



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 30, 2017 – 06:39 PM EDT

PDB ID : 3RQJ
Title : Structure of the neuronal nitric oxide synthase heme domain in complex with 6-(((3R,4R)-4-(2-((1S,2R)-2-(3-Fluorophenyl)cyclopropylamino)ethoxy)pyrrolidin-3-yl)methyl)-4-methylpyridin-2-amine
Authors : Li, H.; Delker, S.L.; Poulos, T.L.
Deposited on : unknown
Resolution : 1.84 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

<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

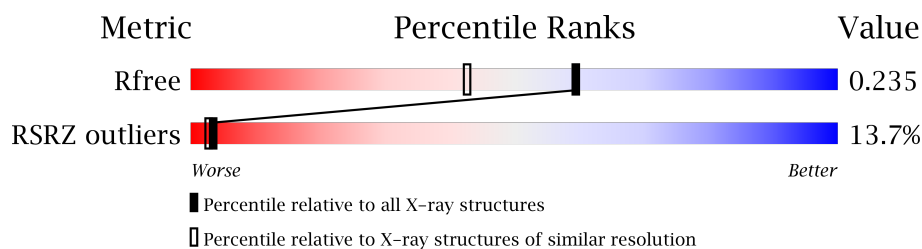
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.84 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	2964 (1.86-1.82)
RSRZ outliers	101464	2973 (1.86-1.82)

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

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
4	ACT	A	860	-	-	-	X

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 7189 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, brain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	407	Total	C	N	O	S	0	2	0
			3322	2127	566	608	21			
1	B	411	Total	C	N	O	S	0	2	0
			3354	2146	574	612	22			

- 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		
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: $C_9H_{15}N_5O_3$).



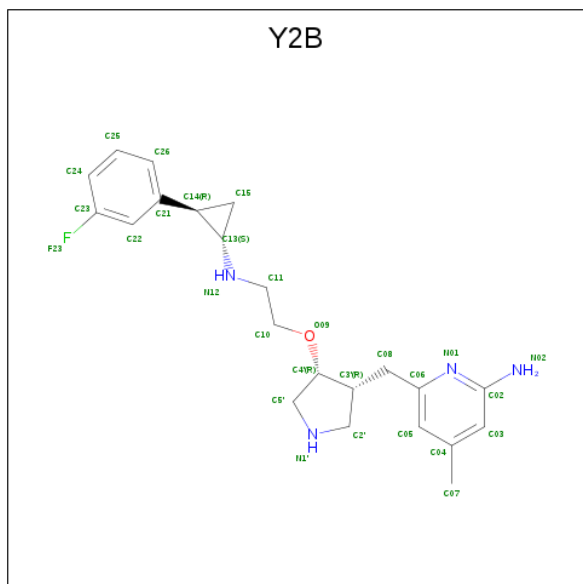
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 5 is 6-{[(3R,4R)-4-(2-{[(1S,2R)-2-(3-fluorophenyl)cyclopropyl]amino}ethoxy)pyrrolidin-3-yl]methyl}-4-methylpyridin-2-amine (three-letter code: Y2B) (formula: C₂₂H₂₉FN₄O).



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

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	138	Total	O	0	0
			138	138		
7	B	190	Total	O	0	0
			190	190		

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3 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	51.84Å 110.74Å 164.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.11 – 1.84 37.84 – 1.84	Depositor EDS
% Data completeness (in resolution range)	98.3 (38.11-1.84) 98.3 (37.84-1.84)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 1.84Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.189 , 0.221 0.208 , 0.235	Depositor DCC
R_{free} test set	4057 reflections (5.20%)	DCC
Wilson B-factor (Å ²)	36.5	Xtriage
Anisotropy	0.302	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 39.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7189	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% 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](#)

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4.2 Too-close contacts [i](#)

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4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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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 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 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	750	1	28,50,50	2.26	8 (28%)	17,82,82	2.26	5 (29%)
3	H4B	A	760	-	14,18,18	0.77	0	12,26,26	2.28	4 (33%)
5	Y2B	A	800	-	26,31,31	0.91	0	30,43,43	2.31	8 (26%)
4	ACT	A	860	-	1,3,3	1.41	0	0,3,3	0.00	-
2	HEM	B	750	1	28,50,50	2.17	12 (42%)	17,82,82	2.39	3 (17%)
3	H4B	B	760	-	14,18,18	1.11	0	12,26,26	2.47	5 (41%)
5	Y2B	B	800	-	26,31,31	0.83	0	30,43,43	2.17	9 (30%)
4	ACT	B	860	-	1,3,3	1.88	0	0,3,3	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	750	1	-	0/6/54/54	0/0/8/8
3	H4B	A	760	-	-	0/8/17/17	0/2/2/2
5	Y2B	A	800	-	-	0/13/30/30	0/3/4/4
4	ACT	A	860	-	-	0/0/0/0	0/0/0/0
2	HEM	B	750	1	-	0/6/54/54	0/0/8/8
3	H4B	B	760	-	-	0/8/17/17	0/2/2/2
5	Y2B	B	800	-	-	0/13/30/30	0/3/4/4
4	ACT	B	860	-	-	0/0/0/0	0/0/0/0

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	750	HEM	C3B-C2B	-5.57	1.33	1.40
2	B	750	HEM	C3C-C2C	-4.36	1.34	1.40
2	B	750	HEM	C3B-C2B	-4.08	1.35	1.40
2	A	750	HEM	C3C-C2C	-2.92	1.36	1.40
2	B	750	HEM	C4B-NB	2.07	1.40	1.36
2	B	750	HEM	CMB-C2B	2.07	1.56	1.51
2	B	750	HEM	C4A-NA	2.10	1.40	1.36
2	A	750	HEM	C1C-NC	2.13	1.39	1.36
2	B	750	HEM	CAA-C2A	2.27	1.55	1.52
2	B	750	HEM	CMA-C3A	2.38	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	750	HEM	CMA-C3A	2.64	1.57	1.51
2	B	750	HEM	C3B-CAB	2.64	1.53	1.47
2	B	750	HEM	C3C-CAC	2.79	1.53	1.47
2	A	750	HEM	C1B-NB	3.03	1.40	1.36
2	A	750	HEM	C3B-CAB	3.12	1.54	1.47
2	B	750	HEM	CAD-C3D	3.33	1.58	1.52
2	A	750	HEM	C3C-CAC	3.68	1.55	1.47
2	B	750	HEM	C4D-ND	3.84	1.41	1.36
2	B	750	HEM	C3D-C2D	4.36	1.50	1.37
2	A	750	HEM	C3D-C2D	5.12	1.52	1.37

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	800	Y2B	C15-C14-C21	-6.86	109.73	122.31
2	B	750	HEM	CBA-CAA-C2A	-6.79	99.51	112.48
5	A	800	Y2B	C15-C14-C21	-6.76	109.91	122.31
2	A	750	HEM	CBD-CAD-C3D	-6.02	100.99	112.47
2	B	750	HEM	CBD-CAD-C3D	-5.16	102.63	112.47
2	A	750	HEM	CBA-CAA-C2A	-4.48	103.92	112.48
5	A	800	Y2B	C26-C25-C24	-3.80	114.90	120.24
3	B	760	H4B	N3-C2-N1	-3.21	120.24	125.45
3	A	760	H4B	N3-C2-N1	-3.17	120.31	125.45
5	A	800	Y2B	C05-C06-N01	-2.85	119.82	122.91
5	B	800	Y2B	C04-C05-C06	-2.48	118.70	120.26
5	B	800	Y2B	C05-C06-N01	-2.16	120.57	122.91
5	B	800	Y2B	C24-C23-C22	-2.12	120.51	123.29
2	A	750	HEM	C3C-C4C-NC	-2.11	106.95	110.94
2	B	750	HEM	CMA-C3A-C4A	-2.10	125.24	128.46
5	A	800	Y2B	C24-C23-C22	-2.05	120.60	123.29
5	B	800	Y2B	C22-C21-C14	2.01	123.79	120.10
5	B	800	Y2B	C10-C11-N12	2.06	116.77	111.55
5	A	800	Y2B	C26-C21-C22	2.14	121.28	118.79
3	B	760	H4B	C2-N1-C8A	2.27	119.62	114.51
5	A	800	Y2B	C25-C24-C23	2.31	123.11	118.19
2	A	750	HEM	C4C-C3C-C2C	2.34	108.53	106.90
5	B	800	Y2B	C2'-N1'-C5'	2.46	111.14	105.40
5	B	800	Y2B	N02-C02-N01	2.49	120.84	116.64
2	A	750	HEM	CMC-C2C-C3C	2.64	129.79	124.89
3	B	760	H4B	N2-C2-N1	2.69	121.54	117.24
3	A	760	H4B	C4-N3-C2	2.93	120.27	116.06
5	A	800	Y2B	C2'-N1'-C5'	3.11	112.63	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	760	H4B	C2-N1-C8A	3.23	121.79	114.51
3	B	760	H4B	C4-N3-C2	3.83	121.57	116.06
3	A	760	H4B	C4-C4A-C8A	4.30	118.45	114.56
3	B	760	H4B	C4-C4A-C8A	5.33	119.39	114.56
5	B	800	Y2B	C02-N01-C06	5.81	122.28	118.17
5	A	800	Y2B	C02-N01-C06	6.42	122.71	118.17

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

5.1 Protein, DNA and RNA chains

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	407/422 (96%)	0.97	78 (19%) 1 1	28, 53, 92, 121	0
1	B	411/422 (97%)	0.47	34 (8%) 12 11	28, 41, 66, 80	0
All	All	818/844 (96%)	0.72	112 (13%) 3 3	28, 47, 86, 121	0

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	300	PHE	8.6
1	A	488	PRO	8.3
1	A	716	TRP	8.1
1	A	713	THR	5.9
1	A	351	LYS	5.9
1	A	355	PHE	5.8
1	B	619	ARG	5.5
1	A	352	ASP	5.5
1	A	486	LYS	5.3
1	A	388	ILE	4.7
1	A	506	ILE	4.5
1	A	300	PHE	4.3
1	B	348	VAL	4.3
1	A	715	VAL	4.2
1	B	350	THR	4.1
1	A	514	ARG	4.0
1	A	491	SER	3.7
1	A	714	HIS	3.7
1	A	487	GLN	3.7
1	A	507	GLN	3.7
1	A	567	VAL	3.7
1	A	678	TRP	3.6
1	B	667	ARG	3.6
1	A	385	ASN	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	389	GLU	3.5
1	B	616	LEU	3.5
1	A	386	LYS	3.4
1	A	392	SER	3.4
1	A	490	GLY	3.4
1	A	592[A]	GLU	3.3
1	A	551	PHE	3.3
1	A	479	LEU	3.3
1	A	390	SER	3.3
1	A	552	ASP	3.2
1	A	503	GLU	3.2
1	A	593	ILE	3.2
1	A	469	LYS	3.2
1	A	299	ARG	3.1
1	B	620	LYS	3.1
1	A	619	ARG	3.1
1	B	677	VAL	3.1
1	B	567	VAL	3.1
1	A	511	LYS	3.1
1	A	391	THR	3.0
1	B	680	VAL	3.0
1	A	480	ILE	3.0
1	B	691	PHE	2.9
1	A	680	VAL	2.9
1	B	479	LEU	2.9
1	A	489	ASP	2.9
1	A	584	PHE	2.9
1	A	591	THR	2.8
1	B	561	TRP	2.8
1	A	382	GLU	2.8
1	B	310	VAL	2.8
1	A	321	THR	2.8
1	A	682	PRO	2.8
1	A	350	THR	2.8
1	B	566	ALA	2.8
1	A	676	TRP	2.8
1	B	592[A]	GLU	2.8
1	B	302	LYS	2.7
1	A	561	TRP	2.7
1	B	591	THR	2.7
1	A	492	THR	2.7
1	B	713	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	416	VAL	2.7
1	A	415	CYS	2.7
1	A	677	VAL	2.6
1	B	715	VAL	2.6
1	A	588	TYR	2.6
1	B	480	ILE	2.6
1	A	712	ASN	2.6
1	B	617	ASP	2.6
1	A	508	GLN	2.6
1	B	682	PRO	2.6
1	A	505	CYS	2.6
1	B	299	ARG	2.5
1	A	681	PRO	2.5
1	A	595	VAL	2.5
1	B	352	ASP	2.5
1	A	566	ALA	2.4
1	B	615	ASP	2.4
1	A	499	VAL	2.4
1	A	565	PRO	2.4
1	A	667	ARG	2.4
1	A	467	ASP	2.3
1	B	389	GLU	2.3
1	B	321	THR	2.3
1	A	683	MET	2.3
1	A	470	HIS	2.3
1	A	550	LYS	2.3
1	B	681	PRO	2.3
1	A	370	LYS	2.2
1	B	679	ILE	2.2
1	A	322	LEU	2.2
1	A	686	SER	2.2
1	B	375	LYS	2.2
1	A	679	ILE	2.2
1	A	446	VAL	2.2
1	A	572	LEU	2.2
1	A	328	GLU	2.2
1	B	678	TRP	2.1
1	A	485	TYR	2.1
1	B	676	TRP	2.1
1	A	704	PHE	2.1
1	A	568	SER	2.1
1	A	617	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	593	ILE	2.1
1	A	618	MET	2.0
1	A	710	PRO	2.0
1	A	711	TRP	2.0

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	ACT	A	860	4/4	0.93	0.22	5.24	51,53,53,55	0
3	H4B	A	760	17/17	0.95	0.20	0.72	32,35,39,40	0
3	H4B	B	760	17/17	0.96	0.18	0.66	32,34,38,39	0
4	ACT	B	860	4/4	0.97	0.10	0.26	47,47,49,49	0
2	HEM	A	750	43/43	0.97	0.21	0.16	26,34,41,44	0
2	HEM	B	750	43/43	0.98	0.17	0.14	24,31,41,46	0
5	Y2B	B	800	28/28	0.83	0.17	-0.16	31,38,42,47	0
5	Y2B	A	800	28/28	0.81	0.20	-0.26	33,42,44,44	0
6	ZN	A	900	1/1	0.99	0.07	-1.09	38,38,38,38	0

5.5 Other polymers [i](#)

There are no such residues in this entry.