



wwPDB X-ray Structure Validation Summary Report ⓘ

May 2, 2016 – 06:13 PM EDT

PDB ID : 5ER0
Title : Water-forming NADH oxidase from Lactobacillus brevis (LbNOX)
Authors : Cracan, V.; Grabarek, Z.
Deposited on : 2015-11-13
Resolution : 2.41 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
<http://wwpdb.org/validation/2016/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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027457
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : rb-20027457

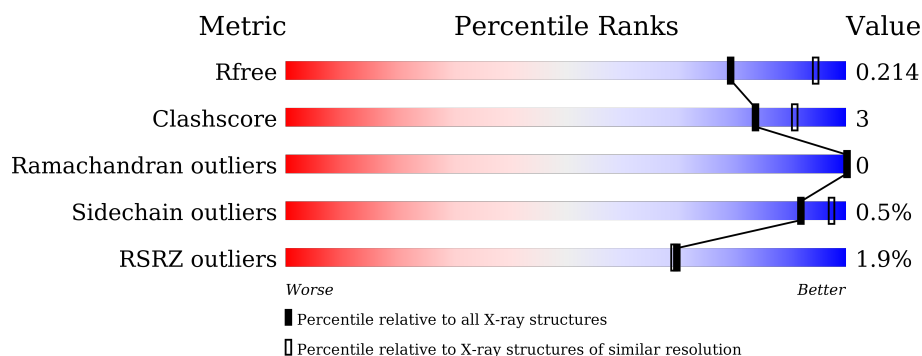
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.41 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}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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. 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	518	<div> <div>2%</div> <div>80% 7% 13%</div> </div>
1	B	518	<div> <div>2%</div> <div>80% 6% 13%</div> </div>
1	C	518	<div> <div>2%</div> <div>79% 8% 13%</div> </div>
1	D	518	<div> <div>2%</div> <div>80% 7% 13%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	OXY	A	502	-	-	-	X
3	OXY	B	502	-	-	-	X
3	OXY	C	502	-	-	-	X
3	OXY	D	502	-	-	-	X
4	EDO	C	503	-	-	-	X
4	EDO	D	506	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14950 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 NADH oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	450	Total	C	N	O	S	0	0	0
			3434	2160	574	682	18			
1	B	450	Total	C	N	O	S	0	0	0
			3434	2160	574	682	18			
1	C	450	Total	C	N	O	S	0	0	0
			3434	2160	574	682	18			
1	D	450	Total	C	N	O	S	0	0	0
			3434	2160	574	682	18			

There are 272 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-49	MET	-	initiating methionine	UNP M5B0V2
A	-48	HIS	-	expression tag	UNP M5B0V2
A	-47	HIS	-	expression tag	UNP M5B0V2
A	-46	HIS	-	expression tag	UNP M5B0V2
A	-45	HIS	-	expression tag	UNP M5B0V2
A	-44	HIS	-	expression tag	UNP M5B0V2
A	-43	HIS	-	expression tag	UNP M5B0V2
A	-42	SER	-	expression tag	UNP M5B0V2
A	-41	SER	-	expression tag	UNP M5B0V2
A	-40	GLY	-	expression tag	UNP M5B0V2
A	-39	LEU	-	expression tag	UNP M5B0V2
A	-38	VAL	-	expression tag	UNP M5B0V2
A	-37	PRO	-	expression tag	UNP M5B0V2
A	-36	ARG	-	expression tag	UNP M5B0V2
A	-35	GLY	-	expression tag	UNP M5B0V2
A	-34	SER	-	expression tag	UNP M5B0V2
A	-33	GLY	-	expression tag	UNP M5B0V2
A	-32	MET	-	expression tag	UNP M5B0V2
A	-31	LYS	-	expression tag	UNP M5B0V2
A	-30	GLU	-	expression tag	UNP M5B0V2
A	-29	THR	-	expression tag	UNP M5B0V2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-28	ALA	-	expression tag	UNP M5B0V2
A	-27	ALA	-	expression tag	UNP M5B0V2
A	-26	ALA	-	expression tag	UNP M5B0V2
A	-25	LYS	-	expression tag	UNP M5B0V2
A	-24	PHE	-	expression tag	UNP M5B0V2
A	-23	GLU	-	expression tag	UNP M5B0V2
A	-22	ARG	-	expression tag	UNP M5B0V2
A	-21	GLN	-	expression tag	UNP M5B0V2
A	-20	HIS	-	expression tag	UNP M5B0V2
A	-19	MET	-	expression tag	UNP M5B0V2
A	-18	ASP	-	expression tag	UNP M5B0V2
A	-17	SER	-	expression tag	UNP M5B0V2
A	-16	PRO	-	expression tag	UNP M5B0V2
A	-15	ASP	-	expression tag	UNP M5B0V2
A	-14	LEU	-	expression tag	UNP M5B0V2
A	-13	GLY	-	expression tag	UNP M5B0V2
A	-12	THR	-	expression tag	UNP M5B0V2
A	-11	ASP	-	expression tag	UNP M5B0V2
A	-10	ASP	-	expression tag	UNP M5B0V2
A	-9	ASP	-	expression tag	UNP M5B0V2
A	-8	ASP	-	expression tag	UNP M5B0V2
A	-7	LYS	-	expression tag	UNP M5B0V2
A	-6	ALA	-	expression tag	UNP M5B0V2
A	-5	MET	-	expression tag	UNP M5B0V2
A	-4	ALA	-	expression tag	UNP M5B0V2
A	-3	ASP	-	expression tag	UNP M5B0V2
A	-2	ILE	-	expression tag	UNP M5B0V2
A	-1	GLY	-	expression tag	UNP M5B0V2
A	0	SER	-	expression tag	UNP M5B0V2
A	451	GLY	-	expression tag	UNP M5B0V2
A	452	GLY	-	expression tag	UNP M5B0V2
A	453	SER	-	expression tag	UNP M5B0V2
A	454	GLY	-	expression tag	UNP M5B0V2
A	455	GLY	-	expression tag	UNP M5B0V2
A	456	SER	-	expression tag	UNP M5B0V2
A	457	GLY	-	expression tag	UNP M5B0V2
A	458	GLY	-	expression tag	UNP M5B0V2
A	459	SER	-	expression tag	UNP M5B0V2
A	460	MET	-	expression tag	UNP M5B0V2
A	461	ASP	-	expression tag	UNP M5B0V2
A	462	TYR	-	expression tag	UNP M5B0V2
A	463	LYS	-	expression tag	UNP M5B0V2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	464	ASP	-	expression tag	UNP M5B0V2
A	465	ASP	-	expression tag	UNP M5B0V2
A	466	ASP	-	expression tag	UNP M5B0V2
A	467	ASP	-	expression tag	UNP M5B0V2
A	468	LYS	-	expression tag	UNP M5B0V2
B	-49	MET	-	initiating methionine	UNP M5B0V2
B	-48	HIS	-	expression tag	UNP M5B0V2
B	-47	HIS	-	expression tag	UNP M5B0V2
B	-46	HIS	-	expression tag	UNP M5B0V2
B	-45	HIS	-	expression tag	UNP M5B0V2
B	-44	HIS	-	expression tag	UNP M5B0V2
B	-43	HIS	-	expression tag	UNP M5B0V2
B	-42	SER	-	expression tag	UNP M5B0V2
B	-41	SER	-	expression tag	UNP M5B0V2
B	-40	GLY	-	expression tag	UNP M5B0V2
B	-39	LEU	-	expression tag	UNP M5B0V2
B	-38	VAL	-	expression tag	UNP M5B0V2
B	-37	PRO	-	expression tag	UNP M5B0V2
B	-36	ARG	-	expression tag	UNP M5B0V2
B	-35	GLY	-	expression tag	UNP M5B0V2
B	-34	SER	-	expression tag	UNP M5B0V2
B	-33	GLY	-	expression tag	UNP M5B0V2
B	-32	MET	-	expression tag	UNP M5B0V2
B	-31	LYS	-	expression tag	UNP M5B0V2
B	-30	GLU	-	expression tag	UNP M5B0V2
B	-29	THR	-	expression tag	UNP M5B0V2
B	-28	ALA	-	expression tag	UNP M5B0V2
B	-27	ALA	-	expression tag	UNP M5B0V2
B	-26	ALA	-	expression tag	UNP M5B0V2
B	-25	LYS	-	expression tag	UNP M5B0V2
B	-24	PHE	-	expression tag	UNP M5B0V2
B	-23	GLU	-	expression tag	UNP M5B0V2
B	-22	ARG	-	expression tag	UNP M5B0V2
B	-21	GLN	-	expression tag	UNP M5B0V2
B	-20	HIS	-	expression tag	UNP M5B0V2
B	-19	MET	-	expression tag	UNP M5B0V2
B	-18	ASP	-	expression tag	UNP M5B0V2
B	-17	SER	-	expression tag	UNP M5B0V2
B	-16	PRO	-	expression tag	UNP M5B0V2
B	-15	ASP	-	expression tag	UNP M5B0V2
B	-14	LEU	-	expression tag	UNP M5B0V2
B	-13	GLY	-	expression tag	UNP M5B0V2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-12	THR	-	expression tag	UNP M5B0V2
B	-11	ASP	-	expression tag	UNP M5B0V2
B	-10	ASP	-	expression tag	UNP M5B0V2
B	-9	ASP	-	expression tag	UNP M5B0V2
B	-8	ASP	-	expression tag	UNP M5B0V2
B	-7	LYS	-	expression tag	UNP M5B0V2
B	-6	ALA	-	expression tag	UNP M5B0V2
B	-5	MET	-	expression tag	UNP M5B0V2
B	-4	ALA	-	expression tag	UNP M5B0V2
B	-3	ASP	-	expression tag	UNP M5B0V2
B	-2	ILE	-	expression tag	UNP M5B0V2
B	-1	GLY	-	expression tag	UNP M5B0V2
B	0	SER	-	expression tag	UNP M5B0V2
B	451	GLY	-	expression tag	UNP M5B0V2
B	452	GLY	-	expression tag	UNP M5B0V2
B	453	SER	-	expression tag	UNP M5B0V2
B	454	GLY	-	expression tag	UNP M5B0V2
B	455	GLY	-	expression tag	UNP M5B0V2
B	456	SER	-	expression tag	UNP M5B0V2
B	457	GLY	-	expression tag	UNP M5B0V2
B	458	GLY	-	expression tag	UNP M5B0V2
B	459	SER	-	expression tag	UNP M5B0V2
B	460	MET	-	expression tag	UNP M5B0V2
B	461	ASP	-	expression tag	UNP M5B0V2
B	462	TYR	-	expression tag	UNP M5B0V2
B	463	LYS	-	expression tag	UNP M5B0V2
B	464	ASP	-	expression tag	UNP M5B0V2
B	465	ASP	-	expression tag	UNP M5B0V2
B	466	ASP	-	expression tag	UNP M5B0V2
B	467	ASP	-	expression tag	UNP M5B0V2
B	468	LYS	-	expression tag	UNP M5B0V2
C	-49	MET	-	initiating methionine	UNP M5B0V2
C	-48	HIS	-	expression tag	UNP M5B0V2
C	-47	HIS	-	expression tag	UNP M5B0V2
C	-46	HIS	-	expression tag	UNP M5B0V2
C	-45	HIS	-	expression tag	UNP M5B0V2
C	-44	HIS	-	expression tag	UNP M5B0V2
C	-43	HIS	-	expression tag	UNP M5B0V2
C	-42	SER	-	expression tag	UNP M5B0V2
C	-41	SER	-	expression tag	UNP M5B0V2
C	-40	GLY	-	expression tag	UNP M5B0V2
C	-39	LEU	-	expression tag	UNP M5B0V2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-38	VAL	-	expression tag	UNP M5B0V2
C	-37	PRO	-	expression tag	UNP M5B0V2
C	-36	ARG	-	expression tag	UNP M5B0V2
C	-35	GLY	-	expression tag	UNP M5B0V2
C	-34	SER	-	expression tag	UNP M5B0V2
C	-33	GLY	-	expression tag	UNP M5B0V2
C	-32	MET	-	expression tag	UNP M5B0V2
C	-31	LYS	-	expression tag	UNP M5B0V2
C	-30	GLU	-	expression tag	UNP M5B0V2
C	-29	THR	-	expression tag	UNP M5B0V2
C	-28	ALA	-	expression tag	UNP M5B0V2
C	-27	ALA	-	expression tag	UNP M5B0V2
C	-26	ALA	-	expression tag	UNP M5B0V2
C	-25	LYS	-	expression tag	UNP M5B0V2
C	-24	PHE	-	expression tag	UNP M5B0V2
C	-23	GLU	-	expression tag	UNP M5B0V2
C	-22	ARG	-	expression tag	UNP M5B0V2
C	-21	GLN	-	expression tag	UNP M5B0V2
C	-20	HIS	-	expression tag	UNP M5B0V2
C	-19	MET	-	expression tag	UNP M5B0V2
C	-18	ASP	-	expression tag	UNP M5B0V2
C	-17	SER	-	expression tag	UNP M5B0V2
C	-16	PRO	-	expression tag	UNP M5B0V2
C	-15	ASP	-	expression tag	UNP M5B0V2
C	-14	LEU	-	expression tag	UNP M5B0V2
C	-13	GLY	-	expression tag	UNP M5B0V2
C	-12	THR	-	expression tag	UNP M5B0V2
C	-11	ASP	-	expression tag	UNP M5B0V2
C	-10	ASP	-	expression tag	UNP M5B0V2
C	-9	ASP	-	expression tag	UNP M5B0V2
C	-8	ASP	-	expression tag	UNP M5B0V2
C	-7	LYS	-	expression tag	UNP M5B0V2
C	-6	ALA	-	expression tag	UNP M5B0V2
C	-5	MET	-	expression tag	UNP M5B0V2
C	-4	ALA	-	expression tag	UNP M5B0V2
C	-3	ASP	-	expression tag	UNP M5B0V2
C	-2	ILE	-	expression tag	UNP M5B0V2
C	-1	GLY	-	expression tag	UNP M5B0V2
C	0	SER	-	expression tag	UNP M5B0V2
C	451	GLY	-	expression tag	UNP M5B0V2
C	452	GLY	-	expression tag	UNP M5B0V2
C	453	SER	-	expression tag	UNP M5B0V2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	454	GLY	-	expression tag	UNP M5B0V2
C	455	GLY	-	expression tag	UNP M5B0V2
C	456	SER	-	expression tag	UNP M5B0V2
C	457	GLY	-	expression tag	UNP M5B0V2
C	458	GLY	-	expression tag	UNP M5B0V2
C	459	SER	-	expression tag	UNP M5B0V2
C	460	MET	-	expression tag	UNP M5B0V2
C	461	ASP	-	expression tag	UNP M5B0V2
C	462	TYR	-	expression tag	UNP M5B0V2
C	463	LYS	-	expression tag	UNP M5B0V2
C	464	ASP	-	expression tag	UNP M5B0V2
C	465	ASP	-	expression tag	UNP M5B0V2
C	466	ASP	-	expression tag	UNP M5B0V2
C	467	ASP	-	expression tag	UNP M5B0V2
C	468	LYS	-	expression tag	UNP M5B0V2
D	-49	MET	-	initiating methionine	UNP M5B0V2
D	-48	HIS	-	expression tag	UNP M5B0V2
D	-47	HIS	-	expression tag	UNP M5B0V2
D	-46	HIS	-	expression tag	UNP M5B0V2
D	-45	HIS	-	expression tag	UNP M5B0V2
D	-44	HIS	-	expression tag	UNP M5B0V2
D	-43	HIS	-	expression tag	UNP M5B0V2
D	-42	SER	-	expression tag	UNP M5B0V2
D	-41	SER	-	expression tag	UNP M5B0V2
D	-40	GLY	-	expression tag	UNP M5B0V2
D	-39	LEU	-	expression tag	UNP M5B0V2
D	-38	VAL	-	expression tag	UNP M5B0V2
D	-37	PRO	-	expression tag	UNP M5B0V2
D	-36	ARG	-	expression tag	UNP M5B0V2
D	-35	GLY	-	expression tag	UNP M5B0V2
D	-34	SER	-	expression tag	UNP M5B0V2
D	-33	GLY	-	expression tag	UNP M5B0V2
D	-32	MET	-	expression tag	UNP M5B0V2
D	-31	LYS	-	expression tag	UNP M5B0V2
D	-30	GLU	-	expression tag	UNP M5B0V2
D	-29	THR	-	expression tag	UNP M5B0V2
D	-28	ALA	-	expression tag	UNP M5B0V2
D	-27	ALA	-	expression tag	UNP M5B0V2
D	-26	ALA	-	expression tag	UNP M5B0V2
D	-25	LYS	-	expression tag	UNP M5B0V2
D	-24	PHE	-	expression tag	UNP M5B0V2
D	-23	GLU	-	expression tag	UNP M5B0V2

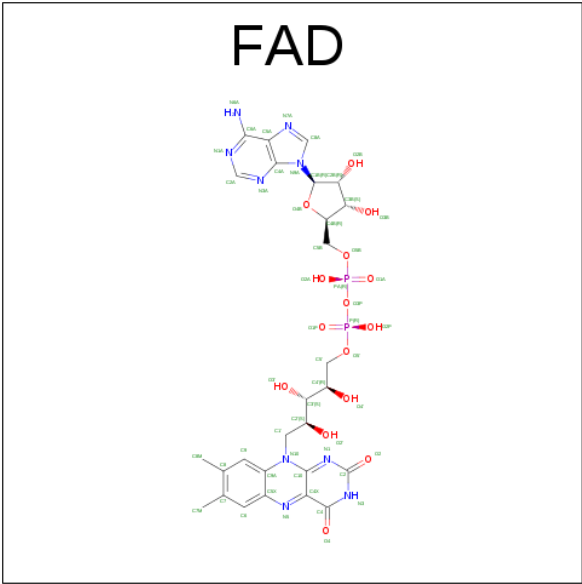
Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	-22	ARG	-	expression tag	UNP M5B0V2
D	-21	GLN	-	expression tag	UNP M5B0V2
D	-20	HIS	-	expression tag	UNP M5B0V2
D	-19	MET	-	expression tag	UNP M5B0V2
D	-18	ASP	-	expression tag	UNP M5B0V2
D	-17	SER	-	expression tag	UNP M5B0V2
D	-16	PRO	-	expression tag	UNP M5B0V2
D	-15	ASP	-	expression tag	UNP M5B0V2
D	-14	LEU	-	expression tag	UNP M5B0V2
D	-13	GLY	-	expression tag	UNP M5B0V2
D	-12	THR	-	expression tag	UNP M5B0V2
D	-11	ASP	-	expression tag	UNP M5B0V2
D	-10	ASP	-	expression tag	UNP M5B0V2
D	-9	ASP	-	expression tag	UNP M5B0V2
D	-8	ASP	-	expression tag	UNP M5B0V2
D	-7	LYS	-	expression tag	UNP M5B0V2
D	-6	ALA	-	expression tag	UNP M5B0V2
D	-5	MET	-	expression tag	UNP M5B0V2
D	-4	ALA	-	expression tag	UNP M5B0V2
D	-3	ASP	-	expression tag	UNP M5B0V2
D	-2	ILE	-	expression tag	UNP M5B0V2
D	-1	GLY	-	expression tag	UNP M5B0V2
D	0	SER	-	expression tag	UNP M5B0V2
D	451	GLY	-	expression tag	UNP M5B0V2
D	452	GLY	-	expression tag	UNP M5B0V2
D	453	SER	-	expression tag	UNP M5B0V2
D	454	GLY	-	expression tag	UNP M5B0V2
D	455	GLY	-	expression tag	UNP M5B0V2
D	456	SER	-	expression tag	UNP M5B0V2
D	457	GLY	-	expression tag	UNP M5B0V2
D	458	GLY	-	expression tag	UNP M5B0V2
D	459	SER	-	expression tag	UNP M5B0V2
D	460	MET	-	expression tag	UNP M5B0V2
D	461	ASP	-	expression tag	UNP M5B0V2
D	462	TYR	-	expression tag	UNP M5B0V2
D	463	LYS	-	expression tag	UNP M5B0V2
D	464	ASP	-	expression tag	UNP M5B0V2
D	465	ASP	-	expression tag	UNP M5B0V2
D	466	ASP	-	expression tag	UNP M5B0V2
D	467	ASP	-	expression tag	UNP M5B0V2
D	468	LYS	-	expression tag	UNP M5B0V2

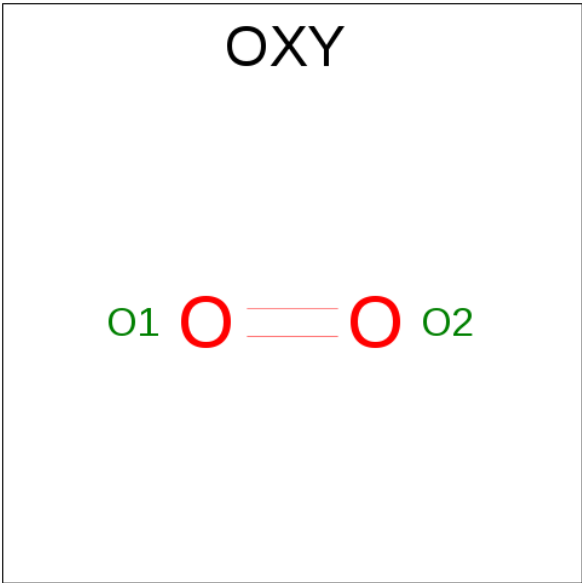
- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:

C₂₇H₃₃N₉O₁₅P₂).



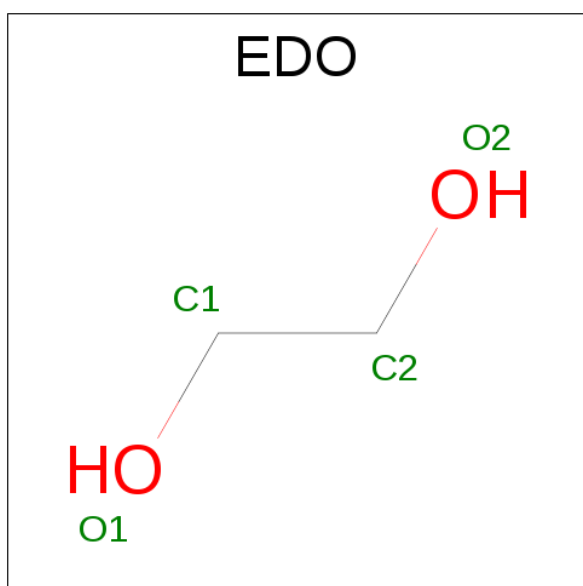
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O 2 2	0	0
3	B	1	Total O 2 2	0	0
3	C	1	Total O 2 2	0	0
3	D	1	Total O 2 2	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0

Continued on next page...

Continued from previous page...

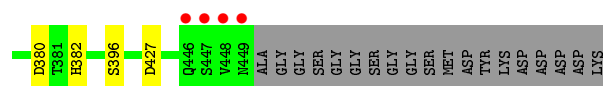
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	255	Total	O	0	0
			255	255		
5	B	264	Total	O	0	0
			264	264		
5	C	192	Total	O	0	0
			192	192		
5	D	235	Total	O	0	0
			235	235		

- Molecule 1: NADH oxidase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	67.97Å 86.35Å 93.33Å 96.92° 94.07° 92.40°	Depositor
Resolution (Å)	48.03 – 2.41 48.03 – 2.41	Depositor EDS
% Data completeness (in resolution range)	98.0 (48.03-2.41) 94.6 (48.03-2.41)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 2.39Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.172 , 0.215 0.171 , 0.214	Depositor DCC
R_{free} test set	4044 reflections (5.07%)	DCC
Wilson B-factor (Å ²)	25.0	Xtriage
Anisotropy	0.486	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 44.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14950	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

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: OXY, FAD, EDO

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	0.24	0/3497	0.44	0/4761
1	B	0.24	0/3497	0.44	0/4761
1	C	0.24	0/3497	0.43	0/4761
1	D	0.24	0/3497	0.43	0/4761
All	All	0.24	0/13988	0.44	0/19044

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3434	0	3389	21	0
1	B	3434	0	3389	22	0
1	C	3434	0	3389	21	0
1	D	3434	0	3389	20	0
2	A	53	0	29	1	0
2	B	53	0	30	1	0
2	C	53	0	29	0	0
2	D	53	0	29	0	0
3	A	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	16	0	24	0	0
4	B	12	0	18	0	0
4	C	4	0	6	0	0
4	D	16	0	24	0	0
5	A	255	0	0	1	0
5	B	264	0	0	3	0
5	C	192	0	0	1	0
5	D	235	0	0	3	0
All	All	14950	0	13745	83	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.

The worst 5 of 83 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:C:157:TYR:HB2	1:C:327:LEU:HD21	1.72	0.71
1:D:294:ILE:HD13	1:D:323:SER:HB2	1.74	0.69
1:A:294:ILE:HD13	1:A:323:SER:HB2	1.75	0.68
1:B:397:GLN:NE2	5:B:602:HOH:O	2.25	0.67
1:C:335:VAL:HG11	1:C:396:SER:HA	1.79	0.65

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	448/518 (86%)	436 (97%)	12 (3%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	448/518 (86%)	432 (96%)	16 (4%)	0	100	100
1	C	448/518 (86%)	436 (97%)	12 (3%)	0	100	100
1	D	448/518 (86%)	433 (97%)	15 (3%)	0	100	100
All	All	1792/2072 (86%)	1737 (97%)	55 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	376/427 (88%)	376 (100%)	0	100	100
1	B	376/427 (88%)	374 (100%)	2 (0%)	92	97
1	C	376/427 (88%)	372 (99%)	4 (1%)	80	92
1	D	376/427 (88%)	374 (100%)	2 (0%)	92	97
All	All	1504/1708 (88%)	1496 (100%)	8 (0%)	92	97

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	232	GLU
1	D	382	HIS
1	C	449	ASN
1	C	220	THR
1	C	447	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	347	GLN
1	D	205	GLN
1	D	289	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	382	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

20 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	$\# Z > 2$
2	FAD	A	501	-	52,58,58	3.97	20 (38%)	52,89,89	2.54	13 (25%)
3	OXY	A	502	-	1,1,1	0.31	0	0,0,0	0.00	-
4	EDO	A	503	-	3,3,3	0.44	0	2,2,2	0.36	0
4	EDO	A	504	-	3,3,3	0.44	0	2,2,2	0.42	0
4	EDO	A	505	-	3,3,3	0.44	0	2,2,2	0.39	0
4	EDO	A	506	-	3,3,3	0.44	0	2,2,2	0.43	0
2	FAD	B	501	-	52,58,58	3.97	20 (38%)	52,89,89	2.54	13 (25%)
3	OXY	B	502	-	1,1,1	0.31	0	0,0,0	0.00	-
4	EDO	B	503	-	3,3,3	0.45	0	2,2,2	0.41	0
4	EDO	B	504	-	3,3,3	0.43	0	2,2,2	0.45	0
4	EDO	B	505	-	3,3,3	0.45	0	2,2,2	0.39	0
2	FAD	C	501	-	52,58,58	3.98	20 (38%)	52,89,89	2.55	13 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OXY	C	502	-	1,1,1	0.31	0	0,0,0	0.00	-
4	EDO	C	503	-	3,3,3	0.44	0	2,2,2	0.40	0
2	FAD	D	501	-	52,58,58	3.98	20 (38%)	52,89,89	2.54	13 (25%)
3	OXY	D	502	-	1,1,1	0.31	0	0,0,0	0.00	-
4	EDO	D	503	-	3,3,3	0.41	0	2,2,2	0.55	0
4	EDO	D	504	-	3,3,3	0.44	0	2,2,2	0.44	0
4	EDO	D	505	-	3,3,3	0.44	0	2,2,2	0.43	0
4	EDO	D	506	-	3,3,3	0.46	0	2,2,2	0.31	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
2	FAD	A	501	-	-	0/30/50/50	0/6/6/6
3	OXY	A	502	-	-	0/0/0/0	0/0/0/0
4	EDO	A	503	-	-	0/1/1/1	0/0/0/0
4	EDO	A	504	-	-	0/1/1/1	0/0/0/0
4	EDO	A	505	-	-	0/1/1/1	0/0/0/0
4	EDO	A	506	-	-	0/1/1/1	0/0/0/0
2	FAD	B	501	-	-	0/30/50/50	0/6/6/6
3	OXY	B	502	-	-	0/0/0/0	0/0/0/0
4	EDO	B	503	-	-	0/1/1/1	0/0/0/0
4	EDO	B	504	-	-	0/1/1/1	0/0/0/0
4	EDO	B	505	-	-	0/1/1/1	0/0/0/0
2	FAD	C	501	-	-	0/30/50/50	0/6/6/6
3	OXY	C	502	-	-	0/0/0/0	0/0/0/0
4	EDO	C	503	-	-	0/1/1/1	0/0/0/0
2	FAD	D	501	-	-	0/30/50/50	0/6/6/6
3	OXY	D	502	-	-	0/0/0/0	0/0/0/0
4	EDO	D	503	-	-	0/1/1/1	0/0/0/0
4	EDO	D	504	-	-	0/1/1/1	0/0/0/0
4	EDO	D	505	-	-	0/1/1/1	0/0/0/0
4	EDO	D	506	-	-	0/1/1/1	0/0/0/0

The worst 5 of 80 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	FAD	C2B-C1B	-16.09	1.28	1.53
2	C	501	FAD	C2B-C1B	-16.06	1.28	1.53
2	D	501	FAD	C2B-C1B	-16.00	1.28	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	FAD	C2B-C1B	-15.98	1.28	1.53
2	C	501	FAD	O4B-C4B	-6.62	1.29	1.45

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	FAD	N3A-C2A-N1A	-11.56	119.79	128.87
2	A	501	FAD	N3A-C2A-N1A	-11.49	119.85	128.87
2	C	501	FAD	N3A-C2A-N1A	-11.46	119.87	128.87
2	D	501	FAD	N3A-C2A-N1A	-11.45	119.87	128.87
2	D	501	FAD	N6A-C6A-N1A	-7.37	106.16	118.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	FAD	1	0
2	B	501	FAD	1	0

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, 95th 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 ²)	Q<0.9
1	A	450/518 (86%)	-0.33	7 (1%) 74 74	12, 25, 42, 68	0
1	B	450/518 (86%)	-0.26	7 (1%) 74 74	15, 25, 43, 76	0
1	C	450/518 (86%)	-0.18	10 (2%) 65 64	16, 30, 52, 75	0
1	D	450/518 (86%)	-0.30	10 (2%) 65 64	17, 26, 48, 83	0
All	All	1800/2072 (86%)	-0.27	34 (1%) 70 69	12, 26, 47, 83	0

The worst 5 of 34 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	449	ASN	4.5
1	C	449	ASN	4.4
1	C	220	THR	4.3
1	B	449	ASN	4.2
1	B	448	VAL	3.7

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](#)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	LLDF	B-factors(Å ²)	Q<0.9
4	EDO	C	503	4/4	0.89	0.22	4.84	34,35,37,50	0
3	OXY	B	502	2/2	1.00	0.21	4.65	16,16,16,16	0
4	EDO	D	506	4/4	0.82	0.22	4.01	26,33,33,37	0
3	OXY	D	502	2/2	0.98	0.16	3.21	17,17,17,17	0
3	OXY	A	502	2/2	0.99	0.15	3.16	22,22,22,22	0
3	OXY	C	502	2/2	0.99	0.17	2.66	24,24,24,27	0
4	EDO	B	505	4/4	0.92	0.16	1.42	28,31,31,45	0
4	EDO	A	506	4/4	0.94	0.15	1.35	22,30,32,36	0
4	EDO	B	504	4/4	0.93	0.18	1.17	27,31,37,44	0
4	EDO	D	505	4/4	0.95	0.15	0.00	27,27,29,35	0
4	EDO	A	503	4/4	0.94	0.16	-0.01	28,35,38,40	0
2	FAD	B	501	53/53	0.97	0.11	-0.33	13,20,25,26	0
2	FAD	D	501	53/53	0.98	0.11	-0.41	17,22,26,27	0
2	FAD	A	501	53/53	0.97	0.11	-0.46	17,22,27,30	0
2	FAD	C	501	53/53	0.97	0.10	-0.67	19,25,31,32	0
4	EDO	A	505	4/4	0.97	0.14	-0.78	18,23,25,29	0
4	EDO	D	504	4/4	0.97	0.14	-	23,23,28,31	0
4	EDO	D	503	4/4	0.91	0.17	-	19,26,28,38	0
4	EDO	B	503	4/4	0.96	0.10	-	19,20,21,22	0
4	EDO	A	504	4/4	0.98	0.15	-	20,22,27,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.