



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 05:06 AM GMT

PDB ID : 1RS6  
Title : Rat neuronal NOS heme domain with D-lysine-D-nitroarginineamide bound  
Authors : Flinspach, M.; Li, H.; Jamal, J.; Yang, W.; Huang, H.; Silverman, R.B.; Poulos, T.L.  
Deposited on : 2003-12-09  
Resolution : 1.95 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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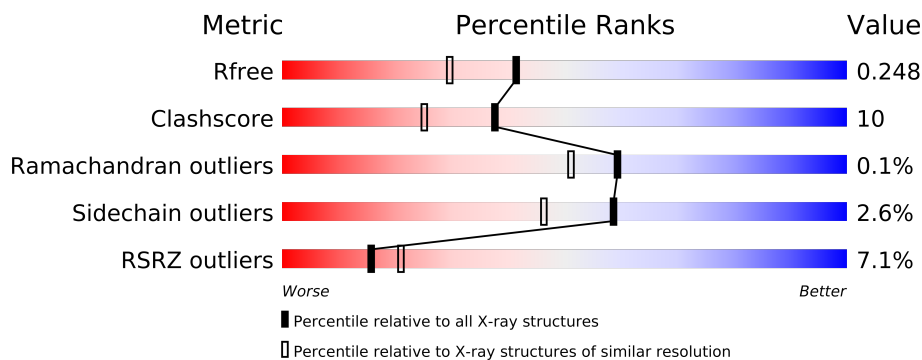
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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))
$R_{free}$	66092	1321 (1.96-1.96)
Clashscore	79885	1488 (1.96-1.96)
Ramachandran outliers	78287	1475 (1.96-1.96)
Sidechain outliers	78261	1475 (1.96-1.96)
RSRZ outliers	66119	1321 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	421	
1	B	421	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	MTL	A	870	-	X
2	MTL	B	871	-	X
3	ACT	A	860	-	X

## 2 Entry composition i

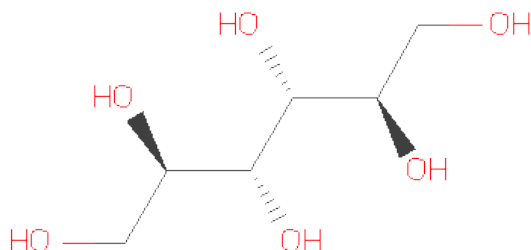
There are 8 unique types of molecules in this entry. The entry contains 7401 atoms, of which 0 are hydrogen and 0 are deuterium.

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
			3315	2121	566	606	22			
1	B	410	Total	C	N	O	S	0	2	0
			3343	2138	573	611	21			

- Molecule 2 is D-MANNITOL (three-letter code: MTL) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		
2	B	1	Total	C	O	0	0
			12	6	6		

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

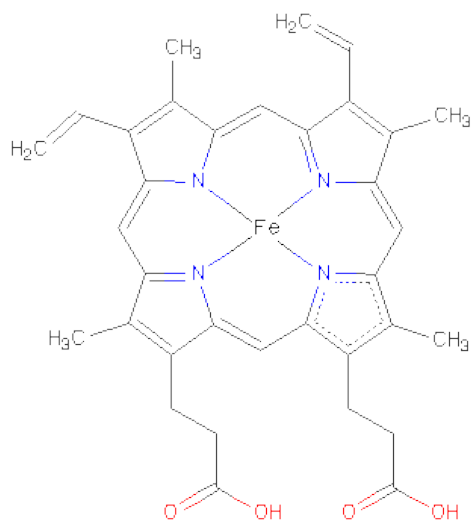


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

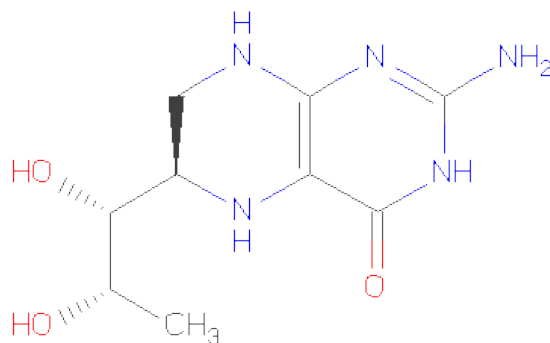
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).



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

- Molecule 6 is 5,6,7,8-TETRAHYDROBIOPTERIN (three-letter code: H4B) (formula:  $C_9H_{15}N_5O_3$ ).



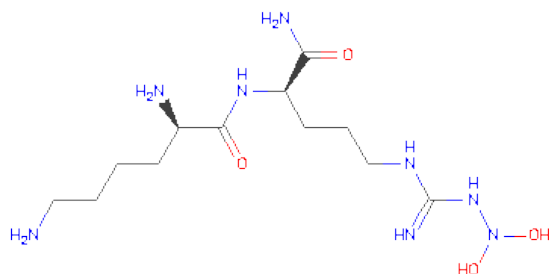
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			17	9	5	3		

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

- Molecule 7 is L-LYSYL-N 5 -[(Z)-(2,2-DIHYDROXYHYDRAZINO)(IMINO)METHYL]-L-ORNITHINAMIDE (three-letter code: DP2) (formula: C<sub>12</sub>H<sub>28</sub>N<sub>8</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			24	12	8	4		
7	B	1	Total	C	N	O	0	0
			24	12	8	4		

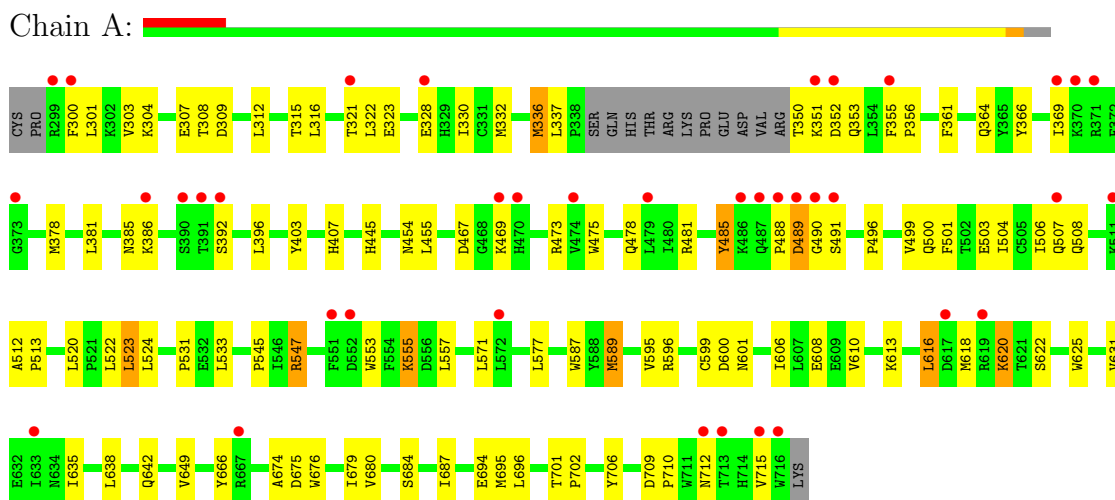
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	230	Total	O	0	0
			230	230		
8	B	312	Total	O	0	0
			312	312		

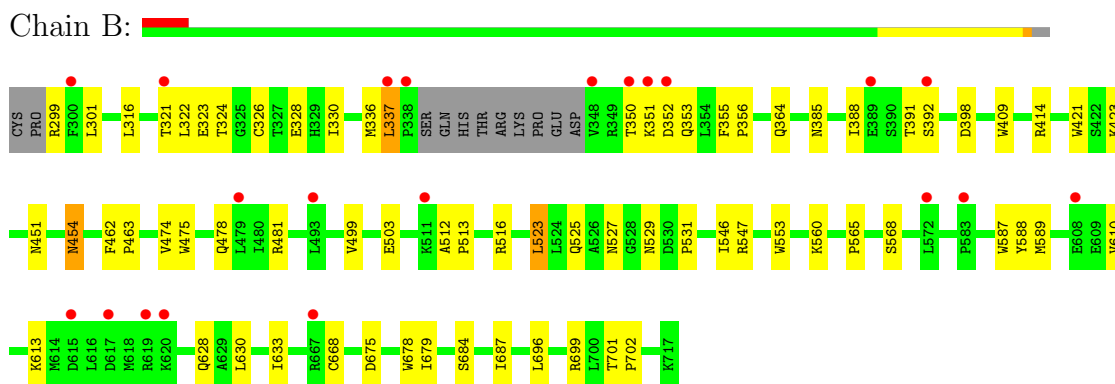
### 3 Residue-property plots

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, $\alpha$ , $\beta$ , $\gamma$	51.59Å 109.81Å 164.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.08 – 1.95 27.08 – 1.90	Depositor EDS
% Data completeness (in resolution range)	92.4 (27.08-1.95) 91.8 (27.08-1.90)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.47 (at 1.89Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.221 , 0.254 0.218 , 0.248	Depositor DCC
$R_{free}$ test set	3434 reflections (5.25%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.9	Xtriage
Anisotropy	0.736	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 44.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 68862 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7401	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.04% of the height of the origin peak. No significant pseudotranslation is detected.*

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



## 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: ZN, DP2, MTL, ACT, HEM, H4B

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	0.45	0/3418	0.67	1/4637 (0.0%)
1	B	0.47	0/3446	0.68	2/4672 (0.0%)
All	All	0.46	0/6864	0.67	3/9309 (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	-5.91	95.04	111.00
1	B	326	CYS	CA-CB-SG	5.88	124.59	114.00
1	A	589	MET	N-CA-C	-5.46	96.26	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3315	0	3223	89	0
1	B	3343	0	3258	51	0
2	A	12	0	14	1	0
2	B	12	0	14	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	4	0	3	0	0
3	B	4	0	3	0	0
4	A	1	0	0	0	0
5	A	43	0	30	2	0
5	B	43	0	30	3	0
6	A	17	0	15	0	0
6	B	17	0	15	1	0
7	A	24	0	28	1	0
7	B	24	0	27	0	0
8	A	230	0	0	7	0
8	B	312	0	0	8	0
All	All	7401	0	6660	135	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 10.

All (135) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:523:LEU:HD22	1:B:531:PRO:HB2	1.43	1.00
1:A:523:LEU:HD22	1:A:531:PRO:HB2	1.55	0.89
1:B:350:THR:HB	1:B:353:GLN:OE1	1.79	0.82
1:B:350:THR:HG22	1:B:352:ASP:H	1.47	0.78
1:A:350:THR:HB	1:A:353:GLN:HG3	1.64	0.78
1:B:610:VAL:HG21	1:B:633:ILE:HD11	1.68	0.74
1:A:350:THR:HG22	1:A:352:ASP:H	1.53	0.73
1:B:699:ARG:HB3	8:B:1090:HOH:O	1.90	0.71
1:A:332:MET:HE1	1:B:301:LEU:HD22	1.75	0.69
1:B:478:GLN:HB2	1:B:481:ARG:HG3	1.77	0.67
1:A:696:LEU:HD22	1:B:330:ILE:HD11	1.78	0.65
1:A:478:GLN:HB2	1:A:481:ARG:HG3	1.80	0.64
1:A:350:THR:HB	1:A:353:GLN:CG	2.30	0.62
1:B:299:ARG:HB3	1:B:299:ARG:NH1	2.14	0.62
1:B:475:TRP:HB2	1:B:523:LEU:HB3	1.83	0.61
1:A:503:GLU:HG3	8:A:1013:HOH:O	2.00	0.60
1:A:545:PRO:HG2	1:A:547:ARG:NH1	2.16	0.60
1:A:467:ASP:OD1	1:A:469:LYS:HB2	2.02	0.60
1:B:668:CYS:HB3	8:B:998:HOH:O	2.02	0.59
1:B:355:PHE:N	1:B:356:PRO:HD2	2.17	0.59
1:A:303:VAL:HG13	1:A:694:GLU:HB2	1.84	0.59
1:B:351:LYS:HE2	1:B:392:SER:OG	2.03	0.59
1:B:299:ARG:HB3	1:B:299:ARG:HH11	1.68	0.59
1:A:308:THR:O	1:A:309:ASP:HB2	2.04	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:A:941:HOH:O	1:B:337:LEU:HD23	2.05	0.57
1:A:485:TYR:CE2	1:A:512:ALA:HB1	2.40	0.57
1:A:684:SER:HB3	1:A:687:ILE:HD11	1.87	0.56
1:B:337:LEU:N	1:B:337:LEU:HD23	2.21	0.56
1:A:307:GLU:HG3	8:B:951:HOH:O	2.03	0.56
1:A:553:TRP:CE3	1:A:613:LYS:HD3	2.40	0.56
1:B:699:ARG:HG2	8:B:1160:HOH:O	2.05	0.55
1:A:489:ASP:HB2	1:A:491:SER:OG	2.07	0.55
1:A:353:GLN:O	1:A:356:PRO:HD2	2.07	0.55
1:B:336:MET:HG2	1:B:337:LEU:HD22	1.89	0.55
1:A:330:ILE:HD11	1:B:696:LEU:HD22	1.89	0.55
1:A:396:LEU:HG	1:A:577:LEU:HD12	1.88	0.55
1:A:616:LEU:HD13	1:A:625:TRP:HB2	1.89	0.54
1:B:565:PRO:HB3	1:B:588:TYR:CZ	2.44	0.53
1:A:328:GLU:O	1:B:324:THR:HG23	2.08	0.52
1:A:555:LYS:HB3	1:A:555:LYS:HZ2	1.74	0.52
1:B:322:LEU:HD12	8:B:1090:HOH:O	2.09	0.52
5:A:750:HEM:HMC1	5:A:750:HEM:HBC2	1.91	0.52
1:A:485:TYR:HA	8:A:1099:HOH:O	2.10	0.51
1:A:606:ILE:O	1:A:610:VAL:HG23	2.09	0.51
1:A:330:ILE:HD11	1:B:696:LEU:HB3	1.92	0.50
1:A:675:ASP:O	1:A:679:ILE:HG12	2.12	0.50
1:A:321:THR:HG21	8:A:1107:HOH:O	2.10	0.49
1:A:321:THR:HG23	1:A:322:LEU:HG	1.94	0.49
1:A:638:LEU:O	1:A:642:GLN:HG3	2.11	0.49
1:A:620:LYS:HE3	1:A:622:SER:OG	2.13	0.49
1:A:488:PRO:C	1:A:490:GLY:H	2.16	0.49
1:A:715:VAL:HG23	1:A:715:VAL:O	2.12	0.49
1:B:391:THR:O	1:B:392:SER:HB2	2.12	0.49
1:A:351:LYS:HE2	1:A:392:SER:HA	1.94	0.49
1:A:488:PRO:C	1:A:490:GLY:N	2.66	0.49
1:A:485:TYR:HE2	1:A:512:ALA:HB1	1.78	0.49
1:A:522:LEU:O	1:A:533:LEU:HA	2.13	0.48
1:A:491:SER:HB2	8:A:1100:HOH:O	2.14	0.47
5:B:750:HEM:HBC2	5:B:750:HEM:CMC	2.44	0.47
1:A:304:LYS:O	1:A:694:GLU:HG3	2.15	0.47
5:A:750:HEM:CMC	5:A:750:HEM:HBC2	2.44	0.47
1:B:675:ASP:O	1:B:679:ILE:HG12	2.15	0.47
1:A:706:TYR:CE2	7:A:792:DP2:HD'2	2.50	0.47
1:A:303:VAL:CG1	1:A:694:GLU:O	2.63	0.47
1:A:496:PRO:O	1:A:499:VAL:HG23	2.14	0.46
1:A:524:LEU:O	1:A:531:PRO:HA	2.16	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:553:TRP:HZ3	1:A:557:LEU:HD11	1.81	0.46
1:A:300:PHE:CD2	1:A:315:THR:HG22	2.51	0.46
1:A:601:ASN:HB2	8:A:970:HOH:O	2.15	0.46
1:B:409:TRP:CE3	1:B:421:TRP:HA	2.50	0.46
1:A:571:LEU:C	1:A:571:LEU:HD23	2.36	0.46
1:A:488:PRO:O	1:A:490:GLY:N	2.49	0.46
1:B:587:TRP:H	5:B:750:HEM:HAB	1.80	0.46
1:A:545:PRO:HG2	1:A:547:ARG:HH11	1.81	0.45
1:B:388:ILE:O	1:B:392:SER:N	2.43	0.45
1:A:403:TYR:CE1	1:A:407:HIS:CE1	3.05	0.45
1:A:366:TYR:CD2	1:A:369:ILE:HD11	2.52	0.45
1:A:336:MET:HE1	8:A:989:HOH:O	2.16	0.45
1:B:525:GLN:HG3	1:B:529:ASN:O	2.17	0.45
1:A:608:GLU:HG3	1:A:618:MET:HE1	1.98	0.44
1:A:555:LYS:HB3	1:A:555:LYS:NZ	2.32	0.44
1:A:351:LYS:HE2	1:A:392:SER:CA	2.46	0.44
1:B:546:ILE:HG12	1:B:560:LYS:HA	1.99	0.44
1:B:462:PHE:HB3	1:B:463:PRO:HD2	1.99	0.44
1:A:350:THR:HB	1:A:353:GLN:CD	2.38	0.44
1:A:475:TRP:CE2	1:A:710:PRO:HB2	2.52	0.44
1:A:512:ALA:HA	1:A:513:PRO:HD3	1.88	0.44
5:B:750:HEM:HBC2	5:B:750:HEM:HMC1	2.00	0.44
1:A:674:ALA:HB3	1:A:695:MET:HB3	1.99	0.43
1:A:496:PRO:HA	1:A:499:VAL:HG23	2.00	0.43
1:B:355:PHE:CE1	1:B:385:ASN:HB2	2.54	0.43
1:A:631:VAL:HG11	1:B:628:GLN:HG2	1.99	0.43
1:A:676:TRP:CZ2	1:A:680:VAL:HG21	2.54	0.43
1:A:301:LEU:CD1	1:B:330:ILE:HD13	2.48	0.43
1:A:500:GLN:O	1:A:504:ILE:HG13	2.19	0.43
1:B:364:GLN:NE2	8:B:1119:HOH:O	2.52	0.43
1:B:684:SER:HB3	1:B:687:ILE:CG1	2.49	0.43
1:A:321:THR:HG23	1:A:322:LEU:N	2.34	0.43
1:A:366:TYR:HA	1:A:369:ILE:HG12	2.01	0.43
1:B:553:TRP:CH2	1:B:613:LYS:HB2	2.54	0.43
1:A:684:SER:HB3	1:A:687:ILE:CG1	2.49	0.43
1:B:398:ASP:HB2	8:B:1080:HOH:O	2.19	0.42
1:A:701:THR:HA	1:A:702:PRO:C	2.39	0.42
1:B:337:LEU:N	1:B:337:LEU:CD2	2.82	0.42
1:A:596:ARG:O	1:A:600:ASP:HB2	2.19	0.42
1:A:595:VAL:O	1:A:599:CYS:HB2	2.19	0.42
1:A:323:GLU:HA	1:B:328:GLU:O	2.19	0.42
1:B:299:ARG:CB	1:B:299:ARG:NH1	2.83	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:516:ARG:HG3	8:B:1033:HOH:O	2.19	0.42
1:A:687:ILE:HD13	1:B:630:LEU:HD22	2.01	0.42
1:B:414:ARG:HD3	1:B:678:TRP:CD2	2.55	0.42
1:A:361:PHE:O	1:A:364:GLN:HG2	2.19	0.42
1:B:323:GLU:O	1:B:699:ARG:HD3	2.20	0.42
1:A:501:PHE:HD2	1:A:520:LEU:HD13	1.84	0.41
1:A:501:PHE:HB2	2:A:870:MTL:H61	2.01	0.41
1:B:451:ASN:HB3	1:B:454:ASN:O	2.20	0.41
1:B:499:VAL:O	1:B:503:GLU:HG3	2.19	0.41
1:A:378:MET:HE2	1:A:378:MET:HA	2.02	0.41
1:A:303:VAL:HG11	1:A:694:GLU:O	2.19	0.41
1:B:678:TRP:HA	6:B:761:H4B:N1	2.35	0.41
1:A:709:ASP:HB2	1:A:712:ASN:ND2	2.35	0.41
1:A:300:PHE:N	1:A:300:PHE:CD1	2.89	0.41
1:A:473:ARG:CZ	1:A:710:PRO:HG3	2.50	0.41
1:B:512:ALA:HA	1:B:513:PRO:HD3	1.92	0.41
1:A:355:PHE:CZ	1:A:385:ASN:ND2	2.89	0.41
1:A:312:LEU:HB3	1:A:666:TYR:CD2	2.56	0.41
1:B:701:THR:HA	1:B:702:PRO:C	2.41	0.41
1:B:474:VAL:HG11	1:B:568:SER:HB2	2.03	0.41
1:A:445:HIS:C	1:A:445:HIS:CD2	2.94	0.41
1:A:381:LEU:HA	1:A:381:LEU:HD12	1.95	0.41
1:A:455:LEU:HD12	1:A:587:TRP:HB3	2.02	0.40
1:A:507:GLN:HG2	1:A:507:GLN:O	2.21	0.40
1:A:506:ILE:C	1:A:508:GLN:H	2.24	0.40
1:A:589:MET:HA	1:A:649:VAL:O	2.20	0.40
1:A:386:LYS:HA	1:A:386:LYS:HD3	1.92	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	405/421 (96%)	384 (95%)	20 (5%)	1 (0%)	56 46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	408/421 (97%)	394 (97%)	14 (3%)	0	100	100
All	All	813/842 (97%)	778 (96%)	34 (4%)	1 (0%)	59	51

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	489	ASP

### 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%)	354 (97%)	11 (3%)	53	39
1	B	368/377 (98%)	360 (98%)	8 (2%)	64	55
All	All	733/754 (97%)	714 (97%)	19 (3%)	59	46

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	316	LEU
1	A	336	MET
1	A	337	LEU
1	A	454	ASN
1	A	485	TYR
1	A	523	LEU
1	A	547	ARG
1	A	555	LYS
1	A	616	LEU
1	A	620	LYS
1	A	635	ILE
1	B	316	LEU
1	B	321	THR
1	B	337	LEU
1	B	423	LYS
1	B	454	ASN
1	B	523	LEU

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Mol	Chain	Res	Type
1	B	527	ASN
1	B	547	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	440	ASN
1	A	454	ASN
1	A	487	GLN
1	A	697	ASN
1	A	712	ASN
1	B	364	GLN
1	B	425	GLN
1	B	440	ASN
1	B	454	ASN
1	B	507	GLN
1	B	527	ASN
1	B	535	GLN
1	B	664	ASN
1	B	697	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 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	$\# Z  > 2$
5	HEM	A	750	1	49,50,50	2.18	14 (28%)	46,82,82	1.60	6 (13%)
6	H4B	A	760	-	18,18,18	1.94	4 (22%)	24,26,26	2.49	9 (37%)
7	DP2	A	792	-	20,23,23	0.93	0	24,28,28	1.20	2 (8%)
3	ACT	A	860	-	1,3,3	2.93	1 (100%)	0,3,3	0.00	-
2	MTL	A	870	-	11,11,11	1.02	0	14,14,14	0.62	0
5	HEM	B	750	1	49,50,50	2.13	14 (28%)	46,82,82	1.80	9 (19%)
6	H4B	B	761	-	18,18,18	1.78	4 (22%)	24,26,26	2.45	7 (29%)
7	DP2	B	793	-	20,23,23	1.08	3 (15%)	24,28,28	1.44	3 (12%)
3	ACT	B	861	-	1,3,3	2.53	1 (100%)	0,3,3	0.00	-
2	MTL	B	871	-	11,11,11	1.02	0	14,14,14	0.58	0

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
5	HEM	A	750	1	-	0/14/114/114	0/0/8/8
6	H4B	A	760	-	-	0/8/17/17	0/0/2/2
7	DP2	A	792	-	-	0/24/28/28	0/0/0/0
3	ACT	A	860	-	-	0/0/0/0	0/0/0/0
2	MTL	A	870	-	-	0/16/16/16	0/0/0/0
5	HEM	B	750	1	-	0/14/114/114	0/0/8/8
6	H4B	B	761	-	-	0/8/17/17	0/0/2/2
7	DP2	B	793	-	-	0/24/28/28	0/0/0/0
3	ACT	B	861	-	-	0/0/0/0	0/0/0/0
2	MTL	B	871	-	-	0/16/16/16	0/0/0/0

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	750	HEM	C2D-C1D	8.59	1.46	1.44
5	B	750	HEM	CHB-C1B	6.14	1.44	1.35
5	A	750	HEM	C4A-C3A	5.76	1.47	1.40
5	B	750	HEM	C3C-C2C	-4.52	1.35	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	750	HEM	C2B-C1B	-4.49	1.43	1.44
6	A	760	H4B	C4-N3	4.39	1.44	1.37
5	A	750	HEM	C3B-C2B	-4.26	1.36	1.43
6	A	760	H4B	C6-N5	4.21	1.54	1.46
6	B	761	H4B	C6-N5	4.19	1.54	1.46
5	B	750	HEM	C2D-C1D	-4.13	1.43	1.44
5	B	750	HEM	C3D-C4D	3.97	1.45	1.44
5	B	750	HEM	C3D-C2D	-3.97	1.36	1.43
5	B	750	HEM	C3B-C2B	-3.88	1.37	1.43
5	A	750	HEM	C3D-C2D	-3.82	1.37	1.43
5	B	750	HEM	CHD-C4C	3.61	1.43	1.36
6	B	761	H4B	C4-N3	3.33	1.42	1.37
6	A	760	H4B	C4A-N5	3.18	1.49	1.38
5	B	750	HEM	CMD-C2D	3.04	1.56	1.47
3	A	860	ACT	CH3-C	2.93	1.53	1.48
5	A	750	HEM	CHC-C1C	2.74	1.41	1.36
6	A	760	H4B	C8A-N1	2.67	1.39	1.34
6	B	761	H4B	C2-N1	2.63	1.36	1.33
5	A	750	HEM	CMC-C2C	2.63	1.55	1.47
6	B	761	H4B	C4A-N5	2.61	1.47	1.38
3	B	861	ACT	CH3-C	2.53	1.52	1.48
5	B	750	HEM	C4A-NA	2.52	1.41	1.36
5	A	750	HEM	C3D-C4D	2.43	1.45	1.44
5	A	750	HEM	CHB-C1B	2.43	1.39	1.35
5	B	750	HEM	FE-NA	2.41	2.02	1.92
5	A	750	HEM	CMD-C2D	2.40	1.54	1.47
5	B	750	HEM	CMC-C2C	2.37	1.54	1.47
5	A	750	HEM	CHD-C4C	2.36	1.40	1.36
5	A	750	HEM	C1A-NA	2.28	1.41	1.36
5	A	750	HEM	C4C-NC	2.18	1.41	1.38
7	B	793	DP2	O-C	-2.15	1.19	1.23
5	B	750	HEM	CMB-C2B	2.11	1.54	1.47
7	B	793	DP2	CA-C	2.10	1.56	1.52
5	A	750	HEM	C1C-NC	2.06	1.41	1.38
5	A	750	HEM	C3C-C2C	-2.05	1.40	1.43
5	B	750	HEM	C3B-C4B	2.04	1.46	1.44
7	B	793	DP2	C'-N	2.03	1.38	1.34

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	761	H4B	C4-C4A-C8A	8.76	122.68	114.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	760	H4B	C4-C4A-C8A	8.22	122.18	114.56
5	B	750	HEM	C3B-C4B-NB	-5.12	110.34	114.00
5	A	750	HEM	C3B-C4B-NB	-4.83	110.54	114.00
5	B	750	HEM	C4A-CHB-C1B	-4.47	121.59	127.47
5	B	750	HEM	C3A-C4A-NA	4.44	112.77	109.41
7	B	793	DP2	O-C-N2	-4.19	115.94	123.03
5	A	750	HEM	CBA-CAA-C2A	-4.14	105.41	112.69
5	A	750	HEM	CBD-CAD-C3D	-4.12	105.39	114.37
6	A	760	H4B	C2-N1-C8A	3.83	123.05	117.61
5	B	750	HEM	C4C-NC-C1C	-3.63	101.76	105.53
6	A	760	H4B	C4A-N5-C6	-3.43	111.82	121.16
7	A	792	DP2	O-C-N2	-3.38	117.31	123.03
5	B	750	HEM	C4A-NA-C1A	-3.34	102.36	106.76
5	B	750	HEM	CBA-CAA-C2A	-3.25	106.97	112.69
6	A	760	H4B	N3-C2-N1	-3.20	117.30	121.78
6	B	761	H4B	C4A-N5-C6	-3.18	112.50	121.16
6	B	761	H4B	C2-N1-C8A	3.15	122.09	117.61
5	A	750	HEM	C3A-C4A-NA	3.11	111.76	109.41
6	A	760	H4B	C4-N3-C2	3.11	124.95	119.51
5	A	750	HEM	C4A-NA-C1A	-2.92	102.92	106.76
6	B	761	H4B	C4-N3-C2	2.90	124.58	119.51
7	B	793	DP2	CA-C-N2	2.85	122.28	116.78
5	B	750	HEM	CBD-CAD-C3D	-2.80	108.27	114.37
6	B	761	H4B	C4A-C8A-N8	2.68	122.91	119.23
6	A	760	H4B	C4A-C8A-N8	2.39	122.51	119.23
5	B	750	HEM	C1A-CHA-C4D	-2.38	124.33	127.47
6	B	761	H4B	N3-C2-N1	-2.36	118.47	121.78
5	B	750	HEM	C4D-ND-C1D	-2.22	102.89	105.16
6	A	760	H4B	N2-C2-N3	2.18	120.25	117.86
5	A	750	HEM	C4C-NC-C1C	-2.10	103.35	105.53
6	A	760	H4B	N8-C8A-N1	2.09	118.88	115.82
7	B	793	DP2	CD-NE-CZ	2.05	127.64	124.03
6	A	760	H4B	O9-C9-C6	2.05	114.04	109.07
7	A	792	DP2	CA-C-N2	2.03	120.70	116.78
6	B	761	H4B	C9-C6-N5	-2.00	105.95	109.69

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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%)	0.64	38 (9%) 9 11	23, 38, 62, 77	0
1	B	410/421 (97%)	0.29	21 (5%) 27 33	22, 33, 54, 70	0
All	All	817/842 (97%)	0.46	59 (7%) 16 20	22, 36, 59, 77	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	300	PHE	5.1
1	B	348	VAL	5.1
1	B	619	ARG	4.8
1	A	299	ARG	4.6
1	A	486	LYS	4.5
1	B	300	PHE	4.2
1	A	488	PRO	4.2
1	A	715	VAL	4.0
1	B	351	LYS	3.6
1	B	352	ASP	3.6
1	A	489	ASP	3.6
1	A	552	ASP	3.5
1	A	667	ARG	3.4
1	A	355	PHE	3.4
1	B	350	THR	3.3
1	A	716	TRP	3.1
1	B	615	ASP	3.1
1	A	619	ARG	3.0
1	A	511	LYS	2.9
1	A	470	HIS	2.9
1	B	620	LYS	2.9
1	A	351	LYS	2.9
1	A	712	ASN	2.7
1	A	713	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	392	SER	2.7
1	A	370	LYS	2.7
1	A	386	LYS	2.7
1	A	469	LYS	2.7
1	A	390	SER	2.6
1	A	321	THR	2.6
1	B	338	PRO	2.5
1	A	633	ILE	2.5
1	A	487	GLN	2.5
1	A	490	GLY	2.5
1	A	352	ASP	2.5
1	A	491	SER	2.4
1	A	328	GLU	2.4
1	B	583	PRO	2.4
1	B	321	THR	2.4
1	B	572	LEU	2.3
1	B	389	GLU	2.3
1	A	391	THR	2.3
1	B	667	ARG	2.3
1	A	373	GLY	2.3
1	A	551	PHE	2.2
1	A	479	LEU	2.2
1	B	337	LEU	2.2
1	A	507	GLN	2.2
1	A	617	ASP	2.2
1	A	371	ARG	2.1
1	B	617	ASP	2.1
1	A	474	VAL	2.1
1	B	511	LYS	2.1
1	A	392	SER	2.1
1	A	572	LEU	2.1
1	B	479	LEU	2.0
1	B	493	LEU	2.0
1	A	369	ILE	2.0
1	B	608	GLU	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

There are no carbohydrates in this entry.

### 6.4 Ligands

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	MTL	A	870	12/12	0.26	5.16	46,50,52,52	0
3	ACT	A	860	4/4	0.19	4.15	57,58,58,58	0
2	MTL	B	871	12/12	0.20	4.06	45,49,50,50	0
7	DP2	A	792	24/24	0.17	1.48	33,39,42,43	0
7	DP2	B	793	24/24	0.15	0.17	29,39,42,43	0
5	HEM	B	750	43/43	0.10	-0.37	22,23,26,28	0
3	ACT	B	861	4/4	0.08	-0.41	38,38,39,39	0
5	HEM	A	750	43/43	0.10	-0.80	23,26,27,28	0
6	H4B	B	761	17/17	0.09	-0.84	24,25,27,28	0
6	H4B	A	760	17/17	0.09	-1.25	23,25,27,28	0
4	ZN	A	900	1/1	0.05	-2.38	33,33,33,33	0

### 6.5 Other polymers

There are no such residues in this entry.