



Full wwPDB X-ray Structure Validation Report

Mar 12, 2014 – 06:55 PM GMT

PDB ID : 4CDT
Title : Structure of rat neuronal nitric oxide synthase heme domain in complex with
7-((3-Fluorophenethylamino)ethyl)quinolin-2-amine
Authors : Li, H.; Poulos, T.L.
Deposited on : 2013-11-05
Resolution : 2.00 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

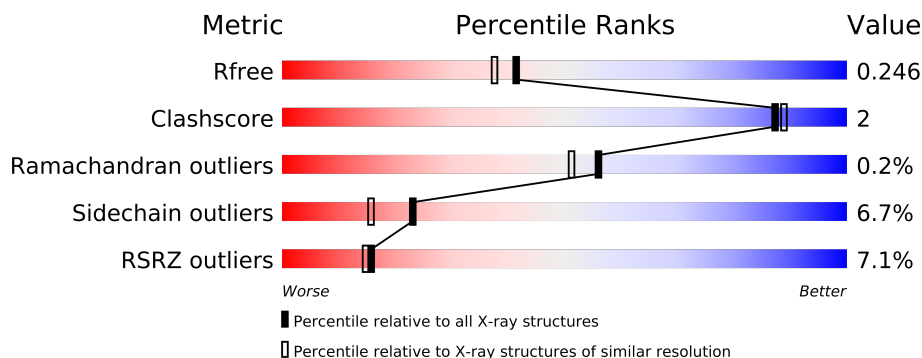
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1323
EDS : trunk22714
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) : trunk22714

1 Overall quality at a glance

The reported resolution of this entry is 2.00 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	4888 (2.00-2.00)
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (2.00-2.00)

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 ≥ 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
5	ACT	A	860	-	X

2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 7017 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.

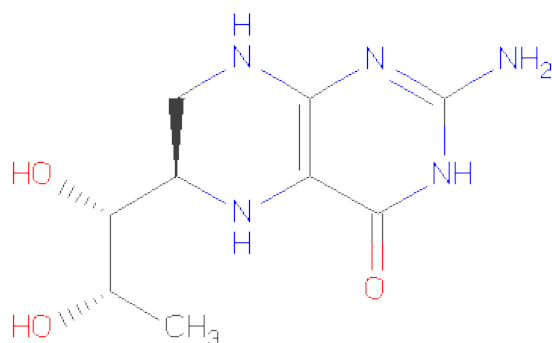
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	408	Total	C	N	O	S	0	0	1
			3314	2121	567	605	21			
1	B	411	Total	C	N	O	S	0	0	0
			3345	2140	574	610	21			

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



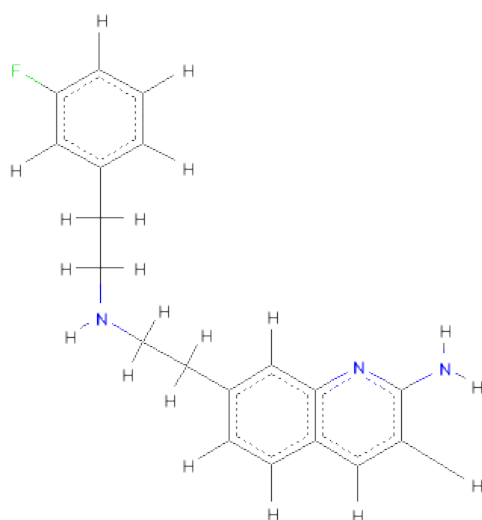
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- 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 7-[2-[2-(3-FLUOROPHENYL)ETHYLAMINO]ETHYL]QUINOLIN-2-AMIN E (three-letter code: M48) (formula: C₁₉H₂₀FN₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	F	N	0	0
			23	19	1	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	F	N	0	0
			23	19	1	3		

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



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.

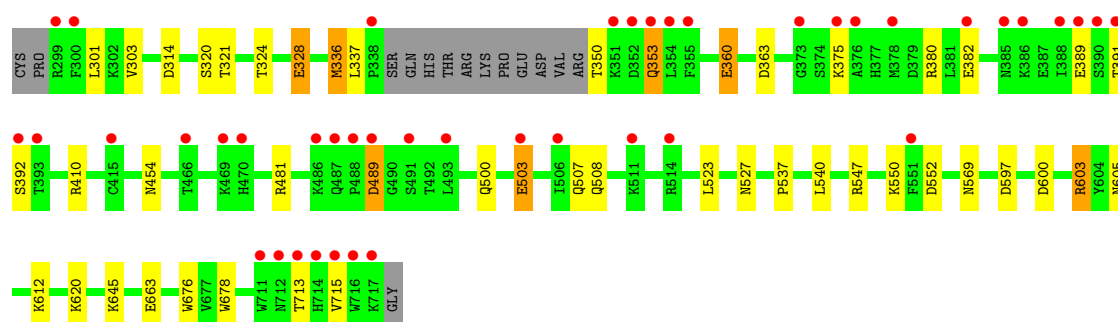
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	91	Total	O	0	0
			91	91		
7	B	92	Total	O	0	0
			92	92		

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.

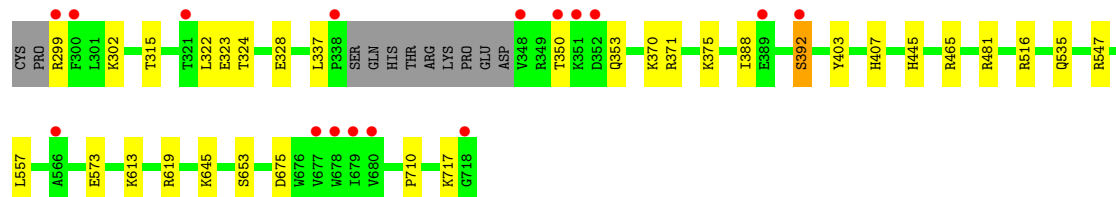
• Molecule 1: NITRIC OXIDE SYNTHASE, BRAIN

Chain A: 



• Molecule 1: NITRIC OXIDE SYNTHASE, BRAIN

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	52.37Å 111.82Å 165.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	92.65 – 2.00 46.32 – 2.00	Depositor EDS
% Data completeness (in resolution range)	92.4 (92.65-2.00) 92.5 (46.32-2.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.74 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.196 , 0.247 0.197 , 0.246	Depositor DCC
R_{free} test set	3061 reflections (5.22%)	DCC
Wilson B-factor (Å ²)	32.2	Xtriage
Anisotropy	0.632	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 45.3	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	3 of 61671 reflections (0.005%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7017	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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, M48, 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	0.84	2/3407 (0.1%)	0.91	5/4623 (0.1%)
1	B	0.85	0/3438	0.89	3/4661 (0.1%)
All	All	0.84	2/6845 (0.0%)	0.90	8/9284 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	360	GLU	CG-CD	6.52	1.61	1.51
1	A	676	TRP	CE3-CZ3	5.24	1.47	1.38

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	410	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	B	675	ASP	CB-CG-OD1	6.33	124.00	118.30
1	A	410	ARG	NE-CZ-NH2	-6.27	117.17	120.30
1	A	603	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	A	363	ASP	CB-CG-OD1	5.72	123.44	118.30
1	A	600	ASP	CB-CG-OD1	5.44	123.20	118.30
1	B	557	LEU	CB-CG-CD1	-5.42	101.79	111.00
1	B	371	ARG	NE-CZ-NH1	5.27	122.94	120.30

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	3314	0	0	13	0
1	B	3345	0	0	6	0
2	A	43	0	0	0	0
2	B	43	0	0	0	0
3	A	17	0	0	0	0
3	B	17	0	0	0	0
4	A	23	0	0	0	0
4	B	23	0	0	0	0
5	A	4	0	0	0	0
5	B	4	0	0	0	0
6	A	1	0	0	0	0
7	A	91	0	0	2	0
7	B	92	0	0	1	0
All	All	7017	0	0	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)
1:A:500:GLN:CA	1:A:503:GLU:OE2	2.40	0.69
1:A:350:THR:N	1:A:353:GLN:NE2	2.52	0.57
1:B:465:ARG:NH2	7:B:2040:HOH:O	2.41	0.53
1:A:328:GLU:O	1:B:324:THR:N	2.42	0.52
1:A:336:MET:CE	1:A:678:TRP:CZ2	2.92	0.52
1:A:605:ASN:ND2	7:A:2062:HOH:O	2.44	0.49
1:B:388:ILE:O	1:B:392:SER:N	2.46	0.48
1:A:324:THR:N	1:B:328:GLU:O	2.46	0.48
1:B:403:TYR:CE1	1:B:407:HIS:CE1	3.02	0.48
1:B:619:ARG:CB	1:B:619:ARG:NH1	2.78	0.47
1:A:391:THR:O	1:A:392:SER:OG	2.34	0.46
1:A:328:GLU:N	1:A:328:GLU:CD	2.70	0.44
1:A:508:GLN:CA	1:A:508:GLN:NE2	2.80	0.43
1:A:301:LEU:O	1:A:314:ASP:N	2.52	0.42
1:A:597:ASP:OD1	1:A:603:ARG:NH2	2.53	0.42
1:A:481:ARG:NE	7:A:2042:HOH:O	2.52	0.41
1:A:537:PRO:O	1:A:540:LEU:N	2.54	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%)	382 (95%)	21 (5%)	1 (0%)	56	51
1	B	407/422 (96%)	398 (98%)	8 (2%)	1 (0%)	56	51
All	All	811/844 (96%)	780 (96%)	29 (4%)	2 (0%)	56	51

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	489	ASP
1	B	322	LEU

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	363/377 (96%)	335 (92%)	28 (8%)	18	11
1	B	366/377 (97%)	345 (94%)	21 (6%)	29	21
All	All	729/754 (97%)	680 (93%)	49 (7%)	23	16

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	303	VAL
1	A	320	SER
1	A	321	THR
1	A	328	GLU

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Mol	Chain	Res	Type
1	A	336	MET
1	A	337	LEU
1	A	353	GLN
1	A	360	GLU
1	A	375	LYS
1	A	380	ARG
1	A	382	GLU
1	A	389	GLU
1	A	454	ASN
1	A	489	ASP
1	A	503	GLU
1	A	507	GLN
1	A	523	LEU
1	A	527	ASN
1	A	547	ARG
1	A	550	LYS
1	A	552	ASP
1	A	569	ASN
1	A	612	LYS
1	A	620	LYS
1	A	645	LYS
1	A	663	GLU
1	A	713	THR
1	A	715	VAL
1	B	299	ARG
1	B	302	LYS
1	B	315	THR
1	B	323	GLU
1	B	337	LEU
1	B	350	THR
1	B	353	GLN
1	B	370	LYS
1	B	375	LYS
1	B	392	SER
1	B	445	HIS
1	B	481	ARG
1	B	516	ARG
1	B	535	GLN
1	B	547	ARG
1	B	573	GLU
1	B	613	LYS
1	B	645	LYS

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Mol	Chain	Res	Type
1	B	653	SER
1	B	710	PRO
1	B	717	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	750	1	50,50,50	2.49	17 (34%)	46,82,82	2.58	14 (30%)
3	H4B	A	760	-	18,18,18	1.86	4 (22%)	24,26,26	2.06	8 (33%)
4	M48	A	801	-	25,25,25	1.14	2 (8%)	33,33,33	1.45	5 (15%)
5	ACT	A	860	-	1,3,3	1.24	0	0,3,3	0.00	-
2	HEM	B	750	1	50,50,50	2.68	18 (36%)	46,82,82	2.68	9 (19%)
3	H4B	B	760	-	18,18,18	1.76	4 (22%)	24,26,26	1.81	5 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	M48	B	801	-	25,25,25	1.11	3 (12%)	33,33,33	1.74	8 (24%)
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	-	0/14/114/114	0/0/8/8
3	H4B	A	760	-	-	0/8/17/17	0/2/2/2
4	M48	A	801	-	-	0/8/8/8	0/3/3/3
5	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	0/2/2/2
4	M48	B	801	-	-	0/8/8/8	0/3/3/3
5	ACT	B	860	-	-	0/0/0/0	0/0/0/0

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	750	HEM	C3D-C2D	-9.33	1.34	1.44
2	A	750	HEM	C3D-C2D	-7.25	1.36	1.44
2	B	750	HEM	C3B-C2B	-6.92	1.36	1.45
2	A	750	HEM	C3B-C2B	-6.50	1.37	1.45
2	A	750	HEM	CHA-C4D	5.52	1.43	1.35
2	B	750	HEM	C2D-C1D	5.09	1.49	1.45
2	B	750	HEM	CHA-C4D	5.02	1.42	1.35
2	A	750	HEM	C2B-C1B	-4.85	1.41	1.45
2	B	750	HEM	C3C-C2C	-4.79	1.39	1.45
3	A	760	H4B	C2-N1	4.68	1.39	1.33
3	B	760	H4B	C2-N1	4.49	1.39	1.33
2	A	750	HEM	CHB-C1B	4.20	1.41	1.35
2	B	750	HEM	FE-NC	3.93	2.11	1.95
2	A	750	HEM	FE-NC	3.87	2.11	1.95
2	A	750	HEM	FE-NB	3.85	2.11	1.96
2	A	750	HEM	C3C-C2C	-3.65	1.40	1.45
2	A	750	HEM	CHC-C1C	3.42	1.41	1.36
2	B	750	HEM	C3D-C4D	3.37	1.48	1.45
2	B	750	HEM	C2B-C1B	-3.28	1.42	1.45
2	B	750	HEM	CHB-C1B	3.26	1.40	1.35
3	B	760	H4B	C6-N5	3.25	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	760	H4B	C2-N2	3.19	1.37	1.32
2	A	750	HEM	C3B-CAB	2.90	1.49	1.40
2	A	750	HEM	C2D-C1D	2.86	1.47	1.45
2	B	750	HEM	C3B-C4B	2.78	1.51	1.43
2	B	750	HEM	FE-NB	2.76	2.07	1.96
2	B	750	HEM	C3C-CAC	2.74	1.49	1.40
2	A	750	HEM	CMC-C2C	2.67	1.56	1.47
4	A	801	M48	C06-C07	2.67	1.42	1.36
2	A	750	HEM	C4C-NC	-2.66	1.34	1.38
2	B	750	HEM	CMD-C2D	2.65	1.55	1.47
2	B	750	HEM	CMC-C2C	2.64	1.55	1.47
2	A	750	HEM	C1B-NB	-2.62	1.34	1.39
3	A	760	H4B	C7-C6	-2.52	1.49	1.52
2	A	750	HEM	CMD-C2D	2.48	1.55	1.47
4	B	801	M48	C04-C03	2.41	1.41	1.36
2	A	750	HEM	C3C-CAC	2.40	1.48	1.40
2	B	750	HEM	C1A-NA	2.38	1.40	1.36
2	B	750	HEM	CMB-C2B	2.35	1.55	1.47
2	B	750	HEM	C3B-CAB	2.27	1.47	1.40
4	B	801	M48	C22-C23	2.26	1.41	1.37
3	B	760	H4B	C7-C6	2.25	1.54	1.52
4	B	801	M48	C24-C23	2.22	1.41	1.37
3	A	760	H4B	C2-N3	-2.18	1.33	1.36
4	A	801	M48	C22-C23	2.12	1.41	1.37
2	B	750	HEM	C2C-C1C	-2.10	1.41	1.45
2	A	750	HEM	CMB-C2B	2.08	1.54	1.47
3	B	760	H4B	C8A-N8	2.05	1.39	1.34

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	750	HEM	C3B-C4B-NB	-10.23	106.68	114.00
2	A	750	HEM	C1A-CHA-C4D	-8.76	115.94	127.47
2	A	750	HEM	C3B-C4B-NB	-8.57	107.87	114.00
2	B	750	HEM	C1A-CHA-C4D	-8.08	116.84	127.47
2	B	750	HEM	C4A-CHB-C1B	-6.02	119.55	127.47
2	A	750	HEM	CBA-CAA-C2A	-4.96	104.38	112.63
2	B	750	HEM	CBA-CAA-C2A	-4.80	104.64	112.63
2	A	750	HEM	CHA-C4D-ND	4.70	130.89	124.28
3	B	760	H4B	C4-C4A-C8A	4.51	118.65	114.56
4	B	801	M48	N02-C02-N01	4.39	120.58	118.11
3	A	760	H4B	C9-C6-N5	4.14	117.54	111.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	760	H4B	C4-C4A-C8A	4.13	118.31	114.56
2	B	750	HEM	CHD-C1D-ND	4.08	129.21	124.47
2	B	750	HEM	CHC-C4B-NB	4.07	129.20	124.47
3	A	760	H4B	C7-C6-C9	-3.70	107.72	113.45
3	B	760	H4B	C4A-C8A-N8	3.65	122.72	118.43
4	B	801	M48	C02-N01-C10	3.55	121.75	118.08
4	A	801	M48	C21-C22-C23	3.52	121.63	118.86
2	A	750	HEM	C4C-NC-C1C	3.41	108.98	105.51
3	B	760	H4B	C7-N8-C8A	-3.26	117.65	121.36
2	A	750	HEM	C4A-NA-C1A	-3.19	104.04	107.12
4	A	801	M48	C12-N13-C14	3.18	124.32	113.25
2	A	750	HEM	CHC-C4B-NB	3.16	128.14	124.47
4	A	801	M48	C12-C11-C08	3.02	119.48	112.84
2	B	750	HEM	C1B-NB-C4B	2.93	108.15	105.11
2	A	750	HEM	CHD-C1D-ND	2.90	127.84	124.47
4	B	801	M48	C24-C23-C22	-2.87	119.50	123.32
2	A	750	HEM	C4A-CHB-C1B	-2.87	123.70	127.47
3	A	760	H4B	C4A-C8A-N8	2.83	121.76	118.43
2	A	750	HEM	CHC-C1C-NC	2.82	127.60	124.38
2	A	750	HEM	O2D-CGD-CBD	2.82	123.94	114.19
3	A	760	H4B	O9-C9-C6	-2.79	102.31	109.07
4	B	801	M48	C03-C04-C05	-2.73	116.56	120.83
4	A	801	M48	C24-C23-C22	-2.71	119.72	123.32
4	B	801	M48	C12-N13-C14	2.62	122.36	113.25
3	B	760	H4B	C4A-N5-C6	-2.59	114.11	121.16
4	B	801	M48	C21-C22-C23	2.58	120.89	118.86
3	B	760	H4B	C9-C6-N5	2.56	115.07	111.10
3	A	760	H4B	C4A-N5-C6	-2.49	114.39	121.16
2	B	750	HEM	C4A-NA-C1A	-2.26	104.94	107.12
3	A	760	H4B	C7-N8-C8A	-2.22	118.84	121.36
2	B	750	HEM	C4D-ND-C1D	-2.21	102.82	105.11
2	A	750	HEM	C1B-NB-C4B	2.21	107.40	105.11
4	A	801	M48	C14-C15-C21	2.19	117.66	112.84
2	A	750	HEM	C2D-C1D-ND	-2.18	110.35	112.93
4	B	801	M48	C03-C02-N01	-2.18	119.58	122.13
2	A	750	HEM	C2A-C1A-CHA	-2.10	122.02	126.00
4	B	801	M48	C08-C09-C10	-2.08	119.32	121.09
3	A	760	H4B	N8-C8A-N1	2.03	118.80	115.82

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, 95th 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 ²)	Q<0.9
1	A	408/422 (96%)	0.54	43 (10%) 7 6	25, 51, 89, 127	0
1	B	411/422 (97%)	0.26	16 (3%) 37 37	27, 42, 73, 101	0
All	All	819/844 (97%)	0.40	59 (7%) 16 14	25, 46, 85, 127	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	300	PHE	6.4
1	A	715	VAL	5.0
1	A	716	TRP	4.9
1	A	355	PHE	4.8
1	A	299	ARG	4.5
1	B	348	VAL	4.1
1	B	718	GLY	4.1
1	A	385	ASN	3.8
1	A	489	ASP	3.8
1	A	338	PRO	3.7
1	B	350	THR	3.7
1	A	506	ILE	3.7
1	B	352	ASP	3.4
1	B	321	THR	3.4
1	A	713	THR	3.4
1	A	488	PRO	3.3
1	A	352	ASP	3.3
1	A	514	ARG	3.2
1	A	382	GLU	3.1
1	A	503	GLU	3.1
1	A	487	GLN	3.1
1	A	493	LEU	3.1
1	A	378	MET	3.0
1	A	351	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	711	TRP	2.9
1	B	299	ARG	2.8
1	A	717	LYS	2.8
1	A	486	LYS	2.8
1	A	373	GLY	2.7
1	B	389	GLU	2.7
1	B	677	VAL	2.6
1	A	388	ILE	2.6
1	A	714	HIS	2.6
1	A	491	SER	2.5
1	A	470	HIS	2.5
1	A	712	ASN	2.4
1	A	354	LEU	2.4
1	A	376	ALA	2.4
1	A	469	LYS	2.4
1	A	391	THR	2.4
1	A	551	PHE	2.4
1	B	338	PRO	2.4
1	A	415	CYS	2.3
1	A	466	THR	2.3
1	A	511	LYS	2.3
1	A	390	SER	2.2
1	B	392	SER	2.2
1	B	678	TRP	2.2
1	A	392	SER	2.1
1	A	300	PHE	2.1
1	A	353	GLN	2.1
1	A	393	THR	2.1
1	B	566	ALA	2.1
1	B	351	LYS	2.1
1	A	389	GLU	2.1
1	B	679	ILE	2.1
1	B	680	VAL	2.1
1	A	375	LYS	2.1
1	A	386	LYS	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, 95th 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 ²)	Q<0.9
5	ACT	A	860	4/4	0.23	5.93	67,73,74,75	0
2	HEM	B	750	43/43	0.20	1.15	24,30,40,49	0
2	HEM	A	750	43/43	0.17	0.63	27,32,41,43	0
6	ZN	A	1717	1/1	0.13	0.53	40,40,40,40	0
3	H4B	B	760	17/17	0.17	0.28	28,30,37,38	0
5	ACT	B	860	4/4	0.14	0.12	54,58,58,62	0
3	H4B	A	760	17/17	0.13	-0.21	28,32,40,43	0
4	M48	A	801	23/23	0.14	-0.46	13,22,81,84	0
4	M48	B	801	23/23	0.14	-0.82	16,26,76,84	0

6.5 Other polymers ⓘ

There are no such residues in this entry.