



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:21 PM GMT

PDB ID : 1OM5  
Title : STRUCTURE OF RAT NEURONAL NOS HEME DOMAIN WITH 3-BROMO-7-NITROINDAZOLE BOUND  
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Deposited on : 2003-02-24  
Resolution : 2.30 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

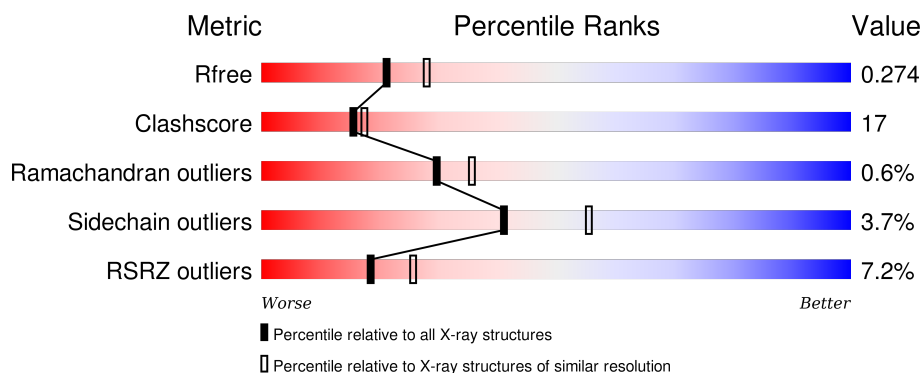
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	421	<div> <div>10%</div> <div>61%</div> <div>32%</div> <div>• •</div> </div>
1	B	421	<div> <div>4%</div> <div>67%</div> <div>30%</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
2	ACT	A	860	-	-	X	-

## 2 Entry composition [i](#)

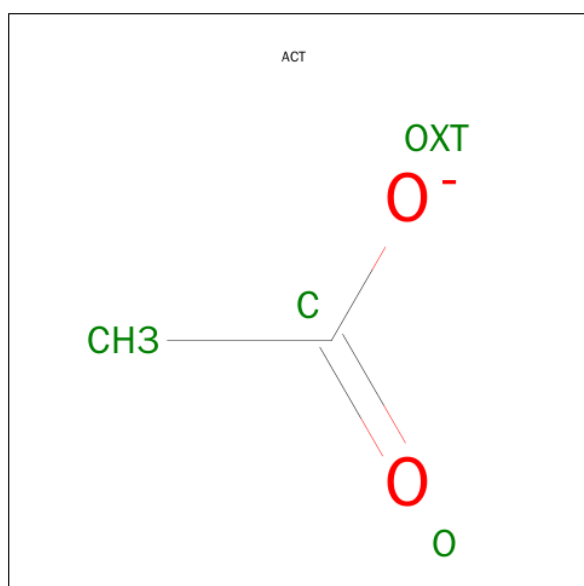
There are 7 unique types of molecules in this entry. The entry contains 7055 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	410	Total	C	N	O	S	0	0	0
			3341	2138	573	609	21			

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

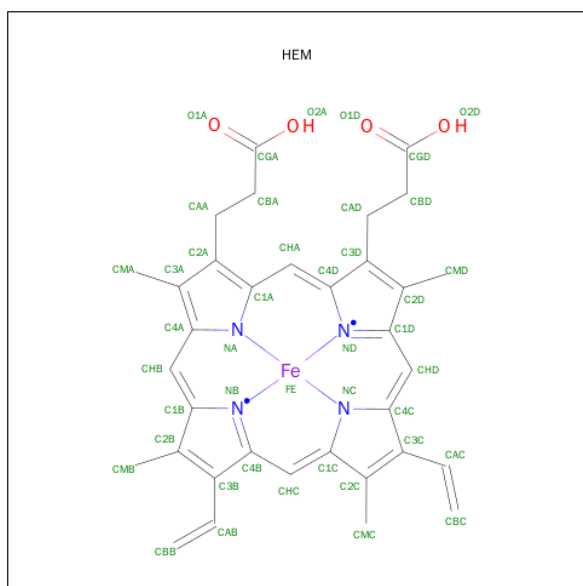


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

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

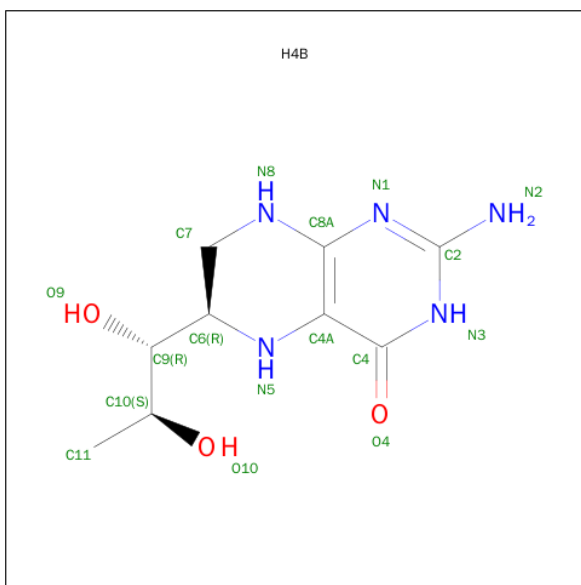
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Zn 1 1	0	0

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



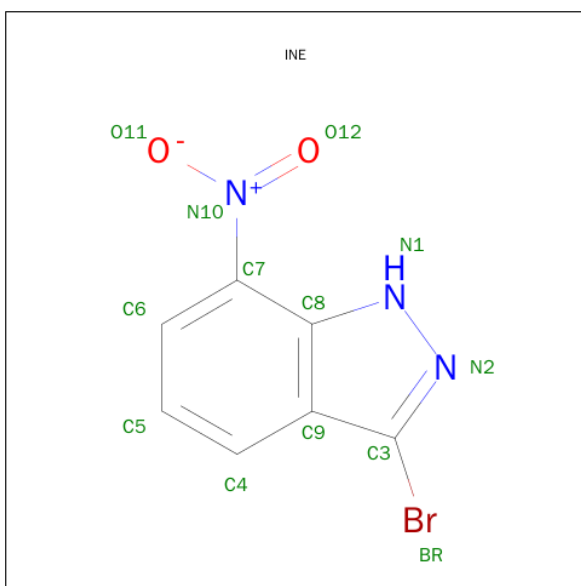
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- 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 17	C 9	N 5	O 3	0	0
5	B	1	Total 17	C 9	N 5	O 3	0	0

- Molecule 6 is 3-BROMO-7-NITROINDAZOLE (three-letter code: INE) (formula:  $\text{C}_7\text{H}_4\text{BrN}_3\text{O}_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total 13	Br 1	C 7	N 3	O 2	0	0
6	B	1	Total 13	Br 1	C 7	N 3	O 2	0	0

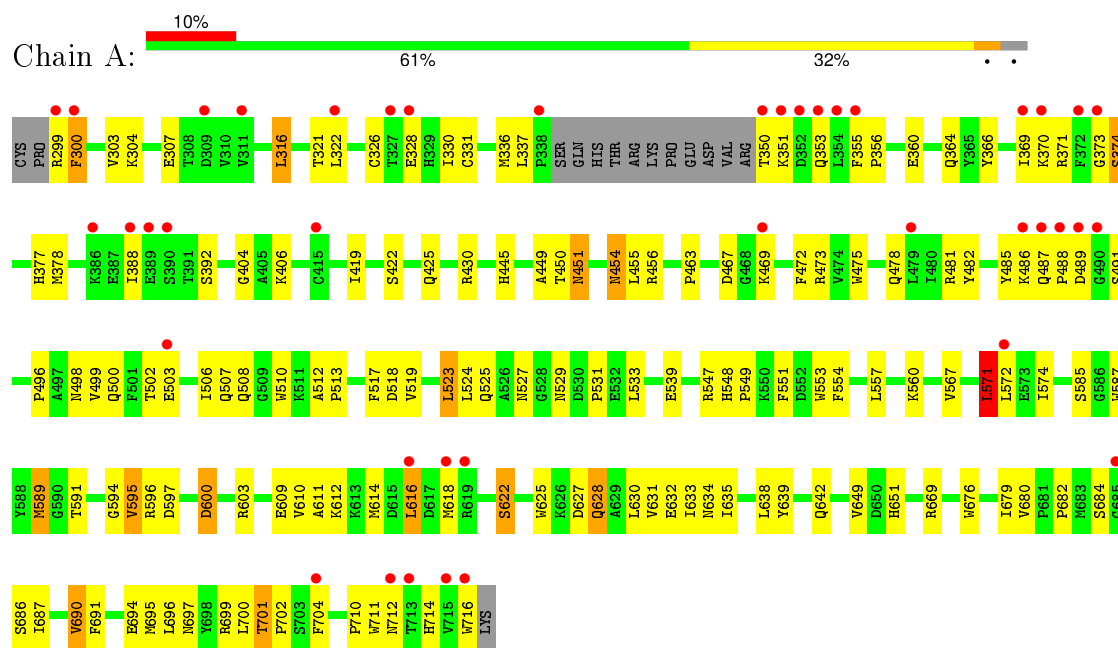
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	111	Total 111	O 111	0	0
7	B	135	Total 135	O 135	0	0

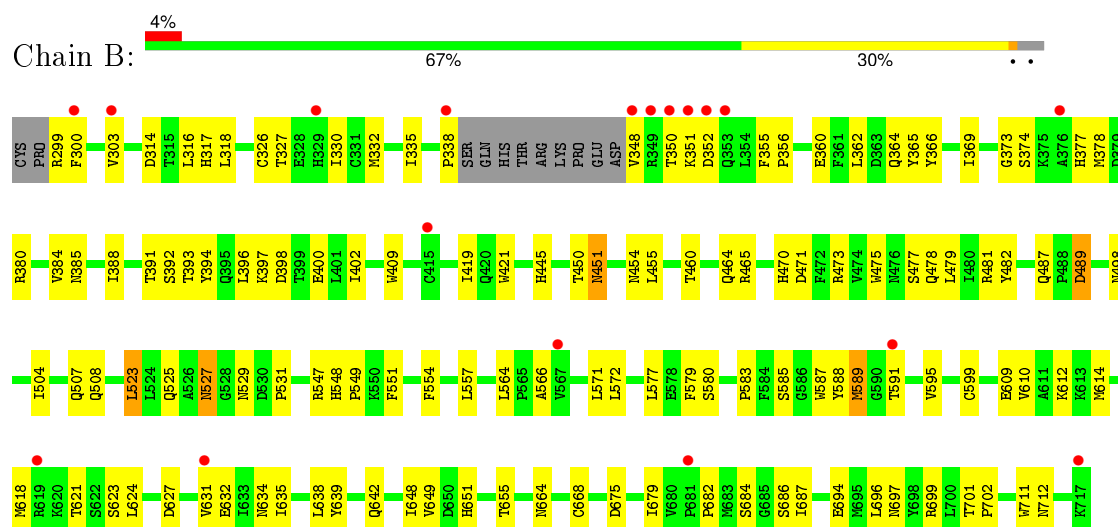
### 3 Residue-property plots

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, $\alpha$ , $\beta$ , $\gamma$	51.70Å 110.78Å 164.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.56 – 2.30 29.56 – 2.30	Depositor EDS
% Data completeness (in resolution range)	91.5 (29.56-2.30) 91.5 (29.56-2.30)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.62 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.231 , 0.280 0.227 , 0.274	Depositor DCC
$R_{free}$ test set	1978 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	38.6	Xtriage
Anisotropy	0.827	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 49.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 39328 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7055	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% 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: INE, ZN, H4B, HEM, 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	0.39	0/3406	0.66	3/4621 (0.1%)
1	B	0.40	0/3434	0.65	2/4656 (0.0%)
All	All	0.39	0/6840	0.66	5/9277 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	326	CYS	CA-CB-SG	8.22	128.80	114.00
1	A	326	CYS	CA-CB-SG	7.87	128.17	114.00
1	B	589	MET	N-CA-C	-5.34	96.59	111.00
1	A	589	MET	N-CA-C	-5.22	96.91	111.00
1	A	571	LEU	CA-CB-CG	5.19	127.25	115.30

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	128	0
1	B	3341	0	3256	112	0
2	A	4	0	3	3	0
2	B	4	0	3	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
4	A	43	0	30	2	0
4	B	43	0	30	5	0
5	A	17	0	15	0	0
5	B	17	0	15	0	0
6	A	13	0	4	1	0
6	B	13	0	4	1	0
7	A	111	0	0	7	0
7	B	135	0	0	5	0
All	All	7055	0	6581	230	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 17.

All (230) 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:523:LEU:HD22	1:B:531:PRO:HB2	1.35	1.04
1:B:373:GLY:H	1:B:377:HIS:CD2	1.86	0.92
1:B:373:GLY:H	1:B:377:HIS:HD2	0.97	0.91
1:A:696:LEU:HD22	1:B:330:ILE:HD11	1.51	0.91
1:A:523:LEU:HD22	1:A:531:PRO:HB2	1.49	0.91
1:A:596:ARG:O	1:A:600:ASP:HB2	1.77	0.83
1:A:549:PRO:HG3	1:A:639:TYR:CG	2.14	0.82
1:B:614:MET:HE3	1:B:632:GLU:HG3	1.62	0.80
1:B:373:GLY:N	1:B:377:HIS:HD2	1.77	0.79
1:B:612:LYS:HA	1:B:618:MET:HE1	1.65	0.78
1:B:610:VAL:O	1:B:614:MET:HG3	1.85	0.77
1:A:322:LEU:HB2	1:A:699:ARG:NH1	1.99	0.77
1:B:631:VAL:O	1:B:635:ILE:HG12	1.85	0.76
4:A:750:HEM:HMC2	4:A:750:HEM:HBC2	1.67	0.76
1:B:470:HIS:HB3	1:B:527:ASN:ND2	2.01	0.76
1:B:566:ALA:HB2	1:B:585:SER:HB3	1.69	0.74
1:A:611:ALA:HB1	1:A:616:LEU:HD11	1.69	0.73
1:B:299:ARG:HH11	1:B:299:ARG:HG2	1.53	0.72
1:A:684:SER:HB3	1:A:687:ILE:HG12	1.72	0.72
1:A:508:GLN:HE22	1:A:716:TRP:HZ3	1.38	0.72
1:B:478:GLN:HB2	1:B:481:ARG:HG3	1.73	0.70
1:B:360:GLU:O	1:B:364:GLN:HG3	1.92	0.70
1:A:322:LEU:HB3	1:A:699:ARG:HD3	1.72	0.70
1:A:491:SER:HB2	7:A:200:HOH:O	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:504:ILE:O	1:B:508:GLN:HG2	1.93	0.69
1:A:350:THR:HB	1:A:353:GLN:HG3	1.75	0.68
1:B:332:MET:HB3	1:B:335:ILE:HG13	1.74	0.68
1:B:548:HIS:ND1	1:B:549:PRO:HD2	2.09	0.67
1:A:322:LEU:HB2	1:A:699:ARG:HH11	1.58	0.67
1:A:485:TYR:CE2	1:A:512:ALA:HB1	2.30	0.67
1:B:299:ARG:HG3	1:B:300:PHE:N	2.09	0.67
1:A:595:VAL:HB	1:A:630:LEU:HD11	1.75	0.66
1:A:373:GLY:H	1:A:377:HIS:CD2	2.12	0.66
1:A:485:TYR:HE2	1:A:512:ALA:HB1	1.61	0.66
1:A:517:PHE:HB2	1:A:560:LYS:HE2	1.78	0.65
1:A:328:GLU:H	1:A:328:GLU:CD	1.99	0.65
1:A:635:ILE:HD11	1:B:624:LEU:HB2	1.78	0.65
1:B:350:THR:HB	1:B:352:ASP:OD1	1.97	0.65
1:B:549:PRO:HG3	1:B:639:TYR:CG	2.32	0.65
1:A:571:LEU:HD12	1:A:571:LEU:C	2.18	0.64
1:B:398:ASP:O	1:B:402:ILE:HG13	1.98	0.64
1:B:303:VAL:HG13	1:B:694:GLU:HB2	1.80	0.64
1:B:523:LEU:CD2	1:B:531:PRO:HB2	2.20	0.63
4:B:750:HEM:HMC1	4:B:750:HEM:HBC2	1.80	0.63
1:B:473:ARG:CD	1:B:580:SER:HB2	2.30	0.62
1:B:397:LYS:HB2	1:B:400:GLU:HG3	1.82	0.61
1:A:330:ILE:HD11	1:B:696:LEU:HD22	1.81	0.61
1:A:591:THR:O	1:A:595:VAL:HG13	2.01	0.61
1:A:690:VAL:HG22	1:A:695:MET:CE	2.31	0.61
1:B:335:ILE:HB	1:B:338:PRO:HG3	1.82	0.61
1:A:682:PRO:HB2	1:B:686:SER:OG	2.01	0.60
1:B:355:PHE:CE1	1:B:385:ASN:HB2	2.37	0.60
1:B:473:ARG:HD3	1:B:580:SER:HB2	1.82	0.60
1:B:591:THR:O	1:B:595:VAL:HG13	2.02	0.59
1:A:631:VAL:O	1:A:635:ILE:HG12	2.02	0.59
1:A:553:TRP:CZ3	1:A:557:LEU:HD11	2.37	0.59
4:B:750:HEM:CMC	4:B:750:HEM:HBC2	2.32	0.59
1:B:571:LEU:HD12	1:B:572:LEU:N	2.17	0.59
1:B:362:LEU:HD11	1:B:384:VAL:HG21	1.83	0.59
1:B:475:TRP:HB2	1:B:523:LEU:HB3	1.84	0.58
1:A:496:PRO:HA	1:A:499:VAL:HG23	1.85	0.58
1:A:548:HIS:ND1	1:A:549:PRO:HD2	2.19	0.58
1:B:651:HIS:O	1:B:655:THR:HG23	2.04	0.58
1:B:638:LEU:O	1:B:642:GLN:HG3	2.04	0.58
1:B:380:ARG:O	1:B:384:VAL:HG23	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:451:ASN:HB3	1:B:454:ASN:O	2.04	0.57
1:B:525:GLN:HG3	1:B:529:ASN:O	2.04	0.57
1:A:554:PHE:O	1:A:557:LEU:HD13	2.04	0.57
1:A:304:LYS:O	1:A:694:GLU:HG3	2.05	0.57
1:A:587:TRP:NE1	2:A:860:ACT:H1	2.20	0.57
1:A:525:GLN:HG3	1:A:529:ASN:O	2.04	0.56
1:B:482:TYR:O	1:B:498:ASN:ND2	2.36	0.56
1:B:464:GLN:HB3	1:B:579:PHE:CE2	2.39	0.56
1:A:303:VAL:HG13	1:A:694:GLU:HB2	1.88	0.56
1:A:714:HIS:HB3	7:A:209:HOH:O	2.05	0.56
1:B:566:ALA:CB	1:B:585:SER:HB3	2.35	0.56
1:B:348:VAL:O	1:B:348:VAL:HG22	2.05	0.56
1:A:508:GLN:OE1	1:A:508:GLN:HA	2.06	0.55
1:B:409:TRP:CE3	1:B:421:TRP:HA	2.42	0.55
1:A:610:VAL:HG21	1:A:633:ILE:HD11	1.89	0.55
1:A:487:GLN:HB3	1:A:488:PRO:HD2	1.88	0.55
1:A:549:PRO:HG3	1:A:639:TYR:CD1	2.42	0.54
1:B:564:LEU:HD11	1:B:585:SER:HB2	1.89	0.54
1:A:635:ILE:CD1	1:B:624:LEU:HB2	2.38	0.54
1:A:690:VAL:HG22	1:A:695:MET:HE1	1.89	0.54
1:A:478:GLN:HB2	1:A:481:ARG:HG3	1.88	0.54
1:B:327:THR:OG1	1:B:330:ILE:HG22	2.07	0.54
1:A:684:SER:HB3	1:A:687:ILE:CG1	2.37	0.54
1:B:299:ARG:NH1	1:B:299:ARG:HG2	2.23	0.54
1:B:699:ARG:HG2	1:B:699:ARG:HH11	1.72	0.54
1:A:616:LEU:HD13	1:A:625:TRP:HB2	1.90	0.54
1:B:332:MET:HB3	1:B:335:ILE:CG1	2.38	0.53
1:B:450:THR:HA	1:B:455:LEU:HD22	1.90	0.53
1:A:507:GLN:O	1:A:507:GLN:HG2	2.09	0.53
1:A:686:SER:HA	1:A:691:PHE:CG	2.44	0.52
1:B:419:ILE:HD13	7:B:235:HOH:O	2.09	0.52
1:A:299:ARG:CG	1:A:300:PHE:H	2.22	0.52
1:A:467:ASP:OD2	1:A:469:LYS:HB2	2.09	0.52
1:A:330:ILE:CD1	1:B:696:LEU:HD22	2.40	0.52
1:B:711:TRP:CD1	1:B:712:ASN:ND2	2.77	0.52
1:A:463:PRO:HB2	1:A:472:PHE:CE1	2.45	0.52
1:A:322:LEU:CD2	1:A:699:ARG:HD3	2.40	0.51
1:A:478:GLN:HB2	1:A:481:ARG:CG	2.40	0.51
1:B:445:HIS:HD2	1:B:460:THR:OG1	1.92	0.51
1:A:307:GLU:HG3	7:B:32:HOH:O	2.09	0.51
1:A:622:SER:HB3	7:A:48:HOH:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:LEU:CB	1:A:699:ARG:HD3	2.40	0.51
1:B:314:ASP:OD1	1:B:317:HIS:ND1	2.43	0.51
1:B:299:ARG:HB3	1:B:318:LEU:HD21	1.93	0.50
1:A:614:MET:CE	1:A:632:GLU:HG3	2.41	0.50
1:B:391:THR:O	1:B:392:SER:HB2	2.11	0.50
1:B:487:GLN:NE2	7:B:234:HOH:O	2.45	0.50
1:B:595:VAL:HG12	1:B:634:ASN:HD21	1.77	0.50
1:A:404:GLY:HA3	1:A:574:ILE:HD13	1.94	0.50
1:A:567:VAL:CG2	6:A:790:INE:H41	2.41	0.50
1:A:450:THR:HA	1:A:455:LEU:CD2	2.42	0.49
1:A:696:LEU:HD22	1:B:330:ILE:CD1	2.31	0.49
1:B:595:VAL:O	1:B:599:CYS:HB2	2.11	0.49
1:B:523:LEU:HD22	1:B:531:PRO:CB	2.25	0.49
1:A:627:ASP:O	1:A:631:VAL:HG23	2.13	0.49
1:B:350:THR:HG22	1:B:351:LYS:N	2.28	0.49
1:B:701:THR:HA	1:B:702:PRO:C	2.32	0.49
1:A:638:LEU:O	1:A:642:GLN:HG3	2.13	0.49
1:B:299:ARG:HH11	1:B:299:ARG:CG	2.25	0.49
1:A:587:TRP:O	4:A:750:HEM:HMB3	2.12	0.49
1:A:686:SER:OG	1:B:682:PRO:HB2	2.13	0.49
1:A:587:TRP:HE1	2:A:860:ACT:H1	1.78	0.49
1:A:594:GLY:HA3	1:A:634:ASN:ND2	2.27	0.49
1:B:557:LEU:HD23	1:B:609:GLU:OE2	2.13	0.48
1:A:373:GLY:O	1:A:374:SER:O	2.31	0.48
1:A:554:PHE:HA	1:A:557:LEU:HD13	1.95	0.48
1:B:632:GLU:O	1:B:635:ILE:HB	2.12	0.48
1:A:680:VAL:HB	7:A:23:HOH:O	2.14	0.48
1:A:711:TRP:CD1	1:A:712:ASN:ND2	2.82	0.48
1:A:701:THR:HA	1:A:702:PRO:C	2.34	0.48
1:B:587:TRP:O	4:B:750:HEM:HMB3	2.13	0.48
1:B:473:ARG:HD2	1:B:580:SER:HB2	1.96	0.48
1:A:473:ARG:NH2	1:A:710:PRO:HD3	2.28	0.48
1:A:373:GLY:H	1:A:377:HIS:HD2	1.57	0.47
1:B:711:TRP:HD1	1:B:712:ASN:ND2	2.13	0.47
1:B:479:LEU:HD21	1:B:583:PRO:HB3	1.95	0.47
1:A:553:TRP:HZ3	1:A:557:LEU:HD11	1.80	0.47
1:B:588:TYR:HA	6:B:791:INE:O12	2.15	0.47
1:A:366:TYR:HA	1:A:369:ILE:HG12	1.96	0.47
1:A:597:ASP:OD1	1:A:603:ARG:NH1	2.46	0.47
1:A:510:TRP:HB2	1:A:533:LEU:HD13	1.97	0.47
1:A:330:ILE:HD11	1:B:696:LEU:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:LYS:O	1:A:371:ARG:HD3	2.14	0.46
1:A:553:TRP:CE3	1:A:557:LEU:HD11	2.50	0.46
1:A:571:LEU:CD1	1:A:571:LEU:C	2.83	0.46
1:A:614:MET:HE3	1:A:632:GLU:HG3	1.97	0.46
1:A:589:MET:HA	1:A:649:VAL:O	2.15	0.46
1:A:388:ILE:O	1:A:392:SER:HA	2.15	0.46
1:A:548:HIS:HB2	1:A:554:PHE:CG	2.51	0.46
1:A:628:GLN:NE2	1:B:632:GLU:OE2	2.49	0.46
1:B:397:LYS:HD2	7:B:217:HOH:O	2.16	0.46
1:A:539:GLU:HG3	7:A:55:HOH:O	2.16	0.46
1:B:366:TYR:CD2	1:B:369:ILE:HD11	2.51	0.46
1:A:679:ILE:HG21	1:A:690:VAL:HG21	1.97	0.46
1:B:489:ASP:HB3	7:B:11:HOH:O	2.15	0.45
1:B:465:ARG:HG3	1:B:471:ASP:OD1	2.17	0.45
1:B:614:MET:HE3	1:B:632:GLU:CG	2.41	0.45
1:B:548:HIS:HB3	1:B:551:PHE:HB2	1.98	0.45
1:B:675:ASP:O	1:B:679:ILE:HG12	2.15	0.45
1:B:612:LYS:CA	1:B:618:MET:HE1	2.43	0.45
1:A:451:ASN:HB3	1:A:454:ASN:O	2.17	0.45
1:B:355:PHE:N	1:B:356:PRO:HD2	2.31	0.45
1:A:487:GLN:HB3	1:A:488:PRO:CD	2.47	0.45
1:A:618:MET:HA	1:A:625:TRP:CD1	2.52	0.45
1:B:684:SER:HB3	1:B:687:ILE:HD11	1.99	0.45
1:A:587:TRP:CE2	2:A:860:ACT:H1	2.52	0.45
1:B:388:ILE:O	1:B:392:SER:N	2.50	0.45
1:A:322:LEU:CB	1:A:699:ARG:HH11	2.28	0.45
1:A:548:HIS:CE1	1:A:549:PRO:HD2	2.51	0.44
1:A:635:ILE:CD1	1:B:623:SER:O	2.65	0.44
1:A:524:LEU:O	1:A:531:PRO:HA	2.17	0.44
1:A:551:PHE:HB3	1:A:553:TRP:NE1	2.32	0.44
1:A:355:PHE:N	1:A:356:PRO:HD2	2.32	0.44
1:B:548:HIS:CE1	1:B:549:PRO:HD2	2.51	0.44
1:A:676:TRP:CZ2	1:A:680:VAL:HG21	2.52	0.44
1:A:430:ARG:O	1:A:463:PRO:HG3	2.17	0.44
1:B:299:ARG:HG3	1:B:300:PHE:H	1.80	0.44
1:A:316:LEU:HD22	1:A:700:LEU:HD11	1.99	0.44
1:A:378:MET:HE2	1:A:378:MET:HA	2.00	0.44
1:A:475:TRP:CE2	1:A:710:PRO:HB2	2.53	0.44
1:B:299:ARG:CG	1:B:299:ARG:NH1	2.80	0.43
1:A:611:ALA:O	1:A:612:LYS:C	2.56	0.43
1:B:621:THR:C	1:B:623:SER:H	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:684:SER:HB3	1:B:687:ILE:CG1	2.48	0.43
1:B:595:VAL:HG21	1:B:682:PRO:HG2	2.00	0.43
1:A:449:ALA:O	1:A:455:LEU:HA	2.19	0.43
1:A:331:CYS:HB3	1:B:697:ASN:HB3	2.00	0.43
1:A:502:THR:O	1:A:506:ILE:HG13	2.18	0.43
1:A:350:THR:HG22	1:A:351:LYS:N	2.34	0.43
1:B:445:HIS:HE1	1:B:585:SER:OG	2.01	0.43
1:A:456:ARG:HG2	7:A:61:HOH:O	2.19	0.43
1:B:571:LEU:HD12	1:B:572:LEU:H	1.83	0.42
1:B:393:THR:OG1	1:B:394:TYR:N	2.52	0.42
4:B:750:HEM:HBA1	4:B:750:HEM:HMA2	2.01	0.42
1:B:591:THR:HA	1:B:634:ASN:HD21	1.83	0.42
1:A:500:GLN:O	1:A:503:GLU:HB2	2.19	0.42
1:A:635:ILE:HD12	1:B:623:SER:O	2.19	0.42
1:B:393:THR:O	1:B:394:TYR:HB3	2.20	0.42
1:A:551:PHE:CD1	1:A:553:TRP:CZ2	3.08	0.42
1:B:396:LEU:HG	1:B:577:LEU:HD12	2.02	0.42
1:A:486:LYS:HE3	1:A:503:GLU:OE1	2.19	0.42
1:B:589:MET:HA	1:B:649:VAL:O	2.20	0.42
1:A:510:TRP:HB2	1:A:533:LEU:CD1	2.49	0.42
1:B:664:ASN:O	1:B:668:CYS:HB2	2.20	0.42
1:B:548:HIS:HB2	1:B:554:PHE:CG	2.55	0.42
1:B:507:GLN:HG2	1:B:507:GLN:O	2.20	0.42
1:A:353:GLN:O	1:A:356:PRO:HG2	2.21	0.41
1:A:498:ASN:O	1:A:499:VAL:C	2.58	0.41
1:A:406:LYS:HE2	1:A:422:SER:O	2.20	0.41
1:A:482:TYR:HA	1:A:518:ASP:O	2.21	0.41
1:A:651:HIS:NE2	1:B:627:ASP:OD2	2.44	0.41
1:B:587:TRP:H	4:B:750:HEM:HAB	1.86	0.41
1:A:551:PHE:HB3	1:A:553:TRP:CE2	2.56	0.41
1:B:364:GLN:O	1:B:365:TYR:C	2.60	0.41
1:A:513:PRO:HG2	1:A:518:ASP:CG	2.41	0.41
1:A:445:HIS:HE1	1:A:585:SER:OG	2.03	0.41
1:A:419:ILE:O	1:A:419:ILE:HG12	2.20	0.40
1:B:332:MET:HE3	1:B:338:PRO:HB3	2.03	0.40
1:B:351:LYS:HG3	1:B:352:ASP:N	2.36	0.40
1:A:711:TRP:HD1	1:A:712:ASN:ND2	2.19	0.40
1:A:425:GLN:NE2	1:A:425:GLN:HA	2.37	0.40
1:A:519:VAL:HG23	7:A:201:HOH:O	2.21	0.40
1:A:697:ASN:HD22	1:A:697:ASN:HA	1.65	0.40
1:A:572:LEU:HD13	1:A:704:PHE:CE2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:GLU:O	1:A:364:GLN:HG3	2.21	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	403/421 (96%)	369 (92%)	31 (8%)	3 (1%)	26	31
1	B	406/421 (96%)	377 (93%)	27 (7%)	2 (0%)	34	41
All	All	809/842 (96%)	746 (92%)	58 (7%)	5 (1%)	30	36

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	374	SER
1	B	374	SER
1	A	489	ASP
1	A	669	ARG
1	B	648	ILE

### 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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	363/377 (96%)	344 (95%)	19 (5%)	29	38
1	B	366/377 (97%)	358 (98%)	8 (2%)	60	77
All	All	729/754 (97%)	702 (96%)	27 (4%)	41	55

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	300	PHE
1	A	316	LEU
1	A	321	THR
1	A	336	MET
1	A	337	LEU
1	A	451	ASN
1	A	454	ASN
1	A	523	LEU
1	A	527	ASN
1	A	547	ARG
1	A	571	LEU
1	A	595	VAL
1	A	600	ASP
1	A	609	GLU
1	A	616	LEU
1	A	622	SER
1	A	628	GLN
1	A	690	VAL
1	A	701	THR
1	B	316	LEU
1	B	378	MET
1	B	451	ASN
1	B	477	SER
1	B	489	ASP
1	B	523	LEU
1	B	527	ASN
1	B	547	ARG

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	364	GLN
1	A	425	GLN
1	A	445	HIS
1	A	451	ASN
1	A	454	ASN
1	A	628	GLN
1	A	634	ASN
1	A	697	ASN
1	A	712	ASN
1	B	377	HIS
1	B	425	GLN
1	B	445	HIS
1	B	451	ASN
1	B	454	ASN
1	B	508	GLN
1	B	527	ASN
1	B	634	ASN
1	B	664	ASN
1	B	697	ASN
1	B	712	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	30,50,50	2.83	11 (36%)	24,82,82	2.40	8 (33%)
5	H4B	A	760	-	13,18,18	2.26	3 (23%)	11,26,26	4.08	6 (54%)
6	INE	A	790	-	10,14,14	2.89	2 (20%)	6,20,20	1.32	1 (16%)
2	ACT	A	860	-	1,3,3	2.71	1 (100%)	0,3,3	0.00	-
4	HEM	B	750	1	30,50,50	2.72	9 (30%)	24,82,82	2.71	9 (37%)
5	H4B	B	761	-	13,18,18	2.21	3 (23%)	11,26,26	4.12	6 (54%)
6	INE	B	791	-	10,14,14	2.90	2 (20%)	6,20,20	1.30	1 (16%)
2	ACT	B	861	-	1,3,3	3.04	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	-	0/10/54/54	0/0/8/8
5	H4B	A	760	-	-	0/8/17/17	0/2/2/2
6	INE	A	790	-	-	0/3/4/4	0/2/2/2
2	ACT	A	860	-	-	0/0/0/0	0/0/0/0
4	HEM	B	750	1	-	0/10/54/54	0/0/8/8
5	H4B	B	761	-	-	0/8/17/17	0/2/2/2
6	INE	B	791	-	-	0/3/4/4	0/2/2/2
2	ACT	B	861	-	-	0/0/0/0	0/0/0/0

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	750	HEM	C3D-C4D	-6.58	1.43	1.51
4	B	750	HEM	C3B-CAB	-6.37	1.39	1.51
4	A	750	HEM	C2D-C3D	-5.99	1.36	1.54
4	B	750	HEM	C3C-CAC	-5.96	1.40	1.51
4	B	750	HEM	C3D-C4D	-5.90	1.44	1.51
4	B	750	HEM	C2D-C3D	-5.87	1.36	1.54
4	A	750	HEM	C3B-CAB	-5.71	1.40	1.51
4	A	750	HEM	C3C-CAC	-5.63	1.40	1.51
4	A	750	HEM	C3B-C4B	-5.39	1.47	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	750	HEM	C2C-C1C	-4.31	1.44	1.52
4	B	750	HEM	C3B-C4B	-4.16	1.48	1.51
4	A	750	HEM	C2C-C1C	-3.72	1.45	1.52
6	A	790	INE	C8-N1	-2.57	1.31	1.37
6	B	791	INE	C8-N1	-2.56	1.31	1.37
4	A	750	HEM	C2D-C1D	-2.30	1.44	1.51
4	B	750	HEM	C2D-C1D	-2.21	1.44	1.51
4	A	750	HEM	C2B-C1B	-2.10	1.45	1.51
4	A	750	HEM	CHD-C4C	2.07	1.41	1.36
4	A	750	HEM	C1C-NC	2.23	1.38	1.36
2	A	860	ACT	CH3-C	2.71	1.52	1.48
2	B	861	ACT	CH3-C	3.04	1.53	1.48
4	B	750	HEM	C4C-NC	3.23	1.40	1.36
5	B	761	H4B	C4A-N5	3.53	1.46	1.38
4	B	750	HEM	C1C-NC	3.75	1.40	1.36
5	A	760	H4B	C4A-N5	3.97	1.47	1.38
4	A	750	HEM	C4C-NC	4.16	1.41	1.36
5	B	761	H4B	C6-N5	4.46	1.54	1.45
5	A	760	H4B	C6-N5	4.48	1.54	1.45
5	A	760	H4B	C4-N3	4.84	1.42	1.33
5	B	761	H4B	C4-N3	4.85	1.42	1.33
6	B	791	INE	C3-N2	8.45	1.45	1.34
6	A	790	INE	C3-N2	8.51	1.45	1.34

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	750	HEM	CBA-CAA-C2A	-7.81	98.53	112.53
4	A	750	HEM	CBA-CAA-C2A	-5.62	102.46	112.53
5	A	760	H4B	N3-C2-N1	-4.73	117.79	125.53
5	B	761	H4B	N3-C2-N1	-4.71	117.81	125.53
4	B	750	HEM	C1D-CHD-C4C	-2.82	121.10	125.82
4	A	750	HEM	CBD-CAD-C3D	-2.01	107.71	113.55
4	B	750	HEM	C3B-C4B-CHC	2.07	126.07	123.16
4	A	750	HEM	CMD-C2D-C3D	2.09	123.58	114.35
6	B	791	INE	C6-C7-N10	2.84	120.27	116.59
6	A	790	INE	C6-C7-N10	2.89	120.33	116.59
5	A	760	H4B	N2-C2-N1	3.03	122.22	117.20
5	B	761	H4B	N2-C2-N1	3.16	122.42	117.20
4	B	750	HEM	CMD-C2D-C3D	3.28	128.84	114.35
4	B	750	HEM	C2D-C3D-C4D	3.32	107.13	101.50
4	B	750	HEM	CAD-C3D-C4D	3.40	124.45	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	761	H4B	C2-N1-C8A	3.54	122.50	114.54
4	A	750	HEM	CAD-C3D-C4D	3.75	125.70	112.47
5	A	760	H4B	C2-N1-C8A	3.76	122.99	114.54
5	B	761	H4B	C4A-C8A-N8	3.86	122.97	118.43
5	A	760	H4B	C4A-C8A-N8	3.86	122.98	118.43
4	B	750	HEM	CMB-C2B-C3B	3.99	126.50	116.53
4	A	750	HEM	CMB-C2B-C3B	4.14	126.86	116.53
4	A	750	HEM	CMC-C2C-C3C	4.15	126.89	116.53
4	A	750	HEM	CAD-C3D-C2D	4.18	125.24	113.22
4	B	750	HEM	CMC-C2C-C3C	4.41	127.54	116.53
4	A	750	HEM	C2D-C3D-C4D	4.46	109.05	101.50
4	B	750	HEM	CAD-C3D-C2D	5.26	128.33	113.22
5	B	761	H4B	C4-N3-C2	6.47	124.93	115.94
5	A	760	H4B	C4-N3-C2	6.56	125.04	115.94
5	A	760	H4B	C4-C4A-C8A	8.69	122.43	114.56
5	B	761	H4B	C4-C4A-C8A	9.02	122.73	114.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	750	HEM	2	0
6	A	790	INE	1	0
2	A	860	ACT	3	0
4	B	750	HEM	5	0
6	B	791	INE	1	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, 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	407/421 (96%)	0.57	41 (10%) 9 13	30, 51, 80, 98	0
1	B	410/421 (97%)	0.33	18 (4%) 38 47	23, 47, 75, 95	0
All	All	817/842 (97%)	0.45	59 (7%) 18 26	23, 49, 78, 98	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	351	LYS	6.2
1	A	352	ASP	5.1
1	A	715	VAL	4.6
1	B	350	THR	4.6
1	A	351	LYS	4.4
1	A	488	PRO	4.3
1	A	299	ARG	4.2
1	B	300	PHE	4.2
1	A	388	ILE	4.2
1	B	352	ASP	3.9
1	A	489	ASP	3.7
1	A	716	TRP	3.5
1	B	619	ARG	3.5
1	A	490	GLY	3.4
1	A	350	THR	3.3
1	A	486	LYS	3.3
1	B	329	HIS	3.2
1	A	322	LEU	3.2
1	A	355	PHE	3.1
1	B	717	LYS	3.1
1	B	349	ARG	3.1
1	B	348	VAL	2.9
1	A	713	THR	2.9
1	A	389	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	369	ILE	2.8
1	A	712	ASN	2.8
1	A	370	LYS	2.8
1	A	469	LYS	2.7
1	A	327	THR	2.6
1	A	311	VAL	2.6
1	A	300	PHE	2.5
1	A	353	GLN	2.5
1	A	487	GLN	2.4
1	A	503	GLU	2.4
1	A	618	MET	2.4
1	A	338	PRO	2.4
1	B	353	GLN	2.3
1	A	386	LYS	2.3
1	B	681	PRO	2.3
1	A	704	PHE	2.3
1	A	415	CYS	2.3
1	A	572	LEU	2.2
1	A	373	GLY	2.2
1	B	338	PRO	2.2
1	B	415	CYS	2.2
1	A	372	PHE	2.2
1	A	616	LEU	2.2
1	A	390	SER	2.1
1	B	591	THR	2.1
1	B	567	VAL	2.1
1	A	619	ARG	2.1
1	B	376	ALA	2.1
1	B	631	VAL	2.1
1	A	354	LEU	2.1
1	A	479	LEU	2.1
1	A	328	GLU	2.0
1	A	685	GLY	2.0
1	A	309	ASP	2.0
1	B	303	VAL	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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



### 6.3 Carbohydrates [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( $\text{\AA}^2$ )	Q<0.9
4	HEM	A	750	43/43	0.97	0.20	0.75	31,38,45,52	0
5	H4B	A	760	17/17	0.94	0.16	0.68	46,49,51,52	0
4	HEM	B	750	43/43	0.97	0.19	0.50	27,33,41,47	0
6	INE	B	791	13/13	0.98	0.17	-0.37	50,53,56,58	0
5	H4B	B	761	17/17	0.94	0.13	-0.51	39,45,50,50	0
3	ZN	A	900	1/1	0.99	0.09	-0.78	44,44,44,44	0
2	ACT	B	861	4/4	0.99	0.10	-0.95	30,31,33,35	0
6	INE	A	790	13/13	0.98	0.15	-1.33	38,48,52,53	0
2	ACT	A	860	4/4	0.98	0.08	-2.73	41,43,43,47	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.