



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 11:14 AM GMT

PDB ID : 1RS7  
Title : Rat neuronal NOS heme domain with D-phenylalanine-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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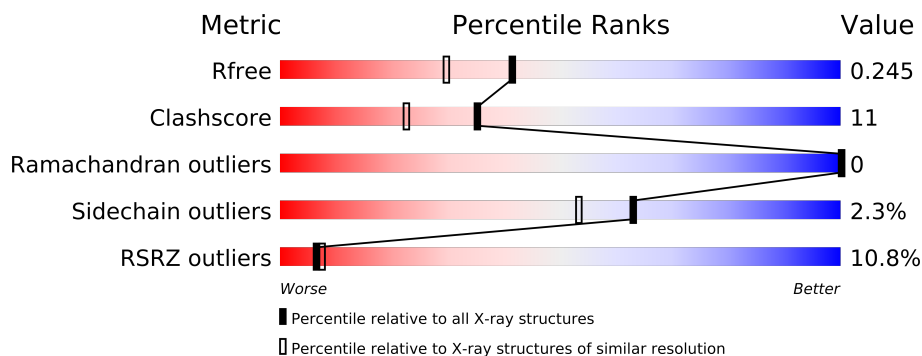
The following versions of software and data (see [references](#)) were used in the production of this report:

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
7	D7P	B	798	-	X

## 2 Entry composition (i)

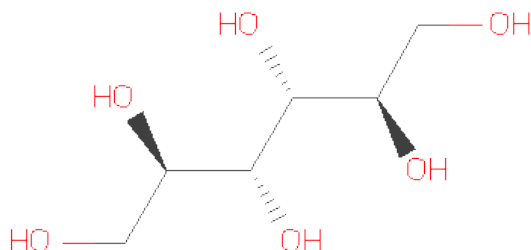
There are 8 unique types of molecules in this entry. The entry contains 7408 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

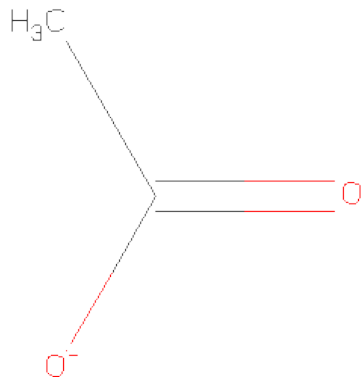
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	407	Total	C	N	O	S	0	0	0
			3313	2121	566	605	21			
1	B	410	Total	C	N	O	S	0	0	0
			3341	2138	573	609	21			

- Molecule 2 is 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	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).

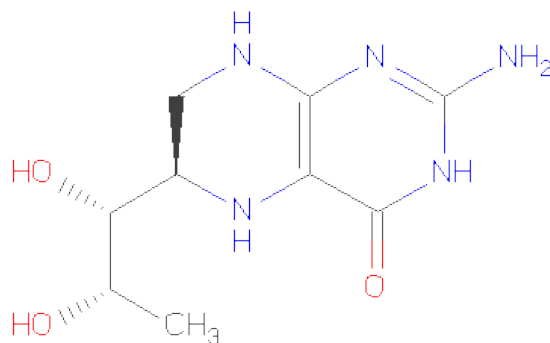
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		

- 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
			43	34	1	4	4	
5	B	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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



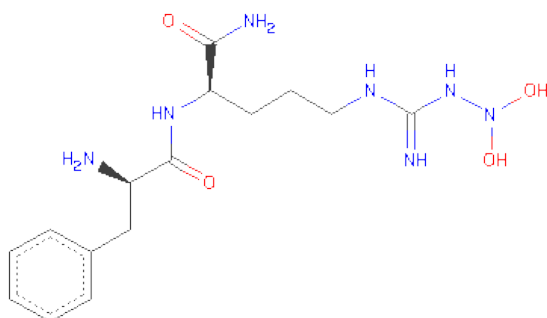
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			17	9	5	3		

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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 D-PHENYLALANYL-N 5 -[(2,2-DIHYDROXYHYDRAZINO)(IMINO)METHYL]-D-ORNITHINAMIDE (three-letter code: D7P) (formula: C<sub>15</sub>H<sub>25</sub>N<sub>7</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			26	15	7	4		
7	B	1	Total	C	N	O	0	0
			26	15	7	4		

- Molecule 8 is water.

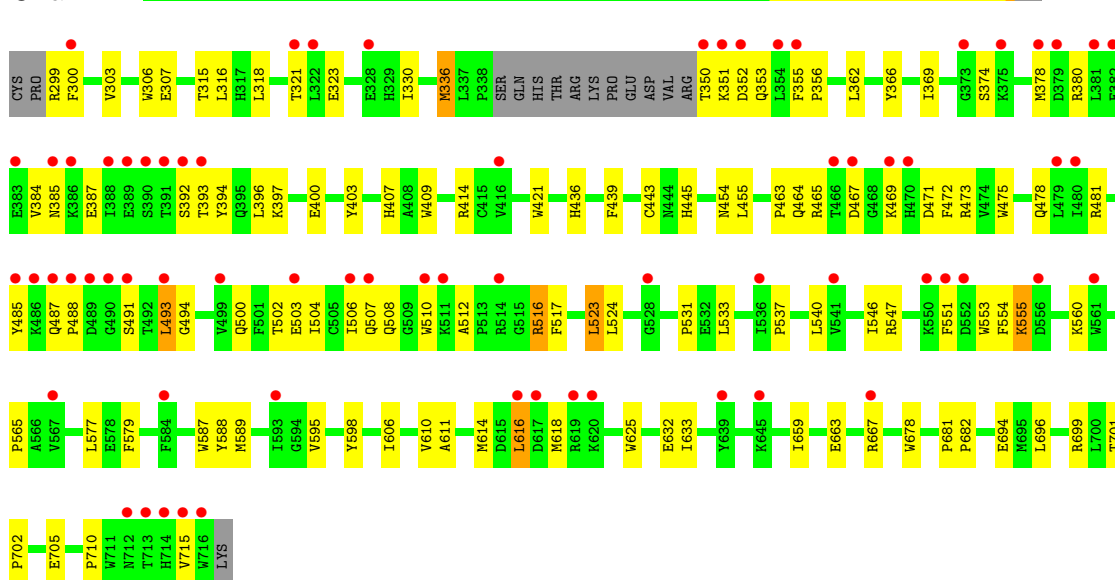
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	257	Total	O	0	0
			257	257		
8	B	304	Total	O	0	0
			304	304		

### 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.

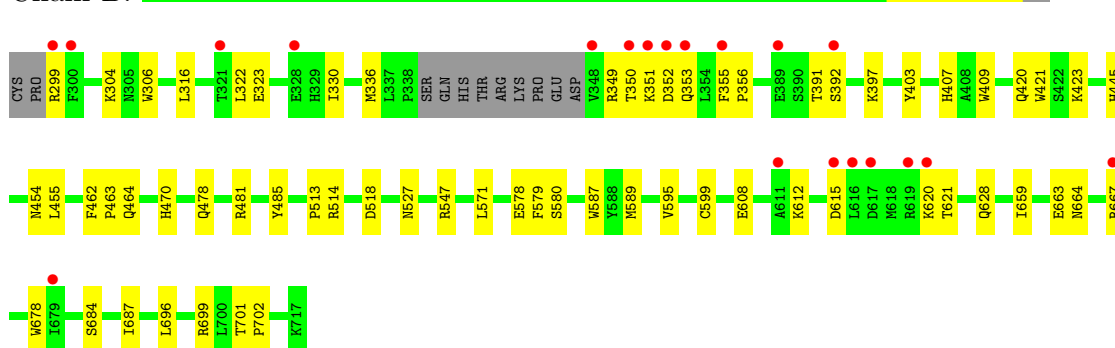
- Molecule 1: Nitric-oxide synthase, brain

Chain A:



- Molecule 1: Nitric-oxide synthase, brain

Chain B:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	52.09Å 110.91Å 165.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.06 – 1.95 39.05 – 1.95	Depositor EDS
% Data completeness (in resolution range)	91.2 (39.06-1.95) 91.4 (39.05-1.95)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.50 (at 1.95Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.216 , 0.251 0.214 , 0.245	Depositor DCC
$R_{free}$ test set	3221 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.7	Xtriage
Anisotropy	0.670	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 45.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 64184 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7408	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% of the height of the origin peak. No significant pseudotranslation is detected.*

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



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: D7P, H4B, ZN, MTL, ACT, HEM

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	0.48	0/3406	0.66	1/4621 (0.0%)
1	B	0.52	0/3434	0.68	1/4656 (0.0%)
All	All	0.50	0/6840	0.67	2/9277 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	589	MET	N-CA-C	-5.37	96.50	111.00
1	A	589	MET	N-CA-C	-5.13	97.14	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 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	3313	0	3221	99	0
1	B	3341	0	3256	50	0
2	B	12	0	14	0	0
3	A	4	0	3	1	0
3	B	4	0	3	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	1	0	0	0	0
5	A	43	0	30	1	0
5	B	43	0	30	1	0
6	A	17	0	15	1	0
6	B	17	0	15	1	0
7	A	26	0	24	0	0
7	B	26	0	24	0	0
8	A	257	0	0	10	0
8	B	304	0	0	8	0
All	All	7408	0	6635	143	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 11.

All (143) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:523:LEU:HD22	1:A:531:PRO:HB2	1.50	0.94
1:B:699:ARG:HG2	8:B:1175:HOH:O	1.73	0.88
1:A:396:LEU:CD2	1:A:577:LEU:HD12	2.10	0.81
1:A:611:ALA:HB1	1:A:616:LEU:HD11	1.65	0.77
1:A:595:VAL:HG11	1:A:682:PRO:HB2	1.67	0.76
1:A:667:ARG:HD3	8:A:1155:HOH:O	1.87	0.74
1:A:350:THR:HG22	1:A:352:ASP:H	1.52	0.74
1:B:350:THR:HG22	1:B:352:ASP:H	1.53	0.73
1:A:321:THR:HG21	8:A:1014:HOH:O	1.89	0.73
1:B:351:LYS:HE2	1:B:392:SER:OG	1.89	0.72
1:A:336:MET:HG3	1:B:306:TRP:NE1	2.05	0.71
1:A:502:THR:O	1:A:506:ILE:HG12	1.93	0.69
1:A:504:ILE:HA	1:A:507:GLN:HG2	1.76	0.67
1:A:350:THR:HB	1:A:353:GLN:HG3	1.77	0.67
1:A:306:TRP:NE1	1:B:336:MET:HG3	2.13	0.64
1:B:391:THR:O	1:B:392:SER:HB2	1.98	0.63
1:A:659:ILE:O	1:A:663:GLU:HG3	1.99	0.62
1:A:396:LEU:HD23	1:A:577:LEU:HD12	1.81	0.61
1:B:455:LEU:HD12	1:B:587:TRP:HB3	1.83	0.61
1:B:336:MET:HE3	8:B:878:HOH:O	2.00	0.61
1:B:664:ASN:O	1:B:667:ARG:HG2	2.00	0.61
1:B:323:GLU:O	1:B:699:ARG:HD3	2.01	0.60
1:A:396:LEU:HD21	1:A:577:LEU:HD12	1.84	0.59
1:A:478:GLN:HB2	1:A:481:ARG:HG3	1.85	0.58
1:A:350:THR:HB	1:A:353:GLN:CG	2.34	0.57
1:A:551:PHE:HB3	1:A:553:TRP:NE1	2.19	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:513:PRO:HG2	1:B:518:ASP:CG	2.23	0.57
1:A:350:THR:HG22	1:A:352:ASP:N	2.19	0.57
1:A:500:GLN:NE2	8:A:1116:HOH:O	2.38	0.56
1:B:659:ILE:O	1:B:663:GLU:HG3	2.05	0.56
1:A:374:SER:O	1:A:378:MET:HG2	2.06	0.56
1:A:467:ASP:OD1	1:A:469:LYS:HB2	2.06	0.55
1:A:611:ALA:CB	1:A:616:LEU:HD11	2.36	0.55
1:A:473:ARG:NH2	1:A:710:PRO:HD3	2.21	0.55
1:B:478:GLN:HB2	1:B:481:ARG:HG3	1.88	0.55
1:A:616:LEU:HD13	1:A:625:TRP:HB2	1.88	0.55
1:A:611:ALA:HB1	1:A:616:LEU:CD1	2.36	0.55
1:A:504:ILE:HA	1:A:507:GLN:CG	2.36	0.54
1:A:715:VAL:HG22	8:A:1142:HOH:O	2.08	0.53
1:A:299:ARG:HG3	1:A:318:LEU:HD21	1.90	0.53
1:A:436:HIS:HB2	8:A:994:HOH:O	2.08	0.53
1:A:351:LYS:HE2	1:A:392:SER:HA	1.90	0.53
1:A:560:LYS:NZ	8:A:1129:HOH:O	2.41	0.53
1:B:455:LEU:HD12	1:B:587:TRP:CB	2.39	0.53
3:A:860:ACT:H1	5:A:750:HEM:HMB2	1.90	0.52
1:B:684:SER:HB3	1:B:687:ILE:HD11	1.91	0.52
1:B:608:GLU:HG3	8:B:1052:HOH:O	2.09	0.52
1:A:551:PHE:HB3	1:A:553:TRP:CE2	2.45	0.52
1:A:396:LEU:HD12	1:A:400:GLU:HB3	1.92	0.52
1:A:614:MET:CE	1:A:632:GLU:HG3	2.41	0.51
1:A:614:MET:HE3	1:A:632:GLU:HG3	1.91	0.51
1:B:684:SER:HB3	1:B:687:ILE:CG1	2.41	0.51
1:A:351:LYS:HE2	1:A:392:SER:CB	2.41	0.50
1:A:464:GLN:HB3	1:A:579:PHE:CE2	2.47	0.50
1:A:565:PRO:HB3	1:A:588:TYR:CZ	2.47	0.50
1:A:504:ILE:O	1:A:508:GLN:HB2	2.11	0.50
1:A:475:TRP:HB2	1:A:523:LEU:HB3	1.93	0.50
1:A:715:VAL:HG23	1:A:715:VAL:O	2.12	0.49
1:A:516:ARG:HG2	1:A:517:PHE:CE1	2.48	0.49
1:B:571:LEU:HD11	1:B:578:GLU:HB3	1.95	0.49
1:A:439:PHE:CZ	1:A:443:CYS:SG	3.06	0.49
1:A:300:PHE:CD2	1:A:315:THR:HG22	2.48	0.49
1:A:696:LEU:HB3	1:B:330:ILE:HD11	1.93	0.49
1:A:504:ILE:CA	1:A:507:GLN:HG2	2.42	0.49
1:A:362:LEU:HD11	1:A:384:VAL:HG21	1.95	0.48
1:A:351:LYS:HE2	1:A:392:SER:CA	2.44	0.48
1:A:546:ILE:HG12	1:A:560:LYS:HA	1.95	0.48
1:B:355:PHE:N	1:B:356:PRO:HD2	2.27	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:523:LEU:HG	1:A:533:LEU:HD23	1.94	0.48
1:B:621:THR:HG22	8:B:1035:HOH:O	2.13	0.48
1:B:403:TYR:CE1	1:B:407:HIS:CE1	3.01	0.48
1:A:524:LEU:O	1:A:531:PRO:HA	2.14	0.48
1:B:350:THR:O	1:B:353:GLN:HG2	2.14	0.48
1:A:560:LYS:NZ	8:A:1128:HOH:O	2.47	0.47
1:A:307:GLU:HG3	8:B:965:HOH:O	2.14	0.47
1:A:506:ILE:HD11	1:A:512:ALA:HB2	1.96	0.47
1:A:503:GLU:O	1:A:507:GLN:HG2	2.14	0.47
1:B:595:VAL:O	1:B:599:CYS:HB2	2.14	0.47
1:A:491:SER:HB2	8:A:1045:HOH:O	2.14	0.47
1:A:465:ARG:NE	1:A:471:ASP:OD2	2.47	0.47
1:A:355:PHE:N	1:A:356:PRO:HD2	2.30	0.47
1:A:300:PHE:HD2	1:A:315:THR:HG22	1.80	0.47
1:A:523:LEU:HG	1:A:533:LEU:CD2	2.45	0.47
1:A:336:MET:HG3	1:B:306:TRP:CD1	2.50	0.47
1:B:612:LYS:O	1:B:615:ASP:N	2.42	0.46
1:B:684:SER:HB3	1:B:687:ILE:HG12	1.97	0.46
1:B:304:LYS:NZ	8:B:1072:HOH:O	2.46	0.46
1:A:387:GLU:OE2	1:A:394:TYR:HA	2.15	0.46
1:B:391:THR:O	1:B:392:SER:CB	2.63	0.46
1:A:555:LYS:HB3	1:A:555:LYS:HZ1	1.81	0.46
1:B:336:MET:HE1	1:B:678:TRP:CZ2	2.51	0.45
1:A:403:TYR:CE1	1:A:407:HIS:CE1	3.04	0.45
1:B:620:LYS:NZ	8:B:1163:HOH:O	2.48	0.45
1:A:523:LEU:CD2	1:A:531:PRO:HB2	2.33	0.45
1:A:350:THR:HB	1:A:353:GLN:OE1	2.16	0.45
1:B:409:TRP:CE3	1:B:421:TRP:HA	2.51	0.45
1:A:306:TRP:CD1	1:B:336:MET:HG3	2.52	0.45
1:A:366:TYR:HA	1:A:369:ILE:HG12	1.99	0.44
1:A:681:PRO:HA	1:A:682:PRO:HD3	1.77	0.44
1:A:350:THR:HG23	8:A:1078:HOH:O	2.17	0.44
1:A:330:ILE:HD11	1:B:696:LEU:HB3	1.98	0.44
1:A:396:LEU:HD12	1:A:400:GLU:CB	2.47	0.44
1:A:598:TYR:O	1:A:606:ILE:HG12	2.18	0.44
1:B:445:HIS:CD2	1:B:445:HIS:C	2.91	0.43
1:B:684:SER:HB3	1:B:687:ILE:CD1	2.48	0.43
1:B:420:GLN:HG2	3:B:861:ACT:H2	2.01	0.43
1:B:678:TRP:HA	6:B:761:H4B:N1	2.33	0.43
1:A:699:ARG:HH21	1:A:705:GLU:CD	2.22	0.43
1:A:618:MET:HA	1:A:625:TRP:CD1	2.54	0.43
1:A:299:ARG:HG3	1:A:318:LEU:CD2	2.48	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:455:LEU:HD12	1:A:587:TRP:HB3	2.00	0.43
1:A:493:LEU:HD23	1:A:494:GLY:N	2.33	0.43
1:B:485:TYR:CE1	1:B:514:ARG:HA	2.53	0.43
1:B:464:GLN:HB3	1:B:579:PHE:CE2	2.54	0.43
1:B:608:GLU:O	1:B:612:LYS:HG3	2.19	0.43
1:A:487:GLN:HB3	1:A:488:PRO:CD	2.49	0.43
1:A:487:GLN:HB3	1:A:488:PRO:HD2	2.01	0.42
1:A:610:VAL:HG21	1:A:633:ILE:HD11	2.02	0.42
1:B:701:THR:HA	1:B:702:PRO:C	2.40	0.42
1:A:409:TRP:CE3	1:A:421:TRP:HA	2.54	0.42
1:A:463:PRO:HB2	1:A:472:PHE:CE1	2.55	0.42
1:A:414:ARG:HD3	1:A:678:TRP:CD2	2.55	0.42
1:A:682:PRO:HG3	8:A:902:HOH:O	2.19	0.41
1:A:546:ILE:HG22	1:A:554:PHE:HE2	1.85	0.41
1:B:462:PHE:HB3	1:B:463:PRO:CD	2.50	0.41
1:B:322:LEU:HD13	1:B:699:ARG:NH2	2.36	0.41
1:B:571:LEU:HD13	1:B:580:SER:HA	2.03	0.41
1:A:393:THR:OG1	1:A:394:TYR:N	2.52	0.41
1:B:397:LYS:HD3	8:B:1043:HOH:O	2.19	0.41
1:A:537:PRO:HB2	1:A:540:LEU:HG	2.03	0.41
5:B:750:HEM:HBC2	5:B:750:HEM:CMC	2.50	0.41
1:A:510:TRP:HB2	1:A:533:LEU:HD13	2.02	0.41
1:B:351:LYS:HE2	1:B:392:SER:HG	1.84	0.41
1:A:323:GLU:O	1:A:699:ARG:HD3	2.21	0.41
1:A:678:TRP:HA	6:A:760:H4B:N1	2.35	0.41
1:A:523:LEU:HD22	1:A:531:PRO:CB	2.36	0.40
1:A:306:TRP:CE2	1:B:336:MET:HG3	2.55	0.40
1:A:701:THR:HA	1:A:702:PRO:C	2.42	0.40
1:A:380:ARG:NH1	1:A:397:LYS:HE2	2.37	0.40
1:B:470:HIS:HB3	1:B:527:ASN:ND2	2.37	0.40
1:A:445:HIS:C	1:A:445:HIS:CD2	2.95	0.40
1:A:632:GLU:OE2	1:B:628:GLN:NE2	2.53	0.40
1:A:303:VAL:CG1	1:A:694:GLU:O	2.70	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries

of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	403/421 (96%)	383 (95%)	20 (5%)	0	100	100
1	B	406/421 (96%)	394 (97%)	12 (3%)	0	100	100
All	All	809/842 (96%)	777 (96%)	32 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	363/377 (96%)	352 (97%)	11 (3%)	53	39
1	B	366/377 (97%)	360 (98%)	6 (2%)	75	69
All	All	729/754 (97%)	712 (98%)	17 (2%)	63	53

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	316	LEU
1	A	336	MET
1	A	385	ASN
1	A	454	ASN
1	A	485	TYR
1	A	493	LEU
1	A	516	ARG
1	A	523	LEU
1	A	547	ARG
1	A	555	LYS
1	A	616	LEU
1	B	299	ARG
1	B	316	LEU
1	B	349	ARG
1	B	423	LYS
1	B	454	ASN
1	B	547	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	385	ASN
1	A	454	ASN
1	A	500	GLN
1	A	697	ASN
1	A	712	ASN
1	B	364	GLN
1	B	454	ASN
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 10 ligands modelled in this entry, 1 is monoatomic - leaving 9 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	1.94	15 (30%)	46,82,82	1.75	8 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	H4B	A	760	-	18,18,18	1.76	3 (16%)	24,26,26	2.55	7 (29%)
7	D7P	A	797	-	23,26,26	1.14	1 (4%)	29,33,33	1.25	4 (13%)
3	ACT	A	860	-	1,3,3	2.34	1 (100%)	0,3,3	0.00	-
5	HEM	B	750	1	49,50,50	2.41	13 (26%)	46,82,82	1.64	9 (19%)
6	H4B	B	761	-	18,18,18	2.09	6 (33%)	24,26,26	2.56	9 (37%)
7	D7P	B	798	-	23,26,26	1.14	2 (8%)	29,33,33	1.35	4 (13%)
3	ACT	B	861	-	1,3,3	2.39	1 (100%)	0,3,3	0.00	-
2	MTL	B	871	-	11,11,11	1.00	0	14,14,14	0.86	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	D7P	A	797	-	-	0/23/27/27	0/1/1/1
3	ACT	A	860	-	-	0/0/0/0	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	D7P	B	798	-	-	0/23/27/27	0/1/1/1
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 (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	750	HEM	C2D-C1D	7.69	1.46	1.44
5	B	750	HEM	CHB-C1B	6.64	1.45	1.35
5	A	750	HEM	C3D-C4D	-5.82	1.43	1.44
6	B	761	H4B	C6-N5	5.13	1.56	1.46
5	B	750	HEM	C2B-C1B	4.74	1.45	1.44
5	B	750	HEM	C3C-C2C	-4.73	1.35	1.43
5	B	750	HEM	C3D-C4D	-4.69	1.43	1.44
5	A	750	HEM	C4A-C3A	4.15	1.45	1.40
5	B	750	HEM	C3B-C2B	-4.15	1.36	1.43
5	B	750	HEM	C3D-C2D	-3.92	1.36	1.43
6	B	761	H4B	C4-N3	3.92	1.43	1.37
6	A	760	H4B	C6-N5	3.81	1.54	1.46
6	A	760	H4B	C4-N3	3.74	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	750	HEM	CMD-C2D	3.64	1.58	1.47
5	A	750	HEM	CHA-C4D	3.62	1.41	1.35
5	A	750	HEM	C3C-C2C	-3.40	1.37	1.43
6	A	760	H4B	C4A-N5	3.24	1.49	1.38
5	A	750	HEM	C3B-C2B	-3.16	1.38	1.43
6	B	761	H4B	C4A-N5	3.13	1.48	1.38
5	B	750	HEM	CAA-C2A	3.13	1.57	1.52
5	A	750	HEM	CHD-C4C	3.01	1.41	1.36
5	A	750	HEM	C3D-C2D	-2.90	1.38	1.43
5	A	750	HEM	FE-NA	2.86	2.04	1.92
5	B	750	HEM	CMC-C2C	2.75	1.56	1.47
5	A	750	HEM	CMC-C2C	2.70	1.55	1.47
5	A	750	HEM	CMB-C2B	2.57	1.55	1.47
7	A	797	D7P	CA-N	2.49	1.51	1.45
5	A	750	HEM	C4A-NA	2.46	1.41	1.36
5	B	750	HEM	C3B-C4B	2.45	1.47	1.44
5	A	750	HEM	CMA-C3A	2.44	1.56	1.51
5	A	750	HEM	CMD-C2D	2.40	1.54	1.47
3	B	861	ACT	CH3-C	2.39	1.52	1.48
6	B	761	H4B	C8A-N1	2.37	1.39	1.34
5	B	750	HEM	FE-NA	2.36	2.02	1.92
3	A	860	ACT	CH3-C	2.34	1.52	1.48
6	B	761	H4B	C9-C10	2.30	1.57	1.52
5	A	750	HEM	CHC-C1C	2.19	1.40	1.36
5	B	750	HEM	C4C-NC	2.16	1.41	1.38
7	B	798	D7P	CD2-CG'	2.15	1.43	1.38
5	A	750	HEM	C1A-NA	2.15	1.40	1.36
7	B	798	D7P	CA-N	2.10	1.50	1.45
6	B	761	H4B	C7-N8	2.06	1.49	1.46

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	761	H4B	C4-C4A-C8A	8.39	122.34	114.56
6	A	760	H4B	C4-C4A-C8A	8.39	122.33	114.56
5	A	750	HEM	C3B-C4B-NB	-7.19	108.85	114.00
5	B	750	HEM	C3B-C4B-NB	-4.87	110.51	114.00
5	B	750	HEM	C3A-C4A-NA	4.55	112.85	109.41
5	A	750	HEM	CBD-CAD-C3D	-4.45	104.67	114.37
6	A	760	H4B	C2-N1-C8A	3.89	123.14	117.61
6	B	761	H4B	C4A-N5-C6	-3.88	110.61	121.16
5	A	750	HEM	CBA-CAA-C2A	-3.74	106.10	112.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	760	H4B	C4A-N5-C6	-3.64	111.25	121.16
5	B	750	HEM	C4A-NA-C1A	-3.37	102.32	106.76
7	B	798	D7P	CD-NE-CZ	3.31	129.84	124.03
6	B	761	H4B	C4-N3-C2	3.28	125.25	119.51
6	B	761	H4B	N3-C2-N1	-3.19	117.30	121.78
6	B	761	H4B	C2-N1-C8A	3.19	122.15	117.61
6	A	760	H4B	N3-C2-N1	-3.19	117.32	121.78
7	B	798	D7P	O-C-N1'	-3.11	117.76	123.03
5	A	750	HEM	C4A-NA-C1A	-2.96	102.87	106.76
7	A	797	D7P	O-C-N1'	-2.94	118.05	123.03
7	B	798	D7P	CB-CA-N	-2.92	105.28	110.83
7	A	797	D7P	CD-NE-CZ	2.87	129.06	124.03
6	A	760	H4B	C4-N3-C2	2.86	124.52	119.51
5	B	750	HEM	C4C-NC-C1C	-2.84	102.58	105.53
5	B	750	HEM	CMA-C3A-C4A	-2.82	124.29	128.62
6	A	760	H4B	N2-C2-N3	2.75	120.89	117.86
5	B	750	HEM	CBA-CAA-C2A	-2.72	107.90	112.69
5	B	750	HEM	CBD-CAD-C3D	-2.56	108.78	114.37
7	A	797	D7P	CB-CA-N	-2.52	106.03	110.83
6	B	761	H4B	O9-C9-C6	2.51	115.16	109.07
6	B	761	H4B	C4A-C8A-N8	2.50	122.66	119.23
5	B	750	HEM	C4A-CHB-C1B	-2.49	124.20	127.47
5	A	750	HEM	C2D-C1D-ND	-2.43	110.06	112.93
6	A	760	H4B	C4A-C8A-N8	2.40	122.52	119.23
5	A	750	HEM	C4C-NC-C1C	-2.35	103.09	105.53
5	A	750	HEM	C2A-C1A-NA	2.22	112.82	109.73
6	B	761	H4B	C8A-C4A-N5	2.20	121.51	118.50
5	B	750	HEM	CMA-C3A-C2A	2.17	129.03	124.94
7	A	797	D7P	CB'-CA'-C'	2.08	112.40	108.33
6	B	761	H4B	C4-C4A-N5	-2.03	116.15	119.10
7	B	798	D7P	CB'-CA'-C'	2.02	112.28	108.33
5	A	750	HEM	C3A-C4A-NA	2.01	110.93	109.41

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%)	1.07	69 (16%) 2 2	18, 38, 61, 75	0
1	B	410/421 (97%)	0.42	20 (4%) 28 35	18, 29, 51, 65	0
All	All	817/842 (97%)	0.74	89 (10%) 6 7	18, 32, 58, 75	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	355	PHE	7.1
1	A	715	VAL	5.8
1	B	300	PHE	5.7
1	A	716	TRP	5.4
1	A	470	HIS	5.4
1	A	491	SER	5.1
1	A	489	ASP	5.1
1	A	490	GLY	5.1
1	A	392	SER	5.0
1	A	488	PRO	4.8
1	A	351	LYS	4.8
1	A	390	SER	4.8
1	B	348	VAL	4.7
1	A	391	THR	4.7
1	B	350	THR	4.7
1	A	486	LYS	4.5
1	A	388	ILE	4.5
1	B	619	ARG	4.1
1	A	386	LYS	4.1
1	A	381	LEU	4.0
1	A	506	ILE	3.9
1	B	321	THR	3.9
1	A	389	GLU	3.8
1	A	385	ASN	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	373	GLY	3.7
1	A	352	ASP	3.6
1	A	469	LYS	3.5
1	A	487	GLN	3.4
1	A	499	VAL	3.4
1	B	667	ARG	3.4
1	A	300	PHE	3.3
1	A	551	PHE	3.3
1	B	620	LYS	3.2
1	B	299	ARG	3.2
1	A	393	THR	3.2
1	A	639	TYR	3.1
1	A	479	LEU	3.1
1	A	619	ARG	3.1
1	A	552	ASP	3.0
1	A	616	LEU	2.9
1	A	493	LEU	2.8
1	A	378	MET	2.8
1	A	375	LYS	2.7
1	B	351	LYS	2.7
1	A	354	LEU	2.7
1	A	507	GLN	2.7
1	A	713	THR	2.7
1	A	379	ASP	2.6
1	A	511	LYS	2.6
1	A	514	ARG	2.6
1	B	617	ASP	2.6
1	A	620	LYS	2.5
1	A	485	TYR	2.5
1	A	567	VAL	2.5
1	A	584	PHE	2.5
1	B	392	SER	2.5
1	A	528	GLY	2.5
1	A	561	TRP	2.4
1	A	321	THR	2.4
1	A	550	LYS	2.4
1	B	353	GLN	2.4
1	A	617	ASP	2.4
1	A	593	ILE	2.4
1	A	503	GLU	2.4
1	A	714	HIS	2.4
1	A	712	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	467	ASP	2.3
1	A	350	THR	2.2
1	A	480	ILE	2.2
1	A	382	GLU	2.2
1	B	352	ASP	2.2
1	A	328	GLU	2.2
1	B	389	GLU	2.2
1	A	322	LEU	2.2
1	A	536	ILE	2.2
1	A	556	ASP	2.2
1	A	645	LYS	2.2
1	B	355	PHE	2.2
1	A	667	ARG	2.2
1	B	616	LEU	2.2
1	B	615	ASP	2.2
1	A	466	THR	2.1
1	A	510	TRP	2.1
1	B	679	ILE	2.1
1	B	328	GLU	2.1
1	A	416	VAL	2.1
1	B	611	ALA	2.1
1	A	541	VAL	2.0
1	A	383	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( $\text{\AA}^2$ )	Q<0.9
7	D7P	B	798	26/26	0.20	2.31	30,32,35,35	0
7	D7P	A	797	26/26	0.23	1.92	31,35,39,40	0
2	MTL	B	871	12/12	0.13	1.12	29,32,34,34	0
6	H4B	A	760	17/17	0.17	1.04	19,21,24,24	0
6	H4B	B	761	17/17	0.15	0.51	16,18,21,21	0
3	ACT	A	860	4/4	0.13	0.46	54,54,54,54	0
5	HEM	A	750	43/43	0.17	0.29	19,20,21,22	0
5	HEM	B	750	43/43	0.13	0.15	17,18,21,21	0
3	ACT	B	861	4/4	0.10	-0.14	40,40,40,40	0
4	ZN	A	900	1/1	0.06	-2.35	31,31,31,31	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.