



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:48 PM GMT

PDB ID : 4FVW  
Title : Structure of rat nNOS heme domain in complex with N(omega)-methoxy-L-arginine  
Authors : Li, H.; Poulos, T.L.  
Deposited on : 2012-06-29  
Resolution : 1.81 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  
<http://wwpdb.org/validation/2016/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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

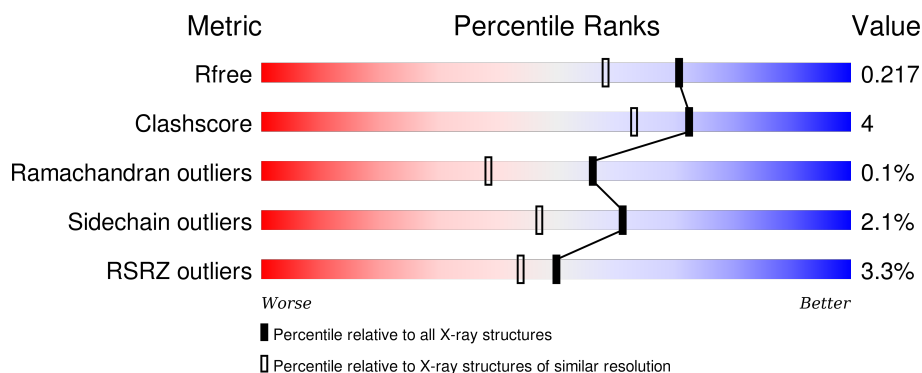
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*



The reported resolution of this entry is 1.81 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))
$R_{free}$	91344	5422 (1.84-1.80)
Clashscore	102246	6347 (1.84-1.80)
Ramachandran outliers	100387	6276 (1.84-1.80)
Sidechain outliers	100360	6276 (1.84-1.80)
RSRZ outliers	91569	5439 (1.84-1.80)

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	 4% 85% 9% . .
1	B	422	 2% 91% 6% . .

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	1KJ	A	803[A]	-	-	-	X
4	1KJ	A	803[B]	-	-	X	X
5	ACT	A	804	-	-	-	X

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 7229 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	3	6	0
			3336	2136	567	611	22			
1	B	411	Total	C	N	O	S	0	4	0
			3360	2150	574	614	22			

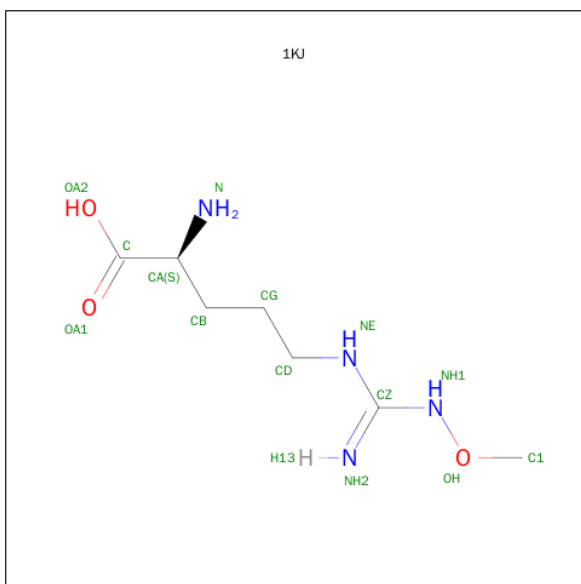
- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).





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

- Molecule 4 is N 5 -(N-METHOXYCARBAMIMIDOYL)-L-ORNITHINE (three-letter code: 1KJ) (formula:  $C_7H_{16}N_4O_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	1
			15	8	4	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	1
			15	8	4	3		

- 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		

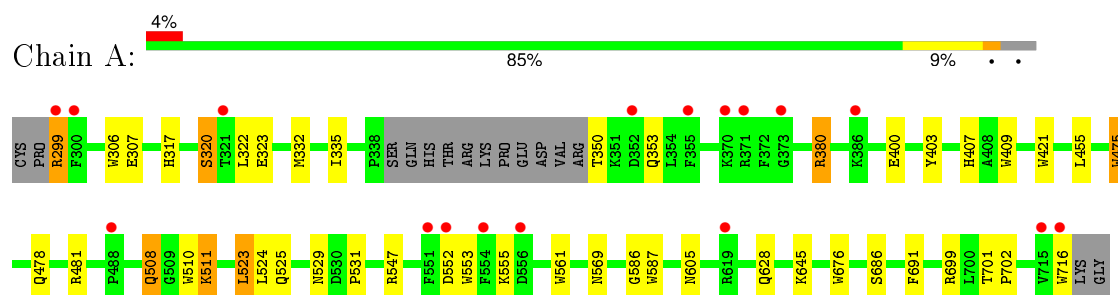
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	159	Total	O	0	1
			159	159		
7	B	215	Total	O	0	1
			215	215		

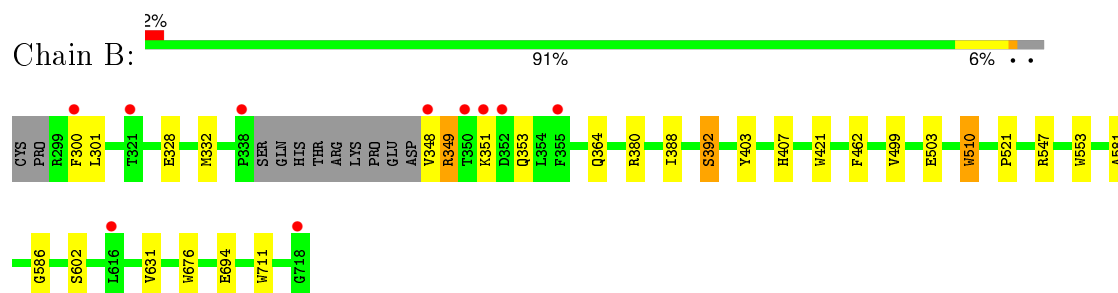
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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, 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, $\alpha$ , $\beta$ , $\gamma$	52.15Å 111.00Å 165.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.81 49.73 – 1.81	Depositor EDS
% Data completeness (in resolution range)	99.3 (50.00-1.81) 99.4 (49.73-1.81)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.15 (at 1.81Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.181 , 0.218 0.180 , 0.217	Depositor DCC
$R_{free}$ test set	4379 reflections (5.23%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.5	Xtriage
Anisotropy	0.569	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 43.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 88358 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	7229	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.74% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 1KJ, ZN, H4B, HEM, 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	0.74	9/3447 (0.3%)	0.69	0/4676
1	B	0.79	5/3465 (0.1%)	0.73	1/4697 (0.0%)
All	All	0.77	14/6912 (0.2%)	0.71	1/9373 (0.0%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	409	TRP	CD2-CE2	5.56	1.48	1.41
1	B	676	TRP	CD2-CE2	5.42	1.47	1.41
1	A	421	TRP	CD2-CE2	5.37	1.47	1.41
1	A	306	TRP	CD2-CE2	5.34	1.47	1.41
1	A	676	TRP	CD2-CE2	5.31	1.47	1.41
1	A	561	TRP	CD2-CE2	5.28	1.47	1.41
1	A	553	TRP	CD2-CE2	5.24	1.47	1.41
1	B	421	TRP	CD2-CE2	5.19	1.47	1.41
1	B	553	TRP	CD2-CE2	5.19	1.47	1.41
1	B	510	TRP	CD2-CE2	5.19	1.47	1.41
1	A	716	TRP	CD2-CE2	5.19	1.47	1.41
1	B	711	TRP	CD2-CE2	5.14	1.47	1.41
1	A	510	TRP	CD2-CE2	5.13	1.47	1.41
1	A	475	TRP	CD2-CE2	5.13	1.47	1.41

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	380	ARG	NE-CZ-NH2	-5.33	117.64	120.30

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	3336	0	3253	35	0
1	B	3360	0	3280	22	0
2	A	43	0	30	4	0
2	B	43	0	30	3	0
3	A	17	0	15	0	0
3	B	17	0	15	0	0
4	A	15	0	6	7	0
4	B	15	0	6	5	0
5	A	4	0	3	0	0
5	B	4	0	3	0	0
6	A	1	0	0	0	0
7	A	159	0	0	2	0
7	B	215	0	0	2	0
All	All	7229	0	6641	57	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 4.

All (57) 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:B:586:GLY:H	4:B:803[B]:1KJ:H16	1.24	1.02
1:A:307[B]:GLU:OE1	1:B:602[B]:SER:CB	2.16	0.93
1:B:586:GLY:N	4:B:803[B]:1KJ:H16	1.82	0.93
1:A:307[B]:GLU:OE1	1:B:602[B]:SER:OG	1.89	0.89
1:A:307[B]:GLU:OE1	1:B:602[B]:SER:HB3	1.78	0.82
1:A:508:GLN:HA	1:A:508:GLN:HE21	1.46	0.80
2:A:801:HEM:HMC2	2:A:801:HEM:HBC2	1.69	0.73
1:A:508:GLN:HE21	1:A:508:GLN:CA	2.01	0.71
1:A:508:GLN:HA	1:A:508:GLN:NE2	2.07	0.70
2:A:801:HEM:C4B	4:A:803[B]:1KJ:H18	2.26	0.70
1:B:348:VAL:O	1:B:349:ARG:HB2	1.92	0.68
1:B:586:GLY:CA	4:B:803[B]:1KJ:H16	2.27	0.65
1:A:586:GLY:CA	4:A:803[B]:1KJ:H16	2.29	0.63
1:B:300:PHE:HB3	7:B:1084:HOH:O	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:586:GLY:N	4:A:803[B]:1KJ:H16	2.17	0.59
1:B:499:VAL:O	1:B:503:GLU:HG3	2.02	0.59
1:A:523:LEU:HD22	1:A:531:PRO:HB2	1.85	0.58
1:A:586:GLY:H	4:A:803[B]:1KJ:H16	1.71	0.56
2:A:801:HEM:CHC	4:A:803[B]:1KJ:H18	2.36	0.56
1:B:586:GLY:CA	4:B:803[B]:1KJ:C1	2.85	0.54
1:A:525:GLN:HG3	1:A:529:ASN:O	2.08	0.54
1:A:508:GLN:NE2	1:A:508:GLN:CA	2.70	0.54
1:A:323:GLU:HG2	1:B:328:GLU:HB3	1.90	0.54
1:A:455:LEU:HD12	1:A:587:TRP:HB3	1.91	0.53
1:A:380:ARG:HD3	1:A:400:GLU:OE1	2.09	0.52
1:A:299:ARG:O	1:A:299:ARG:HG2	2.10	0.52
1:A:322:LEU:HD13	1:A:699:ARG:HH21	1.76	0.49
1:A:628:GLN:HG2	1:B:631:VAL:HG11	1.93	0.49
2:A:801:HEM:CMC	2:A:801:HEM:HBC2	2.42	0.49
1:B:403:TYR:CE1	1:B:407:HIS:CE1	3.01	0.48
1:B:388:ILE:O	1:B:392:SER:HA	2.13	0.48
1:B:586:GLY:HA3	4:B:803[B]:1KJ:C1	2.44	0.48
2:B:801:HEM:HBC2	2:B:801:HEM:CMC	2.44	0.48
1:A:335:ILE:HD13	1:B:694:GLU:HB3	1.95	0.47
1:A:317:HIS:O	1:A:320:SER:HB3	2.16	0.46
1:A:332:MET:HE3	1:B:301:LEU:HD22	1.98	0.45
1:A:475:TRP:HB2	1:A:523:LEU:HB3	1.98	0.44
1:A:350:THR:N	1:A:353:GLN:HE21	2.15	0.44
1:A:701:THR:HA	1:A:702:PRO:C	2.38	0.44
1:A:350:THR:OG1	1:A:353:GLN:HG3	2.17	0.43
1:A:686:SER:HA	1:A:691:PHE:CG	2.53	0.43
1:B:462:PHE:HB2	1:B:581:ALA:HB3	1.99	0.43
2:B:801:HEM:CBB	2:B:801:HEM:HHC	2.49	0.43
1:A:332:MET:CE	1:B:301:LEU:HD22	2.48	0.42
1:A:403:TYR:CE1	1:A:407:HIS:CE1	3.07	0.42
1:A:478:GLN:HB2	1:A:481:ARG:HG3	2.00	0.42
1:A:511:LYS:HG3	1:A:511:LYS:O	2.19	0.42
1:B:348:VAL:O	1:B:349:ARG:CB	2.64	0.41
1:A:555:LYS:N	7:A:1025:HOH:O	2.53	0.41
2:B:801:HEM:HBB2	2:B:801:HEM:HHC	2.03	0.41
1:B:510:TRP:CE2	1:B:521:PRO:HD3	2.56	0.41
1:B:364:GLN:NE2	7:B:1031:HOH:O	2.50	0.41
1:A:455:LEU:HD12	1:A:587:TRP:CB	2.49	0.40
1:A:605:ASN:ND2	7:A:916:HOH:O	2.48	0.40
1:A:586:GLY:HA3	4:A:803[B]:1KJ:H16	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:524:LEU:O	1:A:531:PRO:HA	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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	409/422 (97%)	400 (98%)	9 (2%)	0	100	100
1	B	411/422 (97%)	403 (98%)	7 (2%)	1 (0%)	52	35
All	All	820/844 (97%)	803 (98%)	16 (2%)	1 (0%)	56	38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	349	ARG

### 5.3.2 Protein sidechains [i](#)

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	369/377 (98%)	359 (97%)	10 (3%)	52	36
1	B	370/377 (98%)	365 (99%)	5 (1%)	74	65
All	All	739/754 (98%)	724 (98%)	15 (2%)	61	49

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	299	ARG
1	A	320	SER
1	A	380	ARG
1	A	508	GLN
1	A	511	LYS
1	A	523	LEU
1	A	547	ARG
1	A	552	ASP
1	A	569	ASN
1	A	645	LYS
1	B	332	MET
1	B	351	LYS
1	B	353	GLN
1	B	392	SER
1	B	547	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	454	ASN
1	A	508	GLN
1	A	527	ASN
1	A	569	ASN
1	A	605	ASN
1	A	628	GLN
1	A	697	ASN
1	B	364	GLN
1	B	454	ASN
1	B	535	GLN
1	B	601	ASN
1	B	605	ASN
1	B	697	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules 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 11 ligands modelled in this entry, 1 is 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	30,50,50	2.79	13 (43%)	24,82,82	2.77	9 (37%)
3	H4B	A	802	-	13,18,18	0.97	0	11,26,26	2.95	6 (54%)
4	1KJ	A	803[A]	-	6,13,13	0.44	0	3,15,15	0.56	0
4	1KJ	A	803[B]	-	6,13,13	0.35	0	3,15,15	0.56	0
5	ACT	A	804	-	1,3,3	1.69	0	0,3,3	0.00	-
2	HEM	B	801	1	30,50,50	2.56	11 (36%)	24,82,82	2.94	10 (41%)
3	H4B	B	802	-	13,18,18	1.20	1 (7%)	11,26,26	2.67	6 (54%)
4	1KJ	B	803[A]	-	6,13,13	0.58	0	3,15,15	0.15	0
4	1KJ	B	803[B]	-	6,13,13	0.49	0	3,15,15	0.15	0
5	ACT	B	804	-	1,3,3	1.40	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	801	1	-	0/10/54/54	0/0/8/8
3	H4B	A	802	-	-	0/8/17/17	0/2/2/2
4	1KJ	A	803[A]	-	-	0/5/14/14	0/0/0/0
4	1KJ	A	803[B]	-	-	0/5/14/14	0/0/0/0
5	ACT	A	804	-	-	0/0/0/0	0/0/0/0
2	HEM	B	801	1	-	0/10/54/54	0/0/8/8
3	H4B	B	802	-	-	0/8/17/17	0/2/2/2
4	1KJ	B	803[A]	-	-	0/5/14/14	0/0/0/0
4	1KJ	B	803[B]	-	-	0/5/14/14	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ACT	B	804	-	-	0/0/0/0	0/0/0/0

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	HEM	C3B-C4B	-4.48	1.47	1.51
2	B	801	HEM	C3B-C4B	-3.66	1.48	1.51
2	A	801	HEM	C3D-C4D	-3.47	1.47	1.51
2	B	801	HEM	C2D-C3D	-2.89	1.45	1.54
2	B	801	HEM	C3D-C4D	-2.82	1.48	1.51
2	A	801	HEM	C2D-C3D	-2.78	1.46	1.54
2	B	801	HEM	C2C-C1C	-2.72	1.47	1.52
3	B	802	H4B	C7-N8	2.07	1.48	1.46
2	A	801	HEM	FE-ND	2.23	2.09	1.97
2	B	801	HEM	C1A-CHA	2.29	1.46	1.39
2	A	801	HEM	FE-NB	2.55	2.11	1.97
2	B	801	HEM	CHC-C4B	2.56	1.46	1.38
2	B	801	HEM	CHC-C1C	2.62	1.42	1.36
2	A	801	HEM	C4A-CHB	2.70	1.47	1.39
2	A	801	HEM	CHD-C1D	2.72	1.46	1.38
2	A	801	HEM	CHC-C4B	2.82	1.46	1.38
2	B	801	HEM	C2A-C3A	3.17	1.47	1.37
2	A	801	HEM	C2A-C3A	3.44	1.47	1.37
2	A	801	HEM	CHC-C1C	4.19	1.46	1.36
2	B	801	HEM	CHD-C4C	4.25	1.46	1.36
2	B	801	HEM	C4C-NC	5.03	1.42	1.36
2	A	801	HEM	CHD-C4C	5.44	1.49	1.36
2	A	801	HEM	C4C-NC	6.08	1.43	1.36
2	A	801	HEM	C1C-NC	6.86	1.44	1.36
2	B	801	HEM	C1C-NC	7.86	1.45	1.36

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	HEM	CBA-CAA-C2A	-6.53	100.82	112.53
2	A	801	HEM	CBA-CAA-C2A	-4.46	104.54	112.53
3	A	802	H4B	N3-C2-N1	-3.62	119.60	125.53
2	A	801	HEM	C3C-CAC-CBC	-3.49	119.11	124.46
2	B	801	HEM	CBD-CAD-C3D	-3.35	103.80	113.55
2	A	801	HEM	CBD-CAD-C3D	-3.14	104.42	113.55
3	B	802	H4B	N3-C2-N1	-3.12	120.42	125.53
2	B	801	HEM	C3B-CAB-CBB	-2.54	120.55	124.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	HEM	C3C-CAC-CBC	-2.53	120.57	124.46
3	B	802	H4B	C4A-C8A-N8	2.16	120.98	118.43
3	A	802	H4B	N2-C2-N3	2.20	120.85	117.20
3	B	802	H4B	N2-C2-N1	2.36	121.11	117.20
3	B	802	H4B	C2-N1-C8A	2.63	120.46	114.54
2	B	801	HEM	C2C-C1C-NC	2.74	114.83	110.21
2	A	801	HEM	C2C-C1C-NC	2.76	114.86	110.21
2	B	801	HEM	CMD-C2D-C3D	3.23	128.63	114.35
3	A	802	H4B	C4-N3-C2	3.31	120.53	115.94
3	A	802	H4B	C2-N1-C8A	3.47	122.33	114.54
2	A	801	HEM	CMD-C2D-C3D	3.57	130.16	114.35
3	B	802	H4B	C4-N3-C2	3.72	121.10	115.94
3	A	802	H4B	C4A-C8A-N8	4.05	123.21	118.43
2	A	801	HEM	CAD-C3D-C4D	4.40	127.98	112.47
2	A	801	HEM	CMB-C2B-C3B	4.42	127.55	116.53
2	B	801	HEM	CAD-C3D-C4D	4.67	128.94	112.47
2	B	801	HEM	CMC-C2C-C3C	4.98	128.96	116.53
2	B	801	HEM	CAD-C3D-C2D	5.30	128.45	113.22
2	A	801	HEM	CAD-C3D-C2D	5.66	129.48	113.22
3	A	802	H4B	C4-C4A-C8A	5.79	119.80	114.56
2	B	801	HEM	CMB-C2B-C3B	5.84	131.11	116.53
3	B	802	H4B	C4-C4A-C8A	6.06	120.05	114.56
2	A	801	HEM	CMC-C2C-C3C	6.12	131.80	116.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	HEM	4	0
4	A	803[B]	1KJ	7	0
2	B	801	HEM	3	0
4	B	803[B]	1KJ	5	0

## 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%)	0.17	17 (4%) 40 34	27, 50, 90, 120	0
1	B	411/422 (97%)	-0.00	10 (2%) 62 57	27, 40, 66, 97	0
All	All	818/844 (96%)	0.08	27 (3%) 50 44	27, 44, 84, 120	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	300	PHE	7.5
1	A	355	PHE	5.4
1	B	718	GLY	5.1
1	A	488	PRO	4.2
1	B	348	VAL	4.0
1	A	715	VAL	3.6
1	A	321	THR	3.4
1	B	616	LEU	3.3
1	A	373	GLY	3.3
1	A	552	ASP	3.2
1	B	350	THR	3.1
1	B	352	ASP	3.1
1	A	619	ARG	3.0
1	A	551	PHE	3.0
1	A	716	TRP	2.8
1	A	386	LYS	2.8
1	A	299	ARG	2.7
1	B	355	PHE	2.6
1	A	352	ASP	2.6
1	A	300	PHE	2.5
1	A	370	LYS	2.4
1	B	351	LYS	2.3
1	A	556	ASP	2.2
1	B	321	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	338	PRO	2.2
1	A	371	ARG	2.1
1	A	554	PHE	2.1

## 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. 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	ACT	A	804	4/4	0.97	0.12	2.85	48,54,55,55	0
4	1KJ	A	803[B]	14/14	0.93	0.12	2.38	33,36,49,50	1
4	1KJ	A	803[A]	14/14	0.93	0.12	2.38	33,36,49,49	1
2	HEM	A	801	43/43	0.98	0.12	1.52	27,32,36,39	0
4	1KJ	B	803[B]	14/14	0.94	0.13	1.32	28,31,47,49	1
4	1KJ	B	803[A]	14/14	0.94	0.13	1.32	28,31,45,49	1
2	HEM	B	801	43/43	0.99	0.12	1.00	26,30,38,41	0
3	H4B	A	802	17/17	0.96	0.11	0.57	28,30,34,36	0
3	H4B	B	802	17/17	0.96	0.11	0.25	28,30,33,34	0
6	ZN	A	805	1/1	0.99	0.09	-0.29	35,35,35,35	0
5	ACT	B	804	4/4	0.96	0.09	-1.52	42,42,45,48	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.