



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 12, 2021 – 02:09 PM JST

PDB ID : 7E0O  
Title : Crystal Structure of Human Indoleamine 2,3-dioxygenase 1 (hIDO1) Complexed with 6-Bromo-1H-indazol-4-amine (1)  
Authors : Li, G.-B.; Ning, X.-L.  
Deposited on : 2021-01-28  
Resolution : 3.34 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 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 : 2.22  
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) : 2.22

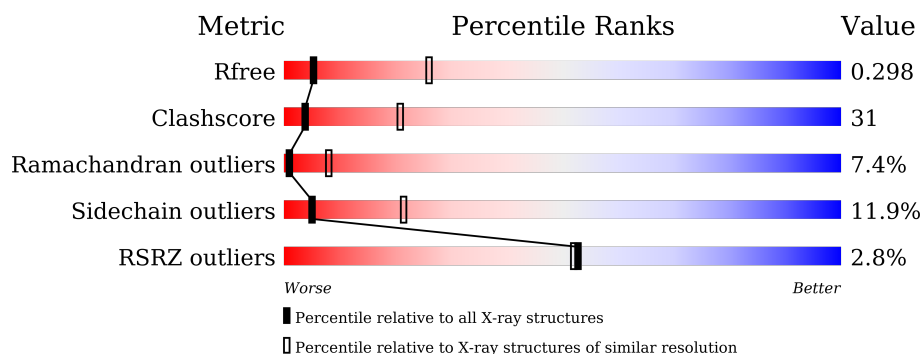
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.34 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	1060 (3.38-3.30)
Clashscore	141614	1111 (3.38-3.30)
Ramachandran outliers	138981	1090 (3.38-3.30)
Sidechain outliers	138945	1089 (3.38-3.30)
RSRZ outliers	127900	1028 (3.38-3.30)

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	392	<div> <div>3%</div> <div>40%</div> <div>43%</div> <div>10%</div> <div>6%</div> </div>
1	B	392	<div> <div>3%</div> <div>42%</div> <div>43%</div> <div>8%</div> <div>6%</div> </div>

## 2 Entry composition [i](#)

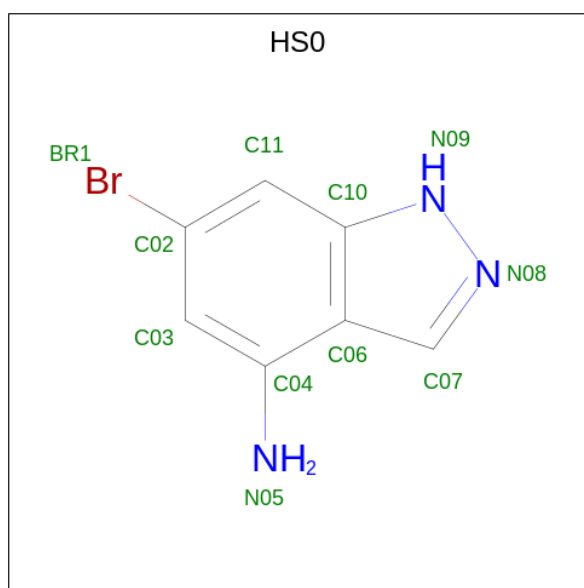
There are 3 unique types of molecules in this entry. The entry contains 5966 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Indoleamine 2,3-dioxygenase 1.

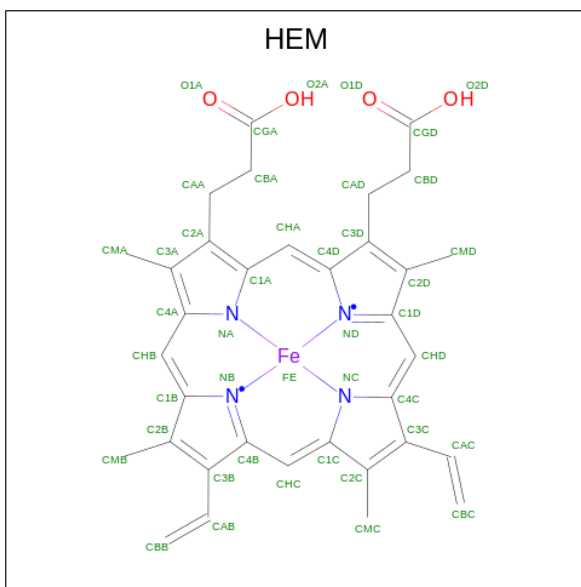
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	370	Total	C	N	O	S	0	0	0
			2929	1883	499	530	17			
1	B	370	Total	C	N	O	S	0	0	0
			2929	1883	499	530	17			

- Molecule 2 is 6-bromanyl-1 {H}-indazol-4-amine (three-letter code: HS0) (formula:  $C_7H_6BrN_3$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	Br	C	N	0	0
			11	1	7	3		
2	B	1	Total	Br	C	N	0	0
			11	1	7	3		

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ) (labeled as "Ligand of Interest" by depositor).

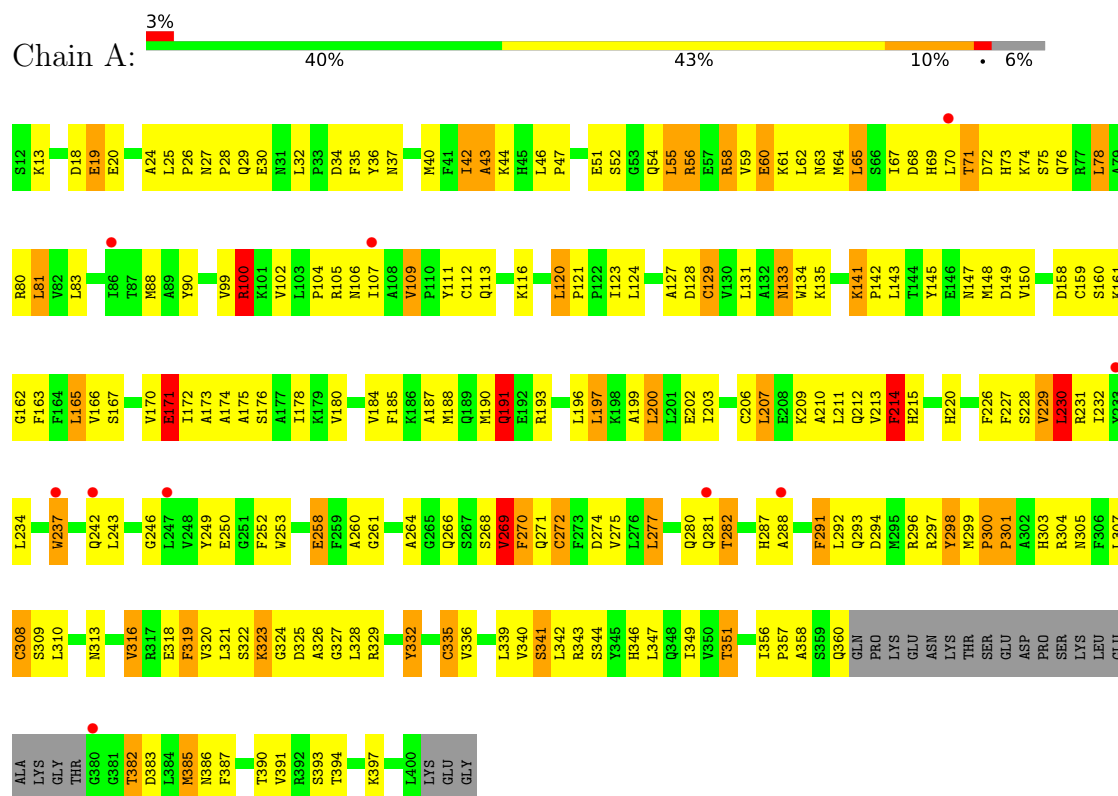


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

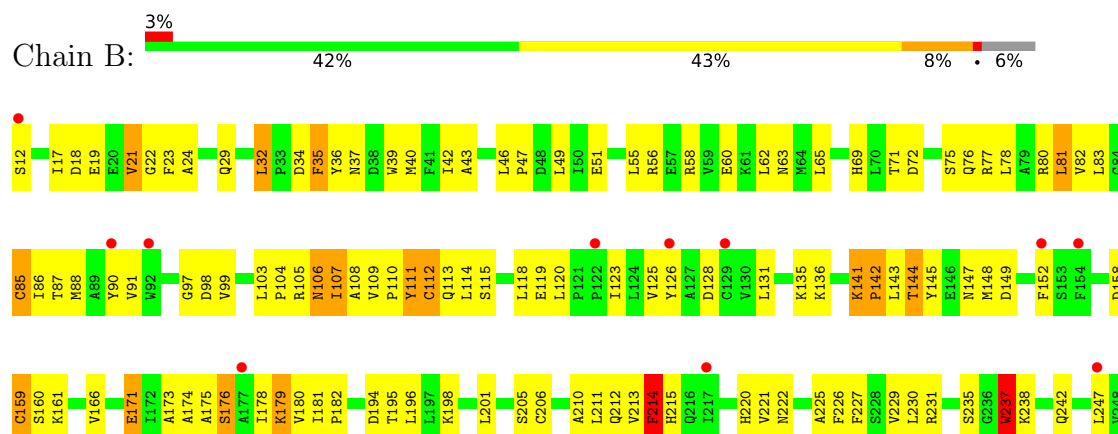
### 3 Residue-property plots

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: Indoleamine 2,3-dioxygenase 1



#### • Molecule 1: Indoleamine 2,3-dioxygenase 1



Y249		F319	THR
F252		V320	G380
W253		L321	G381
		S322	T382
E258		K323	D383
F259		G324	L384
A260		D325	M385
G261		A326	
		G327	L388
A264		L328	
G265		R329	V391
Q266		A330	R392
S267		A331	S393
S268		Y332	
V269		D333	E396
F270		A334	K397
Q271		G335	S398
Q272		V336	L399
F273		K337	L400
D274		A338	LYS
V275		L339	GLU
L276		V340	GLY
L277		S341	
G278		L342	
L279		R343	
Q280		S344	
Q281		Y345	
T282		H346	
A283		L347	
G284		Q348	
G285		I349	
G286		V350	
H287		T351	
A288		K352	
A289		Y353	
Q290		I354	
F291		L355	
L292		I356	
Q293		P357	
		A358	
R296		S359	
R297		Q360	
Y298		GLN	
M299		PRO	
P300		LYS	
P301		GLU	
A302		ASN	
H303		LYS	
		THR	
		SER	
L307		GLU	
G308		ASP	
S309		PRO	
L310		SER	
E311		LYS	
S312		LEU	
		GLU	
V316		ALA	
R317		LYS	
E318		GLY	

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.59Å 96.79Å 130.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	65.49 – 3.34 65.49 – 3.34	Depositor EDS
% Data completeness (in resolution range)	96.3 (65.49-3.34) 96.3 (65.49-3.34)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.14 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, $R_{free}$	0.211 , 0.302 0.218 , 0.298	Depositor DCC
$R_{free}$ test set	1578 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	101.2	Xtriage
Anisotropy	0.614	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 39.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	5966	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.58% 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: HS0, HEM

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	0.80	4/2997 (0.1%)	0.88	3/4055 (0.1%)
1	B	0.78	1/2997 (0.0%)	0.91	4/4055 (0.1%)
All	All	0.79	5/5994 (0.1%)	0.89	7/8110 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	335	CYS	CB-SG	-5.78	1.72	1.81
1	A	316	VAL	CB-CG2	-5.27	1.41	1.52
1	B	237	TRP	CA-CB	5.21	1.65	1.53
1	A	19	GLU	CB-CG	5.10	1.61	1.52
1	A	258	GLU	CB-CG	5.04	1.61	1.52

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	100	ARG	NE-CZ-NH2	-6.17	117.21	120.30
1	B	201	LEU	CB-CG-CD1	-6.04	100.73	111.00
1	B	32	LEU	CB-CG-CD2	-5.26	102.06	111.00
1	A	55	LEU	CA-CB-CG	-5.20	103.35	115.30
1	B	329	ARG	NE-CZ-NH1	5.17	122.89	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen



atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2929	0	2934	185	0
1	B	2929	0	2934	183	0
2	A	11	0	0	0	0
2	B	11	0	0	1	0
3	A	43	0	30	6	0
3	B	43	0	30	5	0
All	All	5966	0	5928	367	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 31.

The worst 5 of 367 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:317:ARG:NH2	1:B:398:SER:O	2.07	0.87
1:A:109:VAL:O	1:A:113:GLN:HG3	1.76	0.84
1:A:80:ARG:NH2	1:A:128:ASP:OD2	2.09	0.84
1:B:274:ASP:OD2	1:B:343:ARG:NH2	2.14	0.79
1:A:64:MET:N	1:A:106:ASN:OD1	2.17	0.78

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	366/392 (93%)	266 (73%)	72 (20%)	28 (8%)	<b>1</b> <b>7</b>
1	B	366/392 (93%)	261 (71%)	79 (22%)	26 (7%)	<b>1</b> <b>9</b>
All	All	732/784 (93%)	527 (72%)	151 (21%)	54 (7%)	<b>1</b> <b>8</b>

5 of 54 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	13	LYS
1	A	160	SER
1	A	171	GLU
1	A	214	PHE
1	A	269	VAL

### 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	319/339 (94%)	281 (88%)	38 (12%)	5	21
1	B	319/339 (94%)	281 (88%)	38 (12%)	5	21
All	All	638/678 (94%)	562 (88%)	76 (12%)	5	21

5 of 76 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	230	LEU
1	B	345	TYR
1	B	242	GLN
1	B	318	GLU
1	B	382	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	HEM	B	502	1,2	27,50,50	2.14	6 (22%)	17,82,82	2.71	8 (47%)
2	HS0	A	501	3	11,12,12	1.03	1 (9%)	12,17,17	1.48	1 (8%)
3	HEM	A	502	1,2	27,50,50	1.93	5 (18%)	17,82,82	2.22	6 (35%)
2	HS0	B	501	3	11,12,12	1.69	5 (45%)	12,17,17	2.71	5 (41%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEM	B	502	1,2	-	2/6/54/54	-
2	HS0	A	501	3	-	-	0/2/2/2
3	HEM	A	502	1,2	-	3/6/54/54	-
2	HS0	B	501	3	-	-	0/2/2/2

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	HEM	C3B-C2B	-4.86	1.33	1.40
3	B	502	HEM	CAA-C2A	4.43	1.58	1.52
3	A	502	HEM	C3C-C2C	-4.16	1.34	1.40
3	A	502	HEM	C3B-CAB	4.14	1.56	1.47
3	B	502	HEM	C3C-C2C	-4.14	1.34	1.40

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502	HEM	CMA-C3A-C4A	-5.08	120.66	128.46
3	A	502	HEM	CAA-CBA-CGA	-5.01	104.27	112.67
2	B	501	HS0	BR1-C02-C03	4.80	125.93	119.27
3	B	502	HEM	CAD-CBD-CGD	-4.74	104.72	112.67
2	B	501	HS0	C03-C04-C06	4.38	120.99	117.96

There are no chirality outliers.

All (5) torsion outliers are listed below:

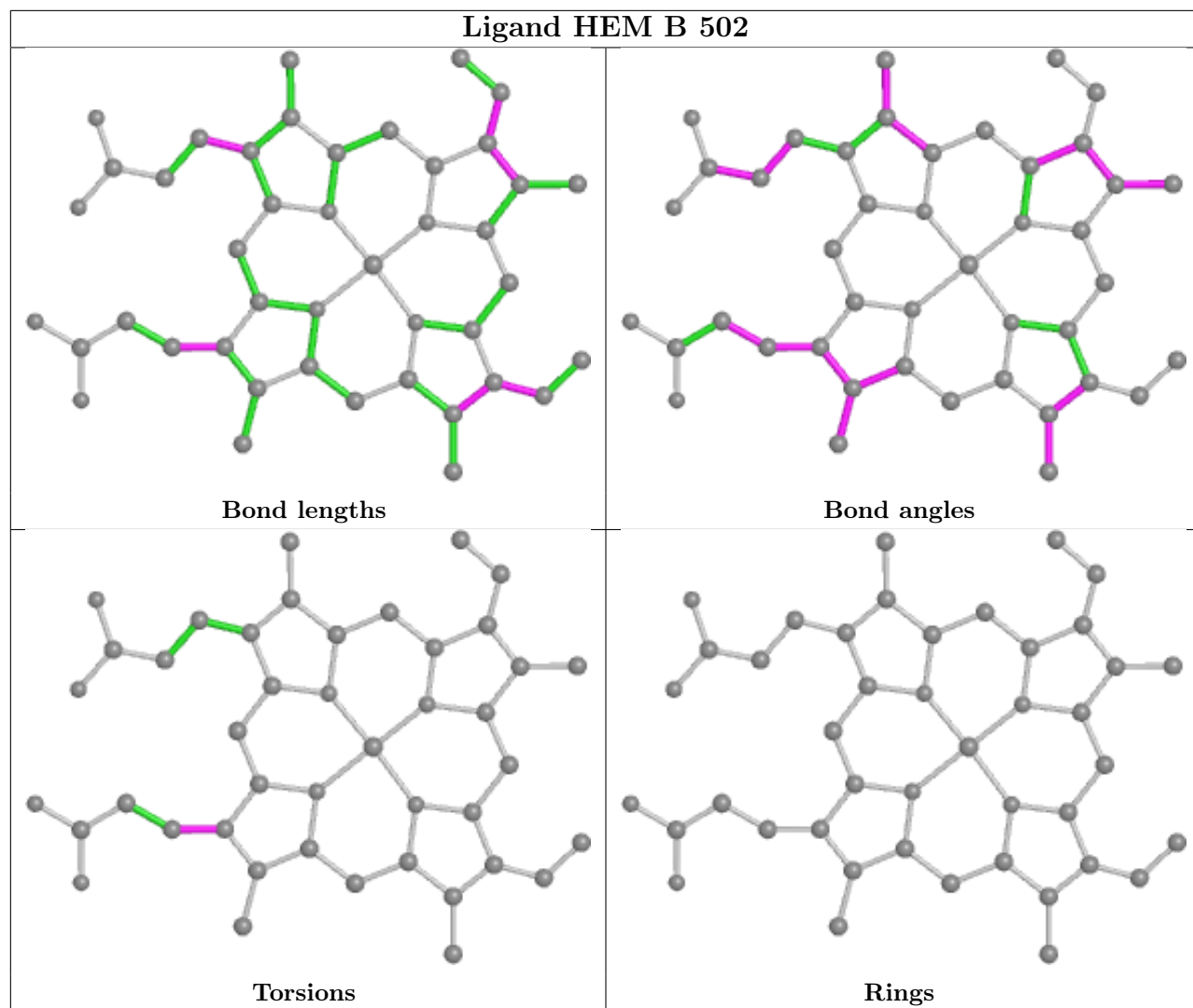
Mol	Chain	Res	Type	Atoms
3	B	502	HEM	C1A-C2A-CAA-CBA
3	B	502	HEM	C3A-C2A-CAA-CBA
3	A	502	HEM	C2D-C3D-CAD-CBD
3	A	502	HEM	C4D-C3D-CAD-CBD
3	A	502	HEM	C3D-CAD-CBD-CGD

There are no ring outliers.

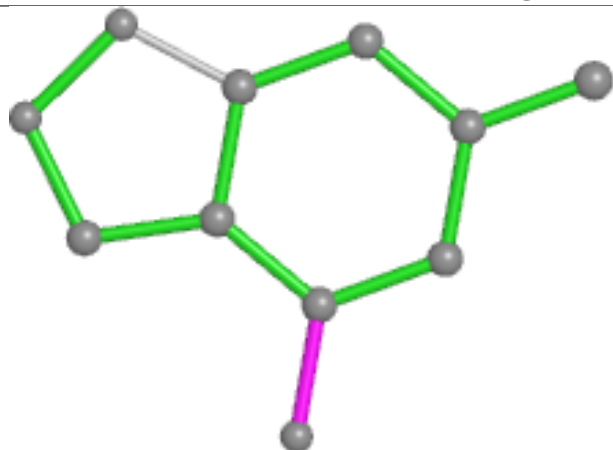
3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502	HEM	5	0
3	A	502	HEM	6	0
2	B	501	HS0	1	0

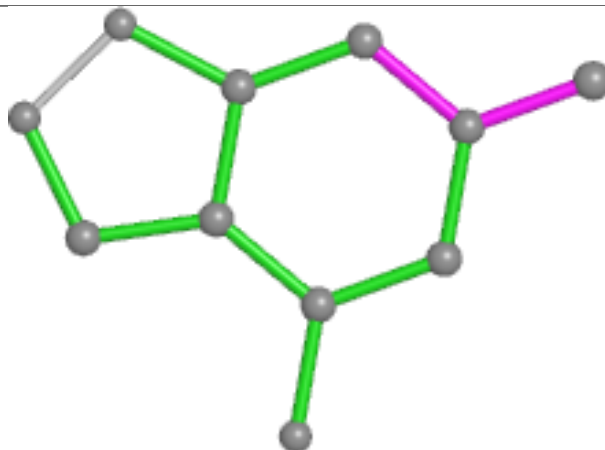
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



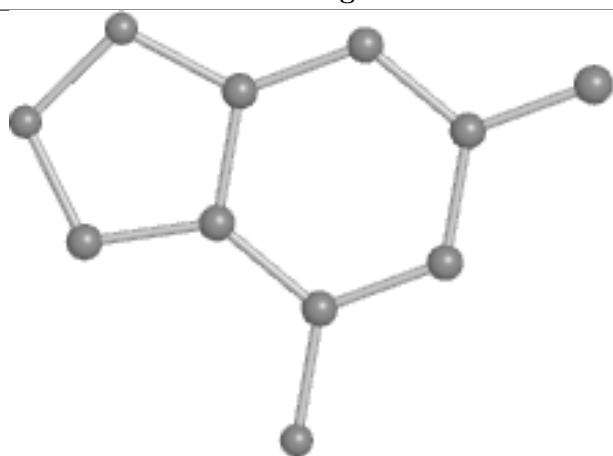
## Ligand HS0 A 501



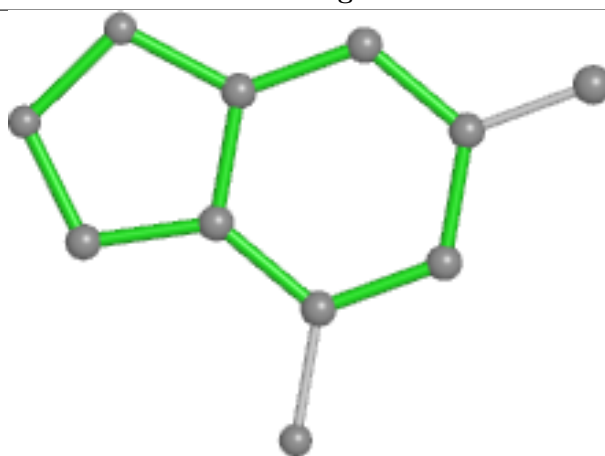
Bond lengths



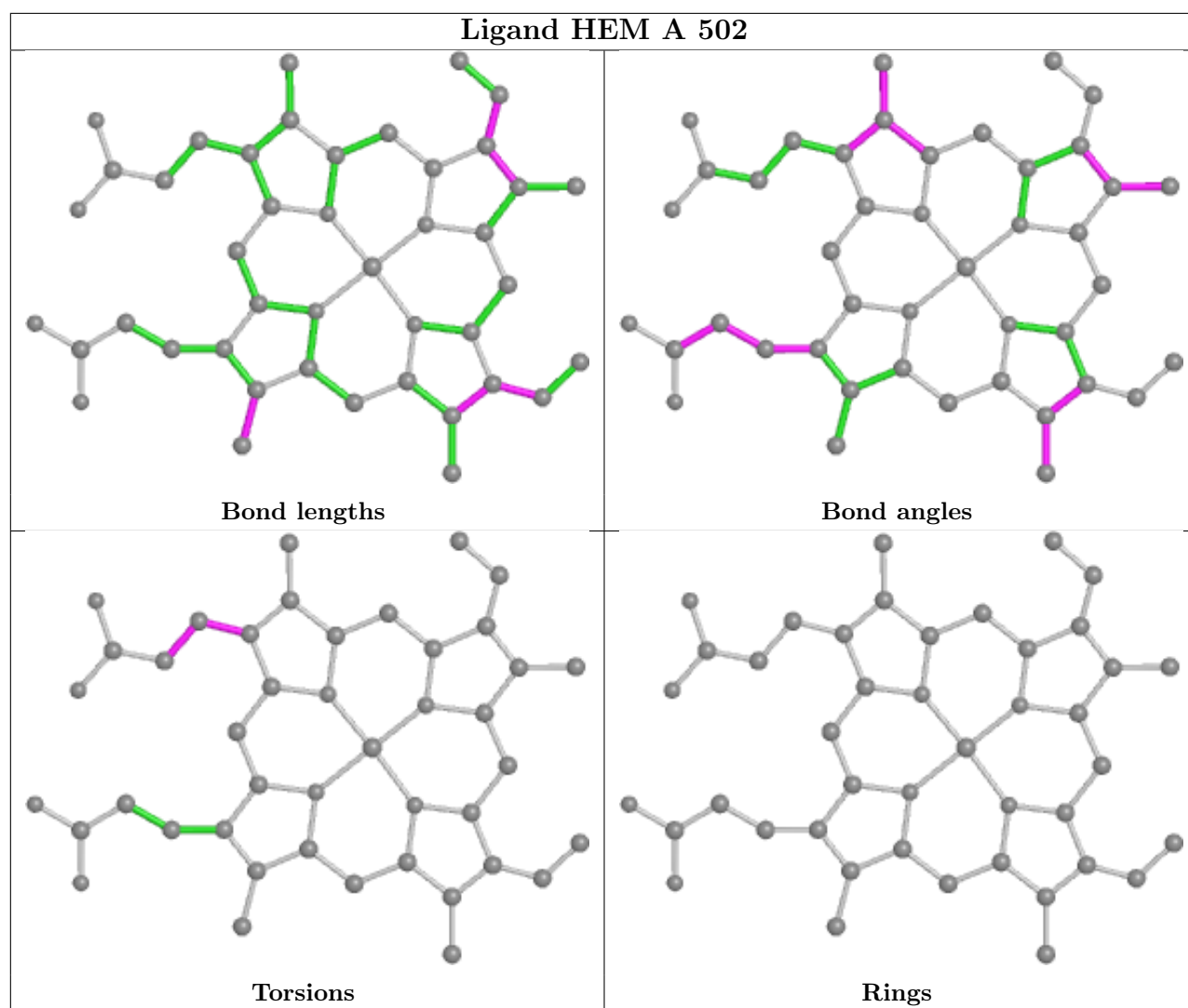
Bond angles

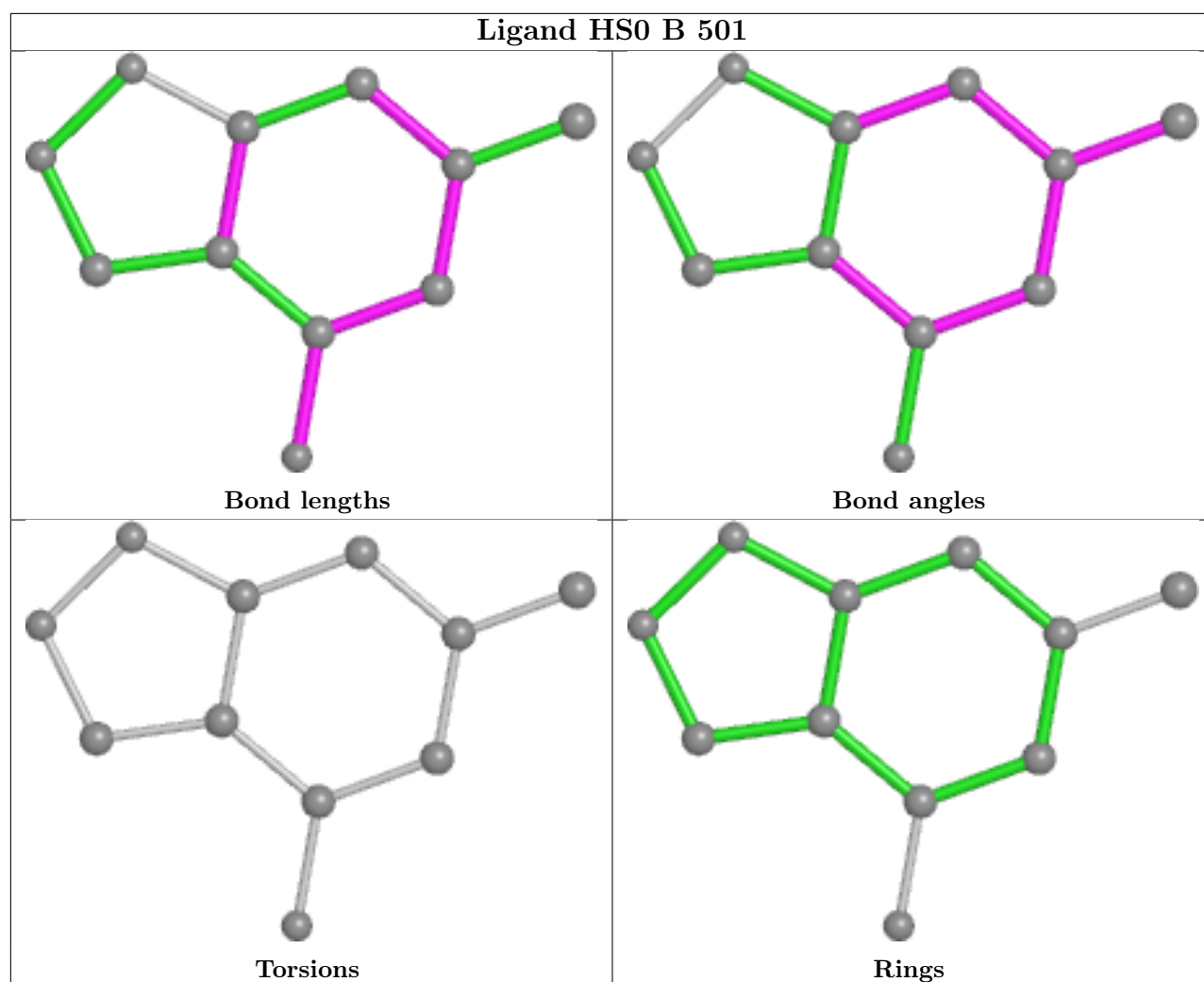


Torsions



Rings





## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	370/392 (94%)	0.07	10 (2%) 54 53	67, 104, 131, 162	0
1	B	370/392 (94%)	0.08	11 (2%) 50 50	72, 103, 131, 152	0
All	All	740/784 (94%)	0.08	21 (2%) 53 52	67, 104, 131, 162	0

The worst 5 of 21 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	12	SER	3.2
1	B	90	TYR	2.9
1	A	107	ILE	2.9
1	B	154	PHE	2.8
1	B	152	PHE	2.7

### 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](#)

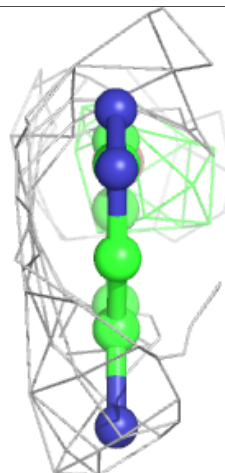
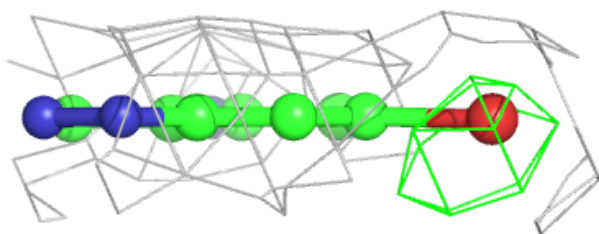
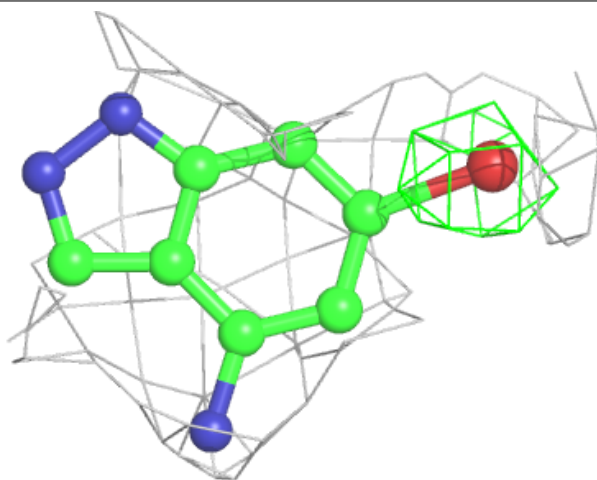
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 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
2	HS0	B	501	11/11	0.88	0.22	93,108,129,192	0
3	HEM	B	502	43/43	0.96	0.36	67,91,117,131	0
3	HEM	A	502	43/43	0.97	0.40	74,91,110,118	0
2	HS0	A	501	11/11	0.97	0.16	88,100,116,128	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.

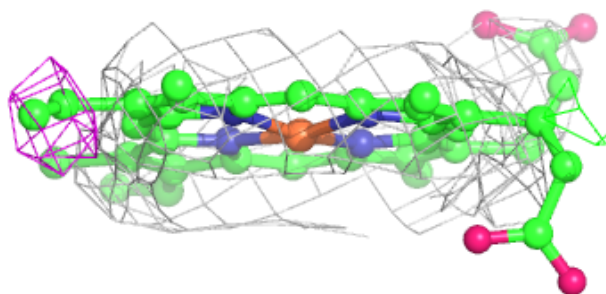
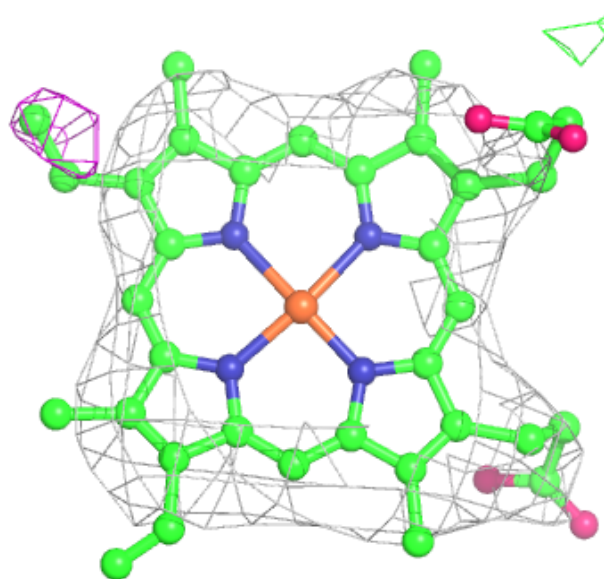
**Electron density around HS0 B 501:**

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)



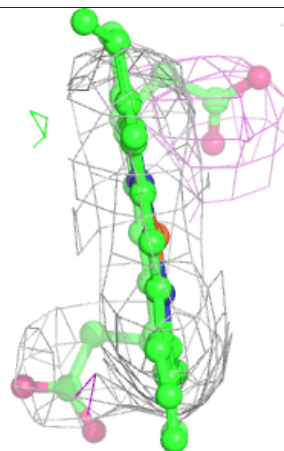
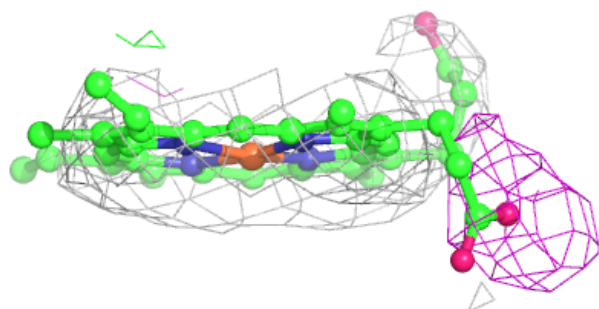
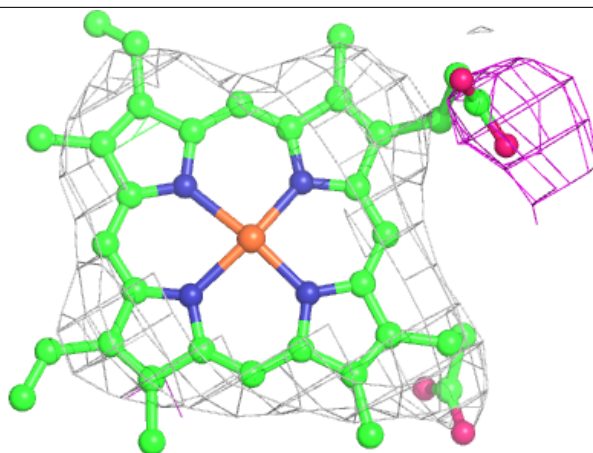
**Electron density around HEM B 502:**

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



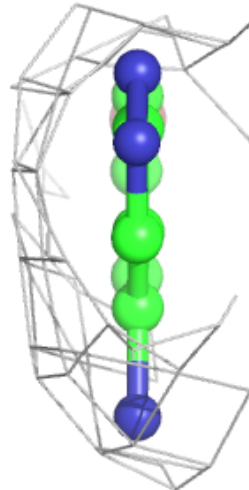
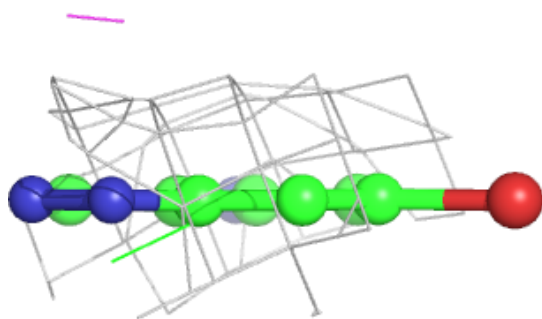
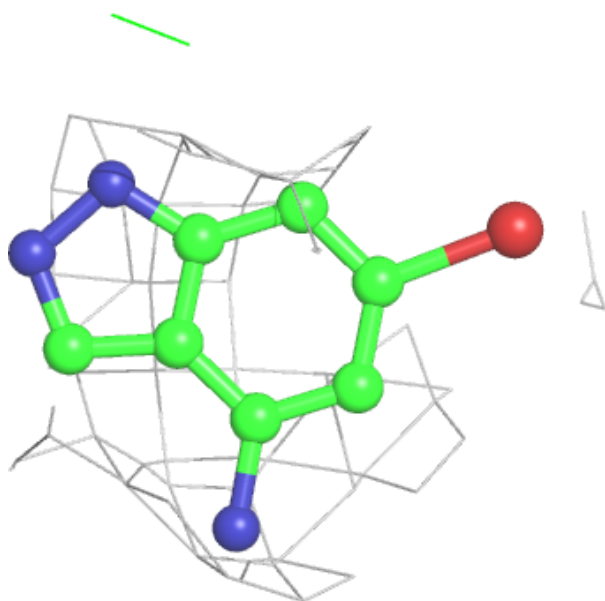
**Electron density around HEM A 502:**

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



**Electron density around HS0 A 501:**

$2mF_o-DF_c$  (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.