Full wwPDB X-ray Structure Validation Report (i)

Dec 14, 2023 – 05:14 pm GMT

PDB ID	:	4UGL
Title	:	Structure of Bacillus subtilis Nitric Oxide Synthase in complex with N1-(3-(2-(6-Amino-4-methylpyridin-2-yl)ethyl)-5-fluorophenyl)-N1- cyclopropyl-N2-methylethane-1,2-diamine
Authors	:	Holden, J.K.; Poulos, T.L.
Deposited on	:	2015-03-22
Resolution	:	1.82 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

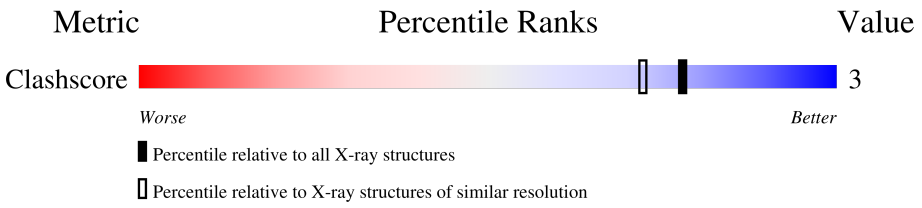
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.82 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	8401 (1.84-1.80)

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	S90	A	904	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 3329 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.

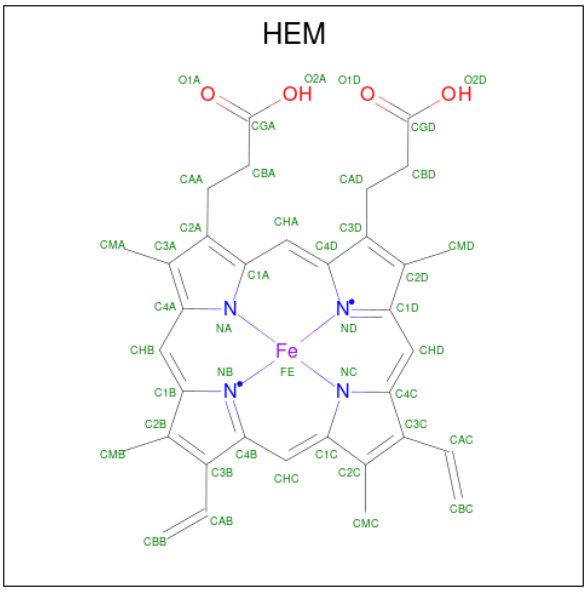
- Molecule 1 is a protein called NITRIC OXIDE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	362	2941	1873	507	553	8	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

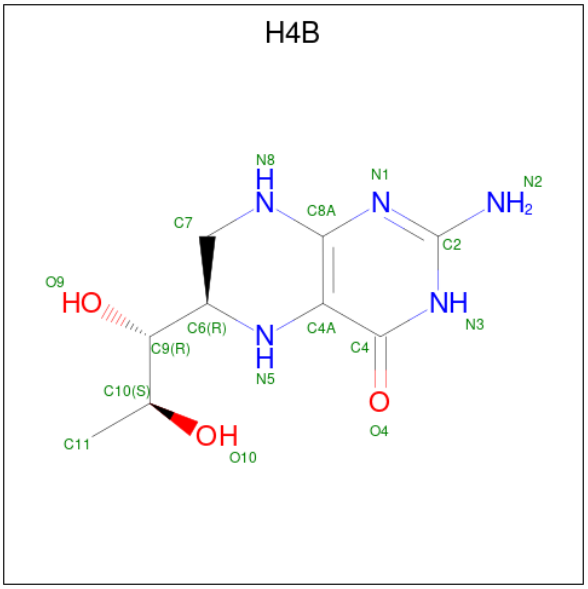
Chain	Residue	Modelled	Actual	Comment	Reference
A	25	ALA	GLU	engineered mutation	UNP O34453
A	26	ALA	GLU	engineered mutation	UNP O34453
A	316	ALA	GLU	engineered mutation	UNP O34453

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
2	A	1	43	34	1	4	4	0	0

- Molecule 3 is 5,6,7,8-TETRAHYDROBIOPTERIN (three-letter code: H4B) (formula: $C_9H_{15}N_5O_3$).

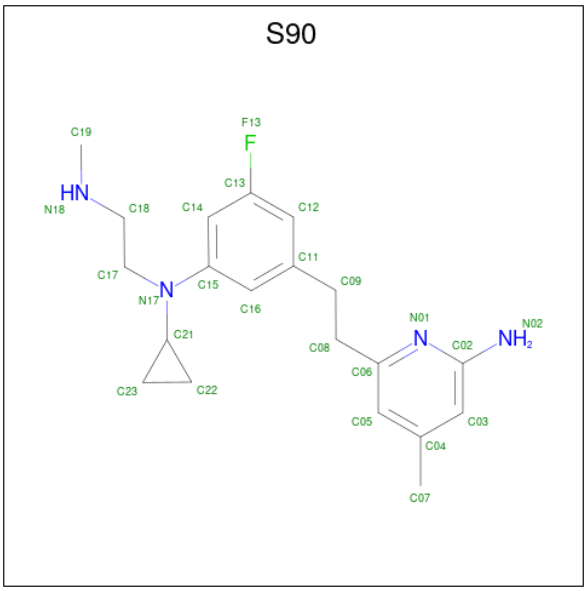


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	17	9	5	3	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

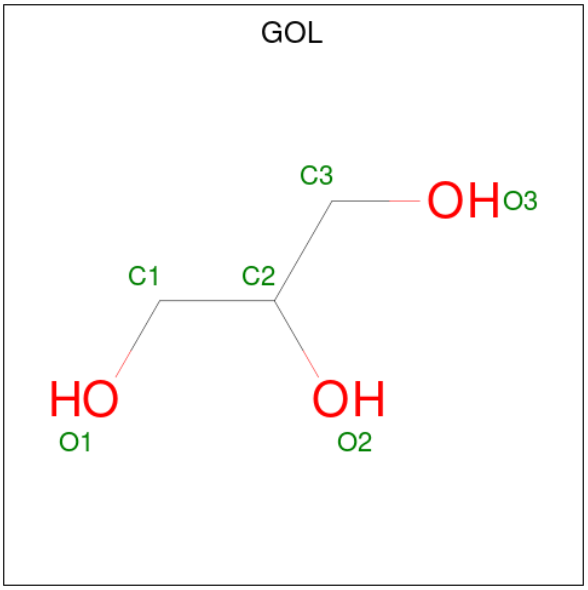
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
4	A	1	1	1	0	0

- Molecule 5 is N1-(3-(2-(6-Amino-4-methylpyridin-2-yl)ethyl)-5-fluorophenyl)-N1-cyclopropyl-N2-methylethane-1,2-diamine (three-letter code: S90) (formula: $C_{20}H_{27}FN_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	F	N		
5	A	1	25	20	1	4	0	0

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



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	296	296	296	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	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	80.74Å 94.78Å 63.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.89 – 1.82	Depositor
% Data completeness (in resolution range)	99.8 (37.89-1.82)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.52 (at 1.82Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.175 , 0.204	Depositor
Wilson B-factor (Å^2)	30.5	Xtriage
Anisotropy	0.712	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3329	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.75% 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 (i)

4.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, H4B, HEM, GOL, S90

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	0.39	0/3017	0.51	0/4088

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	2941	0	2856	12	0
2	A	43	0	30	3	0
3	A	17	0	15	0	0
4	A	1	0	0	0	0
5	A	25	0	27	9	0
6	A	6	0	8	1	0
7	A	296	0	0	1	0
All	All	3329	0	2936	17	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 (17) 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)
2:A:901:HEM:HBA1	5:A:904:S90:H092	1.69	0.74
2:A:901:HEM:HBD1	5:A:904:S90:C13	2.31	0.61
1:A:357:TYR:CE1	5:A:904:S90:H232	2.36	0.60
2:A:901:HEM:HBD1	5:A:904:S90:C14	2.32	0.58
1:A:60:TRP:CE3	1:A:72:TRP:HA	2.41	0.54
1:A:247:ARG:NH1	1:A:251:ASP:OD2	2.41	0.53
1:A:298:SER:HB3	6:A:905:GOL:H11	1.92	0.52
1:A:129:GLN:HG2	1:A:218:ILE:HD13	1.91	0.52
1:A:357:TYR:HE1	5:A:904:S90:H232	1.76	0.50
1:A:105:LYS:HE2	7:A:2086:HOH:O	2.12	0.49
1:A:49:LYS:NZ	1:A:79:ASP:OD2	2.39	0.48
5:A:904:S90:H193	5:A:904:S90:H171	1.67	0.47
5:A:904:S90:H172	5:A:904:S90:H221	1.56	0.46
1:A:32:LEU:HD12	1:A:32:LEU:HA	1.79	0.44
1:A:29:LYS:HD2	1:A:29:LYS:HA	1.69	0.43
1:A:218:ILE:HG13	5:A:904:S90:C13	2.50	0.42
1:A:237:GLY:H	5:A:904:S90:H072	1.86	0.40

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)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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)

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

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

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

5.3 Carbohydrates (i)

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

5.4 Ligands (i)

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

5.5 Other polymers (i)

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