Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2020 – 02:11 PM BST

PDB ID	:	4B68
Title	:	A. fumigatus ornithine hydroxylase (SidA), re-oxidised state bound to NADP and Arg
Authors	:	Franceschini, S.; Fedkenheuer, M.; Vogelaar, N.J.; Robinson, H.H.; Sobrado, P.; Mattevi, A.
Deposited on	:	2012-08-09
Resolution	:	2.29 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 ⓘ symbol.

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

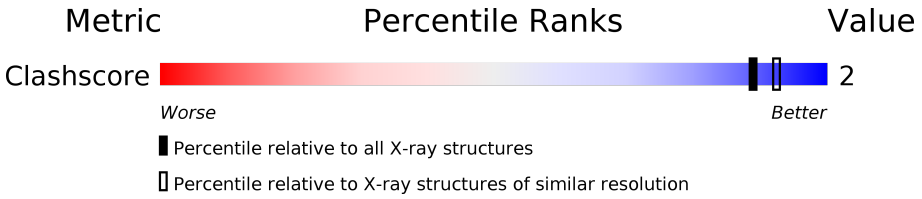
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.4.dev1

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 2.29 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))
Clashscore	141614	5643 (2.30-2.30)

2 Entry composition

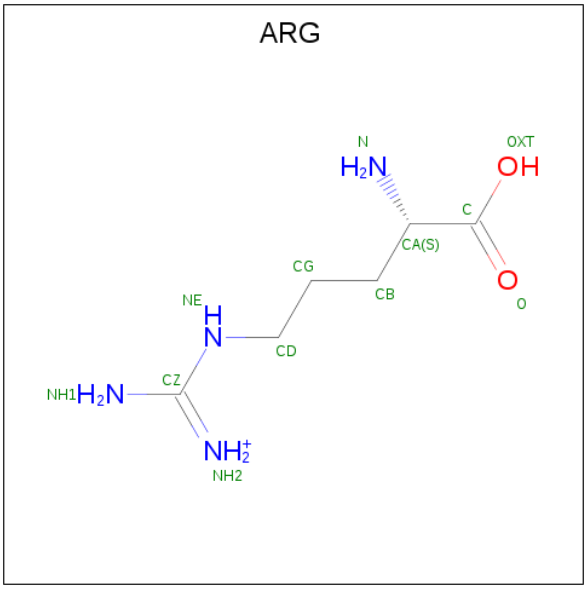
There are 7 unique types of molecules in this entry. The entry contains 3977 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 L-ORNITHINE N5 MONOOXYGENASE.

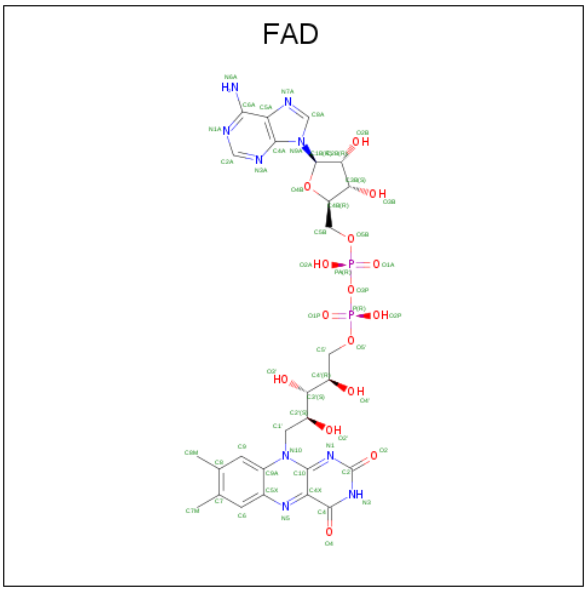
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	454	Total	C	N	O	S	0	4	0
			3576	2255	635	669	17			

- Molecule 2 is ARGININE (three-letter code: ARG) (formula: $C_6H_{15}N_4O_2$).



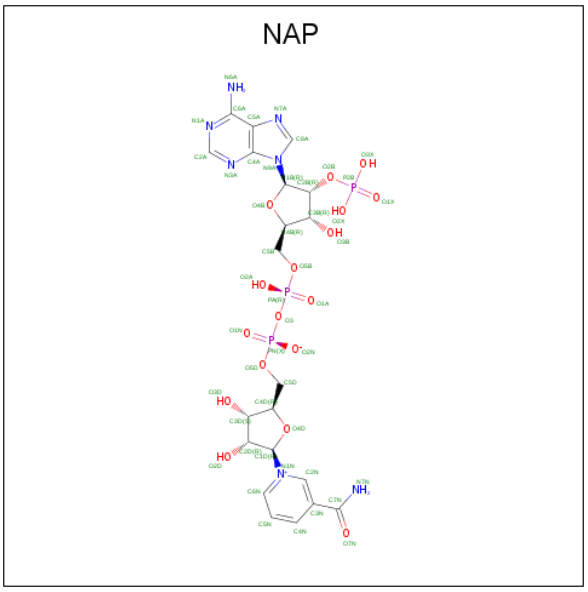
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			12	6	4	2		

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



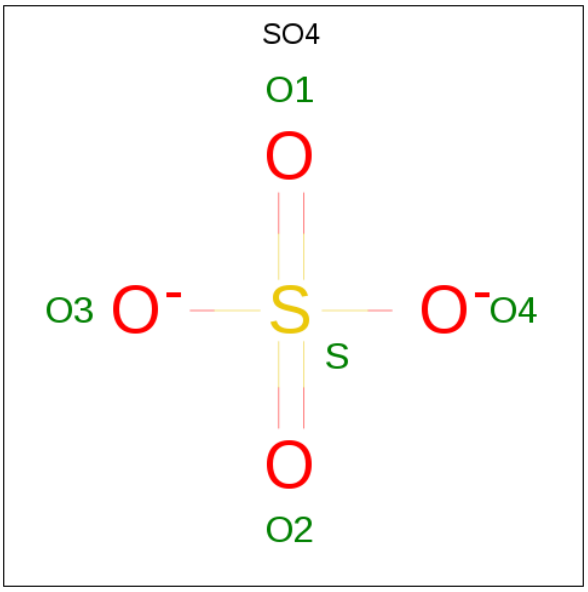
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 4 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



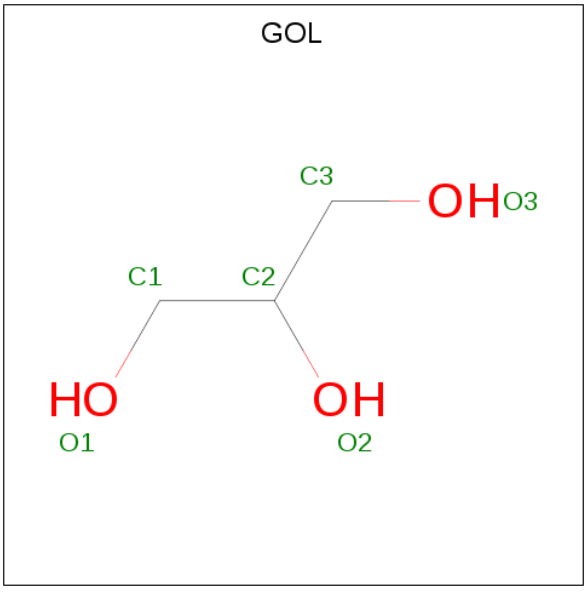
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O S 5 4 1	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	247	Total O 247 247	0	0

SEQUENCE-PLOTS INFOmissingINFO

3 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	77.53Å 84.73Å 145.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	68.39 – 2.29	Depositor
% Data completeness (in resolution range)	92.2 (68.39-2.29)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.95 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.6.0119	Depositor
R, R_{free}	0.217 , 0.269	Depositor
Wilson B-factor (Å^2)	25.8	Xtriage
Anisotropy	0.985	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3977	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.47% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical 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.

4 Model quality

4.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, NAP, SO4, 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	0.43	0/3666	0.48	0/4969

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

4.2 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	3576	0	3491	13	0
2	A	12	0	12	0	0
3	A	53	0	31	1	0
4	A	48	0	25	0	0
5	A	5	0	0	0	0
6	A	36	0	48	2	0
7	A	247	0	0	0	0
All	All	3977	0	3607	14	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 2.

All (14) 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:419:VAL:HG23	1:A:422:LEU:HD12	1.70	0.73
1:A:409:ARG:HH21	6:A:1500:GOL:H31	1.62	0.64
1:A:328:ARG:NH1	1:A:330:GLU:OE1	2.42	0.52
1:A:42:LEU:HD11	1:A:207:VAL:HG23	1.94	0.49
1:A:43:LEU:HD22	1:A:80:CYS:HB3	1.95	0.47
3:A:1492:FAD:O2'	6:A:1500:GOL:H32	2.14	0.47
1:A:375:ARG:HG3	1:A:397:GLU:HG2	1.97	0.46
1:A:103:ILE:HD11	1:A:107:LYS:HD2	1.96	0.46
1:A:74:HIS:CD2	1:A:74:HIS:H	2.34	0.46
1:A:81:PHE:HB2	1:A:162:VAL:HG22	1.99	0.44
1:A:419:VAL:O	1:A:419:VAL:HG22	2.17	0.44
1:A:285:PRO:HA	1:A:327:VAL:O	2.17	0.44
1:A:74:HIS:CG	1:A:75:ALA:H	2.38	0.42
1:A:102:GLN:HE22	1:A:328:ARG:HB2	1.85	0.41

There are no symmetry-related clashes.

4.3 Torsion angles

4.3.1 Protein backbone

There are no protein backbone outliers to report in this entry.

4.3.2 Protein sidechains

There are no protein residues with a non-rotameric sidechain to report in this entry.

4.3.3 RNA

There are no RNA molecules in this entry.

4.4 Non-standard residues in protein, DNA, RNA chains

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

4.5 Carbohydrates

There are no monosaccharides in this entry.

4.6 Ligand geometry (i)

10 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	$\#\|Z\| > 2$
6	GOL	A	1498	-	5,5,5	0.24	0	5,5,5	0.30	0
6	GOL	A	1497	-	5,5,5	0.43	0	5,5,5	0.24	0
6	GOL	A	1500	-	5,5,5	0.28	0	5,5,5	0.28	0
6	GOL	A	1495	-	5,5,5	0.31	0	5,5,5	0.26	0
6	GOL	A	1499	-	5,5,5	0.32	0	5,5,5	0.29	0
2	ARG	A	503	-	7,11,11	0.57	0	6,13,13	0.34	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
6	GOL	A	1498	-	-	0/4/4/4	-
6	GOL	A	1497	-	-	3/4/4/4	-
6	GOL	A	1500	-	-	0/4/4/4	-
6	GOL	A	1495	-	-	2/4/4/4	-
6	GOL	A	1499	-	-	1/4/4/4	-
2	ARG	A	503	-	-	0/7/11/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1497	GOL	C1-C2-C3-O3
6	A	1497	GOL	O2-C2-C3-O3
6	A	1495	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
6	A	1495	GOL	O2-C2-C3-O3
6	A	1497	GOL	O1-C1-C2-O2
6	A	1499	GOL	O1-C1-C2-C3

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1500	GOL	2	0

4.7 Other polymers

There are no such residues in this entry.

4.8 Polymer linkage issues

There are no chain breaks in this entry.

5 Fit of model and data

5.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

5.2 Non-standard residues in protein, DNA, RNA chains

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

5.4 Ligands

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers

EDS failed to run properly - this section is therefore empty.