



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2018 – 12:16 am GMT

PDB ID : 3B3M  
Title : Structure of neuronal NOS heme domain in complex with a inhibitor (+-)-3-{cis-4'-[(6"-aminopyridin-2"-yl)methyl]pyrrolidin-3'-ylamino}propan-1-ol  
Authors : Igarashi, J.; Li, H.; Poulos, T.L.  
Deposited on : 2007-10-22  
Resolution : 1.95 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

<https://www.wwpdb.org/validation/2017/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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

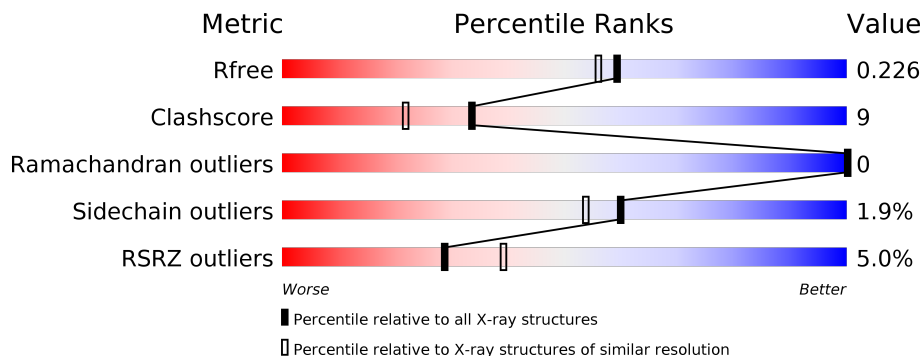
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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))
$R_{free}$	111664	2220 (1.96-1.96)
Clashscore	122126	2333 (1.96-1.96)
Ramachandran outliers	120053	2314 (1.96-1.96)
Sidechain outliers	120020	2314 (1.96-1.96)
RSRZ outliers	108989	2174 (1.96-1.96)

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>7%</div> <div> <div></div> <div>69%</div> <div>26%</div> <div>• •</div> </div> </div>
1	B	422	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>16%</div> <div>•</div> </div> </div>

## 2 Entry composition [i](#)

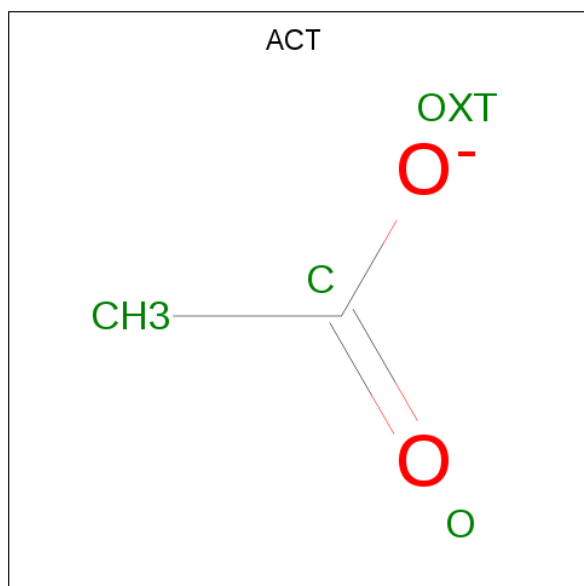
There are 7 unique types of molecules in this entry. The entry contains 7373 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	407	Total	C	N	O	S	0	2	0
			3315	2121	566	606	22			
1	B	411	Total	C	N	O	S	0	2	0
			3347	2140	574	612	21			

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).

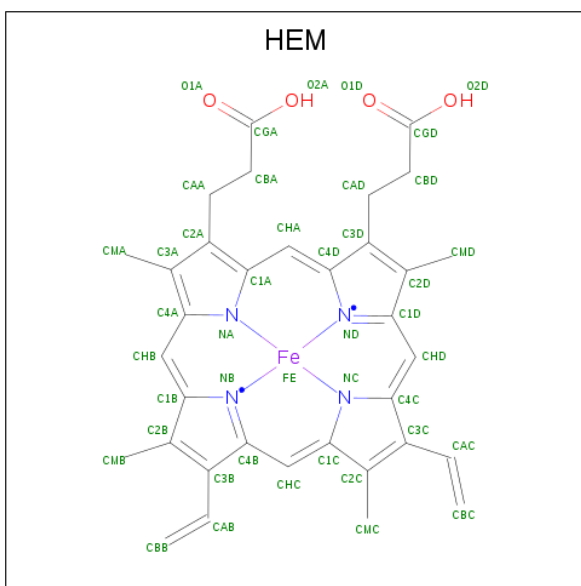


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

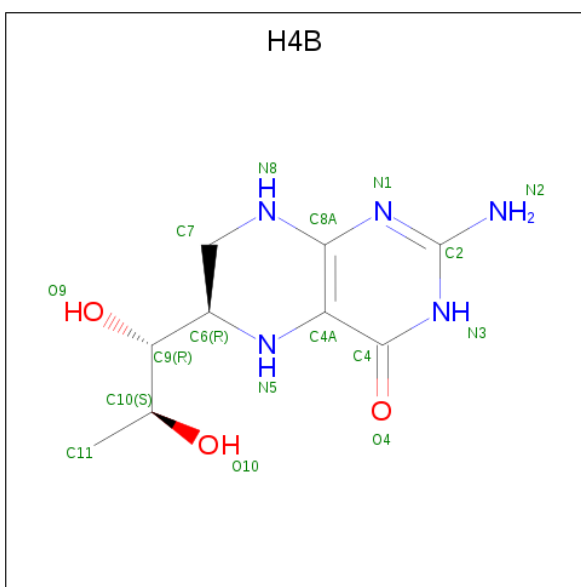
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Zn 1 1	0	0

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



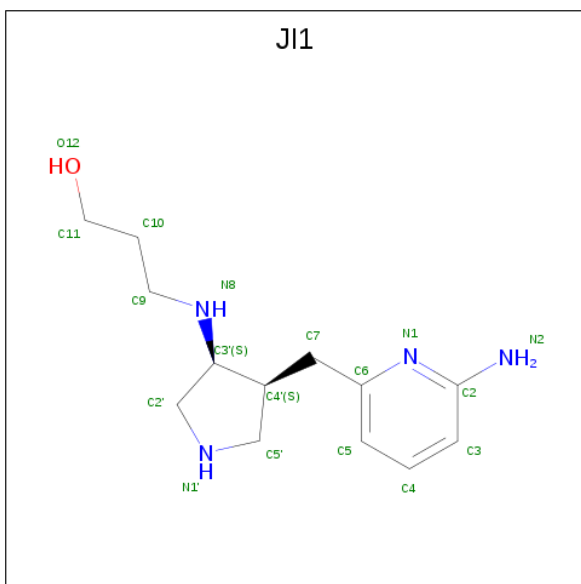
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 5 is 5,6,7,8-TETRAHYDROBIOPTERIN (three-letter code: H4B) (formula:  $\text{C}_9\text{H}_{15}\text{N}_5\text{O}_3$ ).



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

- Molecule 6 is 3-((3S,4S)-4-[(6-aminopyridin-2-yl)methyl]pyrrolidin-3-yl)amino)propan-1-ol (three-letter code: JI1) (formula: C<sub>13</sub>H<sub>22</sub>N<sub>4</sub>O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			18	13	4	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	O	0	0
			18	13	4	1		

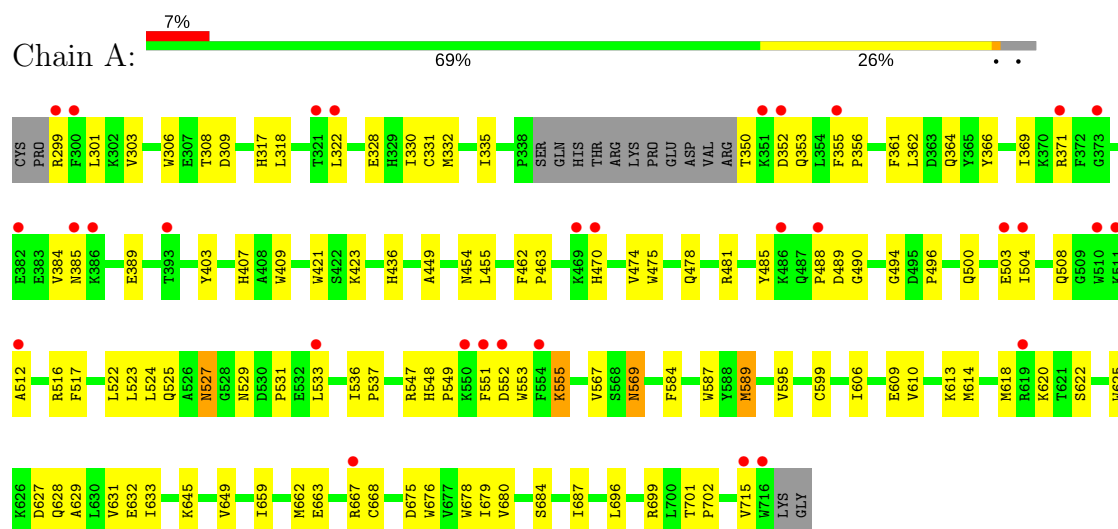
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	223	Total	O	0	0
			223	223		
7	B	323	Total	O	0	0
			323	323		

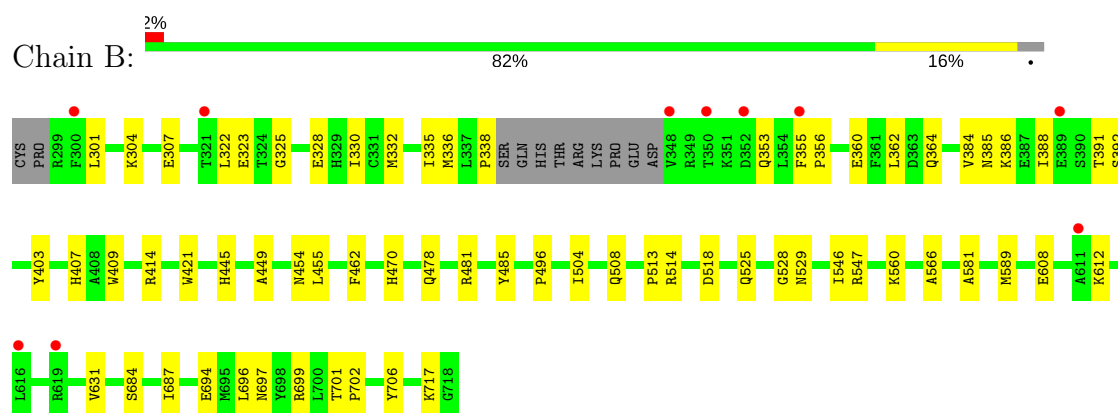
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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



#### • Molecule 1: Nitric-oxide synthase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	51.50Å 109.53Å 163.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.12 – 1.95 49.11 – 1.95	Depositor EDS
% Data completeness (in resolution range)	95.0 (49.12-1.95) 94.8 (49.11-1.95)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.22 (at 1.95Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.204 , 0.233 0.198 , 0.226	Depositor DCC
$R_{free}$ test set	3254 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.2	Xtriage
Anisotropy	0.723	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 50.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7373	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.27% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, ZN, JI1, 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	0.36	0/3418	0.62	2/4637 (0.0%)
1	B	0.39	0/3450	0.64	1/4677 (0.0%)
All	All	0.37	0/6868	0.63	3/9314 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	589	MET	N-CA-C	-6.13	94.44	111.00
1	A	589	MET	N-CA-C	-5.92	95.02	111.00
1	A	474	VAL	N-CA-C	-5.57	95.97	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	3315	0	3223	82	0
1	B	3347	0	3261	47	0
2	A	4	0	3	0	0
2	B	4	0	3	0	0
3	A	1	0	0	0	0
4	A	43	0	30	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	43	0	30	3	0
5	A	17	0	15	1	0
5	B	17	0	15	0	0
6	A	18	0	22	1	0
6	B	18	0	22	2	0
7	A	223	0	0	2	0
7	B	323	0	0	2	0
All	All	7373	0	6624	124	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 9.

All (124) 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:322:LEU:HB3	1:A:699:ARG:HH21	1.49	0.77
1:A:371:ARG:HG3	1:A:371:ARG:HH21	1.52	0.75
1:A:350:THR:HG22	1:A:352:ASP:H	1.54	0.72
1:A:523:LEU:HD22	1:A:531:PRO:HB2	1.74	0.69
1:A:478:GLN:HB2	1:A:481:ARG:HG3	1.76	0.67
4:A:750:HEM:HMC2	4:A:750:HEM:HBC2	1.79	0.64
1:A:659:ILE:O	1:A:663:GLU:HG3	1.98	0.63
1:A:620:LYS:HE3	1:A:622:SER:OG	1.99	0.62
1:A:627:ASP:O	1:A:631:VAL:HG23	2.02	0.59
1:A:478:GLN:HB2	1:A:481:ARG:CG	2.32	0.59
1:A:361:PHE:O	1:A:364:GLN:HG2	2.03	0.59
1:B:478:GLN:HB2	1:B:481:ARG:HG3	1.84	0.58
1:A:328:GLU:H	1:A:328:GLU:CD	2.06	0.58
1:A:470:HIS:HB3	1:A:527:ASN:ND2	2.19	0.57
1:B:386:LYS:HD3	7:B:1268:HOH:O	2.05	0.57
1:A:362:LEU:HD11	1:A:384:VAL:HG21	1.85	0.56
1:B:513:PRO:HG2	1:B:518:ASP:CG	2.25	0.56
1:A:332:MET:HE2	1:B:696:LEU:HD21	1.85	0.56
1:A:614:MET:CE	1:A:632:GLU:HG3	2.36	0.55
1:A:684:SER:HB3	1:A:687:ILE:CG1	2.37	0.55
1:A:504:ILE:O	1:A:508:GLN:HG2	2.08	0.54
1:A:353:GLN:O	1:A:356:PRO:HD2	2.08	0.54
1:B:325:GLY:O	1:B:332:MET:HG3	2.09	0.53
1:A:371:ARG:HG3	1:A:371:ARG:NH2	2.21	0.53
1:A:475:TRP:HB2	1:A:523:LEU:HB3	1.91	0.52
1:A:569:ASN:H	1:A:569:ASN:HD22	1.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:555:LYS:HB3	1:A:555:LYS:NZ	2.25	0.52
1:A:449:ALA:O	1:A:455:LEU:HA	2.11	0.51
1:B:328:GLU:OE1	1:B:328:GLU:N	2.43	0.51
1:A:524:LEU:O	1:A:531:PRO:HA	2.10	0.51
1:B:323:GLU:O	1:B:699:ARG:HD3	2.11	0.50
1:B:409:TRP:CE3	1:B:421:TRP:HA	2.46	0.50
1:A:667:ARG:NH1	1:A:668[A]:CYS:SG	2.84	0.50
1:A:306:TRP:CD2	1:B:336:MET:HE3	2.47	0.50
1:B:684:SER:HB3	1:B:687:ILE:HD11	1.93	0.50
1:A:715:VAL:HG23	1:A:715:VAL:O	2.11	0.50
1:B:608:GLU:O	1:B:612:LYS:HG3	2.12	0.50
1:A:606:ILE:O	1:A:610:VAL:HG23	2.12	0.50
1:A:618:MET:HA	1:A:625:TRP:CD1	2.47	0.50
1:B:684:SER:HB3	1:B:687:ILE:CG1	2.42	0.49
1:A:455:LEU:HD12	1:A:587:TRP:HB3	1.94	0.49
1:A:684:SER:HB3	1:A:687:ILE:HD11	1.93	0.49
1:B:485:TYR:CE1	1:B:514:ARG:HA	2.48	0.49
1:A:629:ALA:O	1:A:633:ILE:HG13	2.12	0.49
1:B:362:LEU:HD11	1:B:384:VAL:HG21	1.94	0.49
4:B:750:HEM:HBA2	6:B:800:JI1:H72	1.95	0.49
1:A:455:LEU:HD12	1:A:587:TRP:CB	2.43	0.48
1:A:589:MET:HA	1:A:649:VAL:O	2.12	0.48
1:A:330:ILE:HD11	1:B:696:LEU:HD22	1.96	0.48
1:A:569:ASN:N	1:A:569:ASN:HD22	2.12	0.48
1:B:525:GLN:HG3	1:B:529:ASN:O	2.13	0.47
1:B:322:LEU:HB2	1:B:699:ARG:HB2	1.95	0.47
1:A:409:TRP:CE3	1:A:421:TRP:HA	2.48	0.47
1:B:391:THR:O	1:B:392:SER:HB2	2.15	0.47
1:A:525:GLN:HG3	1:A:529:ASN:O	2.15	0.47
1:B:478:GLN:HB2	1:B:481:ARG:CG	2.44	0.47
1:A:436:HIS:ND1	7:A:1106:HOH:O	2.36	0.46
1:B:485:TYR:CZ	1:B:514:ARG:HA	2.51	0.46
1:B:355:PHE:HD1	1:B:388:ILE:HD12	1.81	0.46
1:A:332:MET:HE1	1:B:301:LEU:HD22	1.98	0.46
1:A:516:ARG:HD3	1:A:517:PHE:CE1	2.51	0.45
1:A:610:VAL:HG21	1:A:633:ILE:HD11	1.98	0.45
1:B:701:THR:HA	1:B:702:PRO:C	2.37	0.45
1:A:485:TYR:CE2	1:A:512:ALA:HB1	2.51	0.45
1:B:403:TYR:CE1	1:B:407:HIS:CE1	3.05	0.45
1:B:478:GLN:HA	1:B:566:ALA:O	2.17	0.45
1:B:304:LYS:O	1:B:694:GLU:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:ARG:O	1:A:317:HIS:CE1	2.70	0.45
7:A:1095:HOH:O	1:B:307:GLU:HG3	2.17	0.45
1:A:569:ASN:H	1:A:569:ASN:ND2	2.13	0.45
1:A:494:GLY:O	1:A:496:PRO:HD3	2.17	0.44
1:A:536:ILE:O	1:A:537:PRO:C	2.55	0.44
1:A:551:PHE:HB3	1:A:553:TRP:CE2	2.52	0.44
1:A:610:VAL:O	1:A:614:MET:HG3	2.16	0.44
1:B:364:GLN:NE2	7:B:1164:HOH:O	2.49	0.44
1:B:355:PHE:N	1:B:356:PRO:HD2	2.32	0.44
1:B:546:ILE:HG12	1:B:560:LYS:HA	1.98	0.44
1:A:308:THR:O	1:A:309:ASP:HB2	2.17	0.44
1:A:551:PHE:CD2	1:A:551:PHE:N	2.83	0.44
1:A:488:PRO:C	1:A:490:GLY:N	2.71	0.44
1:A:628:GLN:HG3	1:B:631:VAL:HG11	1.99	0.44
1:A:500:GLN:O	1:A:504:ILE:HG13	2.18	0.43
1:A:489:ASP:O	1:A:489:ASP:OD2	2.36	0.43
1:A:488:PRO:C	1:A:490:GLY:H	2.22	0.43
1:A:371:ARG:CG	1:A:371:ARG:NH2	2.81	0.43
1:A:403:TYR:CE1	1:A:407:HIS:CE1	3.07	0.43
1:A:595:VAL:O	1:A:599:CYS:HB2	2.18	0.43
1:B:449:ALA:O	1:B:455:LEU:HA	2.19	0.43
1:A:678:TRP:HA	5:A:760:H4B:N1	2.33	0.43
4:A:750:HEM:CBA	6:A:800:JI1:H72	2.49	0.43
4:B:750:HEM:CBA	6:B:800:JI1:H72	2.48	0.43
1:A:335:ILE:HD13	1:B:694:GLU:HB3	2.01	0.42
1:A:350:THR:HB	1:A:353:GLN:HG3	2.01	0.42
1:A:552:ASP:O	1:A:555:LYS:HG2	2.18	0.42
1:B:462:PHE:HB2	1:B:581:ALA:HB3	2.01	0.42
1:B:470:HIS:HA	1:B:528:GLY:HA3	2.01	0.42
1:B:355:PHE:CE1	1:B:385:ASN:HB2	2.54	0.42
1:B:504:ILE:O	1:B:508:GLN:HG2	2.19	0.42
1:A:299:ARG:HG3	1:A:318:LEU:HD21	2.01	0.42
1:A:548:HIS:ND1	1:A:549:PRO:HD2	2.34	0.42
1:A:306:TRP:CE2	1:B:336:MET:HE3	2.55	0.42
1:B:445:HIS:C	1:B:445:HIS:CD2	2.93	0.42
1:B:356:PRO:O	1:B:360:GLU:HG3	2.19	0.42
1:A:350:THR:HB	1:A:353:GLN:CD	2.39	0.41
1:A:331:CYS:HB3	1:B:697:ASN:HB3	2.02	0.41
1:B:322:LEU:HD13	1:B:699:ARG:HH21	1.85	0.41
1:B:414:ARG:NH1	1:B:706:TYR:OH	2.52	0.41
4:B:750:HEM:HBC2	4:B:750:HEM:CMC	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:TYR:HA	1:A:369:ILE:HG12	2.03	0.41
1:A:462:PHE:HB3	1:A:463:PRO:CD	2.51	0.41
1:A:522:LEU:O	1:A:533:LEU:HA	2.21	0.41
1:A:301:LEU:CD1	1:B:330:ILE:HD13	2.51	0.41
1:A:701:THR:HA	1:A:702:PRO:C	2.41	0.41
1:A:609:GLU:O	1:A:613:LYS:HG2	2.21	0.41
1:A:350:THR:HB	1:A:353:GLN:CG	2.50	0.41
1:A:355:PHE:CE1	1:A:385:ASN:HB2	2.56	0.41
1:A:675:ASP:O	1:A:679:ILE:HG12	2.21	0.40
1:B:335:ILE:HB	1:B:338:PRO:HG3	2.02	0.40
1:A:303:VAL:CG1	1:A:696:LEU:HG	2.51	0.40
1:A:567:VAL:HB	1:A:584:PHE:CZ	2.56	0.40
1:A:676:TRP:CZ2	1:A:680:VAL:HG21	2.57	0.40
1:A:684:SER:HB3	1:A:687:ILE:CD1	2.51	0.40
1:A:330:ILE:HD11	1:B:696:LEU:HB3	2.03	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%)	391 (96%)	14 (4%)	0	100	100
1	B	409/422 (97%)	395 (97%)	14 (3%)	0	100	100
All	All	814/844 (96%)	786 (97%)	28 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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%)	355 (97%)	10 (3%)	48	37
1	B	368/377 (98%)	364 (99%)	4 (1%)	76	73
All	All	733/754 (97%)	719 (98%)	14 (2%)	60	54

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	389	GLU
1	A	423	LYS
1	A	454	ASN
1	A	503	GLU
1	A	527	ASN
1	A	547	ARG
1	A	555	LYS
1	A	569	ASN
1	A	645	LYS
1	A	662	MET
1	B	353	GLN
1	B	454	ASN
1	B	547	ARG
1	B	717	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	353	GLN
1	A	425	GLN
1	A	454	ASN
1	A	507	GLN
1	A	508	GLN
1	A	527	ASN
1	A	569	ASN
1	A	605	ASN
1	A	697	ASN
1	A	712	ASN
1	B	364	GLN
1	B	385	ASN

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Mol	Chain	Res	Type
1	B	425	GLN
1	B	440	ASN
1	B	454	ASN
1	B	527	ASN
1	B	529	ASN
1	B	535	GLN
1	B	601	ASN
1	B	605	ASN
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	$\# Z  > 2$
4	HEM	A	750	1	27,50,50	1.53	5 (18%)	17,82,82	2.01	4 (23%)
5	H4B	A	760	-	15,18,18	2.07	4 (26%)	11,26,26	4.16	8 (72%)
6	JI1	A	800	-	15,19,19	1.34	2 (13%)	17,24,24	1.93	2 (11%)
2	ACT	A	860	-	1,3,3	3.08	1 (100%)	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	HEM	B	750	1	27,50,50	1.54	5 (18%)	17,82,82	2.27	4 (23%)
5	H4B	B	760	-	15,18,18	2.17	4 (26%)	11,26,26	4.20	8 (72%)
6	JI1	B	800	-	15,19,19	1.36	1 (6%)	17,24,24	1.89	2 (11%)
2	ACT	B	860	-	1,3,3	3.76	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
4	HEM	A	750	1	-	0/6/54/54	0/0/8/8
5	H4B	A	760	-	-	0/8/17/17	0/2/2/2
6	JI1	A	800	-	-	0/9/19/19	0/2/2/2
2	ACT	A	860	-	-	0/0/0/0	0/0/0/0
4	HEM	B	750	1	-	0/6/54/54	0/0/8/8
5	H4B	B	760	-	-	0/8/17/17	0/2/2/2
6	JI1	B	800	-	-	0/9/19/19	0/2/2/2
2	ACT	B	860	-	-	0/0/0/0	0/0/0/0

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	750	HEM	C3B-CAB	-3.93	1.40	1.47
4	A	750	HEM	C3B-CAB	-3.59	1.40	1.47
4	A	750	HEM	C3B-C2B	-3.45	1.35	1.40
4	B	750	HEM	C3B-C2B	-3.29	1.35	1.40
4	B	750	HEM	C3C-C2C	-2.76	1.36	1.40
4	A	750	HEM	C3C-C2C	-2.05	1.37	1.40
5	A	760	H4B	C8A-N1	2.00	1.37	1.34
4	B	750	HEM	C4B-NB	2.15	1.40	1.36
4	A	750	HEM	C4B-NB	2.26	1.40	1.36
6	A	800	JI1	C4'-C3'	2.33	1.56	1.53
5	B	760	H4B	C8A-N1	2.52	1.38	1.34
4	A	750	HEM	C1D-ND	2.55	1.41	1.36
4	B	750	HEM	C4A-NA	2.73	1.41	1.36
6	B	800	JI1	C7-C4'	3.00	1.58	1.53
6	A	800	JI1	C7-C4'	3.05	1.58	1.53
2	A	860	ACT	CH3-C	3.08	1.52	1.48
5	A	760	H4B	C6-N5	3.33	1.52	1.45
2	B	860	ACT	CH3-C	3.76	1.53	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	760	H4B	C6-N5	3.82	1.53	1.45
5	A	760	H4B	C4A-N5	4.33	1.47	1.38
5	B	760	H4B	C4A-N5	4.36	1.47	1.38
5	A	760	H4B	C4-N3	5.13	1.42	1.33
5	B	760	H4B	C4-N3	5.14	1.42	1.33

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	750	HEM	CBA-CAA-C2A	-6.77	99.53	112.48
4	A	750	HEM	CBA-CAA-C2A	-6.03	100.95	112.48
5	A	760	H4B	N3-C2-N1	-4.77	117.85	125.43
5	B	760	H4B	N3-C2-N1	-4.69	117.97	125.43
4	B	750	HEM	CBD-CAD-C3D	-3.91	105.01	112.47
4	A	750	HEM	CBD-CAD-C3D	-3.51	105.76	112.47
5	B	760	H4B	C4A-C4-N3	-3.46	113.73	123.91
5	A	760	H4B	C4A-C4-N3	-3.44	113.81	123.91
5	A	760	H4B	C4A-N5-C6	-3.04	112.88	121.16
5	B	760	H4B	C4A-N5-C6	-3.01	112.96	121.16
4	B	750	HEM	C4A-C3A-C2A	-2.44	105.30	107.00
6	B	800	JI1	C2'-C3'-N8	-2.27	109.68	113.73
6	A	800	JI1	C2'-C3'-N8	-2.20	109.82	113.73
4	A	750	HEM	C4C-C3C-C2C	-2.17	105.39	106.90
4	B	750	HEM	CMD-C2D-C1D	-2.10	125.24	128.46
4	A	750	HEM	CMC-C2C-C3C	2.01	128.54	124.88
5	B	760	H4B	O9-C9-C6	2.35	114.59	108.98
5	A	760	H4B	O9-C9-C6	2.45	114.85	108.98
5	A	760	H4B	N2-C2-N1	3.27	122.39	117.25
5	B	760	H4B	N2-C2-N1	3.36	122.53	117.25
5	B	760	H4B	C2-N1-C8A	3.43	122.19	114.50
5	A	760	H4B	C2-N1-C8A	3.78	122.99	114.50
5	A	760	H4B	C4-N3-C2	6.00	124.69	116.06
5	B	760	H4B	C4-N3-C2	6.20	124.98	116.06
6	B	800	JI1	C2-N1-C6	6.32	122.61	118.17
6	A	800	JI1	C2-N1-C6	6.51	122.75	118.17
5	A	760	H4B	C4-C4A-C8A	8.75	122.48	114.56
5	B	760	H4B	C4-C4A-C8A	9.07	122.77	114.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	750	HEM	2	0
5	A	760	H4B	1	0
6	A	800	JI1	1	0
4	B	750	HEM	3	0
6	B	800	JI1	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%)	0.64	31 (7%) 14 21	17, 33, 61, 78	0
1	B	411/422 (97%)	0.28	10 (2%) 59 68	15, 26, 49, 67	0
All	All	818/844 (96%)	0.46	41 (5%) 29 39	15, 29, 57, 78	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	355	PHE	6.7
1	A	300	PHE	4.5
1	B	300	PHE	4.5
1	A	299	ARG	4.1
1	A	488	PRO	3.8
1	B	611	ALA	3.4
1	A	351	LYS	3.4
1	B	348	VAL	3.3
1	B	352	ASP	3.3
1	A	321	THR	3.1
1	A	486	LYS	3.1
1	A	373	GLY	3.1
1	B	321	THR	3.0
1	A	322	LEU	3.0
1	B	355	PHE	3.0
1	A	552	ASP	3.0
1	A	371	ARG	2.9
1	B	616	LEU	2.9
1	A	716	TRP	2.9
1	B	619	ARG	2.8
1	A	385	ASN	2.8
1	A	469	LYS	2.8
1	A	619	ARG	2.8
1	A	386	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	715	VAL	2.6
1	A	352	ASP	2.6
1	A	382	GLU	2.5
1	A	511	LYS	2.4
1	A	550	LYS	2.4
1	A	503	GLU	2.3
1	B	389	GLU	2.3
1	B	350	THR	2.3
1	A	551	PHE	2.3
1	A	533	LEU	2.3
1	A	554	PHE	2.2
1	A	470	HIS	2.2
1	A	512	ALA	2.2
1	A	504	ILE	2.1
1	A	393	THR	2.1
1	A	667	ARG	2.0
1	A	510	TRP	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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
5	H4B	A	760	17/17	0.94	0.13	22,23,26,26	0
6	JI1	B	800	18/18	0.95	0.13	21,23,35,37	0
6	JI1	A	800	18/18	0.95	0.14	18,24,38,41	0
2	ACT	A	860	4/4	0.95	0.27	46,46,46,47	0
2	ACT	B	860	4/4	0.96	0.10	29,31,32,33	0
5	H4B	B	760	17/17	0.96	0.11	21,23,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	HEM	A	750	43/43	0.98	0.11	18,20,23,28	0
4	HEM	B	750	43/43	0.98	0.12	15,18,24,27	0
3	ZN	A	900	1/1	1.00	0.09	24,24,24,24	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.