



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 09:31 PM GMT

PDB ID : 4JSG  
Title : Structure of rat neuronal nitric oxide synthase heme domain in complex with  
6-((3-(3-aminopropoxy)phenoxy)methyl)-4-methylpyridin-2-amine  
Authors : Li, H.; Poulos, T.L.  
Deposited on : 2013-03-22  
Resolution : 1.94 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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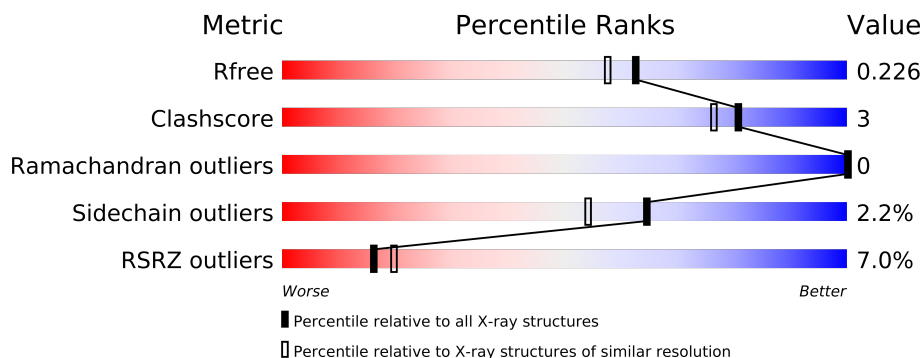
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.94 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	2024 (1.96-1.92)
Clashscore	79885	2281 (1.96-1.92)
Ramachandran outliers	78287	2255 (1.96-1.92)
Sidechain outliers	78261	2255 (1.96-1.92)
RSRZ outliers	66119	2024 (1.96-1.92)

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	803	-	X
5	Q10	A	804	-	X
5	Q10	B	803	-	X

## 2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 7192 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	1	0
			3313	2119	566	606	22			
1	B	411	Total	C	N	O	S	0	3	0
			3351	2142	574	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:  $C_{34}H_{32}FeN_4O_4$ ).



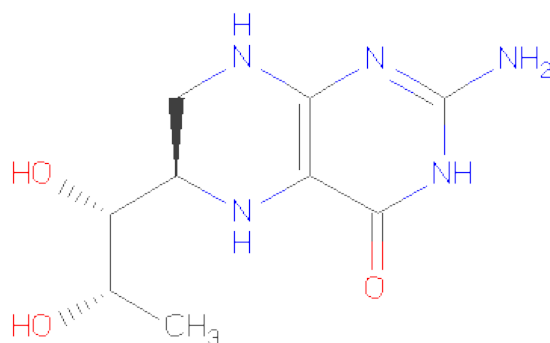
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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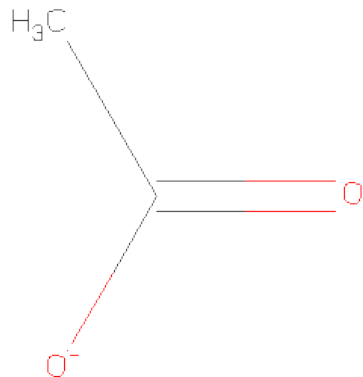
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



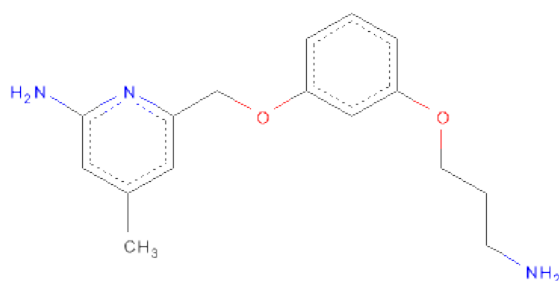
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 4 is 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-{[3-(3-AMINOPROPOXY)PHENOXY]METHYL}-4-METHYLPYRIDIN-2-AMINE (three-letter code: Q10) (formula: C<sub>16</sub>H<sub>21</sub>N<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			21	16	3	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			21	16	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		

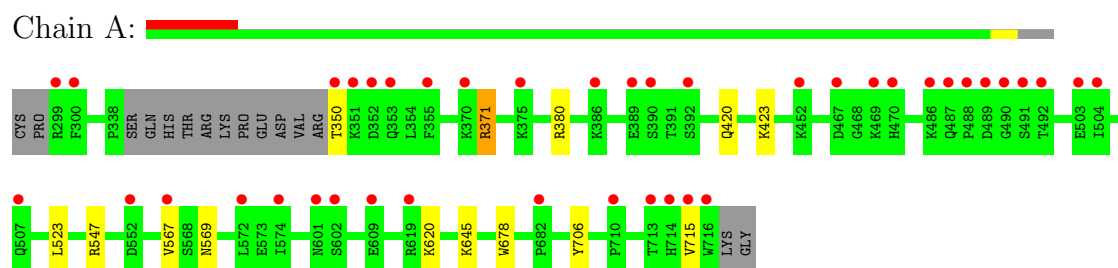
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	123	Total	O	0	0
			123	123		
7	B	234	Total	O	0	0
			234	234		

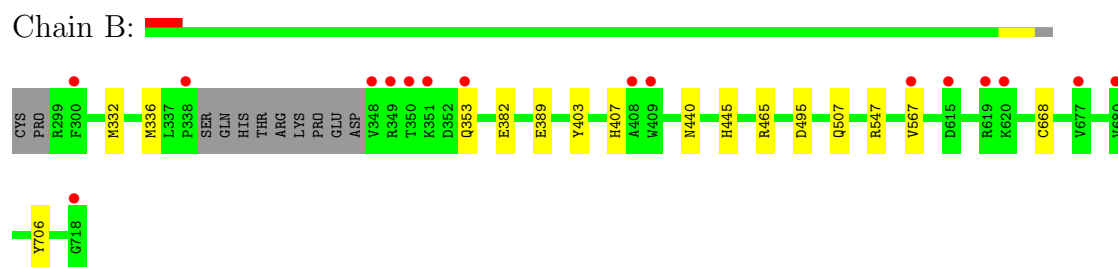
### 3 Residue-property plots

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, $\alpha$ , $\beta$ , $\gamma$	52.25Å 111.18Å 164.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.80 – 1.94 33.78 – 1.94	Depositor EDS
% Data completeness (in resolution range)	99.0 (33.80-1.94) 99.0 (33.78-1.94)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.03 (at 1.94Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.189 , 0.226 0.189 , 0.226	Depositor DCC
$R_{free}$ test set	3508 reflections (5.21%)	DCC
Wilson B-factor (Å <sup>2</sup> )	31.5	Xtriage
Anisotropy	0.682	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 45.0	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 70966 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7192	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.41% 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, Q10

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	0.49	0/3408	0.62	0/4623
1	B	0.55	0/3452	0.66	1/4679 (0.0%)
All	All	0.52	0/6860	0.64	1/9302 (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	495	ASP	CB-CG-OD1	5.17	122.95	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	3313	0	0	6	0
1	B	3351	0	0	8	0
2	A	43	0	0	3	0
2	B	43	0	0	4	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	3	0	0
4	B	4	0	3	0	0
5	A	21	0	21	7	0
5	B	21	0	21	7	0
6	A	1	0	0	0	0
7	A	123	0	0	0	0
7	B	234	0	0	5	0
All	All	7192	0	48	23	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 3.

All (23) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:567:VAL:CG2	5:B:803:Q10:H12	1.76	1.15
2:B:801:HEM:O2A	5:B:803:Q10:H13	1.74	0.87
1:B:668[B]:CYS:SG	7:B:905:HOH:O	2.36	0.82
2:A:801:HEM:O2A	5:A:804:Q10:H13	1.80	0.81
1:B:567:VAL:CG2	5:B:803:Q10:C22	2.65	0.66
5:A:804:Q10:H10	5:A:804:Q10:H7	1.76	0.66
1:B:465:ARG:NH2	7:B:1124:HOH:O	2.30	0.65
1:A:567:VAL:CG2	5:A:804:Q10:H12	2.30	0.61
5:A:804:Q10:C24	5:A:804:Q10:H7	2.35	0.56
1:A:678:TRP:CH2	5:A:804:Q10:H9	2.41	0.55
1:A:706:TYR:OH	2:A:801:HEM:O2D	2.25	0.54
1:B:706:TYR:OH	2:B:801:HEM:O2D	2.26	0.54
5:B:803:Q10:H14	7:B:1014:HOH:O	2.08	0.54
2:B:801:HEM:CBA	5:B:803:Q10:H15	2.39	0.53
1:A:567:VAL:CG2	5:A:804:Q10:C22	2.89	0.51
5:B:803:Q10:H6	7:B:969:HOH:O	2.11	0.50
1:B:403:TYR:CE1	1:B:407:HIS:CE1	3.01	0.49
2:A:801:HEM:C1C	5:A:804:Q10:H22	2.48	0.48
1:A:371:ARG:CG	1:A:371:ARG:NH2	2.76	0.48
2:B:801:HEM:C1C	5:B:803:Q10:H22	2.50	0.47
1:A:420:GLN:OE1	1:A:423:LYS:NZ	2.53	0.42
1:B:440:ASN:ND2	7:B:1067:HOH:O	2.52	0.41
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%)	11 (3%)	0	100	100
1	B	410/422 (97%)	403 (98%)	7 (2%)	0	100	100
All	All	814/844 (96%)	796 (98%)	18 (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	364/377 (97%)	355 (98%)	9 (2%)	60	48
1	B	369/377 (98%)	362 (98%)	7 (2%)	69	60
All	All	733/754 (97%)	717 (98%)	16 (2%)	64	54

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	350	THR
1	A	371	ARG
1	A	380	ARG
1	A	523	LEU
1	A	547	ARG
1	A	569	ASN
1	A	620	LYS
1	A	645	LYS
1	A	715	VAL
1	B	332	MET
1	B	336	MET

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Mol	Chain	Res	Type
1	B	353	GLN
1	B	382	GLU
1	B	389	GLU
1	B	507	GLN
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	801	1	49,50,50	2.70	16 (32%)	46,82,82	2.77	11 (23%)
3	H4B	A	802	-	18,18,18	0.87	1 (5%)	24,26,26	1.68	6 (25%)
4	ACT	A	803	-	1,3,3	1.62	0	0,3,3	0.00	-
5	Q10	A	804	-	22,22,22	0.67	0	28,28,28	1.66	6 (21%)
2	HEM	B	801	1	49,50,50	3.34	15 (30%)	46,82,82	2.85	16 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	H4B	B	802	-	18,18,18	1.18	2 (11%)	24,26,26	1.66	7 (29%)
5	Q10	B	803	-	22,22,22	0.95	0	28,28,28	2.16	6 (21%)
4	ACT	B	804	-	1,3,3	1.63	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	ACT	A	803	-	-	0/0/0/0	0/0/0/0
5	Q10	A	804	-	-	0/10/10/10	0/2/2/2
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
5	Q10	B	803	-	-	0/10/10/10	0/2/2/2
4	ACT	B	804	-	-	0/0/0/0	0/0/0/0

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	HEM	C3D-C4D	15.41	1.48	1.44
2	A	801	HEM	C2D-C1D	12.50	1.47	1.44
2	B	801	HEM	C2D-C1D	10.20	1.47	1.44
2	B	801	HEM	C3B-C4B	5.40	1.50	1.44
2	B	801	HEM	C3D-C2D	-5.12	1.34	1.43
2	A	801	HEM	C3D-C2D	-5.00	1.35	1.43
2	A	801	HEM	C3B-C4B	4.67	1.50	1.44
2	A	801	HEM	C3D-C4D	4.62	1.45	1.44
2	B	801	HEM	C2B-C1B	-4.52	1.43	1.44
2	A	801	HEM	C3B-C2B	-4.19	1.36	1.43
2	B	801	HEM	CHA-C4D	3.93	1.41	1.35
2	B	801	HEM	FE-NB	3.72	2.11	1.97
2	A	801	HEM	FE-NB	3.52	2.10	1.97
2	B	801	HEM	C3B-C2B	-3.52	1.37	1.43
2	B	801	HEM	C3C-CAC	3.02	1.49	1.40
2	A	801	HEM	CHA-C4D	2.86	1.39	1.35
2	A	801	HEM	CHB-C1B	2.85	1.39	1.35
2	B	801	HEM	CHC-C1C	2.84	1.41	1.36
2	A	801	HEM	CHC-C1C	2.84	1.41	1.36
2	A	801	HEM	C3C-CAC	2.67	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	802	H4B	C2-N2	2.66	1.36	1.32
2	A	801	HEM	C1B-NB	-2.65	1.34	1.39
2	B	801	HEM	C3B-CAB	2.63	1.48	1.40
2	A	801	HEM	FE-NC	2.62	2.07	1.97
2	B	801	HEM	C3C-C2C	-2.60	1.39	1.43
3	B	802	H4B	C2-N2	2.59	1.36	1.32
2	A	801	HEM	C3B-CAB	2.54	1.48	1.40
2	B	801	HEM	C1B-NB	-2.45	1.34	1.39
2	A	801	HEM	C2B-C1B	-2.37	1.44	1.44
2	B	801	HEM	FE-NC	2.36	2.06	1.97
3	B	802	H4B	C2-N1	2.30	1.36	1.33
2	A	801	HEM	C3C-C2C	-2.28	1.39	1.43
2	B	801	HEM	CMD-C2D	2.06	1.53	1.47
2	A	801	HEM	FE-ND	-2.05	1.90	1.97

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	HEM	C3B-C4B-NB	-10.20	106.70	114.00
2	A	801	HEM	C3B-C4B-NB	-9.99	106.85	114.00
2	A	801	HEM	CBA-CAA-C2A	-6.97	100.42	112.69
2	A	801	HEM	C1A-CHA-C4D	-6.69	118.67	127.47
5	B	803	Q10	C02-N01-C06	6.31	122.66	118.23
2	B	801	HEM	C4A-CHB-C1B	-5.83	119.80	127.47
2	B	801	HEM	CHD-C1D-ND	5.75	129.36	124.58
2	B	801	HEM	CBA-CAA-C2A	-5.31	103.34	112.69
2	B	801	HEM	CBD-CAD-C3D	-5.21	103.00	114.37
2	B	801	HEM	C1A-CHA-C4D	-5.18	120.65	127.47
2	A	801	HEM	CHC-C4B-NB	5.00	128.74	124.58
5	B	803	Q10	O09-C08-C06	4.98	122.88	109.48
5	A	804	Q10	C02-N01-C06	4.96	121.71	118.23
2	B	801	HEM	CHC-C4B-NB	4.74	128.52	124.58
5	B	803	Q10	C05-C06-N01	-4.64	117.83	122.99
2	A	801	HEM	CHD-C1D-ND	4.55	128.37	124.58
2	A	801	HEM	C1B-NB-C4B	4.44	109.70	105.16
2	B	801	HEM	C1B-NB-C4B	4.34	109.61	105.16
2	A	801	HEM	CBD-CAD-C3D	-4.32	104.94	114.37
3	B	802	H4B	C4-C4A-C8A	4.22	118.47	114.56
2	A	801	HEM	CHA-C4D-ND	4.15	130.01	124.31
3	B	802	H4B	N8-C8A-N1	3.69	121.23	115.82
5	A	804	Q10	C05-C06-N01	-3.65	118.93	122.99
3	A	802	H4B	C4-C4A-C8A	3.58	117.88	114.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	HEM	C4A-CHB-C1B	-3.29	123.15	127.47
2	B	801	HEM	C1D-CHD-C4C	-3.22	118.10	126.57
5	B	803	Q10	C22-C21-C26	-3.21	115.94	120.56
3	A	802	H4B	C2-N1-C8A	3.05	121.95	117.61
5	B	803	Q10	C23-C22-C21	3.02	124.27	118.91
3	A	802	H4B	C4-C4A-N5	2.99	123.45	119.10
2	B	801	HEM	C1A-C2A-C3A	2.91	109.93	106.92
5	A	804	Q10	C11-O10-C25	2.75	124.95	117.94
2	A	801	HEM	C4C-NC-C1C	2.69	108.33	105.53
3	B	802	H4B	C4A-C4-N3	2.46	120.36	114.06
5	A	804	Q10	O09-C08-C06	2.36	115.83	109.48
2	B	801	HEM	CAD-C3D-C4D	2.29	128.65	124.53
3	A	802	H4B	C9-C6-N5	2.24	113.87	109.69
2	B	801	HEM	CHA-C4D-ND	2.20	127.33	124.31
2	B	801	HEM	O1D-CGD-CBD	-2.20	115.47	123.03
2	B	801	HEM	C3A-C4A-NA	2.18	111.05	109.41
5	A	804	Q10	C08-C06-N01	2.17	120.56	115.92
2	A	801	HEM	C1D-CHD-C4C	-2.17	120.86	126.57
3	A	802	H4B	N8-C8A-N1	2.15	118.97	115.82
5	A	804	Q10	C22-C21-C26	-2.13	117.49	120.56
3	B	802	H4B	C2-N1-C8A	2.11	120.61	117.61
3	B	802	H4B	C6-C7-N8	-2.11	108.94	111.66
3	A	802	H4B	C4A-C4-N3	2.09	119.42	114.06
2	B	801	HEM	C4A-C3A-C2A	-2.08	105.55	107.00
5	B	803	Q10	C11-O10-C25	2.07	123.21	117.94
3	B	802	H4B	C4-C4A-N5	2.05	122.08	119.10
3	B	802	H4B	C7-N8-C8A	2.03	123.66	121.36
2	B	801	HEM	O2A-CGA-O1A	-2.02	118.16	123.30

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%)	0.68	41 (10%) 7 9	24, 45, 75, 106	0
1	B	411/422 (97%)	0.26	16 (3%) 37 41	23, 35, 58, 99	0
All	All	818/844 (96%)	0.47	57 (6%) 16 20	23, 39, 70, 106	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	488	PRO	7.5
1	A	716	TRP	7.0
1	A	715	VAL	6.9
1	B	348	VAL	6.0
1	A	352	ASP	5.6
1	B	300	PHE	5.5
1	B	718	GLY	5.1
1	A	713	THR	4.6
1	B	350	THR	4.6
1	A	486	LYS	4.3
1	A	507	GLN	4.1
1	A	351	LYS	4.1
1	B	338	PRO	4.1
1	A	300	PHE	3.9
1	A	489	ASP	3.8
1	A	469	LYS	3.6
1	A	350	THR	3.5
1	A	619	ARG	3.5
1	B	619	ARG	3.4
1	A	601	ASN	3.3
1	A	392	SER	3.0
1	A	389	GLU	2.9
1	A	375	LYS	2.9
1	A	299	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	714	HIS	2.8
1	B	351	LYS	2.8
1	A	470	HIS	2.7
1	A	386	LYS	2.7
1	B	349	ARG	2.7
1	A	491	SER	2.7
1	A	503	GLU	2.7
1	A	602	SER	2.6
1	A	370	LYS	2.6
1	A	390	SER	2.6
1	B	620	LYS	2.6
1	B	353	GLN	2.6
1	A	487	GLN	2.6
1	B	567	VAL	2.5
1	A	490	GLY	2.5
1	A	567	VAL	2.5
1	A	452	LYS	2.3
1	A	355	PHE	2.3
1	B	680	VAL	2.3
1	A	574	ILE	2.3
1	A	552	ASP	2.2
1	A	467	ASP	2.2
1	A	710	PRO	2.2
1	B	409	TRP	2.2
1	B	677	VAL	2.2
1	A	682	PRO	2.1
1	A	609	GLU	2.1
1	A	572	LEU	2.1
1	B	408	ALA	2.1
1	A	504	ILE	2.1
1	A	492	THR	2.0
1	B	615	ASP	2.0
1	A	353	GLN	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	ACT	A	803	4/4	0.19	7.10	47,48,48,51	0
5	Q10	B	803	21/21	0.32	4.92	29,59,80,82	0
5	Q10	A	804	21/21	0.29	3.76	28,61,93,94	0
2	HEM	B	801	43/43	0.20	1.54	23,28,36,39	0
2	HEM	A	801	43/43	0.16	0.53	28,31,43,50	0
4	ACT	B	804	4/4	0.11	0.38	37,40,41,42	0
3	H4B	A	802	17/17	0.12	-0.04	31,33,37,40	0
3	H4B	B	802	17/17	0.10	-0.25	28,31,34,34	0
6	ZN	A	805	1/1	0.07	-0.86	31,31,31,31	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.