



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2018 – 04:59 am GMT

PDB ID : 4D3B  
Title : Structure of rat neuronal nitric oxide synthase heme domain in complex with N1-(2-(1H-imidazol-1-yl)pyrimidin-4-yl)-N2-(3- fluorophenethyl)ethane-1,2-diamine  
Authors : Li, H.; Poulos, T.L.  
Deposited on : 2014-10-20  
Resolution : 1.80 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](mailto: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 ⓘ symbol.

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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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

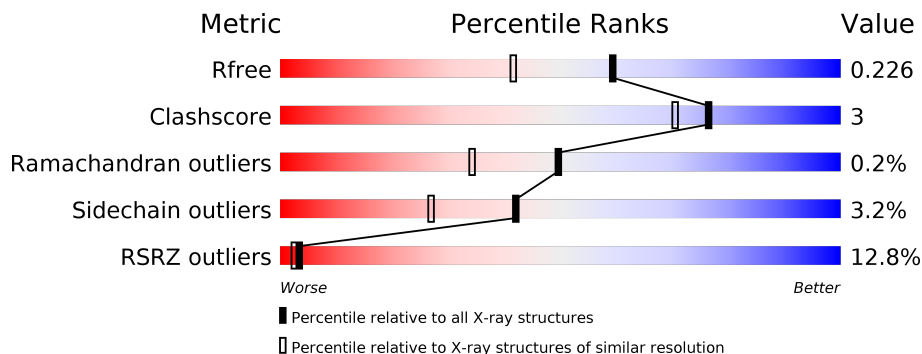
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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))
$R_{free}$	111664	5253 (1.80-1.80)
Clashscore	122126	6077 (1.80-1.80)
Ramachandran outliers	120053	6011 (1.80-1.80)
Sidechain outliers	120020	6010 (1.80-1.80)
RSRZ outliers	108989	5157 (1.80-1.80)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	422	<div> <div>18%</div> <div> <div></div> <div>86%</div> <div>10%</div> <div></div> </div> </div>
1	B	422	<div> <div>7%</div> <div> <div></div> <div>89%</div> <div>7%</div> <div></div> </div> </div>

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 7409 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	408	Total	C	N	O	S	0	4	1
			3329	2131	567	609	22			
1	B	411	Total	C	N	O	S	0	4	0
			3360	2150	574	615	21			

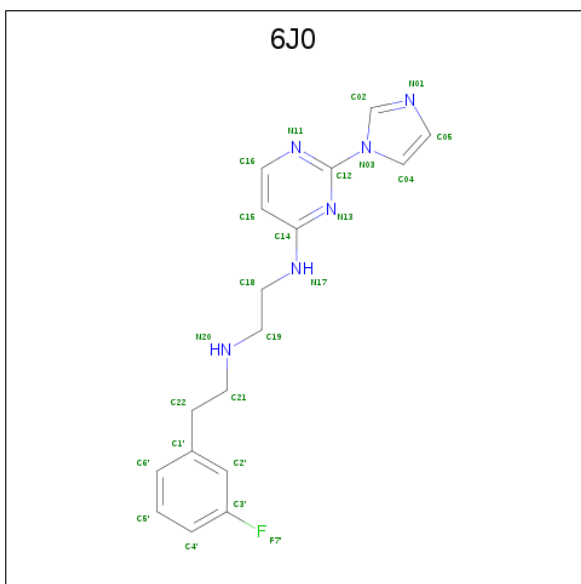
- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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 N-[2-(3-fluorophenyl)ethyl]-N'-[2-(1H-imidazol-1-yl)pyrimidin-4-yl]ethane-1,2-diamine (three-letter code: 6J0) (formula: C<sub>17</sub>H<sub>19</sub>FN<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	F	N	0	0
			24	17	1	6		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	F	N	0	0
			24	17	1	6		

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



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 ZINC ION (three-letter code: ZN) (formula:  $Zn$ ).

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

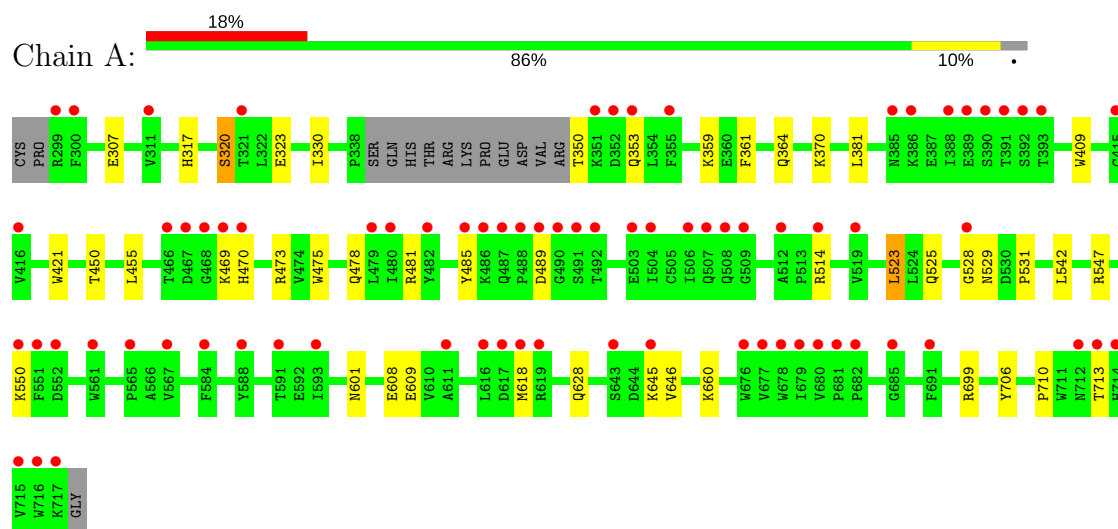
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	245	Total	O	0	0
			245	245		
7	B	298	Total	O	0	0
			298	298		

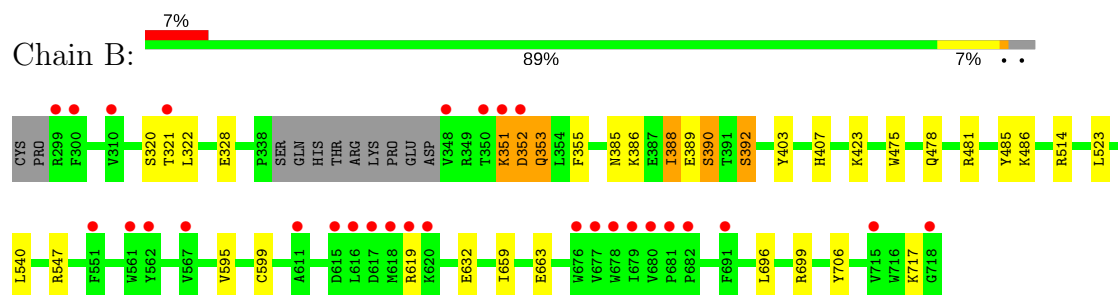
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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, BRAIN



#### • Molecule 1: NITRIC OXIDE SYNTHASE, BRAIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	51.85Å 110.46Å 164.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.87 – 1.80 38.87 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.0 (38.87-1.80) 99.5 (38.87-1.80)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.56 (at 1.79Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.186 , 0.226 0.186 , 0.226	Depositor DCC
$R_{free}$ test set	4381 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.8	Xtriage
Anisotropy	0.695	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 46.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	7409	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.39% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical 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.

## 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, 6J0, H4B, ACT

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	0.35	0/3434	0.51	0/4659
1	B	0.36	0/3465	0.51	0/4697
All	All	0.36	0/6899	0.51	0/9356

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-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 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	3329	0	3242	24	0
1	B	3360	0	3280	17	0
2	A	43	0	30	3	0
2	B	43	0	30	4	0
3	A	17	0	15	0	0
3	B	17	0	15	0	0
4	A	24	0	19	0	0
4	B	24	0	19	1	0
5	A	4	0	3	0	0
5	B	4	0	3	0	0
6	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	245	0	0	2	0
7	B	298	0	0	1	0
All	All	7409	0	6656	44	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 (44) 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)
1:A:706:TYR:OH	2:A:750:HEM:O2D	1.98	0.79
1:B:706:TYR:OH	2:B:750:HEM:O2D	2.00	0.79
1:A:523:LEU:HD22	1:A:531:PRO:HB2	1.62	0.79
1:B:478:GLN:HB2	1:B:481:ARG:HG3	1.70	0.72
2:B:750:HEM:HHC	2:B:750:HEM:HBB2	1.75	0.69
2:B:750:HEM:HBC2	2:B:750:HEM:HMC2	1.78	0.66
1:B:322:LEU:HD13	1:B:699:ARG:HH21	1.61	0.66
1:A:628:GLN:NE2	1:B:632:GLU:OE2	2.28	0.65
2:A:750:HEM:HMC2	2:A:750:HEM:HBC2	1.77	0.64
2:A:750:HEM:HBB2	2:A:750:HEM:HHC	1.82	0.61
1:B:486:LYS:NZ	7:B:2188:HOH:O	2.34	0.61
1:A:307[B]:GLU:OE2	7:A:2010:HOH:O	2.16	0.60
1:A:478:GLN:HB2	1:A:481:ARG:HG3	1.85	0.59
1:B:388:ILE:O	1:B:392:SER:N	2.32	0.56
1:A:475:TRP:HB2	1:A:523:LEU:HB3	1.89	0.54
1:B:355:PHE:CE1	1:B:385:ASN:HB2	2.46	0.51
1:A:323:GLU:HG2	1:B:328:GLU:HB3	1.92	0.50
1:B:386:LYS:O	1:B:390:SER:HB3	2.14	0.48
1:A:330:ILE:HD11	1:B:696:LEU:HB3	1.96	0.48
1:B:485:TYR:CE2	1:B:514:ARG:HA	2.48	0.48
1:B:351:LYS:NZ	1:B:389:GLU:HA	2.29	0.48
1:A:470:HIS:HA	1:A:528:GLY:HA3	1.97	0.47
1:B:403:TYR:CE1	1:B:407:HIS:CE1	3.03	0.47
1:A:370:LYS:HE3	1:A:370:LYS:HB2	1.69	0.45
1:A:361:PHE:O	1:A:364:GLN:HG2	2.17	0.44
2:B:750:HEM:CHC	2:B:750:HEM:HBB2	2.46	0.44
1:B:659:ILE:O	1:B:663:GLU:HG3	2.17	0.44
1:A:473:ARG:NH2	1:A:710:PRO:HD3	2.33	0.43
4:B:800:6J0:H15	4:B:800:6J0:H18	1.86	0.43
1:A:608:GLU:HG3	1:A:618:MET:HE1	2.01	0.43
1:B:595:VAL:O	1:B:599:CYS:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:353:GLN:HG2	1:B:353:GLN:H	1.61	0.42
1:A:359:LYS:HZ3	1:A:381:LEU:HD21	1.84	0.42
1:A:450:THR:HA	1:A:455:LEU:HD22	2.01	0.42
1:A:542:LEU:HD21	1:A:646:VAL:HG22	2.02	0.41
1:A:409:TRP:CE3	1:A:421:TRP:HA	2.55	0.41
1:A:317:HIS:O	1:A:320:SER:HB3	2.21	0.41
1:A:350:THR:N	1:A:353:GLN:HE21	2.19	0.41
1:A:350:THR:OG1	1:A:353:GLN:HG3	2.21	0.41
1:A:525:GLN:HG3	1:A:529:ASN:O	2.21	0.41
1:B:475:TRP:HB2	1:B:523:LEU:HB3	2.03	0.41
1:A:475:TRP:CZ2	1:A:531:PRO:HG3	2.56	0.40
1:A:485:TYR:CE2	1:A:514:ARG:HA	2.57	0.40
1:A:609:GLU:HG3	7:A:2190:HOH:O	2.22	0.40

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	408/422 (97%)	398 (98%)	10 (2%)	0	100	100
1	B	411/422 (97%)	403 (98%)	6 (2%)	2 (0%)	31	16
All	All	819/844 (97%)	801 (98%)	16 (2%)	2 (0%)	49	34

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	352	ASP
1	B	388	ILE

### 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	367/377 (97%)	356 (97%)	11 (3%)	44	29
1	B	370/377 (98%)	358 (97%)	12 (3%)	42	27
All	All	737/754 (98%)	714 (97%)	23 (3%)	42	28

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

Mol	Chain	Res	Type
1	A	320	SER
1	A	469	LYS
1	A	489	ASP
1	A	523	LEU
1	A	547	ARG
1	A	550	LYS
1	A	601	ASN
1	A	645	LYS
1	A	660	LYS
1	A	699	ARG
1	A	713	THR
1	B	320	SER
1	B	321	THR
1	B	351	LYS
1	B	352	ASP
1	B	353	GLN
1	B	390	SER
1	B	392	SER
1	B	423	LYS
1	B	540	LEU
1	B	547	ARG
1	B	619	ARG
1	B	717	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	440	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 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	1,4	27,50,50	2.06	5 (18%)	17,82,82	2.44	4 (23%)
3	H4B	A	760	-	15,18,18	0.84	0	11,26,26	2.61	6 (54%)
4	6J0	A	800	2	25,26,26	1.32	4 (16%)	30,33,33	2.30	13 (43%)
5	ACT	A	860	-	1,3,3	1.16	0	0,3,3	0.00	-
2	HEM	B	750	1,4	27,50,50	2.10	5 (18%)	17,82,82	2.09	4 (23%)
3	H4B	B	760	-	15,18,18	0.83	1 (6%)	11,26,26	2.48	4 (36%)
4	6J0	B	800	2	25,26,26	1.19	4 (16%)	30,33,33	2.34	14 (46%)
5	ACT	B	860	-	1,3,3	1.03	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	1,4	-	0/6/54/54	0/0/8/8
3	H4B	A	760	-	-	0/8/17/17	0/2/2/2
4	6J0	A	800	2	-	0/9/13/13	0/3/3/3
5	ACT	A	860	-	-	0/0/0/0	0/0/0/0
2	HEM	B	750	1,4	-	0/6/54/54	0/0/8/8
3	H4B	B	760	-	-	0/8/17/17	0/2/2/2
4	6J0	B	800	2	-	0/9/13/13	0/3/3/3
5	ACT	B	860	-	-	0/0/0/0	0/0/0/0

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	750	HEM	C3B-C2B	-4.47	1.34	1.40
2	B	750	HEM	C3B-C2B	-4.26	1.34	1.40
2	B	750	HEM	C3C-C2C	-3.92	1.34	1.40
4	A	800	6J0	C04-N03	-3.70	1.33	1.39
2	A	750	HEM	C3C-C2C	-3.47	1.35	1.40
4	B	800	6J0	C04-N03	-3.22	1.34	1.39
4	A	800	6J0	C02-N03	-3.02	1.33	1.36
4	B	800	6J0	C02-N03	-2.90	1.33	1.36
3	B	760	H4B	C4-C4A	-2.17	1.38	1.41
4	B	800	6J0	C12-N13	2.24	1.35	1.32
4	B	800	6J0	C12-N11	2.37	1.35	1.31
4	A	800	6J0	C12-N13	2.71	1.36	1.32
4	A	800	6J0	C12-N11	2.74	1.35	1.31
2	A	750	HEM	C3B-CAB	3.69	1.55	1.47
2	B	750	HEM	C3B-CAB	3.75	1.55	1.47
2	A	750	HEM	C3C-CAC	3.95	1.55	1.47
2	B	750	HEM	C3C-CAC	4.02	1.55	1.47
2	B	750	HEM	C3D-C2D	4.77	1.51	1.37
2	A	750	HEM	C3D-C2D	5.00	1.52	1.37

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	750	HEM	CBD-CAD-C3D	-7.07	98.98	112.47
2	A	750	HEM	CBA-CAA-C2A	-5.34	102.27	112.48
2	B	750	HEM	CBD-CAD-C3D	-4.60	103.69	112.47
4	B	800	6J0	C18-N17-C14	-4.40	116.57	123.51
4	A	800	6J0	N11-C12-N13	-4.24	121.11	126.08
4	B	800	6J0	N11-C12-N13	-3.98	121.41	126.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	750	HEM	CBA-CAA-C2A	-3.97	104.89	112.48
2	B	750	HEM	C1D-C2D-C3D	-3.86	104.31	107.00
4	A	800	6J0	C15-C16-N11	-3.55	119.60	123.92
4	B	800	6J0	C15-C16-N11	-3.23	120.00	123.92
3	A	760	H4B	N3-C2-N1	-3.00	120.67	125.43
3	B	760	H4B	N3-C2-N1	-2.96	120.73	125.43
4	A	800	6J0	C18-N17-C14	-2.88	118.97	123.51
4	A	800	6J0	C04-N03-C12	-2.87	122.25	125.50
4	B	800	6J0	C15-C14-N13	-2.67	118.66	123.18
4	B	800	6J0	C02-N03-C12	-2.64	120.83	126.02
2	A	750	HEM	C1D-C2D-C3D	-2.62	105.17	107.00
2	B	750	HEM	CAD-CBD-CGD	-2.52	108.35	112.66
4	A	800	6J0	C15-C14-N13	-2.21	119.44	123.18
4	A	800	6J0	C02-N03-C12	-2.17	121.76	126.02
4	B	800	6J0	C04-N03-C12	-2.14	123.09	125.50
4	A	800	6J0	C4'-C3'-C2'	-2.06	120.57	123.29
4	B	800	6J0	C4'-C3'-C2'	-2.04	120.61	123.29
4	B	800	6J0	C05-C04-N03	-2.03	102.92	106.50
3	A	760	H4B	C4A-N5-C6	-2.02	115.65	121.16
2	A	750	HEM	CMC-C2C-C3C	2.04	128.60	124.88
3	A	760	H4B	N2-C2-N1	2.11	120.56	117.25
4	A	800	6J0	N17-C14-N13	2.29	120.34	116.39
3	B	760	H4B	C2-N1-C8A	2.44	119.99	114.50
3	A	760	H4B	C2-N1-C8A	2.56	120.25	114.50
4	B	800	6J0	N17-C14-N13	2.64	120.95	116.39
4	A	800	6J0	N11-C12-N03	2.84	119.22	114.81
4	B	800	6J0	N13-C12-N03	3.05	118.73	114.78
4	B	800	6J0	N11-C12-N03	3.24	119.83	114.81
3	B	760	H4B	C4-N3-C2	3.45	121.02	116.06
3	A	760	H4B	C4-N3-C2	3.64	121.29	116.06
4	A	800	6J0	C16-C15-C14	3.73	119.28	116.78
4	B	800	6J0	C16-C15-C14	3.75	119.29	116.78
4	A	800	6J0	N13-C12-N03	3.79	119.68	114.78
4	A	800	6J0	C04-N03-C02	4.13	115.98	108.50
4	B	800	6J0	C04-N03-C02	4.16	116.04	108.50
4	B	800	6J0	C16-N11-C12	4.49	119.98	114.04
4	A	800	6J0	C16-N11-C12	4.93	120.56	114.04
3	B	760	H4B	C4-C4A-C8A	5.49	119.53	114.56
3	A	760	H4B	C4-C4A-C8A	5.78	119.79	114.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	750	HEM	3	0
2	B	750	HEM	4	0
4	B	800	6J0	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

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%)	0.94	76 (18%) <b>1</b> <b>1</b>	13, 33, 69, 101	0
1	B	411/422 (97%)	0.40	29 (7%) <b>16</b> <b>12</b>	11, 25, 52, 77	0
All	All	819/844 (97%)	0.67	105 (12%) <b>3</b> <b>2</b>	11, 28, 65, 101	0

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	717	LYS	8.7
1	A	715	VAL	8.1
1	A	716	TRP	7.2
1	B	300	PHE	7.2
1	A	488	PRO	7.0
1	A	490	GLY	5.4
1	A	355	PHE	5.4
1	A	391	THR	4.9
1	A	388	ILE	4.8
1	B	620	LYS	4.6
1	A	300	PHE	4.5
1	A	619	ARG	4.5
1	A	486	LYS	4.4
1	B	348	VAL	4.4
1	A	677	VAL	4.2
1	A	351	LYS	4.2
1	A	507	GLN	4.1
1	B	619	ARG	4.1
1	A	678	TRP	3.9
1	A	321	THR	3.8
1	A	352	ASP	3.8
1	A	680	VAL	3.8
1	A	676	TRP	3.7
1	A	713	THR	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	551	PHE	3.7
1	A	616	LEU	3.6
1	B	616	LEU	3.6
1	B	321	THR	3.6
1	A	299	ARG	3.5
1	B	350	THR	3.5
1	A	681	PRO	3.4
1	B	611	ALA	3.4
1	A	679	ILE	3.3
1	A	480	ILE	3.3
1	B	679	ILE	3.3
1	A	508	GLN	3.3
1	B	618	MET	3.2
1	A	489	ASP	3.2
1	A	611	ALA	3.2
1	B	677	VAL	3.2
1	A	714	HIS	3.2
1	A	503	GLU	3.2
1	A	567	VAL	3.2
1	A	593	ILE	3.2
1	B	718	GLY	3.2
1	B	680	VAL	3.1
1	B	617	ASP	3.1
1	A	552	ASP	3.0
1	A	588	TYR	3.0
1	A	504	ILE	3.0
1	A	584	PHE	3.0
1	A	528	GLY	2.9
1	A	385	ASN	2.9
1	A	509	GLY	2.9
1	A	386	LYS	2.9
1	B	561	TRP	2.9
1	B	715	VAL	2.8
1	A	390	SER	2.8
1	A	561	TRP	2.8
1	A	712	ASN	2.8
1	B	691	PHE	2.8
1	B	676	TRP	2.8
1	A	506	ILE	2.7
1	A	469	LYS	2.7
1	B	682	PRO	2.7
1	B	352	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	470	HIS	2.6
1	A	487	GLN	2.6
1	B	615	ASP	2.6
1	A	682	PRO	2.6
1	B	310	VAL	2.5
1	A	389	GLU	2.5
1	B	562	TYR	2.4
1	A	416	VAL	2.4
1	B	681	PRO	2.4
1	A	485	TYR	2.4
1	A	643	SER	2.4
1	A	691	PHE	2.4
1	A	491	SER	2.4
1	A	685	GLY	2.4
1	A	466	THR	2.4
1	B	551	PHE	2.3
1	A	468	GLY	2.3
1	A	467	ASP	2.2
1	A	482	TYR	2.2
1	A	311	VAL	2.2
1	B	678	TRP	2.2
1	A	415	CYS	2.2
1	A	645	LYS	2.2
1	A	492	THR	2.2
1	A	618	MET	2.2
1	A	514	ARG	2.2
1	A	512	ALA	2.2
1	A	550	LYS	2.1
1	A	479	LEU	2.1
1	A	591	THR	2.1
1	A	392	SER	2.1
1	B	299	ARG	2.1
1	A	393	THR	2.0
1	A	617	ASP	2.0
1	A	353	GLN	2.0
1	A	565	PRO	2.0
1	B	351	LYS	2.0
1	A	519	VAL	2.0
1	B	567	VAL	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 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. 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	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	ACT	A	860	4/4	0.90	0.14	38,43,44,45	0
4	6J0	A	800	24/24	0.91	0.22	23,33,59,60	0
4	6J0	B	800	24/24	0.94	0.17	20,34,45,54	0
5	ACT	B	860	4/4	0.94	0.11	31,32,37,40	0
3	H4B	A	760	17/17	0.95	0.17	10,15,19,21	0
3	H4B	B	760	17/17	0.96	0.16	11,14,19,20	0
2	HEM	B	750	43/43	0.97	0.15	8,16,28,37	0
2	HEM	A	750	43/43	0.97	0.18	9,17,26,36	0
6	ZN	A	1717	1/1	1.00	0.04	19,19,19,19	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.