



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 12:25 PM GMT

PDB ID : 3NLO
Title : Structure of neuronal nitric oxide synthase R349A mutant heme domain in complex with 6-{{(3'S,4'R)-3'-[2''-(3'''-fluorophenethylamino)ethoxy]pyrrolidin-4'-yl}methyl}-4-methylpyridin-2-amine
Authors : Li, H.; Delker, S.L.; Poulos, T.L.
Deposited on : 2010-06-21
Resolution : 2.30 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>

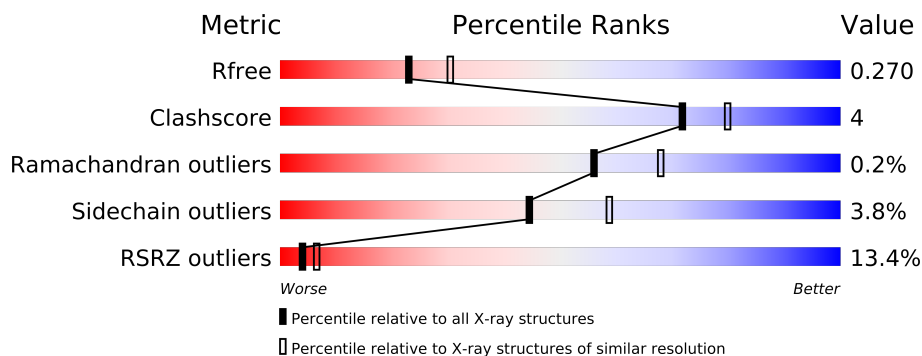
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 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 2.30 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	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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
4	JSR	A	800	-	X
4	JSR	B	800	-	X
5	ACT	A	860	-	X
6	EDO	A	890	-	X

2 Entry composition i

There are 8 unique types of molecules in this entry. The entry contains 6948 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	0	0
			3313	2121	566	605	21			
1	B	411	Total	C	N	O	S	0	0	0
			3339	2137	571	610	21			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	349	ALA	ARG	ENGINEERED MUTATION	UNP P29476
B	349	ALA	ARG	ENGINEERED MUTATION	UNP P29476

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



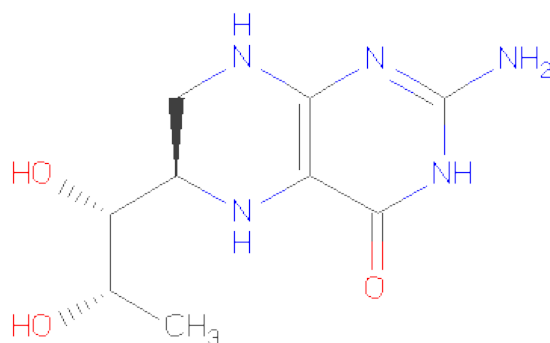
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

Continued on next page...

Continued from previous page...

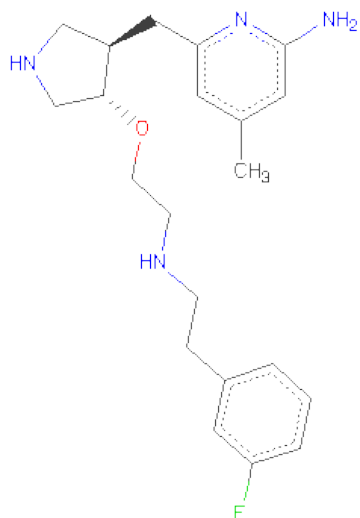
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



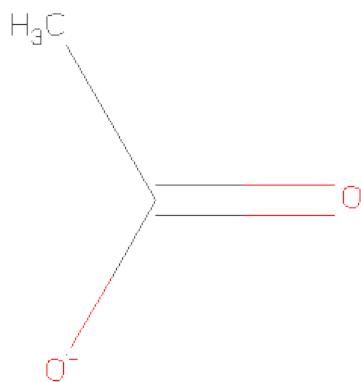
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 4 is 6-{[(3R,4S)-4-(2-{[2-(3-FLUOROPHENYL)ETHYL]AMINO}ETHOXY)PYRROLIDIN-3-YL]METHYL}-4-METHYLPYRIDIN-2-AMINE (three-letter code: JSR) (formula: $C_{21}H_{29}FN_4O$).



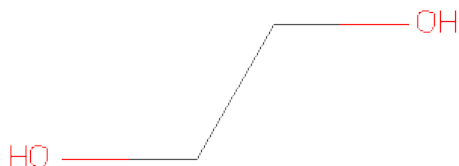
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	0	0
			27	21	1	4	1		
4	B	1	Total	C	F	N	O	0	0
			27	21	1	4	1		

- 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 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

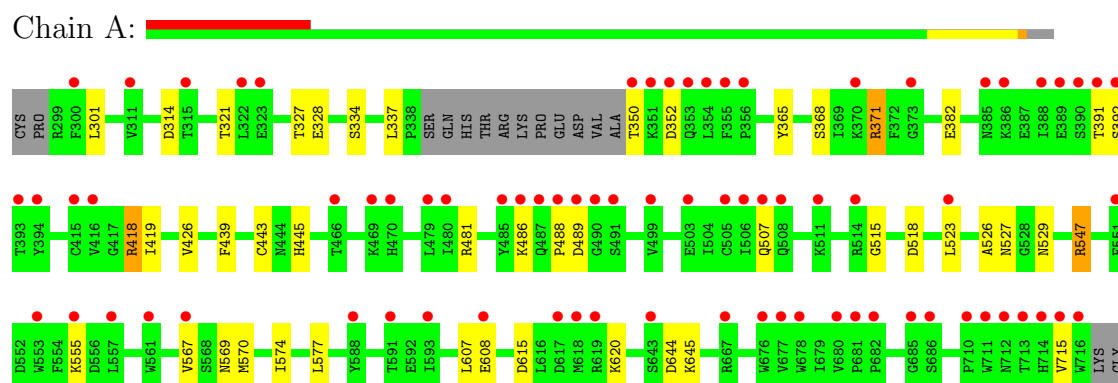
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	43	Total	O	0	0
			43	43		
8	B	62	Total	O	0	0
			62	62		

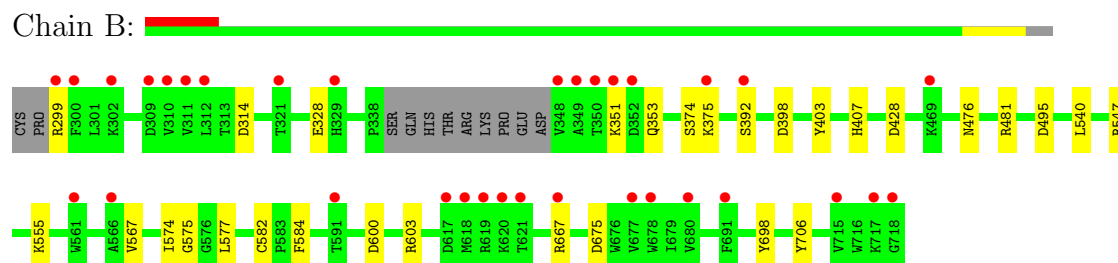
3 Residue-property plots

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, α , β , γ	51.41Å 112.00Å 164.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.62 – 2.30 39.15 – 2.29	Depositor EDS
% Data completeness (in resolution range)	96.6 (40.62-2.30) 96.6 (39.15-2.29)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.197 , 0.262 0.212 , 0.270	Depositor DCC
R_{free} test set	2103 reflections (5.25%)	DCC
Wilson B-factor (Å ²)	53.3	Xtriage
Anisotropy	0.417	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.1	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 42192 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6948	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.75% 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: ZN, H4B, EDO, JSR, ACT, HEM

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	0/3406	0.78	2/4621 (0.0%)
1	B	0.86	1/3432 (0.0%)	0.80	3/4654 (0.1%)
All	All	0.85	1/6838 (0.0%)	0.79	5/9275 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	582	CYS	CB-SG	6.54	1.93	1.82

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	418	ARG	NE-CZ-NH1	-6.68	116.96	120.30
1	B	675	ASP	CB-CG-OD1	5.55	123.30	118.30
1	A	570	MET	CA-CB-CG	-5.42	104.09	113.30
1	B	428	ASP	CB-CG-OD2	5.22	122.99	118.30
1	B	675	ASP	CB-CG-OD2	-5.19	113.63	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	18	0
1	B	3339	0	0	12	0
2	A	43	0	0	0	0
2	B	43	0	0	3	0
3	A	17	0	0	0	0
3	B	17	0	0	0	0
4	A	27	0	0	1	0
4	B	27	0	0	1	0
5	A	4	0	0	0	0
5	B	4	0	0	0	0
6	A	8	0	12	2	0
7	A	1	0	0	0	0
8	A	43	0	0	1	0
8	B	62	0	0	2	0
All	All	6948	0	12	30	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 4.

All (30) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:706:TYR:OH	2:B:750:HEM:O1D	1.86	0.94
1:A:350:THR:N	8:A:1008:HOH:O	2.20	0.75
1:A:371:ARG:CG	1:A:371:ARG:NH2	2.60	0.64
1:A:334:SER:N	6:A:890:EDO:HO1	1.95	0.63
1:A:547:ARG:NH1	1:A:644:ASP:OD1	2.35	0.60
1:B:567:VAL:CG2	4:B:800:JSR:C5'	2.80	0.59
1:A:426:VAL:N	6:A:891:EDO:HO1	2.03	0.57
1:A:567:VAL:CG2	4:A:800:JSR:C5'	2.83	0.56
1:B:495:ASP:OD2	1:B:603:ARG:NH2	2.38	0.56
1:A:301:LEU:O	1:A:314:ASP:N	2.41	0.54
1:B:600:ASP:OD2	8:B:1055:HOH:O	2.19	0.51
1:A:365:TYR:O	1:A:368:SER:OG	2.30	0.50
1:B:299:ARG:CB	1:B:299:ARG:CZ	2.90	0.48
1:B:584:PHE:CD1	2:B:750:HEM:CAC	2.97	0.48
2:B:750:HEM:CBC	2:B:750:HEM:CMC	2.91	0.48
1:B:403:TYR:CE1	1:B:407:HIS:CE1	3.02	0.47
1:A:607:LEU:O	1:A:608:GLU:C	2.52	0.47
1:A:328:GLU:OE2	1:B:328:GLU:OE2	2.33	0.46
1:B:374:SER:O	1:B:375:LYS:C	2.53	0.46
1:A:391:THR:O	1:A:392:SER:OG	2.34	0.46
1:A:418:ARG:O	1:A:419:ILE:C	2.54	0.45
1:A:526:ALA:O	1:A:529:ASN:ND2	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:445:HIS:CD2	1:A:445:HIS:C	2.92	0.43
1:B:574:ILE:O	1:B:577:LEU:N	2.54	0.41
1:B:314:ASP:OD2	1:B:698:TYR:OH	2.37	0.41
1:A:439:PHE:CZ	1:A:443:CYS:SG	3.14	0.41
1:A:391:THR:O	1:A:392:SER:CB	2.69	0.41
1:B:476:ASN:ND2	8:B:1051:HOH:O	2.54	0.40
1:A:515:GLY:N	1:A:518:ASP:OD2	2.54	0.40
1:A:574:ILE:O	1:A:577:LEU:N	2.54	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	403/422 (96%)	378 (94%)	24 (6%)	1 (0%)	56	68
1	B	407/422 (96%)	393 (97%)	13 (3%)	1 (0%)	56	68
All	All	810/844 (96%)	771 (95%)	37 (5%)	2 (0%)	56	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	575	GLY
1	A	488	PRO

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.

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	363/376 (96%)	344 (95%)	19 (5%)	32	42
1	B	365/376 (97%)	356 (98%)	9 (2%)	60	77
All	All	728/752 (97%)	700 (96%)	28 (4%)	44	59

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	321	THR
1	A	327	THR
1	A	337	LEU
1	A	352	ASP
1	A	371	ARG
1	A	382	GLU
1	A	481	ARG
1	A	486	LYS
1	A	489	ASP
1	A	507	GLN
1	A	523	LEU
1	A	527	ASN
1	A	547	ARG
1	A	555	LYS
1	A	569	ASN
1	A	615	ASP
1	A	620	LYS
1	A	645	LYS
1	A	715	VAL
1	B	351	LYS
1	B	353	GLN
1	B	392	SER
1	B	398	ASP
1	B	481	ARG
1	B	540	LEU
1	B	547	ARG
1	B	555	LYS
1	B	667	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 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	750	1	49,50,50	2.48	16 (32%)	46,82,82	2.27	11 (23%)
3	H4B	A	760	-	18,18,18	1.22	1 (5%)	24,26,26	2.55	8 (33%)
4	JSR	A	800	-	29,29,29	0.96	2 (6%)	38,38,38	2.02	8 (21%)
5	ACT	A	860	-	1,3,3	1.27	0	0,3,3	0.00	-
6	EDO	A	890	-	3,3,3	0.90	0	2,2,2	0.35	0
6	EDO	A	891	-	3,3,3	0.54	0	2,2,2	0.62	0
2	HEM	B	750	1	49,50,50	2.82	16 (32%)	46,82,82	1.97	9 (19%)
3	H4B	B	760	-	18,18,18	1.50	3 (16%)	24,26,26	2.08	10 (41%)
4	JSR	B	800	-	29,29,29	1.01	2 (6%)	38,38,38	2.36	10 (26%)
5	ACT	B	860	-	1,3,3	2.90	1 (100%)	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	0/0/2/2
4	JSR	A	800	-	-	0/13/23/23	0/3/3/3
5	ACT	A	860	-	-	0/0/0/0	0/0/0/0
6	EDO	A	890	-	-	0/1/1/1	0/0/0/0
6	EDO	A	891	-	-	0/1/1/1	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	0/0/2/2
4	JSR	B	800	-	-	0/13/23/23	0/3/3/3
5	ACT	B	860	-	-	0/0/0/0	0/0/0/0

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	750	HEM	C2D-C1D	9.93	1.47	1.44
2	B	750	HEM	C3D-C4D	6.62	1.46	1.44
2	A	750	HEM	C4A-C3A	6.37	1.48	1.40
2	A	750	HEM	C2D-C1D	6.26	1.46	1.44
2	B	750	HEM	C3B-C2B	-5.51	1.34	1.43
2	A	750	HEM	C3B-C2B	-5.35	1.34	1.43
2	B	750	HEM	C3D-C2D	5.26	1.53	1.43
2	B	750	HEM	C3C-C2C	-5.15	1.34	1.43
2	B	750	HEM	C4A-C3A	5.09	1.46	1.40
2	A	750	HEM	FE-ND	5.08	2.16	1.97
2	A	750	HEM	C3C-C2C	-4.82	1.35	1.43
2	A	750	HEM	C3B-CAB	4.69	1.55	1.40
2	B	750	HEM	C3C-CAC	4.42	1.54	1.40
2	A	750	HEM	C3D-C2D	4.38	1.51	1.43
2	A	750	HEM	C3C-CAC	4.06	1.53	1.40
2	B	750	HEM	C3B-CAB	3.90	1.52	1.40
3	A	760	H4B	C2-N2	3.66	1.38	1.32
2	B	750	HEM	CMC-C2C	3.55	1.58	1.47
2	A	750	HEM	CMC-C2C	3.28	1.57	1.47
3	B	760	H4B	C2-N2	3.08	1.37	1.32
2	B	750	HEM	C2B-C1B	2.97	1.45	1.44
3	B	760	H4B	C2-N1	2.92	1.37	1.33
2	B	750	HEM	CMB-C2B	2.90	1.56	1.47
5	B	860	ACT	CH3-C	2.90	1.52	1.48
2	B	750	HEM	CAA-C2A	2.78	1.56	1.52
2	B	750	HEM	FE-ND	2.77	2.07	1.97
2	A	750	HEM	FE-NC	2.75	2.08	1.97
2	B	750	HEM	CMD-C2D	2.74	1.55	1.47
2	A	750	HEM	CMD-C2D	2.68	1.55	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	750	HEM	FE-NA	2.63	2.03	1.92
2	A	750	HEM	CMB-C2B	2.63	1.55	1.47
4	B	800	JSR	C12-C13	2.51	1.42	1.37
2	B	750	HEM	C3B-C4B	2.41	1.47	1.44
3	B	760	H4B	C4A-C8A	-2.34	1.37	1.41
2	A	750	HEM	CHD-C4C	2.28	1.40	1.36
4	A	800	JSR	C12-C13	2.28	1.41	1.37
4	B	800	JSR	C14-C13	2.27	1.41	1.36
2	B	750	HEM	FE-NA	2.23	2.02	1.92
2	A	750	HEM	O1A-CGA	2.13	1.29	1.22
2	A	750	HEM	CAA-C2A	2.10	1.55	1.52
4	A	800	JSR	C14-C13	2.07	1.41	1.36

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	750	HEM	C3B-C4B-NB	-9.20	107.42	114.00
2	A	750	HEM	C3B-C4B-NB	-8.49	107.93	114.00
4	B	800	JSR	C6A-N1A-C2A	7.39	123.42	118.23
4	B	800	JSR	C3A-C2A-N1A	-6.89	115.33	122.99
4	A	800	JSR	C6A-N1A-C2A	6.66	122.91	118.23
4	B	800	JSR	C2'-C3'-C4'	6.32	108.42	103.48
3	A	760	H4B	N2-C2-N3	5.58	124.00	117.86
3	A	760	H4B	C4-C4A-C8A	5.41	119.57	114.56
2	A	750	HEM	C4D-ND-C1D	5.31	110.60	105.16
2	A	750	HEM	CBA-CAA-C2A	-5.19	103.55	112.69
4	A	800	JSR	C3A-C2A-N1A	-5.17	117.24	122.99
4	A	800	JSR	C2'-C3'-C4'	4.78	107.21	103.48
3	B	760	H4B	C2-N1-C8A	4.18	123.55	117.61
3	B	760	H4B	C4-C4A-C8A	4.16	118.41	114.56
2	A	750	HEM	C4C-NC-C1C	4.15	109.85	105.53
3	A	760	H4B	C2-N1-C8A	4.09	123.42	117.61
2	B	750	HEM	CHC-C1C-NC	-3.98	121.27	124.73
2	A	750	HEM	C1A-CHA-C4D	-3.94	122.29	127.47
3	A	760	H4B	C7-C6-C9	-3.82	107.77	113.66
3	A	760	H4B	C6-C7-N8	-3.59	107.02	111.66
2	A	750	HEM	C2D-C1D-ND	-3.52	108.77	112.93
3	A	760	H4B	C4-C4A-N5	3.47	124.14	119.10
2	B	750	HEM	CBD-CAD-C3D	-3.25	107.29	114.37
4	A	800	JSR	C5'-C4'-C7A	-3.18	101.60	114.26
3	B	760	H4B	C6-C7-N8	-3.18	107.56	111.66
3	A	760	H4B	C4A-C8A-N8	3.12	123.51	119.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	750	HEM	C4A-C3A-C2A	3.06	109.13	107.00
3	B	760	H4B	C4-C4A-N5	3.06	123.55	119.10
4	B	800	JSR	C4A-C3A-C2A	2.99	122.29	120.29
4	A	800	JSR	C3-N2-C2	2.82	123.51	113.30
2	A	750	HEM	CHD-C4C-NC	2.81	127.17	124.73
3	B	760	H4B	N2-C2-N3	2.76	120.90	117.86
2	B	750	HEM	C4D-ND-C1D	2.67	107.90	105.16
3	B	760	H4B	C4A-C4-N3	2.63	120.82	114.06
4	B	800	JSR	C14-C13-C12	-2.62	119.71	123.32
2	A	750	HEM	C1B-NB-C4B	2.60	107.82	105.16
2	B	750	HEM	CHD-C4C-NC	2.58	126.97	124.73
4	B	800	JSR	C3-N2-C2	2.57	122.62	113.30
2	B	750	HEM	CBA-CAA-C2A	-2.56	108.19	112.69
3	A	760	H4B	N2-C2-N1	-2.54	116.88	120.31
2	A	750	HEM	C3A-C4A-NA	-2.53	107.50	109.41
3	B	760	H4B	N8-C8A-N1	2.44	119.40	115.82
4	B	800	JSR	C2A-C7A-C4'	2.42	125.05	115.57
4	A	800	JSR	C4'-C5'-N1'	2.42	110.63	105.75
4	B	800	JSR	C5'-C4'-C7A	-2.41	104.67	114.26
4	A	800	JSR	C14-C13-C12	-2.39	120.04	123.32
2	B	750	HEM	CHB-C1B-NB	2.32	127.49	124.31
2	A	750	HEM	CBD-CAD-C3D	-2.28	109.40	114.37
3	B	760	H4B	C7-C6-C9	-2.23	110.21	113.66
2	B	750	HEM	C1B-NB-C4B	2.19	107.40	105.16
2	B	750	HEM	C1A-CHA-C4D	-2.13	124.67	127.47
3	B	760	H4B	N3-C2-N1	-2.11	118.82	121.78
4	B	800	JSR	C7A-C4'-C3'	2.10	116.73	113.47
4	A	800	JSR	O1-C3'-C4'	2.07	115.50	109.38
3	B	760	H4B	C4A-C8A-N8	2.06	122.06	119.23
4	B	800	JSR	O1-C3'-C2'	-2.02	105.08	110.63

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	407/422 (96%)	0.94	76 (18%) 2 3	40, 71, 127, 163	0
1	B	411/422 (97%)	0.48	33 (8%) 12 19	40, 60, 89, 115	0
All	All	818/844 (96%)	0.71	109 (13%) 4 6	40, 64, 117, 163	0

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	348	VAL	6.5
1	B	300	PHE	6.1
1	A	352	ASP	5.9
1	A	713	THR	5.5
1	A	716	TRP	5.3
1	B	351	LYS	5.0
1	A	351	LYS	4.8
1	A	389	GLU	4.8
1	A	486	LYS	4.6
1	A	354	LEU	4.6
1	A	488	PRO	4.5
1	A	470	HIS	4.5
1	A	390	SER	4.4
1	B	680	VAL	4.3
1	A	715	VAL	4.2
1	A	618	MET	4.2
1	A	619	ARG	4.1
1	A	712	ASN	4.0
1	A	388	ILE	3.9
1	A	506	ILE	3.8
1	A	415	CYS	3.8
1	A	391	THR	3.8
1	A	678	TRP	3.8
1	B	619	ARG	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	350	THR	3.7
1	B	329	HIS	3.6
1	A	490	GLY	3.6
1	A	355	PHE	3.6
1	A	680	VAL	3.6
1	A	682	PRO	3.6
1	A	485	TYR	3.5
1	B	352	ASP	3.5
1	A	507	GLN	3.5
1	A	394	TYR	3.4
1	B	321	THR	3.4
1	A	714	HIS	3.3
1	B	667	ARG	3.3
1	A	479	LEU	3.2
1	A	503	GLU	3.1
1	A	385	ASN	3.1
1	A	553	TRP	3.1
1	A	551	PHE	3.1
1	B	299	ARG	3.1
1	A	489	ASP	3.1
1	A	677	VAL	3.0
1	B	677	VAL	3.0
1	A	416	VAL	2.9
1	A	681	PRO	2.9
1	A	710	PRO	2.8
1	B	718	GLY	2.8
1	A	555	LYS	2.8
1	A	350	THR	2.8
1	A	676	TRP	2.7
1	A	353	GLN	2.7
1	A	511	LYS	2.7
1	B	375	LYS	2.7
1	A	393	THR	2.7
1	A	591	THR	2.7
1	A	392	SER	2.7
1	A	300	PHE	2.7
1	A	469	LYS	2.7
1	A	514	ARG	2.7
1	A	505	CYS	2.6
1	B	618	MET	2.6
1	B	620	LYS	2.6
1	B	621	THR	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	469	LYS	2.6
1	B	591	THR	2.5
1	A	311	VAL	2.5
1	B	561	TRP	2.5
1	A	480	ILE	2.5
1	B	691	PHE	2.5
1	A	487	GLN	2.4
1	A	711	TRP	2.4
1	A	557	LEU	2.4
1	A	561	TRP	2.4
1	A	667	ARG	2.4
1	A	356	PRO	2.4
1	A	322	LEU	2.4
1	A	386	LYS	2.4
1	A	685	GLY	2.3
1	B	392	SER	2.3
1	B	715	VAL	2.3
1	B	311	VAL	2.3
1	A	373	GLY	2.3
1	A	567	VAL	2.2
1	A	499	VAL	2.2
1	A	323	GLU	2.2
1	A	466	THR	2.2
1	B	717	LYS	2.2
1	A	523	LEU	2.2
1	A	491	SER	2.2
1	A	593	ILE	2.2
1	B	617	ASP	2.2
1	A	643	SER	2.2
1	B	566	ALA	2.2
1	A	588	TYR	2.2
1	B	678	TRP	2.2
1	B	302	LYS	2.1
1	B	349	ALA	2.1
1	B	309	ASP	2.1
1	B	312	LEU	2.1
1	B	310	VAL	2.1
1	A	617	ASP	2.0
1	A	370	LYS	2.0
1	A	508	GLN	2.0
1	A	686	SER	2.0
1	A	315	THR	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	608	GLU	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	0.33	9.48	71,73,73,75	0
4	JSR	A	800	27/27	0.56	6.46	60,90,136,138	0
6	EDO	A	890	4/4	0.40	4.28	59,60,61,61	0
4	JSR	B	800	27/27	0.38	3.94	64,88,107,108	0
5	ACT	B	860	4/4	0.18	1.89	73,77,78,79	0
6	EDO	A	891	4/4	0.16	1.61	66,68,68,68	0
3	H4B	A	760	17/17	0.26	0.99	53,57,61,61	0
2	HEM	A	750	43/43	0.26	0.92	40,47,70,77	0
3	H4B	B	760	17/17	0.24	0.88	48,52,59,64	0
2	HEM	B	750	43/43	0.18	0.45	42,46,66,72	0
7	ZN	A	900	1/1	0.10	-1.72	54,54,54,54	0

6.5 Other polymers ⓘ

There are no such residues in this entry.