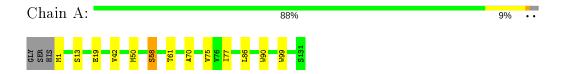
4.2.10 Score per residue for model 10

• Molecule 1: Arsenate reductase

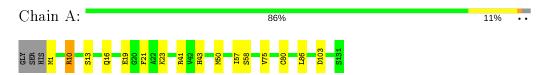


4.2.11 Score per residue for model 11

• Molecule 1: Arsenate reductase



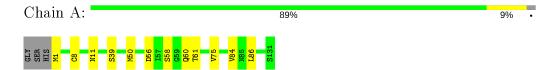
4.2.12 Score per residue for model 12





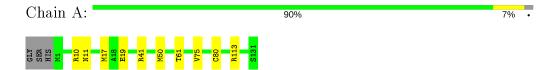
4.2.13 Score per residue for model 13

• Molecule 1: Arsenate reductase



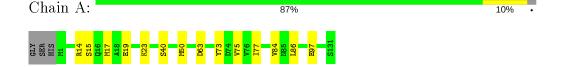
4.2.14 Score per residue for model 14

• Molecule 1: Arsenate reductase



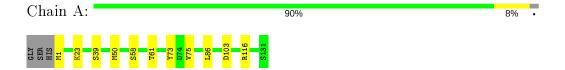
4.2.15 Score per residue for model 15

• Molecule 1: Arsenate reductase

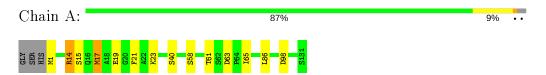


4.2.16 Score per residue for model 16

• Molecule 1: Arsenate reductase



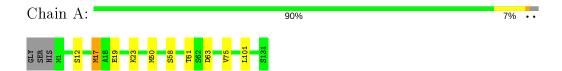
4.2.17 Score per residue for model 17





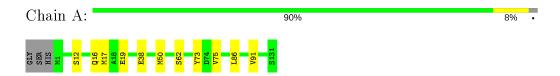
4.2.18 Score per residue for model 18

• Molecule 1: Arsenate reductase

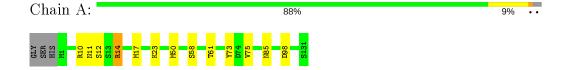


4.2.19 Score per residue for model 19

• Molecule 1: Arsenate reductase



4.2.20 Score per residue for model 20





5 Refinement protocol and experimental data overview (i)



The models were refined using the following method: molecular dynamics.

Of the 200 calculated structures, 20 were deposited, based on the following criterion: structures with the lowest energy.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
CYANA	structure solution	
AMBER	refinement	

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

COVALENT-GEOMETRY INFOmissingINFO

5.1Too-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 each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1007	990	992	1±1
All	All	20140	19800	19840	11

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 0.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom 2	Clash(Å)	Distance(Å)	Models	
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total
1:A:70:ALA:HB2	1:A:90:TRP:CD2	0.48	2.43	11	4
1:A:77:ILE:HD12	1:A:97:GLU:HB2	0.45	1.88	10	4
1:A:77:ILE:HG21	1:A:99:TRP:CZ3	0.44	2.48	11	2
1:A:17:MET:SD	1:A:21:PHE:CD2	0.42	3.12	17	1



5.2 Torsion angles (i)

5.2.1 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 PDB entries followed by that with respect to all NMR entries. 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 A		Allowed	Outliers	Perce	entiles
1	A	129/134 (96%)	116±3 (90±2%)	$11\pm 3 \ (9\pm 2\%)$	2±1 (2±1%)	13	57
All	All	$2580/2680 \ (96\%)$	2316 (90%)	223 (9%)	41 (2%)	13	57

All 19 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	84	VAL	6
1	A	58	SER	4
1	A	13	SER	4
1	A	14	ARG	4
1	A	17	MET	3
1	A	79	LEU	2
1	A	10	ARG	2
1	A	39	SER	2
1	A	40	SER	2
1	A	85	ASN	2
1	A	80	CYS	2
1	A	65	ILE	1
1	A	16	GLN	1
1	A	103	ASP	1
1	A	38	GLU	1
1	A	9	LYS	1
1	A	11	ASN	1
1	A	62	SER	1
1	A	15	SER	1

5.2.2 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 PDB entries followed by that with respect to all NMR entries. 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	113/115 (98%)	104±2 (92±2%)	9±2 (8±2%)	16 64		
All	All	$2260/2300 \ (98\%)$	2086 (92%)	174 (8%)	16 64		

All 33 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	75	VAL	19
1	A	50	MET	18
1	A	86	LEU	14
1	A	19	GLU	13
1	A	17	MET	13
1	A	58	SER	12
1	A	61	THR	12
1	A	23	LYS	11
1	A	1	MET	6
1	A	11	ASN	5
1	A	63	ASP	5
1	A	12	SER	5
1	A	60	GLN	4
1	A	14	ARG	4
1	A	98	ASP	3
1	A	41	ARG	3
1	A	15	SER	3
1	A	16	GLN	3
1	A	56	ASP	2
1	A	79	LEU	2
1	A	43	HIS	2
1	A	101	LEU	2
1	A	80	CYS	2
1	A	103	ASP	2
1	A	99	TRP	1
1	A	8	CYS	1
1	A	91	VAL	1
1	A	57	ILE	1
1	A	35	SER	1
1	A	110	GLU	1
1	A	113	ARG	1
1	A	42	VAL	1
1	A	21	PHE	1



5.2.3 RNA (i)

There are no RNA molecules in this entry.

5.3 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.4 Carbohydrates (i)

There are no carbohydrates in this entry.

5.5 Ligand geometry (i)

There are no ligands in this entry.

5.6 Other polymers (i)

There are no such molecules in this entry.

5.7 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Chemical shift validation (i)

No chemical shift data were provided

