



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 16, 2024 – 06:49 PM EDT

PDB ID : 5MNS  
Title : Structural and functional characterization of OleP in complex with 6DEB in sodium formate  
Authors : Parisi, G.; Savino, C.; Montemiglio, L.C.; Vallone, B.  
Deposited on : 2016-12-13  
Resolution : 2.62 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 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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
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)	:	2.37.1

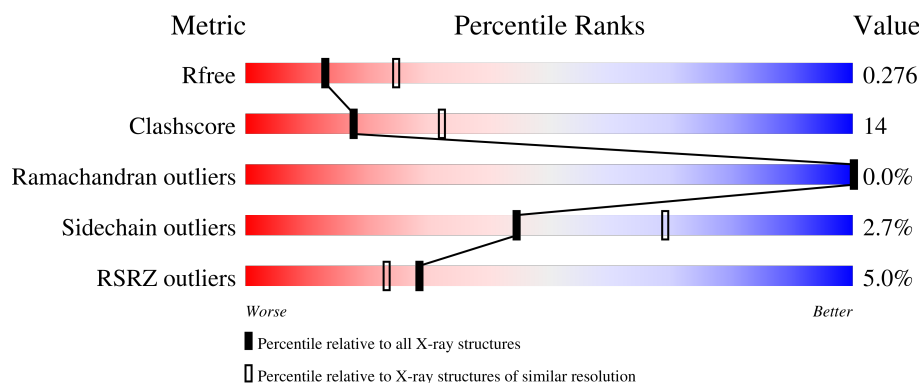
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.62 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	3797 (2.64-2.60)
Clashscore	141614	4168 (2.64-2.60)
Ramachandran outliers	138981	4093 (2.64-2.60)
Sidechain outliers	138945	4093 (2.64-2.60)
RSRZ outliers	127900	3731 (2.64-2.60)

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	407	 2% 78% 18% ..
1	B	407	 % 81% 15% ..
1	C	407	 % 83% 13% ..
1	D	407	 2% 72% 24% ..
1	E	407	 7% 78% 18% ..

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Mol	Chain	Length	Quality of chain
1	F	407	<div><div></div><div>16%</div><div></div><div>72%</div><div></div><div>22%</div><div></div><div></div></div>

## 2 Entry composition [i](#)

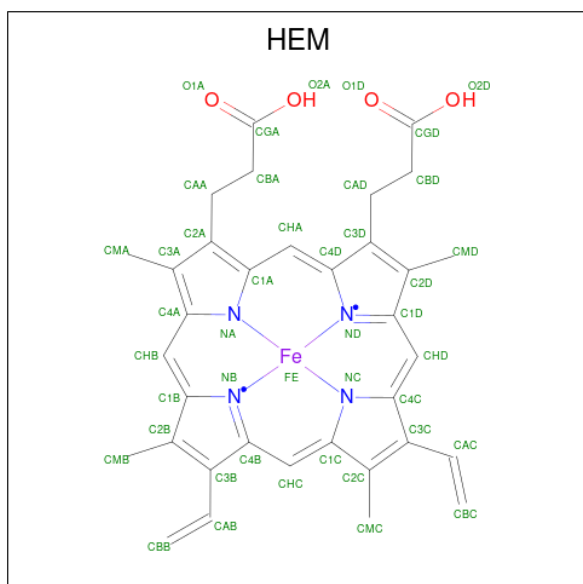
There are 4 unique types of molecules in this entry. The entry contains 19457 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Cytochrome P-450.

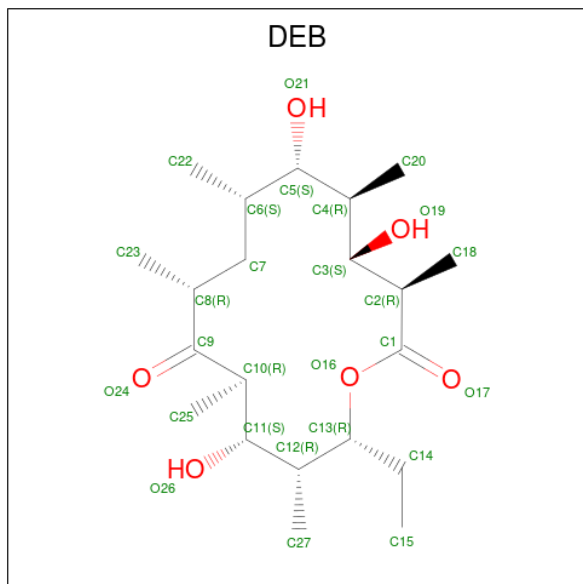
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	395	Total	C	N	O	S	0	0	0
			3077	1937	552	575	13			
1	B	395	Total	C	N	O	S	0	2	0
			3094	1947	556	578	13			
1	C	395	Total	C	N	O	S	0	0	0
			3077	1937	552	575	13			
1	D	395	Total	C	N	O	S	0	0	0
			3077	1937	552	575	13			
1	E	395	Total	C	N	O	S	0	1	0
			3085	1942	555	575	13			
1	F	393	Total	C	N	O	S	0	0	0
			3062	1928	550	571	13			

- 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	
2	E	1	Total	C	Fe	N	O	
			43	34	1	4	4	
2	F	1	Total	C	Fe	N	O	
			43	34	1	4	4	

- Molecule 3 is 6-DEOXYERYTHRONOLIDE B (three-letter code: DEB) (formula:  $C_{21}H_{38}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O		
			27	21	6		
3	B	1	Total	C	O		
			27	21	6		
3	C	1	Total	C	O		
			27	21	6		
3	D	1	Total	C	O		
			27	21	6		
3	E	1	Total	C	O		
			27	21	6		
3	F	1	Total	C	O		
			27	21	6		

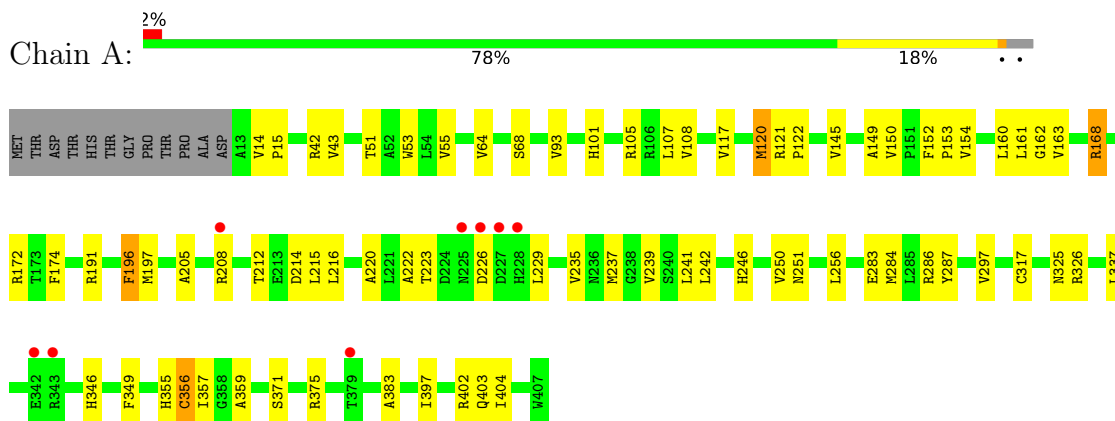
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	89	Total 89	O 89	0	0
4	B	126	Total 126	O 126	0	0
4	C	184	Total 184	O 184	0	0
4	D	56	Total 56	O 56	0	0
4	E	53	Total 53	O 53	0	0
4	F	57	Total 57	O 57	0	0

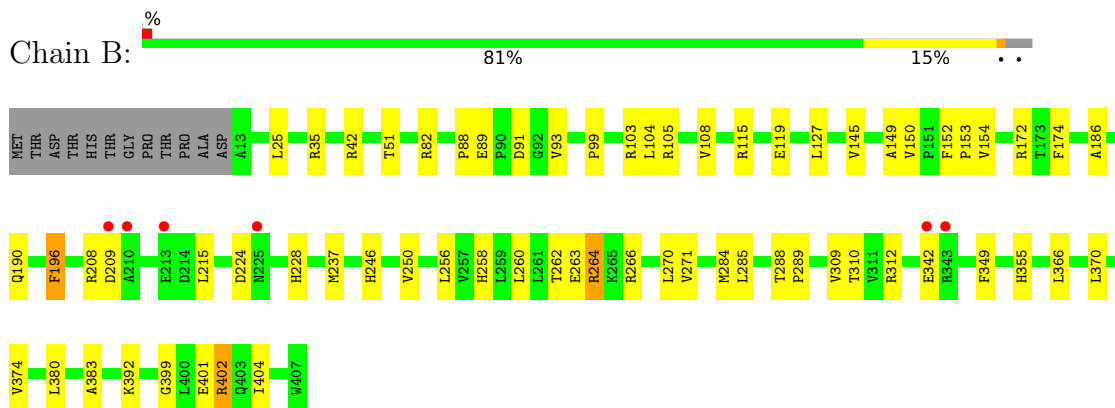
### 3 Residue-property plots [i](#)

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.

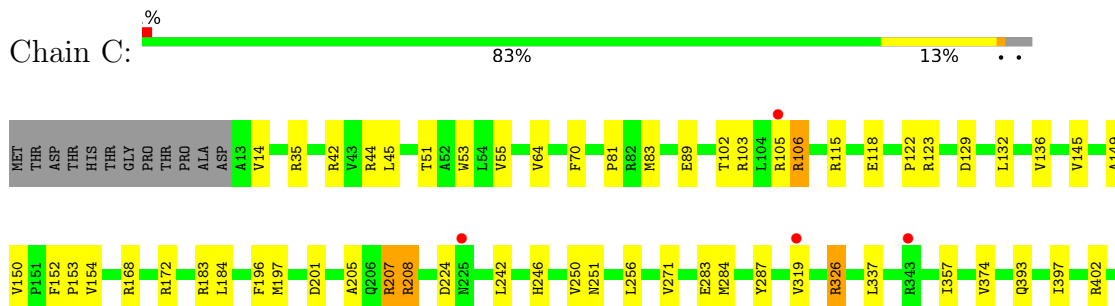
#### • Molecule 1: Cytochrome P-450



#### • Molecule 1: Cytochrome P-450



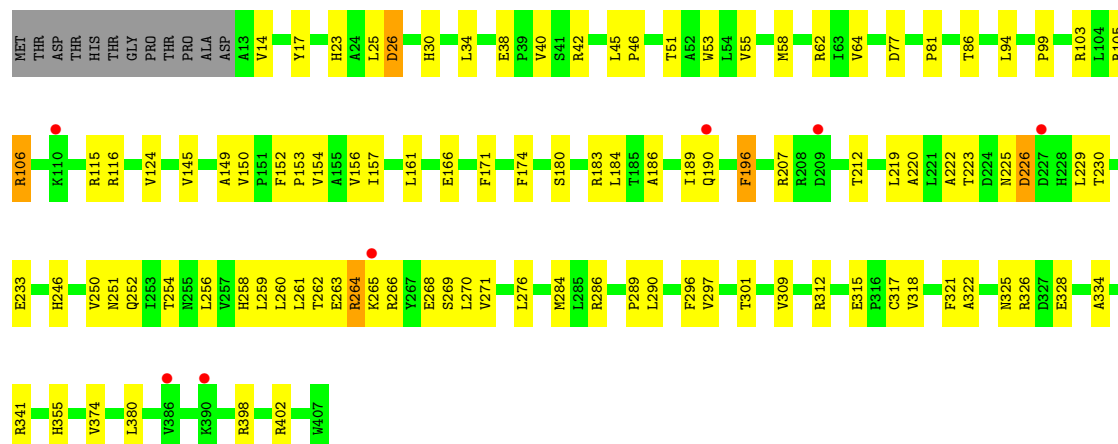
#### • Molecule 1: Cytochrome P-450




W407

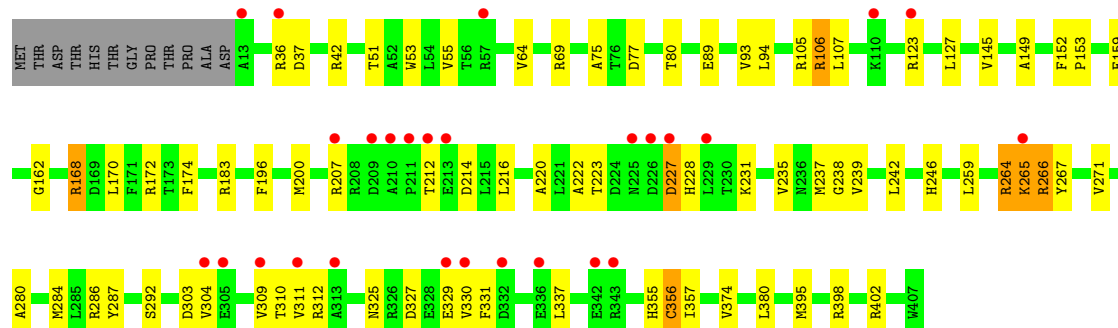
- Molecule 1: Cytochrome P-450

Chain D: 



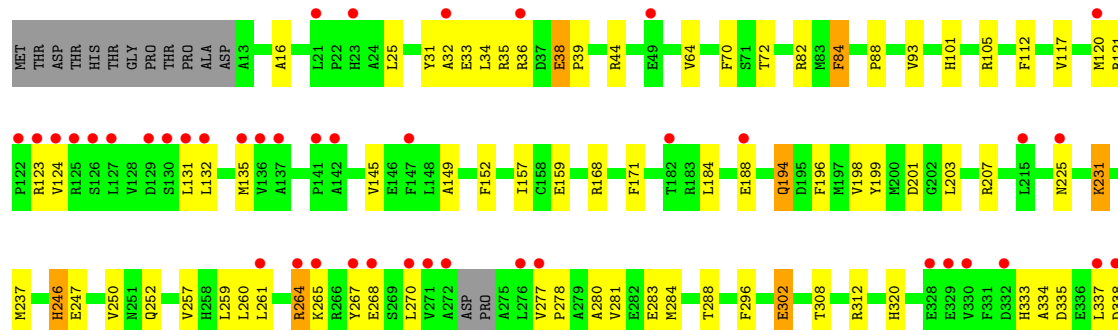
- Molecule 1: Cytochrome P-450

Chain E: 

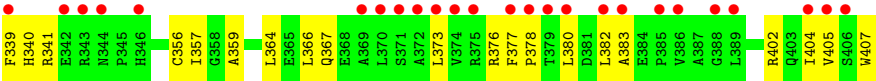


- Molecule 1: Cytochrome P-450

Chain F: 







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	247.60Å 110.80Å 159.10Å 90.00° 129.60° 90.00°	Depositor
Resolution (Å)	120.00 – 2.62 47.91 – 2.62	Depositor EDS
% Data completeness (in resolution range)	99.6 (120.00-2.62) 99.7 (47.91-2.62)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.50 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.208 , 0.258 0.234 , 0.276	Depositor DCC
$R_{free}$ test set	4932 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.4	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 40.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.019 for -h-2*k,l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	19457	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.57 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.4422e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: DEB, 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	0.50	0/3144	0.72	0/4284
1	B	0.50	0/3164	0.74	0/4310
1	C	0.51	0/3144	0.74	2/4284 (0.0%)
1	D	0.51	0/3144	0.75	1/4284 (0.0%)
1	E	0.49	0/3155	0.74	1/4298 (0.0%)
1	F	0.48	0/3127	0.74	0/4258
All	All	0.50	0/18878	0.74	4/25718 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	26	ASP	N-CA-C	-5.44	96.32	111.00
1	C	103	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	C	123	ARG	NE-CZ-NH2	5.04	122.82	120.30
1	E	266	ARG	NE-CZ-NH1	5.03	122.81	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	3077	0	3056	75	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3094	0	3074	65	0
1	C	3077	0	3056	49	0
1	D	3077	0	3056	95	1
1	E	3085	0	3070	109	0
1	F	3062	0	3044	118	1
2	A	43	0	30	6	0
2	B	43	0	30	4	0
2	C	43	0	30	2	0
2	D	43	0	30	4	0
2	E	43	0	30	12	0
2	F	43	0	30	4	0
3	A	27	0	38	0	0
3	B	27	0	38	1	0
3	C	27	0	38	0	0
3	D	27	0	38	1	0
3	E	27	0	38	0	0
3	F	27	0	38	0	0
4	A	89	0	0	0	0
4	B	126	0	0	3	1
4	C	184	0	0	6	0
4	D	56	0	0	5	0
4	E	53	0	0	1	0
4	F	57	0	0	4	0
All	All	19457	0	18764	511	3

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 14.

The worst 5 of 511 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:E:356:CYS:SG	2:E:501:HEM:FE	0.96	1.56
1:A:42:ARG:HH11	1:A:51:THR:CG2	1.30	1.44
1:E:123:ARG:NH1	1:E:127:LEU:HD12	1.42	1.35
1:E:356:CYS:SG	2:E:501:HEM:ND	2.00	1.34
1:E:42:ARG:HD2	1:E:51:THR:OG1	1.34	1.25

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:723:HOH:O	4:B:723:HOH:O[2_656]	2.11	0.09
1:A:208:ARG:NH1	1:D:301:THR:OG1[4_445]	2.16	0.04
1:A:68:SER:OG	1:F:231:LYS:NZ[4_546]	2.19	0.01

## 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	393/407 (97%)	383 (98%)	10 (2%)	0	100	100
1	B	395/407 (97%)	384 (97%)	11 (3%)	0	100	100
1	C	393/407 (97%)	380 (97%)	13 (3%)	0	100	100
1	D	393/407 (97%)	371 (94%)	22 (6%)	0	100	100
1	E	394/407 (97%)	378 (96%)	15 (4%)	1 (0%)	41	62
1	F	389/407 (96%)	372 (96%)	17 (4%)	0	100	100
All	All	2357/2442 (96%)	2268 (96%)	88 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	265	LYS

### 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	331/341 (97%)	325 (98%)	6 (2%)	59	79
1	B	333/341 (98%)	330 (99%)	3 (1%)	78	90
1	C	331/341 (97%)	323 (98%)	8 (2%)	49	72
1	D	331/341 (97%)	319 (96%)	12 (4%)	35	59
1	E	332/341 (97%)	321 (97%)	11 (3%)	38	62
1	F	329/341 (96%)	315 (96%)	14 (4%)	29	53
All	All	1987/2046 (97%)	1933 (97%)	54 (3%)	44	69

5 of 54 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	402	ARG
1	E	264	ARG
1	F	264	ARG
1	E	89	GLU
1	E	168	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	246	HIS
1	D	246	HIS
1	E	246	HIS
1	D	252	GLN
1	C	206	GLN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry

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
3	DEB	A	502	-	27,27,27	1.13	1 (3%)	35,39,39	1.18	2 (5%)
3	DEB	F	502	-	27,27,27	1.12	1 (3%)	35,39,39	1.16	4 (11%)
2	HEM	A	501	-	41,50,50	1.39	7 (17%)	45,82,82	1.99	16 (35%)
2	HEM	D	501	1	41,50,50	1.47	5 (12%)	45,82,82	2.05	14 (31%)
2	HEM	B	501	1	41,50,50	1.35	6 (14%)	45,82,82	2.00	14 (31%)
3	DEB	C	502	-	27,27,27	1.10	1 (3%)	35,39,39	1.06	2 (5%)
3	DEB	D	502	-	27,27,27	1.16	1 (3%)	35,39,39	1.27	2 (5%)
2	HEM	F	501	1	41,50,50	1.36	5 (12%)	45,82,82	1.84	11 (24%)
2	HEM	E	501	-	41,50,50	1.78	14 (34%)	45,82,82	1.79	8 (17%)
3	DEB	E	502	-	27,27,27	1.52	4 (14%)	35,39,39	1.56	7 (20%)
3	DEB	B	502	-	27,27,27	1.55	3 (11%)	35,39,39	1.38	3 (8%)
2	HEM	C	501	1	41,50,50	1.40	6 (14%)	45,82,82	2.11	16 (35%)

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	DEB	A	502	-	-	7/50/50/50	0/1/1/1
3	DEB	F	502	-	-	10/50/50/50	0/1/1/1
2	HEM	A	501	-	-	2/12/54/54	-
2	HEM	D	501	1	-	5/12/54/54	-
2	HEM	B	501	1	-	2/12/54/54	-
3	DEB	C	502	-	-	10/50/50/50	0/1/1/1
3	DEB	D	502	-	-	8/50/50/50	0/1/1/1
2	HEM	F	501	1	-	0/12/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	E	501	-	-	1/12/54/54	-
3	DEB	E	502	-	-	6/50/50/50	0/1/1/1
3	DEB	B	502	-	-	8/50/50/50	0/1/1/1
2	HEM	C	501	1	-	2/12/54/54	-

The worst 5 of 54 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	DEB	O16-C1	5.54	1.47	1.34
3	D	502	DEB	O16-C1	5.46	1.47	1.34
3	F	502	DEB	O16-C1	5.20	1.46	1.34
2	E	501	HEM	C1B-NB	-4.82	1.32	1.40
2	D	501	HEM	C1B-NB	-4.79	1.32	1.40

The worst 5 of 99 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	HEM	C1B-NB-C4B	5.89	111.16	105.07
2	C	501	HEM	CHC-C4B-NB	5.65	130.57	124.43
2	B	501	HEM	C1B-NB-C4B	5.46	110.72	105.07
2	A	501	HEM	C1B-NB-C4B	5.41	110.66	105.07
2	A	501	HEM	CHC-C4B-NB	5.19	130.07	124.43

There are no chirality outliers.

5 of 61 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	DEB	C3-C4-C5-O21
3	A	502	DEB	C20-C4-C5-O21
3	C	502	DEB	C18-C2-C3-C4
3	D	502	DEB	C3-C4-C5-O21
3	E	502	DEB	C3-C4-C5-O21

There are no ring outliers.

8 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	HEM	6	0
2	D	501	HEM	4	0
2	B	501	HEM	4	0

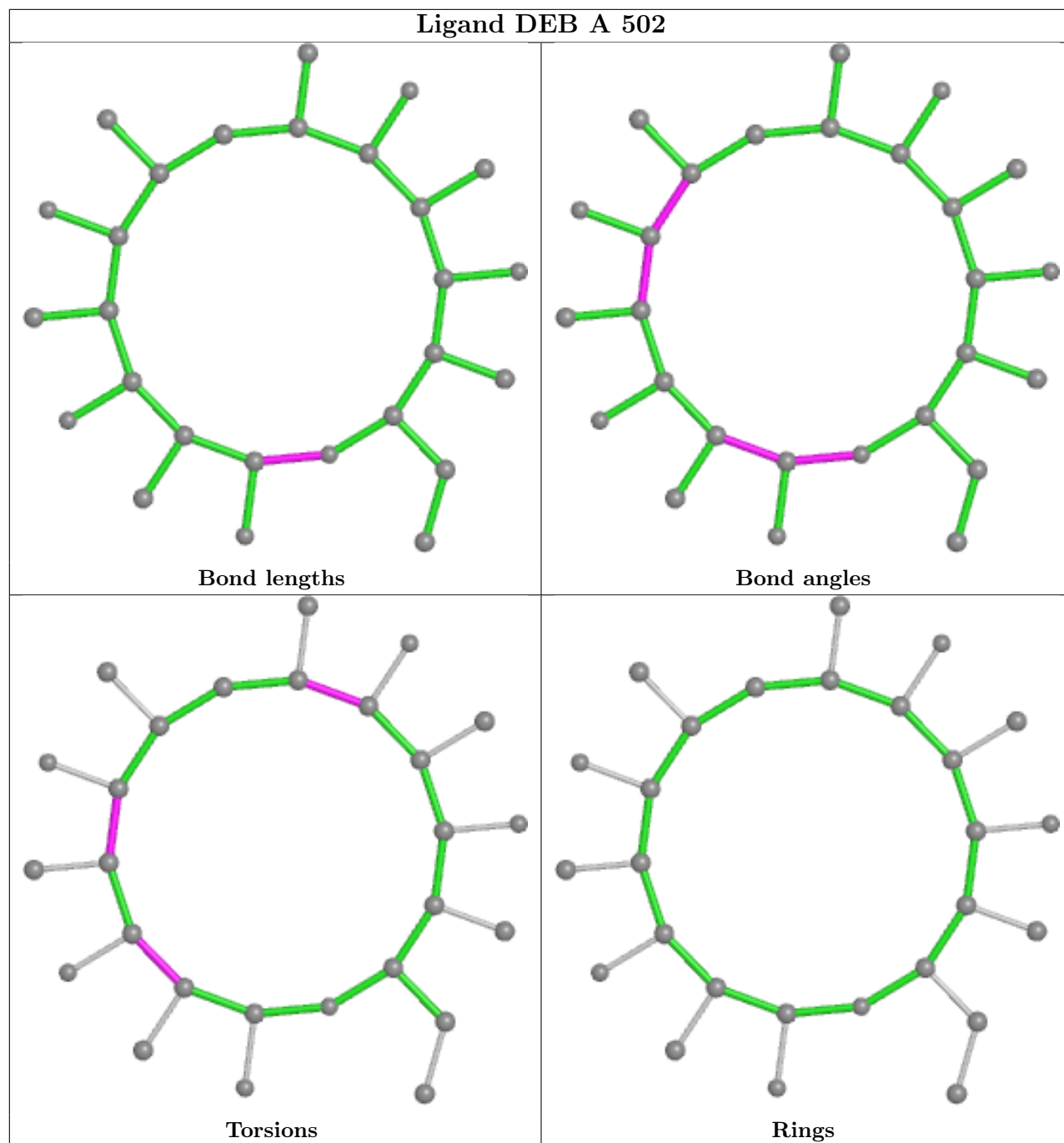
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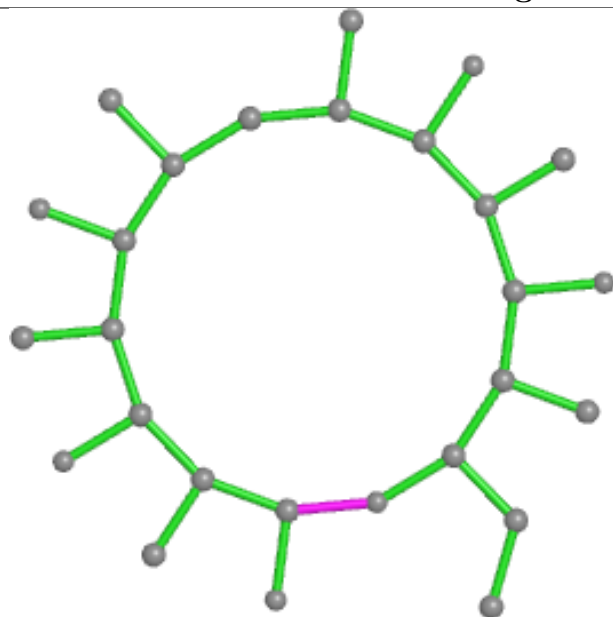
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	502	DEB	1	0
2	F	501	HEM	4	0
2	E	501	HEM	12	0
3	B	502	DEB	1	0
2	C	501	HEM	2	0

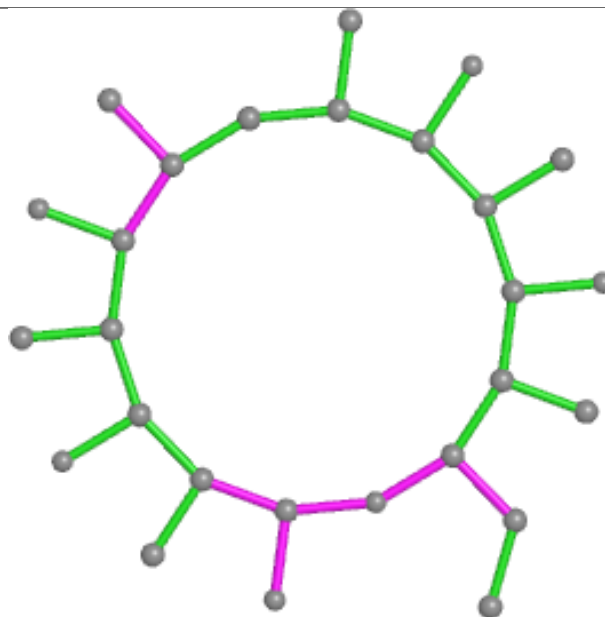
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



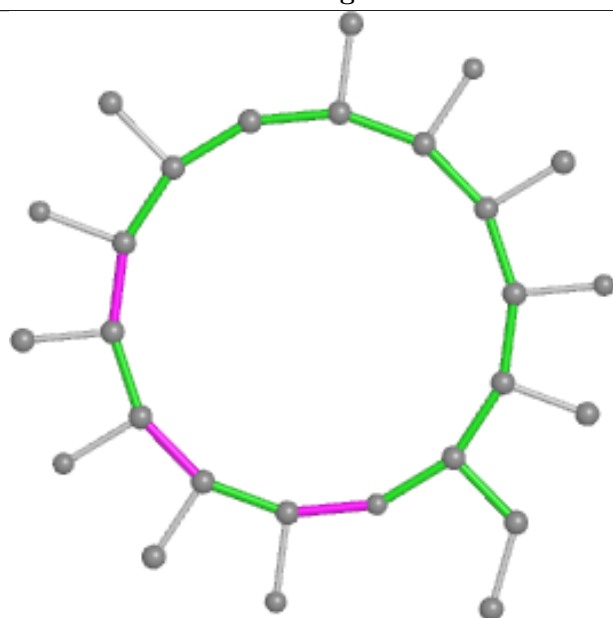
## Ligand DEB F 502



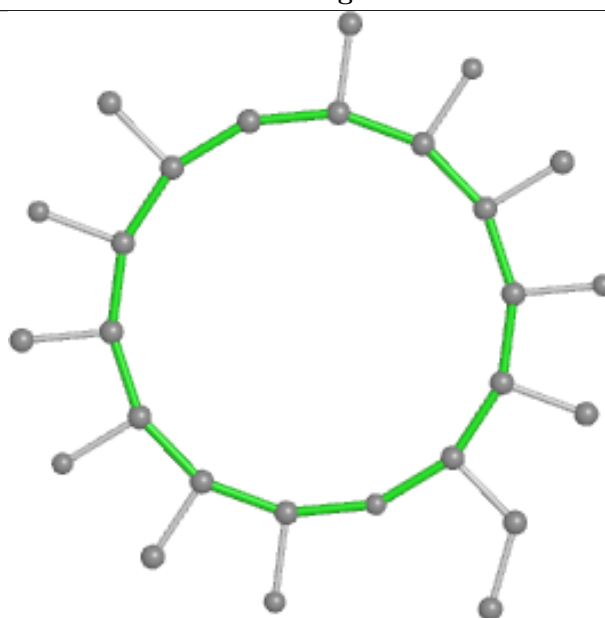
Bond lengths



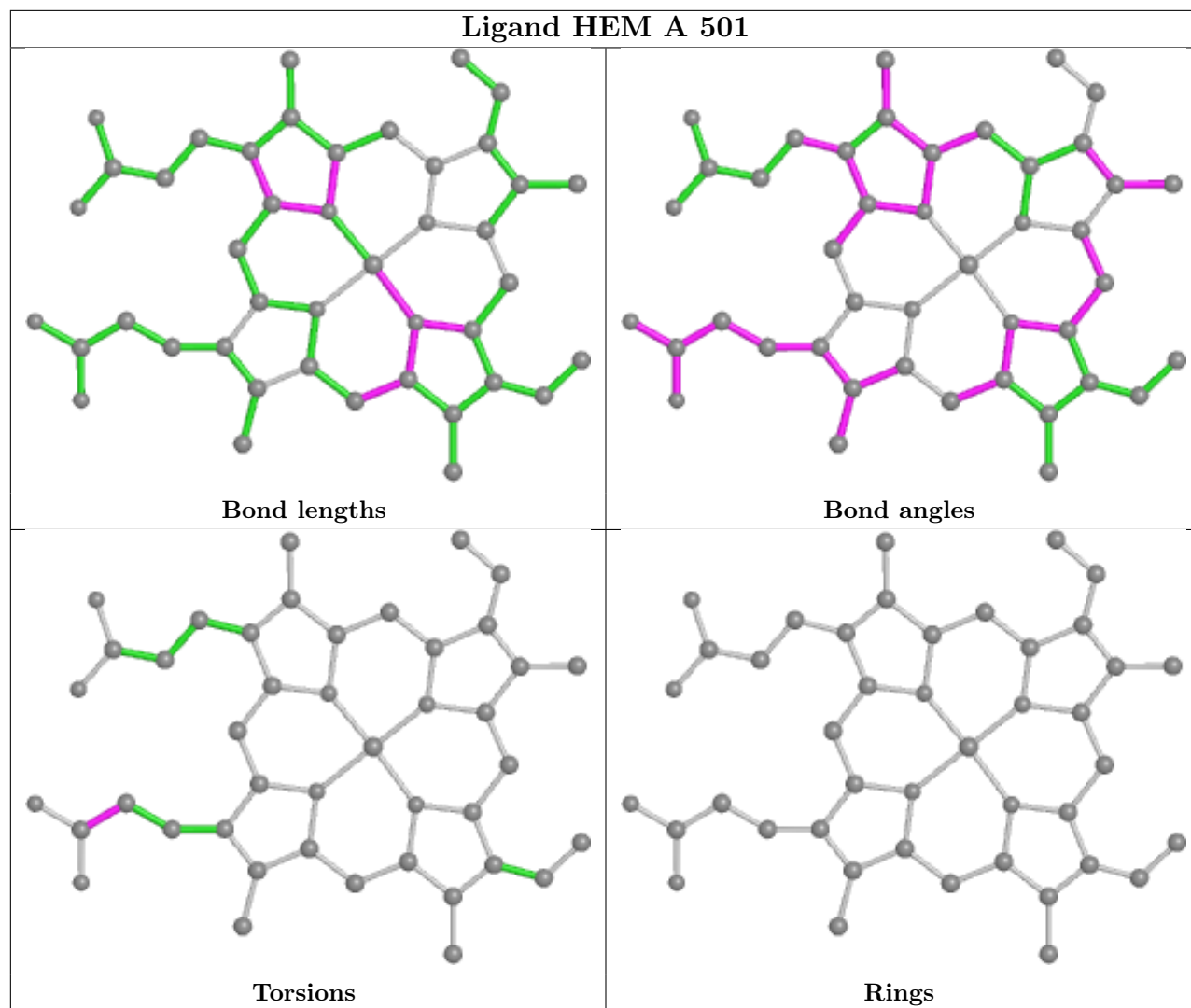
Bond angles

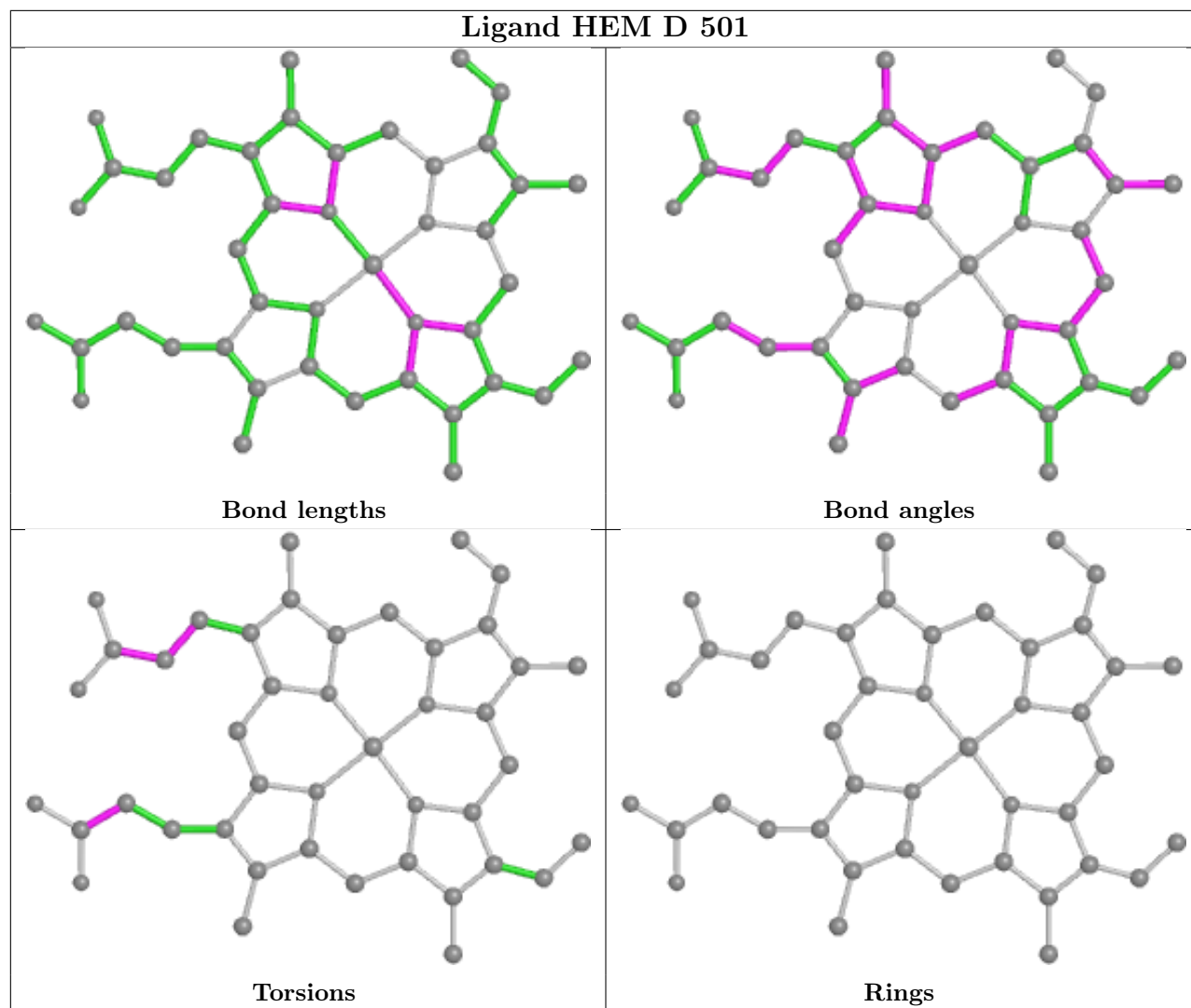


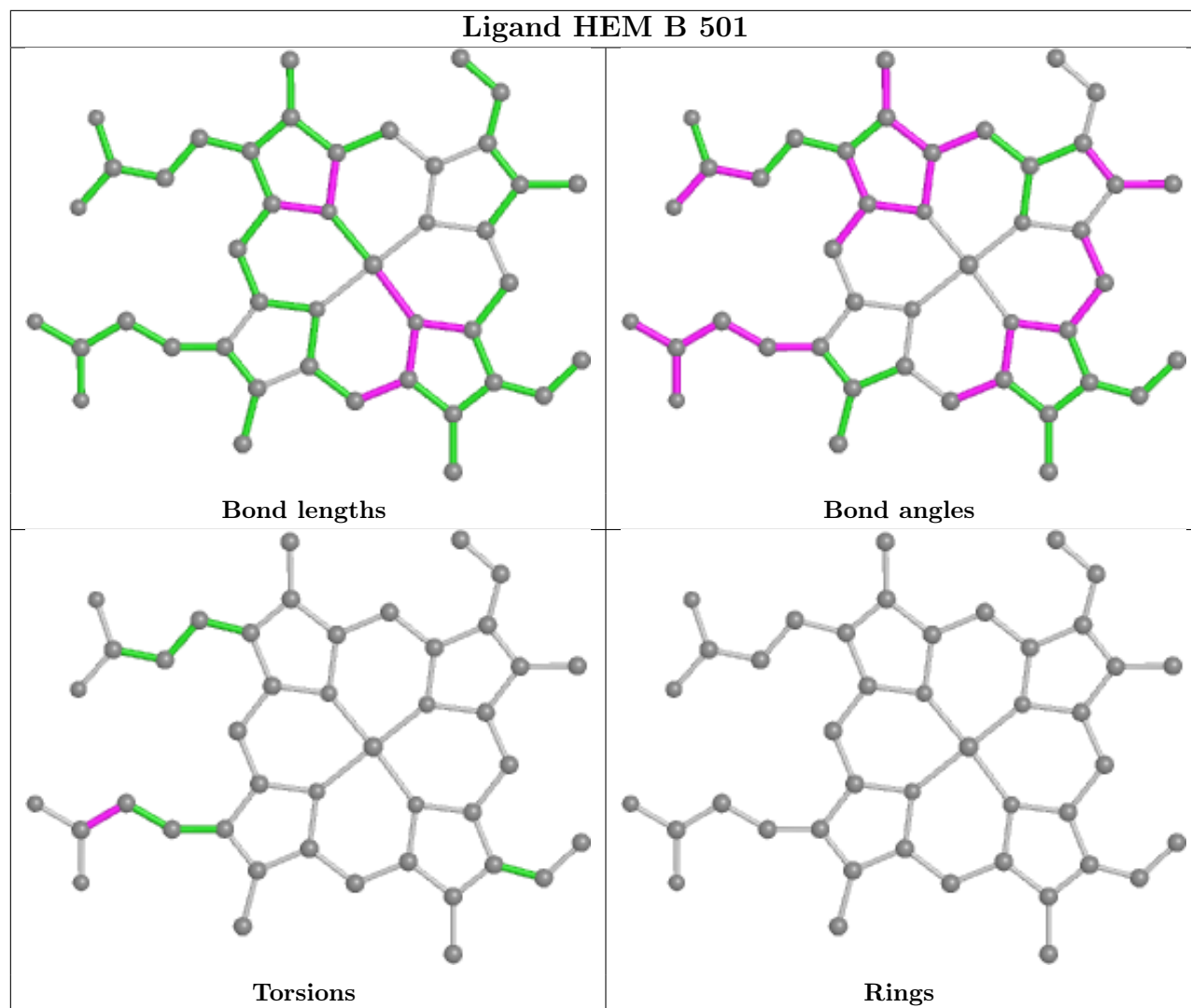
Torsions

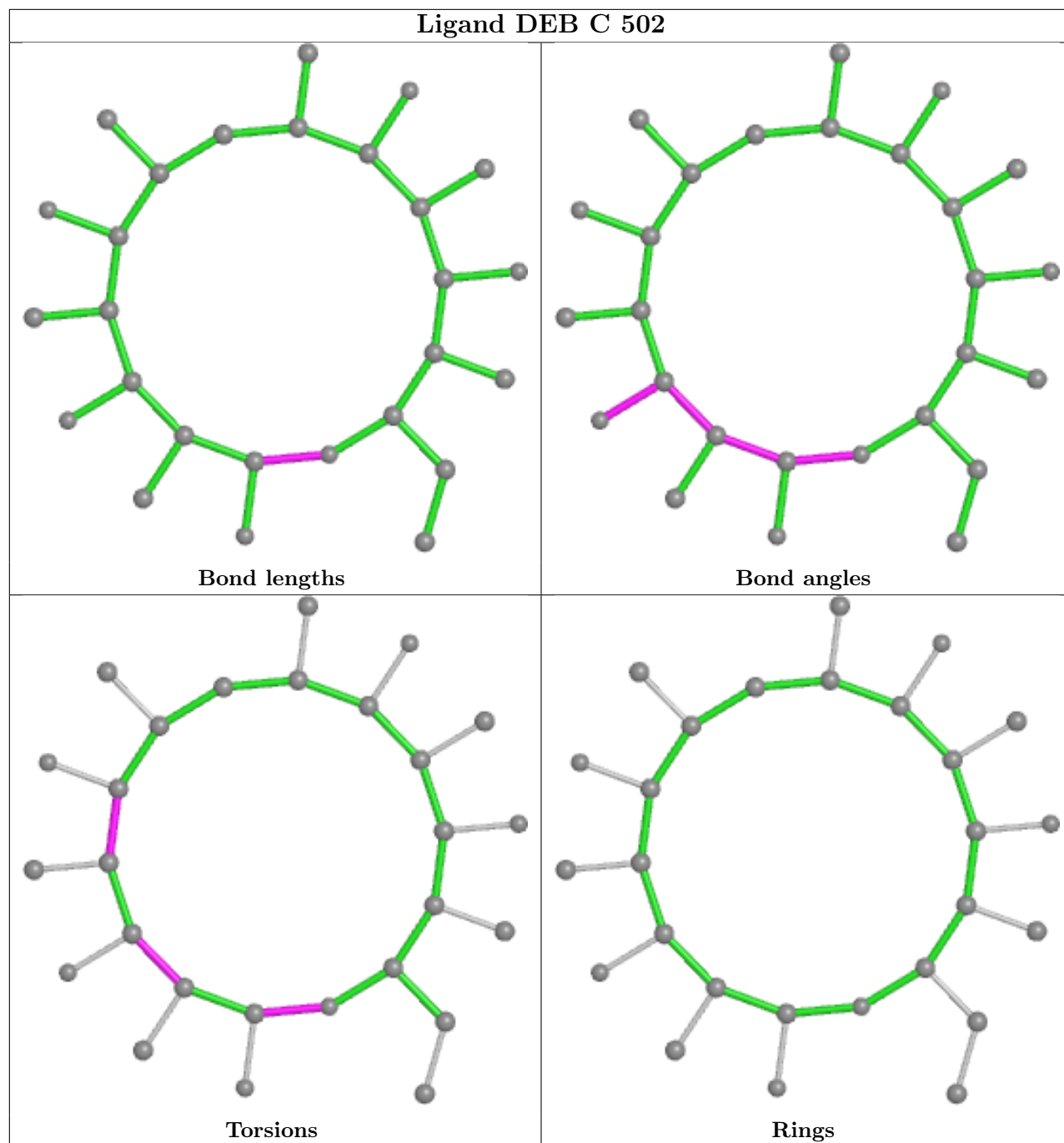


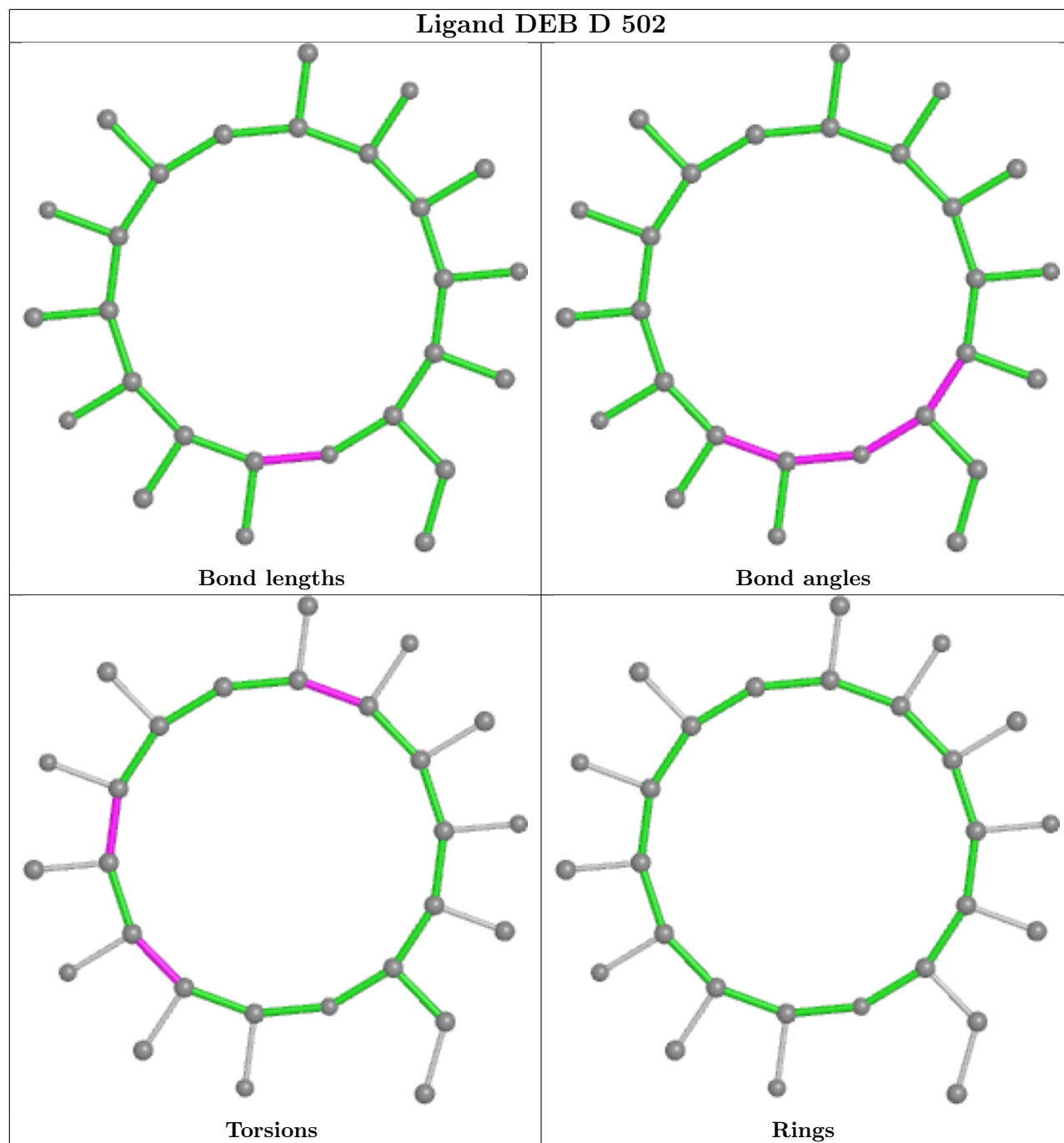
Rings



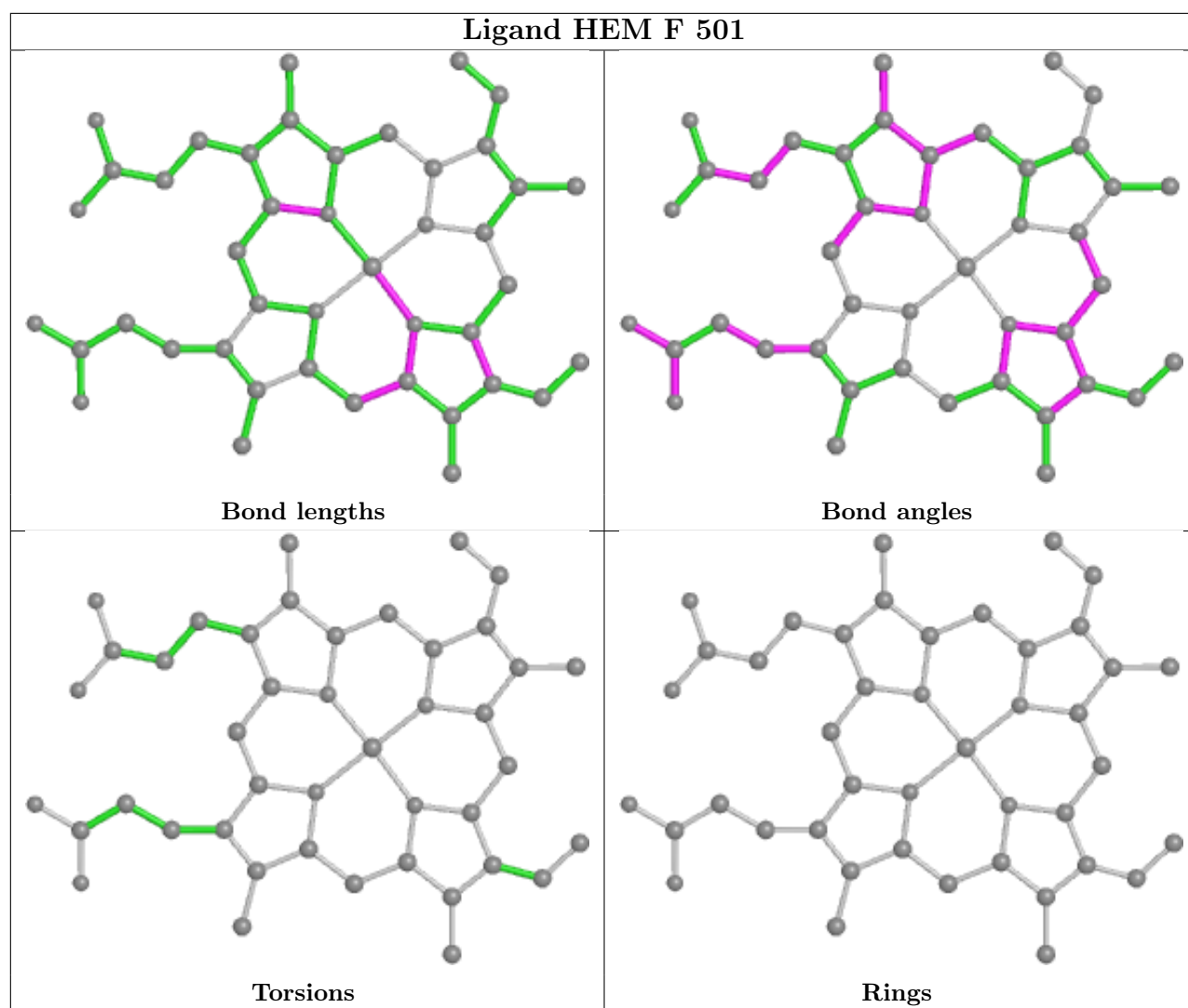


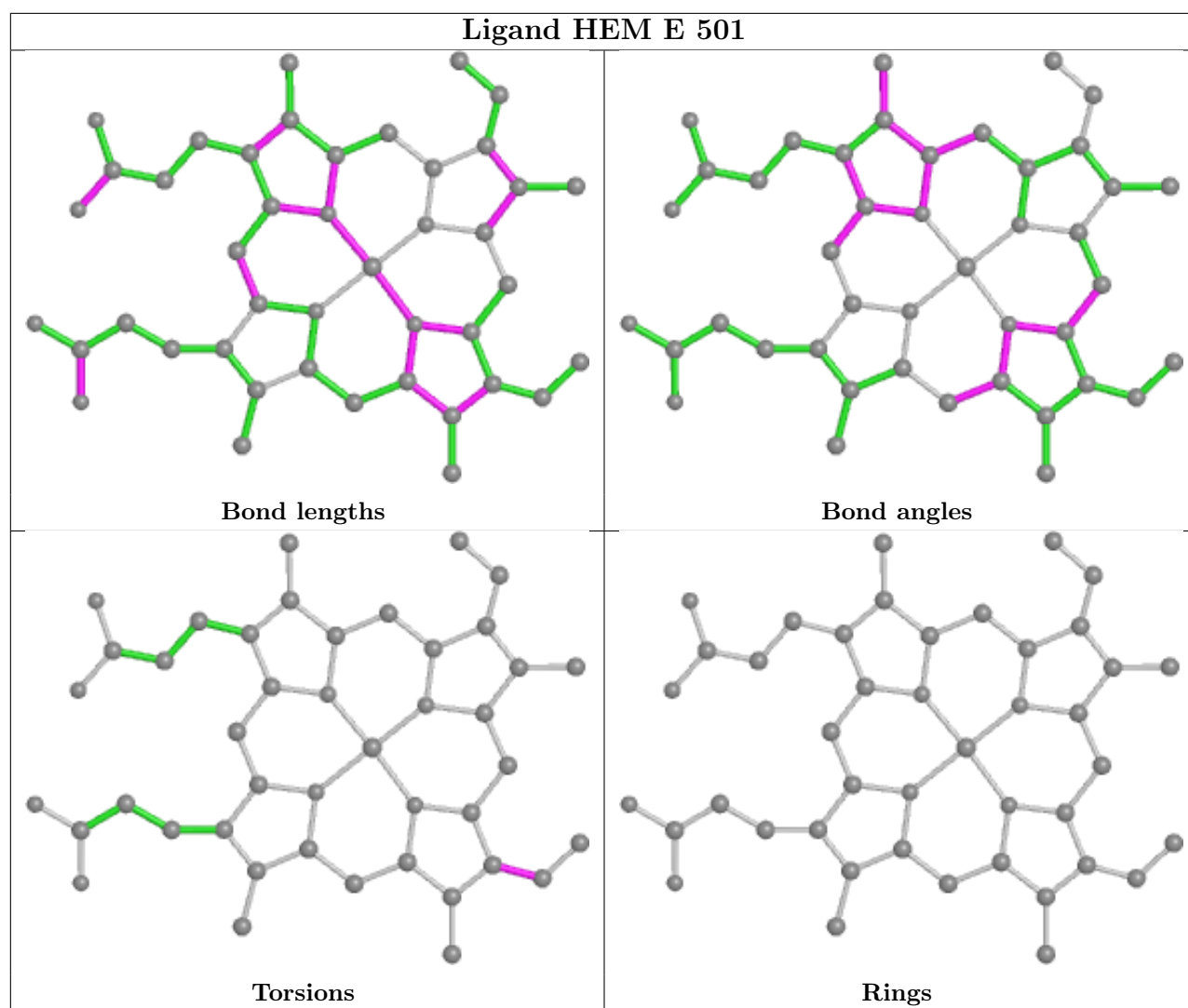




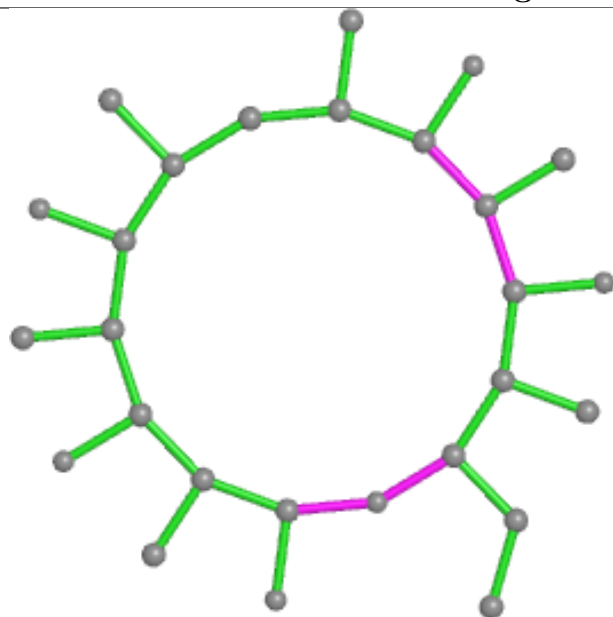




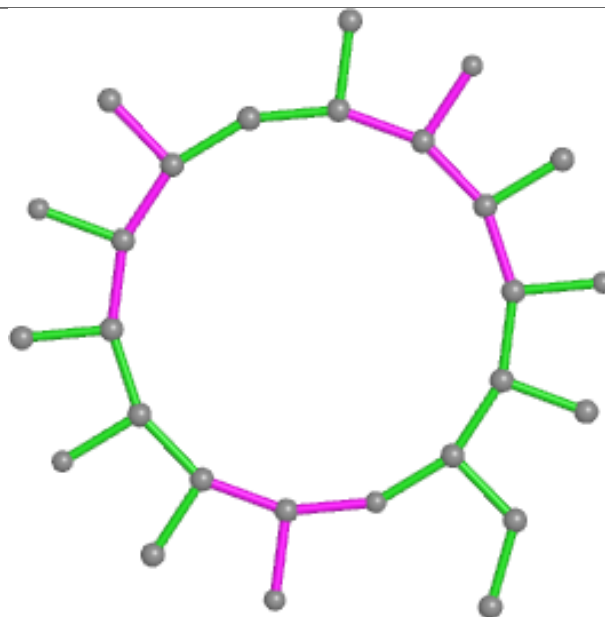




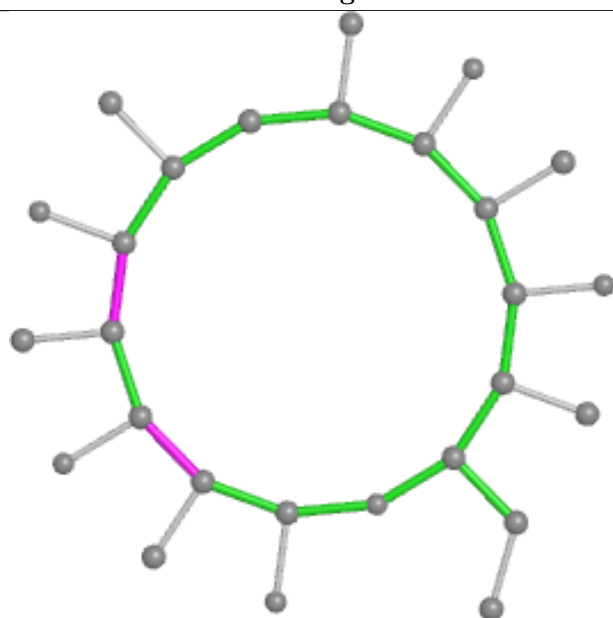
## Ligand DEB E 502



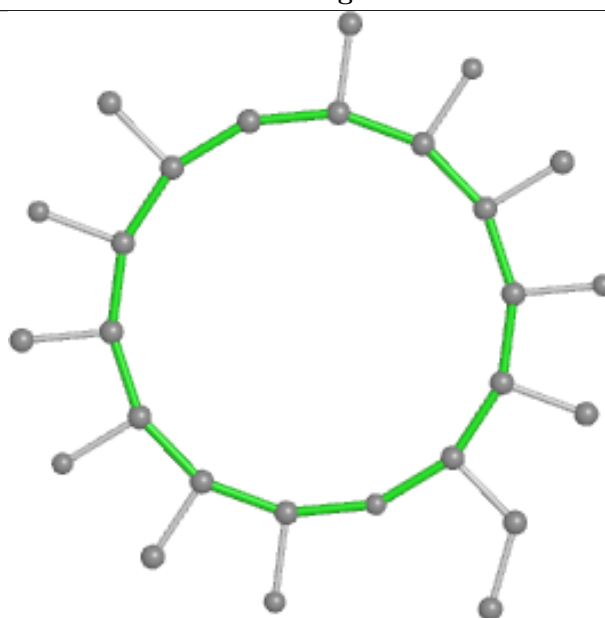
Bond lengths



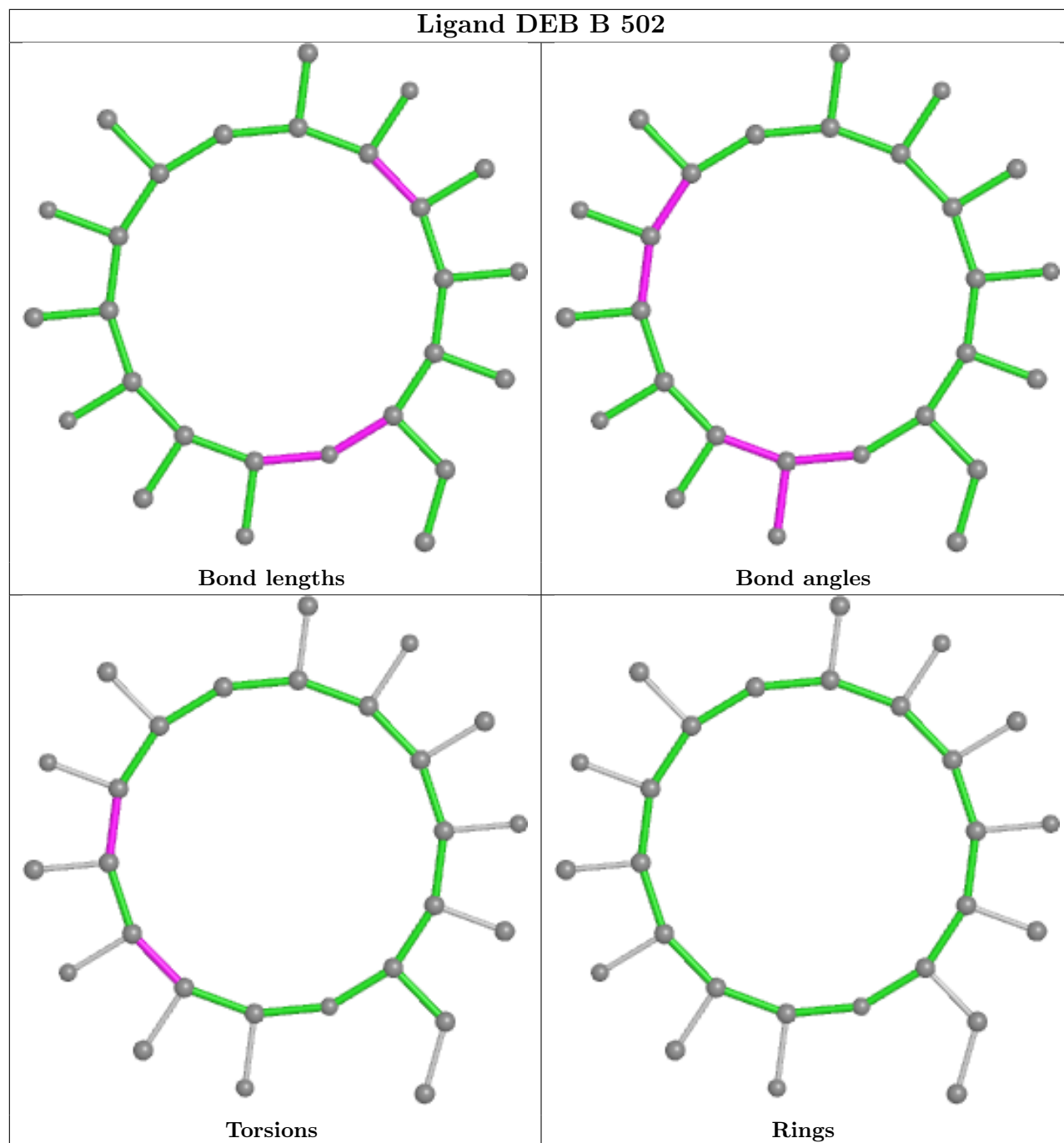
Bond angles

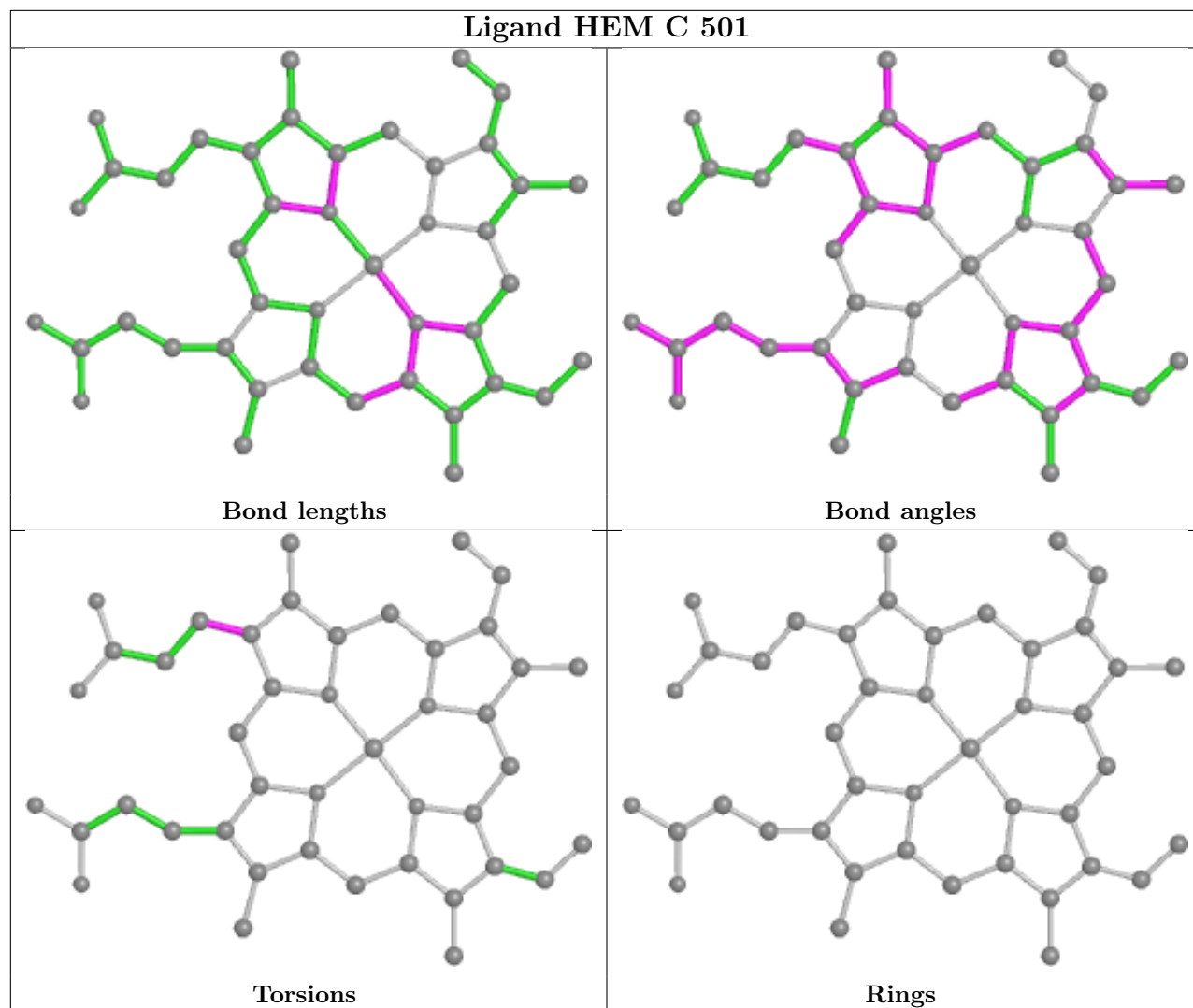


Torsions



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	395/407 (97%)	-0.07	8 (2%) 65 60	26, 48, 75, 102	0
1	B	395/407 (97%)	-0.21	6 (1%) 73 70	25, 43, 66, 111	0
1	C	395/407 (97%)	-0.32	4 (1%) 82 80	24, 37, 54, 88	0
1	D	395/407 (97%)	0.11	7 (1%) 68 64	33, 58, 86, 121	0
1	E	395/407 (97%)	0.23	27 (6%) 17 13	37, 64, 93, 120	0
1	F	393/407 (96%)	0.68	67 (17%) 1 1	42, 72, 106, 121	0
All	All	2368/2442 (96%)	0.07	119 (5%) 28 23	24, 53, 91, 121	0

The worst 5 of 119 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	131	LEU	6.3
1	F	261	LEU	6.3
1	F	267	TYR	5.4
1	F	405	VAL	5.3
1	E	209	ASP	5.3

### 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

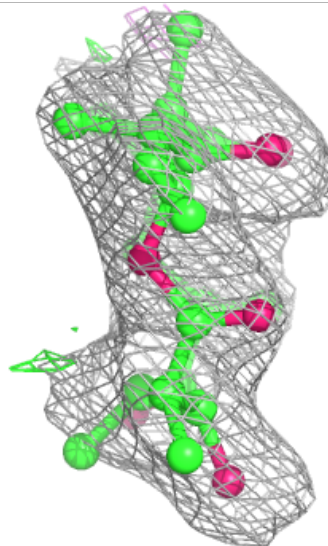
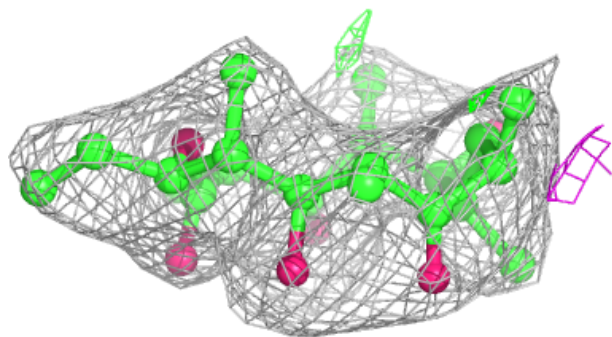
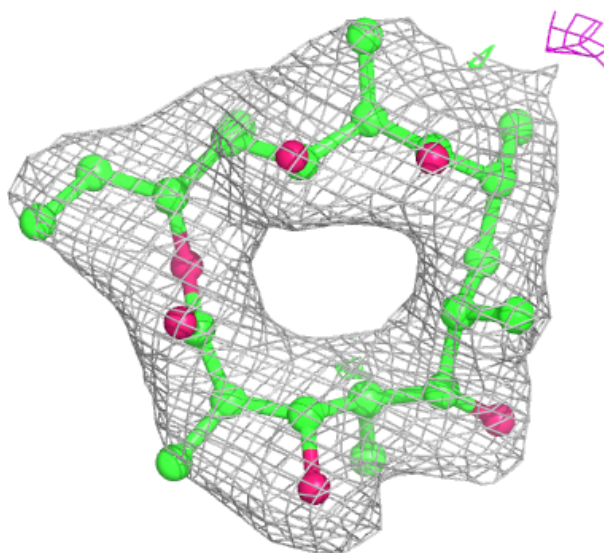
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	DEB	D	502	27/27	0.94	0.19	39,43,47,50	0
2	HEM	F	501	43/43	0.95	0.16	50,70,76,84	0
3	DEB	E	502	27/27	0.95	0.16	40,43,45,45	0
3	DEB	F	502	27/27	0.95	0.17	54,58,61,61	0
2	HEM	E	501	43/43	0.96	0.11	39,44,50,60	0
2	HEM	A	501	43/43	0.96	0.14	24,26,29,34	0
3	DEB	B	502	27/27	0.96	0.17	29,32,33,33	0
3	DEB	A	502	27/27	0.97	0.19	27,28,29,30	0
2	HEM	D	501	43/43	0.97	0.17	22,24,36,44	0
3	DEB	C	502	27/27	0.97	0.16	25,28,31,32	0
2	HEM	C	501	43/43	0.98	0.16	23,25,29,36	0
2	HEM	B	501	43/43	0.98	0.17	20,22,26,29	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 DEB D 502:**

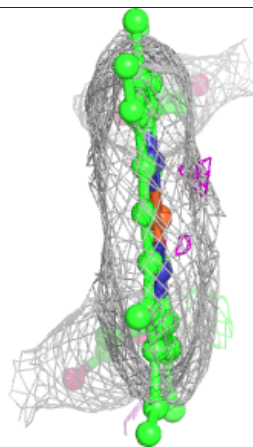
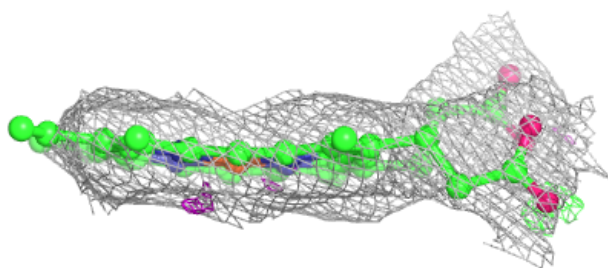
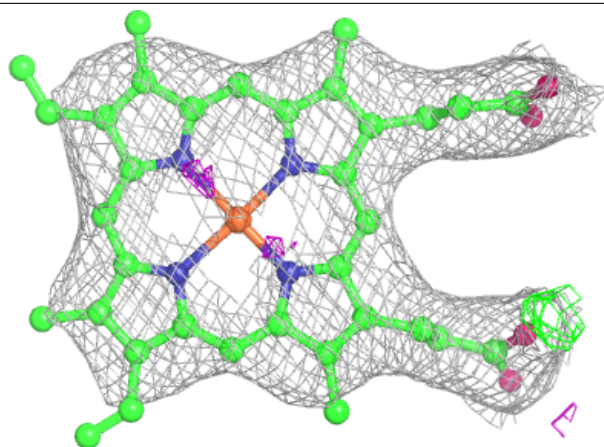
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





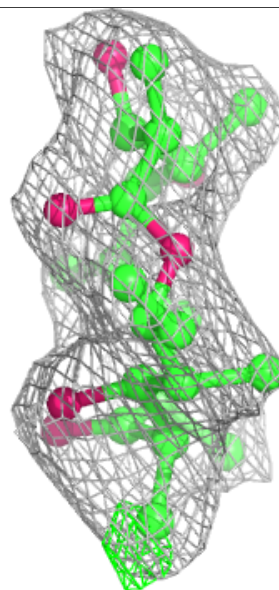
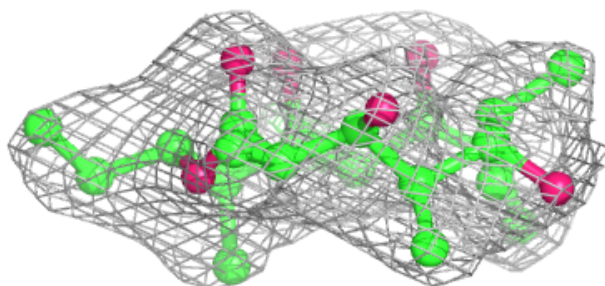
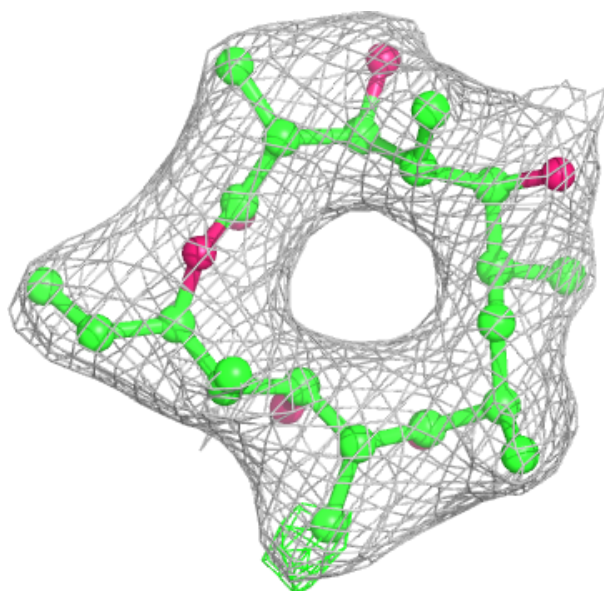
**Electron density around HEM F 501:**

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



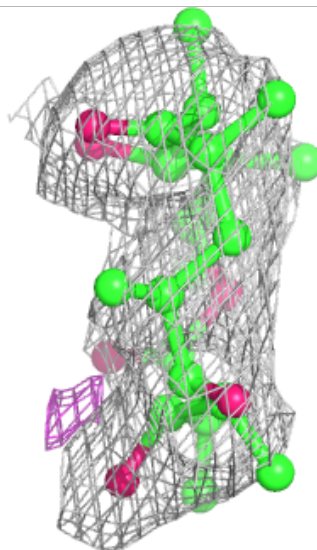
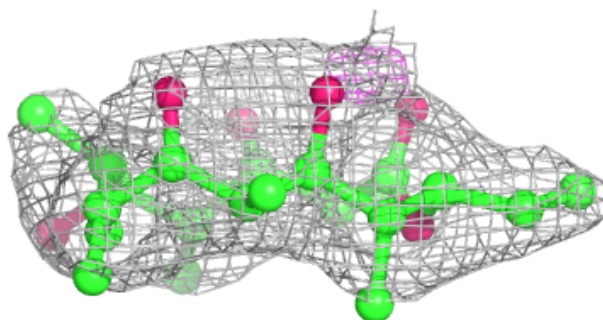
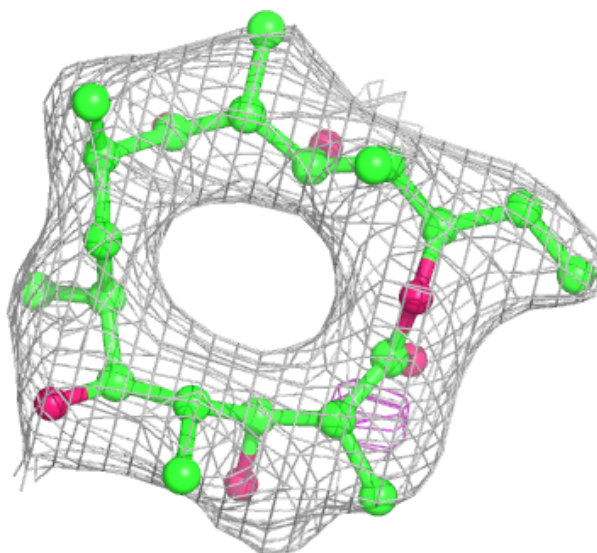
**Electron density around DEB E 502:**

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



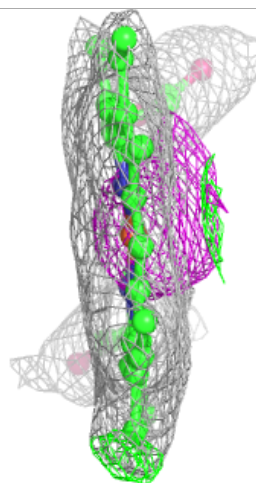
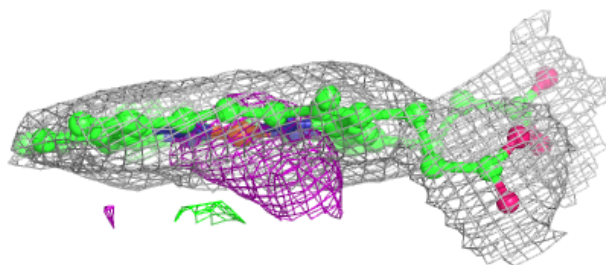
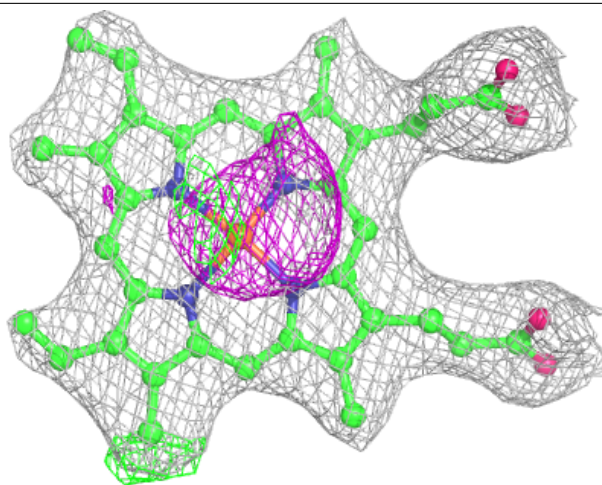
**Electron density around DEB F 502:**

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



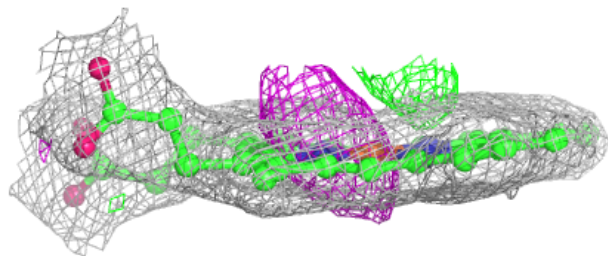
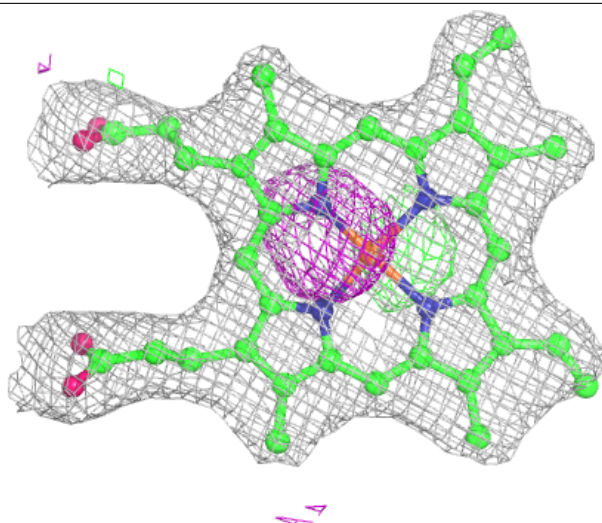
**Electron density around HEM E 501:**

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



**Electron density around HEM A 501:**

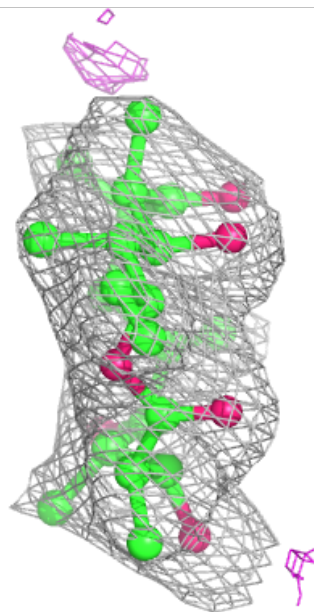
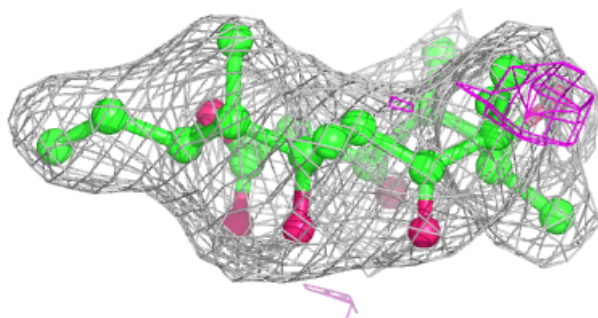
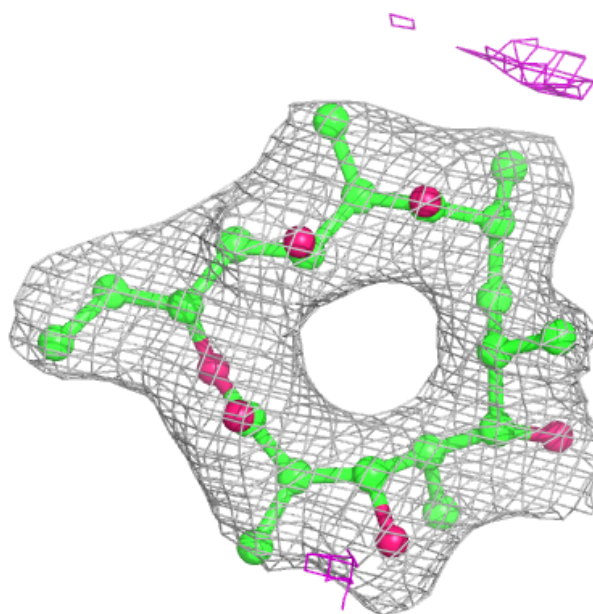
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





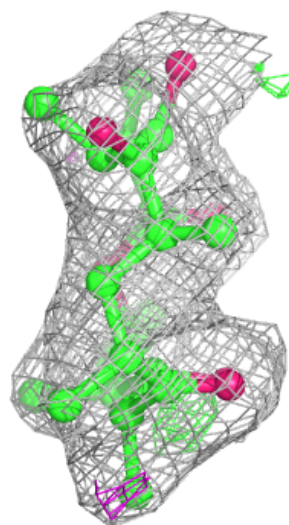
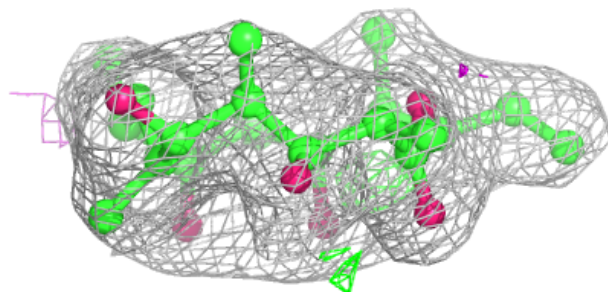
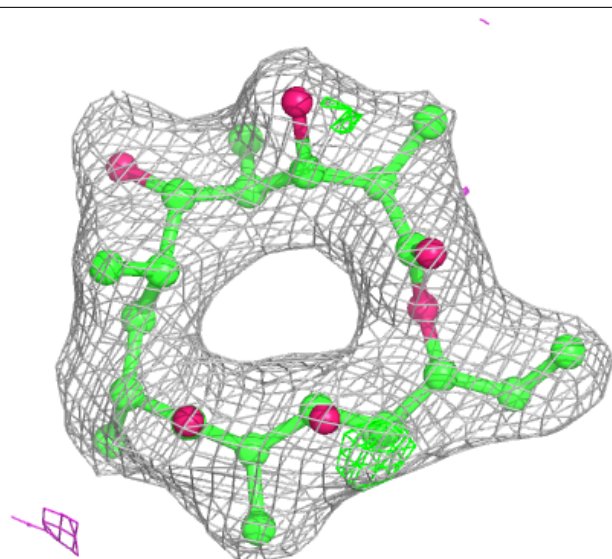
**Electron density around DEB B 502:**

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



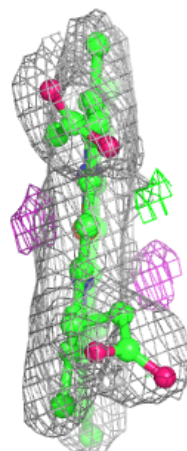
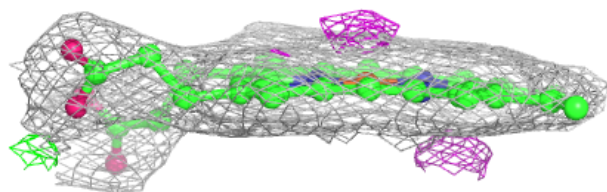
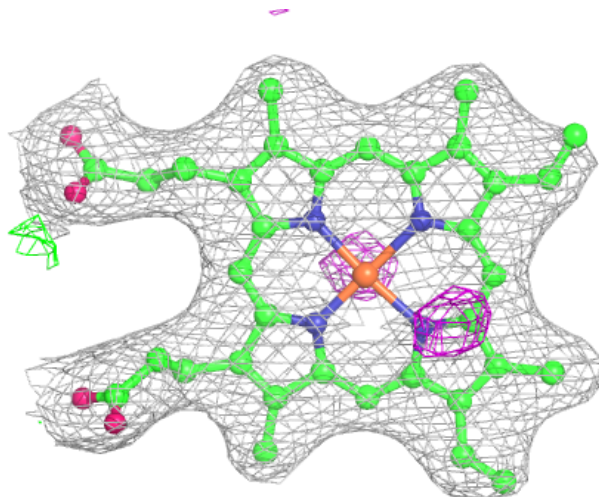
**Electron density around DEB A 502:**

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



**Electron density around HEM D 501:**

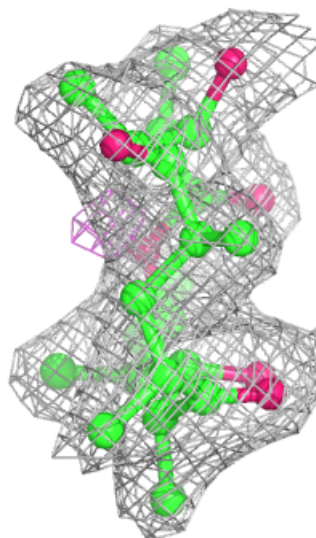
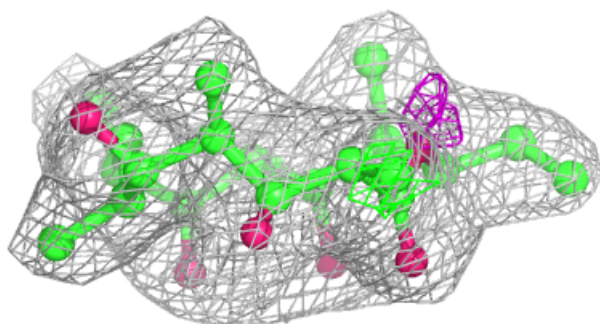
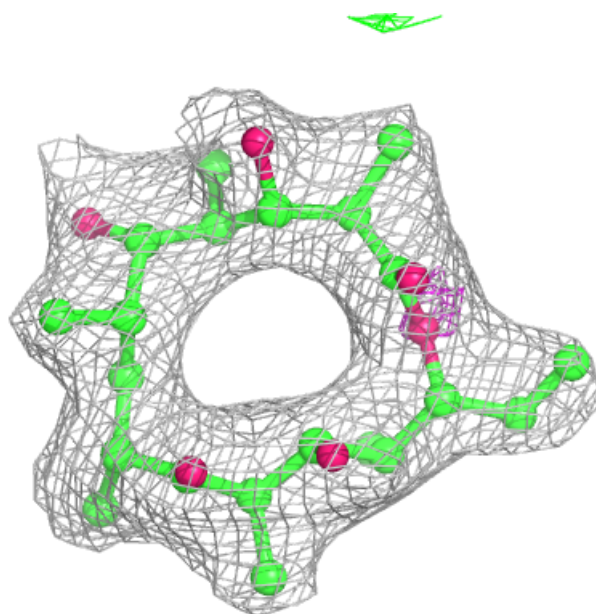
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





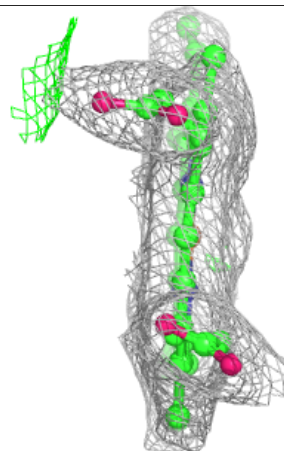
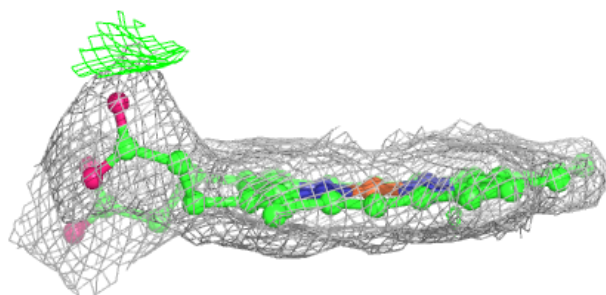
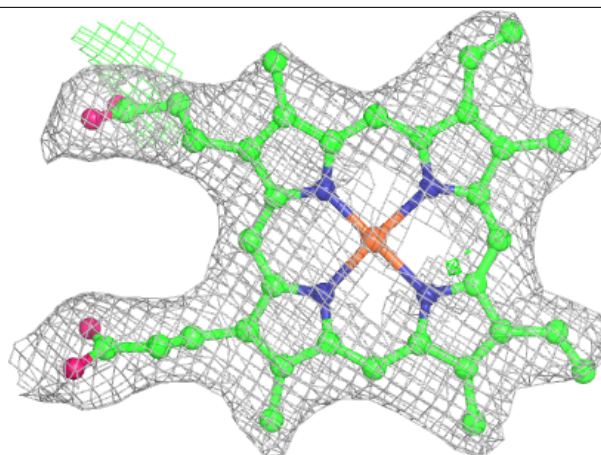
**Electron density around DEB C 502:**

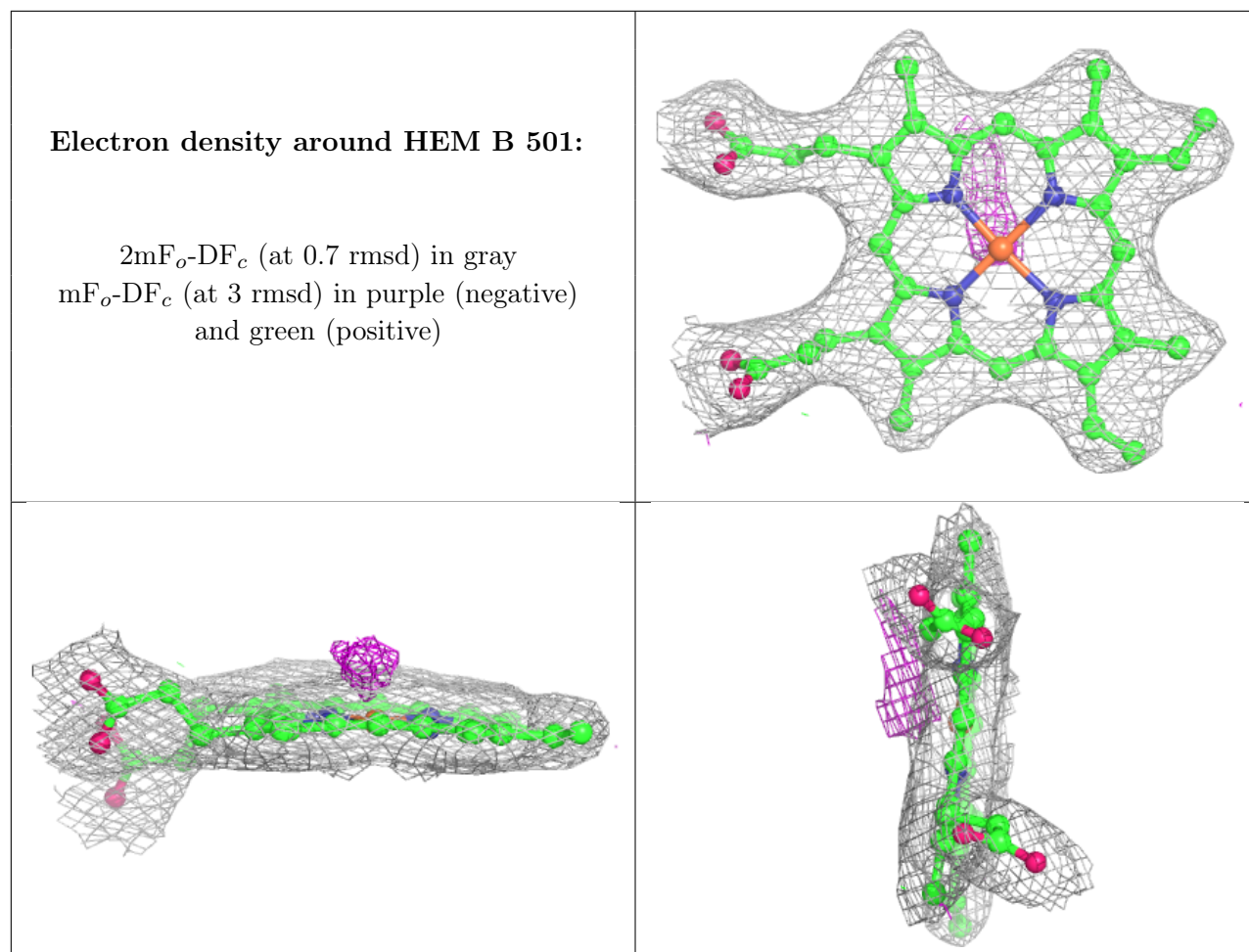
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEM C 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.