



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:41 PM GMT

PDB ID : 4D2Z
Title : Structure of rat neuronal nitric oxide synthase heme domain in complex with (1S,2S)-2-(3-fluorobenzyl)-N-{2-[2-(1H-imidazol-1-yl)pyrimidin-4-yl]ethyl} cyclopropanamine
Authors : Li, H.; Poulos, T.L.
Deposited on : 2014-10-20
Resolution : 1.89 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

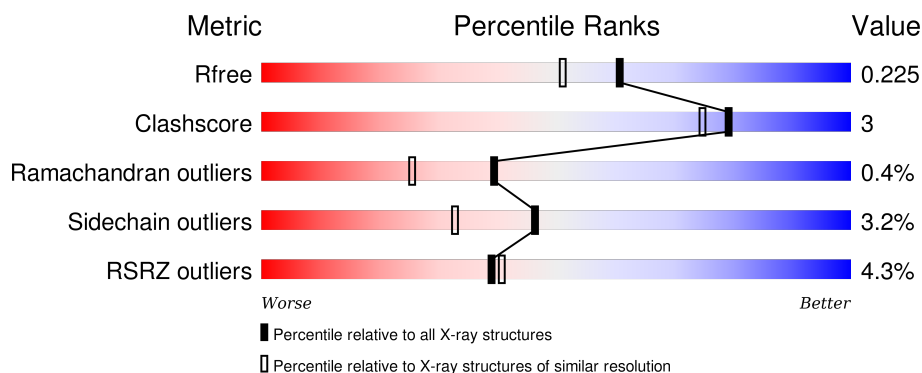
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.89 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}	91344	6965 (1.90-1.86)
Clashscore	102246	7778 (1.90-1.86)
Ramachandran outliers	100387	7691 (1.90-1.86)
Sidechain outliers	100360	7692 (1.90-1.86)
RSRZ outliers	91569	6979 (1.90-1.86)

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. 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	<div> <div>7%</div> <div>84%</div> <div>11%</div> <div>••</div> </div>
1	B	422	<div> <div>2%</div> <div>88%</div> <div>9%</div> <div>•</div> </div>

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	K9L	A	800	-	-	-	X
5	ACT	A	860	-	-	-	X

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 7247 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	408	Total	C	N	O	S	0	1	1
			3317	2123	567	605	22			
1	B	411	Total	C	N	O	S	0	2	0
			3356	2150	574	611	21			

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



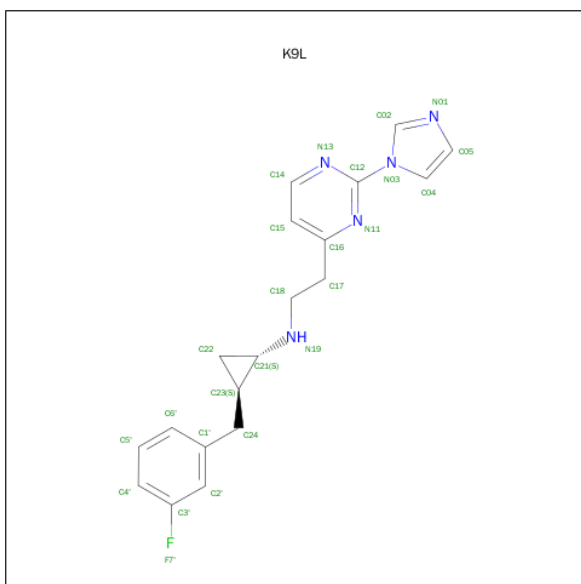
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- 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 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 (1S,2S)-2-(3-FLUOROBENZYL)-N-{2-[2-(1H-IMIDAZOL-1-YL)PYRIMIDIN-4-YL]ETHYL}CYCLOPROPANAMINE (three-letter code: K9L) (formula: C₁₉H₂₀FN₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	F	N	0	0
			25	19	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	F	N	0	0
			25	19	1	5		

- 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		

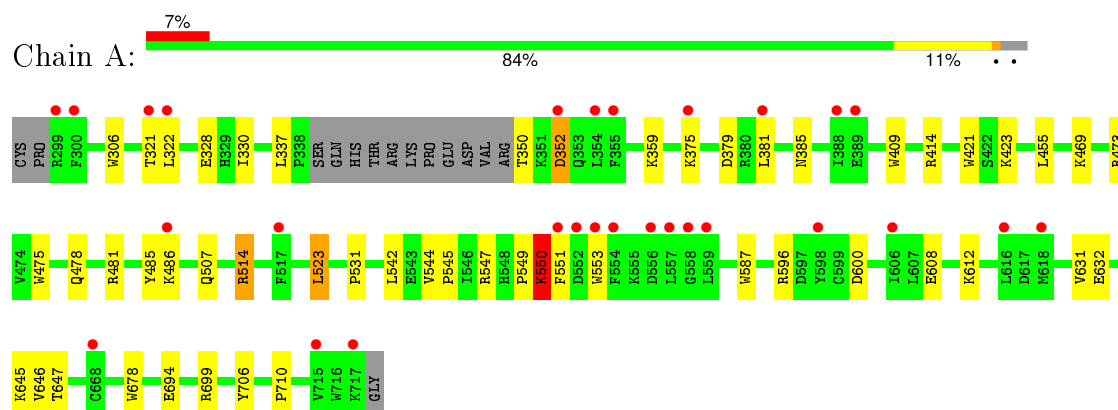
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	162	Total	O	0	0
			162	162		
7	B	233	Total	O	0	0
			233	233		

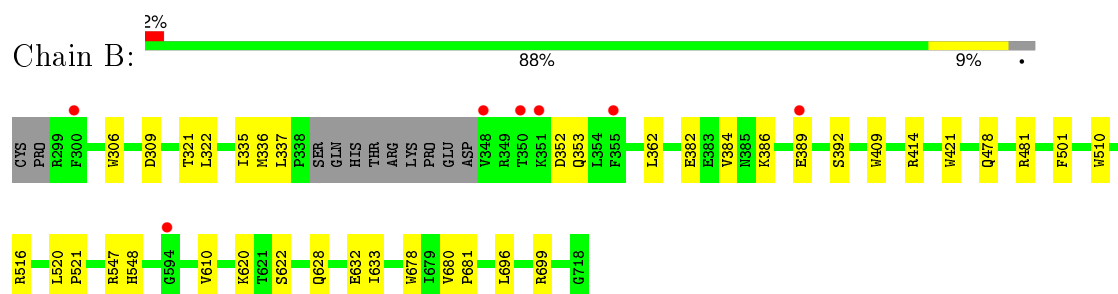
3 Residue-property plots [i](#)

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, α , β , γ	51.82Å 111.32Å 164.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.42 – 1.89 49.42 – 1.96	Depositor EDS
% Data completeness (in resolution range)	75.3 (49.42-1.89) 98.6 (49.42-1.96)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 1.95Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.178 , 0.227 0.184 , 0.225	Depositor DCC
R_{free} test set	3398 reflections (5.21%)	DCC
Wilson B-factor (Å ²)	37.2	Xtriage
Anisotropy	0.954	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 54.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	3 of 68591 reflections (0.004%)	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7247	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.71% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, ZN, ACT, H4B, K9L

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	0.40	0/3413	0.54	0/4631
1	B	0.42	0/3456	0.56	0/4686
All	All	0.41	0/6869	0.55	0/9317

There are no bond length outliers.

There are no bond angle outliers.

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	3317	0	3226	27	0
1	B	3356	0	3273	19	0
2	A	43	0	30	3	0
2	B	43	0	30	1	0
3	A	17	0	15	0	0
3	B	17	0	15	0	0
4	A	25	0	20	2	0
4	B	25	0	20	3	0
5	A	4	0	3	0	0
5	B	4	0	3	0	0
6	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	162	0	0	0	0
7	B	233	0	0	1	0
All	All	7247	0	6635	47	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 3.

All (47) 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:A:523:LEU:HD22	1:A:531:PRO:HB2	1.65	0.78
1:A:549:PRO:O	1:A:550:LYS:NZ	2.20	0.73
2:B:750:HEM:HHC	2:B:750:HEM:HBB2	1.71	0.72
2:A:750:HEM:HMC2	2:A:750:HEM:HBC2	1.76	0.68
1:A:359:LYS:HZ3	1:A:381:LEU:HD21	1.68	0.58
1:A:486:LYS:O	1:A:514:ARG:NH2	2.38	0.56
1:A:478:GLN:HB2	1:A:481:ARG:HG3	1.88	0.55
2:A:750:HEM:HBB2	2:A:750:HEM:HHC	1.89	0.54
1:B:478:GLN:HB2	1:B:481:ARG:HG3	1.89	0.53
1:B:322:LEU:HB3	1:B:699:ARG:HH21	1.72	0.52
1:A:473:ARG:NH2	1:A:710:PRO:HD3	2.25	0.51
4:A:800:K9L:H4'	1:B:306:TRP:CH2	2.46	0.51
1:B:336:MET:HE2	4:B:800:K9L:C3'	2.41	0.50
1:A:475:TRP:HB2	1:A:523:LEU:HB3	1.94	0.49
1:A:455:LEU:HG	1:A:647:THR:HB	1.94	0.48
1:A:475:TRP:CZ2	1:A:531:PRO:HG3	2.49	0.48
1:A:322:LEU:HB2	1:A:699:ARG:HB2	1.95	0.47
1:A:631:VAL:HG11	1:B:628:GLN:HG3	1.96	0.47
1:A:409:TRP:CE3	1:A:421:TRP:HA	2.49	0.47
1:B:620:LYS:HD3	1:B:622:SER:H	1.80	0.47
1:A:306:TRP:CH2	4:B:800:K9L:H4'	2.50	0.46
1:A:350:THR:OG1	1:A:352:ASP:OD1	2.30	0.46
1:B:409:TRP:CE3	1:B:421:TRP:HA	2.50	0.46
1:B:414:ARG:HD3	1:B:678:TRP:CD2	2.51	0.45
4:A:800:K9L:H2'	4:A:800:K9L:H23	1.77	0.45
1:B:510:TRP:CE2	1:B:521:PRO:HD3	2.52	0.45
1:A:414:ARG:HD3	1:A:678:TRP:CD2	2.52	0.45
4:B:800:K9L:H22	7:B:2197:HOH:O	2.17	0.44
1:A:330:ILE:HD11	1:B:696:LEU:HD22	2.00	0.44
1:B:680:VAL:HA	1:B:681:PRO:HD3	1.87	0.44
1:A:375:LYS:NZ	1:A:379:ASP:OD2	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:596:ARG:O	1:A:600:ASP:HB2	2.18	0.43
1:B:501:PHE:CD2	1:B:520:LEU:HD13	2.53	0.43
1:A:455:LEU:HD12	1:A:587:TRP:HB3	2.01	0.43
1:A:632:GLU:OE2	1:B:628:GLN:NE2	2.51	0.43
1:A:544:VAL:HA	1:A:545:PRO:HD2	1.92	0.43
1:A:321:THR:HG23	1:A:322:LEU:HG	2.01	0.43
1:A:542:LEU:HD21	1:A:646:VAL:HG22	2.01	0.43
1:A:596:ARG:NH2	1:A:600:ASP:OD2	2.47	0.42
1:B:501:PHE:HD2	1:B:520:LEU:HD13	1.84	0.42
1:B:386:LYS:HA	1:B:386:LYS:HD3	1.84	0.41
1:A:551:PHE:HB3	1:A:553:TRP:CE2	2.55	0.41
1:B:548:HIS:NE2	1:B:632:GLU:OE1	2.53	0.41
1:A:694:GLU:HB3	1:B:335:ILE:HD13	2.03	0.41
1:B:362:LEU:HD11	1:B:384:VAL:HG21	2.02	0.40
1:B:610:VAL:HG21	1:B:633:ILE:HD11	2.03	0.40
1:A:706:TYR:OH	2:A:750:HEM:O2D	2.18	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	405/422 (96%)	389 (96%)	14 (4%)	2 (0%)	34	20
1	B	409/422 (97%)	401 (98%)	7 (2%)	1 (0%)	52	40
All	All	814/844 (96%)	790 (97%)	21 (3%)	3 (0%)	39	25

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	514	ARG
1	B	352	ASP

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Mol	Chain	Res	Type
1	A	550	LYS

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%)	350 (96%)	14 (4%)	40	25
1	B	368/377 (98%)	359 (98%)	9 (2%)	57	46
All	All	732/754 (97%)	709 (97%)	23 (3%)	46	34

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	328	GLU
1	A	337	LEU
1	A	352	ASP
1	A	385	ASN
1	A	423	LYS
1	A	469	LYS
1	A	485	TYR
1	A	507	GLN
1	A	523	LEU
1	A	547	ARG
1	A	550	LYS
1	A	608	GLU
1	A	612	LYS
1	A	645	LYS
1	B	309	ASP
1	B	321	THR
1	B	337	LEU
1	B	353	GLN
1	B	382	GLU
1	B	389	GLU
1	B	392	SER
1	B	516	ARG

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Mol	Chain	Res	Type
1	B	547	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	407	HIS
1	B	508	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	1,4	30,50,50	2.22	11 (36%)	24,82,82	2.46	9 (37%)
3	H4B	A	760	-	13,18,18	0.79	0	11,26,26	2.52	5 (45%)
4	K9L	A	800	2	24,28,28	1.40	3 (12%)	32,38,38	2.39	13 (40%)
5	ACT	A	860	-	1,3,3	1.32	0	0,3,3	0.00	-
2	HEM	B	750	1,4	30,50,50	2.02	7 (23%)	24,82,82	2.44	10 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	H4B	B	760	-	13,18,18	0.85	0	11,26,26	2.36	4 (36%)
4	K9L	B	800	2	24,28,28	1.41	3 (12%)	32,38,38	2.41	15 (46%)
5	ACT	B	860	-	1,3,3	1.01	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	1,4	-	0/10/54/54	0/0/8/8
3	H4B	A	760	-	-	0/8/17/17	0/2/2/2
4	K9L	A	800	2	-	0/8/19/19	0/3/4/4
5	ACT	A	860	-	-	0/0/0/0	0/0/0/0
2	HEM	B	750	1,4	-	0/10/54/54	0/0/8/8
3	H4B	B	760	-	-	0/8/17/17	0/2/2/2
4	K9L	B	800	2	-	0/8/19/19	0/3/4/4
5	ACT	B	860	-	-	0/0/0/0	0/0/0/0

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	750	HEM	C3B-C4B	-6.70	1.45	1.51
2	B	750	HEM	C3B-C4B	-5.74	1.46	1.51
2	B	750	HEM	C3D-C4D	-5.27	1.44	1.51
2	A	750	HEM	C3D-C4D	-5.16	1.45	1.51
2	A	750	HEM	C2C-C1C	-3.74	1.45	1.52
2	B	750	HEM	C2C-C1C	-3.73	1.45	1.52
4	A	800	K9L	C04-N03	-3.65	1.33	1.39
4	B	800	K9L	C04-N03	-3.59	1.34	1.39
2	A	750	HEM	C2B-C1B	-2.06	1.45	1.51
2	B	750	HEM	C2D-C1D	-2.03	1.45	1.51
2	A	750	HEM	FE-ND	2.04	2.08	1.97
2	B	750	HEM	C4C-NC	2.06	1.38	1.36
2	A	750	HEM	CAA-C2A	2.08	1.55	1.52
2	B	750	HEM	C1C-NC	2.12	1.38	1.36
2	A	750	HEM	C3B-CAB	2.21	1.55	1.51
2	A	750	HEM	C3C-CAC	2.43	1.55	1.51
4	B	800	K9L	C12-N11	2.52	1.36	1.32
2	A	750	HEM	FE-NB	2.63	2.11	1.97
2	B	750	HEM	C3C-CAC	2.73	1.56	1.51
2	A	750	HEM	C1C-NC	2.79	1.39	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	750	HEM	C4C-NC	2.81	1.39	1.36
4	A	800	K9L	C12-N11	3.23	1.36	1.32
4	A	800	K9L	C12-N13	4.13	1.35	1.31
4	B	800	K9L	C12-N13	4.39	1.36	1.31

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	800	K9L	C22-C23-C24	-6.45	105.47	121.01
4	A	800	K9L	C22-C23-C24	-4.92	109.16	121.01
4	B	800	K9L	N13-C12-N11	-4.13	121.25	126.44
4	A	800	K9L	C15-C14-N13	-4.13	119.18	123.90
2	A	750	HEM	CBA-CAA-C2A	-4.09	105.19	112.53
4	A	800	K9L	N13-C12-N11	-3.90	121.54	126.44
2	B	750	HEM	CBA-CAA-C2A	-3.66	105.96	112.53
4	A	800	K9L	C04-N03-C12	-3.66	121.60	125.61
4	B	800	K9L	C15-C14-N13	-3.56	119.84	123.90
4	B	800	K9L	C22-C21-N19	-3.48	108.68	118.20
4	A	800	K9L	C18-N19-C21	-3.48	108.64	113.89
2	A	750	HEM	CBD-CAD-C3D	-3.46	103.49	113.55
4	A	800	K9L	C22-C21-N19	-3.10	109.74	118.20
3	A	760	H4B	N3-C2-N1	-3.00	120.61	125.53
4	B	800	K9L	C04-N03-C12	-2.97	122.36	125.61
3	B	760	H4B	N3-C2-N1	-2.60	121.27	125.53
2	B	750	HEM	CBD-CAD-C3D	-2.53	106.18	113.55
4	A	800	K9L	C4'-C3'-C2'	-2.53	120.08	123.35
4	A	800	K9L	C1'-C24-C23	-2.42	109.60	113.75
4	B	800	K9L	C4'-C3'-C2'	-2.42	120.23	123.35
4	B	800	K9L	C02-N03-C12	-2.40	121.31	126.02
2	B	750	HEM	CMA-C3A-C4A	-2.30	124.55	128.36
4	B	800	K9L	C18-N19-C21	-2.30	110.42	113.89
4	B	800	K9L	C15-C16-N11	-2.23	119.69	122.41
4	B	800	K9L	C05-C04-N03	-2.21	102.61	106.50
4	A	800	K9L	C05-C04-N03	-2.02	102.93	106.50
4	B	800	K9L	N11-C12-N03	2.07	117.88	114.82
3	B	760	H4B	C2-N1-C8A	2.24	119.57	114.54
2	A	750	HEM	CMD-C2D-C3D	2.46	125.25	114.35
2	A	750	HEM	C2D-C3D-C4D	2.48	105.71	101.50
4	B	800	K9L	C17-C16-N11	2.49	119.37	115.69
4	A	800	K9L	C12-N11-C16	2.64	118.71	115.26
3	A	760	H4B	C2-N1-C8A	2.73	120.67	114.54
4	A	800	K9L	C17-C16-N11	2.76	119.77	115.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	750	HEM	C2D-C3D-C4D	2.91	106.44	101.50
2	B	750	HEM	CMD-C2D-C3D	2.96	127.45	114.35
3	A	760	H4B	C4A-C8A-N8	2.99	121.96	118.43
2	B	750	HEM	C3B-C4B-CHC	3.17	127.62	123.16
3	B	760	H4B	C4-N3-C2	3.27	120.48	115.94
2	A	750	HEM	CMB-C2B-C3B	3.47	125.20	116.53
4	B	800	K9L	N13-C12-N03	3.48	120.83	115.16
3	A	760	H4B	C4-N3-C2	3.54	120.85	115.94
4	B	800	K9L	C12-N11-C16	3.67	120.06	115.26
2	B	750	HEM	CAD-C3D-C4D	3.97	126.48	112.47
4	A	800	K9L	N11-C12-N03	3.99	120.72	114.82
2	B	750	HEM	CMB-C2B-C3B	4.13	126.85	116.53
4	B	800	K9L	C04-N03-C02	4.14	116.24	108.53
4	A	800	K9L	C04-N03-C02	4.14	116.24	108.53
2	A	750	HEM	C3B-C4B-CHC	4.14	129.00	123.16
2	A	750	HEM	CAD-C3D-C4D	4.15	127.09	112.47
2	B	750	HEM	CMC-C2C-C3C	4.36	127.40	116.53
2	A	750	HEM	CMC-C2C-C3C	4.80	128.52	116.53
2	B	750	HEM	CAD-C3D-C2D	4.82	127.07	113.22
2	A	750	HEM	CAD-C3D-C2D	4.86	127.19	113.22
3	A	760	H4B	C4-C4A-C8A	5.18	119.25	114.56
3	B	760	H4B	C4-C4A-C8A	5.61	119.64	114.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	750	HEM	3	0
4	A	800	K9L	2	0
2	B	750	HEM	1	0
4	B	800	K9L	3	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, 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%)	0.62	28 (6%) 20 21	14, 45, 89, 127	0
1	B	411/422 (97%)	0.31	7 (1%) 73 75	16, 33, 67, 96	0
All	All	819/844 (97%)	0.47	35 (4%) 39 41	14, 38, 82, 127	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	717	LYS	8.0
1	A	355	PHE	4.7
1	A	554	PHE	4.6
1	B	348	VAL	4.4
1	A	352	ASP	4.2
1	B	300	PHE	4.1
1	A	322	LEU	3.7
1	A	715	VAL	3.6
1	A	558	GLY	3.4
1	A	551	PHE	3.3
1	A	668[A]	CYS	3.2
1	A	553	TRP	3.2
1	A	559	LEU	3.1
1	A	381	LEU	2.8
1	A	300	PHE	2.8
1	A	299	ARG	2.6
1	B	355[A]	PHE	2.6
1	A	552	ASP	2.6
1	A	557	LEU	2.5
1	A	517	PHE	2.5
1	A	388	ILE	2.5
1	B	389	GLU	2.5
1	B	350	THR	2.5
1	A	321	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	598	TYR	2.4
1	A	354	LEU	2.3
1	A	556	ASP	2.2
1	A	618	MET	2.2
1	A	486	LYS	2.2
1	A	616	LEU	2.2
1	A	375	LYS	2.2
1	B	351	LYS	2.1
1	A	606	ILE	2.1
1	A	389	GLU	2.1
1	B	594	GLY	2.0

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, 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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	ACT	A	860	4/4	0.97	0.36	15.75	52,55,55,56	0
4	K9L	A	800	25/25	0.97	0.17	2.53	16,36,90,95	0
4	K9L	B	800	25/25	0.95	0.16	1.68	15,30,97,101	0
6	ZN	A	1717	1/1	1.00	0.11	1.27	28,28,28,28	0
5	ACT	B	860	4/4	0.97	0.16	1.26	48,48,52,52	0
2	HEM	B	750	43/43	0.99	0.15	0.95	13,21,31,40	0
2	HEM	A	750	43/43	0.98	0.13	0.69	10,22,33,38	0
3	H4B	B	760	17/17	0.97	0.12	-0.17	18,24,31,38	0
3	H4B	A	760	17/17	0.97	0.10	-1.08	22,26,33,36	0

6.5 Other polymers

There are no such residues in this entry.