



wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 02:42 am BST

PDB ID : 6NLK
Title : 1.85 Å resolution structure of WT BfrB from *Pseudomonas aeruginosa* in complex with a protein-protein interaction inhibitor (analog 13)
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 : 1.85 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

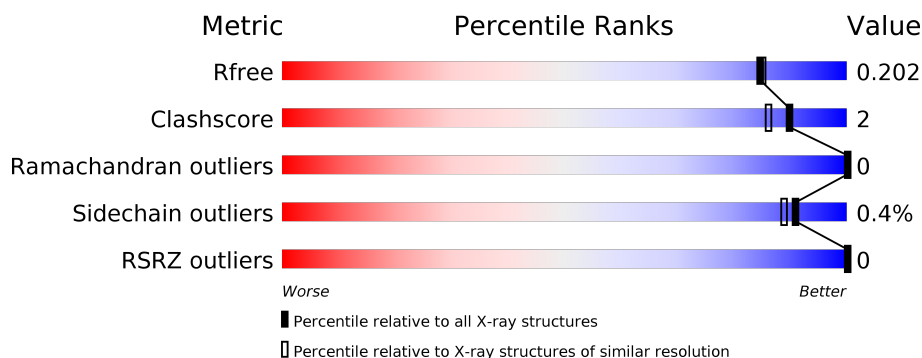
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	<div> <div>93%</div> <div>5% ..</div> </div>
1	B	158	<div> <div>96%</div> <div>..</div> </div>
1	C	158	<div> <div>97%</div> <div>..</div> </div>
1	D	158	<div> <div>97%</div> <div>..</div> </div>
1	E	158	<div> <div>94%</div> <div>5% .</div> </div>
1	F	158	<div> <div>94%</div> <div>5% .</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	158	<div><div></div><div>94%</div><div>5% .</div></div>
1	H	158	<div><div></div><div>96%</div><div>. .</div></div>
1	I	158	<div><div></div><div>96%</div><div>. .</div></div>
1	J	158	<div><div></div><div>96%</div><div>. .</div></div>
1	K	158	<div><div></div><div>92%</div><div>6% .</div></div>
1	L	158	<div><div></div><div>96%</div><div>. .</div></div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17552 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	2	0
			1278	809	218	244	7			
1	B	156	Total	C	N	O	S	0	2	0
			1275	807	217	244	7			
1	C	156	Total	C	N	O	S	0	2	0
			1267	802	216	242	7			
1	D	156	Total	C	N	O	S	0	2	0
			1277	807	217	246	7			
1	E	156	Total	C	N	O	S	0	3	0
			1280	811	218	244	7			
1	F	156	Total	C	N	O	S	0	2	0
			1267	804	216	240	7			
1	G	156	Total	C	N	O	S	0	2	0
			1272	806	216	243	7			
1	H	156	Total	C	N	O	S	0	3	0
			1274	808	217	242	7			
1	I	156	Total	C	N	O	S	0	2	0
			1270	805	215	243	7			
1	J	156	Total	C	N	O	S	0	2	0
			1274	806	217	244	7			
1	K	156	Total	C	N	O	S	0	2	0
			1277	809	218	243	7			
1	L	156	Total	C	N	O	S	0	3	0
			1280	811	218	244	7			

- Molecule 2 is FE (II) ION (three-letter code: FE2) (formula: Fe).

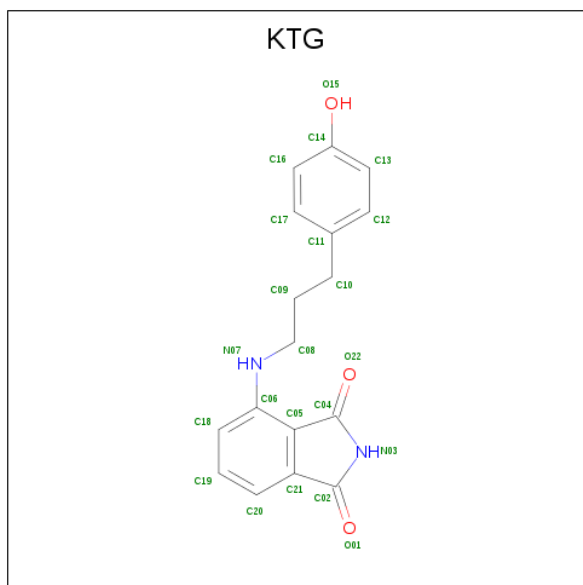
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Fe	0	0
			1	1		
2	A	1	Total	Fe	0	0
			1	1		

Continued on next page...

Continued from previous page...

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

- Molecule 3 is 4-{[3-(4-hydroxyphenyl)propyl]amino}-1H-isoindole-1,3(2H)-dione (three-letter code: KTG) (formula: C₁₇H₁₆N₂O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			13	9	2	2		
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
			13	9	2	2		
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
			15	11	2	2		
3	I	1	Total	C	N	O	0	0
			22	17	2	3		
3	J	1	Total	C	N	O	0	0
			22	17	2	3		

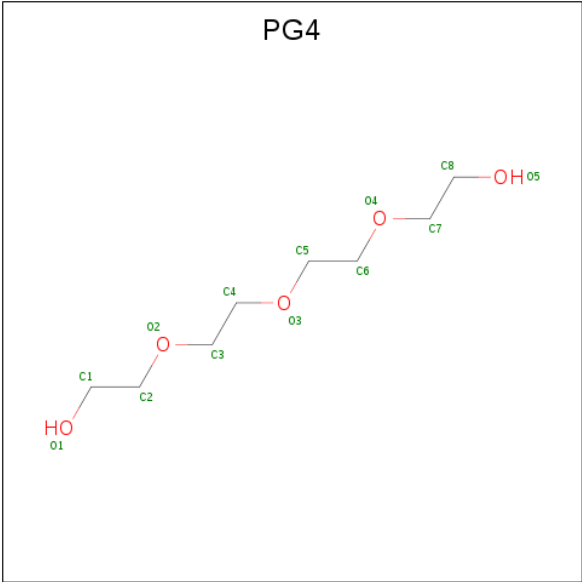
Continued on next page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	K	1	Total 22	C 17	N 2	O 3	0	0
3	L	1	Total 22	C 17	N 2	O 3	0	0

- # HEM

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	H	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	L	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- WORLDWIDE
PDB
PROTEIN DATA BANK



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
			13	8	5		
5	C	1	Total	C	O	0	0
			11	7	4		
5	C	1	Total	C	O	0	0
			10	6	4		
5	D	1	Total	C	O	0	0
			13	8	5		
5	D	1	Total	C	O	0	0
			10	6	4		
5	E	1	Total	C	O	0	0
			13	8	5		
5	E	1	Total	C	O	0	0
			8	5	3		
5	G	1	Total	C	O	0	0
			13	8	5		
5	H	1	Total	C	O	0	0
			13	8	5		
5	H	1	Total	C	O	0	0
			8	5	3		
5	I	1	Total	C	O	0	0
			13	8	5		
5	I	1	Total	C	O	0	0
			8	5	3		
5	J	1	Total	C	O	0	0
			13	8	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	J	1	Total	C	O	0	0
			13	8	5		
5	K	1	Total	C	O	0	0
			13	8	5		
5	L	1	Total	C	O	0	0
			13	8	5		

- Molecule 6 is water.

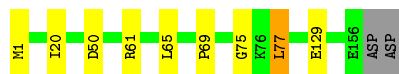
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	124	Total	O	0	0
			124	124		
6	B	135	Total	O	0	0
			135	135		
6	C	144	Total	O	0	0
			144	144		
6	D	109	Total	O	0	0
			109	109		
6	E	156	Total	O	0	0
			156	156		
6	F	133	Total	O	0	0
			133	133		
6	G	115	Total	O	0	0
			115	115		
6	H	122	Total	O	0	0
			122	122		
6	I	104	Total	O	0	0
			104	104		
6	J	127	Total	O	0	0
			127	127		
6	K	133	Total	O	0	0
			133	133		
6	L	118	Total	O	0	0
			118	118		

3 Residue-property plots [i](#)

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

- Molecule 1: Ferroxidase

Chain A:  93% 5% ..



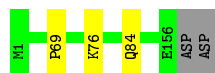
- Molecule 1: Ferroxidase

Chain B:  96% ..

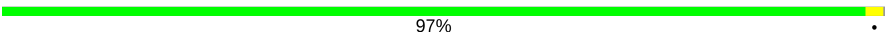


- Molecule 1: Ferroxidase

Chain C:  97% ..



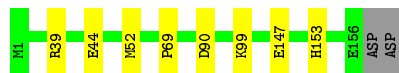
- Molecule 1: Ferroxidase

Chain D:  97% ..



- Molecule 1: Ferroxidase

Chain E:  94% 5% ..



- Molecule 1: Ferroxidase

Chain F:  94% 5% ..



- Molecule 1: Ferroxidase

Chain G: 94% 5% .



- Molecule 1: Ferroxidase

Chain H: 96% . .



- Molecule 1: Ferroxidase

Chain I: 96% . .



- Molecule 1: Ferroxidase

Chain J: 96% . .



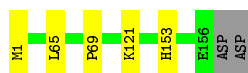
- Molecule 1: Ferroxidase

Chain K: 92% 6% .



- Molecule 1: Ferroxidase

Chain L: 96% . .



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	129.81Å 194.56Å 203.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.31 – 1.85 48.64 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.6 (47.31-1.85) 99.6 (48.64-1.85)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 1.86Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.162 , 0.195 0.172 , 0.202	Depositor DCC
R_{free} test set	10820 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	23.8	Xtriage
Anisotropy	0.571	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 53.4	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	0.96	EDS
Total number of atoms	17552	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% 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, KTG, FE2

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	0.45	0/1305	0.56	0/1758
1	B	0.43	0/1302	0.54	0/1755
1	C	0.45	0/1294	0.57	0/1746
1	D	0.42	0/1304	0.54	0/1758
1	E	0.54	0/1310	0.56	0/1765
1	F	0.45	0/1294	0.54	0/1745
1	G	0.46	0/1299	0.54	0/1751
1	H	0.42	0/1304	0.52	0/1758
1	I	0.49	0/1297	0.56	1/1749 (0.1%)
1	J	0.49	0/1301	0.56	0/1754
1	K	0.45	0/1304	0.56	0/1756
1	L	0.41	0/1310	0.51	0/1765
All	All	0.46	0/15624	0.55	1/21060 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	30	ARG	NE-CZ-NH2	-5.17	117.72	120.30

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	1278	0	1256	7	0
1	B	1275	0	1247	3	0
1	C	1267	0	1232	3	0
1	D	1277	0	1247	2	0
1	E	1280	0	1258	6	0
1	F	1267	0	1236	5	0
1	G	1272	0	1243	5	0
1	H	1274	0	1247	3	0
1	I	1270	0	1236	2	0
1	J	1274	0	1245	2	0
1	K	1277	0	1259	7	0
1	L	1280	0	1258	3	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	D	1	0	0	0	0
3	A	13	0	0	1	0
3	B	22	0	0	1	0
3	C	22	0	0	1	0
3	D	13	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	15	0	0	1	0
3	I	22	0	0	1	0
3	J	22	0	0	1	0
3	K	22	0	0	1	0
3	L	22	0	0	1	0
4	A	43	0	30	0	0
4	C	43	0	30	1	0
4	D	43	0	30	0	0
4	E	43	0	30	2	0
4	F	43	0	30	3	0
4	H	43	0	30	1	0
4	L	43	0	30	0	0
5	A	26	0	36	3	0
5	C	21	0	26	1	0
5	D	23	0	31	0	0
5	E	21	0	27	0	0
5	G	13	0	18	0	0
5	H	21	0	27	0	0
5	I	21	0	27	3	0
5	J	26	0	36	0	0
5	K	13	0	18	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	L	13	0	18	0	0
6	A	124	0	0	0	0
6	B	135	0	0	1	0
6	C	144	0	0	3	0
6	D	109	0	0	1	0
6	E	156	0	0	1	0
6	F	133	0	0	1	0
6	G	115	0	0	1	0
6	H	122	0	0	1	0
6	I	104	0	0	2	0
6	J	127	0	0	0	0
6	K	133	0	0	2	0
6	L	118	0	0	1	0
All	All	17552	0	15438	55	0

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

The worst 5 of 55 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:D:84:GLN:NE2	6:D:301:HOH:O	2.24	0.68
1:F:69:PRO:O	3:F:201:KTG:N03	2.34	0.61
1:B:69:PRO:O	3:B:202:KTG:N03	2.34	0.61
1:I:69:PRO:O	3:I:201:KTG:N03	2.34	0.61
1:H:69:PRO:O	3:H:201:KTG:N03	2.34	0.61

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	156/158 (99%)	154 (99%)	2 (1%)	0	100	100
1	B	156/158 (99%)	156 (100%)	0	0	100	100
1	C	156/158 (99%)	156 (100%)	0	0	100	100
1	D	156/158 (99%)	154 (99%)	2 (1%)	0	100	100
1	E	157/158 (99%)	157 (100%)	0	0	100	100
1	F	156/158 (99%)	156 (100%)	0	0	100	100
1	G	156/158 (99%)	156 (100%)	0	0	100	100
1	H	157/158 (99%)	157 (100%)	0	0	100	100
1	I	156/158 (99%)	156 (100%)	0	0	100	100
1	J	156/158 (99%)	155 (99%)	1 (1%)	0	100	100
1	K	156/158 (99%)	155 (99%)	1 (1%)	0	100	100
1	L	157/158 (99%)	157 (100%)	0	0	100	100
All	All	1875/1896 (99%)	1869 (100%)	6 (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	139/144 (96%)	137 (99%)	2 (1%)	67	55
1	B	138/144 (96%)	138 (100%)	0	100	100
1	C	136/144 (94%)	136 (100%)	0	100	100
1	D	139/144 (96%)	138 (99%)	1 (1%)	84	79
1	E	139/144 (96%)	139 (100%)	0	100	100
1	F	135/144 (94%)	134 (99%)	1 (1%)	84	79
1	G	137/144 (95%)	137 (100%)	0	100	100
1	H	137/144 (95%)	137 (100%)	0	100	100
1	I	136/144 (94%)	135 (99%)	1 (1%)	84	79

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	138/144 (96%)	137 (99%)	1 (1%)	84	79
1	K	139/144 (96%)	139 (100%)	0	100	100
1	L	139/144 (96%)	138 (99%)	1 (1%)	84	79
All	All	1652/1728 (96%)	1645 (100%)	7 (0%)	91	89

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	121	LYS
1	L	121	LYS
1	I	121	LYS
1	A	77	LEU
1	J	121	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 39 ligands modelled in this entry, 3 are monoatomic - leaving 36 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	C	204	-	9,9,12	0.57	0	8,8,11	0.47	0
3	KTG	H	201	-	16,16,24	1.94	5 (31%)	22,22,33	1.66	3 (13%)
4	HEM	A	203	1	27,50,50	1.86	6 (22%)	17,82,82	2.20	7 (41%)
3	KTG	I	201	-	24,24,24	1.78	4 (16%)	33,33,33	0.95	1 (3%)
5	PG4	H	204	-	7,7,12	0.58	0	6,6,11	0.31	0
5	PG4	H	203	-	12,12,12	0.47	0	11,11,11	0.49	0
3	KTG	J	201	-	24,24,24	1.84	5 (20%)	33,33,33	1.25	3 (9%)
5	PG4	E	204	-	7,7,12	0.63	0	6,6,11	0.17	0
5	PG4	J	202	-	12,12,12	0.53	0	11,11,11	0.43	0
5	PG4	A	204	-	12,12,12	0.62	0	11,11,11	0.49	0
3	KTG	E	201	-	24,24,24	1.72	4 (16%)	33,33,33	1.12	3 (9%)
5	PG4	A	205	-	12,12,12	0.48	0	11,11,11	0.39	0
4	HEM	H	202	1	27,50,50	1.87	6 (22%)	17,82,82	2.10	7 (41%)
5	PG4	C	203	-	10,10,12	0.53	0	9,9,11	0.46	0
5	PG4	G	202	-	12,12,12	0.50	0	11,11,11	0.57	0
3	KTG	L	201	-	24,24,24	1.84	4 (16%)	33,33,33	1.21	2 (6%)
3	KTG	F	201	-	24,24,24	1.66	5 (20%)	33,33,33	1.02	3 (9%)
4	HEM	D	203	1	27,50,50	1.83	5 (18%)	17,82,82	1.65	2 (11%)
5	PG4	D	204	-	12,12,12	0.52	0	11,11,11	0.35	0
3	KTG	D	202	-	14,14,24	2.35	5 (35%)	19,20,33	1.26	2 (10%)
5	PG4	I	202	-	12,12,12	0.36	0	11,11,11	0.81	0
3	KTG	C	201	-	24,24,24	1.71	4 (16%)	33,33,33	1.19	3 (9%)
5	PG4	K	202	-	12,12,12	0.59	0	11,11,11	0.35	0
3	KTG	K	201	-	24,24,24	1.83	4 (16%)	33,33,33	1.08	2 (6%)
5	PG4	I	203	-	7,7,12	0.56	0	6,6,11	0.21	0
5	PG4	J	203	-	12,12,12	0.39	0	11,11,11	0.58	0
4	HEM	L	202	1	27,50,50	1.75	4 (14%)	17,82,82	1.75	4 (23%)
5	PG4	L	203	-	12,12,12	0.47	0	11,11,11	0.42	0
3	KTG	G	201	-	24,24,24	1.73	5 (20%)	33,33,33	1.09	2 (6%)
5	PG4	E	203	-	12,12,12	0.59	0	11,11,11	0.53	0
4	HEM	C	202	1	27,50,50	1.73	5 (18%)	17,82,82	2.37	9 (52%)
4	HEM	F	202	1	27,50,50	1.83	4 (14%)	17,82,82	2.03	8 (47%)
4	HEM	E	202	1	27,50,50	1.70	6 (22%)	17,82,82	1.90	7 (41%)
5	PG4	D	205	-	9,9,12	0.63	0	8,8,11	0.29	0
3	KTG	B	202	-	24,24,24	1.70	6 (25%)	33,33,33	1.07	2 (6%)
3	KTG	A	202	-	14,14,24	2.53	5 (35%)	19,20,33	1.35	2 (10%)

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	C	204	-	-	3/7/7/10	-
3	KTG	H	201	-	-	1/4/16/19	0/2/2/3
4	HEM	A	203	1	-	0/6/54/54	-
3	KTG	I	201	-	-	0/7/19/19	0/3/3/3
5	PG4	H	204	-	-	0/5/5/10	-
5	PG4	H	203	-	-	4/10/10/10	-
3	KTG	J	201	-	-	0/7/19/19	0/3/3/3
5	PG4	E	204	-	-	0/5/5/10	-
5	PG4	J	202	-	-	1/10/10/10	-
5	PG4	A	204	-	-	5/10/10/10	-
3	KTG	E	201	-	-	0/7/19/19	0/3/3/3
5	PG4	A	205	-	-	1/10/10/10	-
4	HEM	H	202	1	-	0/6/54/54	-
5	PG4	C	203	-	-	0/8/8/10	-
5	PG4	G	202	-	-	5/10/10/10	-
3	KTG	L	201	-	-	0/7/19/19	0/3/3/3
3	KTG	F	201	-	-	0/7/19/19	0/3/3/3
4	HEM	D	203	1	-	2/6/54/54	-
5	PG4	D	204	-	-	3/10/10/10	-
3	KTG	D	202	-	-	0/2/14/19	0/2/2/3
5	PG4	I	202	-	-	3/10/10/10	-
3	KTG	C	201	-	-	1/7/19/19	0/3/3/3
5	PG4	K	202	-	-	2/10/10/10	-
3	KTG	K	201	-	-	0/7/19/19	0/3/3/3
5	PG4	I	203	-	-	1/5/5/10	-
5	PG4	J	203	-	-	0/10/10/10	-
4	HEM	L	202	1	-	0/6/54/54	-
5	PG4	L	203	-	-	3/10/10/10	-
3	KTG	G	201	-	-	0/7/19/19	0/3/3/3
5	PG4	E	203	-	-	1/10/10/10	-
4	HEM	C	202	1	-	0/6/54/54	-
4	HEM	F	202	1	-	0/6/54/54	-
4	HEM	E	202	1	-	0/6/54/54	-
5	PG4	D	205	-	-	0/7/7/10	-
3	KTG	B	202	-	-	2/7/19/19	0/3/3/3
3	KTG	A	202	-	-	0/2/14/19	0/2/2/3

The worst 5 of 92 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	203	HEM	C3C-C2C	-4.96	1.33	1.40
3	I	201	KTG	C21-C02	4.87	1.56	1.48
3	D	202	KTG	C06-N07	4.80	1.46	1.37
3	A	202	KTG	C06-N07	4.76	1.46	1.37
3	C	201	KTG	C21-C02	4.75	1.55	1.48

The worst 5 of 72 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	201	KTG	C05-C06-N07	-4.96	115.44	121.32
4	A	203	HEM	CMC-C2C-C3C	4.44	132.98	124.68
3	L	201	KTG	C04-N03-C02	-4.20	108.94	112.52
4	F	202	HEM	CMC-C2C-C3C	4.11	132.37	124.68
3	J	201	KTG	C05-C06-N07	-4.11	116.45	121.32

There are no chirality outliers.

5 of 38 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	204	PG4	O2-C3-C4-O3
5	H	203	PG4	O4-C7-C8-O5
3	B	202	KTG	N07-C08-C09-C10
5	C	204	PG4	O3-C5-C6-O4
5	G	202	PG4	O4-C7-C8-O5

There are no ring outliers.

21 monomers are involved in 26 short contacts:

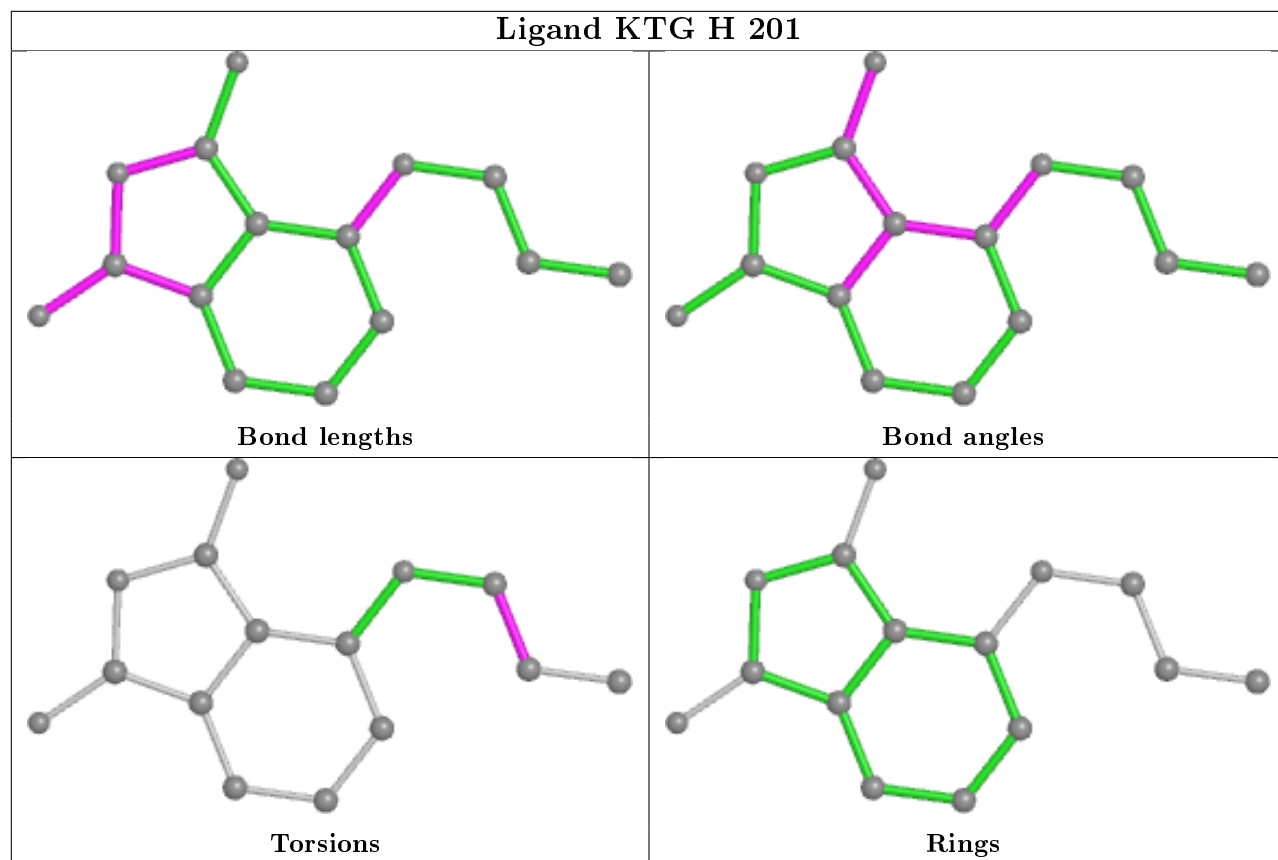
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	204	PG4	1	0
3	H	201	KTG	1	0
3	I	201	KTG	1	0
3	J	201	KTG	1	0
5	A	204	PG4	1	0
3	E	201	KTG	1	0
5	A	205	PG4	2	0
4	H	202	HEM	1	0
3	L	201	KTG	1	0
3	F	201	KTG	1	0
3	D	202	KTG	1	0

Continued on next page...

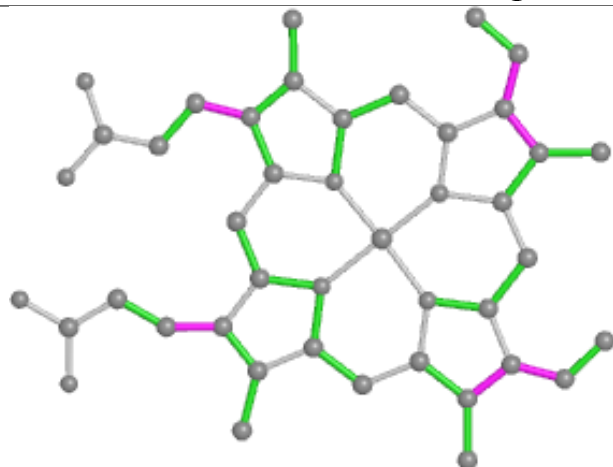
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	I	202	PG4	2	0
3	C	201	KTG	1	0
3	K	201	KTG	1	0
5	I	203	PG4	1	0
3	G	201	KTG	1	0
4	C	202	HEM	1	0
4	F	202	HEM	3	0
4	E	202	HEM	2	0
3	B	202	KTG	1	0
3	A	202	KTG	1	0

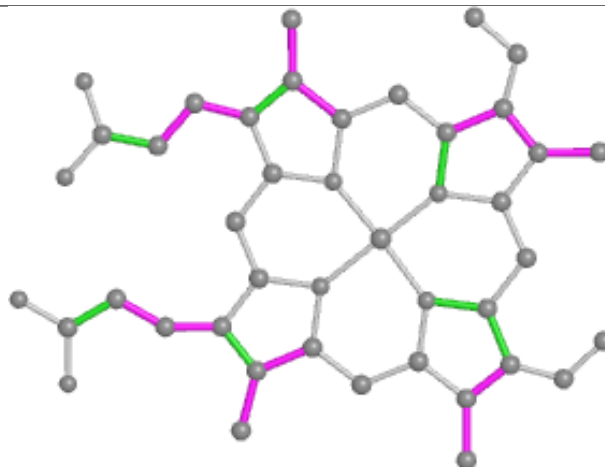
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



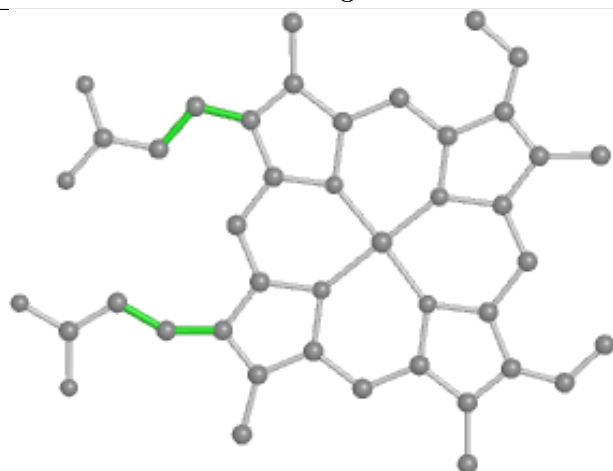
Ligand HEM A 203



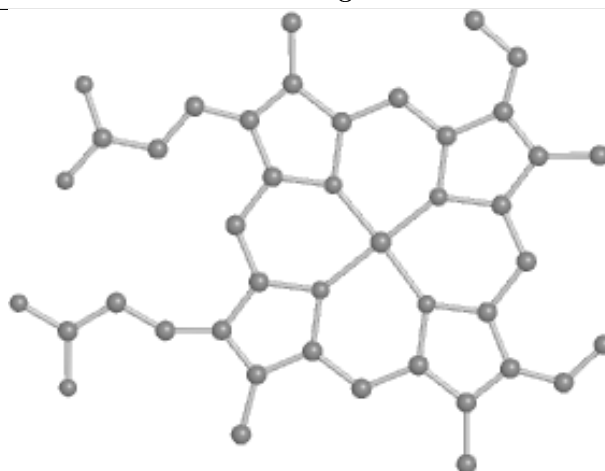
Bond lengths



Bond angles

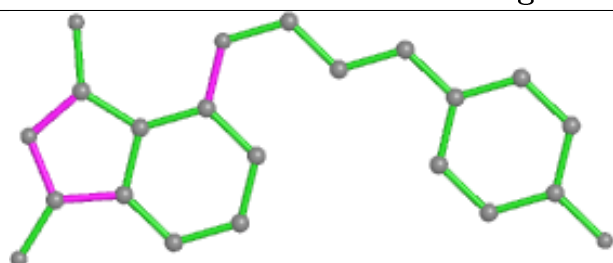


Torsions

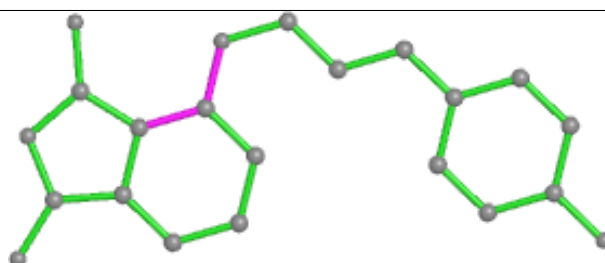


Rings

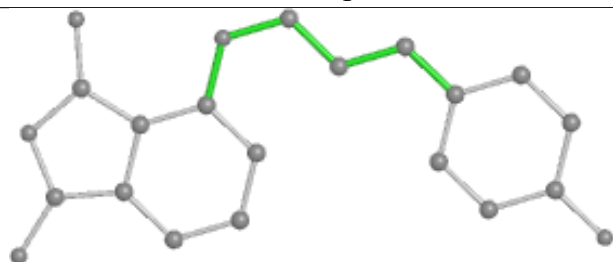
Ligand KTG I 201



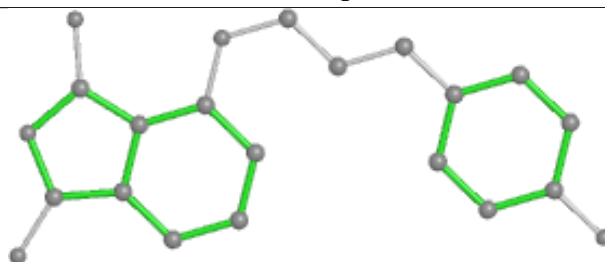
Bond lengths



Bond angles

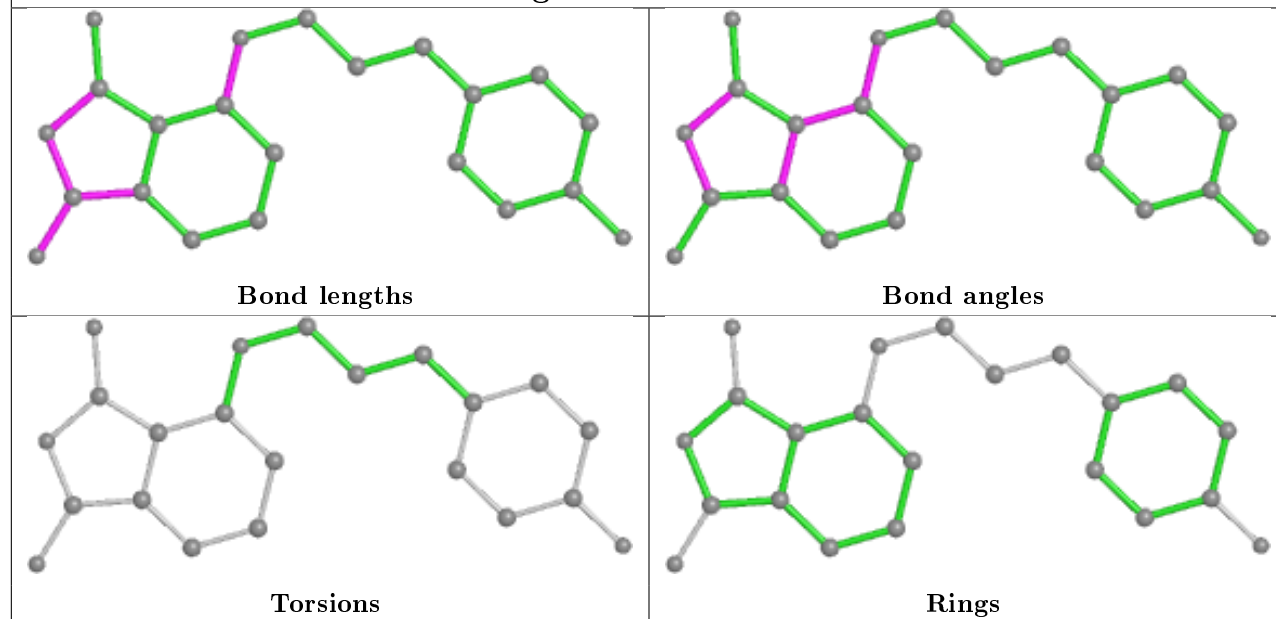


Torsions

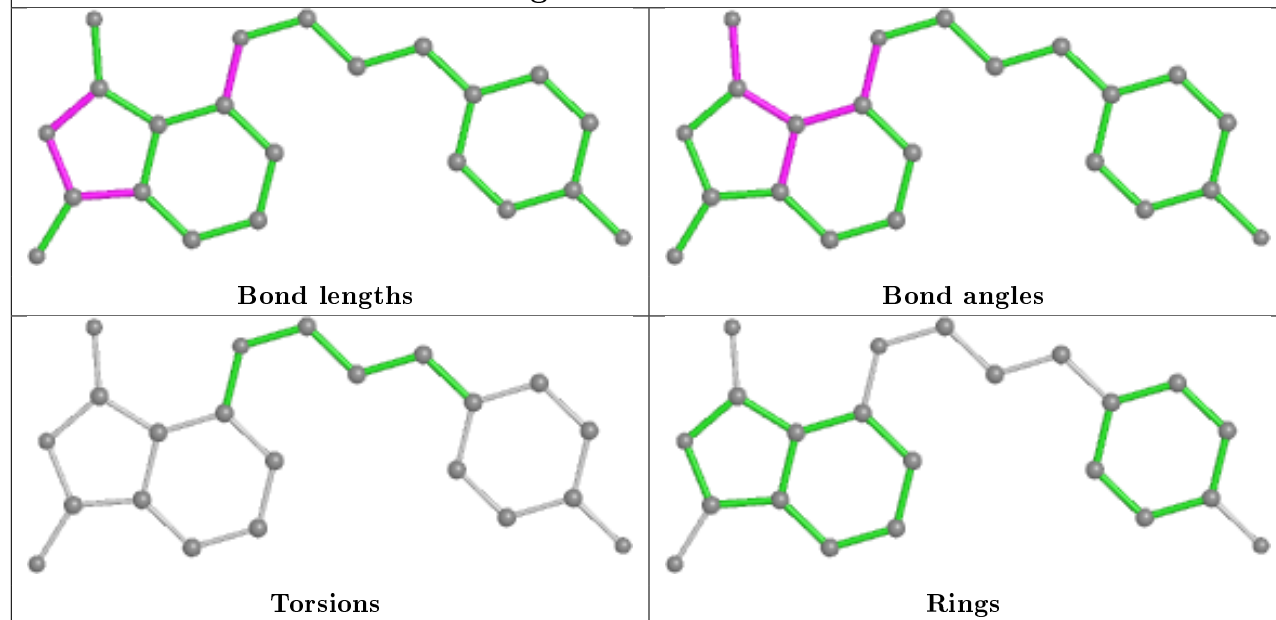


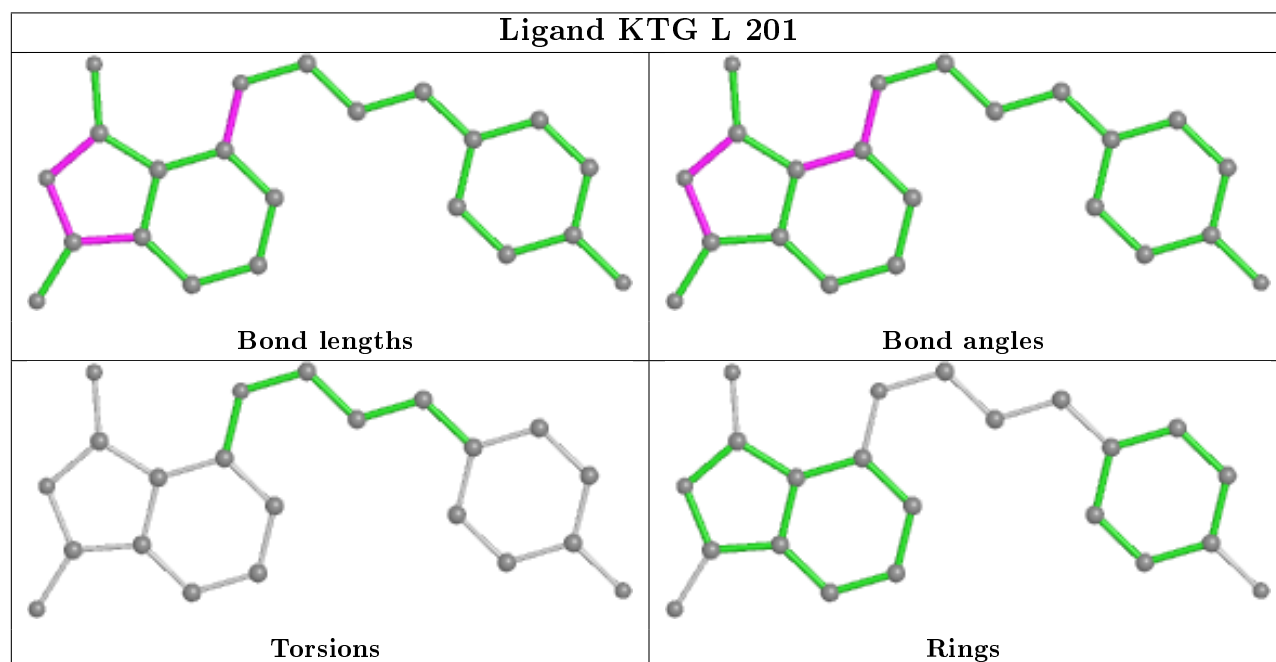
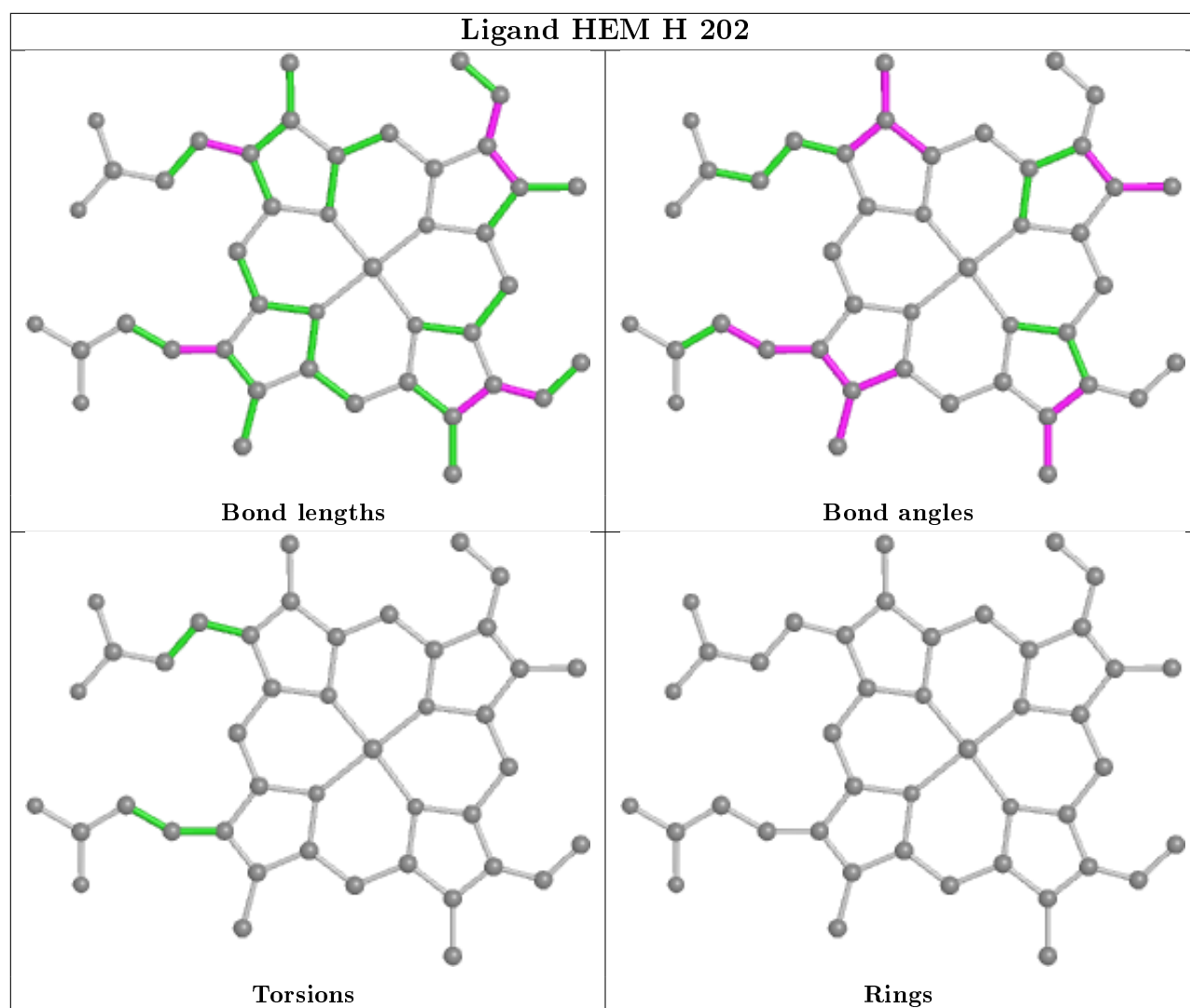
Rings

Ligand KTG J 201

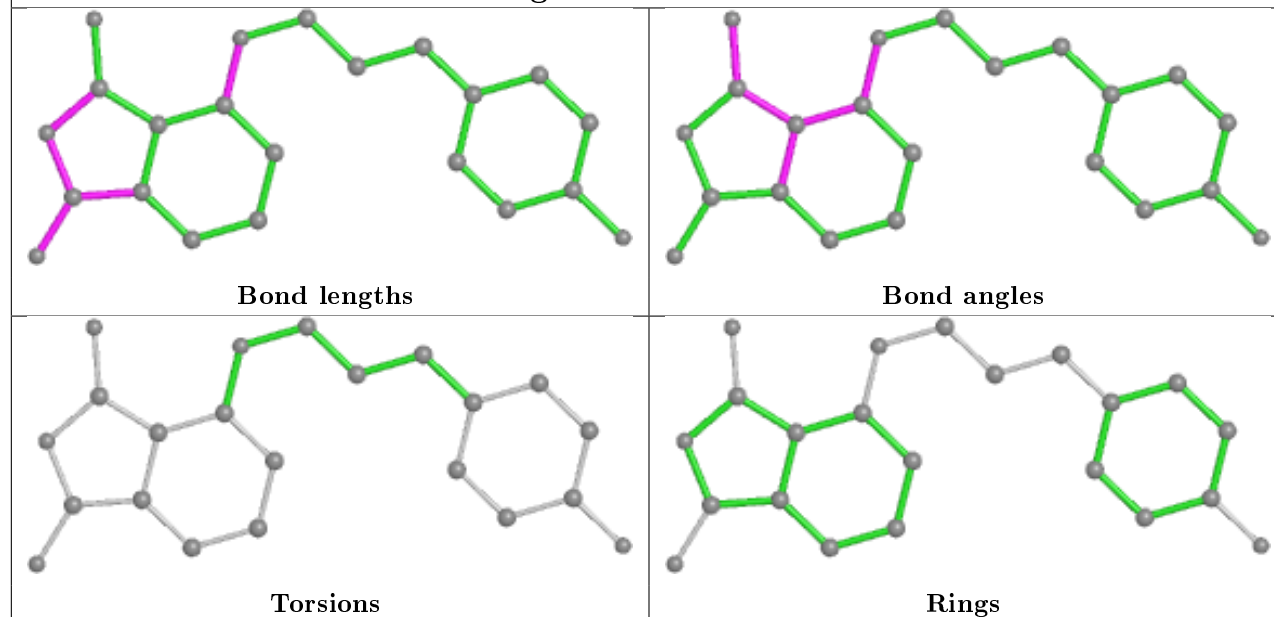


Ligand KTG E 201

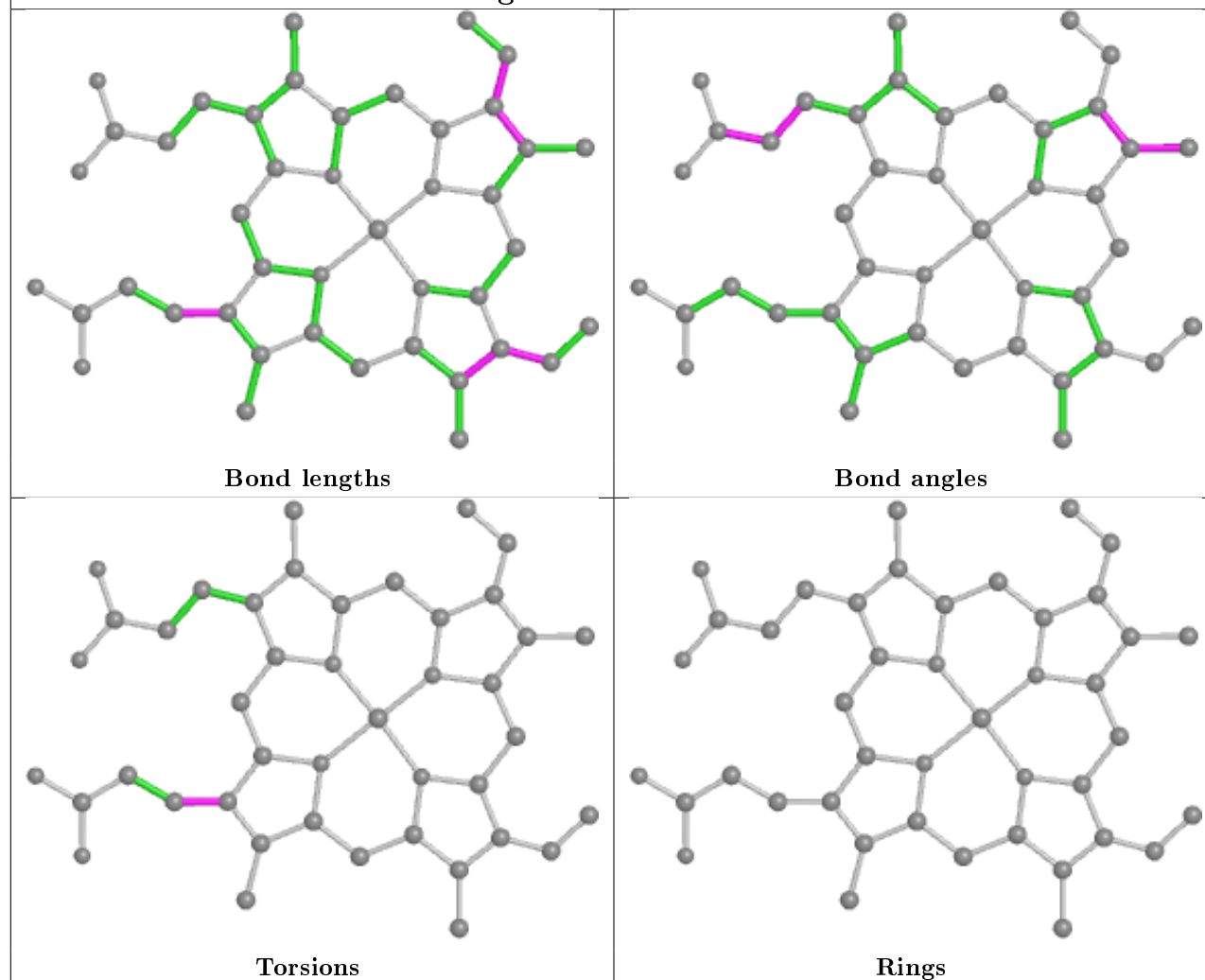


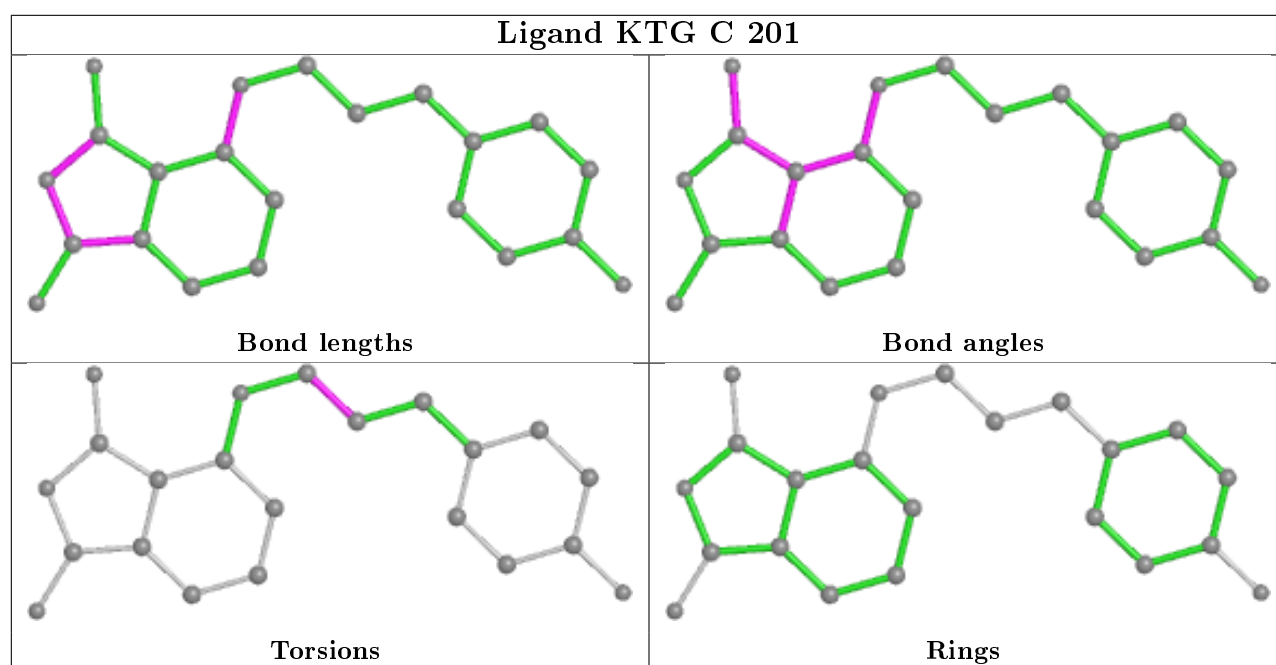
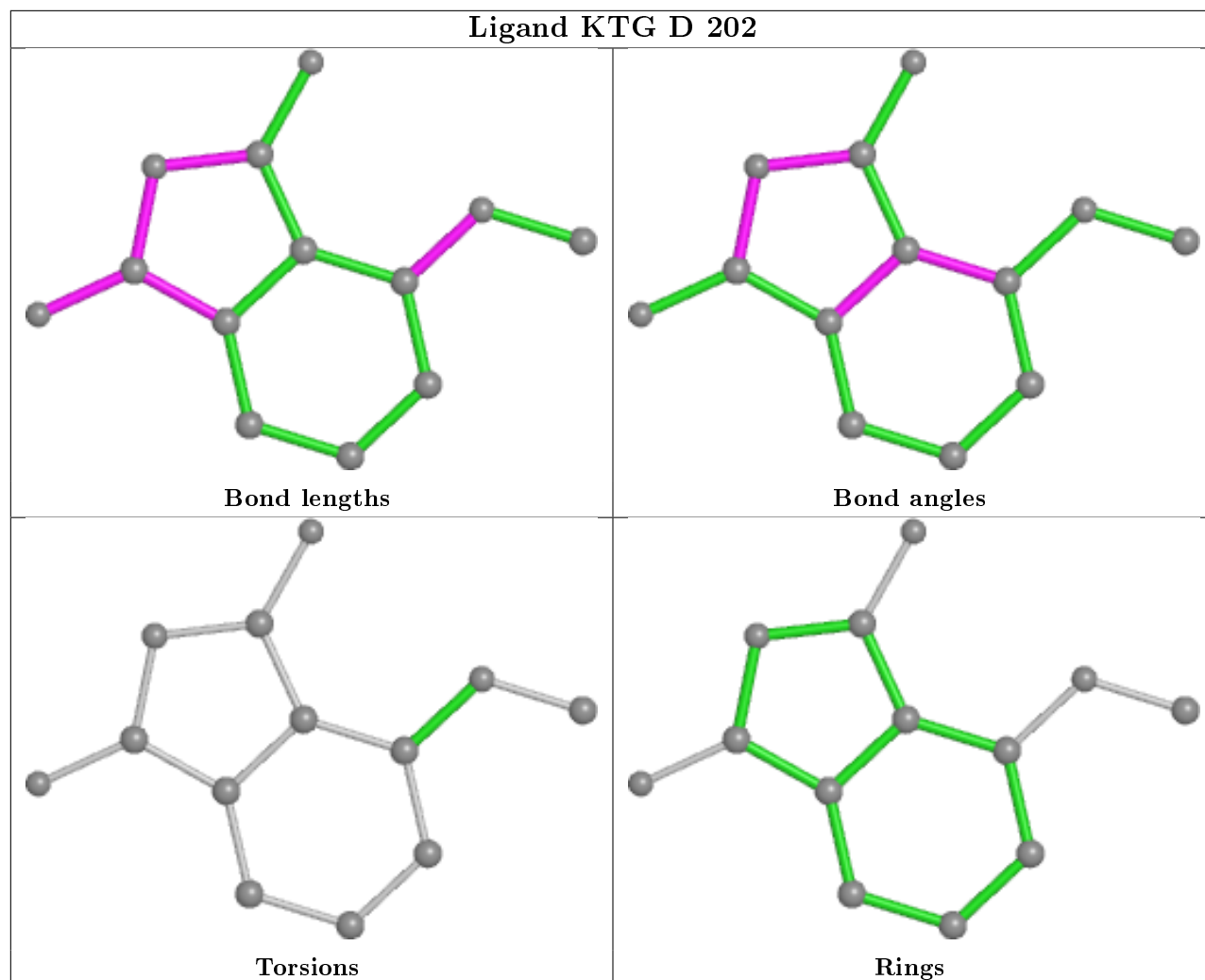


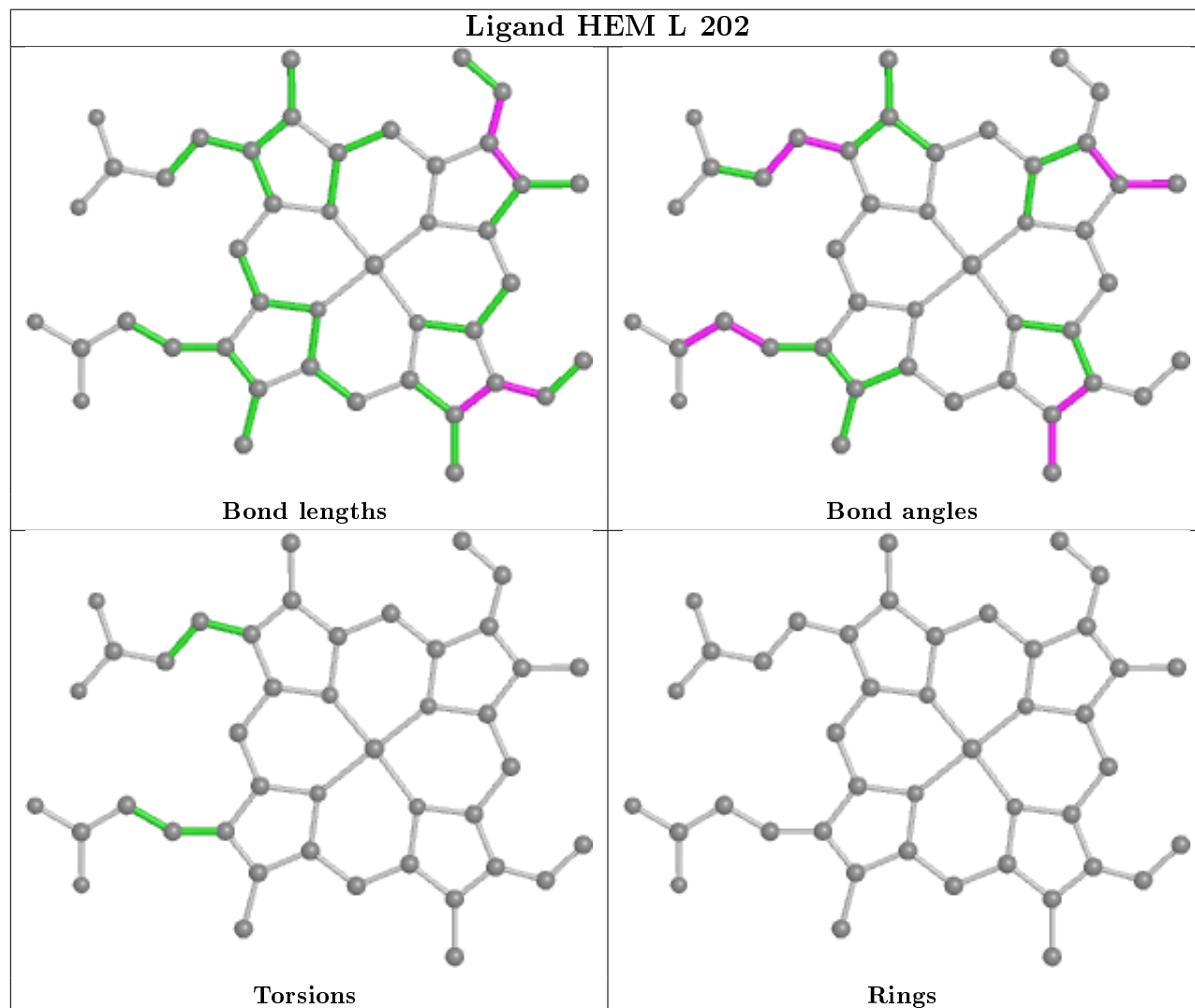
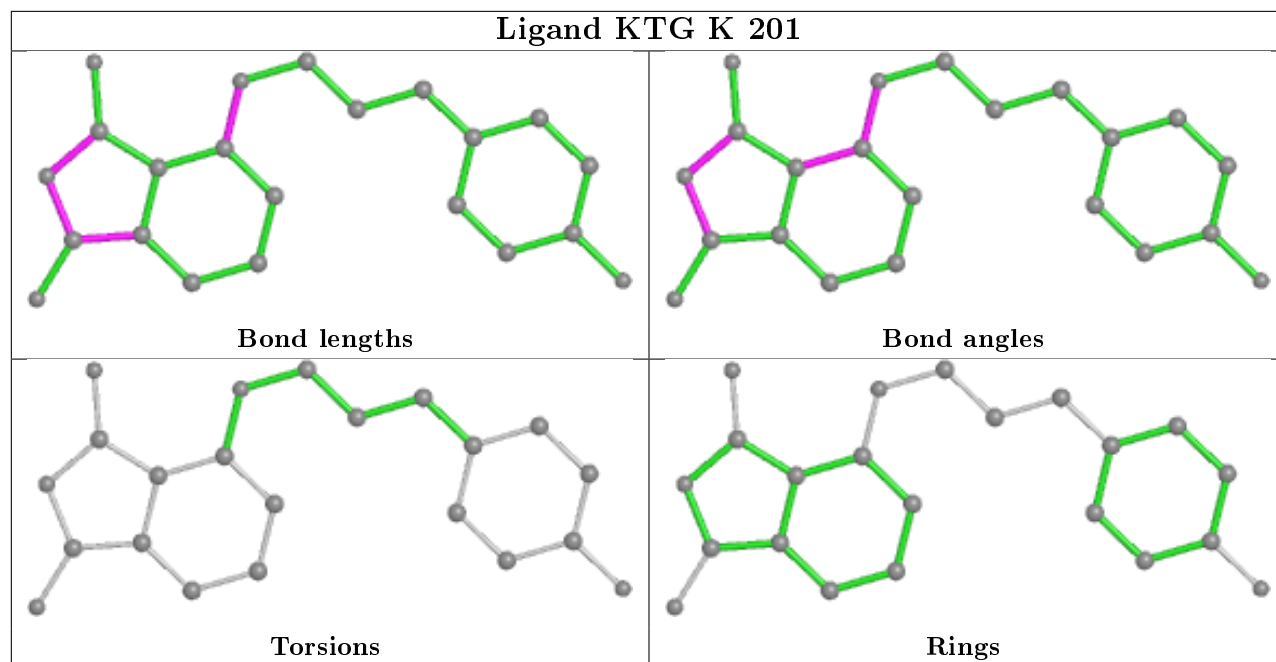
Ligand KTG F 201

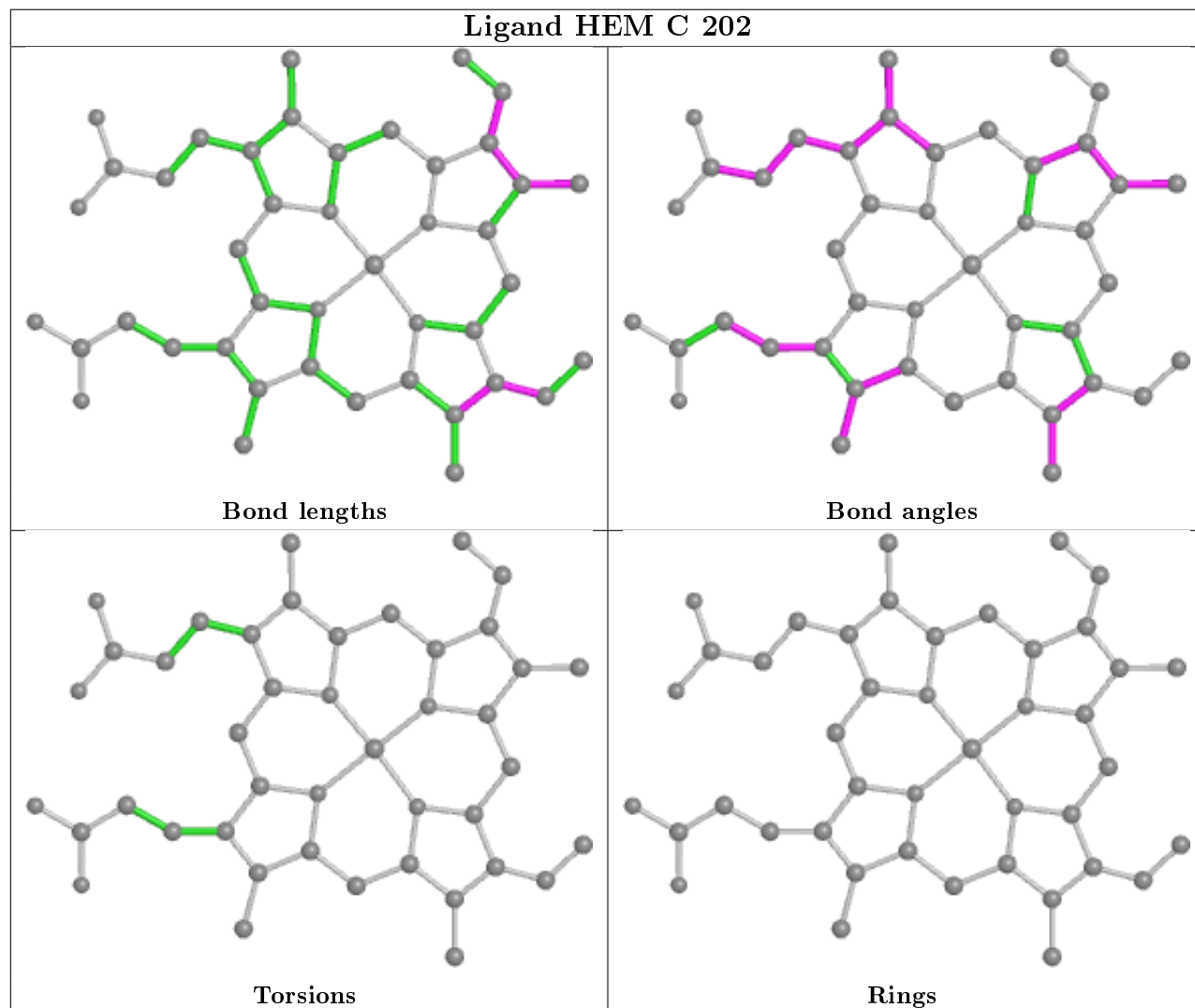
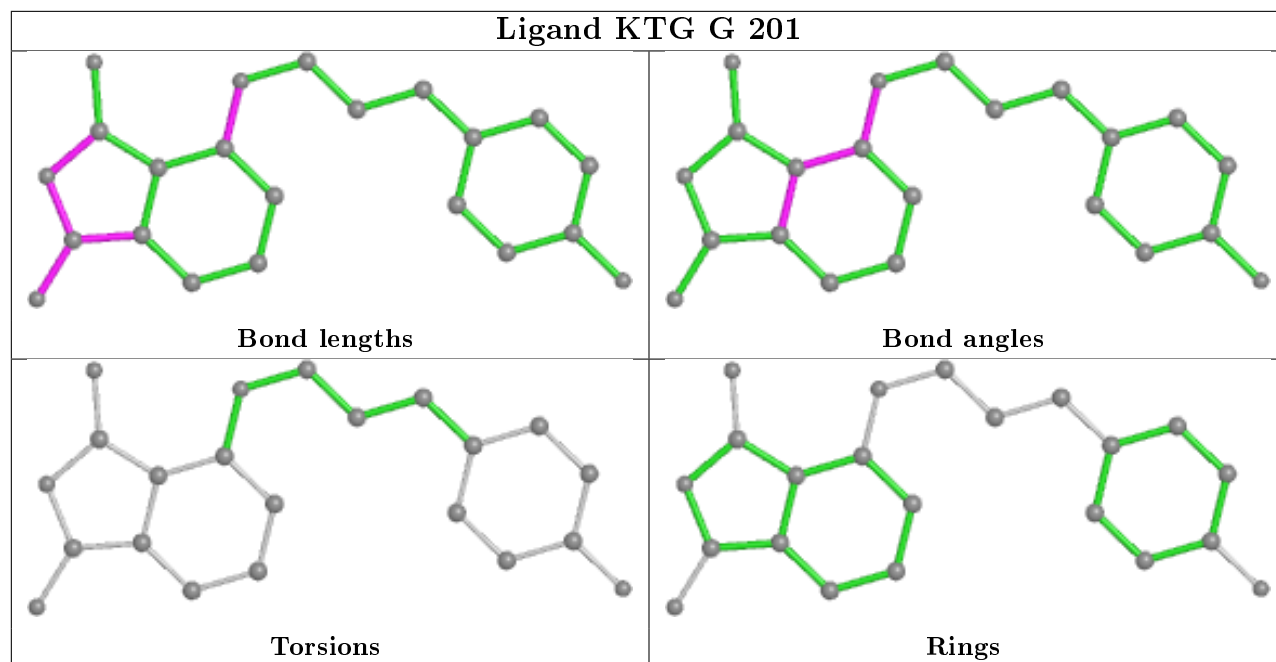


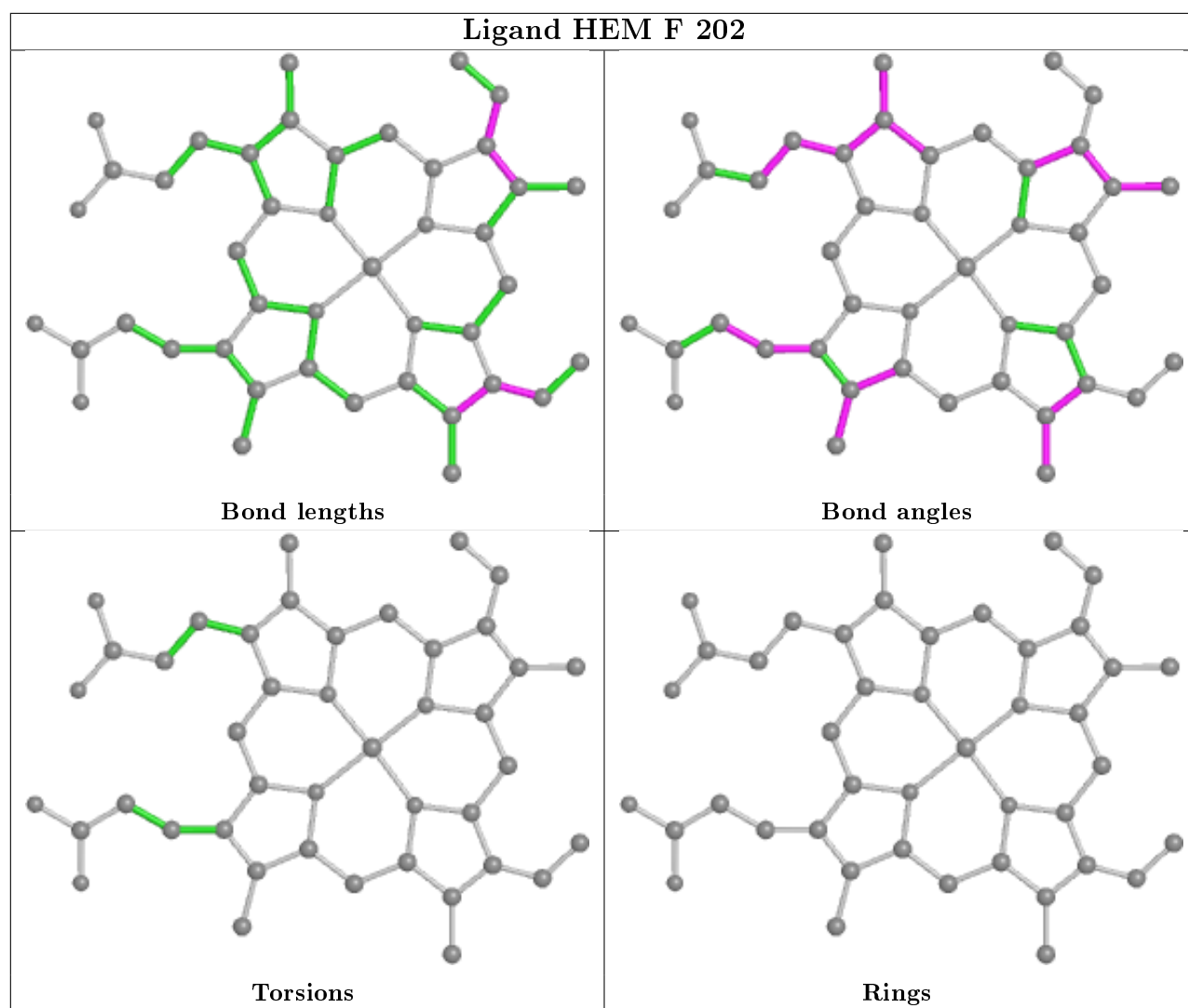
Ligand HEM D 203

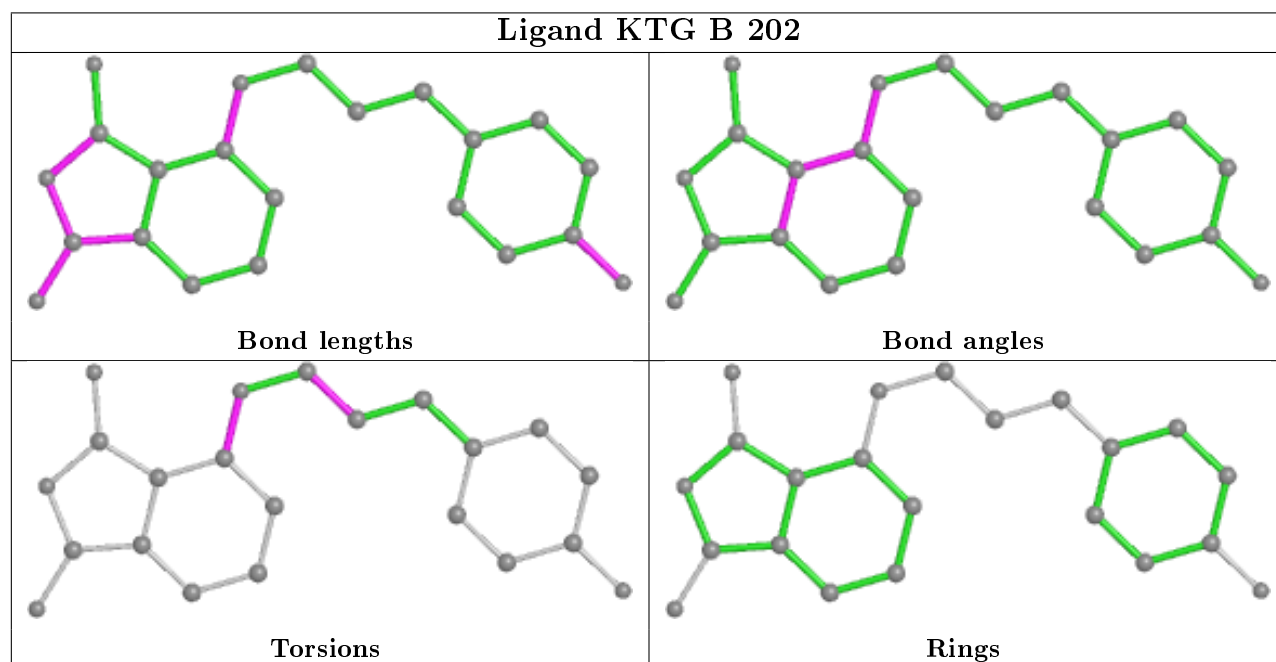
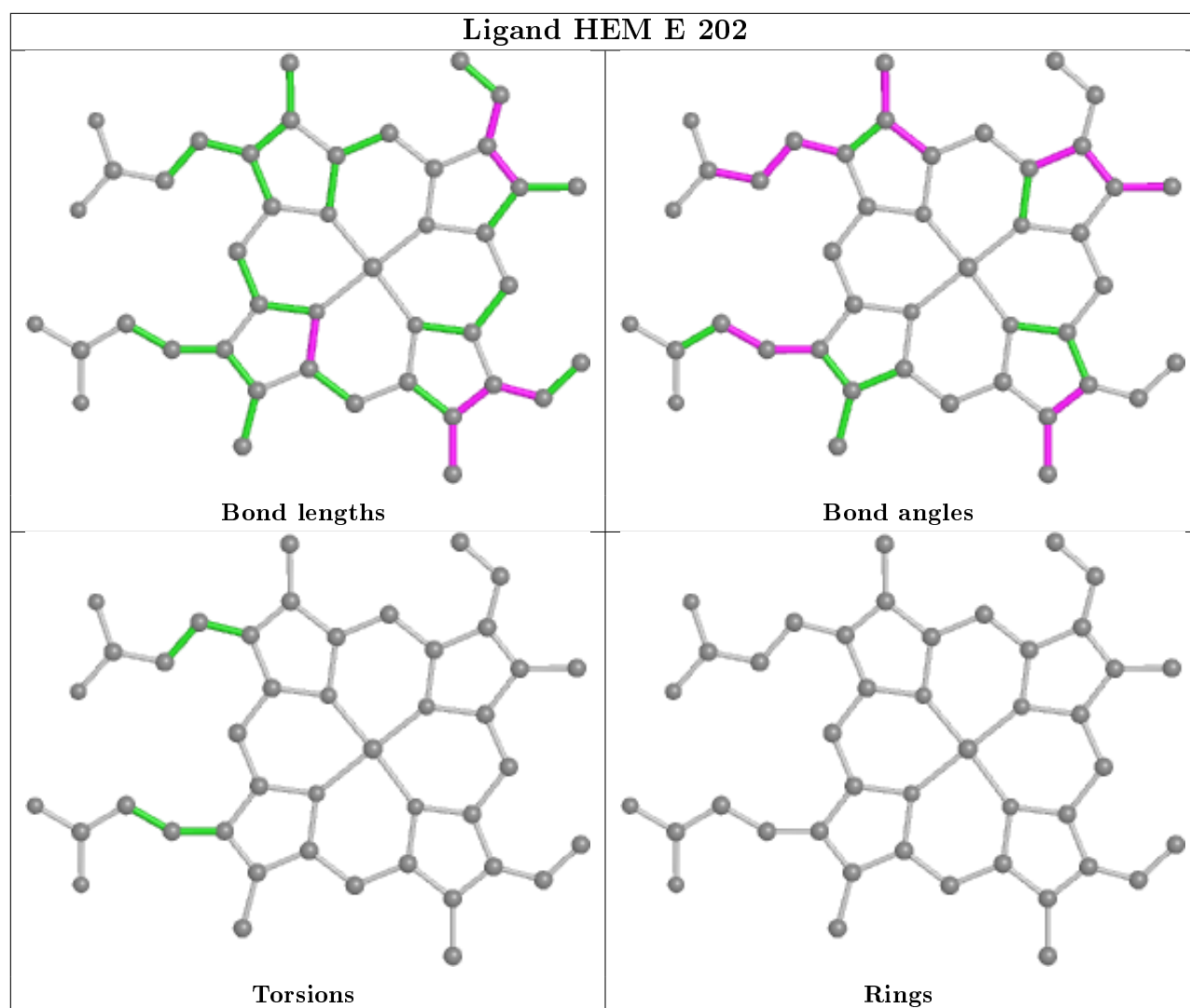


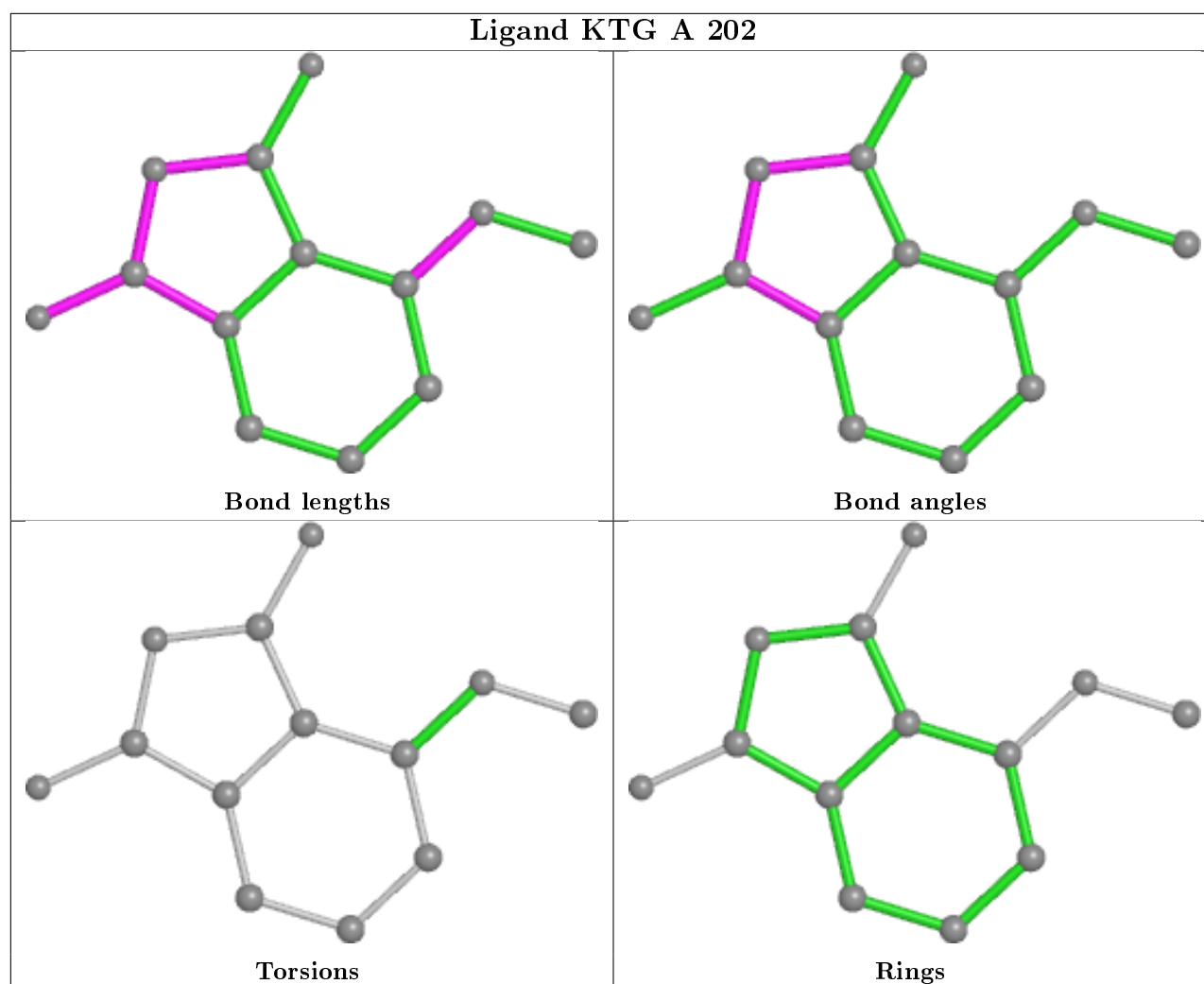












5.7 Other polymers [i](#)

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	156/158 (98%)	-0.39	0 100 100	17, 23, 35, 48	0
1	B	156/158 (98%)	-0.41	0 100 100	18, 23, 34, 51	0
1	C	156/158 (98%)	-0.42	0 100 100	17, 22, 31, 50	0
1	D	156/158 (98%)	-0.30	0 100 100	22, 27, 38, 54	0
1	E	156/158 (98%)	-0.43	0 100 100	17, 20, 29, 47	0
1	F	156/158 (98%)	-0.37	0 100 100	17, 23, 31, 51	0
1	G	156/158 (98%)	-0.41	0 100 100	19, 24, 34, 52	0
1	H	156/158 (98%)	-0.25	0 100 100	20, 25, 35, 51	0
1	I	156/158 (98%)	-0.41	0 100 100	19, 24, 34, 51	0
1	J	156/158 (98%)	-0.35	0 100 100	18, 23, 34, 49	0
1	K	156/158 (98%)	-0.42	0 100 100	18, 24, 34, 50	0
1	L	156/158 (98%)	-0.25	0 100 100	19, 26, 39, 54	0
All	All	1872/1896 (98%)	-0.37	0 100 100	17, 24, 34, 54	0

There are no RSRZ outliers to report.

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 ⓘ

There are no carbohydrates 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.

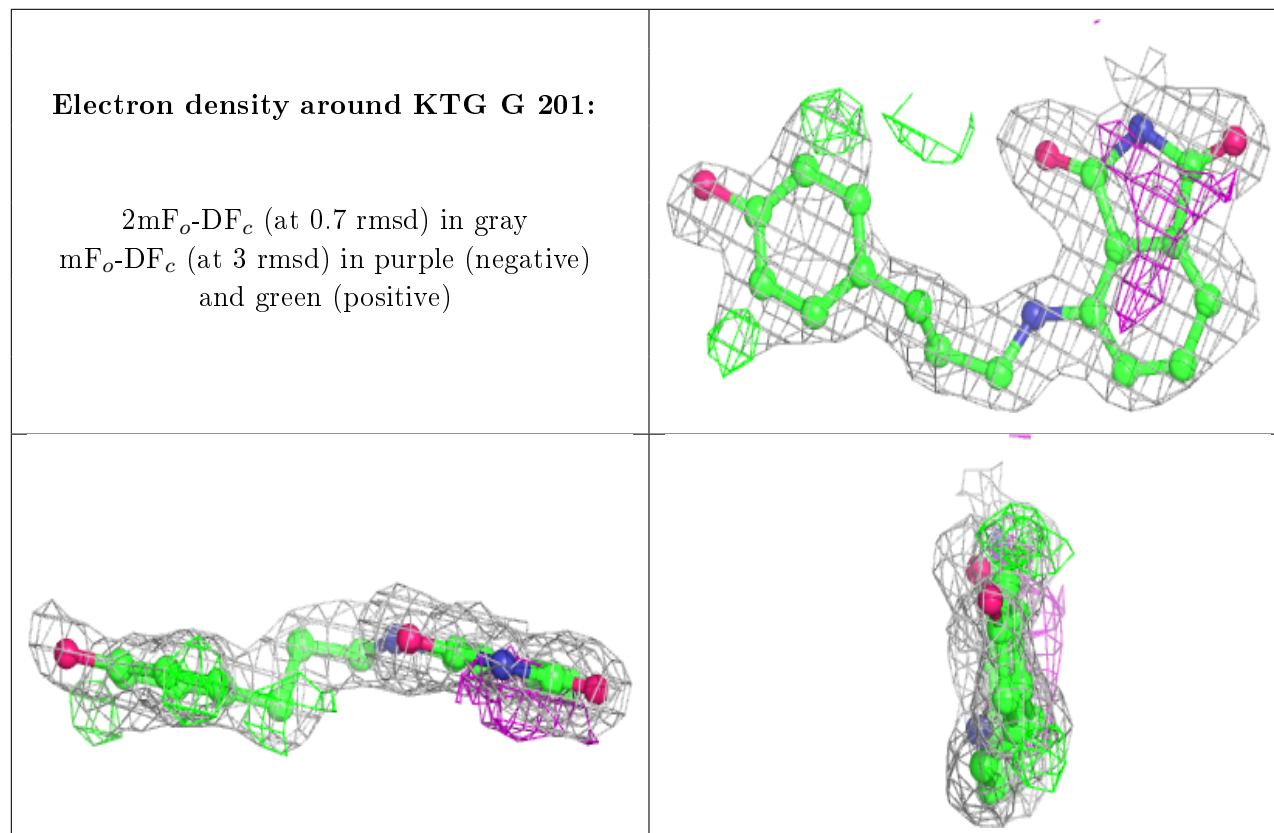
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	PG4	I	203	8/13	0.75	0.21	40,50,56,60	0
3	KTG	G	201	22/22	0.75	0.25	27,43,53,63	0
3	KTG	I	201	22/22	0.77	0.26	31,41,56,70	0
5	PG4	A	204	13/13	0.78	0.19	29,42,50,59	0
3	KTG	K	201	22/22	0.78	0.23	36,45,60,70	0
3	KTG	C	201	22/22	0.79	0.23	30,46,59,68	0
5	PG4	G	202	13/13	0.79	0.19	31,42,49,59	0
5	PG4	H	204	8/13	0.80	0.21	44,50,55,60	0
3	KTG	E	201	22/22	0.81	0.25	27,40,55,63	0
5	PG4	E	204	8/13	0.81	0.22	39,46,53,53	0
3	KTG	H	201	15/22	0.81	0.22	28,36,44,46	0
5	PG4	D	205	10/13	0.81	0.18	45,47,55,60	0
5	PG4	D	204	13/13	0.82	0.18	30,41,58,58	0
3	KTG	F	201	22/22	0.83	0.23	28,41,55,65	0
3	KTG	B	202	22/22	0.83	0.21	27,37,55,64	0
5	PG4	C	204	10/13	0.84	0.19	31,38,50,50	0
5	PG4	C	203	11/13	0.85	0.15	31,41,53,56	0
5	PG4	K	202	13/13	0.86	0.17	30,39,51,53	0
5	PG4	A	205	13/13	0.86	0.15	33,41,48,53	0
5	PG4	H	203	13/13	0.86	0.15	31,44,50,57	0
5	PG4	J	202	13/13	0.87	0.15	26,37,49,51	0
3	KTG	J	201	22/22	0.88	0.18	29,39,49,56	0
5	PG4	E	203	13/13	0.88	0.14	29,36,47,52	0
5	PG4	L	203	13/13	0.89	0.13	24,40,45,46	0
3	KTG	L	201	22/22	0.89	0.16	30,40,55,56	0
5	PG4	I	202	13/13	0.90	0.13	29,44,49,51	0
3	KTG	A	202	13/22	0.92	0.17	26,31,42,46	0
4	HEM	L	202	43/43	0.93	0.14	21,25,30,35	43
3	KTG	D	202	13/22	0.93	0.14	29,35,44,46	0
5	PG4	J	203	13/13	0.95	0.09	26,33,38,44	0
4	HEM	H	202	43/43	0.95	0.11	19,23,38,44	0
4	HEM	F	202	43/43	0.95	0.12	17,22,37,39	0
4	HEM	C	202	43/43	0.96	0.12	18,24,36,41	0
4	HEM	D	203	43/43	0.96	0.11	21,25,33,34	43
4	HEM	E	202	43/43	0.96	0.11	16,21,37,39	0
4	HEM	A	203	43/43	0.97	0.10	18,23,37,39	0
2	FE2	B	201	1/1	0.99	0.07	19,19,19,19	0

Continued on next page...

Continued from previous page...

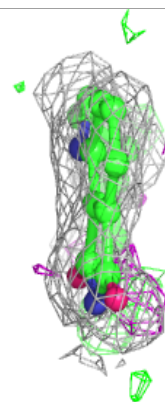
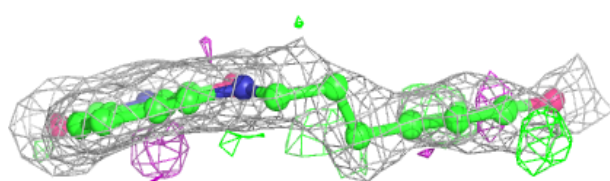
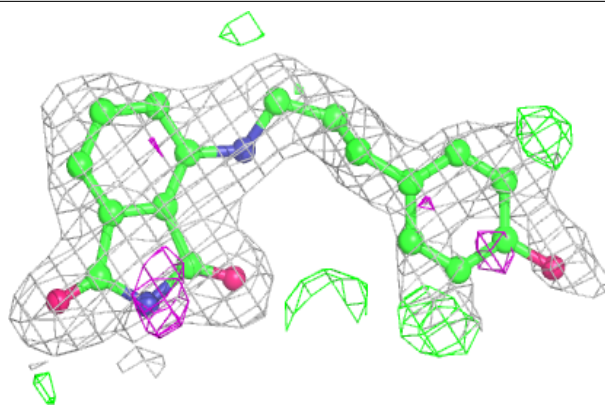
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	FE2	D	201	1/1	0.99	0.08	22,22,22,22	0
2	FE2	A	201	1/1	1.00	0.07	17,17,17,17	0

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.

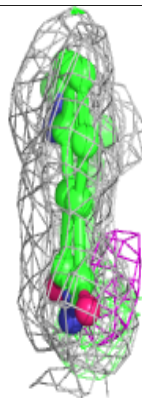
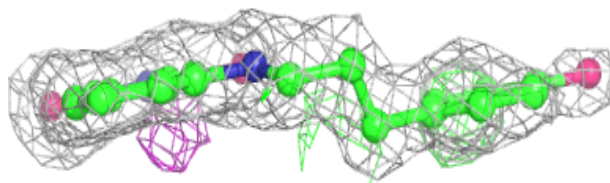
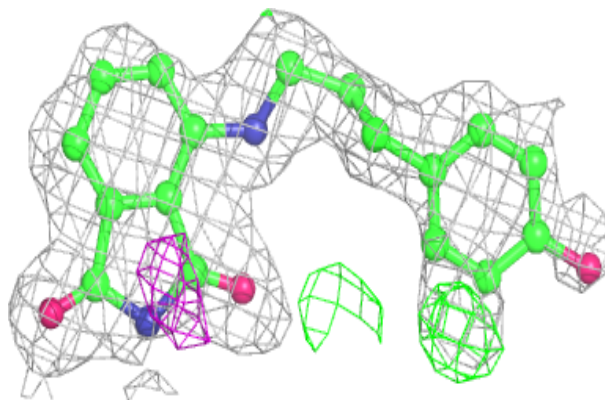


Electron density around KTG I 201:

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

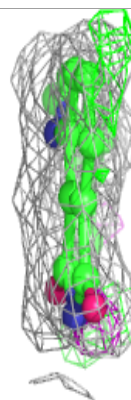
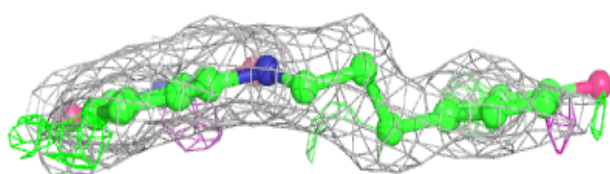
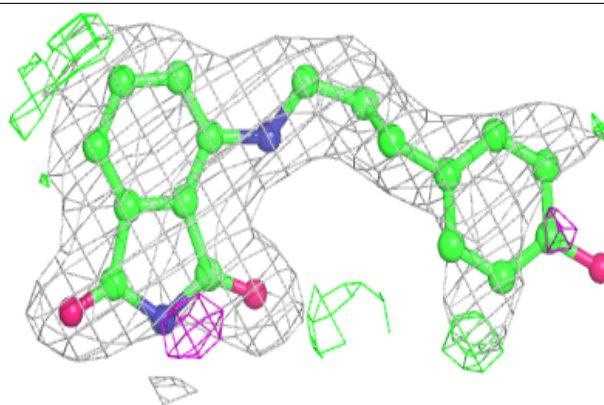
**Electron density around KTG K 201:**

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

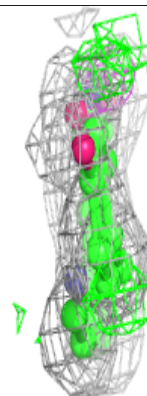
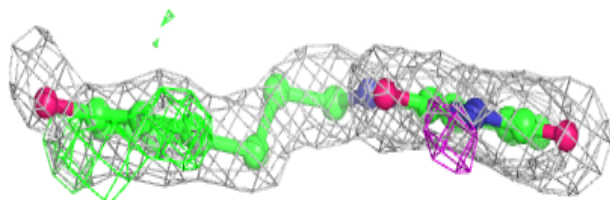
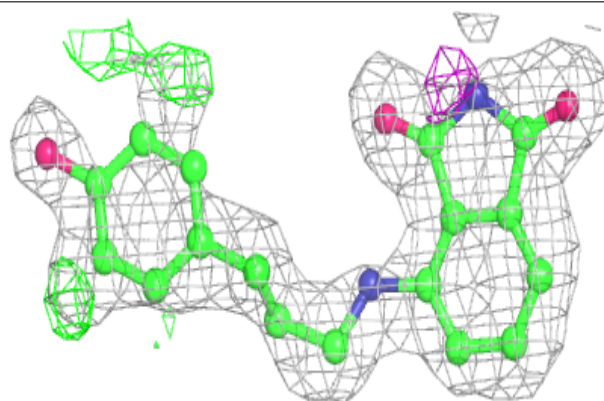


Electron density around KTG C 201:

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

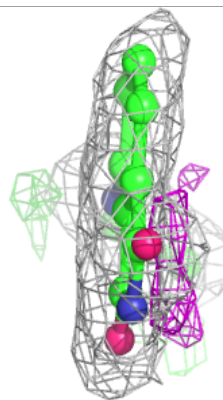
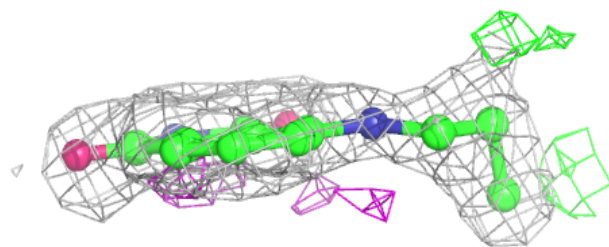
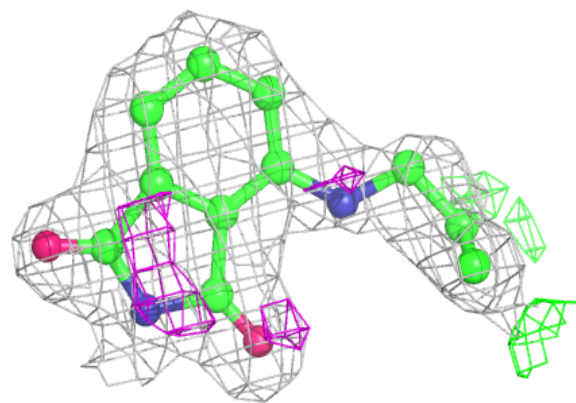
**Electron density around KTG E 201:**

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

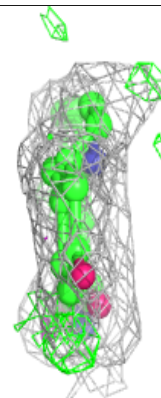
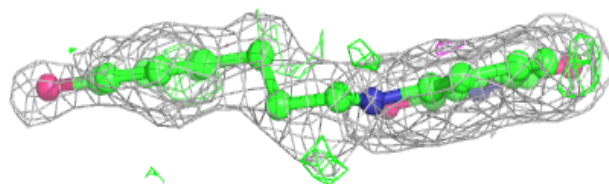
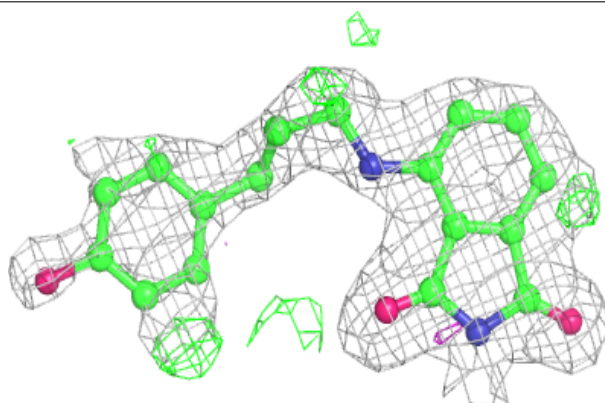


Electron density around KTG H 201:

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

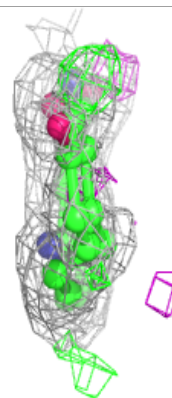
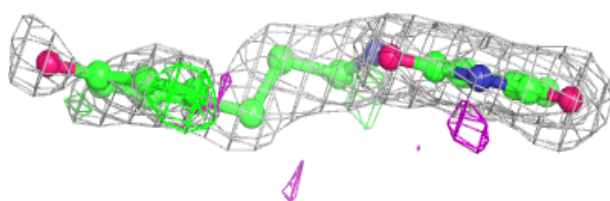
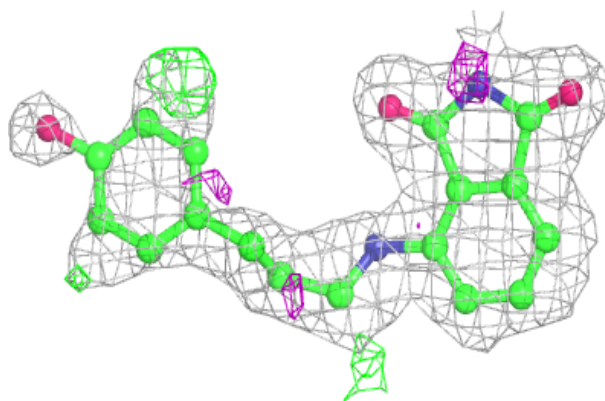
**Electron density around KTG F 201:**

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

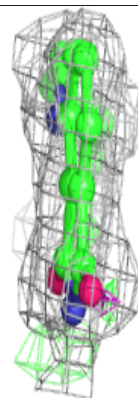
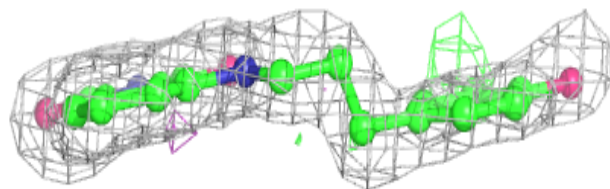
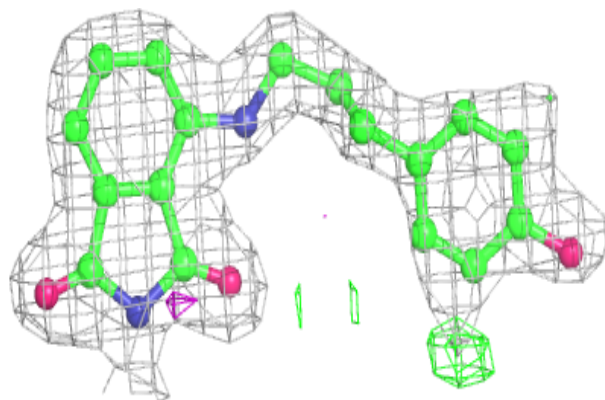


Electron density around KTG B 202:

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

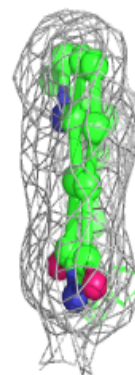
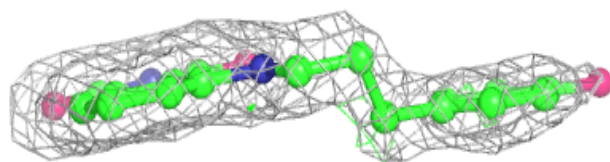
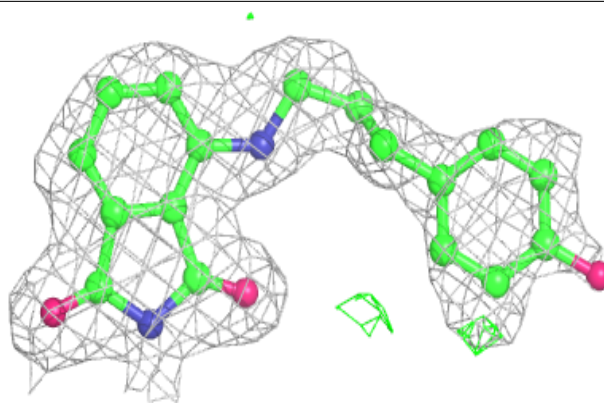
**Electron density around KTG J 201:**

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



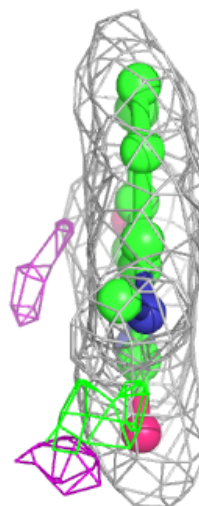
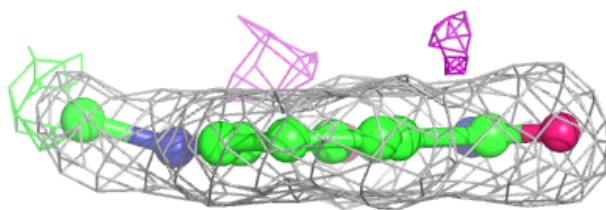
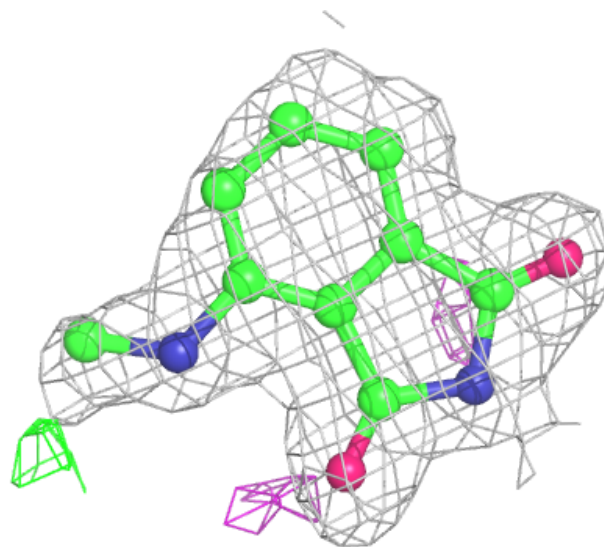
Electron density around KTG L 201:

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



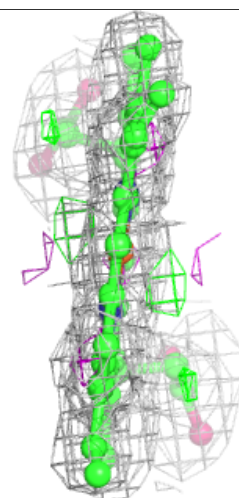
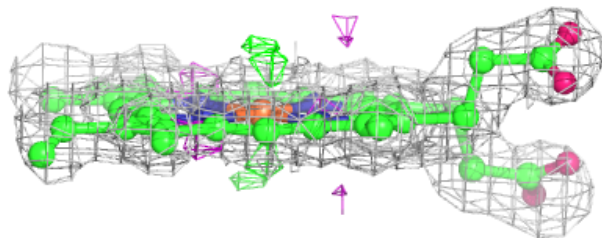
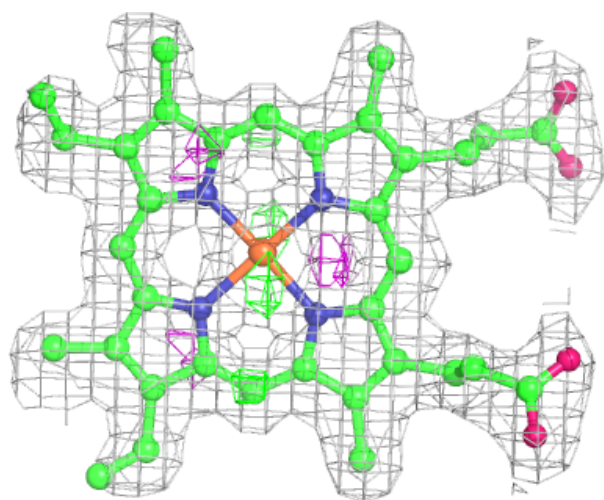
Electron density around KTG A 202:

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



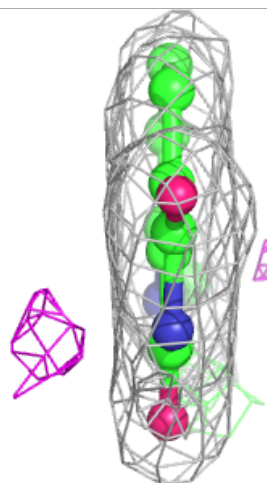
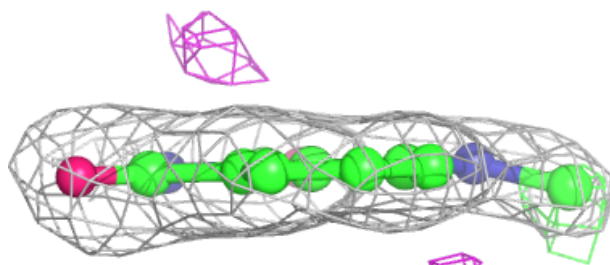
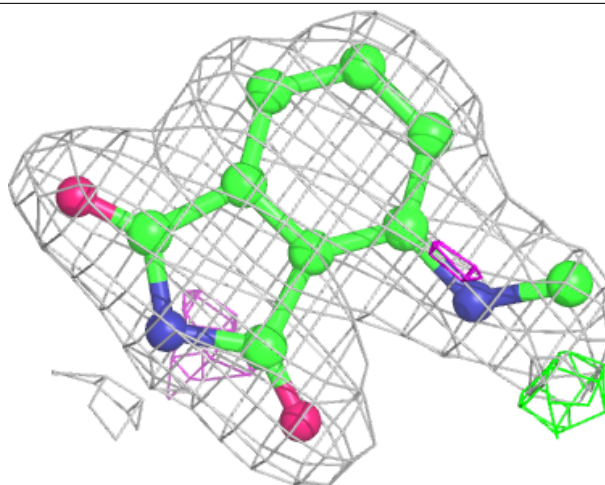
Electron density around HEM L 202:

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



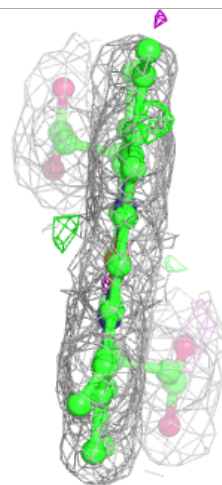
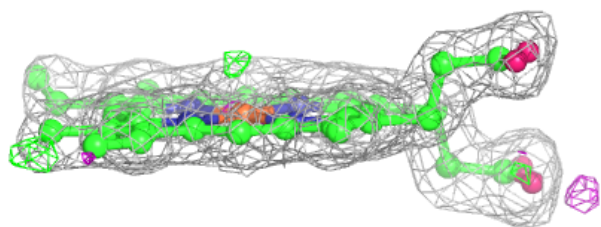
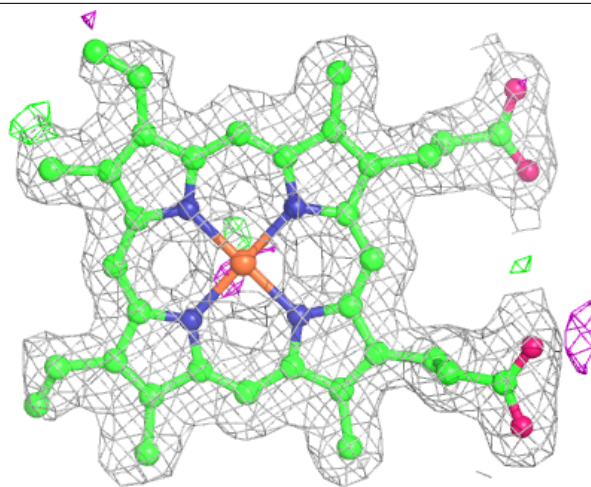
Electron density around KTG D 202:

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



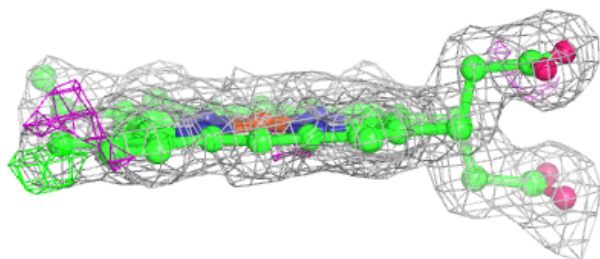
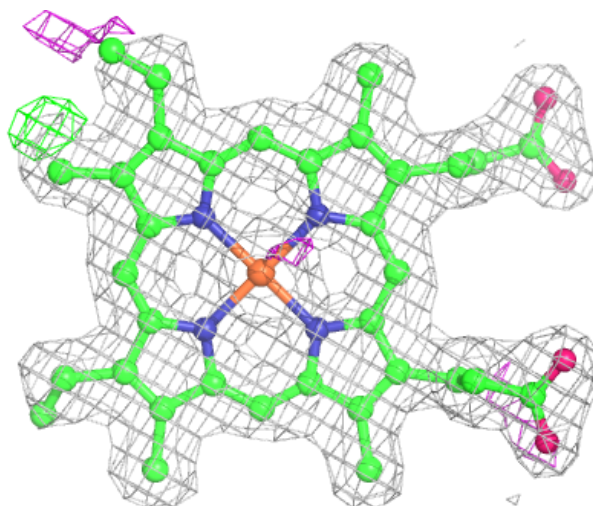
Electron density around HEM H 202:

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



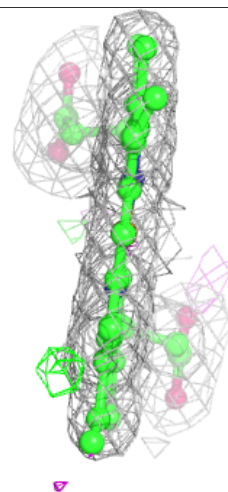
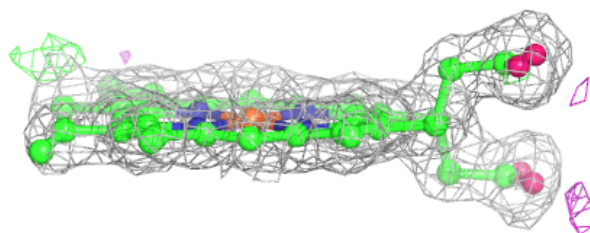
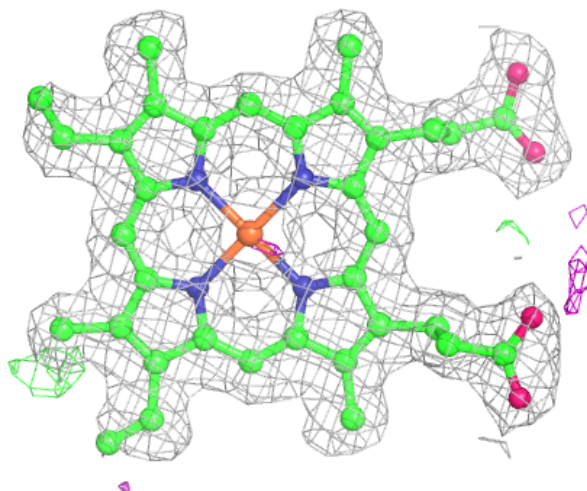
Electron density around HEM F 202:

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



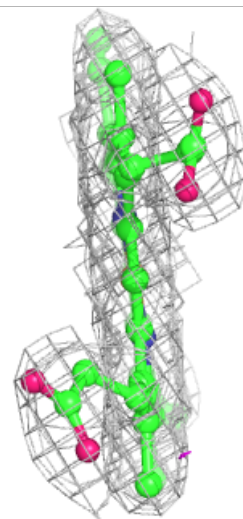
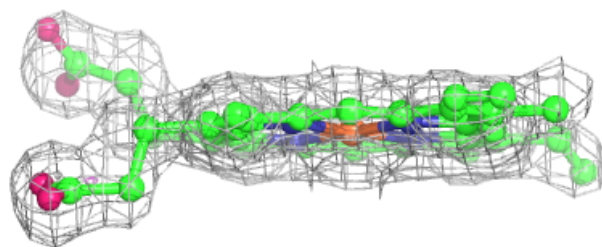
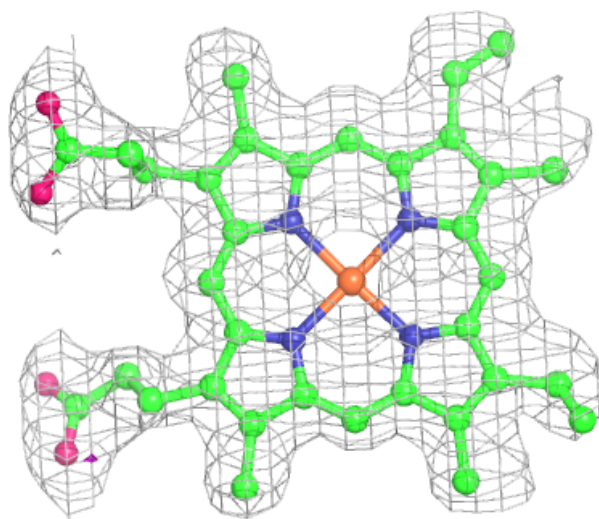
Electron density around HEM C 202:

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



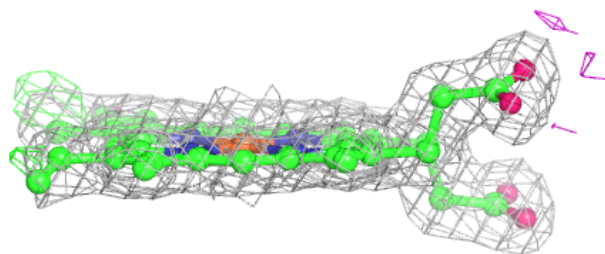
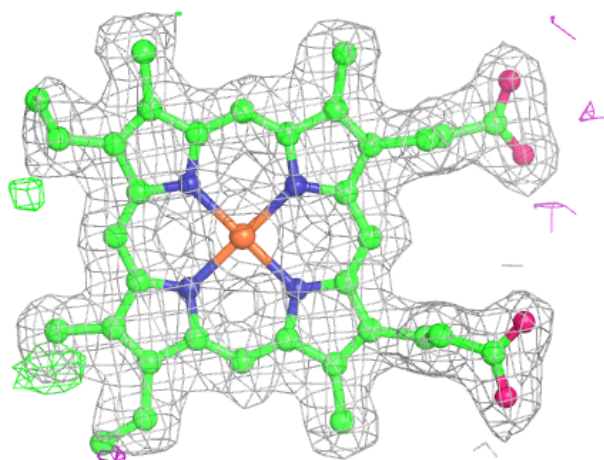
Electron density around HEM D 203:

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



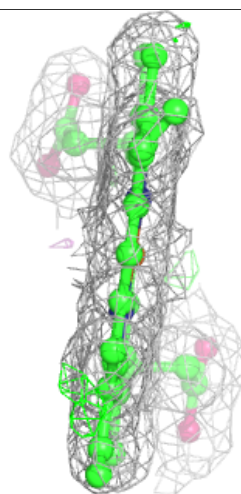
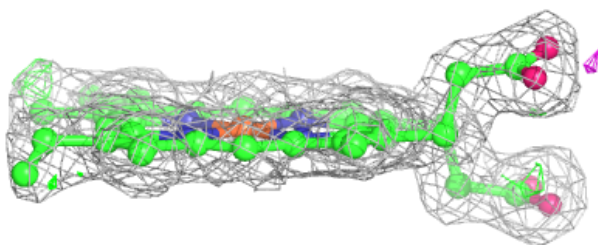
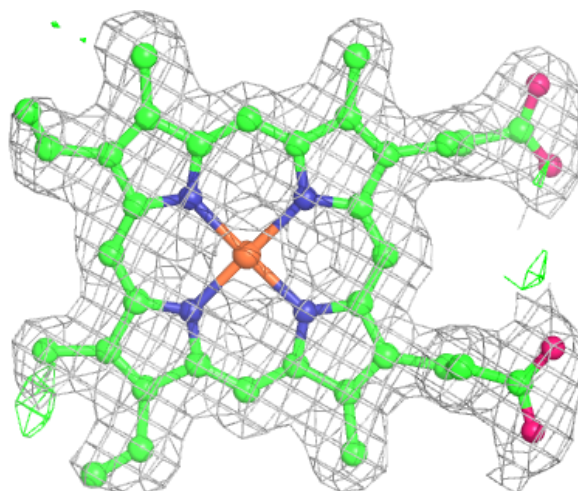
Electron density around HEM E 202:

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



Electron density around HEM 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.