



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 08:32 AM GMT

PDB ID : 3N2R  
Title : Structure of neuronal nitric oxide synthase heme domain in complex with 6-((3R,4R/3S,4S)-4-(3-Phenoxyphenoxy)pyrrolidin-3-yl)methylpyridin-2-amine  
Authors : Li, H.; Poulos, T.L.  
Deposited on : 2010-05-18  
Resolution : 1.90 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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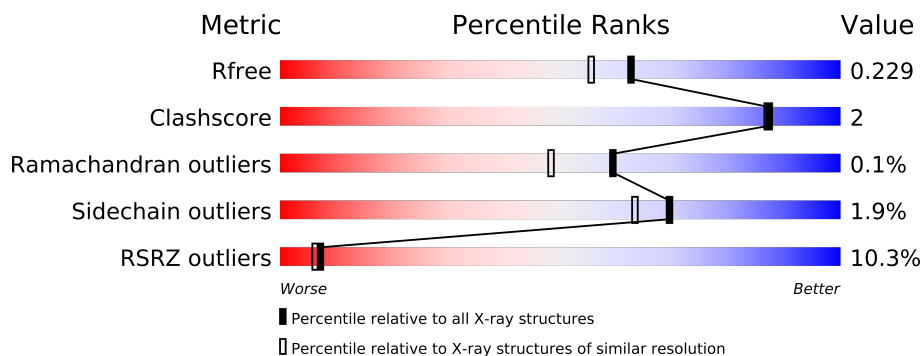
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.90 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	3684 (1.90-1.90)
Clashscore	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)
RSRZ outliers	66119	3686 (1.90-1.90)

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
4	ACT	A	860	-	X
5	XJH	A	800	-	X
5	XJH	B	800	-	X

## 2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 7233 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.

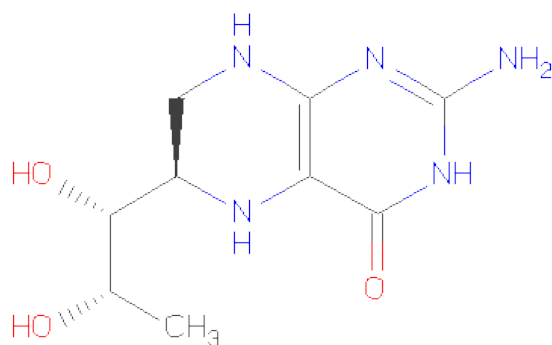
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	407	Total	C	N	O	S	0	1	0
			3316	2123	566	605	22			
1	B	411	Total	C	N	O	S	0	3	0
			3354	2146	574	612	22			

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



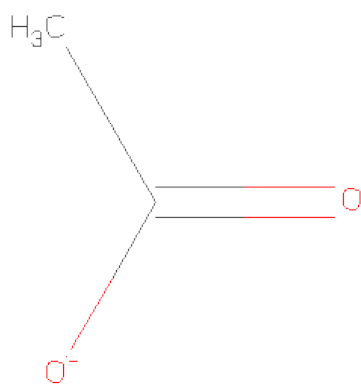
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



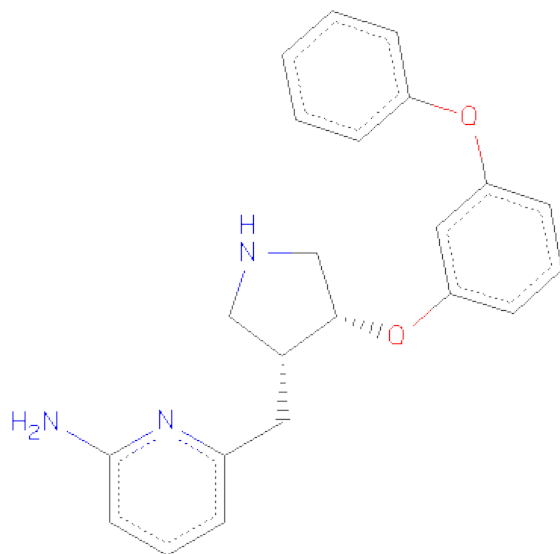
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		

- 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-(3-PHENOXYPHENOXY)PYRROLIDIN-3-YL]METHYL}PYRIDIN-2-AMINE (three-letter code: XJH) (formula: C<sub>22</sub>H<sub>23</sub>N<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			27	22	3	2		
5	B	1	Total	C	N	O	0	0
			27	22	3	2		

- 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		

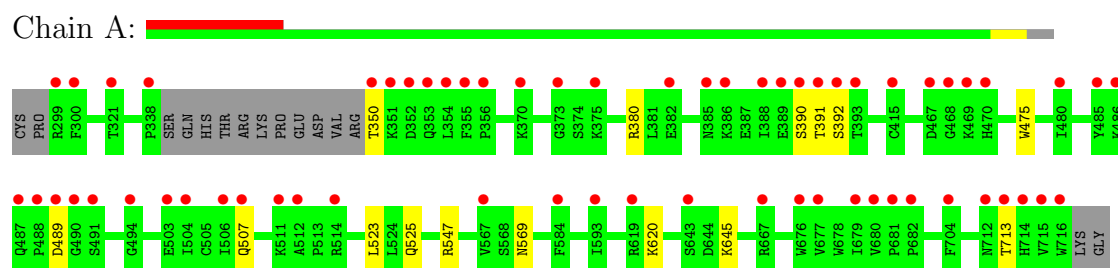
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	161	Total	O	0	0
			161	161		
7	B	219	Total	O	0	0
			219	219		

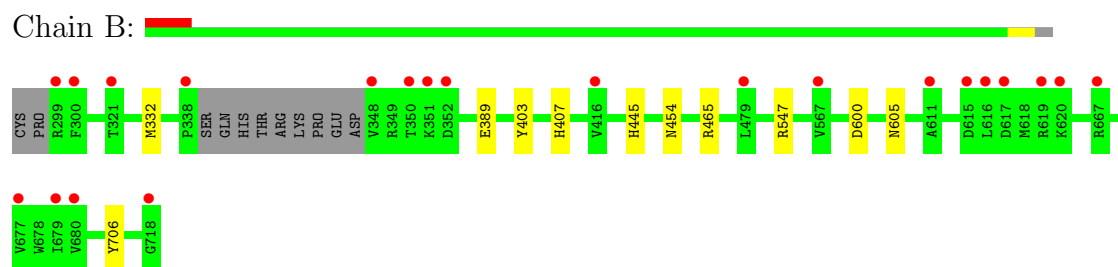
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Nitric oxide synthase



- Molecule 1: Nitric oxide synthase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	52.28Å 111.56Å 164.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.36 – 1.90 38.66 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.8 (47.36-1.90) 98.8 (38.66-1.90)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.39 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.182 , 0.215 0.197 , 0.229	Depositor DCC
$R_{free}$ test set	3757 reflections (5.23%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.5	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 36.5	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	2 of 75631 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7233	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% 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: HEM, ZN, ACT, H4B, XJH

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	0.61	0/3412	0.62	0/4629
1	B	0.70	0/3456	0.65	1/4685 (0.0%)
All	All	0.65	0/6868	0.63	1/9314 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	600	ASP	CB-CG-OD2	5.07	122.86	118.30

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	3316	0	0	2	0
1	B	3354	0	0	5	0
2	A	43	0	0	1	0
2	B	43	0	0	2	0
3	A	17	0	0	0	0
3	B	17	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	4	0	0	0	0
4	B	4	0	0	0	0
5	A	27	0	23	5	0
5	B	27	0	23	5	0
6	A	1	0	0	0	0
7	A	161	0	0	0	0
7	B	219	0	0	2	0
All	All	7233	0	46	17	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 2.

All (17) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:A:800:XJH:H12	5:A:800:XJH:H5'A	1.49	0.94
5:A:800:XJH:H12	5:A:800:XJH:C5'	2.20	0.69
1:B:465:ARG:NH2	7:B:1263:HOH:O	2.30	0.65
5:A:800:XJH:C12	5:A:800:XJH:H5'A	2.28	0.60
5:B:800:XJH:C5'	5:B:800:XJH:C12	2.80	0.56
5:B:800:XJH:H5'	5:B:800:XJH:H12	1.87	0.56
1:B:403:TYR:CE1	1:B:407:HIS:CE1	2.98	0.52
5:A:800:XJH:C12	5:A:800:XJH:C5'	2.88	0.51
2:A:750:HEM:O2D	5:A:800:XJH:H16	2.10	0.51
1:A:391:THR:O	1:A:392:SER:OG	2.28	0.50
5:B:800:XJH:C5'	5:B:800:XJH:H12	2.42	0.49
5:B:800:XJH:H5'	5:B:800:XJH:C12	2.45	0.46
1:B:706:TYR:OH	2:B:750:HEM:O1D	2.35	0.45
1:A:475:TRP:NE1	1:A:525:GLN:OE1	2.51	0.44
2:B:750:HEM:O2A	5:B:800:XJH:H4'	2.18	0.43
1:B:605:ASN:ND2	7:B:1195:HOH:O	2.53	0.42
1:B:445:HIS:C	1:B:445:HIS:CD2	2.94	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	404/422 (96%)	393 (97%)	10 (2%)	1 (0%)	56	44
1	B	410/422 (97%)	405 (99%)	5 (1%)	0	100	100
All	All	814/844 (96%)	798 (98%)	15 (2%)	1 (0%)	59	48

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	489	ASP

### 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	364/377 (97%)	354 (97%)	10 (3%)	57	47
1	B	369/377 (98%)	365 (99%)	4 (1%)	84	82
All	All	733/754 (97%)	719 (98%)	14 (2%)	69	63

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	350	THR
1	A	380	ARG
1	A	390	SER
1	A	507	GLN
1	A	523	LEU
1	A	547	ARG
1	A	569	ASN
1	A	620	LYS
1	A	645	LYS
1	A	713	THR
1	B	332	MET
1	B	389	GLU
1	B	454	ASN
1	B	547	ARG

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 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	49,50,50	2.38	19 (38%)	46,82,82	2.22	8 (17%)
3	H4B	A	760	-	18,18,18	1.34	2 (11%)	24,26,26	1.92	9 (37%)
5	XJH	A	800	-	30,30,30	0.88	0	40,40,40	1.78	8 (20%)
4	ACT	A	860	-	1,3,3	1.50	0	0,3,3	0.00	-
2	HEM	B	750	1	49,50,50	2.34	18 (36%)	46,82,82	2.16	9 (19%)
3	H4B	B	760	-	18,18,18	1.33	2 (11%)	24,26,26	1.60	5 (20%)
5	XJH	B	800	-	30,30,30	0.85	0	40,40,40	1.76	9 (22%)
4	ACT	B	860	-	1,3,3	1.33	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	-	0/14/114/114	0/0/8/8
3	H4B	A	760	-	-	0/8/17/17	0/0/2/2
5	XJH	A	800	-	-	0/12/22/22	0/4/4/4
4	ACT	A	860	-	-	0/0/0/0	0/0/0/0
2	HEM	B	750	1	-	0/14/114/114	0/0/8/8
3	H4B	B	760	-	-	0/8/17/17	0/0/2/2
5	XJH	B	800	-	-	0/12/22/22	0/4/4/4
4	ACT	B	860	-	-	0/0/0/0	0/0/0/0

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	750	HEM	C3C-C2C	-6.20	1.32	1.43
2	A	750	HEM	C3D-C4D	-5.75	1.43	1.44
2	A	750	HEM	C3B-C2B	-5.72	1.33	1.43
2	B	750	HEM	C3B-C2B	-5.38	1.34	1.43
2	B	750	HEM	C3C-CAC	4.93	1.55	1.40
2	A	750	HEM	C3C-C2C	-4.81	1.35	1.43
2	A	750	HEM	C3B-CAB	4.63	1.55	1.40
2	A	750	HEM	C3C-CAC	4.59	1.54	1.40
2	B	750	HEM	C3B-CAB	4.57	1.54	1.40
3	A	760	H4B	C2-N2	4.36	1.39	1.32
2	A	750	HEM	C3D-C2D	4.32	1.51	1.43
2	B	750	HEM	C4A-C3A	4.14	1.45	1.40
2	A	750	HEM	C4A-C3A	4.04	1.45	1.40
2	B	750	HEM	C3D-C2D	3.86	1.50	1.43
2	A	750	HEM	FE-NC	3.63	2.11	1.97
2	B	750	HEM	C2D-C1D	3.60	1.45	1.44
3	B	760	H4B	C7-C6	3.56	1.56	1.52
2	B	750	HEM	CMD-C2D	3.38	1.57	1.47
2	B	750	HEM	C3B-C4B	3.14	1.48	1.44
2	B	750	HEM	FE-NC	2.84	2.08	1.97
2	B	750	HEM	CMC-C2C	2.82	1.56	1.47
2	A	750	HEM	CMB-C2B	2.78	1.56	1.47
2	A	750	HEM	CMD-C2D	2.74	1.55	1.47
2	B	750	HEM	CMB-C2B	2.70	1.55	1.47
2	A	750	HEM	CMC-C2C	2.59	1.55	1.47
2	A	750	HEM	FE-ND	2.53	2.07	1.97
2	A	750	HEM	FE-NA	2.46	2.02	1.92
2	A	750	HEM	C3B-C4B	2.33	1.47	1.44
2	A	750	HEM	CHA-C4D	2.29	1.39	1.35
2	A	750	HEM	C2D-C1D	2.27	1.45	1.44
2	A	750	HEM	FE-NB	2.23	2.06	1.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	750	HEM	C2B-C1B	2.22	1.45	1.44
2	B	750	HEM	CAA-C2A	2.21	1.55	1.52
2	A	750	HEM	CHD-C4C	2.21	1.40	1.36
2	B	750	HEM	CHA-C4D	2.15	1.38	1.35
3	A	760	H4B	C2-N1	2.10	1.36	1.33
2	B	750	HEM	FE-NA	2.09	2.01	1.92
2	B	750	HEM	FE-NB	2.08	2.05	1.97
2	B	750	HEM	FE-ND	2.04	2.05	1.97
3	B	760	H4B	C2-N2	2.02	1.35	1.32
2	B	750	HEM	CHD-C4C	2.01	1.39	1.36

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	750	HEM	C3B-C4B-NB	-9.94	106.89	114.00
2	A	750	HEM	C3B-C4B-NB	-8.70	107.78	114.00
2	A	750	HEM	C4D-ND-C1D	6.02	111.32	105.16
5	B	800	XJH	O10-C4'-C3'	5.00	121.84	108.14
5	B	800	XJH	C07-C3'-C4'	4.66	120.72	113.47
5	A	800	XJH	C02-N01-C06	4.65	121.50	118.23
2	B	750	HEM	CBA-CAA-C2A	-4.64	104.52	112.69
5	A	800	XJH	C07-C3'-C4'	4.57	120.57	113.47
2	A	750	HEM	CBA-CAA-C2A	-4.54	104.69	112.69
3	B	760	H4B	C4-C4A-C8A	4.48	118.71	114.56
2	A	750	HEM	CBD-CAD-C3D	-4.24	105.13	114.37
3	A	760	H4B	C4-C4A-C8A	4.21	118.46	114.56
2	A	750	HEM	C2D-C1D-ND	-4.14	108.04	112.93
2	B	750	HEM	C4A-CHB-C1B	-4.13	122.04	127.47
5	A	800	XJH	O10-C4'-C3'	4.03	119.19	108.14
2	B	750	HEM	C4D-ND-C1D	3.94	109.19	105.16
3	A	760	H4B	C2-N1-C8A	3.59	122.71	117.61
5	B	800	XJH	C02-N01-C06	3.31	120.55	118.23
3	A	760	H4B	N2-C2-N3	3.30	121.49	117.86
2	A	750	HEM	C4A-CHB-C1B	-3.25	123.20	127.47
5	B	800	XJH	C5'-N1'-C2'	3.22	114.04	105.92
5	B	800	XJH	C07-C06-N01	3.05	123.28	116.71
2	B	750	HEM	CMA-C3A-C4A	-3.05	123.94	128.62
2	B	750	HEM	CBD-CAD-C3D	-3.00	107.82	114.37
5	B	800	XJH	C2'-C3'-C4'	2.92	107.70	103.07
5	A	800	XJH	C5'-N1'-C2'	2.84	113.09	105.92
2	A	750	HEM	C4C-NC-C1C	2.84	108.48	105.53
5	A	800	XJH	C05-C06-N01	-2.80	118.58	122.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	800	XJH	C07-C06-N01	2.79	122.71	116.71
2	B	750	HEM	C1B-NB-C4B	2.73	107.95	105.16
5	A	800	XJH	N02-C02-N01	2.64	121.65	116.59
5	B	800	XJH	C5'-C4'-C3'	2.60	105.51	103.48
5	B	800	XJH	N02-C02-N01	2.58	121.54	116.59
3	B	760	H4B	C6-C7-N8	-2.53	108.39	111.66
2	B	750	HEM	CAD-C3D-C4D	2.47	128.97	124.53
3	A	760	H4B	N8-C8A-N1	2.46	119.42	115.82
3	A	760	H4B	C9-C6-N5	2.44	114.23	109.69
3	A	760	H4B	C4-C4A-N5	2.39	122.57	119.10
3	B	760	H4B	N8-C8A-N1	2.38	119.31	115.82
3	B	760	H4B	N2-C2-N3	2.31	120.40	117.86
2	B	750	HEM	C2D-C1D-ND	-2.25	110.28	112.93
5	A	800	XJH	C2'-C3'-C4'	2.19	106.54	103.07
3	A	760	H4B	N3-C2-N1	-2.19	118.72	121.78
3	A	760	H4B	C6-C7-N8	-2.15	108.89	111.66
3	A	760	H4B	C4A-C4-N3	2.10	119.45	114.06
2	A	750	HEM	CHD-C1D-ND	2.07	126.31	124.58
3	B	760	H4B	C4-N3-C2	2.06	123.12	119.51
5	B	800	XJH	C03-C02-N02	-2.03	117.66	121.33

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	407/422 (96%)	0.88	62 (15%) 3 3	24, 47, 85, 107	0
1	B	411/422 (97%)	0.29	22 (5%) 25 25	23, 37, 59, 79	0
All	All	818/844 (96%)	0.58	84 (10%) 7 6	23, 41, 79, 107	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	348	VAL	8.9
1	B	300	PHE	8.1
1	A	715	VAL	7.3
1	A	716	TRP	6.3
1	A	355	PHE	6.1
1	A	300	PHE	5.5
1	A	488	PRO	5.4
1	A	350	THR	5.2
1	A	352	ASP	5.0
1	B	619	ARG	4.9
1	A	351	LYS	4.9
1	A	486	LYS	4.9
1	A	391	THR	4.5
1	B	350	THR	4.2
1	A	386	LYS	4.2
1	A	507	GLN	4.1
1	B	620	LYS	4.1
1	A	388	ILE	4.0
1	A	392	SER	3.9
1	A	490	GLY	3.9
1	A	470	HIS	3.8
1	A	382	GLU	3.8
1	A	714	HIS	3.7
1	B	718	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	338	PRO	3.7
1	A	491	SER	3.6
1	A	385	ASN	3.6
1	A	487	GLN	3.6
1	A	469	LYS	3.5
1	A	321	THR	3.4
1	A	393	THR	3.4
1	B	338	PRO	3.4
1	A	567	VAL	3.3
1	A	503	GLU	3.2
1	A	353	GLN	3.1
1	A	506	ILE	3.1
1	A	713	THR	3.0
1	A	299	ARG	3.0
1	B	680	VAL	3.0
1	A	390	SER	2.9
1	B	352	ASP	2.9
1	B	667	ARG	2.9
1	A	467	ASP	2.9
1	A	619	ARG	2.8
1	A	667	ARG	2.8
1	B	616	LEU	2.8
1	A	415	CYS	2.7
1	B	299	ARG	2.7
1	A	373	GLY	2.7
1	A	679	ILE	2.6
1	A	489	ASP	2.6
1	A	389	GLU	2.5
1	A	682	PRO	2.5
1	B	321	THR	2.5
1	B	615	ASP	2.4
1	A	511	LYS	2.4
1	A	593	ILE	2.4
1	A	584	PHE	2.4
1	A	704	PHE	2.4
1	B	351	LYS	2.4
1	A	676	TRP	2.4
1	B	567	VAL	2.3
1	B	679	ILE	2.3
1	A	712	ASN	2.3
1	A	356	PRO	2.3
1	A	680	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	480	ILE	2.3
1	A	643	SER	2.3
1	A	514	ARG	2.2
1	A	677	VAL	2.2
1	B	617	ASP	2.2
1	B	479	LEU	2.2
1	A	494	GLY	2.2
1	A	504	ILE	2.2
1	A	512	ALA	2.2
1	A	485	TYR	2.1
1	B	416	VAL	2.1
1	A	354	LEU	2.1
1	A	468	GLY	2.1
1	B	611	ALA	2.1
1	A	681	PRO	2.1
1	A	370	LYS	2.1
1	A	375	LYS	2.1
1	B	677	VAL	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	XJH	A	800	27/27	0.36	3.95	28,58,83,83	0
4	ACT	A	860	4/4	0.16	3.17	57,57,57,58	0
5	XJH	B	800	27/27	0.26	2.69	29,58,83,83	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	H4B	B	760	17/17	0.19	1.23	25,28,31,33	0
2	HEM	A	750	43/43	0.20	0.92	24,28,35,38	0
3	H4B	A	760	17/17	0.18	0.91	26,29,34,34	0
2	HEM	B	750	43/43	0.17	0.71	20,25,35,38	0
6	ZN	A	900	1/1	0.09	-0.02	33,33,33,33	0
4	ACT	B	860	4/4	0.10	-0.15	41,41,43,45	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.