



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 30, 2017 – 06:29 PM EDT

PDB ID : 3RQP
Title : Structure of the endothelial nitric oxide synthase heme domain in complex with 6-[[[(3R,4R)-4-(2-[[[(2R/2S)-1-(3-fluorophenyl)propan-2-yl]amino]ethoxy)pyrrolidin-3-yl]methyl]-4-methylpyridin-2-amine
Authors : Li, H.; Delker, S.L.; Poulos, T.L.
Deposited on : unknown
Resolution : 2.35 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 : **FAILED**
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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-20030345

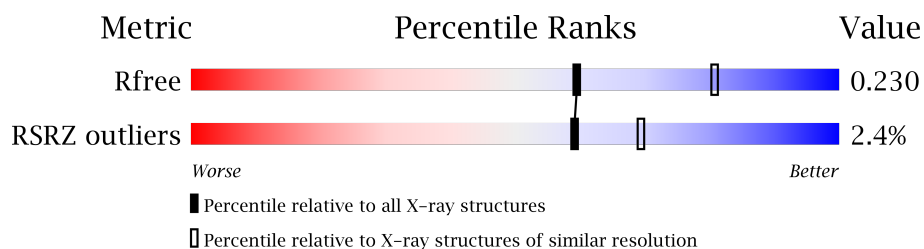
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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}	100719	1522 (2.38-2.34)
RSRZ outliers	101464	1528 (2.38-2.34)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 6920 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, endothelial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	405	Total	C	N	O	S	0	3	0
			3244	2061	572	595	16			
1	B	403	Total	C	N	O	S	0	2	0
			3218	2045	567	590	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	ARG	CYS	SEE REMARK 999	UNP P29473
B	100	ARG	CYS	SEE REMARK 999	UNP P29473

- 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
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

Continued on next page...

Continued from previous page...

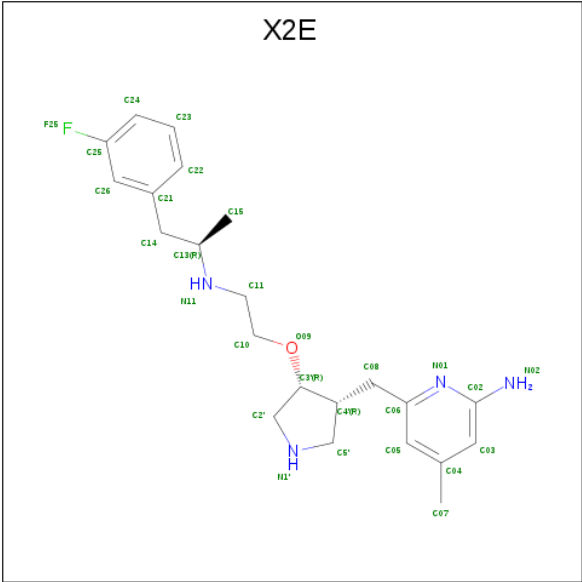
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



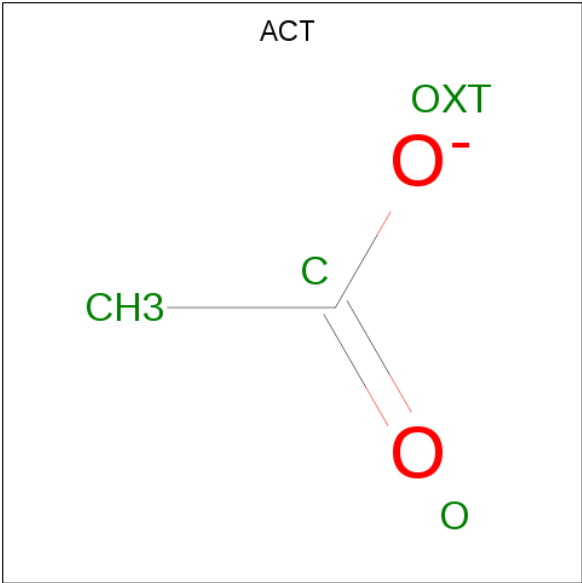
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 4 is 6-[[[(3R,4R)-4-(2-[[[(2R)-1-(3-fluorophenyl)propan-2-yl]amino]ethoxy]pyrrolidin-3-yl)methyl]-4-methylpyridin-2-amine (three-letter code: X2E) (formula: $C_{22}H_{31}FN_4O$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	0	0
			28	22	1	4	1		
4	B	1	Total	C	F	N	O	0	0
			28	22	1	4	1		

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



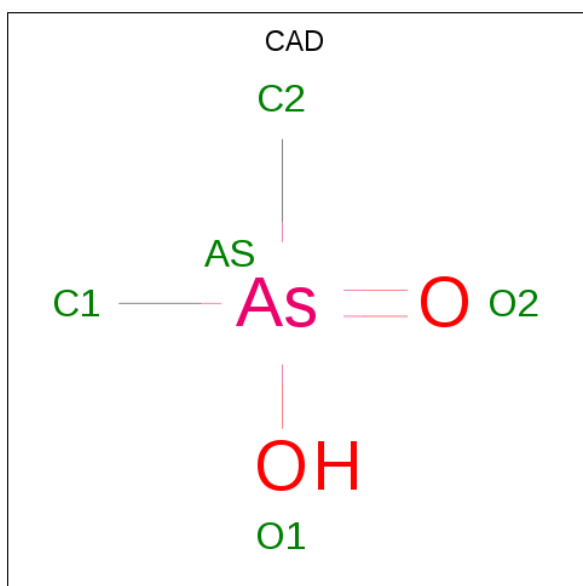
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

- 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	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is CACODYLIC ACID (three-letter code: CAD) (formula: $C_2H_7AsO_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	As	C	0	0
			3	1	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total 3	As 1	C 2	0	0

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total 1	Zn 1	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	128	Total 128	O 128	0	0
9	B	127	Total 127	O 127	0	0

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

3 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.95Å 106.63Å 156.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.43 – 2.35 48.43 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.43-2.35) 99.4 (48.43-2.35)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 2.34Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.178 , 0.228 0.180 , 0.230	Depositor DCC
R_{free} test set	2064 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	37.9	Xtriage
Anisotropy	0.159	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6920	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 3.61% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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

4.2 Too-close contacts [i](#)

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

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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

4.3.2 Protein sidechains [i](#)

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

4.3.3 RNA [i](#)

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

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 carbohydrates in this entry.

4.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 1 is monoatomic - leaving 12 for Mogul analysis.

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	HEM	A	500	1	28,50,50	2.18	8 (28%)	17,82,82	1.81	3 (17%)
3	H4B	A	600	-	14,18,18	0.95	0	12,26,26	2.45	5 (41%)
4	X2E	A	805	-	27,30,30	1.07	2 (7%)	34,40,40	1.75	8 (23%)
5	ACT	A	860	-	1,3,3	1.19	0	0,3,3	0.00	-
6	GOL	A	880	-	5,5,5	0.36	0	5,5,5	0.53	0
7	CAD	A	950	-	0,2,4	0.00	-	0,1,6	0.00	-
2	HEM	B	500	1	28,50,50	2.25	7 (25%)	17,82,82	2.18	3 (17%)
3	H4B	B	600	-	14,18,18	1.27	1 (7%)	12,26,26	2.14	5 (41%)
4	X2E	B	805	-	27,30,30	1.13	2 (7%)	34,40,40	1.88	6 (17%)
5	ACT	B	860	-	1,3,3	1.45	0	0,3,3	0.00	-
6	GOL	B	880	-	5,5,5	0.39	0	5,5,5	1.00	0
7	CAD	B	950	-	0,2,4	0.00	-	0,1,6	0.00	-

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	HEM	A	500	1	-	0/6/54/54	0/0/8/8
3	H4B	A	600	-	-	0/8/17/17	0/2/2/2
4	X2E	A	805	-	-	0/15/25/25	0/3/3/3
5	ACT	A	860	-	-	0/0/0/0	0/0/0/0
6	GOL	A	880	-	-	0/4/4/4	0/0/0/0
7	CAD	A	950	-	-	0/0/0/0	0/0/0/0
2	HEM	B	500	1	-	0/6/54/54	0/0/8/8
3	H4B	B	600	-	-	0/8/17/17	0/2/2/2
4	X2E	B	805	-	-	0/15/25/25	0/3/3/3
5	ACT	B	860	-	-	0/0/0/0	0/0/0/0
6	GOL	B	880	-	-	0/4/4/4	0/0/0/0
7	CAD	B	950	-	-	0/0/0/0	0/0/0/0

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	HEM	C3C-C2C	-5.15	1.33	1.40
2	B	500	HEM	C3B-C2B	-4.78	1.34	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	HEM	C3B-C2B	-4.64	1.34	1.40
2	A	500	HEM	C3C-C2C	-4.42	1.34	1.40
4	B	805	X2E	C13-N11	-4.18	1.42	1.48

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	HEM	CBA-CAA-C2A	-6.66	99.75	112.48
2	A	500	HEM	CBA-CAA-C2A	-5.09	102.75	112.48
4	B	805	X2E	C04-C05-C06	-3.93	117.79	120.26
3	A	600	H4B	N3-C2-N1	-3.62	119.58	125.45
2	B	500	HEM	C1D-C2D-C3D	-3.46	104.59	107.00

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](#)

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	405/443 (91%)	0.01	15 (3%) 42 54	23, 36, 62, 81	0
1	B	403/443 (90%)	-0.18	4 (0%) 82 90	23, 38, 63, 86	0
All	All	808/886 (91%)	-0.09	19 (2%) 59 69	23, 37, 63, 86	0

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	69	LYS	5.0
1	A	259	GLN	4.7
1	A	67	GLY	3.1
1	A	239	GLY	3.1
1	B	477[A]	TYR	3.1

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

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

5.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.4 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(\AA^2)	Q<0.9
4	X2E	B	805	28/28	0.88	0.20	1.32	43,54,56,57	0
6	GOL	A	880	6/6	0.90	0.20	1.31	51,54,54,58	0
7	CAD	A	950	3/5	0.98	0.12	0.83	66,66,67,68	0
4	X2E	A	805	28/28	0.89	0.20	0.51	35,52,55,56	0
2	HEM	A	500	43/43	0.98	0.18	0.50	22,28,38,44	0
5	ACT	A	860	4/4	0.96	0.15	0.39	48,49,50,52	0
6	GOL	B	880	6/6	0.95	0.15	0.36	49,52,52,53	0
2	HEM	B	500	43/43	0.98	0.13	0.26	23,28,36,43	0
5	ACT	B	860	4/4	0.97	0.11	0.17	48,49,50,51	0
3	H4B	B	600	17/17	0.98	0.16	-0.38	28,30,31,31	0
3	H4B	A	600	17/17	0.98	0.16	-0.39	21,26,29,30	0
8	ZN	A	900	1/1	1.00	0.15	-1.25	31,31,31,31	0
7	CAD	B	950	3/5	0.99	0.08	-	56,56,59,60	0

5.5 Other polymers [i](#)

There are no such residues in this entry.