



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 05:35 am BST

PDB ID : 1P6J  
Title : Rat neuronal NOS heme domain with L-N(omega)-nitroarginine-(4R)-amino-L-proline amide bound  
Authors : Flinspach, M.L.; Li, H.; Jamal, J.; Yang, W.; Huang, H.; Hah, J.-M.; Gomez-Vidal, J.A.; Litzinger, E.A.; Silverman, R.B.; Poulos, T.L.  
Deposited on : 2003-04-29  
Resolution : 2.00 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

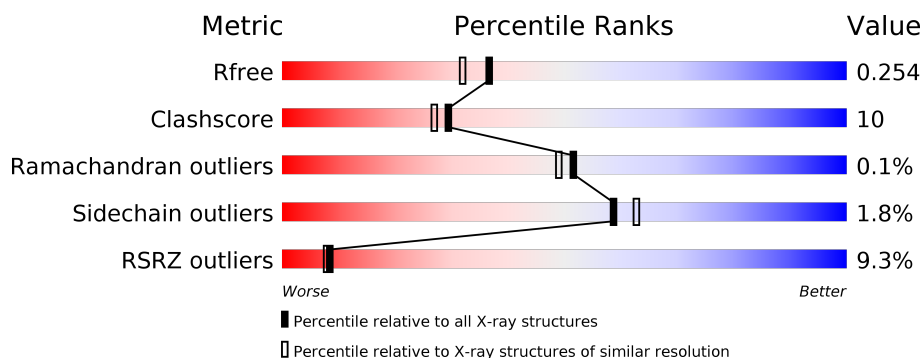
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	421	<div> <div>14%</div> <div> <div></div> <div>71%</div> <div>24%</div> <div>• •</div> </div> </div>
1	B	421	<div> <div>4%</div> <div> <div></div> <div>81%</div> <div>16%</div> <div>•</div> </div> </div>

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 7251 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	410	Total	C	N	O	S	0	0	0
			3341	2138	573	609	21			

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).

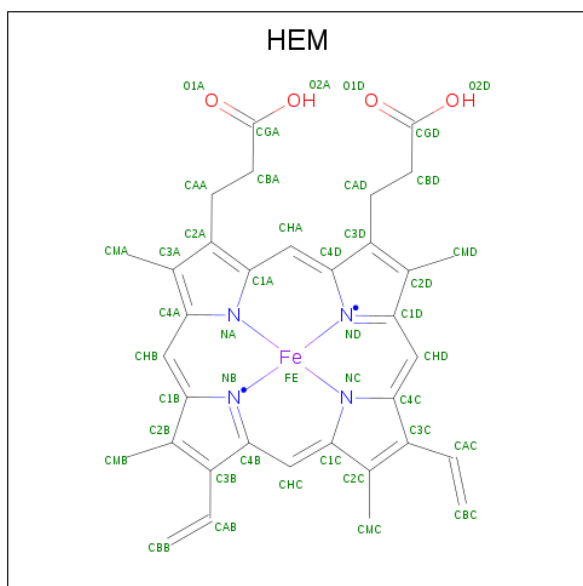


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

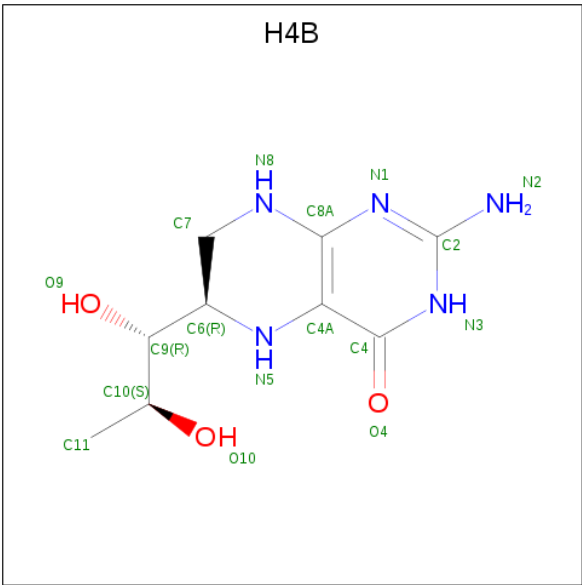
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Zn 1 1	0	0

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



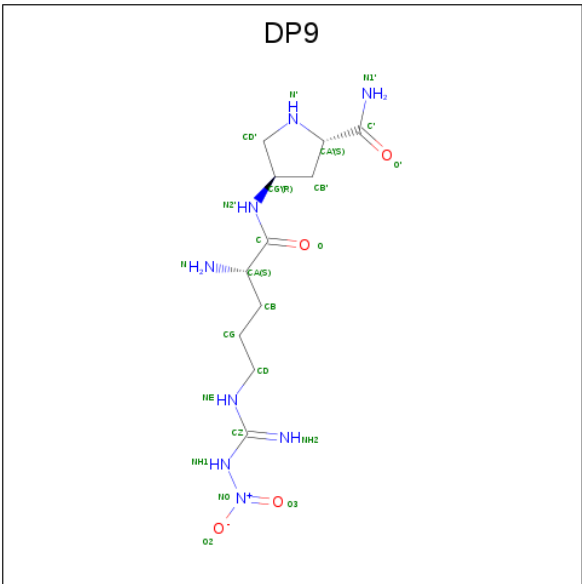
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 5 is 5,6,7,8-TETRAHYDROBIOPTERIN (three-letter code: H4B) (formula:  $\text{C}_9\text{H}_{15}\text{N}_5\text{O}_3$ ).



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

- Molecule 6 is L-N(OMEGA)-NITROARGININE-(4R)-AMINO-L-PROLINE AMIDE (three-letter code: DP9) (formula: C<sub>11</sub>H<sub>22</sub>N<sub>8</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			23	11	8	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	O	0	0
			23	11	8	4		

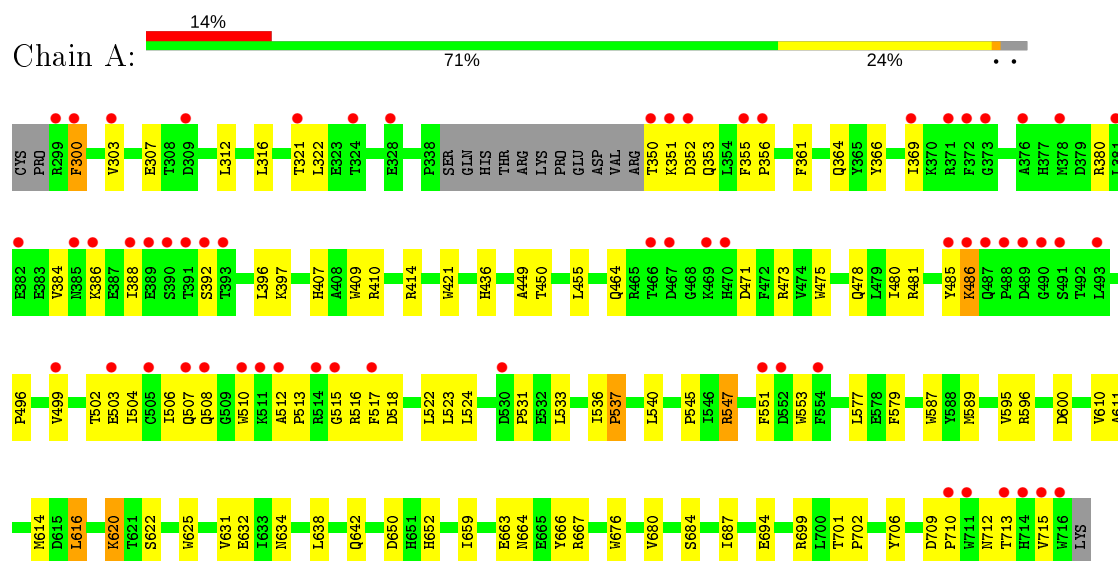
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	160	Total	O	0	0
			160	160		
7	B	262	Total	O	0	0
			262	262		

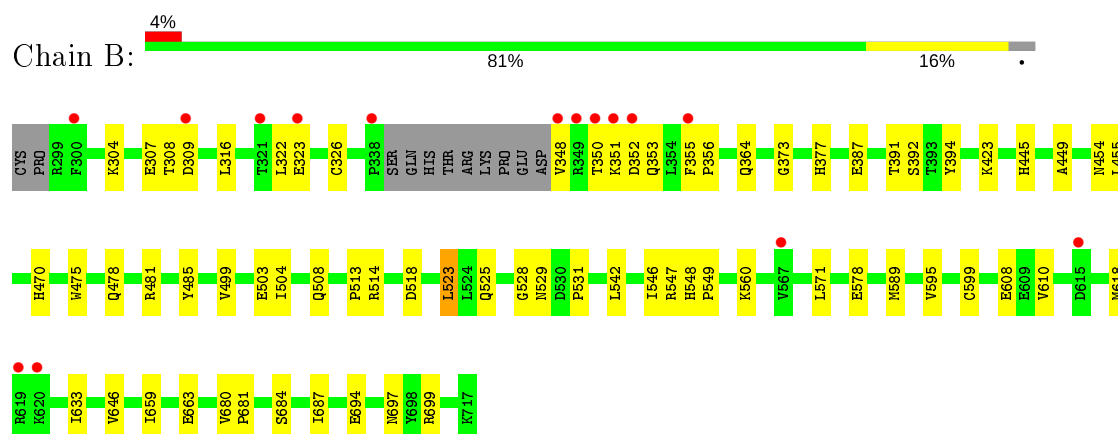
### 3 Residue-property plots [i](#)

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, $\alpha$ , $\beta$ , $\gamma$	52.33Å 111.05Å 164.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.04 – 2.00 46.04 – 2.00	Depositor EDS
% Data completeness (in resolution range)	89.5 (46.04-2.00) 89.5 (46.04-2.00)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.14 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.225 , 0.259 0.219 , 0.254	Depositor DCC
$R_{free}$ test set	2919 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.5	Xtriage
Anisotropy	0.642	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 51.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7251	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% 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: HEM, ZN, H4B, DP9, 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	0.33	0/3406	0.58	1/4621 (0.0%)
1	B	0.35	0/3434	0.61	2/4656 (0.0%)
All	All	0.34	0/6840	0.59	3/9277 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	589	MET	N-CA-C	-5.79	95.37	111.00
1	A	589	MET	N-CA-C	-5.46	96.25	111.00
1	B	326	CYS	CA-CB-SG	5.44	123.79	114.00

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	85	0
1	B	3341	0	3256	40	0
2	A	4	0	3	0	0
2	B	4	0	3	0	0
3	A	1	0	0	0	0
4	A	43	0	30	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	43	0	30	2	0
5	A	17	0	15	0	0
5	B	17	0	15	0	0
6	A	23	0	21	1	0
6	B	23	0	21	0	0
7	A	160	0	0	8	0
7	B	262	0	0	4	0
All	All	7251	0	6615	128	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 10.

All (128) 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:373:GLY:H	1:B:377:HIS:HD2	1.23	0.84
1:B:523:LEU:HD22	1:B:531:PRO:HB2	1.61	0.81
1:A:523:LEU:HD22	1:A:531:PRO:HB2	1.68	0.74
1:A:350:THR:HG22	1:A:352:ASP:H	1.50	0.74
1:B:350:THR:HB	1:B:353:GLN:OE1	1.91	0.70
1:B:373:GLY:H	1:B:377:HIS:CD2	2.10	0.66
1:A:350:THR:HB	1:A:353:GLN:HG3	1.79	0.64
1:A:545:PRO:HG2	1:A:547:ARG:NH1	2.13	0.64
1:A:631:VAL:HA	7:A:982:HOH:O	1.97	0.64
1:A:620:LYS:HE3	1:A:622:SER:OG	1.99	0.62
1:B:499:VAL:O	1:B:503:GLU:HG3	2.00	0.61
1:A:478:GLN:HB2	1:A:481:ARG:HG3	1.82	0.61
1:B:478:GLN:HB2	1:B:481:ARG:HG3	1.83	0.61
1:B:391:THR:O	1:B:392:SER:HB2	2.01	0.60
1:A:380:ARG:NH1	1:A:397:LYS:HE2	2.17	0.60
1:A:486:LYS:HB2	1:A:486:LYS:NZ	2.16	0.60
1:B:659:ILE:O	1:B:663:GLU:HG3	2.02	0.59
1:A:361:PHE:O	1:A:364:GLN:HG2	2.03	0.59
1:A:321:THR:HG21	7:A:990:HOH:O	2.02	0.58
1:A:638:LEU:O	1:A:642:GLN:HG3	2.04	0.58
1:A:436:HIS:HB2	7:A:1040:HOH:O	2.05	0.57
1:A:684:SER:HB3	1:A:687:ILE:HD11	1.87	0.56
1:B:322:LEU:HD13	1:B:699:ARG:HH21	1.70	0.56
1:A:709:ASP:HB2	1:A:712:ASN:HD22	1.69	0.56
1:B:355:PHE:N	1:B:356:PRO:HD2	2.20	0.56
1:A:524:LEU:O	1:A:531:PRO:HA	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:513:PRO:HG2	1:B:518:ASP:CG	2.27	0.55
1:A:449:ALA:O	1:A:455:LEU:HA	2.07	0.55
1:A:659:ILE:O	1:A:663:GLU:HG3	2.07	0.54
1:B:387:GLU:OE2	1:B:394:TYR:HA	2.08	0.54
1:A:595:VAL:HG23	1:A:634:ASN:HD21	1.72	0.54
1:A:486:LYS:HB2	1:A:486:LYS:HZ2	1.73	0.53
1:A:502:THR:O	1:A:506:ILE:HG12	2.09	0.53
1:A:650:ASP:OD2	1:A:652:HIS:HB2	2.08	0.53
1:B:475:TRP:HB2	1:B:523:LEU:HB3	1.92	0.52
1:A:303:VAL:HG13	1:A:694:GLU:HB2	1.92	0.52
1:B:610:VAL:HG21	1:B:633:ILE:HD11	1.93	0.51
1:A:486:LYS:NZ	1:A:499:VAL:HG11	2.24	0.51
1:A:485:TYR:CE2	1:A:512:ALA:HB1	2.47	0.50
1:B:548:HIS:CG	1:B:549:PRO:HD2	2.45	0.50
1:B:684:SER:HB3	1:B:687:ILE:HD11	1.93	0.50
1:A:322:LEU:HB3	1:A:699:ARG:NH1	2.25	0.50
1:A:715:VAL:O	1:A:715:VAL:HG23	2.10	0.50
1:A:634:ASN:HB2	7:A:982:HOH:O	2.12	0.49
1:A:355:PHE:N	1:A:356:PRO:HD2	2.27	0.49
1:A:366:TYR:HA	1:A:369:ILE:HG12	1.94	0.49
1:B:323:GLU:O	1:B:699:ARG:HD3	2.12	0.49
4:B:750:HEM:HBC2	4:B:750:HEM:HMC1	1.95	0.49
1:A:701:THR:HA	1:A:702:PRO:C	2.33	0.49
1:A:610:VAL:O	1:A:614:MET:HG3	2.13	0.48
1:B:485:TYR:CZ	1:B:514:ARG:HA	2.48	0.48
1:A:303:VAL:CG1	1:A:694:GLU:O	2.61	0.48
1:A:407:HIS:CE1	1:A:410:ARG:HH11	2.31	0.48
4:B:750:HEM:HBC2	4:B:750:HEM:CMC	2.44	0.48
1:A:455:LEU:HD12	1:A:587:TRP:HB3	1.95	0.48
1:A:351:LYS:HE2	1:A:392:SER:HA	1.95	0.48
1:A:620:LYS:HB3	7:A:1032:HOH:O	2.13	0.48
1:B:449:ALA:HB1	7:B:918:HOH:O	2.13	0.48
1:A:300:PHE:N	1:A:300:PHE:CD1	2.82	0.47
1:B:364:GLN:NE2	7:B:1097:HOH:O	2.46	0.47
1:A:350:THR:HB	1:A:353:GLN:CG	2.45	0.47
1:B:350:THR:HG22	1:B:352:ASP:H	1.79	0.47
1:A:464:GLN:HB3	1:A:579:PHE:CE2	2.49	0.47
1:A:684:SER:HB3	1:A:687:ILE:CD1	2.45	0.47
1:A:522:LEU:O	1:A:533:LEU:HA	2.14	0.47
1:A:684:SER:HB3	1:A:687:ILE:CG1	2.44	0.47
1:A:506:ILE:C	1:A:508:GLN:H	2.17	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:LYS:O	1:B:694:GLU:HG3	2.15	0.46
1:A:611:ALA:HA	1:A:616:LEU:HD11	1.98	0.46
1:A:475:TRP:HB2	1:A:523:LEU:HB3	1.98	0.46
1:B:307:GLU:HG3	7:B:1026:HOH:O	2.15	0.46
1:A:496:PRO:O	1:A:499:VAL:HG23	2.16	0.45
1:A:504:ILE:O	1:A:508:GLN:HB2	2.17	0.45
1:B:308:THR:O	1:B:309:ASP:HB2	2.15	0.45
1:A:449:ALA:HB1	7:A:903:HOH:O	2.17	0.45
1:A:596:ARG:O	1:A:600:ASP:HB2	2.16	0.45
1:A:614:MET:CE	1:A:632:GLU:HG3	2.46	0.45
1:A:409:TRP:CE3	1:A:421:TRP:HA	2.51	0.45
1:B:542:LEU:HD21	1:B:646:VAL:HG22	1.99	0.45
1:A:414:ARG:NH1	1:A:706:TYR:OH	2.50	0.45
1:B:348:VAL:HG13	1:B:348:VAL:O	2.16	0.45
1:B:445:HIS:C	1:B:445:HIS:CD2	2.91	0.45
1:A:614:MET:HE3	1:A:632:GLU:HG3	1.98	0.44
1:A:450:THR:HA	1:A:455:LEU:CD2	2.48	0.44
1:A:523:LEU:HA	1:A:523:LEU:HD23	1.83	0.44
1:A:684:SER:HB3	1:A:687:ILE:HG12	1.98	0.44
1:B:595:VAL:O	1:B:599:CYS:HB2	2.17	0.44
1:A:616:LEU:HD13	1:A:625:TRP:HB2	1.98	0.44
1:B:608:GLU:HG3	1:B:618:MET:HE3	2.00	0.44
1:A:506:ILE:HD11	1:A:512:ALA:HB2	1.99	0.43
1:B:449:ALA:O	1:B:455:LEU:HA	2.18	0.43
1:A:455:LEU:HD12	1:A:587:TRP:CB	2.49	0.43
1:A:473:ARG:NH2	1:A:710:PRO:HD3	2.33	0.43
1:B:455:LEU:HD23	1:B:455:LEU:N	2.33	0.43
1:A:536:ILE:O	1:A:537:PRO:C	2.56	0.43
1:A:664:ASN:HA	1:A:667:ARG:NH1	2.32	0.43
1:B:504:ILE:O	1:B:508:GLN:HG2	2.18	0.43
1:A:307:GLU:HG3	7:B:951:HOH:O	2.17	0.43
1:A:510:TRP:CZ3	1:A:512:ALA:HB2	2.54	0.43
1:A:396:LEU:HG	1:A:577:LEU:HD12	2.00	0.43
1:A:507:GLN:HG2	1:A:507:GLN:O	2.19	0.43
1:A:515:GLY:N	1:A:518:ASP:OD2	2.44	0.43
1:A:551:PHE:HB3	1:A:553:TRP:NE1	2.34	0.43
1:B:571:LEU:HD11	1:B:578:GLU:HB3	2.01	0.42
1:A:506:ILE:C	1:A:508:GLN:N	2.72	0.42
1:B:470:HIS:HA	1:B:528:GLY:HA3	2.02	0.42
1:A:676:TRP:CZ2	1:A:680:VAL:HG21	2.55	0.42
1:B:323:GLU:O	1:B:699:ARG:NH1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:684:SER:O	1:A:687:ILE:HG12	2.19	0.42
1:A:480:ILE:HA	7:A:989:HOH:O	2.20	0.41
1:B:322:LEU:HD13	1:B:699:ARG:NH2	2.35	0.41
1:A:713:THR:O	1:A:713:THR:HG22	2.20	0.41
1:B:546:ILE:HG12	1:B:560:LYS:HA	2.02	0.41
4:A:750:HEM:HBA2	6:A:799:DP9:HD2	2.02	0.41
1:A:384:VAL:O	1:A:388:ILE:HG13	2.20	0.41
1:B:680:VAL:HA	1:B:681:PRO:HD3	1.91	0.41
1:A:300:PHE:N	1:A:300:PHE:HD1	2.19	0.41
1:A:303:VAL:HG11	1:A:694:GLU:O	2.21	0.41
1:A:351:LYS:HE2	1:A:392:SER:CA	2.50	0.41
1:A:516:ARG:HD3	1:A:517:PHE:CE1	2.56	0.41
1:B:525:GLN:HG3	1:B:529:ASN:O	2.21	0.41
1:A:709:ASP:HB2	1:A:712:ASN:ND2	2.35	0.40
1:B:350:THR:HG22	1:B:351:LYS:N	2.36	0.40
1:A:537:PRO:HB2	1:A:540:LEU:HG	2.03	0.40
1:A:386:LYS:HA	1:A:386:LYS:HD3	1.90	0.40
1:A:512:ALA:HA	1:A:513:PRO:HD3	1.92	0.40
1:A:312:LEU:HB3	1:A:666:TYR:CD2	2.57	0.40
1:A:503:GLU:HG3	7:A:1047:HOH:O	2.21	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	403/421 (96%)	373 (93%)	29 (7%)	1 (0%)	47	44
1	B	406/421 (96%)	391 (96%)	15 (4%)	0	100	100
All	All	809/842 (96%)	764 (94%)	44 (5%)	1 (0%)	51	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	537	PRO

### 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%)	356 (98%)	7 (2%)	57	61
1	B	366/377 (97%)	360 (98%)	6 (2%)	62	67
All	All	729/754 (97%)	716 (98%)	13 (2%)	59	63

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	300	PHE
1	A	316	LEU
1	A	471	ASP
1	A	486	LYS
1	A	547	ARG
1	A	616	LEU
1	A	620	LYS
1	B	316	LEU
1	B	423	LYS
1	B	454	ASN
1	B	523	LEU
1	B	547	ARG
1	B	697	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	407	HIS
1	A	425	GLN
1	A	451	ASN
1	A	454	ASN
1	A	487	GLN

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Mol	Chain	Res	Type
1	A	500	GLN
1	A	634	ASN
1	A	697	ASN
1	A	712	ASN
1	B	364	GLN
1	B	377	HIS
1	B	425	GLN
1	B	451	ASN
1	B	454	ASN
1	B	507	GLN
1	B	508	GLN
1	B	527	ASN
1	B	535	GLN
1	B	634	ASN
1	B	664	ASN
1	B	697	ASN
1	B	712	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
4	HEM	B	750	1	27,50,50	1.77	5 (18%)	17,82,82	1.47	5 (29%)
4	HEM	A	750	1	27,50,50	1.59	4 (14%)	17,82,82	1.45	2 (11%)
5	H4B	A	760	-	16,18,18	2.17	3 (18%)	11,26,26	4.23	9 (81%)
2	ACT	B	861	-	1,3,3	3.19	1 (100%)	0,3,3	0.00	-
6	DP9	A	799	-	18,23,23	0.92	1 (5%)	21,30,30	1.66	4 (19%)
6	DP9	B	800	-	18,23,23	0.84	1 (5%)	21,30,30	1.71	5 (23%)
5	H4B	B	761	-	16,18,18	2.28	3 (18%)	11,26,26	4.26	9 (81%)
2	ACT	A	860	-	1,3,3	3.11	1 (100%)	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
4	HEM	B	750	1	-	0/6/54/54	-
4	HEM	A	750	1	-	0/6/54/54	-
5	H4B	A	760	-	-	0/8/17/17	0/2/2/2
6	DP9	A	799	-	-	1/20/32/32	0/1/1/1
6	DP9	B	800	-	-	2/20/32/32	0/1/1/1
5	H4B	B	761	-	-	0/8/17/17	0/2/2/2

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	761	H4B	C4-N3	5.54	1.42	1.33
5	A	760	H4B	C4-N3	5.22	1.42	1.33
4	B	750	HEM	C3C-C2C	-4.82	1.33	1.40
5	A	760	H4B	C4A-N5	4.63	1.47	1.38
5	B	761	H4B	C6-N5	4.49	1.54	1.45
4	B	750	HEM	C3B-CAB	-4.37	1.39	1.47
5	B	761	H4B	C4A-N5	4.36	1.46	1.38
5	A	760	H4B	C6-N5	4.15	1.54	1.45
4	A	750	HEM	C3B-C2B	-3.94	1.34	1.40
4	A	750	HEM	C3C-CAC	-3.81	1.40	1.47
4	A	750	HEM	C3B-CAB	-3.26	1.41	1.47
4	B	750	HEM	C3C-CAC	-3.25	1.41	1.47
2	B	861	ACT	CH3-C	3.19	1.52	1.48
2	A	860	ACT	CH3-C	3.11	1.52	1.48
4	B	750	HEM	C3B-C2B	-2.92	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	799	DP9	CG'-N2'	2.74	1.52	1.46
6	B	800	DP9	CG'-N2'	2.21	1.51	1.46
4	A	750	HEM	C1D-ND	2.03	1.40	1.36
4	B	750	HEM	C1A-NA	2.02	1.40	1.36

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	761	H4B	C4-C4A-C8A	8.96	122.53	114.57
5	A	760	H4B	C4-C4A-C8A	8.89	122.47	114.57
5	B	761	H4B	C4-N3-C2	5.64	124.90	115.93
5	A	760	H4B	C4-N3-C2	5.60	124.83	115.93
5	A	760	H4B	N3-C2-N1	-4.89	117.75	125.42
5	B	761	H4B	N3-C2-N1	-4.80	117.89	125.42
6	B	800	DP9	CD-NE-CZ	4.38	131.49	123.50
6	A	799	DP9	CD-NE-CZ	4.28	131.30	123.50
5	A	760	H4B	C2-N1-C8A	3.71	122.86	114.54
5	B	761	H4B	C4A-C4-N3	-3.64	113.67	124.01
6	A	799	DP9	O'-C'-N1'	-3.61	116.73	123.00
5	A	760	H4B	C4A-C4-N3	-3.61	113.76	124.01
5	B	761	H4B	C2-N1-C8A	3.59	122.59	114.54
6	B	800	DP9	O'-C'-N1'	-3.51	116.89	123.00
5	A	760	H4B	N2-C2-N1	3.38	122.50	117.25
5	B	761	H4B	N2-C2-N1	3.34	122.45	117.25
5	B	761	H4B	C4A-N5-C6	-3.21	112.44	121.16
5	A	760	H4B	C4A-N5-C6	-3.11	112.69	121.16
5	B	761	H4B	C4-C4A-N5	-3.00	116.61	119.12
4	B	750	HEM	C1D-C2D-C3D	-2.83	105.03	107.00
6	A	799	DP9	CA'-C'-N1'	2.65	121.22	116.69
6	B	800	DP9	CG'-N2'-C	2.61	127.35	123.20
4	A	750	HEM	CMC-C2C-C3C	2.58	129.51	124.68
5	A	760	H4B	C4-C4A-N5	-2.56	116.97	119.12
6	B	800	DP9	CA'-C'-N1'	2.56	121.07	116.69
4	B	750	HEM	CMD-C2D-C3D	2.48	129.63	124.94
4	B	750	HEM	CBA-CAA-C2A	-2.43	108.00	112.49
4	A	750	HEM	CBD-CAD-C3D	-2.41	108.03	112.48
5	B	761	H4B	O9-C9-C6	2.40	114.71	108.98
4	B	750	HEM	CMB-C2B-C3B	2.29	128.96	124.68
5	A	760	H4B	O9-C9-C6	2.25	114.36	108.98
6	A	799	DP9	NE-CZ-NH2	-2.19	116.15	120.26
6	B	800	DP9	NE-CZ-NH2	-2.07	116.38	120.26
4	B	750	HEM	CMD-C2D-C1D	-2.04	125.34	128.46

There are no chirality outliers.

All (3) torsion outliers are listed below:

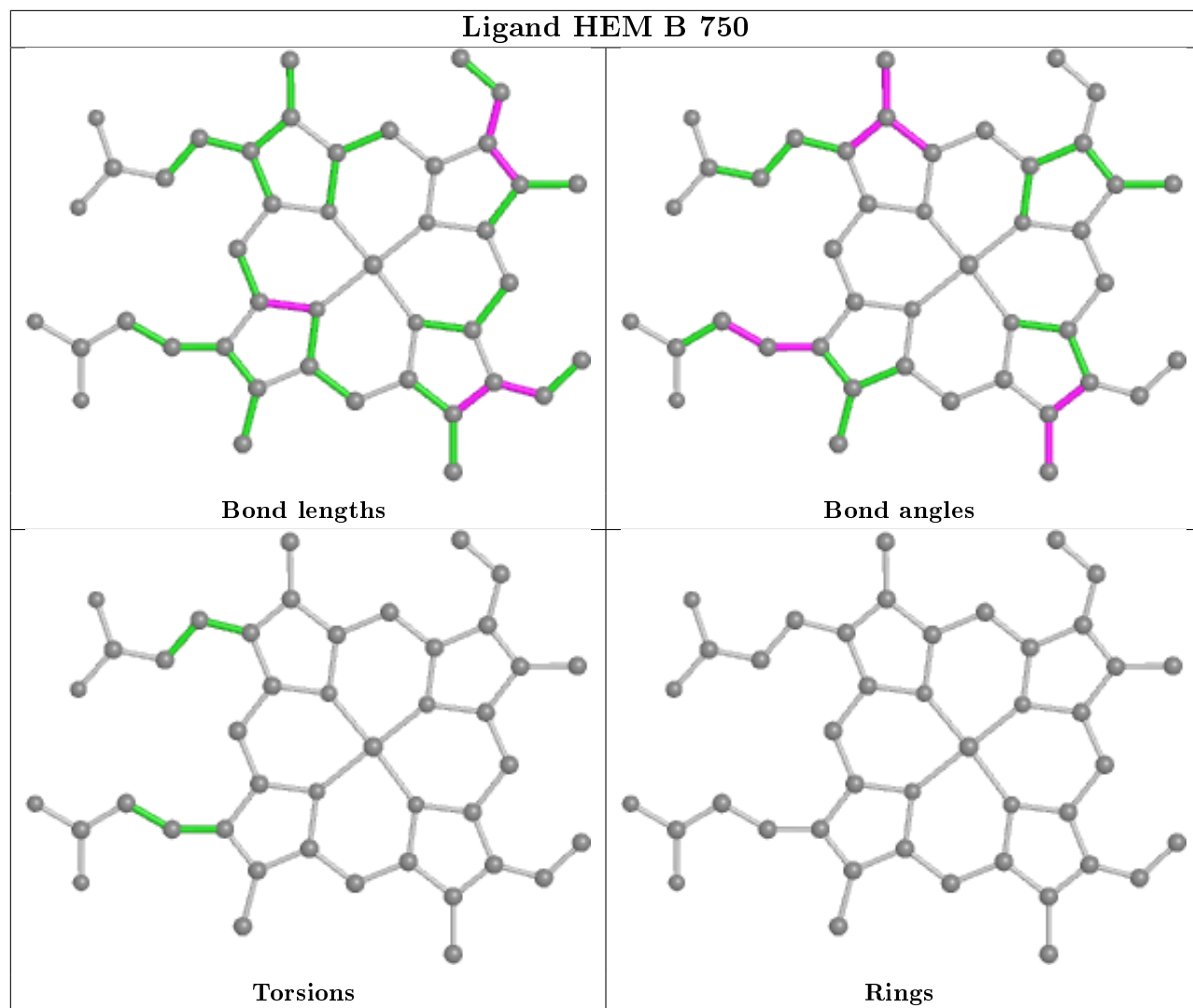
Mol	Chain	Res	Type	Atoms
6	B	800	DP9	C-CA-CB-CG
6	B	800	DP9	N-CA-CB-CG
6	A	799	DP9	CD'-CG'-N2'-C

There are no ring outliers.

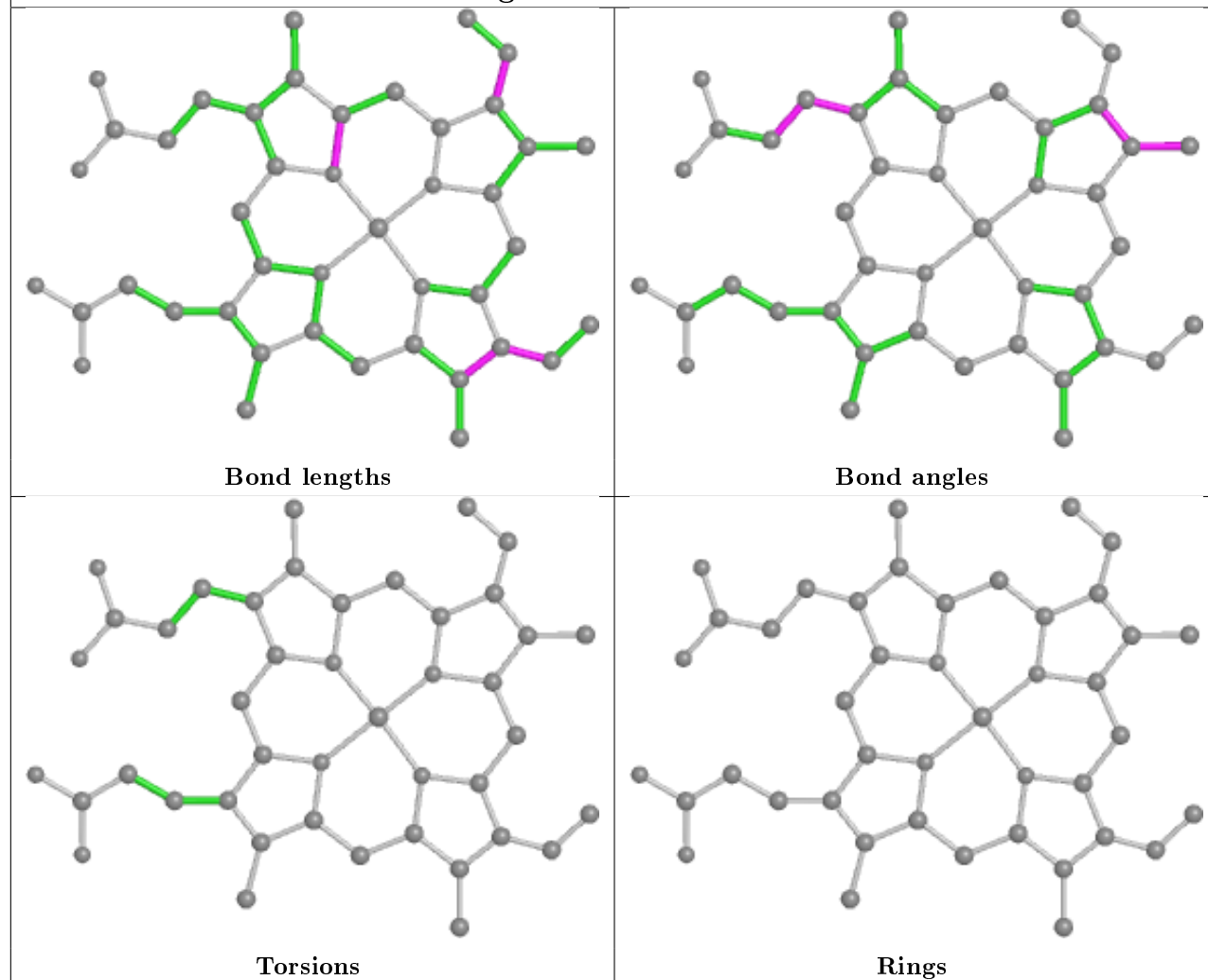
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	750	HEM	2	0
4	A	750	HEM	1	0
6	A	799	DP9	1	0

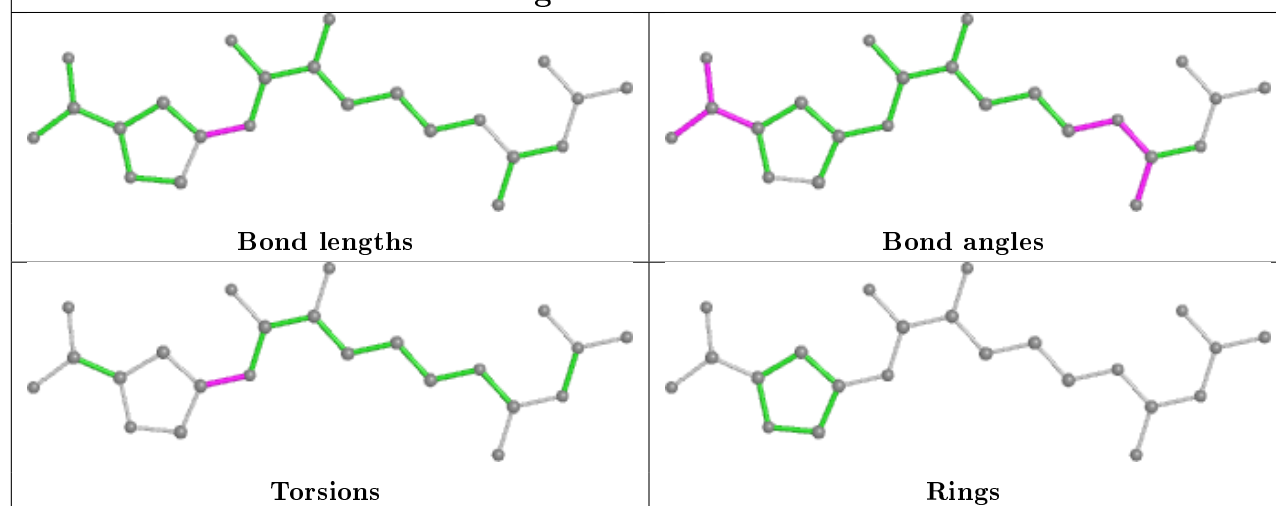
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

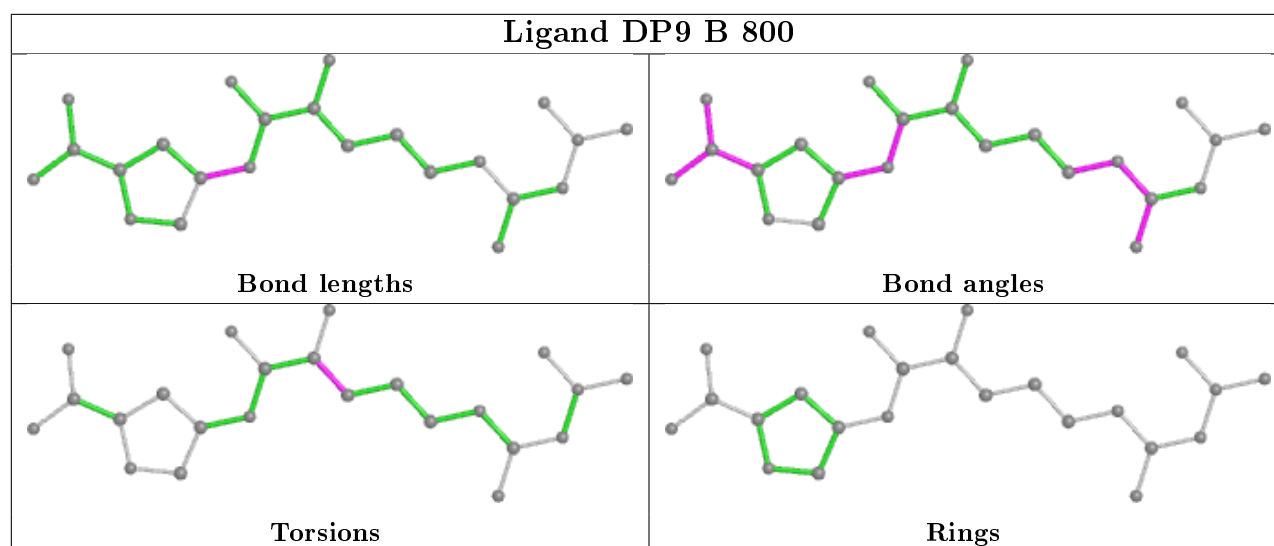


## Ligand HEM A 750



## Ligand DP9 A 799





## 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	407/421 (96%)	0.94	61 (14%) 2 2	16, 41, 62, 76	0
1	B	410/421 (97%)	0.43	15 (3%) 41 41	15, 29, 52, 65	0
All	All	817/842 (97%)	0.68	76 (9%) 8 8	15, 33, 60, 76	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	715	VAL	8.7
1	A	488	PRO	5.6
1	A	355	PHE	5.5
1	B	348	VAL	5.3
1	A	391	THR	5.1
1	B	321	THR	4.8
1	A	352	ASP	4.7
1	A	716	TRP	4.5
1	A	351	LYS	4.5
1	A	466	THR	4.3
1	A	503	GLU	4.1
1	B	350	THR	4.1
1	A	511	LYS	4.1
1	B	300	PHE	3.9
1	B	352	ASP	3.6
1	A	381	LEU	3.6
1	A	512	ALA	3.5
1	A	350	THR	3.5
1	A	487	GLN	3.5
1	A	388	ILE	3.4
1	A	507	GLN	3.3
1	A	385	ASN	3.3
1	A	486	LYS	3.3
1	A	489	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	351	LYS	3.2
1	A	299	ARG	3.2
1	A	321	THR	3.2
1	A	491	SER	3.1
1	A	490	GLY	3.1
1	A	328	GLU	3.1
1	A	300	PHE	2.9
1	A	710	PRO	2.9
1	B	615	ASP	2.9
1	A	711	TRP	2.9
1	A	378	MET	2.7
1	A	554	PHE	2.7
1	A	309	ASP	2.7
1	B	309	ASP	2.7
1	A	324	THR	2.7
1	A	713	THR	2.7
1	A	485	TYR	2.6
1	B	619	ARG	2.6
1	A	393	THR	2.6
1	A	392	SER	2.6
1	A	517	PHE	2.6
1	A	467	ASP	2.5
1	A	386	LYS	2.5
1	A	469	LYS	2.5
1	A	551	PHE	2.5
1	B	338	PRO	2.4
1	B	349	ARG	2.4
1	A	515	GLY	2.4
1	A	371	ARG	2.4
1	A	303	VAL	2.4
1	A	389	GLU	2.4
1	A	373	GLY	2.4
1	B	355	PHE	2.3
1	A	714	HIS	2.3
1	A	369	ILE	2.3
1	A	470	HIS	2.3
1	A	382	GLU	2.3
1	A	552	ASP	2.3
1	A	493	LEU	2.2
1	A	499	VAL	2.2
1	A	356	PRO	2.2
1	A	372	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	508	GLN	2.2
1	B	567	VAL	2.2
1	A	376	ALA	2.1
1	B	323	GLU	2.1
1	B	620	LYS	2.1
1	A	530	ASP	2.1
1	A	390	SER	2.0
1	A	514	ARG	2.0
1	A	510	TRP	2.0
1	A	505	CYS	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. 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.

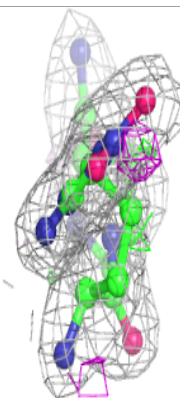
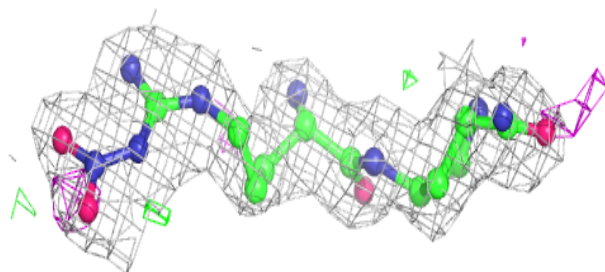
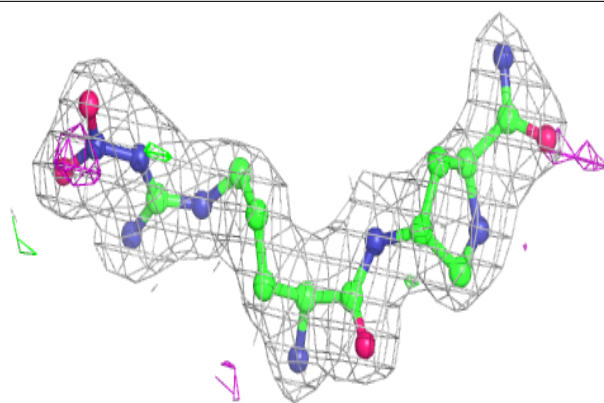
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	DP9	A	799	23/23	0.89	0.15	33,36,39,40	0
2	ACT	B	861	4/4	0.92	0.15	38,38,38,38	0
6	DP9	B	800	23/23	0.93	0.17	34,35,36,36	0
2	ACT	A	860	4/4	0.93	0.15	54,55,55,55	0
5	H4B	A	760	17/17	0.96	0.14	19,19,21,22	0
5	H4B	B	761	17/17	0.97	0.16	17,17,20,20	0
4	HEM	A	750	43/43	0.97	0.16	18,20,24,24	0
4	HEM	B	750	43/43	0.98	0.19	17,18,21,22	0
3	ZN	A	900	1/1	1.00	0.10	36,36,36,36	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.

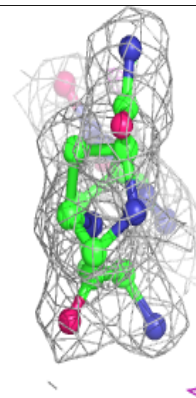
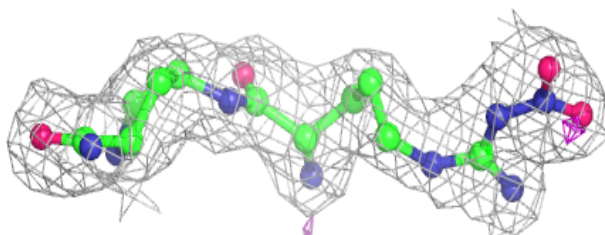
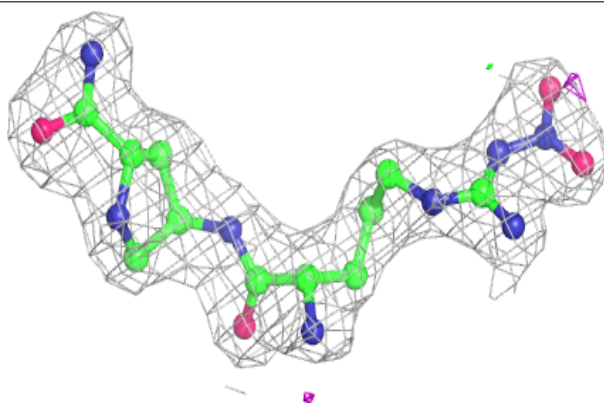


**Electron density around DP9 A 799:**

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

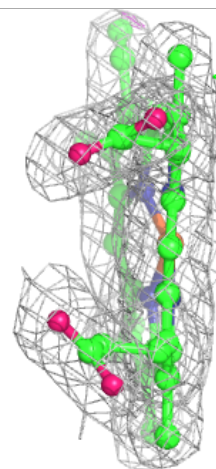
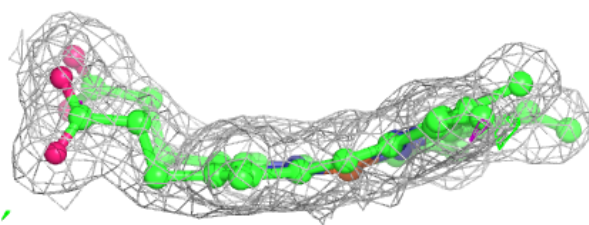
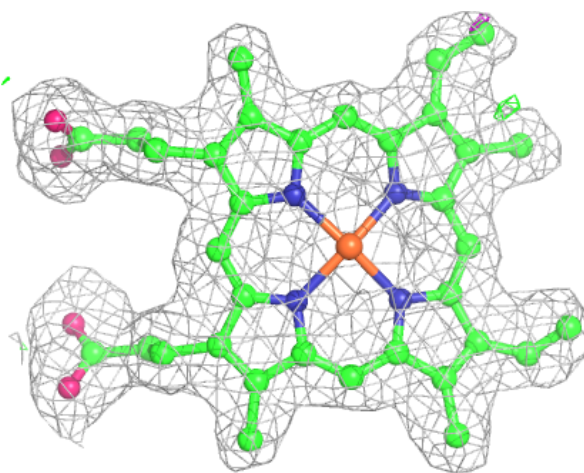
**Electron density around DP9 B 800:**

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



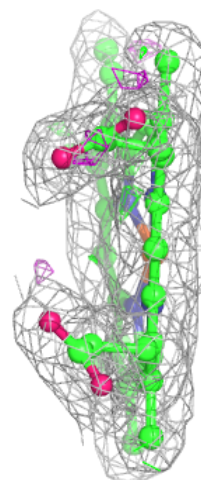
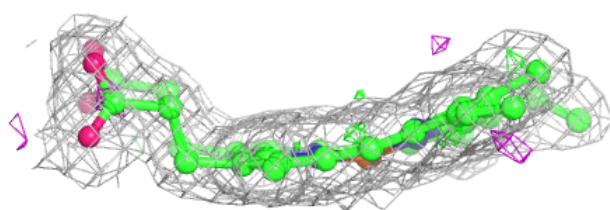
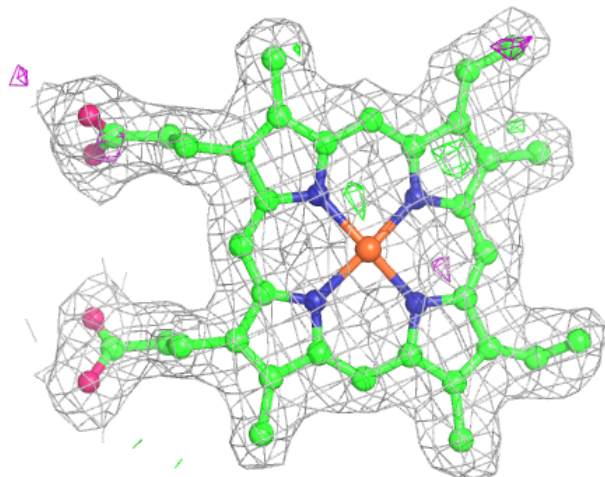
**Electron density around HEM A 750:**

$2mF_o-DF_c$  (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 ⓘ

There are no such residues in this entry.