



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 09:33 PM GMT

PDB ID : 4JSE  
Title : Structure of rat neuronal nitric oxide synthase heme domain in complex with  
6,6'-(pentane-1,5-diyl)bis(4-methylpyridin-2-amine)  
Authors : Li, H.; Poulos, T.L.  
Deposited on : 2013-03-22  
Resolution : 1.97 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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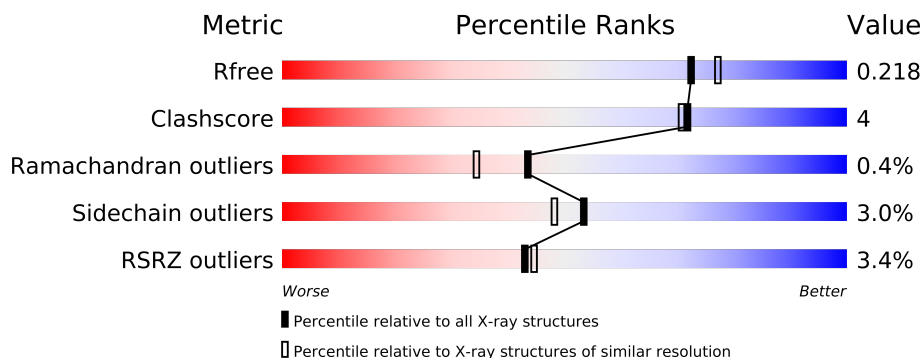
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 1.97 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))
$R_{free}$	66092	6577 (2.00-1.96)
Clashscore	79885	8091 (2.00-1.96)
Ramachandran outliers	78287	7989 (2.00-1.96)
Sidechain outliers	78261	7987 (2.00-1.96)
RSRZ outliers	66119	6578 (2.00-1.96)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	422	
1	B	422	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	ACT	A	802	-	X
4	QJ2	A	803	-	X
4	QJ2	A	805	-	X
4	QJ2	B	805	-	X
5	H4B	A	804	-	X
5	H4B	B	802	-	X

## 2 Entry composition i

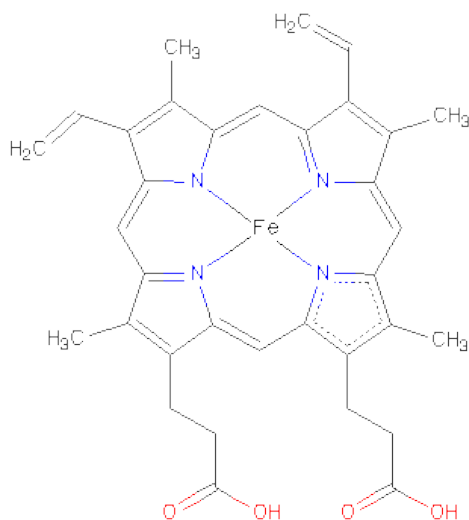
There are 8 unique types of molecules in this entry. The entry contains 7377 atoms, of which 0 are hydrogen and 0 are deuterium.

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	408	Total	C	N	O	S	0	6	0
			3348	2144	570	611	23			
1	B	412	Total	C	N	O	S	0	6	0
			3379	2162	578	616	23			

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



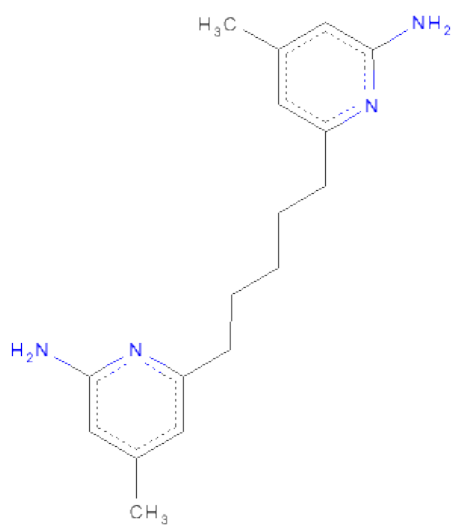
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



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

- Molecule 4 is 6,6'-PENTANE-1,5-DIYLBIS(4-METHYLPYRIDIN-2-AMINE) (three-letter code: QJ2) (formula: C<sub>17</sub>H<sub>24</sub>N<sub>4</sub>).



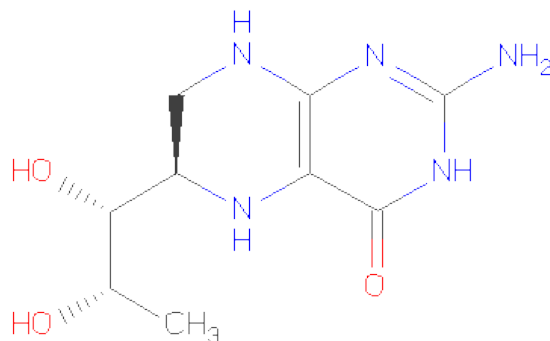
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			21	17	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			21	17	4		
4	B	1	Total	C	N	0	0
			21	17	4		
4	B	1	Total	C	N	0	0
			21	17	4		

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



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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Zn	0	0
			1	1		
6	A	2	Total	Zn	0	1
			2	2		

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	2	Total 2	Cl 2	0	0
7	A	2	Total 2	Cl 2	0	2

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	178	Total 178	O 178	0	0
8	B	253	Total 253	O 253	0	0

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- Molecule 1: Nitric oxide synthase, brain



Chain B:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	51.74Å 110.25Å 163.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.34 – 1.97 49.34 – 1.97	Depositor EDS
% Data completeness (in resolution range)	98.9 (49.34-1.97) 98.9 (49.34-1.97)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.65 (at 1.97Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.170 , 0.205 0.183 , 0.218	Depositor DCC
$R_{free}$ test set	3280 reflections (5.20%)	DCC
Wilson B-factor (Å <sup>2</sup> )	29.3	Xtriage
Anisotropy	0.733	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 34.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 66557 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7377	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, H4B, CL, ACT, HEM, QJ2

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	0.67	0/3459	0.68	0/4692
1	B	0.70	0/3490	0.69	0/4729
All	All	0.68	0/6949	0.68	0/9421

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Close contacts

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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3348	0	0	9	0
1	B	3379	0	0	11	0
2	A	43	0	0	4	0
2	B	43	0	0	5	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
4	A	42	0	48	3	0
4	B	42	0	24	1	0
5	A	17	0	15	6	0
5	B	17	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	2	0	0	0	0
6	B	1	0	0	0	0
7	A	2	0	0	0	0
7	B	2	0	0	0	0
8	A	178	0	0	1	0
8	B	253	0	0	7	0
All	All	7377	0	87	31	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (31) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:801:HEM:O1A	5:B:802:H4B:N2	2.23	0.72
1:A:299:ARG:N	1:A:317:HIS:NE2	2.39	0.70
1:A:371:ARG:CG	1:A:371:ARG:NH2	2.58	0.66
2:A:801:HEM:O1A	5:A:804:H4B:N3	2.27	0.66
1:B:692:HIS:ND1	8:B:1150:HOH:O	2.29	0.64
1:A:336[A]:MET:SD	5:A:804:H4B:H6	2.38	0.63
1:A:336[A]:MET:CA	1:A:336[A]:MET:CE	2.77	0.62
2:B:801:HEM:O1A	5:B:802:H4B:N3	2.36	0.59
1:B:596[B]:ARG:NH1	8:B:1129:HOH:O	2.37	0.58
1:A:336[A]:MET:SD	5:A:804:H4B:H9	2.46	0.56
1:B:364:GLN:NE2	8:B:967:HOH:O	2.39	0.55
1:A:391:THR:O	1:A:392:SER:OG	2.25	0.54
2:A:801:HEM:O1A	5:A:804:H4B:N2	2.39	0.53
1:B:336[A]:MET:CE	8:B:1153:HOH:O	0.82	0.52
2:B:801:HEM:C1C	4:B:805:QJ2:H24	2.45	0.52
1:B:436:HIS:ND1	8:B:1041:HOH:O	2.34	0.52
5:B:802:H4B:C7	5:B:802:H4B:O10	2.57	0.49
1:A:403:TYR:CE1	1:A:407:HIS:CE1	3.02	0.47
1:B:706:TYR:OH	2:B:801:HEM:O1D	2.34	0.46
1:B:596[A]:ARG:NE	8:B:1098:HOH:O	2.49	0.46
4:A:803:QJ2:H20	8:A:1006:HOH:O	2.16	0.46
2:B:801:HEM:O1A	5:B:802:H4B:C2	2.64	0.45
5:A:804:H4B:H71	5:A:804:H4B:O10	2.16	0.44
1:A:352:ASP:OD2	1:A:352:ASP:N	2.51	0.44
2:A:801:HEM:O1A	5:A:804:H4B:C2	2.67	0.42
1:A:592:GLU:OE1	4:A:805:QJ2:N01	2.52	0.42
1:B:414:ARG:NH1	1:B:706:TYR:OH	2.52	0.42
1:B:445:HIS:CD2	1:B:445:HIS:C	2.94	0.41
1:B:596[A]:ARG:NH1	8:B:1119:HOH:O	2.52	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:403:TYR:CE1	1:B:407:HIS:CE1	3.08	0.41
2:A:801:HEM:C1C	4:A:805:QJ2:H24	2.56	0.41

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	410/422 (97%)	398 (97%)	9 (2%)	3 (1%)	30	19
1	B	414/422 (98%)	407 (98%)	7 (2%)	0	100	100
All	All	824/844 (98%)	805 (98%)	16 (2%)	3 (0%)	43	34

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	322	LEU
1	A	300	PHE
1	A	338	PRO

### 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	370/377 (98%)	356 (96%)	14 (4%)	44	37
1	B	373/377 (99%)	364 (98%)	9 (2%)	61	59
All	All	743/754 (98%)	720 (97%)	23 (3%)	53	46

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	300	PHE
1	A	322	LEU
1	A	330	ILE
1	A	336[A]	MET
1	A	336[B]	MET
1	A	350	THR
1	A	352	ASP
1	A	353	GLN
1	A	370	LYS
1	A	371	ARG
1	A	454	ASN
1	A	523	LEU
1	A	547	ARG
1	A	620	LYS
1	B	322	LEU
1	B	360	GLU
1	B	382	GLU
1	B	389	GLU
1	B	390	SER
1	B	454	ASN
1	B	540	LEU
1	B	547	ARG
1	B	717	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

Of 17 ligands modelled in this entry, 7 are monoatomic - leaving 10 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	801	1	49,50,50	2.45	18 (36%)	46,82,82	2.29	10 (21%)
3	ACT	A	802	-	1,3,3	0.98	0	0,3,3	0.00	-
4	QJ2	A	803	-	22,22,22	0.74	0	29,29,29	1.93	7 (24%)
5	H4B	A	804	-	18,18,18	1.09	1 (5%)	24,26,26	2.02	9 (37%)
4	QJ2	A	805	-	22,22,22	0.60	0	29,29,29	1.93	6 (20%)
2	HEM	B	801	1	49,50,50	2.24	18 (36%)	46,82,82	2.13	8 (17%)
5	H4B	B	802	-	18,18,18	1.05	1 (5%)	24,26,26	1.94	9 (37%)
4	QJ2	B	803	-	22,22,22	0.85	0	29,29,29	2.20	6 (20%)
3	ACT	B	804	-	1,3,3	0.97	0	0,3,3	0.00	-
4	QJ2	B	805	-	22,22,22	0.70	0	29,29,29	2.17	8 (27%)

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	801	1	-	0/14/114/114	0/0/8/8
3	ACT	A	802	-	-	0/0/0/0	0/0/0/0
4	QJ2	A	803	-	-	0/8/8/8	0/2/2/2
5	H4B	A	804	-	-	0/8/17/17	0/0/2/2
4	QJ2	A	805	-	-	0/8/8/8	0/2/2/2
2	HEM	B	801	1	-	0/14/114/114	0/0/8/8
5	H4B	B	802	-	-	0/8/17/17	0/0/2/2
4	QJ2	B	803	-	-	0/8/8/8	0/2/2/2
3	ACT	B	804	-	-	0/0/0/0	0/0/0/0
4	QJ2	B	805	-	-	0/8/8/8	0/2/2/2

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	HEM	C2B-C1B	6.31	1.46	1.44
2	B	801	HEM	C3C-C2C	-5.98	1.33	1.43
2	A	801	HEM	C3B-C2B	-5.87	1.33	1.43
2	A	801	HEM	C4A-C3A	5.50	1.47	1.40
2	B	801	HEM	C3B-C2B	-5.32	1.34	1.43
2	A	801	HEM	C3C-C2C	-4.66	1.35	1.43
2	B	801	HEM	C3B-CAB	4.55	1.54	1.40
2	B	801	HEM	C3C-CAC	4.53	1.54	1.40
2	A	801	HEM	C3C-CAC	4.53	1.54	1.40
2	A	801	HEM	C3B-CAB	4.51	1.54	1.40
2	A	801	HEM	C3D-C2D	4.25	1.51	1.43
2	B	801	HEM	C3D-C2D	4.00	1.50	1.43
2	B	801	HEM	C4A-C3A	3.96	1.45	1.40
2	A	801	HEM	CHA-C4D	3.62	1.41	1.35
5	A	804	H4B	C2-N2	3.58	1.38	1.32
2	A	801	HEM	FE-NA	3.43	2.07	1.92
2	A	801	HEM	CMC-C2C	3.23	1.57	1.47
2	B	801	HEM	FE-NA	3.23	2.06	1.92
5	B	802	H4B	C2-N2	3.13	1.37	1.32
2	A	801	HEM	FE-ND	3.12	2.09	1.97
2	B	801	HEM	CMB-C2B	3.08	1.57	1.47
2	B	801	HEM	CHA-C4D	2.83	1.39	1.35
2	A	801	HEM	CMB-C2B	2.65	1.55	1.47
2	B	801	HEM	CMC-C2C	2.63	1.55	1.47
2	B	801	HEM	CMD-C2D	2.63	1.55	1.47
2	A	801	HEM	FE-NB	2.60	2.07	1.97
2	B	801	HEM	CAA-C2A	2.55	1.56	1.52
2	A	801	HEM	CMD-C2D	2.52	1.55	1.47
2	B	801	HEM	FE-ND	2.45	2.06	1.97
2	A	801	HEM	CMA-C3A	2.36	1.56	1.51
2	B	801	HEM	C3B-C4B	2.32	1.47	1.44
2	B	801	HEM	C2B-C1B	-2.25	1.44	1.44
2	B	801	HEM	FE-NC	2.21	2.06	1.97
2	B	801	HEM	CMA-C3A	2.10	1.56	1.51
2	A	801	HEM	CHC-C1C	2.08	1.40	1.36
2	A	801	HEM	CHD-C4C	2.07	1.40	1.36
2	A	801	HEM	CAA-C2A	2.03	1.55	1.52
2	B	801	HEM	C3D-C4D	-2.02	1.44	1.44

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	HEM	C3B-C4B-NB	-9.82	106.97	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	HEM	C3B-C4B-NB	-8.55	107.88	114.00
4	B	803	QJ2	C22-N21-C26	6.61	122.87	118.23
2	A	801	HEM	CBA-CAA-C2A	-6.50	101.24	112.69
4	B	805	QJ2	C22-N21-C26	6.05	122.48	118.23
4	A	803	QJ2	C02-N01-C06	5.78	122.29	118.23
2	A	801	HEM	C4D-ND-C1D	5.72	111.01	105.16
4	B	803	QJ2	C02-N01-C06	5.60	122.16	118.23
4	B	805	QJ2	C02-N01-C06	5.40	122.02	118.23
4	A	805	QJ2	C22-N21-C26	5.18	121.87	118.23
4	A	805	QJ2	C02-N01-C06	4.83	121.62	118.23
2	B	801	HEM	C4D-ND-C1D	4.74	110.01	105.16
4	A	803	QJ2	C22-N21-C26	4.73	121.56	118.23
2	A	801	HEM	CBD-CAD-C3D	-4.69	104.14	114.37
5	B	802	H4B	C10-C9-C6	-4.34	107.09	113.61
4	B	805	QJ2	C05-C06-N01	-4.25	118.26	122.99
4	A	805	QJ2	C05-C06-N01	-4.16	118.36	122.99
4	B	803	QJ2	C08-C06-N01	3.95	121.06	115.69
2	B	801	HEM	CBD-CAD-C3D	-3.82	106.04	114.37
5	A	804	H4B	C4-C4A-N5	3.78	124.60	119.10
4	B	803	QJ2	C25-C26-N21	-3.66	118.92	122.99
2	B	801	HEM	CBA-CAA-C2A	-3.59	106.37	112.69
5	B	802	H4B	C4-C4A-C8A	3.54	117.84	114.56
4	B	803	QJ2	C05-C06-N01	-3.54	119.05	122.99
4	A	803	QJ2	C12-C26-N21	3.34	120.22	115.69
5	A	804	H4B	C10-C9-C6	-3.25	108.72	113.61
2	A	801	HEM	CHA-C4D-ND	3.15	128.63	124.31
5	A	804	H4B	C2-N1-C8A	3.10	122.02	117.61
2	B	801	HEM	C4A-CHB-C1B	-3.06	123.45	127.47
2	A	801	HEM	C2D-C1D-ND	-3.05	109.33	112.93
5	A	804	H4B	C4-C4A-C8A	3.04	117.38	114.56
4	A	803	QJ2	C25-C26-N21	-3.01	119.64	122.99
4	B	805	QJ2	C08-C06-N01	2.93	119.67	115.69
4	A	803	QJ2	C08-C06-N01	2.89	119.62	115.69
2	A	801	HEM	C4C-NC-C1C	2.86	108.51	105.53
5	A	804	H4B	C6-C7-N8	-2.84	107.99	111.66
4	A	803	QJ2	C05-C06-N01	-2.83	119.84	122.99
5	B	802	H4B	C6-C7-N8	-2.83	108.01	111.66
2	B	801	HEM	C2D-C1D-ND	-2.76	109.67	112.93
4	B	805	QJ2	C12-C26-N21	2.71	119.37	115.69
2	B	801	HEM	CMA-C3A-C4A	-2.70	124.46	128.62
4	B	805	QJ2	C27-C24-C25	-2.67	116.63	120.93
4	B	805	QJ2	C25-C26-N21	-2.50	120.21	122.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	804	H4B	N3-C2-N1	-2.47	118.32	121.78
2	A	801	HEM	CHC-C1C-NC	2.46	126.87	124.73
5	A	804	H4B	N2-C2-N3	2.45	120.55	117.86
4	B	803	QJ2	C12-C26-C25	2.43	124.55	121.17
5	B	802	H4B	C4A-N5-C6	-2.37	114.71	121.16
5	B	802	H4B	C7-C6-C9	-2.36	110.02	113.66
5	B	802	H4B	C4-C4A-N5	2.34	122.51	119.10
2	B	801	HEM	CAD-C3D-C4D	2.34	128.74	124.53
2	A	801	HEM	CHD-C4C-NC	2.34	126.77	124.73
5	B	802	H4B	N8-C8A-N1	2.33	119.23	115.82
2	A	801	HEM	CMA-C3A-C4A	-2.31	125.07	128.62
4	A	805	QJ2	C04-C05-C06	2.28	121.82	120.29
4	B	805	QJ2	C11-C12-C26	-2.28	105.10	113.16
5	A	804	H4B	C4A-N5-C6	-2.20	115.17	121.16
5	A	804	H4B	C4A-C4-N3	2.17	119.63	114.06
4	A	805	QJ2	C24-C25-C26	-2.17	118.85	120.29
4	A	805	QJ2	C25-C26-N21	-2.17	120.58	122.99
5	B	802	H4B	N2-C2-N3	2.10	120.17	117.86
5	B	802	H4B	C4A-C4-N3	2.10	119.45	114.06
4	A	803	QJ2	N22-C22-N21	2.09	120.60	116.59

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	408/422 (96%)	0.34	17 (4%) 35 35	24, 39, 63, 85	0
1	B	412/422 (97%)	0.29	11 (2%) 52 54	21, 33, 54, 80	0
All	All	820/844 (97%)	0.31	28 (3%) 43 44	21, 36, 61, 85	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	300	PHE	8.8
1	A	322	LEU	8.0
1	B	322	LEU	7.4
1	B	348	VAL	7.0
1	A	351	LYS	6.8
1	A	299	ARG	5.0
1	B	300	PHE	4.6
1	A	352	ASP	3.8
1	B	718	GLY	3.7
1	A	339	SER	3.4
1	A	355	PHE	3.0
1	B	619	ARG	2.8
1	B	350	THR	2.7
1	A	373	GLY	2.6
1	A	350	THR	2.6
1	B	355	PHE	2.5
1	B	349	ARG	2.5
1	A	370	LYS	2.3
1	B	338	PRO	2.3
1	A	338	PRO	2.3
1	A	715	VAL	2.2
1	B	330	ILE	2.2
1	B	351	LYS	2.2
1	A	716	TRP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	713	THR	2.1
1	A	371	ARG	2.1
1	A	369	ILE	2.0
1	A	386	LYS	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	H4B	A	804	17/17	0.22	5.17	37,43,48,49	0
5	H4B	B	802	17/17	0.21	4.28	44,51,55,56	0
4	QJ2	A	805	21/21	0.16	3.21	21,35,45,46	0
4	QJ2	A	803	21/21	0.44	2.78	37,54,72,72	0
3	ACT	A	802	4/4	0.14	2.36	41,42,42,43	0
4	QJ2	B	805	21/21	0.15	2.11	20,36,48,48	0
2	HEM	A	801	43/43	0.13	1.09	25,29,41,50	0
2	HEM	B	801	43/43	0.15	0.97	22,25,38,48	0
4	QJ2	B	803	21/21	0.21	0.53	35,50,71,73	0
6	ZN	A	809	1/1	0.11	0.20	32,32,32,32	0
7	CL	B	807	1/1	0.12	-0.31	45,45,45,45	1
7	CL	A	807[A]	1/1	0.11	-0.90	35,35,35,35	1
7	CL	B	808	1/1	0.11	-0.97	42,42,42,42	1
6	ZN	A	806[A]	1/1	0.10	-1.26	31,31,31,31	1
3	ACT	B	804	4/4	0.11	-1.61	37,38,39,40	0
7	CL	A	808[A]	1/1	0.07	-2.51	40,40,40,40	1
6	ZN	B	806	1/1	0.08	-2.98	36,36,36,36	1

## 6.5 Other polymers ⓘ

There are no such residues in this entry.