Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:38 PM GMT

PDB ID	:	3UFO
Title	:	Structure of rat nitric oxide synthase heme domain in complex with 6-(((3S,4S)-4-((5-(3-fluorophenyl)pentyl)oxy)pyrrolidin-3-yl)methyl)-4-methylpyridin-2-amine
Authors	:	Li, H.; Poulos, T.L.
Deposited on	:	2011-11-01
Resolution	:	2.17 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:

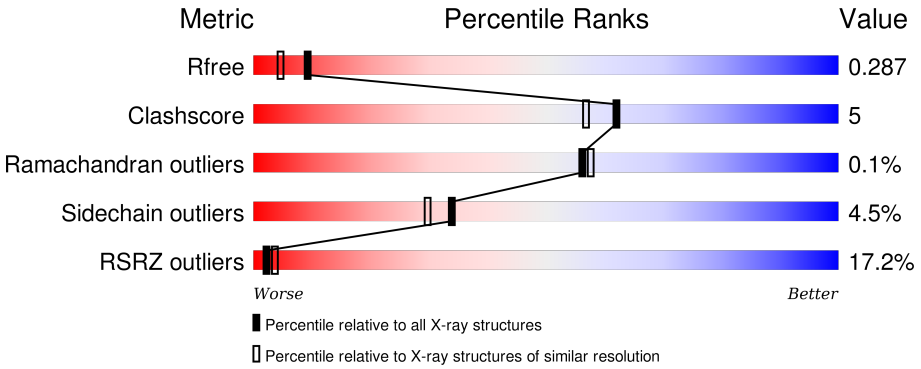
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.17 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	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

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	22% 84% 11%
1	B	422	11% 83% 13%

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
4	ACT	A	860	-	-	-	X
5	HW4	B	800[A]	-	-	-	X
5	HW4	B	800[B]	-	-	-	X

2 Entry composition

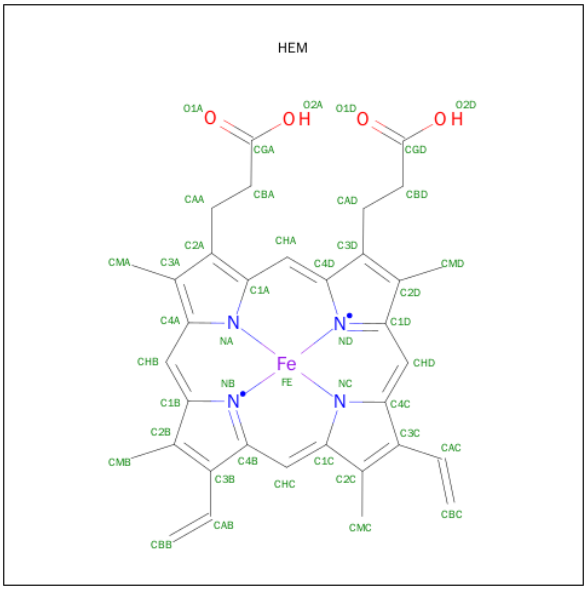
There are 7 unique types of molecules in this entry. The entry contains 7068 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

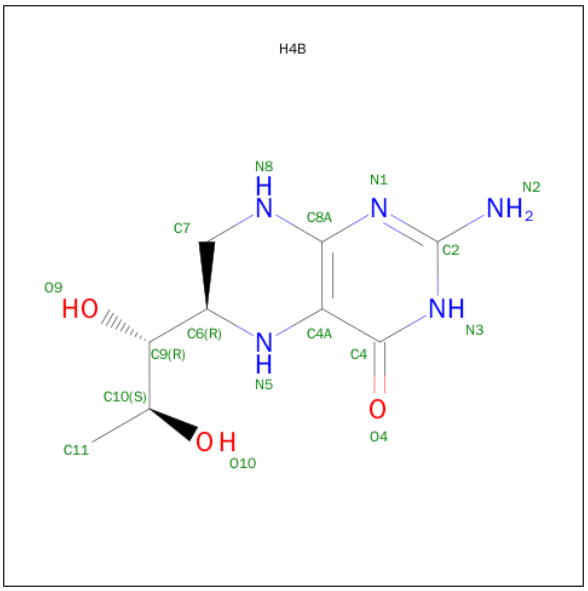
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	407	Total	C	N	O	S	0	2	0
			3322	2127	567	606	22			
1	B	411	Total	C	N	O	S	0	2	0
			3357	2150	574	611	22			

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



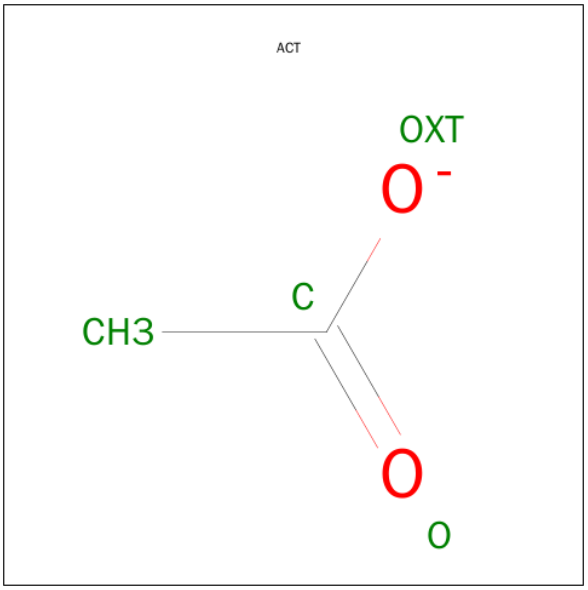
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



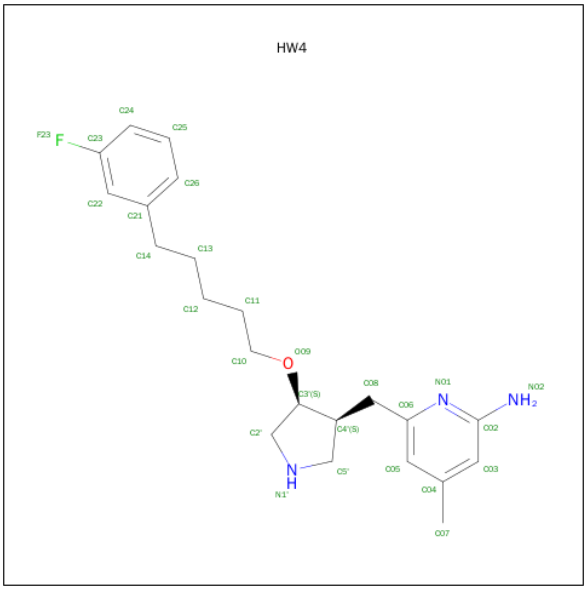
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 17 9 5 3	0	0
3	B	1	Total C N O 17 9 5 3	0	0

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 5 is 6-{[(3S,4S)-4-{[5-(3-FLUOROPHENYL)PENTYL]OXY}PYRROLIDIN-3-YL]METHYL}-4-METHYLPYRIDIN-2-AMINE (three-letter code: HW4) (formula: $C_{22}H_{30}FN_3O$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	F	N	O	0	0
			27	22	1	3	1		
5	B	1	Total	C	F	N	O	0	1
			38	32	2	3	1		

- 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.

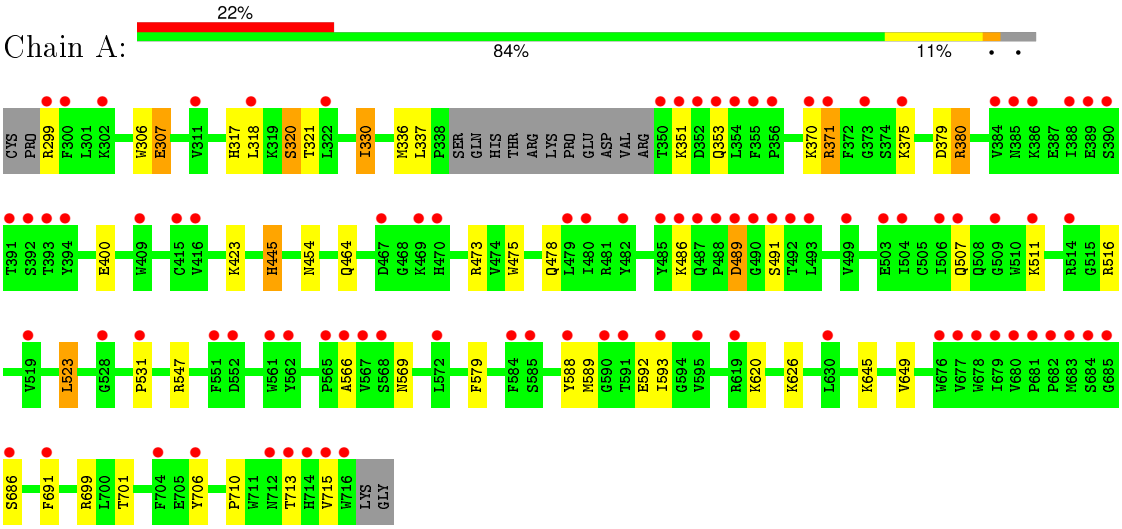
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	81	Total	O	0	0
			81	81		
7	B	114	Total	O	0	0
			114	114		

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.

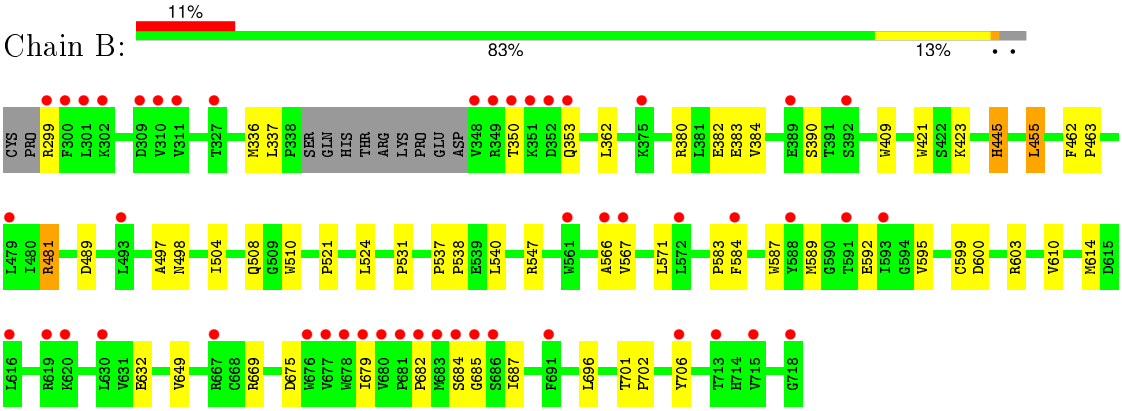
- Molecule 1: Nitric oxide synthase, brain

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	52.19Å 111.58Å 165.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.69 – 2.17 38.69 – 2.17	Depositor EDS
% Data completeness (in resolution range)	96.9 (38.69-2.17) 96.9 (38.69-2.17)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.07 (at 2.18Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.198 , 0.254 0.238 , 0.287	Depositor DCC
R_{free} test set	2525 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	42.2	Xtriage
Anisotropy	0.641	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 48.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	1 of 50397 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7068	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.70% 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: HEM, ZN, HW4, 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	0.72	0/3421	0.72	0/4641
1	B	0.87	1/3457 (0.0%)	0.80	2/4687 (0.0%)
All	All	0.80	1/6878 (0.0%)	0.76	2/9328 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	497	ALA	CA-CB	5.37	1.63	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	489	ASP	CB-CG-OD2	5.79	123.51	118.30
1	B	669	ARG	NE-CZ-NH2	-5.76	117.42	120.30

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	3322	0	3234	32	0
1	B	3357	0	3273	36	0
2	A	43	0	30	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	43	0	30	8	0
3	A	17	0	15	0	0
3	B	17	0	15	1	0
4	A	4	0	3	0	0
4	B	4	0	3	0	0
5	A	27	0	30	3	0
5	B	38	0	28	4	0
6	A	1	0	0	0	0
7	A	81	0	0	0	0
7	B	114	0	0	1	0
All	All	7068	0	6661	73	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 5.

All (73) 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:371:ARG:HH21	1:A:371:ARG:HG2	1.21	1.00
5:B:800[A]:HW4:H3	5:B:800[A]:HW4:H10	1.46	0.98
1:A:371:ARG:CG	1:A:371:ARG:HH21	1.80	0.94
1:A:371:ARG:HG2	1:A:371:ARG:NH2	1.84	0.88
1:A:523:LEU:HD22	1:A:531:PRO:HB2	1.59	0.85
1:A:330:ILE:HD11	1:B:696:LEU:HD22	1.69	0.75
1:A:686:SER:HB3	1:B:682:PRO:HB2	1.71	0.70
1:A:317:HIS:O	1:A:320:SER:HB3	1.92	0.69
1:A:380:ARG:HD3	1:A:400:GLU:OE1	1.95	0.66
1:B:706[A]:TYR:OH	2:B:750:HEM:O2D	2.17	0.59
1:A:626:LYS:HB3	1:B:687:ILE:HD12	1.85	0.58
1:A:475:TRP:HB2	1:A:523:LEU:HB3	1.85	0.58
1:A:523:LEU:CD2	1:A:531:PRO:HB2	2.33	0.57
1:A:592:GLU:OE1	5:A:800:HW4:H21	2.04	0.57
1:A:706:TYR:OH	2:A:750:HEM:O2D	2.19	0.56
5:B:800[A]:HW4:H3	5:B:800[A]:HW4:C12	2.29	0.56
1:B:504:ILE:O	1:B:508:GLN:HG2	2.06	0.55
5:B:800[A]:HW4:H10	5:B:800[A]:HW4:C26	2.27	0.55
1:B:445:HIS:C	1:B:445:HIS:CD2	2.81	0.54
1:A:473:ARG:NH2	1:A:710:PRO:HD3	2.22	0.54
1:B:409:TRP:CE3	1:B:421:TRP:HA	2.44	0.53
1:B:299:ARG:HB3	1:B:299:ARG:NH1	2.25	0.51
1:B:337:LEU:HD21	1:B:706[B]:TYR:CD2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:750:HEM:HBA2	5:A:800:HW4:H23	1.92	0.51
1:B:584:PHE:CD1	2:B:750:HEM:HAC	2.45	0.51
1:A:306:TRP:CD1	1:B:336:MET:HE2	2.46	0.50
1:B:380:ARG:NH1	1:B:383:GLU:OE2	2.43	0.50
1:B:587:TRP:H	2:B:750:HEM:HAB	1.77	0.50
2:A:750:HEM:C1C	5:A:800:HW4:H31	2.47	0.50
1:B:706[A]:TYR:OH	2:B:750:HEM:CGD	2.60	0.49
1:B:675:ASP:O	1:B:679:ILE:HG12	2.13	0.49
1:A:699:ARG:HG3	1:A:699:ARG:NH1	2.28	0.48
1:A:307:GLU:HG2	7:B:32:HOH:O	2.14	0.48
1:B:589:MET:HA	1:B:649:VAL:O	2.14	0.48
1:B:701:THR:HA	1:B:702:PRO:C	2.34	0.48
1:A:489:ASP:HB3	1:A:491:SER:OG	2.13	0.47
1:A:686:SER:HA	1:A:691:PHE:CG	2.50	0.47
1:A:321:THR:HG21	1:A:701:THR:HG22	1.96	0.47
1:B:614:MET:CE	1:B:632:GLU:HG3	2.45	0.47
2:B:750:HEM:O1A	3:B:760:H4B:N2	2.44	0.46
1:A:699:ARG:HH11	1:A:699:ARG:HG3	1.81	0.46
1:A:299:ARG:HE	1:A:318:LEU:HD13	1.81	0.45
1:A:478:GLN:HA	1:A:566:ALA:O	2.17	0.45
1:A:464:GLN:HB3	1:A:579:PHE:CE2	2.52	0.45
1:B:510:TRP:CD1	1:B:521:PRO:HG3	2.52	0.45
1:B:537:PRO:HA	1:B:538:PRO:HD3	1.90	0.45
1:B:362:LEU:HD11	1:B:384:VAL:HG21	1.99	0.45
1:B:571:LEU:HD23	1:B:571:LEU:C	2.37	0.44
1:B:600:ASP:HB2	1:B:603:ARG:HG2	1.98	0.44
1:B:584:PHE:CD1	2:B:750:HEM:CAC	3.01	0.44
1:A:445:HIS:C	1:A:445:HIS:CD2	2.90	0.44
1:A:686:SER:CB	1:B:682:PRO:HB2	2.43	0.43
5:B:800[B]:HW4:H8	5:B:800[B]:HW4:H4	1.76	0.43
1:A:423:LYS:HE2	1:A:423:LYS:HB2	1.96	0.43
1:B:455:LEU:HD23	1:B:587:TRP:HB3	2.00	0.43
1:B:684:SER:O	1:B:685:GLY:C	2.57	0.43
1:A:588:TYR:CD1	1:A:593:ILE:HD11	2.54	0.42
1:B:595:VAL:O	1:B:599:CYS:HB2	2.19	0.42
1:B:610:VAL:O	1:B:614:MET:HG3	2.19	0.42
1:A:371:ARG:CG	1:A:371:ARG:NH2	2.50	0.42
1:A:375:LYS:NZ	1:A:379:ASP:OD1	2.53	0.41
1:B:462:PHE:HB3	1:B:463:PRO:CD	2.50	0.41
1:B:567:VAL:O	1:B:583:PRO:HA	2.20	0.41
2:A:750:HEM:CMC	2:A:750:HEM:HBC2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:614:MET:HE1	1:B:632:GLU:HG3	2.01	0.41
1:B:566:ALA:HA	1:B:584:PHE:O	2.21	0.41
1:A:706:TYR:OH	2:A:750:HEM:CGD	2.69	0.41
1:B:481:ARG:HD3	1:B:498:ASN:ND2	2.36	0.41
1:A:589:MET:HA	1:A:649:VAL:O	2.21	0.40
1:B:524:LEU:O	1:B:531:PRO:HA	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	405/422 (96%)	386 (95%)	18 (4%)	1 (0%)	52 51
1	B	409/422 (97%)	388 (95%)	21 (5%)	0	100 100
All	All	814/844 (96%)	774 (95%)	39 (5%)	1 (0%)	56 57

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	351	LYS

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%)	342 (94%)	23 (6%)	22 16
1	B	368/377 (98%)	358 (97%)	10 (3%)	52 53
All	All	733/754 (97%)	700 (96%)	33 (4%)	34 30

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	307	GLU
1	A	320	SER
1	A	330	ILE
1	A	336	MET
1	A	337	LEU
1	A	353	GLN
1	A	370	LYS
1	A	371	ARG
1	A	380	ARG
1	A	445	HIS
1	A	454	ASN
1	A	486	LYS
1	A	489	ASP
1	A	507	GLN
1	A	511	LYS
1	A	516	ARG
1	A	523	LEU
1	A	547	ARG
1	A	569	ASN
1	A	620	LYS
1	A	645	LYS
1	A	713	THR
1	A	715	VAL
1	B	350	THR
1	B	353	GLN
1	B	382	GLU
1	B	390	SER
1	B	423	LYS
1	B	445	HIS
1	B	455	LEU
1	B	481	ARG
1	B	540	LEU
1	B	547	ARG

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	454	ASN
1	A	507	GLN
1	A	527	ASN
1	A	569	ASN
1	A	642	GLN
1	A	697	ASN
1	A	712	ASN
1	B	353	GLN
1	B	364	GLN
1	B	385	ASN
1	B	425	GLN
1	B	454	ASN
1	B	508	GLN
1	B	601	ASN
1	B	605	ASN
1	B	642	GLN
1	B	697	ASN

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 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	$\#\|Z\|>2$
2	HEM	A	750	1	30,50,50	2.56	8 (26%)	24,82,82	2.58	10 (41%)
3	H4B	A	760	-	13,18,18	0.82	0	11,26,26	2.70	6 (54%)
5	HW4	A	800	-	26,29,29	0.82	2 (7%)	29,38,38	1.23	3 (10%)
4	ACT	A	860	-	1,3,3	2.14	1 (100%)	0,3,3	0.00	-
2	HEM	B	750	1	30,50,50	2.10	8 (26%)	24,82,82	2.67	12 (50%)
3	H4B	B	760	-	13,18,18	1.31	2 (15%)	11,26,26	2.97	6 (54%)
5	HW4	B	800[A]	-	26,29,29	0.76	0	29,38,38	1.62	5 (17%)
5	HW4	B	800[B]	-	26,29,29	0.74	0	29,38,38	1.72	5 (17%)
4	ACT	B	860	-	1,3,3	1.88	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	-	0/10/54/54	0/0/8/8
3	H4B	A	760	-	-	0/8/17/17	0/2/2/2
5	HW4	A	800	-	-	0/13/23/23	0/3/3/3
4	ACT	A	860	-	-	0/0/0/0	0/0/0/0
2	HEM	B	750	1	-	0/10/54/54	0/0/8/8
3	H4B	B	760	-	-	0/8/17/17	0/2/2/2
5	HW4	B	800[A]	-	-	0/13/23/23	0/3/3/3
5	HW4	B	800[B]	-	-	0/13/23/23	0/3/3/3
4	ACT	B	860	-	-	0/0/0/0	0/0/0/0

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	750	HEM	C3B-C4B	-7.59	1.45	1.51
2	A	750	HEM	C3D-C4D	-7.36	1.42	1.51
2	B	750	HEM	C3B-C4B	-6.65	1.45	1.51
2	A	750	HEM	C2C-C1C	-4.29	1.44	1.52
2	B	750	HEM	C3D-C4D	-4.19	1.46	1.51
2	B	750	HEM	C2C-C1C	-3.56	1.45	1.52
2	B	750	HEM	C2B-C1B	-2.35	1.44	1.51
2	A	750	HEM	C2D-C1D	-2.10	1.45	1.51
5	A	800	HW4	C24-C23	2.07	1.41	1.37
2	B	750	HEM	C4C-NC	2.12	1.38	1.36
4	A	860	ACT	CH3-C	2.14	1.51	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	760	H4B	C4-N3	2.17	1.37	1.33
5	A	800	HW4	C22-C23	2.28	1.41	1.37
2	A	750	HEM	CAA-C2A	2.29	1.55	1.52
2	A	750	HEM	CMA-C3A	2.33	1.56	1.51
2	A	750	HEM	C3B-CAB	2.44	1.55	1.51
2	B	750	HEM	FE-NC	2.51	2.05	1.95
3	B	760	H4B	C7-N8	2.63	1.49	1.46
2	B	750	HEM	FE-ND	2.79	2.12	1.97
2	B	750	HEM	C3C-CAC	2.99	1.56	1.51
2	A	750	HEM	C1C-NC	3.33	1.40	1.36

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	750	HEM	C3C-CAC-CBC	-5.47	116.07	124.46
2	B	750	HEM	CAA-CBA-CGA	-4.14	105.17	112.75
2	A	750	HEM	C3C-CAC-CBC	-4.06	118.23	124.46
2	A	750	HEM	CBA-CAA-C2A	-4.04	105.28	112.53
5	B	800[B]	HW4	C05-C06-N01	-3.75	118.72	122.96
5	B	800[A]	HW4	C05-C06-N01	-3.75	118.72	122.96
2	B	750	HEM	CAA-C2A-C1A	-3.36	123.36	127.01
5	B	800[B]	HW4	C24-C23-C22	-3.12	119.33	123.35
3	B	760	H4B	N3-C2-N1	-3.07	120.50	125.53
5	A	800	HW4	C05-C06-N01	-2.91	119.67	122.96
3	A	760	H4B	N3-C2-N1	-2.84	120.88	125.53
2	B	750	HEM	C3B-CAB-CBB	-2.63	120.42	124.46
5	A	800	HW4	C24-C23-C22	-2.44	120.20	123.35
2	B	750	HEM	C3B-C4B-NB	-2.25	107.33	111.63
5	B	800[A]	HW4	C24-C23-C22	-2.23	120.47	123.35
5	B	800[B]	HW4	C07-C04-C05	-2.20	117.60	120.95
5	B	800[A]	HW4	C07-C04-C05	-2.20	117.60	120.95
5	A	800	HW4	C07-C04-C05	-2.13	117.71	120.95
2	A	750	HEM	CAD-CBD-CGD	-2.11	104.43	113.02
3	A	760	H4B	C2-N1-C8A	2.18	119.45	114.54
2	B	750	HEM	CMD-C2D-C3D	2.20	124.06	114.35
5	B	800[B]	HW4	C5'-C4'-C3'	2.21	106.21	103.35
5	B	800[A]	HW4	C5'-C4'-C3'	2.21	106.21	103.35
2	B	750	HEM	C3B-C4B-CHC	2.39	126.53	123.16
2	B	750	HEM	C2C-C1C-CHC	2.46	127.42	123.68
2	A	750	HEM	CMD-C2D-C3D	2.48	125.34	114.35
3	A	760	H4B	N2-C2-N3	2.62	121.53	117.20
3	B	760	H4B	C2-N1-C8A	2.70	120.61	114.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	760	H4B	C4A-C8A-N8	2.72	121.63	118.43
2	A	750	HEM	CMB-C2B-C3B	2.91	123.80	116.53
2	A	750	HEM	CAD-C3D-C4D	2.94	122.84	112.47
3	A	760	H4B	C4A-C8A-N8	3.35	122.38	118.43
2	A	750	HEM	C3B-C4B-CHC	3.39	127.93	123.16
2	A	750	HEM	C2D-C3D-C4D	3.45	107.36	101.50
3	B	760	H4B	N2-C2-N3	3.68	123.30	117.20
2	B	750	HEM	CMC-C2C-C3C	4.02	126.56	116.53
3	B	760	H4B	C4-N3-C2	4.12	121.66	115.94
2	B	750	HEM	CAD-C3D-C2D	4.22	125.35	113.22
2	B	750	HEM	CMB-C2B-C3B	4.37	127.44	116.53
3	A	760	H4B	C4-N3-C2	4.42	122.07	115.94
2	B	750	HEM	CAD-C3D-C4D	5.00	130.09	112.47
3	A	760	H4B	C4-C4A-C8A	5.27	119.34	114.56
2	A	750	HEM	CMC-C2C-C3C	5.32	129.82	116.53
5	B	800[B]	HW4	C02-N01-C06	5.75	122.32	118.23
5	B	800[A]	HW4	C02-N01-C06	5.75	122.32	118.23
2	A	750	HEM	CAD-C3D-C2D	5.76	129.77	113.22
3	B	760	H4B	C4-C4A-C8A	6.06	120.05	114.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	750	HEM	5	0
5	A	800	HW4	3	0
2	B	750	HEM	8	0
3	B	760	H4B	1	0
5	B	800[A]	HW4	3	0
5	B	800[B]	HW4	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

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	407/422 (96%)	1.17	93 (22%) 1 2	31, 61, 103, 131	0
1	B	411/422 (97%)	0.67	48 (11%) 6 10	31, 48, 74, 95	0
All	All	818/844 (96%)	0.92	141 (17%) 2 4	31, 53, 95, 131	0

All (141) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	716	TRP	8.4
1	B	300	PHE	7.7
1	B	348	VAL	6.7
1	A	488	PRO	6.4
1	A	486	LYS	5.7
1	A	352	ASP	5.6
1	B	718	GLY	5.6
1	A	355	PHE	5.6
1	A	351	LYS	5.4
1	B	706[A]	TYR	5.1
1	B	351	LYS	5.0
1	A	300	PHE	4.7
1	A	390	SER	4.7
1	A	714	HIS	4.7
1	A	415	CYS	4.5
1	A	715	VAL	4.4
1	B	350	THR	4.4
1	B	677	VAL	4.4
1	A	567	VAL	4.4
1	A	388	ILE	4.3
1	B	681	PRO	4.2
1	A	713	THR	4.2
1	A	350	THR	4.1
1	A	679	ILE	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	489	ASP	4.1
1	A	392	SER	3.9
1	A	681	PRO	3.9
1	A	370	LYS	3.7
1	A	386	LYS	3.7
1	A	593	ILE	3.7
1	A	490	GLY	3.7
1	A	677	VAL	3.7
1	B	619	ARG	3.6
1	B	310	VAL	3.6
1	A	678	TRP	3.6
1	A	503	GLU	3.5
1	A	385	ASN	3.5
1	A	561	TRP	3.5
1	A	299	ARG	3.4
1	B	667	ARG	3.4
1	B	715	VAL	3.4
1	A	391	THR	3.3
1	A	591	THR	3.3
1	B	299	ARG	3.3
1	A	506	ILE	3.3
1	A	619	ARG	3.3
1	B	479	LEU	3.3
1	B	616	LEU	3.3
1	B	680	VAL	3.2
1	A	588	TYR	3.2
1	A	469	LYS	3.2
1	A	480	ILE	3.2
1	A	584	PHE	3.2
1	A	682	PRO	3.1
1	A	511	LYS	3.1
1	A	479	LEU	3.1
1	A	389	GLU	3.1
1	B	349	ARG	3.1
1	B	375	LYS	3.0
1	A	373	GLY	3.0
1	A	470	HIS	3.0
1	B	353	GLN	3.0
1	A	566	ALA	3.0
1	B	561	TRP	2.9
1	A	356	PRO	2.9
1	A	630	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	507	GLN	2.9
1	B	302	LYS	2.9
1	B	691	PHE	2.9
1	A	487	GLN	2.9
1	B	684	SER	2.9
1	A	528	GLY	2.9
1	A	311	VAL	2.9
1	B	352	ASP	2.8
1	A	393	THR	2.8
1	A	322	LEU	2.8
1	A	706	TYR	2.8
1	B	685	GLY	2.8
1	B	567	VAL	2.7
1	B	620	LYS	2.7
1	B	686	SER	2.7
1	A	302	LYS	2.7
1	A	416	VAL	2.7
1	B	566	ALA	2.7
1	A	482	TYR	2.7
1	B	682	PRO	2.6
1	A	552	ASP	2.6
1	A	491	SER	2.6
1	A	467	ASP	2.6
1	A	704	PHE	2.6
1	B	584	PHE	2.6
1	A	499	VAL	2.6
1	A	514	ARG	2.6
1	A	595	VAL	2.6
1	A	683	MET	2.6
1	B	679	ILE	2.6
1	A	680	VAL	2.5
1	A	493	LEU	2.5
1	B	678	TRP	2.5
1	A	354	LEU	2.5
1	A	676	TRP	2.5
1	A	712	ASN	2.5
1	A	685	GLY	2.5
1	A	572	LEU	2.5
1	A	531	PRO	2.5
1	B	389	GLU	2.4
1	B	591	THR	2.4
1	B	676	TRP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	394	TYR	2.4
1	A	585	SER	2.4
1	A	590	GLY	2.4
1	A	384	VAL	2.4
1	A	485	TYR	2.4
1	A	492	THR	2.4
1	A	551	PHE	2.4
1	B	392	SER	2.4
1	A	565	PRO	2.3
1	A	318	LEU	2.3
1	A	568	SER	2.3
1	B	630	LEU	2.3
1	A	684	SER	2.3
1	A	353	GLN	2.2
1	B	683	MET	2.2
1	B	593	ILE	2.2
1	A	409	TRP	2.2
1	B	327	THR	2.2
1	A	504	ILE	2.2
1	A	691	PHE	2.2
1	B	713	THR	2.1
1	B	572	LEU	2.1
1	B	309	ASP	2.1
1	A	371	ARG	2.1
1	B	301	LEU	2.1
1	A	562	TYR	2.1
1	B	493	LEU	2.0
1	A	509	GLY	2.0
1	A	686	SER	2.0
1	A	519	VAL	2.0
1	B	311	VAL	2.0
1	B	588	TYR	2.0
1	A	375	LYS	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

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	HW4	B	800[A]	27/27	0.89	0.51	6.93	36,55,70,73	11
4	ACT	A	860	4/4	0.95	0.24	3.17	59,59,59,61	0
5	HW4	B	800[B]	27/27	0.89	0.51	3.03	36,55,75,75	11
2	HEM	A	750	43/43	0.96	0.26	0.84	36,41,58,63	0
4	ACT	B	860	4/4	0.97	0.12	0.44	53,54,55,55	0
2	HEM	B	750	43/43	0.97	0.20	0.27	33,39,52,55	0
3	H4B	A	760	17/17	0.95	0.18	0.05	42,49,53,55	0
3	H4B	B	760	17/17	0.95	0.17	-0.12	37,41,46,47	0
5	HW4	A	800	27/27	0.86	0.21	-0.22	9,25,65,66	0
6	ZN	A	900	1/1	0.98	0.09	-1.40	46,46,46,46	0

6.5 Other polymers

There are no such residues in this entry.