



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 10, 2023 – 01:45 AM EDT

PDB ID : 7M8V
Title : Human CYP11B2 in complex with LCI699
Authors : Scott, E.E.; Brixius-Anderko, S.
Deposited on : 2021-03-30
Resolution : 3.08 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

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>.

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)
Xtrriage (Phenix) : 1.13
EDS : 2.35.1
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) : 2.35.1

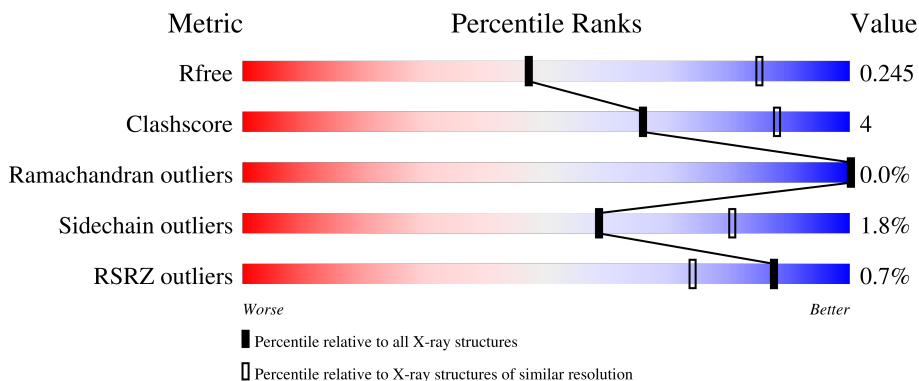
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.08 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	1447 (3.10-3.06)
Clashscore	141614	1546 (3.10-3.06)
Ramachandran outliers	138981	1487 (3.10-3.06)
Sidechain outliers	138945	1486 (3.10-3.06)
RSRZ outliers	127900	1416 (3.10-3.06)

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 ≥ 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	484	 82% 13% .
1	B	484	 84% 11% 5%
1	C	484	 85% 11% .
1	D	484	 83% 12% .
1	E	484	 86% 9% 5%

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Mol	Chain	Length	Quality of chain
1	F	484	 86% 9% 5%
1	G	484	 84% 10% 5%
1	H	484	 82% 13% 5%
1	I	484	 86% 10% 5%
1	J	484	 85% 10% 5%
1	K	484	 88% 8% 5%
1	L	484	 85% 9% 5%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 91890 atoms, of which 46055 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 11B2, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	464	7603	2443	3823	670	647	20	0	0	0
1	B	462	7560	2431	3799	665	645	20	0	0	0
1	C	465	7594	2441	3817	668	648	20	0	0	0
1	D	463	7562	2431	3801	666	644	20	0	0	0
1	E	461	7546	2426	3792	664	644	20	0	0	0
1	F	461	7546	2426	3792	664	644	20	0	0	0
1	G	461	7546	2427	3792	664	643	20	0	0	0
1	H	464	7578	2436	3807	667	648	20	0	0	0
1	I	462	7548	2427	3794	665	642	20	0	0	0
1	J	459	7521	2418	3782	662	639	20	0	0	0
1	K	464	7570	2435	3801	667	647	20	0	0	0
1	L	459	7510	2417	3775	659	639	20	0	0	0

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	MET	-	initiating methionine	UNP P19099
A	25	ALA	-	expression tag	UNP P19099
A	26	LYS	-	expression tag	UNP P19099
A	27	LYS	-	expression tag	UNP P19099
A	28	THR	-	expression tag	UNP P19099

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Chain	Residue	Modelled	Actual	Comment	Reference
A	29	SER	-	expression tag	UNP P19099
A	30	SER	-	expression tag	UNP P19099
A	504	HIS	-	expression tag	UNP P19099
A	505	HIS	-	expression tag	UNP P19099
A	506	HIS	-	expression tag	UNP P19099
A	507	HIS	-	expression tag	UNP P19099
B	24	MET	-	initiating methionine	UNP P19099
B	25	ALA	-	expression tag	UNP P19099
B	26	LYS	-	expression tag	UNP P19099
B	27	LYS	-	expression tag	UNP P19099
B	28	THR	-	expression tag	UNP P19099
B	29	SER	-	expression tag	UNP P19099
B	30	SER	-	expression tag	UNP P19099
B	504	HIS	-	expression tag	UNP P19099
B	505	HIS	-	expression tag	UNP P19099
B	506	HIS	-	expression tag	UNP P19099
B	507	HIS	-	expression tag	UNP P19099
C	24	MET	-	initiating methionine	UNP P19099
C	25	ALA	-	expression tag	UNP P19099
C	26	LYS	-	expression tag	UNP P19099
C	27	LYS	-	expression tag	UNP P19099
C	28	THR	-	expression tag	UNP P19099
C	29	SER	-	expression tag	UNP P19099
C	30	SER	-	expression tag	UNP P19099
C	504	HIS	-	expression tag	UNP P19099
C	505	HIS	-	expression tag	UNP P19099
C	506	HIS	-	expression tag	UNP P19099
C	507	HIS	-	expression tag	UNP P19099
D	24	MET	-	initiating methionine	UNP P19099
D	25	ALA	-	expression tag	UNP P19099
D	26	LYS	-	expression tag	UNP P19099
D	27	LYS	-	expression tag	UNP P19099
D	28	THR	-	expression tag	UNP P19099
D	29	SER	-	expression tag	UNP P19099
D	30	SER	-	expression tag	UNP P19099
D	504	HIS	-	expression tag	UNP P19099
D	505	HIS	-	expression tag	UNP P19099
D	506	HIS	-	expression tag	UNP P19099
D	507	HIS	-	expression tag	UNP P19099
E	24	MET	-	initiating methionine	UNP P19099
E	25	ALA	-	expression tag	UNP P19099
E	26	LYS	-	expression tag	UNP P19099

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Chain	Residue	Modelled	Actual	Comment	Reference
E	27	LYS	-	expression tag	UNP P19099
E	28	THR	-	expression tag	UNP P19099
E	29	SER	-	expression tag	UNP P19099
E	30	SER	-	expression tag	UNP P19099
E	504	HIS	-	expression tag	UNP P19099
E	505	HIS	-	expression tag	UNP P19099
E	506	HIS	-	expression tag	UNP P19099
E	507	HIS	-	expression tag	UNP P19099
F	24	MET	-	initiating methionine	UNP P19099
F	25	ALA	-	expression tag	UNP P19099
F	26	LYS	-	expression tag	UNP P19099
F	27	LYS	-	expression tag	UNP P19099
F	28	THR	-	expression tag	UNP P19099
F	29	SER	-	expression tag	UNP P19099
F	30	SER	-	expression tag	UNP P19099
F	504	HIS	-	expression tag	UNP P19099
F	505	HIS	-	expression tag	UNP P19099
F	506	HIS	-	expression tag	UNP P19099
F	507	HIS	-	expression tag	UNP P19099
G	24	MET	-	initiating methionine	UNP P19099
G	25	ALA	-	expression tag	UNP P19099
G	26	LYS	-	expression tag	UNP P19099
G	27	LYS	-	expression tag	UNP P19099
G	28	THR	-	expression tag	UNP P19099
G	29	SER	-	expression tag	UNP P19099
G	30	SER	-	expression tag	UNP P19099
G	504	HIS	-	expression tag	UNP P19099
G	505	HIS	-	expression tag	UNP P19099
G	506	HIS	-	expression tag	UNP P19099
G	507	HIS	-	expression tag	UNP P19099
H	24	MET	-	initiating methionine	UNP P19099
H	25	ALA	-	expression tag	UNP P19099
H	26	LYS	-	expression tag	UNP P19099
H	27	LYS	-	expression tag	UNP P19099
H	28	THR	-	expression tag	UNP P19099
H	29	SER	-	expression tag	UNP P19099
H	30	SER	-	expression tag	UNP P19099
H	504	HIS	-	expression tag	UNP P19099
H	505	HIS	-	expression tag	UNP P19099
H	506	HIS	-	expression tag	UNP P19099
H	507	HIS	-	expression tag	UNP P19099
I	24	MET	-	initiating methionine	UNP P19099

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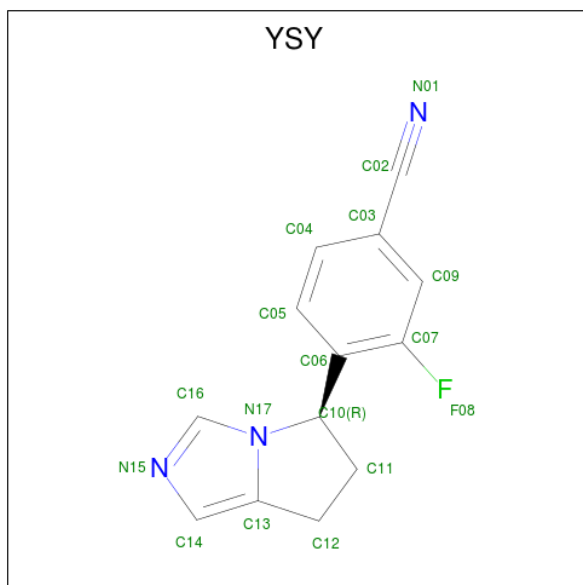
Chain	Residue	Modelled	Actual	Comment	Reference
I	25	ALA	-	expression tag	UNP P19099
I	26	LYS	-	expression tag	UNP P19099
I	27	LYS	-	expression tag	UNP P19099
I	28	THR	-	expression tag	UNP P19099
I	29	SER	-	expression tag	UNP P19099
I	30	SER	-	expression tag	UNP P19099
I	504	HIS	-	expression tag	UNP P19099
I	505	HIS	-	expression tag	UNP P19099
I	506	HIS	-	expression tag	UNP P19099
I	507	HIS	-	expression tag	UNP P19099
J	24	MET	-	initiating methionine	UNP P19099
J	25	ALA	-	expression tag	UNP P19099
J	26	LYS	-	expression tag	UNP P19099
J	27	LYS	-	expression tag	UNP P19099
J	28	THR	-	expression tag	UNP P19099
J	29	SER	-	expression tag	UNP P19099
J	30	SER	-	expression tag	UNP P19099
J	504	HIS	-	expression tag	UNP P19099
J	505	HIS	-	expression tag	UNP P19099
J	506	HIS	-	expression tag	UNP P19099
J	507	HIS	-	expression tag	UNP P19099
K	24	MET	-	initiating methionine	UNP P19099
K	25	ALA	-	expression tag	UNP P19099
K	26	LYS	-	expression tag	UNP P19099
K	27	LYS	-	expression tag	UNP P19099
K	28	THR	-	expression tag	UNP P19099
K	29	SER	-	expression tag	UNP P19099
K	30	SER	-	expression tag	UNP P19099
K	504	HIS	-	expression tag	UNP P19099
K	505	HIS	-	expression tag	UNP P19099
K	506	HIS	-	expression tag	UNP P19099
K	507	HIS	-	expression tag	UNP P19099
L	24	MET	-	initiating methionine	UNP P19099
L	25	ALA	-	expression tag	UNP P19099
L	26	LYS	-	expression tag	UNP P19099
L	27	LYS	-	expression tag	UNP P19099
L	28	THR	-	expression tag	UNP P19099
L	29	SER	-	expression tag	UNP P19099
L	30	SER	-	expression tag	UNP P19099
L	504	HIS	-	expression tag	UNP P19099
L	505	HIS	-	expression tag	UNP P19099
L	506	HIS	-	expression tag	UNP P19099

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Chain	Residue	Modelled	Actual	Comment	Reference
L	507	HIS	-	expression tag	UNP P19099

- Molecule 2 is 4-[(4R,5R)-6,7-dihydro-5H-pyrrolo[1,2-c]imidazol-5-yl]-3-fluorobenzonitrile (three-letter code: YSY) (formula: C₁₃H₁₀FN₃) (labeled as "Ligand of Interest" by depositor).



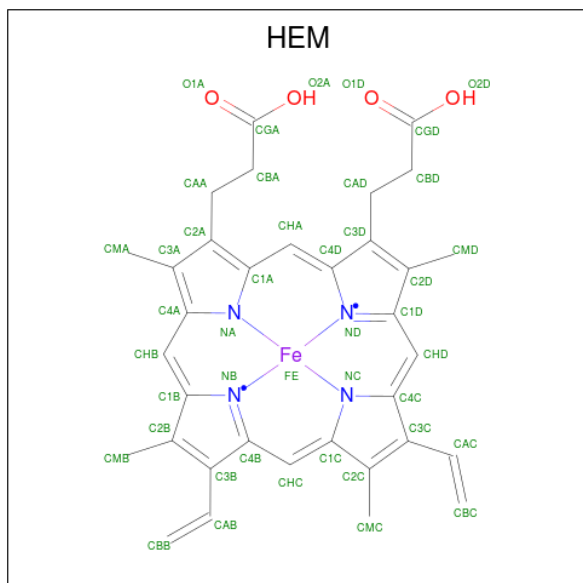
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	H	N		
2	A	1	Total	C	F	H	N	0	0
			27	13	1	10	3		
2	B	1	Total	C	F	H	N	0	0
			27	13	1	10	3		
2	C	1	Total	C	F	H	N	0	0
			27	13	1	10	3		
2	D	1	Total	C	F	H	N	0	0
			27	13	1	10	3		
2	E	1	Total	C	F	H	N	0	0
			27	13	1	10	3		
2	F	1	Total	C	F	H	N	0	0
			27	13	1	10	3		
2	G	1	Total	C	F	H	N	0	0
			27	13	1	10	3		
2	H	1	Total	C	F	H	N	0	0
			27	13	1	10	3		
2	I	1	Total	C	F	H	N	0	0
			27	13	1	10	3		
2	J	1	Total	C	F	H	N	0	0
			27	13	1	10	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	K	1	Total	C	F	H	N	0	0
			27	13	1	10	3		
2	L	1	Total	C	F	H	N	0	0
			27	13	1	10	3		

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
3	B	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
3	C	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
3	D	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
3	E	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
3	F	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
3	G	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
3	H	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
3	I	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
3	J	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
3	K	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
3	L	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

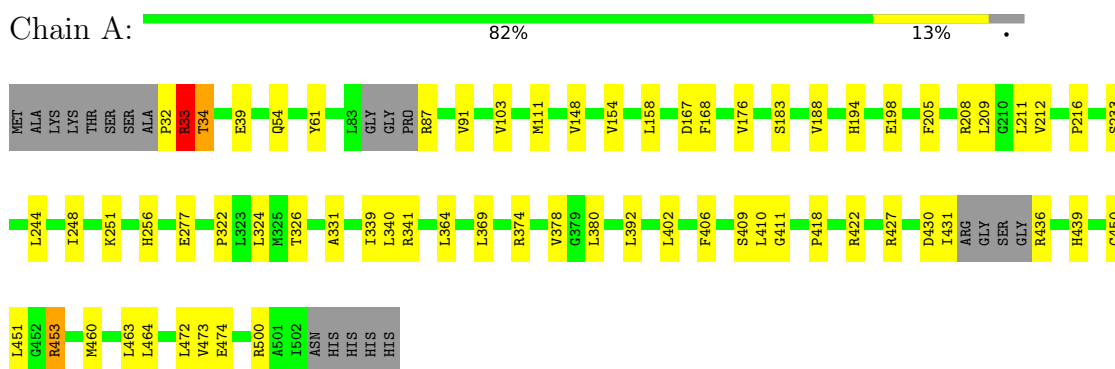
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O	0	0
			1	1		
4	B	1	Total	O	0	0
			1	1		
4	C	1	Total	O	0	0
			1	1		
4	E	1	Total	O	0	0
			1	1		
4	F	1	Total	O	0	0
			1	1		
4	G	1	Total	O	0	0
			1	1		

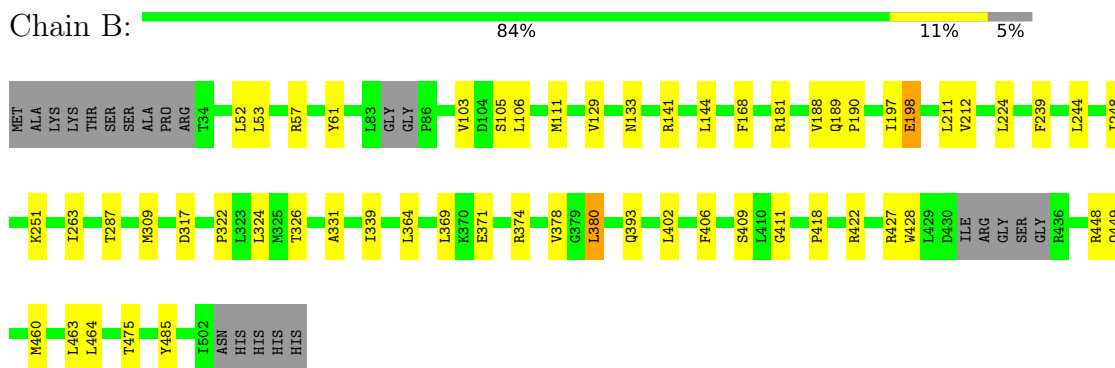
3 Residue-property plots [i](#)

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.

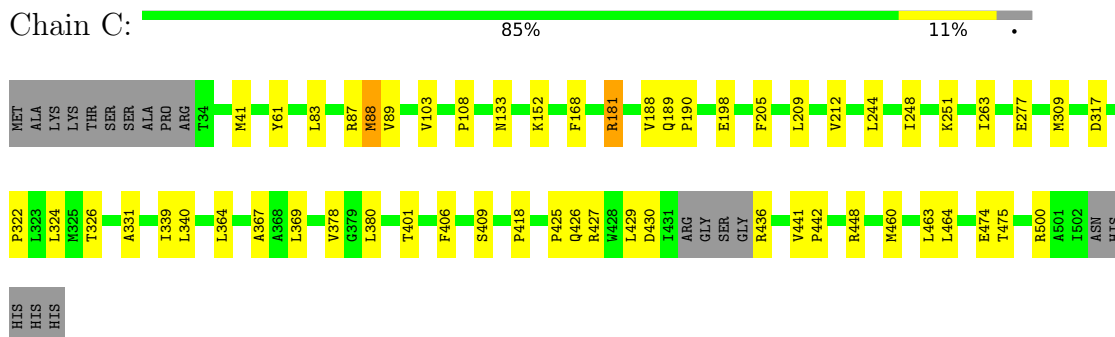
- Molecule 1: Cytochrome P450 11B2, mitochondrial



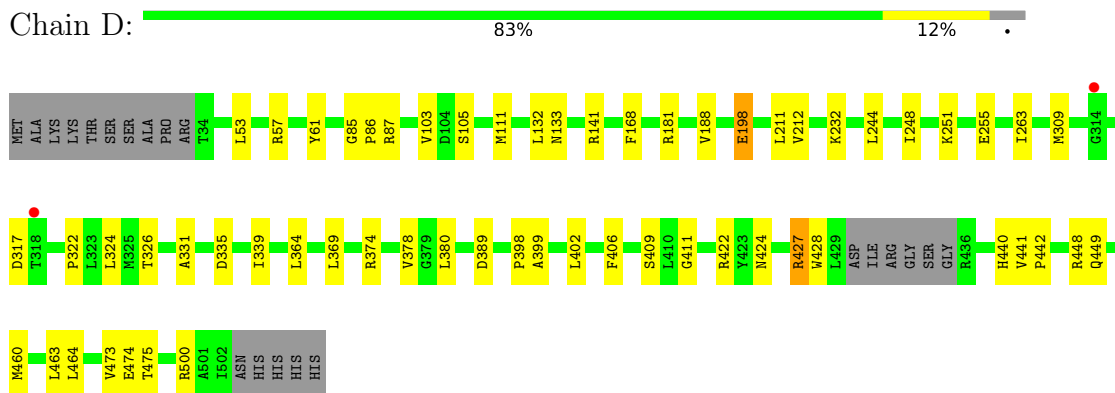
- Molecule 1: Cytochrome P450 11B2, mitochondrial



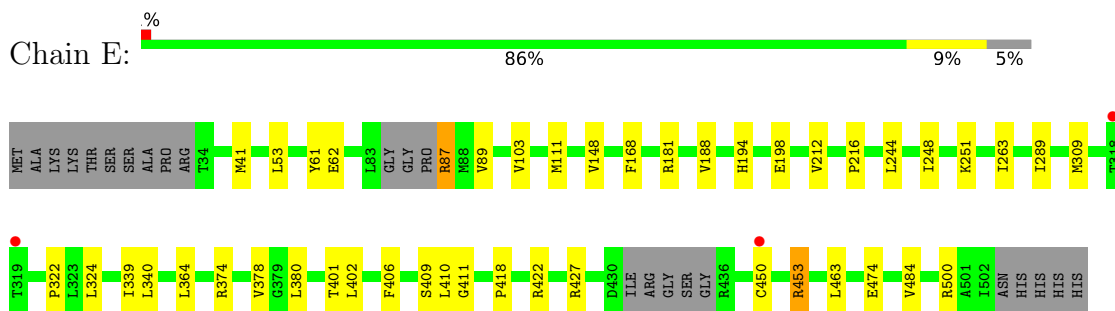
- Molecule 1: Cytochrome P450 11B2, mitochondrial



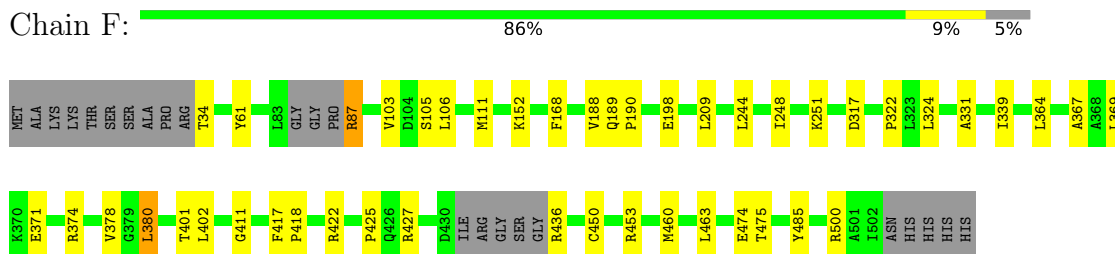
• Molecule 1: Cytochrome P450 11B2, mitochondrial



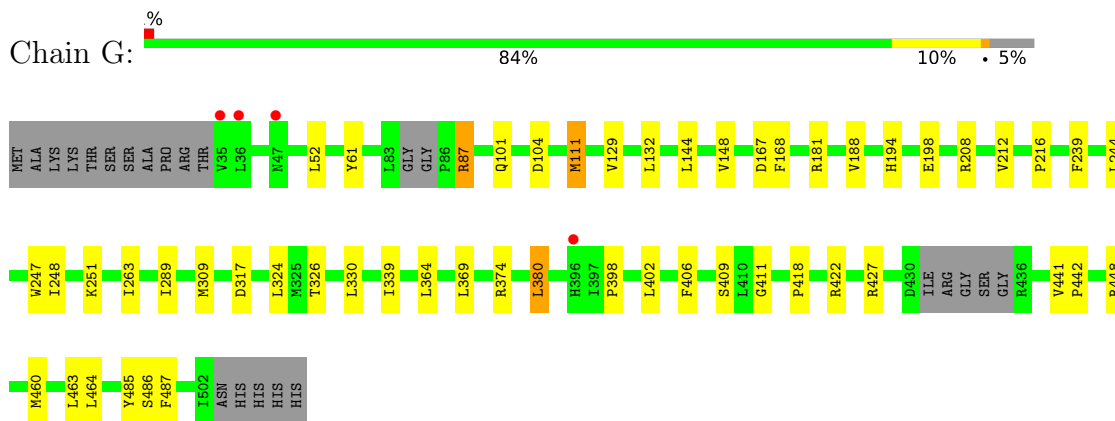
• Molecule 1: Cytochrome P450 11B2, mitochondrial



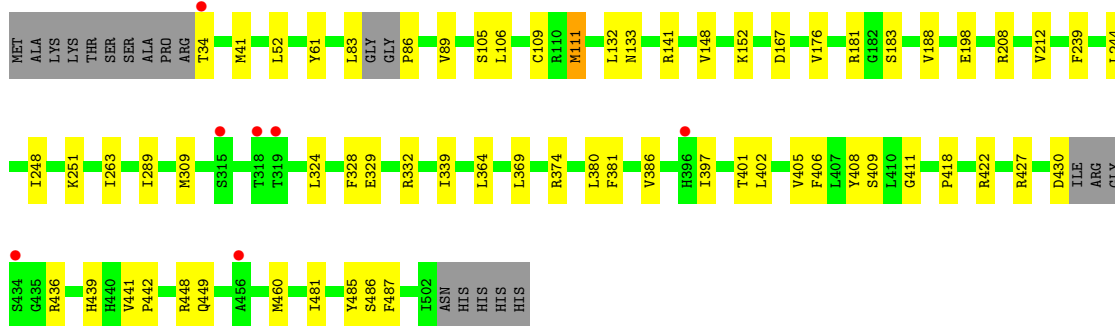
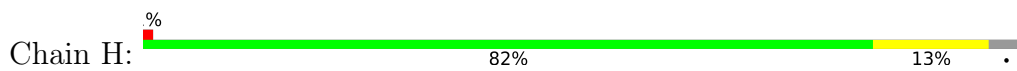
• Molecule 1: Cytochrome P450 11B2, mitochondrial



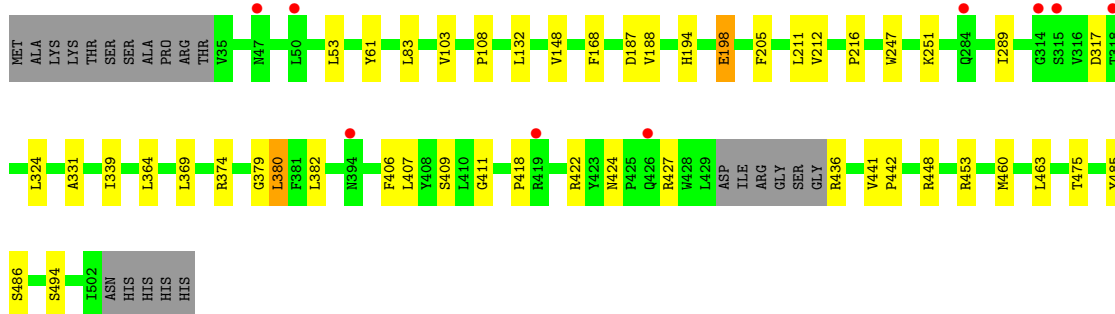
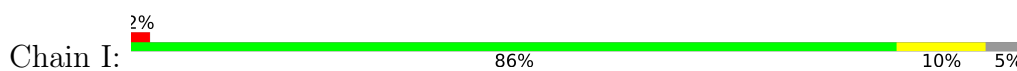
• Molecule 1: Cytochrome P450 11B2, mitochondrial



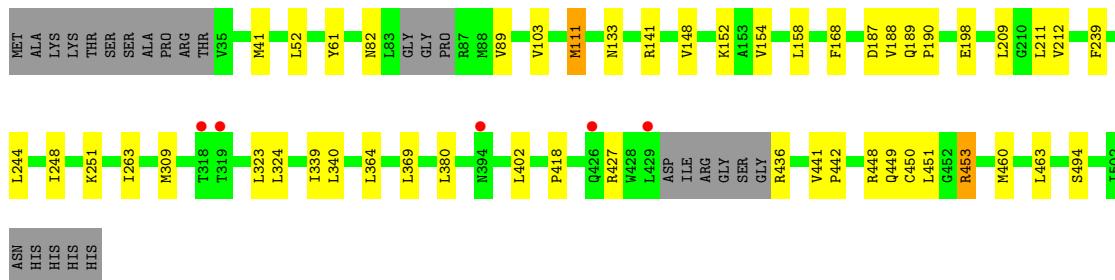
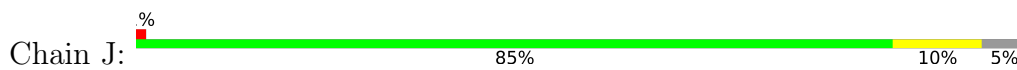
• Molecule 1: Cytochrome P450 11B2, mitochondrial



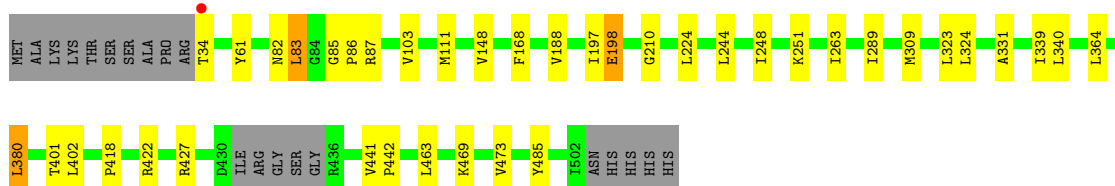
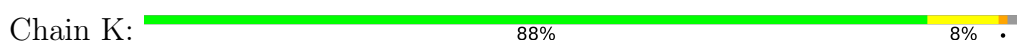
• Molecule 1: Cytochrome P450 11B2, mitochondrial



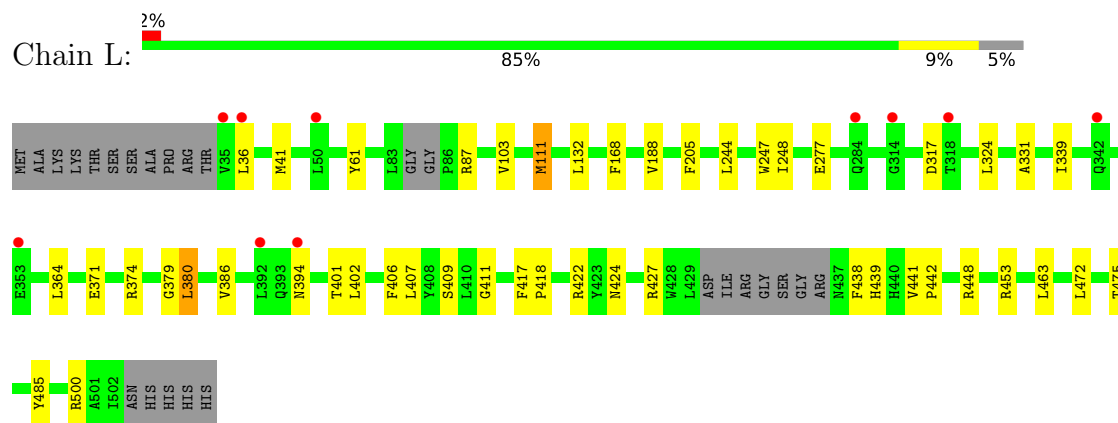
• Molecule 1: Cytochrome P450 11B2, mitochondrial



• Molecule 1: Cytochrome P450 11B2, mitochondrial



- Molecule 1: Cytochrome P450 11B2, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	123.95Å 126.42Å 174.93Å 82.81° 70.03° 79.37°	Depositor
Resolution (Å)	37.95 – 3.08 37.95 – 3.08	Depositor EDS
% Data completeness (in resolution range)	79.8 (37.95-3.08) 51.7 (37.95-3.08)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 3.06Å)	Xtrriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.202 , 0.242 0.202 , 0.245	Depositor DCC
R_{free} test set	1394 reflections (1.42%)	wwPDB-VP
Wilson B-factor (Å ²)	63.6	Xtrriage
Anisotropy	0.011	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 28.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	91890	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.30% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: HEM, YSY

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	0.27	0/3879	0.45	0/5260
1	B	0.28	0/3860	0.44	0/5235
1	C	0.27	0/3877	0.43	0/5260
1	D	0.29	0/3861	0.43	0/5238
1	E	0.27	0/3852	0.43	0/5224
1	F	0.27	0/3852	0.42	0/5224
1	G	0.27	0/3853	0.42	0/5225
1	H	0.27	0/3870	0.42	0/5248
1	I	0.30	0/3854	0.43	0/5228
1	J	0.26	0/3837	0.42	0/5203
1	K	0.28	0/3869	0.44	0/5249
1	L	0.26	0/3834	0.43	0/5200
All	All	0.27	0/46298	0.43	0/62794

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	3780	3823	3822	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3761	3799	3798	31	0
1	C	3777	3817	3815	30	0
1	D	3761	3801	3800	34	0
1	E	3754	3792	3790	24	0
1	F	3754	3792	3790	23	0
1	G	3754	3792	3791	28	0
1	H	3771	3807	3806	32	0
1	I	3754	3794	3793	28	0
1	J	3739	3782	3780	26	0
1	K	3769	3801	3804	21	0
1	L	3735	3775	3774	24	0
2	A	17	10	0	0	0
2	B	17	10	0	0	0
2	C	17	10	0	0	0
2	D	17	10	0	0	0
2	E	17	10	0	0	0
2	F	17	10	0	0	0
2	G	17	10	0	0	0
2	H	17	10	0	0	0
2	I	17	10	0	0	0
2	J	17	10	0	0	0
2	K	17	10	0	0	0
2	L	17	10	0	0	0
3	A	43	30	30	4	0
3	B	43	30	30	4	0
3	C	43	30	30	2	0
3	D	43	30	30	4	0
3	E	43	30	30	4	0
3	F	43	30	30	4	0
3	G	43	30	30	4	0
3	H	43	30	30	4	0
3	I	43	30	30	4	0
3	J	43	30	30	4	0
3	K	43	30	30	4	0
3	L	43	30	30	4	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
All	All	45835	46055	45923	370	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 4.

The worst 5 of 370 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:430:ASP:O	1:A:431:ILE:HG13	1.84	0.77
1:J:198:GLU:HG3	1:J:212:VAL:HG23	1.66	0.77
1:A:277:GLU:OE1	1:D:181:ARG:NH1	2.20	0.74
1:H:418:PRO:O	1:H:427:ARG:NH2	2.24	0.71
1:G:181:ARG:NH1	1:L:277:GLU:OE1	2.24	0.70

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	458/484 (95%)	438 (96%)	18 (4%)	2 (0%)	34	66
1	B	456/484 (94%)	436 (96%)	20 (4%)	0	100	100
1	C	461/484 (95%)	443 (96%)	18 (4%)	0	100	100
1	D	459/484 (95%)	438 (95%)	21 (5%)	0	100	100
1	E	455/484 (94%)	436 (96%)	19 (4%)	0	100	100
1	F	455/484 (94%)	440 (97%)	15 (3%)	0	100	100
1	G	455/484 (94%)	435 (96%)	20 (4%)	0	100	100
1	H	458/484 (95%)	440 (96%)	18 (4%)	0	100	100
1	I	458/484 (95%)	433 (94%)	25 (6%)	0	100	100
1	J	453/484 (94%)	438 (97%)	15 (3%)	0	100	100
1	K	460/484 (95%)	444 (96%)	16 (4%)	0	100	100
1	L	453/484 (94%)	434 (96%)	19 (4%)	0	100	100
All	All	5481/5808 (94%)	5255 (96%)	224 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	33	ARG
1	A	34	THR

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	411/425 (97%)	404 (98%)	7 (2%)	60	82
1	B	409/425 (96%)	401 (98%)	8 (2%)	55	78
1	C	410/425 (96%)	401 (98%)	9 (2%)	52	76
1	D	408/425 (96%)	400 (98%)	8 (2%)	55	78
1	E	408/425 (96%)	402 (98%)	6 (2%)	65	84
1	F	408/425 (96%)	401 (98%)	7 (2%)	60	82
1	G	408/425 (96%)	401 (98%)	7 (2%)	60	82
1	H	410/425 (96%)	402 (98%)	8 (2%)	55	78
1	I	407/425 (96%)	400 (98%)	7 (2%)	60	82
1	J	406/425 (96%)	399 (98%)	7 (2%)	60	82
1	K	409/425 (96%)	402 (98%)	7 (2%)	60	82
1	L	406/425 (96%)	397 (98%)	9 (2%)	52	76
All	All	4900/5100 (96%)	4810 (98%)	90 (2%)	59	80

5 of 90 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	251	LYS
1	J	251	LYS
1	H	430	ASP
1	I	422	ARG
1	K	83	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such

sidechains are listed below:

Mol	Chain	Res	Type
1	G	82	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

24 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	HEM	A	602	2	41,50,50	1.45	3 (7%)	45,82,82	1.11	1 (2%)
2	YSY	L	601	3	14,19,19	1.09	1 (7%)	19,27,27	1.46	3 (15%)
2	YSY	A	601	3	14,19,19	1.17	1 (7%)	19,27,27	1.42	2 (10%)
2	YSY	C	601	3	14,19,19	1.04	1 (7%)	19,27,27	1.41	2 (10%)
3	HEM	K	602	2	41,50,50	1.46	3 (7%)	45,82,82	1.20	3 (6%)
3	HEM	H	602	2	41,50,50	1.47	3 (7%)	45,82,82	1.21	4 (8%)
3	HEM	E	602	2	41,50,50	1.45	3 (7%)	45,82,82	1.20	4 (8%)
2	YSY	I	601	3	14,19,19	1.10	1 (7%)	19,27,27	1.37	2 (10%)
3	HEM	F	602	2	41,50,50	1.48	4 (9%)	45,82,82	1.22	3 (6%)
2	YSY	E	601	3	14,19,19	1.20	1 (7%)	19,27,27	1.32	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	YSY	B	601	3	14,19,19	1.22	2 (14%)	19,27,27	1.37	2 (10%)
3	HEM	L	602	2	41,50,50	1.47	4 (9%)	45,82,82	1.25	5 (11%)
3	HEM	C	602	2,1	41,50,50	1.47	4 (9%)	45,82,82	1.22	5 (11%)
3	HEM	I	602	2	41,50,50	1.46	3 (7%)	45,82,82	1.18	3 (6%)
2	YSY	H	601	3	14,19,19	1.13	1 (7%)	19,27,27	1.44	2 (10%)
2	YSY	F	601	3	14,19,19	1.10	1 (7%)	19,27,27	1.39	2 (10%)
2	YSY	D	601	3	14,19,19	1.13	1 (7%)	19,27,27	1.47	2 (10%)
2	YSY	G	601	3	14,19,19	1.14	1 (7%)	19,27,27	1.33	2 (10%)
3	HEM	B	602	2,1	41,50,50	1.47	4 (9%)	45,82,82	1.15	2 (4%)
2	YSY	J	601	3	14,19,19	1.14	1 (7%)	19,27,27	1.51	2 (10%)
2	YSY	K	601	3	14,19,19	1.17	1 (7%)	19,27,27	1.36	2 (10%)
3	HEM	D	602	2	41,50,50	1.48	4 (9%)	45,82,82	1.17	2 (4%)
3	HEM	J	602	2	41,50,50	1.46	3 (7%)	45,82,82	1.32	6 (13%)
3	HEM	G	602	2	41,50,50	1.46	4 (9%)	45,82,82	1.24	4 (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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEM	A	602	2	-	1/12/54/54	-
2	YSY	L	601	3	-	0/6/15/15	0/3/3/3
2	YSY	A	601	3	-	0/6/15/15	0/3/3/3
2	YSY	C	601	3	-	0/6/15/15	0/3/3/3
3	HEM	K	602	2	-	0/12/54/54	-
3	HEM	H	602	2	-	1/12/54/54	-
3	HEM	E	602	2	-	0/12/54/54	-
2	YSY	I	601	3	-	0/6/15/15	0/3/3/3
3	HEM	F	602	2	-	2/12/54/54	-
2	YSY	E	601	3	-	0/6/15/15	0/3/3/3
2	YSY	B	601	3	-	0/6/15/15	0/3/3/3
3	HEM	L	602	2	-	2/12/54/54	-
3	HEM	C	602	2,1	-	0/12/54/54	-
3	HEM	I	602	2	-	1/12/54/54	-
2	YSY	H	601	3	-	0/6/15/15	0/3/3/3
2	YSY	F	601	3	-	0/6/15/15	0/3/3/3
2	YSY	D	601	3	-	0/6/15/15	0/3/3/3
2	YSY	G	601	3	-	0/6/15/15	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEM	B	602	2,1	-	0/12/54/54	-
2	YSY	J	601	3	-	0/6/15/15	0/3/3/3
2	YSY	K	601	3	-	0/6/15/15	0/3/3/3
3	HEM	D	602	2	-	1/12/54/54	-
3	HEM	J	602	2	-	2/12/54/54	-
3	HEM	G	602	2	-	1/12/54/54	-

The worst 5 of 55 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	602	HEM	C3C-C2C	-4.54	1.34	1.40
3	L	602	HEM	C3C-C2C	-4.46	1.34	1.40
3	B	602	HEM	C3C-C2C	-4.45	1.34	1.40
3	C	602	HEM	C3C-C2C	-4.37	1.34	1.40
3	F	602	HEM	C3C-C2C	-4.31	1.34	1.40

The worst 5 of 67 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	601	YSY	C06-C10-N17	4.09	118.26	113.04
2	H	601	YSY	C06-C10-N17	3.73	117.80	113.04
2	D	601	YSY	C06-C10-N17	3.66	117.72	113.04
2	C	601	YSY	C06-C10-N17	3.65	117.70	113.04
2	L	601	YSY	C06-C10-N17	3.58	117.61	113.04

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	J	602	HEM	C2A-CAA-CBA-CGA
3	L	602	HEM	CAD-CBD-CGD-O2D
3	D	602	HEM	CAD-CBD-CGD-O2D
3	F	602	HEM	CAD-CBD-CGD-O2D
3	G	602	HEM	CAD-CBD-CGD-O2D

There are no ring outliers.

12 monomers are involved in 46 short contacts:

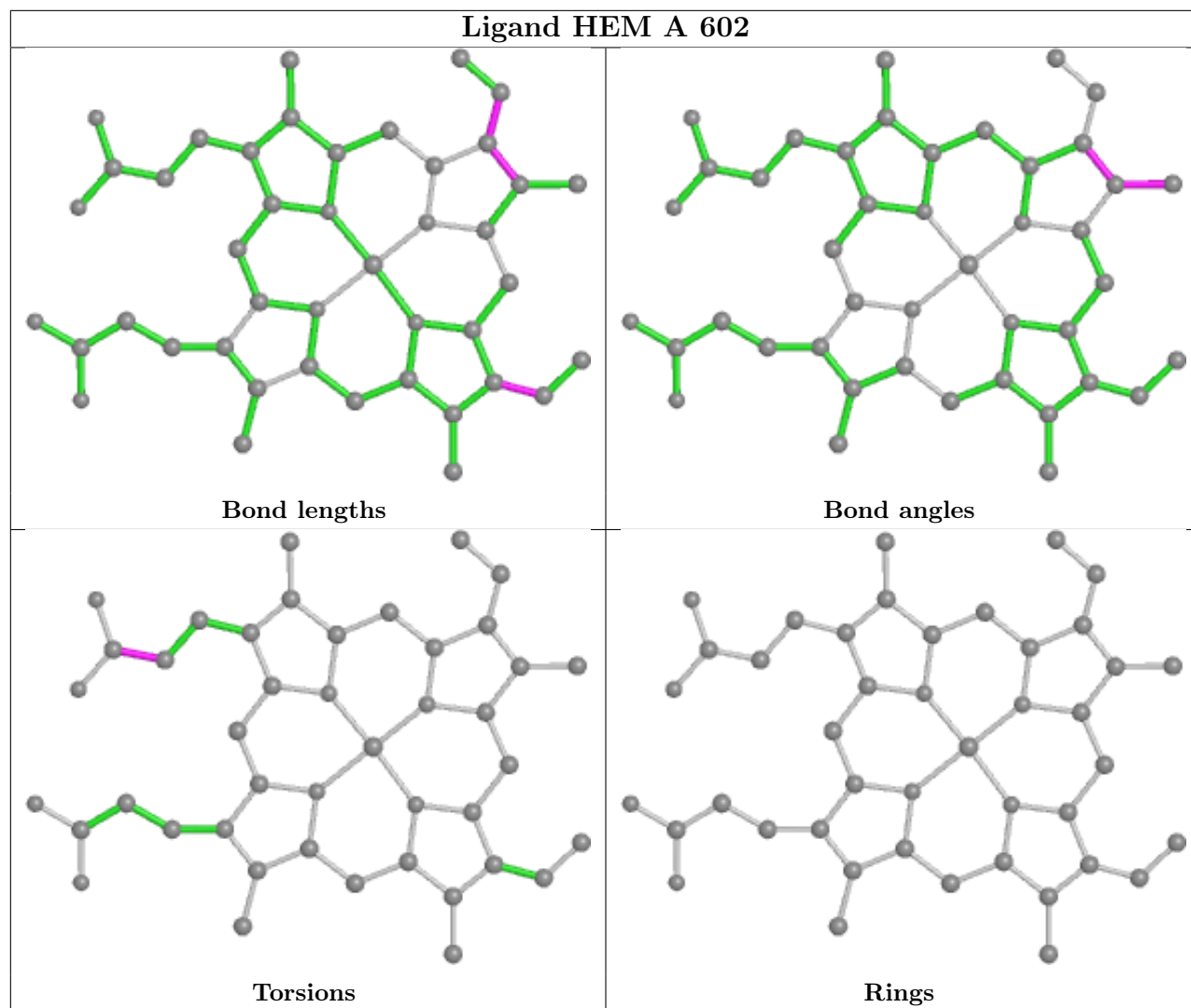
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	HEM	4	0
3	K	602	HEM	4	0

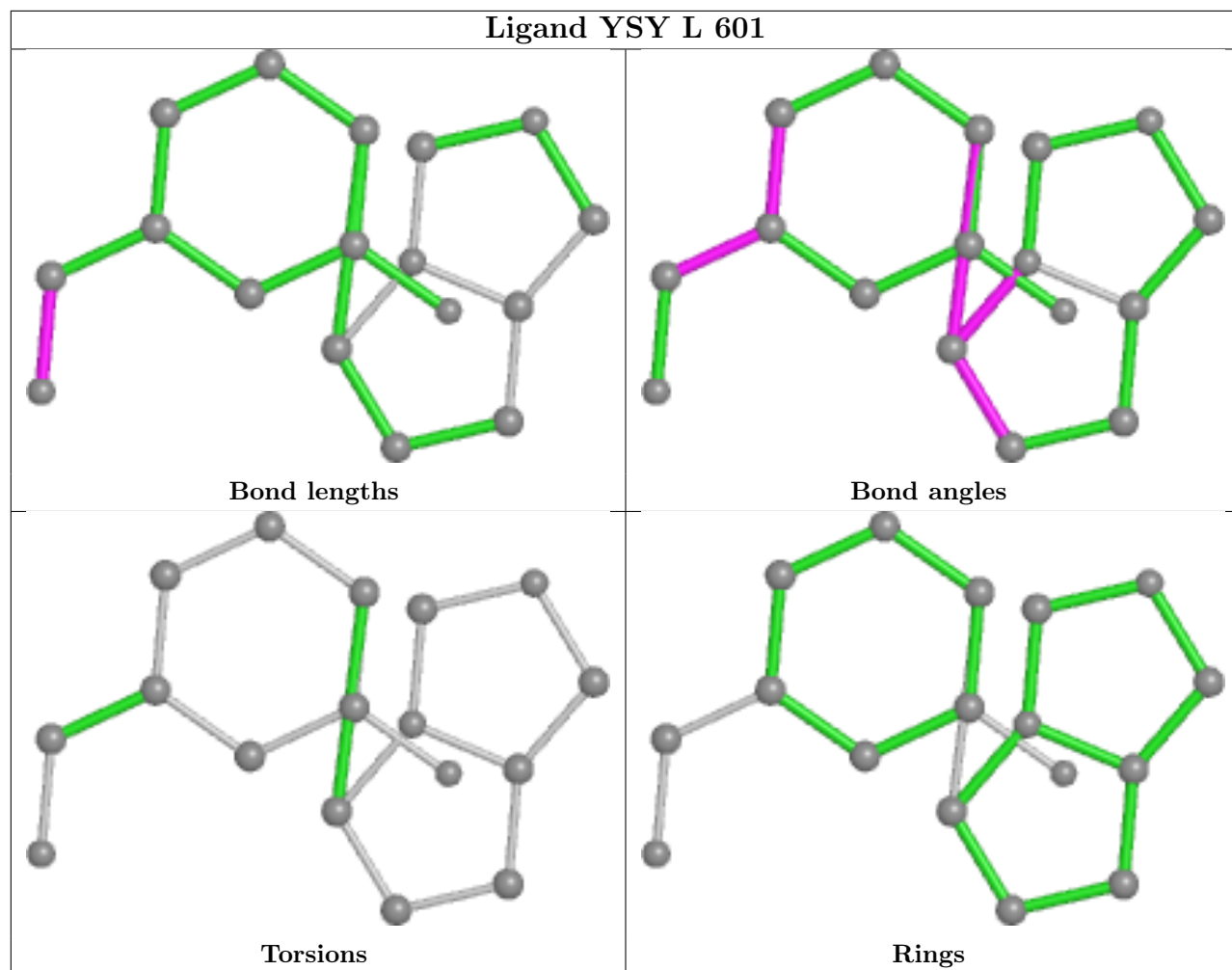
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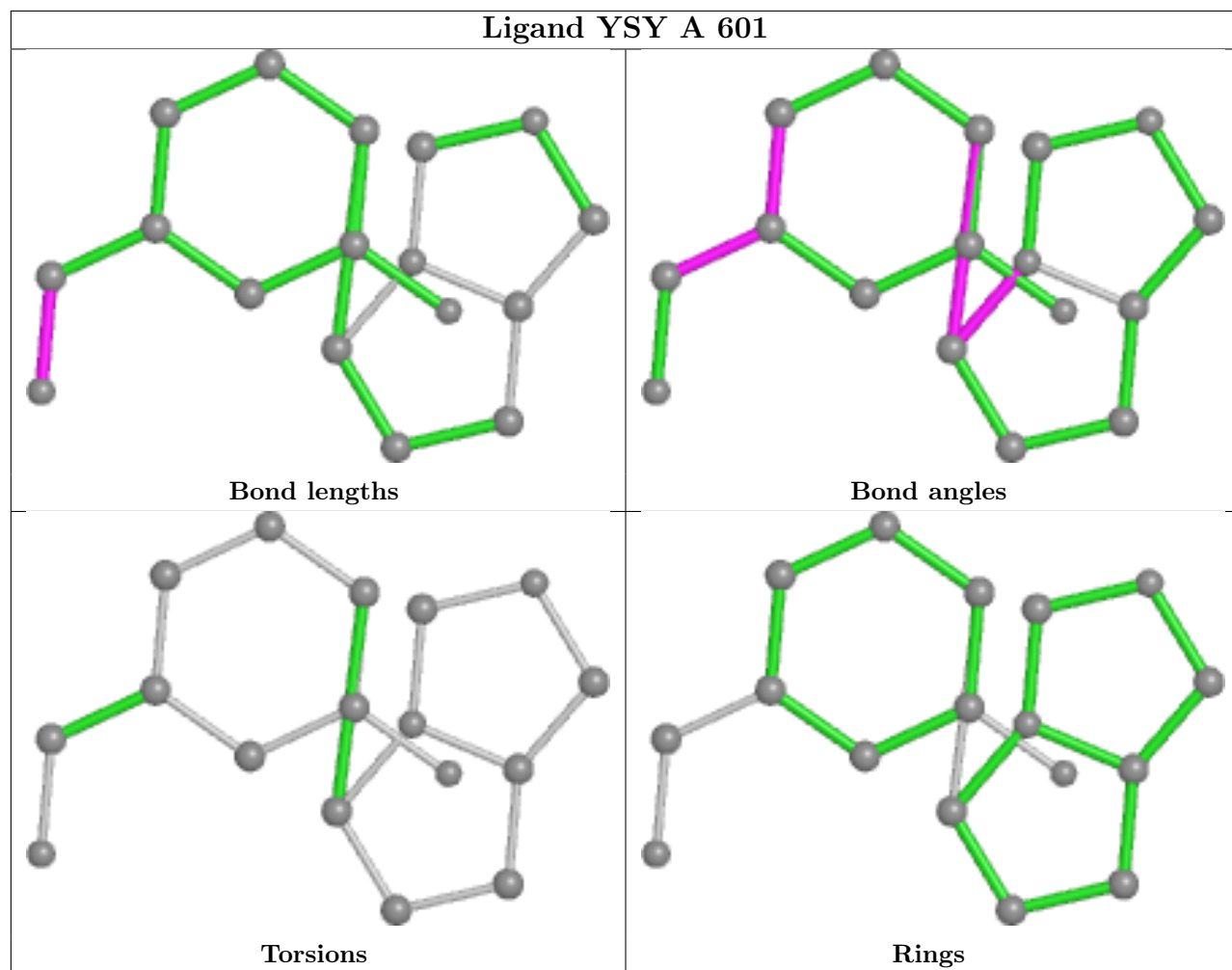
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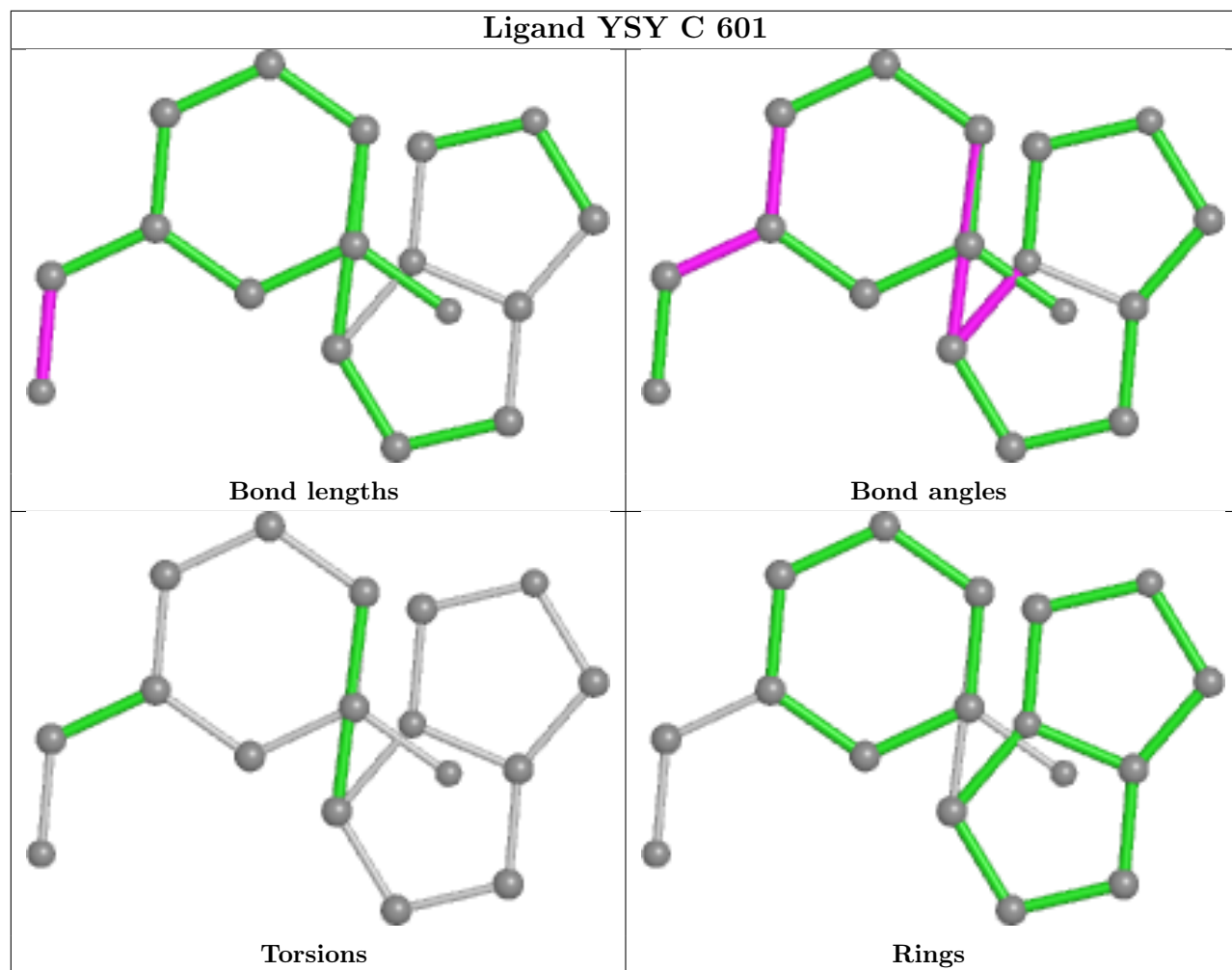
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	602	HEM	4	0
3	E	602	HEM	4	0
3	F	602	HEM	4	0
3	L	602	HEM	4	0
3	C	602	HEM	2	0
3	I	602	HEM	4	0
3	B	602	HEM	4	0
3	D	602	HEM	4	0
3	J	602	HEM	4	0
3	G	602	HEM	4	0

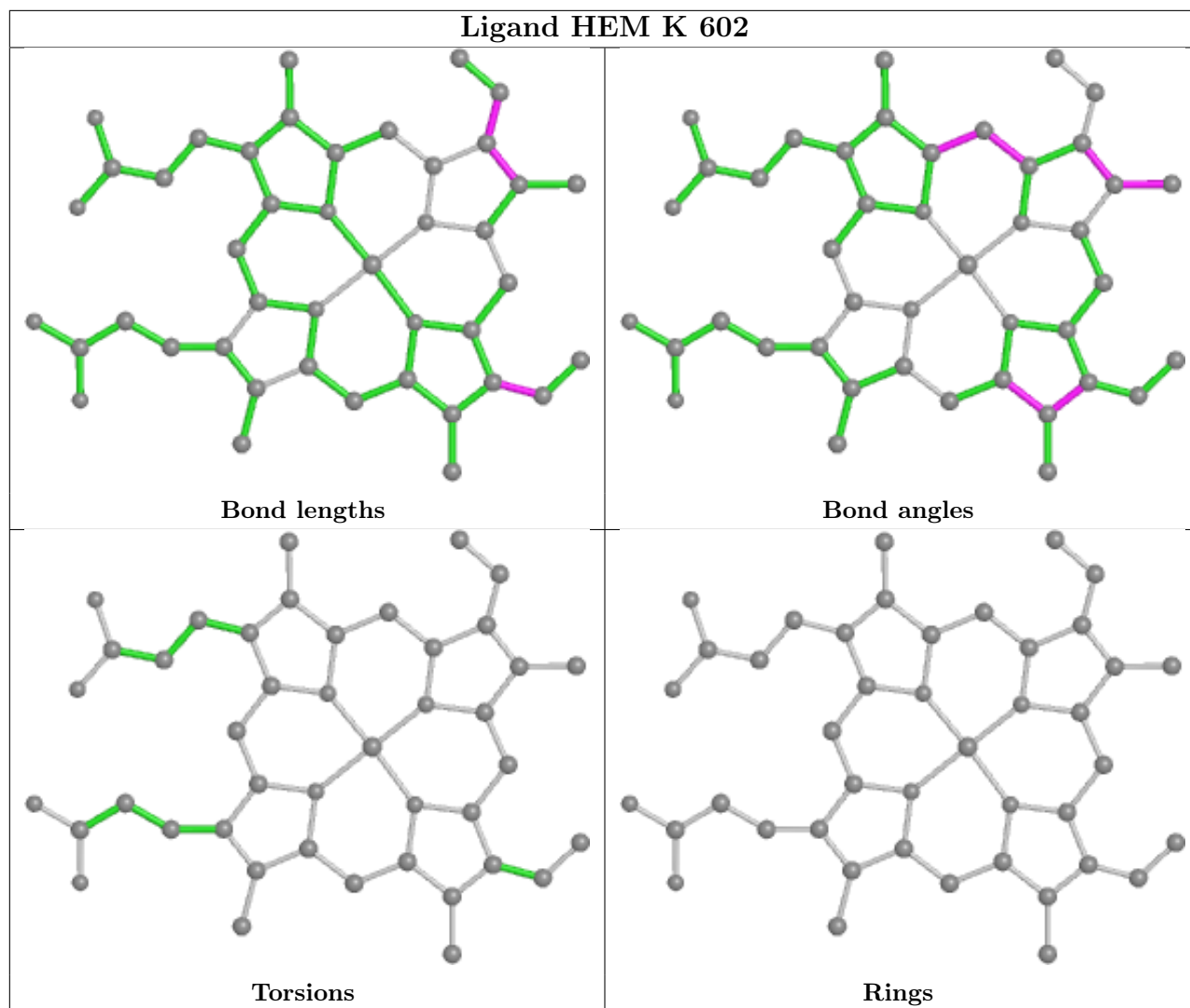
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

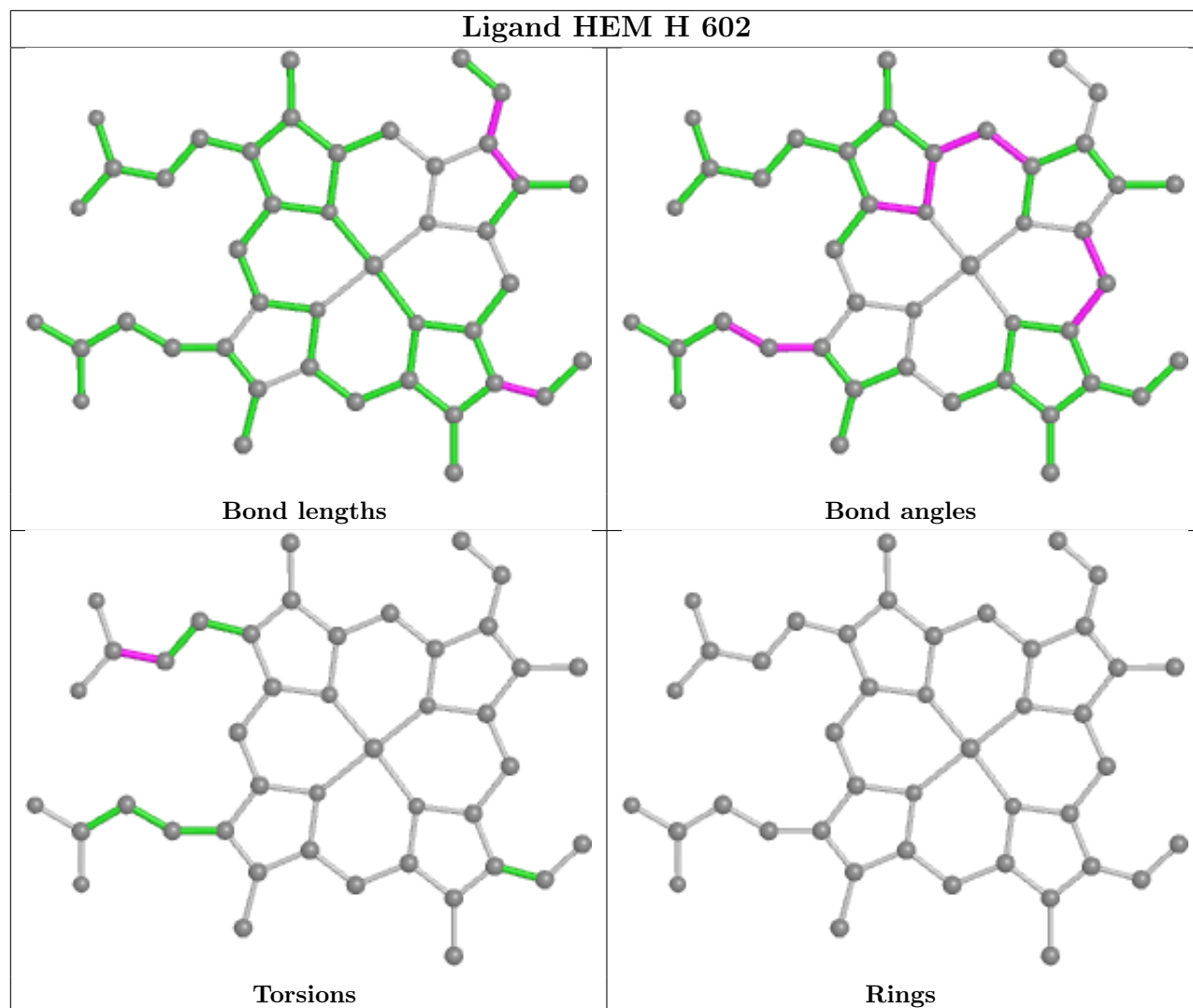


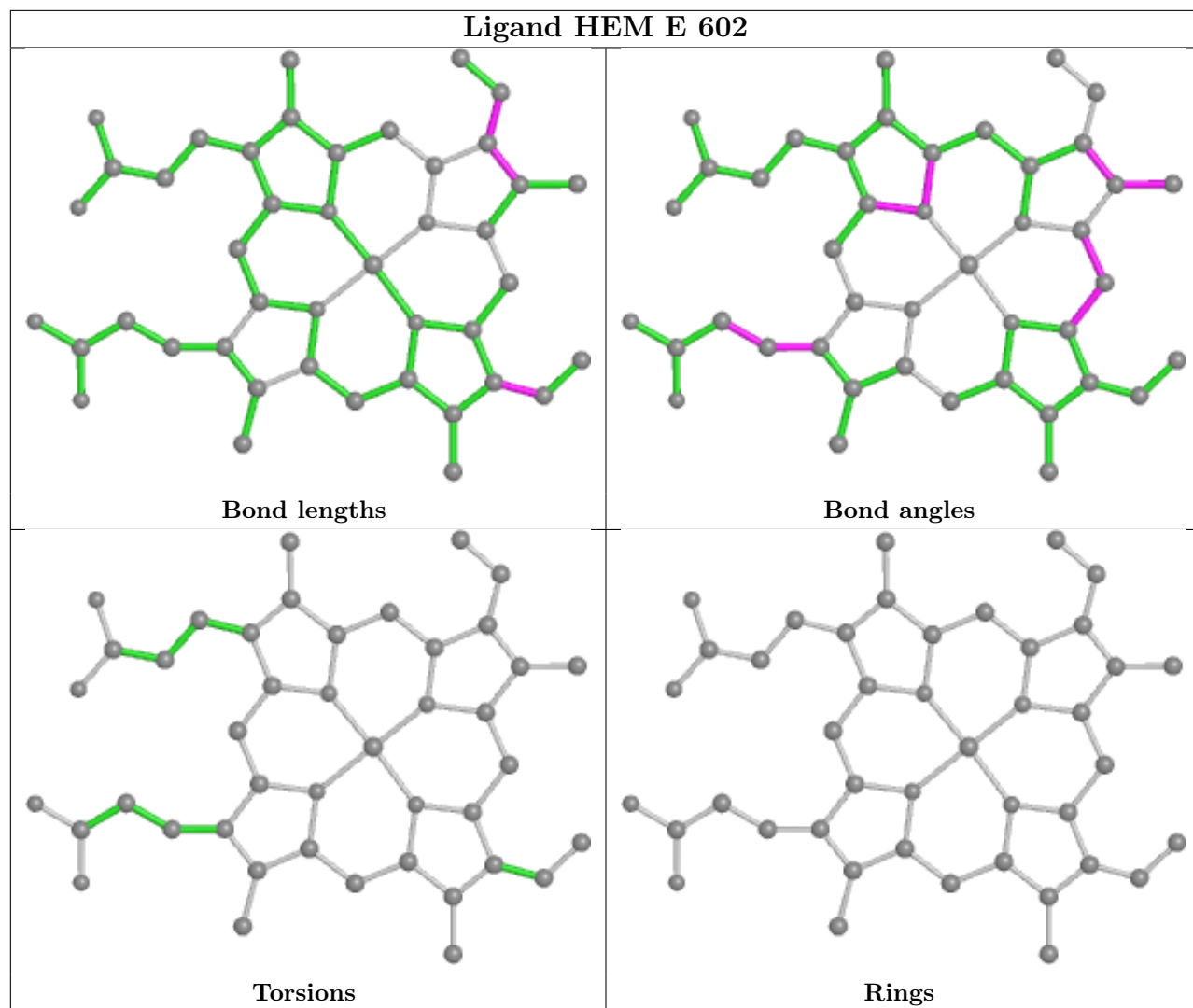


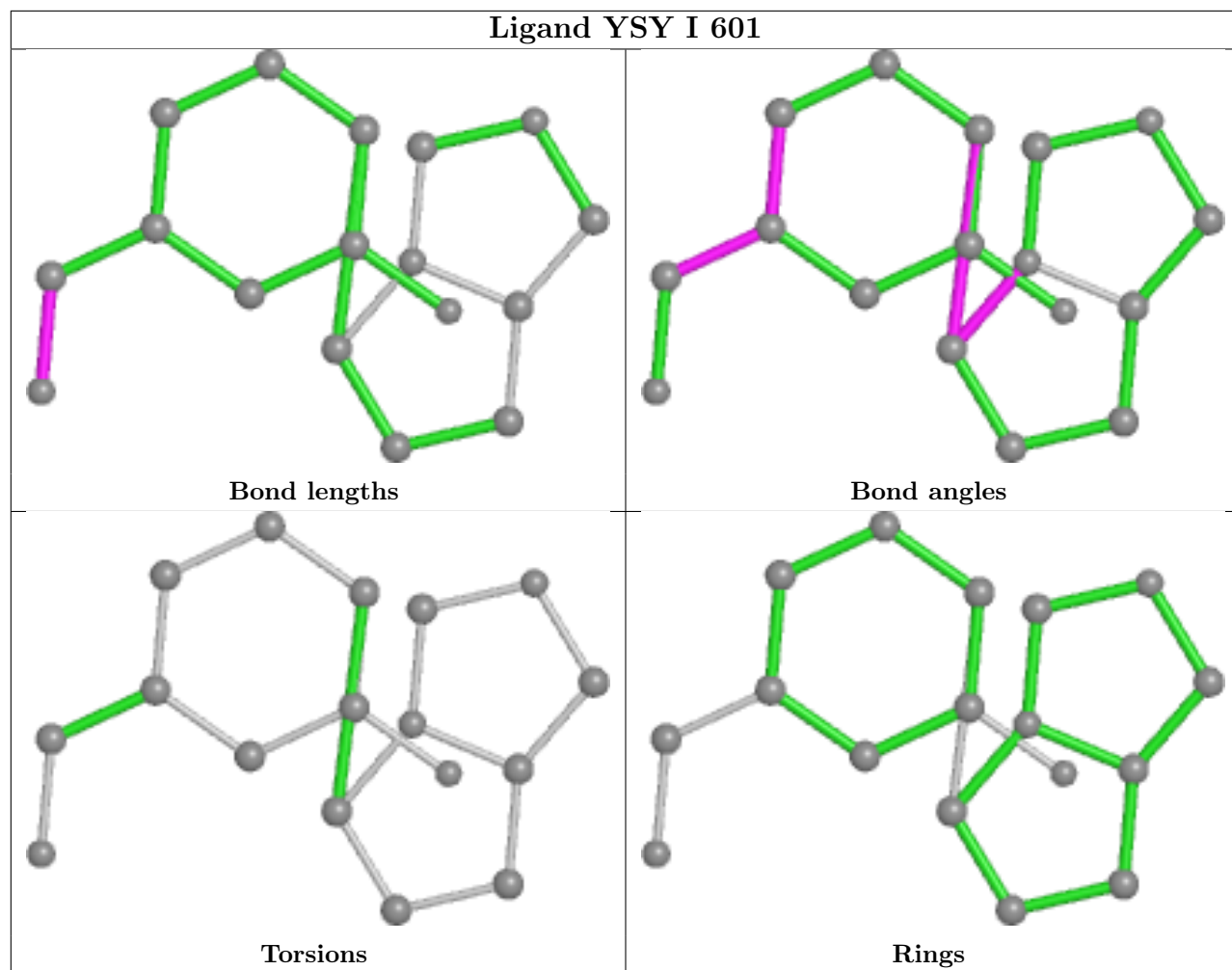


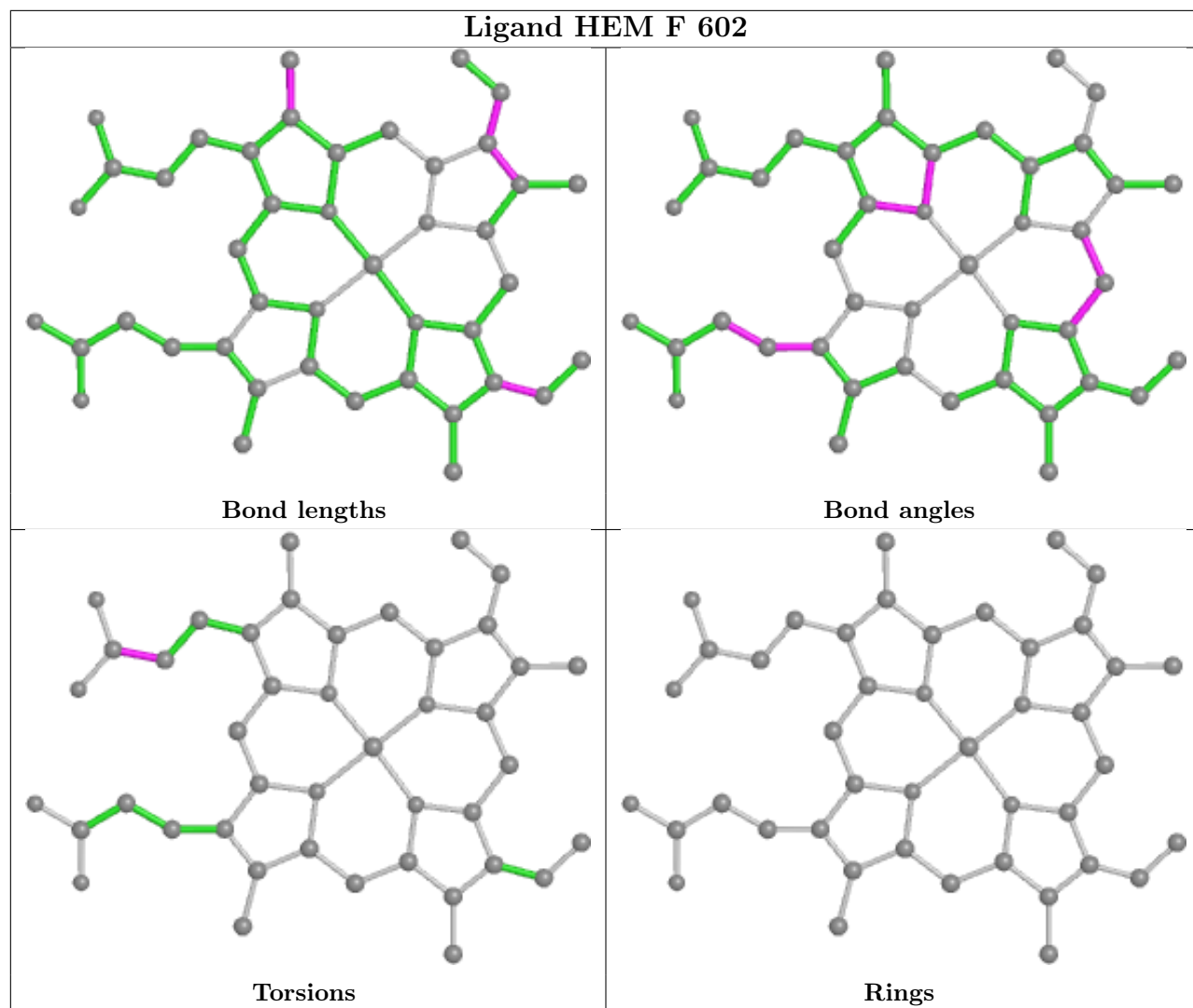


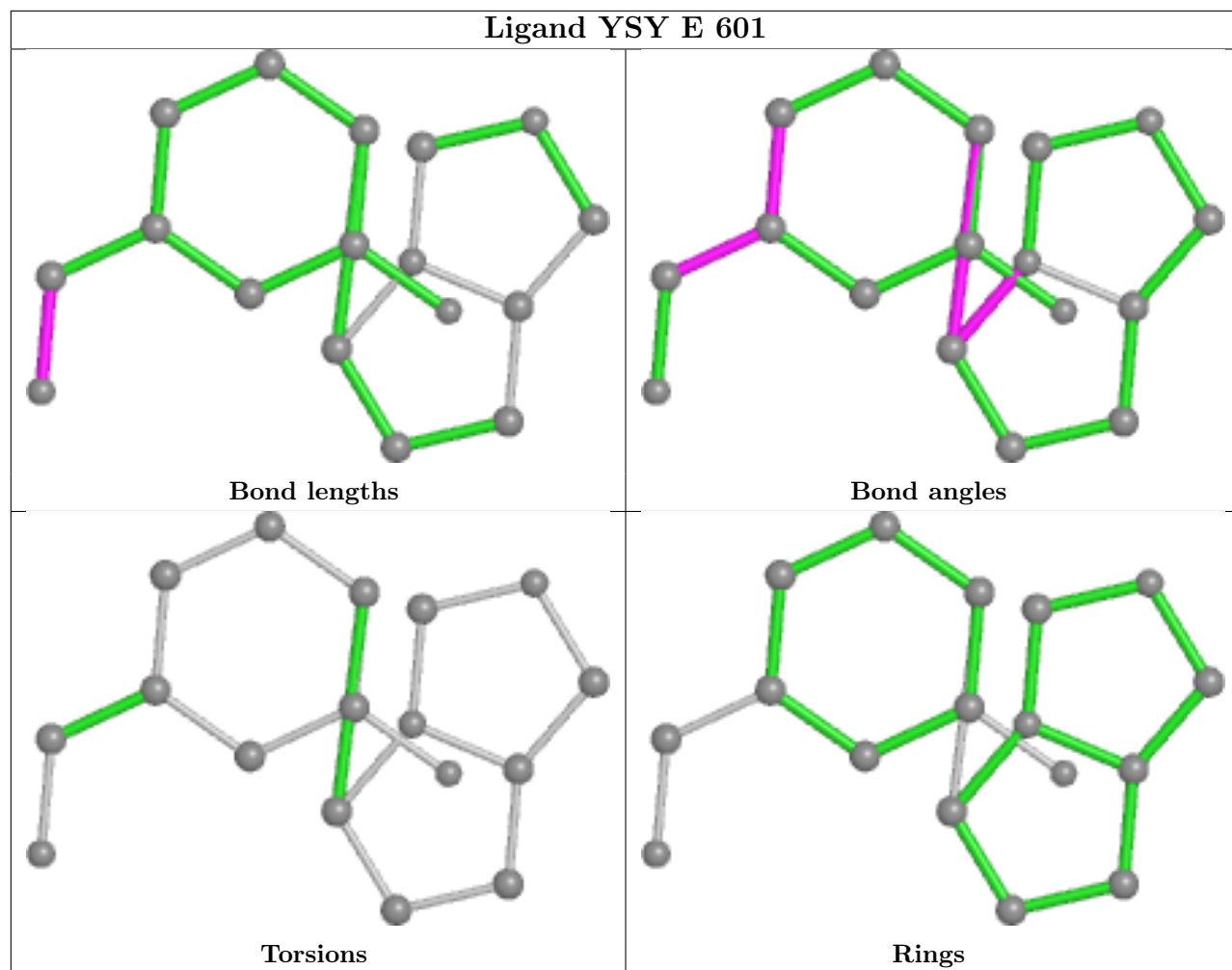


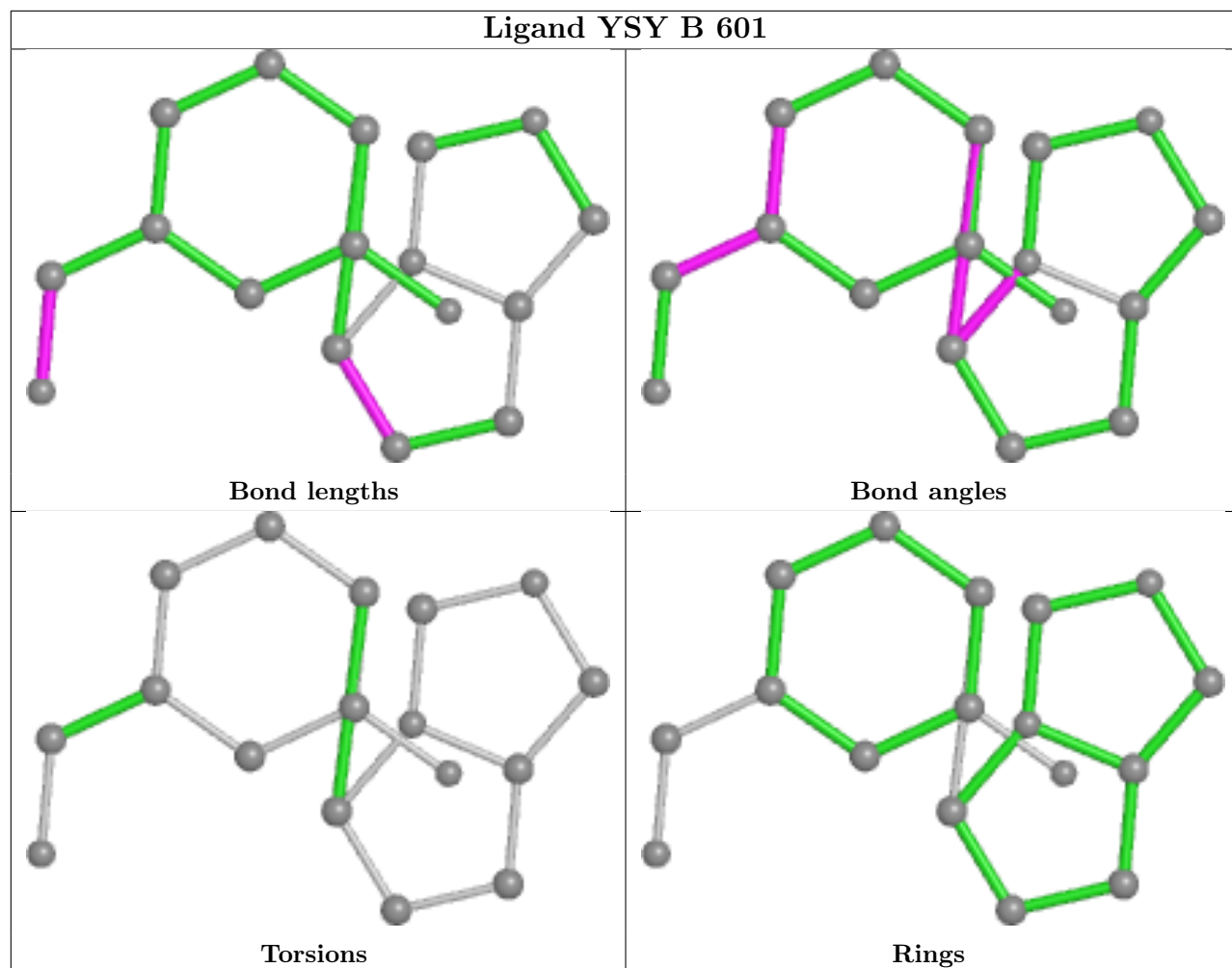


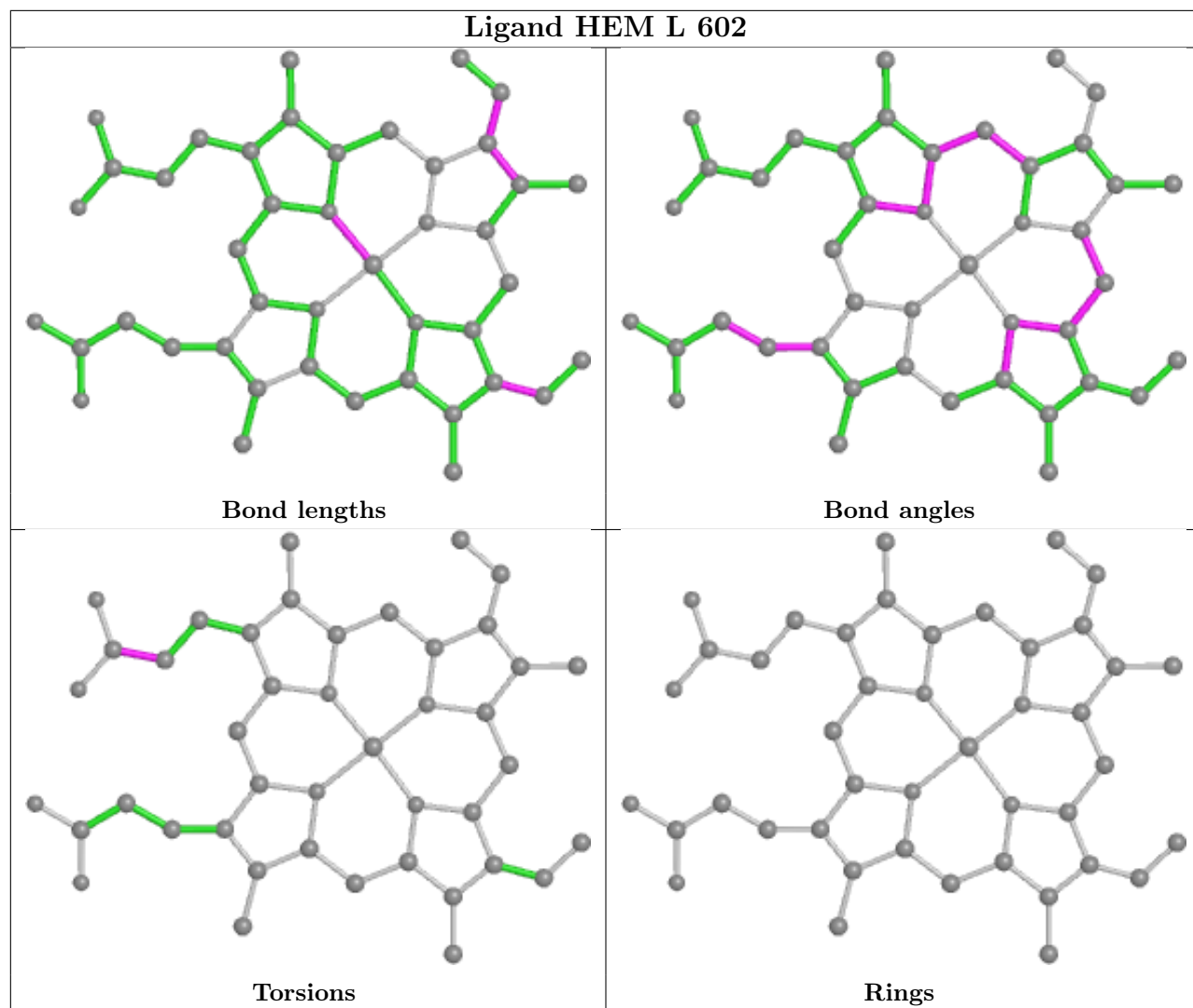


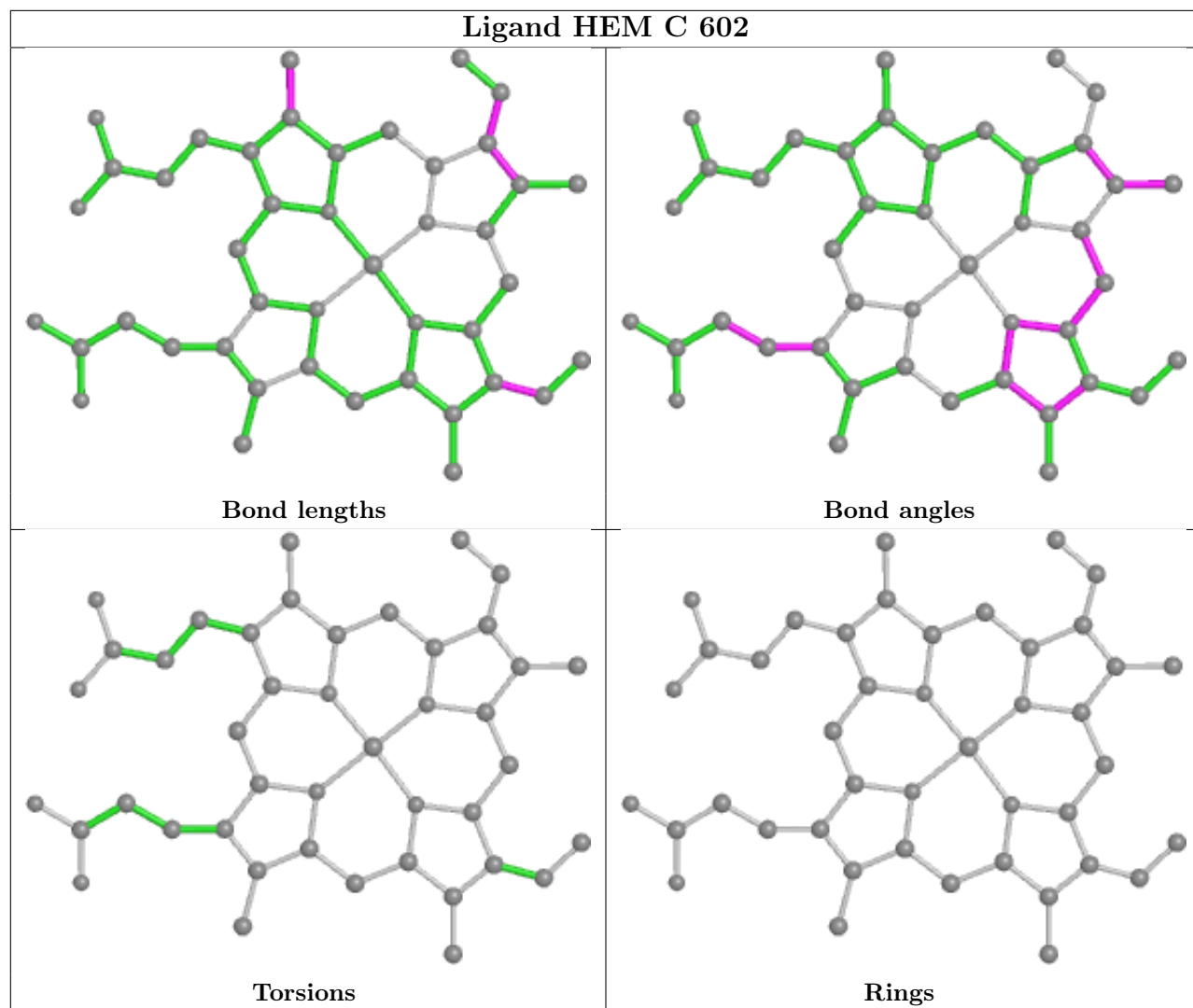


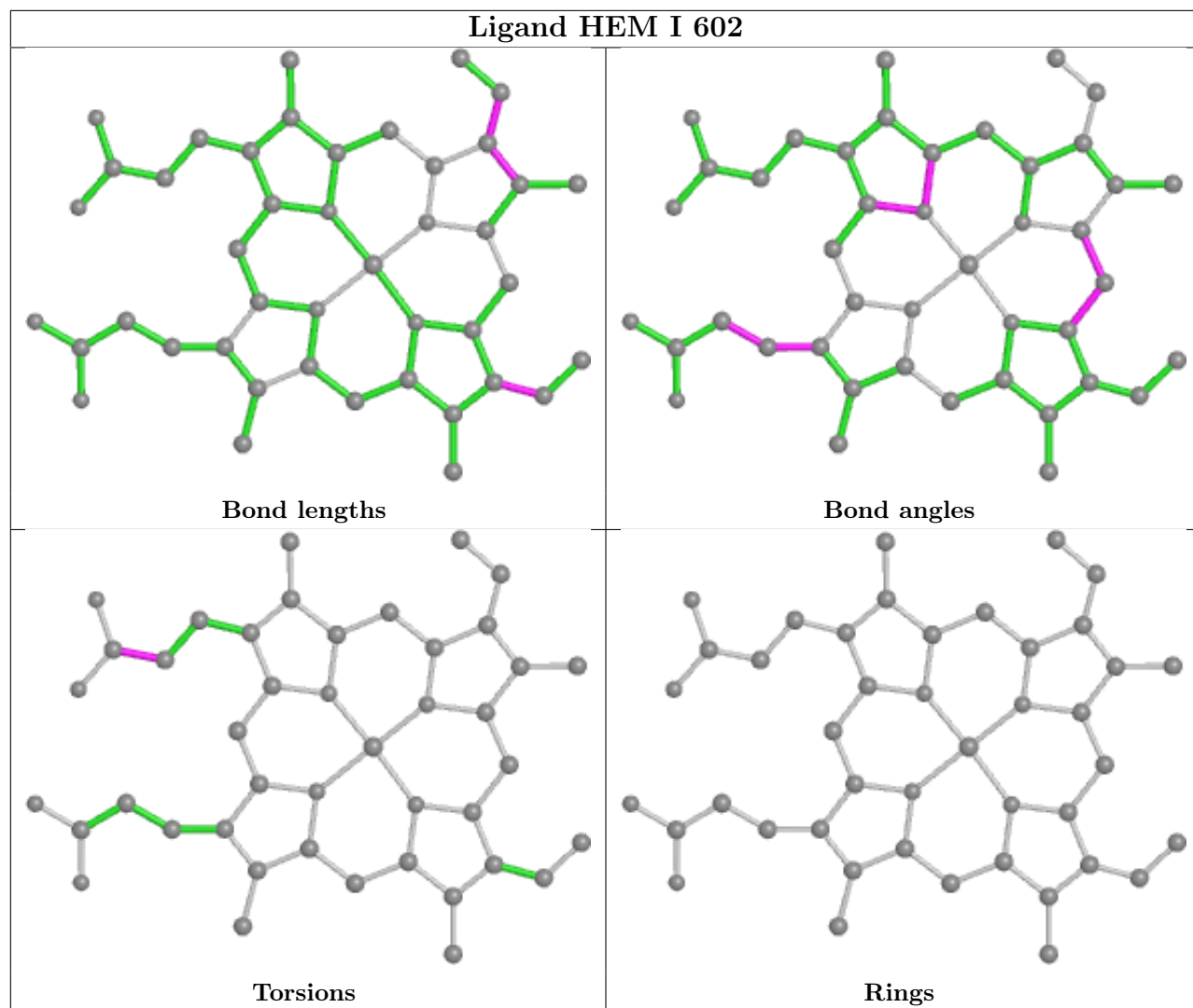


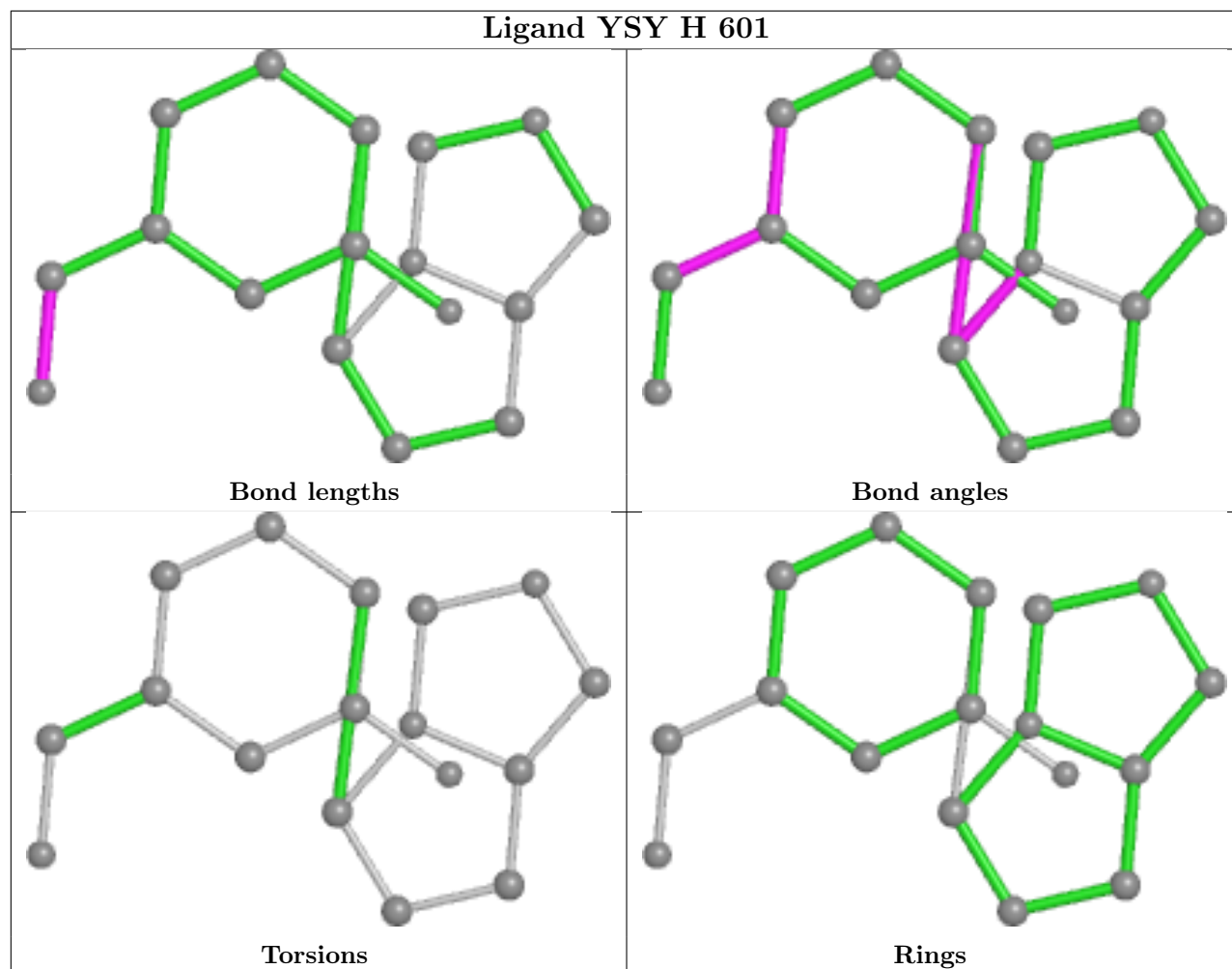


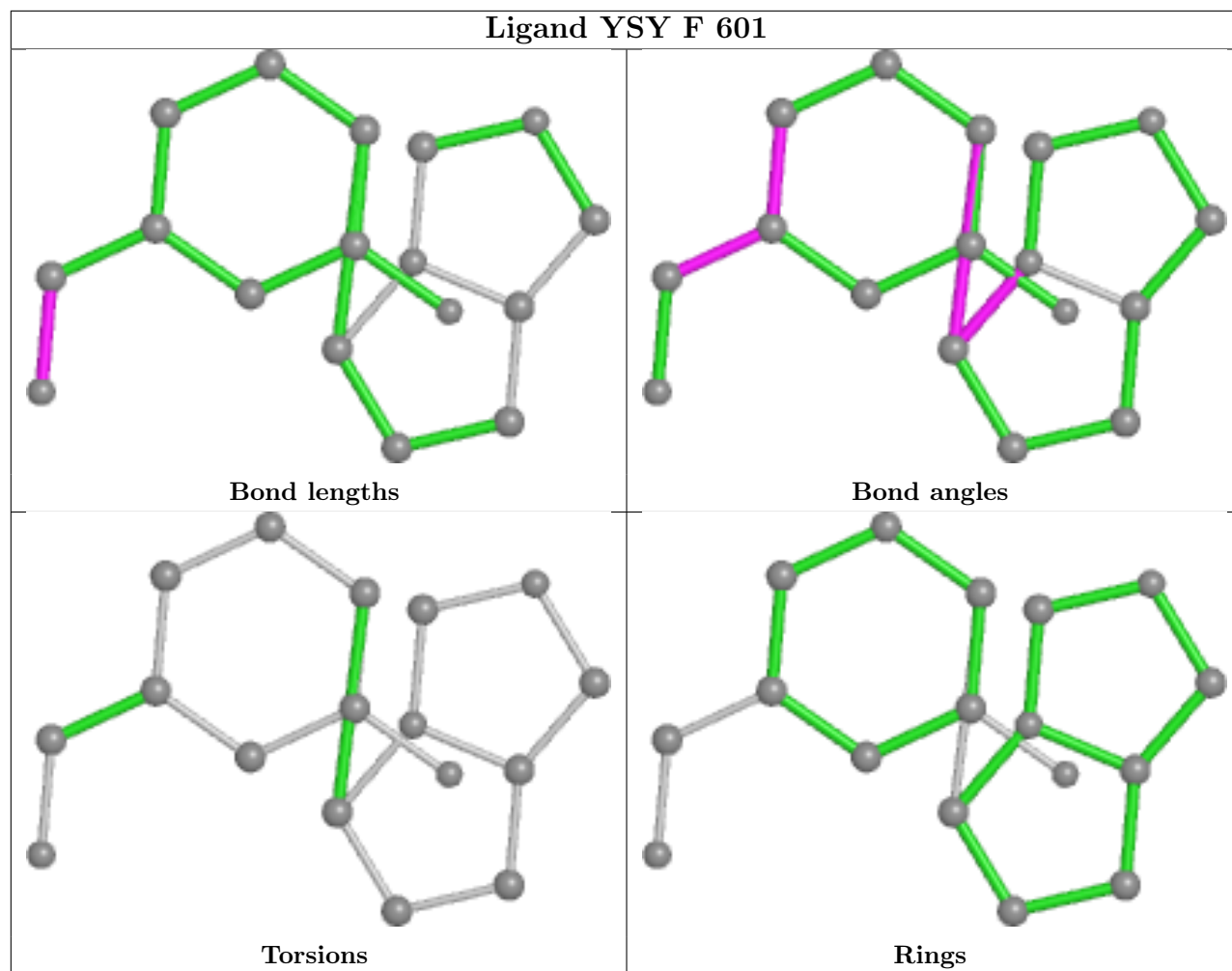


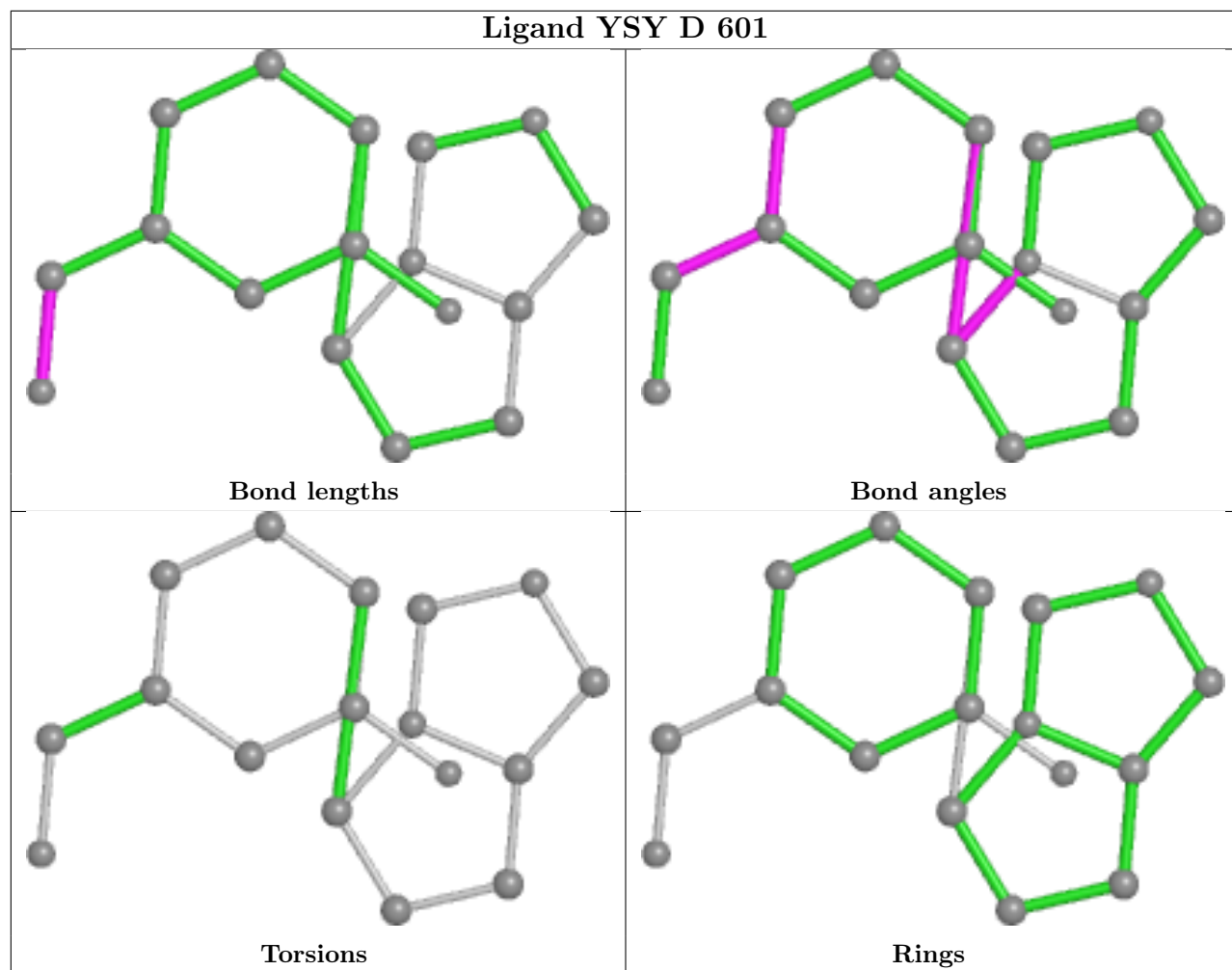


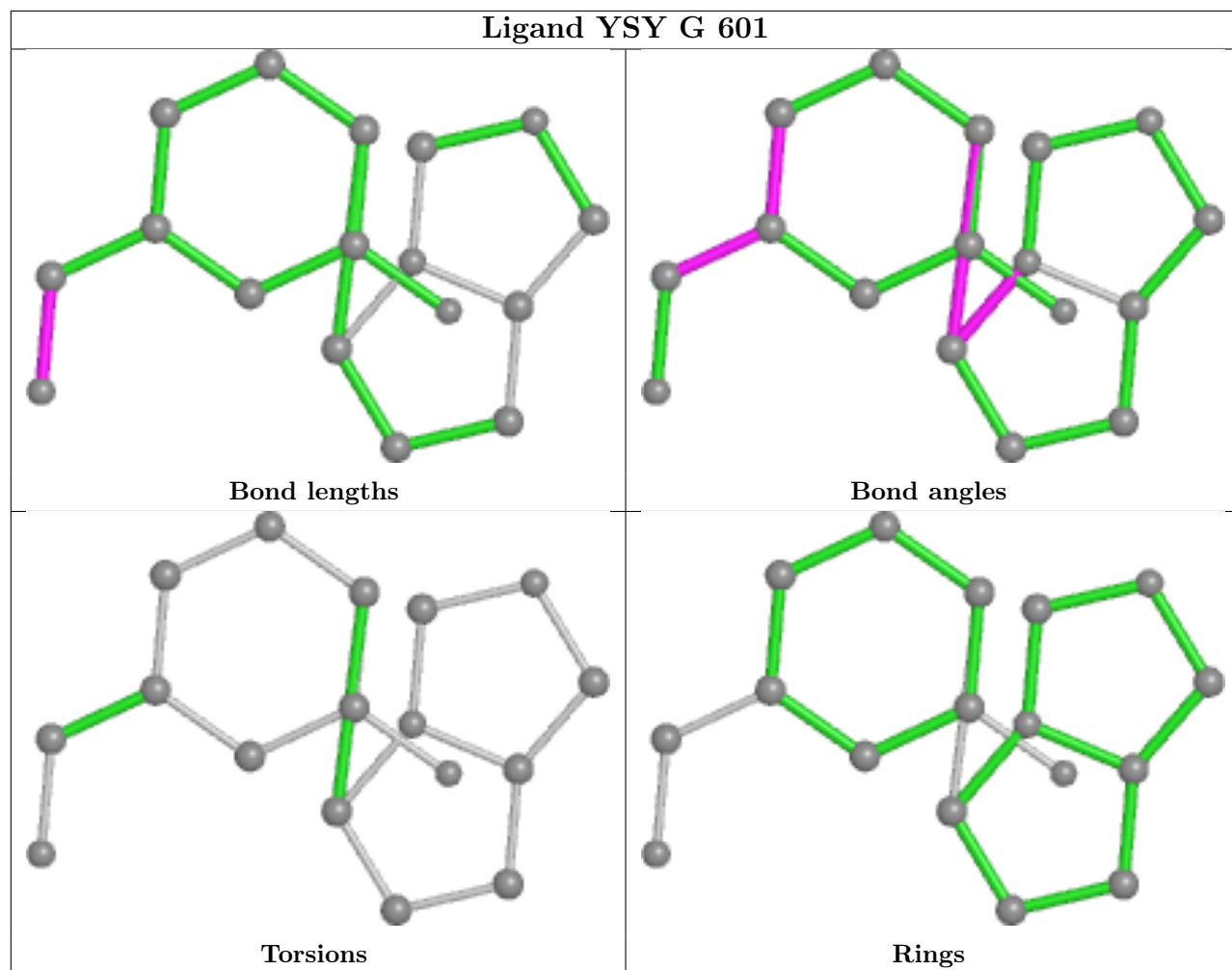


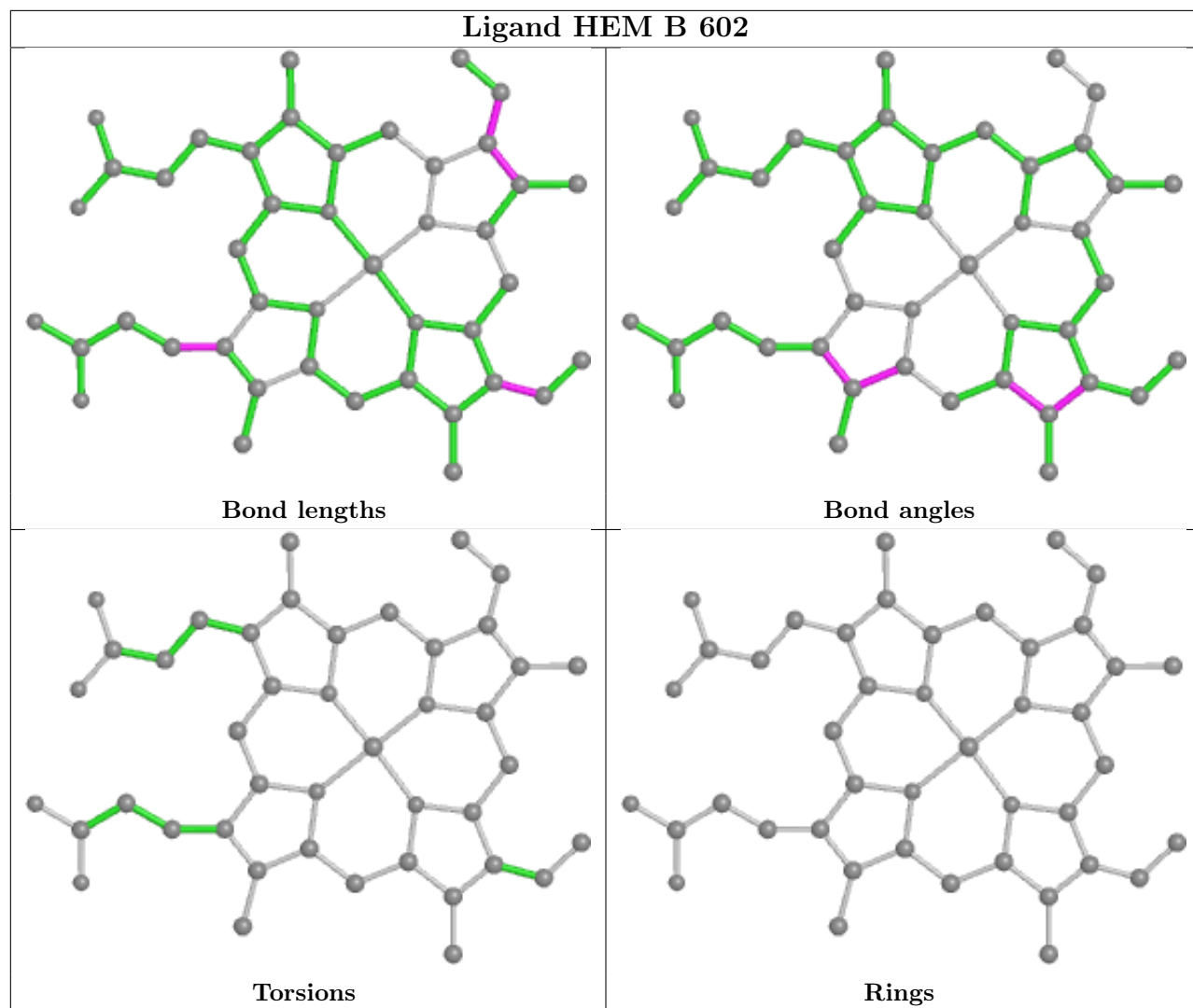


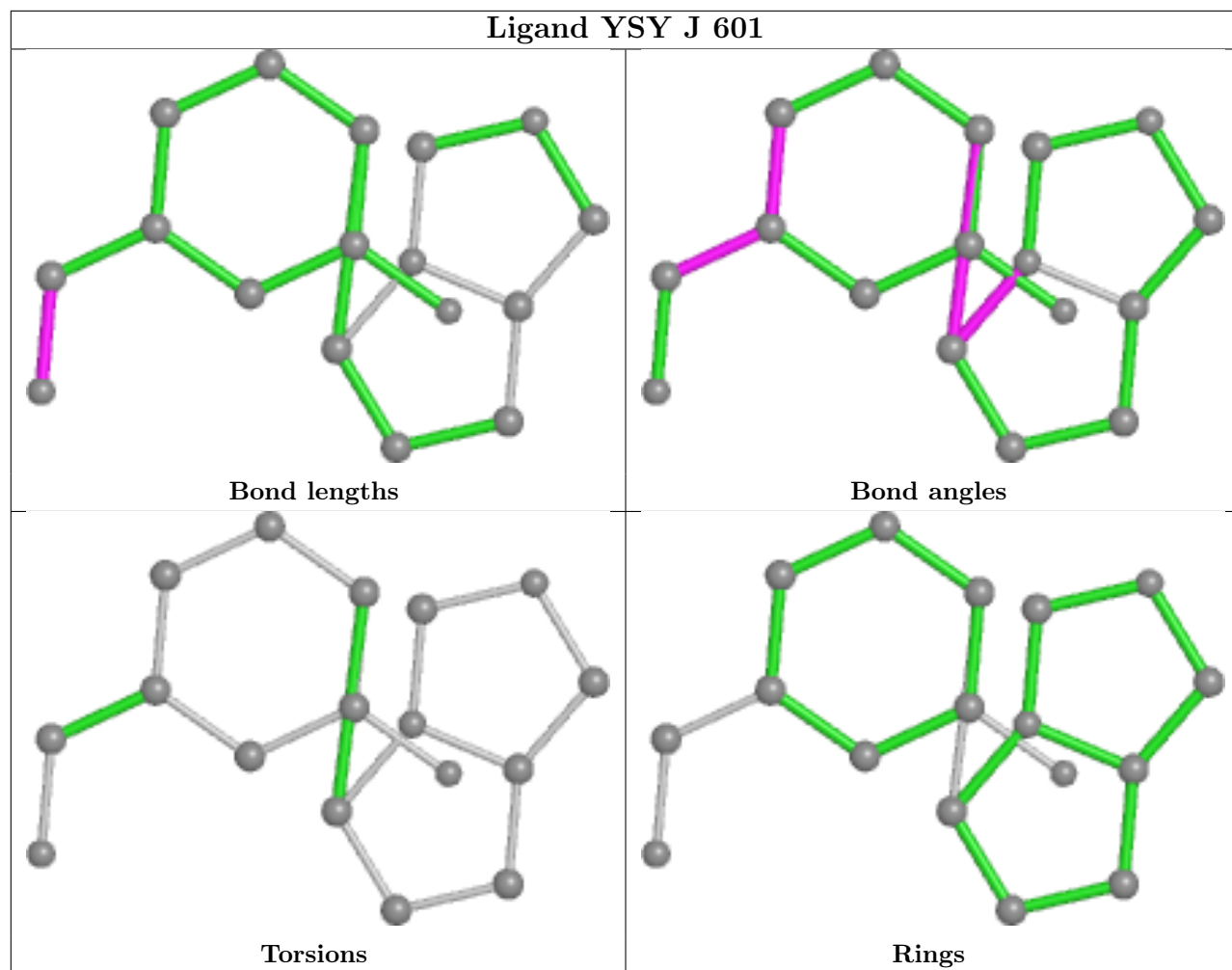


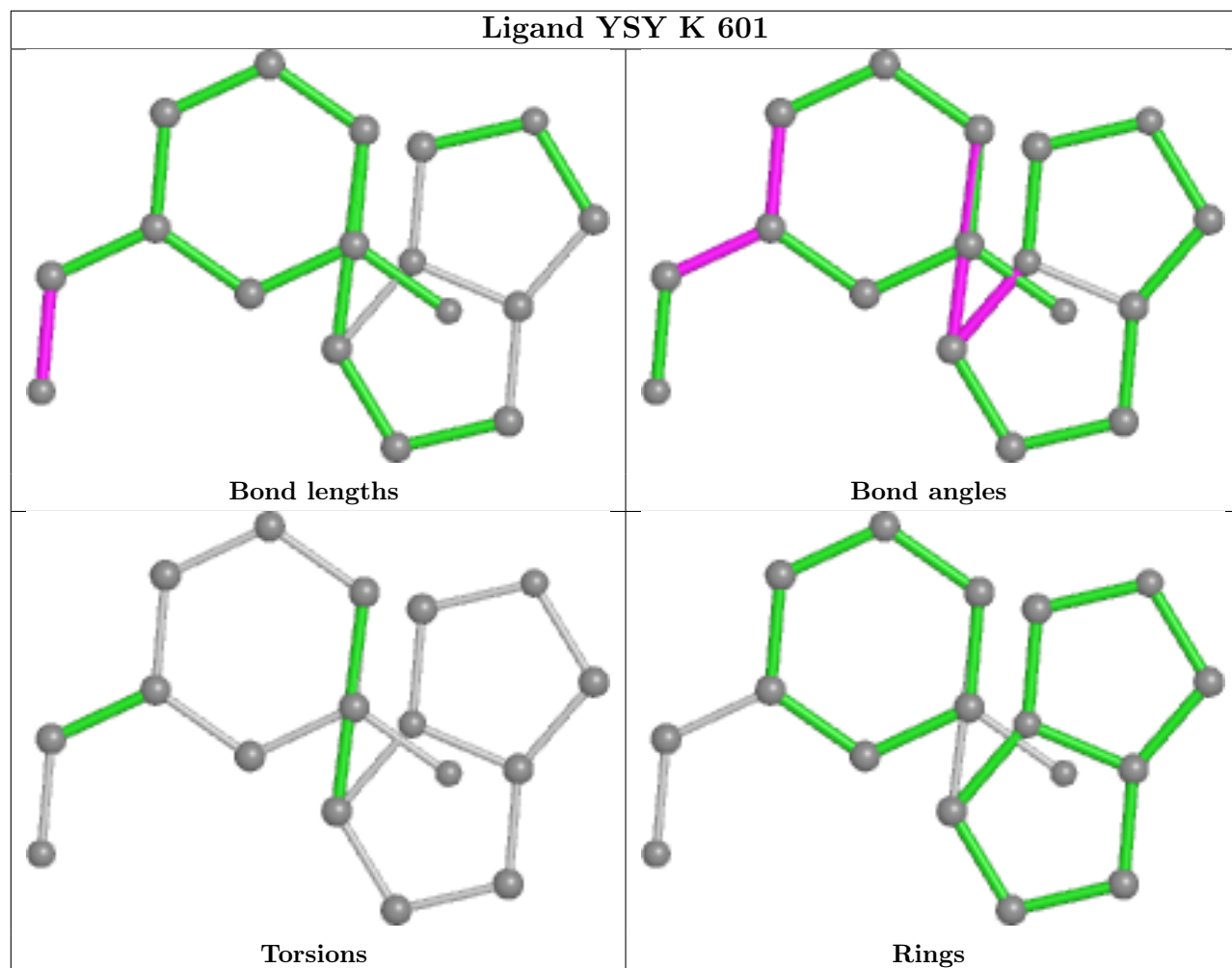


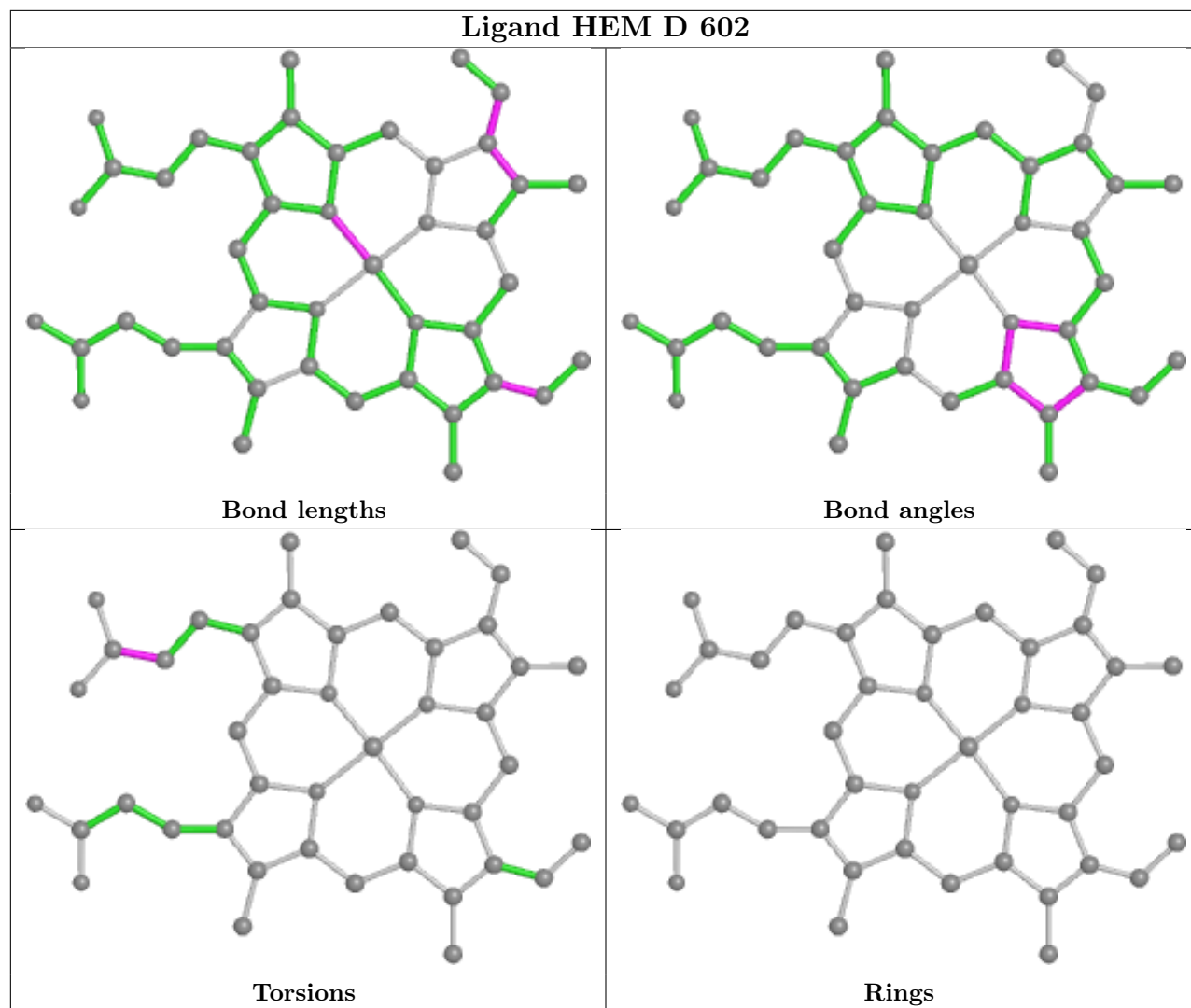


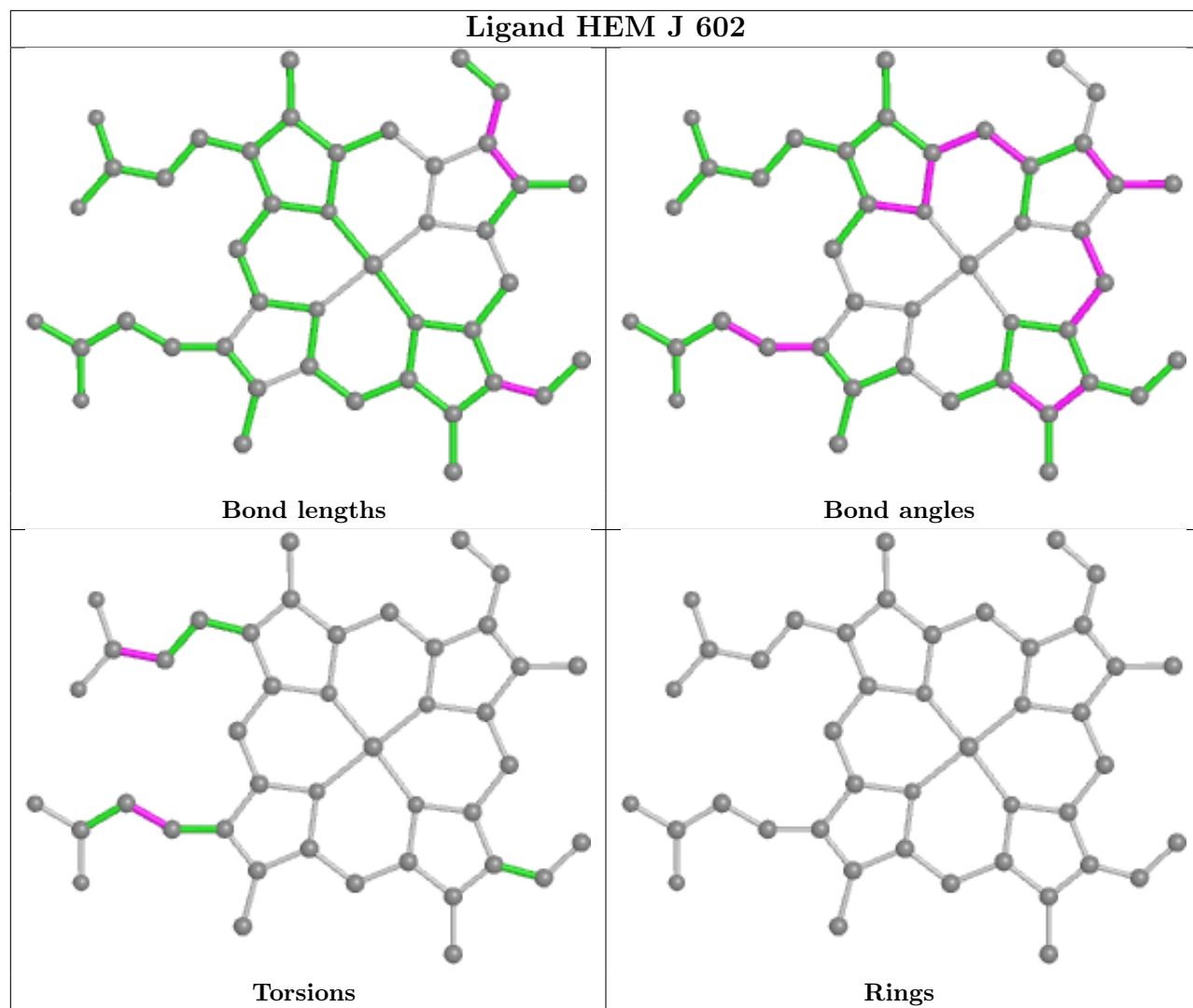


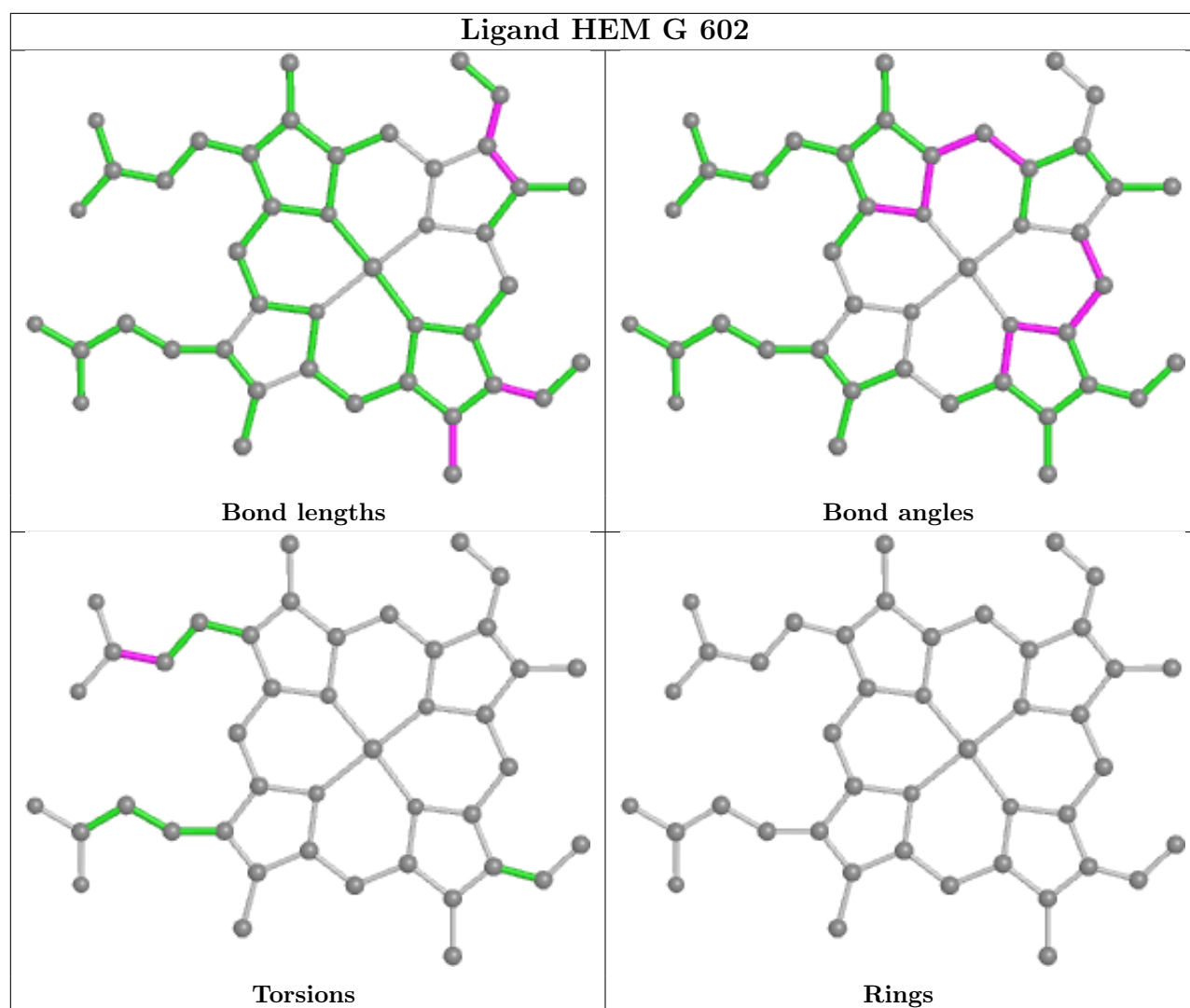












5.7 Other polymers [i](#)

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, 95th 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 ²)	Q<0.9
1	A	464/484 (95%)	-0.54	0 100 100	34, 47, 66, 93	0
1	B	462/484 (95%)	-0.42	0 100 100	38, 55, 78, 97	0
1	C	465/484 (96%)	-0.42	0 100 100	36, 55, 85, 101	0
1	D	463/484 (95%)	-0.41	2 (0%) 92 84	39, 55, 80, 94	0
1	E	461/484 (95%)	-0.43	3 (0%) 87 74	35, 52, 72, 90	0
1	F	461/484 (95%)	-0.39	0 100 100	40, 60, 88, 103	0
1	G	461/484 (95%)	-0.31	4 (0%) 84 68	42, 63, 84, 107	0
1	H	464/484 (95%)	-0.23	7 (1%) 73 53	42, 64, 84, 112	0
1	I	462/484 (95%)	-0.24	9 (1%) 66 45	47, 65, 92, 110	0
1	J	459/484 (94%)	-0.28	5 (1%) 80 62	44, 68, 95, 118	0
1	K	464/484 (95%)	-0.32	1 (0%) 95 89	45, 67, 96, 126	0
1	L	459/484 (94%)	-0.18	10 (2%) 62 39	46, 67, 99, 117	0
All	All	5545/5808 (95%)	-0.35	41 (0%) 87 74	34, 60, 89, 126	0

The worst 5 of 41 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	34	THR	3.5
1	H	34	THR	3.3
1	H	318	THR	3.1
1	E	318	THR	2.9
1	G	35	VAL	2.8

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](#)

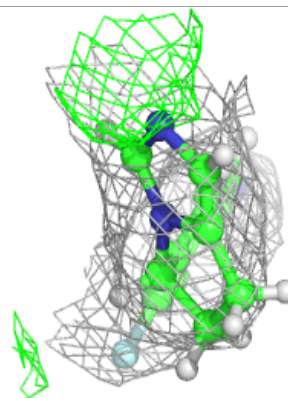
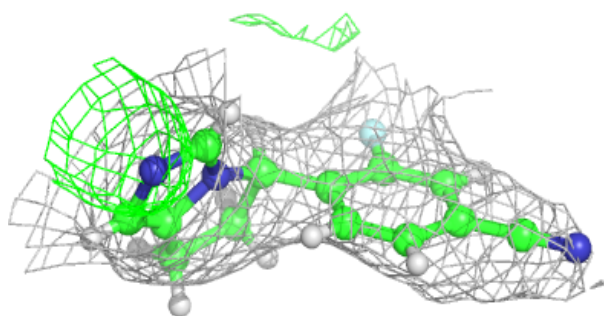
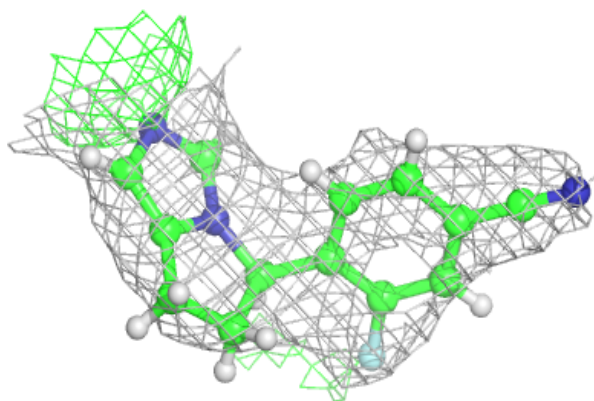
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	YSY	B	601	17/17	0.93	0.33	36,46,57,59	0
2	YSY	A	601	17/17	0.94	0.32	34,45,53,55	0
2	YSY	E	601	17/17	0.94	0.38	35,45,55,73	0
2	YSY	J	601	17/17	0.94	0.32	48,54,63,68	0
2	YSY	K	601	17/17	0.94	0.28	44,50,58,66	0
2	YSY	L	601	17/17	0.94	0.40	44,61,77,83	0
3	HEM	J	602	43/43	0.94	0.35	41,58,76,102	0
2	YSY	F	601	17/17	0.95	0.28	45,55,65,75	0
2	YSY	G	601	17/17	0.95	0.34	50,55,68,71	0
2	YSY	H	601	17/17	0.95	0.37	50,58,70,73	0
3	HEM	B	602	43/43	0.95	0.32	39,50,61,92	0
2	YSY	I	601	17/17	0.95	0.38	42,52,65,65	0
3	HEM	L	602	43/43	0.95	0.39	37,61,75,88	0
3	HEM	H	602	43/43	0.96	0.40	38,57,72,74	0
3	HEM	I	602	43/43	0.96	0.39	45,58,73,83	0
3	HEM	F	602	43/43	0.96	0.36	40,54,68,80	0
3	HEM	K	602	43/43	0.96	0.32	40,54,65,77	0
3	HEM	G	602	43/43	0.96	0.36	39,54,67,74	0
3	HEM	A	602	43/43	0.97	0.32	30,46,55,60	0
2	YSY	C	601	17/17	0.97	0.25	35,45,53,55	0
3	HEM	C	602	43/43	0.97	0.28	31,44,54,59	0
3	HEM	D	602	43/43	0.97	0.30	33,46,57,59	0
3	HEM	E	602	43/43	0.97	0.34	29,44,52,58	0
2	YSY	D	601	17/17	0.97	0.33	36,43,51,59	0

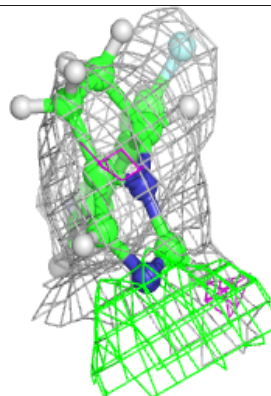
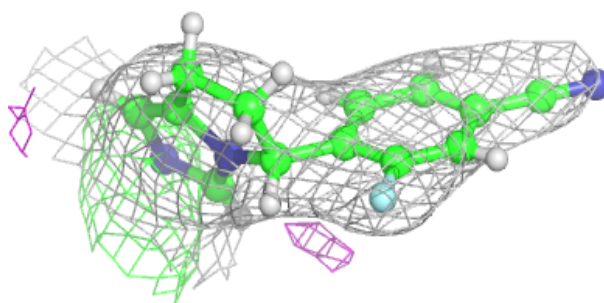
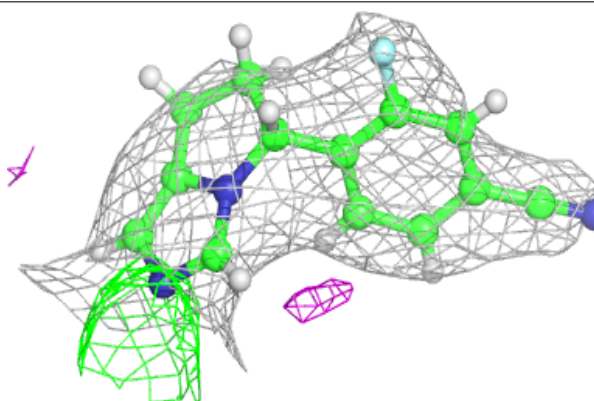
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around YSY 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)

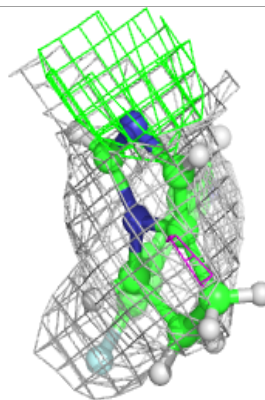
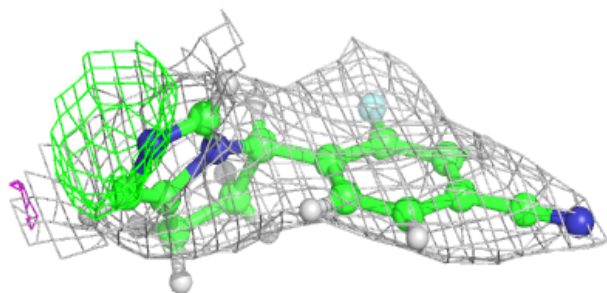
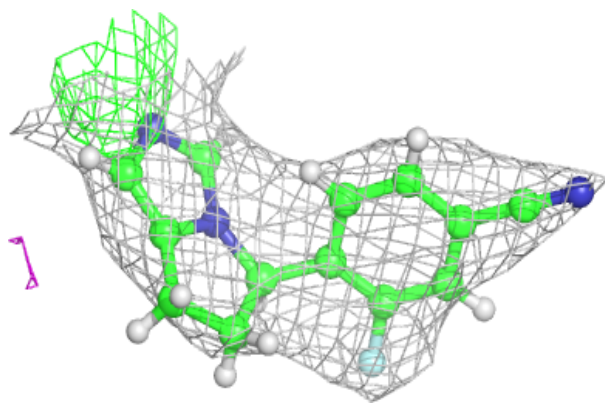
**Electron density around YSY A 601:**

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

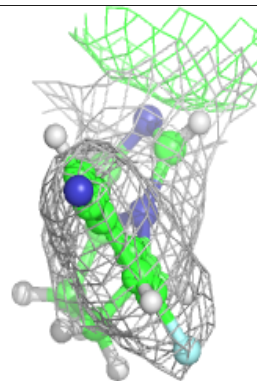
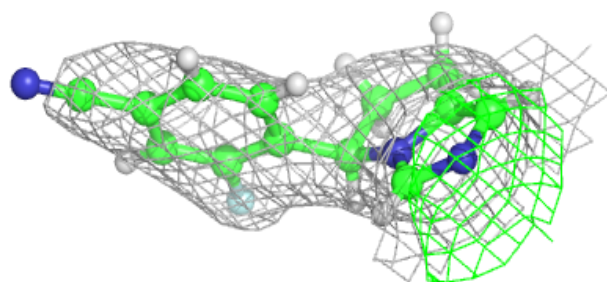
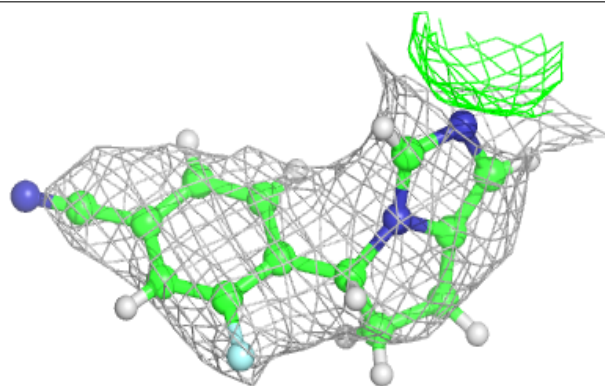


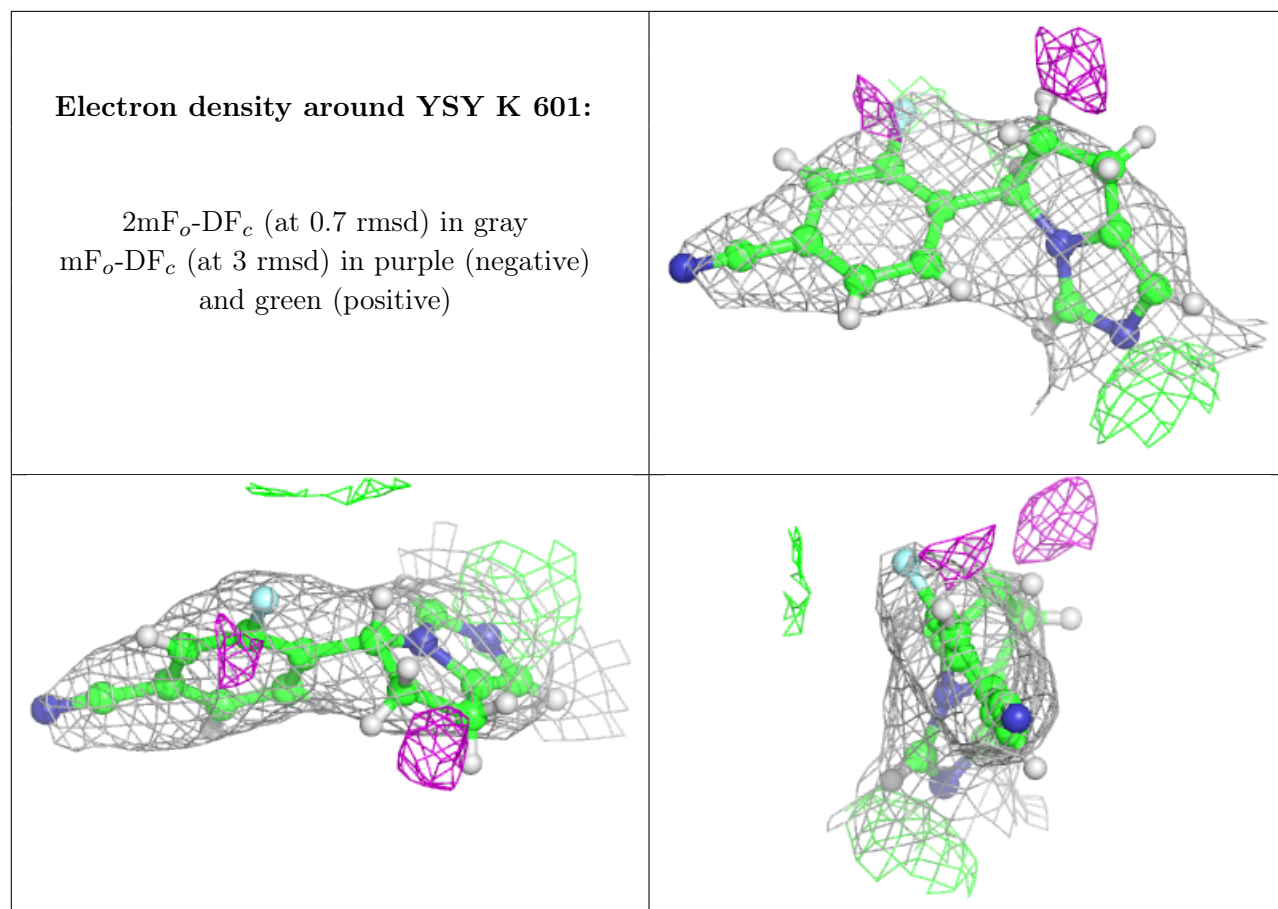
Electron density around YSY E 601:

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

**Electron density around YSY J 601:**

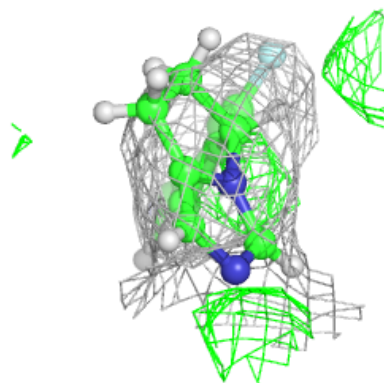
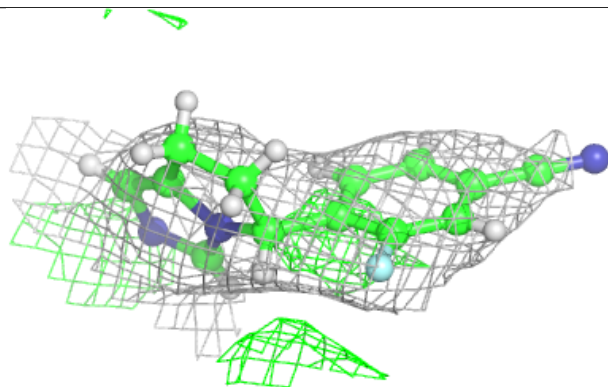
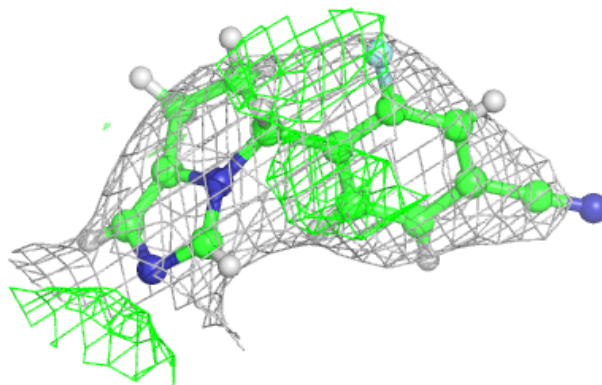
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





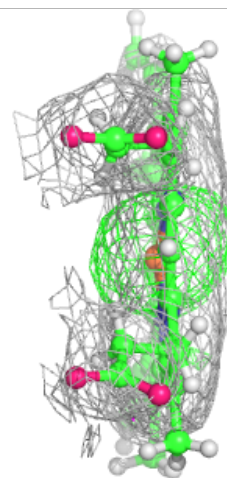
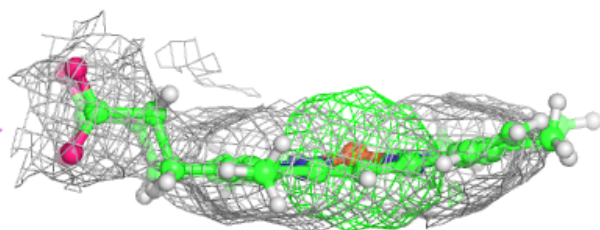
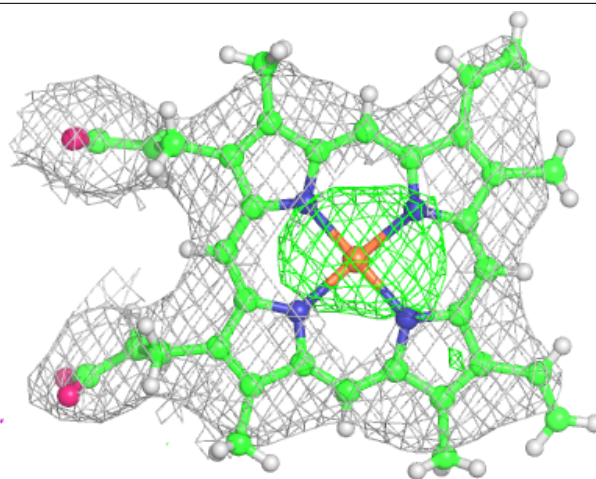
Electron density around YSY L 601:

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and green (positive)



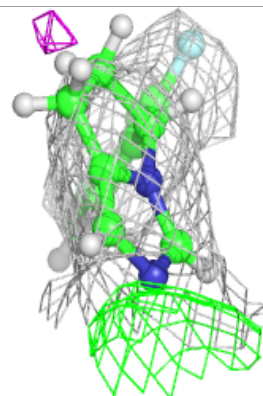
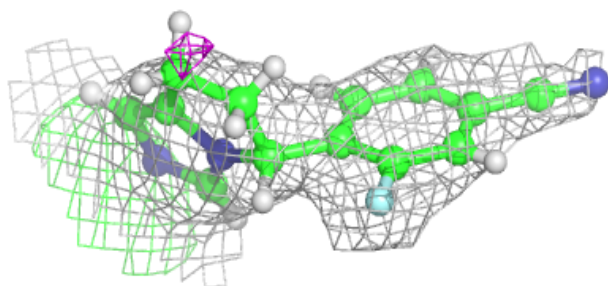
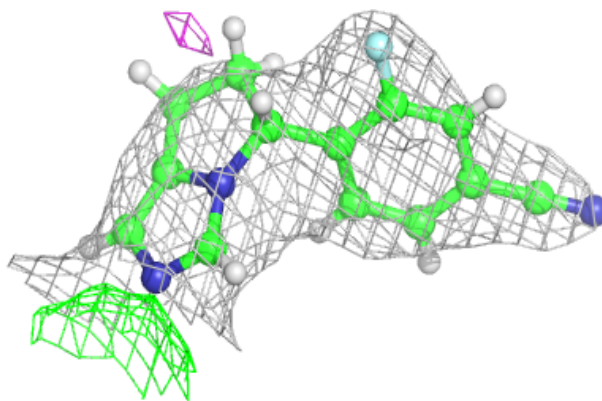
Electron density around HEM J 602:

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

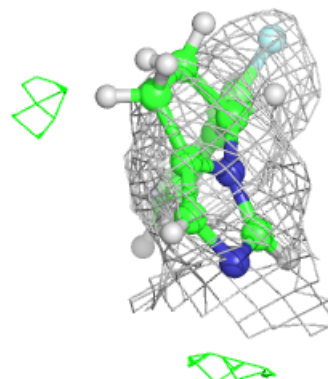
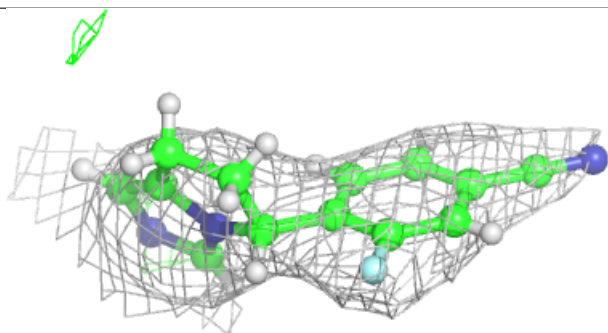
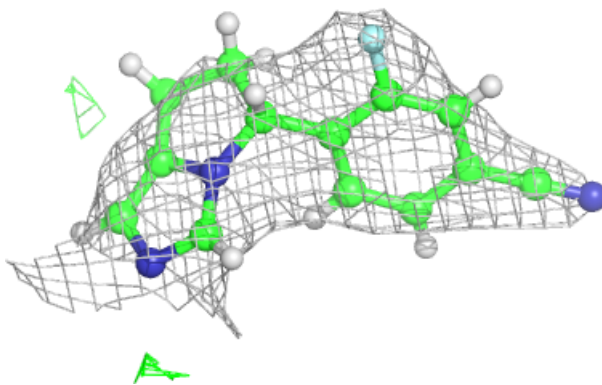


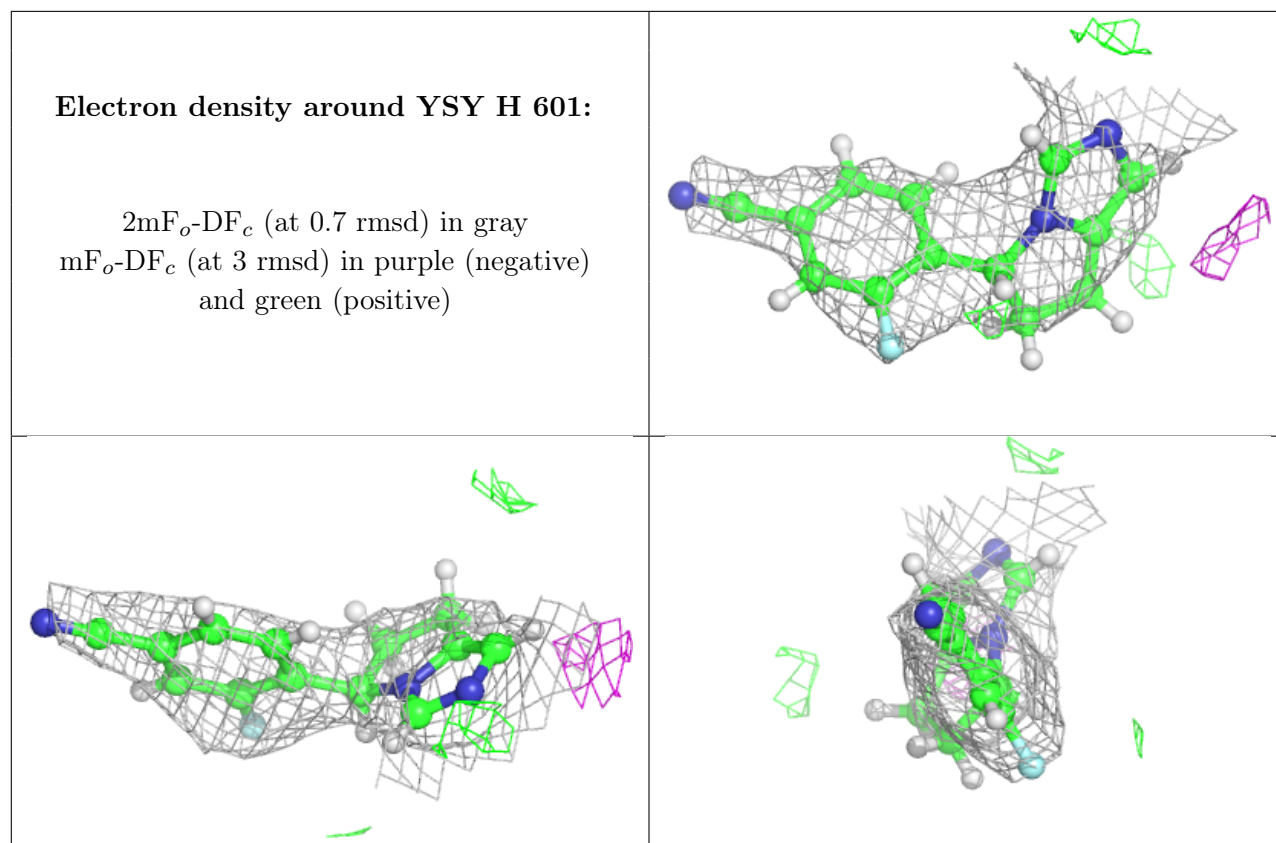
Electron density around YSY F 601:

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and green (positive)

**Electron density around YSY G 601:**

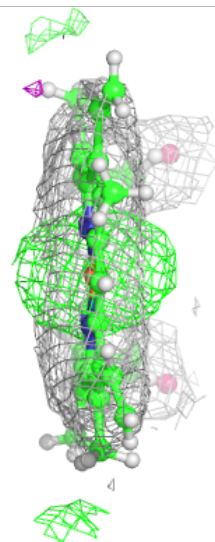
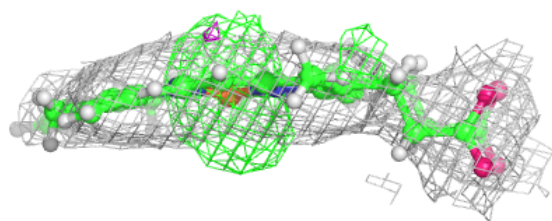
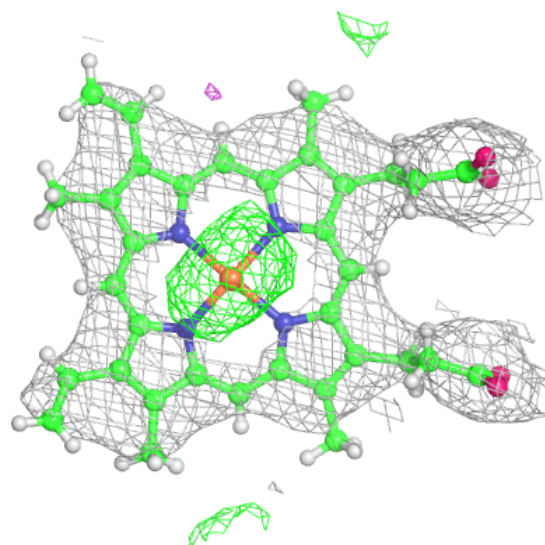
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





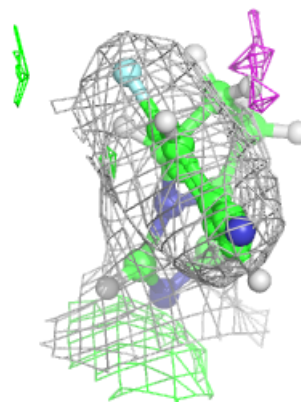
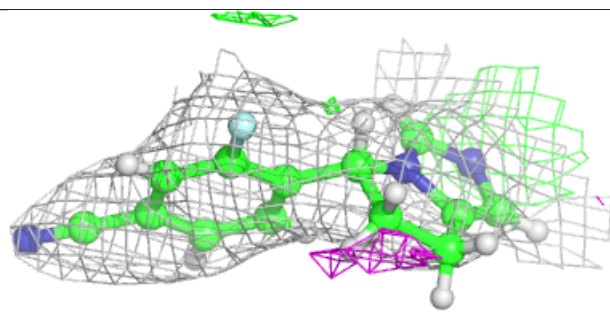
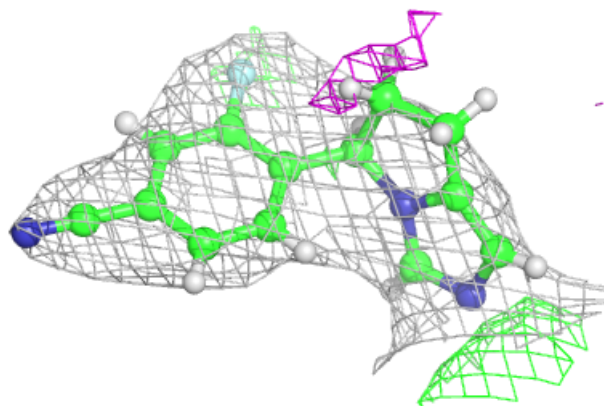
Electron density around HEM B 602:

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



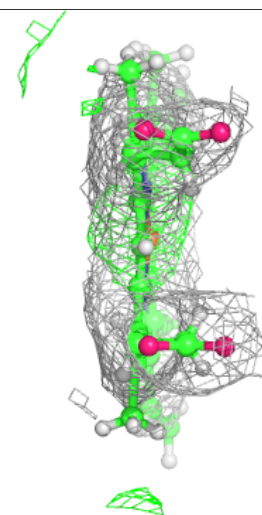
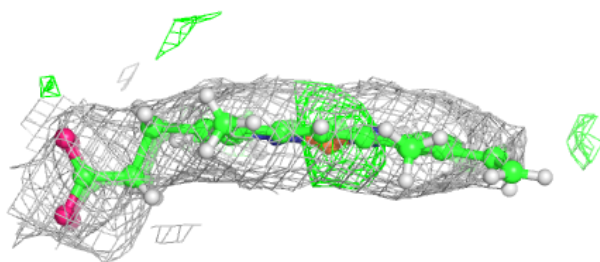
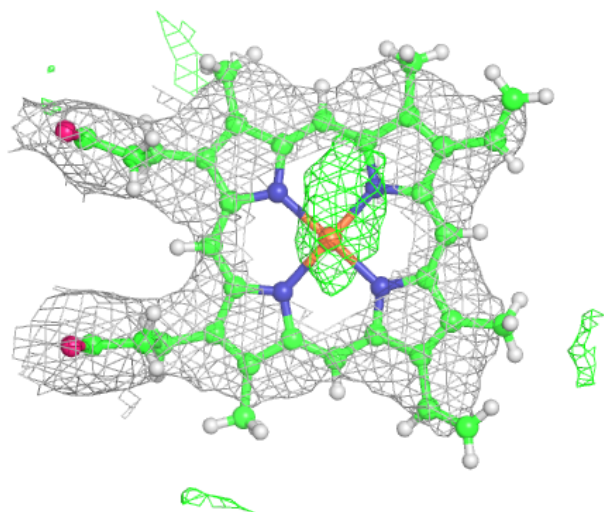
Electron density around YSY I 601:

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and green (positive)



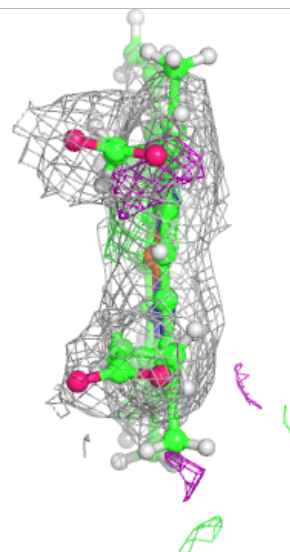
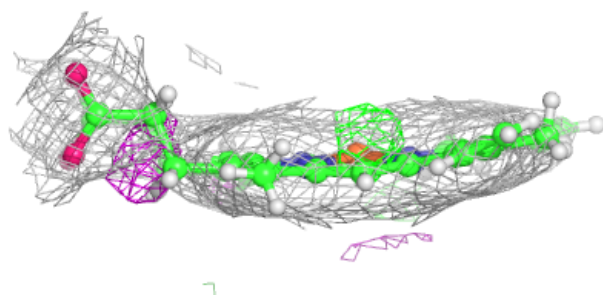
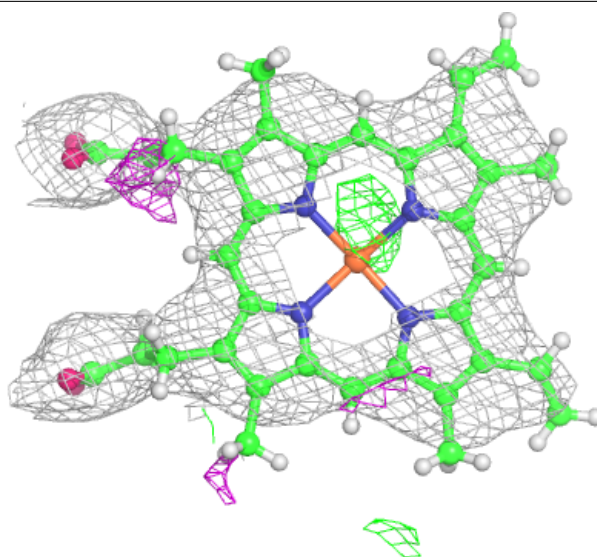
Electron density around HEM L 602:

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and green (positive)



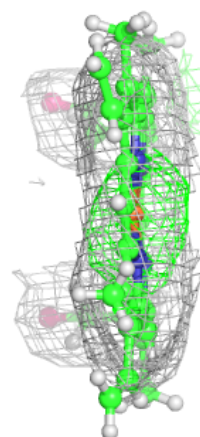
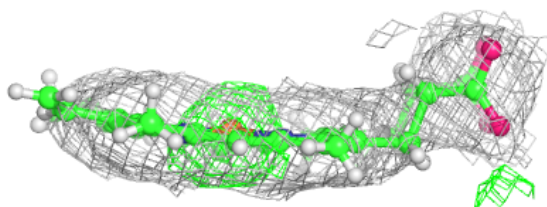
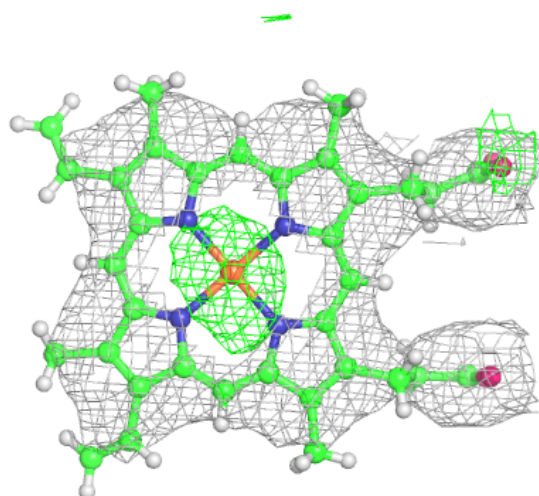
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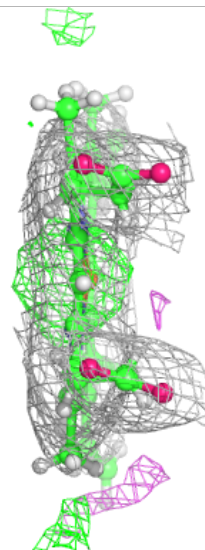
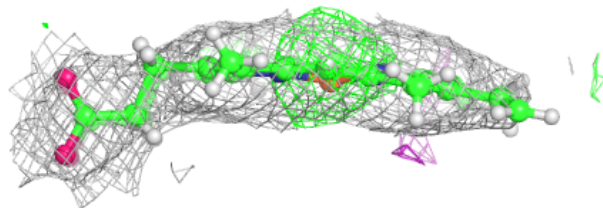
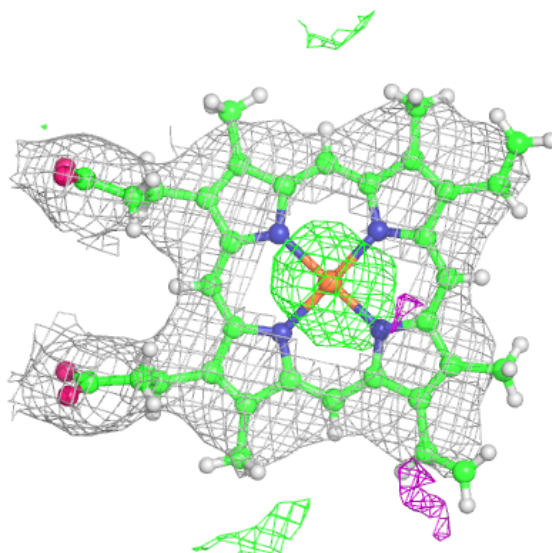
Electron density around HEM I 602:

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and green (positive)



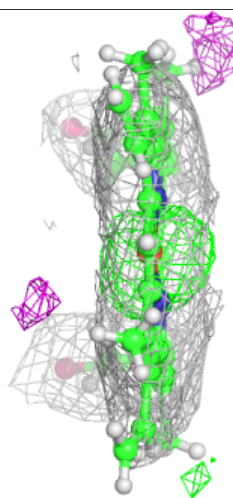
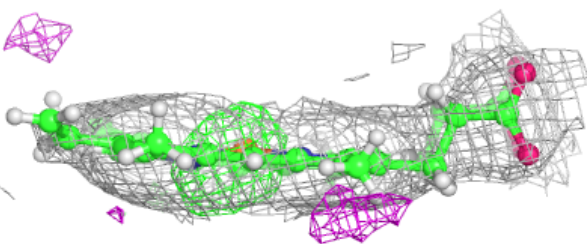
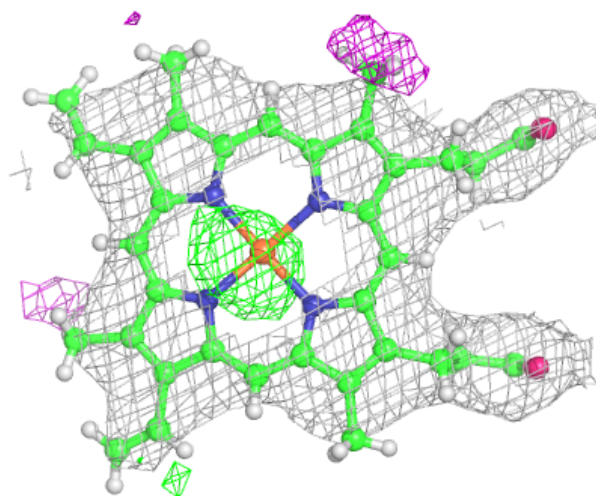
Electron density around HEM F 602:

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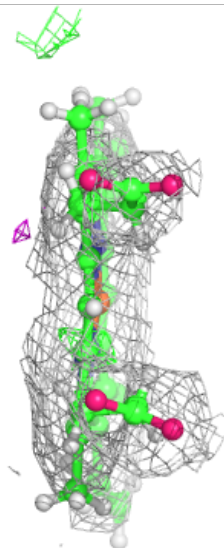
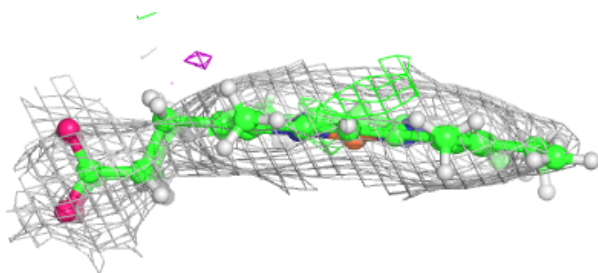
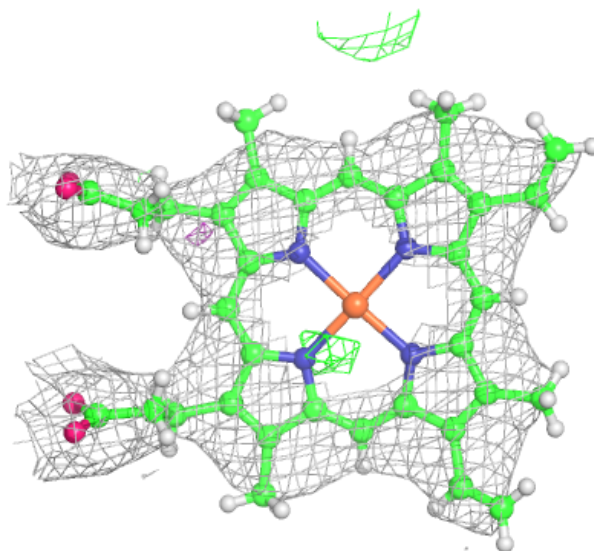
Electron density around HEM K 602:

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and green (positive)



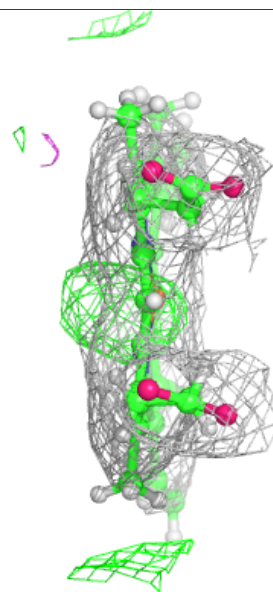
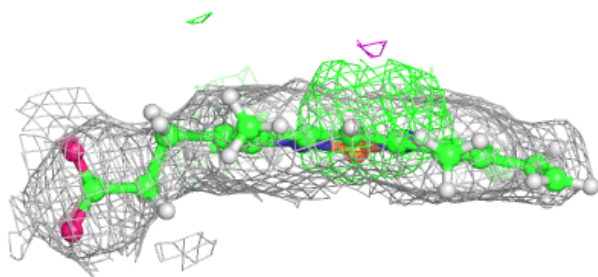
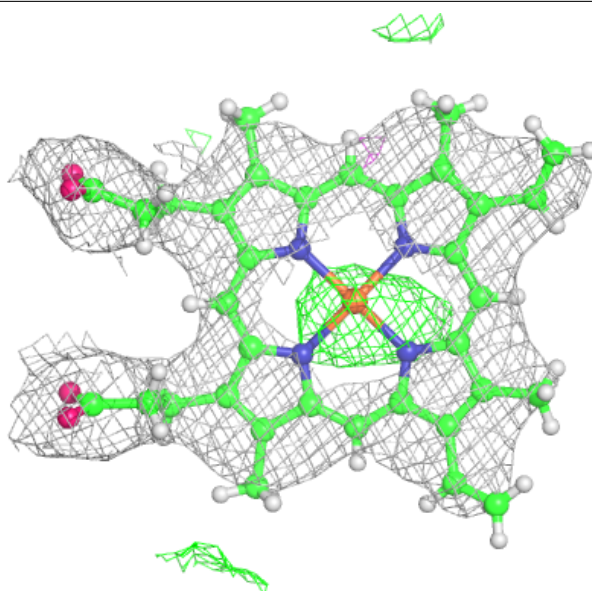
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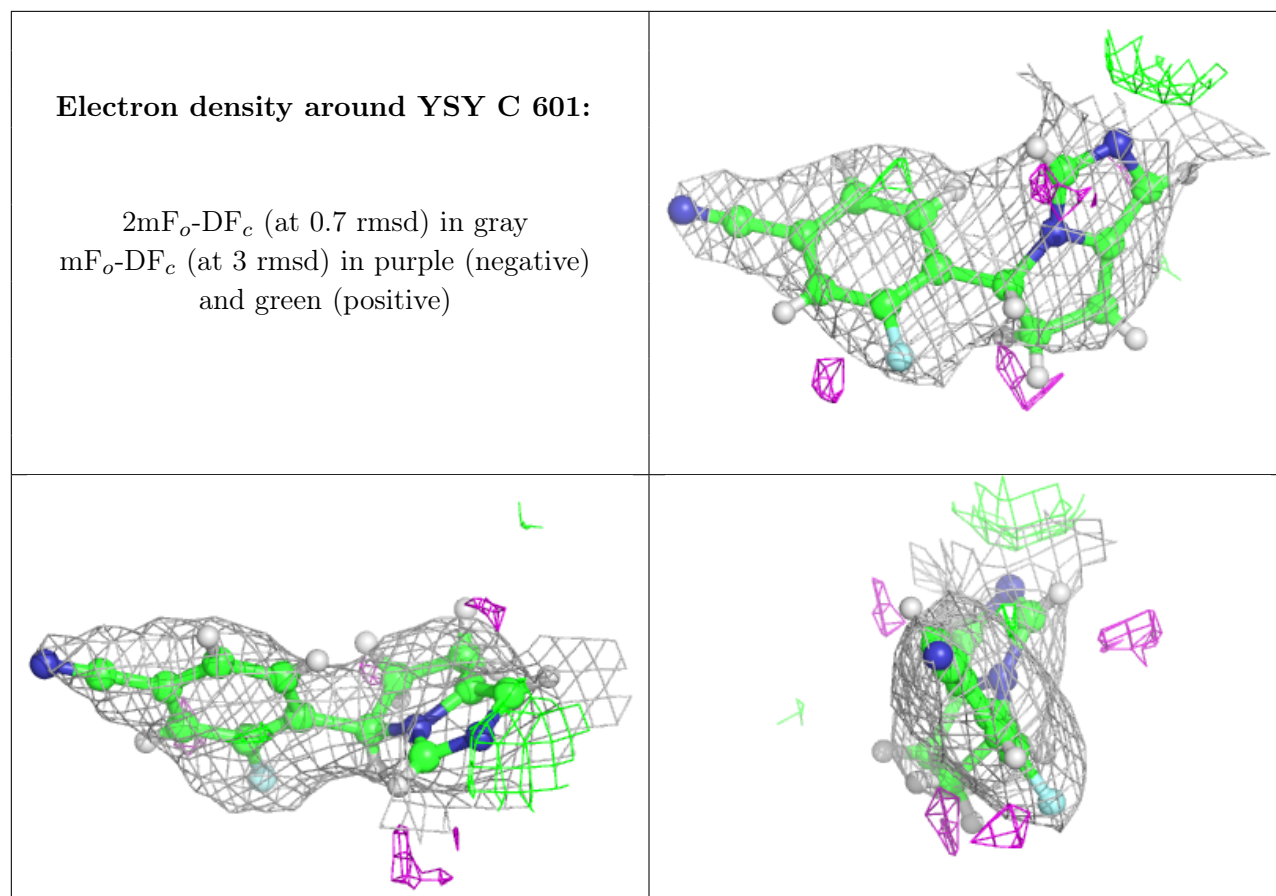
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and green (positive)



Electron density around HEM A 602:

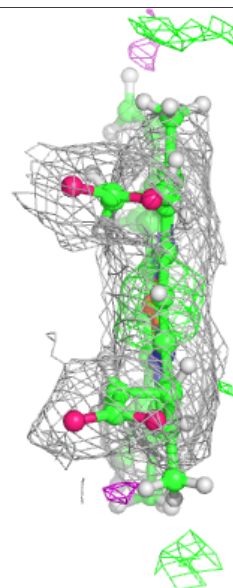
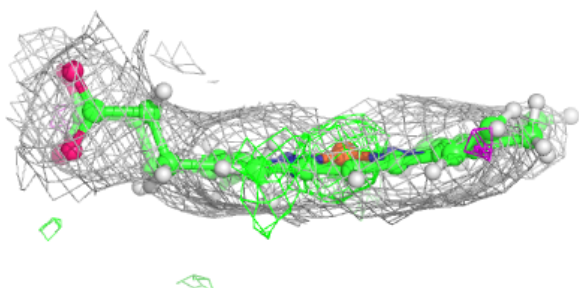
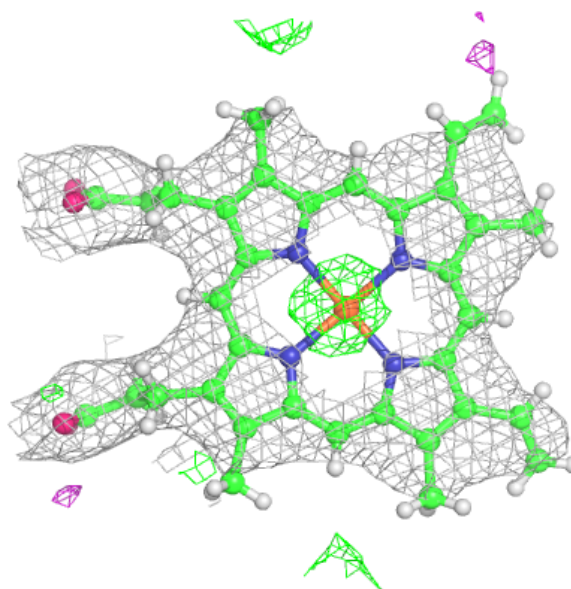
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and green (positive)





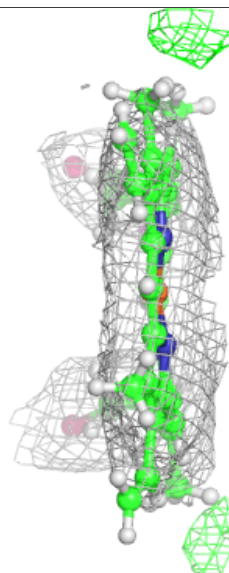
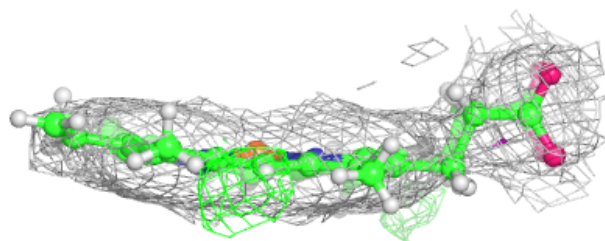
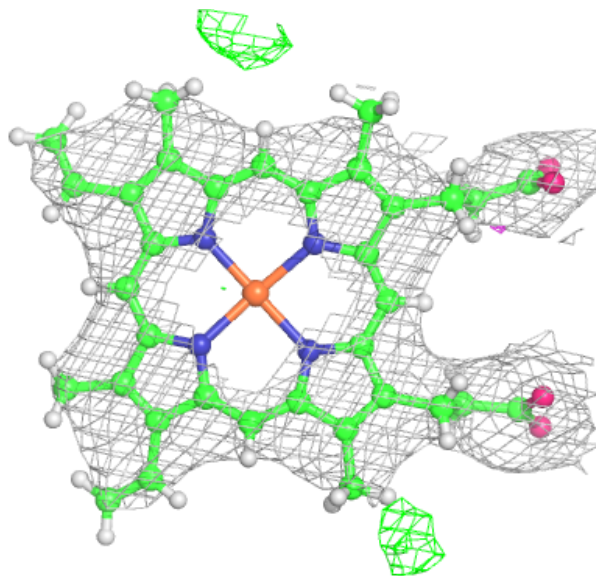
Electron density around HEM C 602:

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



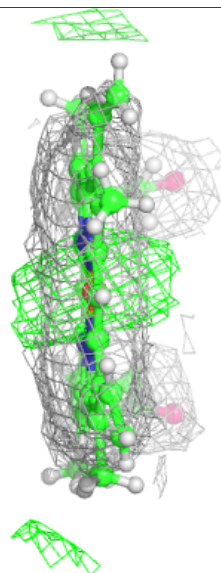
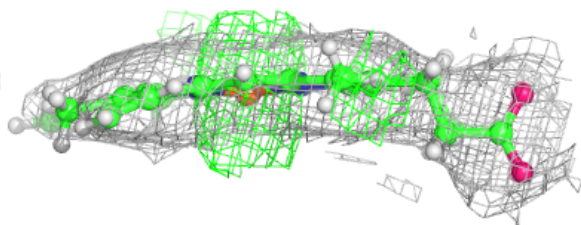
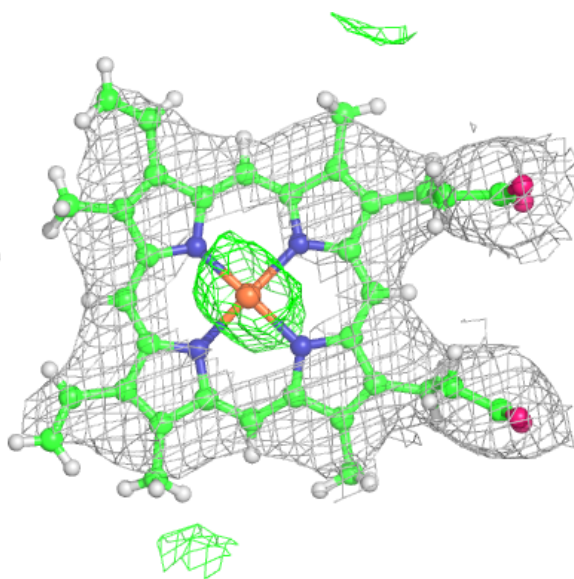
Electron density around HEM D 602:

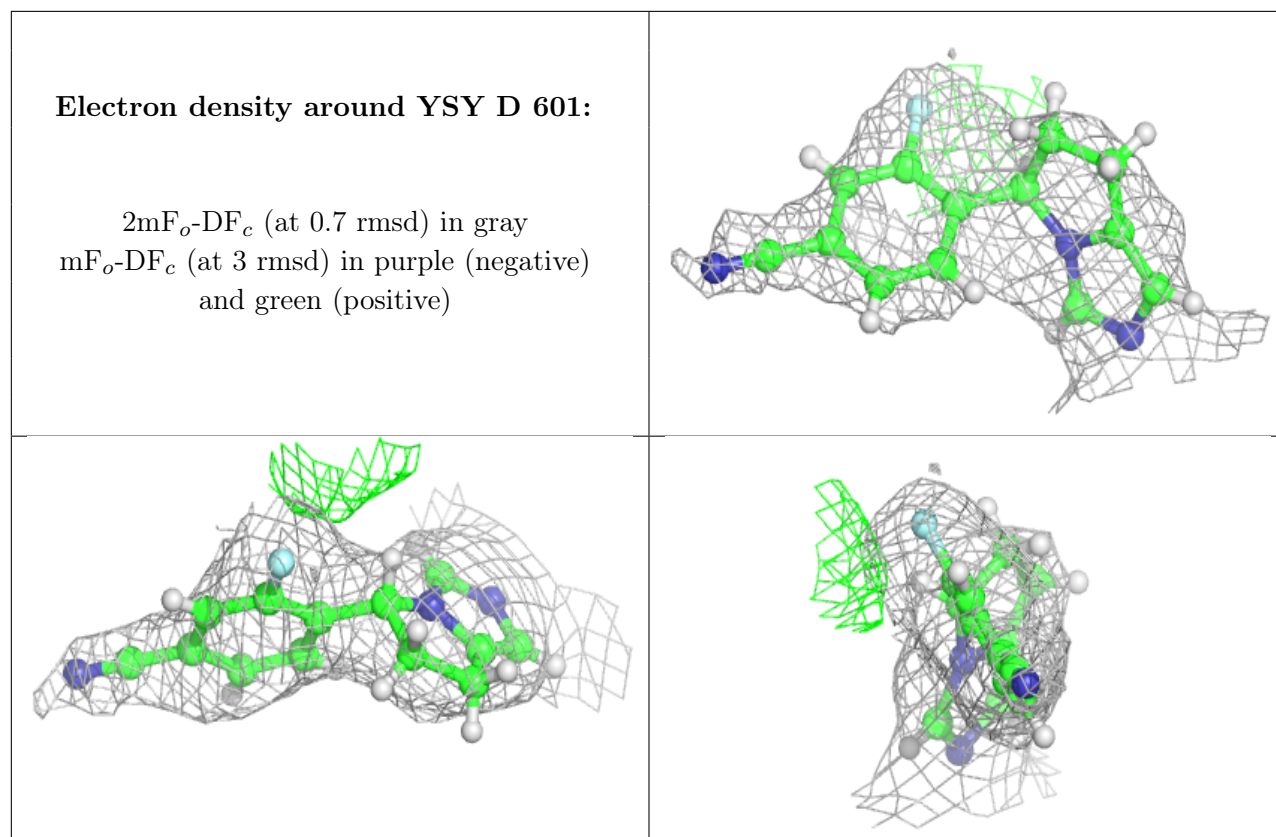
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM E 602:

$2mF_o-DF_c$ (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.