



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 03:43 AM UTC

PDB ID : 6NLN / pdb_00006nlh
Title : 1.60 Å resolution structure of WT BfrB from *Pseudomonas aeruginosa* in complex with a protein-protein interaction inhibitor (analog 16)
Authors : Lovell, S.; Punchi-Hewage, A.; Battaile, K.P.; Yao, H.; Nammalwar, B.; Gnanasekaran, K.K.; Bunce, R.A.; Reitz, A.B.; Rivera, M.
Deposited on : 2019-01-08
Resolution : 1.60 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

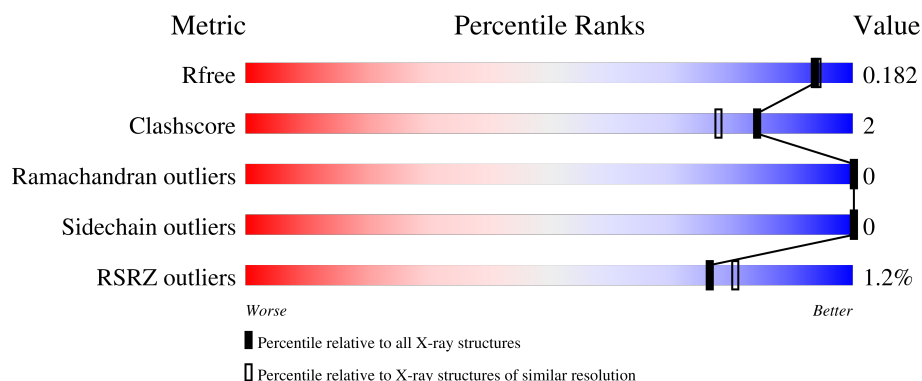
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	158	% 96% ..
1	B	158	% 96% ..
1	C	158	% 96% ..
1	D	158	% 96% ..

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Mol	Chain	Length	Quality of chain
1	E	158	 A horizontal bar chart showing the quality of chain E. The bar is 96% green, with a small red segment at the beginning and a small yellow segment at the end. The percentage '96%' is displayed in the center of the bar. To the right of the bar, there are two dots: a single dot and a double dot.
1	F	158	 A horizontal bar chart showing the quality of chain F. The bar is 97% green, with a small red segment at the beginning and a small yellow segment at the end. The percentage '97%' is displayed in the center of the bar. To the right of the bar, there are two dots: a single dot and a double dot.
1	G	158	 A horizontal bar chart showing the quality of chain G. The bar is 96% green, with a small red segment at the beginning and a small yellow segment at the end. The percentage '96%' is displayed in the center of the bar. To the right of the bar, there are two dots: a single dot and a double dot.
1	H	158	 A horizontal bar chart showing the quality of chain H. The bar is 97% green, with a small red segment at the beginning and a small yellow segment at the end. The percentage '97%' is displayed in the center of the bar. To the right of the bar, there are two dots: a single dot and a double dot.
1	I	158	 A horizontal bar chart showing the quality of chain I. The bar is 96% green, with a small red segment at the beginning and a small yellow segment at the end. The percentage '96%' is displayed in the center of the bar. To the right of the bar, there are two dots: a single dot and a double dot.
1	J	158	 A horizontal bar chart showing the quality of chain J. The bar is 97% green, with a small red segment at the beginning and a small yellow segment at the end. The percentage '97%' is displayed in the center of the bar. To the right of the bar, there are two dots: a single dot and a double dot.
1	K	158	 A horizontal bar chart showing the quality of chain K. The bar is 95% green, with a small red segment at the beginning and a small yellow segment at the end. The percentage '95%' is displayed in the center of the bar. To the right of the bar, there are two dots: a single dot and a double dot.
1	L	158	 A horizontal bar chart showing the quality of chain L. The bar is 94% green, with a small red segment at the beginning and a small yellow segment at the end. The percentage '94%' is displayed in the center of the bar. To the right of the bar, there are two dots: a single dot and a double dot.

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17890 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 Ferroxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	156	Total	C	N	O	S	0	1	0
			1272	807	218	240	7			
1	B	156	Total	C	N	O	S	0	1	0
			1272	805	217	243	7			
1	C	156	Total	C	N	O	S	0	1	0
			1275	807	218	243	7			
1	D	156	Total	C	N	O	S	0	1	0
			1281	810	219	245	7			
1	E	156	Total	C	N	O	S	0	2	0
			1278	810	218	243	7			
1	F	156	Total	C	N	O	S	0	1	0
			1264	802	216	239	7			
1	G	156	Total	C	N	O	S	0	1	0
			1269	804	216	242	7			
1	H	156	Total	C	N	O	S	0	2	0
			1267	804	217	239	7			
1	I	156	Total	C	N	O	S	0	1	0
			1267	803	216	241	7			
1	J	156	Total	C	N	O	S	0	1	0
			1268	803	217	241	7			
1	K	156	Total	C	N	O	S	0	1	0
			1269	804	216	242	7			
1	L	156	Total	C	N	O	S	0	1	0
			1266	803	216	240	7			

- Molecule 2 is FE (II) ION (CCD ID: FE2) (formula: Fe).

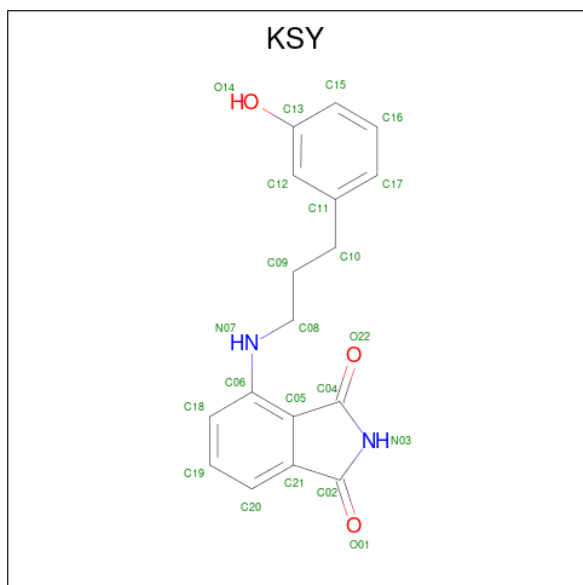
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Fe	0	0
			1	1		
2	B	1	Total	Fe	0	0
			1	1		

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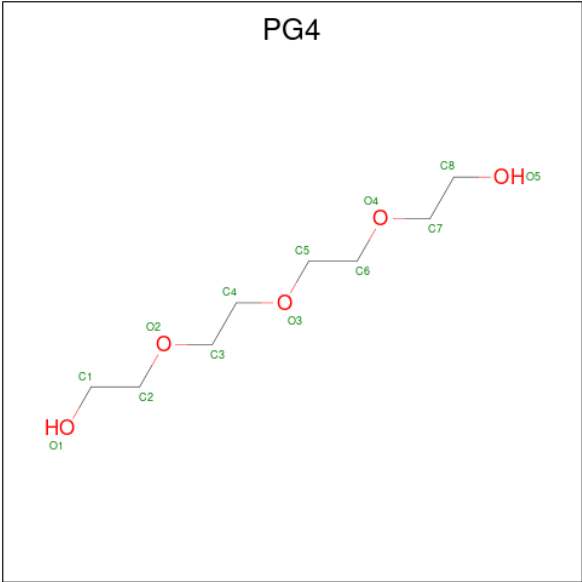
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Fe	0	0
			1	1		

- Molecule 3 is 4-{{[3-(3-hydroxyphenyl)propyl]amino}-1H-isindole-1,3(2H)-dione (CCD ID: KSY) (formula: C₁₇H₁₆N₂O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			22	17	2	3		
3	A	1	Total	C	N	O	0	0
			22	17	2	3		
3	B	1	Total	C	N	O	0	0
			22	17	2	3		
3	C	1	Total	C	N	O	0	0
			22	17	2	3		
3	D	1	Total	C	N	O	0	0
			22	17	2	3		
3	E	1	Total	C	N	O	0	0
			22	17	2	3		
3	F	1	Total	C	N	O	0	0
			22	17	2	3		
3	G	1	Total	C	N	O	0	0
			22	17	2	3		
3	H	1	Total	C	N	O	0	0
			16	12	2	2		
3	I	1	Total	C	N	O	0	0
			22	17	2	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			13	8	5		
5	A	1	Total	C	O	0	0
			10	6	4		
5	B	1	Total	C	O	0	0
			8	5	3		
5	B	1	Total	C	O	0	0
			6	4	2		
5	C	1	Total	C	O	0	0
			13	8	5		
5	C	1	Total	C	O	0	0
			8	5	3		
5	D	1	Total	C	O	0	0
			13	8	5		
5	D	1	Total	C	O	0	0
			10	6	4		
5	D	1	Total	C	O	0	0
			8	5	3		
5	E	1	Total	C	O	0	0
			13	8	5		
5	E	1	Total	C	O	0	0
			10	6	4		
5	E	1	Total	C	O	0	0
			8	5	3		
5	F	1	Total	C	O	0	0
			13	8	5		
5	F	1	Total	C	O	0	0
			10	6	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	F	1	Total	C	O	0	0
			9	6	3		
5	G	1	Total	C	O	0	0
			13	8	5		
5	G	1	Total	C	O	0	0
			10	6	4		
5	H	1	Total	C	O	0	0
			8	5	3		
5	I	1	Total	C	O	0	0
			10	6	4		
5	I	1	Total	C	O	0	0
			8	5	3		
5	I	1	Total	C	O	0	0
			8	5	3		
5	J	1	Total	C	O	0	0
			13	8	5		
5	J	1	Total	C	O	0	0
			13	8	5		
5	K	1	Total	C	O	0	0
			8	5	3		
5	K	1	Total	C	O	0	0
			13	8	5		
5	K	1	Total	C	O	0	0
			8	5	3		
5	L	1	Total	C	O	0	0
			13	8	5		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	159	Total	O	0	0
			159	159		
6	B	147	Total	O	0	0
			147	147		
6	C	159	Total	O	0	0
			159	159		
6	D	154	Total	O	0	0
			154	154		
6	E	152	Total	O	0	0
			152	152		
6	F	156	Total	O	0	0
			156	156		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	144	Total 144	O 144	0	0
6	H	152	Total 152	O 152	0	0
6	I	129	Total 129	O 129	0	0
6	J	154	Total 154	O 154	0	0
6	K	154	Total 154	O 154	0	0
6	L	136	Total 136	O 136	0	0

3 Residue-property plots [i](#)

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

- Molecule 1: Ferrooxidase



- Molecule 1: Ferrooxidase



- Molecule 1: Ferrooxidase



- Molecule 1: Ferrooxidase



- Molecule 1: Ferrooxidase



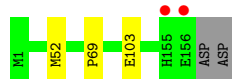
- Molecule 1: Ferrooxidase



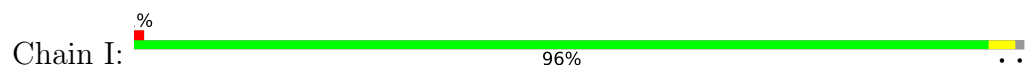
● Molecule 1: Ferroxidase



● Molecule 1: Ferroxidase



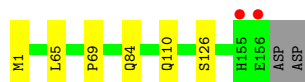
● Molecule 1: Ferroxidase



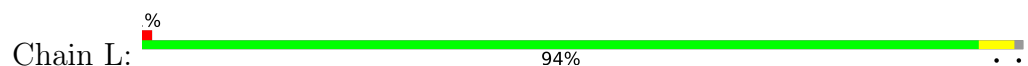
● Molecule 1: Ferroxidase



● Molecule 1: Ferroxidase



● Molecule 1: Ferroxidase



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	129.91Å 194.88Å 203.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.72 – 1.60 48.72 – 1.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.72-1.60) 100.0 (48.72-1.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 1.60Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.147 , 0.169 0.161 , 0.182	Depositor DCC
R_{free} test set	16764 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	18.2	Xtriage
Anisotropy	0.316	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 38.2	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	0.97	EDS
Total number of atoms	17890	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, PG4, FE2, KSY

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	0.37	0/1296	0.52	0/1745
1	B	0.36	0/1296	0.51	0/1747
1	C	0.37	0/1299	0.50	0/1750
1	D	0.36	0/1305	0.51	0/1757
1	E	0.37	0/1305	0.54	0/1758
1	F	0.38	0/1288	0.52	0/1737
1	G	0.36	0/1293	0.51	0/1743
1	H	0.36	0/1294	0.50	0/1745
1	I	0.37	0/1291	0.49	0/1741
1	J	0.39	0/1292	0.54	0/1742
1	K	0.35	0/1293	0.53	0/1743
1	L	0.34	0/1290	0.49	0/1739
All	All	0.36	0/15542	0.51	0/20947

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1272	0	1254	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1272	0	1242	3	0
1	C	1275	0	1251	3	0
1	D	1281	0	1262	4	0
1	E	1278	0	1255	4	0
1	F	1264	0	1231	3	0
1	G	1269	0	1238	4	0
1	H	1267	0	1238	3	0
1	I	1267	0	1233	3	0
1	J	1268	0	1238	3	0
1	K	1269	0	1238	6	0
1	L	1266	0	1236	6	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	D	1	0	0	0	0
3	A	44	0	0	2	0
3	B	22	0	0	1	0
3	C	22	0	0	1	0
3	D	22	0	0	1	0
3	E	22	0	0	1	0
3	F	22	0	0	1	0
3	G	22	0	0	1	0
3	H	16	0	0	1	0
3	I	22	0	0	1	0
3	J	22	0	0	1	0
3	K	15	0	0	1	0
3	L	14	0	0	1	0
4	A	43	0	30	2	0
4	B	43	0	30	4	0
4	C	43	0	30	5	0
4	D	43	0	30	0	0
4	F	43	0	30	3	0
4	H	43	0	30	3	0
4	L	43	0	30	2	0
5	A	23	0	31	1	0
5	B	14	0	13	0	0
5	C	21	0	26	1	0
5	D	31	0	39	0	0
5	E	31	0	40	0	0
5	F	32	0	42	3	0
5	G	23	0	31	2	0
5	H	8	0	9	0	0
5	I	26	0	30	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	J	26	0	36	0	0
5	K	29	0	35	1	0
5	L	13	0	18	2	0
6	A	159	0	0	2	0
6	B	147	0	0	0	0
6	C	159	0	0	3	0
6	D	154	0	0	3	2
6	E	152	0	0	1	0
6	F	156	0	0	2	0
6	G	144	0	0	3	1
6	H	152	0	0	1	0
6	I	129	0	0	3	0
6	J	154	0	0	2	0
6	K	154	0	0	4	0
6	L	136	0	0	5	0
All	All	17890	0	15476	71	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

The worst 5 of 71 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)
4:A:204:HEM:HMC1	4:A:204:HEM:HBC2	1.69	0.75
1:K:126[A]:SER:OG	6:K:301:HOH:O	2.09	0.69
4:B:203:HEM:HBC2	4:B:203:HEM:HMC1	1.75	0.69
4:F:202:HEM:HMC1	4:F:202:HEM:HBC2	1.77	0.66
4:L:202:HEM:O1D	6:L:301:HOH:O	2.13	0.65

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:305:HOH:O	6:D:399:HOH:O[3_554]	1.83	0.37
6:D:391:HOH:O	6:G:348:HOH:O[7_444]	2.11	0.09

5.3 Torsion angles

5.3.1 Protein backbone

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	155/158 (98%)	154 (99%)	1 (1%)	0	100	100
1	B	155/158 (98%)	155 (100%)	0	0	100	100
1	C	155/158 (98%)	155 (100%)	0	0	100	100
1	D	155/158 (98%)	155 (100%)	0	0	100	100
1	E	156/158 (99%)	156 (100%)	0	0	100	100
1	F	155/158 (98%)	155 (100%)	0	0	100	100
1	G	155/158 (98%)	155 (100%)	0	0	100	100
1	H	156/158 (99%)	155 (99%)	1 (1%)	0	100	100
1	I	155/158 (98%)	155 (100%)	0	0	100	100
1	J	155/158 (98%)	154 (99%)	1 (1%)	0	100	100
1	K	155/158 (98%)	154 (99%)	1 (1%)	0	100	100
1	L	155/158 (98%)	155 (100%)	0	0	100	100
All	All	1862/1896 (98%)	1858 (100%)	4 (0%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	137/144 (95%)	137 (100%)	0	100	100
1	B	137/144 (95%)	137 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	138/144 (96%)	138 (100%)	0	100	100
1	D	140/144 (97%)	140 (100%)	0	100	100
1	E	138/144 (96%)	138 (100%)	0	100	100
1	F	134/144 (93%)	134 (100%)	0	100	100
1	G	136/144 (94%)	136 (100%)	0	100	100
1	H	135/144 (94%)	135 (100%)	0	100	100
1	I	135/144 (94%)	135 (100%)	0	100	100
1	J	136/144 (94%)	136 (100%)	0	100	100
1	K	136/144 (94%)	136 (100%)	0	100	100
1	L	135/144 (94%)	135 (100%)	0	100	100
All	All	1637/1728 (95%)	1637 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	88	GLN
1	L	88	GLN
1	I	88	GLN
1	L	151	GLN
1	K	137	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 50 ligands modelled in this entry, 3 are monoatomic - leaving 47 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	PG4	F	204	-	9,9,12	0.55	0	8,8,11	0.31	0
5	PG4	F	205	-	8,8,12	0.45	0	7,7,11	0.48	0
5	PG4	B	204	-	7,7,12	0.57	0	6,6,11	0.21	0
5	PG4	C	203	-	12,12,12	0.51	0	11,11,11	0.58	0
5	PG4	G	203	-	9,9,12	0.51	0	8,8,11	0.16	0
5	PG4	D	204	-	12,12,12	0.50	0	11,11,11	0.44	0
3	KSY	G	201	-	24,24,24	1.66	6 (25%)	33,33,33	1.20	3 (9%)
3	KSY	I	201	-	24,24,24	1.64	5 (20%)	33,33,33	1.52	3 (9%)
4	HEM	A	204	1	50,50,50	1.33	7 (14%)	67,82,82	1.12	4 (5%)
5	PG4	E	202	-	12,12,12	0.52	0	11,11,11	0.42	0
5	PG4	I	204	-	7,7,12	0.38	0	6,6,11	0.45	0
5	PG4	D	206	-	7,7,12	0.41	0	6,6,11	0.32	0
5	PG4	K	204	-	7,7,12	0.51	0	6,6,11	0.38	0
4	HEM	C	202	1	50,50,50	1.33	8 (16%)	67,82,82	1.27	8 (11%)
5	PG4	J	203	-	12,12,12	0.43	0	11,11,11	0.48	0
5	PG4	L	203	-	12,12,12	0.40	0	11,11,11	0.56	0
4	HEM	L	202	1	50,50,50	1.31	8 (16%)	67,82,82	1.08	3 (4%)
3	KSY	F	201	-	24,24,24	1.59	4 (16%)	33,33,33	1.43	3 (9%)
5	PG4	F	203	-	12,12,12	0.49	0	11,11,11	0.53	0
5	PG4	D	205	-	9,9,12	0.53	0	8,8,11	0.25	0
5	PG4	E	204	-	7,7,12	0.50	0	6,6,11	0.34	0
3	KSY	L	201	-	15,15,24	2.27	5 (33%)	21,21,33	1.98	4 (19%)
5	PG4	A	205	-	12,12,12	0.46	0	11,11,11	0.41	0
5	PG4	K	202	-	7,7,12	0.49	0	6,6,11	0.22	0
3	KSY	A	203	-	24,24,24	1.75	4 (16%)	33,33,33	1.30	4 (12%)
3	KSY	K	201	-	16,16,24	2.02	5 (31%)	22,22,33	1.39	3 (13%)
4	HEM	B	203	1	50,50,50	1.36	7 (14%)	67,82,82	1.27	8 (11%)
3	KSY	B	202	-	24,24,24	1.54	5 (20%)	33,33,33	1.45	4 (12%)
5	PG4	I	203	-	7,7,12	0.57	0	6,6,11	0.29	0
5	PG4	I	202	-	9,9,12	0.38	0	8,8,11	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PG4	E	203	-	9,9,12	0.54	0	8,8,11	0.29	0
5	PG4	C	204	-	7,7,12	0.51	0	6,6,11	0.25	0
5	PG4	A	206	-	9,9,12	0.44	0	8,8,11	0.58	0
5	PG4	G	202	-	12,12,12	0.52	0	11,11,11	0.41	0
5	PG4	H	203	-	7,7,12	0.52	0	6,6,11	0.27	0
3	KSY	D	202	-	24,24,24	1.78	5 (20%)	33,33,33	1.78	6 (18%)
5	PG4	B	205	-	5,5,12	0.52	0	4,4,11	0.14	0
5	PG4	K	203	-	12,12,12	0.49	0	11,11,11	0.31	0
3	KSY	A	202	-	24,24,24	1.91	5 (20%)	33,33,33	2.14	6 (18%)
4	HEM	F	202	1	50,50,50	1.24	8 (16%)	67,82,82	1.13	5 (7%)
4	HEM	H	202	1	50,50,50	1.36	8 (16%)	67,82,82	1.32	9 (13%)
5	PG4	J	202	-	12,12,12	0.51	0	11,11,11	0.44	0
3	KSY	H	201	-	17,17,24	1.95	6 (35%)	23,23,33	2.24	7 (30%)
3	KSY	E	201	-	24,24,24	1.64	5 (20%)	33,33,33	1.32	4 (12%)
4	HEM	D	203	1	50,50,50	1.36	9 (18%)	67,82,82	1.09	4 (5%)
3	KSY	J	201	-	24,24,24	1.70	5 (20%)	33,33,33	1.74	4 (12%)
3	KSY	C	201	-	24,24,24	1.69	6 (25%)	33,33,33	1.39	5 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PG4	F	204	-	-	0/7/7/10	-
5	PG4	F	205	-	-	2/6/6/10	-
5	PG4	B	204	-	-	1/5/5/10	-
5	PG4	C	203	-	-	7/10/10/10	-
5	PG4	G	203	-	-	1/7/7/10	-
5	PG4	D	204	-	-	2/10/10/10	-
3	KSY	G	201	-	-	0/7/19/19	0/3/3/3
3	KSY	I	201	-	-	0/7/19/19	0/3/3/3
4	HEM	A	204	1	-	4/14/54/54	-
5	PG4	E	202	-	-	1/10/10/10	-
5	PG4	I	204	-	-	0/5/5/10	-
5	PG4	D	206	-	-	0/5/5/10	-
5	PG4	K	204	-	-	3/5/5/10	-
4	HEM	C	202	1	-	4/14/54/54	-
5	PG4	J	203	-	-	0/10/10/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PG4	L	203	-	-	3/10/10/10	-
4	HEM	L	202	1	-	4/14/54/54	-
3	KSY	F	201	-	-	0/7/19/19	0/3/3/3
5	PG4	F	203	-	-	5/10/10/10	-
5	PG4	D	205	-	-	0/7/7/10	-
5	PG4	E	204	-	-	0/5/5/10	-
3	KSY	L	201	-	-	0/3/15/19	0/2/2/3
5	PG4	A	205	-	-	1/10/10/10	-
5	PG4	K	202	-	-	2/5/5/10	-
3	KSY	A	203	-	-	0/7/19/19	0/3/3/3
3	KSY	K	201	-	-	0/4/16/19	0/2/2/3
4	HEM	B	203	1	-	4/14/54/54	-
3	KSY	B	202	-	-	2/7/19/19	0/3/3/3
5	PG4	I	203	-	-	0/5/5/10	-
5	PG4	I	202	-	-	4/7/7/10	-
5	PG4	E	203	-	-	0/7/7/10	-
5	PG4	C	204	-	-	0/5/5/10	-
5	PG4	A	206	-	-	4/7/7/10	-
5	PG4	G	202	-	-	3/10/10/10	-
5	PG4	H	203	-	-	0/5/5/10	-
3	KSY	D	202	-	-	3/7/19/19	0/3/3/3
5	PG4	B	205	-	-	0/3/3/10	-
5	PG4	K	203	-	-	4/10/10/10	-
3	KSY	A	202	-	-	3/7/19/19	0/3/3/3
4	HEM	F	202	1	-	4/14/54/54	-
4	HEM	H	202	1	-	4/14/54/54	-
5	PG4	J	202	-	-	2/10/10/10	-
3	KSY	H	201	-	-	4/5/17/19	0/2/2/3
3	KSY	E	201	-	-	2/7/19/19	0/3/3/3
4	HEM	D	203	1	-	4/14/54/54	-
3	KSY	J	201	-	-	0/7/19/19	0/3/3/3
3	KSY	C	201	-	-	2/7/19/19	0/3/3/3

The worst 5 of 121 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	202	KSY	C04-N03	5.02	1.46	1.38
3	A	202	KSY	C21-C02	4.78	1.55	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	201	KSY	C21-C02	4.74	1.55	1.48
3	L	201	KSY	C21-C02	4.69	1.55	1.48
3	I	201	KSY	C21-C02	4.48	1.54	1.48

The worst 5 of 97 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	202	KSY	C04-N03-C02	-8.16	105.49	112.59
3	H	201	KSY	C21-C05-C06	-7.27	118.11	121.88
3	D	202	KSY	C04-N03-C02	-6.97	106.53	112.59
3	L	201	KSY	C04-N03-C02	-5.94	107.43	112.59
3	J	201	KSY	C05-C06-N07	-5.51	114.77	121.34

There are no chirality outliers.

5 of 89 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	201	KSY	C05-C06-N07-C08
3	H	201	KSY	C18-C06-N07-C08
3	H	201	KSY	N07-C08-C09-C10
5	I	202	PG4	O3-C5-C6-O4
5	A	206	PG4	O2-C3-C4-O3

There are no ring outliers.

28 monomers are involved in 45 short contacts:

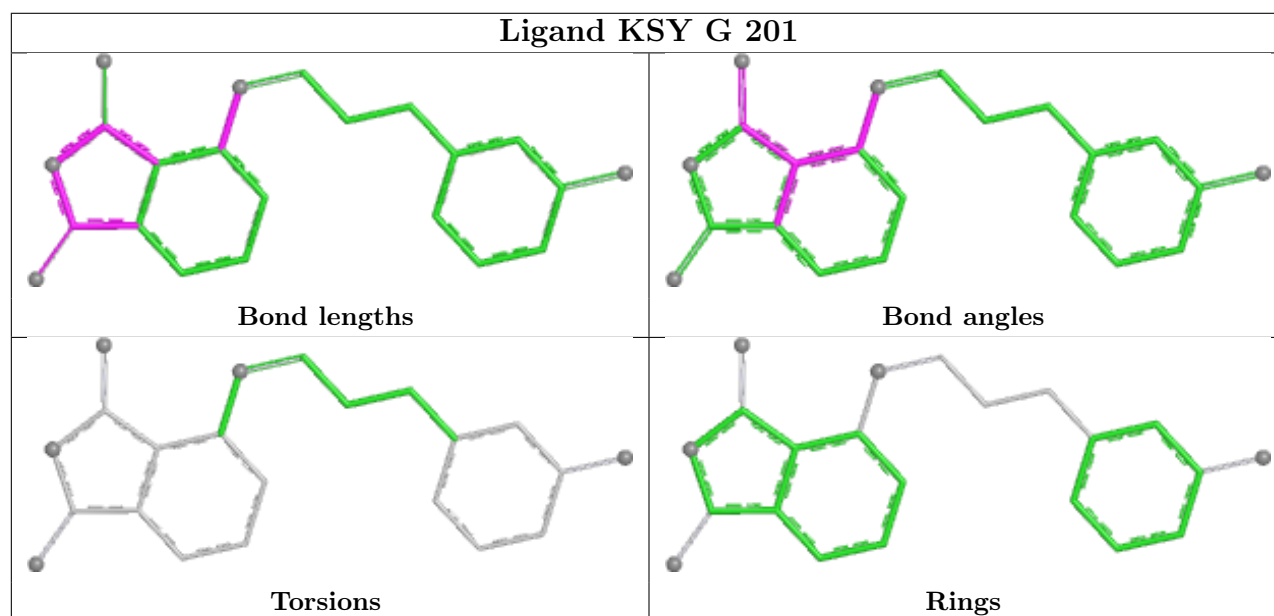
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	205	PG4	1	0
5	C	203	PG4	1	0
5	G	203	PG4	1	0
3	G	201	KSY	1	0
3	I	201	KSY	1	0
4	A	204	HEM	2	0
4	C	202	HEM	5	0
5	L	203	PG4	2	0
4	L	202	HEM	2	0
3	F	201	KSY	1	0
5	F	203	PG4	2	0
3	L	201	KSY	1	0
3	A	203	KSY	1	0
3	K	201	KSY	1	0

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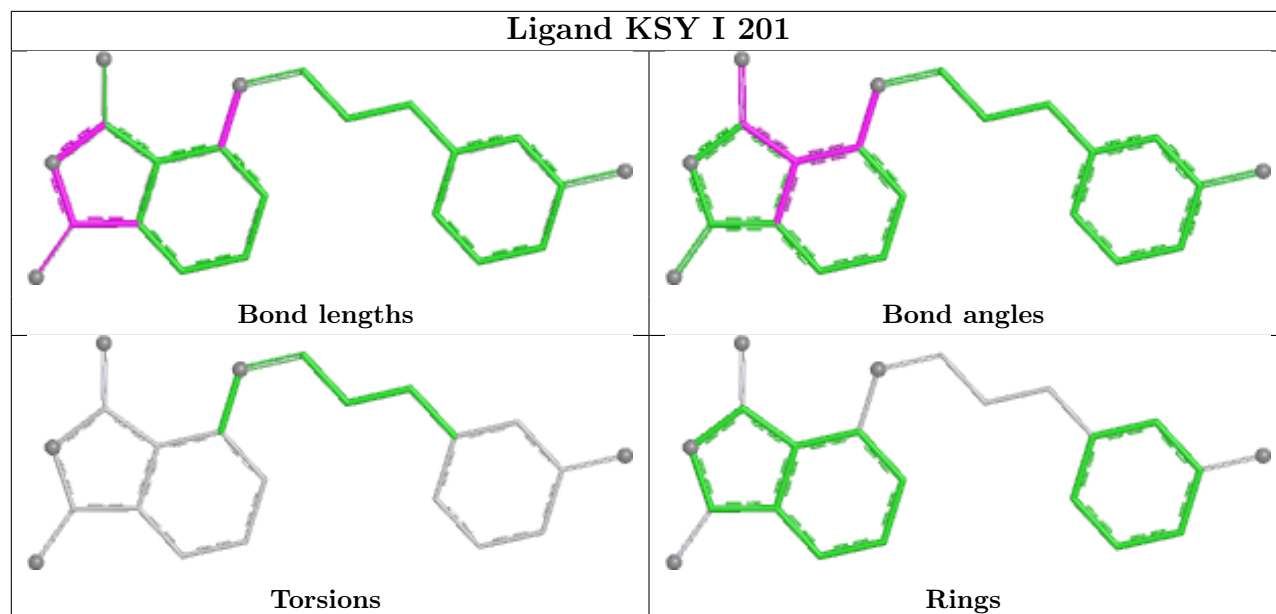
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	203	HEM	4	0
3	B	202	KSY	1	0
5	I	202	PG4	3	0
5	A	206	PG4	1	0
5	G	202	PG4	1	0
3	D	202	KSY	1	0
5	K	203	PG4	1	0
3	A	202	KSY	1	0
4	F	202	HEM	3	0
4	H	202	HEM	3	0
3	H	201	KSY	1	0
3	E	201	KSY	1	0
3	J	201	KSY	1	0
3	C	201	KSY	1	0

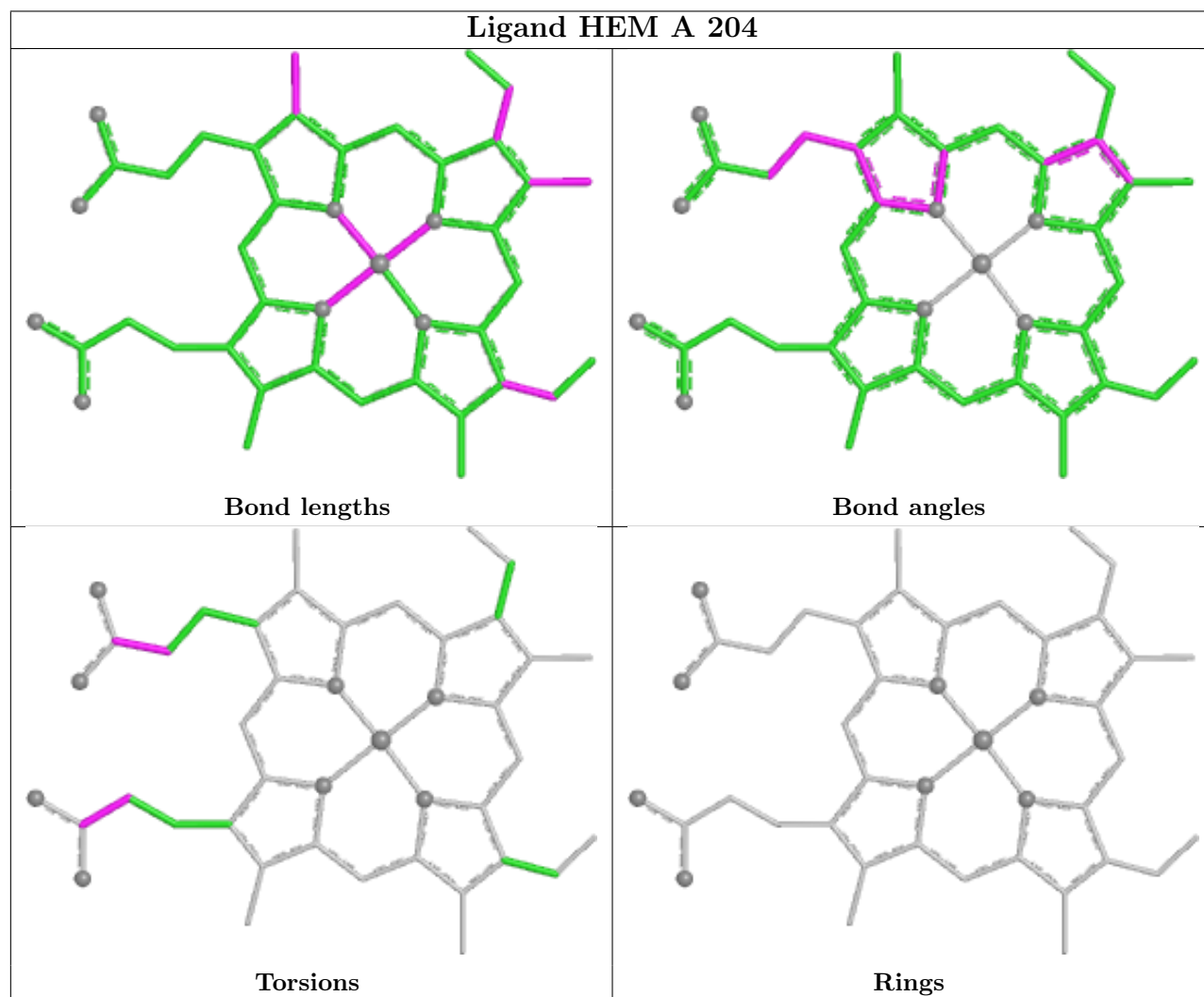
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

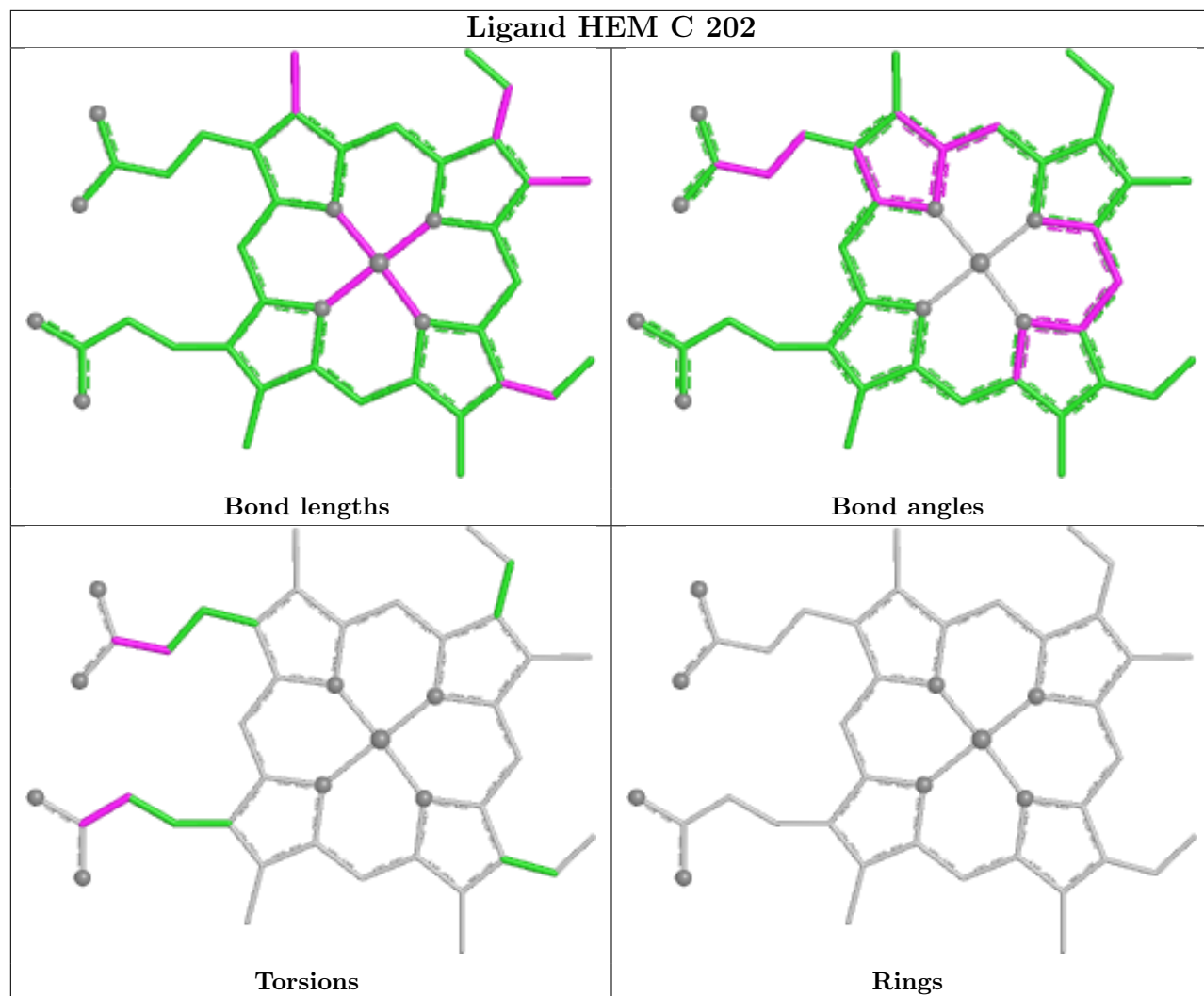


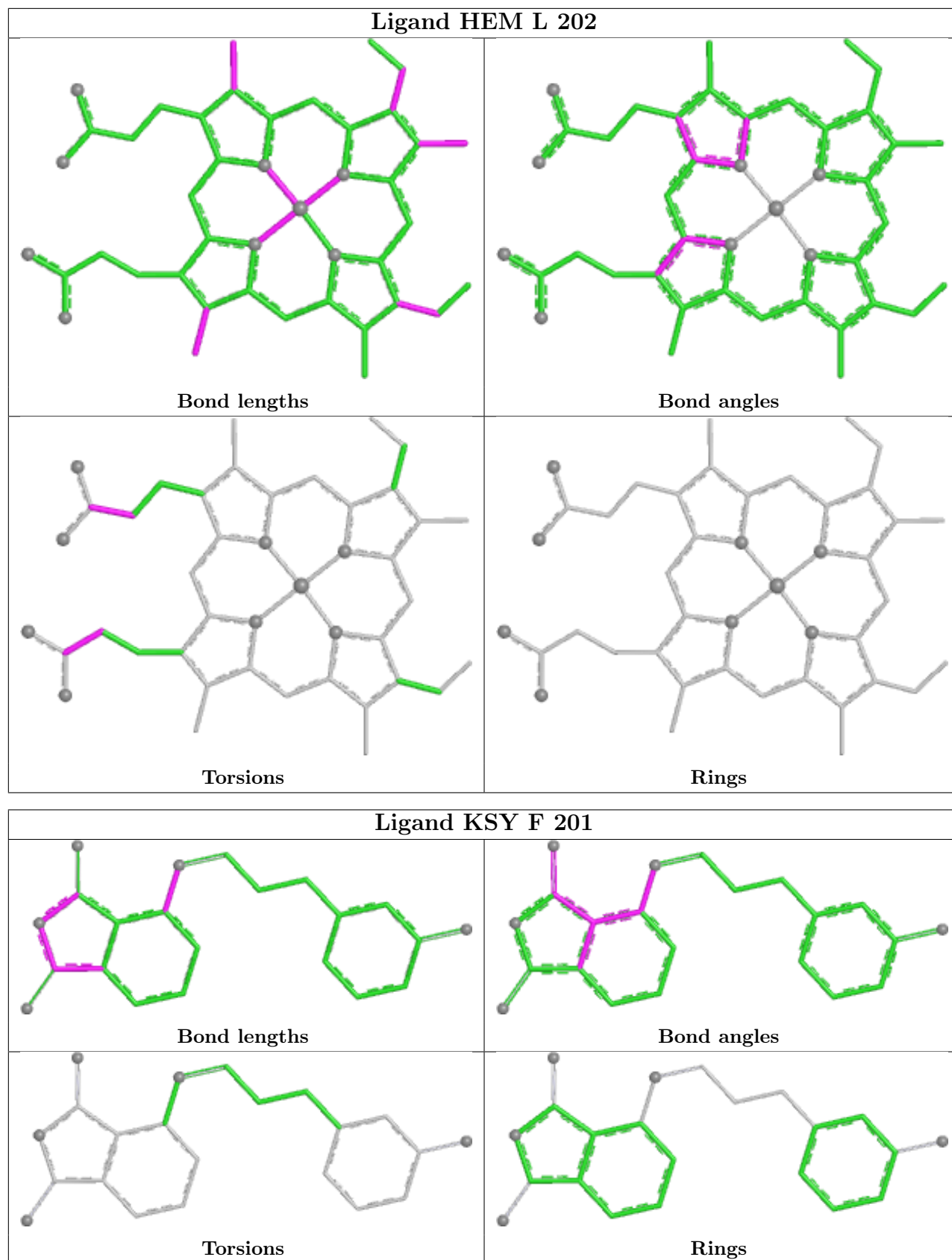
Ligand KSY I 201



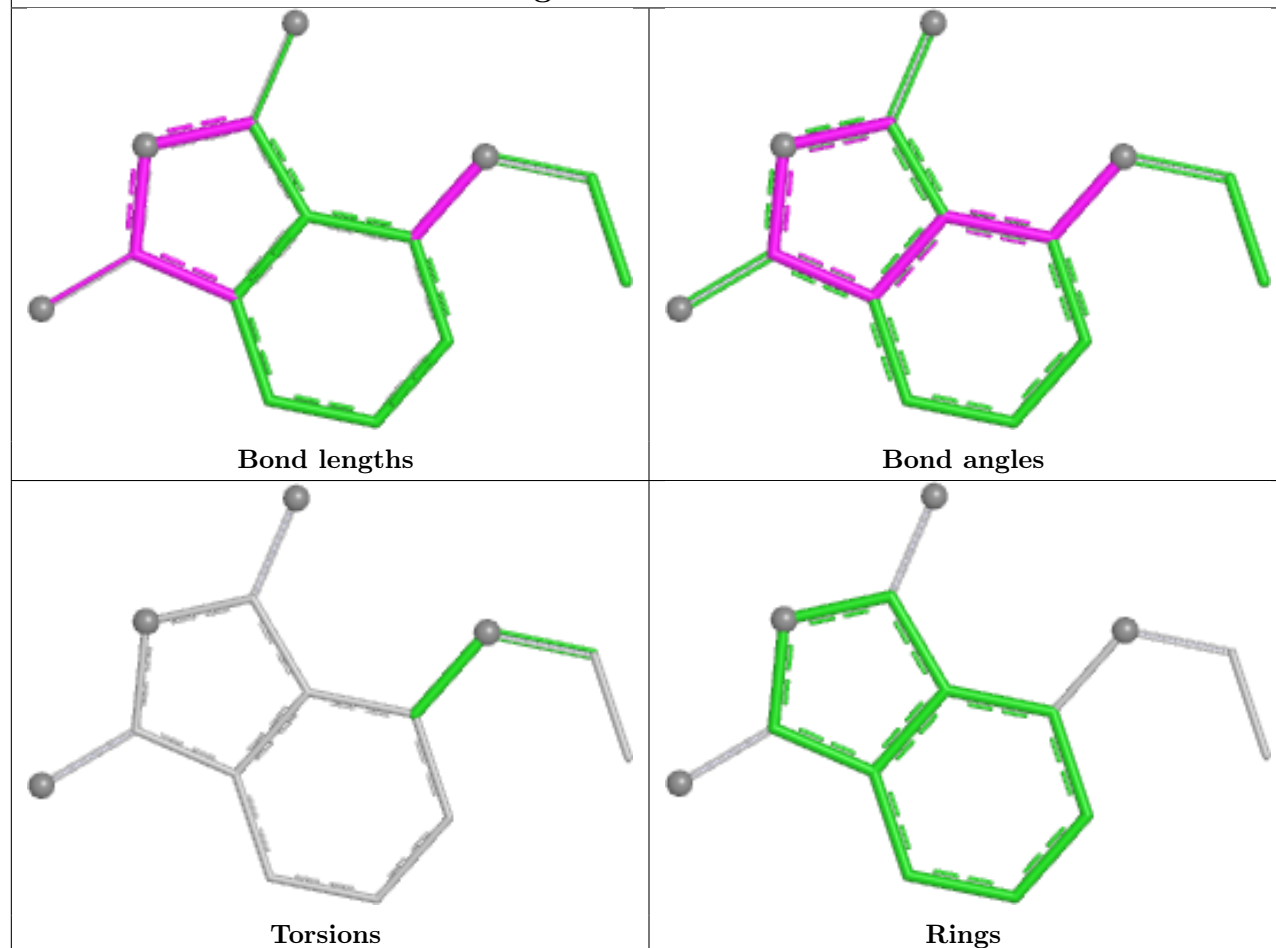
Ligand HEM A 204



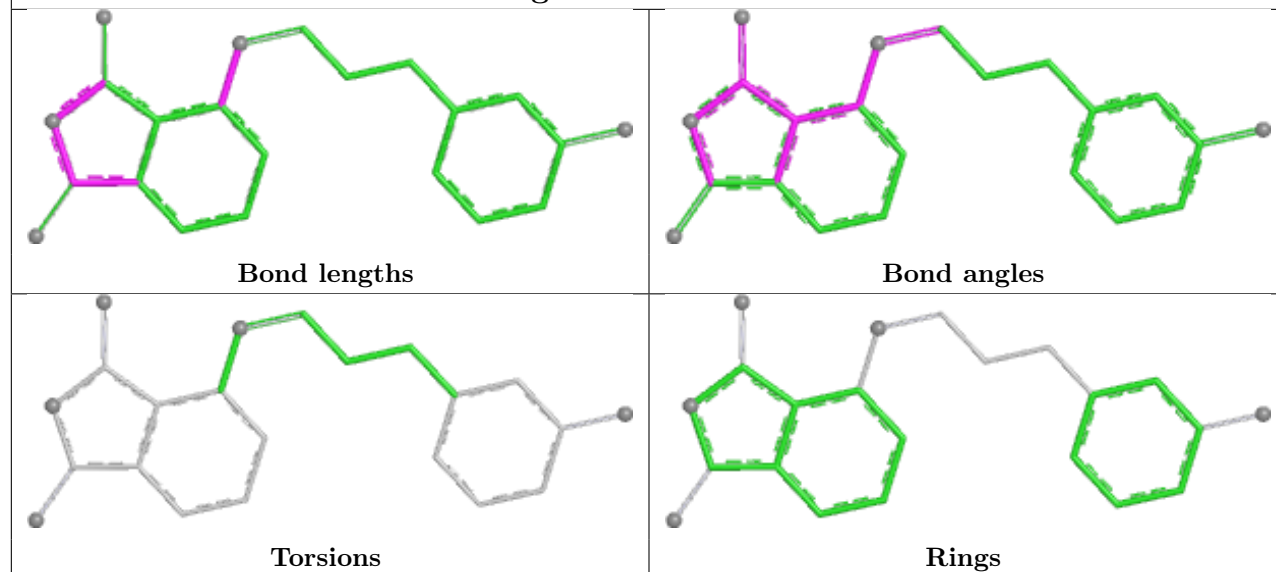


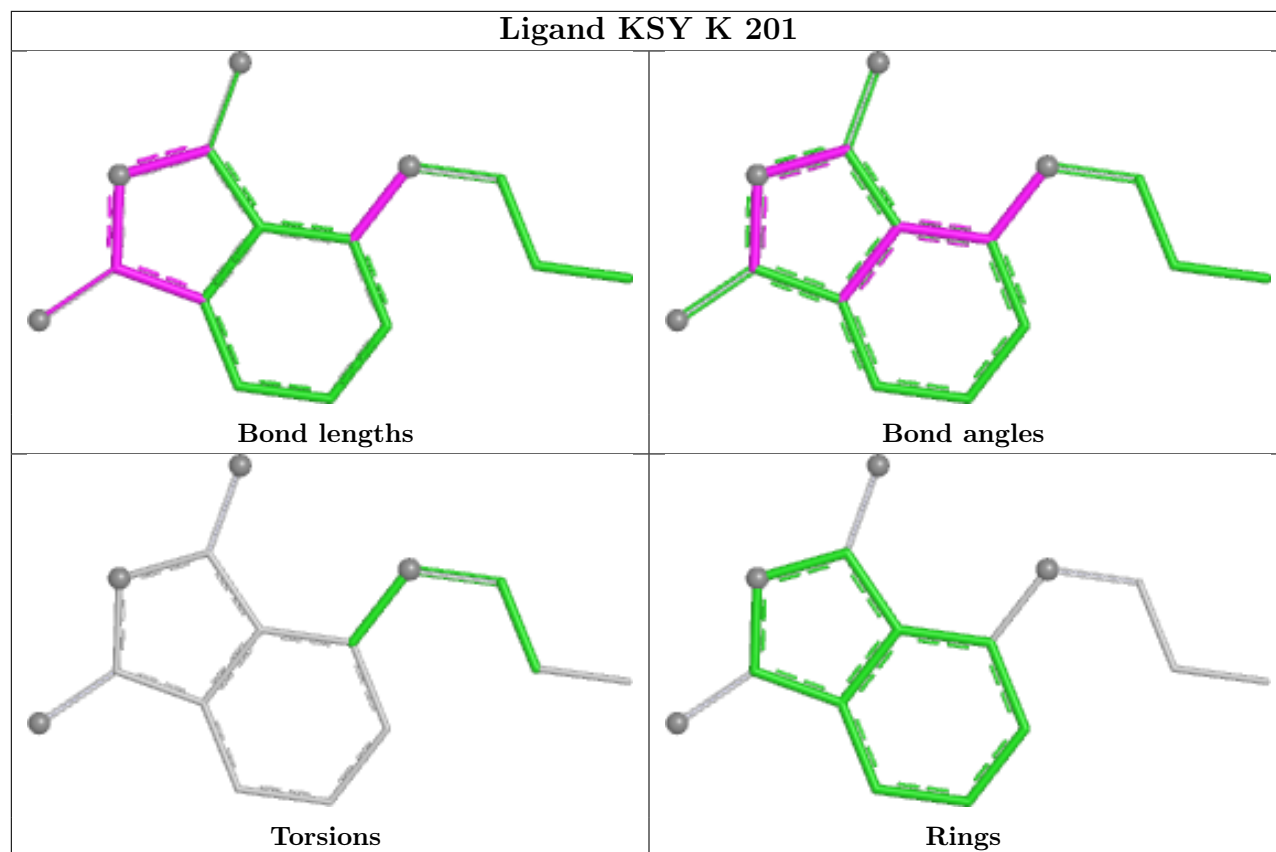


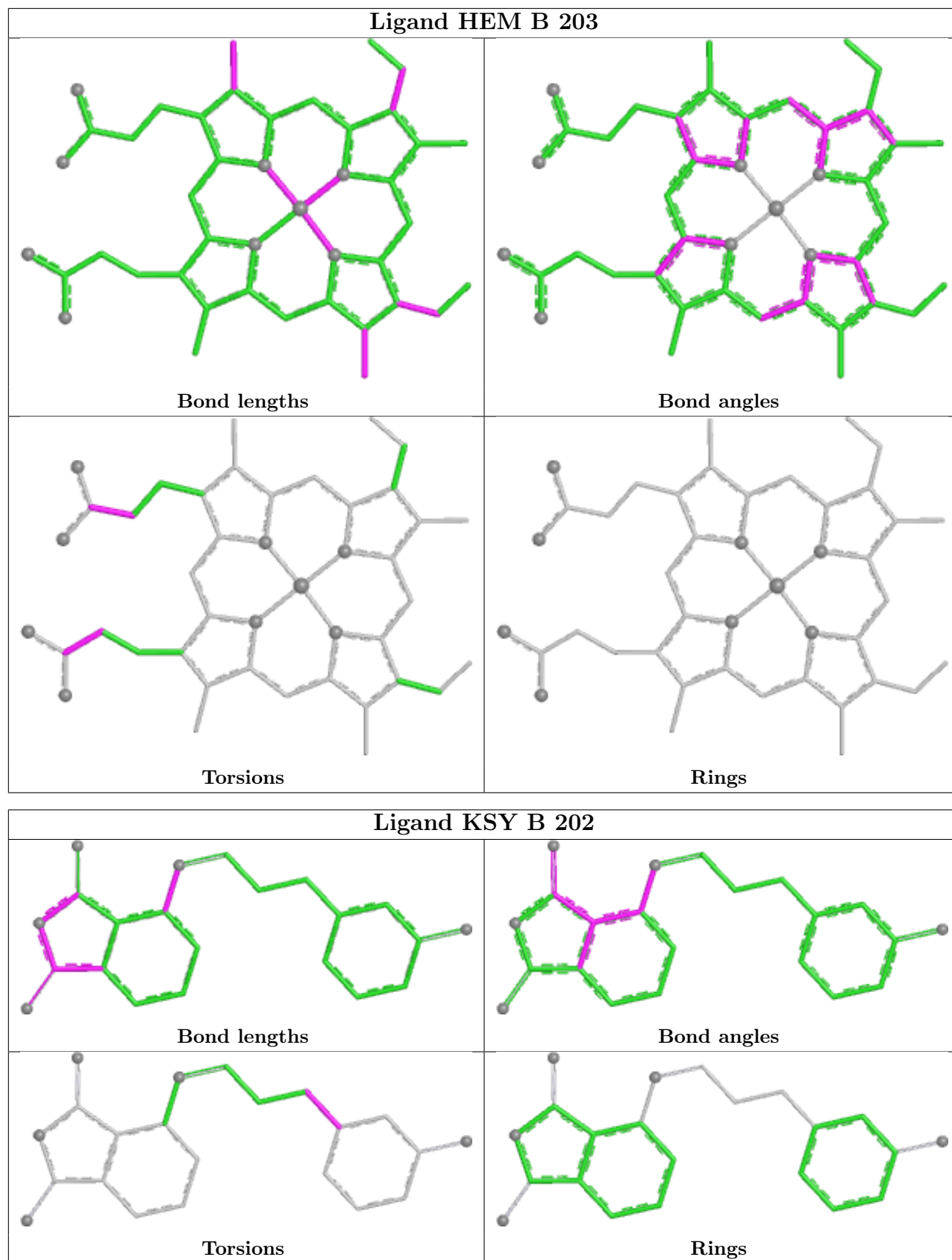
Ligand KSY L 201



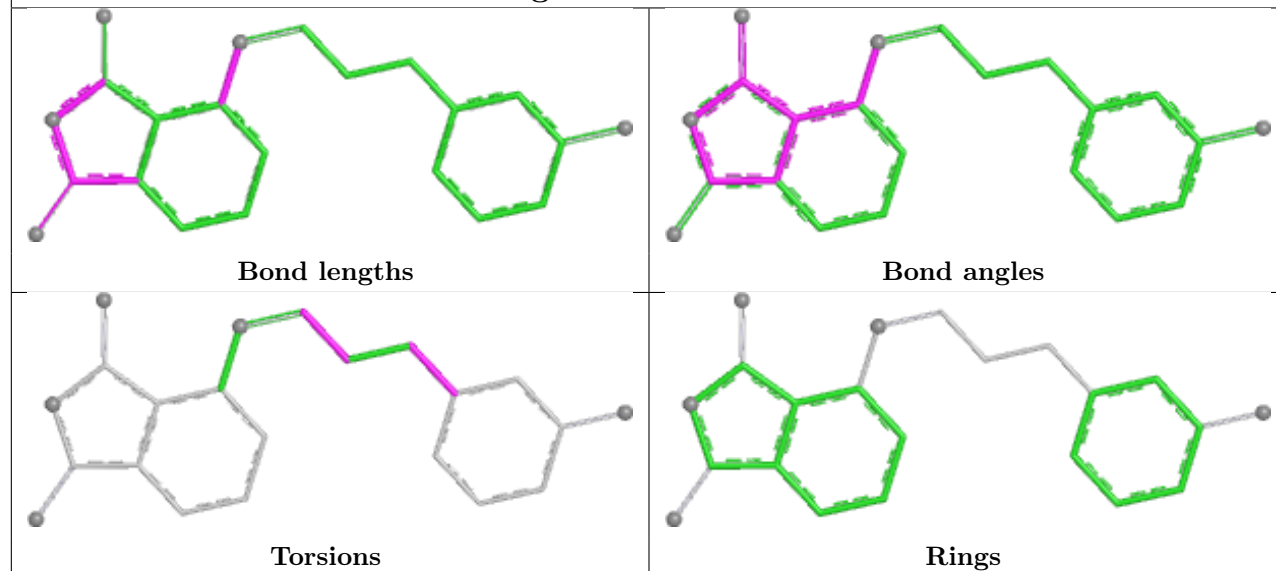
Ligand KSY A 203



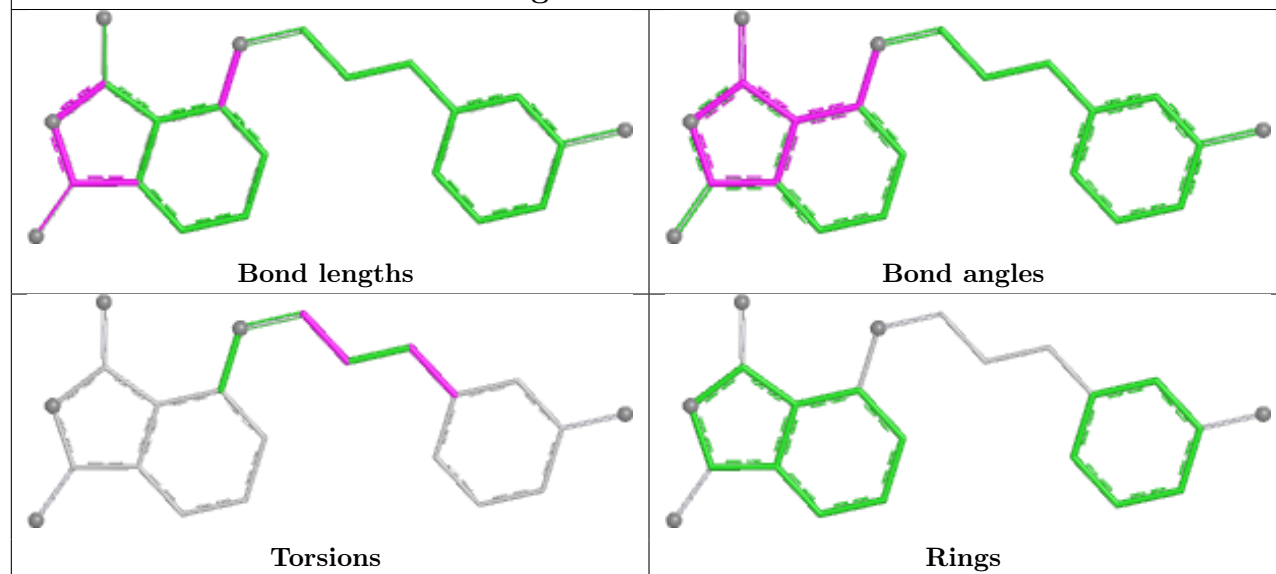


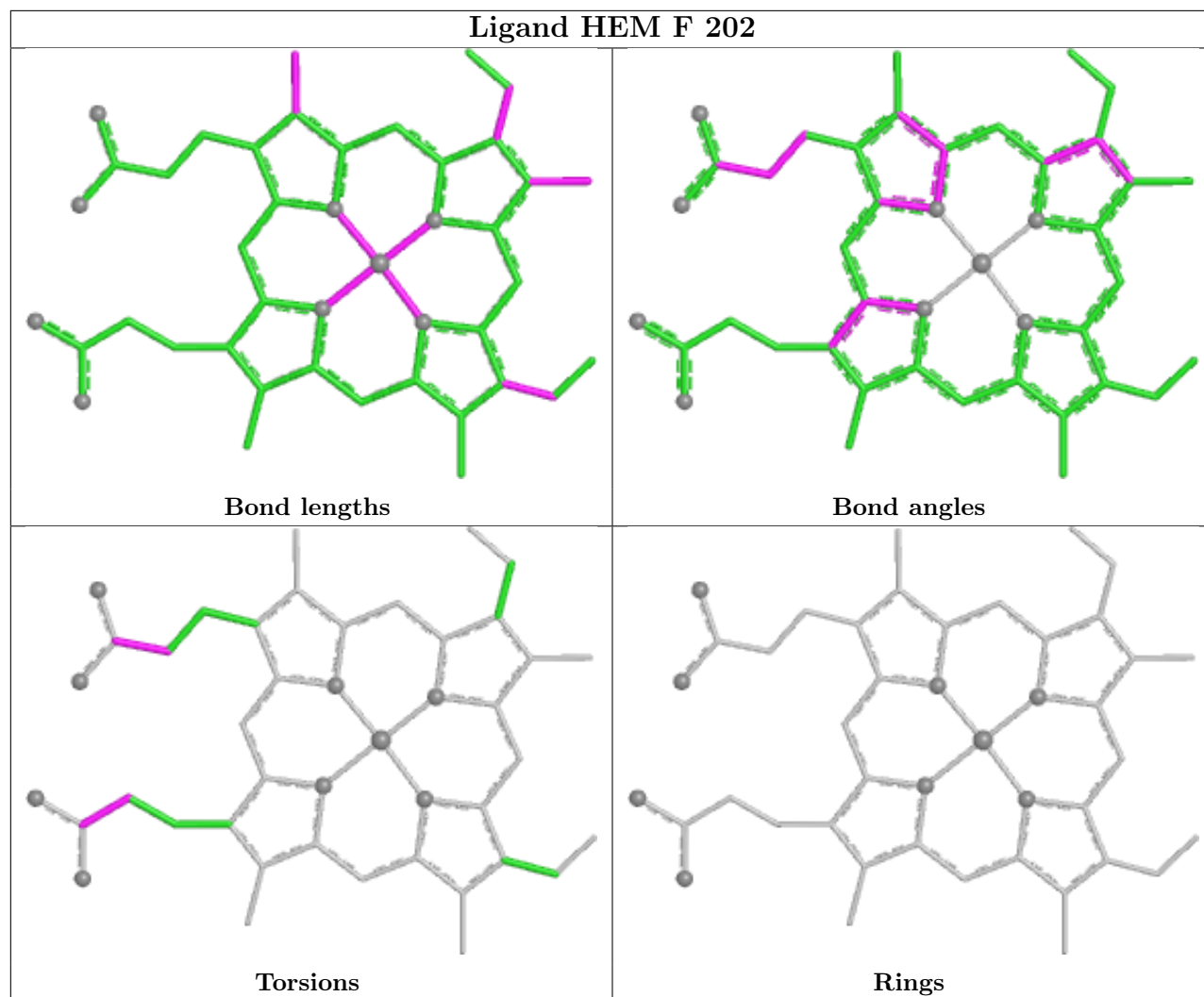


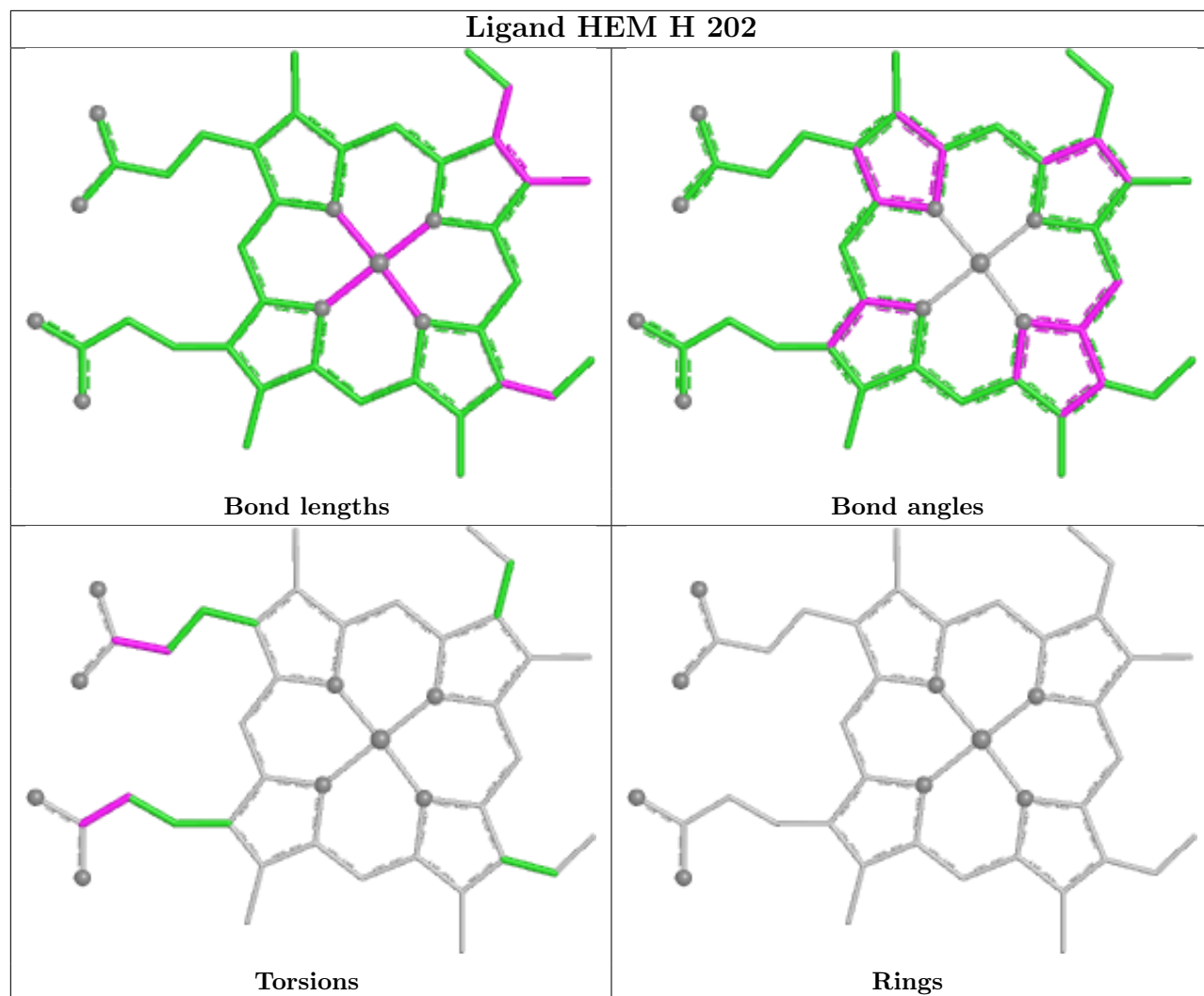
Ligand KSY D 202



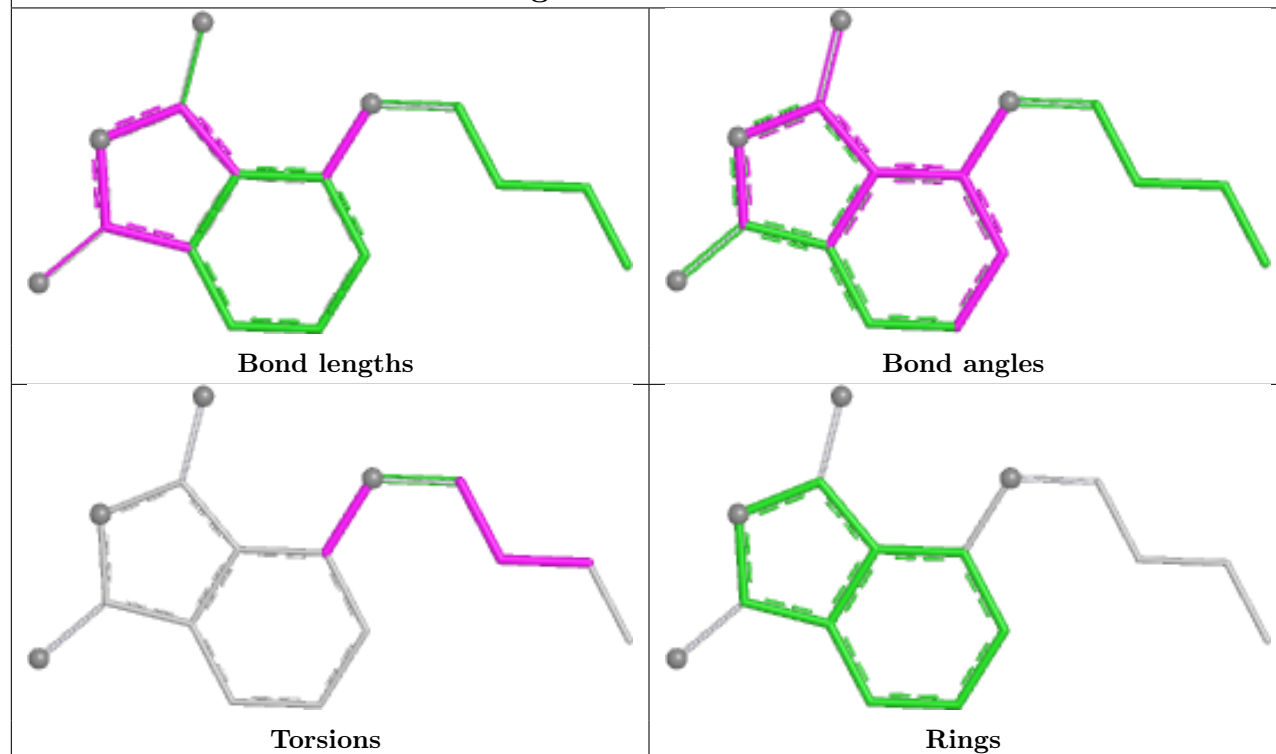
Ligand KSY A 202



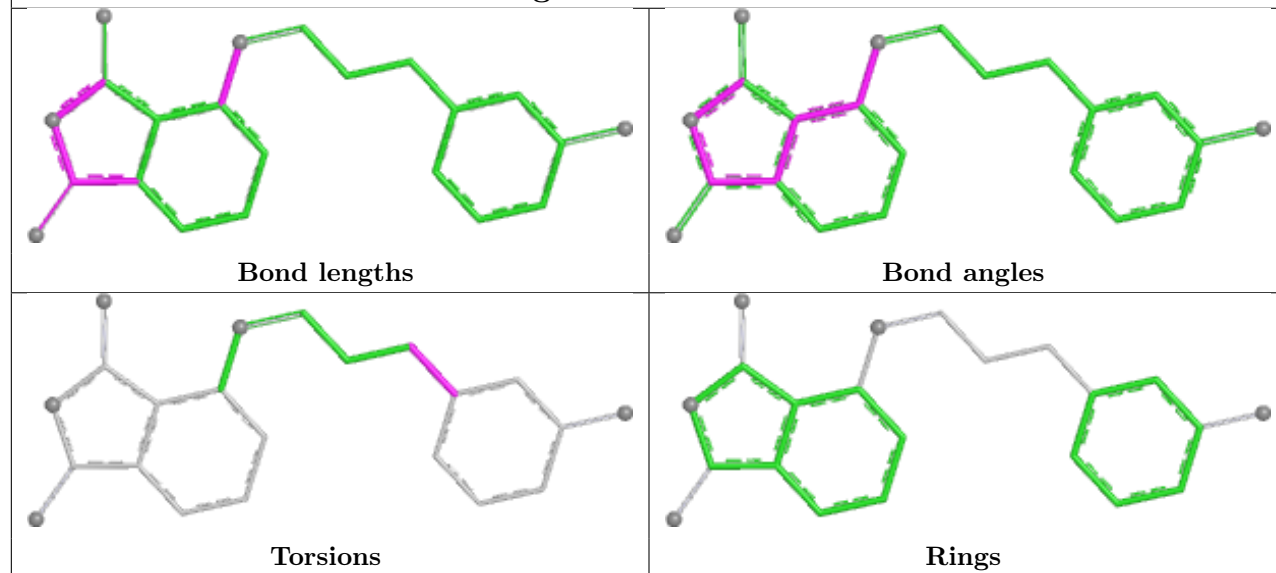




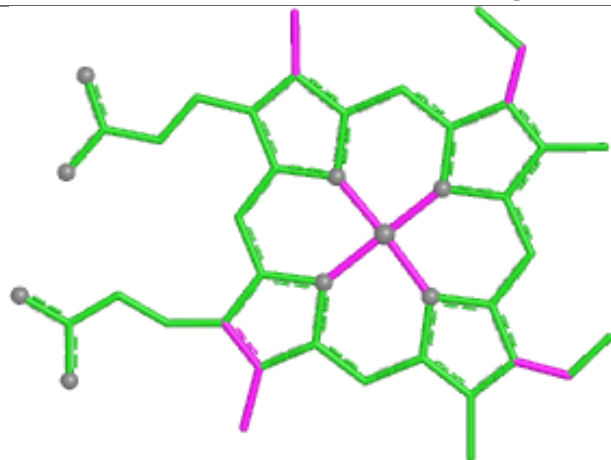
Ligand KSY H 201



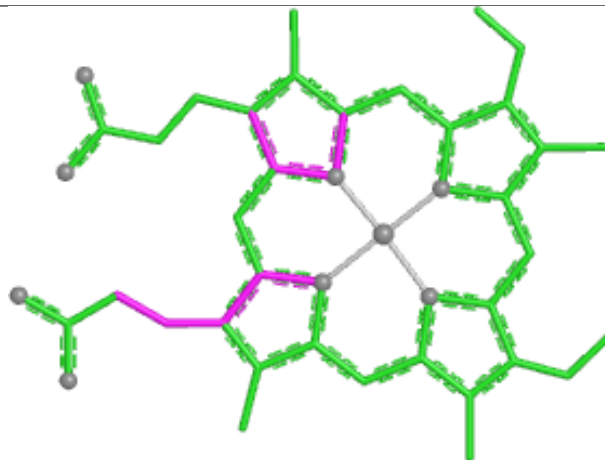
Ligand KSY E 201



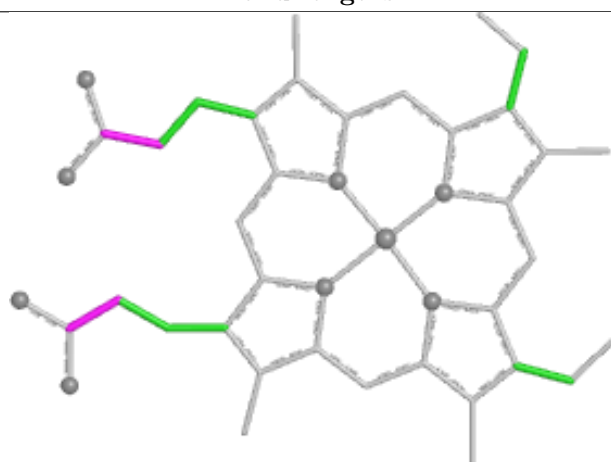
Ligand HEM D 203



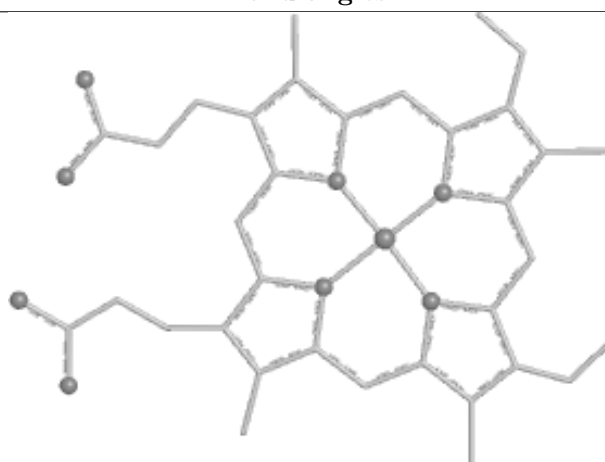
Bond lengths



Bond angles

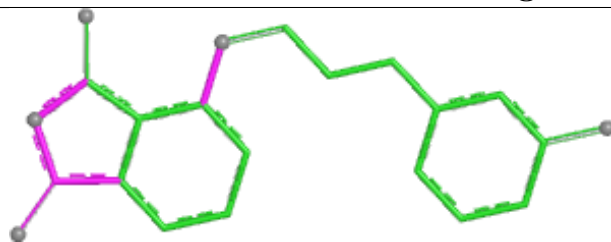


Torsions

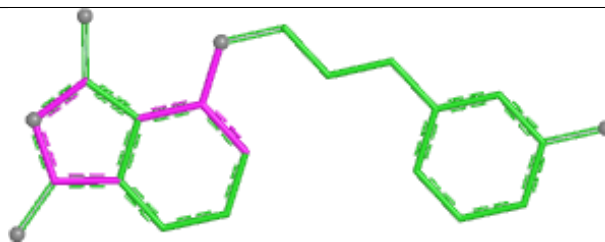


Rings

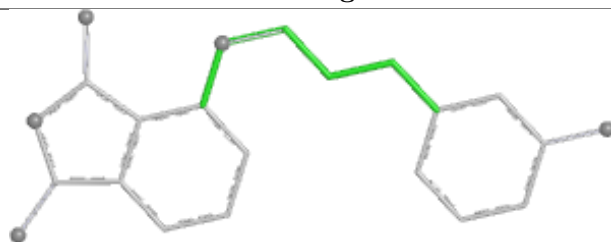
Ligand KSY J 201



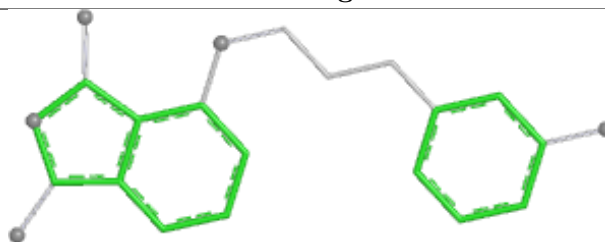
Bond lengths



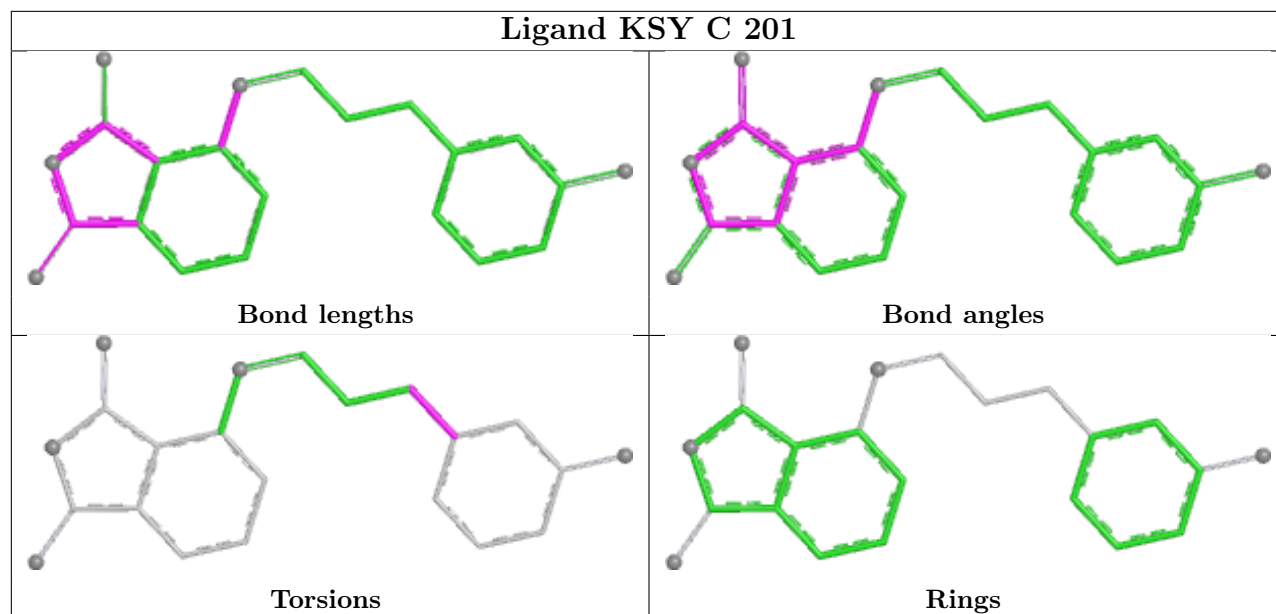
Bond angles



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	156/158 (98%)	-0.32	2 (1%) 75 79	12, 18, 27, 45	1 (0%)
1	B	156/158 (98%)	-0.35	2 (1%) 75 79	12, 18, 27, 47	1 (0%)
1	C	156/158 (98%)	-0.33	2 (1%) 75 79	11, 18, 27, 52	1 (0%)
1	D	156/158 (98%)	-0.36	2 (1%) 75 79	11, 18, 28, 49	1 (0%)
1	E	156/158 (98%)	-0.44	2 (1%) 75 79	10, 16, 25, 45	2 (1%)
1	F	156/158 (98%)	-0.37	2 (1%) 75 79	11, 17, 25, 48	1 (0%)
1	G	156/158 (98%)	-0.32	2 (1%) 75 79	11, 19, 27, 47	1 (0%)
1	H	156/158 (98%)	-0.34	2 (1%) 75 79	11, 18, 27, 43	2 (1%)
1	I	156/158 (98%)	-0.27	1 (0%) 85 88	11, 19, 28, 46	1 (0%)
1	J	156/158 (98%)	-0.32	2 (1%) 75 79	12, 18, 27, 46	1 (0%)
1	K	156/158 (98%)	-0.31	2 (1%) 75 79	11, 18, 27, 47	1 (0%)
1	L	156/158 (98%)	-0.28	2 (1%) 75 79	12, 19, 28, 47	1 (0%)
All	All	1872/1896 (98%)	-0.33	23 (1%) 76 80	10, 18, 27, 52	14 (0%)

The worst 5 of 23 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	155	HIS	3.5
1	K	155	HIS	3.3
1	K	156	GLU	3.2
1	G	155	HIS	3.0
1	E	155	HIS	2.8

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

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

6.3 Carbohydrates ⓘ

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
5	PG4	K	204	8/13	0.67	0.22	33,43,46,47	0
5	PG4	I	204	8/13	0.72	0.21	35,41,45,48	0
5	PG4	I	203	8/13	0.74	0.19	32,38,44,45	0
5	PG4	B	204	8/13	0.75	0.20	33,38,41,43	0
5	PG4	K	203	13/13	0.76	0.19	27,36,46,48	0
5	PG4	D	206	8/13	0.76	0.19	36,43,48,48	0
5	PG4	E	204	8/13	0.77	0.17	32,39,42,43	0
5	PG4	G	203	10/13	0.77	0.19	31,41,47,55	0
5	PG4	H	203	8/13	0.77	0.18	36,38,43,45	0
5	PG4	C	203	13/13	0.77	0.20	24,39,46,48	0
5	PG4	D	205	10/13	0.77	0.17	32,36,48,48	0
3	KSY	G	201	22/22	0.77	0.17	26,35,47,49	0
5	PG4	E	203	10/13	0.77	0.18	32,37,44,49	0
5	PG4	B	205	6/13	0.78	0.18	30,40,41,42	0
5	PG4	A	206	10/13	0.79	0.18	38,41,51,54	0
5	PG4	G	202	13/13	0.79	0.18	29,37,41,44	0
5	PG4	F	204	10/13	0.80	0.17	33,38,41,50	0
5	PG4	D	204	13/13	0.80	0.17	28,40,45,48	0
5	PG4	C	204	8/13	0.81	0.17	32,36,42,47	0
3	KSY	A	203	22/22	0.81	0.16	33,42,48,51	0
3	KSY	H	201	16/22	0.82	0.14	24,30,42,43	0
5	PG4	J	202	13/13	0.82	0.17	26,38,43,46	0
5	PG4	K	202	8/13	0.82	0.16	28,35,40,42	0
5	PG4	F	205	9/13	0.82	0.17	40,44,48,51	0
3	KSY	K	201	15/22	0.82	0.16	26,30,40,43	0
3	KSY	C	201	22/22	0.83	0.17	25,34,55,57	0
5	PG4	I	202	10/13	0.83	0.15	29,39,42,48	0
5	PG4	L	203	13/13	0.83	0.16	32,37,45,46	0
3	KSY	B	202	22/22	0.84	0.17	23,34,52,57	0
3	KSY	E	201	22/22	0.84	0.17	24,33,53,56	0
3	KSY	I	201	22/22	0.84	0.16	26,35,51,57	0
5	PG4	E	202	13/13	0.85	0.14	28,33,41,42	0

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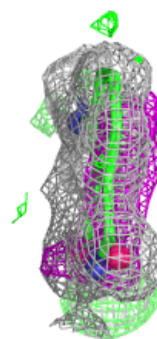
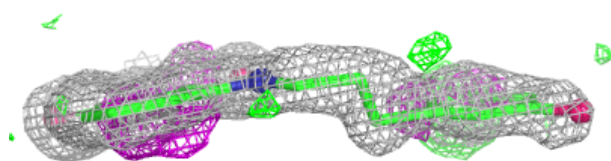
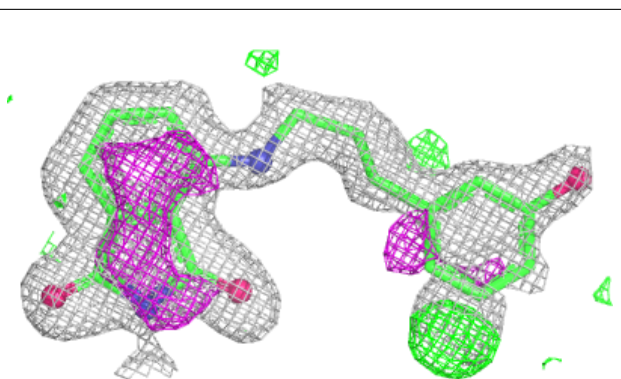
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	PG4	A	205	13/13	0.85	0.15	29,37,47,48	0
5	PG4	F	203	13/13	0.86	0.15	28,38,47,50	0
3	KSY	F	201	22/22	0.86	0.15	23,30,47,50	0
3	KSY	J	201	22/22	0.90	0.14	20,30,49,52	0
3	KSY	L	201	14/22	0.94	0.09	22,27,35,40	0
5	PG4	J	203	13/13	0.94	0.10	23,26,35,37	0
3	KSY	A	202	22/22	0.94	0.10	17,25,38,44	0
3	KSY	D	202	22/22	0.95	0.09	19,22,35,42	0
4	HEM	C	202	43/43	0.97	0.08	15,18,33,34	0
4	HEM	F	202	43/43	0.98	0.08	15,18,32,37	0
4	HEM	H	202	43/43	0.98	0.08	14,18,33,36	0
4	HEM	L	202	43/43	0.98	0.07	16,18,26,31	43
4	HEM	B	203	43/43	0.98	0.07	14,17,31,35	0
4	HEM	A	204	43/43	0.98	0.08	15,18,34,36	0
4	HEM	D	203	43/43	0.98	0.07	13,16,26,29	43
2	FE2	D	201	1/1	1.00	0.01	15,15,15,15	0
2	FE2	A	201	1/1	1.00	0.02	14,14,14,14	0
2	FE2	B	201	1/1	1.00	0.01	15,15,15,15	0

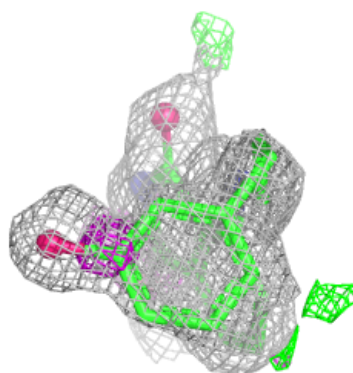
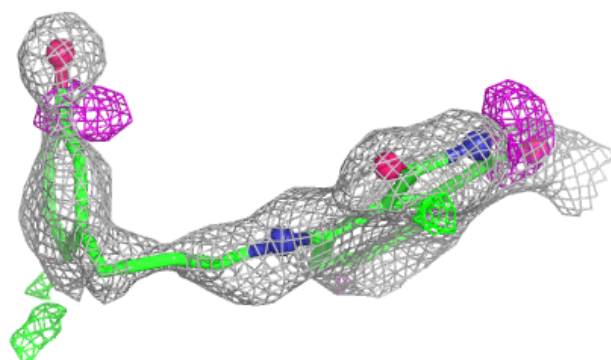
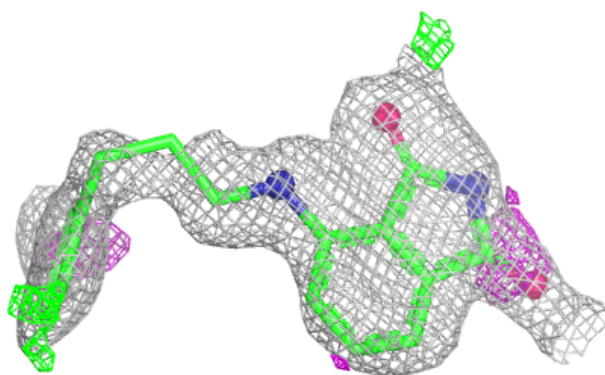
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around KSY G 201:

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

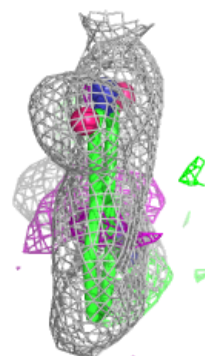
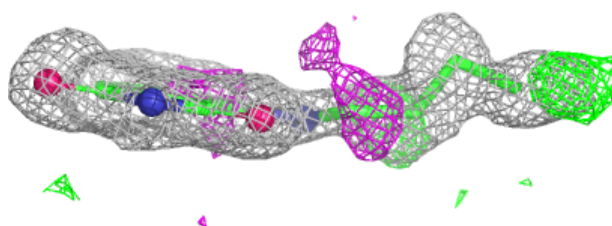
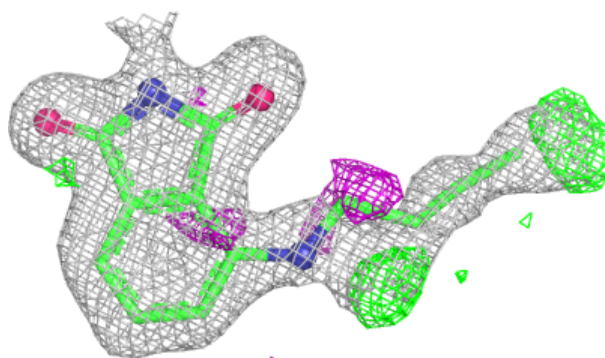
**Electron density around KSY A 203:**

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

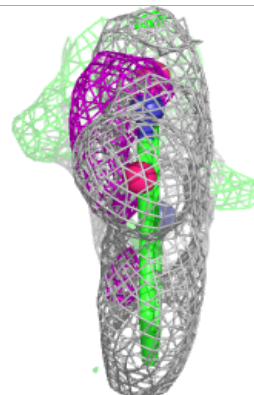
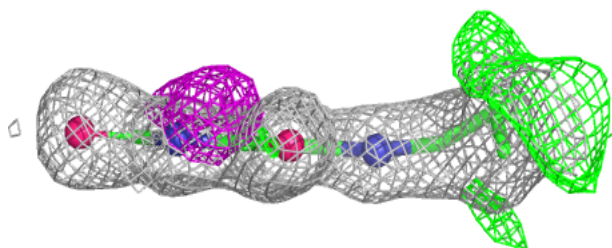
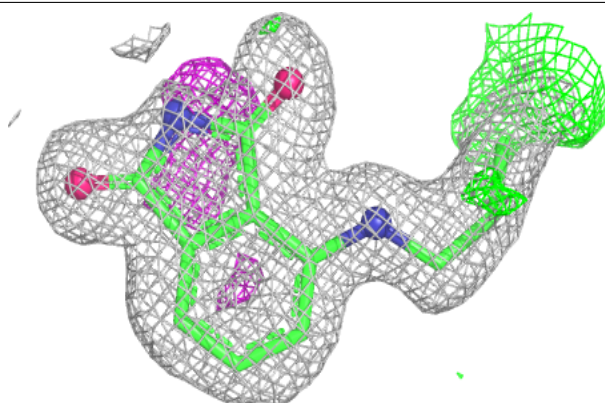


Electron density around KSY H 201:

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

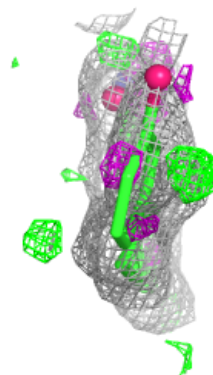
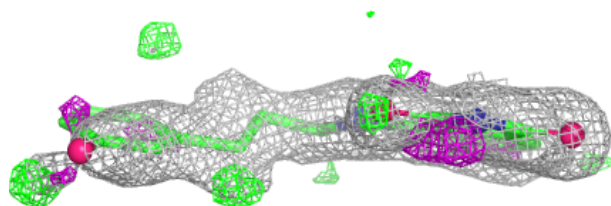
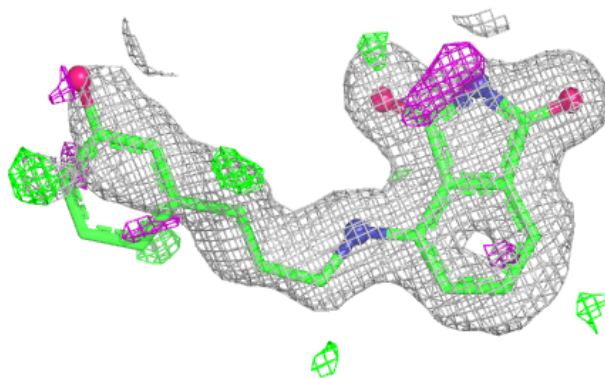
**Electron density around KSY K 201:**

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

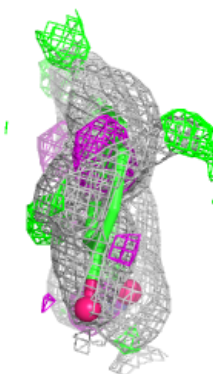
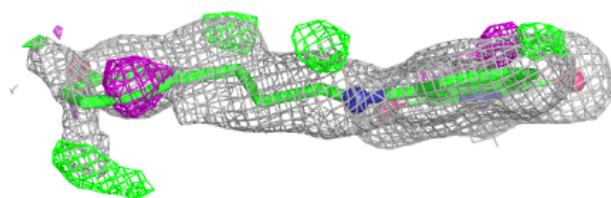
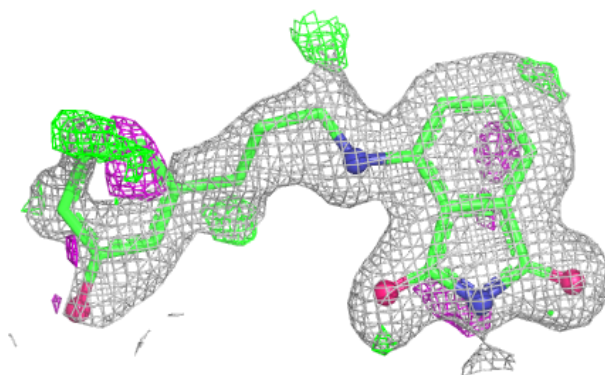


Electron density around KSY C 201:

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

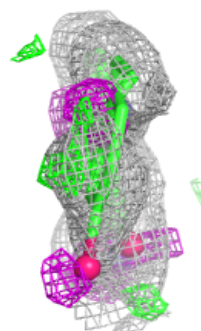
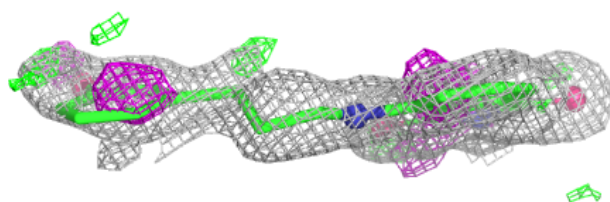
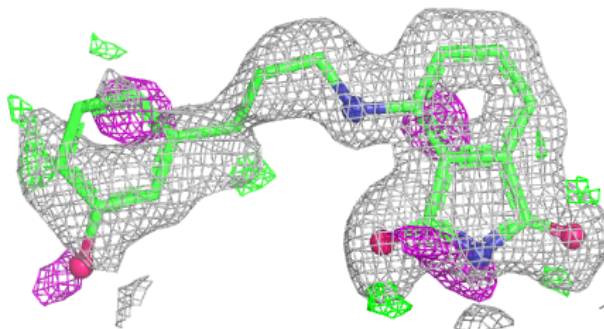
**Electron density around KSY B 202:**

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

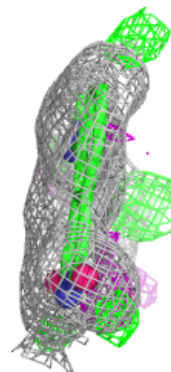
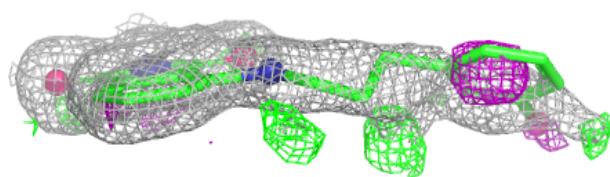
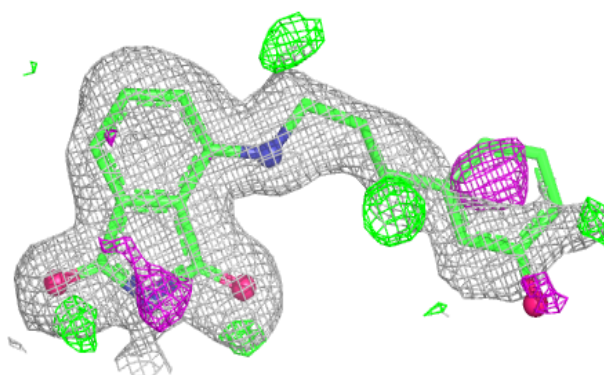


Electron density around KSY E 201:

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

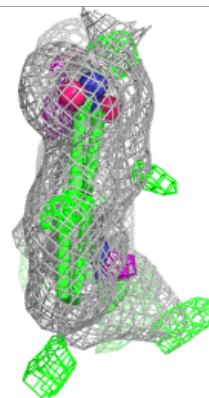
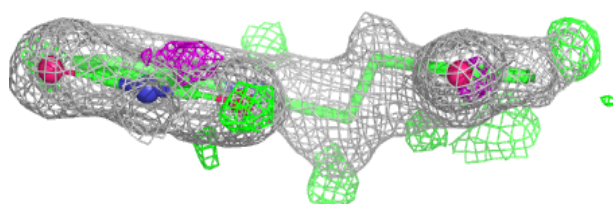
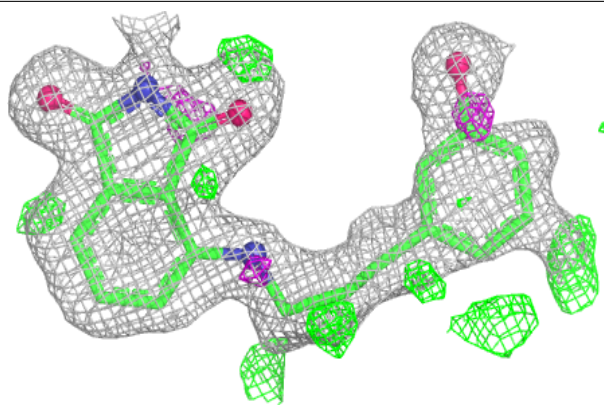
**Electron density around KSY I 201:**

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

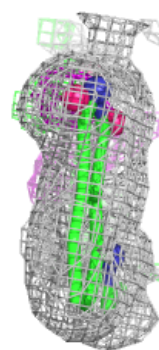
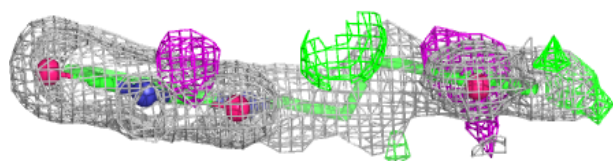
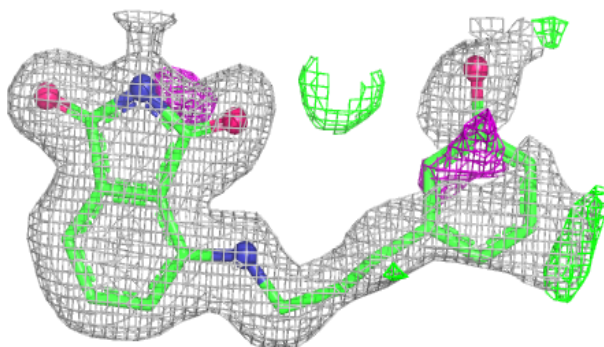


Electron density around KSY F 201:

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

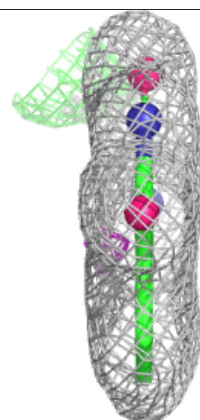
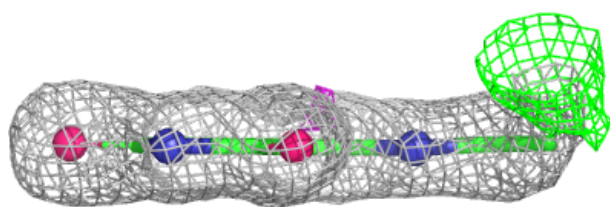
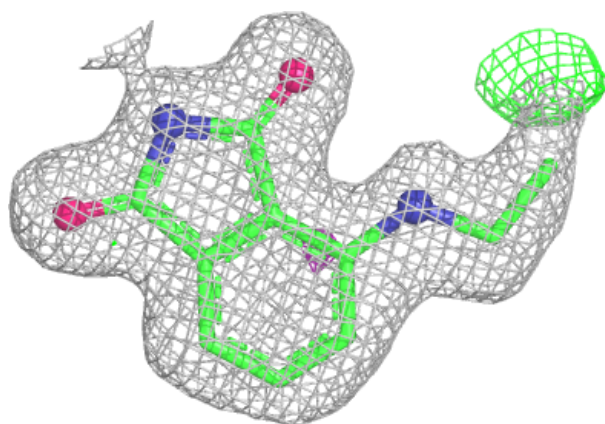
**Electron density around KSY J 201:**

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

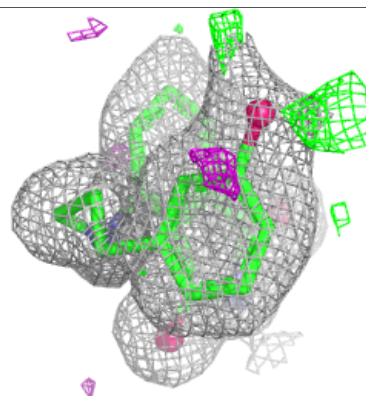
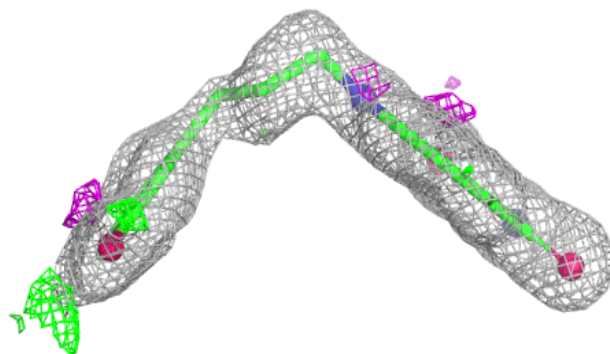
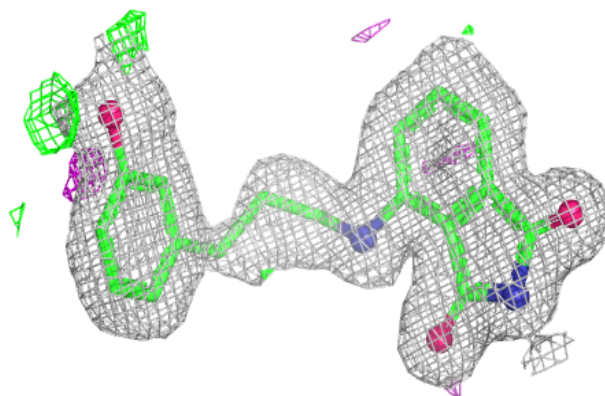


Electron density around KSY L 201:

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

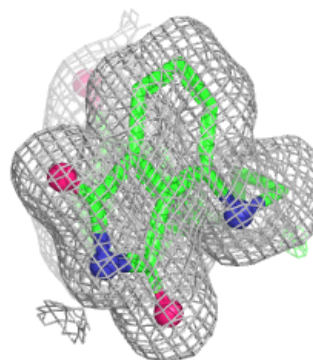
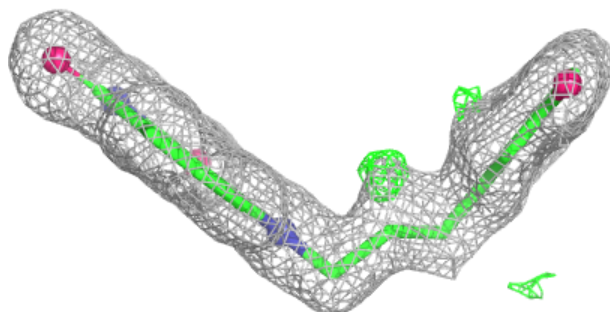
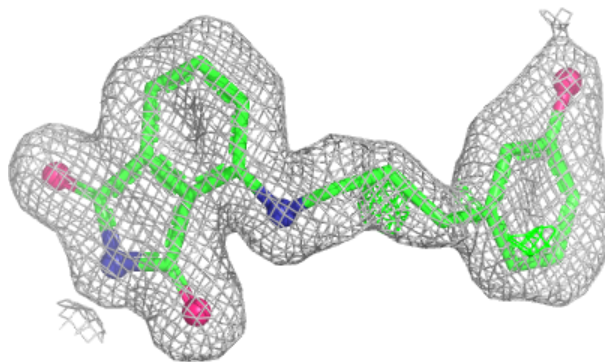
**Electron density around KSY A 202:**

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



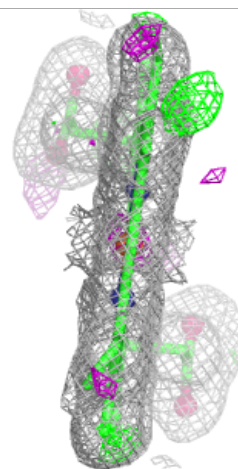
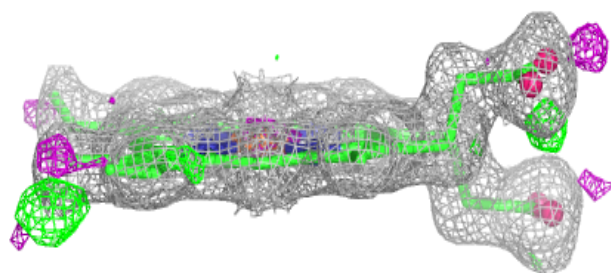
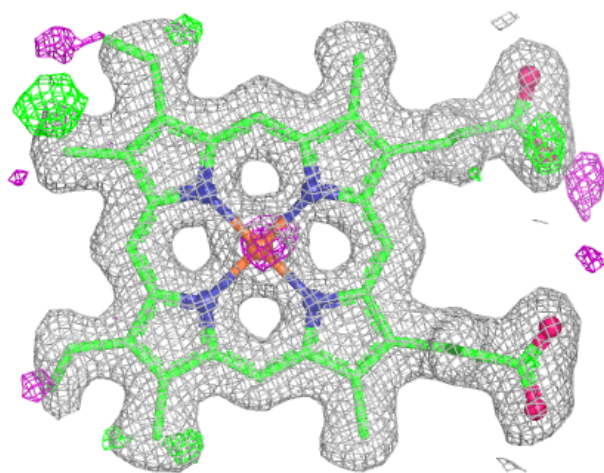
Electron density around KSY D 202:

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



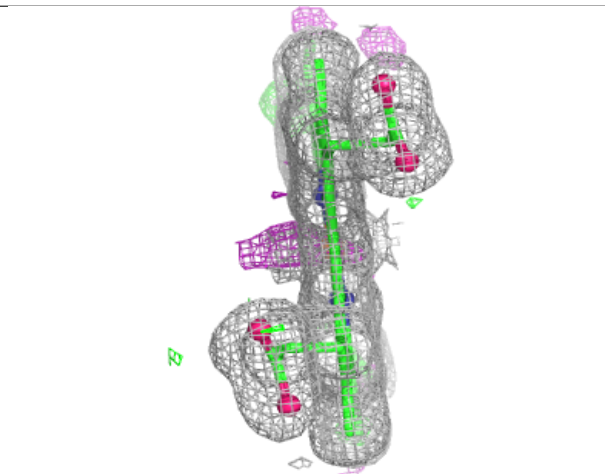
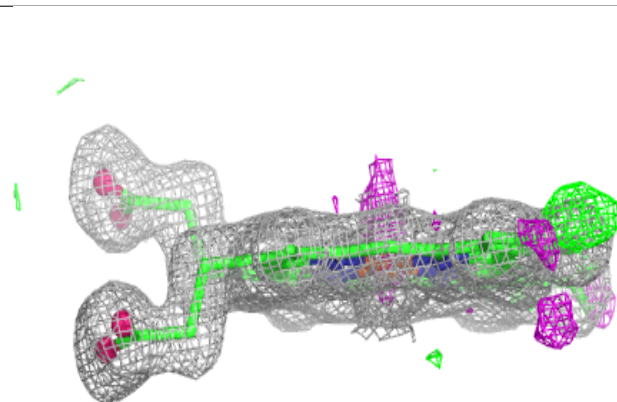
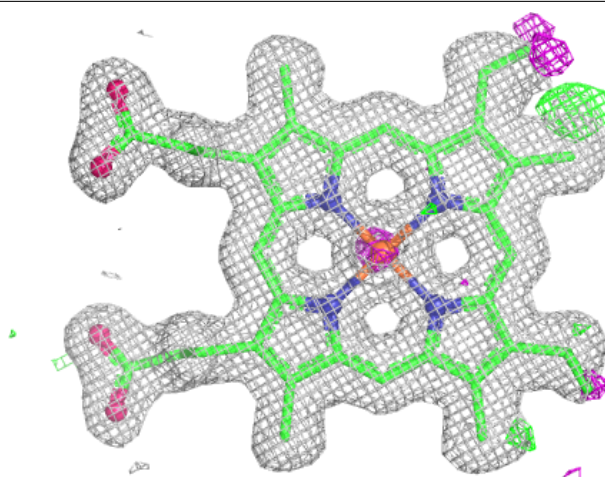
Electron density around HEM C 202:

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



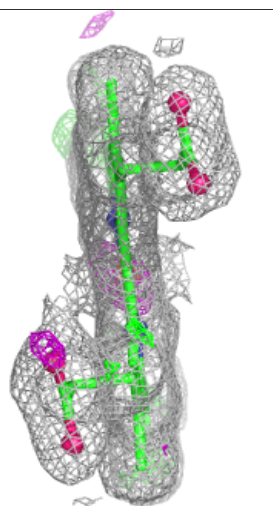
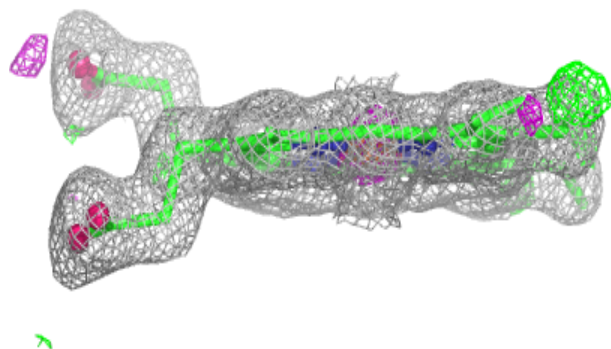
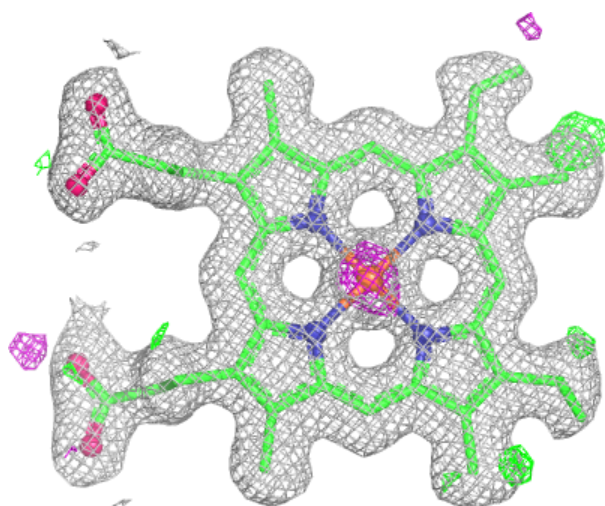
Electron density around HEM F 202:

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



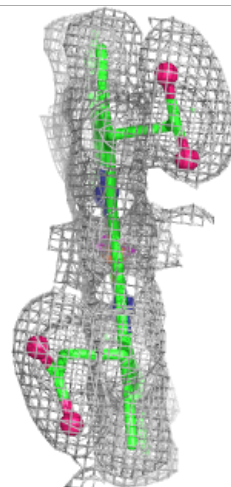
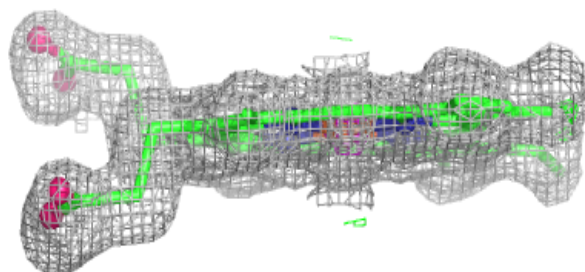
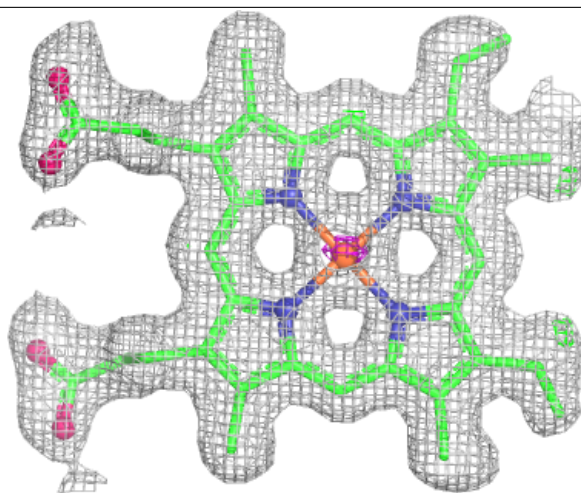
Electron density around HEM H 202:

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



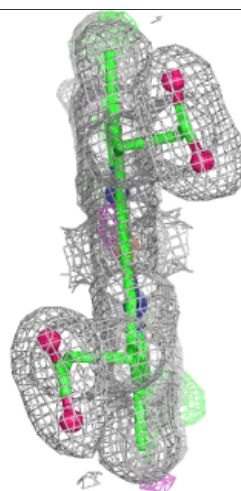
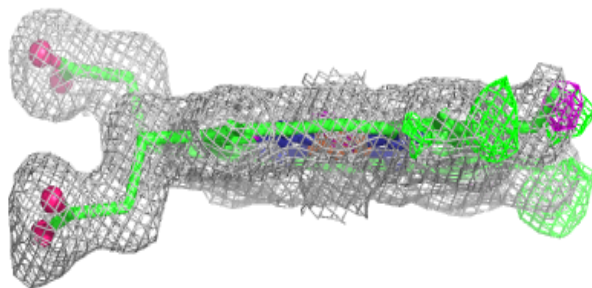
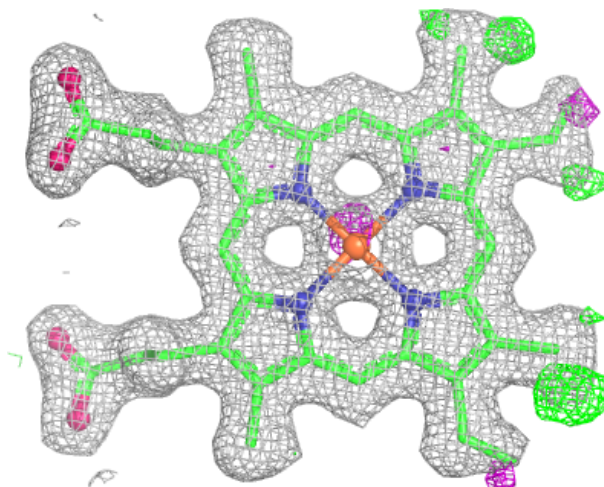
Electron density around HEM L 202:

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



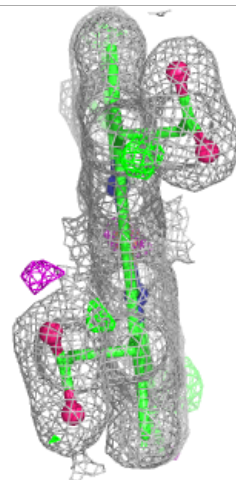
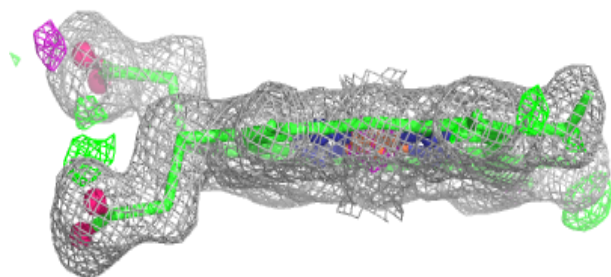
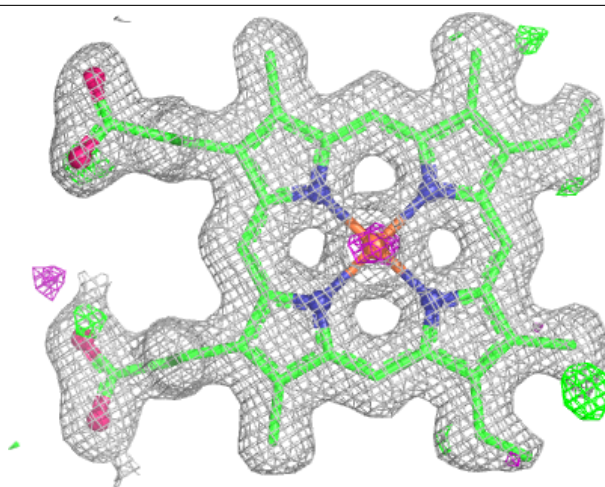
Electron density around HEM B 203:

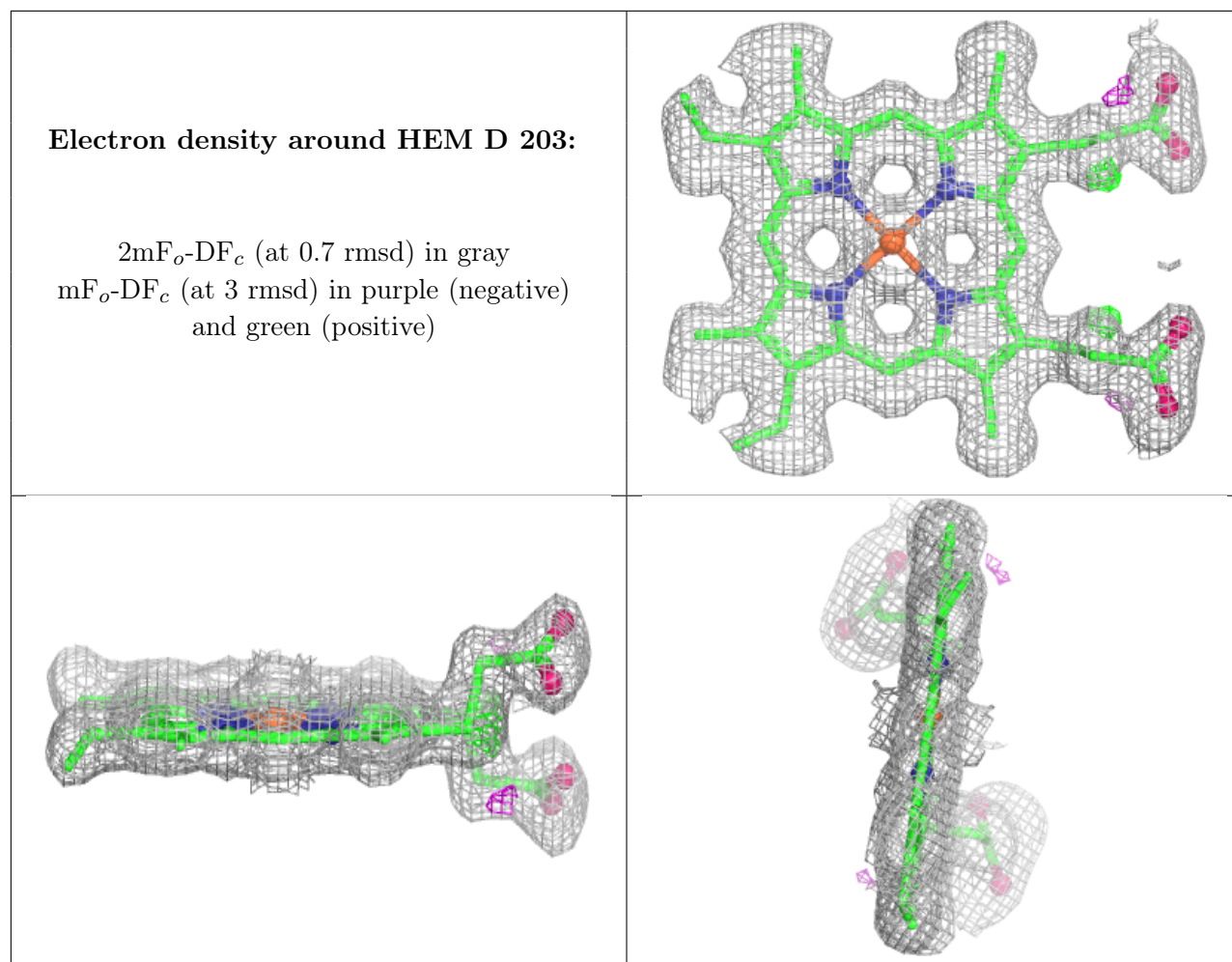
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM A 204:

$2mF_o-DF_c$ (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.