Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 09:10 PM GMT

PDB ID	:	4V3Y
Title	:	Structure of rat neuronal nitric oxide synthase heme domain in complex with N-2-(2-(1H-imidazol-1-yl)pyrimidin-4-yl)ethyl-3-(3- chlorophenyl)propan-1-amine
Authors	:	Li, H.; Poulos, T.L.
Deposited on	:	2014-10-20
Resolution	:	1.96 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

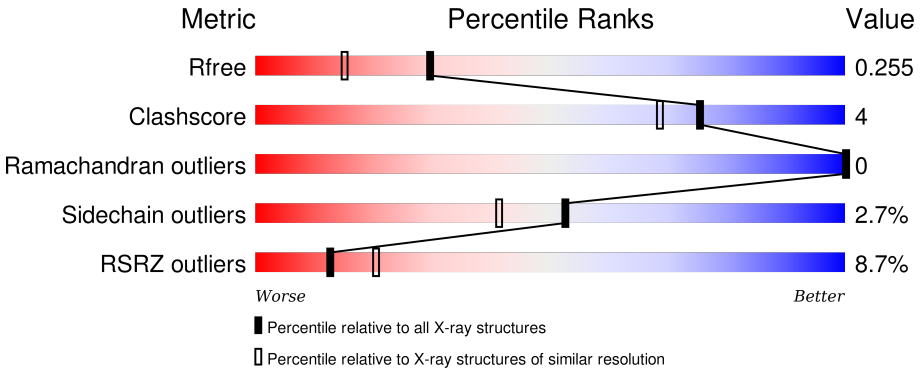
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.96 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (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 >=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	422	13% 82% 14%
1	B	422	4% 90% 7%

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	ACT	A	860	-	-	-	X

2 Entry composition

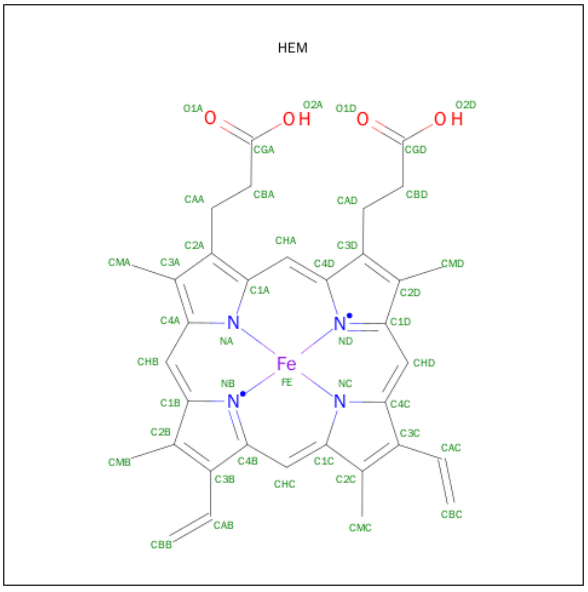
There are 7 unique types of molecules in this entry. The entry contains 7263 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called NITRIC OXIDE SYNTHASE, BRAIN.

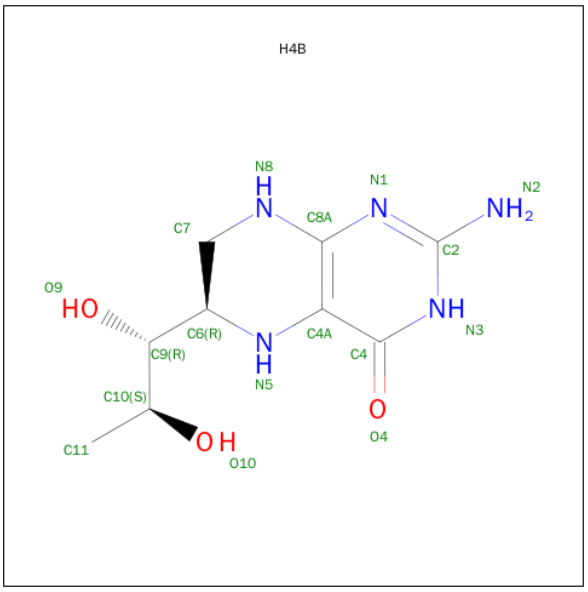
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	408	Total	C	N	O	S	0	3	1
			3323	2127	567	607	22			
1	B	411	Total	C	N	O	S	0	3	0
			3357	2148	574	614	21			

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



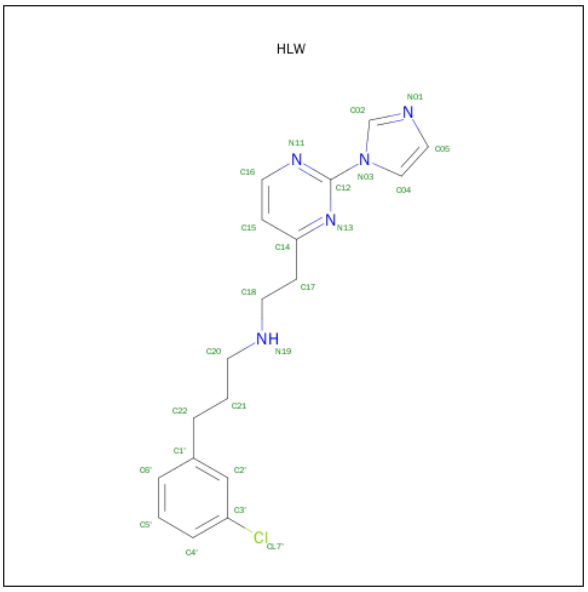
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is 5,6,7,8-TETRAHYDROBIOPTERIN (three-letter code: H4B) (formula: $C_9H_{15}N_5O_3$).



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

- Molecule 4 is 3-(3-CHLOROPHENYL)-N-{2-[2-(1H-IMIDAZOL-1-YL)PYRIMIDIN-4-YL] ETHYL}PROPAN-1-AMINE (three-letter code: HLW) (formula: $C_{18}H_{20}ClN_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C Cl N 24 18 1 5	0	0

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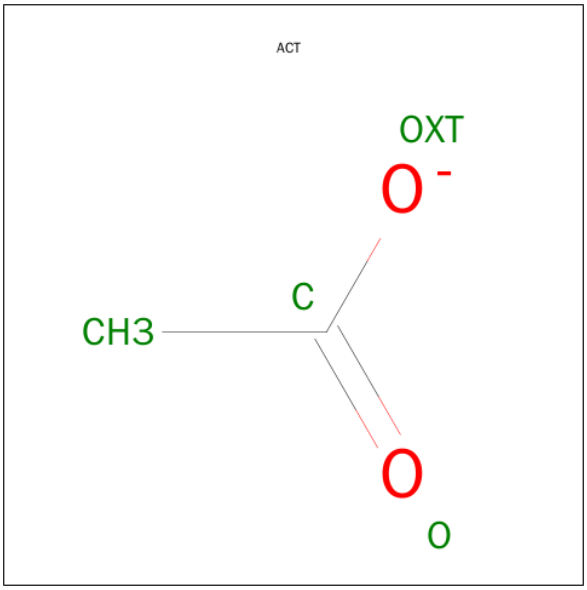
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	Cl	N	0	0
			24	18	1	5		

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 7 is water.

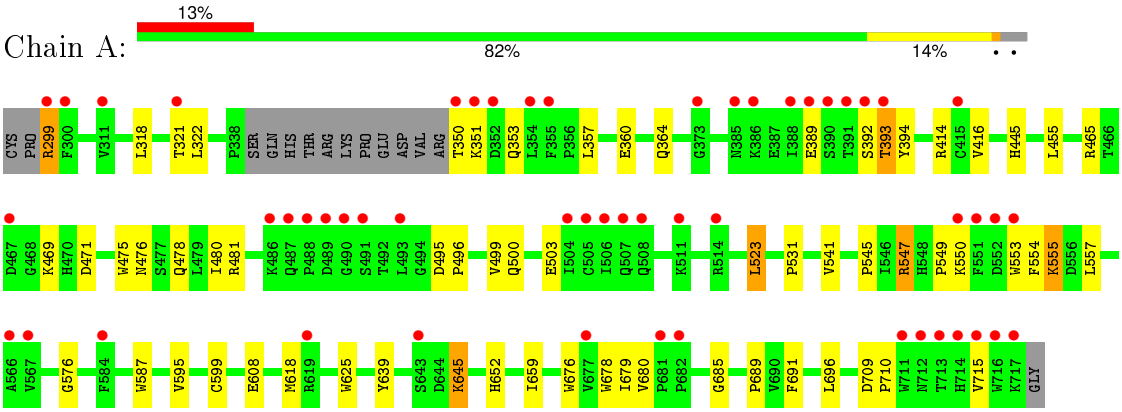
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	178	Total	O	0	0
			178	178		
7	B	228	Total	O	0	0
			228	228		

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 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.

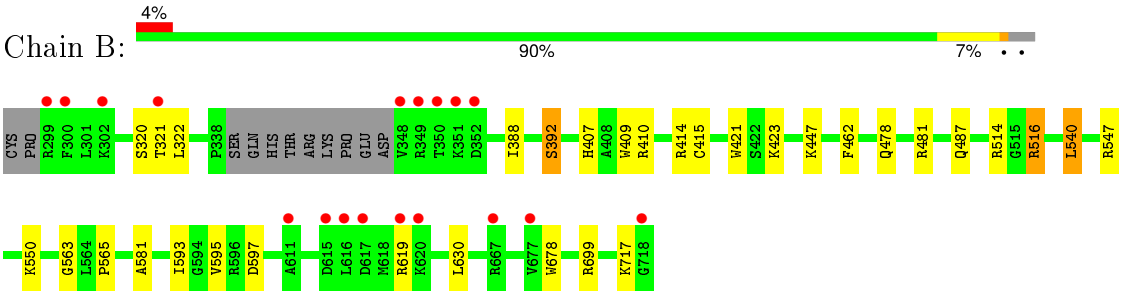
- Molecule 1: NITRIC OXIDE SYNTHASE, BRAIN

Chain A:



- Molecule 1: NITRIC OXIDE SYNTHASE, BRAIN

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	51.85Å 111.05Å 164.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.48 – 1.96 38.49 – 1.96	Depositor EDS
% Data completeness (in resolution range)	78.4 (38.48-1.96) 78.4 (38.49-1.96)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.98 (at 1.97Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.191 , 0.248 0.200 , 0.255	Depositor DCC
R_{free} test set	2656 reflections (5.18%)	DCC
Wilson B-factor (Å^2)	23.9	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 49.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	1 of 53953 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7263	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.93% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.39	0/3422	0.54	0/4643
1	B	0.41	0/3459	0.54	0/4689
All	All	0.40	0/6881	0.54	0/9332

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3323	0	3232	35	0
1	B	3357	0	3275	14	0
2	A	43	0	30	2	0
2	B	43	0	30	3	0
3	A	17	0	15	0	0
3	B	17	0	15	0	0
4	A	24	0	20	0	0
4	B	24	0	20	0	0
5	A	4	0	3	0	0
5	B	4	0	3	0	0
6	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	178	0	0	3	0
7	B	228	0	0	1	0
All	All	7263	0	6643	53	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 4.

All (53) 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)
2:A:750:HEM:HBB2	2:A:750:HEM:HHC	1.70	0.74
1:B:478:GLN:HB2	1:B:481:ARG:HG3	1.73	0.70
2:B:750:HEM:HHC	2:B:750:HEM:HBB2	1.75	0.67
1:B:322:LEU:HD13	1:B:699:ARG:HH21	1.59	0.67
1:A:478:GLN:HB2	1:A:481:ARG:HG3	1.77	0.67
1:A:480:ILE:HD13	1:A:541:VAL:HG13	1.77	0.67
2:B:750:HEM:HBC2	2:B:750:HEM:HMC2	1.76	0.66
2:A:750:HEM:HMC2	2:A:750:HEM:HBC2	1.79	0.65
1:A:523:LEU:HD22	1:A:531:PRO:HB2	1.80	0.63
1:A:652:HIS:ND1	7:A:2152:HOH:O	2.31	0.59
1:A:393:THR:OG1	1:A:394:TYR:N	2.35	0.58
1:A:496:PRO:HA	1:A:499:VAL:HG23	1.86	0.57
1:B:487:GLN:OE1	1:B:514:ARG:NH2	2.38	0.56
1:B:447:LYS:HD2	1:B:540:LEU:HD11	1.87	0.56
1:A:360:GLU:O	1:A:364:GLN:HG3	2.07	0.54
1:A:351:LYS:NZ	1:A:389:GLU:O	2.37	0.53
1:B:593:ILE:HA	1:B:597:ASP:HB2	1.91	0.53
1:A:416:VAL:HG23	1:A:679:ILE:HG23	1.91	0.52
1:A:554:PHE:HB3	7:A:2114:HOH:O	2.10	0.52
1:B:414:ARG:HD3	1:B:678:TRP:CD2	2.44	0.52
1:A:351:LYS:HE2	1:A:392:SER:HA	1.94	0.49
1:A:555:LYS:N	7:A:2114:HOH:O	2.46	0.48
1:A:465:ARG:NH2	1:A:471:ASP:OD2	2.46	0.48
1:B:407:HIS:CE1	1:B:410:ARG:HH11	2.31	0.47
1:A:475:TRP:HB2	1:A:523:LEU:HB3	1.97	0.46
1:A:659:ILE:HG13	1:A:689:PRO:HB2	1.97	0.45
1:A:645:LYS:HB2	1:A:645:LYS:HE3	1.72	0.44
1:B:409:TRP:CE3	1:B:421:TRP:HA	2.53	0.44
1:A:350:THR:N	1:A:353:GLN:OE1	2.50	0.44
1:A:299:ARG:HE	1:A:318:LEU:HD13	1.83	0.44
1:B:516:ARG:HD2	7:B:2140:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:388:ILE:O	1:B:392:SER:N	2.43	0.43
1:A:545:PRO:HG2	1:A:547:ARG:NH1	2.33	0.43
1:A:455:LEU:HD12	1:A:587:TRP:HB3	2.00	0.43
1:A:618:MET:HG2	1:A:625:TRP:CD2	2.54	0.43
1:A:414:ARG:HD3	1:A:678:TRP:CD2	2.54	0.43
1:A:676:TRP:CE2	1:A:680:VAL:HG21	2.54	0.42
1:A:445:HIS:C	1:A:445:HIS:CD2	2.92	0.42
1:B:415:CYS:HB2	2:B:750:HEM:ND	2.34	0.42
1:A:553:TRP:HZ3	1:A:557:LEU:HD11	1.85	0.42
1:A:608:GLU:HG3	1:A:618:MET:HE1	2.02	0.42
1:A:321:THR:HG23	1:A:322:LEU:HG	2.02	0.42
1:B:563:GLY:O	1:B:565:PRO:HD3	2.20	0.41
1:A:696:LEU:HA	1:A:696:LEU:HD23	1.95	0.41
1:A:685:GLY:O	1:A:691:PHE:HB2	2.21	0.41
1:A:709:ASP:HA	1:A:710:PRO:HD3	1.89	0.41
1:A:495:ASP:HA	1:A:496:PRO:HD3	1.93	0.41
1:A:500:GLN:O	1:A:503:GLU:HB2	2.21	0.40
1:A:595:VAL:O	1:A:599:CYS:HB2	2.21	0.40
1:A:549:PRO:HB3	1:A:639:TYR:CE1	2.56	0.40
1:B:462:PHE:HB2	1:B:581:ALA:HB3	2.02	0.40
1:B:595:VAL:HG13	1:B:630:LEU:HD11	2.04	0.40
1:A:357:LEU:HD13	1:A:576:GLY:HA2	2.03	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	406/422 (96%)	392 (97%)	14 (3%)	0	100	100
1	B	410/422 (97%)	396 (97%)	14 (3%)	0	100	100
All	All	816/844 (97%)	788 (97%)	28 (3%)	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	365/377 (97%)	355 (97%)	10 (3%)	52	41
1	B	369/377 (98%)	359 (97%)	10 (3%)	52	41
All	All	734/754 (97%)	714 (97%)	20 (3%)	52	41

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	299	ARG
1	A	393	THR
1	A	469	LYS
1	A	476	ASN
1	A	523	LEU
1	A	547	ARG
1	A	550	LYS
1	A	555	LYS
1	A	645	LYS
1	A	715	VAL
1	B	320	SER
1	B	321	THR
1	B	392	SER
1	B	423	LYS
1	B	516	ARG
1	B	540	LEU
1	B	547	ARG
1	B	550	LYS
1	B	619	ARG
1	B	717	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	407	HIS

5.3.3 RNA

There are no RNA molecules 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 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	HEM	A	750	1,4	30,50,50	2.10	9 (30%)	24,82,82	2.60	11 (45%)
3	H4B	A	760	-	13,18,18	0.92	0	11,26,26	2.43	6 (54%)
4	HLW	A	800	2	24,26,26	1.06	1 (4%)	30,33,33	1.73	7 (23%)
5	ACT	A	860	-	1,3,3	1.29	0	0,3,3	0.00	-
2	HEM	B	750	1,4	30,50,50	1.96	7 (23%)	24,82,82	2.38	11 (45%)
3	H4B	B	760	-	13,18,18	0.77	0	11,26,26	2.39	4 (36%)
4	HLW	B	800	2	24,26,26	1.07	1 (4%)	30,33,33	1.59	4 (13%)
5	ACT	B	860	-	1,3,3	1.08	0	0,3,3	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means

no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	750	1,4	-	0/10/54/54	0/0/8/8
3	H4B	A	760	-	-	0/8/17/17	0/2/2/2
4	HLW	A	800	2	-	0/9/13/13	0/3/3/3
5	ACT	A	860	-	-	0/0/0/0	0/0/0/0
2	HEM	B	750	1,4	-	0/10/54/54	0/0/8/8
3	H4B	B	760	-	-	0/8/17/17	0/2/2/2
4	HLW	B	800	2	-	0/9/13/13	0/3/3/3
5	ACT	B	860	-	-	0/0/0/0	0/0/0/0

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	750	HEM	C3B-C4B	-6.36	1.46	1.51
2	A	750	HEM	C3D-C4D	-5.53	1.44	1.51
2	B	750	HEM	C3B-C4B	-5.38	1.47	1.51
2	B	750	HEM	C3D-C4D	-4.98	1.45	1.51
2	B	750	HEM	C2C-C1C	-3.85	1.45	1.52
2	A	750	HEM	C2C-C1C	-3.78	1.45	1.52
4	A	800	HLW	C04-N03	-3.22	1.34	1.39
4	B	800	HLW	C04-N03	-2.83	1.35	1.39
2	B	750	HEM	C2D-C1D	-2.39	1.44	1.51
2	A	750	HEM	C2D-C1D	-2.20	1.44	1.51
2	A	750	HEM	C2B-C1B	-2.09	1.45	1.51
2	B	750	HEM	C3B-CAB	2.05	1.55	1.51
2	A	750	HEM	C3C-CAC	2.10	1.55	1.51
2	A	750	HEM	C3B-CAB	2.11	1.55	1.51
2	B	750	HEM	C1C-NC	2.15	1.38	1.36
2	A	750	HEM	FE-ND	2.16	2.08	1.97
2	A	750	HEM	FE-NC	2.23	2.04	1.95
2	B	750	HEM	C3C-CAC	2.45	1.55	1.51

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	800	HLW	C15-C16-N11	-5.17	118.00	123.90
4	B	800	HLW	C15-C16-N11	-4.27	119.02	123.90
2	A	750	HEM	CBA-CAA-C2A	-3.95	105.44	112.53
3	A	760	H4B	N3-C2-N1	-3.73	119.42	125.53
2	A	750	HEM	CBD-CAD-C3D	-3.69	102.82	113.55
2	B	750	HEM	CBD-CAD-C3D	-3.61	103.04	113.55
4	B	800	HLW	N11-C12-N13	-2.91	122.79	126.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	750	HEM	CBA-CAA-C2A	-2.78	107.54	112.53
4	A	800	HLW	C04-N03-C12	-2.74	122.61	125.61
3	B	760	H4B	N3-C2-N1	-2.37	121.64	125.53
4	A	800	HLW	N11-C12-N13	-2.29	123.56	126.44
2	A	750	HEM	CMA-C3A-C4A	-2.18	124.76	128.36
2	A	750	HEM	C3B-C4B-NB	-2.15	107.52	111.63
2	B	750	HEM	C3B-C4B-NB	-2.02	107.76	111.63
3	B	760	H4B	C2-N1-C8A	2.06	119.17	114.54
2	B	750	HEM	C2C-C1C-CHC	2.08	126.84	123.68
4	A	800	HLW	C05-N01-C02	2.18	112.72	106.06
4	A	800	HLW	C17-C14-N13	2.21	118.95	115.69
3	A	760	H4B	N2-C2-N3	2.34	121.08	117.20
3	A	760	H4B	C4A-C8A-N8	2.53	121.41	118.43
2	B	750	HEM	C2D-C3D-C4D	2.60	105.90	101.50
4	A	800	HLW	N13-C12-N03	2.70	118.81	114.82
4	B	800	HLW	N11-C12-N03	2.72	119.58	115.16
4	A	800	HLW	C12-N13-C14	2.80	118.92	115.26
2	A	750	HEM	CMD-C2D-C3D	2.94	127.36	114.35
2	B	750	HEM	C3B-C4B-CHC	3.06	127.48	123.16
2	B	750	HEM	CMD-C2D-C3D	3.16	128.33	114.35
2	A	750	HEM	C2D-C3D-C4D	3.23	106.98	101.50
3	A	760	H4B	C2-N1-C8A	3.30	121.95	114.54
3	A	760	H4B	C4-N3-C2	3.32	120.54	115.94
3	B	760	H4B	C4-N3-C2	3.49	120.79	115.94
2	A	750	HEM	C3B-C4B-CHC	3.52	128.12	123.16
4	B	800	HLW	C12-N13-C14	3.75	120.16	115.26
3	A	760	H4B	C4-C4A-C8A	3.76	117.97	114.56
2	B	750	HEM	CMB-C2B-C3B	3.82	126.08	116.53
2	A	750	HEM	CAD-C3D-C4D	4.02	126.64	112.47
2	B	750	HEM	CAD-C3D-C4D	4.03	126.69	112.47
2	A	750	HEM	CMB-C2B-C3B	4.19	126.99	116.53
2	B	750	HEM	CMC-C2C-C3C	4.32	127.32	116.53
2	A	750	HEM	CAD-C3D-C2D	4.57	126.36	113.22
2	B	750	HEM	CAD-C3D-C2D	4.93	127.39	113.22
2	A	750	HEM	CMC-C2C-C3C	5.03	129.09	116.53
3	B	760	H4B	C4-C4A-C8A	5.74	119.76	114.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	750	HEM	2	0
2	B	750	HEM	3	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

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^{th} 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	408/422 (96%)	0.68	53 (12%) 5 8	13, 35, 71, 104	0
1	B	411/422 (97%)	0.08	18 (4%) 38 49	11, 26, 53, 93	0
All	All	819/844 (97%)	0.38	71 (8%) 13 20	11, 30, 68, 104	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	717	LYS	7.9
1	B	348	VAL	7.6
1	A	715	VAL	7.4
1	B	300	PHE	6.5
1	A	488	PRO	6.1
1	A	716	TRP	5.6
1	B	350	THR	5.0
1	A	352	ASP	4.4
1	A	355	PHE	4.1
1	A	388	ILE	3.8
1	A	351	LYS	3.7
1	B	619	ARG	3.6
1	B	718	GLY	3.6
1	A	506	ILE	3.6
1	A	486	LYS	3.5
1	A	551	PHE	3.5
1	B	620	LYS	3.5
1	A	350	THR	3.4
1	B	351	LYS	3.4
1	A	391	THR	3.4
1	A	712	ASN	3.4
1	A	300	PHE	3.4
1	A	490	GLY	3.3
1	A	508	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	491	SER	3.2
1	A	299	ARG	3.1
1	B	302	LYS	3.1
1	A	489	ASP	3.0
1	A	487	GLN	3.0
1	A	389	GLU	3.0
1	A	321	THR	3.0
1	A	390	SER	3.0
1	A	553	TRP	2.9
1	B	352	ASP	2.9
1	A	511	LYS	2.8
1	A	311	VAL	2.8
1	A	386	LYS	2.7
1	A	493	LEU	2.7
1	A	619	ARG	2.7
1	B	299	ARG	2.7
1	A	514	ARG	2.6
1	A	713	THR	2.5
1	A	504	ILE	2.5
1	A	507	GLN	2.5
1	A	354	LEU	2.4
1	A	714	HIS	2.4
1	B	616	LEU	2.3
1	B	667	ARG	2.3
1	A	567	VAL	2.2
1	B	349	ARG	2.2
1	A	393	THR	2.2
1	B	611	ALA	2.2
1	A	711	TRP	2.2
1	A	392	SER	2.2
1	A	552	ASP	2.1
1	B	615	ASP	2.1
1	A	415	CYS	2.1
1	A	584	PHE	2.1
1	A	643	SER	2.1
1	B	677	VAL	2.1
1	A	385	ASN	2.1
1	A	682	PRO	2.1
1	B	617	ASP	2.1
1	A	550	LYS	2.1
1	A	677	VAL	2.1
1	A	681	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	321	THR	2.0
1	A	373	GLY	2.0
1	A	505	CYS	2.0
1	A	566	ALA	2.0
1	A	467	ASP	2.0

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, 95^{th} 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	ACT	A	860	4/4	0.92	0.18	3.69	37,41,42,46	0
5	ACT	B	860	4/4	0.96	0.13	1.84	27,33,34,41	0
4	HLW	A	800	24/24	0.94	0.20	1.26	10,26,55,77	0
2	HEM	B	750	43/43	0.98	0.14	0.96	5,16,25,31	0
4	HLW	B	800	24/24	0.95	0.15	0.88	11,23,51,67	0
2	HEM	A	750	43/43	0.98	0.16	0.67	9,19,28,30	0
3	H4B	B	760	17/17	0.97	0.14	0.37	11,18,25,26	0
3	H4B	A	760	17/17	0.97	0.13	0.30	10,18,26,27	0
6	ZN	A	1717	1/1	1.00	0.06	-1.28	25,25,25,25	0

6.5 Other polymers (i)

There are no such residues in this entry.