



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 03:45 pm BST

PDB ID : 3UFT  
Title : Structure of rat nitric oxide synthase heme domain in complex with 6-(((3R,4R)-4-(4-(3-chloro-5-fluorophenoxy)butoxy)pyrrolidin-3-yl)methyl)-4-methylpyridin-2-amine  
Authors : Li, H.; Poulos, T.L.  
Deposited on : 2011-11-01  
Resolution : 2.08 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

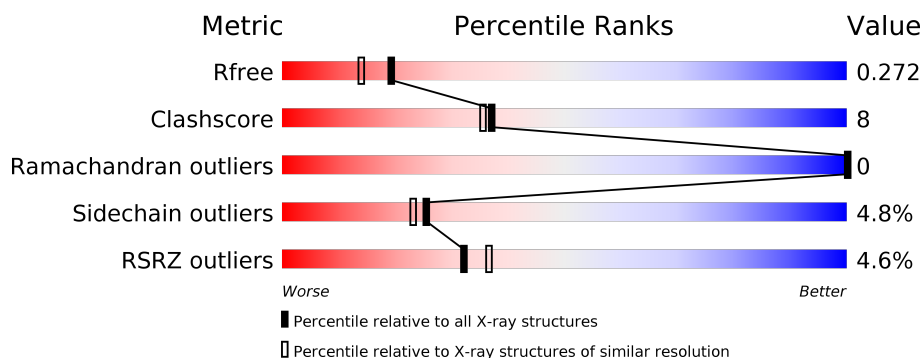
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.08 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))
$R_{free}$	130704	6189 (2.10-2.06)
Clashscore	141614	6738 (2.10-2.06)
Ramachandran outliers	138981	6663 (2.10-2.06)
Sidechain outliers	138945	6664 (2.10-2.06)
RSRZ outliers	127900	6057 (2.10-2.06)

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 respectively. 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>6%</div> <div> <div></div> <div>76%</div> <div>18%</div> <div>• •</div> </div> </div>
1	B	422	<div> <div>3%</div> <div> <div></div> <div>79%</div> <div>17%</div> <div>• •</div> </div> </div>

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 7013 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	1	0
			3348	2142	574	610	22			

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



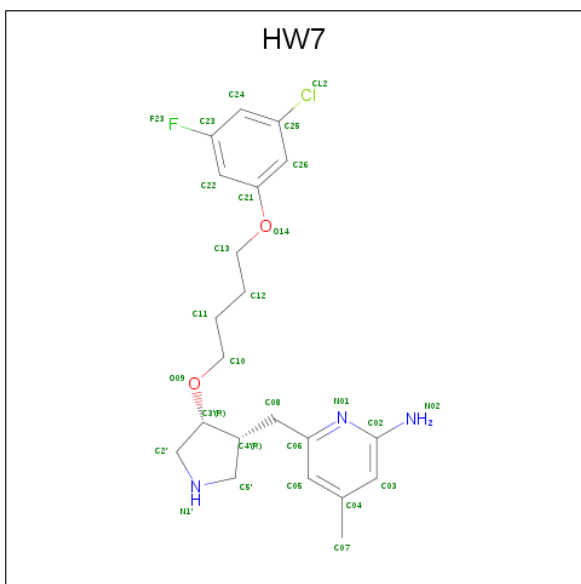
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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

- Molecule 4 is 6-((3R,4R)-4-[4-(3-chloro-5-fluorophenoxy)butoxy]pyrrolidin-3-yl)methyl)-4-methylpyridin-2-amine (three-letter code: HW7) (formula: C<sub>21</sub>H<sub>27</sub>ClFN<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	Cl	F	N	O	0	0
			28	21	1	1	3	2		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	B	1	Total	C	Cl	F	N	O	0	0
			28	21	1	1	3	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		

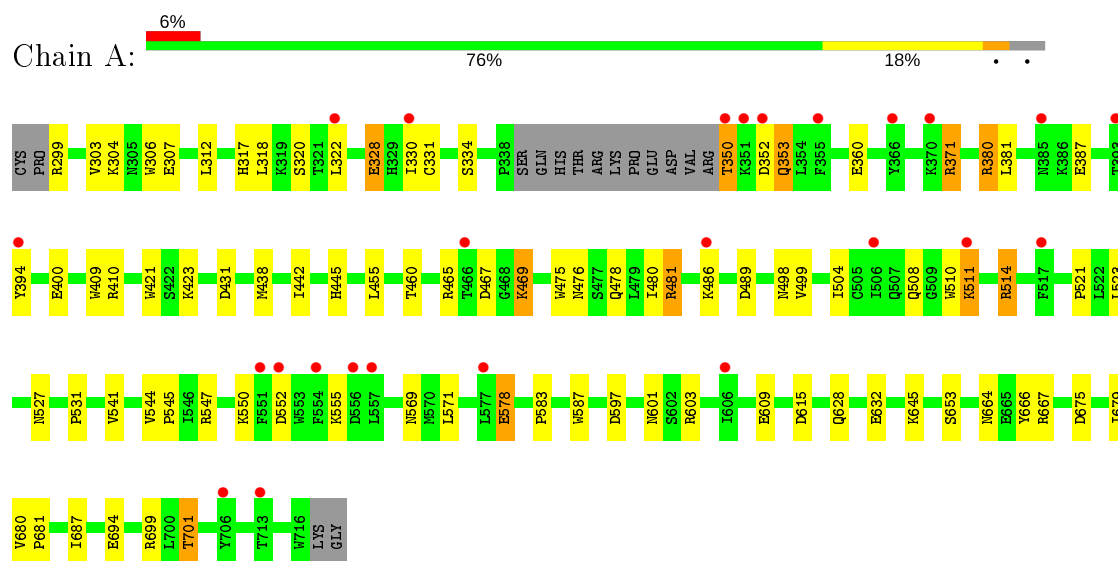
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	69	Total	O	0	0
			69	69		
7	B	98	Total	O	0	0
			98	98		

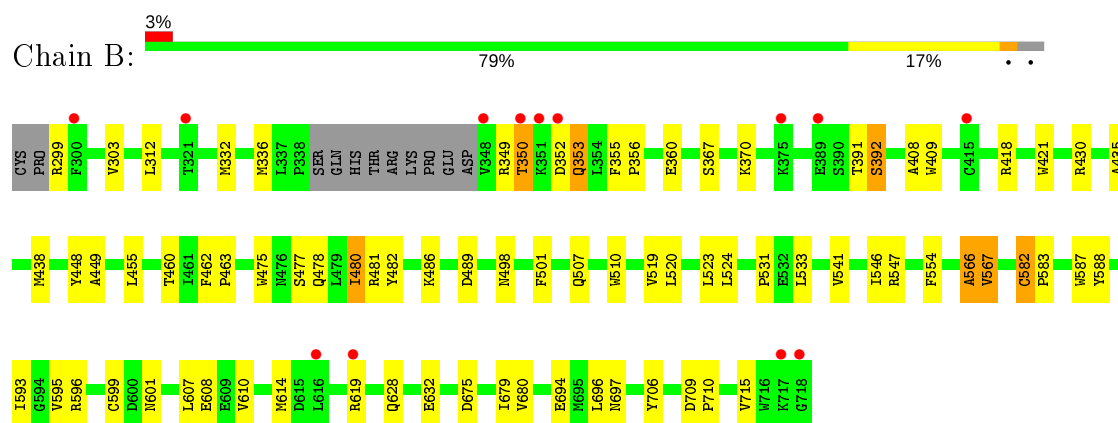
### 3 Residue-property plots [i](#)

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



- 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, $\alpha$ , $\beta$ , $\gamma$	51.84Å 111.22Å 164.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.99 – 2.08 46.99 – 2.08	Depositor EDS
% Data completeness (in resolution range)	99.1 (46.99-2.08) 99.1 (46.99-2.08)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.18 (at 2.08Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.206 , 0.260 0.230 , 0.272	Depositor DCC
$R_{free}$ test set	2848 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.7	Xtriage
Anisotropy	0.391	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 52.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7013	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.77% 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, 0.333 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: HW7, ZN, H4B, HEM, 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	0.84	1/3406 (0.0%)	0.84	1/4621 (0.0%)
1	B	1.02	9/3444 (0.3%)	0.93	4/4669 (0.1%)
All	All	0.94	10/6850 (0.1%)	0.88	5/9290 (0.1%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	421	TRP	CB-CG	7.27	1.63	1.50
1	B	706	TYR	CD1-CE1	6.57	1.49	1.39
1	B	482	TYR	CD2-CE2	-5.88	1.30	1.39
1	B	477	SER	C-O	-5.65	1.12	1.23
1	B	706	TYR	CD2-CE2	5.55	1.47	1.39
1	B	567	VAL	CB-CG1	5.52	1.64	1.52
1	B	582	CYS	CB-SG	5.22	1.91	1.82
1	A	609	GLU	CG-CD	5.12	1.59	1.51
1	B	566	ALA	C-O	5.08	1.33	1.23
1	B	408	ALA	CA-CB	-5.05	1.41	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	489	ASP	CB-CG-OD2	7.64	125.18	118.30
1	A	410	ARG	NE-CZ-NH2	7.59	124.10	120.30
1	B	430	ARG	NE-CZ-NH1	5.81	123.21	120.30
1	B	418	ARG	NE-CZ-NH1	-5.67	117.47	120.30
1	B	596	ARG	NE-CZ-NH2	-5.07	117.77	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	3313	0	3221	61	0
1	B	3348	0	3264	52	0
2	A	43	0	30	1	0
2	B	43	0	30	3	0
3	A	17	0	15	0	0
3	B	17	0	15	0	0
4	A	28	0	27	0	0
4	B	28	0	27	1	0
5	A	4	0	3	0	0
5	B	4	0	3	0	0
6	A	1	0	0	0	0
7	A	69	0	0	1	0
7	B	98	0	0	3	0
All	All	7013	0	6635	105	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 8.

All (105) 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:587:TRP:H	2:B:750:HEM:HAB	1.47	0.79
1:A:511:LYS:O	1:A:511:LYS:HD2	1.86	0.76
1:A:514:ARG:HH21	1:A:514:ARG:CG	2.02	0.73
1:A:460:THR:O	1:A:583:PRO:HD2	1.92	0.69
1:A:322:LEU:HB2	1:A:699:ARG:HB2	1.77	0.67
1:A:478:GLN:HB2	1:A:481:ARG:HG3	1.78	0.66
1:A:481:ARG:HD3	1:A:498:ASN:HD21	1.65	0.61
1:B:610:VAL:O	1:B:614:MET:HG3	2.01	0.61
1:A:475:TRP:HB2	1:A:523:LEU:HB3	1.83	0.60
1:A:514:ARG:HG3	1:A:514:ARG:HH21	1.66	0.59
2:B:750:HEM:O2D	4:B:800:HW7:N01	2.36	0.59
1:A:317:HIS:O	1:A:320:SER:HB3	2.04	0.58
1:B:349:ARG:HG2	1:B:350:THR:H	1.68	0.58
1:A:409:TRP:CE3	1:A:421:TRP:HA	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:480:ILE:HA	7:B:31:HOH:O	2.05	0.57
1:A:571:LEU:HD21	1:A:578:GLU:HB3	1.86	0.56
1:B:391:THR:O	1:B:392:SER:HB2	2.06	0.56
1:B:519:VAL:HG21	1:B:541:VAL:HG11	1.87	0.55
1:A:514:ARG:NH2	1:A:514:ARG:CG	2.68	0.55
1:A:664:ASN:OD1	1:A:667:ARG:NH2	2.40	0.54
1:A:510:TRP:CD1	1:A:511:LYS:HE2	2.43	0.54
1:A:632:GLU:OE2	1:B:628:GLN:NE2	2.40	0.54
1:A:486:LYS:HE2	1:A:499:VAL:HG11	1.89	0.53
1:A:380:ARG:HD3	1:A:400:GLU:OE1	2.08	0.53
1:A:328:GLU:H	1:A:328:GLU:CD	2.10	0.53
1:A:675:ASP:O	1:A:679:ILE:HG12	2.09	0.53
1:A:350:THR:N	1:A:353:GLN:NE2	2.56	0.53
1:B:353:GLN:O	1:B:356:PRO:HG2	2.09	0.52
1:B:299:ARG:CZ	1:B:299:ARG:HB3	2.40	0.52
1:B:462:PHE:HB3	1:B:463:PRO:CD	2.41	0.51
1:A:504:ILE:O	1:A:508:GLN:N	2.43	0.51
1:B:481:ARG:CZ	1:B:498:ASN:OD1	2.59	0.51
1:B:595:VAL:O	1:B:599:CYS:HB2	2.10	0.51
1:A:303:VAL:HG23	1:A:312:LEU:HB2	1.91	0.50
1:A:481:ARG:HD3	1:A:498:ASN:ND2	2.27	0.50
1:A:303:VAL:CG2	1:A:312:LEU:HB2	2.41	0.50
1:A:469:LYS:HA	1:A:469:LYS:NZ	2.27	0.50
1:A:469:LYS:HA	1:A:469:LYS:HZ1	1.77	0.50
1:A:307:GLU:OE1	1:B:601:ASN:HB2	2.12	0.49
1:B:449:ALA:O	1:B:455:LEU:HA	2.13	0.49
1:A:334:SER:O	1:B:694:GLU:HG2	2.14	0.47
1:A:330:ILE:HG23	1:A:330:ILE:O	2.14	0.47
1:B:303:VAL:CG2	1:B:312:LEU:HB2	2.44	0.47
1:A:299:ARG:HG3	1:A:318:LEU:HD21	1.95	0.47
1:A:306:TRP:CD2	1:B:336:MET:HE3	2.49	0.47
1:A:628:GLN:NE2	1:B:632:GLU:OE2	2.48	0.47
1:A:306:TRP:CE2	1:B:336:MET:HE3	2.50	0.47
1:A:371:ARG:CG	1:A:371:ARG:HH21	2.27	0.46
1:A:687:ILE:HG21	1:B:607:LEU:HD11	1.97	0.46
1:A:445:HIS:C	1:A:445:HIS:CD2	2.89	0.46
1:A:438:MET:O	1:A:442:ILE:HG13	2.16	0.46
1:A:317:HIS:O	1:A:320:SER:CB	2.65	0.45
1:A:455:LEU:HD12	1:A:587:TRP:HB3	1.99	0.45
1:B:455:LEU:CD1	1:B:455:LEU:N	2.79	0.45
1:B:355:PHE:N	1:B:356:PRO:HD2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:601:ASN:HB2	7:A:48:HOH:O	2.16	0.45
1:A:330:ILE:HD11	1:B:696:LEU:HB3	1.98	0.45
1:A:571:LEU:C	1:A:571:LEU:HD23	2.37	0.45
1:B:409:TRP:CZ3	2:B:750:HEM:HMC3	2.51	0.45
2:A:750:HEM:CMC	2:A:750:HEM:HBC2	2.47	0.44
1:A:480:ILE:HD13	1:A:541:VAL:HG13	1.99	0.44
1:A:306:TRP:CD1	1:B:336:MET:HE2	2.53	0.44
1:A:514:ARG:HG2	1:A:514:ARG:HH21	1.81	0.44
1:A:360:GLU:OE1	1:A:701:THR:HG22	2.18	0.43
1:B:460:THR:O	1:B:582:CYS:HA	2.18	0.43
1:B:619:ARG:HB2	1:B:619:ARG:HE	1.51	0.43
1:A:597:ASP:OD1	1:A:603:ARG:NH2	2.50	0.43
1:A:523:LEU:HA	1:A:523:LEU:HD23	1.88	0.43
1:A:371:ARG:CG	1:A:371:ARG:NH2	2.82	0.43
1:B:303:VAL:HG23	1:B:312:LEU:HB2	2.01	0.43
1:B:435:ALA:O	1:B:438:MET:HB2	2.19	0.42
1:B:608:GLU:HG3	7:B:58:HOH:O	2.19	0.42
1:B:680:VAL:HB	7:B:167:HOH:O	2.18	0.42
1:A:387:GLU:OE1	1:A:394:TYR:HA	2.19	0.42
1:A:510:TRP:CE2	1:A:521:PRO:HD3	2.54	0.42
1:A:475:TRP:HB2	1:A:523:LEU:CB	2.50	0.42
1:B:350:THR:HG23	1:B:352:ASP:H	1.85	0.42
1:B:524:LEU:O	1:B:531:PRO:HA	2.19	0.42
1:A:467:ASP:C	1:A:467:ASP:OD1	2.58	0.42
1:B:567:VAL:O	1:B:583:PRO:HA	2.19	0.42
1:A:465:ARG:HD2	1:A:578:GLU:OE1	2.20	0.42
1:B:510:TRP:H	1:B:533:LEU:HD11	1.83	0.41
1:A:523:LEU:HD22	1:A:531:PRO:HB2	2.02	0.41
1:A:544:VAL:HA	1:A:545:PRO:HD2	1.93	0.41
1:A:312:LEU:HD13	1:A:666:TYR:CD1	2.55	0.41
1:B:350:THR:CG2	1:B:352:ASP:HB3	2.50	0.41
1:B:697:ASN:HA	1:B:697:ASN:HD22	1.60	0.41
1:B:675:ASP:O	1:B:679:ILE:HG12	2.21	0.41
1:B:478:GLN:HA	1:B:566:ALA:O	2.20	0.41
1:B:588:TYR:CD1	1:B:593:ILE:HD11	2.55	0.41
1:B:607:LEU:HD23	1:B:607:LEU:HA	1.94	0.41
1:A:331:CYS:HB3	1:B:697:ASN:HB3	2.03	0.41
1:B:448:TYR:C	1:B:448:TYR:CD2	2.94	0.41
1:B:510:TRP:H	1:B:533:LEU:CD1	2.34	0.41
1:B:367:SER:O	1:B:370:LYS:HD3	2.20	0.41
1:B:501:PHE:HD2	1:B:520:LEU:HD13	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:709:ASP:HA	1:B:710:PRO:HD3	1.86	0.41
1:B:501:PHE:CD2	1:B:520:LEU:HD13	2.55	0.41
1:B:475:TRP:HB2	1:B:523:LEU:HB3	2.02	0.41
1:B:475:TRP:CZ2	1:B:531:PRO:HG3	2.56	0.40
1:A:304:LYS:O	1:A:694:GLU:HG3	2.22	0.40
1:A:680:VAL:HA	1:A:681:PRO:HD3	1.73	0.40
1:B:455:LEU:H	1:B:455:LEU:CD1	2.34	0.40
1:B:546:ILE:HG22	1:B:554:PHE:CE1	2.57	0.40
1:A:431:ASP:OD2	1:A:431:ASP:C	2.59	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%)	382 (95%)	21 (5%)	0	100	100
1	B	408/422 (97%)	390 (96%)	18 (4%)	0	100	100
All	All	811/844 (96%)	772 (95%)	39 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 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	363/377 (96%)	338 (93%)	25 (7%)	15	12
1	B	367/377 (97%)	357 (97%)	10 (3%)	44	47
All	All	730/754 (97%)	695 (95%)	35 (5%)	25	23

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	328	GLU
1	A	350	THR
1	A	352	ASP
1	A	353	GLN
1	A	371	ARG
1	A	380	ARG
1	A	381	LEU
1	A	423	LYS
1	A	469	LYS
1	A	476	ASN
1	A	481	ARG
1	A	489	ASP
1	A	511	LYS
1	A	514	ARG
1	A	527	ASN
1	A	547	ARG
1	A	550	LYS
1	A	552	ASP
1	A	555	LYS
1	A	569	ASN
1	A	578	GLU
1	A	615	ASP
1	A	645	LYS
1	A	653	SER
1	A	701	THR
1	B	332	MET
1	B	350	THR
1	B	353	GLN
1	B	360	GLU
1	B	392	SER
1	B	480	ILE
1	B	486	LYS
1	B	507	GLN
1	B	547	ARG
1	B	715	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	353	GLN
1	A	454	ASN
1	A	470	HIS
1	A	487	GLN
1	A	569	ASN
1	A	601	ASN
1	A	628	GLN
1	A	697	ASN
1	B	364	GLN
1	B	385	ASN
1	B	425	GLN
1	B	454	ASN
1	B	601	ASN
1	B	605	ASN
1	B	697	ASN

### 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 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
3	H4B	A	760	-	16,18,18	1.04	1 (6%)	11,26,26	2.90	7 (63%)
5	ACT	A	860	-	1,3,3	0.23	0	0,3,3	0.00	-
5	ACT	B	860	-	1,3,3	1.26	0	0,3,3	0.00	-
2	HEM	A	750	1	27,50,50	2.31	8 (29%)	17,82,82	2.74	6 (35%)
3	H4B	B	760	-	16,18,18	1.54	3 (18%)	11,26,26	3.13	8 (72%)
4	HW7	A	800	-	29,30,30	1.19	3 (10%)	34,40,40	2.21	11 (32%)
4	HW7	B	800	-	29,30,30	1.38	3 (10%)	34,40,40	2.00	11 (32%)
2	HEM	B	750	1	27,50,50	2.44	11 (40%)	17,82,82	1.66	3 (17%)

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	H4B	A	760	-	-	0/8/17/17	0/2/2/2
2	HEM	A	750	1	-	0/6/54/54	-
3	H4B	B	760	-	-	0/8/17/17	0/2/2/2
4	HW7	A	800	-	-	3/13/23/23	0/3/3/3
4	HW7	B	800	-	-	7/13/23/23	0/3/3/3
2	HEM	B	750	1	-	0/6/54/54	-

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	750	HEM	C3B-C2B	-5.60	1.32	1.40
2	B	750	HEM	C3C-C2C	-5.20	1.33	1.40
2	A	750	HEM	C3D-C2D	5.02	1.52	1.37
2	B	750	HEM	C3D-C2D	4.62	1.51	1.37
2	B	750	HEM	CAD-C3D	4.54	1.60	1.52
2	A	750	HEM	C3C-C2C	-4.39	1.34	1.40
2	B	750	HEM	C3B-C2B	-4.34	1.34	1.40
4	B	800	HW7	C25-CL2	3.92	1.83	1.74
4	B	800	HW7	C06-N01	3.74	1.40	1.34
2	B	750	HEM	C3C-CAC	3.66	1.55	1.47
4	A	800	HW7	C25-CL2	3.48	1.82	1.74
2	A	750	HEM	C3B-CAB	3.40	1.54	1.47
3	B	760	H4B	C7-N8	3.28	1.50	1.44
4	B	800	HW7	C24-C23	3.15	1.43	1.37
2	A	750	HEM	CAD-C3D	3.03	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	750	HEM	C1A-NA	2.90	1.42	1.36
3	A	760	H4B	C4-C4A	-2.73	1.37	1.41
2	B	750	HEM	C3B-CAB	2.64	1.53	1.47
2	A	750	HEM	C3C-CAC	2.61	1.53	1.47
2	B	750	HEM	C4A-NA	2.50	1.41	1.36
3	B	760	H4B	C2-N2	2.50	1.38	1.33
2	B	750	HEM	CAA-C2A	2.48	1.55	1.52
2	A	750	HEM	CAA-C2A	2.37	1.55	1.52
4	A	800	HW7	C24-C23	2.35	1.41	1.37
4	A	800	HW7	F23-C23	-2.24	1.30	1.36
3	B	760	H4B	O4-C4	2.23	1.30	1.24
2	A	750	HEM	CMC-C2C	2.23	1.56	1.51
2	B	750	HEM	CMB-C2B	2.11	1.56	1.51
2	B	750	HEM	CMA-C3A	2.07	1.55	1.51

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	800	HW7	C02-N01-C06	6.23	122.82	118.10
2	A	750	HEM	CBA-CAA-C2A	-6.11	101.22	112.49
3	B	760	H4B	C4-C4A-C8A	5.87	119.79	114.57
2	A	750	HEM	C4C-C3C-C2C	5.58	110.79	106.90
2	A	750	HEM	CBD-CAD-C3D	-5.37	102.58	112.48
4	A	800	HW7	C24-C25-CL2	5.07	125.48	119.15
4	B	800	HW7	C24-C25-CL2	4.88	125.25	119.15
3	A	760	H4B	N3-C2-N1	-4.28	118.71	125.42
4	B	800	HW7	C21-C26-C25	4.13	122.96	118.14
3	B	760	H4B	C4-N3-C2	3.95	122.21	115.93
3	B	760	H4B	N2-C2-N3	3.91	123.34	117.25
4	B	800	HW7	C02-N01-C06	3.90	121.05	118.10
3	B	760	H4B	N3-C2-N1	-3.89	119.31	125.42
2	B	750	HEM	C4C-C3C-C2C	3.88	109.61	106.90
3	A	760	H4B	C4-C4A-N5	3.85	122.36	119.12
3	A	760	H4B	C4-N3-C2	3.61	121.66	115.93
4	A	800	HW7	F23-C23-C22	-3.61	113.10	118.25
3	A	760	H4B	C4-C4A-C8A	3.53	117.71	114.57
4	A	800	HW7	C5'-N1'-C2'	3.41	113.46	105.42
3	A	760	H4B	N2-C2-N3	3.36	122.48	117.25
4	A	800	HW7	C3'-C2'-N1'	-3.30	99.67	105.20
3	A	760	H4B	C2-N1-C8A	3.30	121.93	114.54
4	A	800	HW7	C21-C26-C25	3.19	121.87	118.14
3	B	760	H4B	C4-C4A-N5	3.19	121.80	119.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	800	HW7	C05-C06-N01	-3.14	119.57	122.90
4	B	800	HW7	O09-C3'-C2'	-3.02	103.37	111.42
3	A	760	H4B	C4A-N5-C6	-2.84	113.42	121.16
4	A	800	HW7	C26-C25-CL2	-2.82	115.63	119.15
4	B	800	HW7	C5'-N1'-C2'	2.72	111.83	105.42
4	B	800	HW7	F23-C23-C24	2.62	122.00	118.25
2	A	750	HEM	CMA-C3A-C4A	-2.56	124.53	128.46
4	B	800	HW7	C3'-C2'-N1'	-2.53	100.95	105.20
4	A	800	HW7	F23-C23-C24	2.53	121.87	118.25
2	A	750	HEM	CAD-CBD-CGD	-2.52	108.44	112.67
4	A	800	HW7	C05-C06-N01	-2.52	120.23	122.90
4	B	800	HW7	C26-C25-C24	-2.47	118.59	121.66
3	B	760	H4B	C2-N1-C8A	2.47	120.08	114.54
2	B	750	HEM	C3C-C4C-NC	-2.43	106.36	110.94
4	B	800	HW7	C26-C25-CL2	-2.42	116.12	119.15
2	A	750	HEM	C4A-C3A-C2A	2.37	108.64	107.00
4	A	800	HW7	C26-C25-C24	-2.23	118.89	121.66
4	B	800	HW7	C10-O09-C3'	2.21	118.99	113.87
4	A	800	HW7	O09-C10-C11	-2.14	102.07	109.56
3	B	760	H4B	C4A-C4-N3	-2.11	118.00	124.01
3	B	760	H4B	C4A-N5-C6	-2.10	115.44	121.16
2	B	750	HEM	CMA-C3A-C4A	-2.01	125.37	128.46

There are no chirality outliers.

All (10) torsion outliers are listed below:

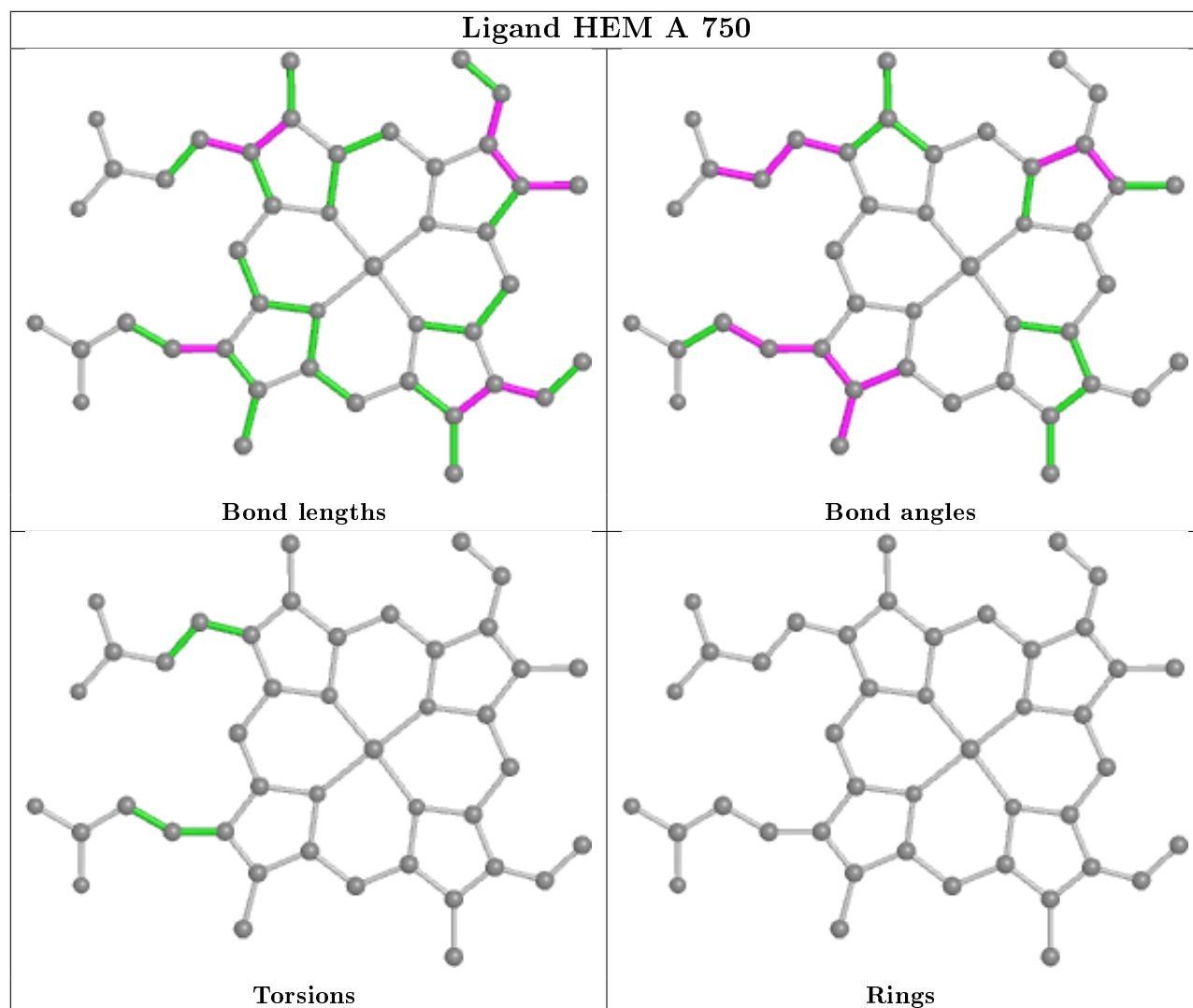
Mol	Chain	Res	Type	Atoms
4	B	800	HW7	N01-C06-C08-C4'
4	A	800	HW7	C22-C21-O14-C13
4	B	800	HW7	C11-C12-C13-O14
4	A	800	HW7	C26-C21-O14-C13
4	B	800	HW7	C11-C10-O09-C3'
4	B	800	HW7	C22-C21-O14-C13
4	B	800	HW7	C26-C21-O14-C13
4	B	800	HW7	C4'-C3'-O09-C10
4	B	800	HW7	C2'-C3'-O09-C10
4	A	800	HW7	C11-C12-C13-O14

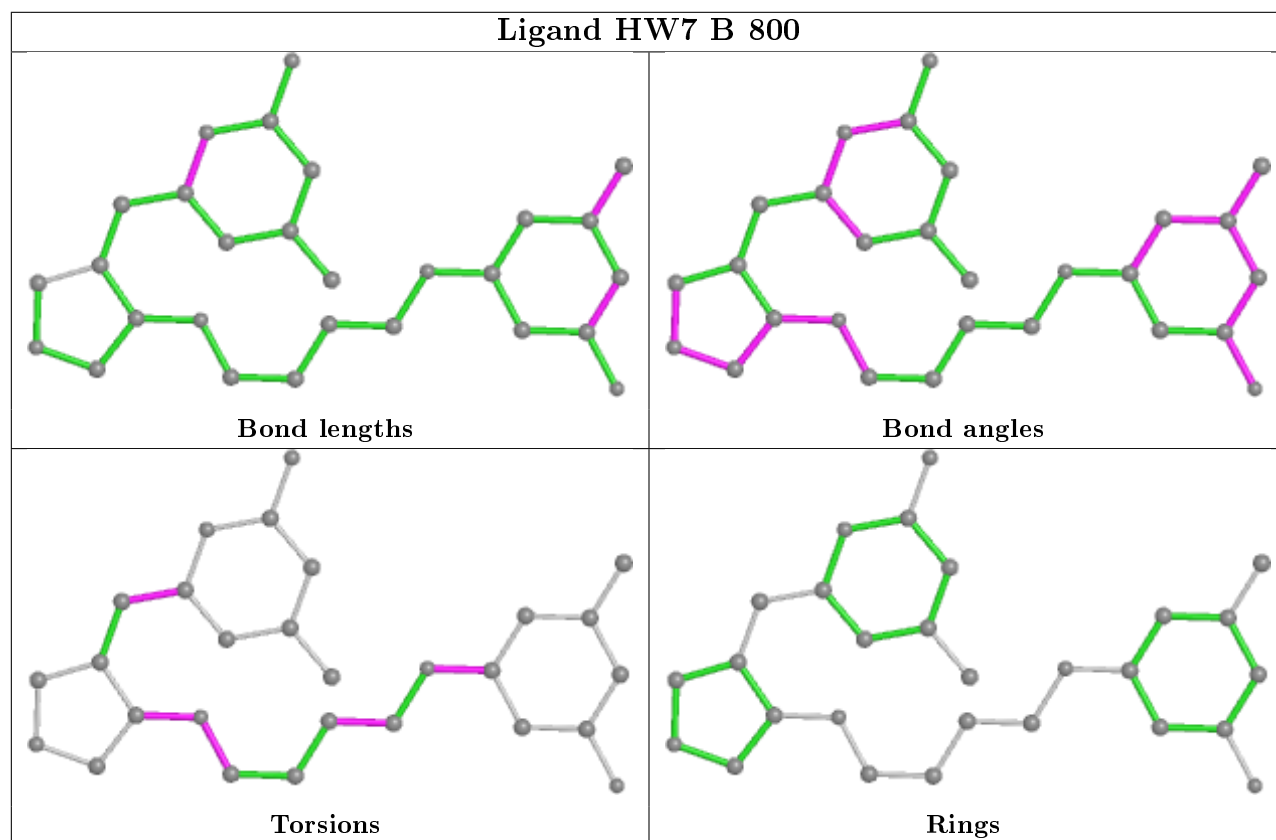
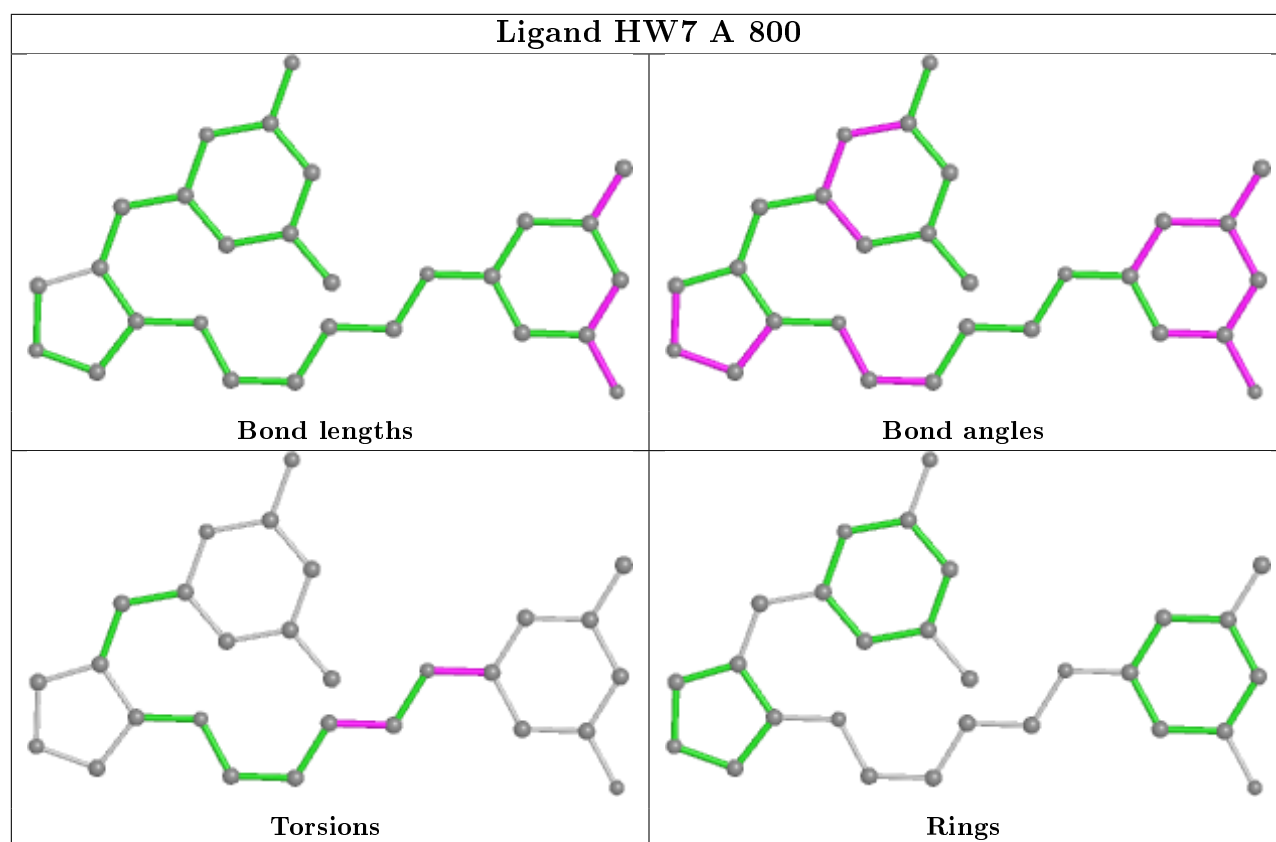
There are no ring outliers.

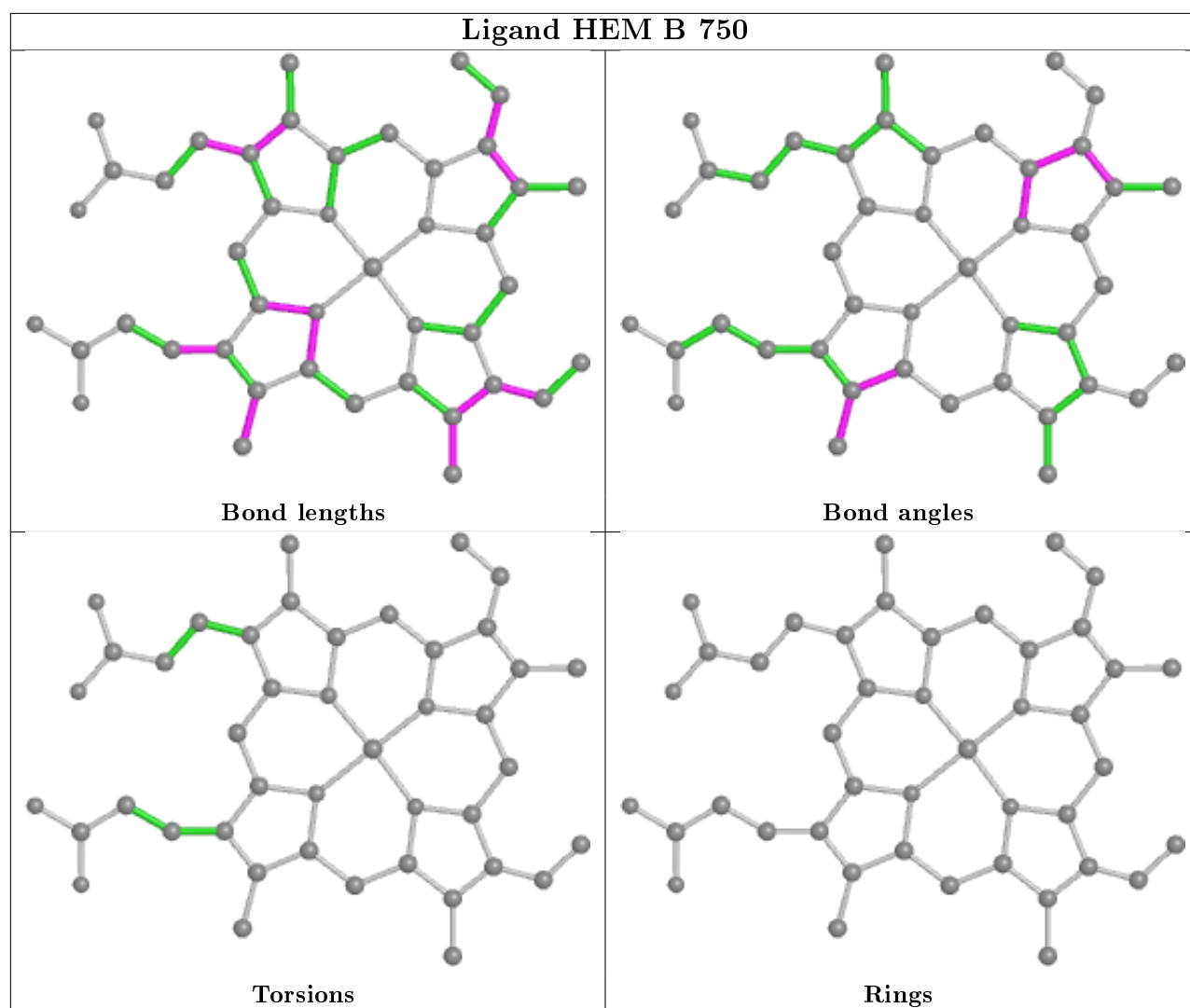
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	750	HEM	1	0
4	B	800	HW7	1	0
2	B	750	HEM	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







## 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%)	0.66	25 (6%) 21 25	33, 62, 99, 125	0
1	B	411/422 (97%)	0.53	13 (3%) 47 53	32, 52, 77, 103	0
All	All	818/844 (96%)	0.59	38 (4%) 32 36	32, 56, 93, 125	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	348	VAL	7.4
1	B	718	GLY	4.2
1	A	554	PHE	3.9
1	B	389	GLU	3.9
1	B	351	LYS	3.7
1	A	351	LYS	3.5
1	B	352	ASP	3.4
1	B	350	THR	3.4
1	A	355	PHE	3.3
1	B	300	PHE	3.3
1	A	393	THR	3.1
1	B	321	THR	3.0
1	A	350	THR	3.0
1	A	551	PHE	2.9
1	A	366	TYR	2.8
1	A	511	LYS	2.7
1	A	394	TYR	2.7
1	A	606	ILE	2.6
1	A	557	LEU	2.4
1	A	552	ASP	2.4
1	A	556	ASP	2.4
1	B	717	LYS	2.3
1	A	352	ASP	2.3
1	A	322	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	385	ASN	2.3
1	B	375	LYS	2.3
1	A	506	ILE	2.3
1	A	330	ILE	2.2
1	A	466	THR	2.2
1	A	370	LYS	2.2
1	A	713	THR	2.2
1	B	616	LEU	2.1
1	A	486	LYS	2.1
1	A	706	TYR	2.1
1	A	577	LEU	2.1
1	A	517	PHE	2.0
1	B	415	CYS	2.0
1	B	619	ARG	2.0

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

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

## 6.3 Carbohydrates ⓘ

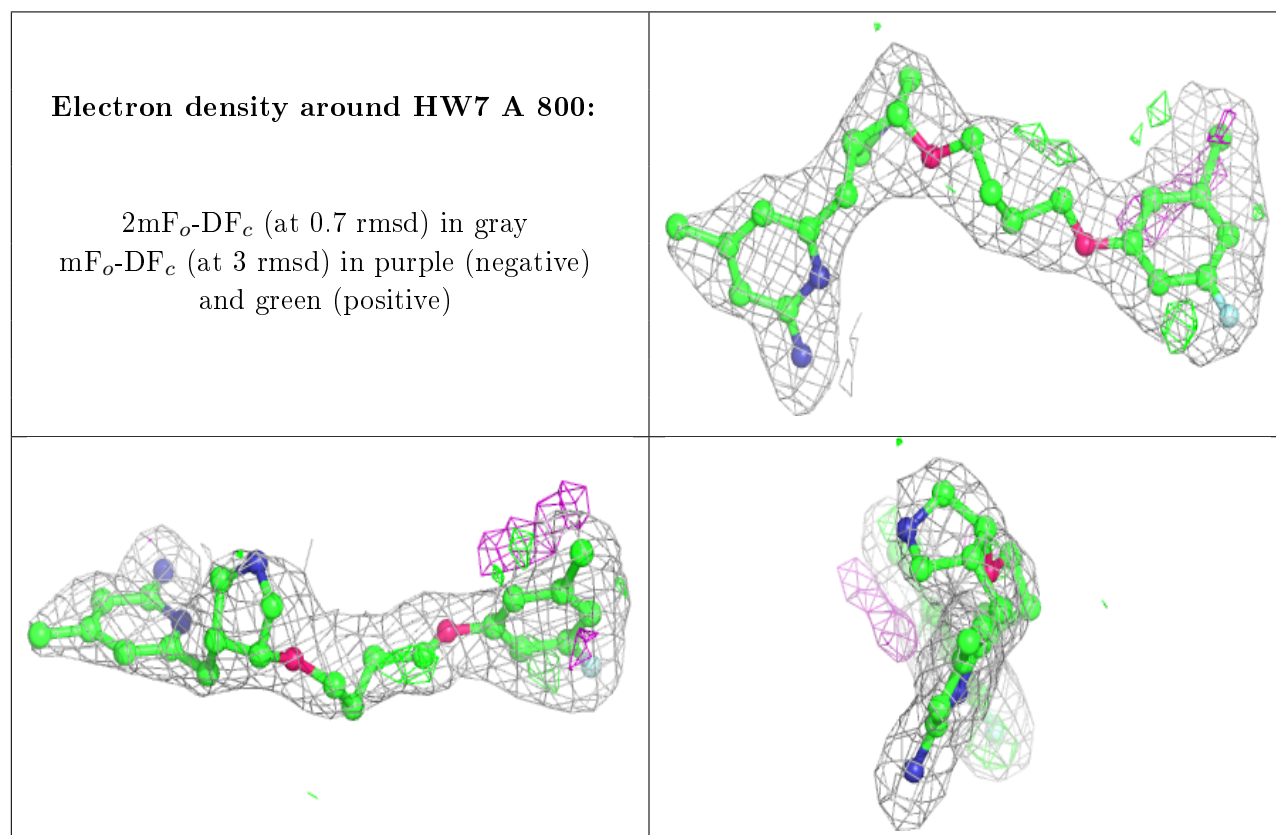
There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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.

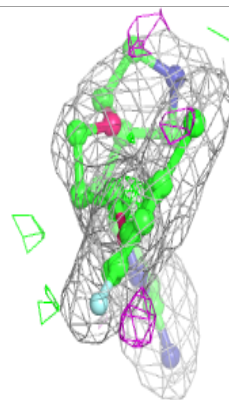
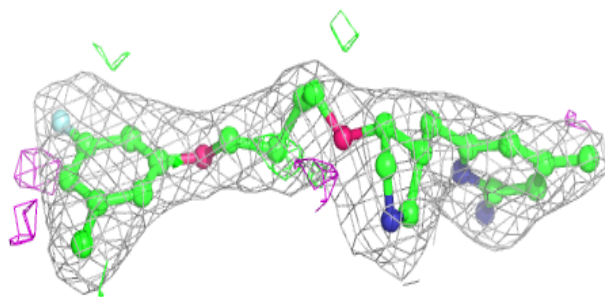
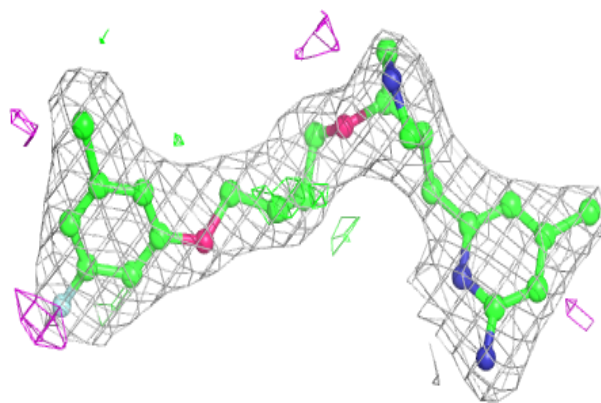
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	HW7	A	800	28/28	0.87	0.18	54,62,73,75	0
4	HW7	B	800	28/28	0.91	0.16	43,55,58,62	0
3	H4B	B	760	17/17	0.93	0.15	35,45,49,50	0
5	ACT	A	860	4/4	0.93	0.31	63,63,63,66	0
5	ACT	B	860	4/4	0.93	0.17	57,59,60,61	0
3	H4B	A	760	17/17	0.95	0.15	49,52,55,59	0
2	HEM	A	750	43/43	0.97	0.16	35,39,57,66	0
2	HEM	B	750	43/43	0.98	0.18	29,44,53,67	0
6	ZN	A	900	1/1	0.99	0.15	50,50,50,50	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



**Electron density around HW7 B 800:**

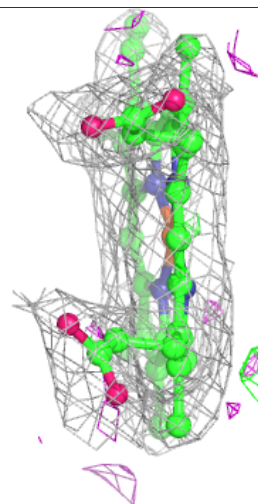
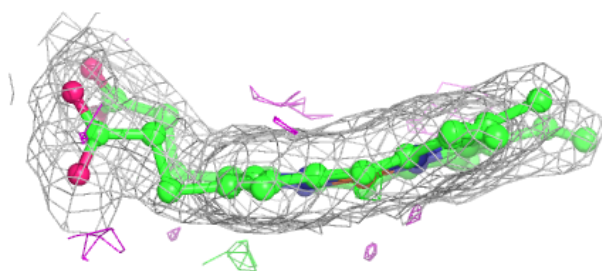
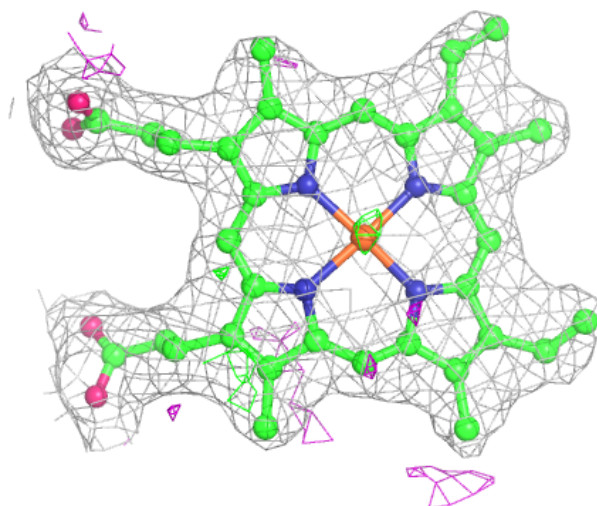
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





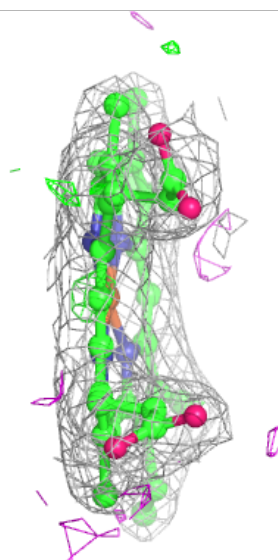
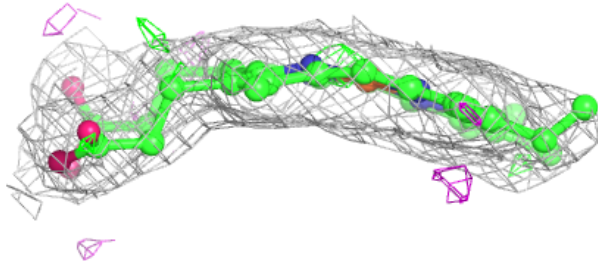
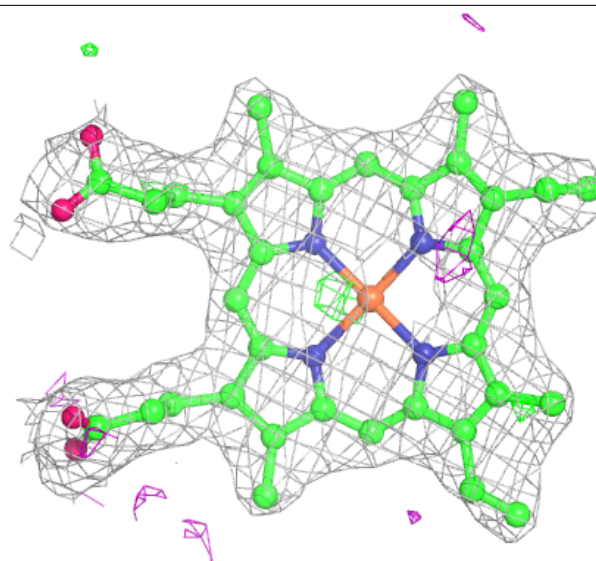
**Electron density around HEM A 750:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEM B 750:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.