



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 04:27 AM GMT

PDB ID : 4K5E  
Title : Structure of neuronal nitric oxide synthase heme domain in complex with (R)  
-1,2-bis((2-amino-4-methylpyridin-6-yl)-methoxy)-propan-3-amine  
Authors : Li, H.; Poulos, T.L.  
Deposited on : 2013-04-14  
Resolution : 1.89 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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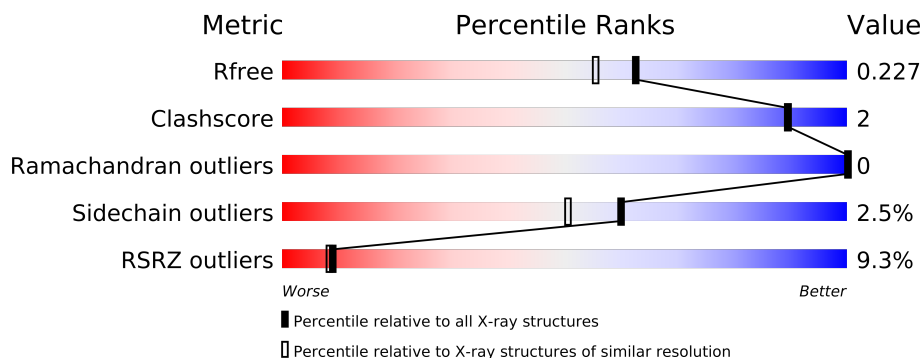
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.89 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	1Q7	A	803	-	X
4	1Q7	B	803	-	X

## 2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 7308 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	407	Total	C	N	O	S	0	2	0
			3316	2121	567	606	22			
1	B	411	Total	C	N	O	S	0	4	0
			3353	2143	575	612	23			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	598	CYS	TYR	CLONING ARTIFACT	UNP P29476
B	598	CYS	TYR	CLONING ARTIFACT	UNP P29476

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



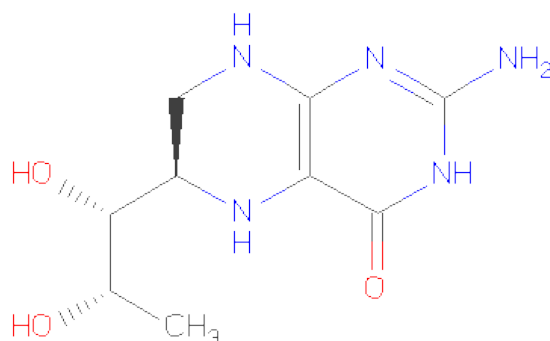
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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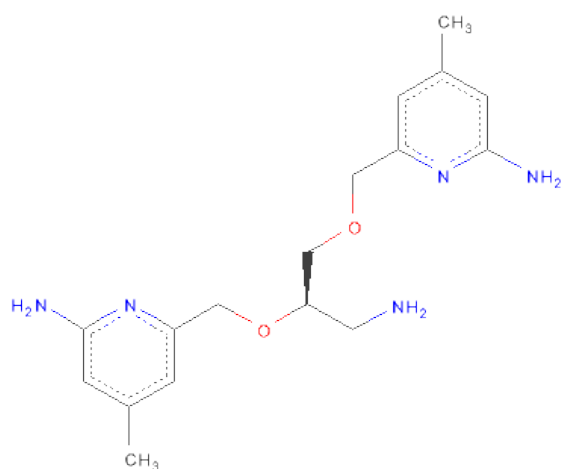
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



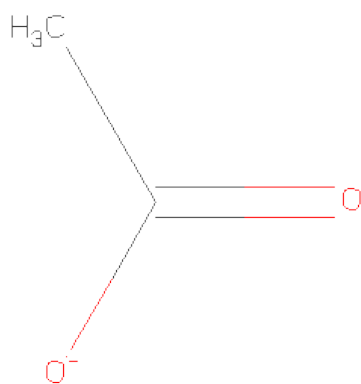
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 4 is 6,6'-{[(2R)-3-AMINOPROPANE-1,2-DIYL]BIS(OXYMETHANEDIYL)}BIS(4-METHYLPYRIDIN-2-AMINE) (three-letter code: 1Q7) (formula:  $C_{17}H_{25}N_5O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			24	17	5	2		
4	B	1	Total	C	N	O	0	0
			24	17	5	2		

- 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 1	Zn 1	0	0

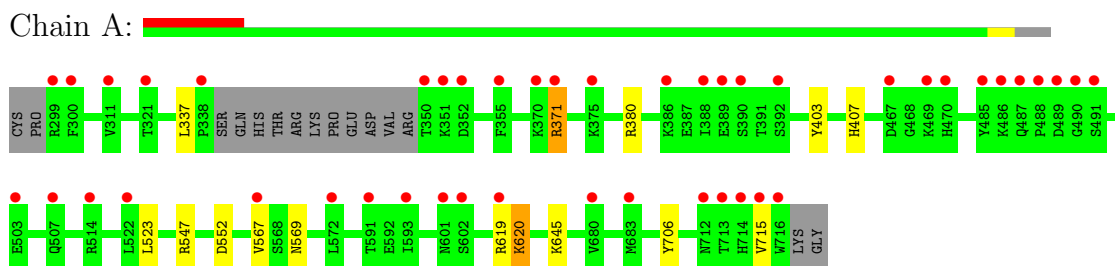
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	178	Total 178	O 178	0	0
7	B	284	Total 284	O 284	0	0

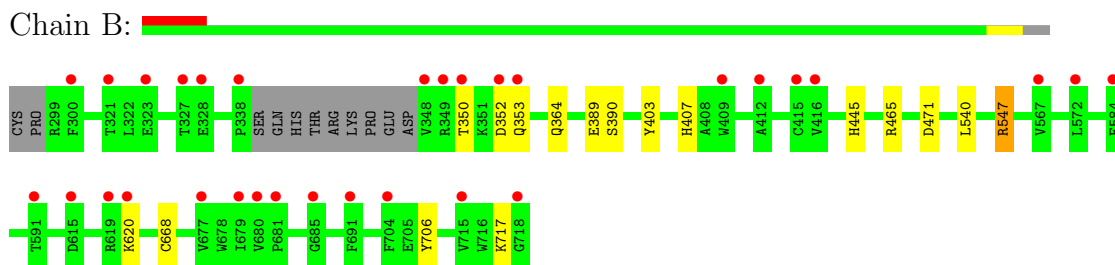
### 3 Residue-property plots

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, 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, $\alpha$ , $\beta$ , $\gamma$	52.00Å 110.67Å 164.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.24 – 1.89 33.65 – 1.89	Depositor EDS
% Data completeness (in resolution range)	98.9 (32.24-1.89) 98.9 (33.65-1.89)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.45 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.180 , 0.212 0.197 , 0.227	Depositor DCC
$R_{free}$ test set	3761 reflections (5.23%)	DCC
Wilson B-factor (Å <sup>2</sup> )	29.6	Xtriage
Anisotropy	0.606	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 32.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 75729 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7308	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.58% 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, 1Q7

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	0.65	0/3414	0.66	0/4633
1	B	0.73	0/3457	0.71	2/4686 (0.0%)
All	All	0.69	0/6871	0.69	2/9319 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	547	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	B	471	ASP	CB-CG-OD2	5.25	123.03	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	6	0
1	B	3353	0	0	7	0
2	A	43	0	0	1	0
2	B	43	0	0	3	0
3	A	17	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	17	0	0	0	0
4	A	24	0	25	1	0
4	B	24	0	25	2	0
5	A	4	0	3	0	0
5	B	4	0	3	0	0
6	A	1	0	0	0	0
7	A	178	0	0	2	0
7	B	284	0	0	4	0
All	All	7308	0	56	15	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 (15) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:668[B]:CYS:SG	7:B:1184:HOH:O	2.20	0.98
1:B:706:TYR:OH	2:B:801:HEM:O1D	2.20	0.60
1:B:465:ARG:NH2	7:B:1113:HOH:O	2.37	0.57
1:A:371:ARG:CG	1:A:371:ARG:NH2	2.67	0.56
1:B:403:TYR:CE1	1:B:407:HIS:CE1	3.00	0.49
1:B:364:GLN:NE2	7:B:1061:HOH:O	2.46	0.49
1:B:717:LYS:NZ	7:B:1176:HOH:O	2.49	0.45
1:A:567:VAL:CG2	4:A:803:1Q7:H16	2.46	0.45
1:A:619:ARG:NH2	7:A:1034:HOH:O	2.50	0.44
1:A:706:TYR:OH	2:A:801:HEM:O1D	2.38	0.42
1:A:620:LYS:NZ	7:A:1035:HOH:O	2.52	0.42
1:B:445:HIS:C	1:B:445:HIS:CD2	2.93	0.41
2:B:801:HEM:CBA	4:B:803:1Q7:H18	2.51	0.41
2:B:801:HEM:C1C	4:B:803:1Q7:H26	2.55	0.41
1:A:403:TYR:CE1	1:A:407:HIS:CE1	3.09	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	405/422 (96%)	393 (97%)	12 (3%)	0	100	100
1	B	411/422 (97%)	406 (99%)	5 (1%)	0	100	100
All	All	816/844 (97%)	799 (98%)	17 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	365/377 (97%)	355 (97%)	10 (3%)	57	47
1	B	370/377 (98%)	362 (98%)	8 (2%)	64	57
All	All	735/754 (98%)	717 (98%)	18 (2%)	60	53

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	337	LEU
1	A	371	ARG
1	A	380	ARG
1	A	523	LEU
1	A	547	ARG
1	A	552	ASP
1	A	569	ASN
1	A	620	LYS
1	A	645	LYS
1	A	715	VAL
1	B	350	THR
1	B	352	ASP
1	B	353	GLN
1	B	389	GLU
1	B	390	SER
1	B	540	LEU
1	B	547	ARG
1	B	620	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 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	801	1	49,50,50	2.36	16 (32%)	46,82,82	2.32	8 (17%)
3	H4B	A	802	-	18,18,18	0.99	1 (5%)	24,26,26	1.75	7 (29%)
4	1Q7	A	803	-	25,25,25	0.63	0	33,33,33	1.96	8 (24%)
5	ACT	A	804	-	1,3,3	1.16	0	0,3,3	0.00	-
2	HEM	B	801	1	49,50,50	2.26	17 (34%)	46,82,82	2.42	12 (26%)
3	H4B	B	802	-	18,18,18	1.29	2 (11%)	24,26,26	1.75	5 (20%)
4	1Q7	B	803	-	25,25,25	0.69	0	33,33,33	1.76	9 (27%)
5	ACT	B	804	-	1,3,3	1.45	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	-	0/14/114/114	0/0/8/8
3	H4B	A	802	-	-	0/8/17/17	0/0/2/2
4	1Q7	A	803	-	-	0/13/13/13	0/2/2/2
5	ACT	A	804	-	-	0/0/0/0	0/0/0/0
2	HEM	B	801	1	-	0/14/114/114	0/0/8/8
3	H4B	B	802	-	-	0/8/17/17	0/0/2/2
4	1Q7	B	803	-	-	0/13/13/13	0/2/2/2
5	ACT	B	804	-	-	0/0/0/0	0/0/0/0

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	HEM	C3B-C2B	-6.06	1.33	1.43
2	B	801	HEM	C3B-C2B	-5.48	1.34	1.43
2	B	801	HEM	C3C-C2C	-5.34	1.34	1.43
2	A	801	HEM	C3D-C2D	4.90	1.52	1.43
2	A	801	HEM	C3C-C2C	-4.87	1.35	1.43
2	A	801	HEM	C2D-C1D	4.85	1.45	1.44
2	B	801	HEM	C3C-CAC	4.82	1.55	1.40
2	A	801	HEM	C3C-CAC	4.73	1.55	1.40
2	A	801	HEM	C3B-CAB	4.52	1.54	1.40
2	A	801	HEM	C4A-C3A	4.29	1.45	1.40
2	B	801	HEM	C3B-CAB	4.21	1.53	1.40
2	B	801	HEM	C4A-C3A	4.07	1.45	1.40
2	B	801	HEM	FE-NA	4.01	2.09	1.92
2	B	801	HEM	C3D-C4D	3.81	1.45	1.44
2	A	801	HEM	FE-NA	3.61	2.07	1.92
2	B	801	HEM	C3D-C2D	3.59	1.50	1.43
2	A	801	HEM	C3D-C4D	-3.34	1.43	1.44
2	A	801	HEM	FE-NC	3.31	2.10	1.97
2	B	801	HEM	FE-NB	2.98	2.08	1.97
2	A	801	HEM	CMC-C2C	2.96	1.56	1.47
2	B	801	HEM	CMD-C2D	2.87	1.56	1.47
2	A	801	HEM	FE-ND	2.86	2.08	1.97
3	B	802	H4B	C2-N2	2.85	1.36	1.32
2	A	801	HEM	CMB-C2B	2.83	1.56	1.47
2	A	801	HEM	CMD-C2D	2.76	1.56	1.47
3	A	802	H4B	C2-N2	2.73	1.36	1.32
2	B	801	HEM	CMA-C3A	2.72	1.57	1.51
2	B	801	HEM	CMB-C2B	2.55	1.55	1.47
2	B	801	HEM	CHA-C4D	2.53	1.39	1.35
2	B	801	HEM	CMC-C2C	2.44	1.55	1.47
2	B	801	HEM	CHB-C1B	2.38	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	HEM	CHA-C4D	2.30	1.39	1.35
2	B	801	HEM	FE-NC	2.24	2.06	1.97
2	B	801	HEM	FE-ND	2.20	2.05	1.97
3	B	802	H4B	C2-N1	2.16	1.36	1.33
2	A	801	HEM	CHD-C4C	2.04	1.39	1.36

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	HEM	C3B-C4B-NB	-9.61	107.12	114.00
2	A	801	HEM	C3B-C4B-NB	-8.36	108.02	114.00
2	A	801	HEM	C4D-ND-C1D	6.69	112.01	105.16
2	A	801	HEM	CBA-CAA-C2A	-5.72	102.62	112.69
2	B	801	HEM	CBA-CAA-C2A	-5.57	102.88	112.69
3	B	802	H4B	C4-C4A-C8A	5.46	119.61	114.56
2	A	801	HEM	CBD-CAD-C3D	-5.36	102.68	114.37
4	A	803	1Q7	C02-N01-C06	5.08	121.80	118.23
2	B	801	HEM	CBD-CAD-C3D	-4.88	103.73	114.37
4	A	803	1Q7	C22-N21-C26	4.80	121.60	118.23
3	A	802	H4B	C4-C4A-C8A	4.72	118.94	114.56
2	B	801	HEM	C4A-CHB-C1B	-4.69	121.31	127.47
2	B	801	HEM	C4D-ND-C1D	4.62	109.89	105.16
2	A	801	HEM	C2D-C1D-ND	-4.40	107.74	112.93
4	A	803	1Q7	C24-C25-C26	-4.14	117.53	120.29
4	A	803	1Q7	O14-C15-C26	-3.85	103.29	111.60
4	B	803	1Q7	C02-N01-C06	3.84	120.93	118.23
4	B	803	1Q7	C22-N21-C26	3.63	120.78	118.23
2	B	801	HEM	CAD-C3D-C4D	3.24	130.35	124.53
2	B	801	HEM	C2D-C1D-ND	-3.09	109.29	112.93
4	A	803	1Q7	C05-C06-N01	-2.97	119.68	122.99
3	A	802	H4B	C9-C6-N5	2.95	115.19	109.69
4	B	803	1Q7	C08-C06-N01	2.93	122.17	115.92
4	A	803	1Q7	C08-C06-N01	2.91	122.13	115.92
2	A	801	HEM	C4C-NC-C1C	2.89	108.54	105.53
3	B	802	H4B	N8-C8A-N1	2.87	120.03	115.82
4	B	803	1Q7	O09-C10-C11	2.83	114.92	109.26
4	B	803	1Q7	C11-C12-N13	-2.75	106.93	113.69
4	B	803	1Q7	C05-C06-N01	-2.69	120.00	122.99
2	B	801	HEM	C1B-NB-C4B	2.66	107.88	105.16
2	B	801	HEM	C1A-C2A-C3A	2.63	109.64	106.92
3	A	802	H4B	C2-N1-C8A	2.61	121.32	117.61
2	A	801	HEM	C4A-CHB-C1B	-2.61	124.03	127.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	803	1Q7	C24-C25-C26	-2.42	118.68	120.29
3	A	802	H4B	N2-C2-N3	2.35	120.45	117.86
3	B	802	H4B	C9-C6-N5	2.30	113.99	109.69
4	A	803	1Q7	C11-C12-N13	-2.28	108.09	113.69
4	B	803	1Q7	C15-C26-N21	2.28	120.78	115.92
3	B	802	H4B	N2-C2-N3	2.20	120.28	117.86
2	B	801	HEM	CHA-C1A-NA	2.18	128.22	124.58
3	A	802	H4B	C10-C9-C6	-2.18	110.34	113.61
2	B	801	HEM	C4C-NC-C1C	2.18	107.80	105.53
4	A	803	1Q7	C07-C04-C05	-2.17	117.43	120.93
2	B	801	HEM	C2A-C1A-NA	-2.14	106.77	109.73
2	A	801	HEM	CHA-C4D-ND	2.12	127.22	124.31
3	A	802	H4B	N8-C8A-N1	2.11	118.91	115.82
3	B	802	H4B	C10-C9-C6	-2.10	110.47	113.61
4	B	803	1Q7	C08-C06-C05	-2.10	117.83	120.69
3	A	802	H4B	C4A-C4-N3	2.00	119.20	114.06

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%)	0.70	45 (11%) 6 5	23, 40, 67, 85	0
1	B	411/422 (97%)	0.35	31 (7%) 14 14	20, 31, 52, 77	0
All	All	818/844 (96%)	0.52	76 (9%) 9 8	20, 35, 62, 85	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	352	ASP	7.2
1	A	715	VAL	6.6
1	A	351	LYS	6.5
1	B	300	PHE	6.3
1	A	716	TRP	6.1
1	A	488	PRO	5.8
1	A	486	LYS	4.9
1	B	348	VAL	4.8
1	A	350	THR	4.7
1	B	350	THR	4.7
1	B	718	GLY	4.6
1	B	338	PRO	3.8
1	A	489	ASP	3.7
1	A	619	ARG	3.7
1	A	355	PHE	3.6
1	B	619	ARG	3.5
1	A	392	SER	3.4
1	A	713	THR	3.3
1	A	321	THR	3.2
1	A	299	ARG	3.2
1	A	469	LYS	3.2
1	B	352	ASP	3.1
1	B	416	VAL	3.1
1	A	389	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	507	GLN	3.0
1	A	490	GLY	3.0
1	A	712	ASN	2.9
1	A	491	SER	2.8
1	B	321	THR	2.8
1	A	386	LYS	2.8
1	A	300	PHE	2.8
1	A	470	HIS	2.7
1	B	591	THR	2.7
1	A	388	ILE	2.7
1	A	714	HIS	2.7
1	A	375	LYS	2.6
1	A	467	ASP	2.6
1	B	349	ARG	2.6
1	B	353	GLN	2.6
1	A	602	SER	2.6
1	A	487	GLN	2.5
1	A	370	LYS	2.5
1	B	415	CYS	2.5
1	A	601[A]	ASN	2.4
1	A	572	LEU	2.4
1	A	338	PRO	2.4
1	B	679	ILE	2.4
1	A	390	SER	2.4
1	B	328	GLU	2.3
1	B	567	VAL	2.3
1	B	584	PHE	2.3
1	A	567	VAL	2.3
1	B	677	VAL	2.3
1	B	680	VAL	2.3
1	B	704	PHE	2.3
1	B	412	ALA	2.2
1	A	591	THR	2.2
1	B	409	TRP	2.2
1	B	681	PRO	2.2
1	B	715	VAL	2.2
1	A	503	GLU	2.2
1	A	485	TYR	2.2
1	B	620	LYS	2.2
1	B	572	LEU	2.2
1	A	311	VAL	2.1
1	A	683	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	691	PHE	2.1
1	A	593	ILE	2.1
1	A	371	ARG	2.1
1	A	514	ARG	2.1
1	A	680	VAL	2.1
1	B	615	ASP	2.1
1	B	327	THR	2.0
1	B	323	GLU	2.0
1	A	522	LEU	2.0
1	B	685	GLY	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
4	1Q7	A	803	24/24	0.26	2.59	28,49,72,73	0
4	1Q7	B	803	24/24	0.28	2.57	26,43,75,75	0
5	ACT	A	804	4/4	0.13	1.95	45,45,46,47	0
2	HEM	B	801	43/43	0.21	0.95	20,23,31,32	0
2	HEM	A	801	43/43	0.17	0.57	22,26,33,37	0
3	H4B	A	802	17/17	0.11	-0.41	28,31,36,36	0
3	H4B	B	802	17/17	0.10	-0.41	26,29,32,33	0
5	ACT	B	804	4/4	0.08	-1.11	33,36,36,37	0
6	ZN	A	805	1/1	0.04	-2.02	29,29,29,29	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.