



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 16, 2020 – 03:16 pm BST

PDB ID : 6DWM  
Title : Structure of Human Cytochrome P450 1A1 with Bergamottin  
Authors : Bart, A.G.; Scott, E.E.  
Deposited on : 2018-06-26  
Resolution : 2.85 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 : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

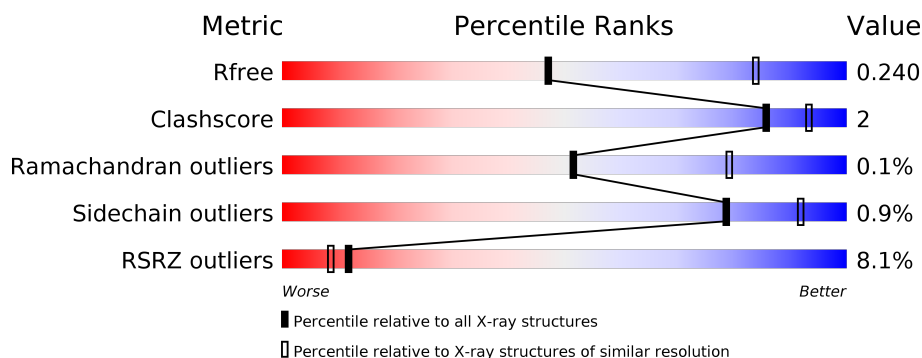
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.85 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	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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	491	<div> <div>4%</div> <div>89%</div> <div>6%</div> <div>•</div> </div>
1	B	491	<div> <div>5%</div> <div>92%</div> <div>5%</div> <div>•</div> </div>
1	C	491	<div> <div>10%</div> <div>90%</div> <div>5%</div> <div>5%</div> </div>
1	D	491	<div> <div>12%</div> <div>91%</div> <div>•</div> <div>5%</div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 30704 atoms, of which 15307 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 P450 1A1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	470	Total	C	H	N	O	S	0	0	0
			7533	2412	3770	655	675	21			
1	B	476	Total	C	H	N	O	S	0	0	0
			7620	2440	3808	663	688	21			
1	C	464	Total	C	H	N	O	S	0	0	0
			7426	2381	3710	646	668	21			
1	D	464	Total	C	H	N	O	S	0	0	0
			7424	2381	3709	645	668	21			

There are 52 discrepancies between the modelled and reference sequences:

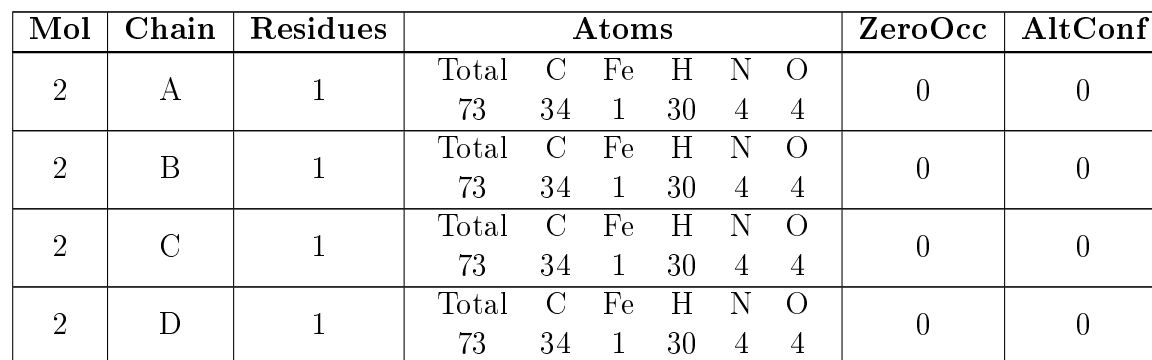
Chain	Residue	Modelled	Actual	Comment	Reference
A	28	MET	-	expression tag	UNP P04798
A	29	ALA	-	expression tag	UNP P04798
A	30	LYS	-	expression tag	UNP P04798
A	31	LYS	-	expression tag	UNP P04798
A	32	THR	-	expression tag	UNP P04798
A	33	SER	-	expression tag	UNP P04798
A	34	SER	-	expression tag	UNP P04798
A	513	HIS	-	expression tag	UNP P04798
A	514	HIS	-	expression tag	UNP P04798
A	515	HIS	-	expression tag	UNP P04798
A	516	HIS	-	expression tag	UNP P04798
A	517	HIS	-	expression tag	UNP P04798
A	518	HIS	-	expression tag	UNP P04798
B	28	MET	-	expression tag	UNP P04798
B	29	ALA	-	expression tag	UNP P04798
B	30	LYS	-	expression tag	UNP P04798
B	31	LYS	-	expression tag	UNP P04798
B	32	THR	-	expression tag	UNP P04798
B	33	SER	-	expression tag	UNP P04798
B	34	SER	-	expression tag	UNP P04798
B	513	HIS	-	expression tag	UNP P04798

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	514	HIS	-	expression tag	UNP P04798
B	515	HIS	-	expression tag	UNP P04798
B	516	HIS	-	expression tag	UNP P04798
B	517	HIS	-	expression tag	UNP P04798
B	518	HIS	-	expression tag	UNP P04798
C	28	MET	-	expression tag	UNP P04798
C	29	ALA	-	expression tag	UNP P04798
C	30	LYS	-	expression tag	UNP P04798
C	31	LYS	-	expression tag	UNP P04798
C	32	THR	-	expression tag	UNP P04798
C	33	SER	-	expression tag	UNP P04798
C	34	SER	-	expression tag	UNP P04798
C	513	HIS	-	expression tag	UNP P04798
C	514	HIS	-	expression tag	UNP P04798
C	515	HIS	-	expression tag	UNP P04798
C	516	HIS	-	expression tag	UNP P04798
C	517	HIS	-	expression tag	UNP P04798
C	518	HIS	-	expression tag	UNP P04798
D	28	MET	-	expression tag	UNP P04798
D	29	ALA	-	expression tag	UNP P04798
D	30	LYS	-	expression tag	UNP P04798
D	31	LYS	-	expression tag	UNP P04798
D	32	THR	-	expression tag	UNP P04798
D	33	SER	-	expression tag	UNP P04798
D	34	SER	-	expression tag	UNP P04798
D	513	HIS	-	expression tag	UNP P04798
D	514	HIS	-	expression tag	UNP P04798
D	515	HIS	-	expression tag	UNP P04798
D	516	HIS	-	expression tag	UNP P04798
D	517	HIS	-	expression tag	UNP P04798
D	518	HIS	-	expression tag	UNP P04798

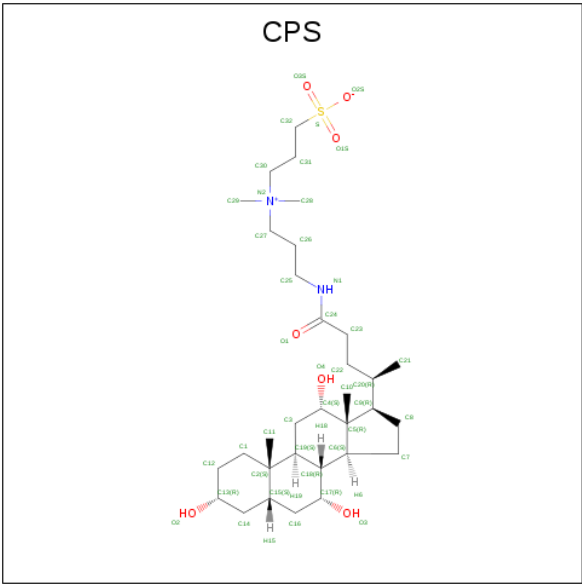
- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



- # HJJ
- 
- ORTEP diagram of the chemical structure, showing thermal ellipsoids at the 50% probability level. The structure is labeled with atom identifiers (O15, O16, C18, O23, C22, C14, C17, C19, C21, C13, C12, C11, C10, C09, C08, C07, C06, C05, C04, C03, C02, C01, C25).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			47	21	22	4		
3	B	1	Total	C	H	O	0	0
			47	21	22	4		
3	C	1	Total	C	H	O	0	0
			47	21	22	4		
3	D	1	Total	C	H	O	0	0
			47	21	22	4		

- Molecule 4 is 3-[(3-CHOLAMIDOPROPYL)DIMETHYLAMMONIO]-1-PROPANESULFO NATE (three-letter code: CPS) (formula: C<sub>32</sub>H<sub>58</sub>N<sub>2</sub>O<sub>7</sub>S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	0
			75	26	44	1	4	
4	D	1	Total	C	H	N	O	0
			72	25	42	1	4	

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	H	O	0	0
			14	3	8	3		
5	D	1	Total	C	H	O	0	0
			14	3	8	3		

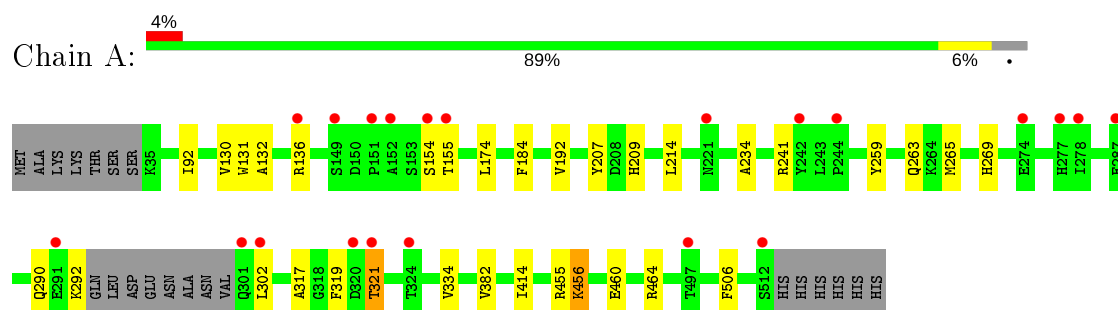
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	19	Total	O	0	0
			19	19		
6	B	27	Total	O	0	0
			27	27		

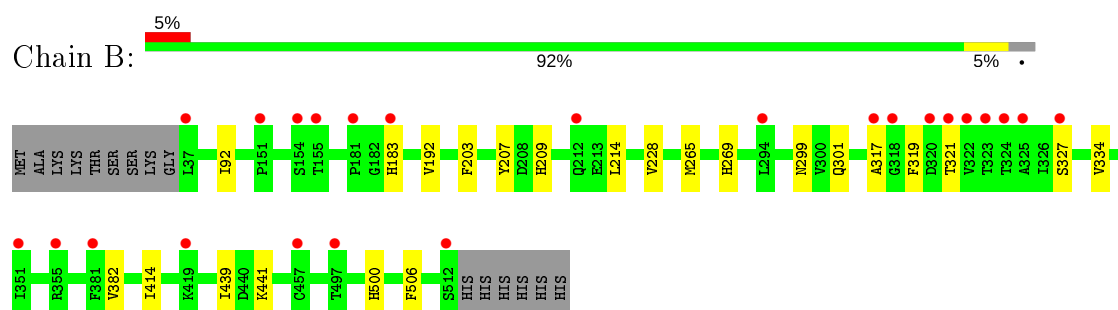
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

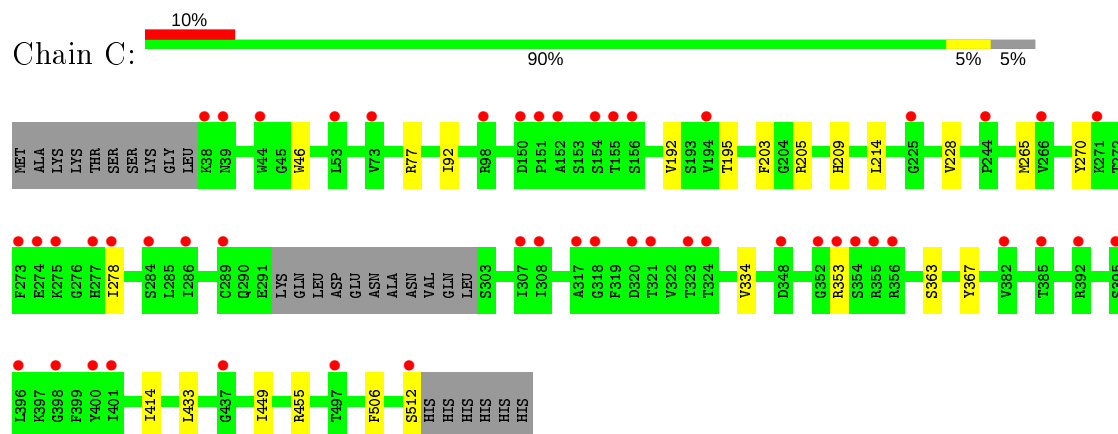
#### • Molecule 1: Cytochrome P450 1A1



#### • Molecule 1: Cytochrome P450 1A1

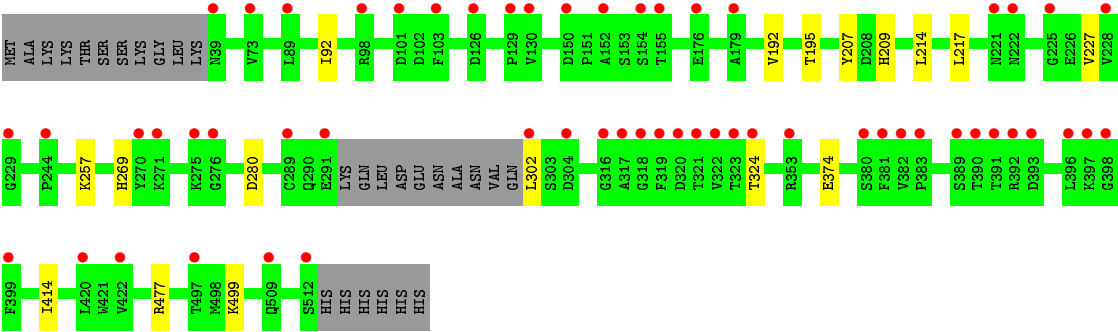
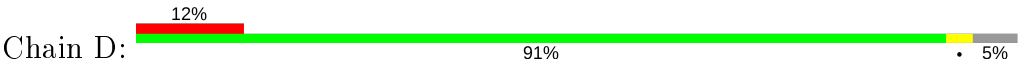


#### • Molecule 1: Cytochrome P450 1A1



#### • Molecule 1: Cytochrome P450 1A1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.33Å 194.76Å 236.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.36 – 2.85 39.36 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.4 (39.36-2.85) 93.9 (39.36-2.85)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.53 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.13 _2998	Depositor
R, $R_{free}$	0.204 , 0.240 0.204 , 0.240	Depositor DCC
$R_{free}$ test set	2000 reflections (2.80%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	65.8	Xtriage
Anisotropy	0.206	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 42.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	30704	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% 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: GOL, CPS, HEM, HJJ

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	0.29	0/3857	0.46	0/5223
1	B	0.30	0/3907	0.47	0/5295
1	C	0.27	0/3810	0.42	0/5162
1	D	0.27	0/3809	0.43	0/5162
All	All	0.28	0/15383	0.45	0/20842

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [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	3763	3770	3766	16	0
1	B	3812	3808	3806	15	0
1	C	3716	3710	3708	11	0
1	D	3715	3709	3705	8	0
2	A	43	30	30	5	0
2	B	43	30	30	7	0
2	C	43	30	30	5	0
2	D	43	30	30	4	0
3	A	25	22	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	25	22	0	0	0
3	C	25	22	0	0	0
3	D	25	22	0	0	0
4	A	31	44	42	0	0
4	D	30	42	40	1	0
5	B	6	8	8	0	0
5	D	6	8	8	0	0
6	A	19	0	0	0	0
6	B	27	0	0	0	0
All	All	15397	15307	15203	67	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 2.

The worst 5 of 67 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:ALA:O	1:A:136:ARG:HG3	1.91	0.70
1:A:292:LYS:NZ	1:A:302:LEU:O	2.19	0.70
2:B:601:HEM:HBC2	2:B:601:HEM:HMC2	1.74	0.69
1:D:92:ILE:HD12	1:D:414:ILE:HD11	1.74	0.69
2:D:601:HEM:HMC2	2:D:601:HEM:HBC2	1.74	0.68

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	466/491 (95%)	453 (97%)	13 (3%)	0	100	100
1	B	474/491 (96%)	462 (98%)	12 (2%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	460/491 (94%)	449 (98%)	10 (2%)	1 (0%)	47	75
1	D	460/491 (94%)	448 (97%)	12 (3%)	0	100	100
All	All	1860/1964 (95%)	1812 (97%)	47 (2%)	1 (0%)	51	79

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	449	ILE

### 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	420/439 (96%)	413 (98%)	7 (2%)	60	83
1	B	426/439 (97%)	424 (100%)	2 (0%)	88	96
1	C	415/439 (94%)	412 (99%)	3 (1%)	84	94
1	D	415/439 (94%)	412 (99%)	3 (1%)	84	94
All	All	1676/1756 (95%)	1661 (99%)	15 (1%)	78	92

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	456	LYS
1	B	183	HIS
1	D	227	VAL
1	A	321	THR
1	C	363	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	255	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	255	ASN
1	C	255	ASN
1	D	99	GLN
1	D	255	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates [i](#)

There are no carbohydrates 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	$\# Z  > 2$
5	GOL	D	604	-	5,5,5	0.82	0	5,5,5	0.97	0
2	HEM	D	601	-	27,50,50	1.87	5 (18%)	17,82,82	1.40	3 (17%)
3	HJJ	D	602	-	21,27,27	2.64	10 (47%)	27,37,37	1.91	6 (22%)
5	GOL	B	603	-	5,5,5	0.95	0	5,5,5	1.08	0
3	HJJ	B	602	-	21,27,27	2.24	7 (33%)	27,37,37	1.94	8 (29%)
3	HJJ	C	602	-	21,27,27	2.65	10 (47%)	27,37,37	1.89	7 (25%)
3	HJJ	A	602	-	21,27,27	2.56	7 (33%)	27,37,37	2.00	8 (29%)
4	CPS	A	603	-	34,34,45	1.05	3 (8%)	52,53,70	2.02	16 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	HEM	C	601	-	27,50,50	1.85	4 (14%)	17,82,82	1.63	3 (17%)
2	HEM	A	601	1	27,50,50	1.87	4 (14%)	17,82,82	1.56	5 (29%)
4	CPS	D	603	-	33,33,45	1.11	3 (9%)	52,52,70	2.16	17 (32%)
2	HEM	B	601	1	27,50,50	1.85	4 (14%)	17,82,82	1.49	4 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	D	604	-	-	1/4/4/4	-
2	HEM	D	601	-	-	0/6/54/54	-
3	HJJ	D	602	-	-	6/12/12/12	0/3/3/3
5	GOL	B	603	-	-	1/4/4/4	-
3	HJJ	B	602	-	-	5/12/12/12	0/3/3/3
3	HJJ	C	602	-	-	2/12/12/12	0/3/3/3
3	HJJ	A	602	-	-	2/12/12/12	0/3/3/3
4	CPS	A	603	-	-	2/12/77/90	0/4/4/4
2	HEM	C	601	-	-	0/6/54/54	-
2	HEM	A	601	1	-	0/6/54/54	-
4	CPS	D	603	-	-	2/11/76/90	0/4/4/4
2	HEM	B	601	1	-	0/6/54/54	-

The worst 5 of 57 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	602	HJJ	C12-C11	5.09	1.52	1.42
3	A	602	HJJ	C12-C11	4.90	1.52	1.42
3	A	602	HJJ	O16-C17	4.86	1.44	1.36
3	A	602	HJJ	C18-C17	4.68	1.46	1.37
3	C	602	HJJ	C18-C17	4.67	1.46	1.37

The worst 5 of 77 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	603	CPS	C5-C9-C20	-5.96	112.38	119.50
4	D	603	CPS	C5-C9-C20	-5.93	112.42	119.50
3	A	602	HJJ	O16-C17-C18	5.49	122.54	116.03
3	C	602	HJJ	O16-C17-C18	5.14	122.13	116.03

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	603	CPS	C7-C6-C18	-5.10	111.20	118.33

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	HJJ	C20-C10-O09-C08
3	A	602	HJJ	C11-C10-O09-C08
4	D	603	CPS	C21-C20-C22-C23
4	D	603	CPS	C9-C20-C22-C23
3	D	602	HJJ	C04-C05-C06-C24

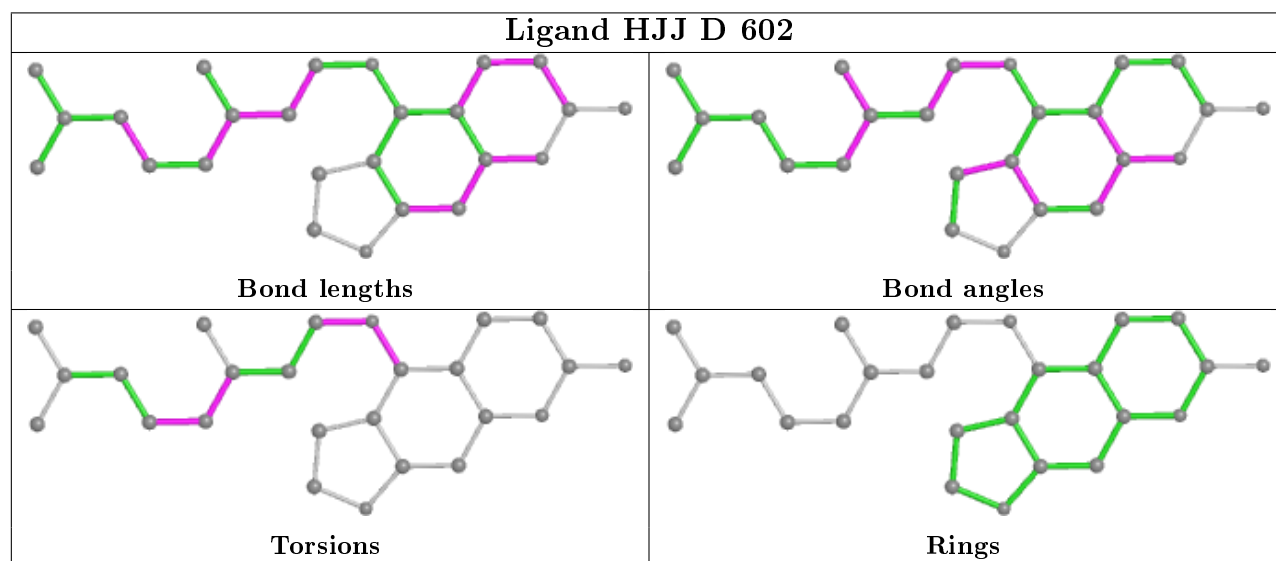
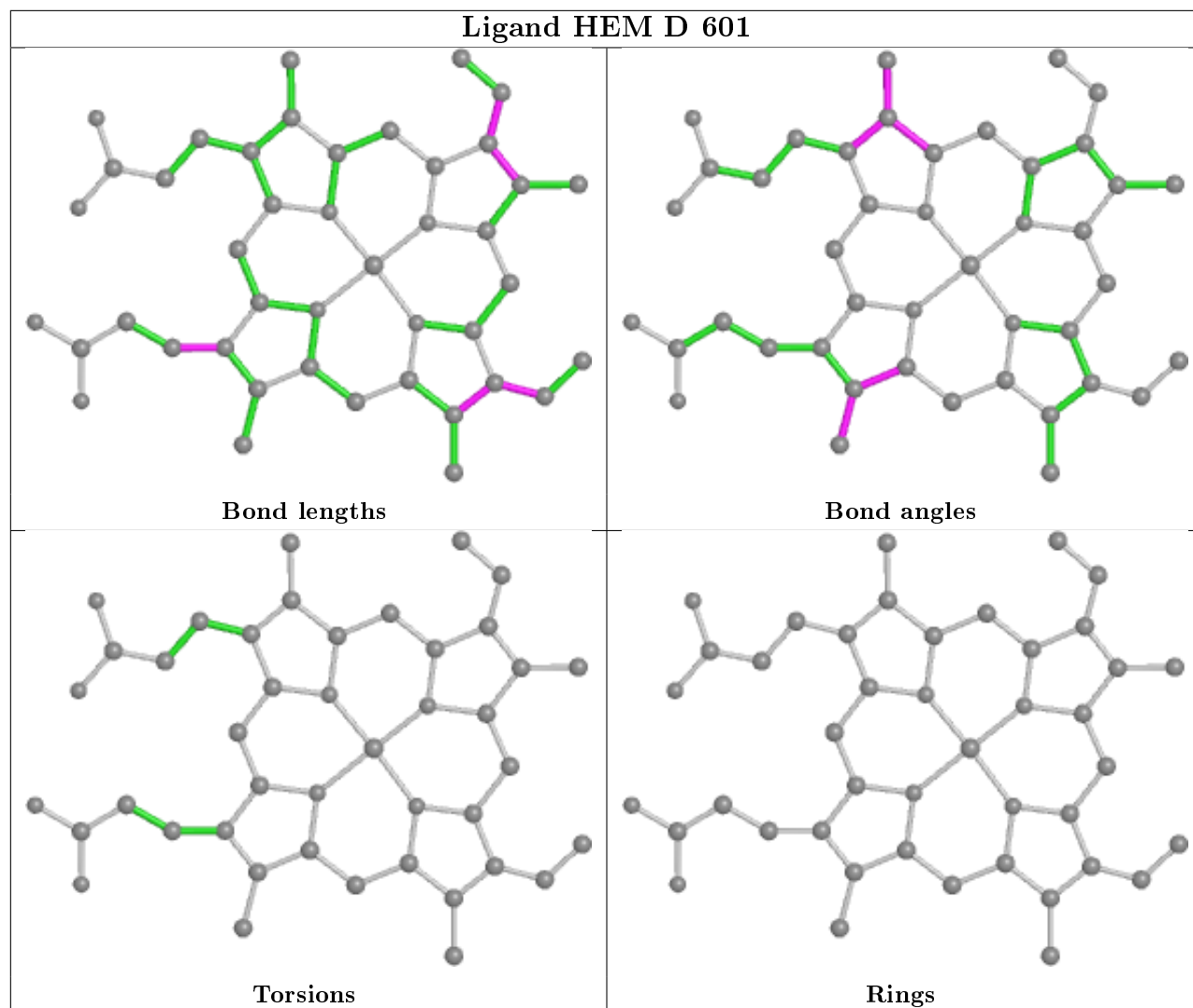
There are no ring outliers.

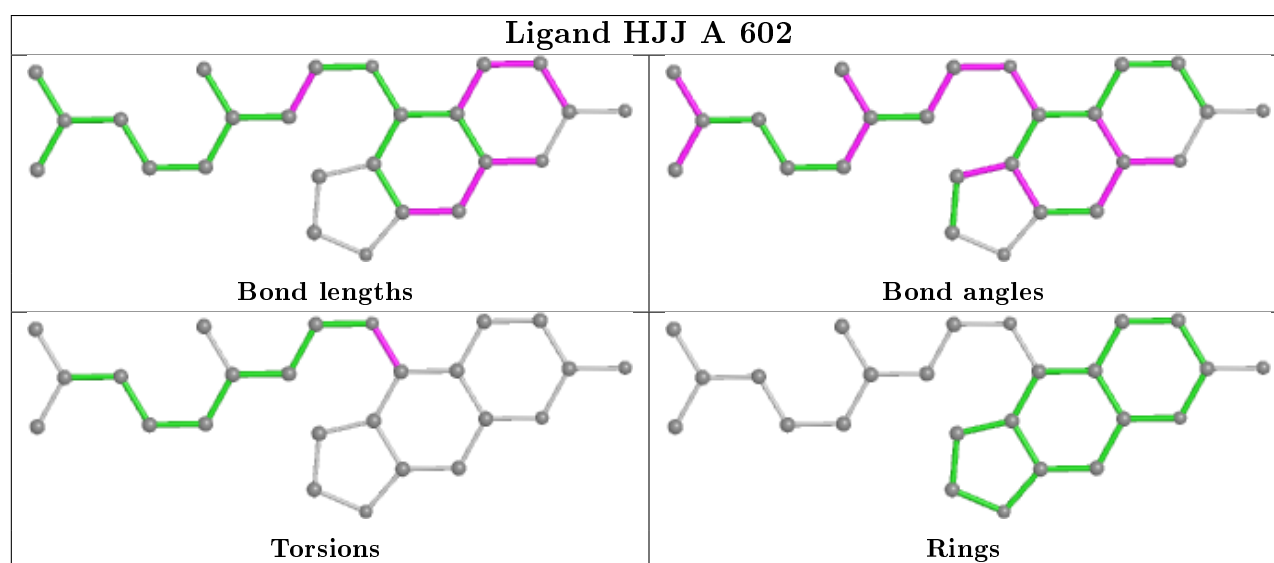
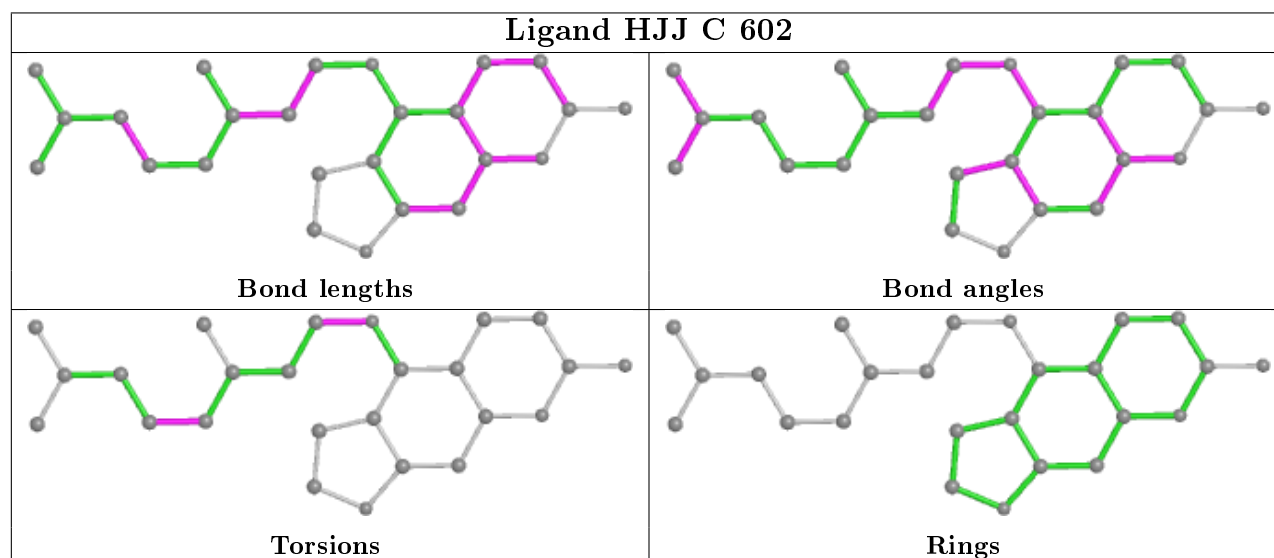
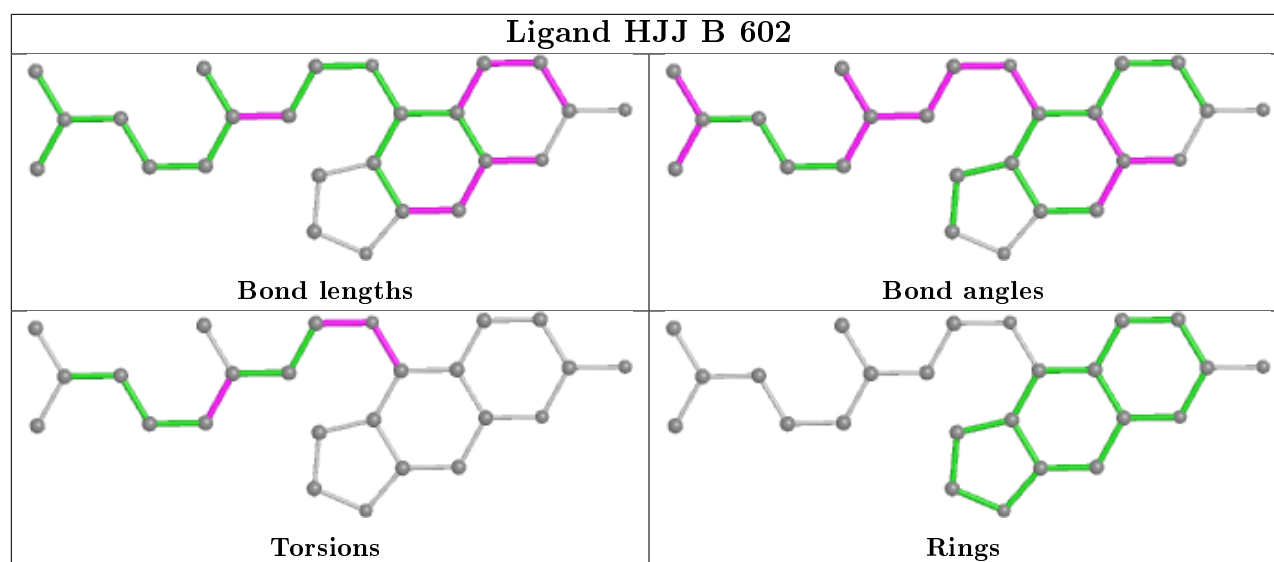
5 monomers are involved in 22 short contacts:

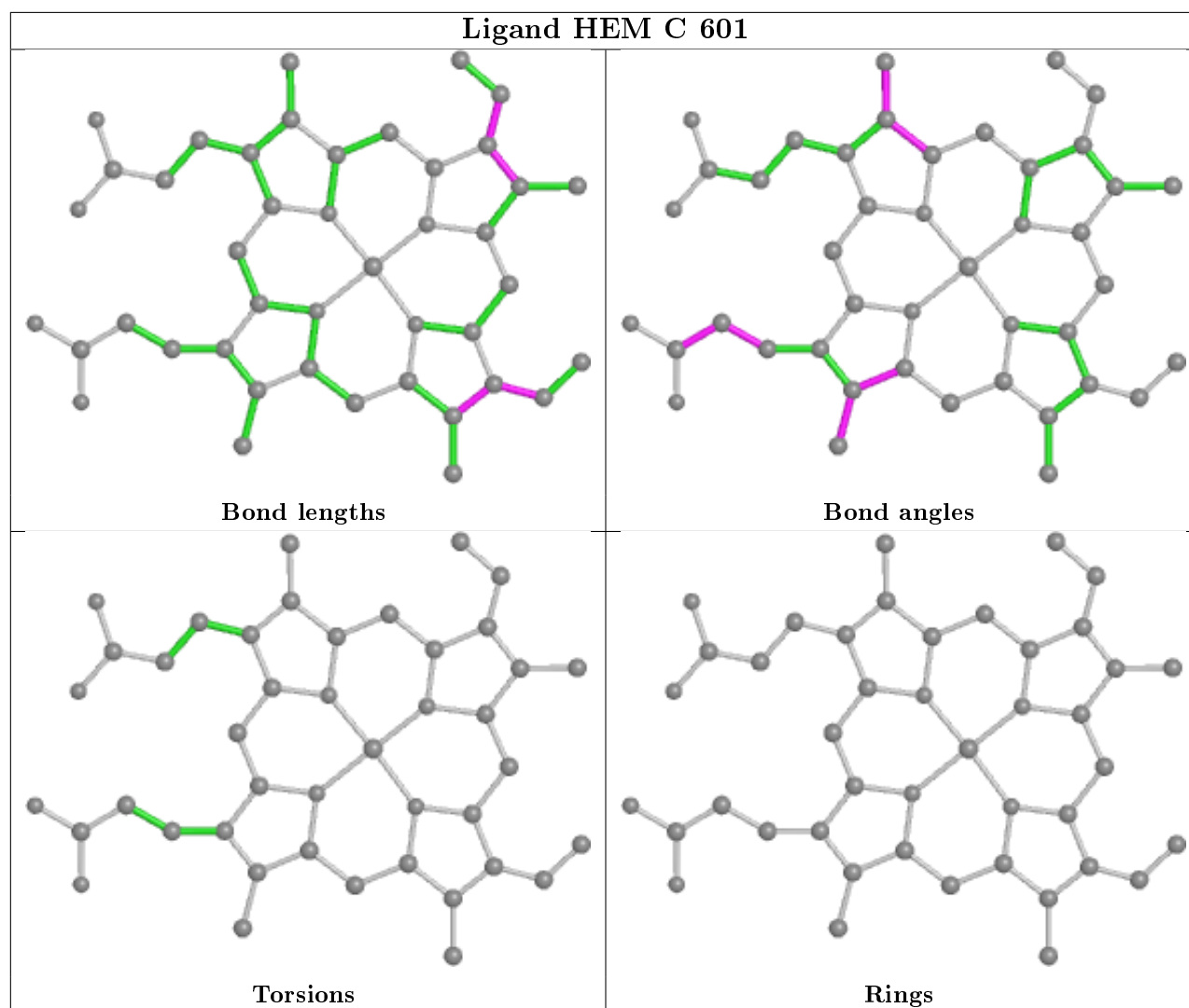
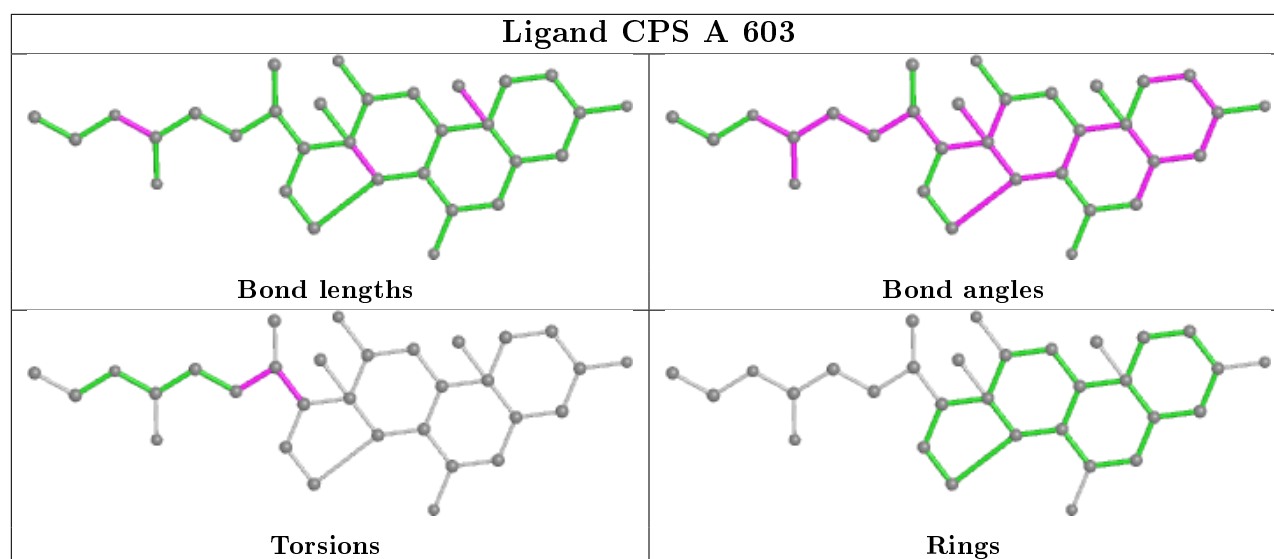
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	601	HEM	4	0
2	C	601	HEM	5	0
2	A	601	HEM	5	0
4	D	603	CPS	1	0
2	B	601	HEM	7	0

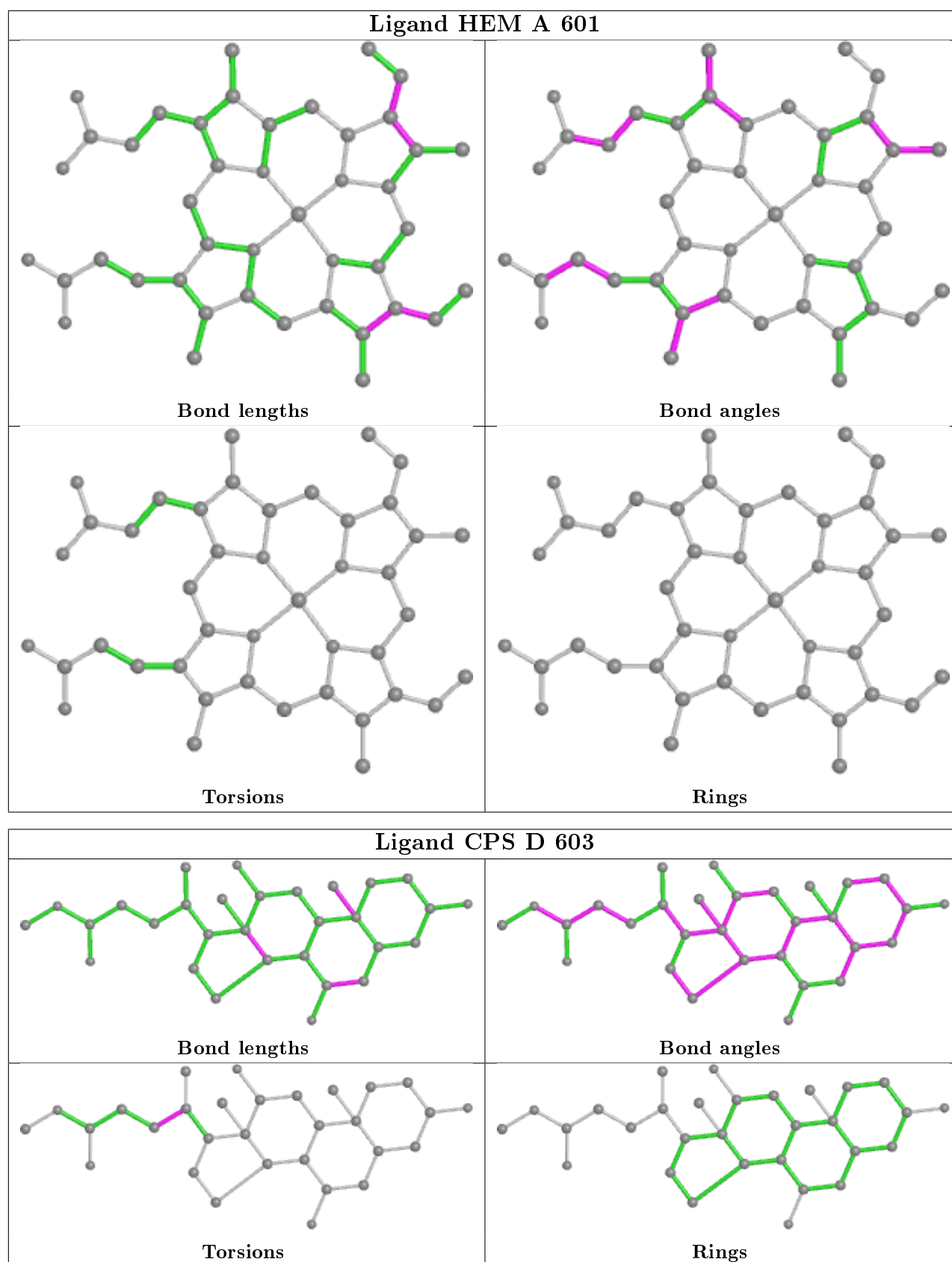
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

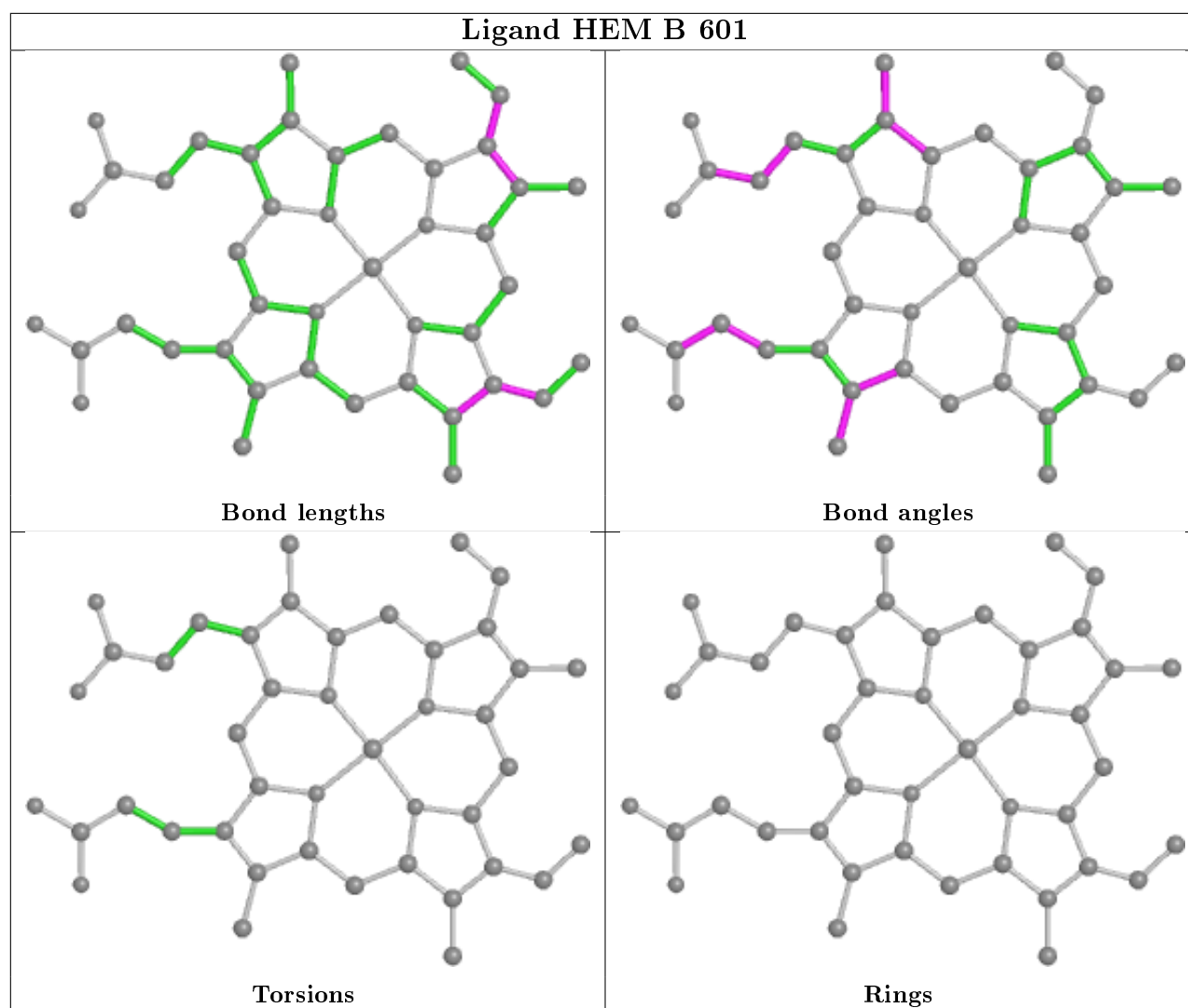












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [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	470/491 (95%)	0.30	21 (4%) 33 28	36, 62, 96, 126	0
1	B	476/491 (96%)	0.40	24 (5%) 28 24	37, 57, 92, 125	0
1	C	464/491 (94%)	0.84	50 (10%) 5 4	62, 91, 112, 135	0
1	D	464/491 (94%)	0.78	57 (12%) 4 2	56, 84, 111, 130	0
All	All	1874/1964 (95%)	0.58	152 (8%) 12 8	36, 75, 107, 135	0

The worst 5 of 152 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	277	HIS	5.1
1	D	244	PRO	4.9
1	A	155	THR	4.6
1	B	320	ASP	4.6
1	C	152	ALA	4.5

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

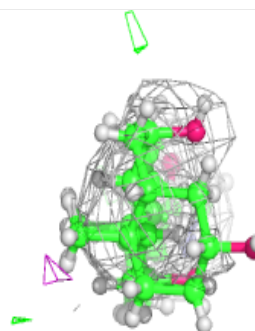
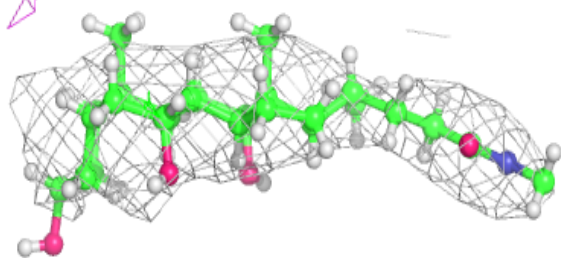
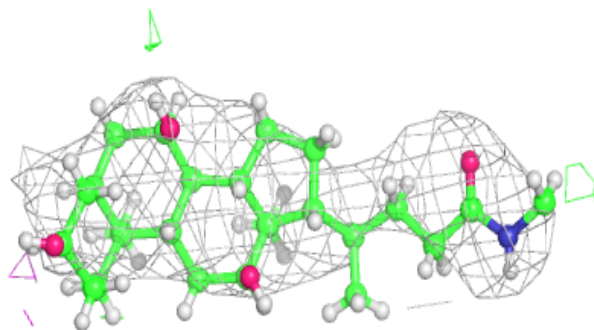
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	GOL	B	603	6/6	0.74	0.23	75,96,115,127	0
4	CPS	D	603	30/42	0.86	0.31	93,124,144,149	0
4	CPS	A	603	31/42	0.91	0.35	75,98,117,121	0
3	HJJ	D	602	25/25	0.92	0.38	64,82,101,113	0
3	HJJ	C	602	25/25	0.92	0.27	70,85,98,104	0
5	GOL	D	604	6/6	0.93	0.22	71,86,100,100	0
3	HJJ	A	602	25/25	0.93	0.29	45,61,69,76	0
2	HEM	D	601	43/43	0.94	0.39	50,65,81,86	0
3	HJJ	B	602	25/25	0.94	0.29	36,52,79,82	0
2	HEM	C	601	43/43	0.96	0.36	56,69,92,95	0
2	HEM	B	601	43/43	0.96	0.36	35,46,56,62	0
2	HEM	A	601	43/43	0.97	0.30	37,50,62,65	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.

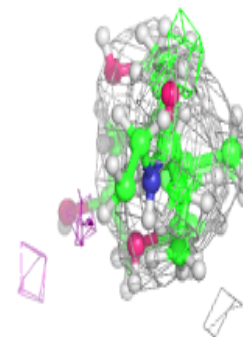
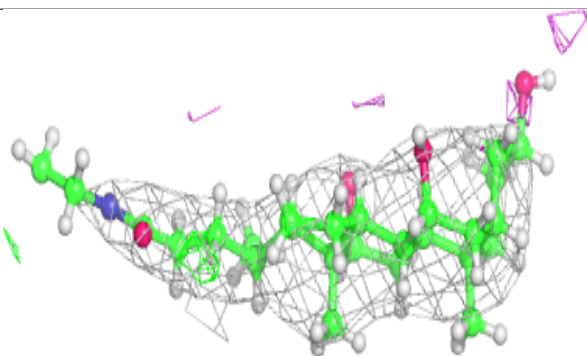
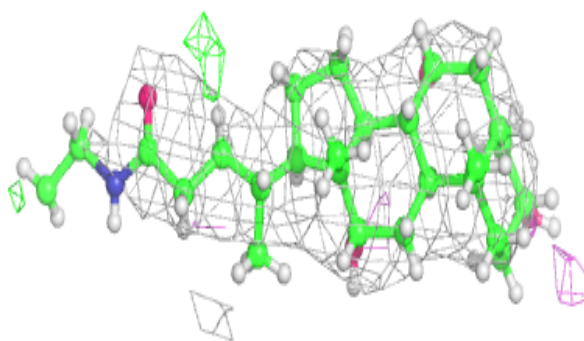
#### Electron density around CPS D 603:

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)

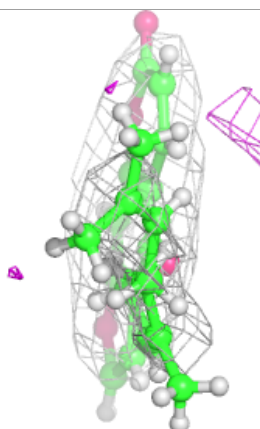
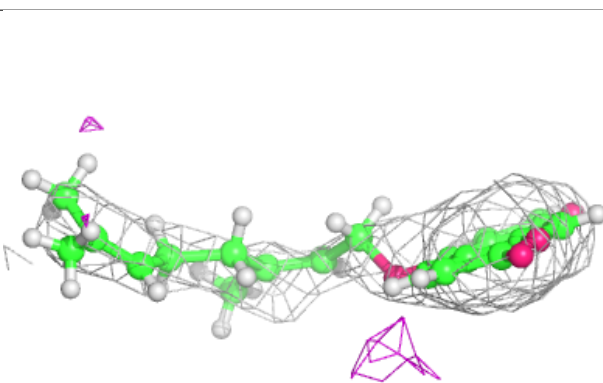
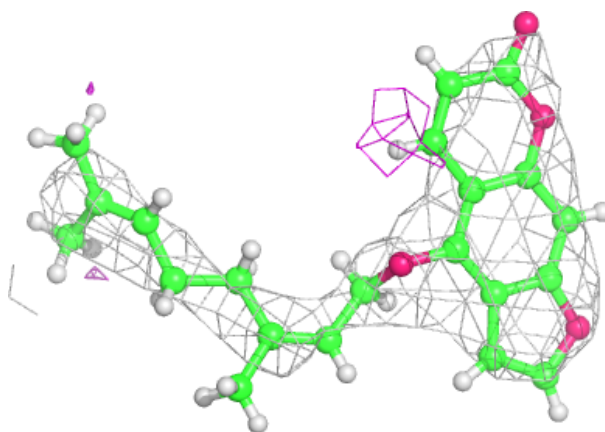


**Electron density around CPS A 603:**

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

**Electron density around HJJ D 602:**

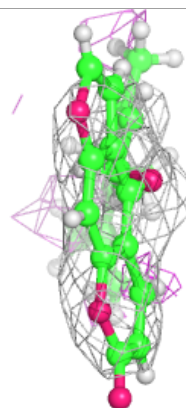
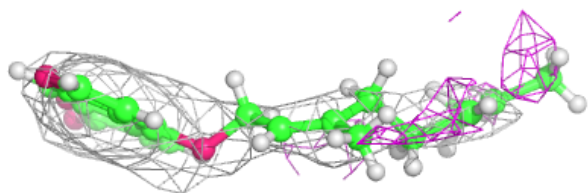
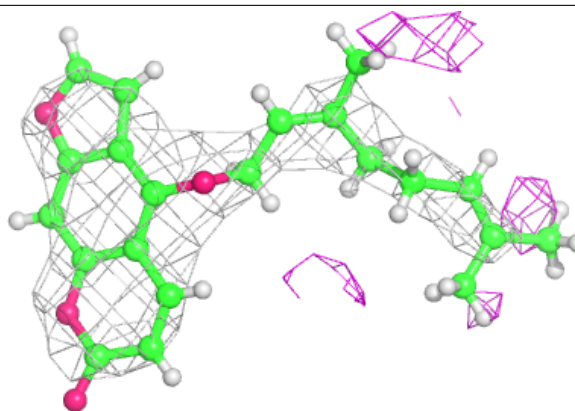
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





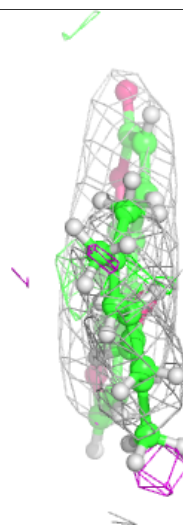
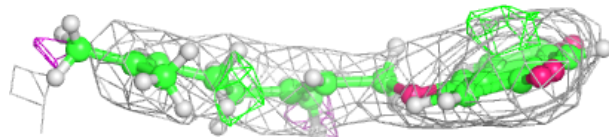
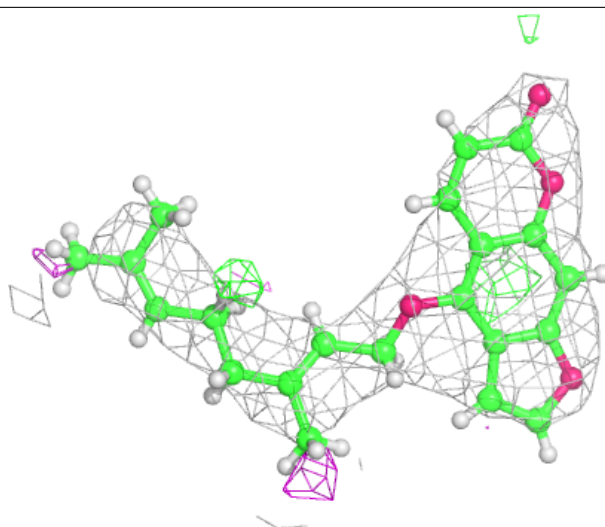
**Electron density around HJJ C 602:**

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



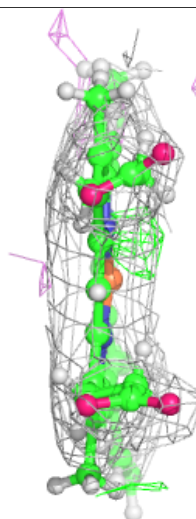
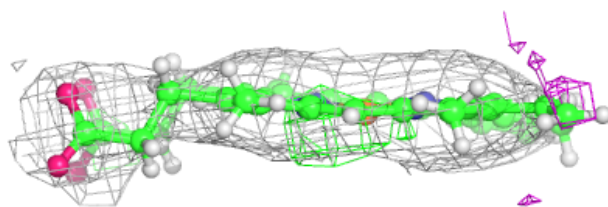
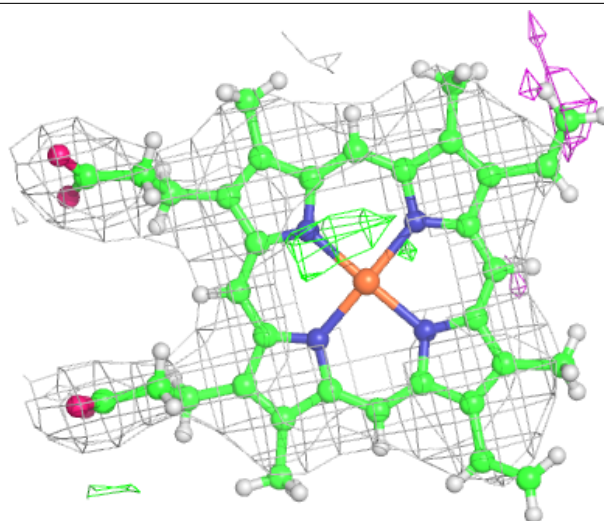
**Electron density around HJJ A 602:**

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



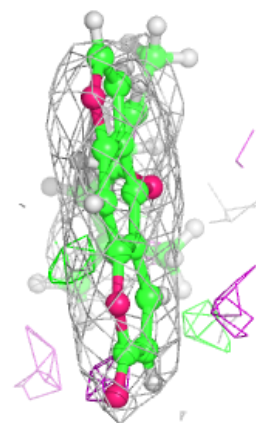
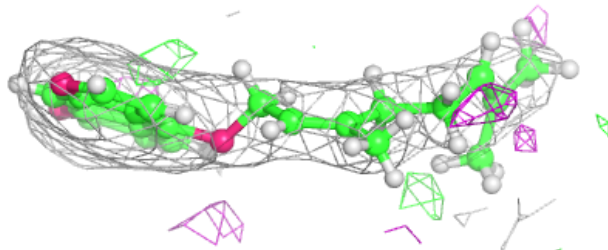
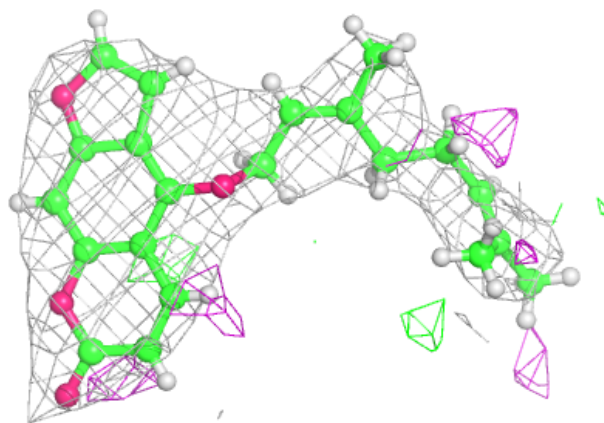
**Electron density around HEM D 601:**

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



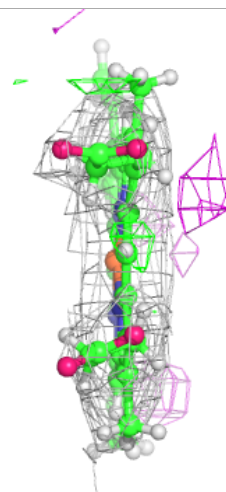
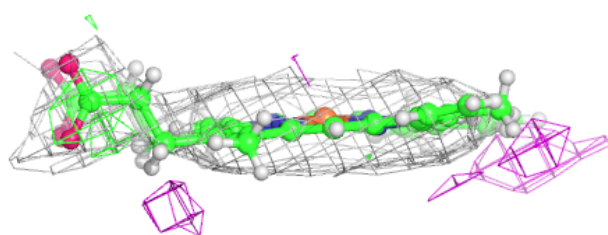
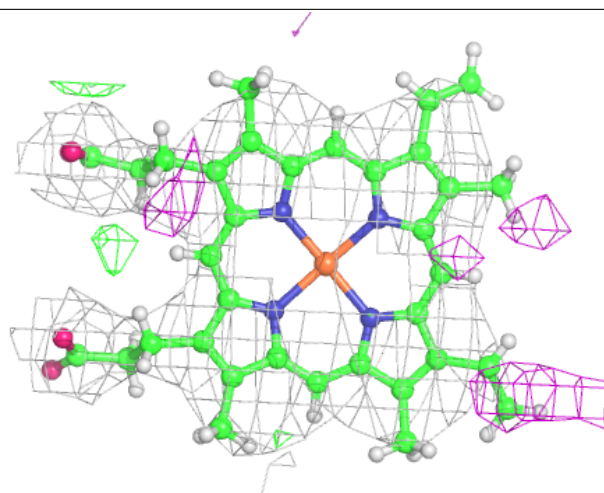
**Electron density around HJJ B 602:**

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



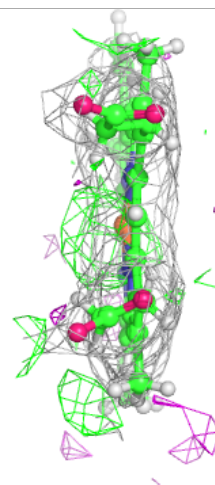
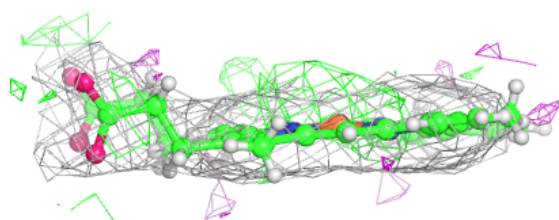
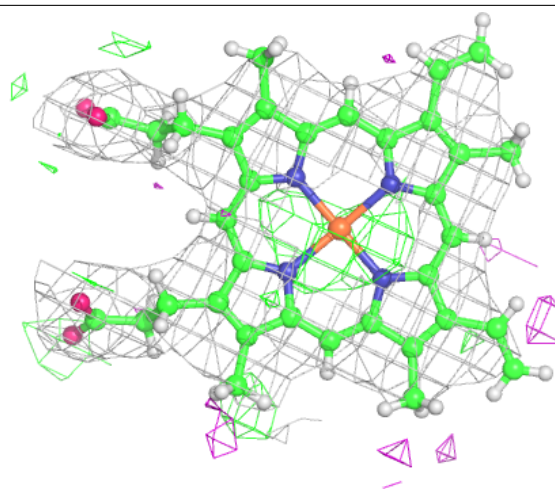
**Electron density around HEM C 601:**

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



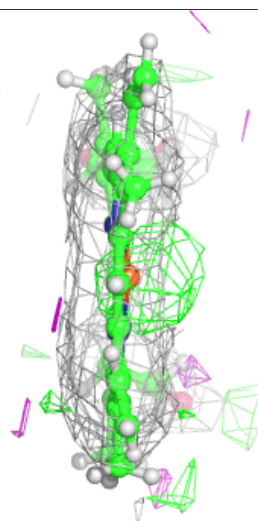
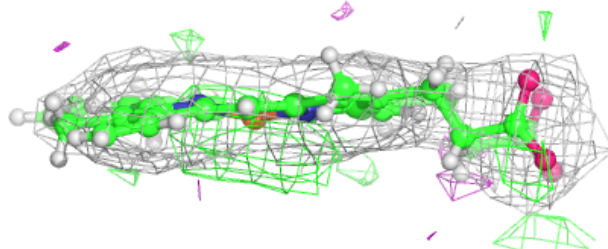
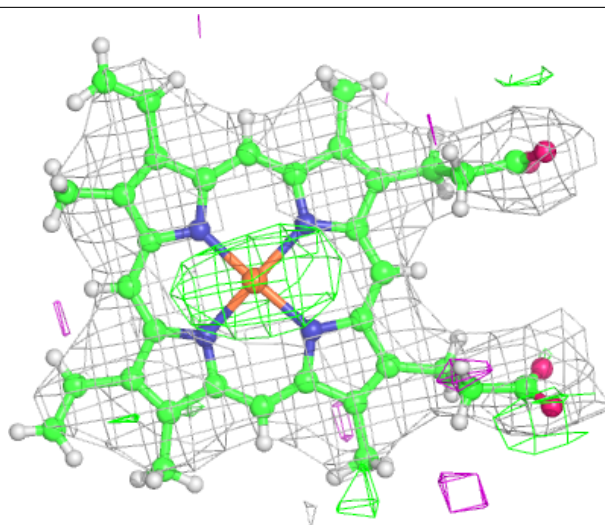
**Electron density around HEM B 601:**

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



**Electron density around HEM A 601:**

$2mF_o-DF_c$  (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.