



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 12:03 PM UTC

PDB ID : 4DVQ / pdb_00004dvq
Title : Structure of human aldosterone synthase, CYP11B2, in complex with deoxy-corticosterone
Authors : Strushkevich, N.; Shen, L.; Tempel, W.; Arrowsmith, C.; Edwards, A.; Usanov, S.A.; Park, H.-W.
Deposited on : 2012-02-23
Resolution : 2.49 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

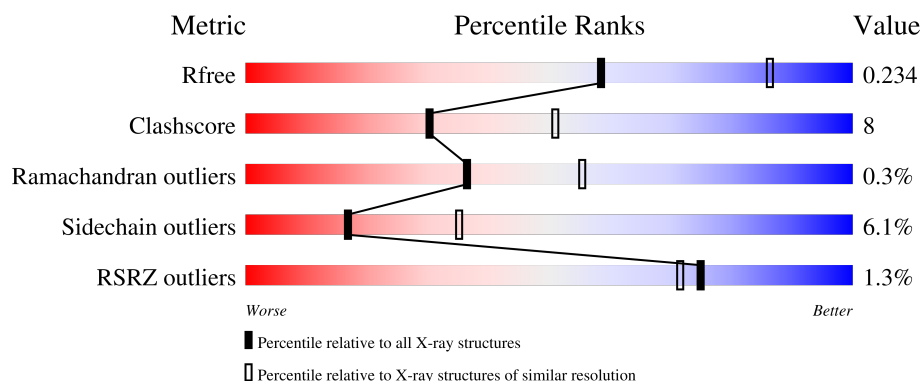
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

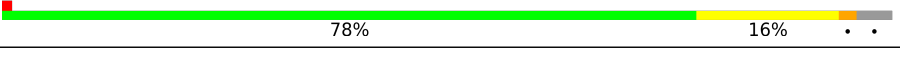
The reported resolution of this entry is 2.49 Å.

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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	483	
1	B	483	
1	C	483	
1	D	483	

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Mol	Chain	Length	Quality of chain
1	E	483	78%16%
1	F	483	73%23%
1	G	483	78%16%
1	H	483	76%18%
1	I	483	73%22%
1	J	483	77%15%
1	K	483	71%22%
1	L	483	75%16%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 46194 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cytochrome P450 11B2, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	463	Total	C	N	O	S	0	0	0
			3758	2431	662	645	20			
1	B	463	Total	C	N	O	S	0	0	0
			3758	2431	662	645	20			
1	C	462	Total	C	N	O	S	0	0	0
			3750	2425	661	644	20			
1	D	462	Total	C	N	O	S	0	0	0
			3750	2425	661	644	20			
1	E	470	Total	C	N	O	S	0	0	0
			3826	2469	683	654	20			
1	F	469	Total	C	N	O	S	0	0	0
			3818	2465	681	652	20			
1	G	462	Total	C	N	O	S	0	0	0
			3750	2425	661	644	20			
1	H	462	Total	C	N	O	S	0	0	0
			3750	2425	661	644	20			
1	I	462	Total	C	N	O	S	0	0	0
			3750	2425	661	644	20			
1	J	462	Total	C	N	O	S	0	0	0
			3750	2425	661	644	20			
1	K	460	Total	C	N	O	S	0	0	0
			3734	2415	659	640	20			
1	L	454	Total	C	N	O	S	0	0	0
			3691	2387	650	634	20			

There are 156 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	MET	-	expression tag	UNP P19099
A	28	ALA	-	expression tag	UNP P19099
A	29	LYS	-	expression tag	UNP P19099
A	30	LYS	-	expression tag	UNP P19099
A	31	THR	-	expression tag	UNP P19099

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Chain	Residue	Modelled	Actual	Comment	Reference
A	32	SER	-	expression tag	UNP P19099
A	33	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
A	508	HIS	-	expression tag	UNP P19099
A	509	HIS	-	expression tag	UNP P19099
B	27	MET	-	expression tag	UNP P19099
B	28	ALA	-	expression tag	UNP P19099
B	29	LYS	-	expression tag	UNP P19099
B	30	LYS	-	expression tag	UNP P19099
B	31	THR	-	expression tag	UNP P19099
B	32	SER	-	expression tag	UNP P19099
B	33	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
B	508	HIS	-	expression tag	UNP P19099
B	509	HIS	-	expression tag	UNP P19099
C	27	MET	-	expression tag	UNP P19099
C	28	ALA	-	expression tag	UNP P19099
C	29	LYS	-	expression tag	UNP P19099
C	30	LYS	-	expression tag	UNP P19099
C	31	THR	-	expression tag	UNP P19099
C	32	SER	-	expression tag	UNP P19099
C	33	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
C	508	HIS	-	expression tag	UNP P19099
C	509	HIS	-	expression tag	UNP P19099
D	27	MET	-	expression tag	UNP P19099
D	28	ALA	-	expression tag	UNP P19099
D	29	LYS	-	expression tag	UNP P19099
D	30	LYS	-	expression tag	UNP P19099
D	31	THR	-	expression tag	UNP P19099
D	32	SER	-	expression tag	UNP P19099
D	33	SER	-	expression tag	UNP P19099
D	504	HIS	-	expression tag	UNP P19099

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Chain	Residue	Modelled	Actual	Comment	Reference
D	505	HIS	-	expression tag	UNP P19099
D	506	HIS	-	expression tag	UNP P19099
D	507	HIS	-	expression tag	UNP P19099
D	508	HIS	-	expression tag	UNP P19099
D	509	HIS	-	expression tag	UNP P19099
E	27	MET	-	expression tag	UNP P19099
E	28	ALA	-	expression tag	UNP P19099
E	29	LYS	-	expression tag	UNP P19099
E	30	LYS	-	expression tag	UNP P19099
E	31	THR	-	expression tag	UNP P19099
E	32	SER	-	expression tag	UNP P19099
E	33	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
E	508	HIS	-	expression tag	UNP P19099
E	509	HIS	-	expression tag	UNP P19099
F	27	MET	-	expression tag	UNP P19099
F	28	ALA	-	expression tag	UNP P19099
F	29	LYS	-	expression tag	UNP P19099
F	30	LYS	-	expression tag	UNP P19099
F	31	THR	-	expression tag	UNP P19099
F	32	SER	-	expression tag	UNP P19099
F	33	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
F	508	HIS	-	expression tag	UNP P19099
F	509	HIS	-	expression tag	UNP P19099
G	27	MET	-	expression tag	UNP P19099
G	28	ALA	-	expression tag	UNP P19099
G	29	LYS	-	expression tag	UNP P19099
G	30	LYS	-	expression tag	UNP P19099
G	31	THR	-	expression tag	UNP P19099
G	32	SER	-	expression tag	UNP P19099
G	33	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

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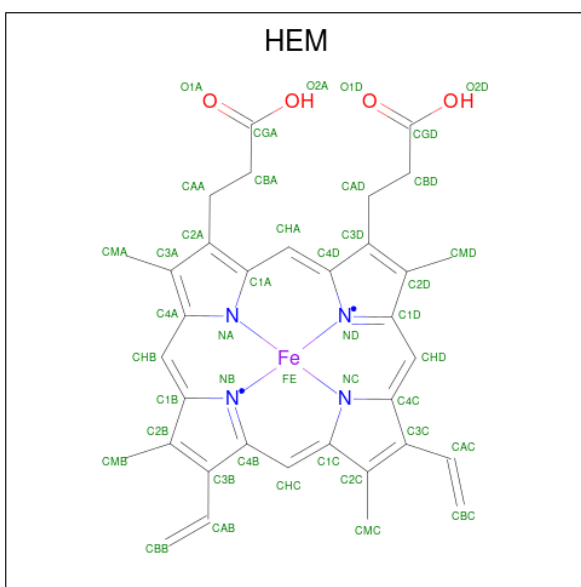
Chain	Residue	Modelled	Actual	Comment	Reference
G	508	HIS	-	expression tag	UNP P19099
G	509	HIS	-	expression tag	UNP P19099
H	27	MET	-	expression tag	UNP P19099
H	28	ALA	-	expression tag	UNP P19099
H	29	LYS	-	expression tag	UNP P19099
H	30	LYS	-	expression tag	UNP P19099
H	31	THR	-	expression tag	UNP P19099
H	32	SER	-	expression tag	UNP P19099
H	33	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
H	508	HIS	-	expression tag	UNP P19099
H	509	HIS	-	expression tag	UNP P19099
I	27	MET	-	expression tag	UNP P19099
I	28	ALA	-	expression tag	UNP P19099
I	29	LYS	-	expression tag	UNP P19099
I	30	LYS	-	expression tag	UNP P19099
I	31	THR	-	expression tag	UNP P19099
I	32	SER	-	expression tag	UNP P19099
I	33	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
I	508	HIS	-	expression tag	UNP P19099
I	509	HIS	-	expression tag	UNP P19099
J	27	MET	-	expression tag	UNP P19099
J	28	ALA	-	expression tag	UNP P19099
J	29	LYS	-	expression tag	UNP P19099
J	30	LYS	-	expression tag	UNP P19099
J	31	THR	-	expression tag	UNP P19099
J	32	SER	-	expression tag	UNP P19099
J	33	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
J	508	HIS	-	expression tag	UNP P19099
J	509	HIS	-	expression tag	UNP P19099
K	27	MET	-	expression tag	UNP P19099

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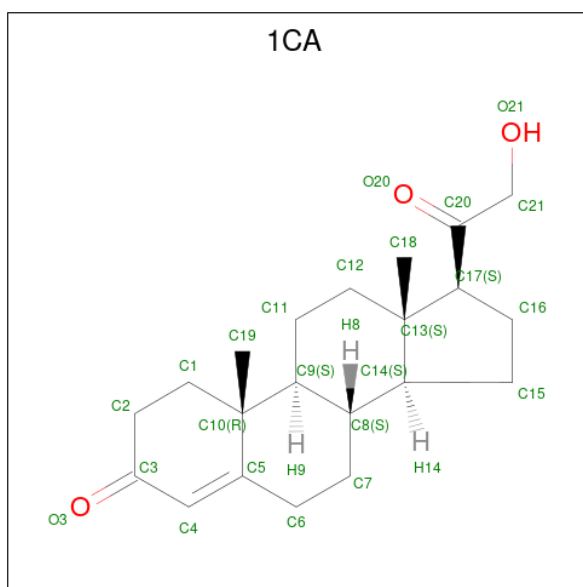
Chain	Residue	Modelled	Actual	Comment	Reference
K	28	ALA	-	expression tag	UNP P19099
K	29	LYS	-	expression tag	UNP P19099
K	30	LYS	-	expression tag	UNP P19099
K	31	THR	-	expression tag	UNP P19099
K	32	SER	-	expression tag	UNP P19099
K	33	SER	-	expression tag	UNP P19099
K	504	HIS	-	expression tag	UNP P19099
K	505	HIS	-	expression tag	UNP P19099
K	506	HIS	-	expression tag	UNP P19099
K	507	HIS	-	expression tag	UNP P19099
K	508	HIS	-	expression tag	UNP P19099
K	509	HIS	-	expression tag	UNP P19099
L	27	MET	-	expression tag	UNP P19099
L	28	ALA	-	expression tag	UNP P19099
L	29	LYS	-	expression tag	UNP P19099
L	30	LYS	-	expression tag	UNP P19099
L	31	THR	-	expression tag	UNP P19099
L	32	SER	-	expression tag	UNP P19099
L	33	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
L	507	HIS	-	expression tag	UNP P19099
L	508	HIS	-	expression tag	UNP P19099
L	509	HIS	-	expression tag	UNP P19099

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



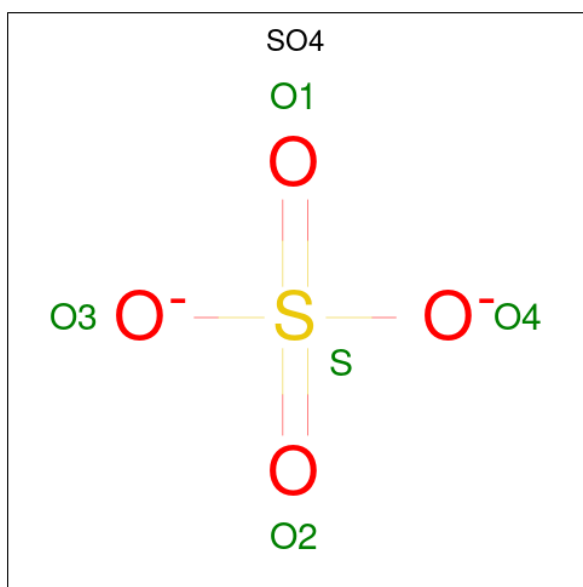
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	G	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	H	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	I	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	J	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	K	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	L	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is DESOXYCORTICOSTERONE (CCD ID: 1CA) (formula: $C_{21}H_{30}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			24	21	3		
3	B	1	Total	C	O	0	0
			24	21	3		
3	C	1	Total	C	O	0	0
			24	21	3		
3	D	1	Total	C	O	0	0
			24	21	3		
3	E	1	Total	C	O	0	0
			24	21	3		
3	F	1	Total	C	O	0	0
			24	21	3		
3	G	1	Total	C	O	0	0
			24	21	3		
3	H	1	Total	C	O	0	0
			24	21	3		
3	I	1	Total	C	O	0	0
			24	21	3		
3	J	1	Total	C	O	0	0
			24	21	3		
3	K	1	Total	C	O	0	0
			24	21	3		
3	L	1	Total	C	O	0	0
			24	21	3		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	K	1	Total	O	S	0	0
			5	4	1		
4	L	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	31	Total	O	0	0
			31	31		
5	B	14	Total	O	0	0
			14	14		
5	C	31	Total	O	0	0
			31	31		

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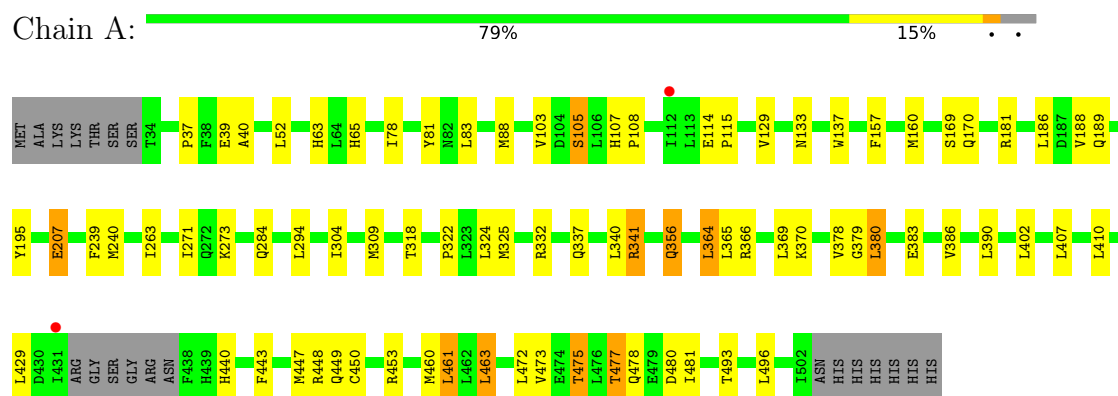
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	34	Total 34	O 34	0	0
5	E	30	Total 30	O 30	0	0
5	F	33	Total 33	O 33	0	0
5	G	18	Total 18	O 18	0	0
5	H	25	Total 25	O 25	0	0
5	I	6	Total 6	O 6	0	0
5	J	6	Total 6	O 6	0	0
5	K	13	Total 13	O 13	0	0
5	L	19	Total 19	O 19	0	0

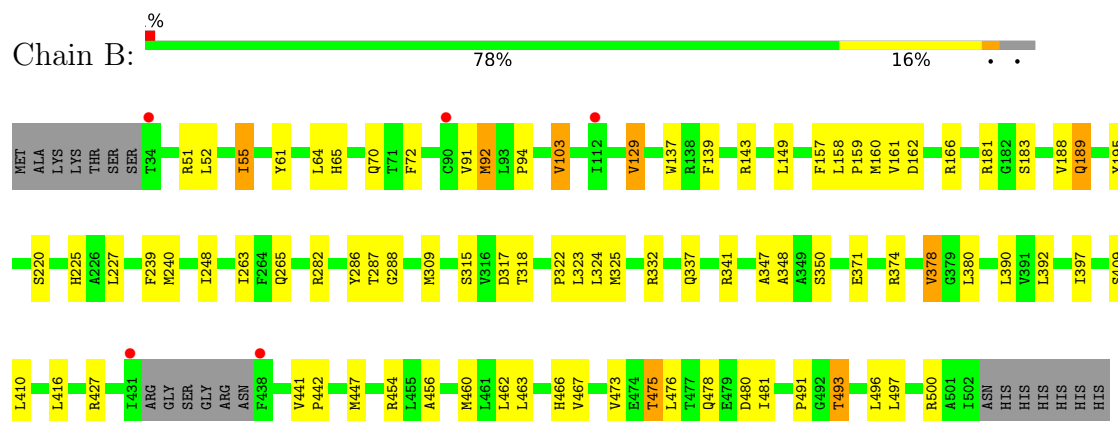
3 Residue-property plots

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.

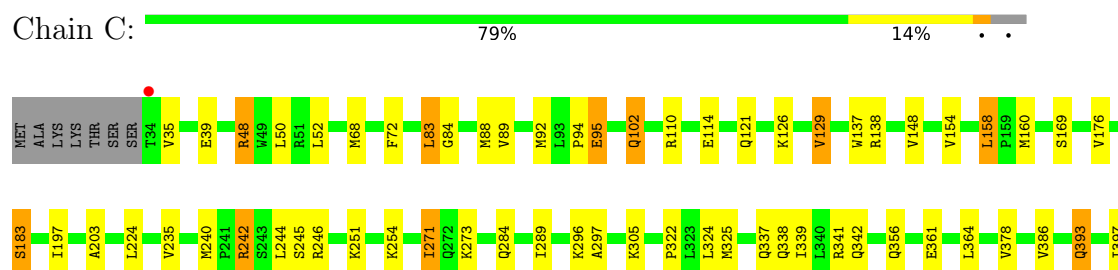
• Molecule 1: Cytochrome P450 11B2, mitochondrial

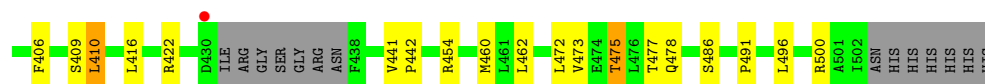


• Molecule 1: Cytochrome P450 11B2, mitochondrial



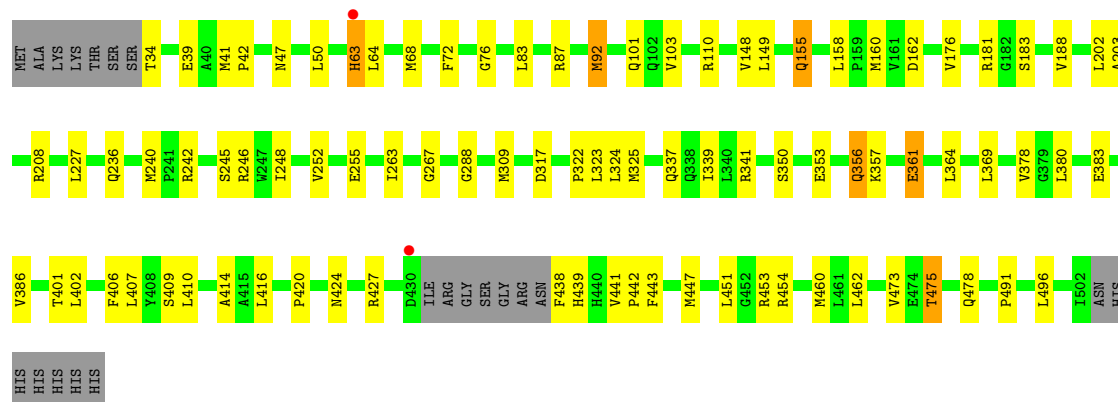
• Molecule 1: Cytochrome P450 11B2, mitochondrial





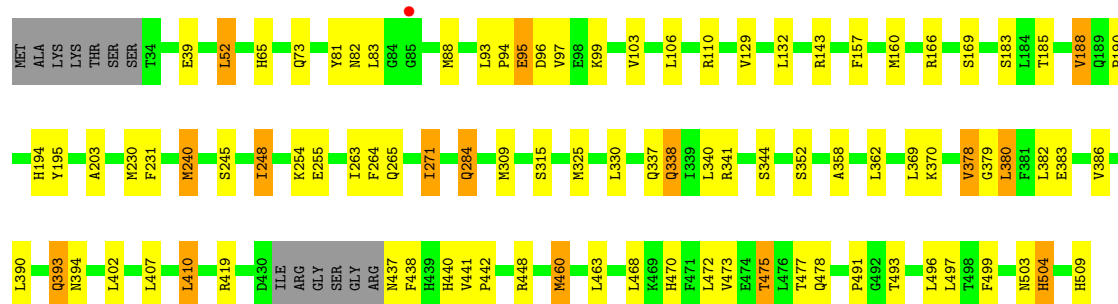
• Molecule 1: Cytochrome P450 11B2, mitochondrial

Chain D: 77% 17% . .



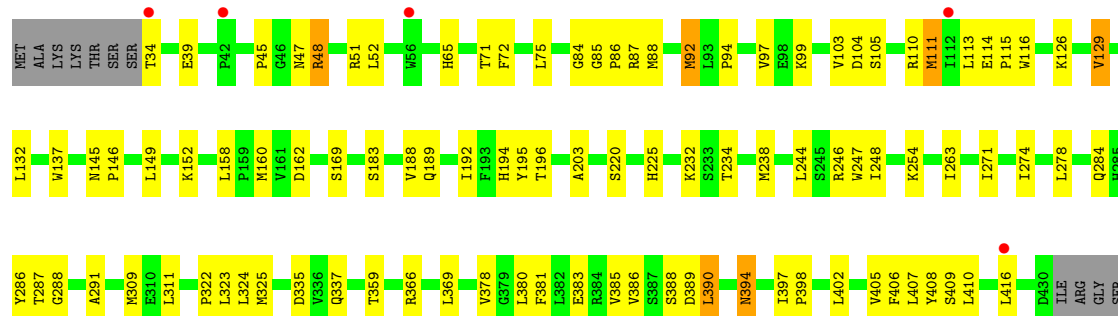
• Molecule 1: Cytochrome P450 11B2, mitochondrial

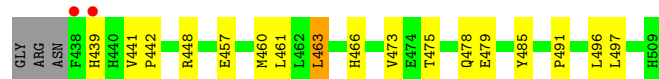
Chain E: 78% 16% . .



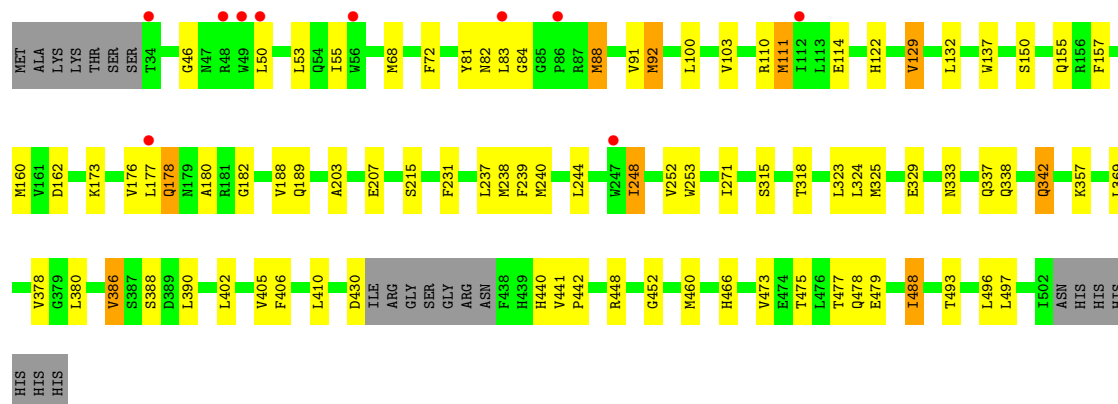
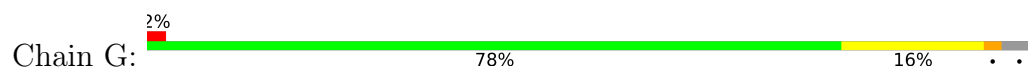
• Molecule 1: Cytochrome P450 11B2, mitochondrial

Chain F: 73% 23% . .

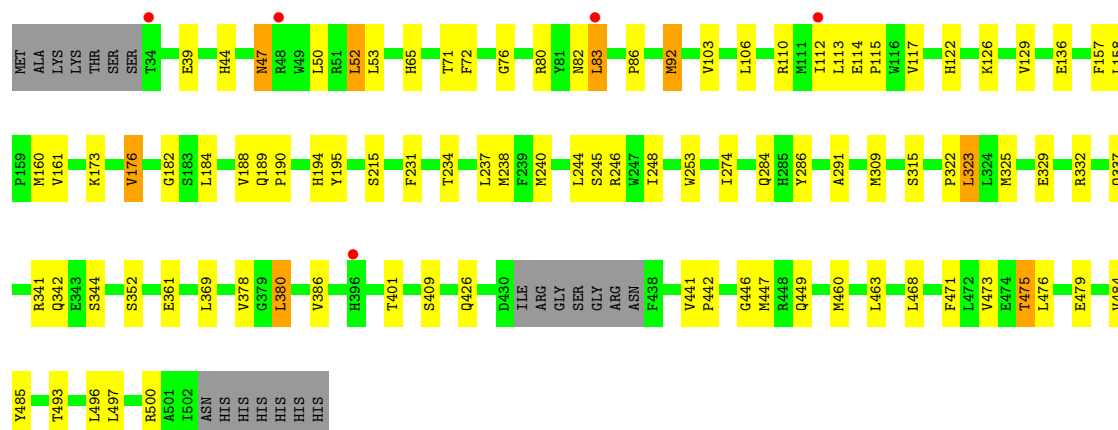
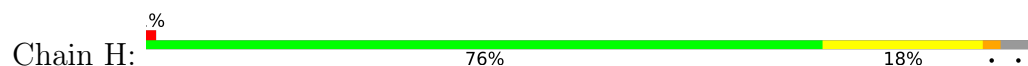




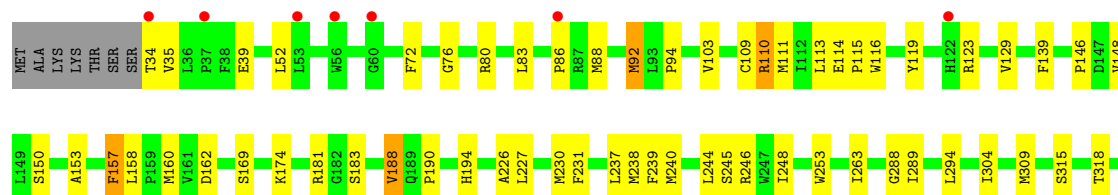
• Molecule 1: Cytochrome P450 11B2, mitochondrial

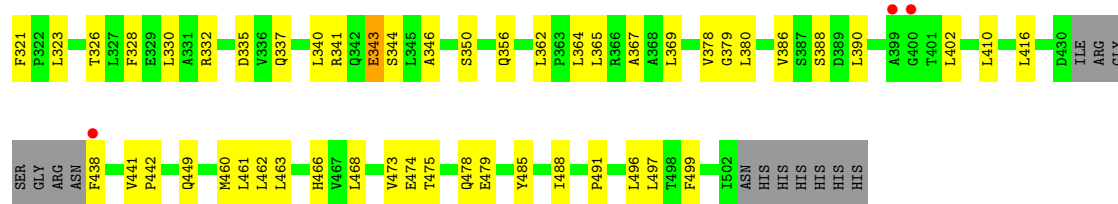


• Molecule 1: Cytochrome P450 11B2, mitochondrial

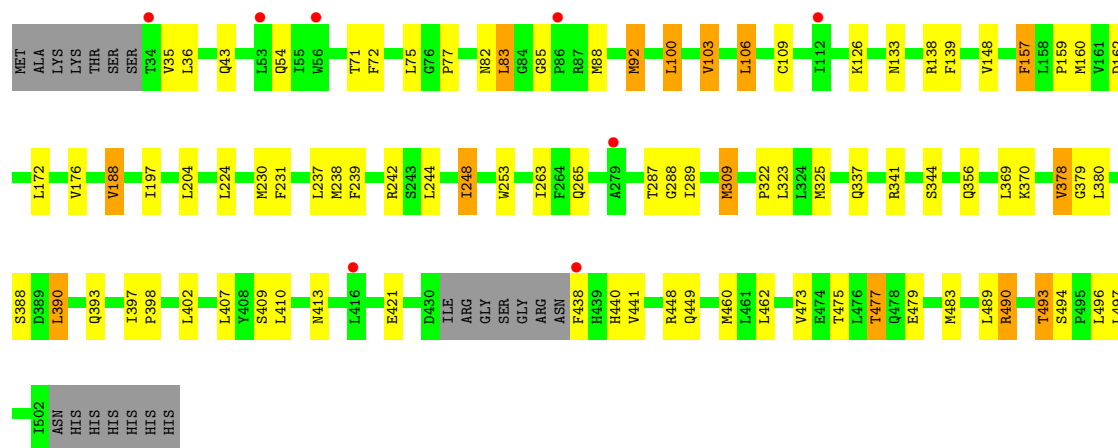
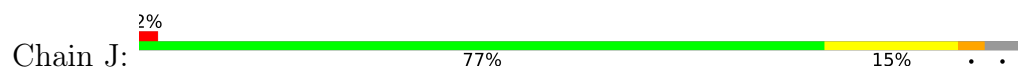


• Molecule 1: Cytochrome P450 11B2, mitochondrial

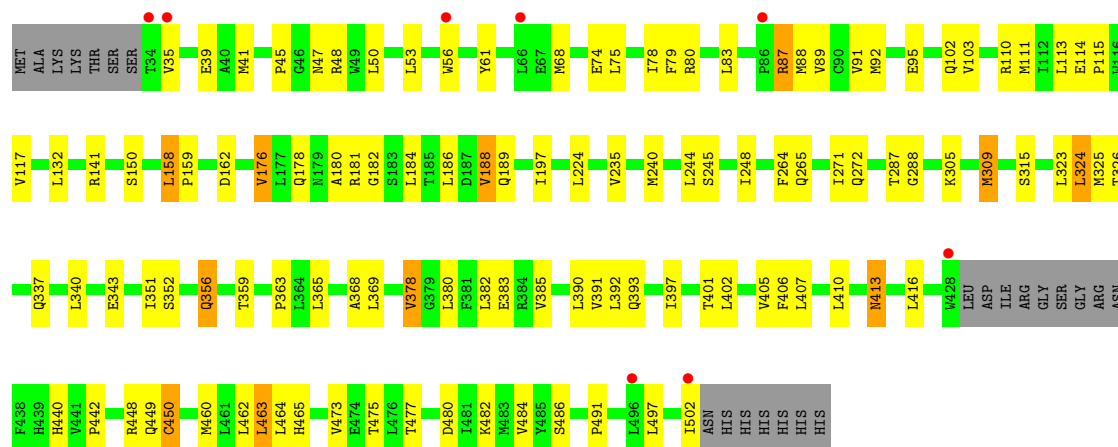




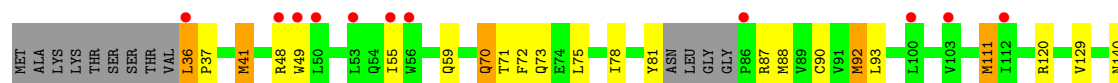
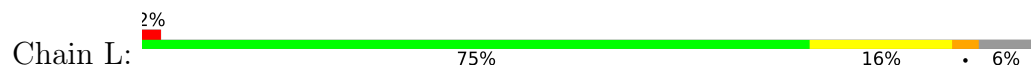
• Molecule 1: Cytochrome P450 11B2, mitochondrial

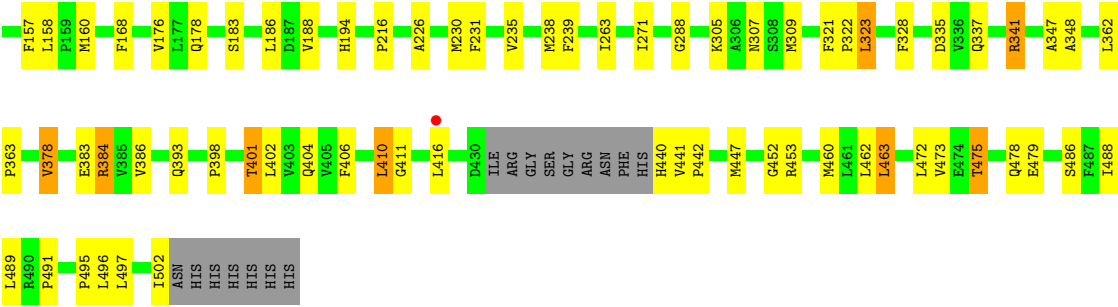


• Molecule 1: Cytochrome P450 11B2, mitochondrial



• Molecule 1: Cytochrome P450 11B2, mitochondrial





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	130.35Å 199.63Å 150.15Å 90.00° 112.18° 90.00°	Depositor
Resolution (Å)	48.07 – 2.49 48.07 – 2.49	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.07-2.49) 99.2 (48.07-2.49)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.19 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.204 , 0.263 (Not available) , 0.234	Depositor DCC
R_{free} test set	12313 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	51.7	Xtriage
Anisotropy	0.001	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 19.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	46194	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 42.03 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.1639e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: HEM, SO4, 1CA

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	0.96	1/3858 (0.0%)	0.87	2/5235 (0.0%)
1	B	0.89	1/3858 (0.0%)	0.86	3/5235 (0.1%)
1	C	0.95	1/3850 (0.0%)	0.86	0/5224
1	D	0.94	1/3850 (0.0%)	0.86	1/5224 (0.0%)
1	E	0.96	0/3932	0.86	1/5336 (0.0%)
1	F	0.95	1/3924 (0.0%)	0.86	3/5325 (0.1%)
1	G	0.87	1/3850 (0.0%)	0.84	0/5224
1	H	0.92	0/3850	0.87	3/5224 (0.1%)
1	I	0.87	0/3850	0.85	3/5224 (0.1%)
1	J	0.87	0/3850	0.85	1/5224 (0.0%)
1	K	0.86	1/3834 (0.0%)	0.83	1/5202 (0.0%)
1	L	0.88	1/3788 (0.0%)	0.86	2/5137 (0.0%)
All	All	0.91	8/46294 (0.0%)	0.86	20/62814 (0.0%)

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	158	LEU	C-O	-6.42	1.18	1.24
1	G	440	HIS	CG-CD2	5.50	1.42	1.35
1	K	440	HIS	CG-CD2	5.32	1.41	1.35
1	B	225	HIS	CG-CD2	5.31	1.41	1.35
1	L	440	HIS	CG-CD2	5.26	1.41	1.35

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	288	GLY	N-CA-C	8.68	120.90	112.04
1	J	288	GLY	N-CA-C	7.56	120.76	112.29
1	A	189	GLN	CA-C-N	-6.45	112.26	118.97
1	A	189	GLN	C-N-CA	-6.45	112.26	118.97
1	F	189	GLN	CA-C-N	-6.42	112.29	118.97

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	3758	0	3796	55	0
1	B	3758	0	3796	60	0
1	C	3750	0	3785	54	0
1	D	3750	0	3785	58	0
1	E	3826	0	3839	60	0
1	F	3818	0	3833	75	0
1	G	3750	0	3785	65	0
1	H	3750	0	3785	64	0
1	I	3750	0	3785	70	0
1	J	3750	0	3785	57	0
1	K	3734	0	3770	91	0
1	L	3691	0	3730	62	0
2	A	43	0	30	6	0
2	B	43	0	30	4	0
2	C	43	0	30	4	0
2	D	43	0	30	2	0
2	E	43	0	30	7	0
2	F	43	0	30	4	0
2	G	43	0	30	5	0
2	H	43	0	30	2	0
2	I	43	0	30	4	0
2	J	43	0	30	0	0
2	K	43	0	30	3	0
2	L	43	0	30	9	0
3	A	24	0	30	0	0
3	B	24	0	30	0	0
3	C	24	0	30	1	0
3	D	24	0	30	0	0
3	E	24	0	30	0	0
3	F	24	0	30	0	0
3	G	24	0	30	0	0
3	H	24	0	30	0	0
3	I	24	0	30	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	24	0	30	0	0
3	K	24	0	30	0	0
3	L	24	0	30	1	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
4	E	5	0	0	0	0
4	F	5	0	0	0	0
4	G	5	0	0	0	0
4	K	5	0	0	0	0
4	L	5	0	0	0	0
5	A	31	0	0	0	0
5	B	14	0	0	1	0
5	C	31	0	0	0	0
5	D	34	0	0	1	0
5	E	30	0	0	0	0
5	F	33	0	0	2	0
5	G	18	0	0	0	0
5	H	25	0	0	0	0
5	I	6	0	0	0	0
5	J	6	0	0	0	0
5	K	13	0	0	1	0
5	L	19	0	0	0	0
All	All	46194	0	46194	778	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 8.

The worst 5 of 778 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:H:240:MET:HE1	1:H:248:ILE:HD12	1.26	1.10
1:B:322:PRO:HB2	1:B:460:MET:HE1	1.26	1.09
1:J:369:LEU:HD22	1:J:460:MET:HE2	1.35	1.06
1:I:475:THR:CG2	1:I:497:LEU:HD23	1.87	1.04
1:G:337:GLN:HE22	1:G:473:VAL:H	1.04	1.01

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	459/483 (95%)	444 (97%)	14 (3%)	1 (0%)	43	63
1	B	459/483 (95%)	437 (95%)	21 (5%)	1 (0%)	43	63
1	C	458/483 (95%)	444 (97%)	13 (3%)	1 (0%)	43	63
1	D	458/483 (95%)	435 (95%)	23 (5%)	0	100	100
1	E	466/483 (96%)	445 (96%)	16 (3%)	5 (1%)	11	22
1	F	465/483 (96%)	449 (97%)	15 (3%)	1 (0%)	43	63
1	G	458/483 (95%)	439 (96%)	19 (4%)	0	100	100
1	H	458/483 (95%)	439 (96%)	18 (4%)	1 (0%)	43	63
1	I	458/483 (95%)	429 (94%)	29 (6%)	0	100	100
1	J	458/483 (95%)	435 (95%)	18 (4%)	5 (1%)	11	22
1	K	456/483 (94%)	433 (95%)	21 (5%)	2 (0%)	30	49
1	L	448/483 (93%)	434 (97%)	13 (3%)	1 (0%)	43	63
All	All	5501/5796 (95%)	5263 (96%)	220 (4%)	18 (0%)	36	55

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	504	HIS
1	B	427	ARG
1	F	48	ARG
1	J	477	THR
1	A	477	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	408/425 (96%)	390 (96%)	18 (4%)	25	50
1	B	408/425 (96%)	389 (95%)	19 (5%)	23	47
1	C	407/425 (96%)	380 (93%)	27 (7%)	15	32
1	D	407/425 (96%)	389 (96%)	18 (4%)	25	50
1	E	415/425 (98%)	384 (92%)	31 (8%)	12	26
1	F	414/425 (97%)	384 (93%)	30 (7%)	13	28
1	G	407/425 (96%)	383 (94%)	24 (6%)	18	37
1	H	407/425 (96%)	377 (93%)	30 (7%)	13	27
1	I	407/425 (96%)	386 (95%)	21 (5%)	21	42
1	J	407/425 (96%)	381 (94%)	26 (6%)	16	33
1	K	405/425 (95%)	377 (93%)	28 (7%)	14	30
1	L	401/425 (94%)	373 (93%)	28 (7%)	14	29
All	All	4893/5100 (96%)	4593 (94%)	300 (6%)	17	35

5 of 300 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	265	GLN
1	L	341	ARG
1	J	421	GLU
1	K	356	GLN
1	E	271	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 149 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	82	ASN
1	L	65	HIS
1	J	337	GLN
1	K	102	GLN
1	E	214	HIS

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

33 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	HEM	J	601	1	50,50,50	1.61	8 (16%)	67,82,82	1.39	9 (13%)
2	HEM	G	601	1	50,50,50	1.75	11 (22%)	67,82,82	1.42	9 (13%)
4	SO4	L	603	-	4,4,4	0.43	0	6,6,6	0.30	0
4	SO4	F	603	-	4,4,4	0.44	0	6,6,6	0.28	0
3	1CA	C	602	-	27,27,27	1.07	4 (14%)	42,43,43	1.57	11 (26%)
2	HEM	A	601	1	50,50,50	1.76	8 (16%)	67,82,82	1.40	13 (19%)
3	1CA	L	602	-	27,27,27	0.69	0	42,43,43	1.24	5 (11%)
2	HEM	K	601	1	50,50,50	1.77	8 (16%)	67,82,82	1.33	6 (8%)
4	SO4	E	603	-	4,4,4	0.47	0	6,6,6	0.29	0
4	SO4	G	603	-	4,4,4	0.43	0	6,6,6	0.36	0
2	HEM	F	601	1	50,50,50	1.57	6 (12%)	67,82,82	1.24	7 (10%)
2	HEM	E	601	1	50,50,50	1.66	10 (20%)	67,82,82	1.12	4 (5%)
3	1CA	G	602	-	27,27,27	0.92	0	42,43,43	1.20	4 (9%)
3	1CA	H	602	-	27,27,27	0.90	1 (3%)	42,43,43	1.13	5 (11%)
3	1CA	K	602	-	27,27,27	0.65	0	42,43,43	1.43	8 (19%)
4	SO4	D	603	-	4,4,4	0.45	0	6,6,6	0.23	0
3	1CA	D	602	-	27,27,27	0.92	1 (3%)	42,43,43	1.31	6 (14%)
4	SO4	B	603	-	4,4,4	0.44	0	6,6,6	0.41	0
3	1CA	J	602	-	27,27,27	0.89	1 (3%)	42,43,43	1.32	6 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	1CA	A	602	-	27,27,27	0.88	2 (7%)	42,43,43	1.30	6 (14%)
3	1CA	B	602	-	27,27,27	0.78	0	42,43,43	1.16	3 (7%)
3	1CA	E	602	-	27,27,27	0.87	1 (3%)	42,43,43	1.49	8 (19%)
2	HEM	C	601	1	50,50,50	1.85	8 (16%)	67,82,82	1.29	7 (10%)
2	HEM	D	601	1	50,50,50	1.78	9 (18%)	67,82,82	1.22	7 (10%)
2	HEM	L	601	1	50,50,50	1.95	12 (24%)	67,82,82	1.40	10 (14%)
2	HEM	H	601	1	50,50,50	1.76	9 (18%)	67,82,82	1.31	9 (13%)
3	1CA	F	602	-	27,27,27	1.10	2 (7%)	42,43,43	1.26	7 (16%)
3	1CA	I	602	-	27,27,27	0.89	0	42,43,43	1.46	7 (16%)
4	SO4	A	603	-	4,4,4	0.47	0	6,6,6	0.25	0
4	SO4	K	603	-	4,4,4	0.46	0	6,6,6	0.32	0
2	HEM	I	601	1	50,50,50	1.68	8 (16%)	67,82,82	1.12	5 (7%)
2	HEM	B	601	1	50,50,50	1.61	9 (18%)	67,82,82	1.29	9 (13%)
4	SO4	C	603	-	4,4,4	0.48	0	6,6,6	0.29	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	J	601	1	-	6/14/54/54	-
2	HEM	G	601	1	-	4/14/54/54	-
3	1CA	C	602	-	-	0/6/64/64	0/4/4/4
2	HEM	A	601	1	-	0/14/54/54	-
3	1CA	L	602	-	-	2/6/64/64	0/4/4/4
2	HEM	K	601	1	-	4/14/54/54	-
2	HEM	F	601	1	-	2/14/54/54	-
2	HEM	E	601	1	-	4/14/54/54	-
3	1CA	G	602	-	-	0/6/64/64	0/4/4/4
3	1CA	H	602	-	-	1/6/64/64	0/4/4/4
3	1CA	K	602	-	-	4/6/64/64	0/4/4/4
3	1CA	D	602	-	-	2/6/64/64	0/4/4/4
3	1CA	J	602	-	-	0/6/64/64	0/4/4/4
3	1CA	A	602	-	-	0/6/64/64	0/4/4/4
3	1CA	B	602	-	-	1/6/64/64	0/4/4/4
3	1CA	E	602	-	-	0/6/64/64	0/4/4/4
2	HEM	C	601	1	-	1/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	D	601	1	-	2/14/54/54	-
2	HEM	L	601	1	-	2/14/54/54	-
2	HEM	H	601	1	-	0/14/54/54	-
3	1CA	F	602	-	-	0/6/64/64	0/4/4/4
3	1CA	I	602	-	-	1/6/64/64	0/4/4/4
2	HEM	I	601	1	-	2/14/54/54	-
2	HEM	B	601	1	-	0/14/54/54	-

The worst 5 of 118 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	601	HEM	C3D-C2D	7.39	1.52	1.36
2	H	601	HEM	C3D-C2D	7.34	1.52	1.36
2	K	601	HEM	C3D-C2D	7.33	1.52	1.36
2	D	601	HEM	C3D-C2D	7.31	1.52	1.36
2	F	601	HEM	C3D-C2D	6.98	1.51	1.36

The worst 5 of 171 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	601	HEM	C4D-ND-C1D	5.67	111.92	105.21
2	K	601	HEM	C4D-ND-C1D	4.88	110.99	105.21
2	H	601	HEM	C4D-ND-C1D	4.40	110.42	105.21
2	G	601	HEM	C4D-ND-C1D	4.38	110.39	105.21
2	F	601	HEM	C4D-ND-C1D	4.14	110.10	105.21

There are no chirality outliers.

5 of 38 torsion outliers are listed below:

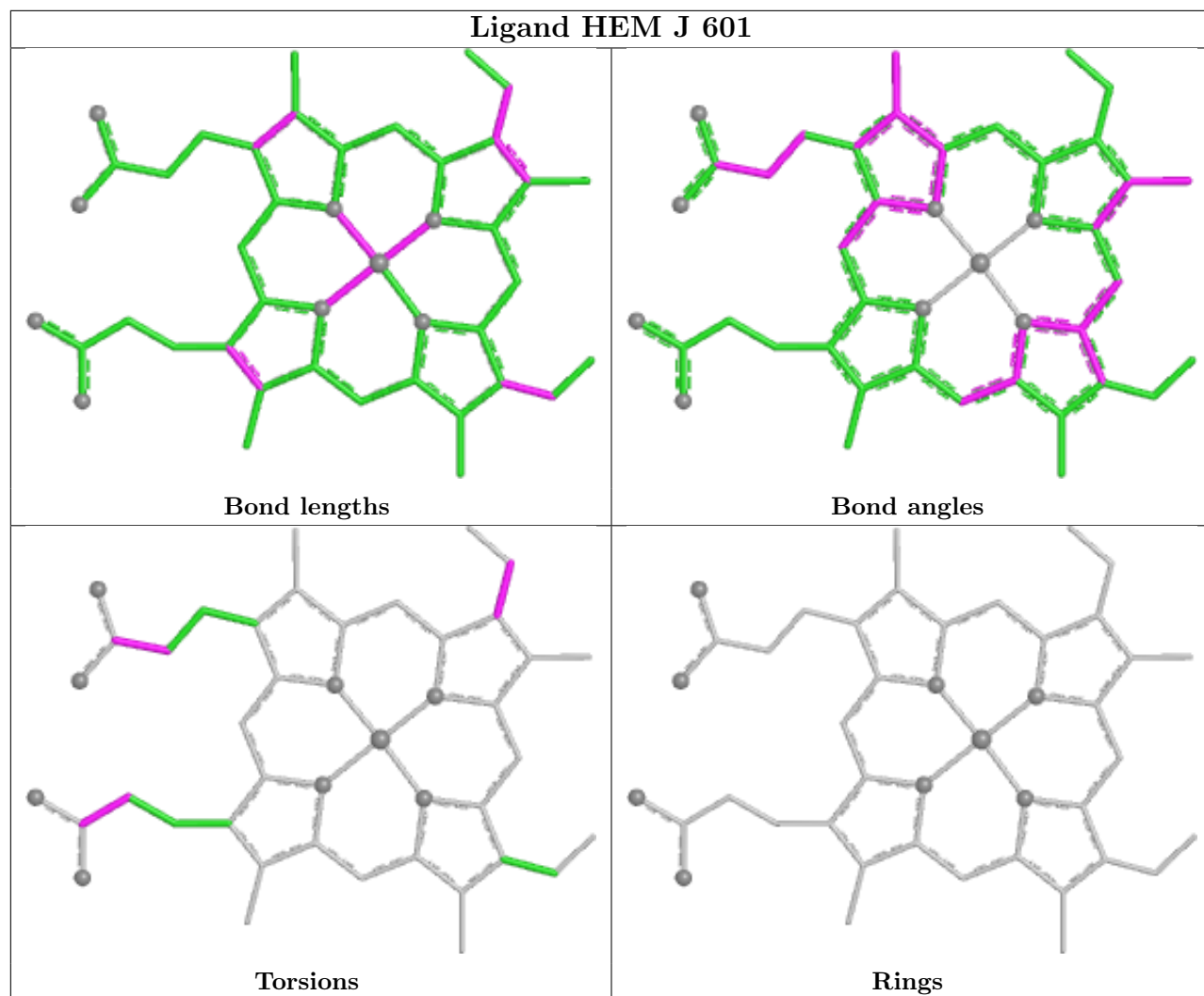
Mol	Chain	Res	Type	Atoms
3	K	602	1CA	C13-C17-C20-O20
3	L	602	1CA	C17-C20-C21-O21
2	K	601	HEM	C2C-C3C-CAC-CBC
3	L	602	1CA	O20-C20-C21-O21
2	G	601	HEM	C2C-C3C-CAC-CBC

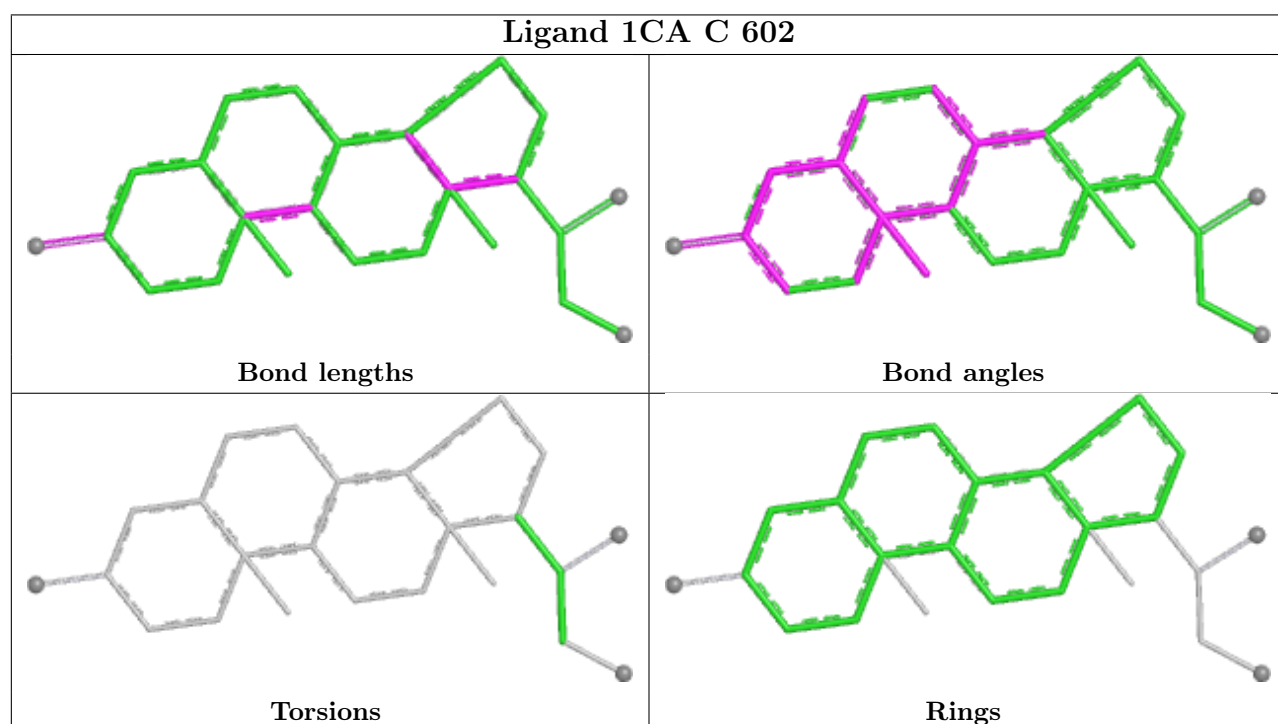
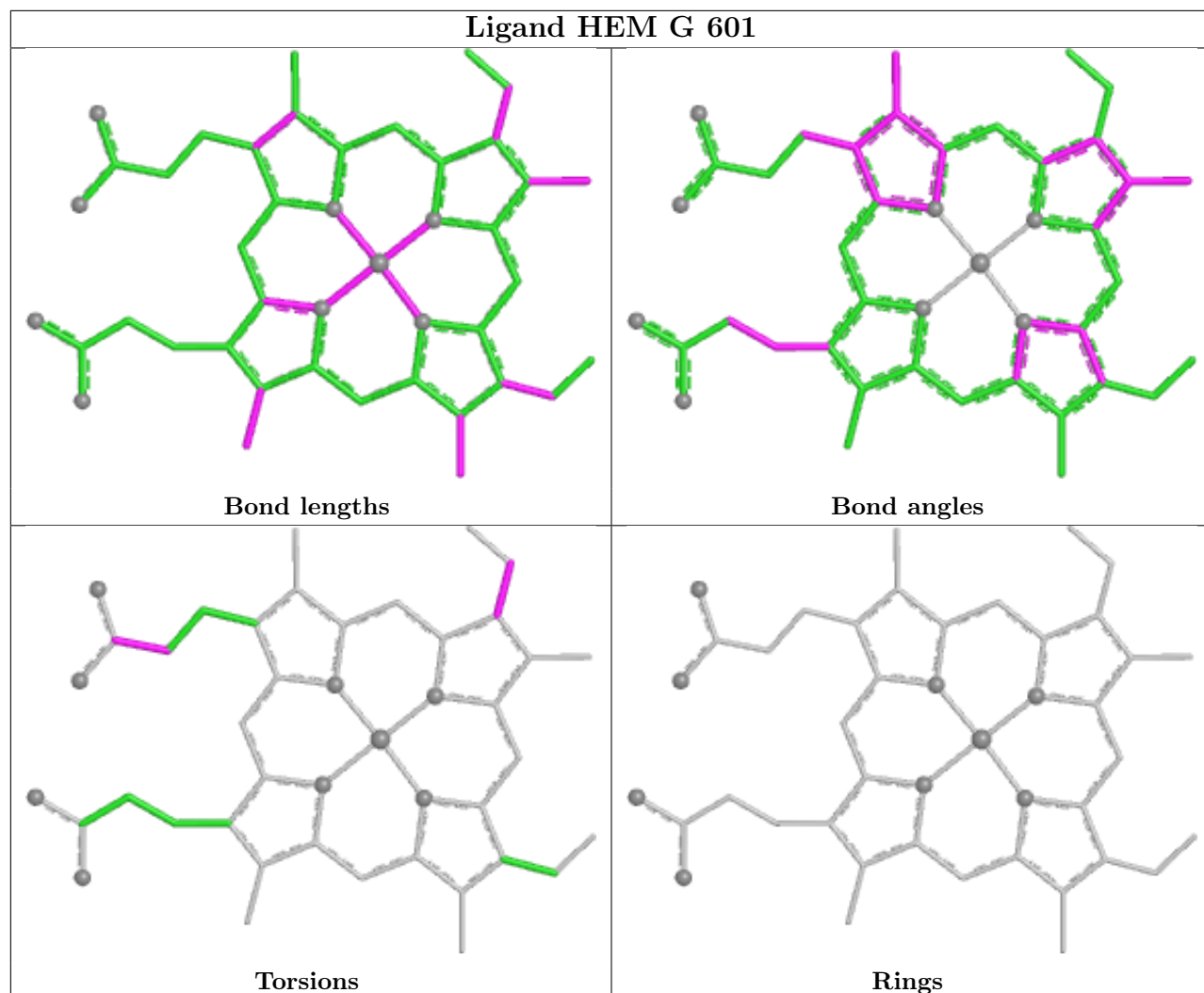
There are no ring outliers.

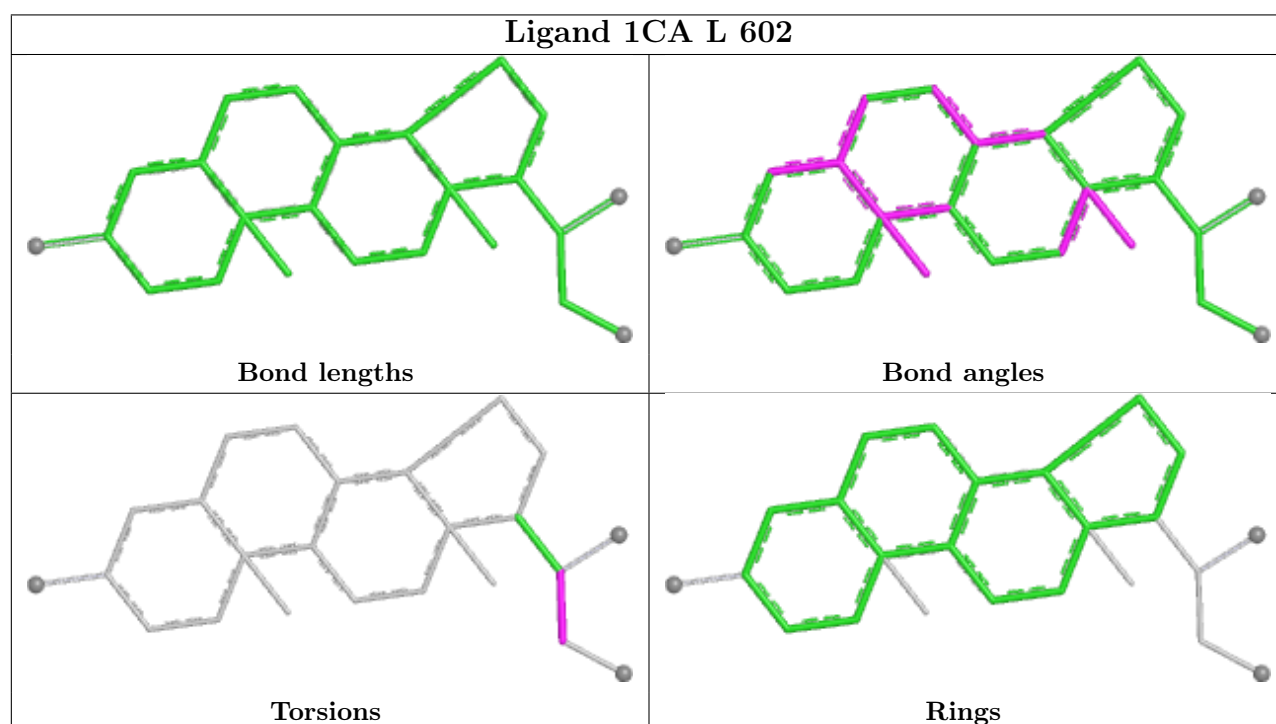
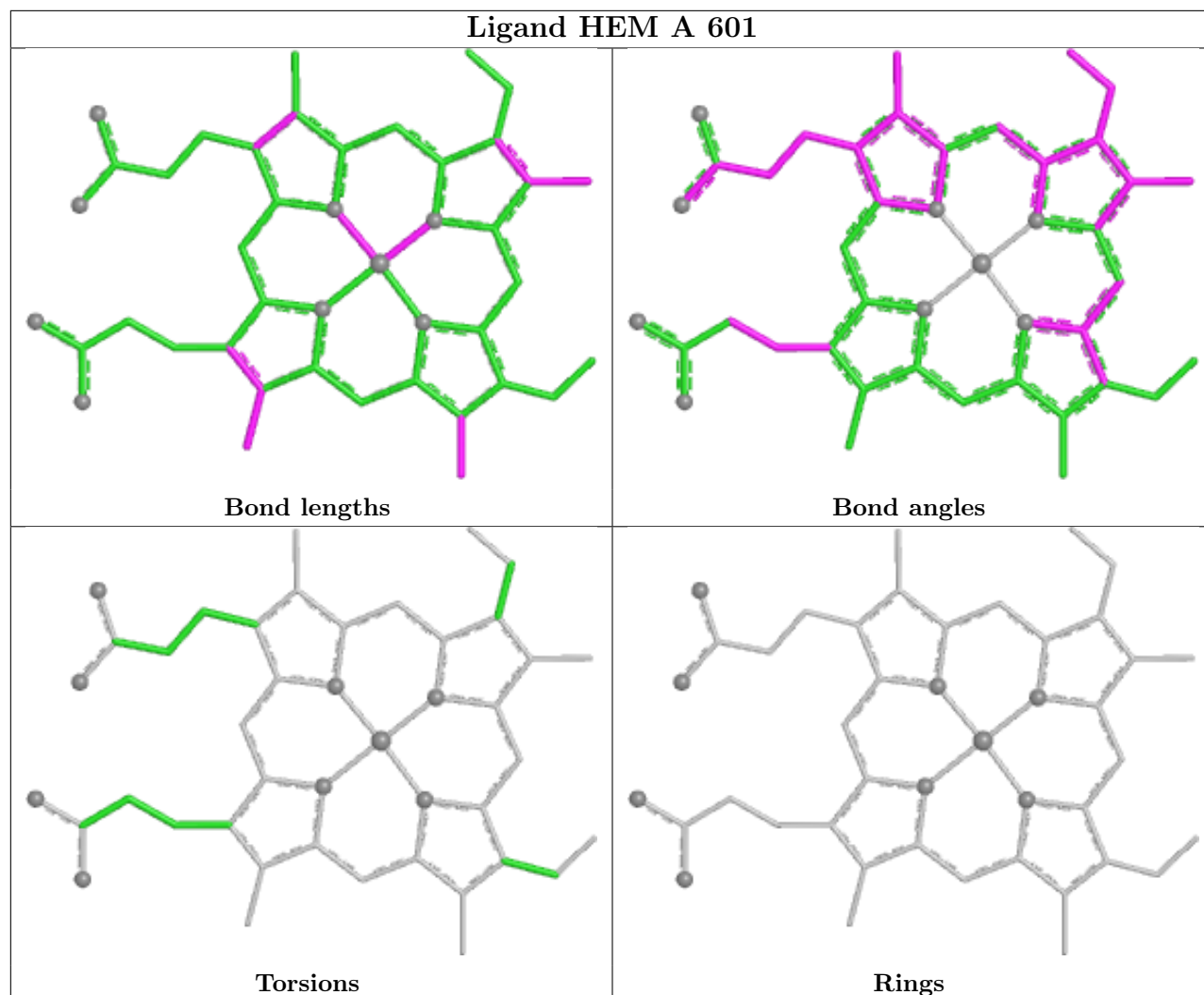
14 monomers are involved in 53 short contacts:

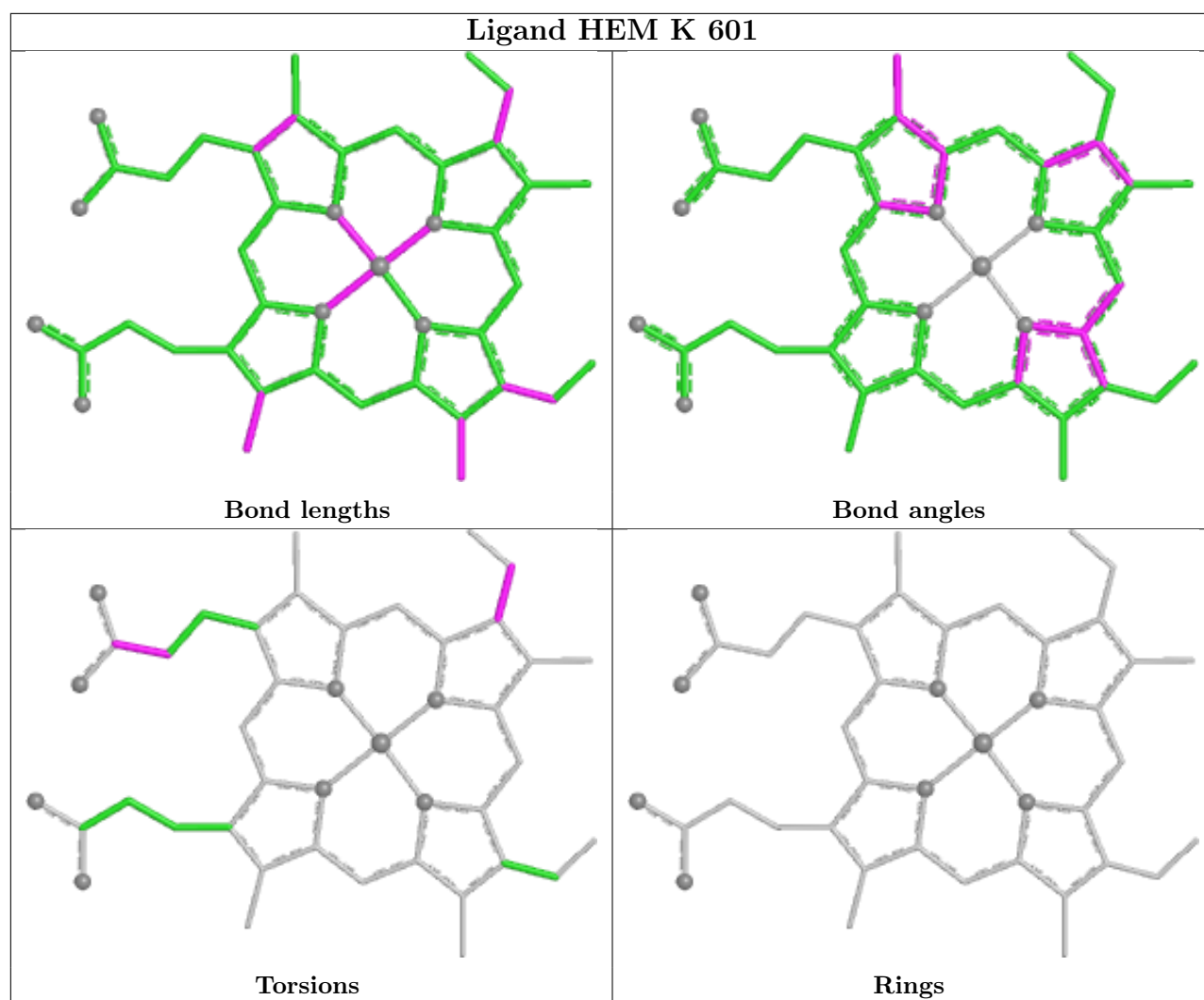
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	601	HEM	5	0
3	C	602	1CA	1	0
2	A	601	HEM	6	0
3	L	602	1CA	1	0
2	K	601	HEM	3	0
2	F	601	HEM	4	0
2	E	601	HEM	7	0
2	C	601	HEM	4	0
2	D	601	HEM	2	0
2	L	601	HEM	9	0
2	H	601	HEM	2	0
3	I	602	1CA	1	0
2	I	601	HEM	4	0
2	B	601	HEM	4	0

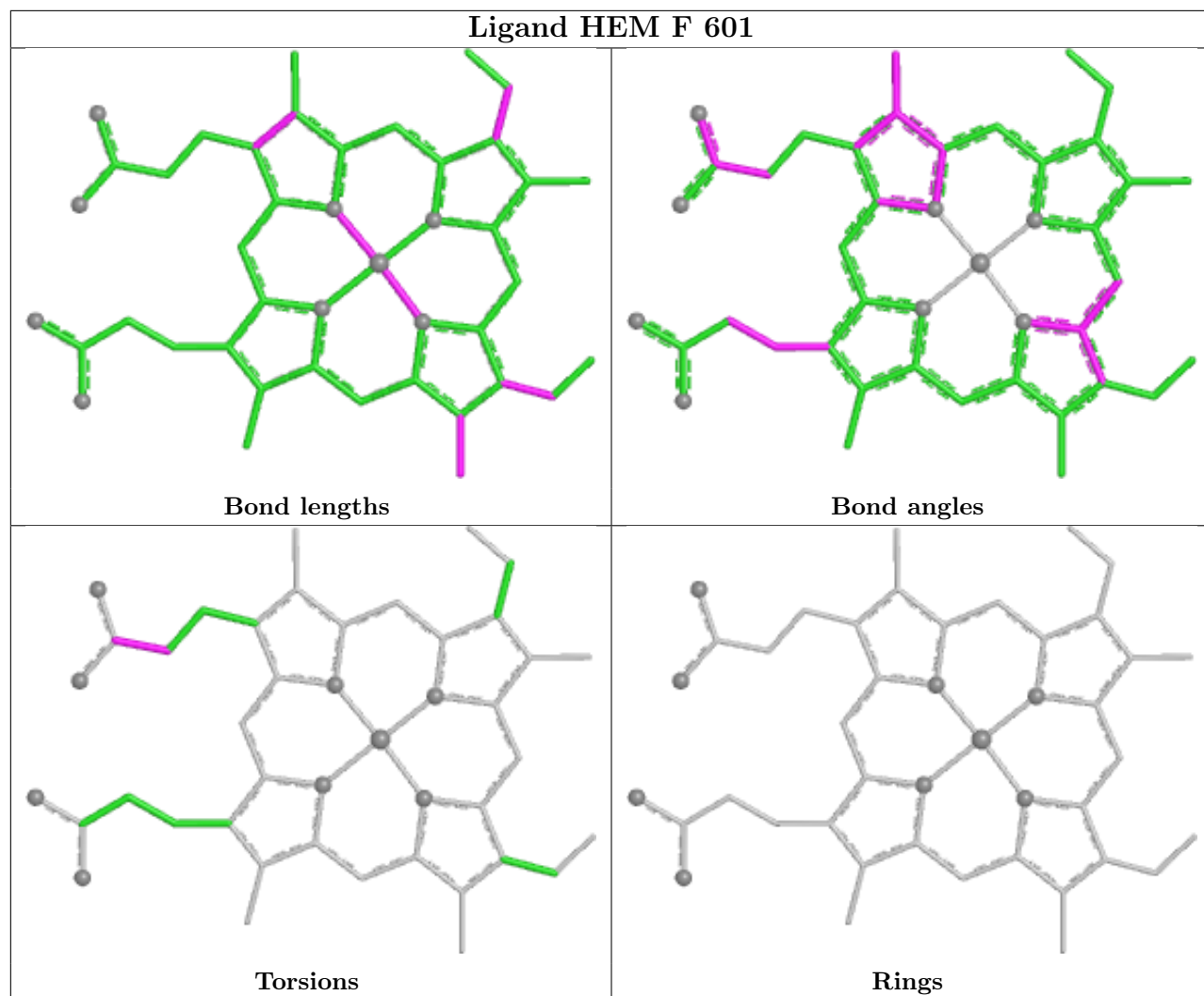
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

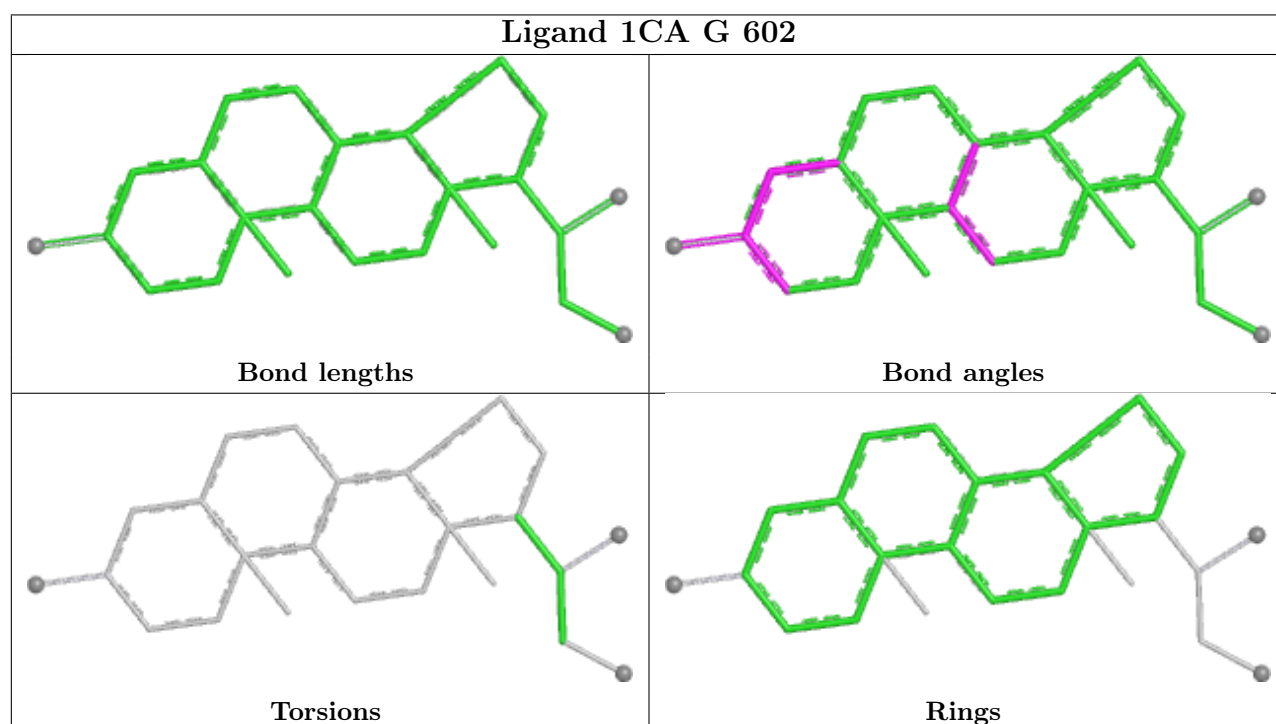
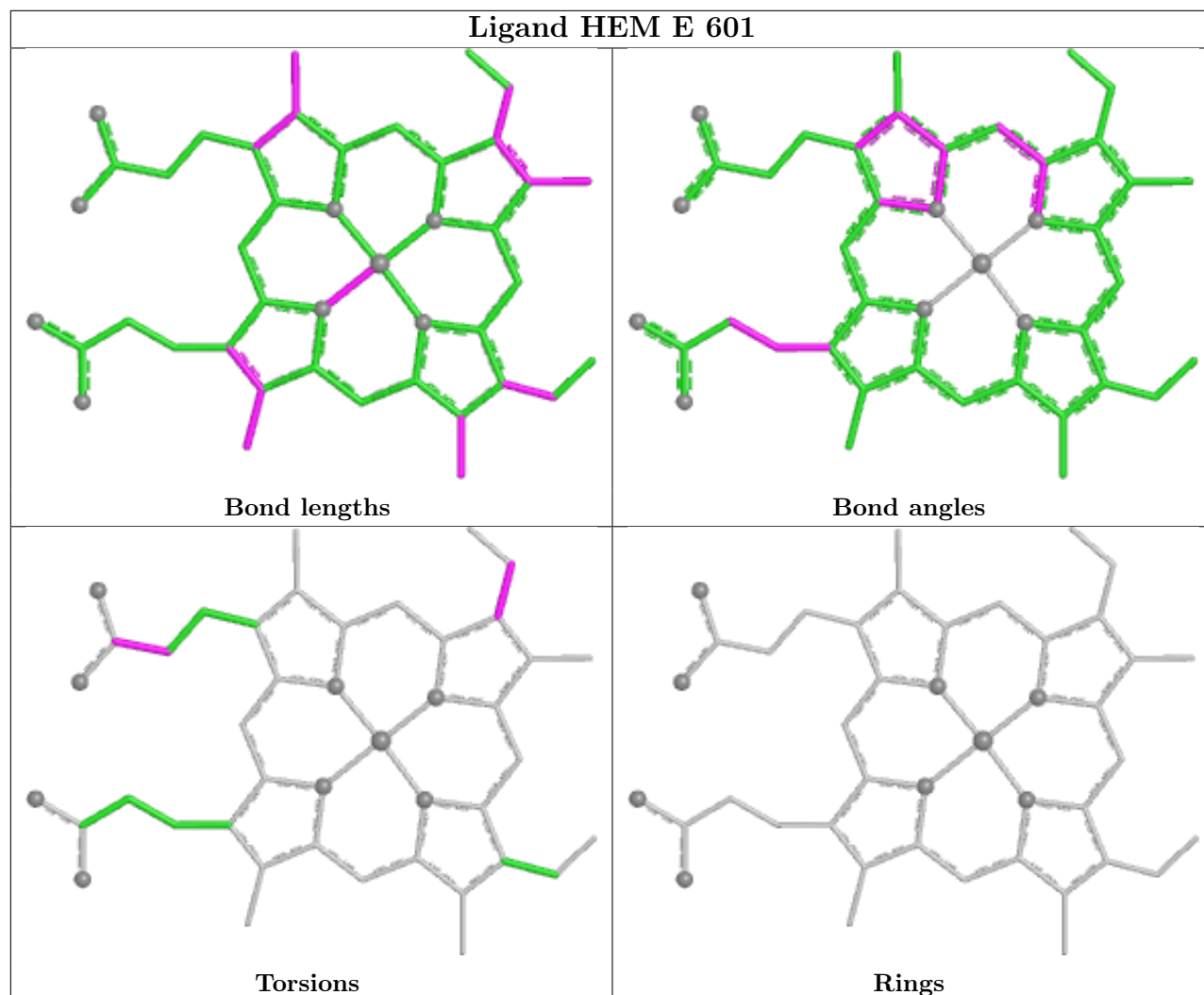




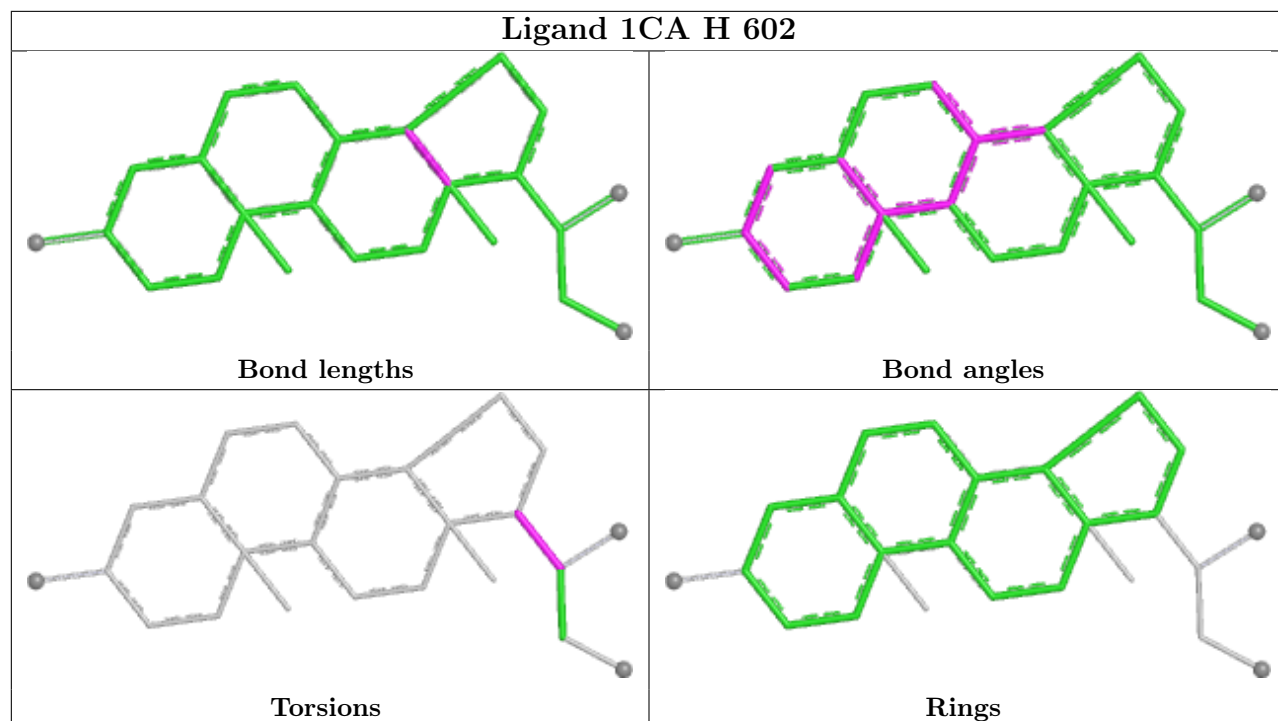




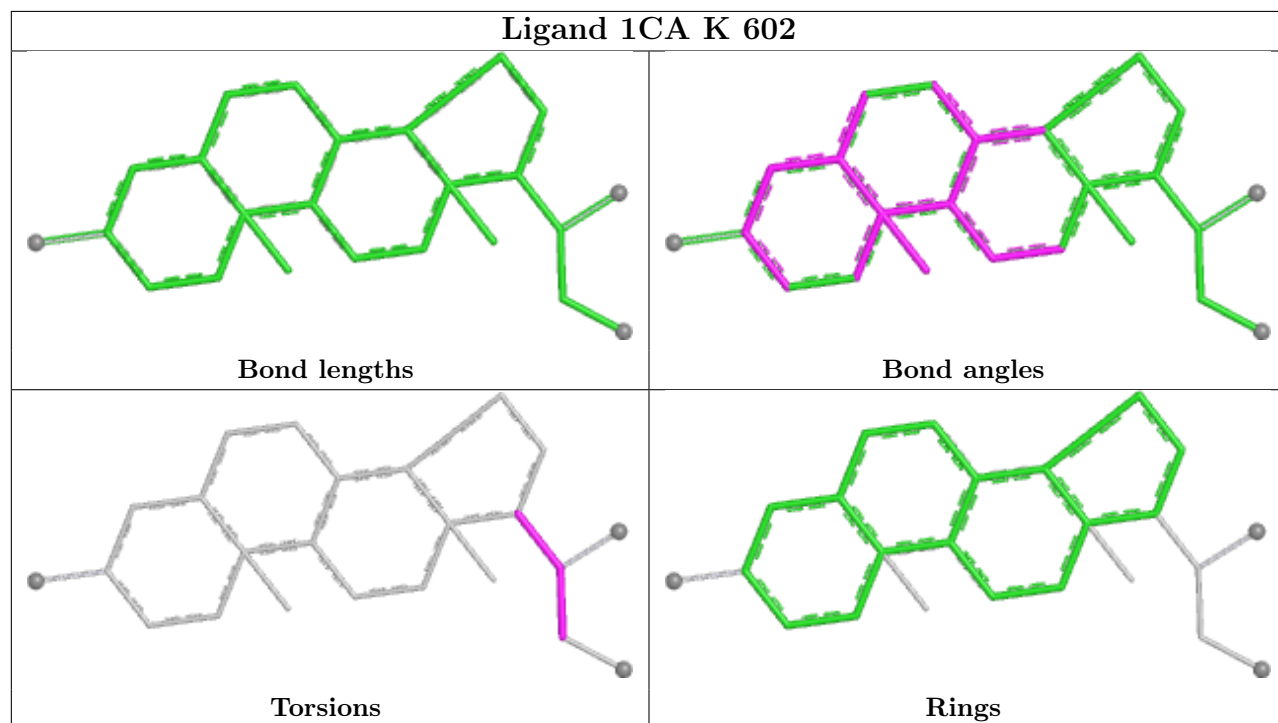




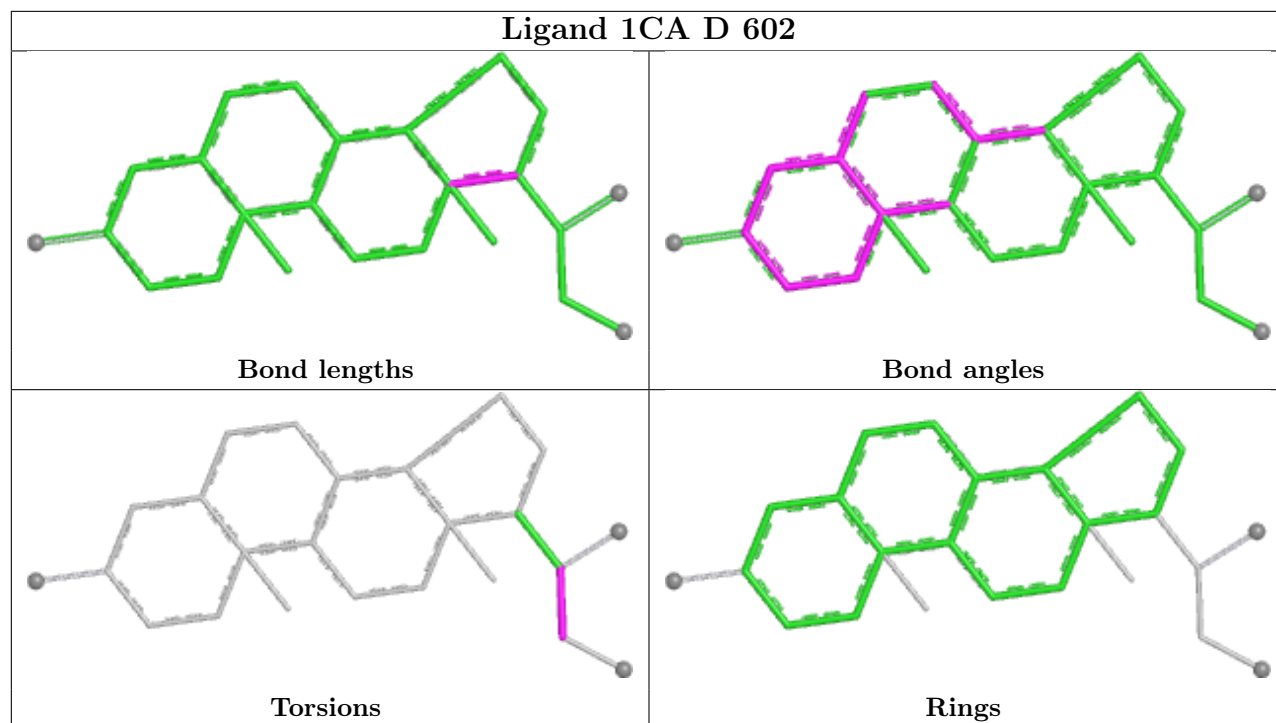
Ligand 1CA H 602



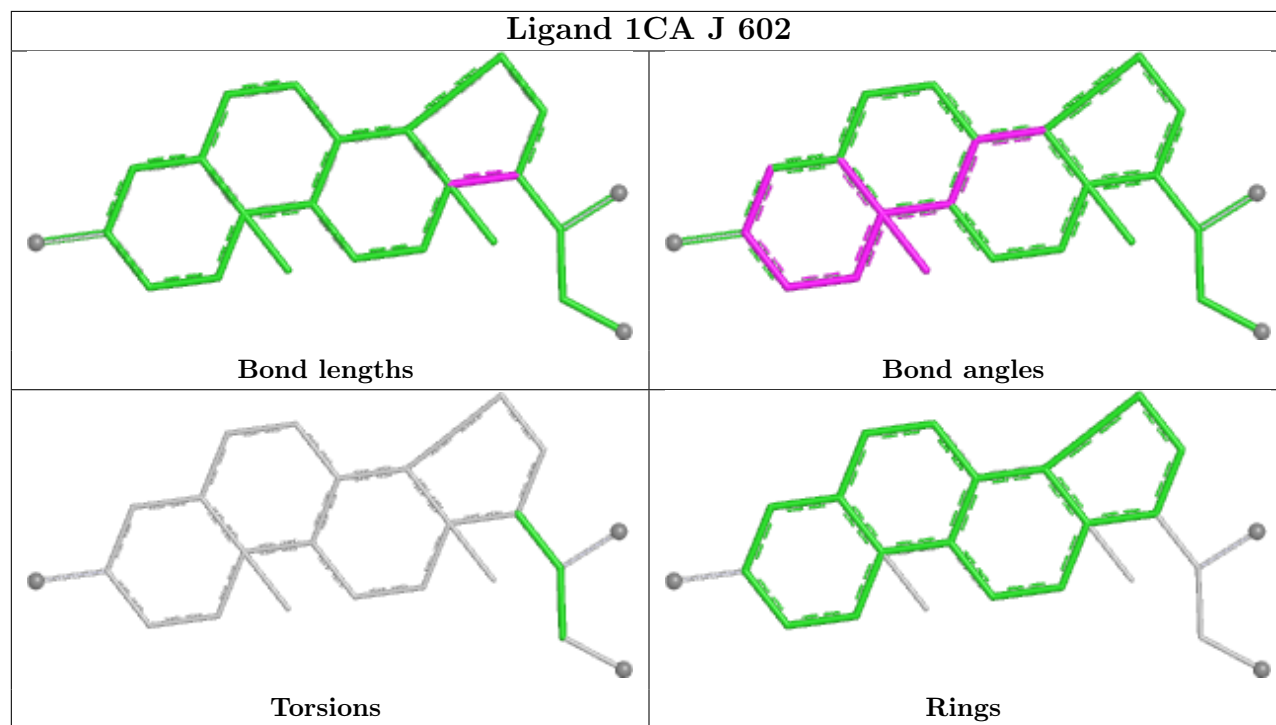
Ligand 1CA K 602



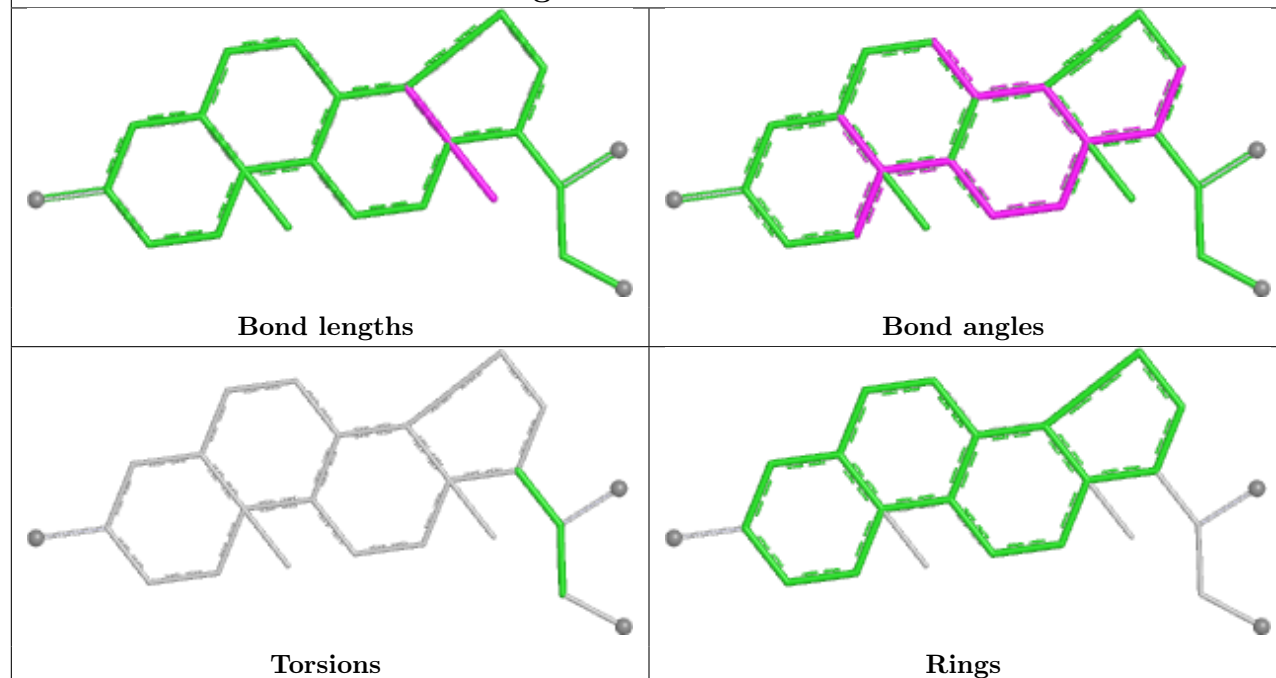
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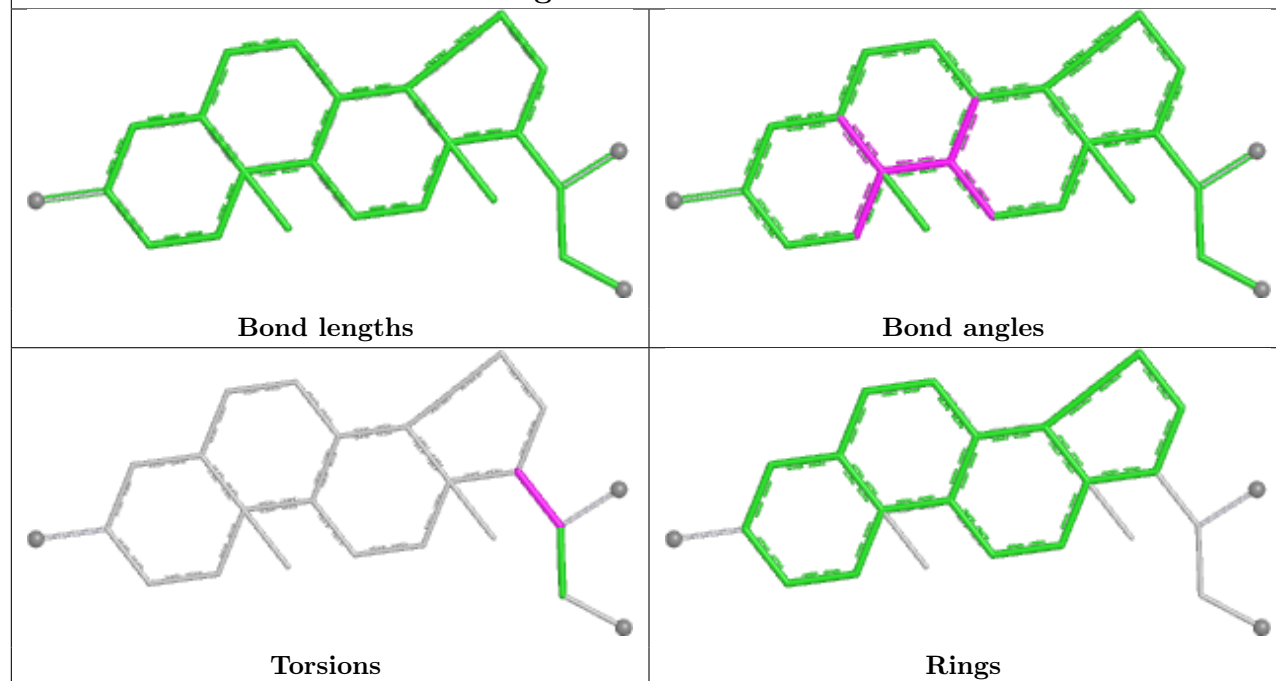
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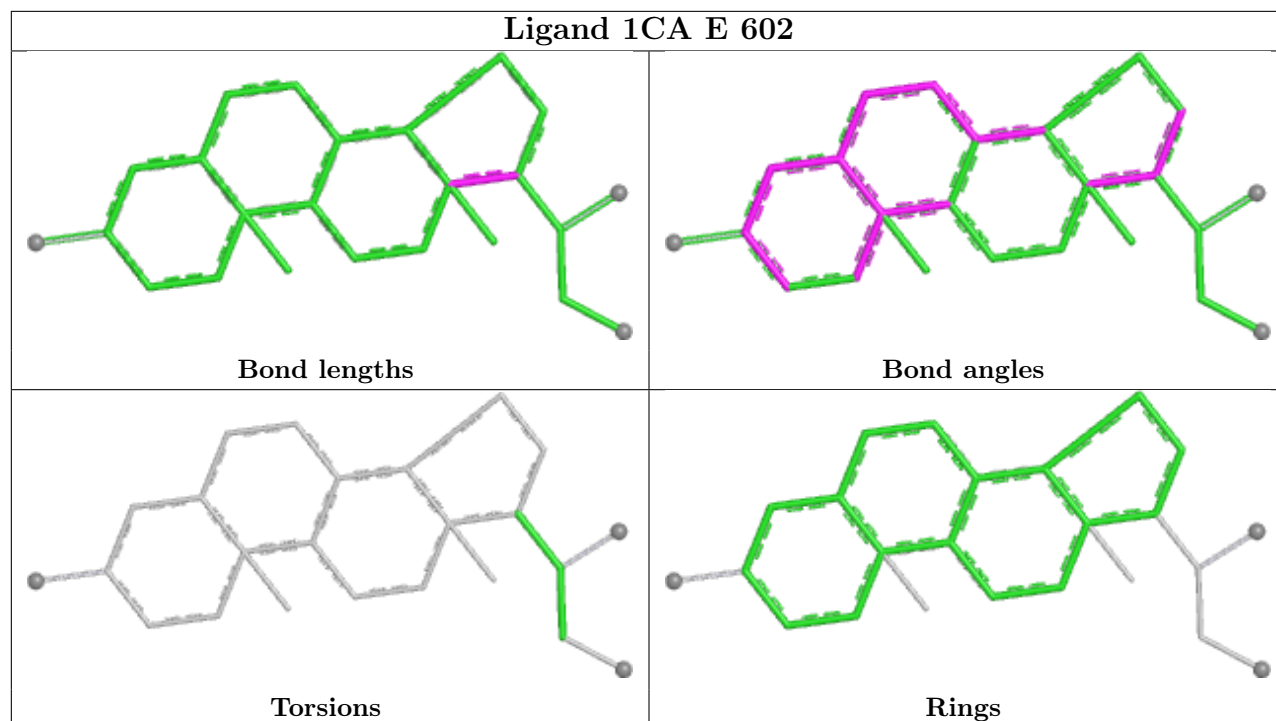
Ligand 1CA A 602



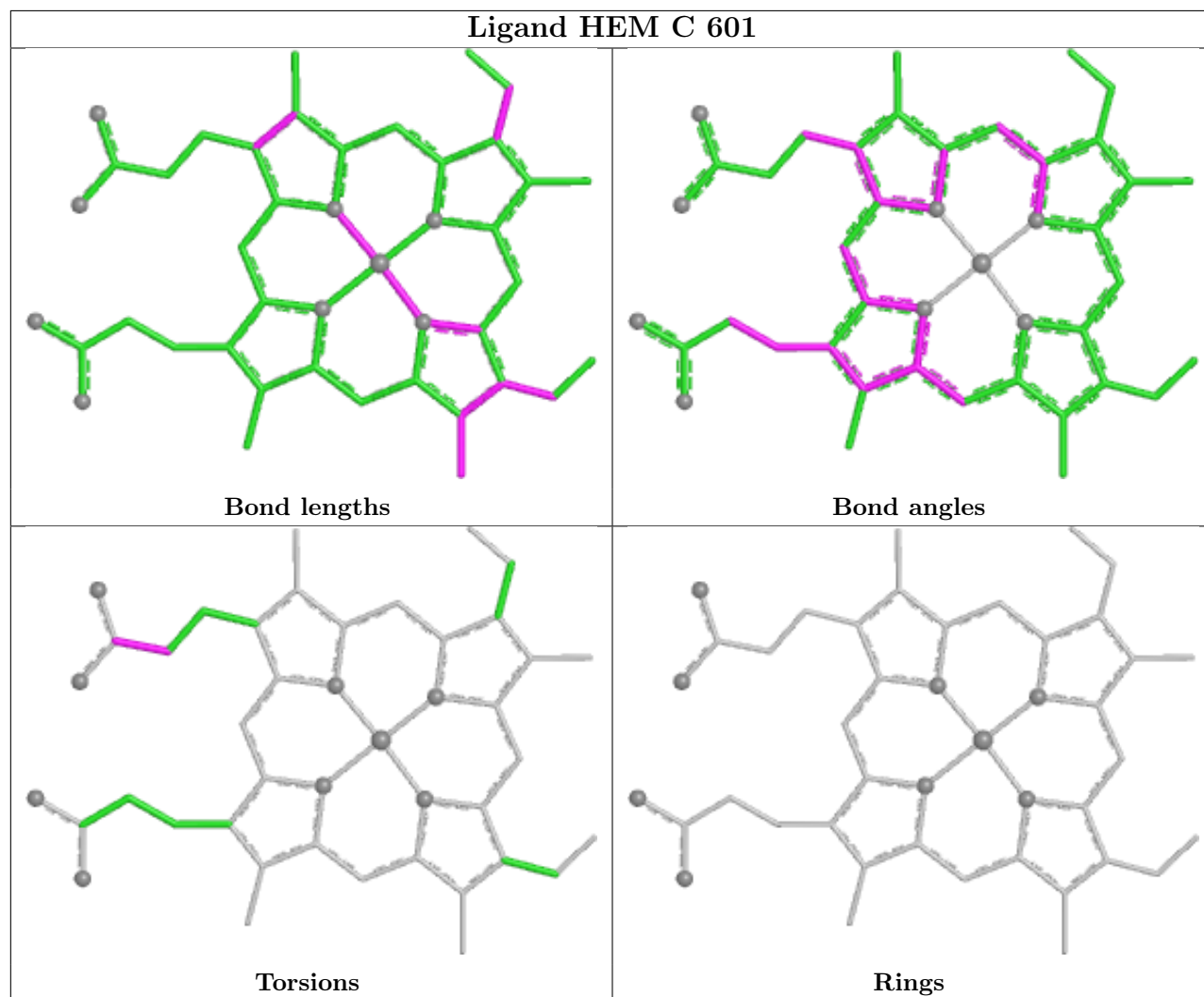
Ligand 1CA B 602

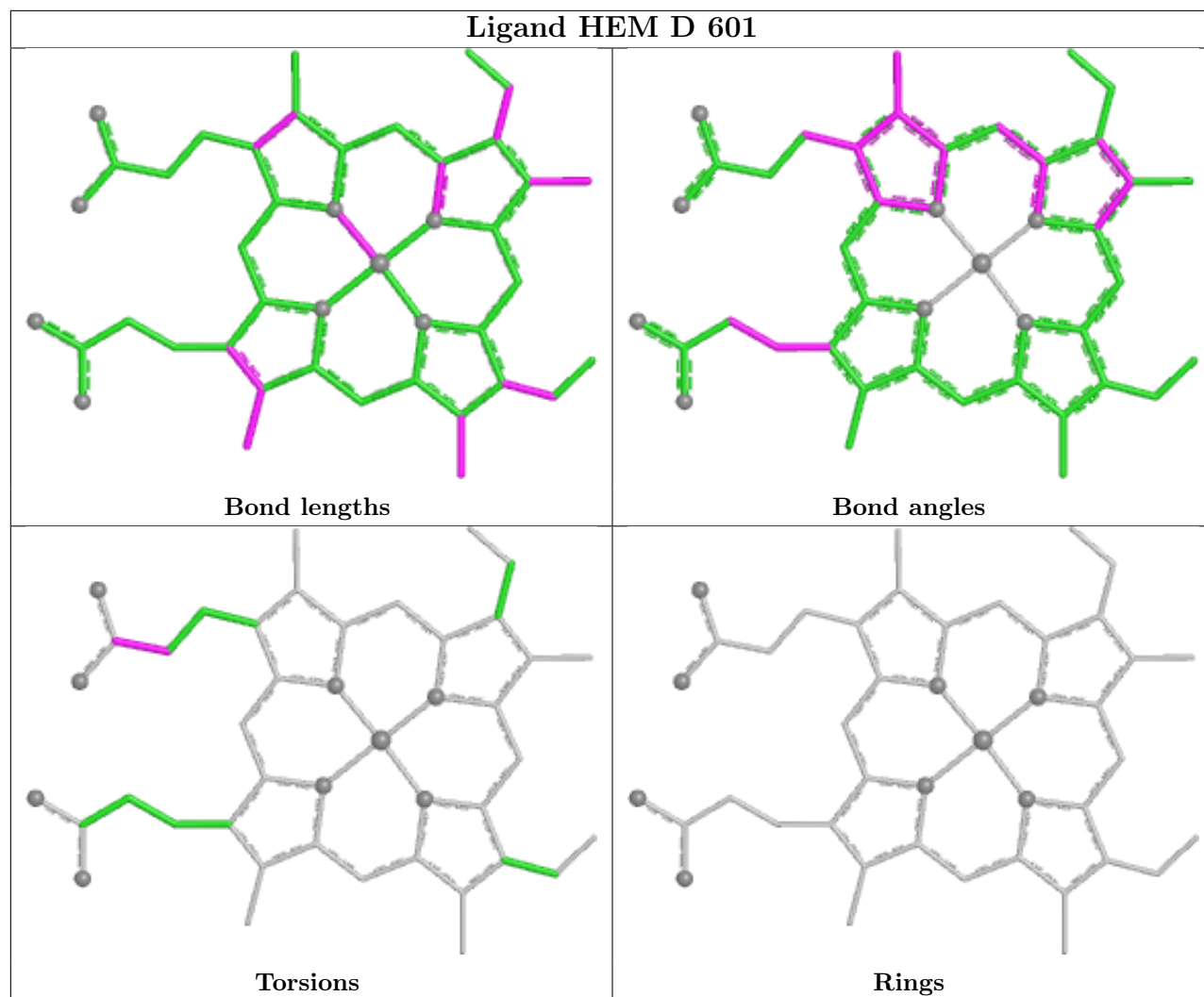


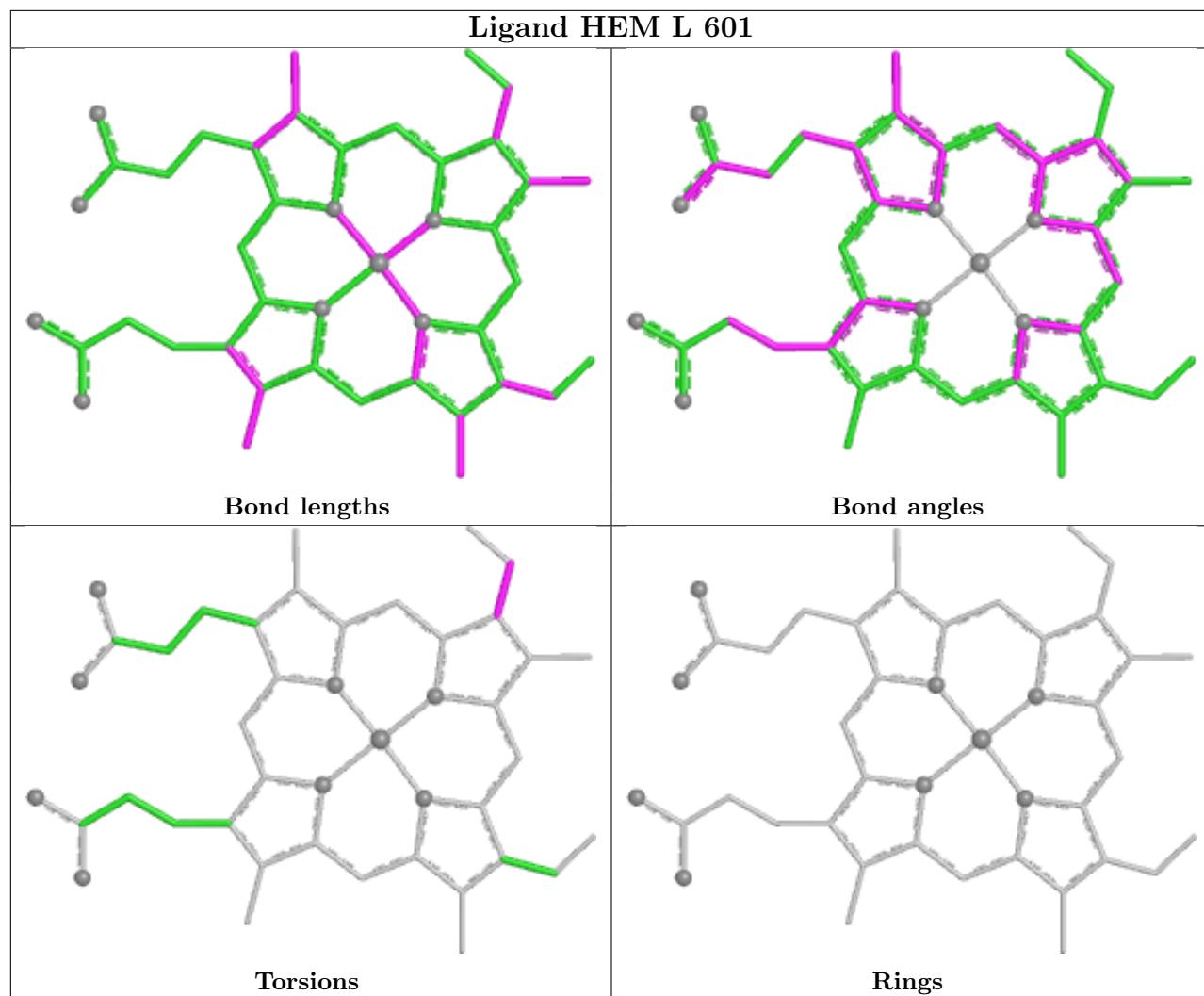
Ligand 1CA E 602

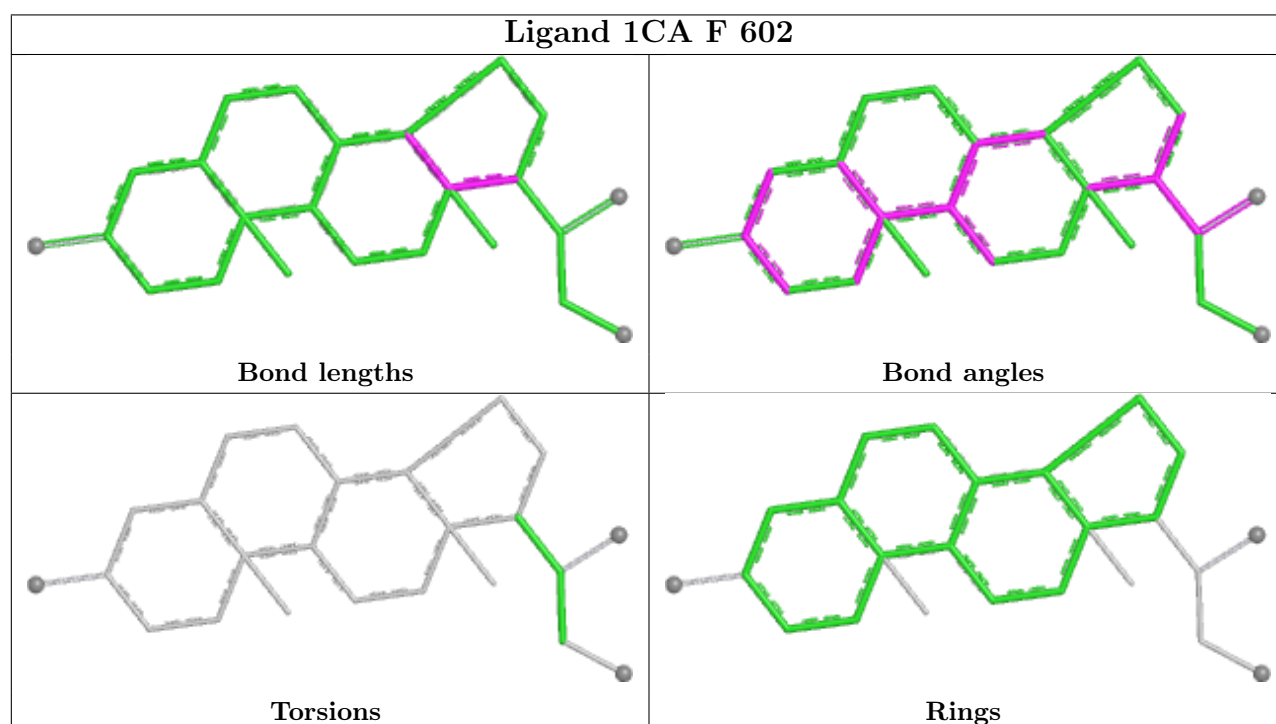
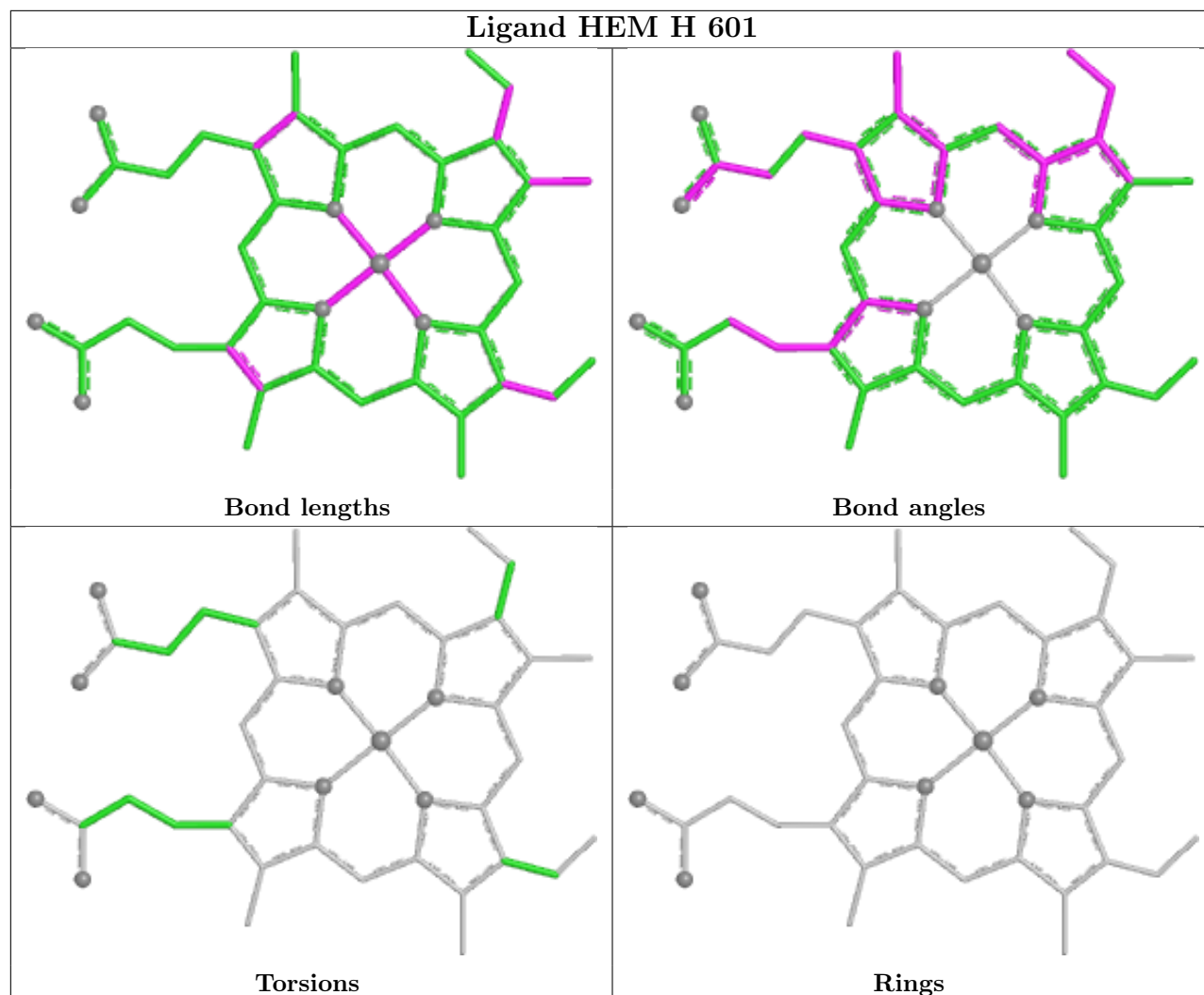


Ligand HEM C 601

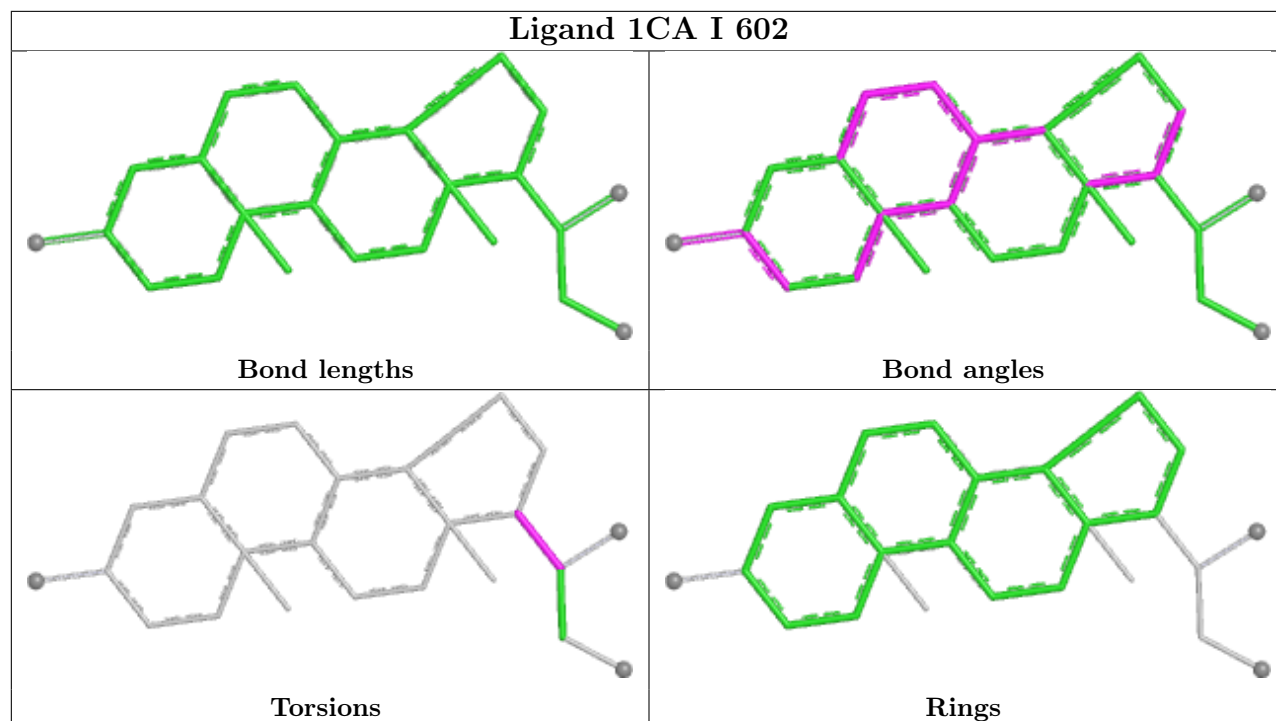




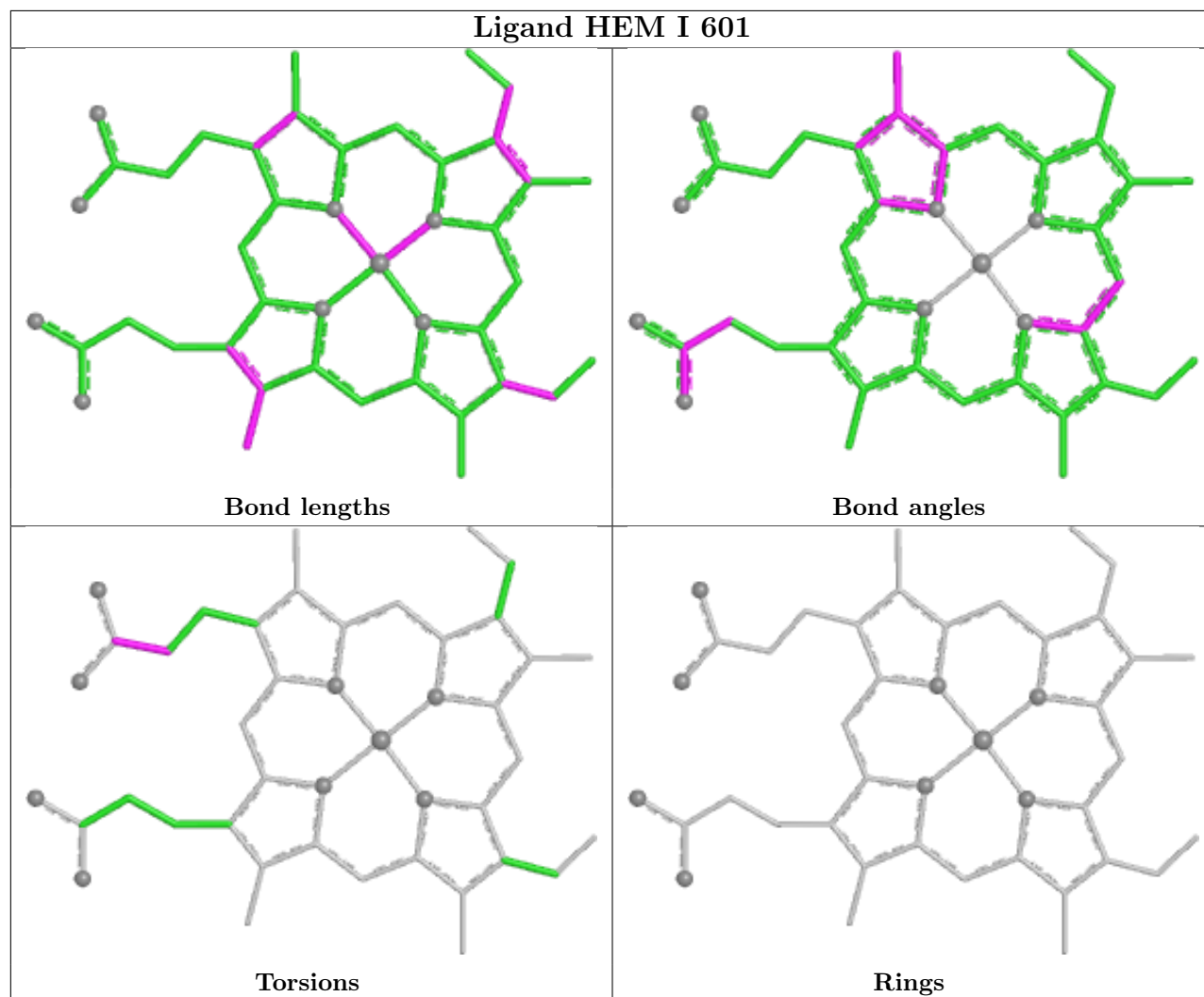


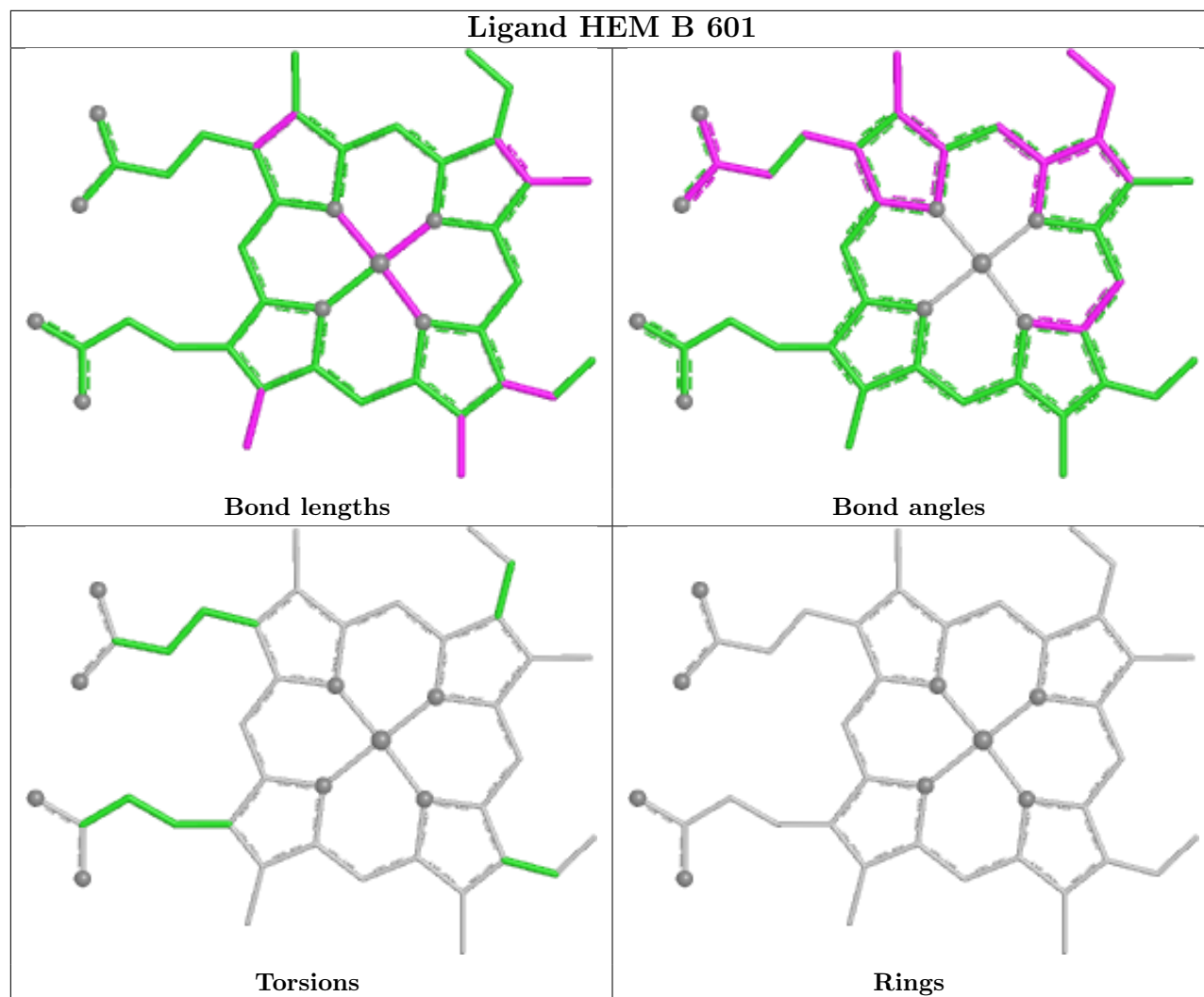


Ligand 1CA I 602



Ligand HEM I 601





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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	463/483 (95%)	-0.34	2 (0%) 88 86	26, 42, 64, 113	0
1	B	463/483 (95%)	-0.11	5 (1%) 78 75	32, 50, 76, 107	0
1	C	462/483 (95%)	-0.30	2 (0%) 88 86	26, 43, 68, 95	0
1	D	462/483 (95%)	-0.26	2 (0%) 88 86	26, 44, 69, 88	0
1	E	470/483 (97%)	-0.29	1 (0%) 91 89	28, 44, 66, 97	0
1	F	469/483 (97%)	-0.12	7 (1%) 72 68	29, 47, 80, 123	0
1	G	462/483 (95%)	-0.11	10 (2%) 62 58	32, 50, 91, 147	0
1	H	462/483 (95%)	-0.14	5 (1%) 78 75	31, 48, 78, 106	0
1	I	462/483 (95%)	0.24	10 (2%) 62 58	35, 60, 101, 121	0
1	J	462/483 (95%)	0.19	8 (1%) 69 65	37, 59, 101, 119	0
1	K	460/483 (95%)	0.17	8 (1%) 69 65	38, 60, 85, 112	0
1	L	454/483 (93%)	0.18	12 (2%) 57 52	36, 55, 95, 154	0
All	All	5551/5796 (95%)	-0.08	72 (1%) 75 71	26, 50, 84, 154	0

The worst 5 of 72 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	438	PHE	6.6
1	A	431	ILE	5.0
1	B	431	ILE	4.9
1	K	502	ILE	4.3
1	A	112	ILE	4.2

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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
4	SO4	B	603	5/5	0.89	0.12	74,74,76,80	0
4	SO4	K	603	5/5	0.91	0.10	64,71,73,75	0
3	1CA	K	602	24/24	0.92	0.09	43,45,52,55	0
4	SO4	F	603	5/5	0.93	0.06	63,65,70,71	0
4	SO4	G	603	5/5	0.93	0.12	58,63,64,64	0
4	SO4	C	603	5/5	0.93	0.09	72,73,76,77	0
4	SO4	L	603	5/5	0.93	0.11	60,66,69,75	0
3	1CA	L	602	24/24	0.94	0.09	42,46,52,57	0
3	1CA	J	602	24/24	0.94	0.09	42,46,52,57	0
3	1CA	B	602	24/24	0.94	0.08	34,36,39,44	0
4	SO4	D	603	5/5	0.94	0.08	67,76,78,81	0
3	1CA	C	602	24/24	0.95	0.07	32,35,39,41	0
4	SO4	E	603	5/5	0.95	0.07	59,61,70,71	0
3	1CA	F	602	24/24	0.96	0.07	35,38,43,49	0
4	SO4	A	603	5/5	0.96	0.09	55,55,56,58	0
3	1CA	I	602	24/24	0.96	0.08	41,45,52,59	0
3	1CA	D	602	24/24	0.96	0.06	30,34,38,43	0
3	1CA	E	602	24/24	0.96	0.07	31,33,39,40	0
3	1CA	H	602	24/24	0.97	0.06	33,36,39,40	0
2	HEM	I	601	43/43	0.97	0.08	36,46,57,62	0
2	HEM	J	601	43/43	0.97	0.08	35,41,53,57	0
2	HEM	K	601	43/43	0.97	0.07	36,45,52,55	0
2	HEM	L	601	43/43	0.97	0.07	38,45,51,56	0
3	1CA	A	602	24/24	0.97	0.07	29,35,38,38	0
3	1CA	G	602	24/24	0.97	0.06	34,38,39,41	0
2	HEM	E	601	43/43	0.98	0.07	25,29,41,42	0
2	HEM	G	601	43/43	0.98	0.07	32,35,39,43	0
2	HEM	H	601	43/43	0.98	0.06	30,35,38,41	0
2	HEM	A	601	43/43	0.98	0.05	25,29,34,38	0
2	HEM	B	601	43/43	0.98	0.06	30,35,47,51	0
2	HEM	C	601	43/43	0.98	0.05	25,30,35,38	0
2	HEM	D	601	43/43	0.98	0.06	27,31,39,44	0

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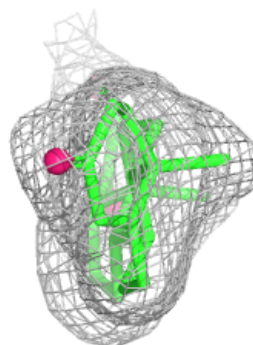
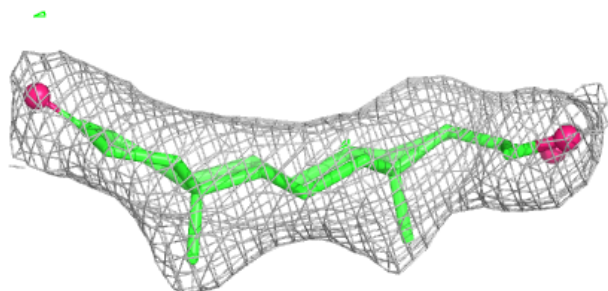
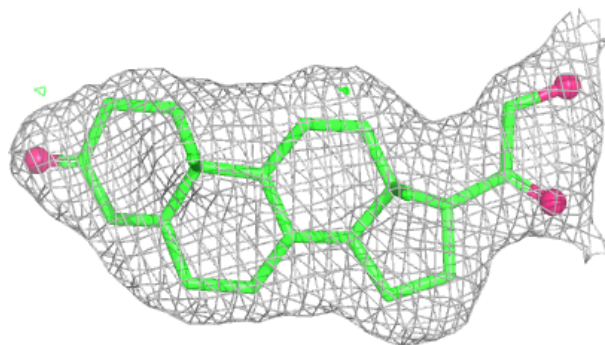
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	HEM	F	601	43/43	0.99	0.05	30,33,39,41	0

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.

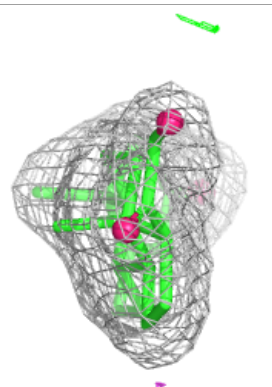
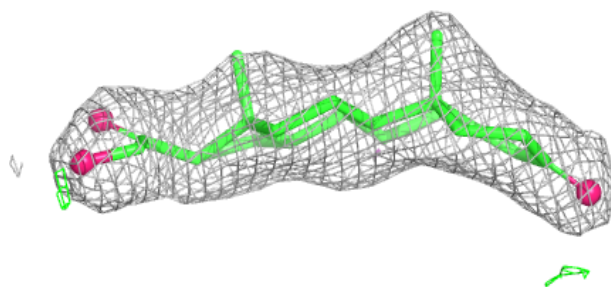
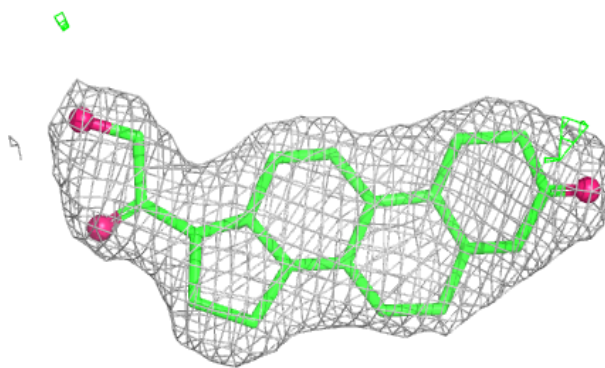
Electron density around 1CA K 602:

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

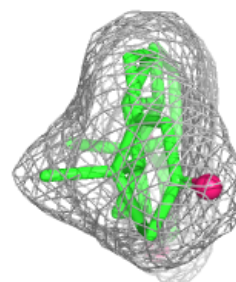
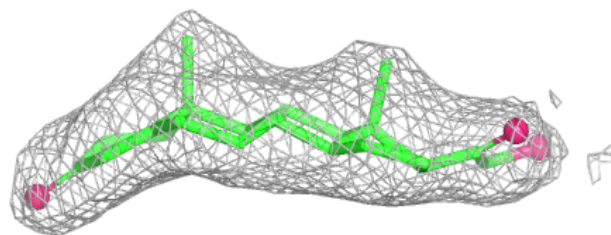
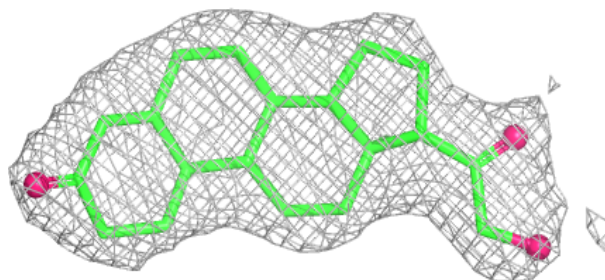


Electron density around 1CA L 602:

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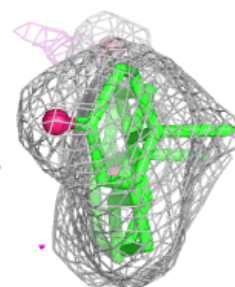
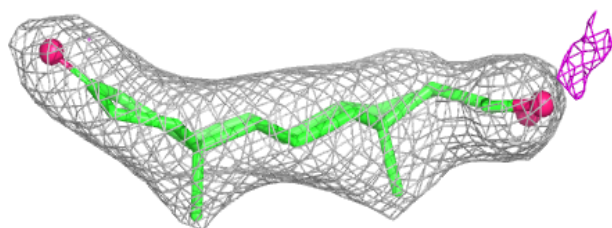
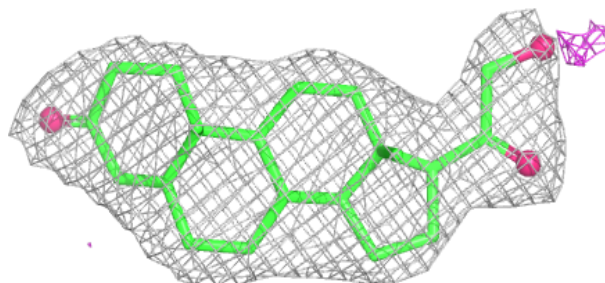
**Electron density around 1CA J 602:**

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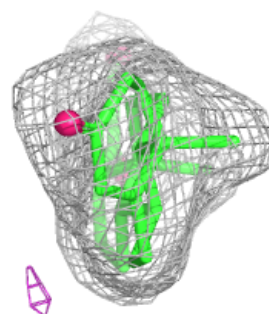
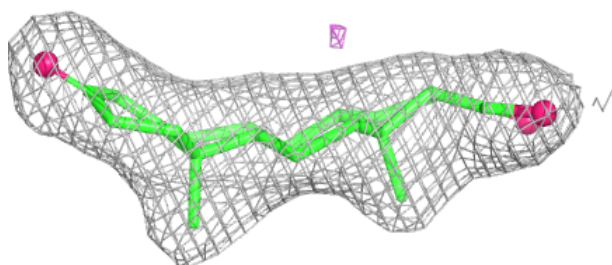
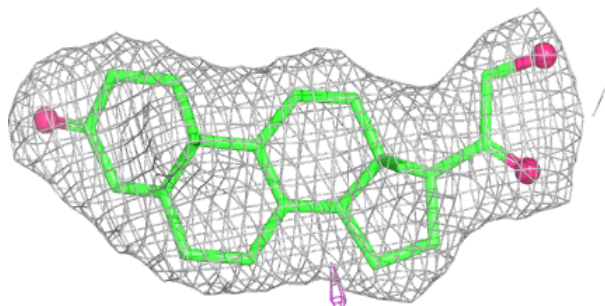


Electron density around 1CA B 602:

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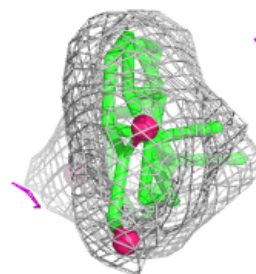
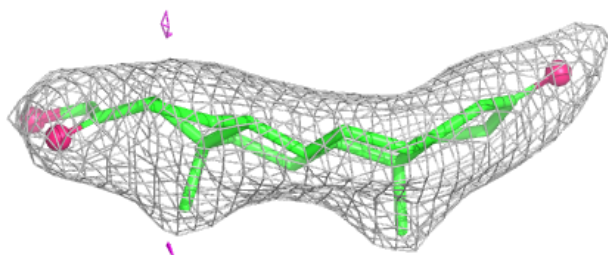
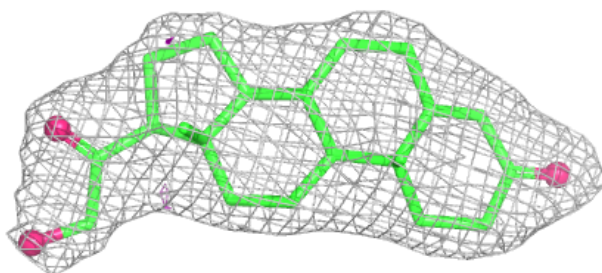
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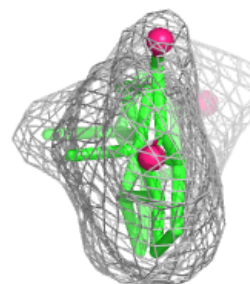
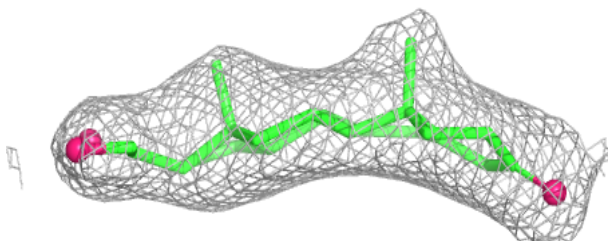
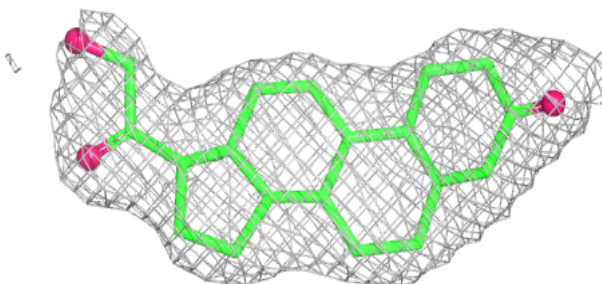


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and green (positive)

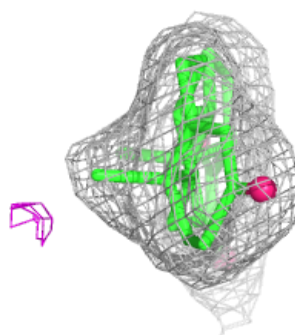
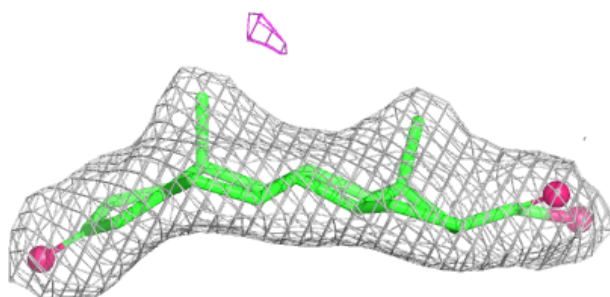
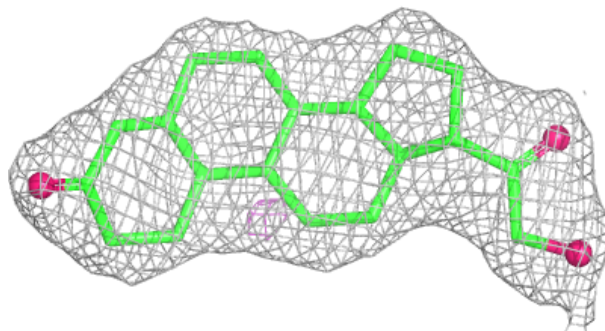
**Electron density around 1CA I 602:**

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and green (positive)

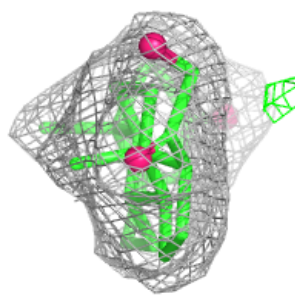
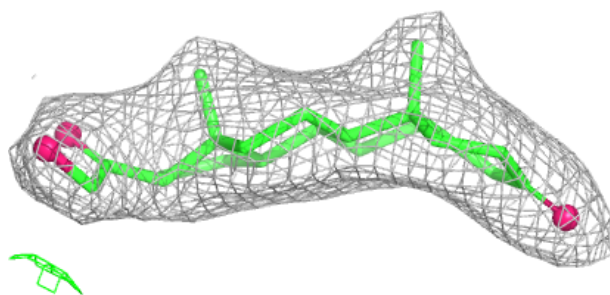
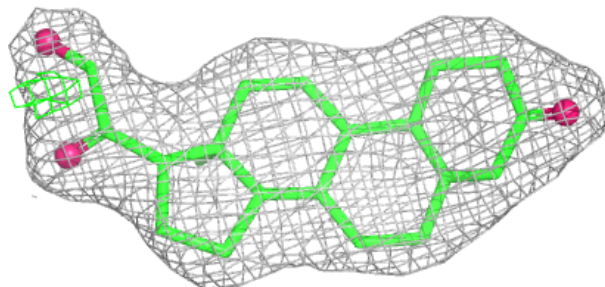


Electron density around 1CA D 602:

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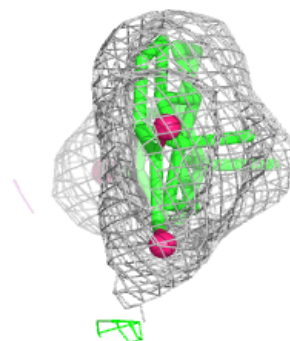
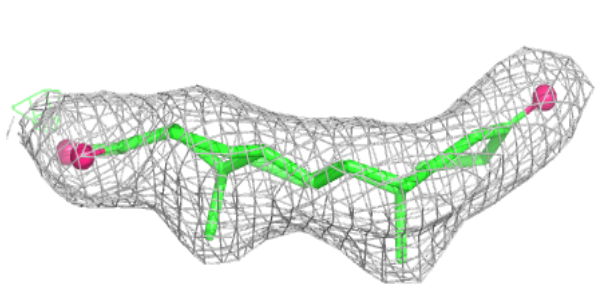
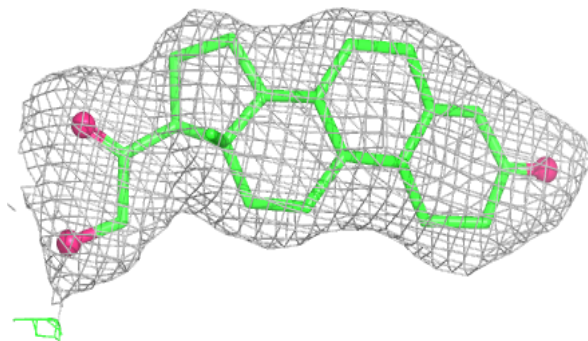
**Electron density around 1CA E 602:**

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and green (positive)



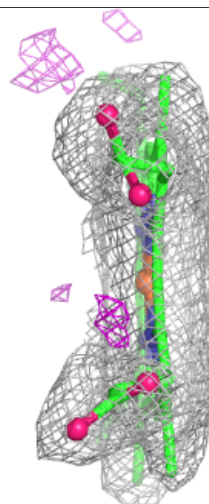
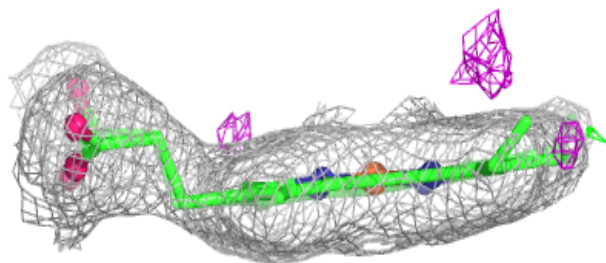
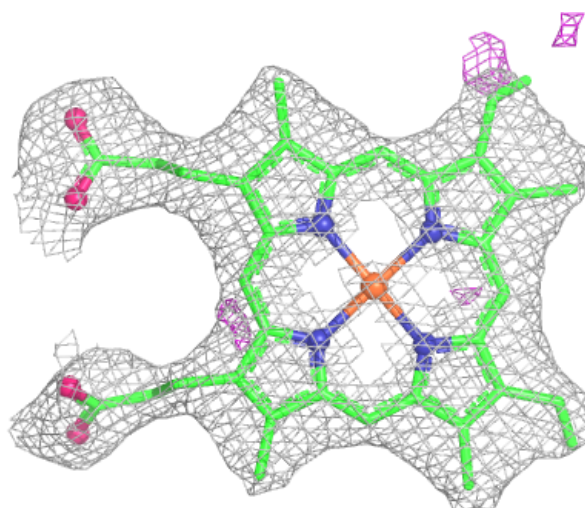
Electron density around 1CA H 602:

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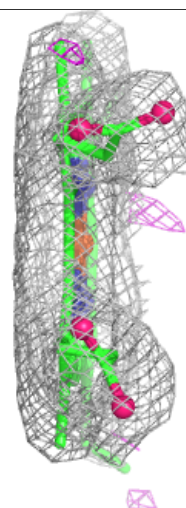
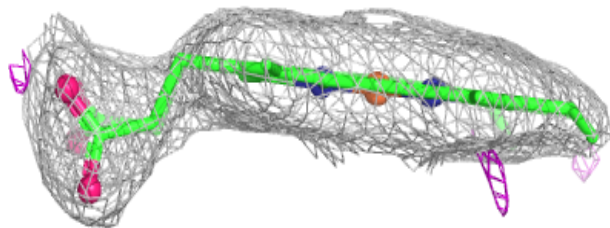
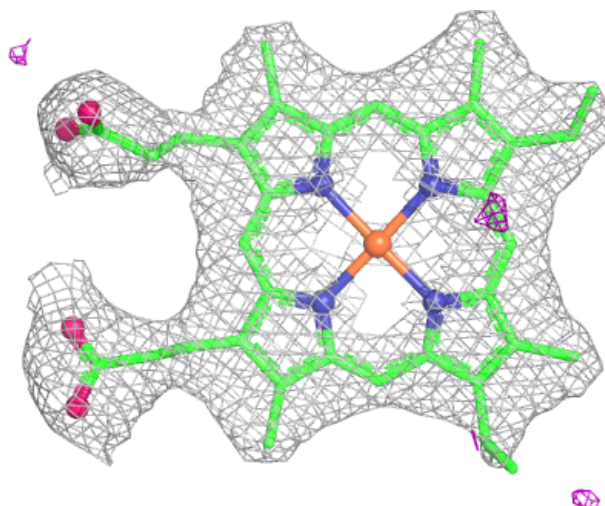
Electron density around HEM I 601:

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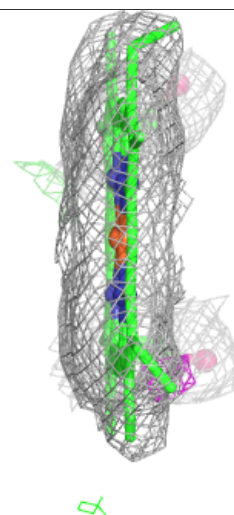
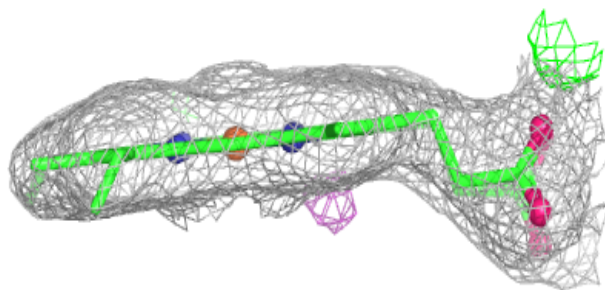
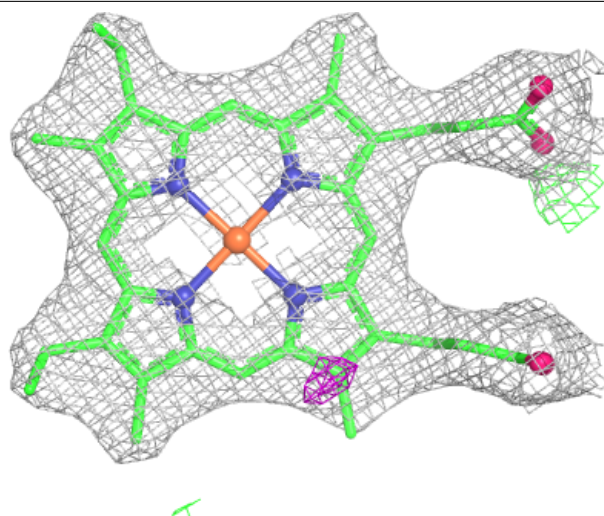
Electron density around HEM J 601:

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



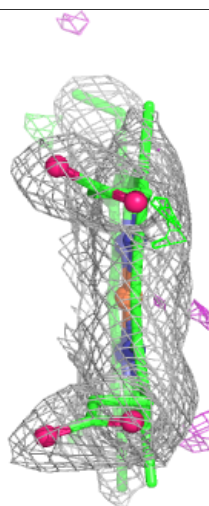
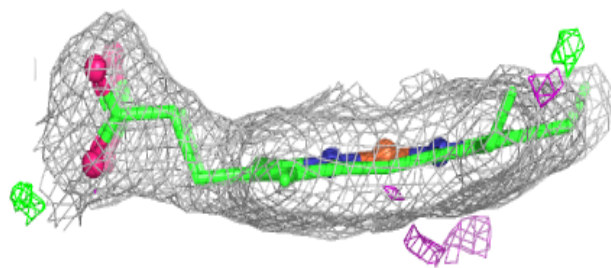
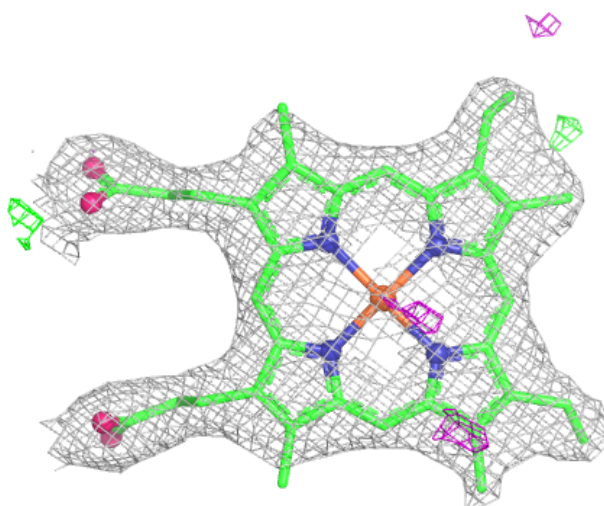
Electron density around HEM K 601:

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



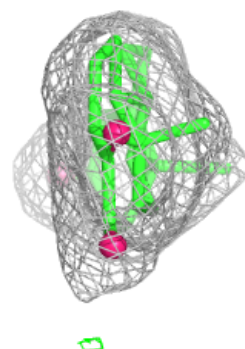
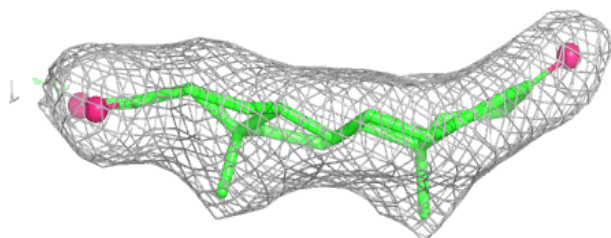
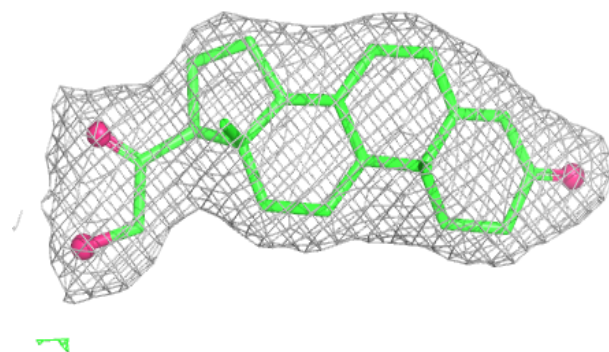
Electron density around HEM L 601:

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

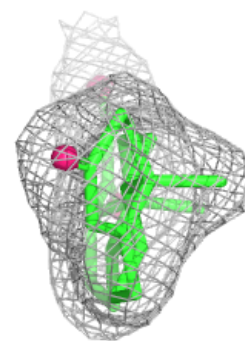
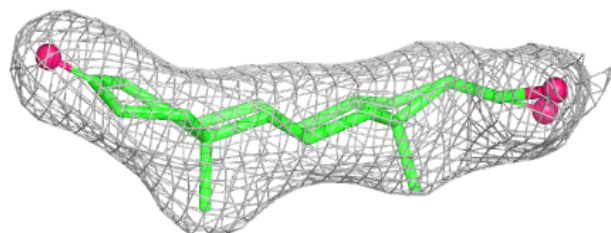
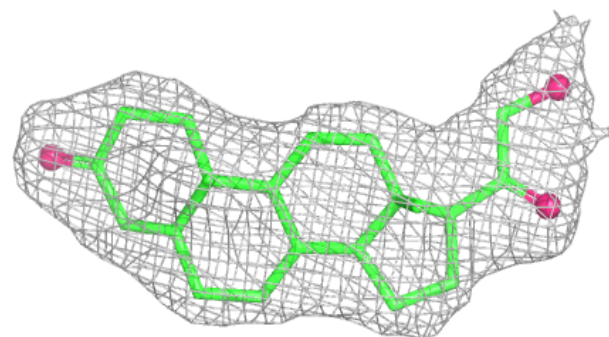


Electron density around 1CA A 602:

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

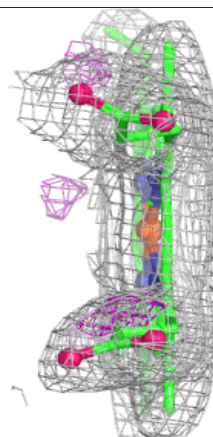
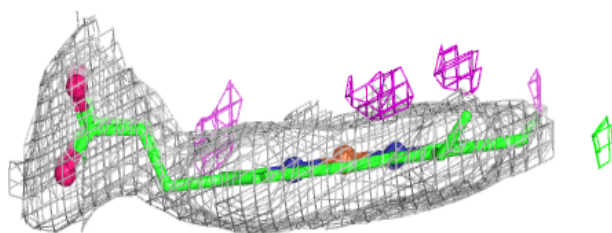
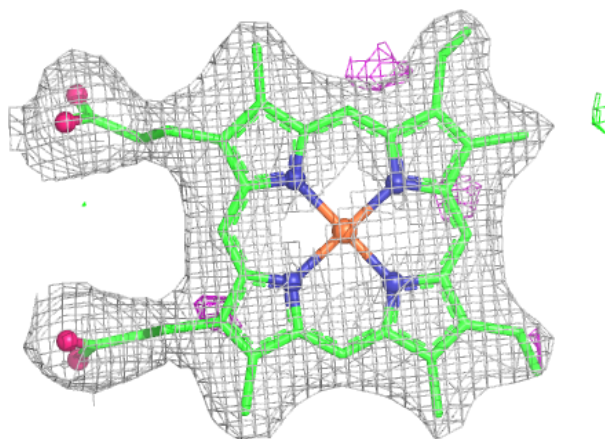
**Electron density around 1CA G 602:**

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



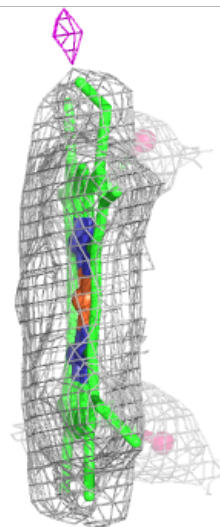
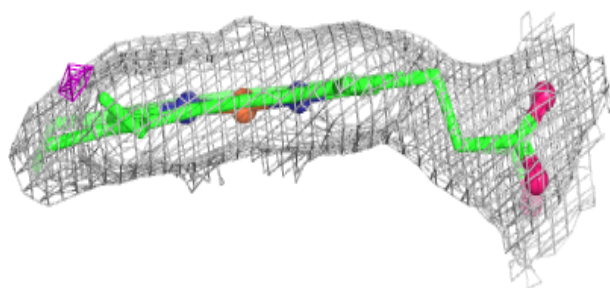
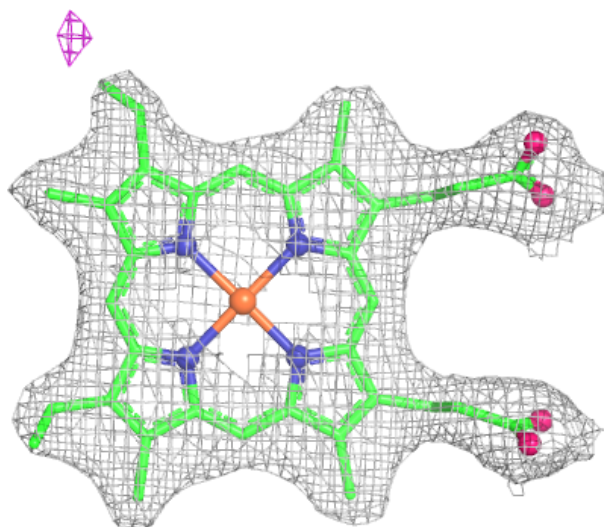
Electron density around HEM E 601:

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



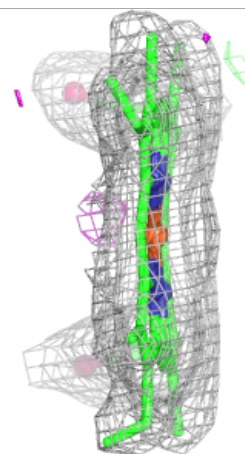
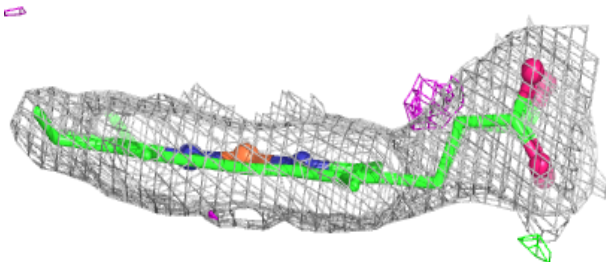
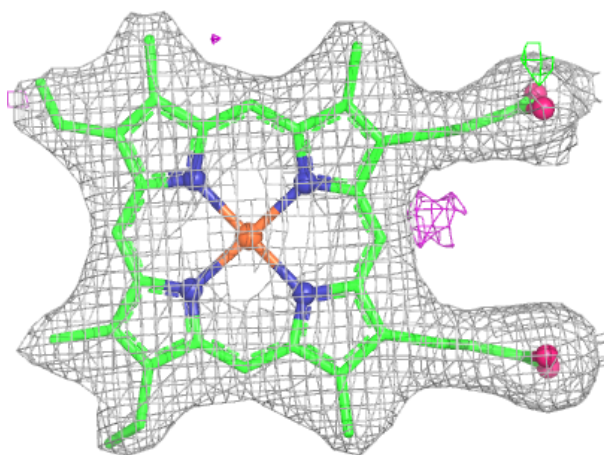
Electron density around HEM G 601:

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



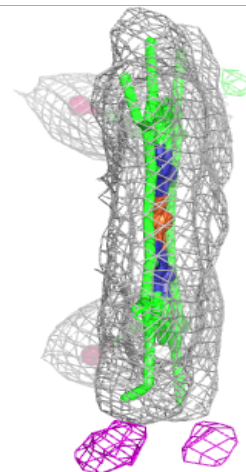
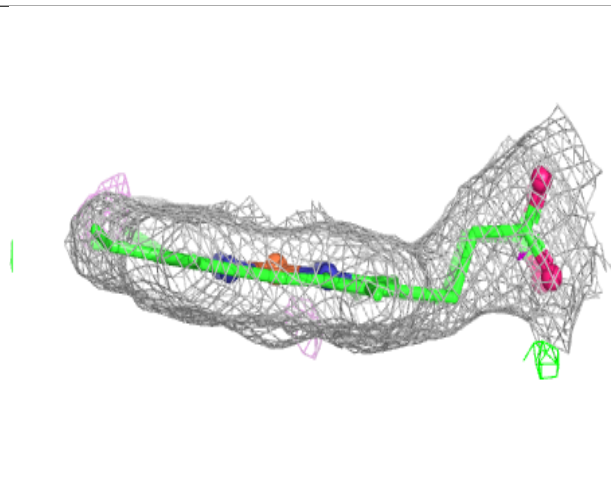
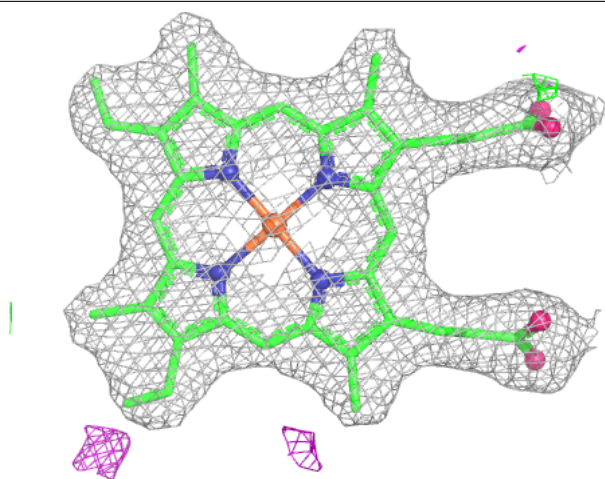
Electron density around HEM H 601:

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



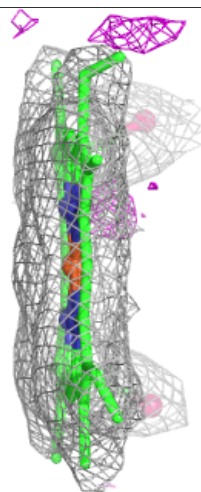
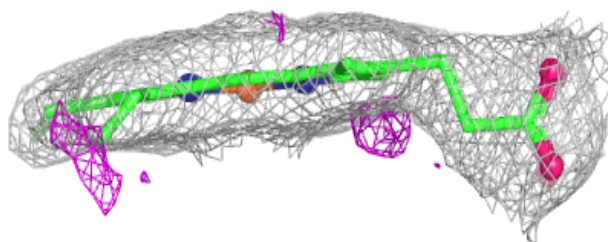
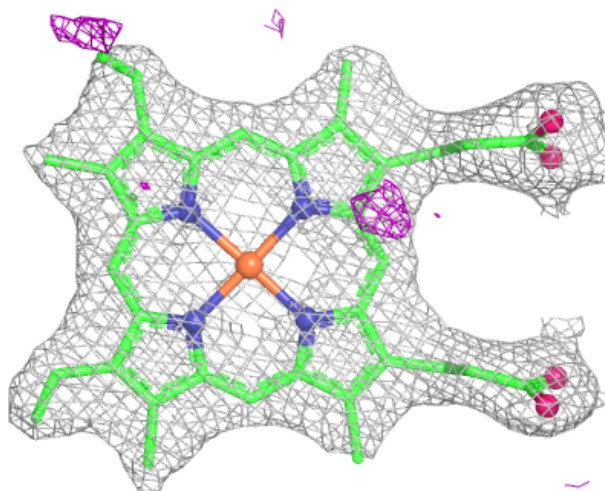
Electron density around HEM A 601:

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



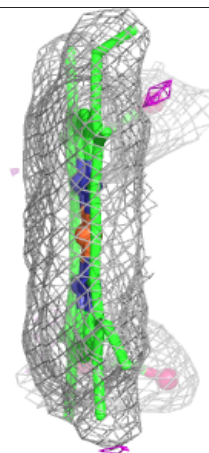
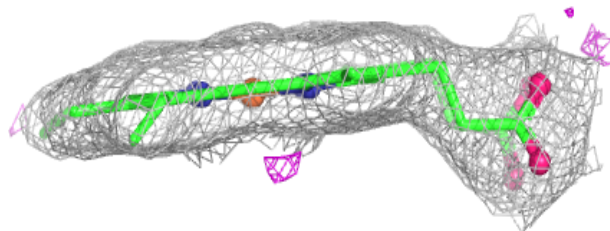
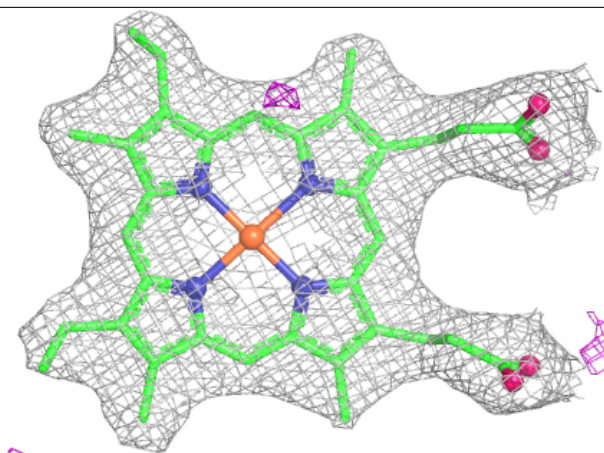
Electron density around HEM B 601:

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



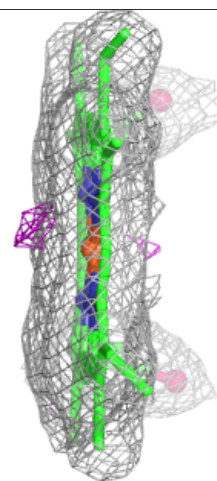
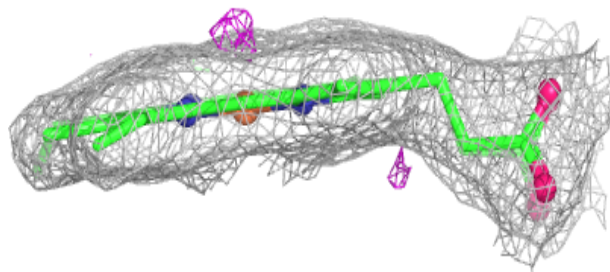
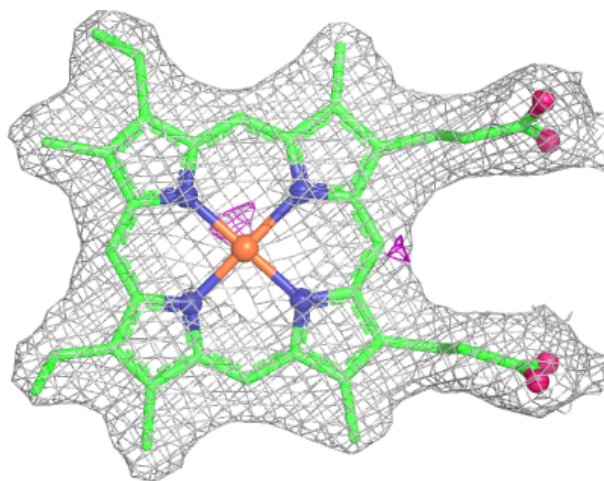
Electron density around HEM C 601:

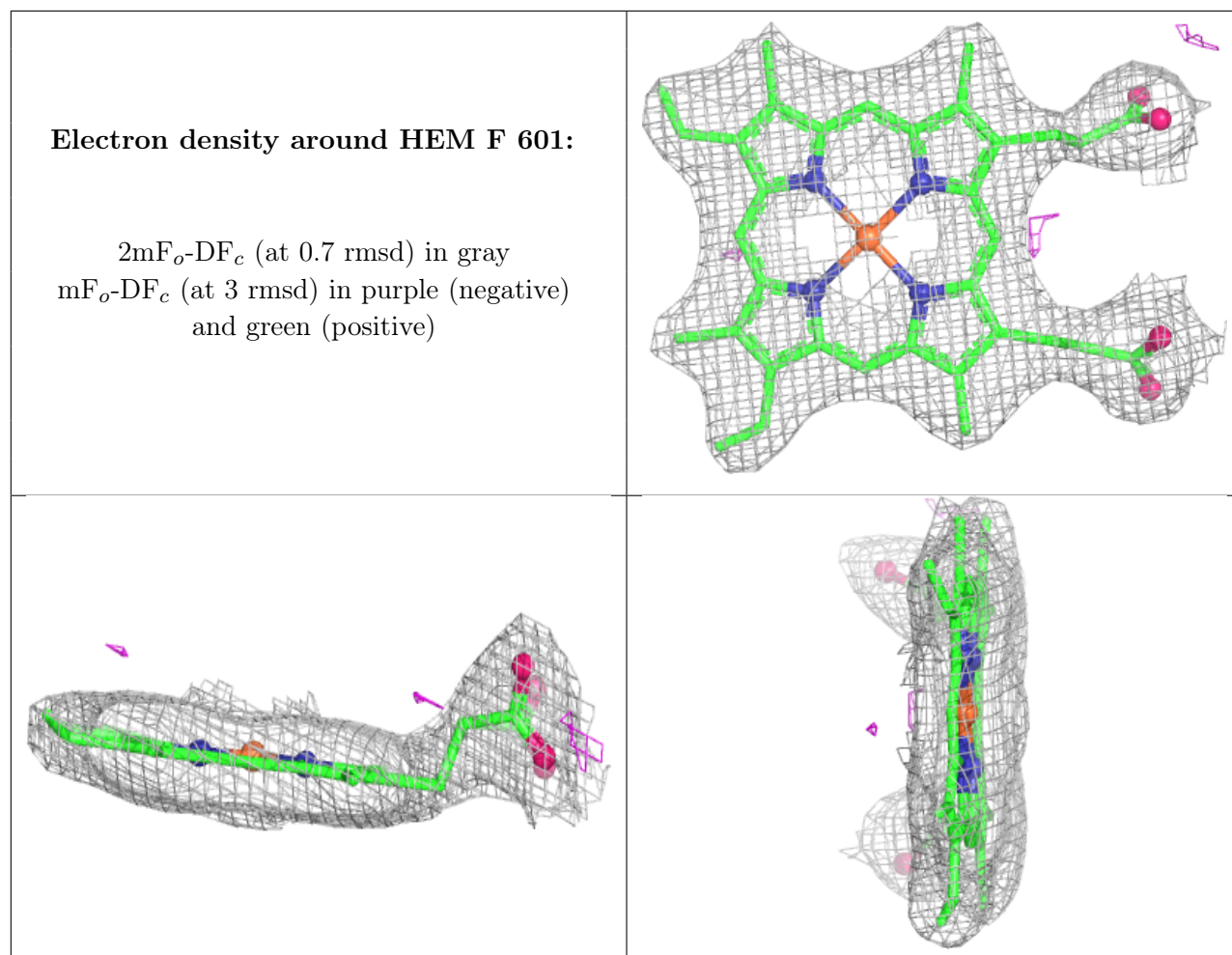
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.