



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2020 – 01:31 am BST

PDB ID : 3JT3  
Title : Structure of neuronal nitric oxide synthase heme domain complexed with N 5  
-[2-(methylsulfanyl)ethanimidoyl]-L-ornithine  
Authors : Li, H.; Poulos, T.L.  
Deposited on : 2009-09-11  
Resolution : 2.15 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

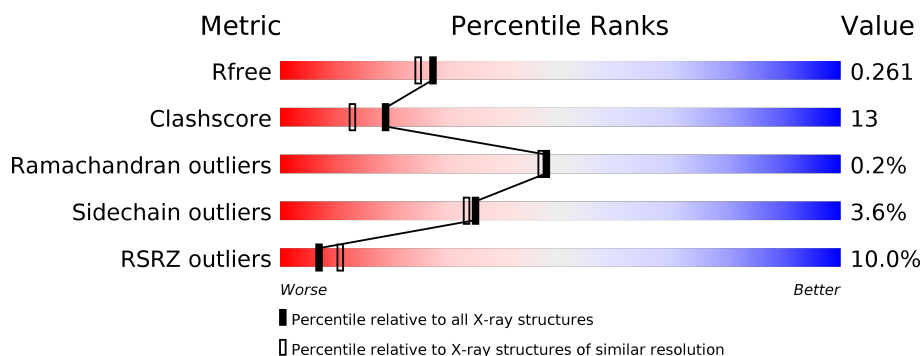
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (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  $\geq 3$ , 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>14%</div> <div> <div></div> <div>71%</div> <div>24%</div> <div>• •</div> </div> </div>
1	B	422	<div> <div>6%</div> <div> <div></div> <div>72%</div> <div>25%</div> <div>• •</div> </div> </div>

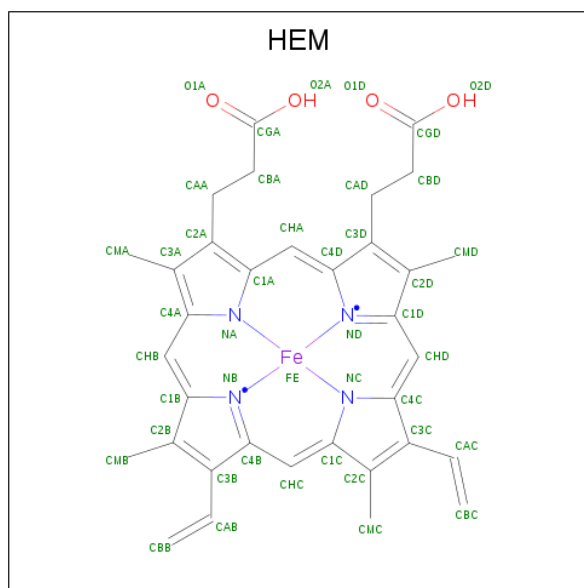


In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Nitric oxide synthase, brain.

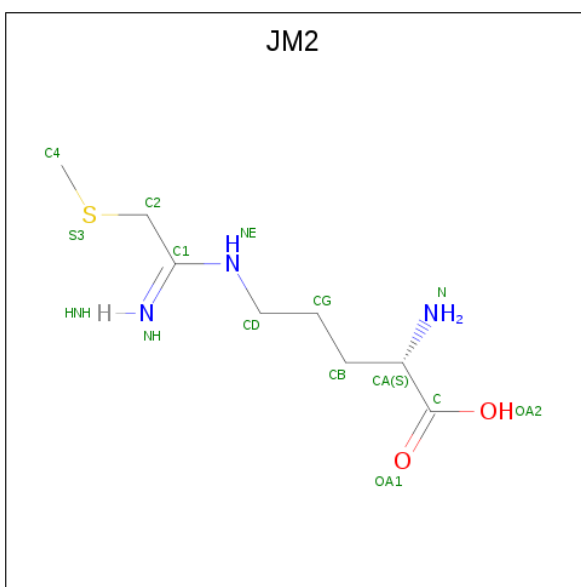
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	407	Total 3313	C 2121	N 566	O 605	S 21	0	0	0
1	B	411	Total 3345	C 2140	N 574	O 610	S 21	0	0	0

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



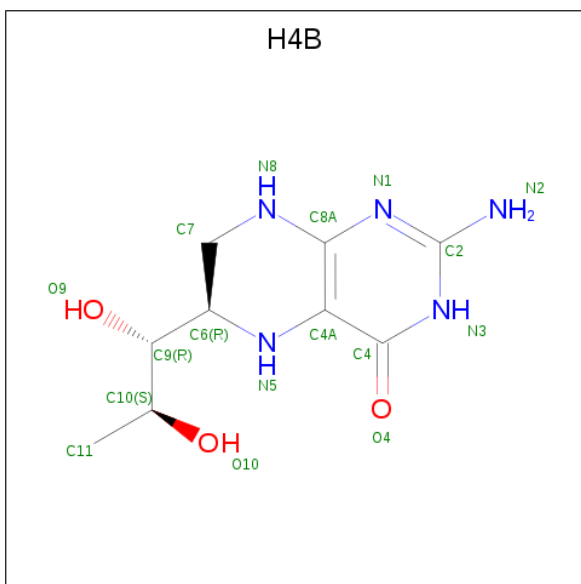
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is N 5 -[2-(methylsulfanyl)ethanimidoyl]-L-ornithine (three-letter code: JM2) (formula: C<sub>8</sub>H<sub>17</sub>N<sub>3</sub>O<sub>2</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			14	8	3	2	1		
3	B	1	Total	C	N	O	S	0	0
			14	8	3	2	1		

- Molecule 4 is 5,6,7,8-TETRAHYDROBIOPTERIN (three-letter code: H4B) (formula:  $C_9H_{15}N_5O_3$ ).



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

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

- 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		

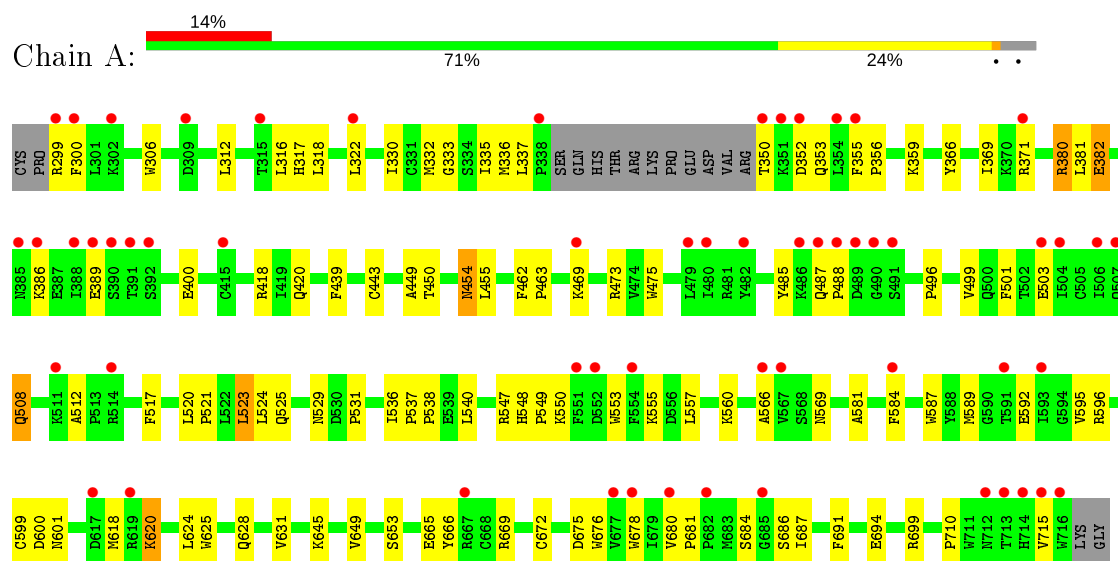
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	62	Total	O	0	0
			62	62		
7	B	101	Total	O	0	0
			101	101		

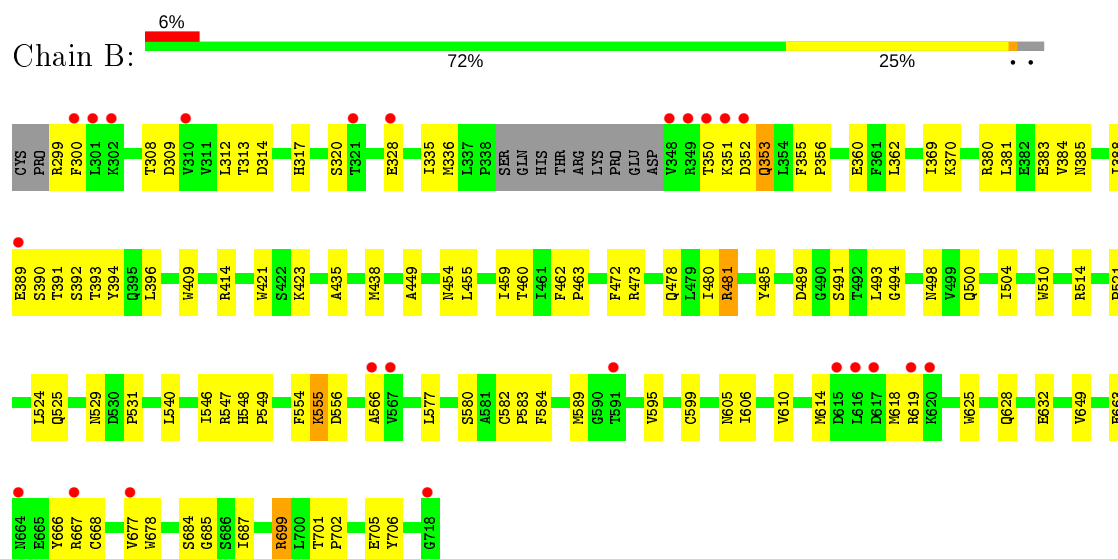
### 3 Residue-property plots [i](#)

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, $\alpha$ , $\beta$ , $\gamma$	51.55Å 111.11Å 164.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.01 – 2.15 37.79 – 2.15	Depositor EDS
% Data completeness (in resolution range)	97.0 (39.01-2.15) 97.0 (37.79-2.15)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	13.46 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.4.0069, CNS	Depositor
R, $R_{free}$	0.194 , 0.248 0.211 , 0.261	Depositor DCC
$R_{free}$ test set	2518 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.0	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 51.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6978	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.31% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: JM2, HEM, ZN, H4B, ACT

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.67	0/3406	0.75	0/4621
1	B	0.69	0/3438	0.74	0/4661
All	All	0.68	0/6844	0.75	0/9282

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3313	0	3221	92	0
1	B	3345	0	3259	82	0
2	A	43	0	30	6	0
2	B	43	0	30	4	0
3	A	14	0	15	1	0
3	B	14	0	15	0	0
4	A	17	0	15	0	0
4	B	17	0	15	0	0
5	A	4	0	3	1	0
5	B	4	0	3	0	0
6	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	62	0	0	0	0
7	B	101	0	0	2	0
All	All	6978	0	6606	176	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 13.

All (176) 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:699:ARG:HH11	1:B:699:ARG:HG2	1.03	1.13
1:B:351:LYS:HE2	1:B:392:SER:OG	1.60	1.01
1:B:353:GLN:H	1:B:353:GLN:NE2	1.71	0.88
1:B:699:ARG:NH1	1:B:699:ARG:HG2	1.75	0.87
1:A:382:GLU:OE1	1:A:382:GLU:HA	1.73	0.87
1:B:350:THR:HG22	1:B:352:ASP:H	1.41	0.86
1:A:350:THR:HG22	1:A:352:ASP:H	1.40	0.84
1:B:353:GLN:H	1:B:353:GLN:HE21	1.25	0.83
1:A:523:LEU:HD22	1:A:531:PRO:HB2	1.62	0.81
1:B:706:TYR:OH	2:B:750:HEM:O1D	1.98	0.81
1:B:473:ARG:HD3	1:B:580:SER:HB2	1.64	0.80
1:B:699:ARG:CG	1:B:699:ARG:HH11	1.90	0.77
1:B:391:THR:O	1:B:392:SER:HB2	1.85	0.75
2:A:750:HEM:HBB2	2:A:750:HEM:HHC	1.69	0.75
1:B:350:THR:HB	1:B:353:GLN:HE22	1.50	0.75
1:B:353:GLN:N	1:B:353:GLN:HE21	1.84	0.74
1:B:299:ARG:HB3	1:B:299:ARG:NH1	2.03	0.74
1:B:699:ARG:NH2	1:B:705:GLU:OE1	2.19	0.74
1:B:473:ARG:CD	1:B:580:SER:HB2	2.19	0.72
1:A:350:THR:HG22	1:A:352:ASP:N	2.05	0.71
1:B:610:VAL:O	1:B:614:MET:HG3	1.91	0.70
1:A:350:THR:HB	1:A:353:GLN:HG3	1.76	0.68
1:A:508:GLN:HA	1:A:508:GLN:HE21	1.58	0.68
1:A:517:PHE:HB2	1:A:560:LYS:HE3	1.75	0.68
1:A:525:GLN:HG3	1:A:529:ASN:O	1.95	0.67
1:A:508:GLN:HE21	1:A:508:GLN:CA	2.07	0.66
1:A:350:THR:HB	1:A:353:GLN:CG	2.24	0.66
2:A:750:HEM:HMC2	2:A:750:HEM:HBC2	1.78	0.65
1:B:299:ARG:HB3	1:B:299:ARG:CZ	2.26	0.65
1:A:336:MET:CE	1:A:678:TRP:HZ2	2.10	0.63
1:B:350:THR:HB	1:B:353:GLN:NE2	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:462:PHE:HB3	1:B:463:PRO:CD	2.30	0.61
1:A:306:TRP:CD1	1:B:336:MET:HE2	2.35	0.61
1:A:508:GLN:HA	1:A:508:GLN:NE2	2.17	0.60
1:A:496:PRO:HA	1:A:499:VAL:HG23	1.83	0.60
1:A:322:LEU:HB3	1:A:699:ARG:HH21	1.67	0.60
1:A:455:LEU:HD12	1:A:587:TRP:HB3	1.83	0.59
1:A:487:GLN:HB3	1:A:488:PRO:HD2	1.84	0.59
1:A:299:ARG:O	1:A:317:HIS:CE1	2.56	0.59
1:B:480:ILE:HA	7:B:145:HOH:O	2.03	0.59
1:B:589:MET:HA	1:B:649:VAL:O	2.04	0.58
1:B:485:TYR:CZ	1:B:514:ARG:HA	2.40	0.56
1:A:336:MET:HE3	1:A:678:TRP:HZ2	1.71	0.56
2:A:750:HEM:HBB2	2:A:750:HEM:CHC	2.35	0.56
1:A:485:TYR:CE2	1:A:512:ALA:HB1	2.41	0.55
1:B:595:VAL:O	1:B:599:CYS:HB2	2.06	0.55
1:A:382:GLU:OE1	1:A:382:GLU:CA	2.49	0.55
1:B:584:PHE:CD1	2:B:750:HEM:HAC	2.42	0.55
1:B:355:PHE:N	1:B:356:PRO:HD2	2.21	0.55
1:B:308:THR:O	1:B:309:ASP:HB2	2.07	0.54
1:B:462:PHE:HB3	1:B:463:PRO:HD2	1.89	0.54
1:B:355:PHE:CE1	1:B:385:ASN:HB2	2.43	0.54
1:A:322:LEU:HD13	1:A:699:ARG:NH2	2.24	0.53
1:B:493:LEU:HD12	1:B:494:GLY:N	2.24	0.53
1:B:546:ILE:HG22	1:B:554:PHE:HE1	1.73	0.53
1:A:524:LEU:O	1:A:531:PRO:HA	2.09	0.53
1:B:485:TYR:CE1	1:B:514:ARG:HA	2.45	0.52
1:A:350:THR:CG2	1:A:352:ASP:H	2.16	0.52
1:A:350:THR:HB	1:A:353:GLN:CD	2.29	0.52
1:A:684:SER:HB3	1:A:687:ILE:CG1	2.40	0.52
1:A:462:PHE:HB2	1:A:581:ALA:HB3	1.93	0.51
1:B:584:PHE:CD1	2:B:750:HEM:CAC	2.94	0.51
1:A:537:PRO:HB2	1:A:540:LEU:HG	1.92	0.51
1:A:312:LEU:HD13	1:A:666:TYR:CD1	2.45	0.51
1:B:389:GLU:HG3	1:B:390:SER:N	2.24	0.51
1:A:675:ASP:OD2	1:A:675:ASP:C	2.49	0.51
1:B:463:PRO:HG2	1:B:472:PHE:CZ	2.46	0.51
1:A:553:TRP:HZ3	1:A:557:LEU:HD11	1.75	0.51
1:B:605:ASN:ND2	7:B:100:HOH:O	2.43	0.50
1:A:508:GLN:NE2	1:A:508:GLN:CA	2.75	0.50
1:B:548:HIS:CG	1:B:549:PRO:HD2	2.47	0.50
1:B:299:ARG:CB	1:B:299:ARG:CZ	2.90	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:450:THR:HA	1:A:455:LEU:HD22	1.94	0.49
1:A:380:ARG:HD3	1:A:400:GLU:OE1	2.12	0.49
1:B:478:GLN:HB2	1:B:481:ARG:HG3	1.94	0.49
1:A:330:ILE:HG23	1:A:330:ILE:O	2.13	0.48
1:A:536:ILE:O	1:A:537:PRO:C	2.50	0.48
1:B:414:ARG:HD3	1:B:678:TRP:CD2	2.48	0.48
1:A:550:LYS:HB2	1:A:550:LYS:HE3	1.32	0.48
1:A:299:ARG:HG3	1:A:318:LEU:HD11	1.94	0.48
1:B:701:THR:HA	1:B:702:PRO:C	2.34	0.48
1:B:566:ALA:HA	1:B:584:PHE:O	2.14	0.47
1:A:487:GLN:CB	1:A:488:PRO:HD2	2.44	0.47
1:B:500:GLN:O	1:B:504:ILE:HG13	2.14	0.47
1:A:455:LEU:HD12	1:A:587:TRP:CB	2.45	0.47
1:A:353:GLN:O	1:A:356:PRO:HD2	2.14	0.47
1:A:473:ARG:NH2	1:A:710:PRO:HD3	2.29	0.47
1:B:489:ASP:OD2	1:B:491:SER:OG	2.26	0.47
1:A:306:TRP:CD2	1:B:336:MET:HE3	2.50	0.47
1:B:473:ARG:HD2	1:B:580:SER:HB2	1.97	0.47
1:A:501:PHE:CD2	1:A:520:LEU:HD13	2.50	0.47
1:A:694:GLU:HB3	1:B:335:ILE:HD13	1.97	0.47
1:B:548:HIS:ND1	1:B:549:PRO:HD2	2.30	0.47
1:B:328:GLU:H	1:B:328:GLU:CD	2.19	0.46
1:A:316:LEU:HD22	1:A:669:ARG:HD3	1.98	0.46
1:B:510:TRP:CE2	1:B:521:PRO:HD3	2.50	0.46
1:B:524:LEU:O	1:B:531:PRO:HA	2.15	0.46
2:B:750:HEM:HBC2	2:B:750:HEM:CMC	2.44	0.46
1:A:599:CYS:O	1:A:600:ASP:C	2.54	0.46
1:B:459:ILE:HG13	1:B:583:PRO:O	2.15	0.46
1:A:517:PHE:CB	1:A:560:LYS:HE3	2.46	0.46
2:A:750:HEM:CBB	2:A:750:HEM:HHC	2.41	0.45
1:A:496:PRO:O	1:A:499:VAL:HG23	2.15	0.45
1:B:460:THR:O	1:B:582:CYS:HA	2.16	0.45
1:A:332:MET:HB3	1:A:335:ILE:HG13	1.97	0.45
1:A:596:ARG:O	1:A:600:ASP:HB2	2.16	0.45
1:B:312:LEU:HB3	1:B:666:TYR:CD2	2.51	0.45
1:A:300:PHE:CD1	1:A:300:PHE:N	2.85	0.45
1:A:439:PHE:CZ	1:A:443:CYS:SG	3.10	0.45
1:A:454:ASN:C	1:A:454:ASN:HD22	2.19	0.45
1:A:485:TYR:HE2	1:A:512:ALA:HB1	1.80	0.45
1:A:352:ASP:N	1:A:352:ASP:OD2	2.50	0.45
1:B:362:LEU:HD12	1:B:381:LEU:HD23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:631:VAL:HG11	1:B:628:GLN:HG3	1.99	0.44
1:A:371:ARG:HG3	1:A:371:ARG:HH21	1.83	0.44
1:B:525:GLN:HG3	1:B:529:ASN:O	2.18	0.44
1:A:592:GLU:O	1:A:596:ARG:HB2	2.17	0.44
1:B:619:ARG:HB2	1:B:619:ARG:HE	1.55	0.44
1:B:435:ALA:O	1:B:438:MET:HB2	2.17	0.44
1:A:537:PRO:HA	1:A:538:PRO:HD2	1.94	0.44
1:A:462:PHE:HB3	1:A:463:PRO:CD	2.48	0.44
1:B:369:ILE:O	1:B:370:LYS:HB2	2.18	0.43
1:A:366:TYR:CD2	1:A:369:ILE:HD11	2.53	0.43
1:A:595:VAL:O	1:A:599:CYS:HB2	2.18	0.43
1:B:356:PRO:O	1:B:360:GLU:HG3	2.18	0.43
1:A:686:SER:HA	1:A:691:PHE:CG	2.53	0.43
1:A:359:LYS:HE2	1:A:381:LEU:HD21	2.01	0.43
1:A:548:HIS:CG	1:A:549:PRO:HD2	2.54	0.43
1:A:449:ALA:O	1:A:455:LEU:HA	2.19	0.43
1:A:501:PHE:HD2	1:A:520:LEU:HD13	1.83	0.43
1:B:449:ALA:O	1:B:455:LEU:HA	2.19	0.43
1:B:663:GLU:O	1:B:667:ARG:HD2	2.18	0.43
1:B:546:ILE:HG22	1:B:554:PHE:CE1	2.53	0.43
1:B:548:HIS:NE2	1:B:632:GLU:OE1	2.51	0.43
1:A:336:MET:CE	1:A:678:TRP:CZ2	2.97	0.43
1:A:330:ILE:O	1:A:330:ILE:CG2	2.66	0.42
1:A:485:TYR:HE2	1:A:512:ALA:CB	2.32	0.42
1:A:618:MET:HA	1:A:625:TRP:CD1	2.53	0.42
1:A:300:PHE:N	1:A:300:PHE:HD1	2.17	0.42
1:A:499:VAL:O	1:A:503:GLU:HG3	2.20	0.42
1:A:350:THR:HB	1:A:353:GLN:NE2	2.34	0.42
1:B:351:LYS:CE	1:B:392:SER:OG	2.47	0.42
1:B:618:MET:HA	1:B:625:TRP:CD1	2.54	0.42
1:A:566:ALA:HA	1:A:584:PHE:O	2.19	0.42
1:A:382:GLU:CD	1:A:386:LYS:HE3	2.40	0.42
1:A:418:ARG:C	1:A:420:GLN:N	2.72	0.42
1:A:520:LEU:HB3	1:A:521:PRO:HD2	2.02	0.42
1:A:355:PHE:N	1:A:356:PRO:CD	2.83	0.42
1:A:589:MET:HA	1:A:649:VAL:O	2.18	0.42
1:B:555:LYS:HG2	1:B:556:ASP:N	2.35	0.42
1:A:439:PHE:CE2	1:A:443:CYS:SG	3.13	0.41
1:B:300:PHE:HD2	1:B:313:THR:CG2	2.33	0.41
1:B:314:ASP:OD1	1:B:317:HIS:ND1	2.48	0.41
1:B:409:TRP:CE3	1:B:421:TRP:HA	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:750:HEM:NB	3:A:800:JM2:H2	2.36	0.41
1:B:481:ARG:HD3	1:B:498:ASN:HD21	1.86	0.41
1:B:388:ILE:O	1:B:392:SER:N	2.49	0.41
1:A:350:THR:HG22	1:A:353:GLN:H	1.85	0.41
1:A:676:TRP:CE3	1:B:677:VAL:HG22	2.56	0.41
1:B:362:LEU:HD11	1:B:384:VAL:HG21	2.03	0.41
1:B:380:ARG:NH1	1:B:383:GLU:OE2	2.46	0.41
1:A:312:LEU:HD13	1:A:666:TYR:CG	2.56	0.41
1:A:680:VAL:HA	1:A:681:PRO:HD3	1.91	0.41
1:A:624:LEU:O	1:A:628:GLN:HG3	2.20	0.40
1:A:299:ARG:HE	1:A:318:LEU:HD13	1.86	0.40
1:A:620:LYS:HB2	1:A:620:LYS:HE3	1.91	0.40
1:A:686:SER:HA	1:A:691:PHE:CB	2.50	0.40
1:B:459:ILE:HD11	1:B:582:CYS:HB2	2.04	0.40
1:B:393:THR:O	1:B:394:TYR:HB3	2.21	0.40
1:B:555:LYS:HG2	1:B:556:ASP:H	1.86	0.40
1:B:684:SER:HB3	1:B:687:ILE:CG1	2.50	0.40
1:A:665:GLU:CB	1:A:672:CYS:HB2	2.52	0.40
2:A:750:HEM:HMB3	5:A:860:ACT:H3	2.03	0.40
1:A:475:TRP:HB2	1:A:523:LEU:HB3	2.04	0.40
1:B:396:LEU:HG	1:B:577:LEU:HD12	2.04	0.40
1:B:606:ILE:O	1:B:610:VAL:HG23	2.21	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%)	383 (95%)	19 (5%)	1 (0%)	47	46
1	B	407/422 (96%)	391 (96%)	15 (4%)	1 (0%)	47	46
All	All	810/844 (96%)	774 (96%)	34 (4%)	2 (0%)	47	46

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	333	GLY
1	B	685	GLY

### 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%)	347 (96%)	16 (4%)	28	25
1	B	366/377 (97%)	356 (97%)	10 (3%)	44	46
All	All	729/754 (97%)	703 (96%)	26 (4%)	35	33

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	337	LEU
1	A	380	ARG
1	A	382	GLU
1	A	389	GLU
1	A	454	ASN
1	A	469	LYS
1	A	508	GLN
1	A	523	LEU
1	A	547	ARG
1	A	555	LYS
1	A	569	ASN
1	A	601	ASN
1	A	620	LYS
1	A	645	LYS
1	A	653	SER
1	A	715	VAL
1	B	320	SER
1	B	353	GLN
1	B	423	LYS
1	B	454	ASN
1	B	481	ARG

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Mol	Chain	Res	Type
1	B	540	LEU
1	B	547	ARG
1	B	555	LYS
1	B	668	CYS
1	B	699	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	353	GLN
1	A	425	GLN
1	A	454	ASN
1	A	508	GLN
1	A	569	ASN
1	A	605	ASN
1	A	642	GLN
1	A	697	ASN
1	B	353	GLN
1	B	385	ASN
1	B	454	ASN
1	B	535	GLN
1	B	601	ASN
1	B	605	ASN
1	B	642	GLN
1	B	661	HIS
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 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	HEM	A	750	1	27,50,50	2.09	6 (22%)	17,82,82	2.80	7 (41%)
2	HEM	B	750	1	27,50,50	2.25	7 (25%)	17,82,82	2.35	4 (23%)
5	ACT	A	860	-	1,3,3	1.68	0	0,3,3	0.00	-
5	ACT	B	860	-	1,3,3	1.76	0	0,3,3	0.00	-
4	H4B	B	760	-	16,18,18	1.01	1 (6%)	11,26,26	2.58	5 (45%)
3	JM2	B	800	-	7,13,13	3.15	2 (28%)	5,15,15	1.60	1 (20%)
3	JM2	A	800	-	7,13,13	3.13	2 (28%)	5,15,15	1.28	1 (20%)
4	H4B	A	760	-	16,18,18	0.98	0	11,26,26	3.08	6 (54%)

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	-	0/6/54/54	-
2	HEM	B	750	1	-	0/6/54/54	-
4	H4B	B	760	-	-	1/8/17/17	0/2/2/2
3	JM2	B	800	-	-	0/9/14/14	-
3	JM2	A	800	-	-	3/9/14/14	-
4	H4B	A	760	-	-	0/8/17/17	0/2/2/2

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	800	JM2	CD-NE	-7.91	1.28	1.46
3	A	800	JM2	CD-NE	-7.90	1.28	1.46
2	A	750	HEM	C3D-C2D	5.23	1.53	1.37
2	B	750	HEM	C3C-C2C	-5.11	1.33	1.40
2	A	750	HEM	C3B-C2B	-5.05	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	750	HEM	C3D-C2D	4.97	1.52	1.37
2	B	750	HEM	C3B-C2B	-4.78	1.33	1.40
2	B	750	HEM	C3C-CAC	3.33	1.54	1.47
2	A	750	HEM	C3C-CAC	3.21	1.54	1.47
2	A	750	HEM	C3B-CAB	2.92	1.53	1.47
2	A	750	HEM	C3C-C2C	-2.91	1.36	1.40
2	B	750	HEM	C3B-CAB	2.83	1.53	1.47
2	B	750	HEM	CMB-C2B	2.70	1.58	1.51
2	A	750	HEM	C1D-ND	2.63	1.41	1.36
3	B	800	JM2	C1-NH	2.46	1.34	1.27
3	A	800	JM2	C1-NH	2.37	1.33	1.27
2	B	750	HEM	CMD-C2D	2.34	1.56	1.51
4	B	760	H4B	C7-C6	2.12	1.54	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	750	HEM	CBA-CAA-C2A	-8.82	96.23	112.49
2	B	750	HEM	CBA-CAA-C2A	-7.08	99.43	112.49
4	A	760	H4B	C4-C4A-N5	5.77	123.97	119.12
4	B	760	H4B	C4-C4A-C8A	5.75	119.68	114.57
4	A	760	H4B	C4-C4A-C8A	4.35	118.44	114.57
2	A	750	HEM	CBD-CAD-C3D	-4.33	104.49	112.48
2	B	750	HEM	C1D-C2D-C3D	-3.84	104.33	107.00
4	A	760	H4B	N3-C2-N1	-3.71	119.60	125.42
4	A	760	H4B	C4-N3-C2	3.57	121.60	115.93
4	B	760	H4B	C2-N1-C8A	3.15	121.61	114.54
4	A	760	H4B	C2-N1-C8A	3.15	121.59	114.54
4	B	760	H4B	C4-C4A-N5	3.07	121.69	119.12
2	A	750	HEM	CMC-C2C-C3C	2.92	130.14	124.68
2	B	750	HEM	CBD-CAD-C3D	-2.90	107.13	112.48
3	B	800	JM2	CG-CD-NE	2.86	120.40	112.21
4	A	760	H4B	N2-C2-N3	2.82	121.64	117.25
2	A	750	HEM	C1D-C2D-C3D	-2.67	105.14	107.00
2	A	750	HEM	C4C-C3C-C2C	2.53	108.66	106.90
4	B	760	H4B	N3-C2-N1	-2.48	121.53	125.42
2	A	750	HEM	C4A-C3A-C2A	2.40	108.67	107.00
2	B	750	HEM	CMB-C2B-C3B	2.30	128.98	124.68
4	B	760	H4B	N2-C2-N3	2.23	120.72	117.25
3	A	800	JM2	CG-CD-NE	2.03	118.00	112.21
2	A	750	HEM	C3C-C4C-NC	-2.02	107.12	110.94

There are no chirality outliers.

All (4) torsion outliers are listed below:

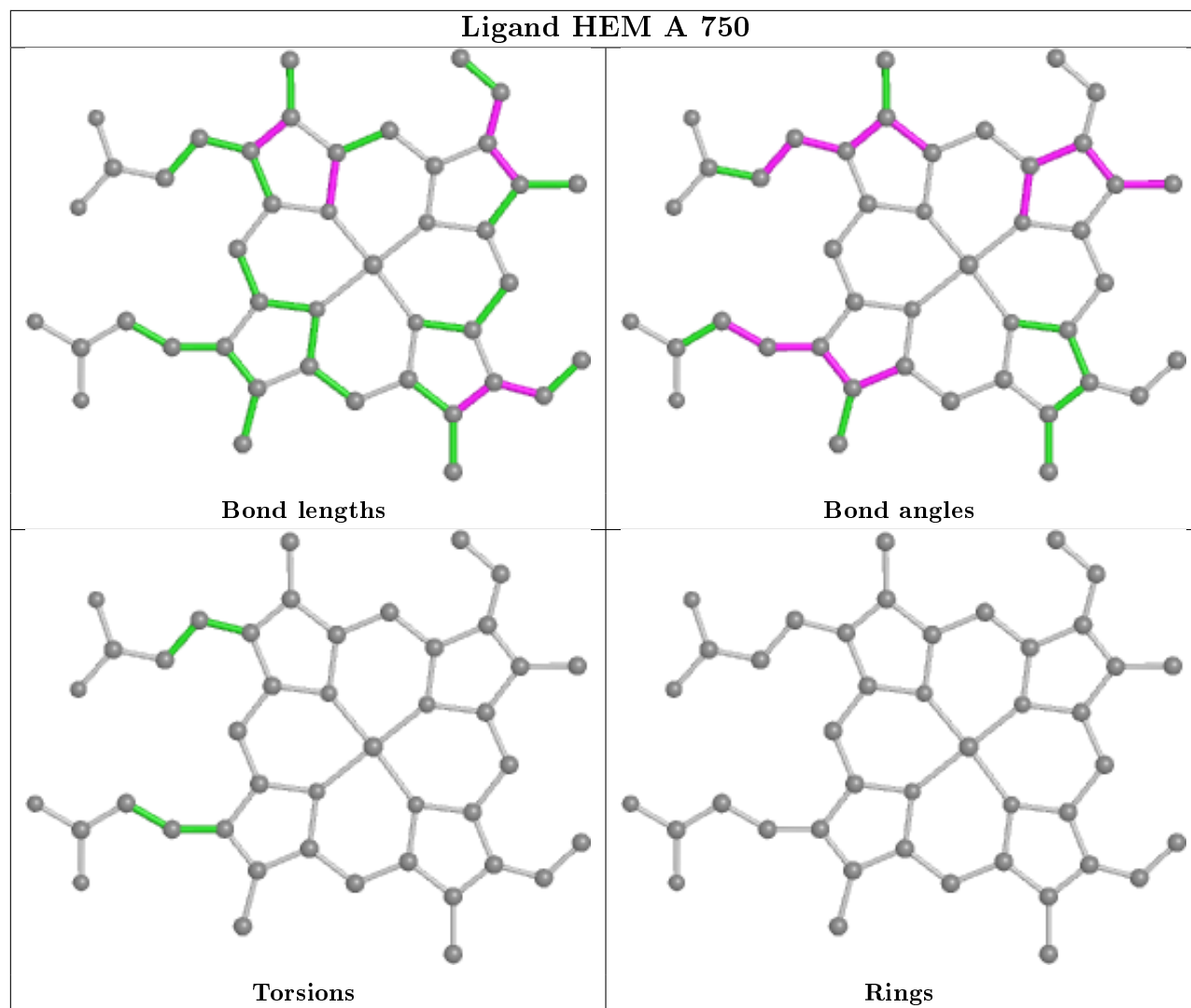
Mol	Chain	Res	Type	Atoms
4	B	760	H4B	O10-C10-C9-O9
3	A	800	JM2	C1-C2-S3-C4
3	A	800	JM2	CA-CB-CG-CD
3	A	800	JM2	NE-CD-CG-CB

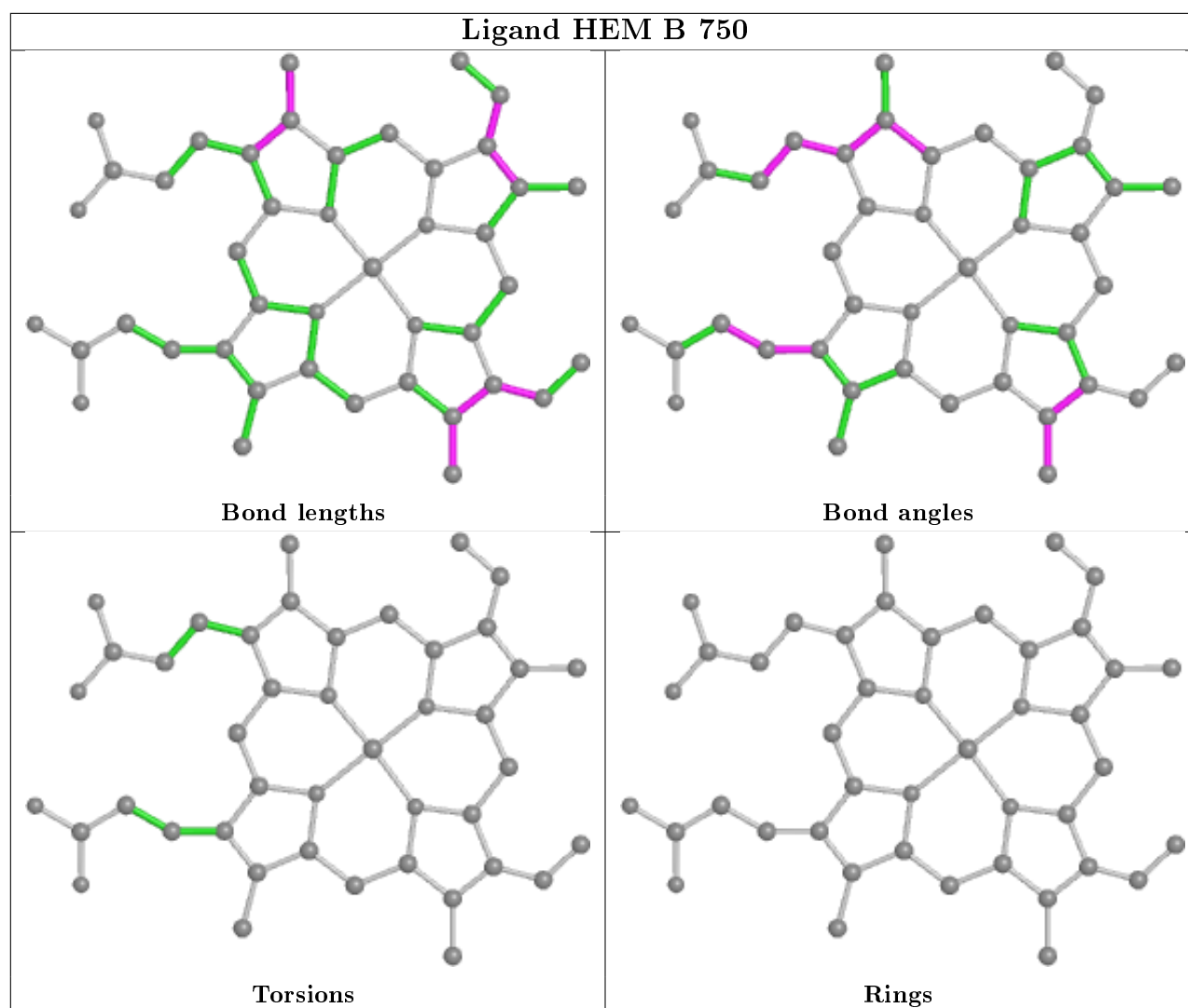
There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	750	HEM	6	0
2	B	750	HEM	4	0
5	A	860	ACT	1	0
3	A	800	JM2	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.





## 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%)	0.76	58 (14%) 2 3	38, 65, 110, 144	0
1	B	411/422 (97%)	0.32	24 (5%) 23 31	38, 56, 86, 106	0
All	All	818/844 (96%)	0.54	82 (10%) 7 11	38, 60, 105, 144	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	300	PHE	9.8
1	A	716	TRP	6.8
1	A	715	VAL	6.5
1	B	718	GLY	6.2
1	A	352	ASP	5.2
1	A	355	PHE	5.1
1	B	350	THR	5.1
1	A	551	PHE	4.8
1	A	488	PRO	4.7
1	A	300	PHE	4.6
1	B	348	VAL	4.2
1	B	615	ASP	4.2
1	A	619	ARG	4.1
1	B	351	LYS	4.0
1	A	511	LYS	4.0
1	A	299	ARG	3.8
1	B	352	ASP	3.8
1	B	619	ARG	3.7
1	A	667	ARG	3.6
1	B	616	LEU	3.6
1	A	388	ILE	3.4
1	A	389	GLU	3.4
1	A	479	LEU	3.4
1	A	506	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	712	ASN	3.3
1	A	386	LYS	3.2
1	A	391	THR	3.2
1	A	338	PRO	3.2
1	A	486	LYS	3.1
1	A	713	THR	3.0
1	B	301	LEU	3.0
1	B	667	ARG	2.9
1	A	371	ARG	2.9
1	A	566	ALA	2.9
1	A	714	HIS	2.8
1	B	591	THR	2.8
1	A	491	SER	2.7
1	A	487	GLN	2.6
1	B	389	GLU	2.6
1	A	390	SER	2.6
1	B	620	LYS	2.6
1	A	480	ILE	2.6
1	A	593	ILE	2.6
1	A	685	GLY	2.6
1	A	554	PHE	2.6
1	A	584	PHE	2.6
1	A	351	LYS	2.6
1	A	682	PRO	2.6
1	A	591	THR	2.5
1	A	385	ASN	2.5
1	B	310	VAL	2.5
1	A	350	THR	2.4
1	A	503	GLU	2.4
1	B	321	THR	2.4
1	A	354	LEU	2.4
1	A	490	GLY	2.4
1	A	392	SER	2.4
1	A	504	ILE	2.4
1	B	302	LYS	2.3
1	B	567	VAL	2.3
1	A	567	VAL	2.3
1	A	315	THR	2.3
1	A	302	LYS	2.3
1	B	328	GLU	2.2
1	B	349	ARG	2.2
1	B	664	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	617	ASP	2.2
1	A	514	ARG	2.2
1	A	415	CYS	2.1
1	A	322	LEU	2.1
1	A	482	TYR	2.1
1	A	680	VAL	2.1
1	A	469	LYS	2.1
1	B	677	VAL	2.1
1	A	617	ASP	2.1
1	A	678	TRP	2.1
1	B	566	ALA	2.0
1	A	489	ASP	2.0
1	A	552	ASP	2.0
1	A	677	VAL	2.0
1	A	309	ASP	2.0
1	A	507	GLN	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
5	ACT	B	860	4/4	0.95	0.18	65,66,66,67	0
3	JM2	B	800	14/14	0.95	0.17	41,47,50,51	0
3	JM2	A	800	14/14	0.95	0.26	39,48,51,52	0
4	H4B	B	760	17/17	0.96	0.15	41,44,48,49	0
4	H4B	A	760	17/17	0.96	0.15	41,45,51,53	0
6	ZN	A	900	1/1	0.97	0.10	54,54,54,54	0
5	ACT	A	860	4/4	0.97	0.16	81,83,83,85	0

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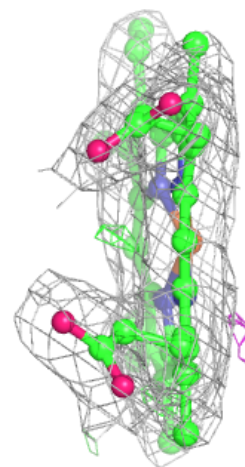
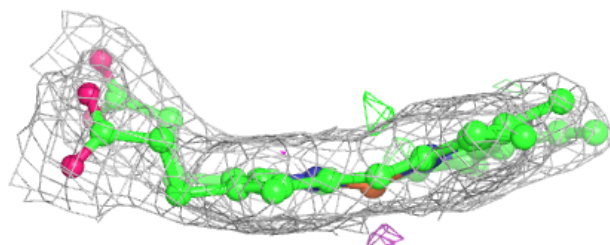
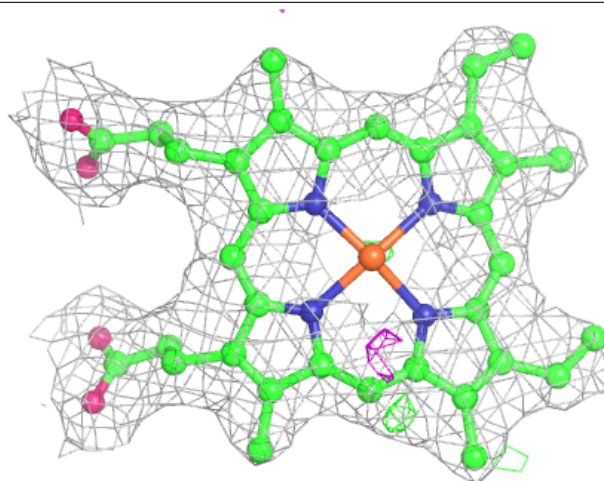
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	HEM	A	750	43/43	0.97	0.23	40,46,52,57	0
2	HEM	B	750	43/43	0.97	0.18	40,44,49,53	0

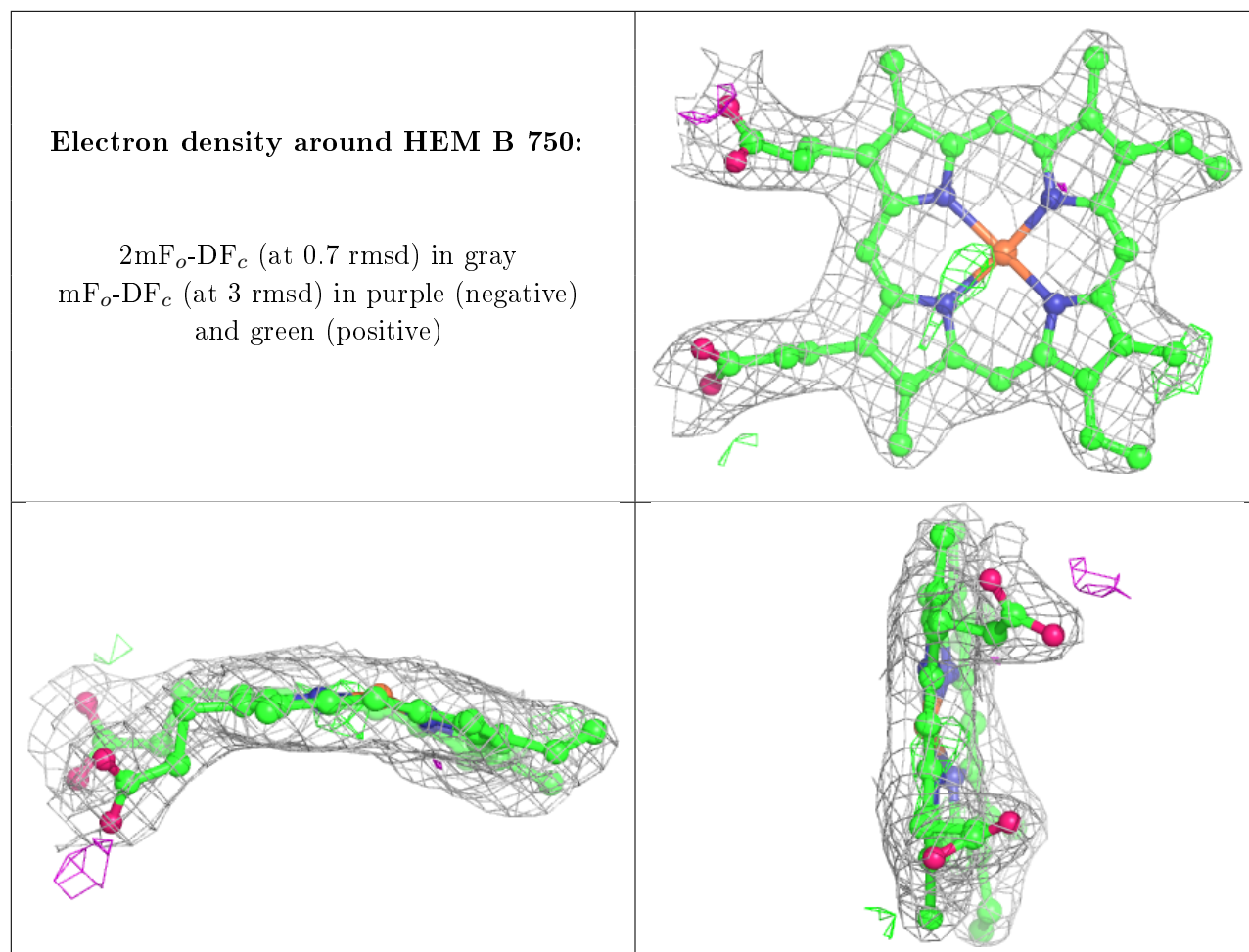
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around HEM A 750:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)







## 6.5 Other polymers [i](#)

There are no such residues in this entry.