



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:48 AM GMT

PDB ID : 3JTA  
Title : Structure of neuronal nitric oxide synthase heme domain in the ferrous state complexed with N 5 -[4-(methylsulfanyl)butanimidoyl]-L-ornithine  
Authors : Li, H.; Poulos, T.L.  
Deposited on : 2009-09-11  
Resolution : 2.18 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

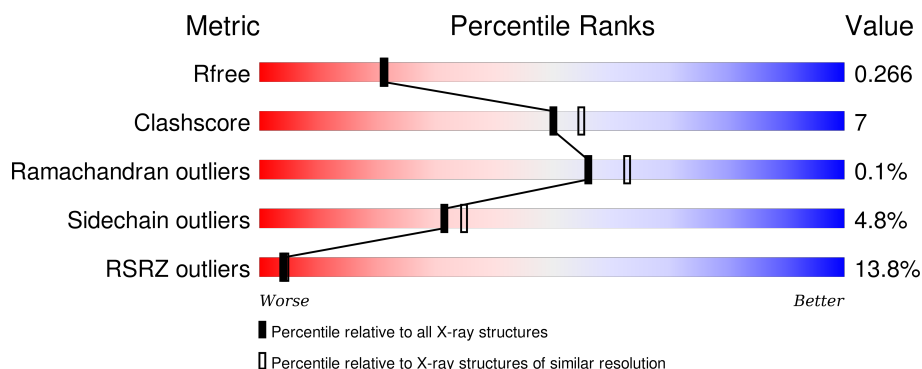
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.18 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	5130 (2.20-2.16)
Clashscore	102246	5965 (2.20-2.16)
Ramachandran outliers	100387	5863 (2.20-2.16)
Sidechain outliers	100360	5864 (2.20-2.16)
RSRZ outliers	91569	5142 (2.20-2.16)

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	
1	B	422	

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	JM6	A	800	-	-	X	-
4	JM6	B	800	-	-	X	-
5	ACT	A	860	-	-	-	X

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 6934 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	2	0
			3322	2127	566	607	22			
1	B	411	Total	C	N	O	S	0	1	0
			3348	2142	574	610	22			

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



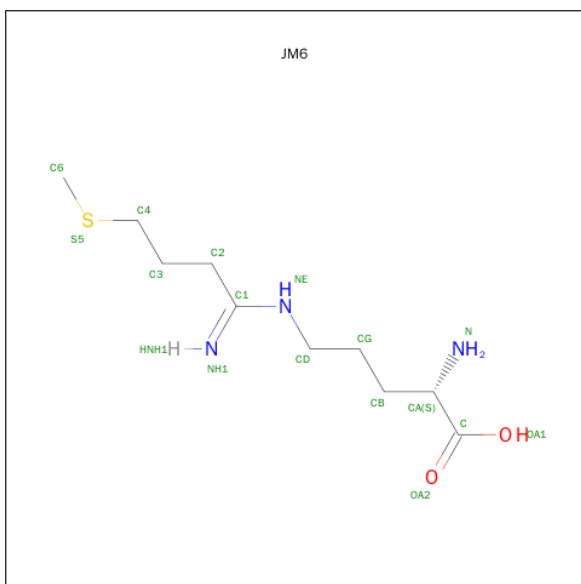
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- 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 N 5 -[4-(METHYLSULFANYL)BUTANIMIDOYL]-L-ORNITHINE (three-letter code: JM6) (formula: C<sub>10</sub>H<sub>21</sub>N<sub>3</sub>O<sub>2</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			16	10	3	2	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	S	0	0
			16	10	3	2	1		

- 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		

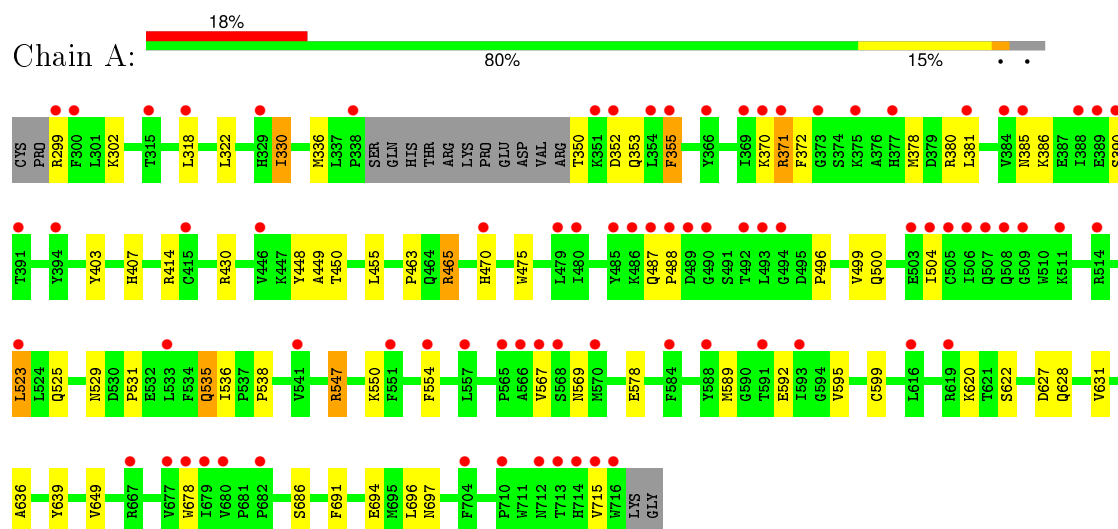
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	42	Total	O	0	0
			42	42		
7	B	61	Total	O	0	0
			61	61		

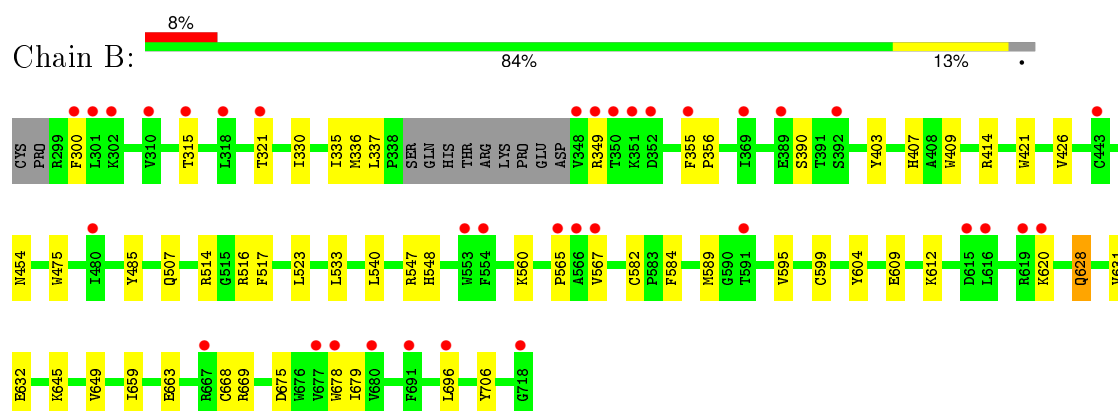
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Nitric oxide synthase, brain



- Molecule 1: Nitric oxide synthase, brain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	51.84Å 111.50Å 164.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.21 – 2.18 40.80 – 2.17	Depositor EDS
% Data completeness (in resolution range)	98.6 (41.21-2.18) 98.7 (40.80-2.17)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.15 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.5.0089	Depositor
R, $R_{free}$	0.190 , 0.245 0.216 , 0.266	Depositor DCC
$R_{free}$ test set	2528 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	50.1	Xtriage
Anisotropy	0.204	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 55.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 50849 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6934	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.99% 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, JM6, 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	0.91	2/3421 (0.1%)	0.84	0/4641
1	B	0.93	3/3444 (0.1%)	0.81	2/4669 (0.0%)
All	All	0.92	5/6865 (0.1%)	0.83	2/9310 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	372	PHE	CG-CD1	7.04	1.49	1.38
1	A	372	PHE	CE1-CZ	6.67	1.50	1.37
1	B	604	TYR	CD1-CE1	5.62	1.47	1.39
1	B	426	VAL	CB-CG2	5.27	1.64	1.52
1	B	582	CYS	CB-SG	5.12	1.91	1.82

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	669	ARG	NE-CZ-NH2	-5.73	117.43	120.30
1	B	533	LEU	CB-CG-CD1	-5.11	102.31	111.00

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	3322	0	3232	52	0
1	B	3348	0	3264	26	0
2	A	43	0	30	5	0
2	B	43	0	30	6	0
3	A	17	0	15	0	0
3	B	17	0	15	0	0
4	A	16	0	19	13	0
4	B	16	0	19	10	0
5	A	4	0	3	0	0
5	B	4	0	3	0	0
6	A	1	0	0	0	0
7	A	42	0	0	5	0
7	B	61	0	0	0	0
All	All	6934	0	6630	94	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 7.

All (94) 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)
4:A:800:JM6:H6A	4:A:800:JM6:H2	1.37	1.06
4:A:800:JM6:HD	4:A:800:JM6:H4A	1.45	0.98
4:A:800:JM6:C6	4:A:800:JM6:H2	1.95	0.94
4:A:800:JM6:CD	4:A:800:JM6:H4A	1.98	0.92
1:A:371:ARG:CG	1:A:371:ARG:HH21	1.85	0.89
2:A:750:HEM:HMC2	2:A:750:HEM:HBC2	1.52	0.89
1:A:371:ARG:HH21	1:A:371:ARG:HG2	1.38	0.87
1:A:355:PHE:CZ	1:A:385:ASN:HB2	2.17	0.79
1:A:567:VAL:HG23	4:A:800:JM6:H6	1.68	0.76
1:B:567:VAL:H	4:B:800:JM6:H6B	1.51	0.75
1:A:350:THR:HG22	1:A:352:ASP:H	1.52	0.73
1:A:487:GLN:HB3	1:A:488:PRO:HD2	1.72	0.71
1:A:535:GLN:HE22	1:A:538:PRO:HD3	1.54	0.71
4:B:800:JM6:H4A	4:B:800:JM6:CD	2.22	0.70
1:A:636:ALA:C	7:A:128:HOH:O	2.29	0.70
4:A:800:JM6:HD	4:A:800:JM6:C4	2.20	0.70
2:A:750:HEM:NB	4:A:800:JM6:H3A	2.06	0.70
1:A:523:LEU:HD22	1:A:531:PRO:HB2	1.76	0.67
4:B:800:JM6:HDA	4:B:800:JM6:H4A	1.77	0.66
1:A:636:ALA:O	7:A:128:HOH:O	2.12	0.66
2:B:750:HEM:HBC2	2:B:750:HEM:CMC	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:VAL:HG23	4:A:800:JM6:C6	2.25	0.66
1:A:299:ARG:HG3	1:A:318:LEU:HD21	1.78	0.64
1:A:330:ILE:HD11	1:B:696:LEU:HD22	1.78	0.63
2:A:750:HEM:CMC	2:A:750:HEM:HBC2	2.25	0.60
1:A:371:ARG:HG2	1:A:371:ARG:NH2	2.13	0.58
1:A:465:ARG:CD	1:A:578:GLU:OE1	2.52	0.58
2:B:750:HEM:HBC2	2:B:750:HEM:HMC1	1.85	0.57
4:B:800:JM6:H4A	4:B:800:JM6:NE	2.18	0.57
1:B:675:ASP:O	1:B:679:ILE:HG12	2.04	0.57
1:A:696:LEU:HD22	1:B:330:ILE:HD11	1.87	0.57
1:A:639:TYR:N	7:A:128:HOH:O	2.37	0.57
4:A:800:JM6:HD	4:A:800:JM6:H6	1.87	0.57
1:B:485:TYR:CZ	1:B:514:ARG:HA	2.40	0.57
1:A:631:VAL:HG11	1:B:628:GLN:HG2	1.87	0.57
1:A:639:TYR:HB3	7:A:128:HOH:O	2.06	0.56
1:A:554:PHE:HB3	7:A:108:HOH:O	2.04	0.56
1:B:565:PRO:HG2	4:B:800:JM6:H2A	1.87	0.56
1:B:300:PHE:HD2	1:B:315:THR:HG22	1.71	0.56
1:A:525:GLN:HG3	1:A:529:ASN:O	2.06	0.56
1:B:517:PHE:HB2	1:B:560:LYS:HE2	1.88	0.55
2:A:750:HEM:HBB2	2:A:750:HEM:HHC	1.89	0.55
1:A:355:PHE:CE2	1:A:385:ASN:ND2	2.75	0.54
1:A:487:GLN:CB	1:A:488:PRO:HD2	2.37	0.54
1:A:547:ARG:HD3	1:A:547:ARG:H	1.73	0.53
1:B:595:VAL:O	1:B:599:CYS:HB2	2.09	0.52
1:A:694:GLU:HB3	1:B:335:ILE:HD13	1.90	0.52
1:A:475:TRP:HB2	1:A:523:LEU:HB3	1.92	0.50
4:A:800:JM6:HD	4:A:800:JM6:C6	2.42	0.50
1:A:465:ARG:HD2	1:A:578:GLU:OE1	2.12	0.49
1:B:409:TRP:CE3	1:B:421:TRP:HA	2.47	0.49
1:A:592:GLU:OE1	4:A:800:JM6:NE	2.45	0.49
1:B:414:ARG:HD3	1:B:678:TRP:CD2	2.48	0.49
1:A:500:GLN:O	1:A:504:ILE:HG13	2.13	0.48
2:B:750:HEM:C4B	4:B:800:JM6:H3A	2.49	0.48
4:A:800:JM6:H4A	4:A:800:JM6:HDA	1.92	0.47
1:B:584:PHE:CE1	4:B:800:JM6:S5	3.08	0.47
1:A:686:SER:HA	1:A:691:PHE:CG	2.48	0.47
1:B:475:TRP:HB2	1:B:523:LEU:HB3	1.95	0.47
1:A:370:LYS:HE3	1:A:370:LYS:HB2	1.71	0.47
1:A:430:ARG:O	1:A:463:PRO:HG3	2.14	0.47
1:A:449:ALA:O	1:A:455:LEU:HA	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:TYR:CD2	1:A:448:TYR:C	2.87	0.47
1:A:535:GLN:NE2	1:A:536:ILE:O	2.48	0.47
1:A:299:ARG:HG3	1:A:318:LEU:CD2	2.45	0.46
1:A:628:GLN:HG2	1:B:631:VAL:HG11	1.97	0.46
1:A:371:ARG:HG3	1:A:371:ARG:HH21	1.78	0.46
1:A:475:TRP:CZ2	1:A:531:PRO:HG3	2.51	0.45
1:B:485:TYR:CE1	1:B:514:ARG:HA	2.50	0.45
1:A:589:MET:HA	1:A:649:VAL:O	2.15	0.45
1:B:517:PHE:CB	1:B:560:LYS:HE2	2.47	0.45
1:B:548:HIS:NE2	1:B:632:GLU:OE1	2.47	0.44
2:B:750:HEM:NC	4:B:800:JM6:H4	2.32	0.44
2:B:750:HEM:CBC	2:B:750:HEM:HMC1	2.46	0.43
1:A:414:ARG:HD3	1:A:678:TRP:CD2	2.53	0.43
1:B:584:PHE:HE1	4:B:800:JM6:S5	2.42	0.43
1:A:450:THR:O	1:A:455:LEU:HD23	2.18	0.43
1:B:589:MET:HA	1:B:649:VAL:O	2.18	0.43
1:A:686:SER:HA	1:A:691:PHE:CB	2.49	0.43
1:A:496:PRO:HA	1:A:499:VAL:HG23	2.01	0.42
1:A:595:VAL:O	1:A:599:CYS:HB2	2.20	0.42
2:A:750:HEM:C1B	4:A:800:JM6:H3A	2.55	0.42
1:A:487:GLN:HB3	1:A:488:PRO:CD	2.47	0.41
1:B:403:TYR:CE1	1:B:407:HIS:CE1	3.08	0.41
1:B:659:ILE:O	1:B:663:GLU:HG3	2.21	0.41
1:A:403:TYR:CE1	1:A:407:HIS:CE1	3.09	0.41
1:A:336:MET:CE	1:A:678:TRP:HZ2	2.34	0.41
1:A:350:THR:N	1:A:353:GLN:HE21	2.18	0.41
1:A:627:ASP:O	1:A:631:VAL:HG23	2.21	0.41
1:B:706:TYR:OH	2:B:750:HEM:O1D	2.16	0.41
1:B:355:PHE:N	1:B:356:PRO:HD2	2.36	0.40
1:A:385:ASN:O	1:A:386:LYS:C	2.58	0.40
1:B:565:PRO:HB2	4:B:800:JM6:H2	2.03	0.40
1:A:465:ARG:HD3	1:A:578:GLU:OE1	2.19	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	405/422 (96%)	385 (95%)	19 (5%)	1 (0%)	52	57
1	B	408/422 (97%)	397 (97%)	11 (3%)	0	100	100
All	All	813/844 (96%)	782 (96%)	30 (4%)	1 (0%)	56	63

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	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	365/377 (97%)	346 (95%)	19 (5%)	29	31
1	B	367/377 (97%)	350 (95%)	17 (5%)	33	37
All	All	732/754 (97%)	696 (95%)	36 (5%)	31	34

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	302	LYS
1	A	330	ILE
1	A	355	PHE
1	A	371	ARG
1	A	378	MET
1	A	380	ARG
1	A	381	LEU
1	A	390	SER
1	A	465	ARG
1	A	470	HIS
1	A	523	LEU

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Mol	Chain	Res	Type
1	A	535	GLN
1	A	547	ARG
1	A	550	LYS
1	A	569	ASN
1	A	620	LYS
1	A	622	SER
1	A	697	ASN
1	A	715	VAL
1	B	321	THR
1	B	336	MET
1	B	337	LEU
1	B	349	ARG
1	B	390	SER
1	B	454	ASN
1	B	507	GLN
1	B	516	ARG
1	B	540	LEU
1	B	547	ARG
1	B	609	GLU
1	B	612	LYS
1	B	620	LYS
1	B	628	GLN
1	B	645	LYS
1	B	668[A]	CYS
1	B	668[B]	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	353	GLN
1	A	385	ASN
1	A	454	ASN
1	A	535	GLN
1	A	569	ASN
1	A	642	GLN
1	A	697	ASN
1	B	364	GLN
1	B	385	ASN
1	B	454	ASN
1	B	470	HIS
1	B	535	GLN
1	B	601	ASN

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Mol	Chain	Res	Type
1	B	605	ASN
1	B	642	GLN
1	B	697	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules 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	30,50,50	2.31	10 (33%)	24,82,82	3.24	12 (50%)
3	H4B	A	760	-	13,18,18	1.06	0	11,26,26	2.70	6 (54%)
4	JM6	A	800	-	10,15,15	0.77	0	8,17,17	2.31	3 (37%)
5	ACT	A	860	-	1,3,3	1.46	0	0,3,3	0.00	-
2	HEM	B	750	1	30,50,50	2.05	7 (23%)	24,82,82	2.90	11 (45%)
3	H4B	B	760	-	13,18,18	1.31	1 (7%)	11,26,26	2.29	5 (45%)
4	JM6	B	800	-	10,15,15	0.73	0	8,17,17	1.54	2 (25%)
5	ACT	B	860	-	1,3,3	1.99	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	JM6	A	800	-	-	0/11/16/16	0/0/0/0
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	JM6	B	800	-	-	0/11/16/16	0/0/0/0
5	ACT	B	860	-	-	0/0/0/0	0/0/0/0

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	750	HEM	C3D-C4D	-6.73	1.42	1.51
2	A	750	HEM	C3B-C4B	-5.56	1.46	1.51
2	B	750	HEM	C3B-C4B	-4.75	1.47	1.51
2	A	750	HEM	C2C-C1C	-4.24	1.44	1.52
2	B	750	HEM	C3D-C4D	-4.13	1.46	1.51
2	B	750	HEM	C2C-C1C	-4.09	1.44	1.52
2	A	750	HEM	C2D-C1D	-2.04	1.45	1.51
2	A	750	HEM	C3B-CAB	2.23	1.55	1.51
2	A	750	HEM	FE-NB	2.29	2.09	1.97
2	B	750	HEM	CMA-C3A	2.33	1.56	1.51
2	A	750	HEM	CMC-C2C	2.36	1.58	1.53
2	B	750	HEM	C4C-NC	2.47	1.39	1.36
2	A	750	HEM	FE-ND	2.53	2.10	1.97
3	B	760	H4B	C4-N3	3.08	1.38	1.33
2	B	750	HEM	FE-ND	3.11	2.14	1.97
2	A	750	HEM	CMA-C3A	3.23	1.58	1.51
2	A	750	HEM	FE-NC	3.24	2.08	1.95
2	B	750	HEM	C1C-NC	3.68	1.40	1.36

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	750	HEM	C3C-CAC-CBC	-7.48	112.99	124.46
2	A	750	HEM	CBA-CAA-C2A	-6.14	101.53	112.53
2	B	750	HEM	CBA-CAA-C2A	-4.94	103.67	112.53
2	A	750	HEM	CBD-CAD-C3D	-4.90	99.30	113.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	750	HEM	C3C-CAC-CBC	-4.60	117.40	124.46
3	A	760	H4B	N3-C2-N1	-4.11	118.79	125.53
4	A	800	JM6	C3-C4-S5	-3.78	99.03	112.37
2	B	750	HEM	CBD-CAD-C3D	-3.40	103.65	113.55
2	A	750	HEM	CAA-C2A-C1A	-2.96	123.79	127.01
4	A	800	JM6	C4-C3-C2	-2.88	103.59	113.28
4	B	800	JM6	C4-C3-C2	-2.52	104.78	113.28
3	B	760	H4B	N3-C2-N1	-2.32	121.73	125.53
2	A	750	HEM	C3B-CAB-CBB	-2.31	120.91	124.46
2	B	750	HEM	C3B-CAB-CBB	-2.13	121.20	124.46
2	B	750	HEM	CAA-C2A-C1A	-2.07	124.76	127.01
3	B	760	H4B	C2-N1-C8A	2.23	119.55	114.54
3	B	760	H4B	C4A-C8A-N8	2.38	121.24	118.43
3	A	760	H4B	N2-C2-N3	2.68	121.63	117.20
2	A	750	HEM	CMD-C2D-C3D	2.70	126.27	114.35
3	A	760	H4B	C4A-C8A-N8	3.00	121.96	118.43
2	A	750	HEM	CMB-C2B-C3B	3.11	124.29	116.53
4	B	800	JM6	C6-S5-C4	3.11	110.98	100.37
3	B	760	H4B	C4-N3-C2	3.19	120.37	115.94
2	B	750	HEM	CMD-C2D-C3D	3.31	128.98	114.35
2	B	750	HEM	C3B-C4B-CHC	3.34	127.87	123.16
2	A	750	HEM	C2D-C3D-C4D	3.35	107.18	101.50
2	A	750	HEM	C3B-C4B-CHC	3.43	127.99	123.16
2	B	750	HEM	CAD-C3D-C4D	3.47	124.70	112.47
3	A	760	H4B	C2-N1-C8A	3.52	122.45	114.54
2	A	750	HEM	CAD-C3D-C4D	3.62	125.24	112.47
3	A	760	H4B	C4-C4A-C8A	3.80	118.00	114.56
4	A	800	JM6	C6-S5-C4	3.82	113.41	100.37
3	A	760	H4B	C4-N3-C2	4.21	121.79	115.94
2	B	750	HEM	CMC-C2C-C3C	4.56	127.90	116.53
2	A	750	HEM	CAD-C3D-C2D	4.97	127.52	113.22
3	B	760	H4B	C4-C4A-C8A	5.05	119.13	114.56
2	B	750	HEM	CMB-C2B-C3B	5.56	130.41	116.53
2	A	750	HEM	CMC-C2C-C3C	5.65	130.63	116.53
2	B	750	HEM	CAD-C3D-C2D	6.11	130.77	113.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	750	HEM	5	0
4	A	800	JM6	13	0
2	B	750	HEM	6	0
4	B	800	JM6	10	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%)	1.05	78 (19%) 2 2	41, 70, 119, 146	0
1	B	411/422 (97%)	0.59	35 (8%) 13 14	40, 59, 86, 111	0
All	All	818/844 (96%)	0.82	113 (13%) 4 4	40, 64, 110, 146	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	716	TRP	8.0
1	A	715	VAL	7.2
1	B	300	PHE	6.3
1	B	718	GLY	6.0
1	B	352	ASP	6.0
1	A	486	LYS	5.4
1	A	366	TYR	5.4
1	A	390	SER	5.0
1	A	355	PHE	4.8
1	A	488	PRO	4.4
1	B	350	THR	4.3
1	B	351	LYS	4.3
1	B	348	VAL	4.3
1	A	371	ARG	4.2
1	A	375	LYS	4.1
1	A	712	ASN	4.1
1	A	551	PHE	4.0
1	B	566	ALA	4.0
1	A	566	ALA	3.9
1	A	388	ILE	3.8
1	A	370	LYS	3.7
1	A	503	GLU	3.7
1	A	485	TYR	3.7
1	A	508	GLN	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	385	ASN	3.7
1	A	299	ARG	3.6
1	A	713	THR	3.6
1	A	480	ILE	3.5
1	B	619	ARG	3.5
1	B	310	VAL	3.5
1	A	565	PRO	3.4
1	A	584	PHE	3.4
1	A	567	VAL	3.4
1	B	567	VAL	3.4
1	A	678	TRP	3.4
1	A	554	PHE	3.3
1	A	352	ASP	3.3
1	A	381	LEU	3.3
1	A	506	ILE	3.3
1	B	667	ARG	3.3
1	A	315	THR	3.2
1	B	554	PHE	3.2
1	A	479	LEU	3.2
1	A	593	ILE	3.2
1	B	615	ASP	3.1
1	A	588	TYR	3.1
1	A	338	PRO	3.0
1	A	354	LEU	3.0
1	A	389	GLU	3.0
1	A	714	HIS	3.0
1	A	533	LEU	2.9
1	A	619	ARG	2.9
1	A	677	VAL	2.9
1	A	394	TYR	2.9
1	A	494	GLY	2.9
1	B	389	GLU	2.8
1	A	679	ILE	2.7
1	B	677	VAL	2.7
1	A	351	LYS	2.7
1	B	318	LEU	2.7
1	B	620	LYS	2.7
1	A	507	GLN	2.7
1	A	523	LEU	2.7
1	A	492	THR	2.6
1	B	301	LEU	2.6
1	A	391	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	302	LYS	2.6
1	B	680	VAL	2.6
1	B	349	ARG	2.6
1	A	300	PHE	2.5
1	A	373	GLY	2.5
1	B	443	CYS	2.5
1	A	489	ASP	2.5
1	A	680	VAL	2.5
1	A	511	LYS	2.5
1	A	541	VAL	2.5
1	B	315	THR	2.5
1	A	493	LEU	2.4
1	B	616	LEU	2.4
1	A	514	ARG	2.4
1	A	415	CYS	2.4
1	A	318	LEU	2.4
1	A	446	VAL	2.4
1	B	355	PHE	2.4
1	A	667	ARG	2.3
1	A	616	LEU	2.3
1	A	487	GLN	2.3
1	B	678	TRP	2.3
1	A	504	ILE	2.3
1	A	710	PRO	2.3
1	A	557	LEU	2.3
1	A	682	PRO	2.2
1	A	505	CYS	2.2
1	B	369	ILE	2.2
1	B	480	ILE	2.2
1	A	470	HIS	2.2
1	A	384	VAL	2.2
1	A	490	GLY	2.2
1	A	591	THR	2.2
1	B	565	PRO	2.2
1	B	392	SER	2.1
1	B	691	PHE	2.1
1	B	321	THR	2.1
1	B	696	LEU	2.1
1	A	377	HIS	2.1
1	A	509	GLY	2.1
1	A	568	SER	2.1
1	B	553	TRP	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	369	ILE	2.0
1	A	704	PHE	2.0
1	B	591	THR	2.0
1	A	329	HIS	2.0
1	A	570	MET	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	0.89	0.30	5.40	93,95,95,96	0
4	JM6	A	800	16/16	0.91	0.33	1.87	47,59,90,94	0
4	JM6	B	800	16/16	0.91	0.25	1.02	39,56,93,94	0
3	H4B	B	760	17/17	0.96	0.19	0.46	40,43,47,51	0
2	HEM	A	750	43/43	0.98	0.21	0.38	44,48,52,57	0
5	ACT	B	860	4/4	0.94	0.14	0.31	77,81,81,84	0
3	H4B	A	760	17/17	0.95	0.18	0.27	43,49,53,56	0
2	HEM	B	750	43/43	0.97	0.16	0.10	37,43,50,55	0
6	ZN	A	900	1/1	0.96	0.11	-0.22	55,55,55,55	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.