



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 13, 2020 – 11:24 PM BST

PDB ID : 6A4I  
Title : Crystal Structure of human TDO inhibitor complex  
Authors : Fu, G.; Wang, J.; Luo, G.; Wu, G.; Qian, K.  
Deposited on : 2018-06-20  
Resolution : 2.65 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.

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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 : 2.14.4.dev1  
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) : 2.14.4.dev1

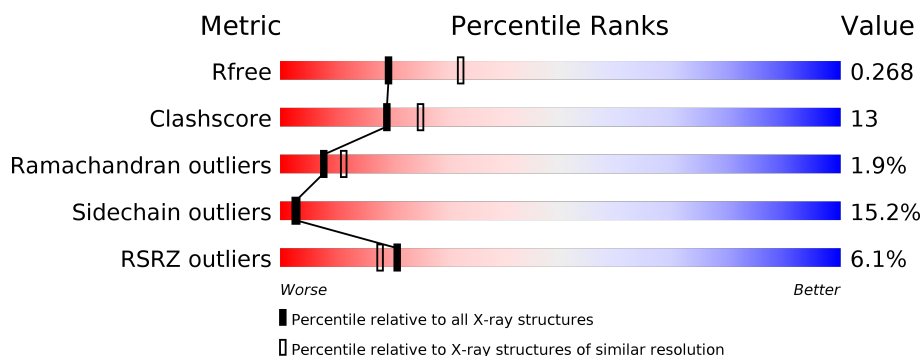
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.65 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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	391	<div> <div>2%</div> <div> <div>57%</div> <div>20%</div> <div>• •</div> <div>18%</div> </div> </div>
1	B	391	<div> <div>4%</div> <div> <div>50%</div> <div>21%</div> <div>8%</div> <div>•</div> <div>21%</div> </div> </div>
1	C	391	<div> <div>6%</div> <div> <div>53%</div> <div>21%</div> <div>7%</div> <div>•</div> <div>17%</div> </div> </div>
1	D	391	<div> <div>7%</div> <div> <div>43%</div> <div>21%</div> <div>7%</div> <div>•</div> <div>26%</div> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10801 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 Tryptophan 2,3-dioxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	322	Total	C	N	O	S	0	0	0
			2710	1745	469	485	11			
1	B	309	Total	C	N	O	S	0	0	0
			2608	1685	451	462	10			
1	C	323	Total	C	N	O	S	0	0	0
			2722	1751	479	481	11			
1	D	290	Total	C	N	O	S	0	1	0
			2463	1594	428	431	10			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	expression tag	UNP P48775
A	-1	GLY	-	expression tag	UNP P48775
A	0	SER	-	expression tag	UNP P48775
A	1	SER	-	expression tag	UNP P48775
A	2	HIS	-	expression tag	UNP P48775
A	3	HIS	-	expression tag	UNP P48775
A	4	HIS	-	expression tag	UNP P48775
A	5	HIS	-	expression tag	UNP P48775
A	6	HIS	-	expression tag	UNP P48775
A	7	HIS	-	expression tag	UNP P48775
A	8	SER	-	expression tag	UNP P48775
A	9	SER	-	expression tag	UNP P48775
A	10	GLY	-	expression tag	UNP P48775
A	11	LEU	-	expression tag	UNP P48775
A	12	VAL	-	expression tag	UNP P48775
A	13	PRO	-	expression tag	UNP P48775
A	14	ARG	-	expression tag	UNP P48775
A	15	GLY	-	expression tag	UNP P48775
A	16	SER	-	expression tag	UNP P48775
A	17	HIS	-	expression tag	UNP P48775
A	18	MET	-	expression tag	UNP P48775

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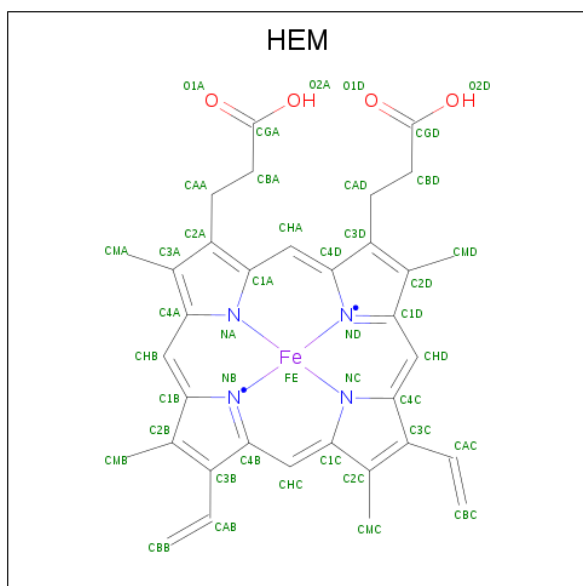
Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	MET	-	expression tag	UNP P48775
B	-1	GLY	-	expression tag	UNP P48775
B	0	SER	-	expression tag	UNP P48775
B	1	SER	-	expression tag	UNP P48775
B	2	HIS	-	expression tag	UNP P48775
B	3	HIS	-	expression tag	UNP P48775
B	4	HIS	-	expression tag	UNP P48775
B	5	HIS	-	expression tag	UNP P48775
B	6	HIS	-	expression tag	UNP P48775
B	7	HIS	-	expression tag	UNP P48775
B	8	SER	-	expression tag	UNP P48775
B	9	SER	-	expression tag	UNP P48775
B	10	GLY	-	expression tag	UNP P48775
B	11	LEU	-	expression tag	UNP P48775
B	12	VAL	-	expression tag	UNP P48775
B	13	PRO	-	expression tag	UNP P48775
B	14	ARG	-	expression tag	UNP P48775
B	15	GLY	-	expression tag	UNP P48775
B	16	SER	-	expression tag	UNP P48775
B	17	HIS	-	expression tag	UNP P48775
B	18	MET	-	expression tag	UNP P48775
C	-2	MET	-	expression tag	UNP P48775
C	-1	GLY	-	expression tag	UNP P48775
C	0	SER	-	expression tag	UNP P48775
C	1	SER	-	expression tag	UNP P48775
C	2	HIS	-	expression tag	UNP P48775
C	3	HIS	-	expression tag	UNP P48775
C	4	HIS	-	expression tag	UNP P48775
C	5	HIS	-	expression tag	UNP P48775
C	6	HIS	-	expression tag	UNP P48775
C	7	HIS	-	expression tag	UNP P48775
C	8	SER	-	expression tag	UNP P48775
C	9	SER	-	expression tag	UNP P48775
C	10	GLY	-	expression tag	UNP P48775
C	11	LEU	-	expression tag	UNP P48775
C	12	VAL	-	expression tag	UNP P48775
C	13	PRO	-	expression tag	UNP P48775
C	14	ARG	-	expression tag	UNP P48775
C	15	GLY	-	expression tag	UNP P48775
C	16	SER	-	expression tag	UNP P48775
C	17	HIS	-	expression tag	UNP P48775
C	18	MET	-	expression tag	UNP P48775

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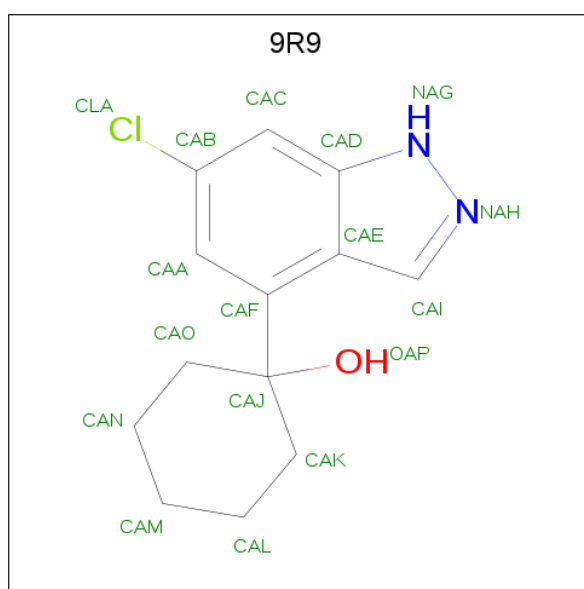
Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	MET	-	expression tag	UNP P48775
D	-1	GLY	-	expression tag	UNP P48775
D	0	SER	-	expression tag	UNP P48775
D	1	SER	-	expression tag	UNP P48775
D	2	HIS	-	expression tag	UNP P48775
D	3	HIS	-	expression tag	UNP P48775
D	4	HIS	-	expression tag	UNP P48775
D	5	HIS	-	expression tag	UNP P48775
D	6	HIS	-	expression tag	UNP P48775
D	7	HIS	-	expression tag	UNP P48775
D	8	SER	-	expression tag	UNP P48775
D	9	SER	-	expression tag	UNP P48775
D	10	GLY	-	expression tag	UNP P48775
D	11	LEU	-	expression tag	UNP P48775
D	12	VAL	-	expression tag	UNP P48775
D	13	PRO	-	expression tag	UNP P48775
D	14	ARG	-	expression tag	UNP P48775
D	15	GLY	-	expression tag	UNP P48775
D	16	SER	-	expression tag	UNP P48775
D	17	HIS	-	expression tag	UNP P48775
D	18	MET	-	expression tag	UNP P48775

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



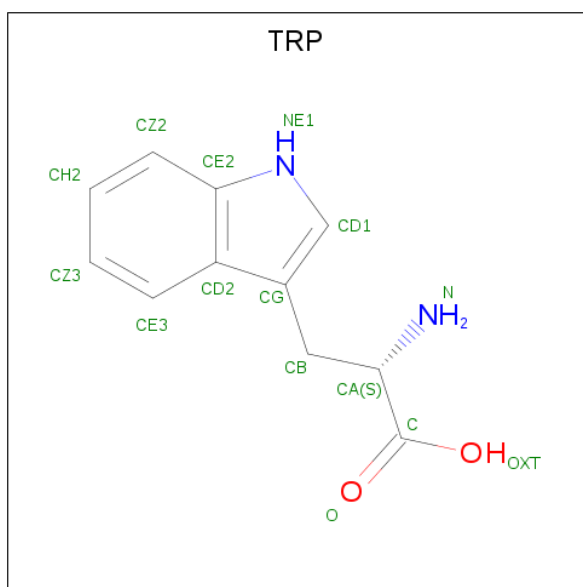
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	
			43	34	1	4	4	
2	B	1	Total	C	Fe	N	O	
			43	34	1	4	4	
2	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	
2	D	1	Total	C	Fe	N	O	
			43	34	1	4	4	

- Molecule 3 is 1-(6-chloro-1H-indazol-4-yl)cyclohexan-1-ol (three-letter code: 9R9) (formula:  $C_{13}H_{15}ClN_2O$ ).



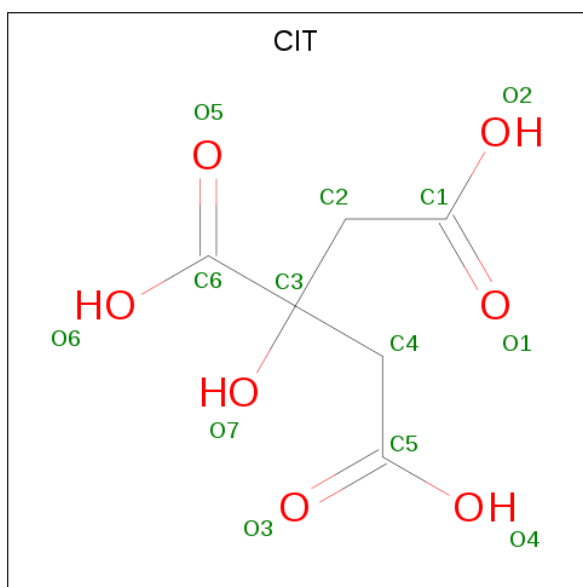
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	
			17	13	1	2	1	
3	B	1	Total	C	Cl	N	O	
			17	13	1	2	1	
3	C	1	Total	C	Cl	N	O	
			17	13	1	2	1	
3	D	1	Total	C	Cl	N	O	
			17	13	1	2	1	

- Molecule 4 is TRYPTOPHAN (three-letter code: TRP) (formula:  $C_{11}H_{12}N_2O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			15	11	2	2		
4	B	1	Total	C	N	O	0	0
			15	11	2	2		
4	D	1	Total	C	N	O	0	0
			15	11	2	2		

- Molecule 5 is CITRIC ACID (three-letter code: CIT) (formula:  $C_6H_8O_7$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			13	6	7		





Chain C:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	156.31Å 144.11Å 89.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	106.17 – 2.65 48.04 – 2.64	Depositor EDS
% Data completeness (in resolution range)	99.7 (106.17-2.65) 99.7 (48.04-2.64)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.55 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.205 , 0.269 0.205 , 0.268	Depositor DCC
$R_{free}$ test set	3058 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	74.8	Xtriage
Anisotropy	0.136	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 56.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10801	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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: HEM, CIT, 9R9

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	1.32	21/2769 (0.8%)	1.23	19/3723 (0.5%)
1	B	1.21	17/2668 (0.6%)	1.11	14/3592 (0.4%)
1	C	1.30	17/2782 (0.6%)	1.15	16/3743 (0.4%)
1	D	1.32	19/2521 (0.8%)	1.22	21/3395 (0.6%)
All	All	1.29	74/10740 (0.7%)	1.18	70/14453 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	2
1	D	0	2
All	All	0	6

The worst 5 of 74 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	248	GLU	N-CA	19.09	1.84	1.46
1	C	243	ALA	N-CA	16.20	1.78	1.46
1	D	286	TYR	CE1-CZ	15.53	1.58	1.38
1	C	227	GLU	CB-CG	14.52	1.79	1.52
1	C	232	ARG	CB-CG	13.79	1.89	1.52

The worst 5 of 70 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	286	TYR	CD1-CE1-CZ	-13.07	108.04	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	377	TRP	CG-CD1-NE1	-10.40	99.70	110.10
1	A	282	ARG	NE-CZ-NH1	10.22	125.41	120.30
1	D	299	ARG	NE-CZ-NH1	9.47	125.03	120.30
1	C	377	TRP	CD1-NE1-CE2	9.42	117.48	109.00

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	251	GLU	Peptide
1	A	347	GLY	Peptide
1	C	103	ARG	Peptide
1	C	253	GLN	Sidechain
1	D	144	ARG	Sidechain

## 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	2710	0	2699	57	0
1	B	2608	0	2605	84	0
1	C	2722	0	2714	74	0
1	D	2463	0	2470	89	0
2	A	43	0	30	4	0
2	B	43	0	30	8	0
2	C	43	0	30	2	0
2	D	43	0	30	2	0
3	A	17	0	0	0	0
3	B	17	0	0	0	0
3	C	17	0	0	0	0
3	D	17	0	0	0	0
4	A	15	0	9	0	0
4	B	15	0	9	0	0
4	D	15	0	9	0	0
5	A	13	0	5	0	0
All	All	10801	0	10640	279	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.

The worst 5 of 279 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:C:227:GLU:CB	1:C:227:GLU:CG	1.79	1.60
1:C:232:ARG:CG	1:C:232:ARG:CB	1.89	1.50
1:C:243:ALA:CA	1:C:243:ALA:N	1.78	1.45
1:A:248:GLU:N	1:A:248:GLU:CA	1.84	1.38
1:B:262:GLU:O	1:B:266:SER:HB3	1.44	1.15

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	314/391 (80%)	296 (94%)	15 (5%)	3 (1%)	15	23
1	B	301/391 (77%)	270 (90%)	24 (8%)	7 (2%)	6	8
1	C	315/391 (81%)	280 (89%)	32 (10%)	3 (1%)	15	23
1	D	283/391 (72%)	247 (87%)	26 (9%)	10 (4%)	3	4
All	All	1213/1564 (78%)	1093 (90%)	97 (8%)	23 (2%)	8	11

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	99	ASN
1	A	241	ILE
1	B	384	THR
1	C	176	ASN
1	D	223	TRP

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	297/356 (83%)	260 (88%)	37 (12%)	4	6
1	B	287/356 (81%)	244 (85%)	43 (15%)	3	3
1	C	297/356 (83%)	250 (84%)	47 (16%)	2	2
1	D	272/356 (76%)	223 (82%)	49 (18%)	1	1
All	All	1153/1424 (81%)	977 (85%)	176 (15%)	3	3

5 of 176 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	382	ASN
1	C	187	GLU
1	D	287	ARG
1	C	44	ASN
1	C	123	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	275	HIS
1	B	386	HIS
1	D	163	ASN
1	B	327	ASN
1	B	349	HIS

### 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](#)

12 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
2	HEM	A	401	1,3	27,50,50	1.14	1 (3%)	17,82,82	2.84	7 (41%)
2	HEM	D	401	1,3	27,50,50	0.96	1 (3%)	17,82,82	2.41	7 (41%)
5	CIT	A	404	-	3,12,12	0.85	0	3,17,17	2.90	1 (33%)
3	9R9	C	402	2	18,19,19	2.79	8 (44%)	19,28,28	1.88	4 (21%)
2	HEM	B	401	1,3	27,50,50	1.13	2 (7%)	17,82,82	2.93	7 (41%)
2	HEM	C	401	1,3	27,50,50	1.02	2 (7%)	17,82,82	2.05	5 (29%)
3	9R9	A	402	2	18,19,19	2.44	7 (38%)	19,28,28	1.34	3 (15%)
4	TRP	D	403	-	12,16,16	2.12	3 (25%)	12,22,22	1.12	1 (8%)
4	TRP	B	403	-	12,16,16	1.99	5 (41%)	12,22,22	1.07	1 (8%)
3	9R9	D	402	2	18,19,19	2.35	7 (38%)	19,28,28	3.88	8 (42%)
3	9R9	B	402	2	18,19,19	3.16	7 (38%)	19,28,28	1.78	5 (26%)
4	TRP	A	403	-	12,16,16	2.24	4 (33%)	12,22,22	1.34	1 (8%)

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	401	1,3	-	2/6/54/54	-
2	HEM	D	401	1,3	-	1/6/54/54	-
5	CIT	A	404	-	-	5/6/16/16	-
3	9R9	C	402	2	-	0/6/16/16	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	B	401	1,3	-	0/6/54/54	-
2	HEM	C	401	1,3	-	0/6/54/54	-
3	9R9	A	402	2	-	0/6/16/16	0/3/3/3
4	TRP	D	403	-	-	0/3/8/8	0/2/2/2
4	TRP	B	403	-	-	0/3/8/8	0/2/2/2
3	9R9	D	402	2	-	0/6/16/16	0/3/3/3
3	9R9	B	402	2	-	0/6/16/16	0/3/3/3
4	TRP	A	403	-	-	1/3/8/8	0/2/2/2

The worst 5 of 47 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	9R9	CAJ-CAF	-8.80	1.43	1.53
3	C	402	9R9	CAJ-CAF	-6.62	1.45	1.53
3	B	402	9R9	CAC-CAD	-5.89	1.32	1.41
3	A	402	9R9	CAC-CAD	-5.61	1.33	1.41
3	C	402	9R9	CAC-CAD	-5.41	1.33	1.41

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	402	9R9	OAP-CAJ-CAF	-10.82	91.41	109.99
3	D	402	9R9	CAO-CAJ-CAK	6.91	118.18	108.80
2	B	401	HEM	CBD-CAD-C3D	-6.87	99.81	112.48
2	B	401	HEM	CAD-CBD-CGD	6.54	123.64	112.67
2	A	401	HEM	CAD-CBD-CGD	6.35	123.33	112.67

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	401	HEM	C3D-CAD-CBD-CGD
5	A	404	CIT	C2-C3-C4-C5
5	A	404	CIT	C6-C3-C4-C5
5	A	404	CIT	C1-C2-C3-C4
5	A	404	CIT	O7-C3-C4-C5

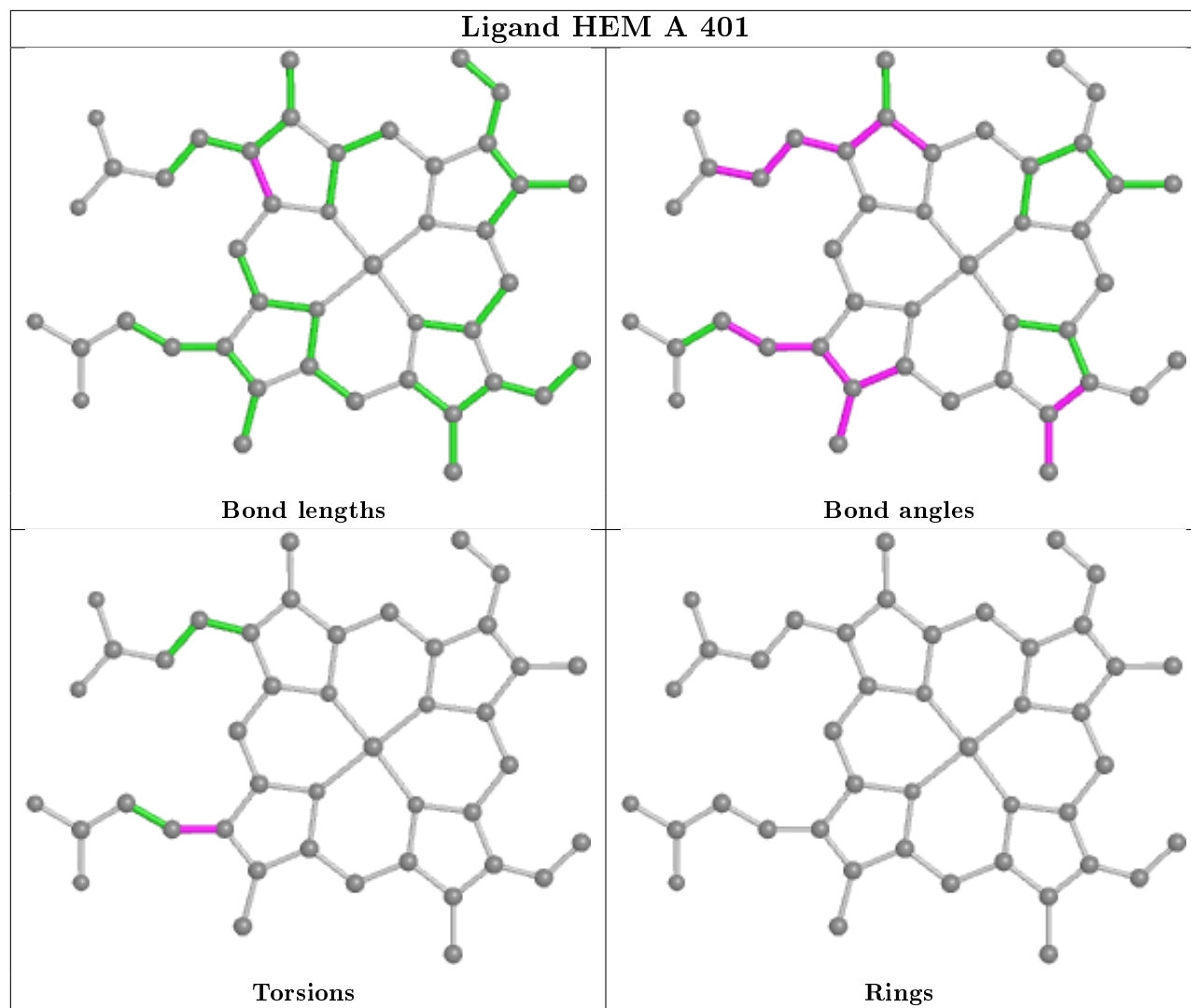
There are no ring outliers.

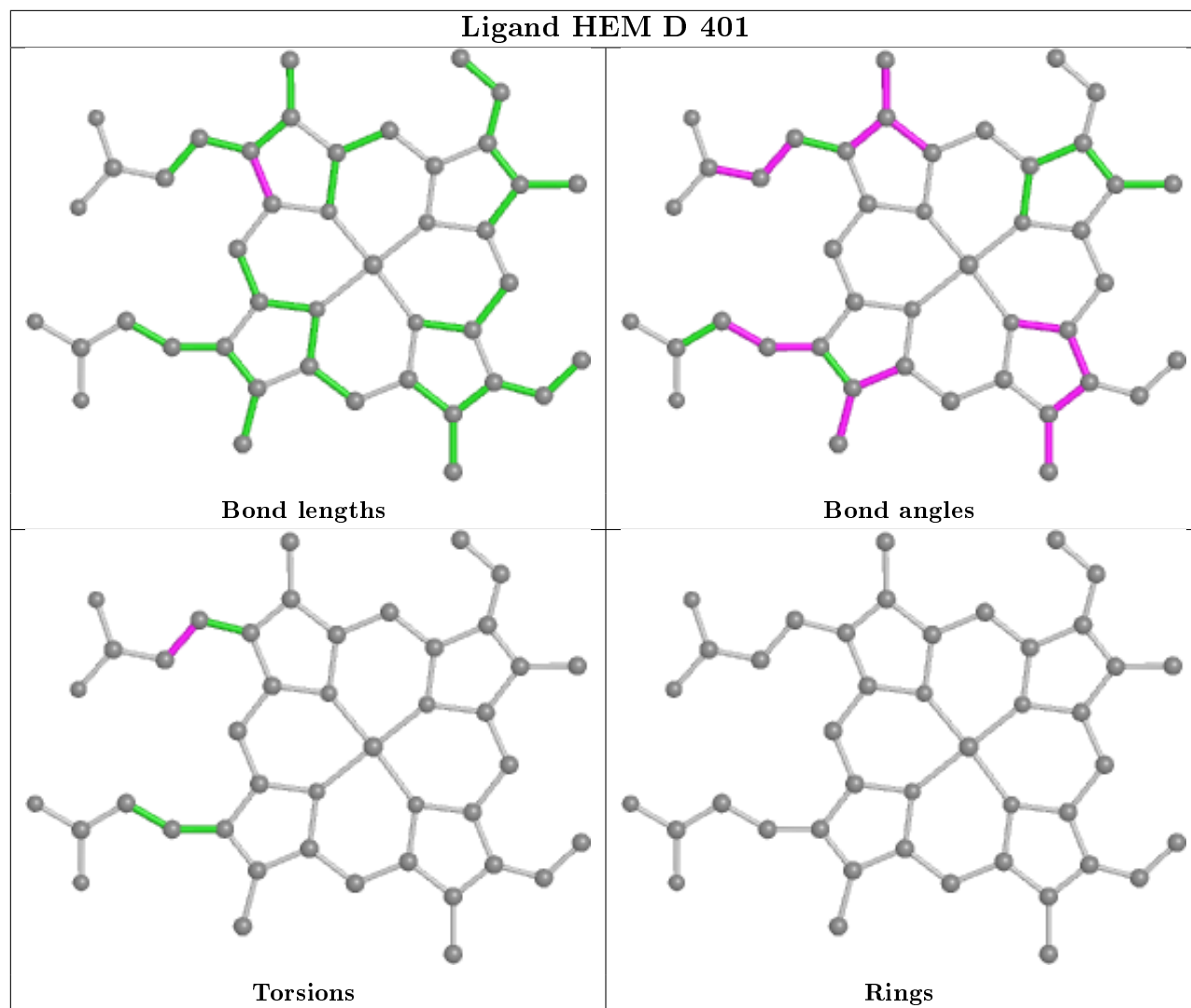
4 monomers are involved in 16 short contacts:



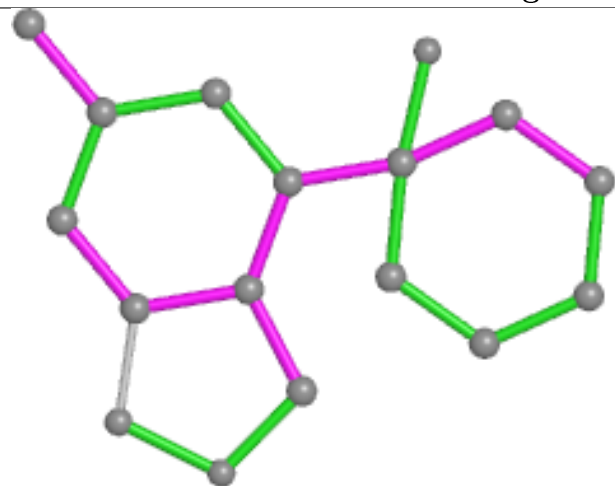
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	HEM	4	0
2	D	401	HEM	2	0
2	B	401	HEM	8	0
2	C	401	HEM	2	0

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.

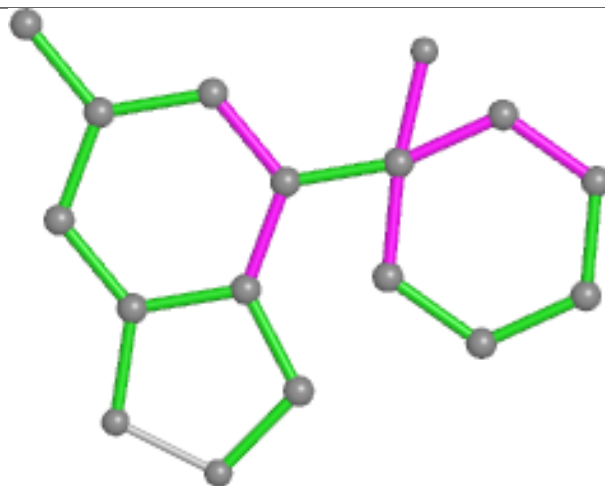




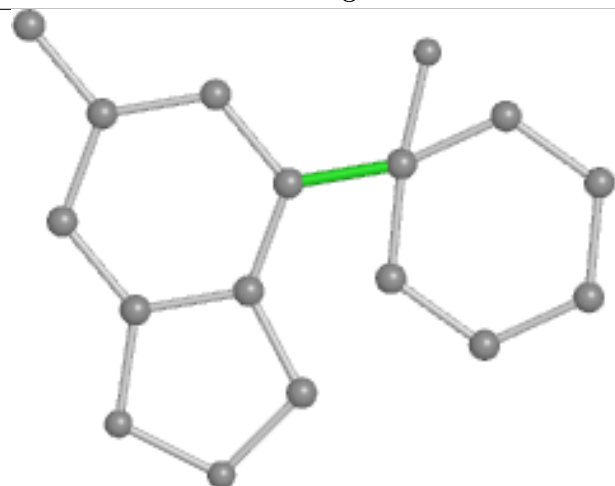
## Ligand 9R9 C 402



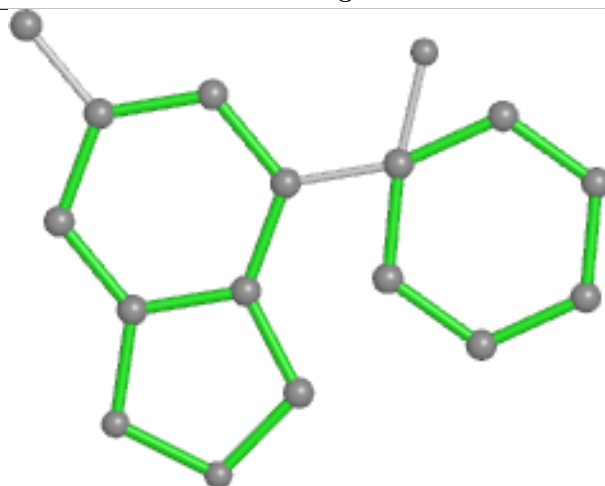
Bond lengths



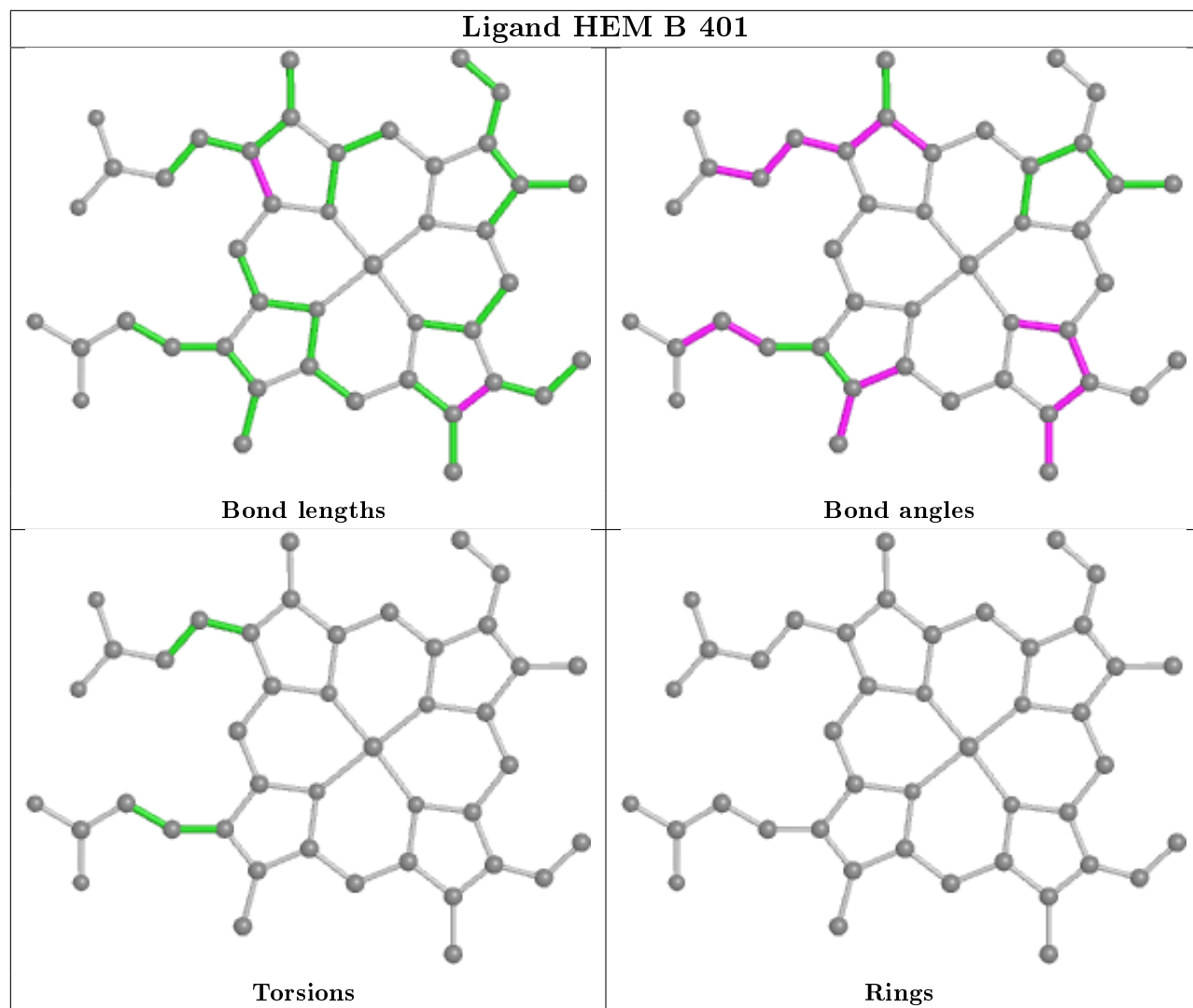
Bond angles

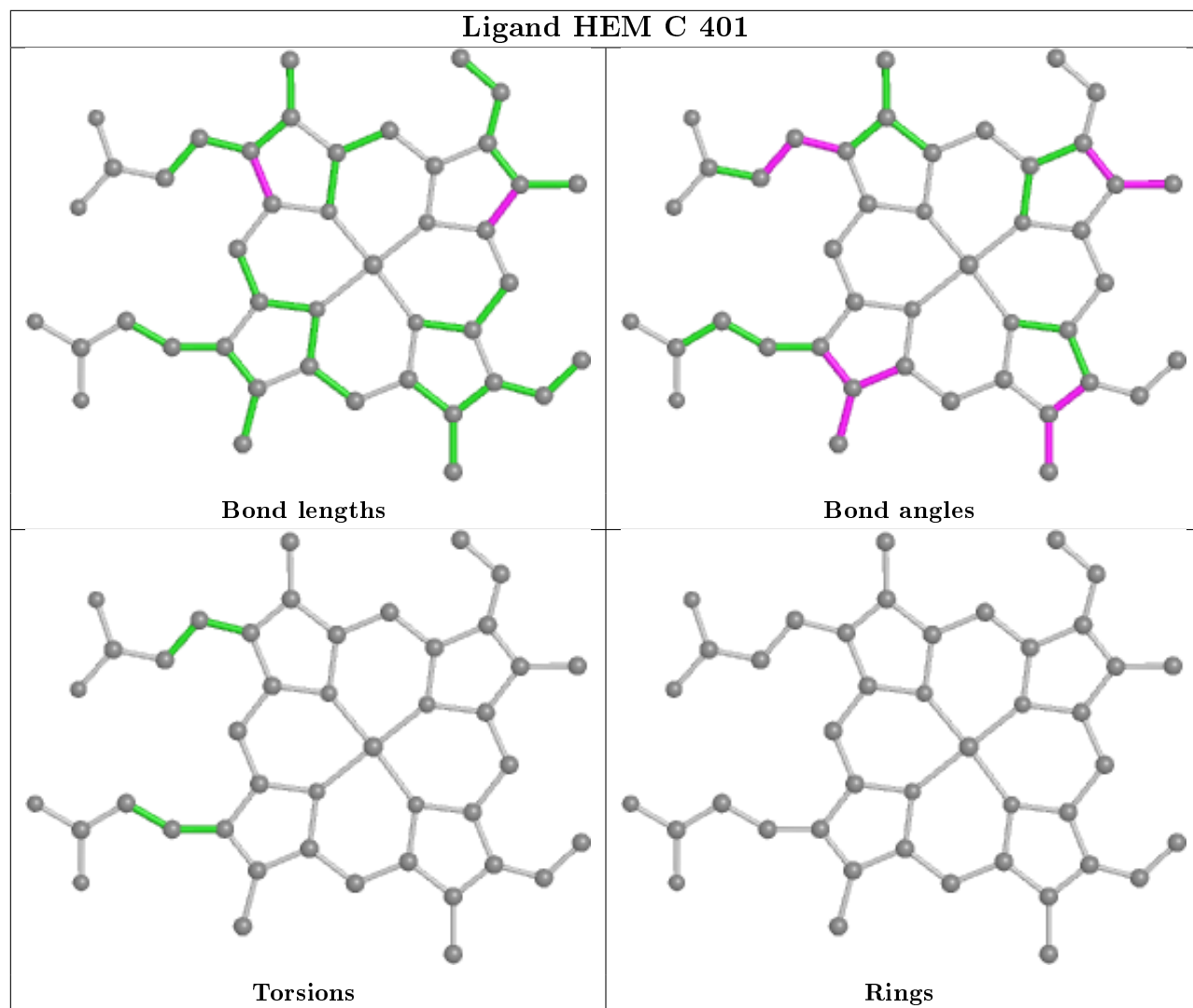


Torsions

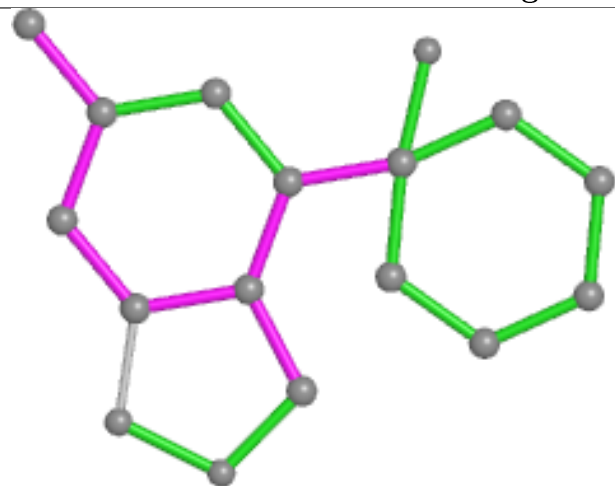


Rings

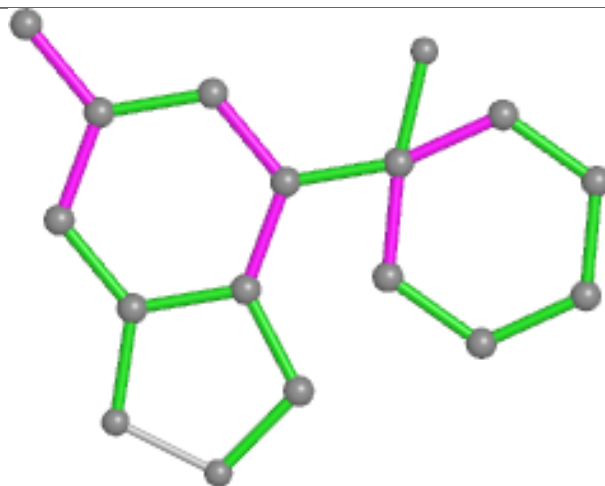




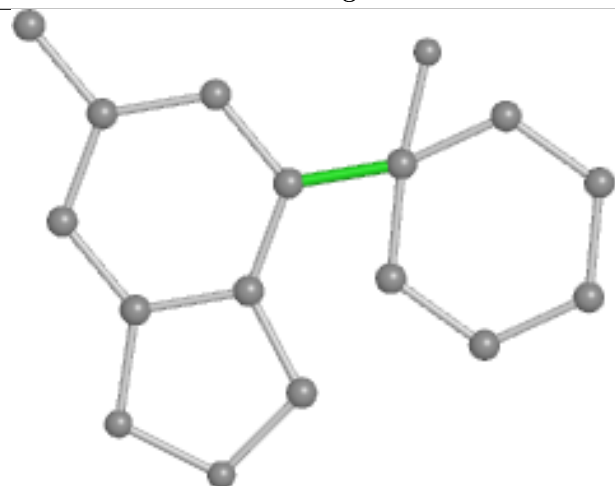
## Ligand 9R9 A 402



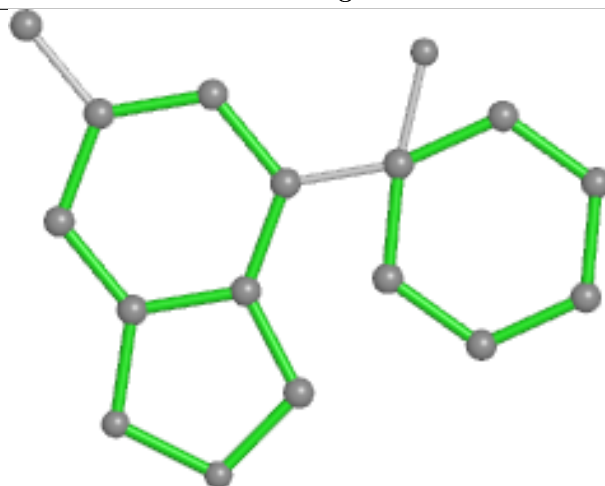
Bond lengths



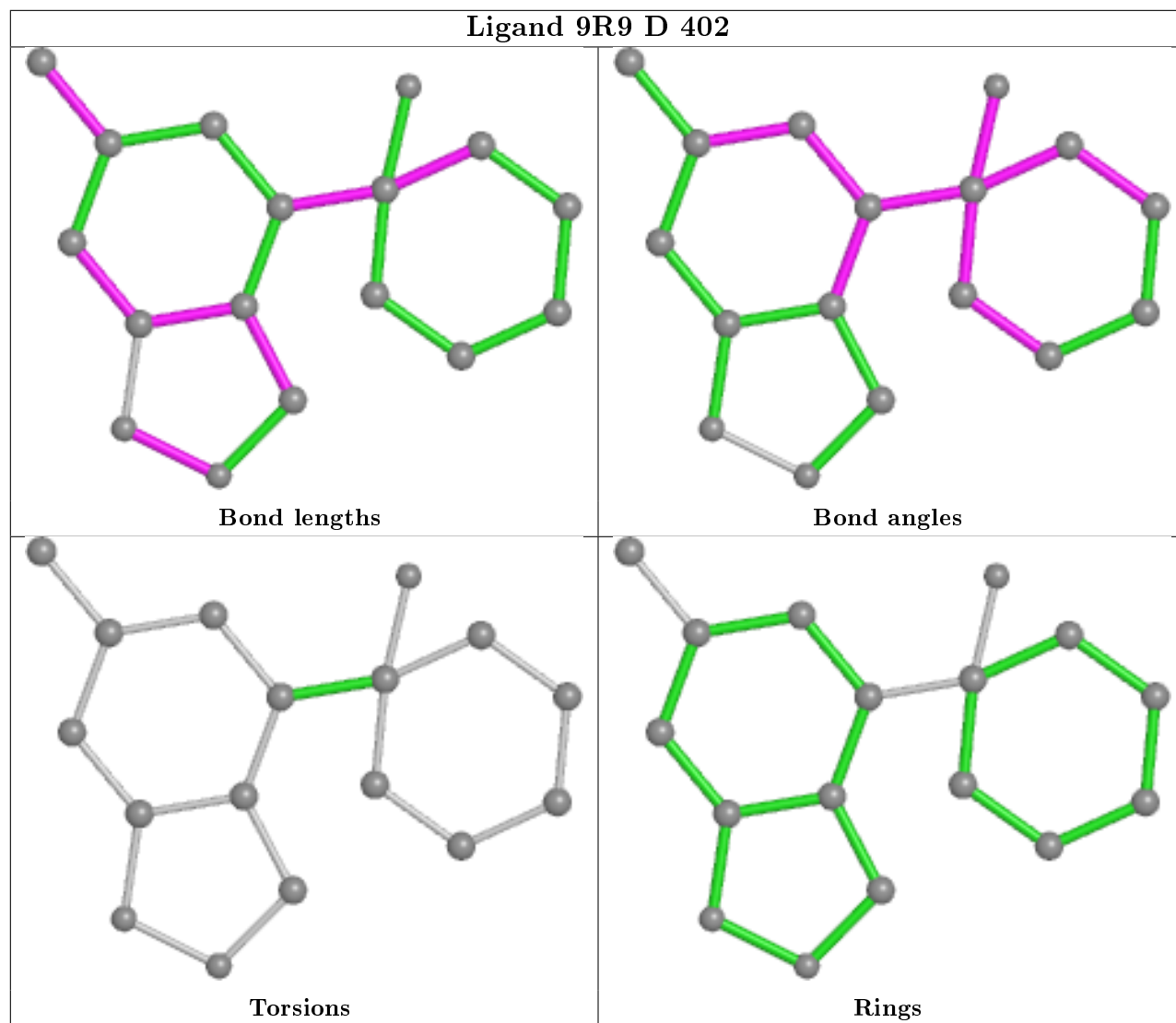
Bond angles



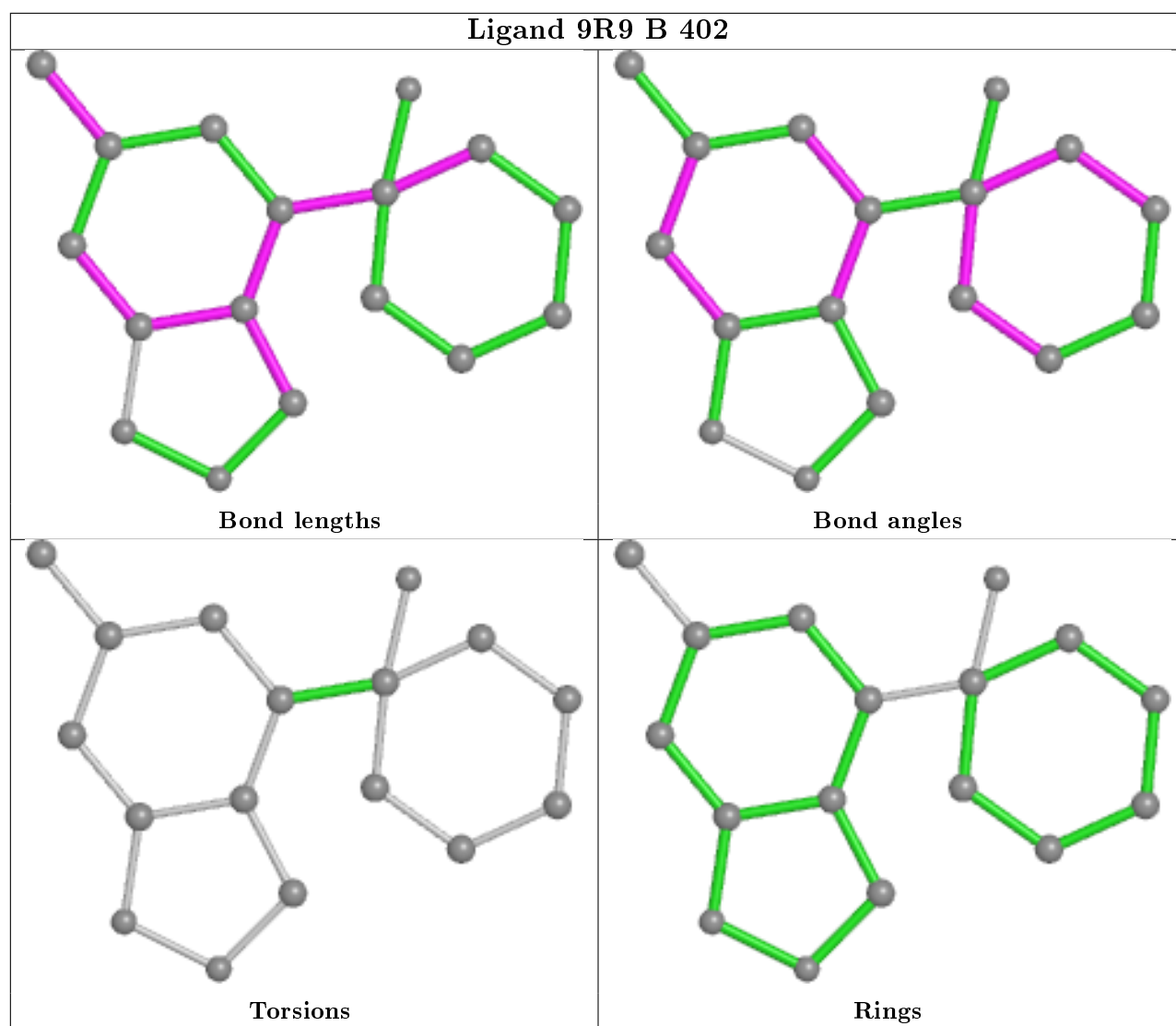
Torsions



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	322/391 (82%)	0.06	7 (2%) 62 57	47, 68, 118, 168	0
1	B	309/391 (79%)	0.12	17 (5%) 25 21	50, 84, 139, 190	0
1	C	323/391 (82%)	0.34	25 (7%) 13 10	58, 97, 146, 170	0
1	D	290/391 (74%)	0.33	27 (9%) 8 7	55, 97, 148, 169	0
All	All	1244/1564 (79%)	0.21	76 (6%) 21 18	47, 86, 144, 190	0

The worst 5 of 76 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	264	LEU	6.8
1	A	345	SER	6.3
1	C	254	VAL	5.6
1	D	265	LEU	5.0
1	D	218	HIS	4.9

### 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](#)

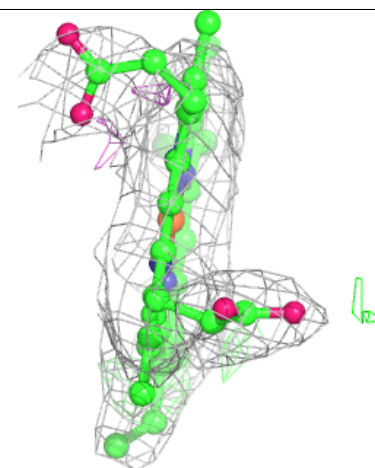
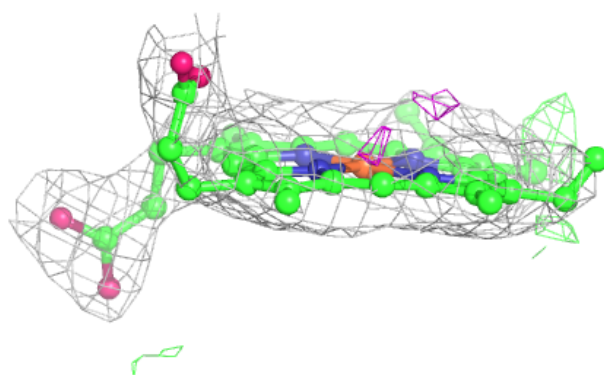
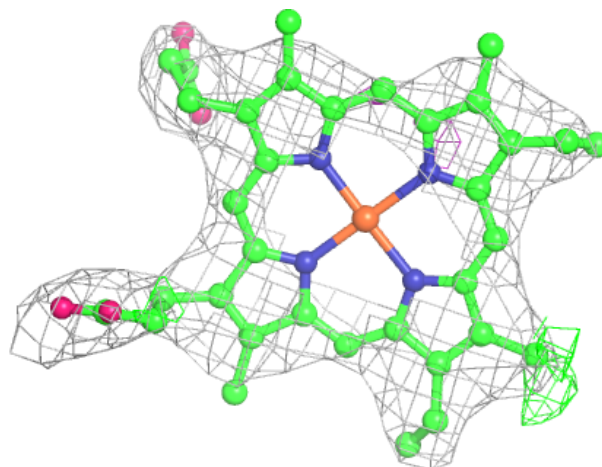
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 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	CIT	A	404	13/13	0.67	0.24	90,121,135,140	0
2	HEM	B	401	43/43	0.96	0.22	68,76,98,107	0
4	TRP	D	403	15/15	0.96	0.13	83,90,109,117	0
2	HEM	D	401	43/43	0.97	0.17	78,88,107,109	0
3	9R9	C	402	17/17	0.97	0.12	61,69,78,92	0
3	9R9	D	402	17/17	0.97	0.12	69,74,84,91	0
4	TRP	B	403	15/15	0.97	0.15	56,66,76,83	0
3	9R9	A	402	17/17	0.98	0.13	49,53,69,70	0
2	HEM	A	401	43/43	0.98	0.16	51,61,82,92	0
2	HEM	C	401	43/43	0.98	0.18	70,80,105,111	0
3	9R9	B	402	17/17	0.98	0.13	63,66,70,82	0
4	TRP	A	403	15/15	0.98	0.15	52,57,68,72	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.

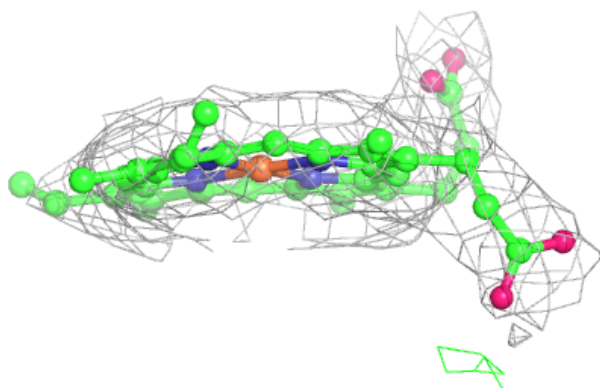
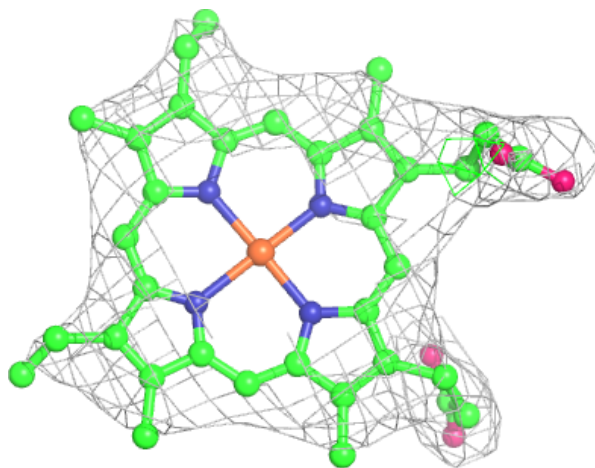
#### Electron density around HEM B 401:

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)



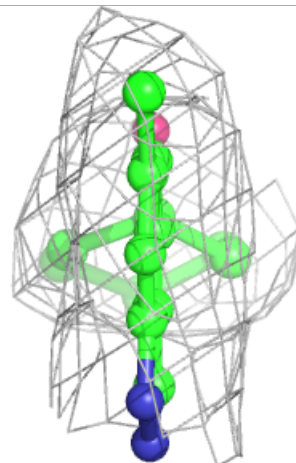
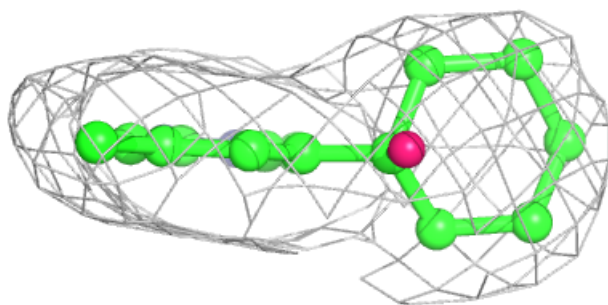
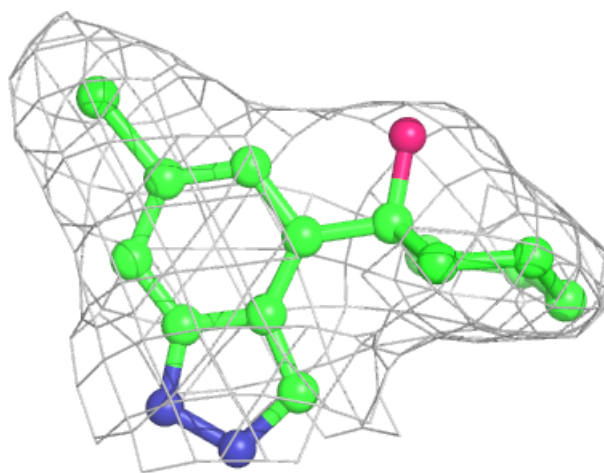
**Electron density around HEM D 401:**

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



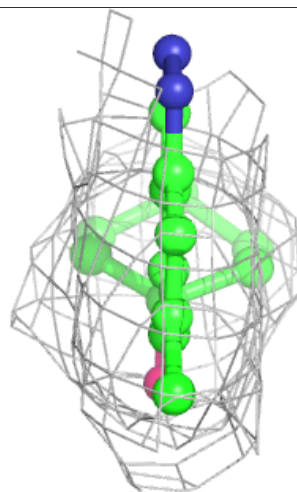
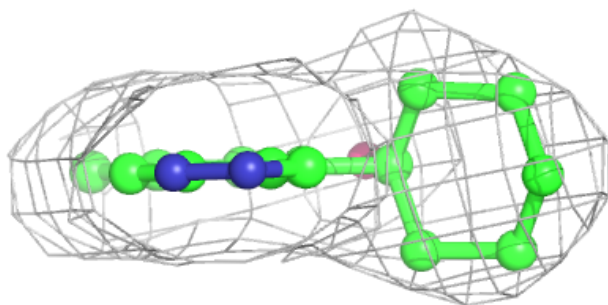
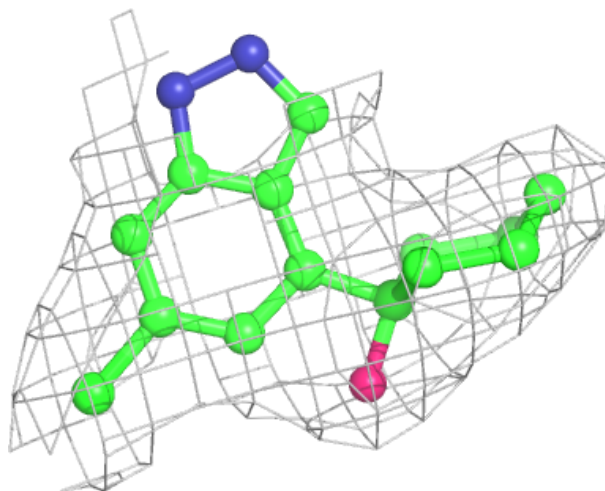
**Electron density around 9R9 C 402:**

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



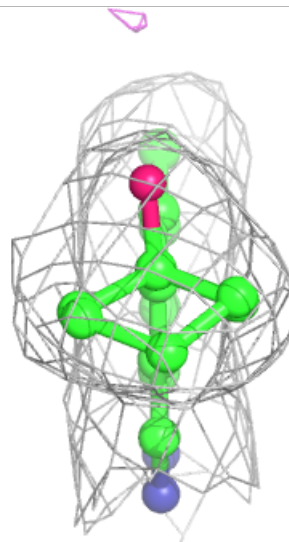
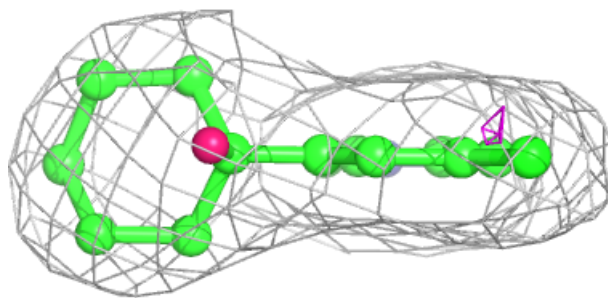
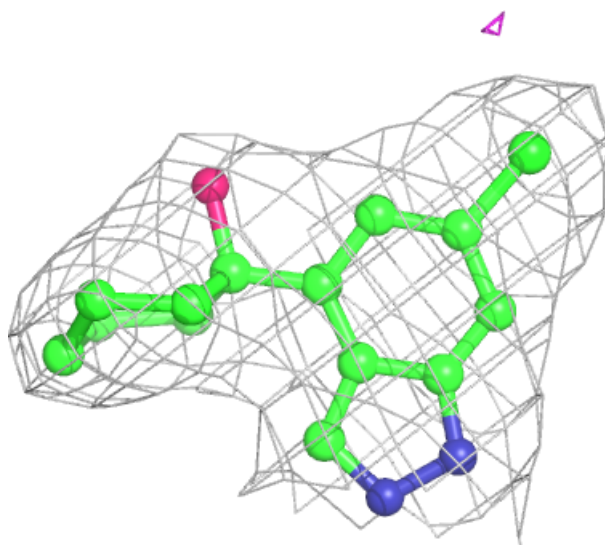
**Electron density around 9R9 D 402:**

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and green (positive)



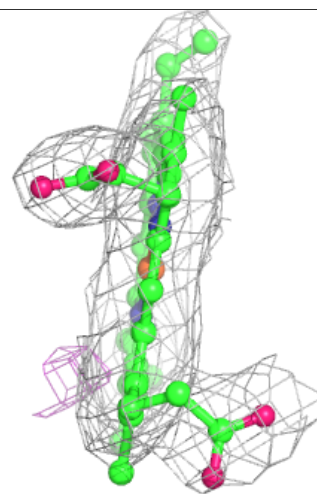
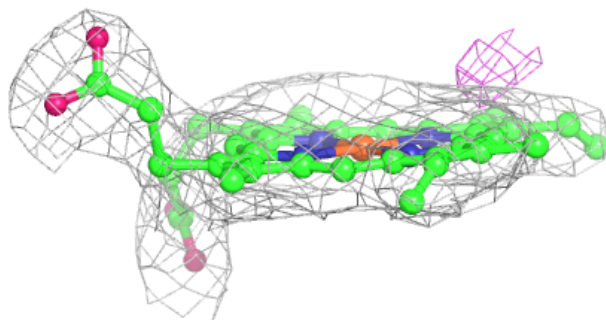
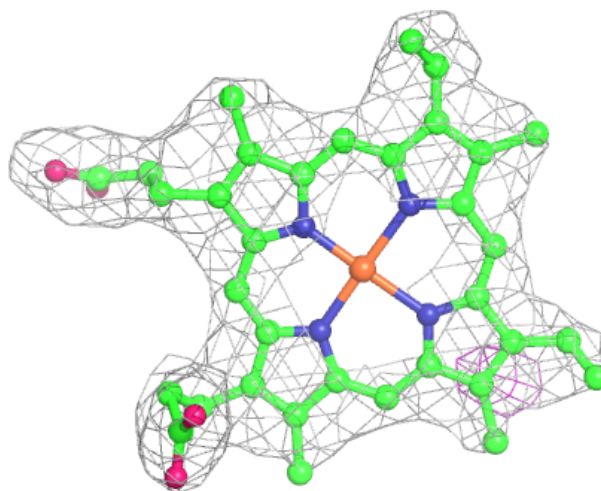
**Electron density around 9R9 A 402:**

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



**Electron density around HEM A 401:**

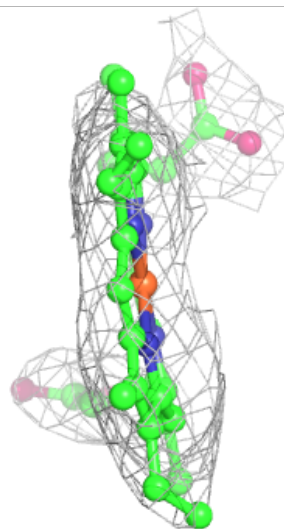
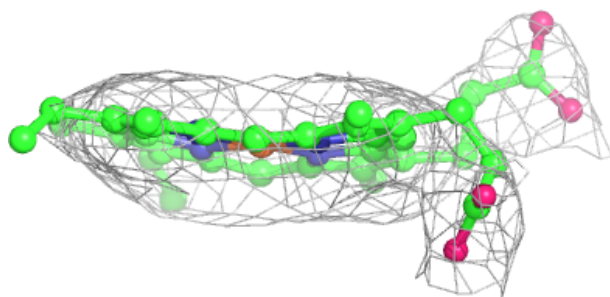
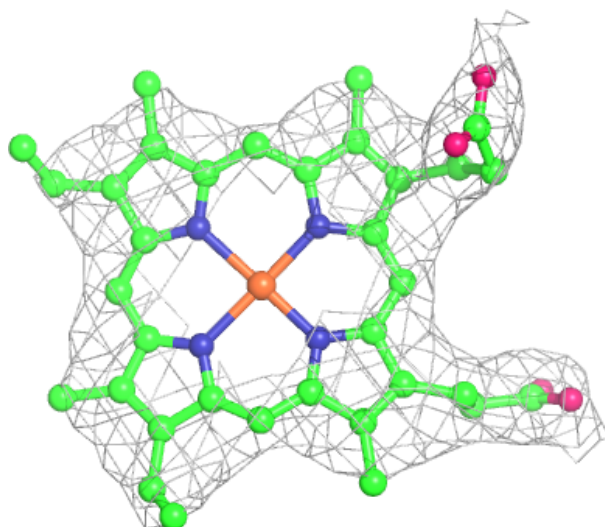
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





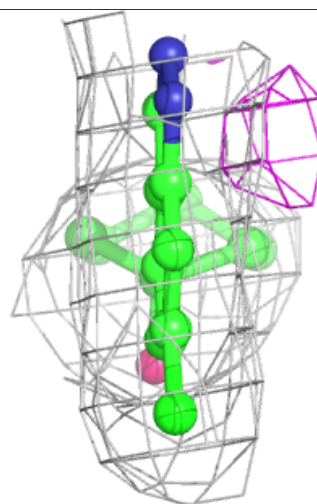
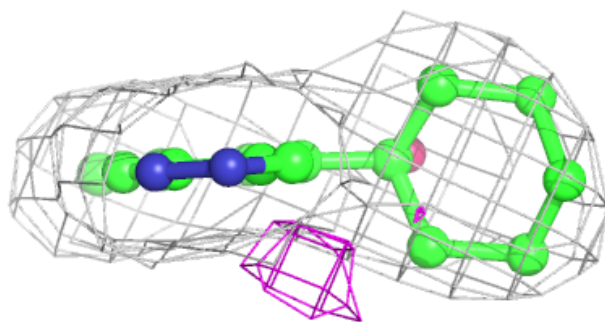
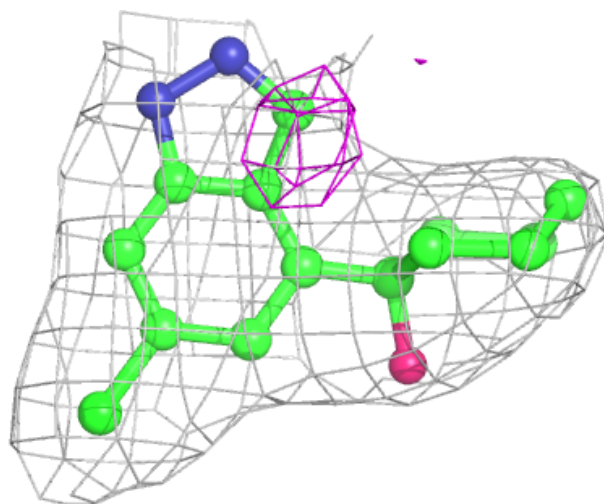
**Electron density around HEM C 401:**

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



**Electron density around 9R9 B 402:**

$2mF_o-DF_c$  (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.