

# wwPDB X-ray Structure Validation Summary Report (i)

#### May 1, 2024 – 01:46 am BST

PDB ID : 8QQ7

Title : Structure of SpNOX: a Bacterial NADPH oxidase

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Deposited on : 2023-10-04

Resolution : 3.62 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
A user guide is available at

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

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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

MolProbity: 4.02b-467

Mogul : 1.8.4, CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : 2.36.2buster-report : 1.1.7 (2018)

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

Refmac : 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) : 2.36.2

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## 1 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3404 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.

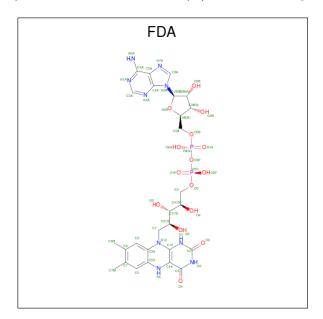
• Molecule 1 is a protein called FAD-binding FR-type domain-containing protein.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Λ	399	Total	С	N	О	S	0	0	0
1	A	399	3265	2167	531	555	12	U		0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference	
A	397	TRP	PHE	engineered mutation	UNP Q8CZ28	

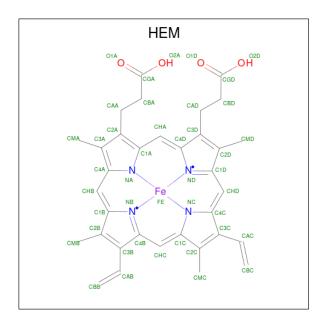
• Molecule 2 is DIHYDROFLAVINE-ADENINE DINUCLEOTIDE (three-letter code: FDA) (formula:  $C_{27}H_{35}N_9O_{15}P_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 53	C 27			P 2	0	0

• Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ) (labeled as "Ligand of Interest" by depositor).





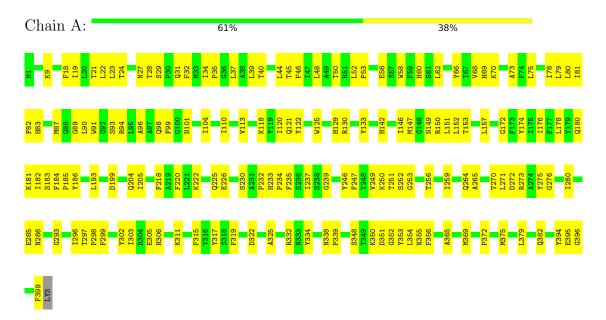
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
2	Λ	1	Total	С	Fe	N	О	0	0	
3	A	1	43	34	1	4	4			
9	Λ	1	Total	С	Fe	N	О	0	0	
3	A	1	43	34	1	4	4	U	U	



# 2 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. 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. 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: FAD-binding FR-type domain-containing protein





# 3 Data and refinement statistics (i)

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants	145.97Å 145.97Å 153.62Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $120.00^{\circ}$	Depositor
Resolution (Å)	47.82 - 3.62	Depositor
Resolution (A)	47.78 - 3.62	EDS
% Data completeness	47.9 (47.82-3.62)	Depositor
(in resolution range)	47.8 (47.78-3.62)	EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.28 (at 3.67Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
D D.	0.262 , 0.320	Depositor
$R, R_{free}$	0.329 , $0.330$	DCC
$R_{free}$ test set	545 reflections (9.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	178.1	Xtriage
Anisotropy	0.122	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.32, 279.8	EDS
L-test for twinning <sup>2</sup>	$ < L > = 0.49, < L^2> = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	3404	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	196.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.66% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

## 4 Model quality (i)

### 4.1 Standard geometry (i)

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

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		
		Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
ſ	1	A	0.37	0/3362	0.85	0/4552	

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 (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	3265	0	3287	201	0
2	A	53	0	33	19	0
3	A	86	0	60	64	0
All	All	3404	0	3380	219	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 32.

The worst 5 of 219 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} \text{Interatomic} \\ \text{distance (Å)} \end{array}$	Clash overlap (Å)
1:A:45:THR:HG21	3:A:1002:HEM:CMC	1.71	1.19

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Atom-1	Atom-2	$egin{aligned} &  ext{Interatomic} \ &  ext{distance} \ &  ext{(Å)} \end{aligned}$	$egin{aligned} \operatorname{Clash} \ \operatorname{overlap}\ (\mathring{\mathbf{A}}) \end{aligned}$
1:A:296:ILE:HD12	1:A:317:TYR:CD2	1.77	1.17
1:A:45:THR:HG21	3:A:1002:HEM:HMC3	1.11	1.07
1:A:101:ASN:HA	3:A:1001:HEM:CBB	1.92	0.99
1:A:125:TRP:HZ2	3:A:1002:HEM:C4A	1.81	0.97

There are no symmetry-related clashes.

#### 4.3 Torsion angles (i)

#### 4.3.1 Protein backbone (i)

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

#### 4.3.2 Protein sidechains (i)

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

#### 4.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

### 4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

#### 4.6 Ligand geometry (i)

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	Bo	ond leng	ths	В	ond ang	gles
MIOI			ites	Lilik	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	HEM	A	1002	1	41,50,50	1.44	7 (17%)	45,82,82	1.85	14 (31%)
3	HEM	A	1001	1	41,50,50	1.45	7 (17%)	45,82,82	1.85	14 (31%)
2	FDA	A	1000	-	52,58,58	0.83	2 (3%)	60,89,89	1.04	6 (10%)

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
3	HEM	A	1002	1	-	5/12/54/54	-
3	HEM	A	1001	1	-	3/12/54/54	-
2	FDA	A	1000	-	-	16/30/50/50	0/6/6/6

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\operatorname{Observed}(\mathring{A})$	Ideal(Å)
3	A	1001	HEM	C1B-NB	-3.93	1.33	1.40
3	A	1002	HEM	C1B-NB	-3.92	1.33	1.40
2	A	1000	FDA	C10-N1	-3.03	1.31	1.37
3	A	1001	HEM	C4D-C3D	2.79	1.49	1.45
3	A	1002	HEM	C4D-C3D	2.77	1.49	1.45

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
3	A	1001	HEM	C1B-NB-C4B	4.88	110.12	105.07
3	A	1002	HEM	C1B-NB-C4B	4.85	110.08	105.07
3	A	1002	HEM	CBA-CAA-C2A	-4.28	105.32	112.62
3	A	1001	HEM	CBA-CAA-C2A	-4.27	105.33	112.62
3	A	1001	HEM	CHC-C4B-NB	3.86	128.62	124.43

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1000	FDA	C5B-O5B-PA-O1A

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Mol	Chain	Res	Type	Atoms
2	A	1000	FDA	C5B-O5B-PA-O2A
2	A	1000	FDA	C5B-O5B-PA-O3P
2	A	1000	FDA	N10-C1'-C2'-O2'
2	A	1000	FDA	N10-C1'-C2'-C3'

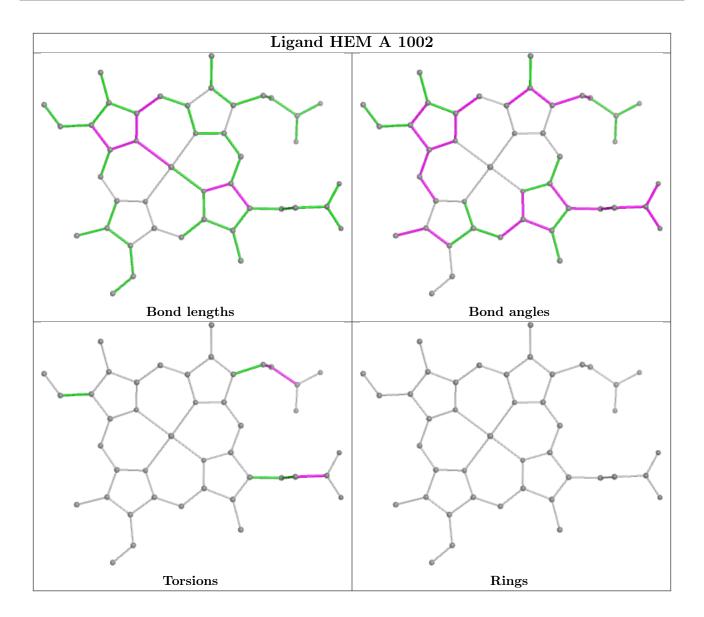
There are no ring outliers.

3 monomers are involved in 83 short contacts:

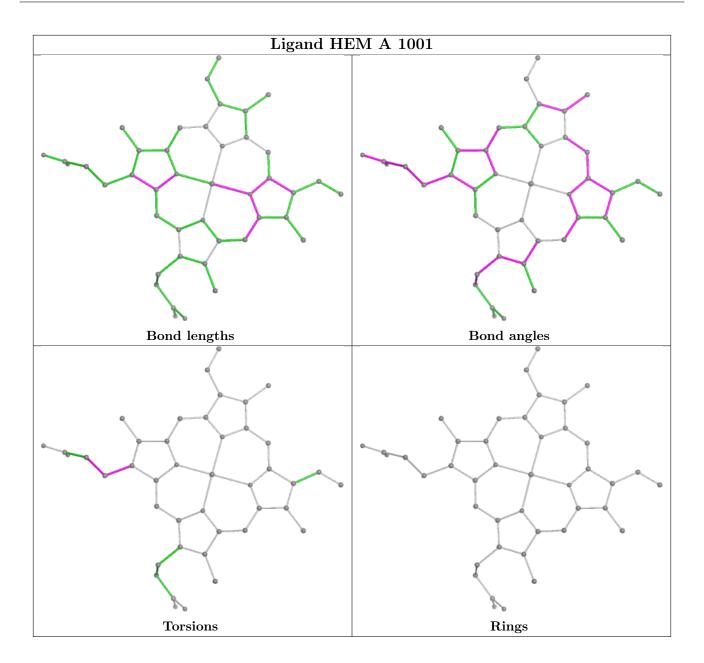
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1002	HEM	30	0
3	A	1001	HEM	34	0
2	A	1000	FDA	19	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

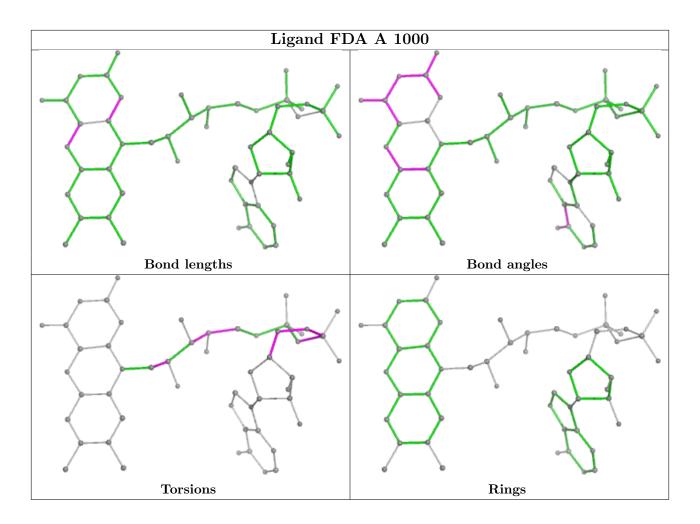












## 4.7 Other polymers (i)

There are no such residues in this entry.

## 4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



# 5 Fit of model and data (i)

#### 5.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 5.3 Carbohydrates (i)

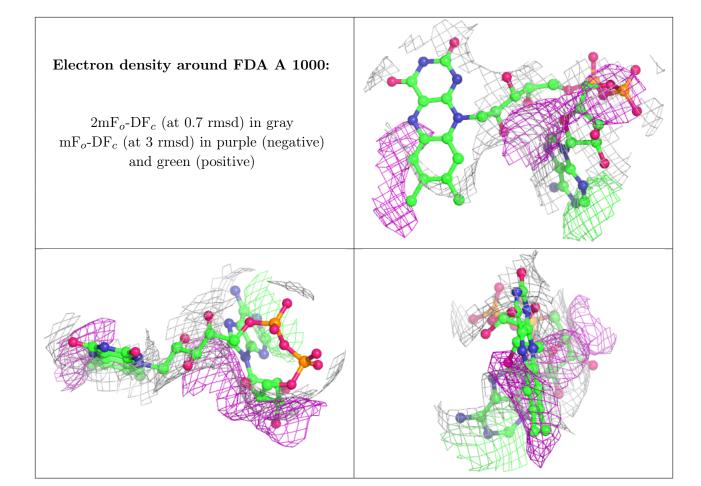
Unable to reproduce the depositors R factor - this section is therefore empty.

#### 5.4 Ligands (i)

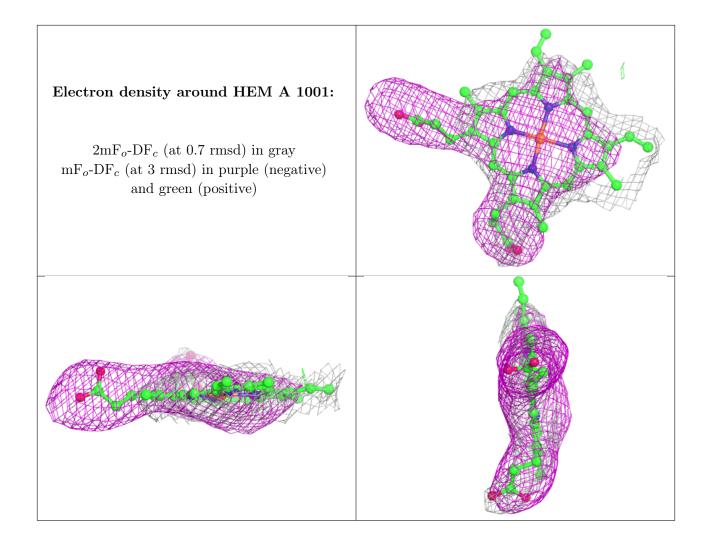
Unable to reproduce the depositors R factor - this section is therefore empty.

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.

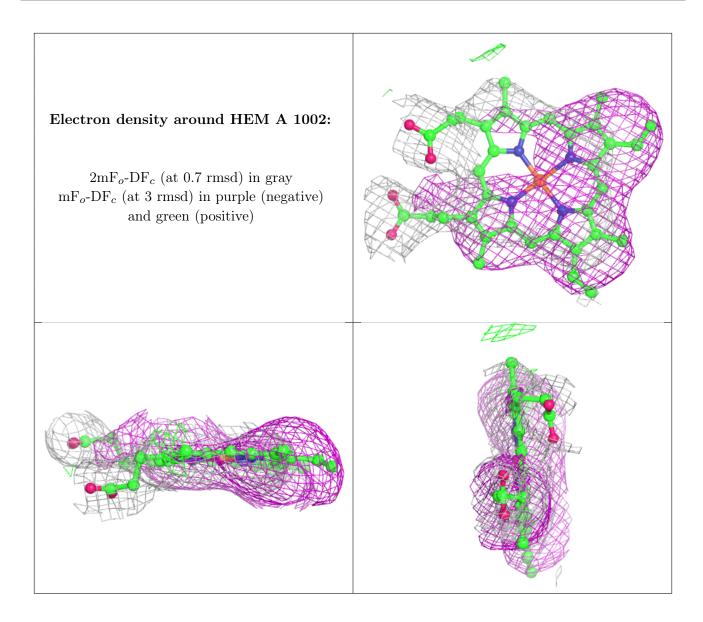












## 5.5 Other polymers (i)

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