



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 02:48 PM GMT

PDB ID : 1ZZR  
Title : Rat nNOS D597N/M336V double mutant with L-N(omega)-Nitroarginine-(4 R)-amino-L-prolineamide bound  
Authors : Li, H.; Flinspach, M.L.; Igarashi, J.; Jamal, J.; Yang, W.; Gomez-Vidal, J.A.; Litzinger, E.A.; Silverman, R.B.; Poulos, T.L.  
Deposited on : 2005-06-14  
Resolution : 2.05 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>

---

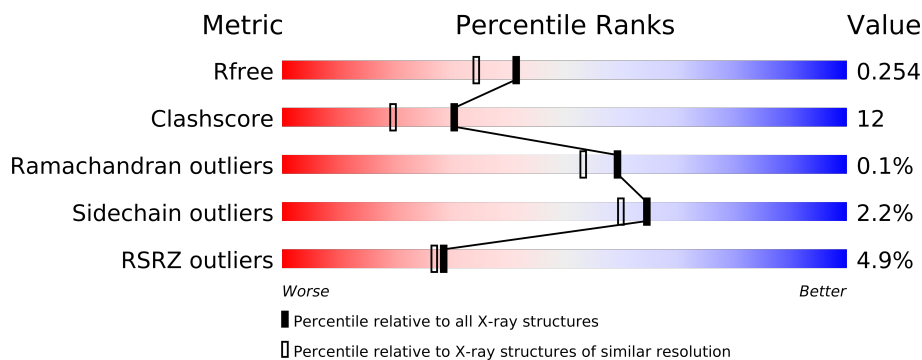
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.05 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	1380 (2.06-2.02)
Clashscore	79885	1577 (2.06-2.02)
Ramachandran outliers	78287	1565 (2.06-2.02)
Sidechain outliers	78261	1565 (2.06-2.02)
RSRZ outliers	66119	1381 (2.06-2.02)

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	420	
1	B	420	

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

Mol	Type	Chain	Res	Geometry	Electron density
5	DP9	A	799	-	X
5	DP9	B	800	-	X
6	TFA	A	865	-	X
6	TFA	B	866	-	X
7	GOL	A	880	-	X
7	GOL	B	881	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 7256 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
			3312	2121	567	604	20			
1	B	411	Total	C	N	O	S	0	0	0
			3344	2140	575	609	20			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	336	VAL	MET	ENGINEERED	UNP P29476
A	597	ASN	ASP	ENGINEERED	UNP P29476
B	336	VAL	MET	ENGINEERED	UNP P29476
B	597	ASN	ASP	ENGINEERED	UNP P29476

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

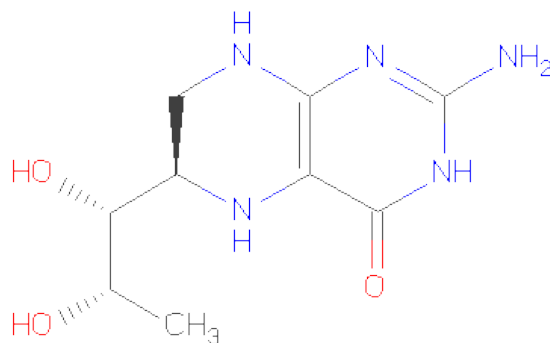
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 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
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 4 is 5,6,7,8-TETRAHYDROBIOPTERIN (three-letter code: H4B) (formula:  $C_9H_{15}N_5O_3$ ).



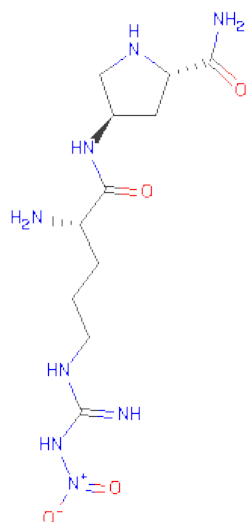
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			17	9	5	3		

*Continued on next page...*

*Continued from previous page...*

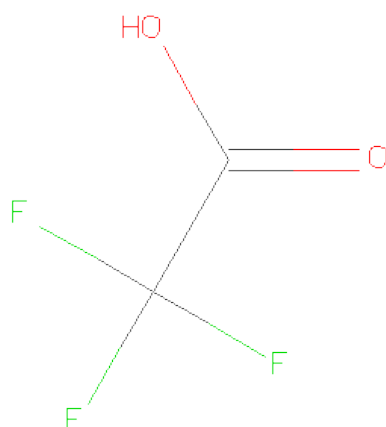
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 5 is L-N(OMEGA)-NITROARGININE-(4R)-AMINO-L-PROLINEAMIDE (three-letter code: DP9) (formula: C<sub>11</sub>H<sub>22</sub>N<sub>8</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			23	11	8	4		
5	B	1	Total	C	N	O	0	0
			23	11	8	4		

- Molecule 6 is TRIFLUOROACETIC ACID (three-letter code: TFA) (formula: C<sub>2</sub>HF<sub>3</sub>O<sub>2</sub>).



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

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

- Molecule 8 is water.

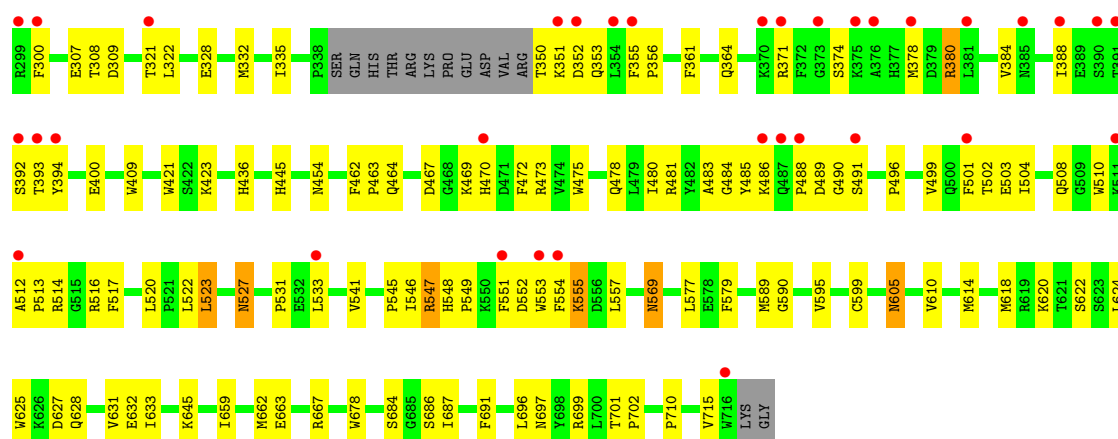
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	162	Total 162	O 162	0	0
8	B	245	Total 245	O 245	0	0

### 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.

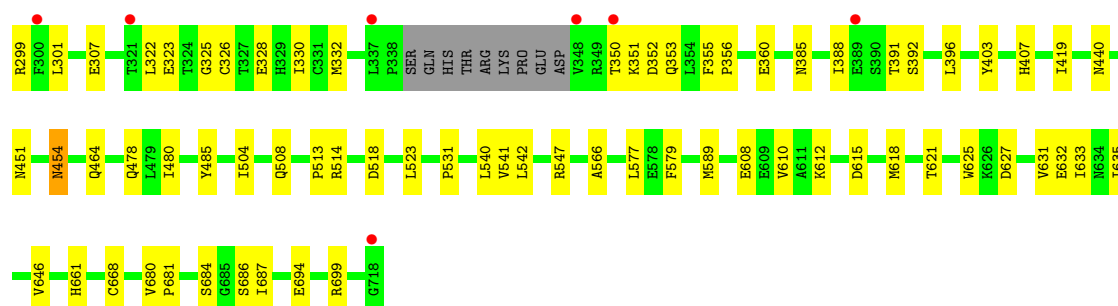
- Molecule 1: Nitric-oxide synthase, brain

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, $\alpha$ , $\beta$ , $\gamma$	52.43Å 111.95Å 164.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.32 – 2.05 49.32 – 2.05	Depositor EDS
% Data completeness (in resolution range)	98.8 (49.32-2.05) 98.9 (49.32-2.05)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.47 (at 2.05Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.227 , 0.260 0.224 , 0.254	Depositor DCC
$R_{free}$ test set	3036 reflections (5.25%)	DCC
Wilson B-factor (Å <sup>2</sup> )	30.3	Xtriage
Anisotropy	0.822	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 45.2	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	3 of 60889 reflections (0.005%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7256	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.33% 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: GOL, ZN, H4B, TFA, DP9, 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	0.43	0/3405	0.64	1/4621 (0.0%)
1	B	0.46	0/3437	0.67	2/4661 (0.0%)
All	All	0.44	0/6842	0.66	3/9282 (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	326	CYS	CA-CB-SG	8.30	128.93	114.00
1	A	589	MET	N-CA-C	-6.22	94.22	111.00
1	B	589	MET	N-CA-C	-5.93	94.98	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	3312	0	3223	115	0
1	B	3344	0	3261	48	0
2	A	1	0	0	0	0
3	A	43	0	30	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	43	0	30	2	0
4	A	17	0	15	1	0
4	B	17	0	15	0	0
5	A	23	0	21	0	0
5	B	23	0	21	0	0
6	A	7	0	0	0	0
6	B	7	0	0	0	0
7	A	6	0	8	0	0
7	B	6	0	8	0	0
8	A	162	0	0	10	0
8	B	245	0	0	4	0
All	All	7256	0	6632	160	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 12.

All (160) 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	1.28	1.14
1:A:523:LEU:CD2	1:A:531:PRO:HB2	2.14	0.75
3:A:750:HEM:HMC2	3:A:750:HEM:HBC2	1.70	0.72
1:A:699:ARG:HD2	8:A:1050:HOH:O	1.90	0.72
1:A:350:THR:HB	1:A:353:GLN:HG3	1.71	0.72
1:A:473:ARG:NH2	1:A:710:PRO:HD3	2.06	0.71
1:A:371:ARG:HG3	1:A:371:ARG:HH21	1.56	0.71
1:A:350:THR:HG22	1:A:352:ASP:H	1.58	0.69
1:A:475:TRP:HB2	1:A:523:LEU:HB3	1.76	0.67
1:A:551:PHE:HB3	1:A:553:TRP:NE1	2.10	0.67
1:A:620:LYS:HE3	1:A:622:SER:OG	1.95	0.66
1:A:322:LEU:HD13	1:A:699:ARG:NH2	2.11	0.66
1:A:436:HIS:HB2	8:A:995:HOH:O	1.96	0.65
1:A:684:SER:HB3	1:A:687:ILE:HD11	1.78	0.65
1:A:478:GLN:HB2	1:A:481:ARG:HG3	1.80	0.64
8:A:979:HOH:O	1:B:307:GLU:HG3	1.98	0.64
1:B:325:GLY:O	1:B:332:MET:HG3	1.98	0.63
1:B:350:THR:HG22	1:B:352:ASP:H	1.64	0.63
1:A:350:THR:HB	1:A:353:GLN:CG	2.30	0.62
1:B:504:ILE:O	1:B:508:GLN:HG2	2.00	0.61
1:A:374:SER:O	1:A:378:MET:HG2	2.00	0.61
1:B:323:GLU:O	1:B:699:ARG:HD3	2.01	0.60
1:A:555:LYS:HB3	1:A:555:LYS:NZ	2.15	0.60
1:A:332:MET:HE1	1:B:301:LEU:HD22	1.86	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:684:SER:HB3	1:A:687:ILE:CD1	2.34	0.57
1:A:350:THR:HB	1:A:353:GLN:CD	2.26	0.57
1:A:496:PRO:HA	1:A:499:VAL:HG23	1.87	0.57
1:B:356:PRO:O	1:B:360:GLU:HG3	2.04	0.57
1:B:621:THR:HG22	8:B:1025:HOH:O	2.06	0.56
1:A:523:LEU:HD22	1:A:531:PRO:CB	2.20	0.56
1:B:388:ILE:O	1:B:392:SER:N	2.36	0.56
1:A:610:VAL:O	1:A:614:MET:HG3	2.06	0.56
1:A:545:PRO:HG2	1:A:547:ARG:NH2	2.21	0.55
1:A:322:LEU:HB2	1:A:699:ARG:HB2	1.87	0.55
1:A:684:SER:HB3	1:A:687:ILE:CG1	2.36	0.55
1:A:322:LEU:HB2	1:A:699:ARG:HE	1.72	0.55
1:A:351:LYS:HE2	1:A:392:SER:CB	2.38	0.54
1:A:351:LYS:HE2	1:A:392:SER:HB3	1.91	0.53
1:B:299:ARG:HD2	8:B:1076:HOH:O	2.08	0.53
1:B:391:THR:O	1:B:392:SER:HB2	2.09	0.53
1:A:322:LEU:CB	1:A:699:ARG:HE	2.23	0.52
1:A:462:PHE:HB3	1:A:463:PRO:CD	2.39	0.52
1:B:322:LEU:HD13	1:B:699:ARG:NH2	2.25	0.52
1:A:488:PRO:HD2	8:A:972:HOH:O	2.10	0.52
1:B:328:GLU:OE1	1:B:328:GLU:N	2.43	0.52
1:A:355:PHE:N	1:A:356:PRO:HD2	2.25	0.52
1:A:485:TYR:CE1	1:A:514:ARG:HA	2.45	0.51
1:A:551:PHE:HB3	1:A:553:TRP:CE2	2.46	0.51
1:A:684:SER:HB3	1:A:687:ILE:HG12	1.92	0.51
1:A:322:LEU:HB3	1:A:699:ARG:HH21	1.75	0.51
1:A:361:PHE:O	1:A:364:GLN:HG2	2.10	0.51
1:A:380:ARG:O	1:A:384:VAL:HG23	2.11	0.51
1:A:464:GLN:HB3	1:A:579:PHE:CE2	2.46	0.50
1:A:475:TRP:CE3	1:A:523:LEU:HD13	2.47	0.50
1:B:440:ASN:ND2	8:B:1091:HOH:O	2.39	0.50
1:A:480:ILE:HD13	1:A:541:VAL:HG13	1.93	0.50
1:A:510:TRP:HB2	1:A:533:LEU:CD1	2.41	0.50
1:A:307:GLU:HG3	8:B:939:HOH:O	2.11	0.50
1:A:659:ILE:O	1:A:663:GLU:HG3	2.12	0.50
1:B:355:PHE:CE1	1:B:385:ASN:HB2	2.47	0.50
1:A:551:PHE:HE1	1:A:614:MET:HE3	1.77	0.49
1:B:351:LYS:HE2	1:B:392:SER:HA	1.94	0.49
1:A:470:HIS:HB3	1:A:527:ASN:ND2	2.26	0.49
1:A:627:ASP:O	1:A:631:VAL:HG23	2.12	0.49
1:A:516:ARG:HD3	1:A:517:PHE:HE1	1.78	0.49
1:B:513:PRO:HG2	1:B:518:ASP:CG	2.33	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:516:ARG:HD3	1:A:517:PHE:CE1	2.48	0.48
1:B:684:SER:HB3	1:B:687:ILE:HD11	1.95	0.48
1:B:403:TYR:CE1	1:B:407:HIS:CE1	3.01	0.48
1:A:371:ARG:HG3	1:A:371:ARG:NH2	2.27	0.48
1:A:380:ARG:HD3	1:A:400:GLU:OE1	2.13	0.48
1:A:489:ASP:O	1:A:489:ASP:OD2	2.31	0.48
1:A:467:ASP:C	1:A:469:LYS:H	2.17	0.48
1:A:504:ILE:O	1:A:508:GLN:HG2	2.13	0.47
1:A:715:VAL:O	1:A:715:VAL:HG23	2.14	0.47
1:B:542:LEU:HD21	1:B:646:VAL:HG22	1.95	0.47
1:A:555:LYS:HZ3	1:A:555:LYS:HB3	1.78	0.47
1:A:569:ASN:H	1:A:569:ASN:HD22	1.61	0.47
1:A:522:LEU:O	1:A:533:LEU:HA	2.15	0.47
1:A:351:LYS:HE2	1:A:392:SER:CA	2.45	0.47
1:B:322:LEU:HB3	1:B:699:ARG:CZ	2.44	0.47
1:B:485:TYR:CE1	1:B:514:ARG:HA	2.50	0.47
1:A:321:THR:HG23	1:A:322:LEU:HG	1.96	0.47
1:A:696:LEU:HD22	1:B:330:ILE:HD11	1.97	0.47
1:B:322:LEU:HB2	1:B:699:ARG:HB2	1.97	0.46
1:A:499:VAL:O	1:A:503:GLU:HG3	2.15	0.46
1:A:483:ALA:HB3	8:A:1041:HOH:O	2.14	0.46
1:A:548:HIS:ND1	1:A:549:PRO:HD2	2.30	0.46
3:B:750:HEM:HMC1	3:B:750:HEM:HBC2	1.98	0.46
1:A:546:ILE:HG22	1:A:554:PHE:HE2	1.81	0.46
1:A:483:ALA:HB1	1:A:502:THR:CG2	2.45	0.46
1:A:701:THR:HA	1:A:702:PRO:C	2.36	0.46
1:A:484:GLY:O	1:A:499:VAL:HA	2.16	0.46
1:A:514:ARG:HG3	1:A:514:ARG:HH21	1.80	0.46
1:B:478:GLN:HA	1:B:566:ALA:O	2.16	0.46
1:A:322:LEU:HD13	1:A:699:ARG:HH21	1.81	0.45
1:A:595:VAL:O	1:A:599:CYS:HB2	2.16	0.45
1:A:485:TYR:CE2	1:A:512:ALA:HB1	2.50	0.45
1:B:322:LEU:HD13	1:B:699:ARG:HH21	1.81	0.45
1:A:351:LYS:HE2	1:A:392:SER:HA	1.97	0.45
1:A:686:SER:HA	1:A:691:PHE:CG	2.51	0.45
1:A:464:GLN:NE2	1:A:577:LEU:HD22	2.31	0.45
1:A:614:MET:CE	1:A:632:GLU:HG3	2.47	0.45
1:B:627:ASP:O	1:B:631:VAL:HG23	2.17	0.45
1:B:355:PHE:N	1:B:356:PRO:HD2	2.32	0.45
3:B:750:HEM:HBC2	3:B:750:HEM:CMC	2.47	0.45
1:B:618:MET:HG2	1:B:625:TRP:CD2	2.52	0.45
1:A:388:ILE:O	1:A:392:SER:N	2.50	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:512:ALA:HA	1:A:513:PRO:HD3	1.82	0.44
1:B:610:VAL:HG21	1:B:633:ILE:HD11	1.98	0.44
1:B:523:LEU:HG	1:B:531:PRO:HB2	1.99	0.44
1:A:463:PRO:HB2	1:A:472:PHE:CE1	2.52	0.44
1:A:618:MET:HG2	1:A:625:TRP:CD2	2.53	0.43
1:B:480:ILE:HD13	1:B:541:VAL:HG13	1.99	0.43
1:A:610:VAL:HG21	1:A:633:ILE:HD11	2.00	0.43
1:A:478:GLN:HB2	1:A:481:ARG:CG	2.48	0.43
1:A:308:THR:O	1:A:309:ASP:HB2	2.19	0.43
1:B:350:THR:HG22	1:B:351:LYS:N	2.34	0.43
1:A:569:ASN:N	1:A:569:ASN:HD22	2.15	0.43
1:A:328:GLU:H	1:A:328:GLU:CD	2.21	0.43
1:A:551:PHE:CD2	1:A:551:PHE:N	2.86	0.43
1:A:335:ILE:HD13	1:B:694:GLU:HB3	1.99	0.43
1:A:501:PHE:CD2	1:A:520:LEU:HD13	2.54	0.43
1:A:501:PHE:HD2	1:A:520:LEU:HD13	1.84	0.43
1:A:552:ASP:O	1:A:555:LYS:HG2	2.19	0.43
1:A:684:SER:O	1:A:687:ILE:HG12	2.19	0.42
1:B:684:SER:HB3	1:B:687:ILE:CG1	2.49	0.42
1:B:485:TYR:CZ	1:B:514:ARG:HA	2.54	0.42
1:A:678:TRP:HA	4:A:760:H4B:N1	2.34	0.42
1:A:321:THR:HG23	1:A:322:LEU:N	2.35	0.42
1:A:701:THR:HB	8:A:980:HOH:O	2.18	0.42
1:B:513:PRO:HG2	1:B:518:ASP:OD2	2.19	0.42
1:A:595:VAL:CG1	1:B:686:SER:OG	2.68	0.42
1:A:393:THR:OG1	1:A:394:TYR:N	2.52	0.42
1:A:523:LEU:HG	1:A:533:LEU:CD2	2.49	0.42
1:B:391:THR:O	1:B:392:SER:CB	2.67	0.42
1:A:554:PHE:HB3	8:A:1056:HOH:O	2.19	0.42
1:A:624:LEU:HD12	1:B:635:ILE:HG13	2.00	0.42
1:B:396:LEU:HG	1:B:577:LEU:HD12	2.02	0.42
1:A:553:TRP:HZ3	1:A:557:LEU:HD11	1.85	0.42
1:B:451:ASN:HB3	1:B:454:ASN:O	2.18	0.42
1:A:545:PRO:HG2	1:A:547:ARG:HH21	1.85	0.41
1:A:590:GLY:HA3	8:A:962:HOH:O	2.19	0.41
1:B:419:ILE:HG13	1:B:661:HIS:HB2	2.02	0.41
1:B:608:GLU:O	1:B:612:LYS:HG3	2.21	0.41
1:A:489:ASP:C	1:A:491:SER:H	2.23	0.41
1:B:464:GLN:HB3	1:B:579:PHE:CE2	2.56	0.41
1:A:605:ASN:ND2	8:A:1058:HOH:O	2.41	0.41
1:A:686:SER:HA	1:A:691:PHE:CB	2.50	0.41
1:B:612:LYS:O	1:B:615:ASP:N	2.48	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:680:VAL:HA	1:B:681:PRO:HD3	1.91	0.41
1:A:423:LYS:NZ	8:A:1014:HOH:O	2.53	0.41
1:A:488:PRO:C	1:A:490:GLY:H	2.24	0.41
1:A:628:GLN:NE2	1:B:632:GLU:OE2	2.54	0.41
1:A:445:HIS:CD2	1:A:445:HIS:C	2.94	0.41
1:A:332:MET:HB3	1:A:335:ILE:HG13	2.03	0.40
1:A:486:LYS:HE2	1:A:499:VAL:HG11	2.03	0.40
1:A:300:PHE:N	1:A:300:PHE:CD1	2.89	0.40
1:A:569:ASN:H	1:A:569:ASN:ND2	2.19	0.40
1:A:409:TRP:CE3	1:A:421:TRP:HA	2.56	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	403/420 (96%)	375 (93%)	27 (7%)	1 (0%)	56	47
1	B	407/420 (97%)	391 (96%)	16 (4%)	0	100	100
All	All	810/840 (96%)	766 (95%)	43 (5%)	1 (0%)	59	53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	605	ASN

### 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	363/375 (97%)	352 (97%)	11 (3%)	53	46
1	B	366/375 (98%)	361 (99%)	5 (1%)	78	77
All	All	729/750 (97%)	713 (98%)	16 (2%)	64	60

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	380	ARG
1	A	454	ASN
1	A	523	LEU
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	A	667	ARG
1	A	697	ASN
1	B	353	GLN
1	B	454	ASN
1	B	540	LEU
1	B	547	ARG
1	B	668	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	364	GLN
1	A	454	ASN
1	A	507	GLN
1	A	527	ASN
1	A	569	ASN
1	A	605	ASN
1	A	642	GLN
1	A	697	ASN
1	A	712	ASN
1	B	364	GLN
1	B	385	ASN
1	B	454	ASN
1	B	527	ASN
1	B	535	GLN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	B	601	ASN
1	B	605	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
3	HEM	A	750	1	49,50,50	2.37	15 (30%)	46,82,82	1.52	6 (13%)
4	H4B	A	760	-	18,18,18	1.50	3 (16%)	24,26,26	2.51	7 (29%)
5	DP9	A	799	-	22,23,23	2.40	3 (13%)	26,30,30	1.75	4 (15%)
6	TFA	A	865	-	6,6,6	1.24	1 (16%)	9,9,9	0.65	0
7	GOL	A	880	-	5,5,5	0.23	0	5,5,5	0.33	0
3	HEM	B	750	1	49,50,50	2.17	14 (28%)	46,82,82	1.70	8 (17%)
4	H4B	B	761	-	18,18,18	1.74	5 (27%)	24,26,26	2.67	11 (45%)
5	DP9	B	800	-	22,23,23	2.13	2 (9%)	26,30,30	1.78	5 (19%)
6	TFA	B	866	-	6,6,6	1.91	1 (16%)	9,9,9	1.13	1 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	GOL	B	881	-	5,5,5	0.21	0	5,5,5	0.36	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
3	HEM	A	750	1	-	0/14/114/114	0/0/8/8
4	H4B	A	760	-	-	0/8/17/17	0/0/2/2
5	DP9	A	799	-	-	0/20/32/32	0/1/1/1
6	TFA	A	865	-	-	0/6/6/6	0/0/0/0
7	GOL	A	880	-	-	0/4/4/4	0/0/0/0
3	HEM	B	750	1	-	0/14/114/114	0/0/8/8
4	H4B	B	761	-	-	0/8/17/17	0/0/2/2
5	DP9	B	800	-	-	0/20/32/32	0/1/1/1
6	TFA	B	866	-	-	0/6/6/6	0/0/0/0
7	GOL	B	881	-	-	0/4/4/4	0/0/0/0

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	799	DP9	O2-NO	10.38	1.29	1.22
3	A	750	HEM	C2B-C1B	9.33	1.46	1.44
5	B	800	DP9	O2-NO	9.01	1.28	1.22
3	B	750	HEM	C3D-C4D	-7.94	1.42	1.44
3	B	750	HEM	C3C-C2C	-4.78	1.35	1.43
3	A	750	HEM	C3B-C2B	-4.66	1.35	1.43
3	A	750	HEM	CHA-C4D	4.57	1.42	1.35
3	B	750	HEM	CHD-C4C	4.29	1.44	1.36
3	B	750	HEM	C3B-C4B	4.01	1.49	1.44
3	A	750	HEM	C3D-C4D	-3.97	1.43	1.44
3	A	750	HEM	C4A-C3A	3.86	1.45	1.40
4	B	761	H4B	C6-N5	3.78	1.53	1.46
6	B	866	TFA	C2-C1	-3.77	1.36	1.52
3	B	750	HEM	C3B-C2B	-3.46	1.37	1.43
4	A	760	H4B	C6-N5	3.42	1.53	1.46
3	B	750	HEM	C2B-C1B	3.32	1.45	1.44
4	B	761	H4B	C2-N1	3.16	1.37	1.33
3	B	750	HEM	CHC-C1C	3.15	1.42	1.36
5	B	800	DP9	CG'-N2'	3.06	1.52	1.46
3	A	750	HEM	CMB-C2B	3.06	1.56	1.47

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	750	HEM	CMD-C2D	3.02	1.56	1.47
3	A	750	HEM	C3B-C4B	3.00	1.48	1.44
3	A	750	HEM	C3C-C2C	-3.00	1.38	1.43
3	B	750	HEM	CMC-C2C	2.98	1.56	1.47
4	B	761	H4B	C4-N3	2.98	1.42	1.37
4	A	760	H4B	C4-N3	2.91	1.42	1.37
5	A	799	DP9	CG'-N2'	2.89	1.52	1.46
3	B	750	HEM	CMB-C2B	2.87	1.56	1.47
3	B	750	HEM	CHB-C1B	2.85	1.39	1.35
3	A	750	HEM	CHD-C4C	2.82	1.41	1.36
3	A	750	HEM	C3D-C2D	-2.81	1.38	1.43
6	A	865	TFA	C2-C1	-2.81	1.40	1.52
4	A	760	H4B	C4A-N5	2.74	1.47	1.38
3	A	750	HEM	FE-NA	2.71	2.04	1.92
3	A	750	HEM	CMC-C2C	2.60	1.55	1.47
3	B	750	HEM	C3D-C2D	-2.59	1.39	1.43
4	B	761	H4B	C7-C6	2.55	1.55	1.52
3	A	750	HEM	C4A-NA	2.49	1.41	1.36
4	B	761	H4B	C4A-N5	2.41	1.46	1.38
3	A	750	HEM	CHC-C1C	2.31	1.40	1.36
3	B	750	HEM	CMD-C2D	2.28	1.54	1.47
3	B	750	HEM	C4A-C3A	2.25	1.43	1.40
3	B	750	HEM	C1A-NA	2.22	1.40	1.36
5	A	799	DP9	CD'-CG'	2.05	1.56	1.53

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	761	H4B	C4-C4A-C8A	9.32	123.19	114.56
4	A	760	H4B	C4-C4A-C8A	8.46	122.39	114.56
3	B	750	HEM	C3B-C4B-NB	-5.23	110.26	114.00
3	A	750	HEM	CBA-CAA-C2A	-4.58	104.62	112.69
5	A	799	DP9	CD-NE-CZ	4.38	131.72	124.03
5	B	800	DP9	CD-NE-CZ	4.27	131.54	124.03
3	B	750	HEM	CBD-CAD-C3D	-4.17	105.28	114.37
3	A	750	HEM	CBD-CAD-C3D	-3.90	105.85	114.37
3	B	750	HEM	C1A-CHA-C4D	-3.89	122.35	127.47
3	A	750	HEM	C3B-C4B-NB	-3.82	111.27	114.00
5	A	799	DP9	O'-C'-N1'	-3.76	116.67	123.03
5	B	800	DP9	C'-CA'-N'	-3.74	104.70	111.72
4	A	760	H4B	C2-N1-C8A	3.68	122.84	117.61
5	B	800	DP9	O'-C'-N1'	-3.51	117.08	123.03

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	761	H4B	C4A-N5-C6	-3.31	112.15	121.16
4	A	760	H4B	C4-N3-C2	3.18	125.07	119.51
3	B	750	HEM	C4A-CHB-C1B	-3.17	123.29	127.47
5	A	799	DP9	C'-CA'-N'	-3.17	105.77	111.72
3	B	750	HEM	C3A-C4A-NA	3.14	111.78	109.41
4	A	760	H4B	C4A-N5-C6	-3.01	112.96	121.16
4	B	761	H4B	C2-N1-C8A	2.99	121.86	117.61
4	B	761	H4B	C4-N3-C2	2.99	124.74	119.51
3	B	750	HEM	CBA-CAA-C2A	-2.93	107.53	112.69
4	A	760	H4B	N3-C2-N1	-2.83	117.81	121.78
4	A	760	H4B	C4A-C8A-N8	2.74	122.98	119.23
6	B	866	TFA	F1-C2-C1	-2.73	101.43	111.79
4	B	761	H4B	C4A-C8A-N8	2.64	122.85	119.23
4	B	761	H4B	O9-C9-C6	2.63	115.45	109.07
3	B	750	HEM	C4C-NC-C1C	-2.59	102.84	105.53
4	B	761	H4B	C4-C4A-N5	-2.53	115.42	119.10
3	A	750	HEM	C4A-CHB-C1B	-2.41	124.30	127.47
4	A	760	H4B	O9-C9-C6	2.41	114.90	109.07
3	B	750	HEM	C4A-NA-C1A	-2.41	103.59	106.76
4	B	761	H4B	N8-C8A-N1	2.35	119.26	115.82
4	B	761	H4B	N3-C2-N1	-2.33	118.51	121.78
3	A	750	HEM	CHC-C4B-NB	-2.32	122.65	124.58
5	B	800	DP9	CA'-C'-N1'	2.27	121.18	116.78
4	B	761	H4B	C4A-C8A-N1	-2.26	117.89	121.50
3	A	750	HEM	C4A-NA-C1A	-2.16	103.92	106.76
4	B	761	H4B	C8A-C4A-N5	2.11	121.39	118.50
5	A	799	DP9	CA'-C'-N1'	2.10	120.85	116.78
5	B	800	DP9	CD'-N'-CA'	2.04	112.88	107.31

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	407/420 (96%)	0.55	34 (8%) 11 10	22, 45, 75, 86	0
1	B	411/420 (97%)	0.13	7 (1%) 67 69	21, 35, 59, 83	0
All	All	818/840 (97%)	0.34	41 (5%) 28 26	21, 39, 71, 86	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	348	VAL	5.6
1	A	355	PHE	4.5
1	B	321	THR	4.3
1	B	300	PHE	3.8
1	A	352	ASP	3.4
1	A	554	PHE	3.4
1	A	321	THR	3.2
1	A	488	PRO	3.1
1	B	718	GLY	3.1
1	A	300	PHE	3.1
1	A	393	THR	3.1
1	A	388	ILE	3.0
1	A	391	THR	3.0
1	A	511	LYS	3.0
1	A	551	PHE	2.9
1	A	553	TRP	2.9
1	B	350	THR	2.9
1	A	373	GLY	2.8
1	B	337	LEU	2.7
1	A	716	TRP	2.6
1	A	392	SER	2.6
1	A	512	ALA	2.6
1	A	533	LEU	2.6
1	A	375	LYS	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	381	LEU	2.6
1	A	486	LYS	2.5
1	A	371	ARG	2.5
1	A	354	LEU	2.4
1	A	351	LYS	2.3
1	A	390	SER	2.2
1	A	299	ARG	2.2
1	A	487	GLN	2.2
1	A	370	LYS	2.2
1	A	501	PHE	2.1
1	A	376	ALA	2.1
1	A	378	MET	2.1
1	A	491	SER	2.1
1	B	389	GLU	2.0
1	A	394	TYR	2.0
1	A	385	ASN	2.0
1	A	470	HIS	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
7	GOL	B	881	6/6	0.25	16.13	55,59,59,60	0
6	TFA	B	866	7/7	0.26	8.80	42,45,48,48	0
6	TFA	A	865	7/7	0.20	4.54	47,48,49,49	0
7	GOL	A	880	6/6	0.15	4.05	49,49,51,52	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	DP9	B	800	23/23	0.16	2.79	29,40,50,52	0
5	DP9	A	799	23/23	0.17	2.48	31,44,52,55	0
3	HEM	B	750	43/43	0.13	0.27	22,26,29,31	0
4	H4B	B	761	17/17	0.12	-0.02	20,23,27,29	0
2	ZN	A	900	1/1	0.11	-0.17	32,32,32,32	0
3	HEM	A	750	43/43	0.11	-0.35	25,28,30,32	0
4	H4B	A	760	17/17	0.10	-1.42	26,29,30,32	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.