Full wwPDB X-ray Structure Validation Report (i)

Oct 2, 2017 – 09:13 AM EDT

PDB ID	:	1QWC
Title	:	Rat neuronal nitric oxide synthase oxygenase domain in complex with W1400 inhibitor.
Authors	:	Fedorov, R.; Hartmann, E.; Ghosh, D.K.; Schlichting, I.
Deposited on	:	unknown
Resolution	:	2.30 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20030345

1 Overall quality at a glance (i)

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	Percentile Ranks	Value
Rfree		0.232
Clashscore		24
Ramachandran outliers		1.9%
Sidechain outliers		8.0%
RSRZ outliers		6.7%

Worse　　　　　　　　　　　　　　　　　　*Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
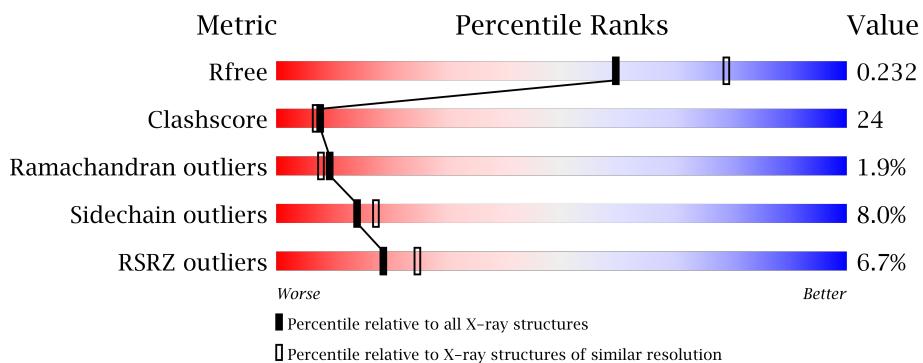
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	100719	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

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 >=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 <=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	420	7% ■ 59% 35% 6% ·
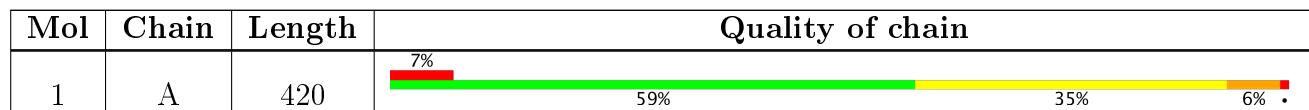
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	14W	A	902	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 3698 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
			Total	C	N	O	S			
1	A	420	3418	2183	589	625	21	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	297	GLY	-	CLONING ARTIFACT	UNP P29476

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

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

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).
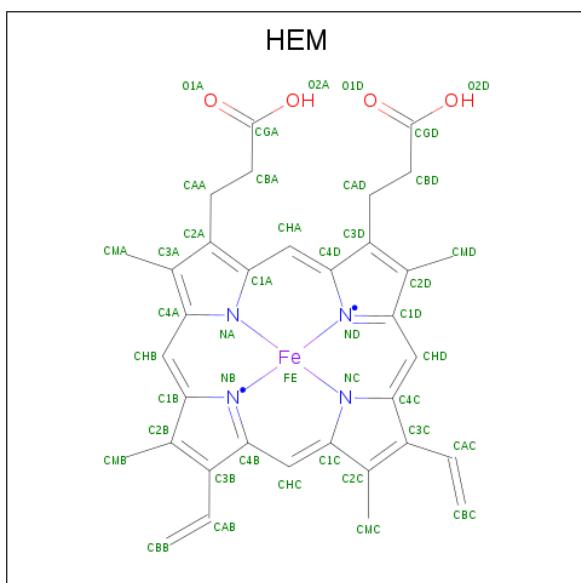
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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

H4B
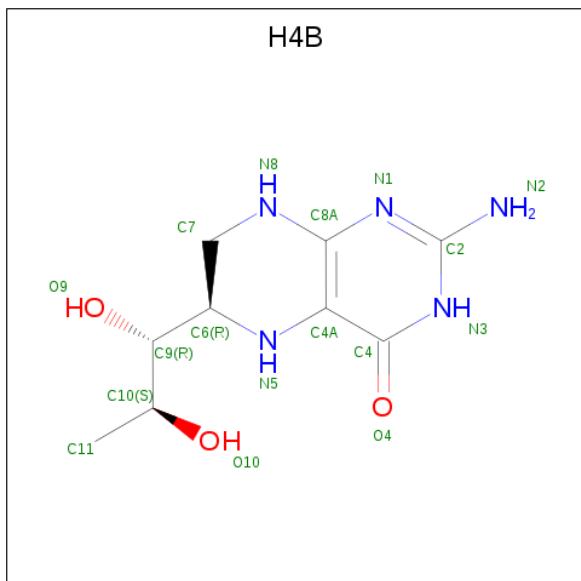
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 5 is N-(3-(AMINOMETHYL)BENZYL)ACETAMIDINE (three-letter code: 14W) (formula: $C_{10}H_{15}N_3$).

14W
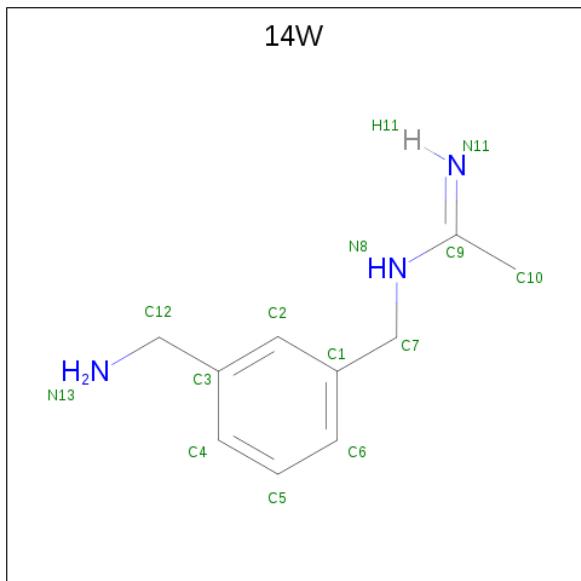
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 13	C 10	N 3	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	206	Total 206	O 206	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Nitric-oxide synthase, brain
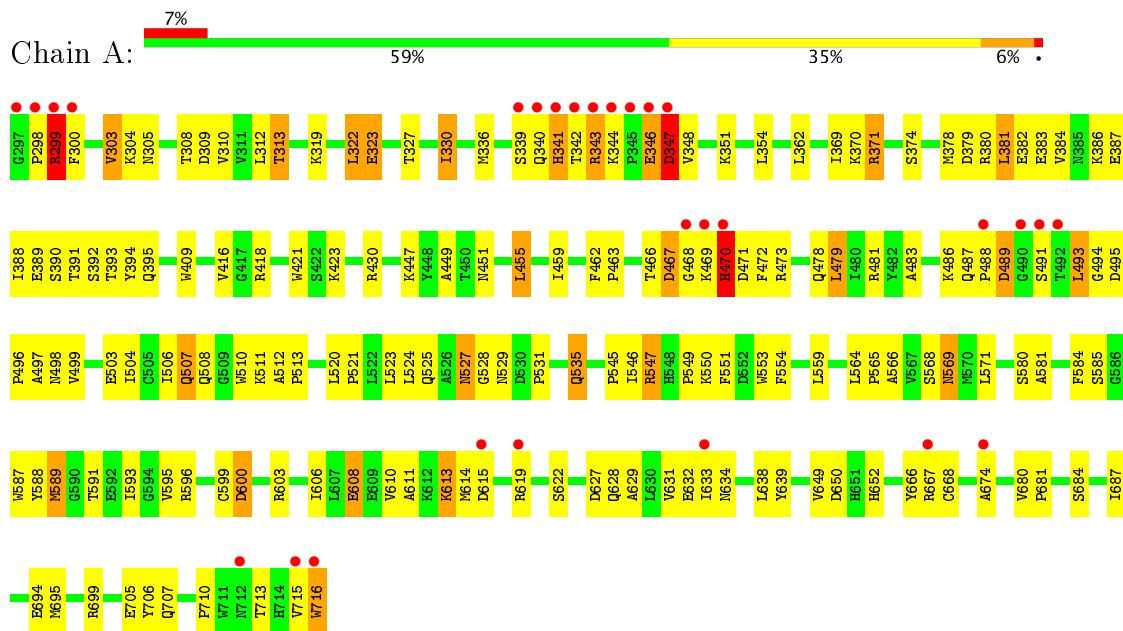
4　Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	44.78Å　　108.78Å　　164.32Å 90.00°　　90.00°　　90.00°	Depositor
Resolution (Å)	8.00　–　2.30 19.64　–　2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.30) 97.3 (19.64-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$<I/\sigma(I)>$ [1]	3.64 (at 2.19Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.193　,　0.235 0.191　,　0.232	Depositor DCC
R_{free} test set	873 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	24.9	Xtriage
Anisotropy	0.994	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 96.0	EDS
L-test for twinning[2]	$<|L|> = 0.47, <L^2> = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	3698	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.97% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, ZN, H4B, 14W

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	0.40	0/3515	0.66	2/4770 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	589	MET	N-CA-C	-5.67	95.70	111.00
1	A	470	HIS	N-CA-C	5.18	124.97	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	470	HIS	Mainchain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3418	0	3324	167	0
2	A	1	0	0	0	0
3	A	43	0	30	1	0
4	A	17	0	15	0	0
5	A	13	0	14	1	0
6	A	206	0	0	12	0
All	All	3698	0	3383	167	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 24.

All (167) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:ARG:HE	1:A:343:ARG:HA	1.25	0.99
1:A:469:LYS:O	1:A:470:HIS:HB2	1.69	0.90
1:A:470:HIS:CG	1:A:528:GLY:HA3	2.10	0.85
1:A:327:THR:HG23	1:A:330:ILE:HG22	1.60	0.84
1:A:481:ARG:NH1	1:A:498:ASN:HD21	1.78	0.80
1:A:488:PRO:HG2	1:A:489:ASP:OD1	1.85	0.76
1:A:343:ARG:HE	1:A:343:ARG:CA	1.99	0.75
1:A:382:GLU:O	1:A:386:LYS:HG3	1.85	0.75
1:A:684:SER:HB3	1:A:687:ILE:HD11	1.68	0.75
1:A:339:SER:HA	1:A:342:THR:OG1	1.86	0.74
1:A:343:ARG:HG2	1:A:706:TYR:O	1.86	0.73
1:A:469:LYS:HD2	6:A:176:HOH:O	1.88	0.72
1:A:351:LYS:HE3	1:A:389:GLU:HA	1.71	0.71
1:A:322:LEU:H	1:A:322:LEU:HD12	1.56	0.70
1:A:322:LEU:HD23	1:A:341:HIS:HD2	1.57	0.70
1:A:481:ARG:HH11	1:A:498:ASN:HD21	1.44	0.65
1:A:343:ARG:HA	1:A:343:ARG:NE	2.02	0.64
1:A:391:THR:O	1:A:392:SER:HB2	1.98	0.64
1:A:511:LYS:O	1:A:511:LYS:HD3	1.98	0.64
1:A:409:TRP:CE3	1:A:421:TRP:HA	2.33	0.64
1:A:379:ASP:O	1:A:383:GLU:HG3	1.98	0.63
1:A:478:GLN:NE2	5:A:902:14W:H5	2.13	0.63
1:A:684:SER:HB3	1:A:687:ILE:CD1	2.29	0.63
1:A:304:LYS:O	1:A:694:GLU:HG3	2.00	0.62
1:A:466:THR:OG1	1:A:469:LYS:HB3	2.00	0.61
1:A:554:PHE:HB3	6:A:9:HOH:O	2.00	0.61
1:A:305:ASN:OD1	1:A:308:THR:HG23	2.01	0.61
1:A:587:TRP:H	3:A:900:HEM:HAB	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:478:GLN:HB2	1:A:481:ARG:HG3	1.82	0.60
1:A:418:ARG:O	1:A:421:TRP:HB3	2.01	0.60
1:A:470:HIS:HB3	1:A:527:ASN:C	2.21	0.60
1:A:463:PRO:HB2	1:A:472:PHE:CE1	2.37	0.60
1:A:343:ARG:HG3	1:A:707:GLN:HB3	1.83	0.60
1:A:299:ARG:HG2	1:A:300:PHE:CD2	2.37	0.60
1:A:470:HIS:HB3	1:A:528:GLY:N	2.16	0.59
1:A:619:ARG:HG3	6:A:161:HOH:O	2.02	0.59
1:A:303:VAL:HG23	1:A:312:LEU:HB2	1.83	0.59
1:A:347:ASP:N	1:A:347:ASP:OD2	2.34	0.59
1:A:298:PRO:HG2	1:A:299:ARG:NH1	2.18	0.59
1:A:299:ARG:N	1:A:299:ARG:HD3	2.16	0.59
1:A:298:PRO:HG2	1:A:299:ARG:CZ	2.33	0.58
1:A:384:VAL:O	1:A:388:ILE:HG13	2.02	0.58
1:A:588:TYR:CD2	1:A:593:ILE:HD11	2.39	0.58
1:A:585:SER:HA	6:A:177:HOH:O	2.01	0.58
1:A:470:HIS:ND1	1:A:528:GLY:HA3	2.17	0.58
1:A:524:LEU:O	1:A:531:PRO:HA	2.04	0.58
1:A:705:GLU:HB3	6:A:131:HOH:O	2.04	0.58
1:A:327:THR:HG21	6:A:78:HOH:O	2.04	0.57
1:A:466:THR:O	1:A:467:ASP:HB2	2.04	0.57
1:A:374:SER:O	1:A:378:MET:HG2	2.04	0.57
1:A:342:THR:O	1:A:342:THR:HG22	2.05	0.57
1:A:354:LEU:HG	1:A:388:ILE:HD13	1.86	0.57
1:A:322:LEU:HD13	1:A:699:ARG:O	2.06	0.56
1:A:596:ARG:O	1:A:600:ASP:HB2	2.05	0.56
1:A:606:ILE:O	1:A:610:VAL:HG23	2.06	0.56
1:A:667:ARG:HG3	1:A:667:ARG:O	2.06	0.55
1:A:479:LEU:HD22	1:A:566:ALA:HB1	1.88	0.55
1:A:479:LEU:HD13	1:A:568:SER:HB3	1.88	0.55
1:A:473:ARG:HD3	1:A:580:SER:HB2	1.87	0.55
1:A:323:GLU:HB2	1:A:340:GLN:OE1	2.06	0.54
1:A:503:GLU:HA	1:A:503:GLU:OE2	2.07	0.54
1:A:545:PRO:HG2	1:A:547:ARG:NH1	2.22	0.54
1:A:606:ILE:HD11	1:A:633:ILE:HD13	1.89	0.54
1:A:343:ARG:CD	1:A:571:LEU:HD13	2.38	0.54
1:A:447:LYS:HE2	6:A:138:HOH:O	2.08	0.53
1:A:638:LEU:HD21	1:A:650:ASP:HB3	1.89	0.53
1:A:510:TRP:CE2	1:A:521:PRO:HD3	2.44	0.53
1:A:380:ARG:O	1:A:383:GLU:HB2	2.08	0.53
1:A:551:PHE:HB3	1:A:553:TRP:CE2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:523:LEU:CD1	1:A:531:PRO:HB2	2.39	0.52
1:A:504:ILE:O	1:A:508:GLN:HG2	2.10	0.51
1:A:462:PHE:HB3	1:A:463:PRO:CD	2.40	0.51
1:A:481:ARG:HB2	6:A:19:HOH:O	2.10	0.51
1:A:449:ALA:O	1:A:455:LEU:HA	2.11	0.51
1:A:546:ILE:HB	1:A:559:LEU:HB2	1.93	0.50
1:A:472:PHE:O	1:A:581:ALA:HB2	2.12	0.50
1:A:710:PRO:HA	1:A:713:THR:OG1	2.12	0.50
1:A:369:ILE:HG13	1:A:371:ARG:HG3	1.94	0.49
1:A:351:LYS:HG2	1:A:388:ILE:HG22	1.94	0.49
1:A:344:LYS:NZ	1:A:346:GLU:CG	2.76	0.48
1:A:348:VAL:HG21	1:A:467:ASP:HA	1.96	0.48
1:A:520:LEU:HD23	1:A:521:PRO:HD2	1.95	0.48
1:A:322:LEU:HB2	1:A:699:ARG:HB2	1.96	0.48
1:A:459:ILE:HG13	1:A:584:PHE:HB3	1.95	0.47
1:A:416:VAL:HG22	1:A:416:VAL:O	2.14	0.47
1:A:343:ARG:CA	1:A:343:ARG:NE	2.68	0.47
1:A:393:THR:HG23	1:A:394:TYR:N	2.29	0.47
1:A:319:LYS:HD3	6:A:112:HOH:O	2.15	0.47
1:A:343:ARG:HH11	1:A:571:LEU:HD22	1.79	0.47
1:A:503:GLU:HG3	1:A:507:GLN:HE22	1.80	0.47
1:A:553:TRP:HD1	6:A:55:HOH:O	1.98	0.47
1:A:308:THR:OG1	1:A:310:VAL:HG23	2.14	0.47
1:A:351:LYS:HD2	1:A:392:SER:HA	1.96	0.47
1:A:523:LEU:HG	1:A:531:PRO:HB2	1.96	0.47
1:A:549:PRO:O	1:A:550:LYS:HG3	2.14	0.47
1:A:298:PRO:HG2	1:A:299:ARG:HD3	1.96	0.46
1:A:389:GLU:OE1	1:A:389:GLU:HA	2.15	0.46
1:A:388:ILE:HA	1:A:393:THR:O	2.15	0.46
1:A:479:LEU:HB2	1:A:566:ALA:HB3	1.97	0.46
1:A:470:HIS:CB	1:A:528:GLY:HA3	2.46	0.46
1:A:569:ASN:H	1:A:569:ASN:HD22	1.63	0.46
1:A:520:LEU:CD2	1:A:521:PRO:HD2	2.45	0.46
1:A:680:VAL:HA	1:A:681:PRO:HD3	1.85	0.46
1:A:493:LEU:HD12	1:A:494:GLY:H	1.81	0.45
1:A:503:GLU:CD	1:A:507:GLN:HE22	2.19	0.45
1:A:551:PHE:CD2	1:A:551:PHE:N	2.84	0.45
1:A:603:ARG:HG3	1:A:603:ARG:HH11	1.80	0.45
1:A:493:LEU:HD12	1:A:494:GLY:N	2.31	0.45
1:A:591:THR:HA	1:A:595:VAL:HG23	1.98	0.45
1:A:430:ARG:O	1:A:463:PRO:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:684:SER:HB3	1:A:687:ILE:CG1	2.47	0.45
1:A:322:LEU:N	1:A:322:LEU:HD12	2.30	0.45
1:A:589:MET:HA	1:A:649:VAL:O	2.16	0.45
1:A:473:ARG:NH2	1:A:710:PRO:HD3	2.32	0.44
1:A:344:LYS:NZ	1:A:346:GLU:HG2	2.33	0.44
1:A:362:LEU:HD13	1:A:381:LEU:HD12	1.99	0.44
1:A:591:THR:HA	1:A:634:ASN:HD21	1.83	0.44
1:A:344:LYS:NZ	1:A:346:GLU:HG3	2.32	0.44
1:A:473:ARG:HD2	1:A:580:SER:O	2.17	0.44
1:A:486:LYS:HD2	1:A:499:VAL:HG11	2.00	0.44
1:A:525:GLN:HG3	1:A:529:ASN:O	2.18	0.44
1:A:483:ALA:HA	1:A:520:LEU:HD11	1.99	0.43
1:A:312:LEU:HB3	1:A:666:TYR:CD1	2.53	0.43
1:A:715:VAL:O	1:A:716:TRP:CB	2.65	0.43
1:A:304:LYS:HG2	1:A:305:ASN:N	2.32	0.43
1:A:308:THR:O	1:A:309:ASP:HB2	2.18	0.43
1:A:470:HIS:CB	1:A:527:ASN:C	2.86	0.43
1:A:629:ALA:O	1:A:633:ILE:HG13	2.18	0.43
1:A:322:LEU:HD22	1:A:699:ARG:HE	1.83	0.43
1:A:549:PRO:HD3	1:A:639:TYR:CG	2.54	0.43
1:A:595:VAL:O	1:A:599:CYS:HB2	2.18	0.43
1:A:470:HIS:HB3	1:A:528:GLY:CA	2.48	0.43
1:A:627:ASP:O	1:A:631:VAL:HG23	2.18	0.42
1:A:521:PRO:HB3	1:A:535:GLN:OE1	2.18	0.42
1:A:455:LEU:H	1:A:455:LEU:CD1	2.33	0.42
1:A:470:HIS:HB3	1:A:528:GLY:HA3	2.02	0.42
1:A:351:LYS:CG	1:A:388:ILE:HG22	2.50	0.42
1:A:569:ASN:N	1:A:569:ASN:HD22	2.18	0.42
1:A:506:ILE:C	1:A:508:GLN:H	2.22	0.42
1:A:614:MET:CE	1:A:632:GLU:HG3	2.50	0.42
1:A:409:TRP:CZ3	1:A:421:TRP:HA	2.54	0.42
1:A:423:LYS:HE3	6:A:40:HOH:O	2.19	0.42
1:A:608:GLU:O	1:A:611:ALA:HB3	2.20	0.42
1:A:614:MET:O	1:A:615:ASP:HB2	2.20	0.41
1:A:300:PHE:HB3	1:A:313:THR:HG22	2.01	0.41
1:A:549:PRO:HB3	1:A:639:TYR:CD1	2.55	0.41
1:A:650:ASP:OD2	1:A:652:HIS:HB2	2.21	0.41
1:A:638:LEU:HD21	1:A:650:ASP:CB	2.50	0.41
1:A:299:ARG:HG2	1:A:300:PHE:CE2	2.55	0.41
1:A:370:LYS:HD2	1:A:370:LYS:N	2.36	0.41
1:A:351:LYS:HE3	1:A:389:GLU:OE1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:LEU:H	1:A:455:LEU:HD12	1.84	0.41
1:A:467:ASP:HB3	1:A:468:GLY:H	1.75	0.41
1:A:588:TYR:O	1:A:649:VAL:HG12	2.20	0.41
1:A:344:LYS:HB3	1:A:344:LYS:NZ	2.36	0.41
1:A:512:ALA:HA	1:A:513:PRO:HD3	1.94	0.41
1:A:495:ASP:HA	1:A:496:PRO:HD3	1.92	0.41
1:A:344:LYS:HZ2	1:A:346:GLU:CG	2.33	0.41
1:A:613:LYS:CA	1:A:613:LYS:HE2	2.50	0.41
1:A:387:GLU:O	1:A:391:THR:OG1	2.38	0.41
1:A:395:GLN:HA	6:A:122:HOH:O	2.20	0.41
1:A:380:ARG:O	1:A:384:VAL:HG22	2.20	0.40
1:A:564:LEU:HA	1:A:565:PRO:HD2	1.97	0.40
1:A:495:ASP:OD1	1:A:497:ALA:HB3	2.22	0.40
1:A:503:GLU:CG	1:A:507:GLN:HE22	2.34	0.40
1:A:478:GLN:HA	1:A:566:ALA:O	2.21	0.40
1:A:674:ALA:HB3	1:A:695:MET:HB3	2.04	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	418/420 (100%)	378 (90%)	32 (8%)	8 (2%)	9 8

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	347	ASP
1	A	467	ASP
1	A	470	HIS
1	A	299	ARG
1	A	346	GLU

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Mol	Chain	Res	Type
1	A	608	GLU
1	A	341	HIS
1	A	455	LEU

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	375/375 (100%)	345 (92%)	30 (8%)	14 17

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	299	ARG
1	A	303	VAL
1	A	313	THR
1	A	322	LEU
1	A	323	GLU
1	A	330	ILE
1	A	336	MET
1	A	343	ARG
1	A	347	ASP
1	A	371	ARG
1	A	381	LEU
1	A	390	SER
1	A	451	ASN
1	A	471	ASP
1	A	479	LEU
1	A	487	GLN
1	A	489	ASP
1	A	491	SER
1	A	493	LEU
1	A	507	GLN
1	A	527	ASN
1	A	535	GLN
1	A	547	ARG

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Mol	Chain	Res	Type
1	A	569	ASN
1	A	600	ASP
1	A	613	LYS
1	A	622	SER
1	A	628	GLN
1	A	668	CYS
1	A	716	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	364	GLN
1	A	451	ASN
1	A	487	GLN
1	A	498	ASN
1	A	500	GLN
1	A	507	GLN
1	A	569	ASN
1	A	628	GLN
1	A	634	ASN
1	A	664	ASN
1	A	707	GLN
1	A	712	ASN
1	A	714	HIS

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 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	900	1	28,50,50	1.91	10 (35%)	17,82,82	0.95	0
4	H4B	A	901	-	14,18,18	2.42	4 (28%)	12,26,26	3.98	7 (58%)
5	14W	A	902	-	12,13,13	0.51	0	13,16,16	0.68	1 (7%)

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	900	1	-	0/6/54/54	0/0/8/8
4	H4B	A	901	-	-	0/8/17/17	0/2/2/2
5	14W	A	902	-	-	0/6/7/7	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	900	HEM	C3B-CAB	-3.55	1.40	1.47
3	A	900	HEM	C3C-CAC	-3.18	1.41	1.47
3	A	900	HEM	C3B-C2B	-2.67	1.36	1.40
3	A	900	HEM	C1D-ND	2.06	1.40	1.36
3	A	900	HEM	C1A-NA	2.08	1.40	1.36
3	A	900	HEM	C1C-NC	2.09	1.39	1.36
3	A	900	HEM	C4B-NB	2.24	1.40	1.36
4	A	901	H4B	C8A-N1	2.97	1.39	1.34
3	A	900	HEM	C4C-NC	2.99	1.40	1.36
3	A	900	HEM	C1B-NB	3.76	1.41	1.36
3	A	900	HEM	C4D-ND	4.05	1.41	1.36
4	A	901	H4B	C6-N5	4.07	1.53	1.45
4	A	901	H4B	C4A-N5	4.33	1.47	1.37
4	A	901	H4B	C4-N3	5.67	1.43	1.33

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All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	901	H4B	N3-C2-N1	-5.12	117.14	125.45
4	A	901	H4B	C4A-C4-N3	-3.51	113.59	123.91
4	A	901	H4B	C4A-N5-C6	-3.06	112.82	121.16
5	A	902	14W	C1-C7-N8	-2.13	108.25	112.96
4	A	901	H4B	N2-C2-N1	3.31	122.53	117.24
4	A	901	H4B	C2-N1-C8A	3.80	123.08	114.51
4	A	901	H4B	C4-N3-C2	6.73	125.74	116.06
4	A	901	H4B	C4-C4A-C8A	8.02	121.82	114.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	900	HEM	1	0
5	A	902	14W	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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^2)	Q<0.9
1	A	420/420 (100%)	0.15	28 (6%)	19	25	10, 30, 64, 100	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	342	THR	9.2
1	A	341	HIS	7.8
1	A	716	TRP	6.2
1	A	343	ARG	5.7
1	A	469	LYS	5.7
1	A	346	GLU	5.4
1	A	344	LYS	4.2
1	A	345	PRO	4.2
1	A	297	GLY	4.0
1	A	488	PRO	3.8
1	A	347	ASP	3.7
1	A	490	GLY	3.6
1	A	340	GLN	3.5
1	A	298	PRO	3.5
1	A	299	ARG	3.3
1	A	619	ARG	3.2
1	A	491	SER	3.0
1	A	339	SER	3.0
1	A	667	ARG	2.9
1	A	715	VAL	2.9
1	A	468	GLY	2.7
1	A	470	HIS	2.6
1	A	300	PHE	2.3
1	A	712	ASN	2.2
1	A	492	THR	2.2
1	A	615	ASP	2.1
1	A	633	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	674	ALA	2.1

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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, 95th 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(Å^2)	Q<0.9
5	14W	A	902	13/13	0.74	0.25	7.14	17,31,36,37	0
3	HEM	A	900	43/43	0.97	0.12	0.28	8,25,43,44	0
4	H4B	A	901	17/17	0.95	0.10	-0.40	9,16,27,33	0
2	ZN	A	950	1/1	0.99	0.04	-	26,26,26,26	1

6.5 Other polymers (i)

There are no such residues in this entry.