



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 02:38 AM UTC

PDB ID : 8GK3 / pdb_00008gk3
Title : Cytochrome P450 3A7 in complex with Dehydroepiandrosterone sulfate
Authors : Liu, J.; Scott, E.E.
Deposited on : 2023-03-16
Resolution : 2.60 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

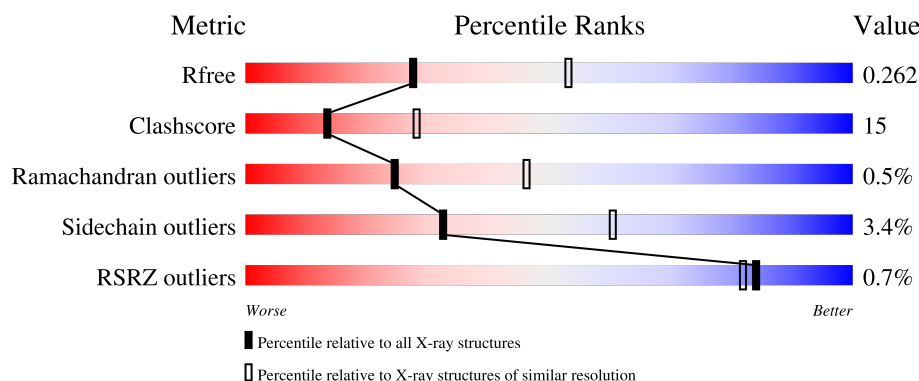
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

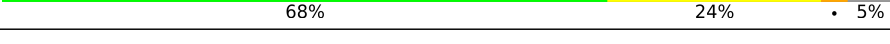
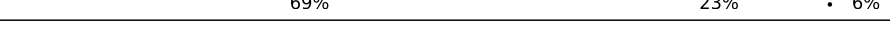
The reported resolution of this entry is 2.60 Å.

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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	486	 75% 21% • •
1	B	486	 70% 24% • 5%
1	C	486	 68% 24% • 5%
1	D	486	 69% 23% • 6%
1	E	486	 65% 27% • 5%

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Mol	Chain	Length	Quality of chain
1	F	486	% 62% 30% • 5%
1	G	486	65% 28% • 5%
1	H	486	65% 27% • 6%
1	I	486	65% 28% • 5%
1	J	486	% 65% 28% • 6%
1	K	486	66% 28% •• 5%
1	L	486	4% 47% 37% 6% • 9%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 91794 atoms, of which 46378 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 3A7.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	473	Total	C	H	N	O	S	0	0	0
			7690	2470	3892	628	681	19			
1	B	462	Total	C	H	N	O	S	0	0	0
			7501	2417	3796	609	660	19			
1	C	463	Total	C	H	N	O	S	0	0	0
			7507	2417	3798	608	665	19			
1	D	459	Total	C	H	N	O	S	0	0	0
			7453	2402	3771	606	655	19			
1	E	460	Total	C	H	N	O	S	0	0	0
			7469	2404	3783	604	659	19			
1	F	461	Total	C	H	N	O	S	0	0	0
			7496	2413	3799	608	657	19			
1	G	462	Total	C	H	N	O	S	0	0	0
			7503	2417	3798	609	660	19			
1	H	458	Total	C	H	N	O	S	0	0	0
			7434	2396	3763	602	654	19			
1	I	463	Total	C	H	N	O	S	0	0	0
			7508	2417	3799	608	665	19			
1	J	458	Total	C	H	N	O	S	0	0	0
			7441	2395	3771	602	654	19			
1	K	462	Total	C	H	N	O	S	0	0	0
			7503	2417	3798	609	660	19			
1	L	440	Total	C	H	N	O	S	0	0	0
			7133	2307	3602	580	626	18			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	MET	-	initiating methionine	UNP P24462
A	23	ALA	-	expression tag	UNP P24462
A	69	GLY	ARG	conflict	UNP P24462
A	77	GLY	CYS	conflict	UNP P24462
A	244	GLU	LYS	conflict	UNP P24462

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Chain	Residue	Modelled	Actual	Comment	Reference
A	421	ALA	LYS	conflict	UNP P24462
A	422	ALA	LYS	conflict	UNP P24462
A	424	ALA	LYS	conflict	UNP P24462
A	504	HIS	-	expression tag	UNP P24462
A	505	HIS	-	expression tag	UNP P24462
A	506	HIS	-	expression tag	UNP P24462
A	507	HIS	-	expression tag	UNP P24462
B	22	MET	-	initiating methionine	UNP P24462
B	23	ALA	-	expression tag	UNP P24462
B	69	GLY	ARG	conflict	UNP P24462
B	77	GLY	CYS	conflict	UNP P24462
B	244	GLU	LYS	conflict	UNP P24462
B	421	ALA	LYS	conflict	UNP P24462
B	422	ALA	LYS	conflict	UNP P24462
B	424	ALA	LYS	conflict	UNP P24462
B	504	HIS	-	expression tag	UNP P24462
B	505	HIS	-	expression tag	UNP P24462
B	506	HIS	-	expression tag	UNP P24462
B	507	HIS	-	expression tag	UNP P24462
C	22	MET	-	initiating methionine	UNP P24462
C	23	ALA	-	expression tag	UNP P24462
C	69	GLY	ARG	conflict	UNP P24462
C	77	GLY	CYS	conflict	UNP P24462
C	244	GLU	LYS	conflict	UNP P24462
C	421	ALA	LYS	conflict	UNP P24462
C	422	ALA	LYS	conflict	UNP P24462
C	424	ALA	LYS	conflict	UNP P24462
C	504	HIS	-	expression tag	UNP P24462
C	505	HIS	-	expression tag	UNP P24462
C	506	HIS	-	expression tag	UNP P24462
C	507	HIS	-	expression tag	UNP P24462
D	22	MET	-	initiating methionine	UNP P24462
D	23	ALA	-	expression tag	UNP P24462
D	69	GLY	ARG	conflict	UNP P24462
D	77	GLY	CYS	conflict	UNP P24462
D	244	GLU	LYS	conflict	UNP P24462
D	421	ALA	LYS	conflict	UNP P24462
D	422	ALA	LYS	conflict	UNP P24462
D	424	ALA	LYS	conflict	UNP P24462
D	504	HIS	-	expression tag	UNP P24462
D	505	HIS	-	expression tag	UNP P24462
D	506	HIS	-	expression tag	UNP P24462

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Chain	Residue	Modelled	Actual	Comment	Reference
D	507	HIS	-	expression tag	UNP P24462
E	22	MET	-	initiating methionine	UNP P24462
E	23	ALA	-	expression tag	UNP P24462
E	69	GLY	ARG	conflict	UNP P24462
E	77	GLY	CYS	conflict	UNP P24462
E	244	GLU	LYS	conflict	UNP P24462
E	421	ALA	LYS	conflict	UNP P24462
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E	504	HIS	-	expression tag	UNP P24462
E	505	HIS	-	expression tag	UNP P24462
E	506	HIS	-	expression tag	UNP P24462
E	507	HIS	-	expression tag	UNP P24462
F	22	MET	-	initiating methionine	UNP P24462
F	23	ALA	-	expression tag	UNP P24462
F	69	GLY	ARG	conflict	UNP P24462
F	77	GLY	CYS	conflict	UNP P24462
F	244	GLU	LYS	conflict	UNP P24462
F	421	ALA	LYS	conflict	UNP P24462
F	422	ALA	LYS	conflict	UNP P24462
F	424	ALA	LYS	conflict	UNP P24462
F	504	HIS	-	expression tag	UNP P24462
F	505	HIS	-	expression tag	UNP P24462
F	506	HIS	-	expression tag	UNP P24462
F	507	HIS	-	expression tag	UNP P24462
G	22	MET	-	initiating methionine	UNP P24462
G	23	ALA	-	expression tag	UNP P24462
G	69	GLY	ARG	conflict	UNP P24462
G	77	GLY	CYS	conflict	UNP P24462
G	244	GLU	LYS	conflict	UNP P24462
G	421	ALA	LYS	conflict	UNP P24462
G	422	ALA	LYS	conflict	UNP P24462
G	424	ALA	LYS	conflict	UNP P24462
G	504	HIS	-	expression tag	UNP P24462
G	505	HIS	-	expression tag	UNP P24462
G	506	HIS	-	expression tag	UNP P24462
G	507	HIS	-	expression tag	UNP P24462
H	22	MET	-	initiating methionine	UNP P24462
H	23	ALA	-	expression tag	UNP P24462
H	69	GLY	ARG	conflict	UNP P24462
H	77	GLY	CYS	conflict	UNP P24462
H	244	GLU	LYS	conflict	UNP P24462

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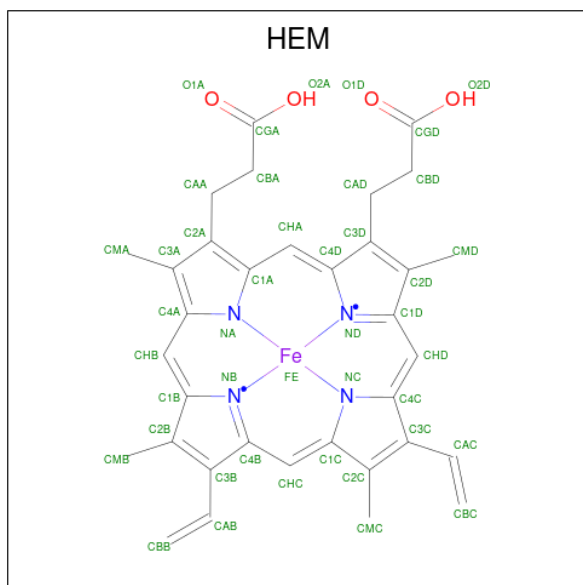
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H	421	ALA	LYS	conflict	UNP P24462
H	422	ALA	LYS	conflict	UNP P24462
H	424	ALA	LYS	conflict	UNP P24462
H	504	HIS	-	expression tag	UNP P24462
H	505	HIS	-	expression tag	UNP P24462
H	506	HIS	-	expression tag	UNP P24462
H	507	HIS	-	expression tag	UNP P24462
I	22	MET	-	initiating methionine	UNP P24462
I	23	ALA	-	expression tag	UNP P24462
I	69	GLY	ARG	conflict	UNP P24462
I	77	GLY	CYS	conflict	UNP P24462
I	244	GLU	LYS	conflict	UNP P24462
I	421	ALA	LYS	conflict	UNP P24462
I	422	ALA	LYS	conflict	UNP P24462
I	424	ALA	LYS	conflict	UNP P24462
I	504	HIS	-	expression tag	UNP P24462
I	505	HIS	-	expression tag	UNP P24462
I	506	HIS	-	expression tag	UNP P24462
I	507	HIS	-	expression tag	UNP P24462
J	22	MET	-	initiating methionine	UNP P24462
J	23	ALA	-	expression tag	UNP P24462
J	69	GLY	ARG	conflict	UNP P24462
J	77	GLY	CYS	conflict	UNP P24462
J	244	GLU	LYS	conflict	UNP P24462
J	421	ALA	LYS	conflict	UNP P24462
J	422	ALA	LYS	conflict	UNP P24462
J	424	ALA	LYS	conflict	UNP P24462
J	504	HIS	-	expression tag	UNP P24462
J	505	HIS	-	expression tag	UNP P24462
J	506	HIS	-	expression tag	UNP P24462
J	507	HIS	-	expression tag	UNP P24462
K	22	MET	-	initiating methionine	UNP P24462
K	23	ALA	-	expression tag	UNP P24462
K	69	GLY	ARG	conflict	UNP P24462
K	77	GLY	CYS	conflict	UNP P24462
K	244	GLU	LYS	conflict	UNP P24462
K	421	ALA	LYS	conflict	UNP P24462
K	422	ALA	LYS	conflict	UNP P24462
K	424	ALA	LYS	conflict	UNP P24462
K	504	HIS	-	expression tag	UNP P24462
K	505	HIS	-	expression tag	UNP P24462
K	506	HIS	-	expression tag	UNP P24462

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Chain	Residue	Modelled	Actual	Comment	Reference
K	507	HIS	-	expression tag	UNP P24462
L	22	MET	-	initiating methionine	UNP P24462
L	23	ALA	-	expression tag	UNP P24462
L	69	GLY	ARG	conflict	UNP P24462
L	77	GLY	CYS	conflict	UNP P24462
L	244	GLU	LYS	conflict	UNP P24462
L	421	ALA	LYS	conflict	UNP P24462
L	422	ALA	LYS	conflict	UNP P24462
L	424	ALA	LYS	conflict	UNP P24462
L	504	HIS	-	expression tag	UNP P24462
L	505	HIS	-	expression tag	UNP P24462
L	506	HIS	-	expression tag	UNP P24462
L	507	HIS	-	expression tag	UNP P24462

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



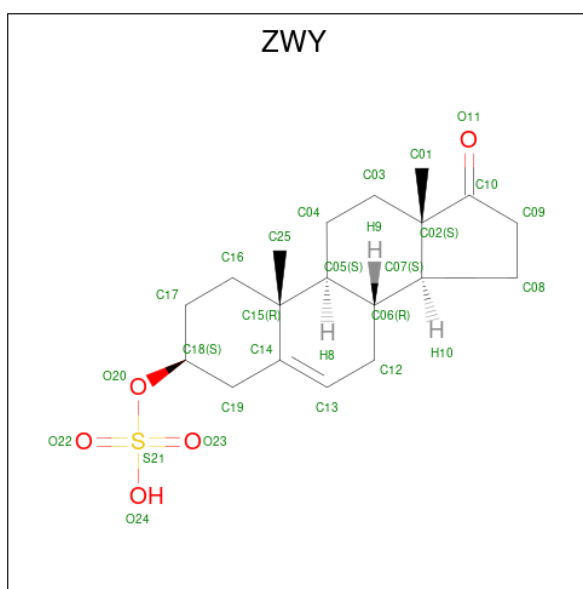
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0	0
2	B	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0	0
2	C	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0	0
2	D	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	E	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
2	F	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
2	G	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
2	H	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
2	I	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
2	J	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
2	K	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
2	L	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

- Molecule 3 is 17-oxoandrost-5-en-3beta-yl hydrogen sulfate (CCD ID: ZWY) (formula: $C_{19}H_{28}O_5S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	O	S	0	0
			52	19	27	5	1		
3	A	1	Total	C	H	O	S	0	0
			52	19	27	5	1		
3	B	1	Total	C	H	O	S	0	0
			52	19	27	5	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	H	O	S	0	0
			52	19	27	5	1		
3	C	1	Total	C	H	O	S	0	0
			52	19	27	5	1		
3	C	1	Total	C	H	O	S	0	0
			52	19	27	5	1		
3	C	1	Total	C	H	O	S	0	0
			52	19	27	5	1		
3	C	1	Total	C	H	O	S	0	0
			52	19	27	5	1		
3	D	1	Total	C	H	O	S	0	0
			52	19	27	5	1		
3	D	1	Total	C	H	O	S	0	0
			52	19	27	5	1		
3	D	1	Total	C	H	O	S	0	0
			52	19	27	5	1		
3	D	1	Total	C	H	O	S	0	0
			52	19	27	5	1		
3	D	1	Total	C	H	O	S	0	0
			52	19	27	5	1		
3	E	1	Total	C	H	O	S	0	0
			52	19	27	5	1		
3	E	1	Total	C	H	O	S	0	0
			52	19	27	5	1		
3	E	1	Total	C	H	O	S	0	0
			52	19	27	5	1		
3	E	1	Total	C	H	O	S	0	0
			52	19	27	5	1		
3	H	1	Total	C	H	O	S	0	0
			52	19	27	5	1		
3	H	1	Total	C	H	O	S	0	0
			52	19	27	5	1		
3	H	1	Total	C	H	O	S	0	0
			52	19	27	5	1		
3	I	1	Total	C	H	O	S	0	0
			52	19	27	5	1		
3	I	1	Total	C	H	O	S	0	0
			52	19	27	5	1		
3	J	1	Total	C	H	O	S	0	0
			52	19	27	5	1		
3	J	1	Total	C	H	O	S	0	0
			52	19	27	5	1		

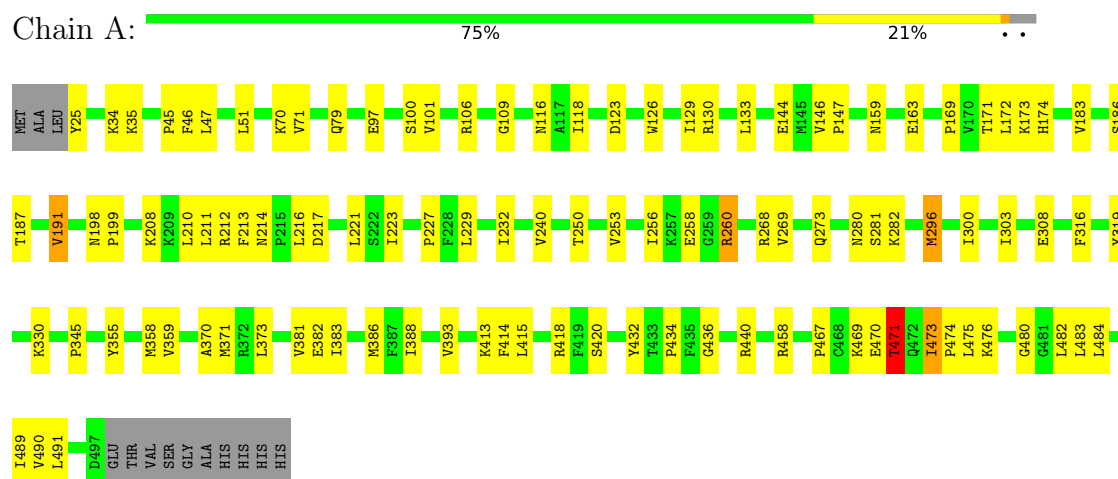
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	5	Total O 5 5	0	0
4	B	7	Total O 7 7	0	0
4	E	2	Total O 2 2	0	0
4	F	4	Total O 4 4	0	0
4	G	5	Total O 5 5	0	0
4	H	2	Total O 2 2	0	0
4	I	1	Total O 1 1	0	0
4	J	1	Total O 1 1	0	0
4	K	5	Total O 5 5	0	0

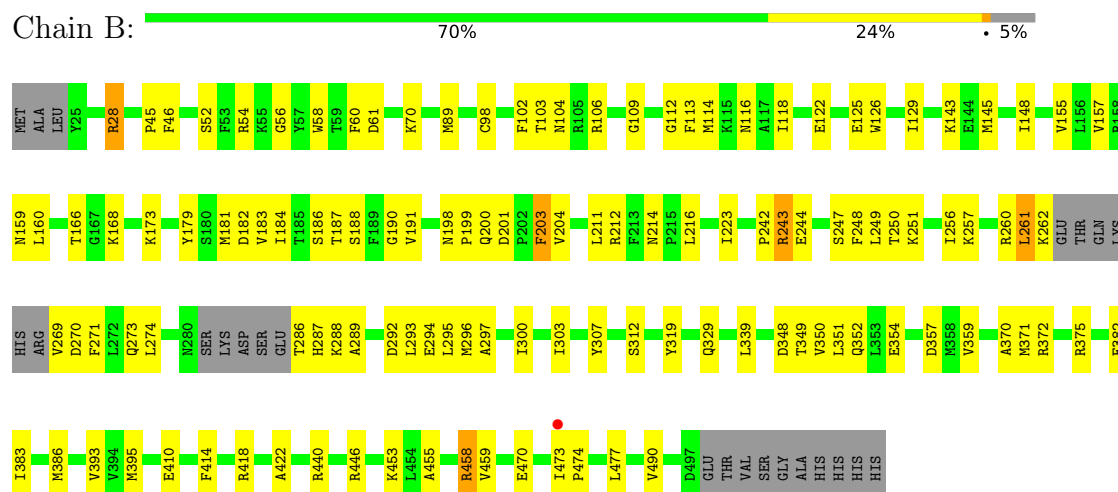
3 Residue-property plots

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

• Molecule 1: Cytochrome P450 3A7

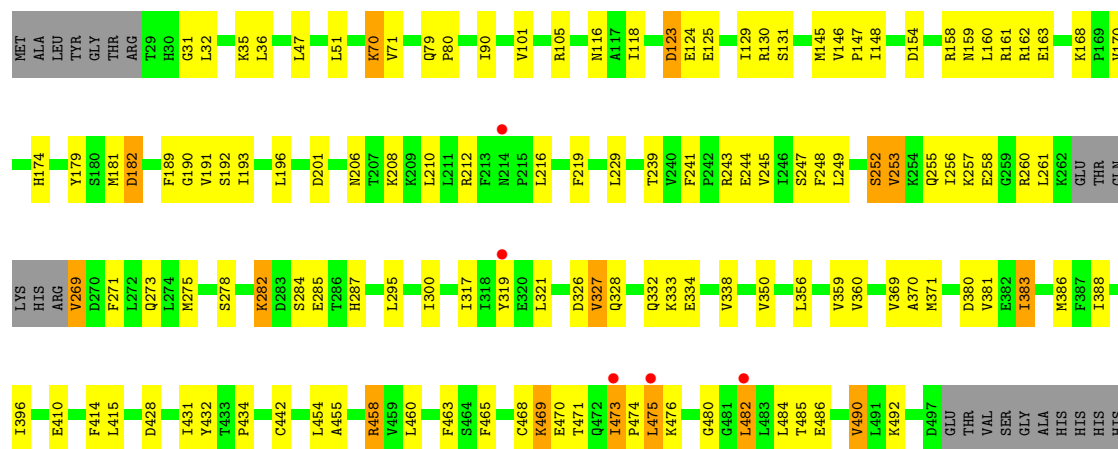


• Molecule 1: Cytochrome P450 3A7



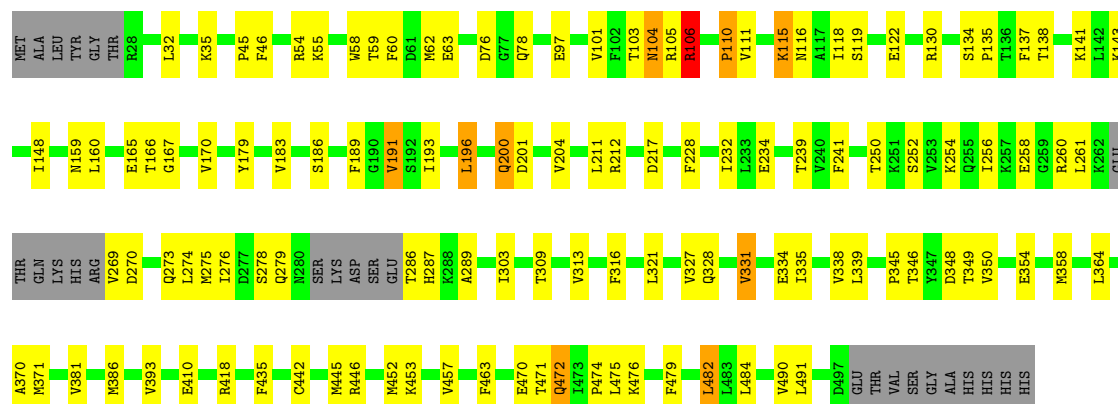
• Molecule 1: Cytochrome P450 3A7





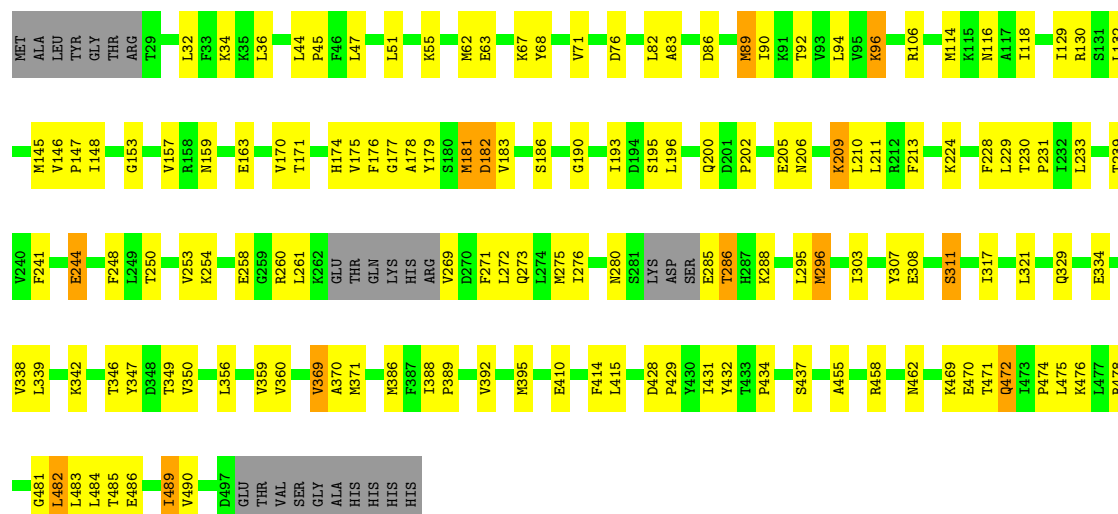
• Molecule 1: Cytochrome P450 3A7

Chain D: 69% 23% 6%

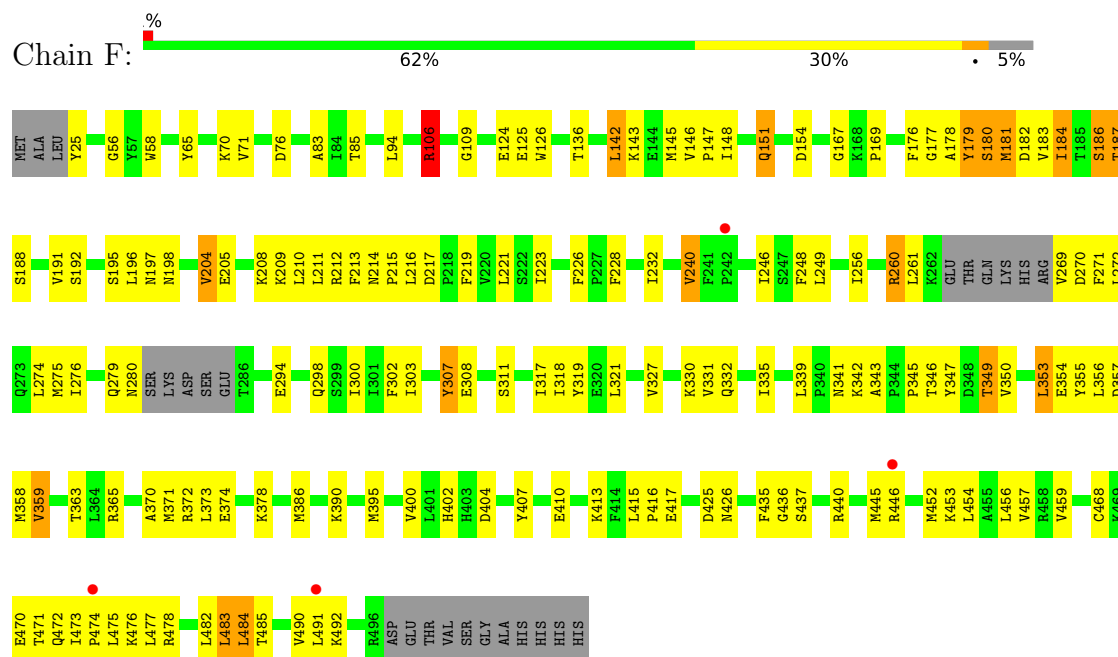


• Molecule 1: Cytochrome P450 3A7

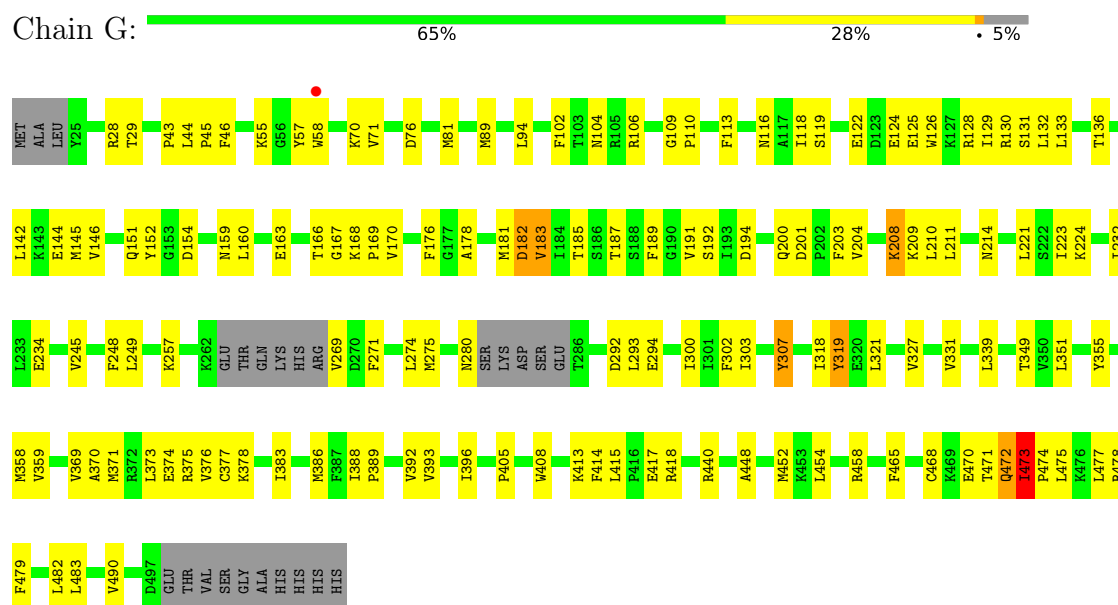
Chain E: 65% 27% 5%



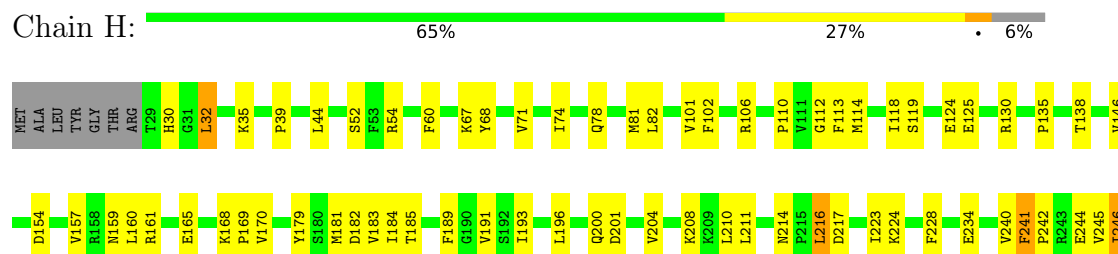
• Molecule 1: Cytochrome P450 3A7

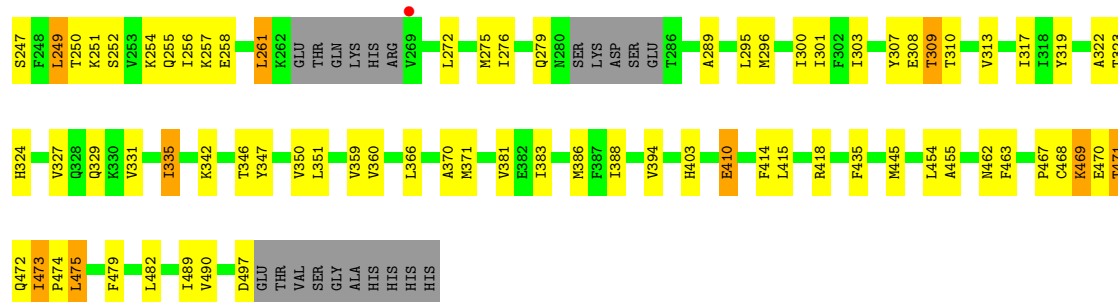


• Molecule 1: Cytochrome P450 3A7



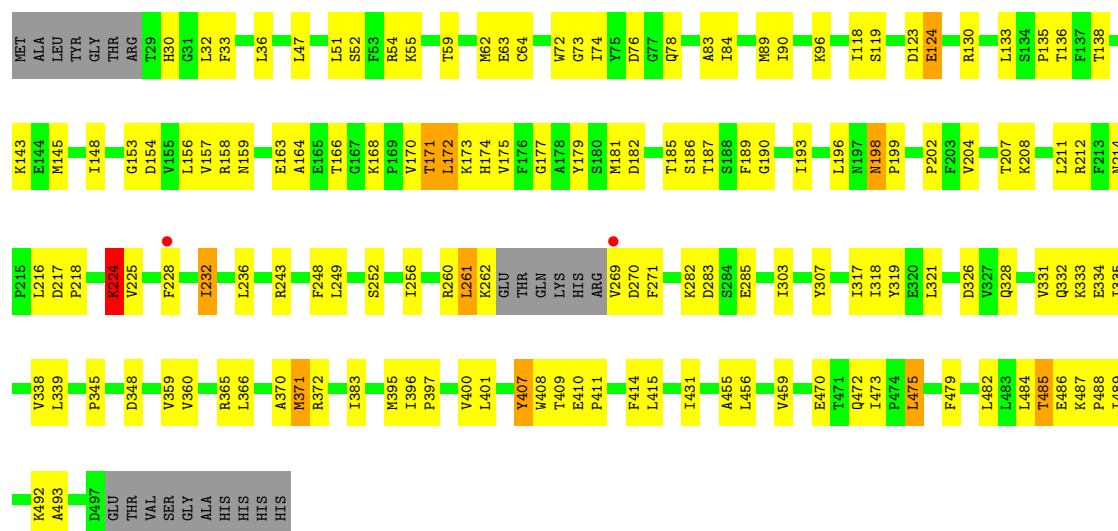
• Molecule 1: Cytochrome P450 3A7





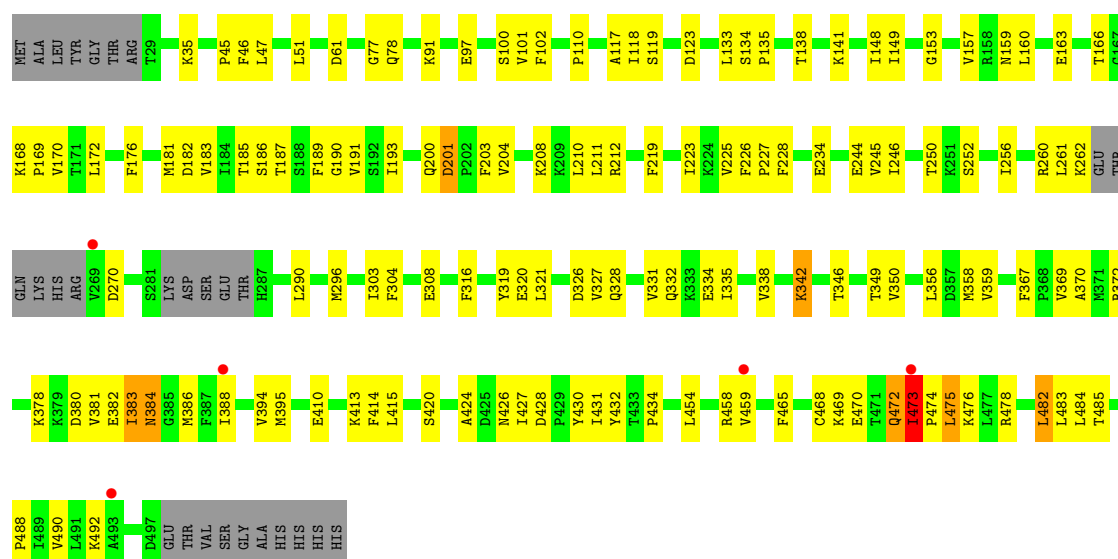
• Molecule 1: Cytochrome P450 3A7

Chain I: 65% 28% 5%



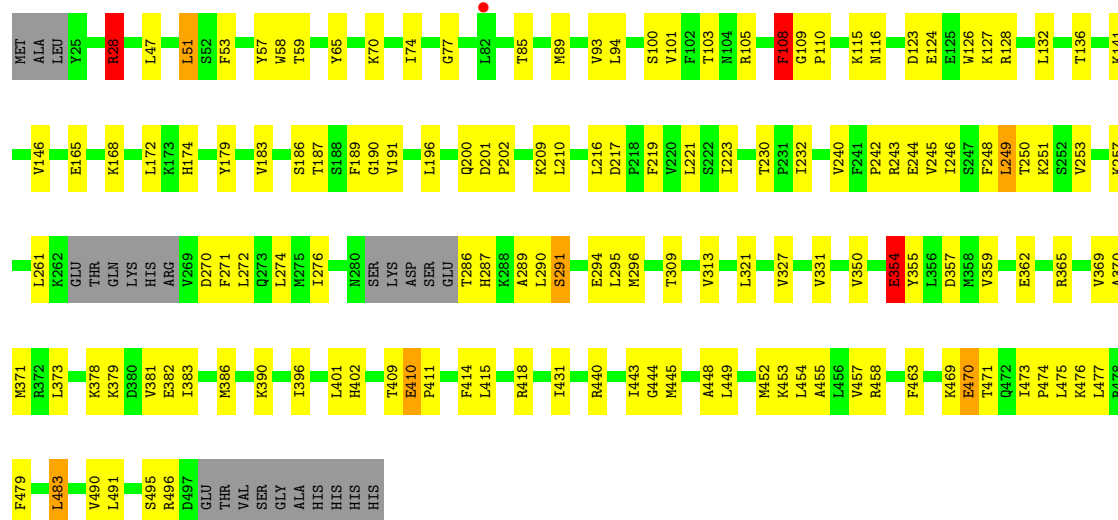
• Molecule 1: Cytochrome P450 3A7

Chain J: 65% 28% 6%



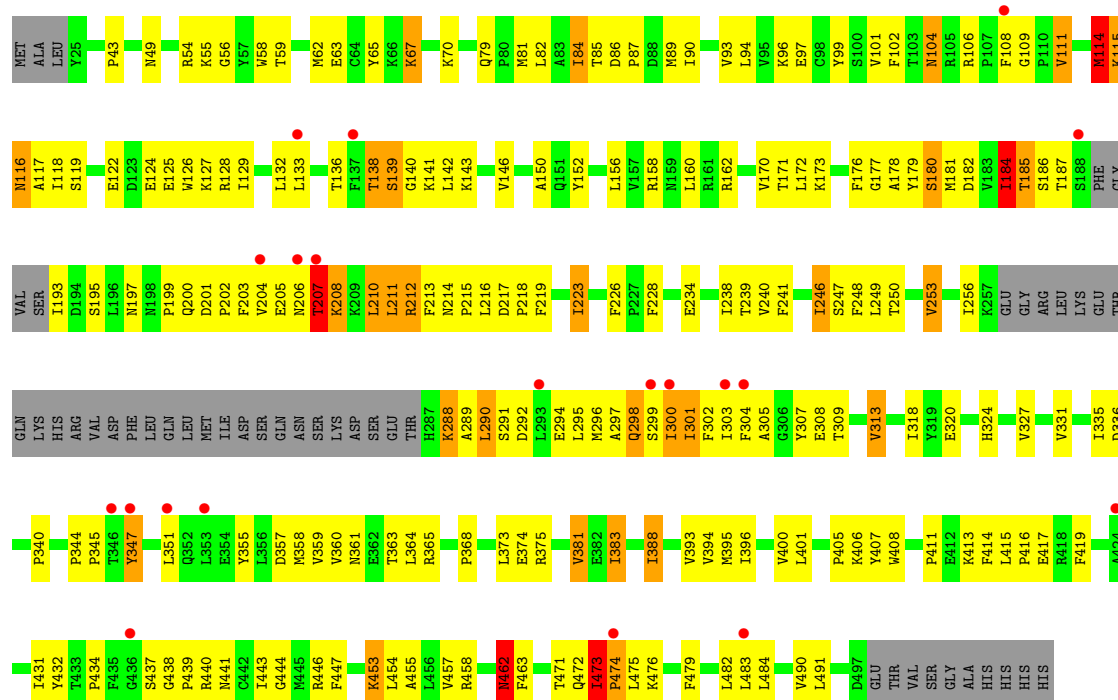
● Molecule 1: Cytochrome P450 3A7

Chain K:  66% 28% 5%



● Molecule 1: Cytochrome P450 3A7

Chain L:  4% 47% 37% 6% 9%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	114.52Å 219.38Å 130.45Å 90.00° 102.17° 90.00°	Depositor
Resolution (Å)	39.94 – 2.60 39.94 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.4 (39.94-2.60) 98.5 (39.94-2.60)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.210 , 0.273 (Not available) , 0.262	Depositor DCC
R_{free} test set	2000 reflections (1.04%)	wwPDB-VP
Wilson B-factor (Å ²)	68.5	Xtriage
Anisotropy	0.447	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	91794	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZWY, HEM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.57	3/3892 (0.1%)	0.61	1/5274 (0.0%)
1	B	0.62	1/3796 (0.0%)	0.71	9/5144 (0.2%)
1	C	0.63	4/3800 (0.1%)	0.68	5/5150 (0.1%)
1	D	0.72	4/3772 (0.1%)	0.69	6/5111 (0.1%)
1	E	0.80	5/3776 (0.1%)	0.69	4/5117 (0.1%)
1	F	0.69	3/3788 (0.1%)	0.72	11/5133 (0.2%)
1	G	0.70	3/3796 (0.1%)	0.75	15/5144 (0.3%)
1	H	0.64	5/3761 (0.1%)	0.68	7/5097 (0.1%)
1	I	0.68	2/3800 (0.1%)	0.73	10/5150 (0.2%)
1	J	0.68	1/3760 (0.0%)	0.73	6/5095 (0.1%)
1	K	0.70	2/3796 (0.1%)	0.73	7/5144 (0.1%)
1	L	0.88	4/3620 (0.1%)	1.05	26/4908 (0.5%)
All	All	0.70	37/45357 (0.1%)	0.74	107/61467 (0.2%)

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	410	GLU	C-O	-10.84	1.18	1.23
1	H	410	GLU	C-O	-10.06	1.19	1.23
1	H	146	VAL	CA-CB	8.35	1.59	1.53
1	F	198	ASN	N-CA	-7.43	1.39	1.46
1	E	410	GLU	C-O	7.09	1.27	1.23

The worst 5 of 107 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	139	SER	N-CA-C	-10.63	99.48	111.71
1	L	152	TYR	N-CA-C	-8.81	101.13	112.23
1	I	30	HIS	N-CA-C	-8.26	103.19	113.18
1	I	472	GLN	N-CA-C	-8.01	97.82	109.59
1	L	417	GLU	N-CA-C	-7.67	103.95	113.38

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3798	3892	3891	82	0
1	B	3705	3796	3802	81	0
1	C	3709	3798	3804	93	0
1	D	3682	3771	3783	91	0
1	E	3686	3783	3781	102	0
1	F	3697	3799	3798	130	0
1	G	3705	3798	3803	101	0
1	H	3671	3763	3770	96	0
1	I	3709	3799	3804	113	0
1	J	3670	3771	3768	114	0
1	K	3705	3798	3802	122	0
1	L	3531	3602	3628	209	0
2	A	43	30	30	2	0
2	B	43	30	30	3	0
2	C	43	30	30	4	0
2	D	43	30	30	6	0
2	E	43	30	30	2	0
2	F	43	30	30	4	0
2	G	43	30	30	5	0
2	H	43	30	30	3	0
2	I	43	30	30	3	0
2	J	43	30	30	2	0
2	K	43	30	30	7	0
2	L	43	30	30	5	0
3	A	50	54	0	1	0
3	B	50	54	0	0	0
3	C	100	108	0	0	0
3	D	125	135	0	2	0
3	E	100	108	0	1	0
3	H	75	81	0	1	0
3	I	50	54	0	0	0
3	J	50	54	0	0	0
4	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	7	0	0	0	0
4	E	2	0	0	0	0
4	F	4	0	0	0	0
4	G	5	0	0	0	0
4	H	2	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
4	K	5	0	0	0	0
All	All	45416	46378	45794	1342	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 15.

The worst 5 of 1342 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:286:THR:HG22	1:G:351:LEU:O	1.40	1.18
1:L:250:THR:HG23	1:L:296:MET:SD	1.84	1.18
1:F:232:ILE:HD11	1:G:232:ILE:HD11	1.15	1.11
1:K:183:VAL:O	1:K:187:THR:HG22	1.54	1.07
1:J:185:THR:HB	1:J:193:ILE:HD11	1.41	1.02

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	471/486 (97%)	435 (92%)	35 (7%)	1 (0%)	43	66
1	B	456/486 (94%)	423 (93%)	30 (7%)	3 (1%)	18	38
1	C	459/486 (94%)	425 (93%)	30 (6%)	4 (1%)	14	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	453/486 (93%)	421 (93%)	30 (7%)	2 (0%)	30	51
1	E	454/486 (93%)	421 (93%)	31 (7%)	2 (0%)	30	51
1	F	455/486 (94%)	425 (93%)	28 (6%)	2 (0%)	30	51
1	G	456/486 (94%)	419 (92%)	36 (8%)	1 (0%)	43	66
1	H	452/486 (93%)	412 (91%)	37 (8%)	3 (1%)	18	38
1	I	459/486 (94%)	432 (94%)	25 (5%)	2 (0%)	30	51
1	J	452/486 (93%)	418 (92%)	32 (7%)	2 (0%)	30	51
1	K	456/486 (94%)	415 (91%)	40 (9%)	1 (0%)	43	66
1	L	434/486 (89%)	376 (87%)	53 (12%)	5 (1%)	10	23
All	All	5457/5832 (94%)	5022 (92%)	407 (8%)	28 (0%)	24	46

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	473	ILE
1	D	166	THR
1	L	212	ARG
1	C	252	SER
1	C	473	ILE

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	428/438 (98%)	422 (99%)	6 (1%)	59	81
1	B	417/438 (95%)	409 (98%)	8 (2%)	50	75
1	C	419/438 (96%)	404 (96%)	15 (4%)	31	58
1	D	415/438 (95%)	406 (98%)	9 (2%)	45	72
1	E	416/438 (95%)	401 (96%)	15 (4%)	31	58
1	F	416/438 (95%)	397 (95%)	19 (5%)	24	49
1	G	417/438 (95%)	405 (97%)	12 (3%)	37	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	414/438 (94%)	393 (95%)	21 (5%)	21	45
1	I	419/438 (96%)	406 (97%)	13 (3%)	35	63
1	J	414/438 (94%)	405 (98%)	9 (2%)	45	72
1	K	417/438 (95%)	404 (97%)	13 (3%)	35	63
1	L	397/438 (91%)	366 (92%)	31 (8%)	11	26
All	All	4989/5256 (95%)	4818 (97%)	171 (3%)	32	60

5 of 171 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	475	LEU
1	L	111	VAL
1	J	342	LYS
1	K	108	PHE
1	L	205	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	159	ASN
1	L	426	ASN
1	K	197	ASN
1	L	255	GLN
1	E	341	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

36 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	ZWY	C	602	-	28,28,28	2.28	8 (28%)	42,46,46	3.80	19 (45%)
2	HEM	K	601	1	50,50,50	1.42	9 (18%)	67,82,82	1.16	5 (7%)
3	ZWY	E	603	-	28,28,28	2.42	10 (35%)	42,46,46	3.73	22 (52%)
2	HEM	L	601	-	50,50,50	1.49	9 (18%)	67,82,82	1.12	4 (5%)
3	ZWY	D	605	-	28,28,28	2.46	10 (35%)	42,46,46	3.84	21 (50%)
3	ZWY	E	602	-	28,28,28	2.47	9 (32%)	42,46,46	3.78	22 (52%)
3	ZWY	A	603	-	28,28,28	2.54	11 (39%)	42,46,46	3.95	22 (52%)
2	HEM	A	601	1	50,50,50	1.44	8 (16%)	67,82,82	1.16	7 (10%)
3	ZWY	C	604	-	28,28,28	2.25	10 (35%)	42,46,46	3.64	19 (45%)
2	HEM	J	601	-	50,50,50	1.39	8 (16%)	67,82,82	1.09	4 (5%)
3	ZWY	B	602	-	28,28,28	2.47	9 (32%)	42,46,46	4.03	20 (47%)
2	HEM	H	601	1	50,50,50	1.35	6 (12%)	67,82,82	1.14	4 (5%)
3	ZWY	D	603	-	28,28,28	2.49	11 (39%)	42,46,46	3.94	21 (50%)
3	ZWY	C	605	-	28,28,28	2.32	9 (32%)	42,46,46	3.75	22 (52%)
3	ZWY	D	604	-	28,28,28	2.46	11 (39%)	42,46,46	3.90	20 (47%)
2	HEM	F	601	-	50,50,50	1.35	8 (16%)	67,82,82	1.01	0
3	ZWY	H	603	-	28,28,28	2.45	10 (35%)	42,46,46	3.86	18 (42%)
3	ZWY	D	606	-	28,28,28	2.56	11 (39%)	42,46,46	3.87	20 (47%)
2	HEM	G	601	-	50,50,50	1.39	8 (16%)	67,82,82	1.00	1 (1%)
3	ZWY	H	604	-	28,28,28	2.23	8 (28%)	42,46,46	3.72	21 (50%)
3	ZWY	C	603	-	28,28,28	2.48	11 (39%)	42,46,46	3.99	20 (47%)
3	ZWY	H	602	-	28,28,28	2.48	10 (35%)	42,46,46	3.75	19 (45%)
3	ZWY	I	603	-	28,28,28	2.34	10 (35%)	42,46,46	3.77	23 (54%)
3	ZWY	J	603	-	28,28,28	2.35	9 (32%)	42,46,46	3.77	23 (54%)
3	ZWY	A	602	-	28,28,28	2.37	11 (39%)	42,46,46	3.66	20 (47%)
3	ZWY	E	605	-	28,28,28	2.37	9 (32%)	42,46,46	3.71	21 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ZWY	B	603	-	28,28,28	2.27	9 (32%)	42,46,46	3.68	19 (45%)
2	HEM	C	601	1	50,50,50	1.41	9 (18%)	67,82,82	1.20	6 (8%)
3	ZWY	E	604	-	28,28,28	2.37	9 (32%)	42,46,46	3.70	18 (42%)
2	HEM	E	601	1	50,50,50	1.42	6 (12%)	67,82,82	1.11	3 (4%)
2	HEM	D	601	1	50,50,50	1.39	9 (18%)	67,82,82	1.15	5 (7%)
3	ZWY	D	602	-	28,28,28	2.33	9 (32%)	42,46,46	3.77	18 (42%)
2	HEM	I	601	1	50,50,50	1.42	10 (20%)	67,82,82	1.10	3 (4%)
3	ZWY	I	602	-	28,28,28	2.32	10 (35%)	42,46,46	3.77	17 (40%)
3	ZWY	J	602	-	28,28,28	2.46	9 (32%)	42,46,46	3.77	17 (40%)
2	HEM	B	601	1	50,50,50	1.40	9 (18%)	67,82,82	1.14	5 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ZWY	C	602	-	-	0/5/63/63	0/4/4/4
2	HEM	K	601	1	-	4/14/54/54	-
3	ZWY	E	603	-	-	1/5/63/63	0/4/4/4
2	HEM	L	601	-	-	3/14/54/54	-
3	ZWY	D	605	-	-	0/5/63/63	0/4/4/4
3	ZWY	E	602	-	-	3/5/63/63	0/4/4/4
3	ZWY	A	603	-	-	0/5/63/63	0/4/4/4
2	HEM	A	601	1	-	1/14/54/54	-
3	ZWY	C	604	-	-	0/5/63/63	0/4/4/4
2	HEM	J	601	-	-	4/14/54/54	-
3	ZWY	B	602	-	-	0/5/63/63	0/4/4/4
2	HEM	H	601	1	-	0/14/54/54	-
3	ZWY	D	603	-	-	2/5/63/63	0/4/4/4
3	ZWY	C	605	-	-	0/5/63/63	0/4/4/4
3	ZWY	D	604	-	-	0/5/63/63	0/4/4/4
2	HEM	F	601	-	-	2/14/54/54	-
3	ZWY	H	603	-	-	0/5/63/63	0/4/4/4
3	ZWY	D	606	-	-	0/5/63/63	0/4/4/4
2	HEM	G	601	-	-	0/14/54/54	-
3	ZWY	H	604	-	-	2/5/63/63	0/4/4/4
3	ZWY	C	603	-	-	0/5/63/63	0/4/4/4
3	ZWY	H	602	-	-	0/5/63/63	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ZWY	I	603	-	-	0/5/63/63	0/4/4/4
3	ZWY	J	603	-	-	0/5/63/63	0/4/4/4
3	ZWY	A	602	-	-	0/5/63/63	0/4/4/4
3	ZWY	E	605	-	-	0/5/63/63	0/4/4/4
3	ZWY	B	603	-	-	0/5/63/63	0/4/4/4
2	HEM	C	601	1	-	2/14/54/54	-
3	ZWY	E	604	-	-	0/5/63/63	0/4/4/4
2	HEM	E	601	1	-	1/14/54/54	-
2	HEM	D	601	1	-	1/14/54/54	-
3	ZWY	D	602	-	-	0/5/63/63	0/4/4/4
2	HEM	I	601	1	-	3/14/54/54	-
3	ZWY	I	602	-	-	0/5/63/63	0/4/4/4
3	ZWY	J	602	-	-	0/5/63/63	0/4/4/4
2	HEM	B	601	1	-	2/14/54/54	-

The worst 5 of 332 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	606	ZWY	C25-C15	-8.22	1.41	1.54
3	E	603	ZWY	C25-C15	-7.97	1.41	1.54
3	A	603	ZWY	C25-C15	-7.78	1.41	1.54
3	D	603	ZWY	C25-C15	-7.71	1.42	1.54
3	C	603	ZWY	C25-C15	-7.68	1.42	1.54

The worst 5 of 529 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	ZWY	C25-C15-C14	-16.94	82.50	108.38
3	A	603	ZWY	C25-C15-C14	-16.77	82.77	108.38
3	C	603	ZWY	C25-C15-C14	-16.76	82.78	108.38
3	C	602	ZWY	C25-C15-C14	-16.72	82.84	108.38
3	D	604	ZWY	C25-C15-C14	-16.71	82.86	108.38

There are no chirality outliers.

5 of 31 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	602	ZWY	C18-O20-S21-O22
2	J	601	HEM	C2C-C3C-CAC-CBC
2	J	601	HEM	C4C-C3C-CAC-CBC
3	E	602	ZWY	C18-O20-S21-O24

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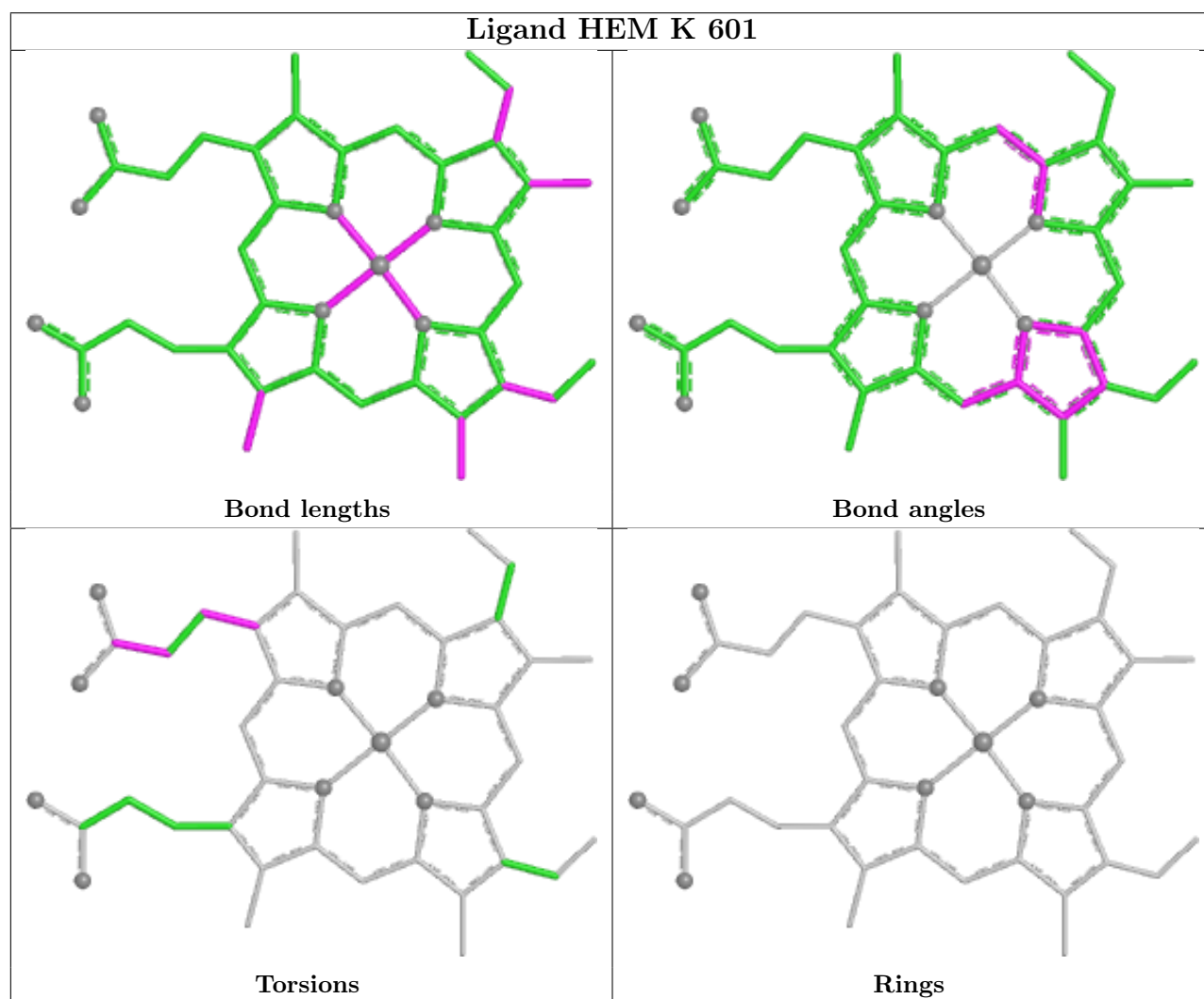
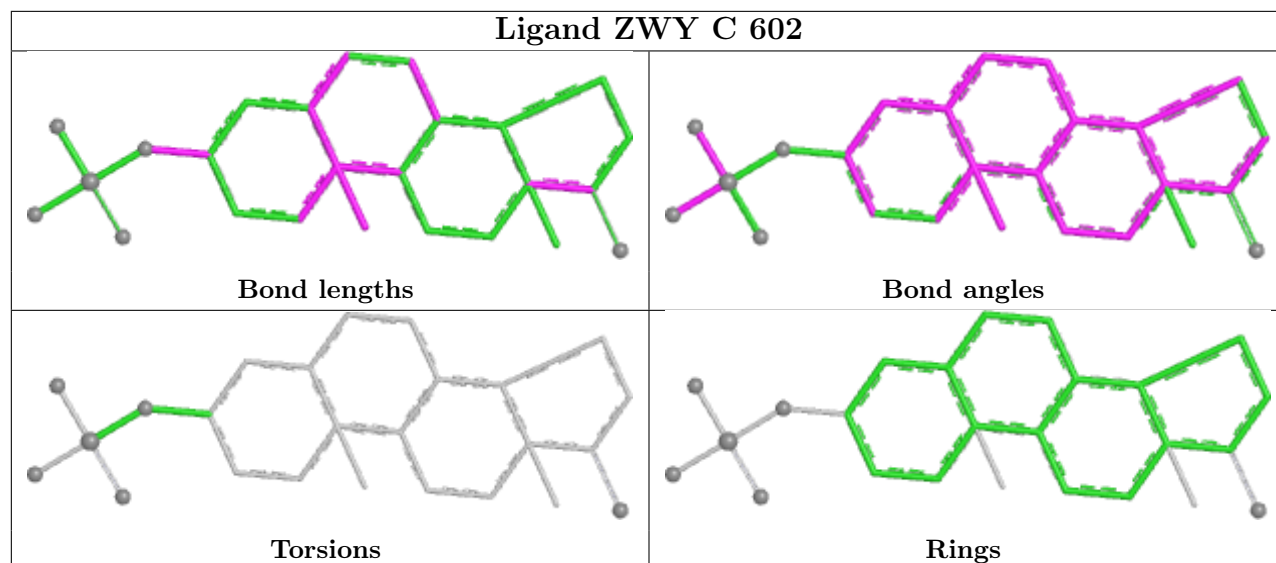
Mol	Chain	Res	Type	Atoms
3	D	603	ZWY	C18-O20-S21-O23

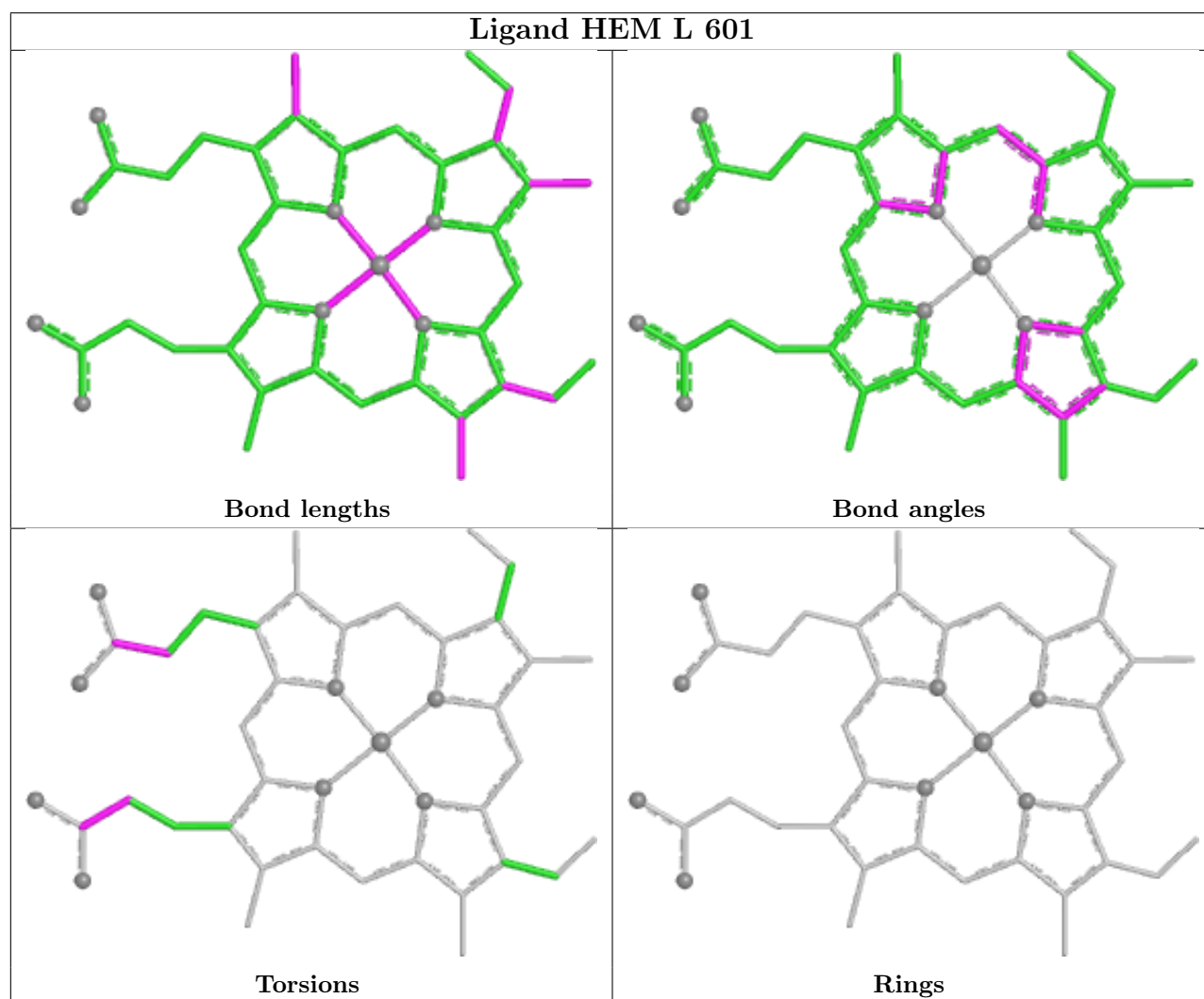
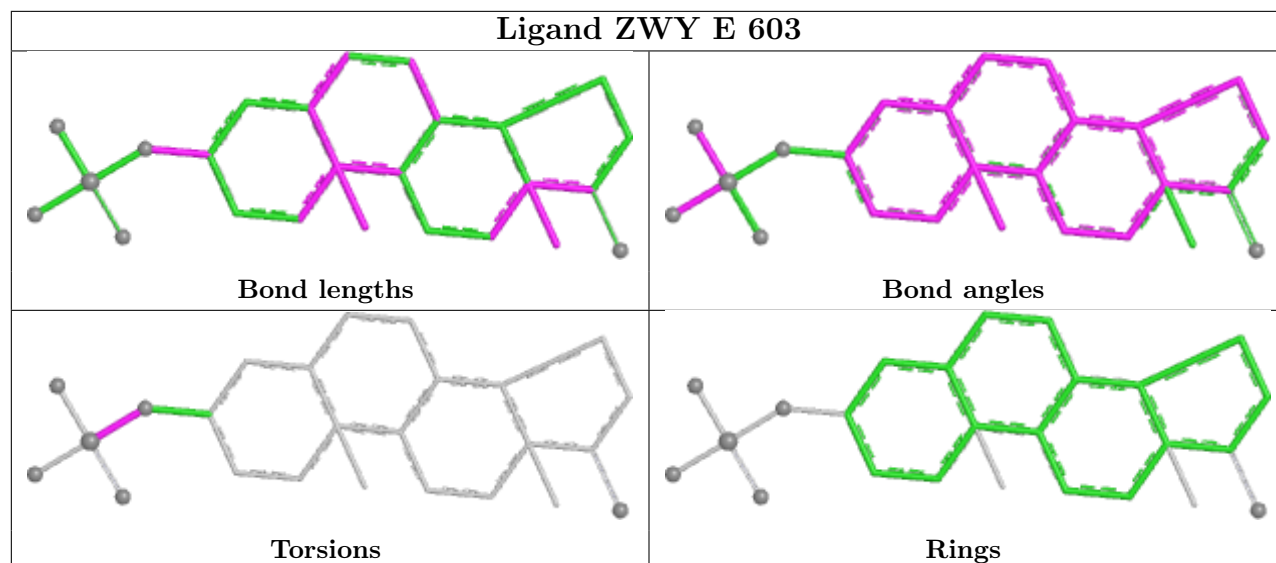
There are no ring outliers.

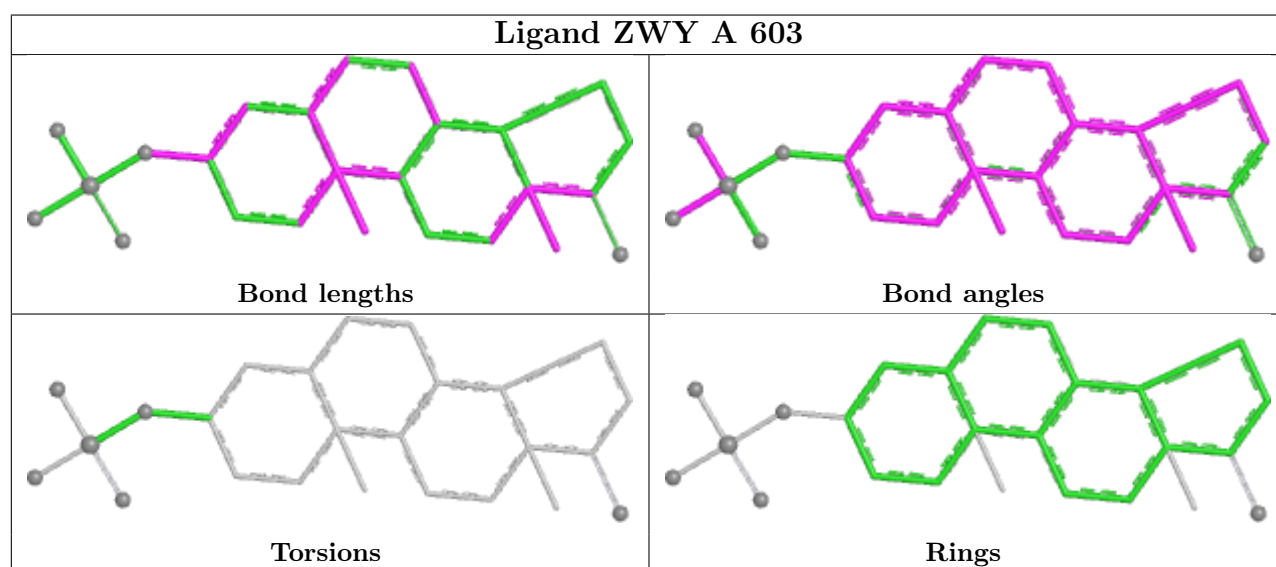
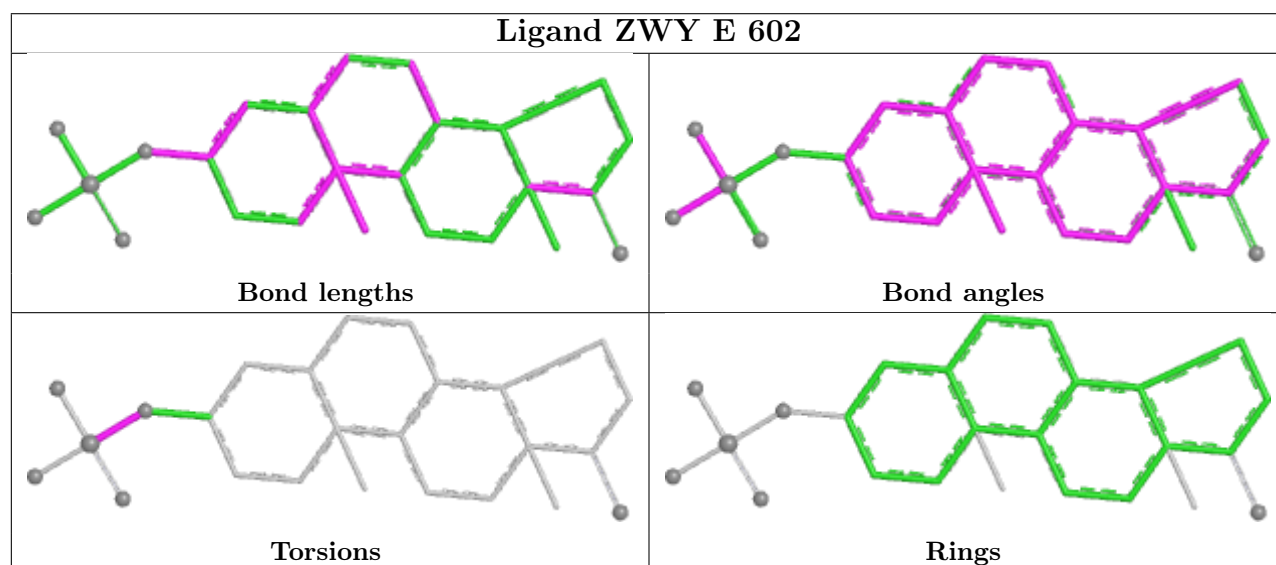
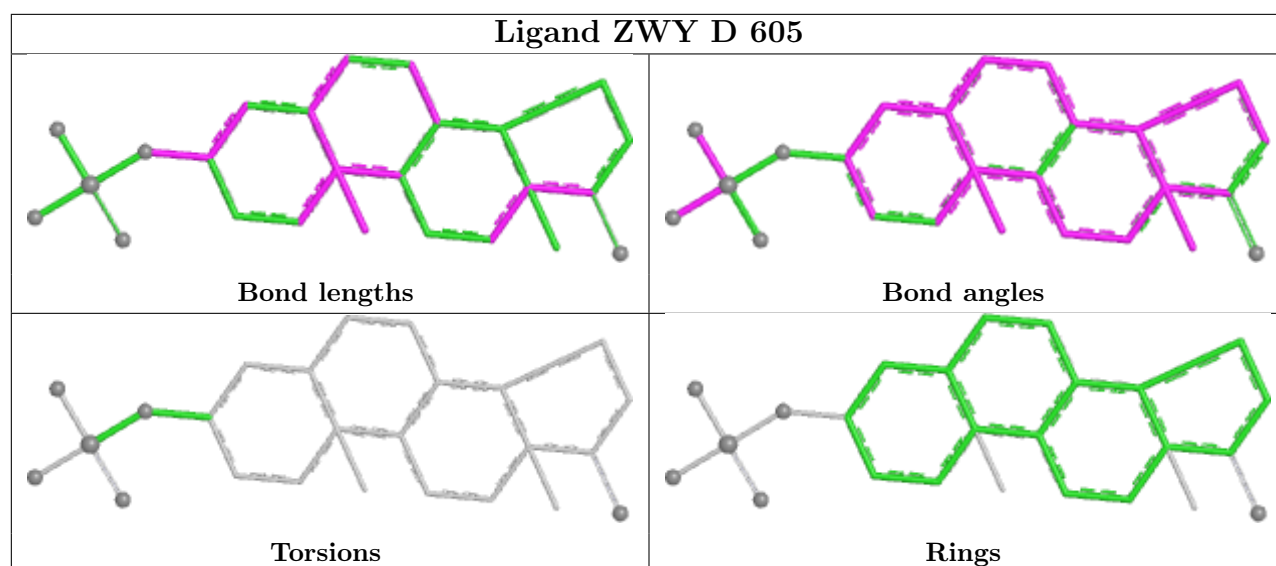
16 monomers are involved in 51 short contacts:

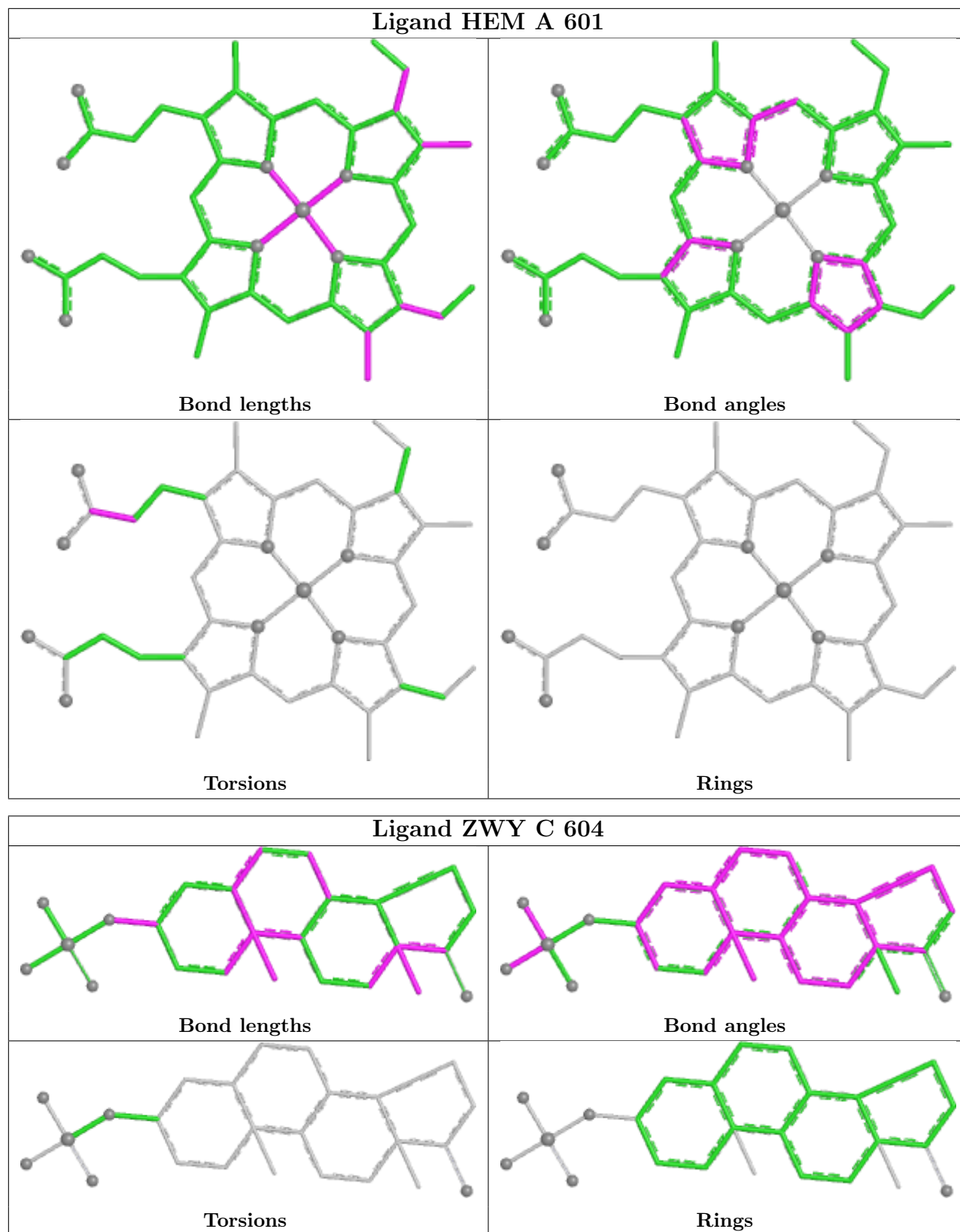
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	601	HEM	7	0
2	L	601	HEM	5	0
2	A	601	HEM	2	0
2	J	601	HEM	2	0
2	H	601	HEM	3	0
2	F	601	HEM	4	0
2	G	601	HEM	5	0
3	H	602	ZWY	1	0
3	A	602	ZWY	1	0
3	E	605	ZWY	1	0
2	C	601	HEM	4	0
2	E	601	HEM	2	0
2	D	601	HEM	6	0
3	D	602	ZWY	2	0
2	I	601	HEM	3	0
2	B	601	HEM	3	0

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

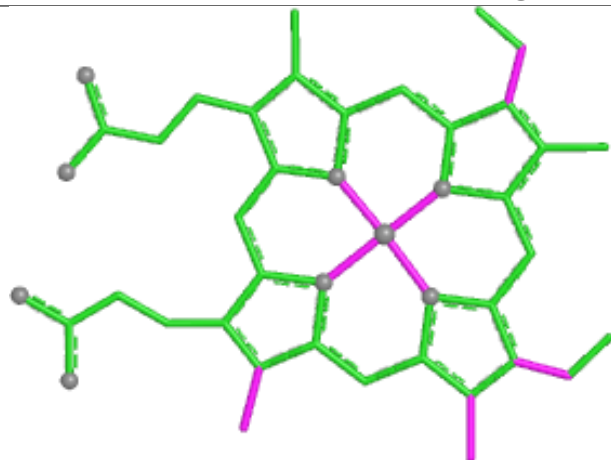




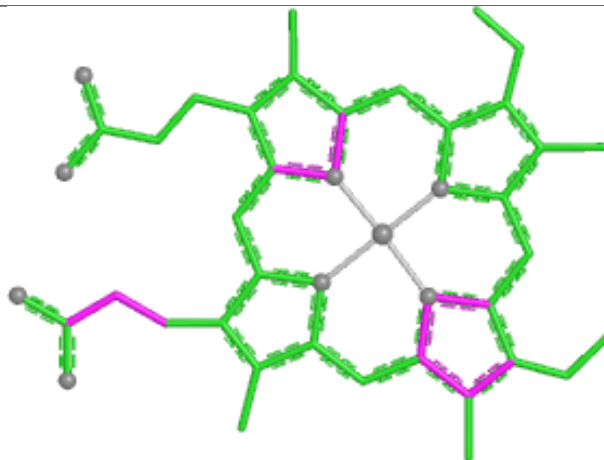




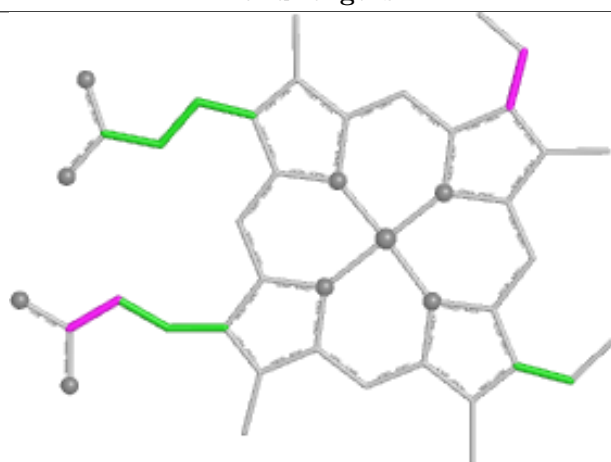
Ligand HEM J 601



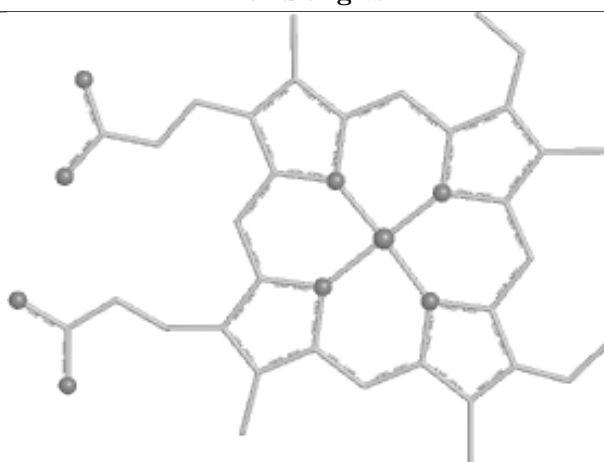
Bond lengths



Bond angles

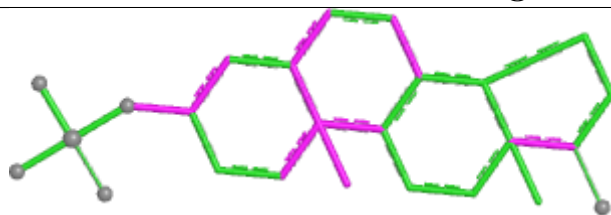


Torsions

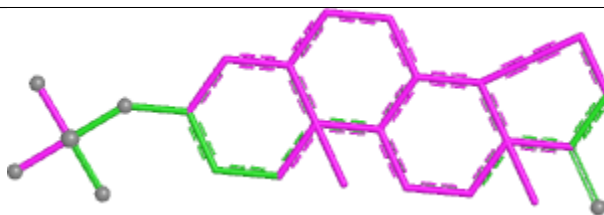


Rings

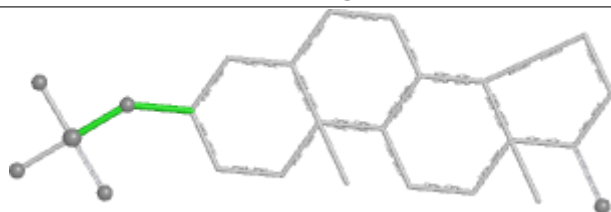
Ligand ZWY B 602



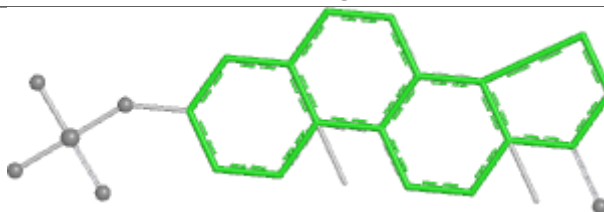
Bond lengths



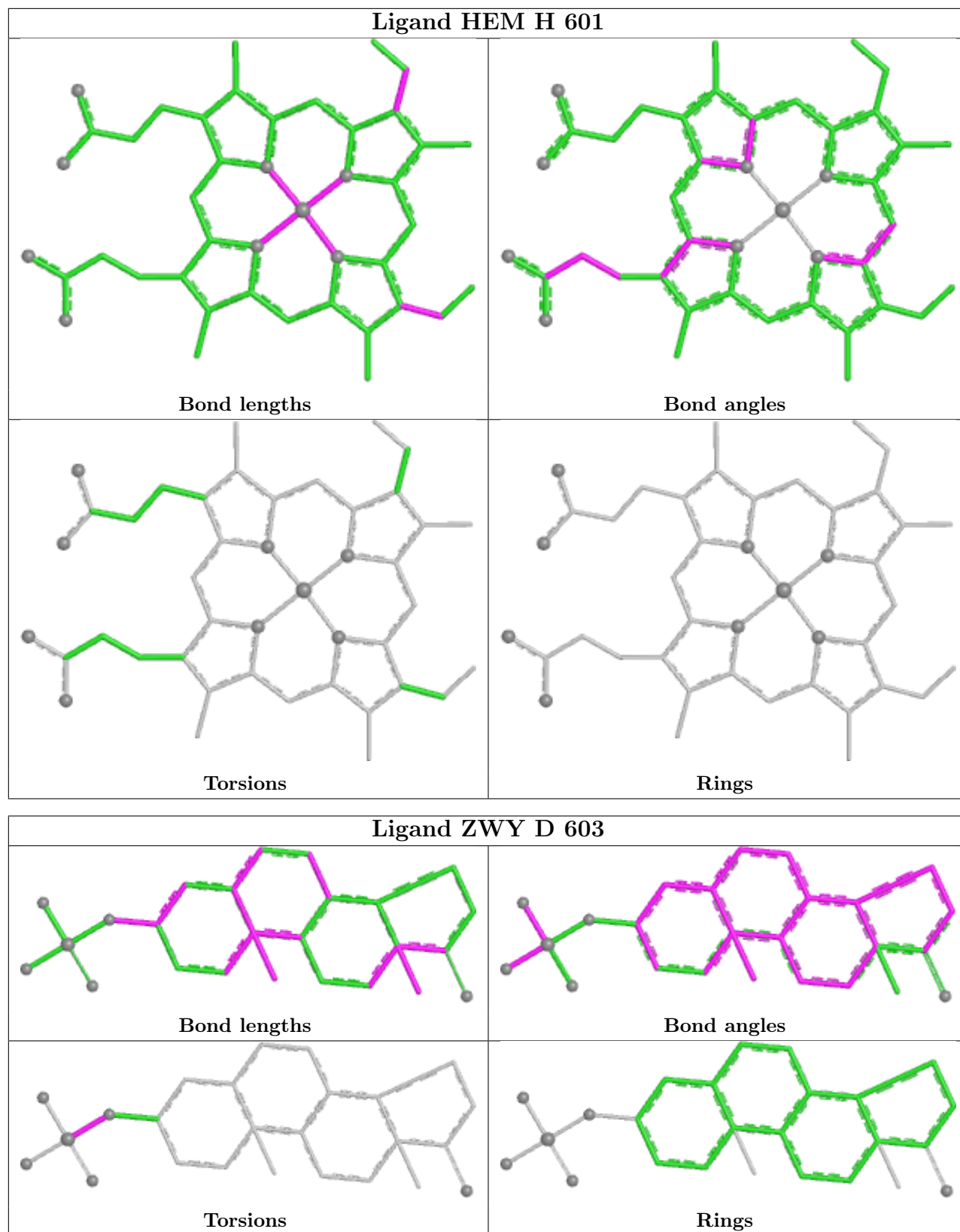
Bond angles

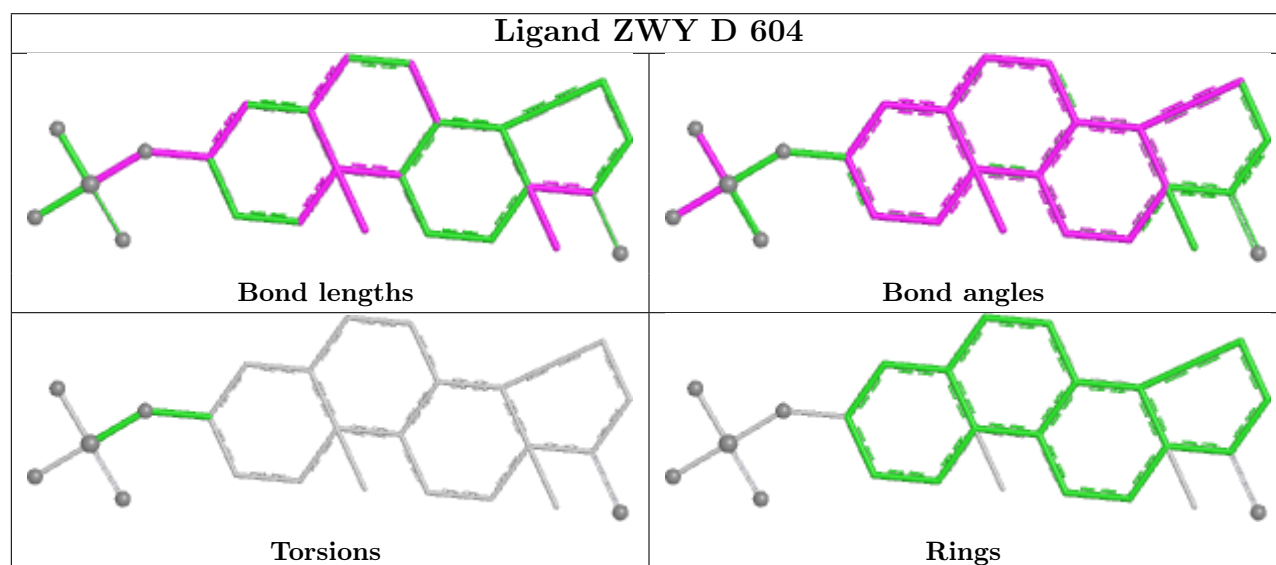
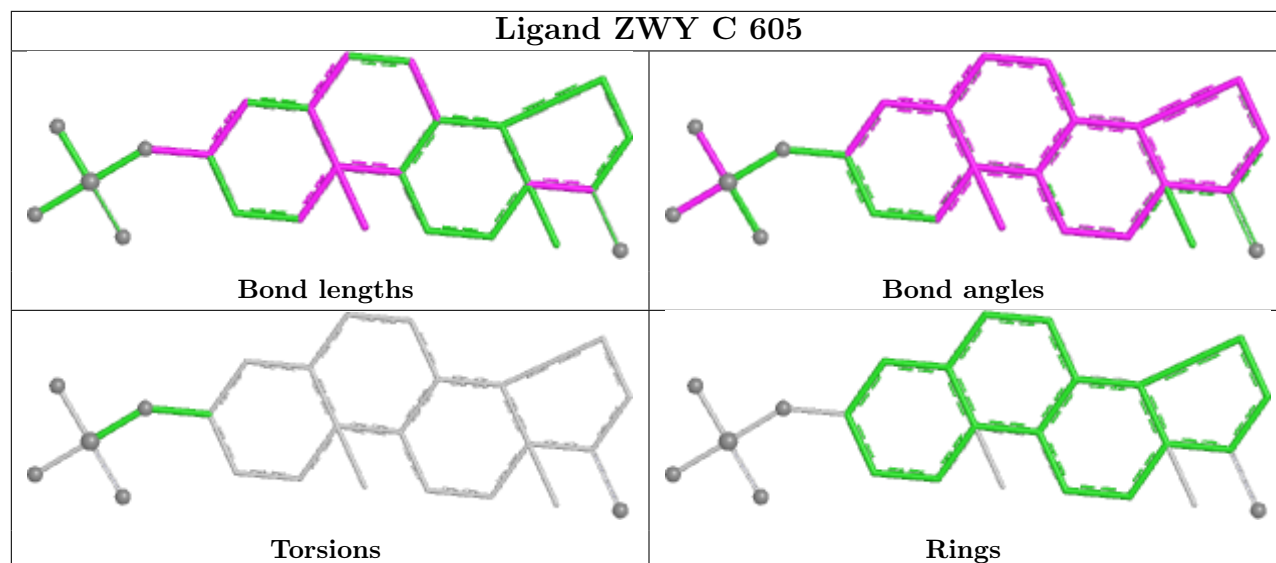


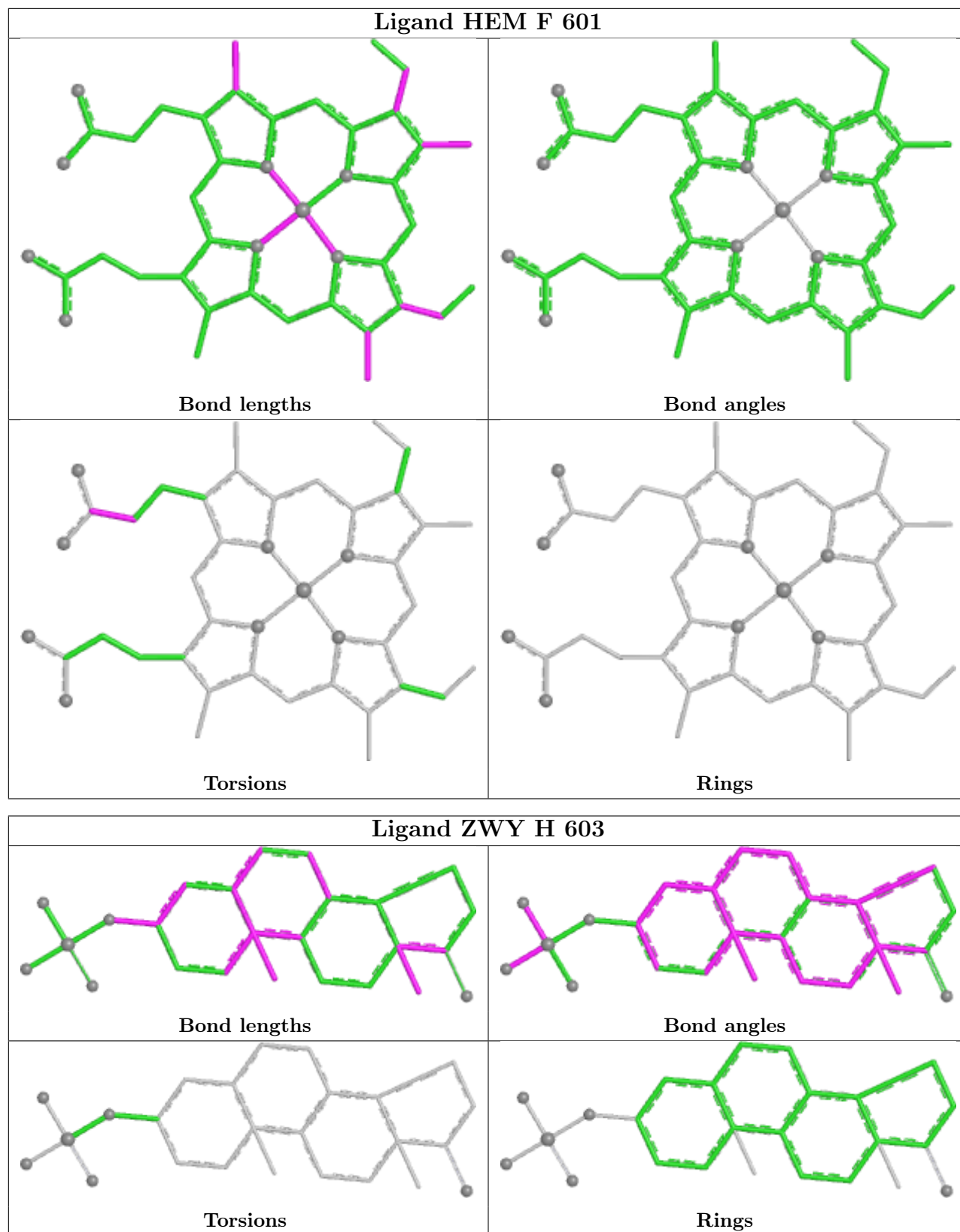
Torsions

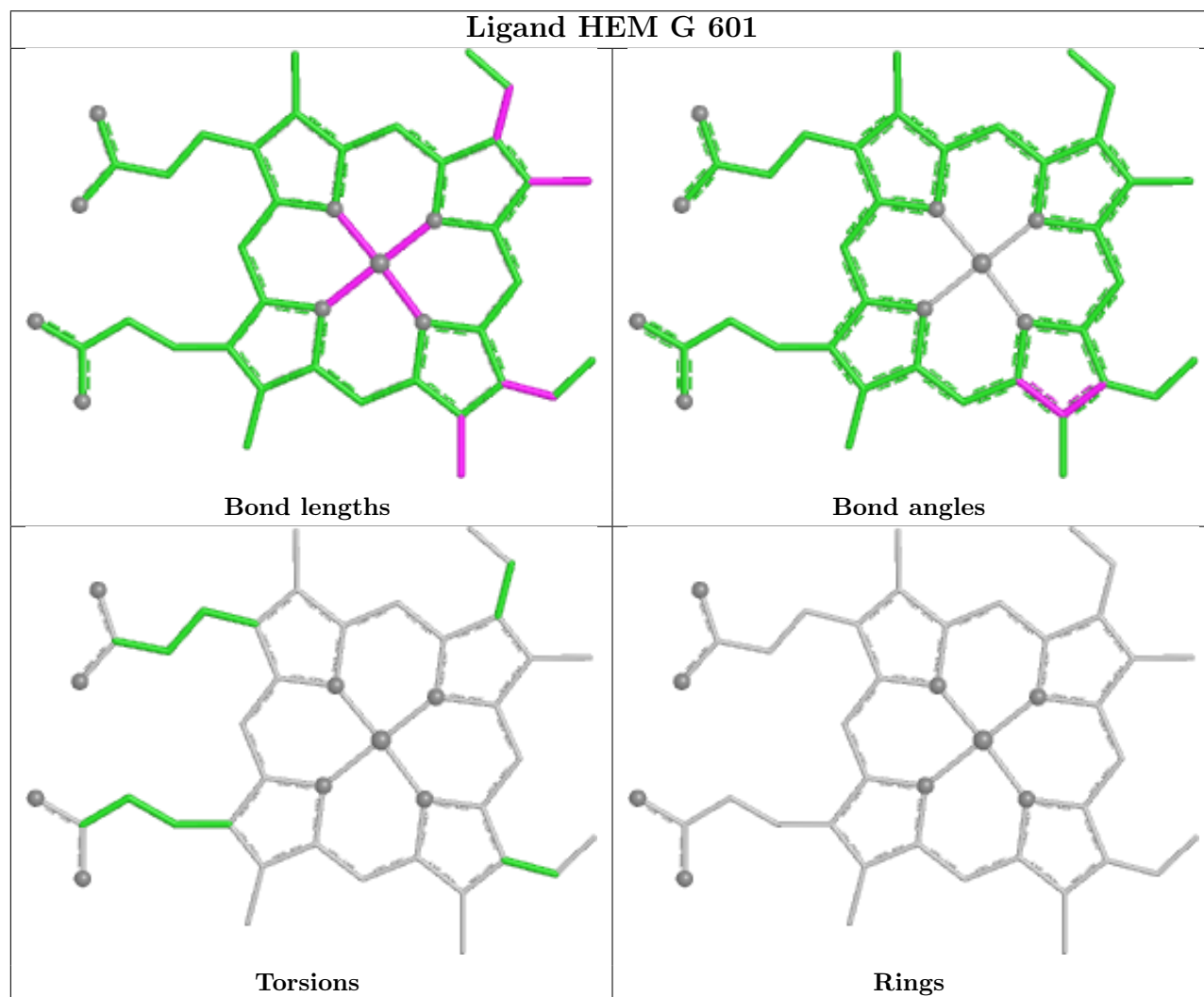
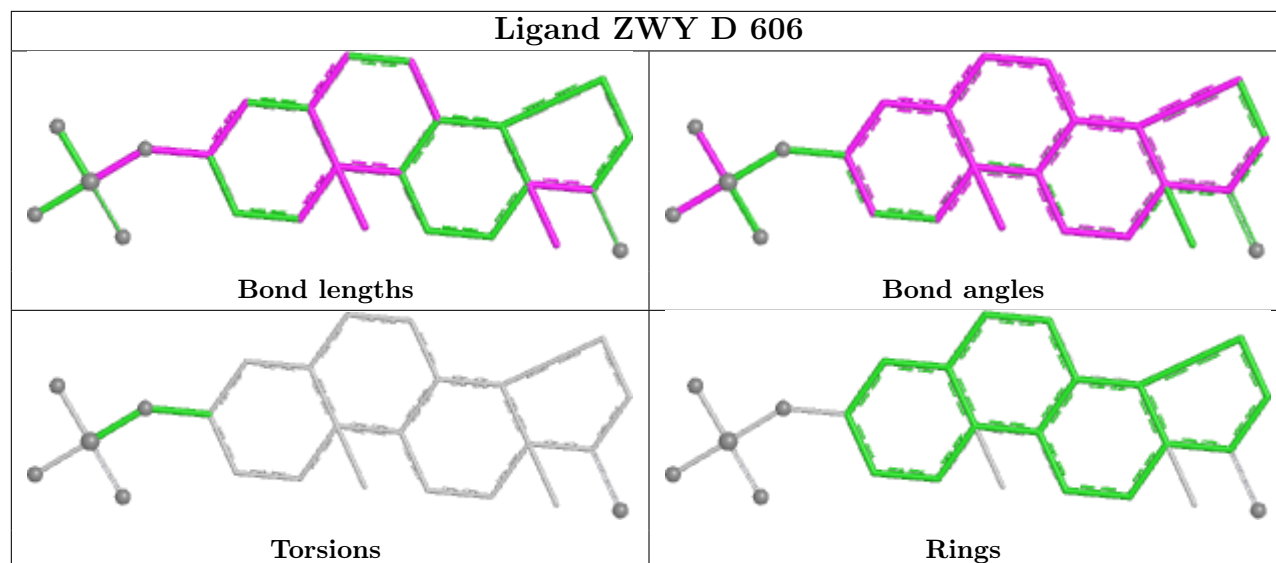


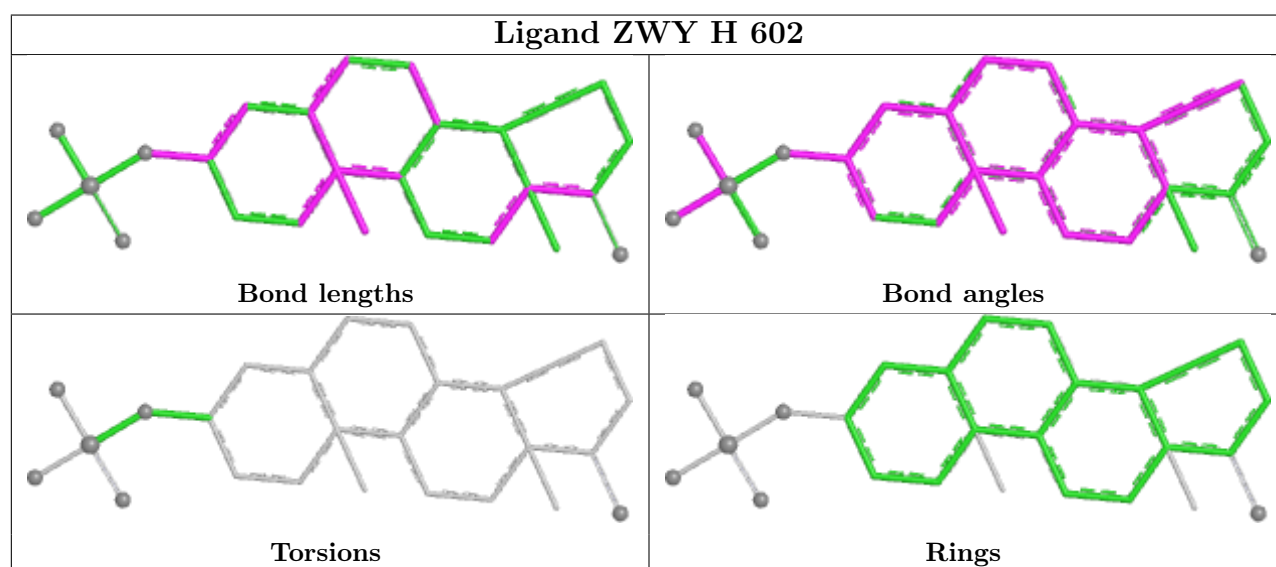
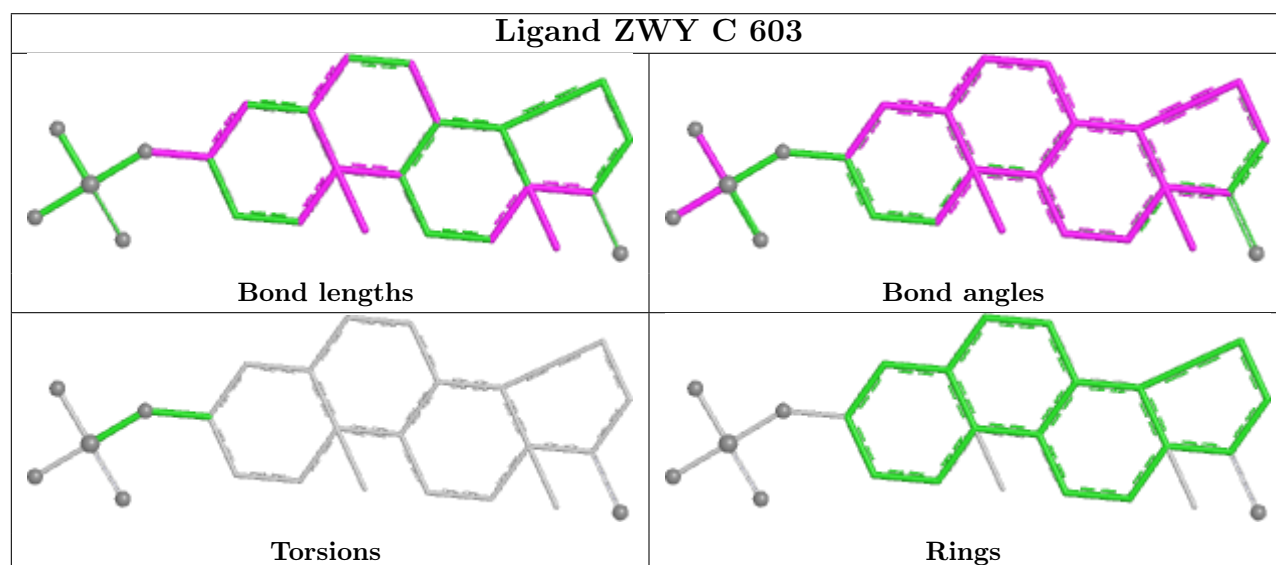
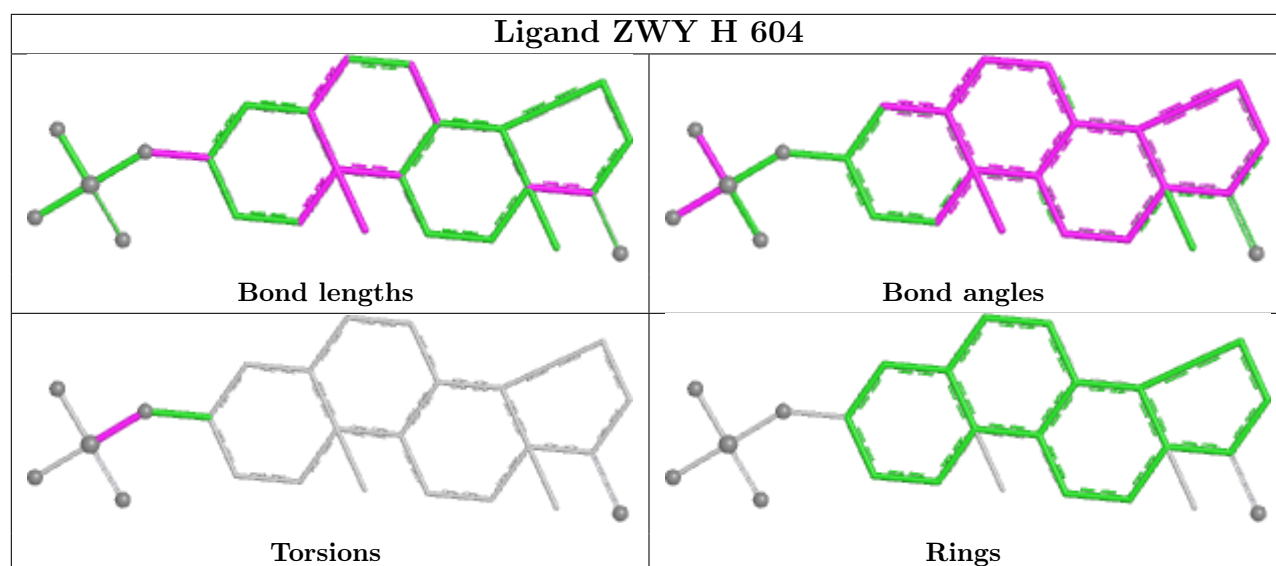
Rings



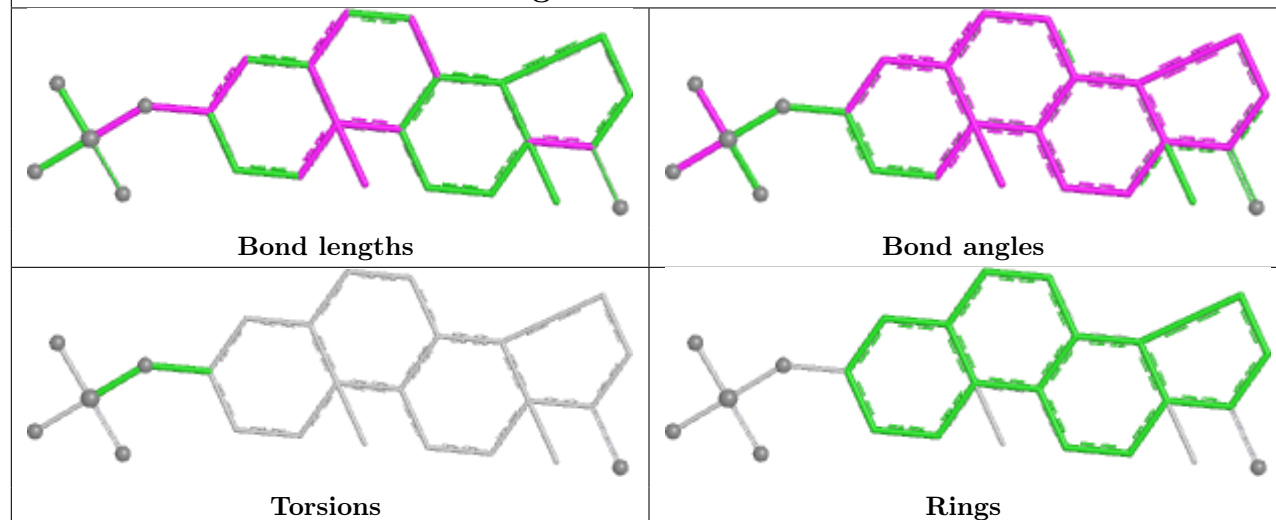




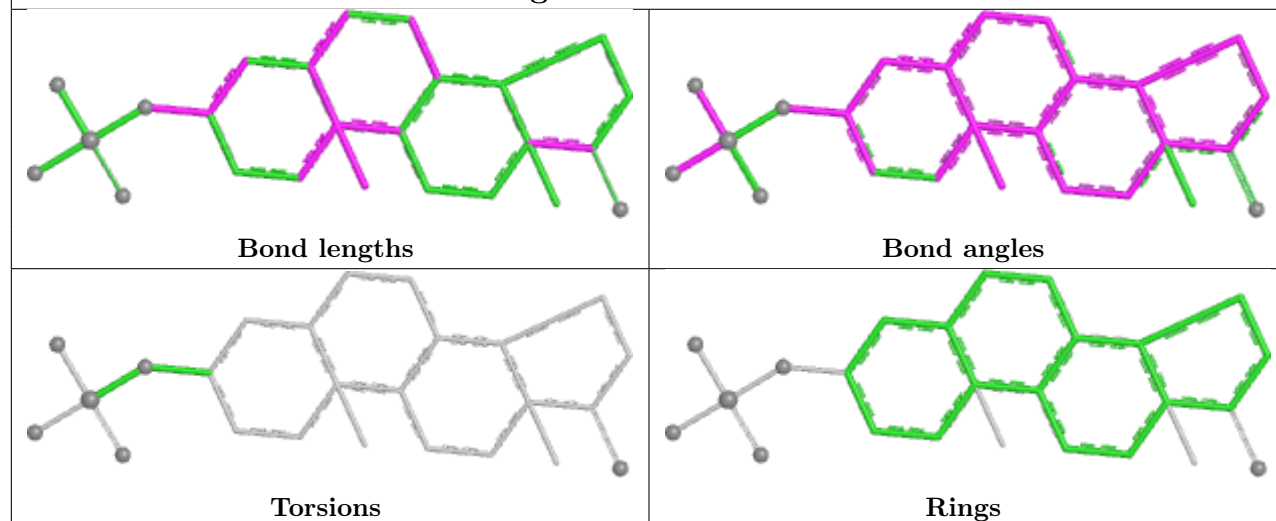




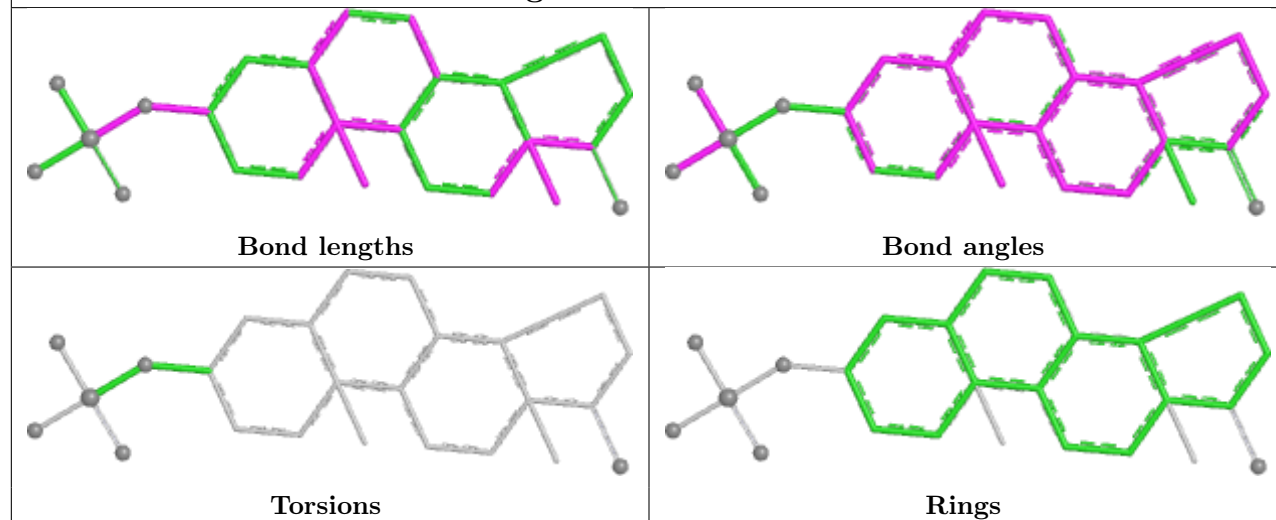
Ligand ZWY I 603

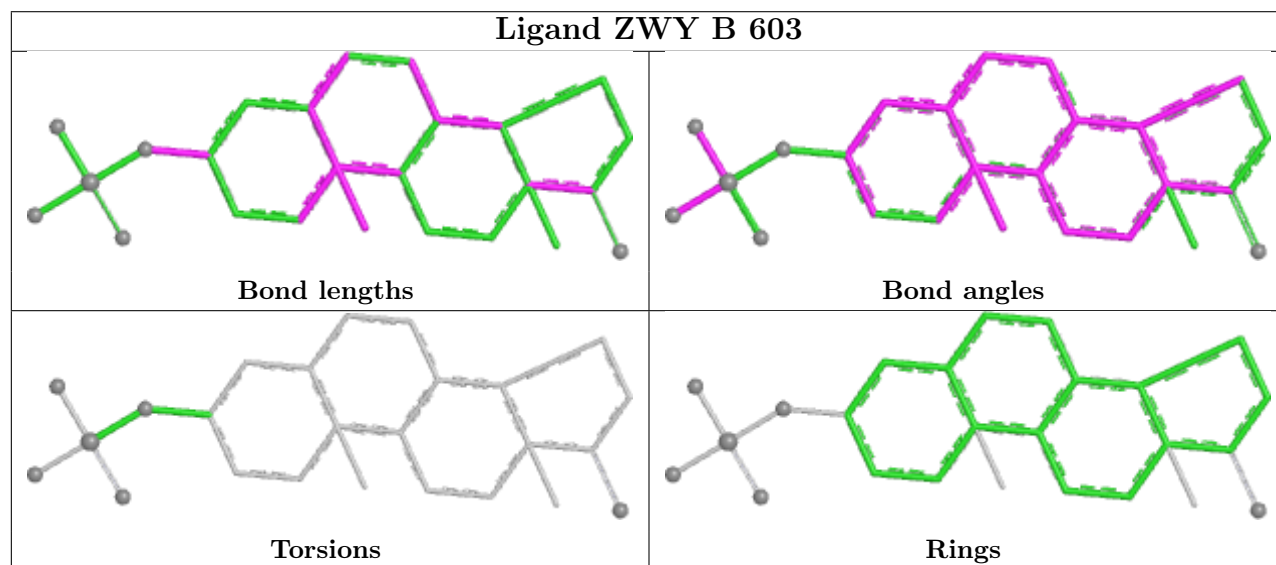
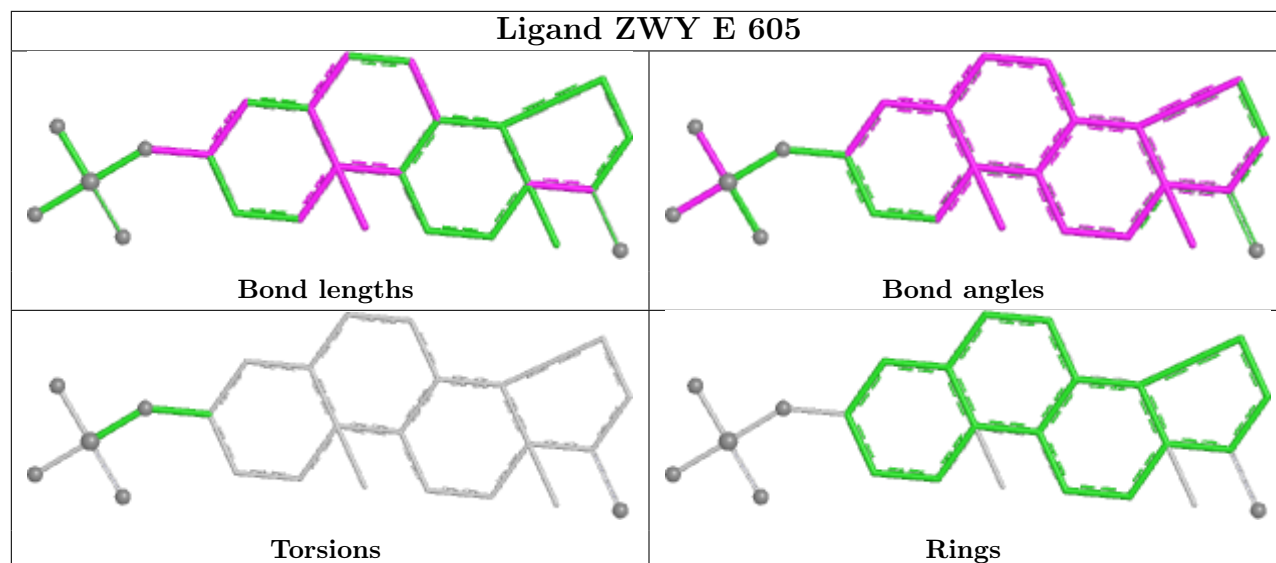


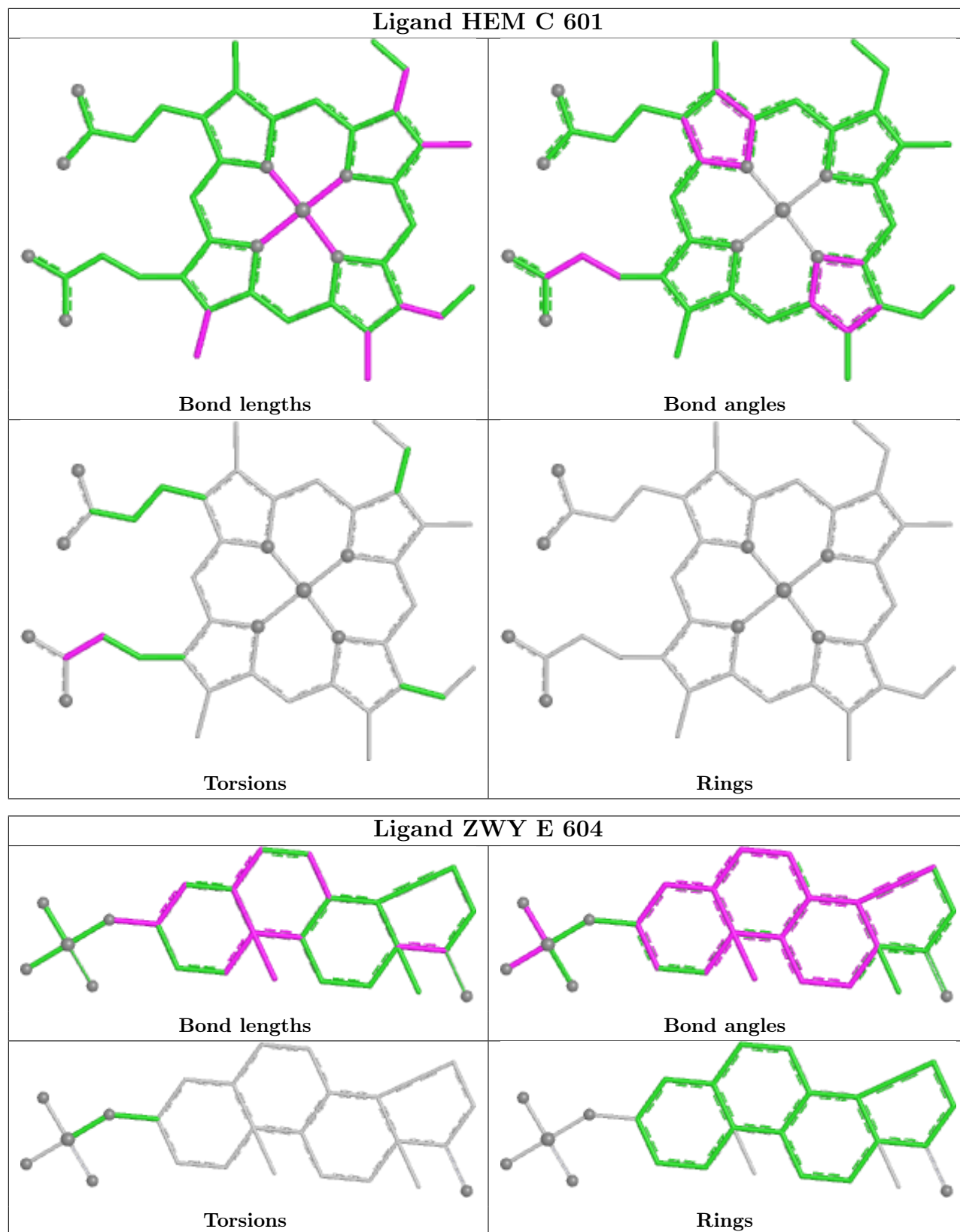
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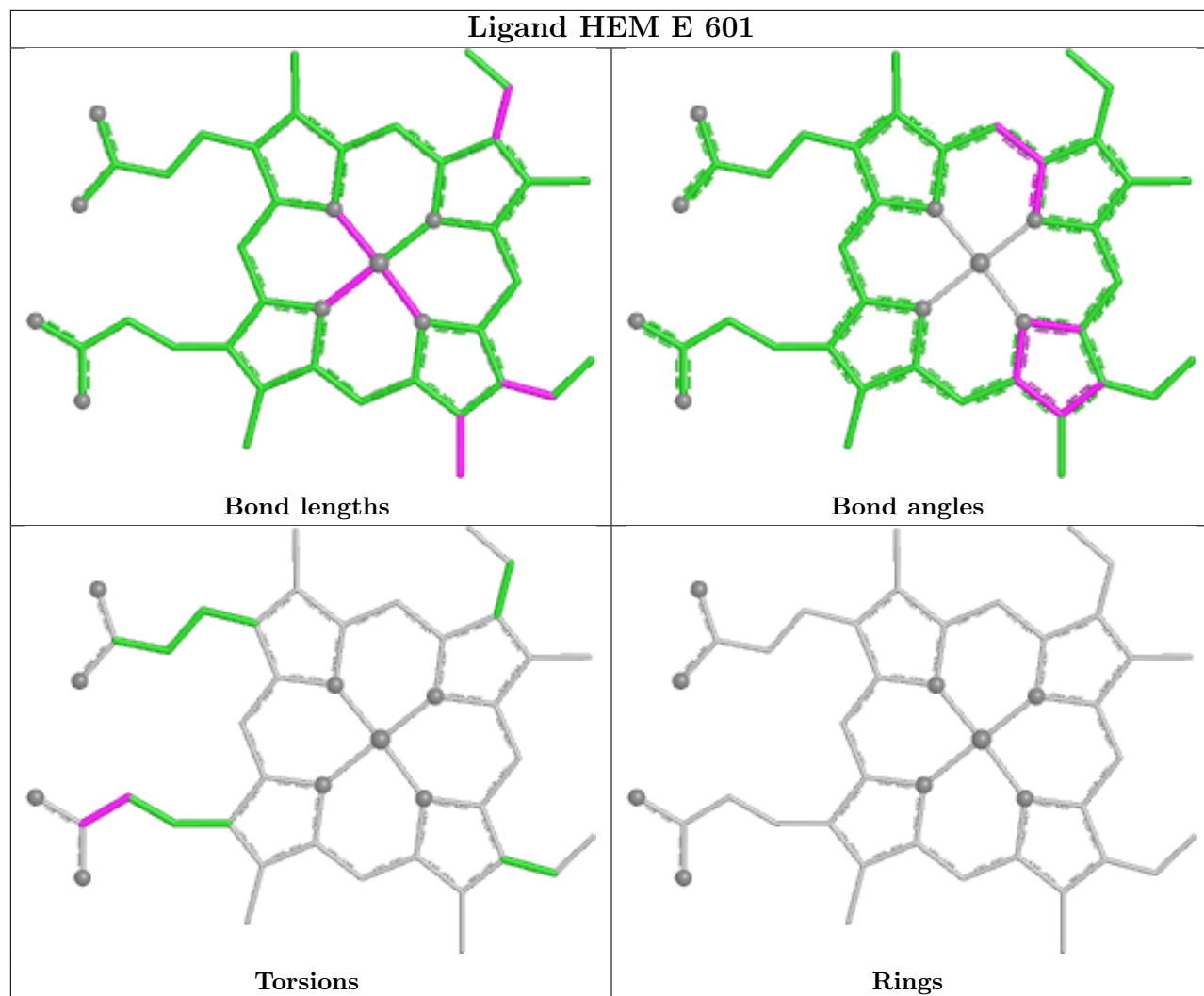


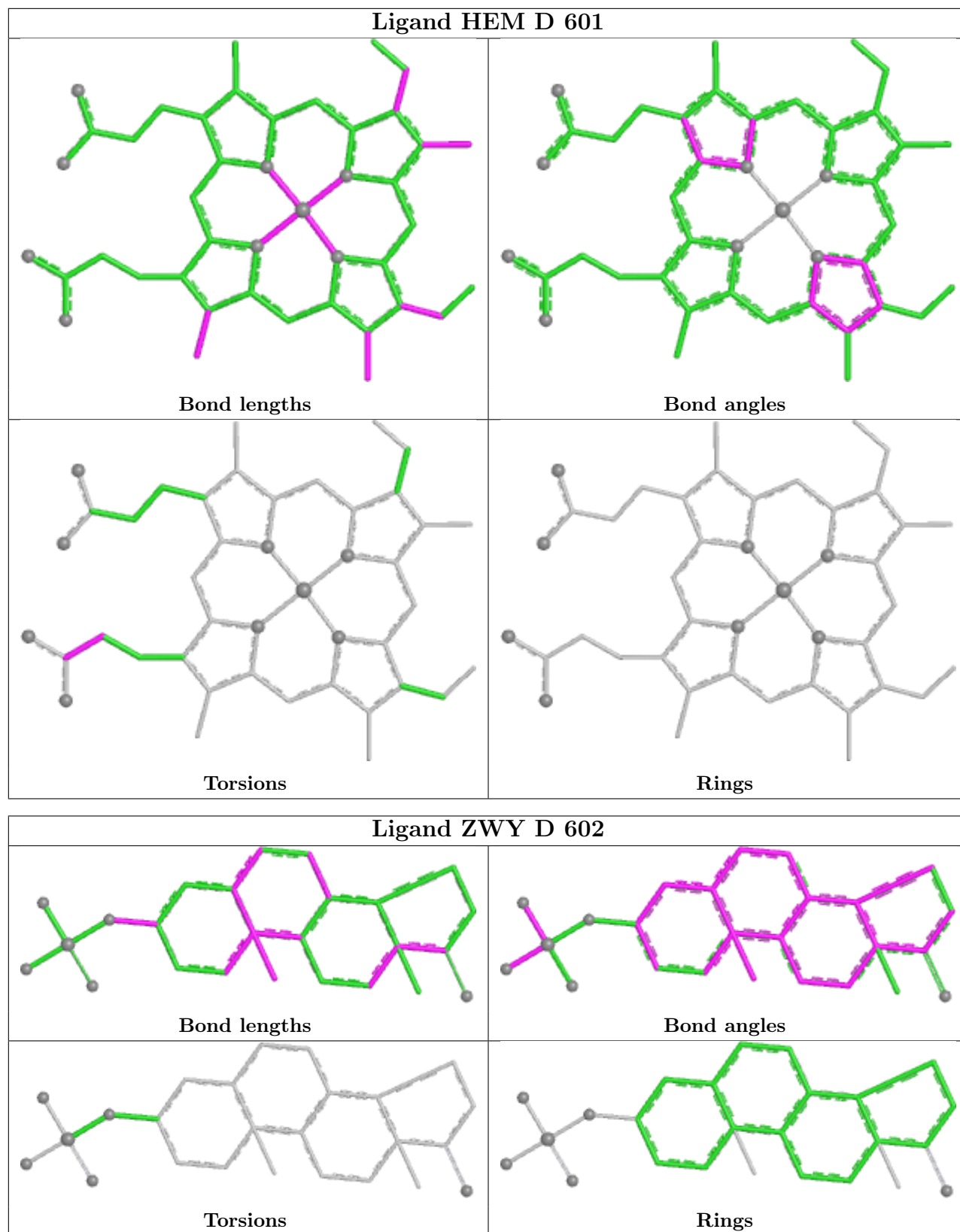
Ligand ZWY A 602



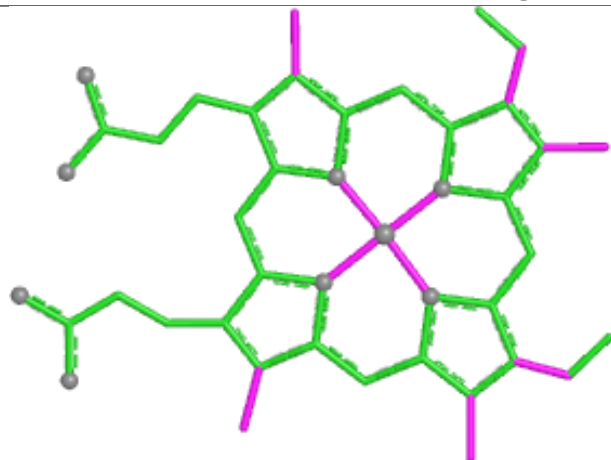




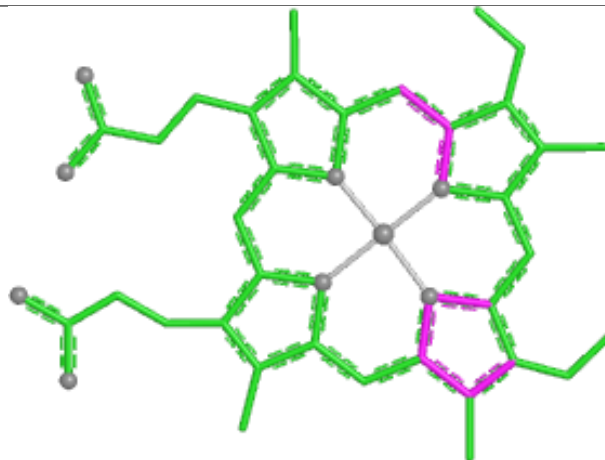




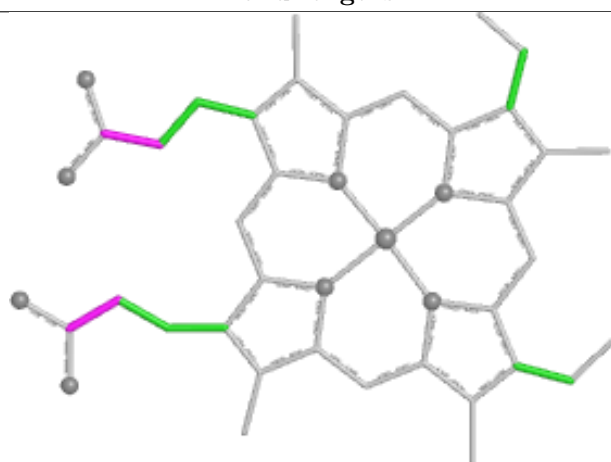
Ligand HEM I 601



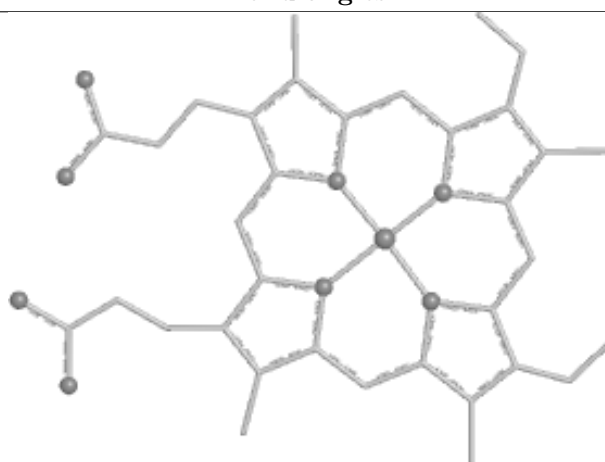
Bond lengths



Bond angles

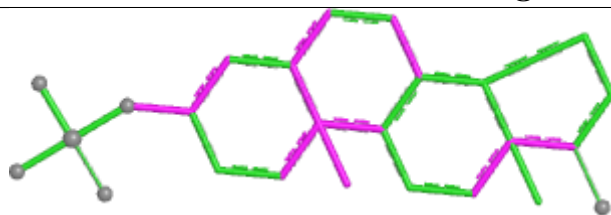


Torsions

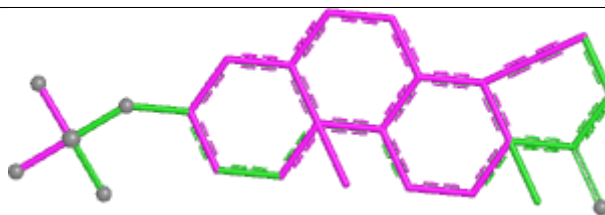


Rings

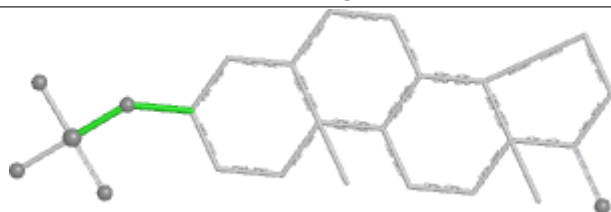
Ligand ZWY I 602



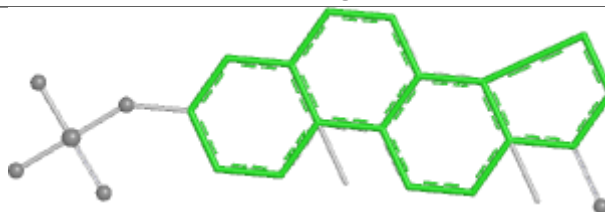
Bond lengths



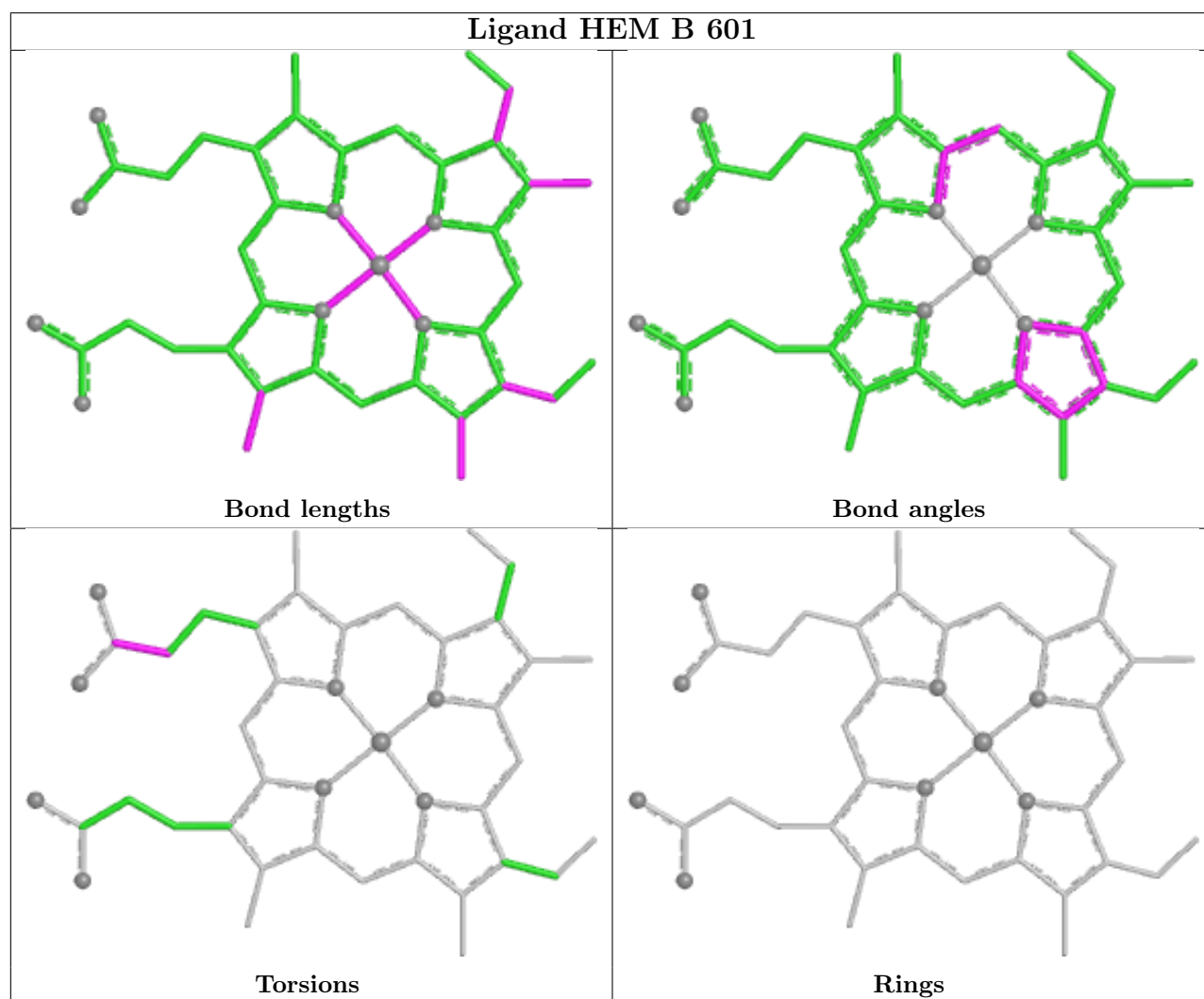
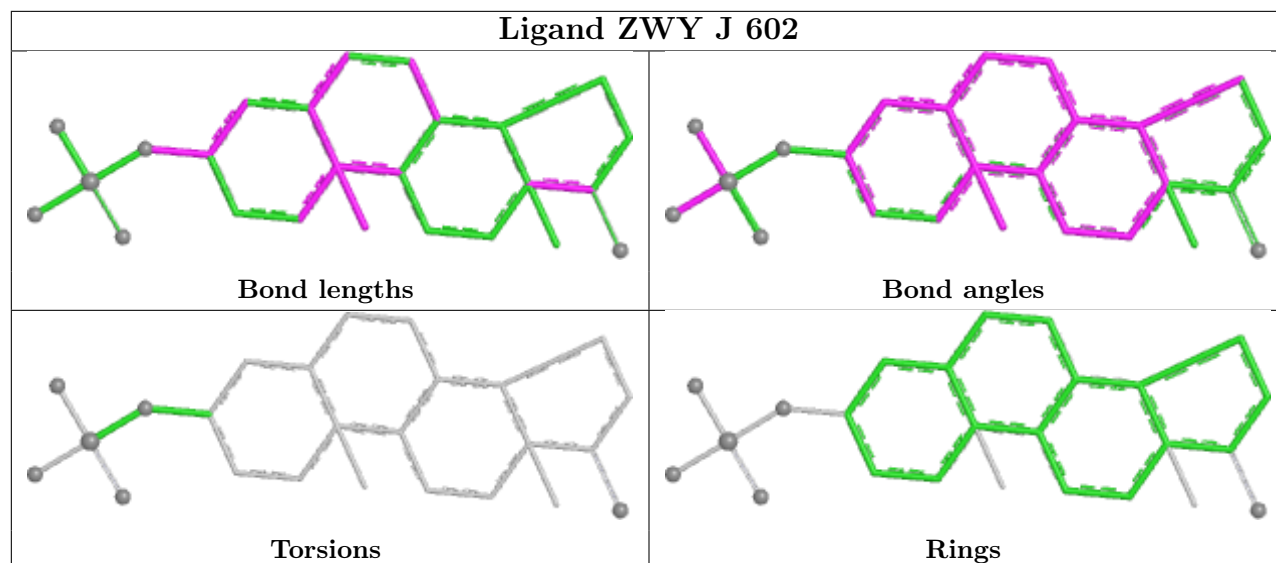
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	473/486 (97%)	-0.31	0 100 100	52, 75, 102, 128	0
1	B	462/486 (95%)	-0.26	1 (0%) 91 90	52, 77, 98, 119	0
1	C	463/486 (95%)	-0.15	5 (1%) 78 74	56, 77, 102, 123	0
1	D	459/486 (94%)	-0.27	0 100 100	57, 78, 104, 121	0
1	E	460/486 (94%)	-0.16	0 100 100	57, 82, 109, 130	0
1	F	461/486 (94%)	-0.06	4 (0%) 81 78	60, 86, 108, 121	0
1	G	462/486 (95%)	-0.09	1 (0%) 91 90	61, 88, 109, 127	0
1	H	458/486 (94%)	-0.11	1 (0%) 91 90	64, 86, 110, 132	0
1	I	463/486 (95%)	-0.03	2 (0%) 88 86	57, 89, 113, 134	0
1	J	458/486 (94%)	-0.09	5 (1%) 78 74	63, 86, 110, 129	0
1	K	462/486 (95%)	-0.04	1 (0%) 91 90	63, 96, 118, 133	0
1	L	440/486 (90%)	0.45	20 (4%) 38 32	66, 108, 129, 137	0
All	All	5521/5832 (94%)	-0.10	40 (0%) 84 82	52, 85, 115, 137	0

The worst 5 of 40 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	347	TYR	4.5
1	L	483	LEU	3.6
1	L	204	VAL	3.6
1	B	473	ILE	3.5
1	L	299	SER	3.2

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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	HEM	E	601	43/43	0.84	0.14	47,62,77,241	0
2	HEM	C	601	43/43	0.88	0.14	45,62,83,157	0
3	ZWY	I	602	25/25	0.89	0.10	32,44,57,78	21
3	ZWY	A	603	25/25	0.90	0.09	30,46,59,90	25
2	HEM	A	601	43/43	0.90	0.12	44,63,92,139	0
3	ZWY	B	603	25/25	0.91	0.12	30,43,53,73	18
3	ZWY	J	602	25/25	0.91	0.10	34,45,53,72	25
3	ZWY	D	603	25/25	0.92	0.07	33,42,54,91	22
3	ZWY	E	603	25/25	0.92	0.07	35,44,55,89	22
3	ZWY	H	603	25/25	0.92	0.07	31,41,54,78	24
3	ZWY	B	602	25/25	0.92	0.07	29,43,55,89	23
3	ZWY	I	603	25/25	0.92	0.10	31,45,56,76	19
3	ZWY	C	603	25/25	0.92	0.08	29,42,56,86	25
3	ZWY	J	603	25/25	0.92	0.09	32,42,56,93	24
3	ZWY	A	602	25/25	0.93	0.09	35,45,54,62	22
3	ZWY	D	602	25/25	0.93	0.08	31,41,52,75	23
2	HEM	G	601	43/43	0.93	0.12	60,76,94,161	0
2	HEM	F	601	43/43	0.94	0.13	61,75,93,143	0
3	ZWY	H	604	25/25	0.94	0.07	30,43,54,87	22
3	ZWY	D	605	25/25	0.94	0.08	33,43,51,85	22
2	HEM	L	601	43/43	0.94	0.11	77,101,125,130	0
3	ZWY	E	605	25/25	0.94	0.08	32,45,54,85	22
3	ZWY	H	602	25/25	0.94	0.07	36,46,52,81	25
3	ZWY	C	602	25/25	0.95	0.06	32,41,50,76	22
3	ZWY	E	602	25/25	0.95	0.07	34,46,52,81	25
3	ZWY	C	605	25/25	0.95	0.07	33,42,55,83	25
3	ZWY	E	604	25/25	0.95	0.06	30,42,51,77	20
3	ZWY	D	606	25/25	0.96	0.06	34,42,51,62	20
2	HEM	J	601	43/43	0.96	0.12	55,75,92,96	0
3	ZWY	D	604	25/25	0.96	0.07	33,45,51,62	24
2	HEM	D	601	43/43	0.96	0.11	44,64,83,93	0
3	ZWY	C	604	25/25	0.97	0.05	32,44,54,65	20

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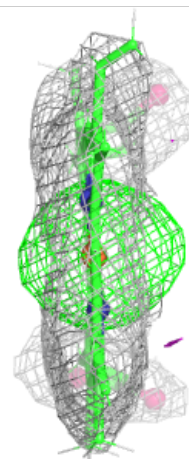
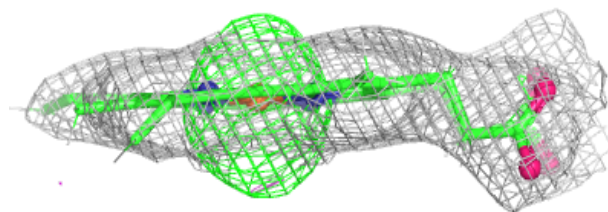
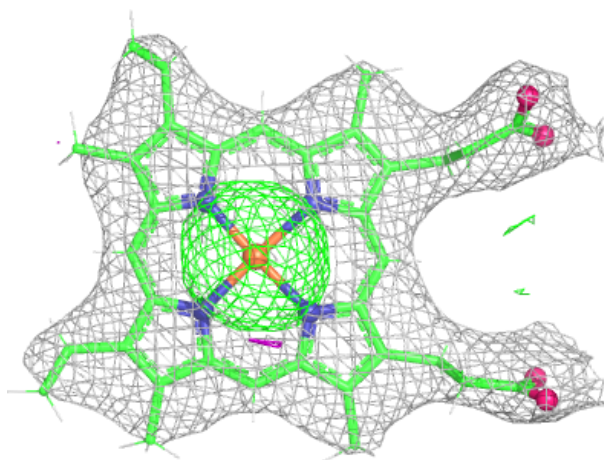
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	HEM	K	601	43/43	0.97	0.10	59,75,102,106	0
2	HEM	I	601	43/43	0.97	0.11	59,75,92,107	0
2	HEM	B	601	43/43	0.98	0.08	47,63,83,91	0
2	HEM	H	601	43/43	0.98	0.10	51,66,86,89	0

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

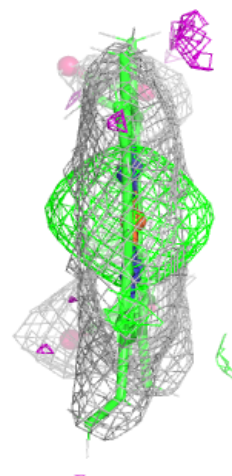
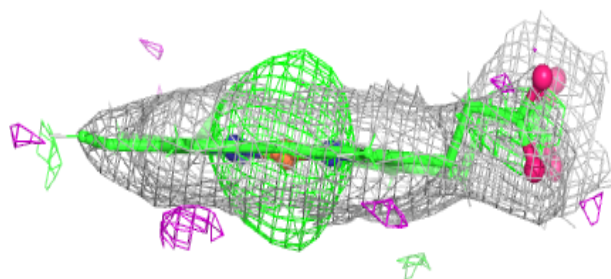
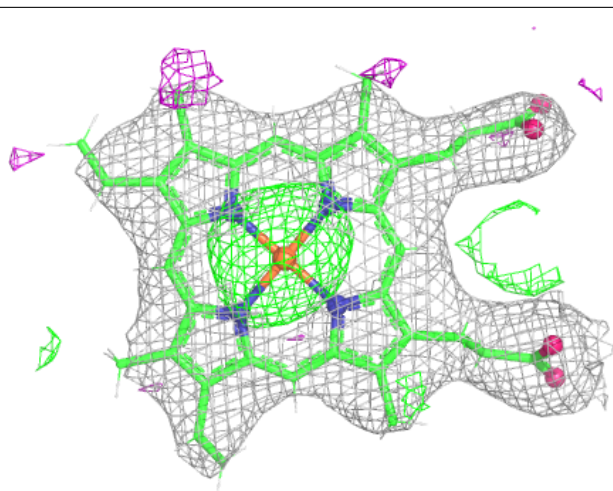
Electron density around HEM E 601:

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



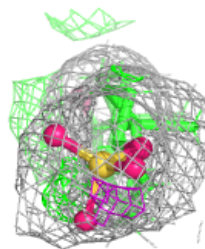
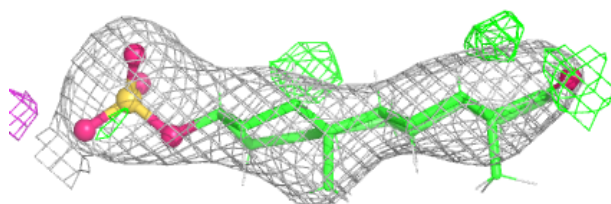
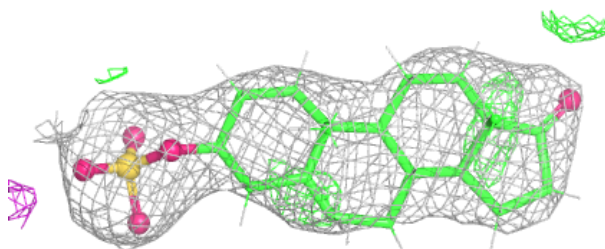
Electron density around HEM C 601:

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and green (positive)

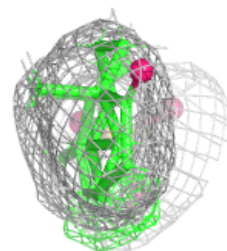
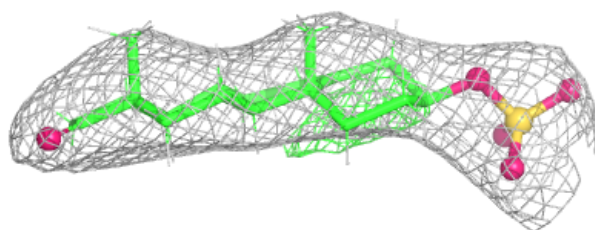
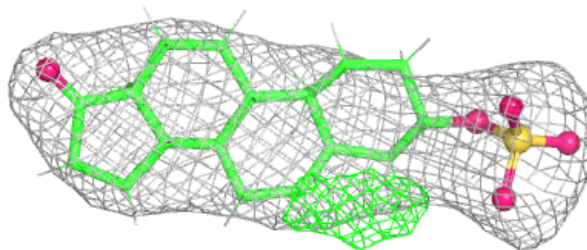


Electron density around ZWY I 602:

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and green (positive)

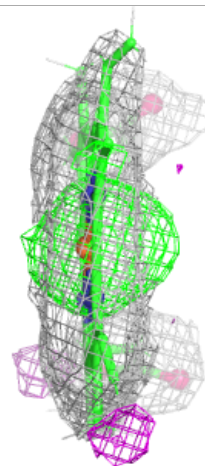
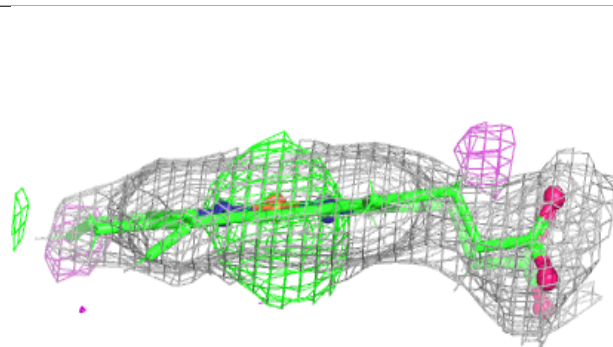
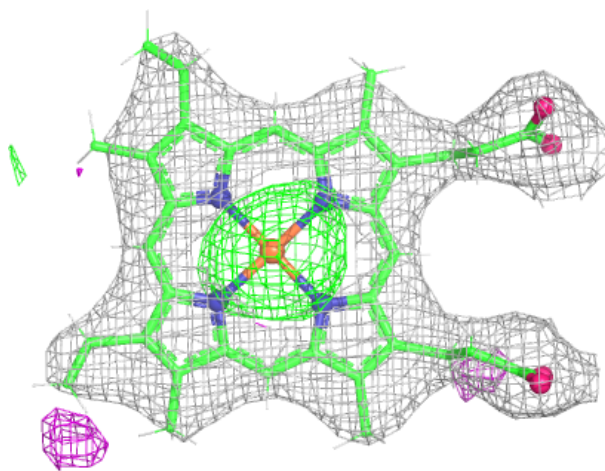
**Electron density around ZWY A 603:**

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and green (positive)



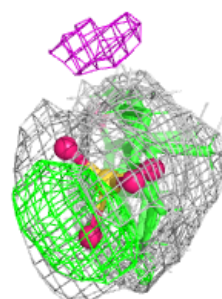
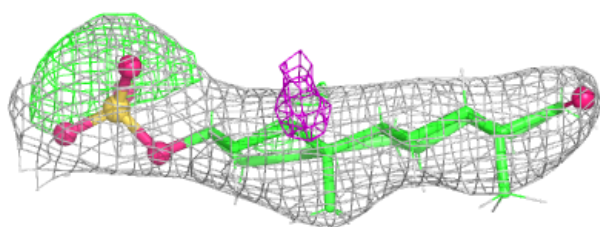
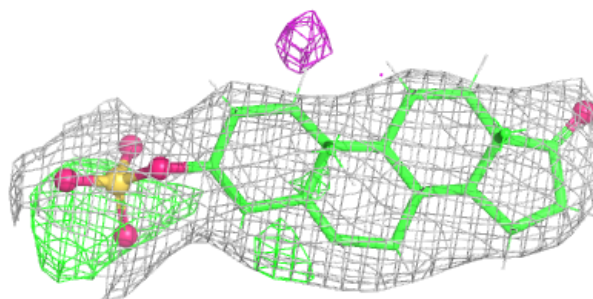
Electron density around HEM A 601:

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and green (positive)

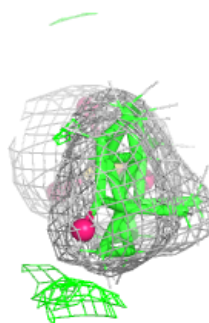
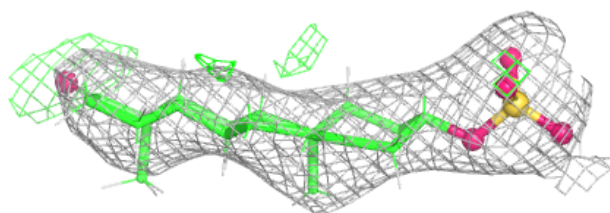
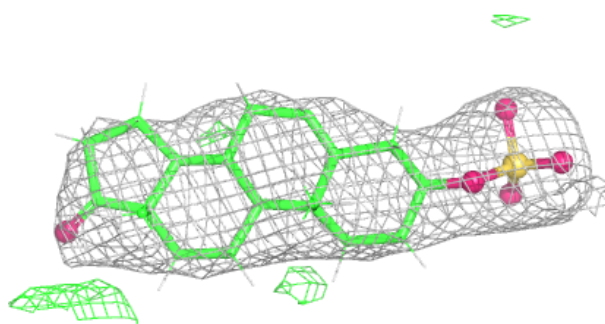


Electron density around ZWY B 603:

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

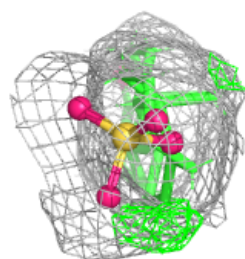
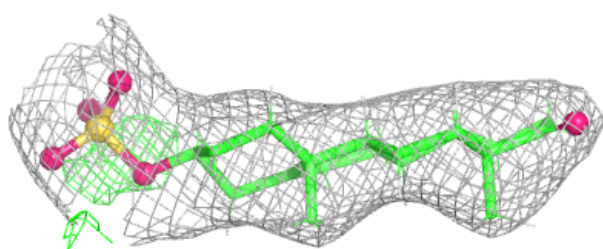
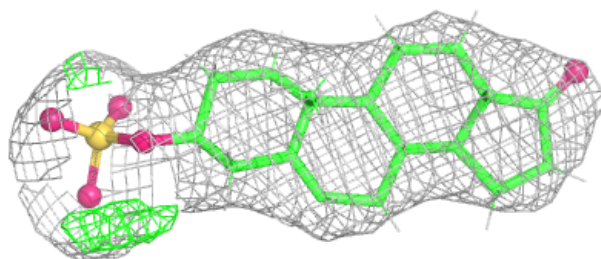
**Electron density around ZWY J 602:**

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

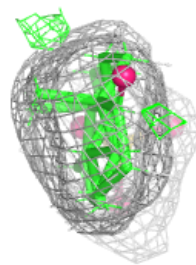
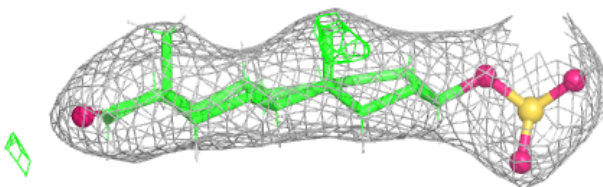
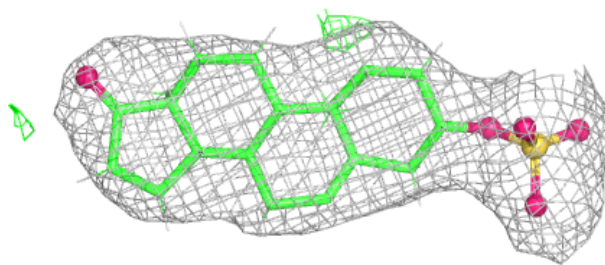


Electron density around ZWY D 603:

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

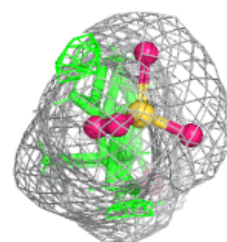
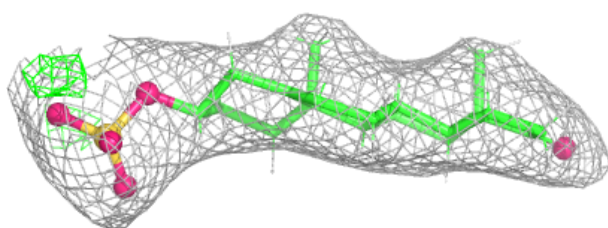
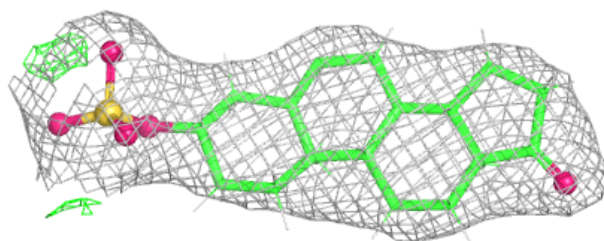
**Electron density around ZWY E 603:**

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

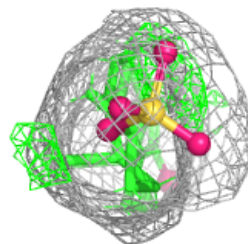
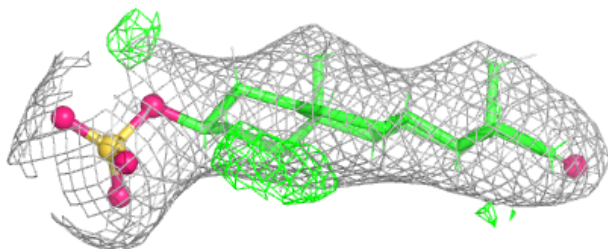
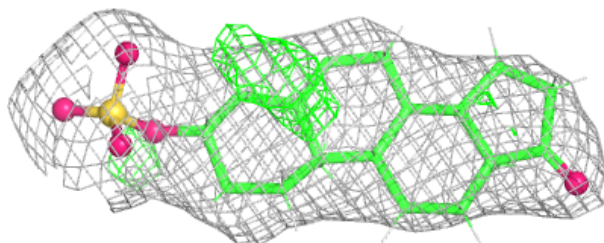


Electron density around ZWY H 603:

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

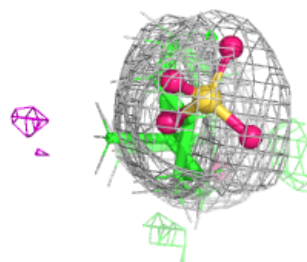
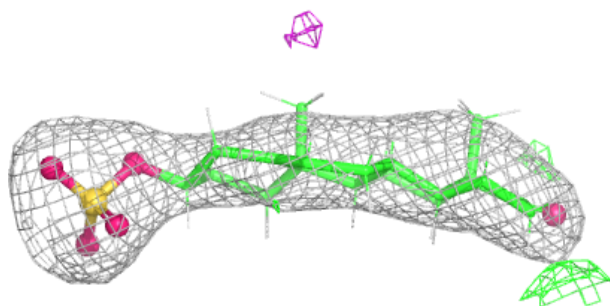
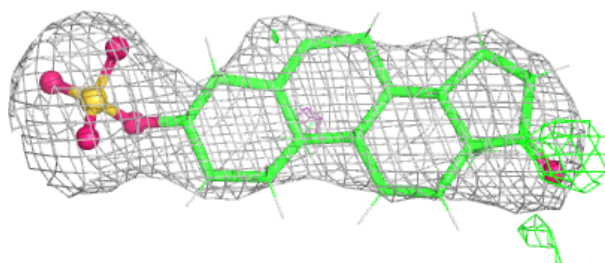
**Electron density around ZWY B 602:**

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

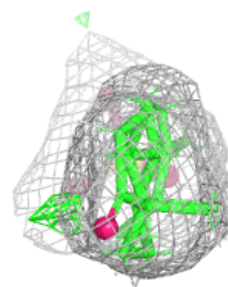
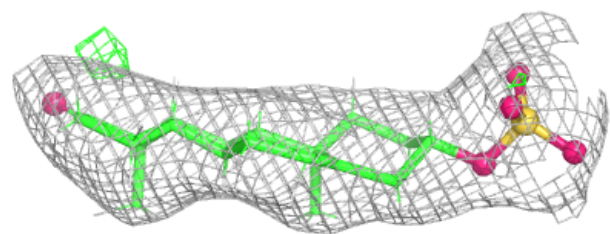
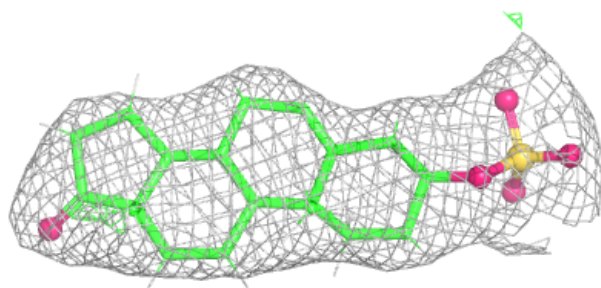


Electron density around ZWY I 603:

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

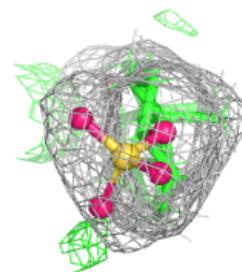
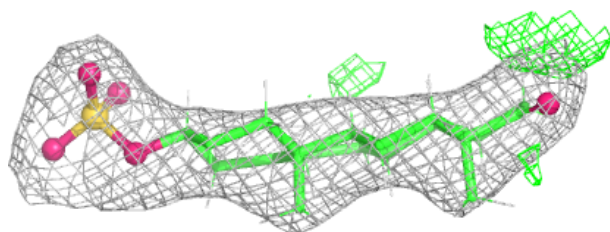
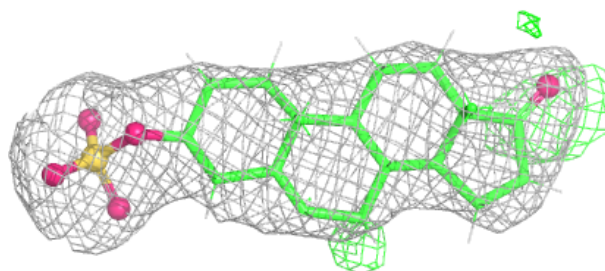
**Electron density around ZWY C 603:**

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

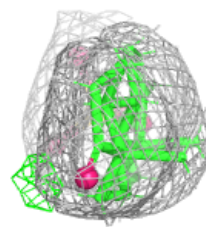
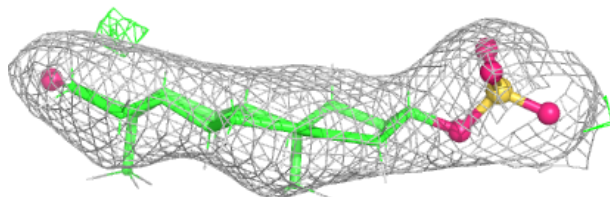
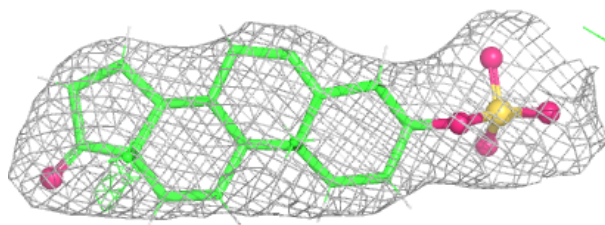


Electron density around ZWY J 603:

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

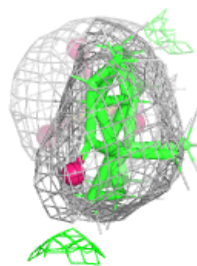
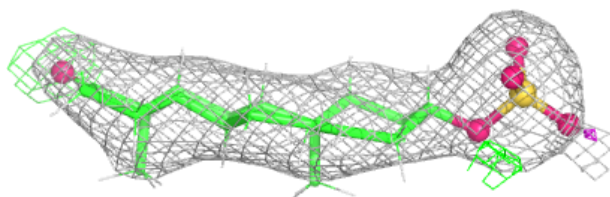
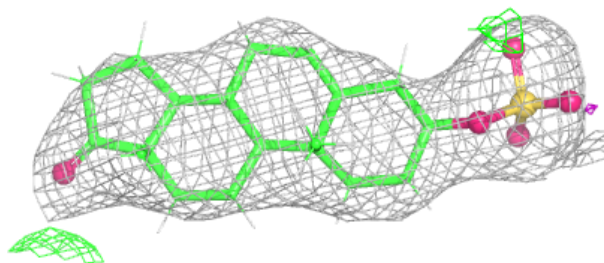
**Electron density around ZWY A 602:**

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



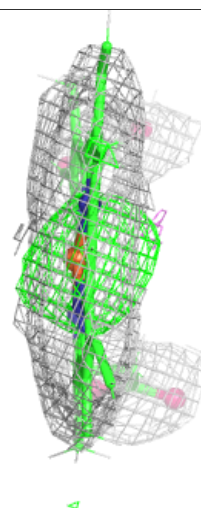
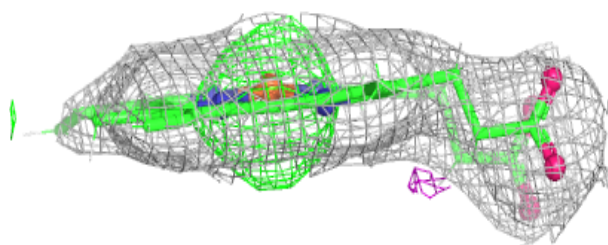
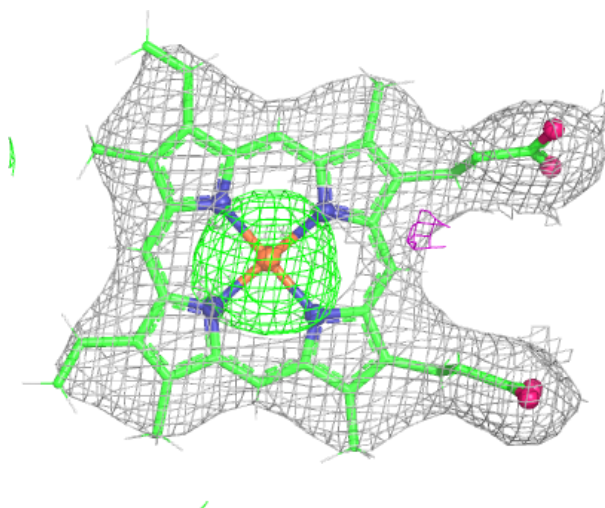
Electron density around ZWY D 602:

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



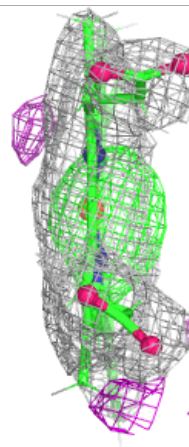
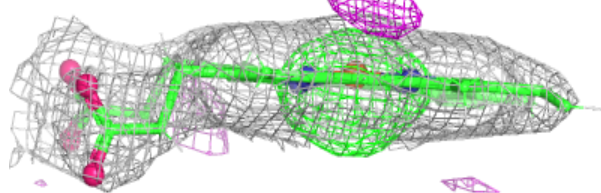
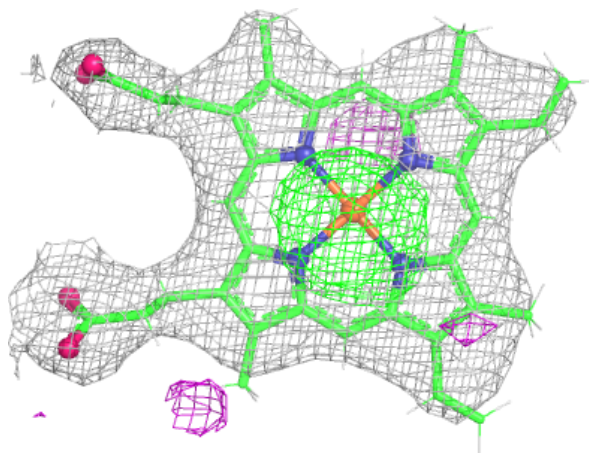
Electron density around HEM G 601:

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



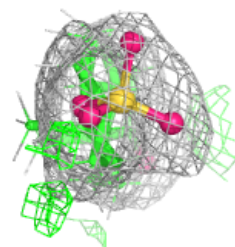
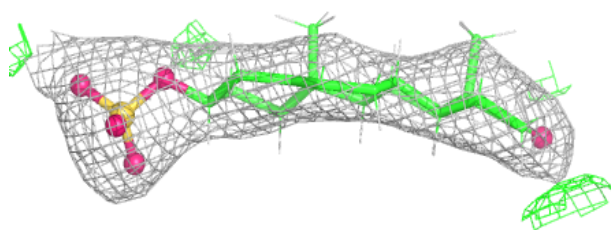
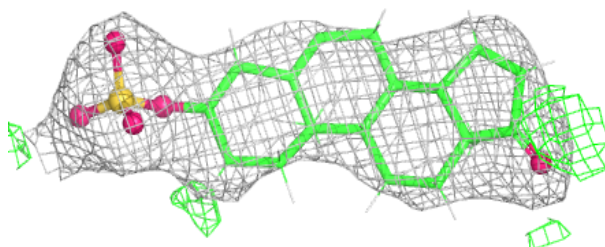
Electron density around HEM F 601:

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

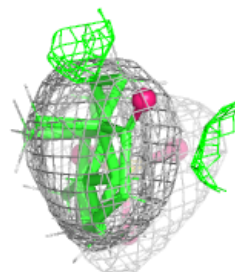
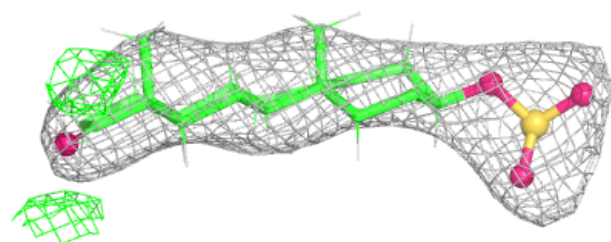
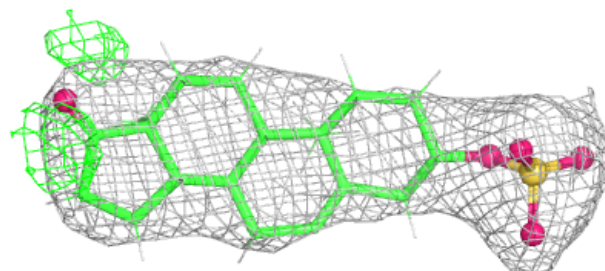


Electron density around ZWY H 604:

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

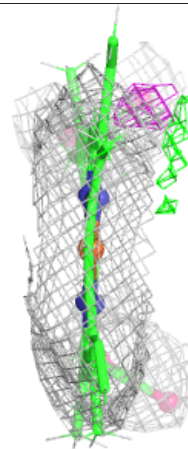
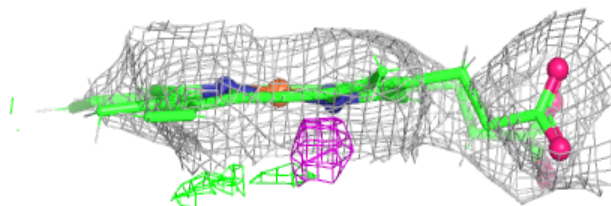
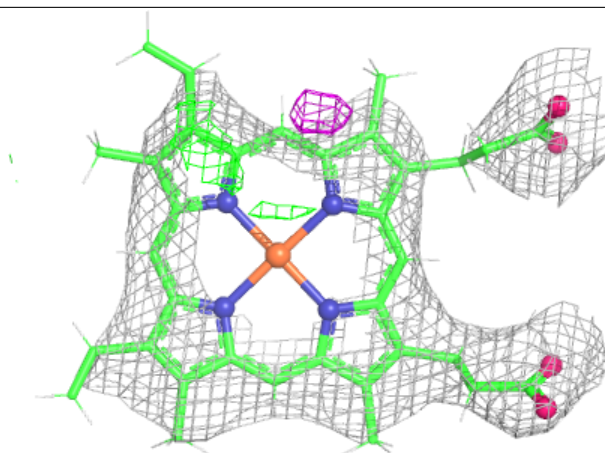
**Electron density around ZWY D 605:**

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



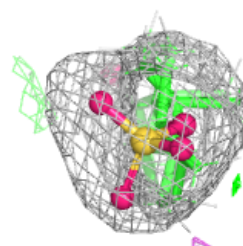
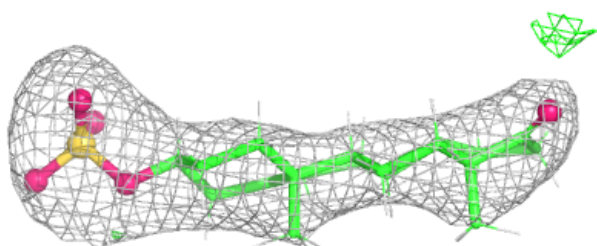
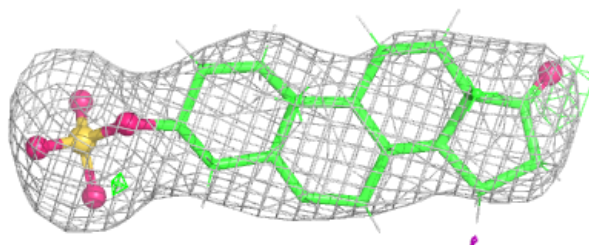
Electron density around HEM L 601:

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

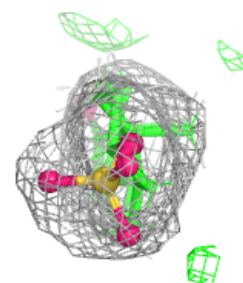
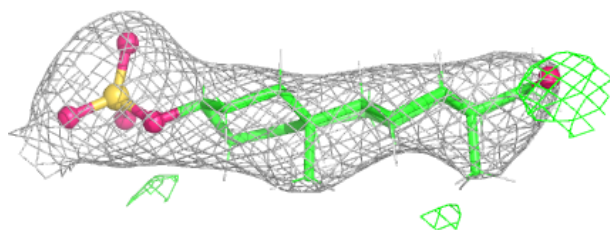
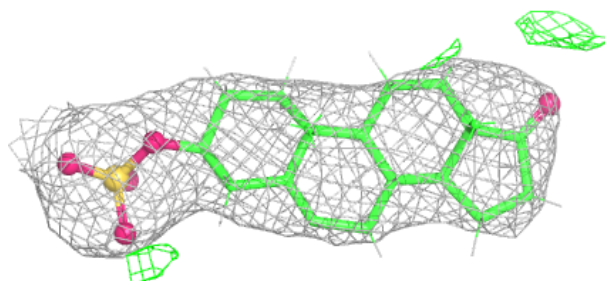


Electron density around ZWY E 605:

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

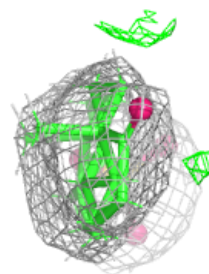
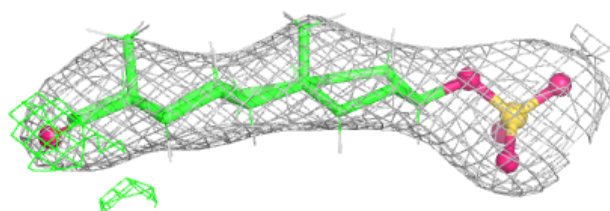
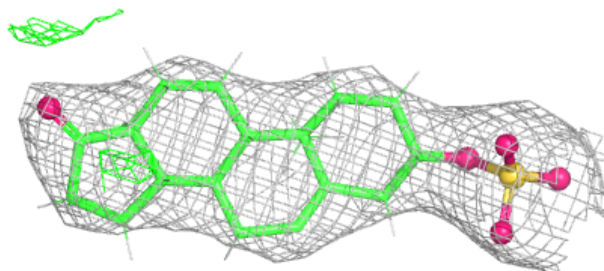
**Electron density around ZWY H 602:**

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

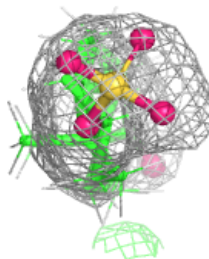
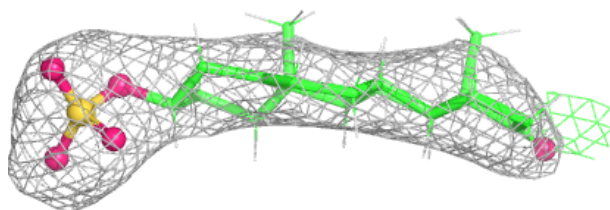
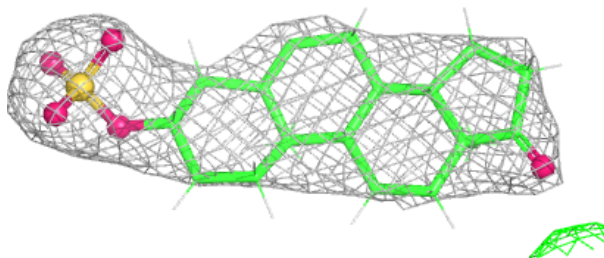


Electron density around ZWY C 602:

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

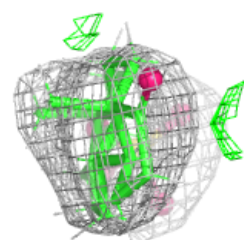
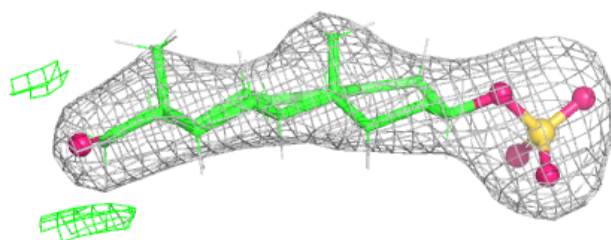
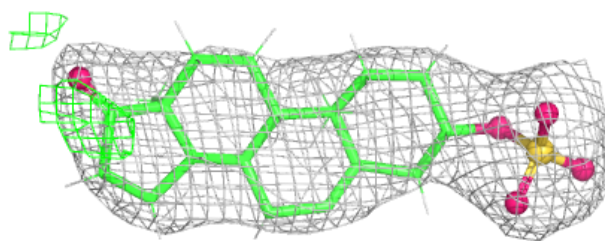
**Electron density around ZWY E 602:**

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

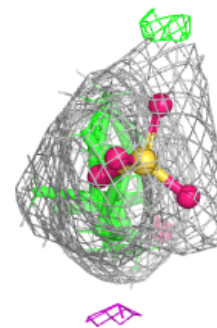
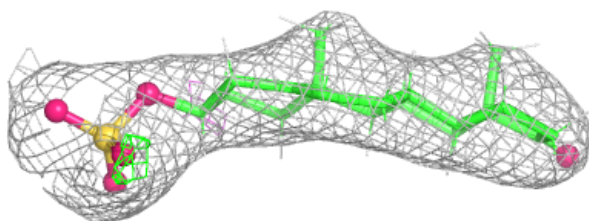
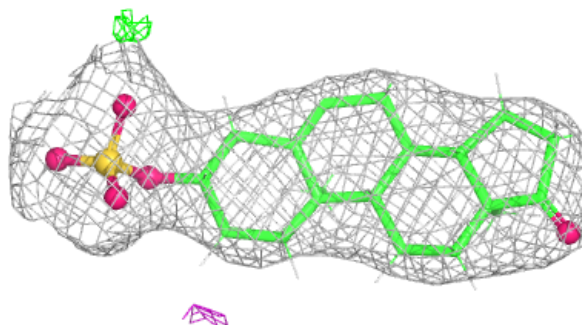


Electron density around ZWY C 605:

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

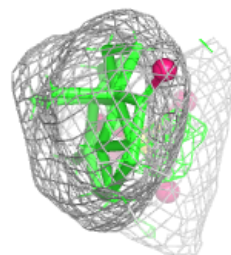
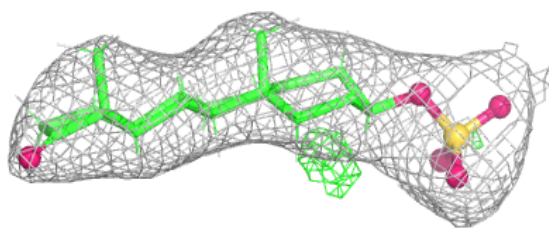
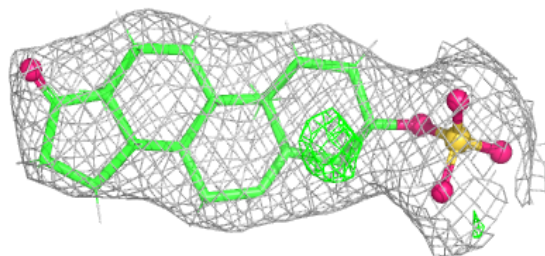
**Electron density around ZWY E 604:**

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



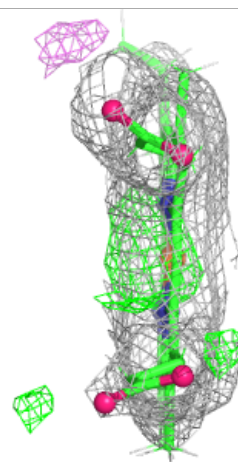
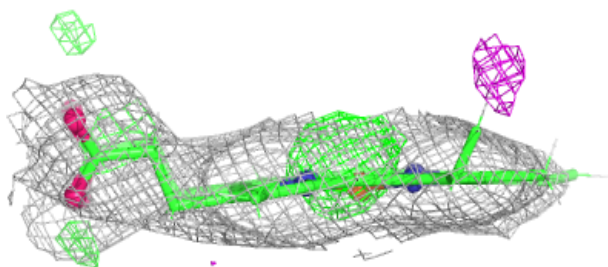
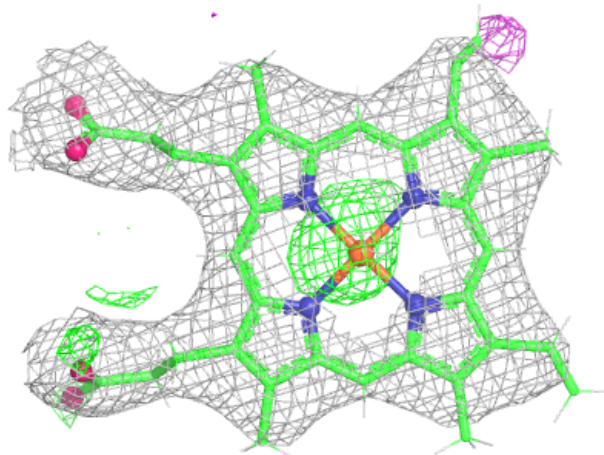
Electron density around ZWY D 606:

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



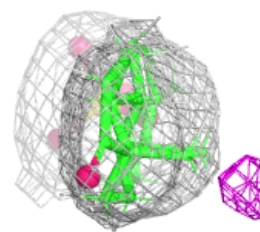
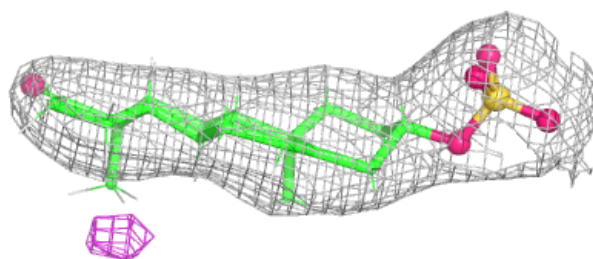
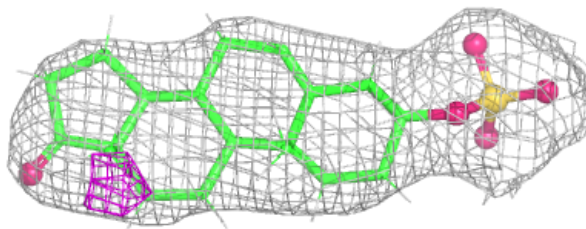
Electron density around HEM J 601:

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



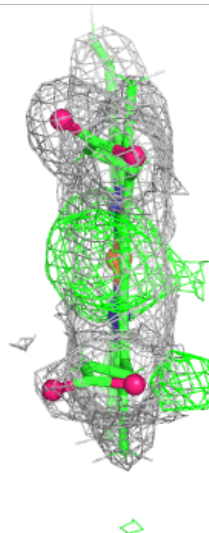
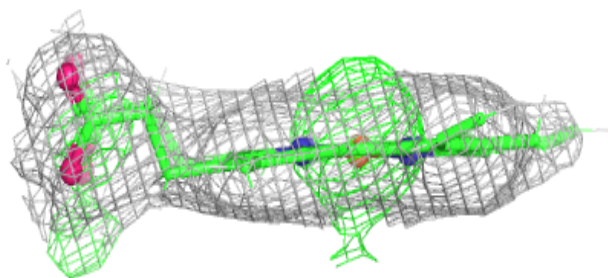
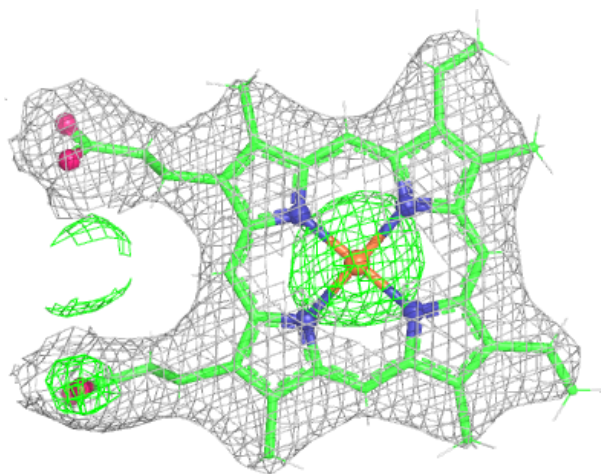
Electron density around ZWY D 604:

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



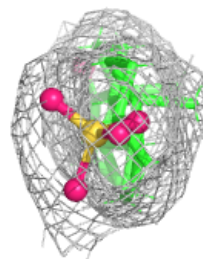
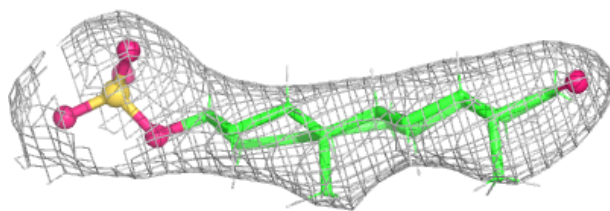
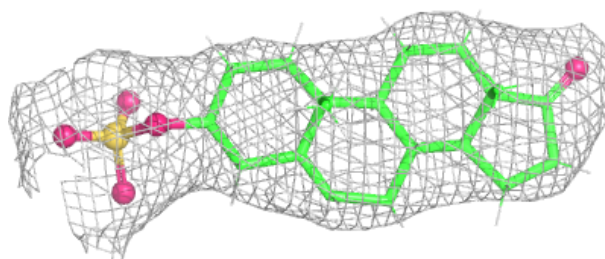
Electron density around HEM D 601:

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



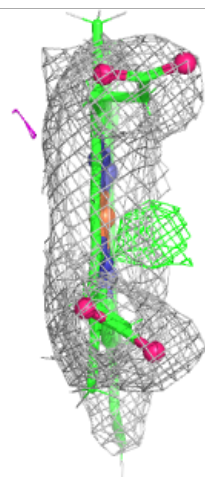
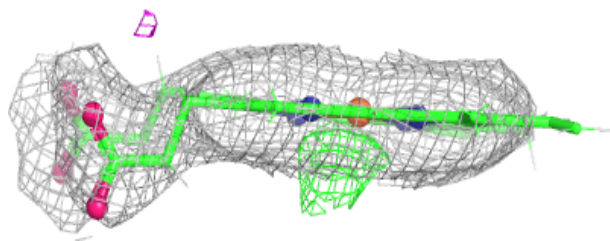
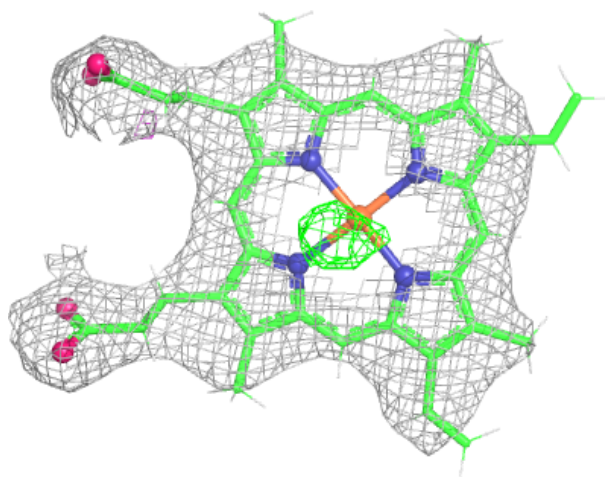
Electron density around ZWY C 604:

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



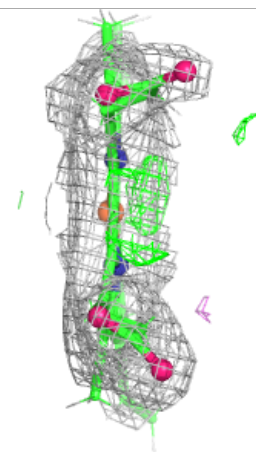
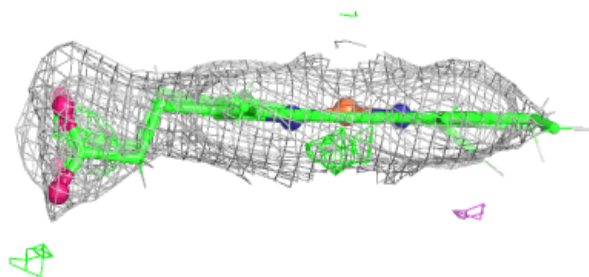
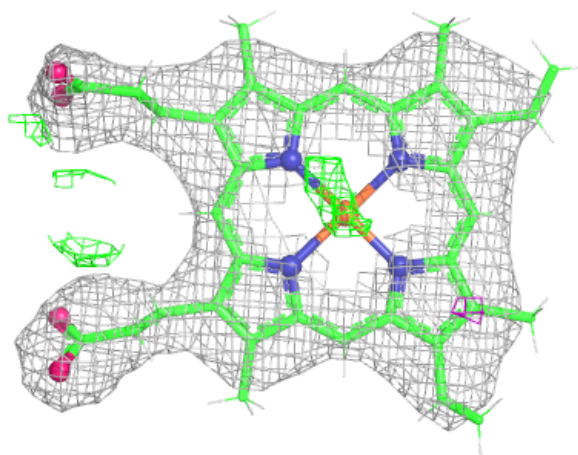
Electron density around HEM K 601:

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



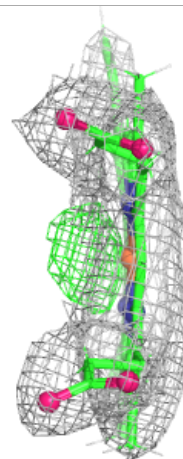
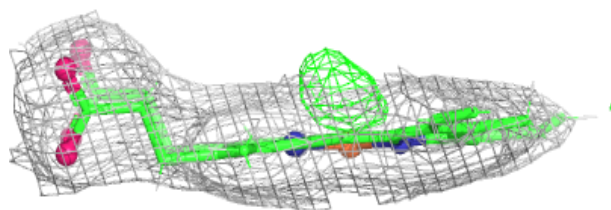
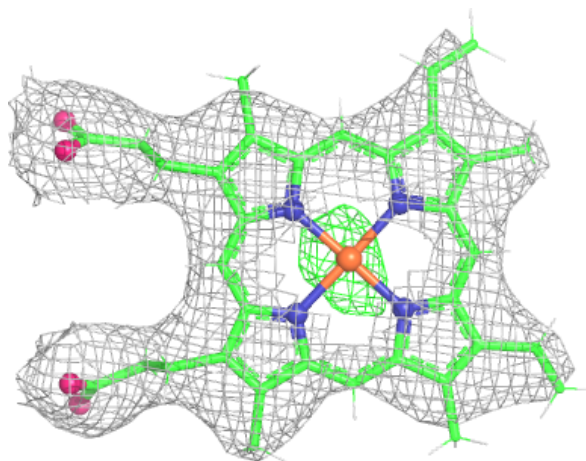
Electron density around HEM I 601:

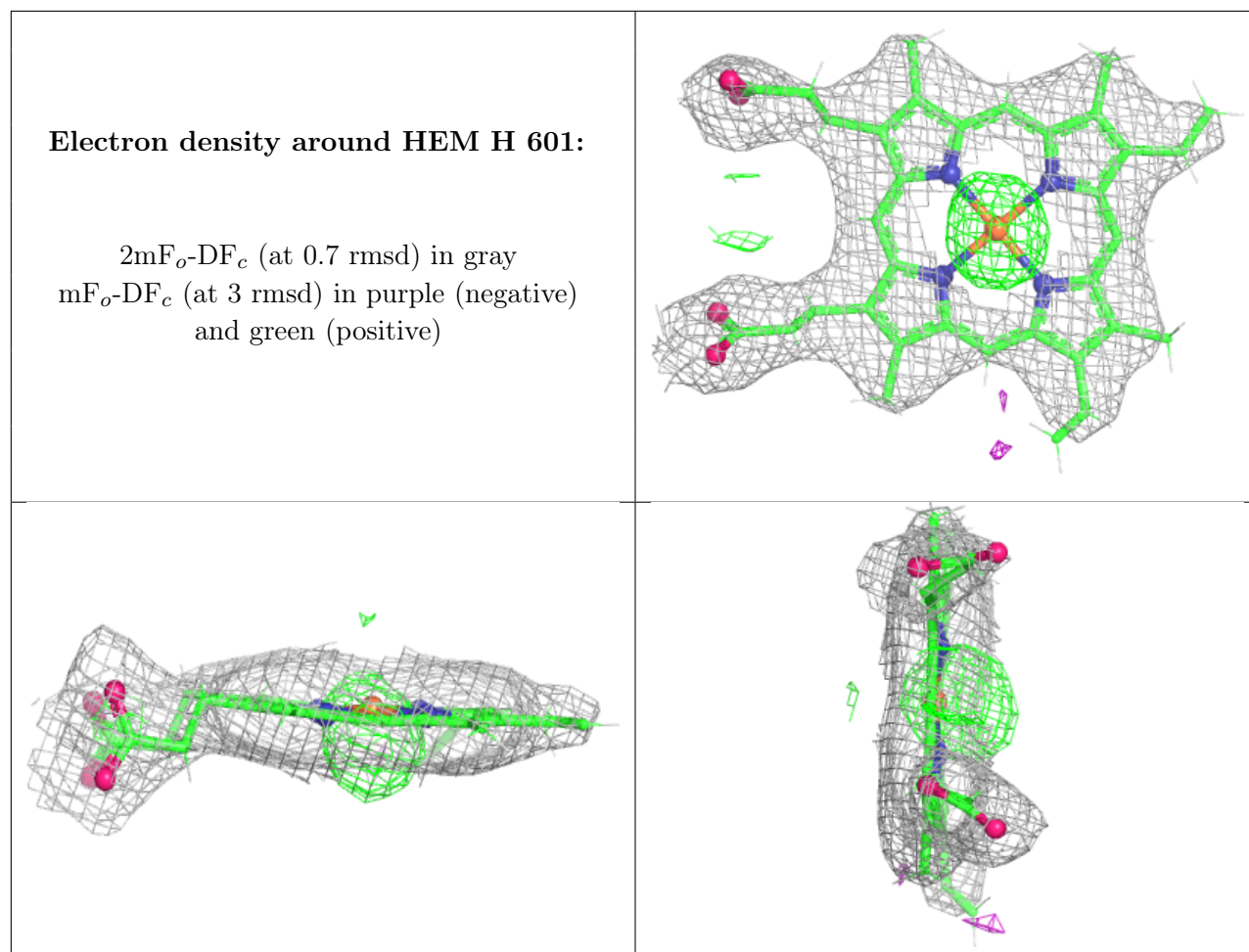
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.5 Other polymers [i](#)

There are no such residues in this entry.