



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:38 PM GMT

PDB ID : 3UFR  
Title : Structure of rat nitric oxide synthase heme domain in complex with 6-(((3R,4R)-4-(((E)-5-(3-fluorophenyl)pent-4-en-1-yl)oxy)pyrrolidin-3-yl)methyl)-4-methylpyridin-2-amine  
Authors : Li, H.; Poulos, T.L.  
Deposited on : 2011-11-01  
Resolution : 2.10 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (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

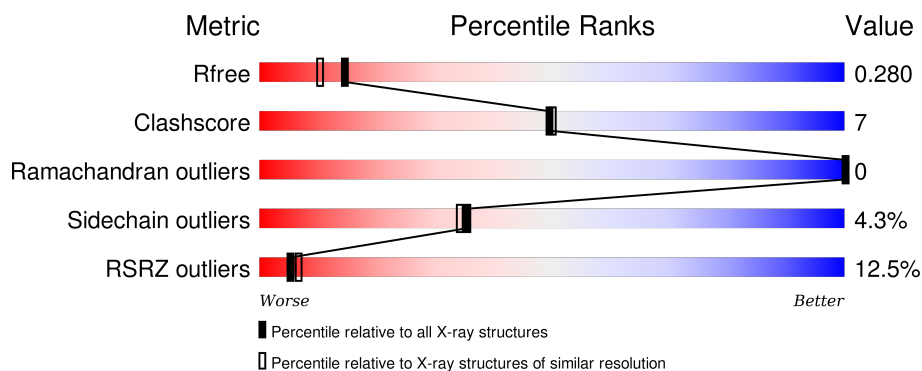
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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. 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  $\leq 5\%$ . 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	<div> <div>15%</div> <div> <div></div> <div>80%</div> <div>15%</div> <div>..</div> </div> </div>
1	B	422	<div> <div>9%</div> <div> <div></div> <div>81%</div> <div>15%</div> <div>..</div> </div> </div>

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	H5W	A	800	-	-	-	X
4	H5W	B	800[A]	-	-	-	X
4	H5W	B	800[B]	-	-	-	X

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 7097 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	0	0
			3313	2121	566	605	21			
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:  $C_{34}H_{32}FeN_4O_4$ ).



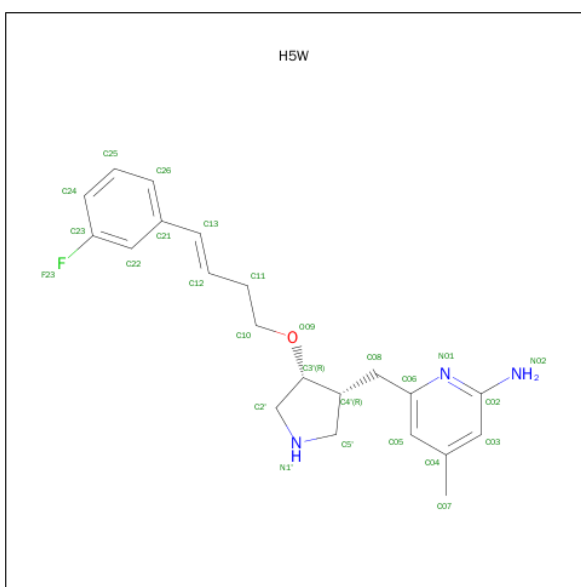
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- 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 17	C 9	N 5	O 3	0	0
3	B	1	Total 17	C 9	N 5	O 3	0	0

- Molecule 4 is 6-{\{[(3R,4R)-4-{\{[(3E)-4-(3-FLUOROPHENYL)BUT-3-EN-1-YL]OXY}PYRROLIDIN-3-YL]METHYL}-4-METHYLPYRIDIN-2-AMINE (three-letter code: H5W) (formula: C<sub>21</sub>H<sub>26</sub>FN<sub>3</sub>O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	0	0
			26	21	1	3	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	F	N	O	0	1
			52	42	2	6	2		

- 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		

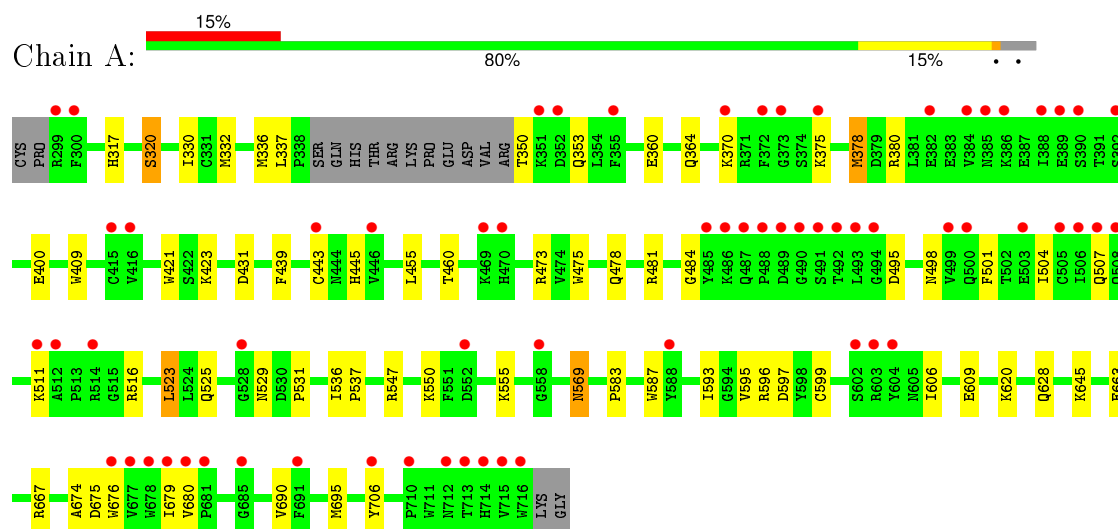
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	84	Total	O	0	0
			84	84		
7	B	136	Total	O	0	0
			136	136		

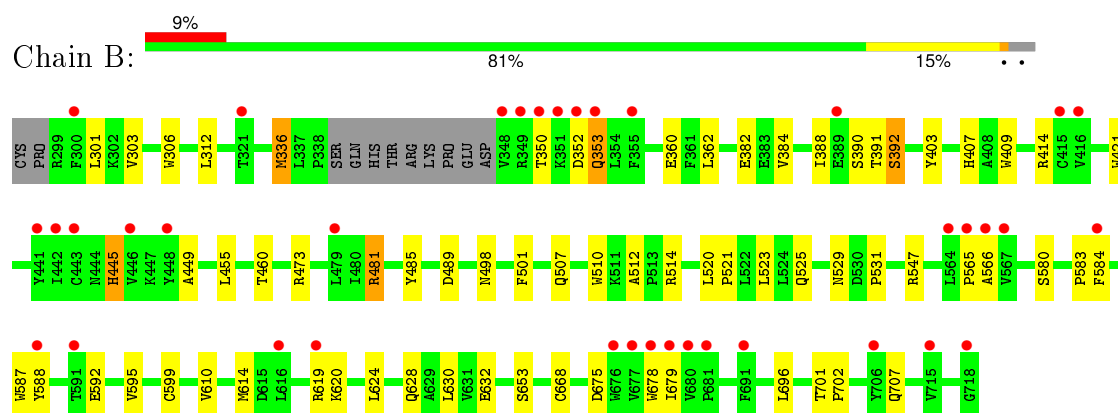
### 3 Residue-property plots

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



- Molecule 1: Nitric oxide synthase, brain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	51.87Å 111.34Å 164.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.10 – 2.10 46.10 – 2.10	Depositor EDS
% Data completeness (in resolution range)	96.8 (46.10-2.10) 96.7 (46.10-2.10)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.31 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.199 , 0.249 0.234 , 0.280	Depositor DCC
$R_{free}$ test set	2704 reflections (5.18%)	DCC
Wilson B-factor (Å <sup>2</sup> )	39.9	Xtriage
Anisotropy	0.417	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 48.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 54933 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7097	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.62% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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, H5W, 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	0/3406	0.73	0/4621
1	B	0.83	0/3457	0.80	1/4687 (0.0%)
All	All	0.78	0/6863	0.77	1/9308 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	489	ASP	CB-CG-OD2	6.45	124.10	118.30

There are no chirality outliers.

There are no planarity outliers.

### 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	3313	0	3221	43	0
1	B	3357	0	3273	49	0
2	A	43	0	30	3	0
2	B	43	0	30	7	0
3	A	17	0	15	1	0
3	B	17	0	15	2	0
4	A	26	0	26	3	0
4	B	52	0	52	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	4	0	3	0	0
5	B	4	0	3	0	0
6	A	1	0	0	0	0
7	A	84	0	0	3	0
7	B	136	0	0	0	0
All	All	7097	0	6668	96	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 7.

All (96) 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:B:592:GLU:OE1	4:B:800[B]:H5W:H3	1.57	1.04
1:B:481:ARG:HD3	1:B:498:ASN:HD21	1.26	0.99
2:A:750:HEM:HMC2	2:A:750:HEM:HBC2	1.55	0.89
1:A:523:LEU:HD22	1:A:531:PRO:HB2	1.58	0.85
1:B:353:GLN:H	1:B:353:GLN:HE21	1.30	0.76
1:B:481:ARG:HD3	1:B:498:ASN:ND2	2.02	0.71
1:A:317:HIS:O	1:A:320:SER:HB3	1.89	0.70
1:B:584:PHE:CD1	2:B:750:HEM:HAC	2.32	0.64
2:B:750:HEM:C1C	4:B:800[A]:H5W:H27	2.33	0.63
1:B:350:THR:HB	1:B:353:GLN:HE22	1.63	0.63
1:B:587:TRP:H	2:B:750:HEM:HAB	1.64	0.63
1:A:596:ARG:HH22	3:A:760:H4B:C4	2.11	0.62
1:A:525:GLN:HG3	1:A:529:ASN:O	2.00	0.62
1:B:336:MET:HG2	4:B:800[B]:H5W:H27	1.83	0.60
1:A:380:ARG:HD3	1:A:400:GLU:OE1	2.02	0.59
1:A:706:TYR:CE2	4:A:800:H5W:H3	2.38	0.58
1:A:478:GLN:HB2	1:A:481:ARG:HG3	1.86	0.57
1:B:350:THR:HB	1:B:353:GLN:NE2	2.20	0.56
1:B:481:ARG:NH1	1:B:498:ASN:OD1	2.37	0.56
1:B:595:VAL:O	1:B:599:CYS:HB2	2.06	0.56
1:A:596:ARG:NH1	1:A:596:ARG:HG3	2.21	0.56
1:B:350:THR:HG22	1:B:352:ASP:H	1.71	0.56
1:A:507:GLN:O	1:A:507:GLN:HG2	2.07	0.55
1:B:460:THR:O	1:B:583:PRO:HD2	2.05	0.55
1:B:584:PHE:CD1	2:B:750:HEM:CAC	2.89	0.55
1:A:330:ILE:HD11	1:B:696:LEU:HB3	1.88	0.55
2:A:750:HEM:CMC	2:A:750:HEM:HBC2	2.34	0.54
1:B:353:GLN:N	1:B:353:GLN:HE21	2.02	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:569:ASN:H	1:A:569:ASN:HD22	1.55	0.54
1:A:674:ALA:HB3	1:A:695:MET:HB3	1.91	0.52
1:A:475:TRP:CZ2	1:A:531:PRO:HG3	2.46	0.51
1:A:336:MET:HG3	1:B:306:TRP:CE2	2.45	0.51
1:A:460:THR:O	1:A:583:PRO:HD2	2.12	0.50
2:A:750:HEM:C1C	4:A:800:H5W:H27	2.46	0.50
2:B:750:HEM:O2D	4:B:800[B]:H5W:N01	2.45	0.49
1:A:501:PHE:HA	1:A:504:ILE:HD12	1.95	0.49
1:A:595:VAL:O	1:A:599:CYS:HB2	2.13	0.49
4:A:800:H5W:H12	4:A:800:H5W:H7	1.95	0.48
1:B:565:PRO:HB3	1:B:588:TYR:CZ	2.48	0.48
1:B:473:ARG:HD2	1:B:580:SER:O	2.13	0.48
1:B:388:ILE:O	1:B:392:SER:HA	2.14	0.47
1:B:675:ASP:O	1:B:679:ILE:HG12	2.15	0.47
1:B:445:HIS:C	1:B:445:HIS:CD2	2.88	0.47
1:B:523:LEU:CD1	1:B:531:PRO:HB2	2.45	0.47
1:A:628:GLN:NE2	1:B:632:GLU:OE2	2.47	0.46
1:A:596:ARG:HH11	1:A:596:ARG:HG3	1.80	0.46
1:A:378:MET:HA	1:A:378:MET:CE	2.45	0.46
1:B:391:THR:O	1:B:392:SER:HB2	2.14	0.46
1:B:353:GLN:H	1:B:353:GLN:NE2	2.08	0.46
1:B:409:TRP:CE3	1:B:421:TRP:HA	2.51	0.46
1:A:596:ARG:NH2	7:A:87:HOH:O	2.48	0.45
1:B:619:ARG:HB2	1:B:619:ARG:CZ	2.46	0.45
2:B:750:HEM:O1A	3:B:760:H4B:N2	2.41	0.45
1:A:439:PHE:CZ	1:A:443:CYS:SG	3.10	0.45
1:B:485:TYR:CE1	1:B:514:ARG:HA	2.51	0.45
1:A:593:ILE:HA	1:A:597:ASP:HB2	1.99	0.44
1:B:303:VAL:HG22	1:B:312:LEU:HB2	1.98	0.44
1:A:439:PHE:CE2	1:A:443:CYS:SG	3.11	0.44
1:B:455:LEU:CD1	1:B:455:LEU:N	2.80	0.44
1:A:445:HIS:C	1:A:445:HIS:CD2	2.90	0.44
1:B:403:TYR:CE1	1:B:407:HIS:CE1	3.06	0.44
1:A:667:ARG:HD3	7:A:136:HOH:O	2.17	0.44
1:B:624:LEU:O	1:B:628:GLN:HG3	2.18	0.44
1:A:536:ILE:O	1:A:537:PRO:C	2.55	0.43
1:B:336:MET:HE1	3:B:760:H4B:H9	2.00	0.43
1:B:388:ILE:O	1:B:392:SER:N	2.51	0.43
1:B:362:LEU:HD11	1:B:384:VAL:HG21	2.00	0.43
1:B:414:ARG:HD3	1:B:678:TRP:CD2	2.53	0.43
1:B:595:VAL:HG22	1:B:630:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:LEU:HD12	1:A:587:TRP:HB3	2.01	0.43
1:B:501:PHE:HD2	1:B:520:LEU:HD13	1.84	0.43
1:B:610:VAL:O	1:B:614:MET:HG3	2.19	0.42
1:B:336:MET:HE2	1:B:336:MET:HB2	1.69	0.42
1:B:566:ALA:HA	1:B:584:PHE:O	2.19	0.42
1:A:676:TRP:CE2	1:A:680:VAL:HG21	2.54	0.42
1:B:525:GLN:HG3	1:B:529:ASN:O	2.19	0.42
1:A:455:LEU:HD12	1:A:587:TRP:CB	2.49	0.42
1:A:550:LYS:HB2	1:A:550:LYS:HE3	1.96	0.42
1:B:701:THR:HA	1:B:702:PRO:C	2.40	0.42
1:A:431:ASP:C	1:A:431:ASP:OD2	2.56	0.42
1:A:484:GLY:HA3	1:A:495:ASP:O	2.20	0.41
1:A:409:TRP:CE3	1:A:421:TRP:HA	2.55	0.41
1:A:569:ASN:N	1:A:569:ASN:HD22	2.17	0.41
1:A:606:ILE:HA	1:A:609:GLU:OE1	2.20	0.41
1:A:473:ARG:NH2	7:A:72:HOH:O	2.54	0.41
1:A:475:TRP:HB2	1:A:523:LEU:HB3	2.03	0.41
1:B:391:THR:O	1:B:392:SER:CB	2.68	0.41
1:B:485:TYR:OH	1:B:512:ALA:HB1	2.21	0.41
1:B:449:ALA:O	1:B:455:LEU:HA	2.21	0.41
1:A:680:VAL:HG22	1:A:690:VAL:HG23	2.03	0.41
1:A:675:ASP:O	1:A:679:ILE:HG12	2.21	0.41
1:A:332:MET:CE	1:B:301:LEU:HD13	2.51	0.40
1:A:481:ARG:HD3	1:A:498:ASN:HD21	1.86	0.40
1:A:360:GLU:O	1:A:364:GLN:HG2	2.21	0.40
2:B:750:HEM:C2C	4:B:800[A]:H5W:H27	2.56	0.40
1:B:510:TRP:CE2	1:B:521:PRO:HD3	2.57	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	403/422 (96%)	386 (96%)	17 (4%)	0	100	100
1	B	409/422 (97%)	391 (96%)	18 (4%)	0	100	100
All	All	812/844 (96%)	777 (96%)	35 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	363/377 (96%)	346 (95%)	17 (5%)	32	30
1	B	368/377 (98%)	353 (96%)	15 (4%)	37	36
All	All	731/754 (97%)	699 (96%)	32 (4%)	35	33

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	320	SER
1	A	337	LEU
1	A	350	THR
1	A	353	GLN
1	A	370	LYS
1	A	375	LYS
1	A	378	MET
1	A	423	LYS
1	A	511	LYS
1	A	516	ARG
1	A	523	LEU
1	A	547	ARG
1	A	555	LYS
1	A	569	ASN
1	A	620	LYS
1	A	645	LYS
1	A	663	GLU
1	B	336	MET

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Mol	Chain	Res	Type
1	B	353	GLN
1	B	360	GLU
1	B	382	GLU
1	B	390	SER
1	B	392	SER
1	B	445	HIS
1	B	481	ARG
1	B	507	GLN
1	B	547	ARG
1	B	620	LYS
1	B	653	SER
1	B	668[A]	CYS
1	B	668[B]	CYS
1	B	707	GLN

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	353	GLN
1	A	454	ASN
1	A	569	ASN
1	A	697	ASN
1	B	353	GLN
1	B	385	ASN
1	B	425	GLN
1	B	454	ASN
1	B	535	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	2.39	7 (23%)	24,82,82	2.71	12 (50%)
3	H4B	A	760	-	13,18,18	0.73	0	11,26,26	2.42	5 (45%)
4	H5W	A	800	-	25,28,28	1.05	3 (12%)	27,37,37	1.47	4 (14%)
5	ACT	A	860	-	1,3,3	2.08	1 (100%)	0,3,3	0.00	-
2	HEM	B	750	1	30,50,50	2.12	9 (30%)	24,82,82	2.69	11 (45%)
3	H4B	B	760	-	13,18,18	1.04	1 (7%)	11,26,26	2.61	5 (45%)
4	H5W	B	800[A]	-	25,28,28	0.97	1 (4%)	27,37,37	1.78	5 (18%)
4	H5W	B	800[B]	-	25,28,28	0.70	0	27,37,37	1.84	6 (22%)
5	ACT	B	860	-	1,3,3	1.50	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
4	H5W	A	800	-	-	0/12/22/22	0/3/3/3
5	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
4	H5W	B	800[A]	-	-	0/12/22/22	0/3/3/3
4	H5W	B	800[B]	-	-	0/12/22/22	0/3/3/3
5	ACT	B	860	-	-	0/0/0/0	0/0/0/0

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	750	HEM	C3D-C4D	-7.42	1.42	1.51
2	A	750	HEM	C3B-C4B	-7.10	1.45	1.51
2	B	750	HEM	C3B-C4B	-6.05	1.46	1.51
2	B	750	HEM	C3D-C4D	-5.32	1.44	1.51
2	B	750	HEM	C2C-C1C	-4.23	1.44	1.52
2	A	750	HEM	C2C-C1C	-3.41	1.46	1.52
2	A	750	HEM	C2D-C1D	-2.20	1.44	1.51
2	B	750	HEM	C2B-C1B	-2.09	1.45	1.51
2	A	750	HEM	C3B-CAB	2.02	1.55	1.51
3	B	760	H4B	C7-N8	2.02	1.48	1.46
2	B	750	HEM	C4C-NC	2.04	1.38	1.36
2	B	750	HEM	FE-ND	2.07	2.08	1.97
5	A	860	ACT	CH3-C	2.08	1.51	1.48
4	A	800	H5W	C22-C23	2.10	1.41	1.37
4	B	800[A]	H5W	C11-C10	2.16	1.54	1.51
2	B	750	HEM	C1C-NC	2.20	1.38	1.36
4	A	800	H5W	C24-C23	2.21	1.41	1.37
2	B	750	HEM	FE-NC	2.46	2.05	1.95
2	A	750	HEM	FE-NC	2.52	2.05	1.95
4	A	800	H5W	C11-C10	2.64	1.55	1.51
2	B	750	HEM	CMA-C3A	2.74	1.57	1.51
2	A	750	HEM	C1C-NC	3.27	1.40	1.36

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	750	HEM	CBA-CAA-C2A	-5.39	102.86	112.53
2	B	750	HEM	C3C-CAC-CBC	-5.23	116.44	124.46
4	B	800[A]	H5W	C05-C06-N01	-4.29	118.12	122.96
2	B	750	HEM	CAA-C2A-C1A	-4.02	122.64	127.01
4	B	800[B]	H5W	C05-C06-N01	-3.86	118.61	122.96
4	A	800	H5W	C05-C06-N01	-3.50	119.00	122.96
4	B	800[B]	H5W	C11-C12-C13	-3.40	118.95	125.24
2	A	750	HEM	C3C-CAC-CBC	-3.33	119.35	124.46
2	A	750	HEM	CBD-CAD-C3D	-3.16	104.37	113.55
4	B	800[A]	H5W	C11-C12-C13	-3.13	119.45	125.24
2	B	750	HEM	C3B-CAB-CBB	-3.08	119.73	124.46
3	B	760	H4B	N3-C2-N1	-2.88	120.82	125.53
4	A	800	H5W	C11-C12-C13	-2.74	120.17	125.24
2	A	750	HEM	CAA-C2A-C1A	-2.74	124.04	127.01
2	B	750	HEM	CBD-CAD-C3D	-2.72	105.65	113.55
2	A	750	HEM	CAA-CBA-CGA	-2.55	108.08	112.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	760	H4B	N3-C2-N1	-2.36	121.67	125.53
2	B	750	HEM	CAA-CBA-CGA	-2.32	108.50	112.75
4	A	800	H5W	C24-C23-C22	-2.29	120.40	123.35
4	B	800[A]	H5W	C24-C23-C22	-2.19	120.52	123.35
2	A	750	HEM	CMA-C3A-C4A	-2.09	124.91	128.36
4	B	800[B]	H5W	C24-C23-C22	-2.02	120.75	123.35
3	B	760	H4B	C2-N1-C8A	2.00	119.04	114.54
2	B	750	HEM	C2D-C3D-C4D	2.11	105.07	101.50
4	B	800[B]	H5W	N02-C02-N01	2.17	120.46	116.50
3	A	760	H4B	C2-N1-C8A	2.22	119.53	114.54
2	B	750	HEM	CMD-C2D-C3D	2.36	124.79	114.35
4	B	800[B]	H5W	C5'-C4'-C3'	2.72	106.88	103.35
3	B	760	H4B	C4A-C8A-N8	2.77	121.70	118.43
2	A	750	HEM	C3B-C4B-CHC	3.07	127.48	123.16
2	A	750	HEM	CMB-C2B-C3B	3.14	124.37	116.53
4	A	800	H5W	C02-N01-C06	3.14	120.46	118.23
2	A	750	HEM	CAD-C3D-C4D	3.41	124.49	112.47
4	B	800[A]	H5W	N02-C02-N01	3.42	122.73	116.50
2	A	750	HEM	C2D-C3D-C4D	3.49	107.42	101.50
3	A	760	H4B	C4A-C8A-N8	3.52	122.57	118.43
3	A	760	H4B	C4-N3-C2	3.83	121.26	115.94
2	B	750	HEM	CMC-C2C-C3C	4.13	126.83	116.53
2	B	750	HEM	CMB-C2B-C3B	4.37	127.45	116.53
2	B	750	HEM	CAD-C3D-C4D	4.52	128.40	112.47
2	B	750	HEM	CAD-C3D-C2D	4.61	126.47	113.22
3	B	760	H4B	C4-N3-C2	4.66	122.41	115.94
2	A	750	HEM	CMC-C2C-C3C	4.72	128.30	116.53
3	A	760	H4B	C4-C4A-C8A	4.74	118.85	114.56
4	B	800[A]	H5W	C02-N01-C06	4.83	121.66	118.23
3	B	760	H4B	C4-C4A-C8A	5.13	119.20	114.56
2	A	750	HEM	CAD-C3D-C2D	5.16	128.04	113.22
4	B	800[B]	H5W	C02-N01-C06	6.20	122.64	118.23

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	750	HEM	3	0
3	A	760	H4B	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	800	H5W	3	0
2	B	750	HEM	7	0
3	B	760	H4B	2	0
4	B	800[A]	H5W	2	0
4	B	800[B]	H5W	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<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	407/422 (96%)	0.92	65 (15%) 3 4	28, 57, 98, 131	0
1	B	411/422 (97%)	0.59	37 (9%) 12 16	29, 46, 69, 95	0
All	All	818/844 (96%)	0.76	102 (12%) 5 7	28, 51, 93, 131	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	350	THR	8.7
1	A	488	PRO	6.9
1	B	300	PHE	6.4
1	A	486	LYS	6.1
1	A	716	TRP	5.9
1	B	718	GLY	5.7
1	A	373	GLY	5.1
1	B	348	VAL	4.9
1	A	505	CYS	4.6
1	A	355	PHE	4.5
1	A	715	VAL	4.3
1	B	706[A]	TYR	4.2
1	A	388	ILE	4.0
1	A	713	THR	3.9
1	A	493	LEU	3.9
1	B	352	ASP	3.9
1	B	677	VAL	3.8
1	A	677	VAL	3.7
1	A	351	LYS	3.6
1	B	567	VAL	3.6
1	A	385	ASN	3.5
1	A	714	HIS	3.5
1	B	619	ARG	3.4
1	A	491	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	375	LYS	3.3
1	A	507	GLN	3.3
1	A	389	GLU	3.2
1	A	506	ILE	3.2
1	B	565	PRO	3.1
1	A	679	ILE	3.1
1	B	566	ALA	3.0
1	A	676	TRP	3.0
1	A	503	GLU	3.0
1	A	386	LYS	2.9
1	A	712	ASN	2.9
1	A	352	ASP	2.9
1	B	584	PHE	2.8
1	B	691	PHE	2.8
1	A	602	SER	2.8
1	B	679	ILE	2.8
1	A	390	SER	2.8
1	B	591	THR	2.8
1	A	678	TRP	2.8
1	B	564	LEU	2.8
1	A	485	TYR	2.7
1	A	490	GLY	2.7
1	B	616	LEU	2.7
1	B	676	TRP	2.7
1	B	446	VAL	2.7
1	A	487	GLN	2.7
1	A	604	TYR	2.7
1	B	321	THR	2.7
1	B	416	VAL	2.6
1	A	494	GLY	2.6
1	A	691	PHE	2.6
1	B	349	ARG	2.6
1	A	446	VAL	2.6
1	B	443	CYS	2.6
1	B	351	LYS	2.6
1	A	528	GLY	2.6
1	A	685	GLY	2.6
1	B	588	TYR	2.5
1	B	353	GLN	2.5
1	A	514	ARG	2.5
1	A	558	GLY	2.5
1	A	299	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	370	LYS	2.5
1	A	489	ASP	2.4
1	A	384	VAL	2.4
1	A	499	VAL	2.4
1	B	715	VAL	2.4
1	B	681	PRO	2.4
1	A	443	CYS	2.4
1	A	372	PHE	2.4
1	A	392	SER	2.4
1	B	389	GLU	2.4
1	A	416	VAL	2.3
1	B	442	ILE	2.3
1	B	680	VAL	2.3
1	A	492	THR	2.3
1	A	508	GLN	2.3
1	B	479	LEU	2.3
1	A	603	ARG	2.3
1	A	710	PRO	2.3
1	A	382	GLU	2.3
1	A	470	HIS	2.2
1	A	588	TYR	2.2
1	B	415	CYS	2.2
1	B	678	TRP	2.2
1	A	511	LYS	2.2
1	B	441	TYR	2.1
1	A	552	ASP	2.1
1	A	300	PHE	2.1
1	A	680	VAL	2.1
1	A	469	LYS	2.1
1	A	500	GLN	2.1
1	A	706	TYR	2.1
1	B	355	PHE	2.1
1	A	415	CYS	2.1
1	A	681	PRO	2.0
1	A	512	ALA	2.0
1	B	448	TYR	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 [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<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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	H5W	B	800[A]	26/26	0.86	0.38	2.83	41,66,86,88	26
4	H5W	B	800[B]	26/26	0.86	0.38	2.78	47,56,64,66	26
4	H5W	A	800	26/26	0.88	0.26	2.20	39,69,96,97	0
5	ACT	A	860	4/4	0.96	0.19	1.30	59,60,60,60	0
2	HEM	B	750	43/43	0.98	0.23	0.60	25,35,47,58	0
3	H4B	A	760	17/17	0.90	0.21	0.58	44,47,55,56	0
3	H4B	B	760	17/17	0.92	0.21	0.52	34,40,46,48	0
2	HEM	A	750	43/43	0.97	0.19	0.43	31,37,50,57	0
6	ZN	A	900	1/1	1.00	0.13	-0.51	40,40,40,40	0
5	ACT	B	860	4/4	0.96	0.11	-0.96	49,49,52,52	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.