



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2024 – 04:46 pm BST

PDB ID : 4V3X  
Title : Structure of rat neuronal nitric oxide synthase heme domain in complex with N-2-(2-(1H-imidazol-1-yl)pyrimidin-4-yl)ethyl-3-(3- fluorophenyl)propan-1-amine  
Authors : Li, H.; Poulos, T.L.  
Deposited on : 2014-10-20  
Resolution : 1.99 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
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)	:	2.36.2

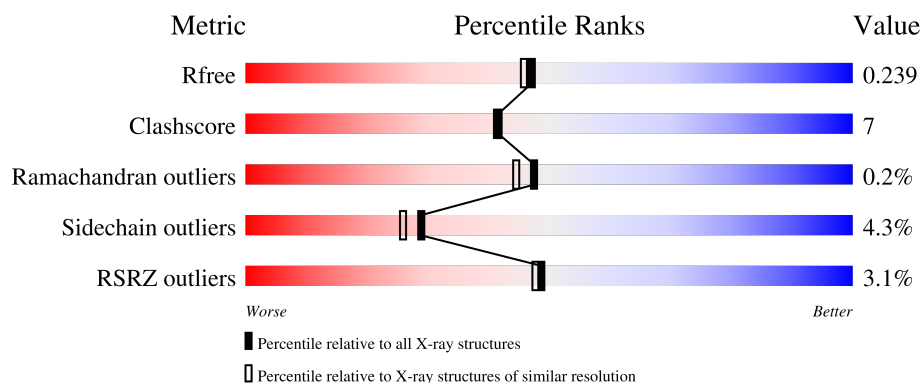
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.99 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 of 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>5%</div> <div> <div></div> <div>79%</div> <div>16%</div> <div>..</div> </div> </div>
1	B	422	<div> <div>%</div> <div> <div></div> <div>81%</div> <div>14%</div> <div>..</div> </div> </div>

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 7078 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	408	Total	C	N	O	S	3	3	1
			3326	2129	567	608	22			
1	B	411	Total	C	N	O	S	0	3	0
			3357	2148	574	614	21			

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



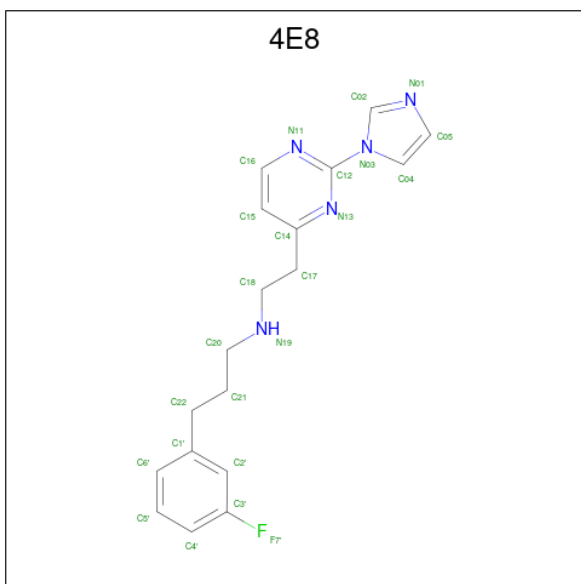
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- 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 3-(3-fluorophenyl)-N-{2-[2-(1H-imidazol-1-yl)pyrimidin-4-yl]ethyl}propan-1-amine (three-letter code: 4E8) (formula: C<sub>18</sub>H<sub>20</sub>FN<sub>5</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	F	N	0	0
			24	18	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	F	N	0	0
			24	18	1	5		

- 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		

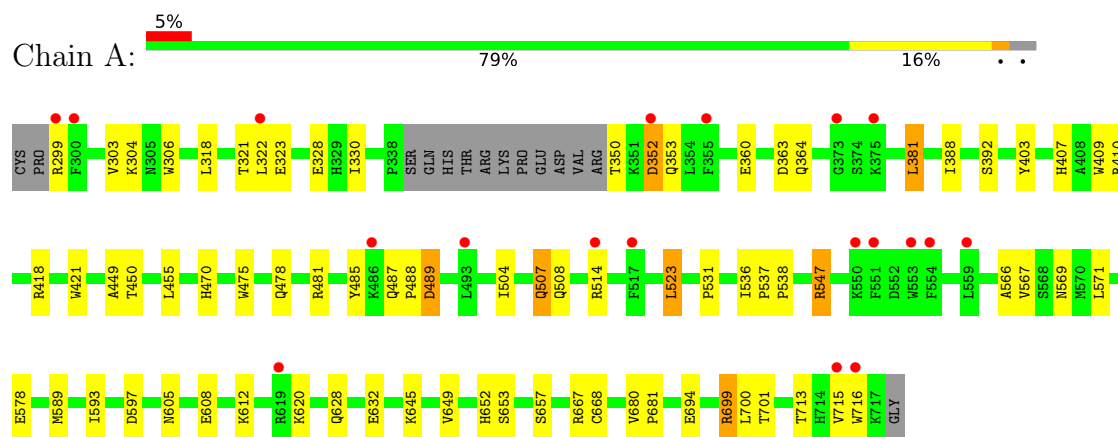
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	89	Total	O	0	0
			89	89		
7	B	129	Total	O	0	0
			129	129		

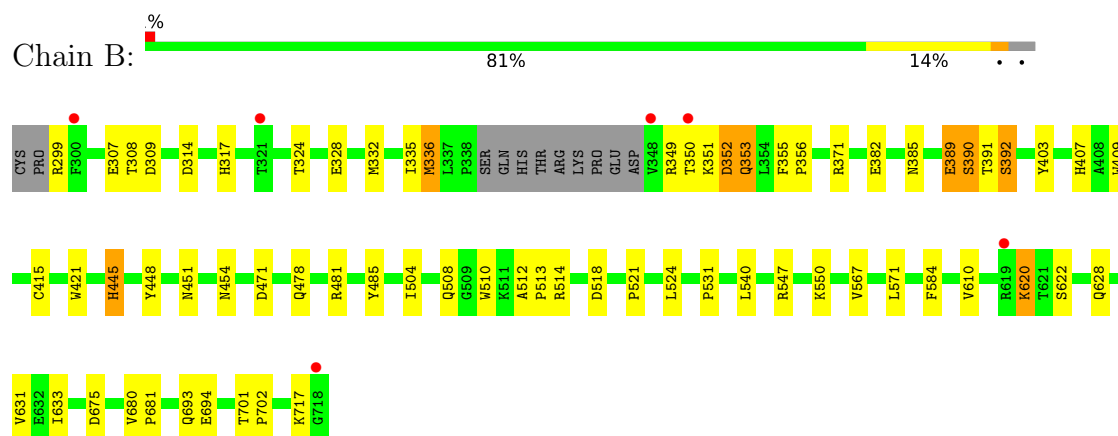
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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, $\alpha$ , $\beta$ , $\gamma$	51.91Å 110.82Å 164.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	92.12 – 1.99 49.51 – 1.99	Depositor EDS
% Data completeness (in resolution range)	98.3 (92.12-1.99) 98.4 (49.51-1.99)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.96 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.186 , 0.239 0.186 , 0.239	Depositor DCC
$R_{free}$ test set	3215 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.4	Xtriage
Anisotropy	0.892	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 47.9	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	0.97	EDS
Total number of atoms	7078	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.70% 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: ACT, 4E8, ZN, HEM, H4B

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	0.85	2/3428 (0.1%)	0.89	6/4651 (0.1%)
1	B	0.85	0/3459	0.87	4/4689 (0.1%)
All	All	0.85	2/6887 (0.0%)	0.88	10/9340 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	657[A]	SER	CA-C	9.90	1.78	1.52
1	A	657[B]	SER	CA-C	9.90	1.78	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	418	ARG	NE-CZ-NH1	-7.11	116.74	120.30
1	A	547	ARG	NE-CZ-NH1	6.85	123.73	120.30
1	A	381	LEU	CA-CB-CG	6.81	130.97	115.30
1	B	675	ASP	CB-CG-OD1	5.87	123.59	118.30
1	A	363	ASP	CB-CG-OD1	5.73	123.45	118.30
1	A	410	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	A	700	LEU	CB-CG-CD2	-5.27	102.05	111.00
1	B	336	MET	CG-SD-CE	-5.19	91.90	100.20
1	B	471	ASP	CB-CG-OD1	5.11	122.90	118.30
1	B	371	ARG	NE-CZ-NH1	5.07	122.83	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	3326	0	3237	52	0
1	B	3357	0	3275	47	0
2	A	43	0	30	2	0
2	B	43	0	30	6	0
3	A	17	0	15	0	0
3	B	17	0	15	0	0
4	A	24	0	20	1	0
4	B	24	0	20	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	89	0	0	2	0
7	B	129	0	0	0	0
All	All	7078	0	6648	95	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (95) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:523:LEU:HD22	1:A:531:PRO:HB2	1.51	0.93
1:A:487:GLN:HB2	1:A:489:ASP:HB3	1.63	0.80
1:B:353:GLN:HE21	1:B:353:GLN:H	1.29	0.80
2:A:750:HEM:HMC2	2:A:750:HEM:HBC2	1.65	0.79
1:A:508:GLN:NE2	1:A:716:TRP:HH2	1.84	0.74
1:A:652:HIS:ND1	7:A:2072:HOH:O	2.21	0.74
1:B:620:LYS:HE3	1:B:622:SER:H	1.53	0.74
1:A:350:THR:N	1:A:353:GLN:NE2	2.38	0.70
1:A:667:ARG:NH1	1:A:668[A]:CYS:SG	2.66	0.68
1:B:355:PHE:CE2	1:B:385:ASN:HB2	2.31	0.64
1:A:628:GLN:HG3	1:B:631:VAL:HG11	1.79	0.64
1:A:323:GLU:HG2	1:B:328:GLU:HB3	1.79	0.64
1:A:508:GLN:NE2	1:A:716:TRP:CH2	2.65	0.63
1:A:299:ARG:HE	1:A:318:LEU:HD13	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:353:GLN:O	1:B:356:PRO:HG2	2.02	0.59
1:A:306:TRP:CD1	1:B:336:MET:HE2	2.38	0.59
1:B:352:ASP:HB3	1:B:353:GLN:HE21	1.68	0.58
1:A:299:ARG:HG2	1:A:318:LEU:HD11	1.85	0.58
2:B:750:HEM:CMC	2:B:750:HEM:HBC2	2.33	0.58
2:B:750:HEM:HBC2	2:B:750:HEM:HMC1	1.87	0.57
1:A:306:TRP:CD2	1:B:336:MET:CE	2.88	0.56
1:A:475:TRP:HB2	1:A:523:LEU:HB3	1.85	0.56
1:A:306:TRP:CD2	1:B:336:MET:HE3	2.41	0.56
1:B:350:THR:OG1	1:B:353:GLN:NE2	2.38	0.56
1:A:306:TRP:CE2	1:B:336:MET:HE3	2.40	0.56
1:B:299:ARG:HB3	1:B:299:ARG:NH1	2.20	0.55
1:A:571:LEU:HD21	1:A:578:GLU:HB3	1.87	0.55
2:B:750:HEM:HHC	2:B:750:HEM:HBB2	1.88	0.55
1:A:306:TRP:CG	1:B:336:MET:HE2	2.41	0.55
1:A:620:LYS:HB2	1:A:620:LYS:NZ	2.22	0.55
1:A:321:THR:HG23	1:A:322:LEU:HG	1.88	0.55
1:A:350:THR:N	1:A:353:GLN:HE21	2.06	0.54
1:A:487:GLN:CB	1:A:489:ASP:HB3	2.36	0.52
1:B:299:ARG:HB3	1:B:299:ARG:CZ	2.40	0.52
2:B:750:HEM:C1C	4:B:800:4E8:H05	2.43	0.52
1:B:308:THR:O	1:B:309:ASP:HB2	2.10	0.51
1:A:504:ILE:HA	1:A:507:GLN:NE2	2.26	0.50
1:B:391:THR:O	1:B:392:SER:CB	2.59	0.50
1:A:299:ARG:HG2	1:A:318:LEU:CD1	2.42	0.50
1:B:403:TYR:CE1	1:B:407:HIS:CE1	2.99	0.50
1:B:409:TRP:CE3	1:B:421:TRP:HA	2.47	0.49
1:A:306:TRP:CG	1:B:336:MET:CE	2.95	0.49
1:B:353:GLN:H	1:B:353:GLN:NE2	2.05	0.49
1:B:478:GLN:HB2	1:B:481:ARG:HG3	1.94	0.48
1:A:632:GLU:OE2	1:B:628:GLN:NE2	2.46	0.48
1:A:388:ILE:O	1:A:392:SER:N	2.41	0.48
1:A:388:ILE:O	1:A:392:SER:HA	2.13	0.48
1:B:352:ASP:HB3	1:B:353:GLN:NE2	2.30	0.47
1:B:448:TYR:CD1	1:B:448:TYR:C	2.88	0.46
1:A:605:ASN:CG	1:A:605:ASN:O	2.53	0.46
1:B:567:VAL:HB	1:B:584:PHE:CZ	2.50	0.46
1:B:349:ARG:HG2	1:B:353:GLN:HG3	1.97	0.46
1:A:409:TRP:CE3	1:A:421:TRP:HA	2.51	0.46
1:B:504:ILE:O	1:B:508:GLN:HG2	2.16	0.45
1:A:360:GLU:O	1:A:364:GLN:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:ASP:OD1	1:A:352:ASP:N	2.49	0.45
1:B:610:VAL:HG21	1:B:633:ILE:HD11	1.99	0.45
1:A:488:PRO:HG2	1:A:489:ASP:H	1.81	0.45
1:A:605:ASN:ND2	7:A:2066:HOH:O	2.44	0.45
2:A:750:HEM:HBC2	2:A:750:HEM:CMC	2.36	0.45
1:B:701:THR:HA	1:B:702:PRO:C	2.37	0.45
1:A:328:GLU:O	1:B:324:THR:N	2.50	0.45
1:A:403:TYR:CE1	1:A:407:HIS:CE1	3.06	0.44
1:B:445:HIS:C	1:B:445:HIS:CD2	2.91	0.44
1:B:512:ALA:HA	1:B:513:PRO:HD2	1.82	0.44
1:A:450:THR:HA	1:A:455:LEU:HD22	2.00	0.43
1:B:485:TYR:CZ	1:B:514:ARG:HA	2.54	0.43
1:A:478:GLN:HA	1:A:566:ALA:O	2.18	0.43
1:A:567:VAL:HG23	4:A:800:4E8:C12	2.49	0.43
1:A:449:ALA:O	1:A:455:LEU:HA	2.19	0.42
1:A:304:LYS:HE2	1:A:306:TRP:CD2	2.54	0.42
1:A:589:MET:HA	1:A:649:VAL:O	2.18	0.42
1:A:536:ILE:O	1:A:537:PRO:C	2.57	0.42
1:B:524:LEU:O	1:B:531:PRO:HA	2.20	0.42
1:A:593:ILE:HA	1:A:597:ASP:HB2	2.02	0.42
1:A:478:GLN:HB2	1:A:481:ARG:HG3	2.01	0.41
1:B:571:LEU:C	1:B:571:LEU:HD23	2.40	0.41
1:A:537:PRO:HA	1:A:538:PRO:HD2	1.87	0.41
1:B:415:CYS:HB2	2:B:750:HEM:ND	2.34	0.41
1:A:322:LEU:HD13	1:A:699:ARG:HH21	1.85	0.41
1:B:510:TRP:CE2	1:B:521:PRO:HD3	2.55	0.41
1:B:451:ASN:HB3	1:B:454:ASN:O	2.21	0.41
1:A:680:VAL:HA	1:A:681:PRO:HD3	1.90	0.41
1:B:389:GLU:HG2	1:B:390:SER:N	2.35	0.41
2:B:750:HEM:HHC	2:B:750:HEM:CBB	2.49	0.41
1:B:513:PRO:HG2	1:B:518:ASP:CG	2.41	0.41
1:A:694:GLU:HB3	1:B:335:ILE:HD13	2.03	0.40
1:B:693:GLN:HG3	1:B:694:GLU:O	2.22	0.40
1:A:523:LEU:CD2	1:A:531:PRO:HB2	2.36	0.40
1:B:680:VAL:HA	1:B:681:PRO:HD3	1.93	0.40
1:A:485:TYR:CZ	1:A:514:ARG:HA	2.57	0.40
1:B:314:ASP:OD1	1:B:317:HIS:ND1	2.51	0.40
1:B:349:ARG:HG2	1:B:353:GLN:CG	2.52	0.40
1:A:523:LEU:HD22	1:A:531:PRO:CB	2.36	0.40
1:B:353:GLN:HE21	1:B:353:GLN:N	2.08	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	407/422 (96%)	386 (95%)	20 (5%)	1 (0%)	47	44
1	B	410/422 (97%)	399 (97%)	10 (2%)	1 (0%)	47	44
All	All	817/844 (97%)	785 (96%)	30 (4%)	2 (0%)	47	44

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	489	ASP
1	B	352	ASP

### 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	366/377 (97%)	349 (95%)	17 (5%)	27	23
1	B	369/377 (98%)	354 (96%)	15 (4%)	30	28
All	All	735/754 (98%)	703 (96%)	32 (4%)	29	25

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

Mol	Chain	Res	Type
1	A	303	VAL
1	A	330	ILE
1	A	352	ASP
1	A	381	LEU

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Mol	Chain	Res	Type
1	A	470	HIS
1	A	507	GLN
1	A	523	LEU
1	A	547	ARG
1	A	569	ASN
1	A	608	GLU
1	A	612	LYS
1	A	645	LYS
1	A	653	SER
1	A	699	ARG
1	A	701	THR
1	A	713	THR
1	A	715	VAL
1	B	307[A]	GLU
1	B	307[B]	GLU
1	B	332	MET
1	B	351	LYS
1	B	353	GLN
1	B	382	GLU
1	B	389	GLU
1	B	390	SER
1	B	392	SER
1	B	445	HIS
1	B	540	LEU
1	B	547	ARG
1	B	550	LYS
1	B	620	LYS
1	B	717	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	353	GLN
1	A	425	GLN
1	A	454	ASN
1	A	507	GLN
1	A	569	ASN
1	A	642	GLN
1	A	697	ASN
1	B	353	GLN
1	B	454	ASN
1	B	507	GLN

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Mol	Chain	Res	Type
1	B	535	GLN
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 monosaccharides 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$
5	ACT	B	860	-	3,3,3	0.64	0	3,3,3	1.39	0
2	HEM	A	750	1,4	41,50,50	1.29	5 (12%)	45,82,82	1.89	12 (26%)
3	H4B	A	760	-	16,18,18	0.92	1 (6%)	11,26,26	2.64	5 (45%)
3	H4B	B	760	-	16,18,18	1.31	2 (12%)	11,26,26	2.46	3 (27%)
2	HEM	B	750	1,4	41,50,50	1.28	4 (9%)	45,82,82	2.19	18 (40%)
5	ACT	A	860	-	3,3,3	0.78	0	3,3,3	0.91	0
4	4E8	A	800	2	25,26,26	1.59	5 (20%)	30,33,33	2.81	15 (50%)
4	4E8	B	800	2	25,26,26	1.34	3 (12%)	30,33,33	2.56	7 (23%)

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	1,4	-	0/12/54/54	-
3	H4B	A	760	-	-	0/8/17/17	0/2/2/2
3	H4B	B	760	-	-	0/8/17/17	0/2/2/2
2	HEM	B	750	1,4	-	2/12/54/54	-
4	4E8	A	800	2	-	1/9/13/13	0/3/3/3
4	4E8	B	800	2	-	0/9/13/13	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	800	4E8	C12-N13	3.84	1.37	1.32
4	B	800	4E8	C12-N13	3.54	1.37	1.32
2	B	750	HEM	C1B-NB	-3.38	1.34	1.40
4	A	800	4E8	C12-N11	3.26	1.36	1.31
4	B	800	4E8	C04-N03	-3.18	1.34	1.39
2	A	750	HEM	C1B-NB	-3.17	1.34	1.40
3	B	760	H4B	C4-N3	3.16	1.38	1.33
4	A	800	4E8	C02-N03	-3.08	1.33	1.36
4	A	800	4E8	C04-N03	-3.04	1.34	1.39
4	A	800	4E8	C4'-C3'	2.80	1.42	1.37
2	A	750	HEM	C4D-ND	-2.80	1.35	1.40
2	B	750	HEM	C4D-ND	-2.54	1.35	1.40
2	B	750	HEM	C3B-C4B	2.50	1.49	1.44
4	B	800	4E8	C4'-C3'	2.46	1.41	1.37
2	A	750	HEM	O1A-CGA	2.45	1.30	1.22
3	B	760	H4B	C7-N8	2.35	1.48	1.44
2	A	750	HEM	C4B-NB	-2.17	1.34	1.38
2	B	750	HEM	C4B-NB	-2.09	1.34	1.38
3	A	760	H4B	C6-N5	2.04	1.49	1.45
2	A	750	HEM	FE-NB	2.01	2.06	1.96

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	800	4E8	N11-C12-N13	-7.21	117.91	126.08
4	A	800	4E8	C16-N11-C12	6.48	122.62	114.04
4	A	800	4E8	N11-C12-N13	-6.19	119.06	126.08
3	B	760	H4B	C8A-C4A-C4	6.09	119.98	114.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	800	4E8	C16-N11-C12	5.61	121.47	114.04
4	A	800	4E8	N13-C12-N03	5.55	121.96	114.78
3	A	760	H4B	C8A-C4A-C4	5.49	119.44	114.57
4	B	800	4E8	N11-C12-N03	5.26	122.97	114.81
4	B	800	4E8	C02-N03-C04	5.06	117.67	108.50
2	A	750	HEM	C1B-NB-C4B	4.95	110.18	105.07
2	B	750	HEM	C1B-NB-C4B	4.92	110.16	105.07
2	B	750	HEM	CBA-CAA-C2A	-4.62	104.74	112.62
4	A	800	4E8	C15-C16-N11	-4.26	118.67	123.96
4	B	800	4E8	C02-N03-C12	-4.09	117.99	126.02
2	A	750	HEM	CHA-C4D-ND	4.02	129.35	124.38
2	B	750	HEM	CHA-C4D-C3D	-3.74	118.31	125.33
4	A	800	4E8	C02-N03-C04	3.72	115.25	108.50
2	B	750	HEM	CHC-C4B-NB	3.70	128.45	124.43
3	A	760	H4B	C2-N1-C8A	3.68	122.79	114.54
4	A	800	4E8	C20-C21-C22	-3.64	106.45	112.95
2	A	750	HEM	CMC-C2C-C3C	3.55	131.31	124.68
2	B	750	HEM	C2D-C1D-ND	3.40	113.95	109.88
3	B	760	H4B	C2-N1-C8A	3.36	122.06	114.54
4	B	800	4E8	N13-C12-N03	3.34	119.10	114.78
3	A	760	H4B	N1-C2-N3	-3.27	120.29	125.42
4	A	800	4E8	C05-C04-N03	-3.26	100.75	106.50
2	B	750	HEM	CHD-C1D-C2D	-3.22	119.94	124.98
2	A	750	HEM	CHD-C1D-ND	3.21	127.91	124.43
2	B	750	HEM	CHA-C4D-ND	3.20	128.33	124.38
2	A	750	HEM	CHA-C4D-C3D	-3.02	119.66	125.33
2	B	750	HEM	O2A-CGA-O1A	-3.02	115.77	123.30
2	B	750	HEM	O2A-CGA-CBA	2.96	123.55	114.03
4	A	800	4E8	C17-C14-N13	2.96	120.36	115.95
2	A	750	HEM	CHC-C4B-NB	2.89	127.57	124.43
2	A	750	HEM	O2D-CGD-CBD	2.89	123.31	114.03
2	B	750	HEM	C3D-C4D-ND	2.86	113.35	110.17
4	A	800	4E8	C02-N03-C12	-2.80	120.53	126.02
4	B	800	4E8	C05-C04-N03	-2.78	101.59	106.50
4	A	800	4E8	F7'-C3'-C4'	2.76	123.23	118.54
4	A	800	4E8	C22-C1'-C2'	-2.67	116.16	120.54
2	B	750	HEM	O2D-CGD-CBD	2.62	122.46	114.03
2	B	750	HEM	C4B-CHC-C1C	2.61	126.00	122.56
2	B	750	HEM	CHB-C1B-NB	2.60	127.59	124.38
4	A	800	4E8	N11-C12-N03	2.57	118.79	114.81
2	A	750	HEM	CHD-C1D-C2D	-2.57	120.96	124.98
3	A	760	H4B	C4A-N5-C6	-2.55	114.21	121.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	800	4E8	C4'-C3'-C2'	-2.55	119.97	123.29
4	A	800	4E8	C16-C15-C14	2.47	118.94	116.62
2	B	750	HEM	CBD-CAD-C3D	-2.47	105.77	112.63
3	A	760	H4B	C2-N3-C4	2.46	119.84	115.93
2	B	750	HEM	C4D-ND-C1D	-2.45	102.54	105.07
2	A	750	HEM	CBA-CAA-C2A	-2.44	108.45	112.62
2	A	750	HEM	CHB-C1B-NB	2.35	127.28	124.38
2	A	750	HEM	CBD-CAD-C3D	-2.35	106.11	112.63
3	B	760	H4B	N1-C2-N3	-2.22	121.93	125.42
2	B	750	HEM	CMA-C3A-C4A	-2.21	125.06	128.46
2	B	750	HEM	CMD-C2D-C1D	2.20	128.40	125.04
2	B	750	HEM	O2D-CGD-O1D	-2.15	117.93	123.30
2	A	750	HEM	CMD-C2D-C1D	2.12	128.27	125.04
4	A	800	4E8	C04-C05-N01	2.05	111.17	107.57

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	800	4E8	N19-C20-C21-C22
2	B	750	HEM	CAA-CBA-CGA-O2A
2	B	750	HEM	CAA-CBA-CGA-O1A

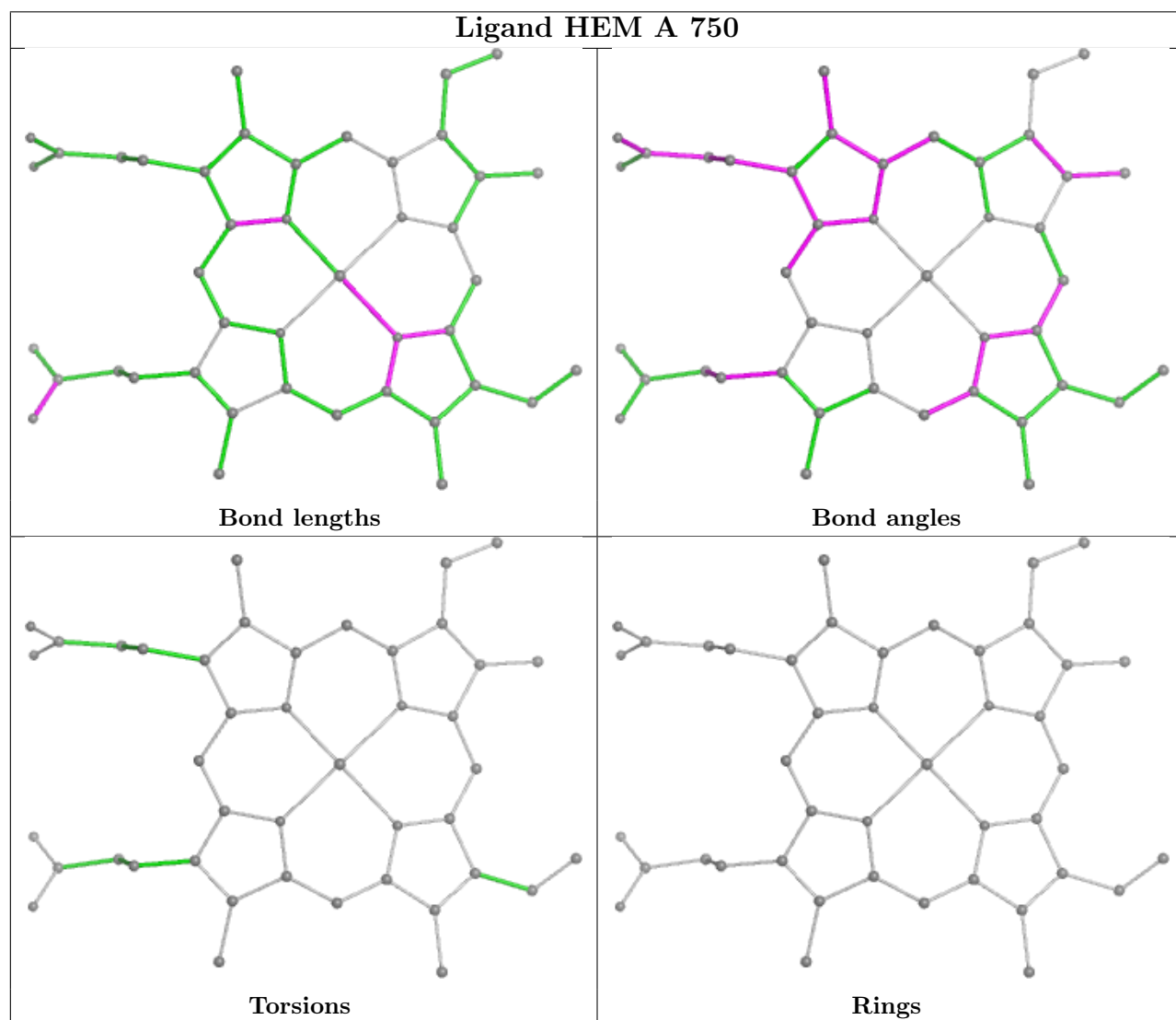
There are no ring outliers.

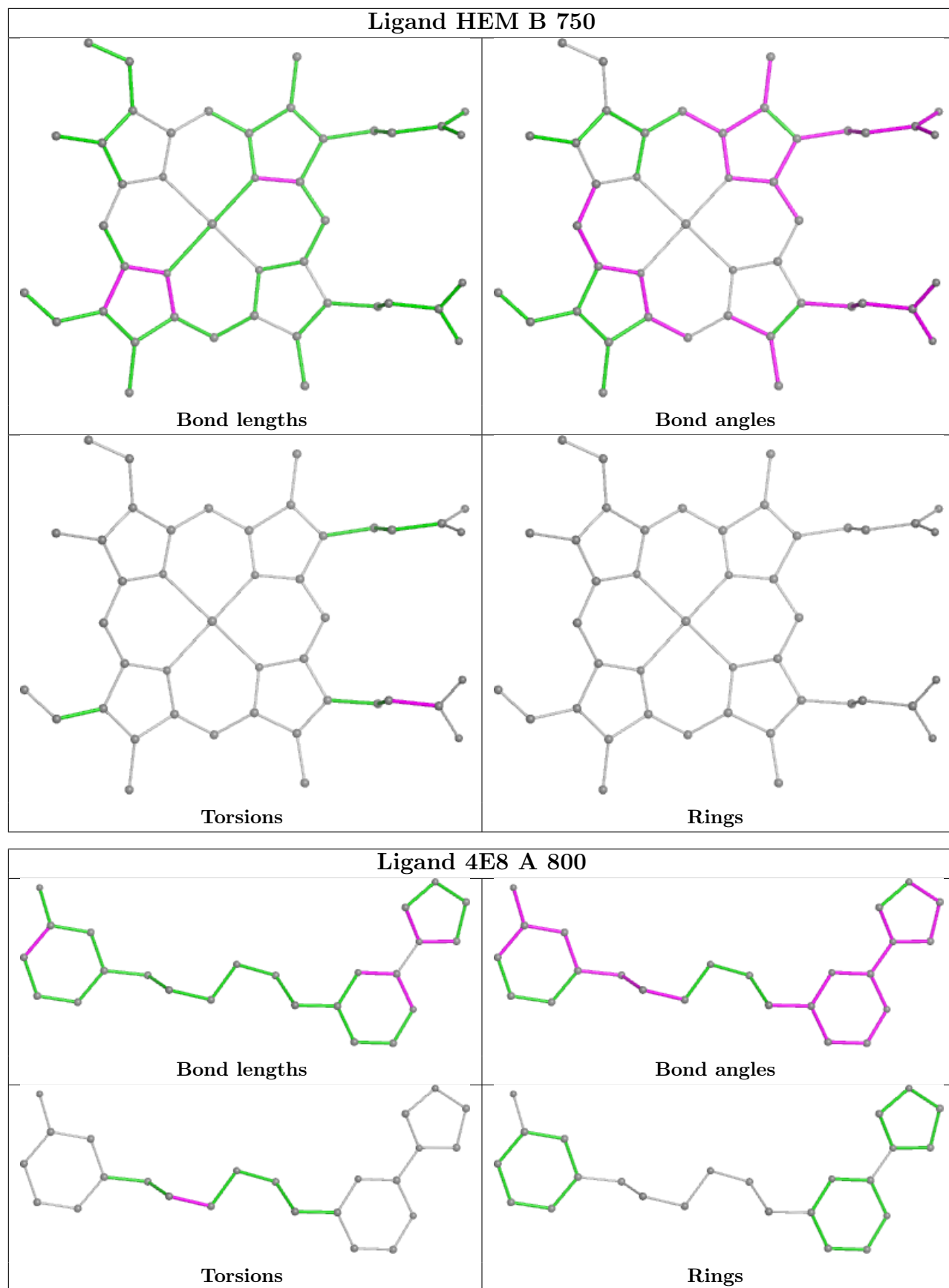
4 monomers are involved in 9 short contacts:

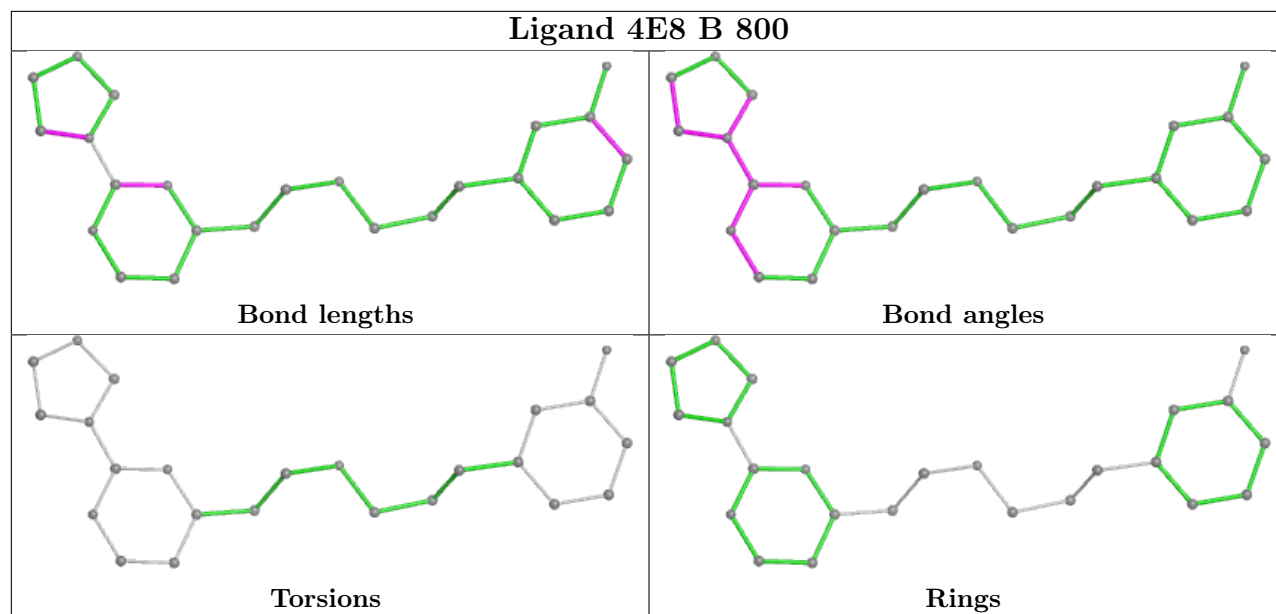
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	750	HEM	2	0
2	B	750	HEM	6	0
4	A	800	4E8	1	0
4	B	800	4E8	1	0

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	408/422 (96%)	0.40	19 (4%) 31 30	34, 56, 91, 117	0
1	B	411/422 (97%)	0.18	6 (1%) 73 72	34, 48, 76, 100	0
All	All	819/844 (97%)	0.29	25 (3%) 49 48	34, 52, 88, 117	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	355	PHE	4.5
1	B	300	PHE	4.4
1	A	554	PHE	4.3
1	A	493	LEU	3.7
1	A	373	GLY	3.3
1	A	551	PHE	3.2
1	A	299	ARG	3.2
1	A	716	TRP	3.1
1	A	715	VAL	3.0
1	A	322	LEU	2.9
1	B	350	THR	2.6
1	A	300	PHE	2.5
1	B	348	VAL	2.5
1	A	352	ASP	2.5
1	A	619	ARG	2.5
1	A	550	LYS	2.4
1	A	553	TRP	2.4
1	A	559	LEU	2.3
1	B	718	GLY	2.3
1	B	619	ARG	2.2
1	A	486	LYS	2.2
1	B	321	THR	2.1
1	A	517	PHE	2.1
1	A	375	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	514	ARG	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

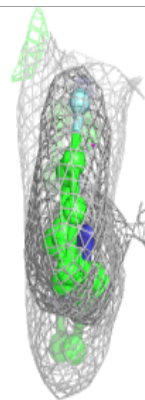
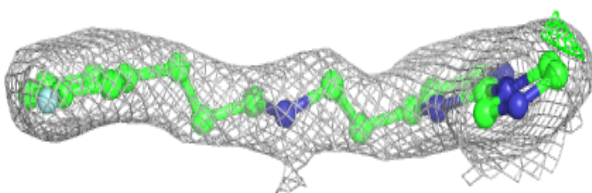
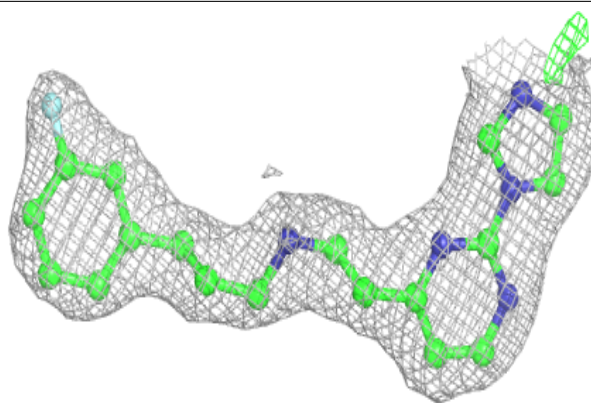
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	A	860	4/4	0.94	0.22	75,77,79,82	0
3	H4B	B	760	17/17	0.95	0.14	37,39,44,44	0
4	4E8	B	800	24/24	0.97	0.11	37,43,55,61	0
3	H4B	A	760	17/17	0.97	0.11	34,39,45,45	0
4	4E8	A	800	24/24	0.98	0.12	39,49,63,65	0
5	ACT	B	860	4/4	0.98	0.15	54,55,57,58	0
2	HEM	A	750	43/43	0.99	0.11	36,40,48,50	0
2	HEM	B	750	43/43	0.99	0.14	31,38,45,50	0
6	ZN	A	900	1/1	0.99	0.14	46,46,46,46	0

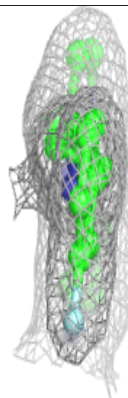
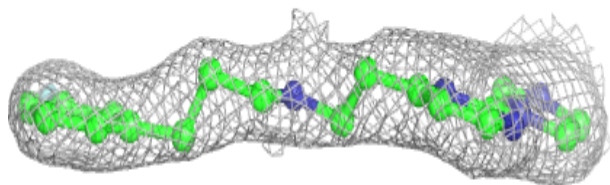
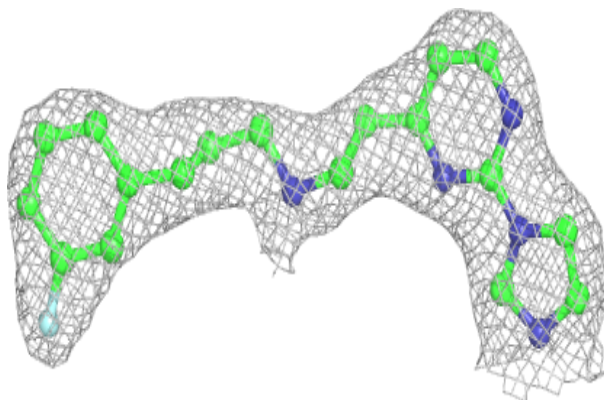
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around 4E8 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)

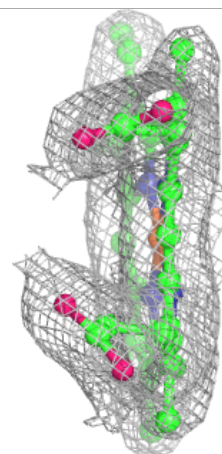
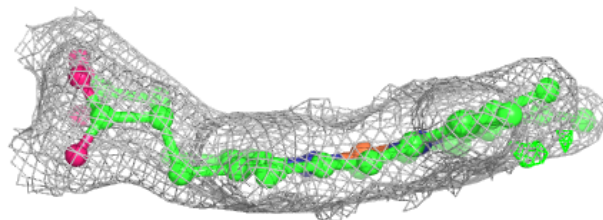
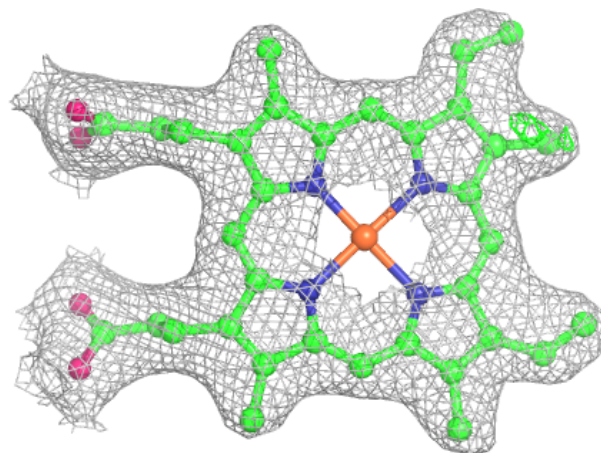
**Electron density around 4E8 A 800:**

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

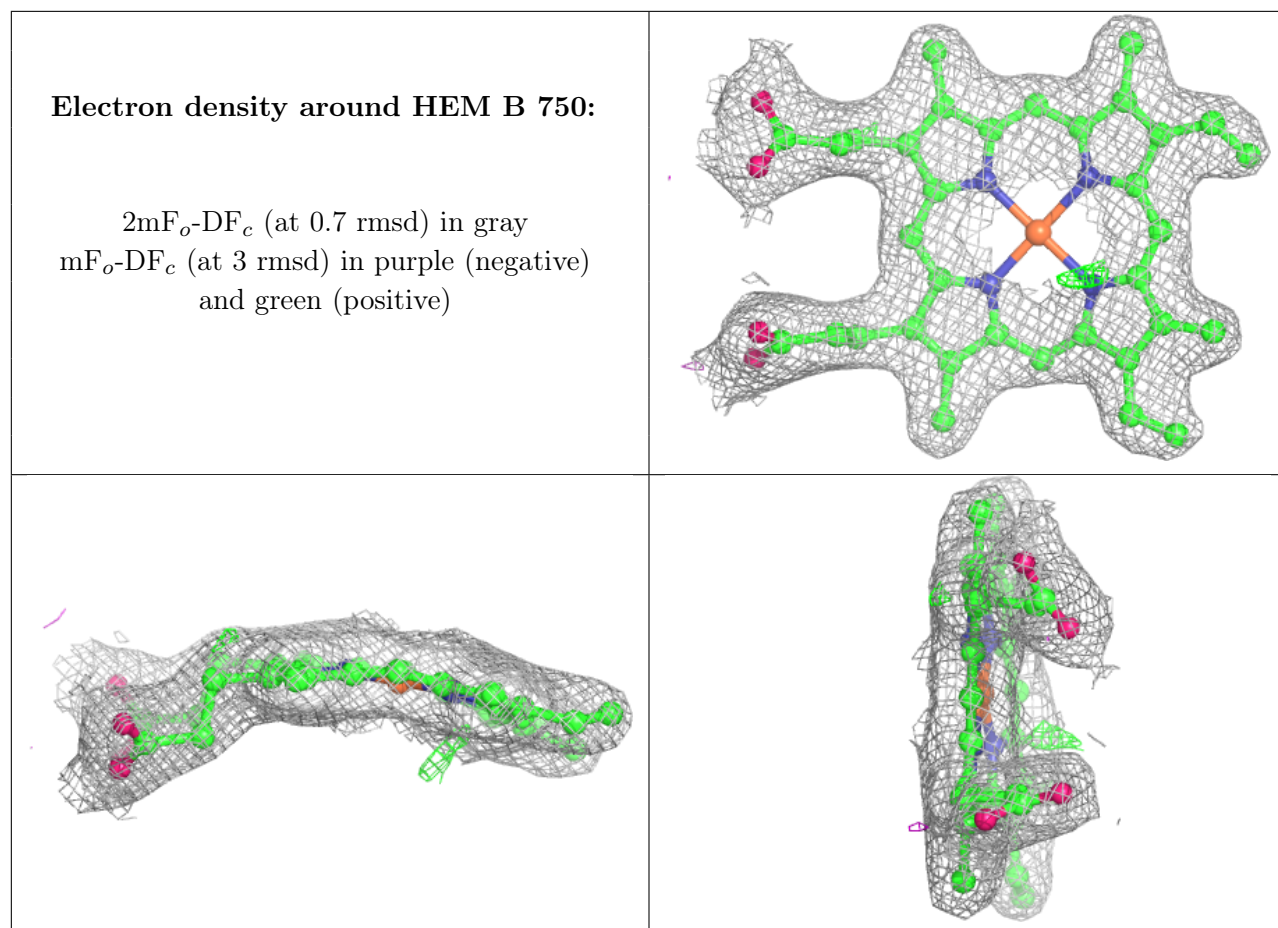


**Electron density around HEM A 750:**

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







## 6.5 Other polymers [i](#)

There are no such residues in this entry.