



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:51 AM GMT

PDB ID : 3JWU  
Title : Structure of rat neuronal nitric oxide synthase R349A mutant heme domain in complex with N1-{(3'R,4'S)-4'-[(6"-amino-4"-methylpyridin-2"-yl)methyl]pyrrolidin-3'-yl}-N2-(3'-fluorophenethyl)ethane-1,2-diamine tetrahydrochloride  
Authors : Delker, S.L.; Li, H.; Poulos, T.L.  
Deposited on : 2009-09-18  
Resolution : 1.93 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](mailto: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.

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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 : 1.7 (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

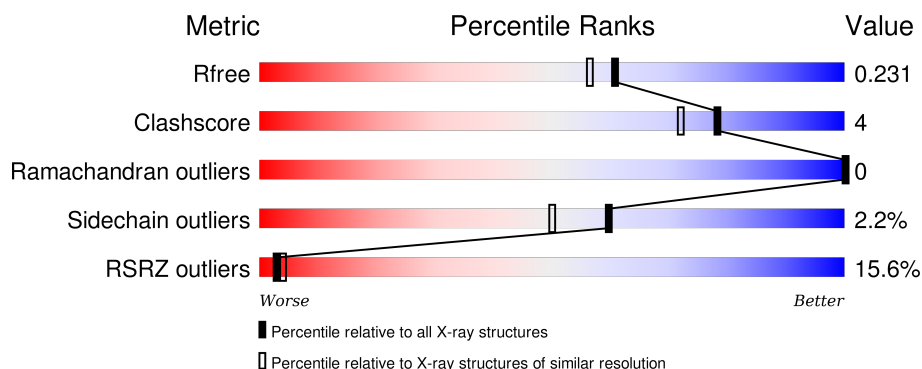
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.93 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	2910 (1.96-1.92)
Clashscore	102246	3095 (1.96-1.92)
Ramachandran outliers	100387	3062 (1.96-1.92)
Sidechain outliers	100360	3062 (1.96-1.92)
RSRZ outliers	91569	2915 (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. 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>21%</div> <div>87%</div> <div>9%</div> <div>.</div> </div>
1	B	422	<div> <div>9%</div> <div>89%</div> <div>8%</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
5	ACT	A	860	-	-	-	X

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 7229 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	407	Total	C	N	O	S	0	0	0
			3313	2121	566	605	21			
1	B	411	Total	C	N	O	S	0	1	0
			3342	2139	571	610	22			

There are 2 discrepancies between the modelled and reference sequences:

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

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



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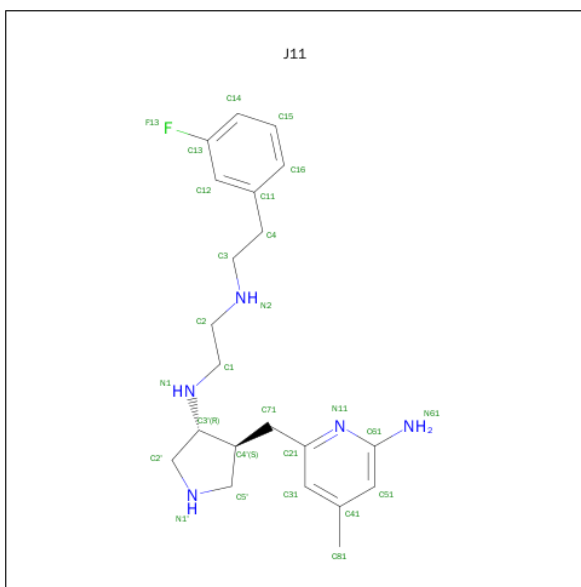
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- 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 N-{(3R,4S)-4-[(6-AMINO-4-METHYLPYRIDIN-2-YL)METHYL]PYRROLIDIN-3-YL}-N'-[2-(3-FLUOROPHENYL)ETHYL]ETHANE-1,2-DIAMINE (three-letter code: J11) (formula:  $C_{21}H_{30}FN_5$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	F	N	0	0
			27	21	1	5		
4	B	1	Total	C	F	N	0	0
			27	21	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 1	Zn 1	0	0

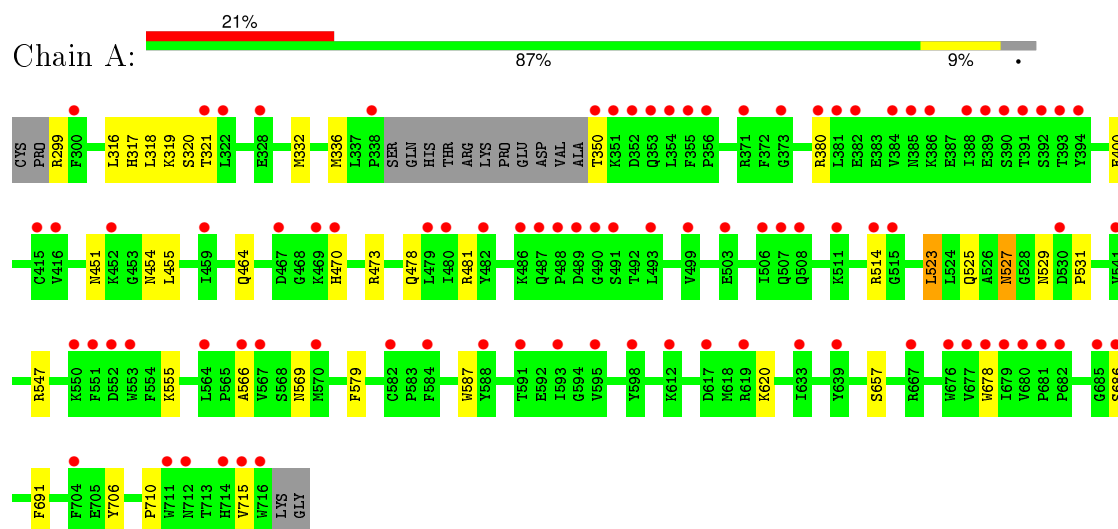
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	147	Total 147	O 147	0	0
7	B	244	Total 244	O 244	0	0

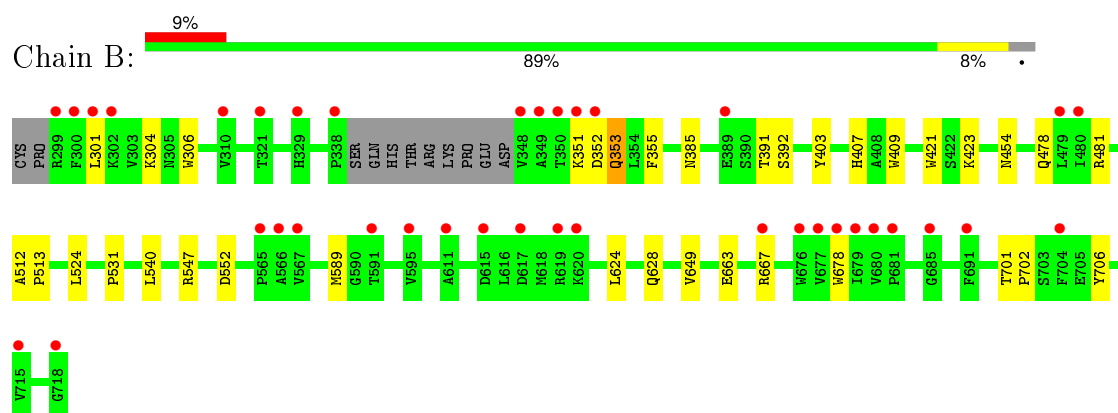
### 3 Residue-property plots [i](#)

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, $\alpha$ , $\beta$ , $\gamma$	51.83Å 111.85Å 164.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.01 – 1.93 38.01 – 1.92	Depositor EDS
% Data completeness (in resolution range)	97.2 (38.01-1.93) 97.2 (38.01-1.92)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.19 (at 1.92Å)	Xtriage
Refinement program	REFMAC 5.5.0089	Depositor
R, $R_{free}$	0.180 , 0.205 0.209 , 0.231	Depositor DCC
$R_{free}$ test set	3560 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.0	Xtriage
Anisotropy	0.684	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 47.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 71830 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7229	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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, J11, 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	0.57	0/3406	0.61	0/4621
1	B	0.59	0/3438	0.62	0/4662
All	All	0.58	0/6844	0.62	0/9283

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	3313	0	3221	21	0
1	B	3342	0	3256	21	0
2	A	43	0	30	5	0
2	B	43	0	30	5	0
3	A	17	0	15	0	0
3	B	17	0	15	0	0
4	A	27	0	30	3	0
4	B	27	0	30	2	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	147	0	0	2	0
7	B	244	0	0	3	0
All	All	7229	0	6633	48	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 4.

All (48) 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:B:706:TYR:OH	2:B:750:HEM:O1D	2.01	0.78
2:A:750:HEM:HBA1	4:A:800:J11:H71A	1.69	0.72
1:A:706:TYR:OH	2:A:750:HEM:O1D	2.04	0.71
2:A:750:HEM:O2D	4:A:800:J11:H2A	1.93	0.69
1:A:478:GLN:HB2	1:A:481:ARG:HG3	1.75	0.68
1:A:380:ARG:HD3	1:A:400:GLU:OE1	1.99	0.61
2:A:750:HEM:HBB2	2:A:750:HEM:HHC	1.82	0.60
2:B:750:HEM:O1A	7:B:1013:HOH:O	2.17	0.60
2:A:750:HEM:O2A	7:A:1101:HOH:O	2.16	0.59
1:A:523:LEU:HD22	1:A:531:PRO:HB2	1.84	0.59
1:B:663:GLU:O	1:B:667:ARG:HD2	2.02	0.59
1:A:299:ARG:HG3	1:A:318:LEU:HD11	1.88	0.55
1:A:473:ARG:NH2	1:A:710:PRO:HD3	2.24	0.53
2:B:750:HEM:HBA1	4:B:800:J11:H71A	1.91	0.52
1:A:455:LEU:HD12	1:A:587:TRP:HB3	1.90	0.52
1:B:706:TYR:OH	2:B:750:HEM:CGD	2.58	0.51
1:B:478:GLN:HB2	1:B:481:ARG:HG3	1.92	0.50
1:A:657:SER:HB2	7:A:1146:HOH:O	2.10	0.50
1:B:403:TYR:CE1	1:B:407:HIS:CE1	3.01	0.49
1:B:423:LYS:NZ	7:B:1220:HOH:O	2.46	0.49
1:A:455:LEU:HD12	1:A:587:TRP:CB	2.43	0.49
1:B:352:ASP:HB3	1:B:353:GLN:HE21	1.77	0.48
1:B:409:TRP:CE3	1:B:421:TRP:HA	2.48	0.48
1:B:701:THR:HA	1:B:702:PRO:C	2.35	0.46
1:B:624:LEU:O	1:B:628:GLN:HG3	2.16	0.45
2:B:750:HEM:HBC2	2:B:750:HEM:CMC	2.46	0.45
1:A:316:LEU:HD12	1:A:319:LYS:HD2	1.99	0.45
1:B:524:LEU:O	1:B:531:PRO:HA	2.16	0.44
1:B:304:LYS:NZ	7:B:1180:HOH:O	2.49	0.44
1:A:299:ARG:O	1:A:317:HIS:CE1	2.71	0.44
1:B:353:GLN:H	1:B:353:GLN:HE21	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:678:TRP:HH2	4:B:800:J11:H4	1.83	0.43
1:A:336:MET:HE3	1:A:678:TRP:HZ2	1.84	0.43
1:A:336:MET:HG3	1:B:306:TRP:NE1	2.34	0.43
1:A:470:HIS:HB3	1:A:527:ASN:ND2	2.33	0.42
4:A:800:J11:H3	4:A:800:J11:H1	1.79	0.42
1:A:451:ASN:HB3	1:A:454:ASN:O	2.20	0.42
1:A:464:GLN:HB3	1:A:579:PHE:CE2	2.54	0.42
1:B:351:LYS:HE3	1:B:392:SER:OG	2.20	0.42
1:A:332:MET:HE1	1:B:301:LEU:HD22	2.02	0.41
1:B:391:THR:O	1:B:392:SER:HB2	2.20	0.41
1:B:355:PHE:CE1	1:B:385:ASN:HB2	2.56	0.41
1:A:525:GLN:HG3	1:A:529:ASN:O	2.21	0.41
1:A:686:SER:HA	1:A:691:PHE:CG	2.56	0.41
1:A:478:GLN:HA	1:A:566:ALA:O	2.22	0.40
1:B:589:MET:HA	1:B:649:VAL:O	2.22	0.40
1:B:512:ALA:HA	1:B:513:PRO:HD3	1.98	0.40
1:A:336:MET:HE3	1:A:678:TRP:CZ2	2.57	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%)	396 (98%)	7 (2%)	0	100	100
1	B	408/422 (97%)	402 (98%)	6 (2%)	0	100	100
All	All	811/844 (96%)	798 (98%)	13 (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	363/376 (96%)	352 (97%)	11 (3%)	48	35
1	B	366/376 (97%)	361 (99%)	5 (1%)	74	68
All	All	729/752 (97%)	713 (98%)	16 (2%)	60	50

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

Mol	Chain	Res	Type
1	A	320	SER
1	A	321	THR
1	A	350	THR
1	A	514	ARG
1	A	523	LEU
1	A	527	ASN
1	A	547	ARG
1	A	555	LYS
1	A	569	ASN
1	A	620	LYS
1	A	715	VAL
1	B	353	GLN
1	B	454	ASN
1	B	540	LEU
1	B	547	ARG
1	B	552	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	425	GLN
1	A	454	ASN
1	A	527	ASN
1	A	569	ASN
1	A	605	ASN
1	A	642	GLN

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Mol	Chain	Res	Type
1	A	697	ASN
1	B	353	GLN
1	B	385	ASN
1	B	454	ASN
1	B	507	GLN
1	B	508	GLN
1	B	527	ASN
1	B	535	GLN
1	B	601	ASN
1	B	605	ASN
1	B	642	GLN
1	B	697	ASN

### 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	30,50,50	2.42	8 (26%)	24,82,82	2.59	12 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	H4B	A	760	-	13,18,18	1.09	2 (15%)	11,26,26	2.73	6 (54%)
4	J11	A	800	-	26,29,29	0.65	0	30,38,38	1.75	6 (20%)
5	ACT	A	860	-	1,3,3	1.26	0	0,3,3	0.00	-
2	HEM	B	750	1	30,50,50	2.12	11 (36%)	24,82,82	2.52	11 (45%)
3	H4B	B	760	-	13,18,18	0.90	1 (7%)	11,26,26	2.56	5 (45%)
4	J11	B	800	-	26,29,29	0.71	0	30,38,38	1.70	5 (16%)
5	ACT	B	860	-	1,3,3	1.25	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	-	0/10/54/54	0/0/8/8
3	H4B	A	760	-	-	0/8/17/17	0/2/2/2
4	J11	A	800	-	-	0/13/23/23	0/3/3/3
5	ACT	A	860	-	-	0/0/0/0	0/0/0/0
2	HEM	B	750	1	-	0/10/54/54	0/0/8/8
3	H4B	B	760	-	-	0/8/17/17	0/2/2/2
4	J11	B	800	-	-	0/13/23/23	0/3/3/3
5	ACT	B	860	-	-	0/0/0/0	0/0/0/0

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	750	HEM	C3D-C4D	-7.42	1.42	1.51
2	A	750	HEM	C3B-C4B	-6.41	1.46	1.51
2	B	750	HEM	C3B-C4B	-5.48	1.47	1.51
2	B	750	HEM	C3D-C4D	-5.34	1.44	1.51
2	A	750	HEM	C2C-C1C	-4.57	1.43	1.52
2	B	750	HEM	C2C-C1C	-3.78	1.45	1.52
2	A	750	HEM	C2D-C1D	-2.53	1.43	1.51
2	B	750	HEM	C2B-C1B	-2.34	1.44	1.51
2	A	750	HEM	C2B-C1B	-2.22	1.44	1.51
2	B	750	HEM	C2D-C1D	-2.06	1.45	1.51
3	A	760	H4B	C4-N3	2.02	1.36	1.33
2	B	750	HEM	CAA-C2A	2.02	1.55	1.52
2	A	750	HEM	FE-NB	2.03	2.08	1.97
3	A	760	H4B	C2-N2	2.03	1.38	1.34
2	B	750	HEM	C1C-NC	2.06	1.38	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	750	HEM	C4C-NC	2.08	1.38	1.36
2	B	750	HEM	C3C-CAC	2.21	1.55	1.51
3	B	760	H4B	C7-N8	2.48	1.49	1.46
2	B	750	HEM	FE-ND	2.57	2.11	1.97
2	A	750	HEM	FE-ND	2.72	2.11	1.97
2	B	750	HEM	FE-NC	3.04	2.07	1.95
2	A	750	HEM	FE-NC	3.22	2.08	1.95

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	750	HEM	CBD-CAD-C3D	-3.62	103.01	113.55
2	A	750	HEM	CBA-CAA-C2A	-3.55	106.17	112.53
2	B	750	HEM	CAA-C2A-C1A	-3.52	123.19	127.01
3	A	760	H4B	N3-C2-N1	-3.35	120.04	125.53
2	A	750	HEM	CAA-C2A-C1A	-3.17	123.56	127.01
2	B	750	HEM	C3C-CAC-CBC	-3.03	119.80	124.46
4	B	800	J11	C31-C21-N11	-2.94	119.64	122.96
2	B	750	HEM	CBD-CAD-C3D	-2.81	105.36	113.55
3	B	760	H4B	N3-C2-N1	-2.46	121.50	125.53
4	A	800	J11	C14-C13-C12	-2.30	120.38	123.35
2	B	750	HEM	CMA-C3A-C4A	-2.24	124.67	128.36
4	A	800	J11	C31-C21-N11	-2.22	120.46	122.96
2	A	750	HEM	C3C-CAC-CBC	-2.16	121.14	124.46
2	A	750	HEM	C3B-C4B-NB	-2.10	107.62	111.63
4	B	800	J11	C3-C4-C11	-2.09	108.50	112.83
4	B	800	J11	C14-C13-C12	-2.05	120.70	123.35
3	B	760	H4B	C2-N1-C8A	2.06	119.17	114.54
3	A	760	H4B	C4A-C8A-N8	2.22	121.05	118.43
3	A	760	H4B	C2-N1-C8A	2.23	119.54	114.54
3	B	760	H4B	C4A-C8A-N8	2.34	121.18	118.43
4	A	800	J11	C3-N2-C2	2.34	121.65	113.35
4	A	800	J11	C5'-C4'-C3'	2.46	107.21	103.80
2	A	750	HEM	C2D-C3D-C4D	2.50	105.73	101.50
2	B	750	HEM	C2D-C3D-C4D	2.52	105.77	101.50
3	A	760	H4B	N2-C2-N3	2.53	121.39	117.20
2	B	750	HEM	C3B-C4B-CHC	2.76	127.05	123.16
2	A	750	HEM	CMD-C2D-C3D	2.96	127.42	114.35
2	B	750	HEM	CMD-C2D-C3D	3.03	127.77	114.35
2	A	750	HEM	C3B-C4B-CHC	3.11	127.54	123.16
3	B	760	H4B	C4-N3-C2	3.78	121.19	115.94
4	B	800	J11	C1-N1-C3'	3.89	119.76	113.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	750	HEM	CAD-C3D-C2D	4.15	125.13	113.22
2	A	750	HEM	CAD-C3D-C4D	4.18	127.22	112.47
4	A	800	J11	C61-N11-C21	4.33	121.31	118.23
2	A	750	HEM	CMB-C2B-C3B	4.40	127.52	116.53
2	B	750	HEM	CMC-C2C-C3C	4.48	127.71	116.53
2	B	750	HEM	CMB-C2B-C3B	4.69	128.24	116.53
2	B	750	HEM	CAD-C3D-C4D	4.70	129.04	112.47
3	A	760	H4B	C4-N3-C2	4.71	122.47	115.94
2	A	750	HEM	CAD-C3D-C2D	4.81	127.04	113.22
2	A	750	HEM	CMC-C2C-C3C	4.83	128.57	116.53
4	B	800	J11	C61-N11-C21	5.03	121.81	118.23
3	A	760	H4B	C4-C4A-C8A	5.51	119.55	114.56
4	A	800	J11	C1-N1-C3'	5.69	122.47	113.89
3	B	760	H4B	C4-C4A-C8A	6.12	120.10	114.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	750	HEM	5	0
4	A	800	J11	3	0
2	B	750	HEM	5	0
4	B	800	J11	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

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%)	1.22	90 (22%) <b>1</b> <b>1</b>	28, 52, 97, 119	0
1	B	411/422 (97%)	0.56	38 (9%) <b>11</b> <b>17</b>	27, 41, 64, 87	0
All	All	818/844 (96%)	0.89	128 (15%) <b>3</b> <b>4</b>	27, 46, 89, 119	0

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	300	PHE	7.8
1	B	350	THR	7.6
1	B	348	VAL	7.6
1	A	488	PRO	7.5
1	A	716	TRP	7.4
1	A	715	VAL	7.1
1	A	355	PHE	6.6
1	A	352	ASP	6.3
1	A	388	ILE	5.9
1	A	506	ILE	5.7
1	A	390	SER	5.5
1	A	392	SER	5.1
1	B	619	ARG	4.8
1	A	351	LYS	4.7
1	A	489	ASP	4.6
1	A	300	PHE	4.5
1	B	349	ALA	4.4
1	A	389	GLU	4.4
1	A	714	HIS	4.3
1	A	321	THR	4.2
1	A	486	LYS	4.2
1	A	490	GLY	4.1
1	B	351	LYS	4.1
1	A	391	THR	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	386	LYS	4.0
1	A	567	VAL	4.0
1	A	503	GLU	3.9
1	A	507	GLN	3.9
1	A	350	THR	3.9
1	A	678	TRP	3.9
1	B	299	ARG	3.8
1	A	394	TYR	3.7
1	A	679	ILE	3.6
1	A	682	PRO	3.6
1	A	470	HIS	3.6
1	A	384	VAL	3.6
1	B	567	VAL	3.6
1	A	511	LYS	3.5
1	A	619	ARG	3.5
1	A	385	ASN	3.5
1	A	711	TRP	3.4
1	A	354	LEU	3.4
1	A	487	GLN	3.4
1	A	712	ASN	3.3
1	B	677	VAL	3.3
1	A	584	PHE	3.3
1	A	479	LEU	3.3
1	B	591	THR	3.3
1	B	611	ALA	3.2
1	B	615	ASP	3.2
1	B	680	VAL	3.2
1	B	620	LYS	3.2
1	A	593	ILE	3.1
1	A	469	LYS	3.1
1	A	393	THR	3.0
1	A	416	VAL	2.9
1	B	667	ARG	2.9
1	A	415	CYS	2.9
1	B	310	VAL	2.9
1	B	352	ASP	2.9
1	B	679	ILE	2.9
1	B	321	THR	2.9
1	B	566	ALA	2.9
1	A	591	THR	2.8
1	A	552	ASP	2.8
1	A	685	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	667	ARG	2.8
1	B	301	LEU	2.8
1	A	639	TYR	2.8
1	A	550	LYS	2.8
1	A	612	LYS	2.8
1	A	499	VAL	2.7
1	B	479	LEU	2.7
1	A	491	SER	2.7
1	B	617	ASP	2.7
1	A	677	VAL	2.7
1	A	680	VAL	2.7
1	B	691	PHE	2.7
1	A	467	ASP	2.6
1	A	541	VAL	2.6
1	A	704	PHE	2.6
1	A	382	GLU	2.6
1	A	530	ASP	2.6
1	A	353	GLN	2.5
1	B	681	PRO	2.5
1	B	676	TRP	2.5
1	A	515	GLY	2.5
1	A	338	PRO	2.5
1	A	514	ARG	2.5
1	A	482	TYR	2.5
1	A	681	PRO	2.5
1	A	371	ARG	2.4
1	A	356	PRO	2.4
1	B	678	TRP	2.4
1	A	582	CYS	2.4
1	A	480	ILE	2.4
1	B	480	ILE	2.4
1	B	389	GLU	2.4
1	B	329	HIS	2.4
1	B	685	GLY	2.3
1	A	595	VAL	2.3
1	B	715	VAL	2.3
1	A	459	ILE	2.3
1	A	566	ALA	2.3
1	A	551	PHE	2.3
1	A	373	GLY	2.3
1	B	718	GLY	2.3
1	A	676	TRP	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	302	LYS	2.3
1	B	595	VAL	2.2
1	A	570	MET	2.2
1	A	588	TYR	2.2
1	A	322	LEU	2.2
1	A	381	LEU	2.2
1	A	508	GLN	2.2
1	A	633	ILE	2.2
1	B	565	PRO	2.2
1	A	493	LEU	2.2
1	A	617	ASP	2.1
1	A	598	TYR	2.1
1	A	564	LEU	2.1
1	A	380	ARG	2.1
1	B	338	PRO	2.1
1	B	704	PHE	2.0
1	A	452	LYS	2.0
1	A	328	GLU	2.0
1	A	553	TRP	2.0
1	A	686	SER	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, 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	ACT	A	860	4/4	0.95	0.20	4.86	57,58,58,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	J11	A	800	27/27	0.91	0.25	1.09	32,48,82,83	0
4	J11	B	800	27/27	0.92	0.19	0.59	33,42,68,70	0
3	H4B	B	760	17/17	0.97	0.18	0.50	32,34,37,37	0
2	HEM	B	750	43/43	0.97	0.16	0.44	29,32,46,52	0
3	H4B	A	760	17/17	0.97	0.18	0.36	35,37,39,41	0
2	HEM	A	750	43/43	0.97	0.20	0.29	29,32,49,58	0
5	ACT	B	860	4/4	0.98	0.10	-1.02	51,52,52,52	0
6	ZN	A	900	1/1	0.99	0.07	-1.14	35,35,35,35	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.