



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 02:54 AM UTC

PDB ID : 6NLL / pdb_00006nll
Title : 1.80 Å resolution structure of WT BfrB from *Pseudomonas aeruginosa* in complex with a protein-protein interaction inhibitor (analog 14)
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 : 1.80 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

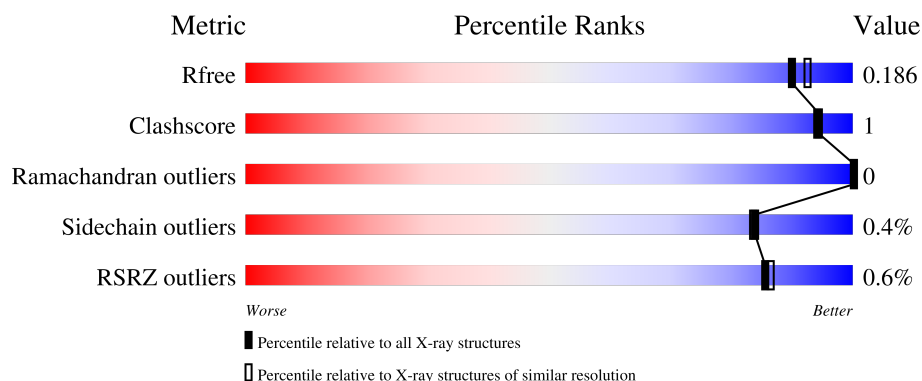
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	% 97% ..
1	D	158	% 97% ..

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Mol	Chain	Length	Quality of chain
1	E	158	% 97% ..
1	F	158	% 95% . .
1	G	158	% 96% . .
1	H	158	96% . . .
1	I	158	% 95% . .
1	J	158	% 94% . . .
1	K	158	% 94% . . .
1	L	158	% 97% ..

2 Entry composition

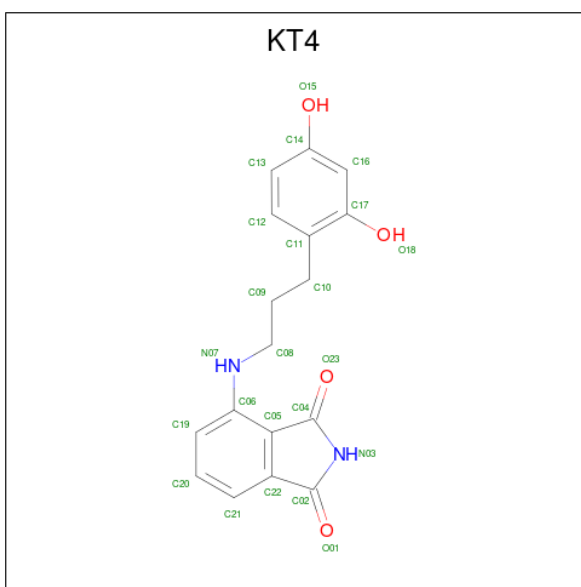
There are 6 unique types of molecules in this entry. The entry contains 17504 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

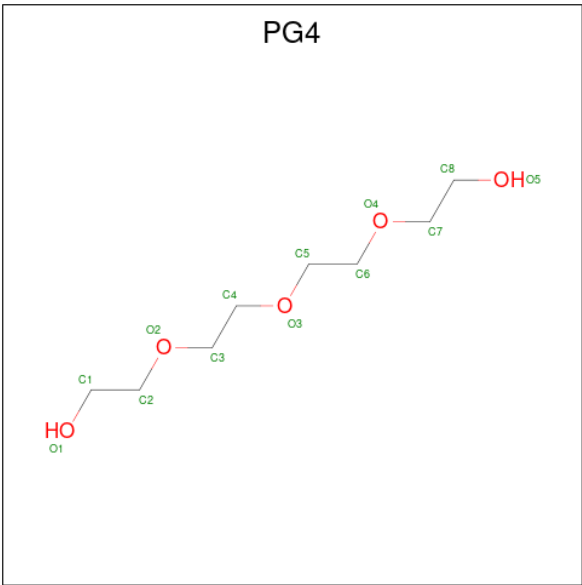
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	156	Total	C	N	O	S	0	1	0
			1271	807	215	242	7			
1	B	155	Total	C	N	O	S	0	2	0
			1265	803	216	239	7			
1	C	155	Total	C	N	O	S	0	1	0
			1254	796	212	239	7			
1	D	155	Total	C	N	O	S	0	1	0
			1268	803	218	240	7			
1	E	155	Total	C	N	O	S	0	1	0
			1266	802	217	240	7			
1	F	156	Total	C	N	O	S	0	2	0
			1272	807	217	241	7			
1	G	155	Total	C	N	O	S	0	2	0
			1260	800	212	241	7			
1	H	155	Total	C	N	O	S	0	2	0
			1264	802	213	242	7			
1	I	155	Total	C	N	O	S	0	1	0
			1256	796	214	239	7			
1	J	155	Total	C	N	O	S	0	2	0
			1267	802	216	242	7			
1	K	155	Total	C	N	O	S	0	2	0
			1260	800	212	241	7			
1	L	156	Total	C	N	O	S	0	2	0
			1271	806	216	242	7			

- Molecule 2 is 4-{{[3-(2,4-dihydroxyphenyl)propyl]amino}-1H-isoindole-1,3(2H)-dione (CCD ID: KT4) (formula: C₁₇H₁₆N₂O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			13	9	2	2		
2	B	1	Total	C	N	O	0	0
			23	17	2	4		
2	C	1	Total	C	N	O	0	0
			23	17	2	4		
2	D	1	Total	C	N	O	0	0
			13	9	2	2		
2	E	1	Total	C	N	O	0	0
			23	17	2	4		
2	F	1	Total	C	N	O	0	0
			23	17	2	4		
2	G	1	Total	C	N	O	0	0
			16	12	2	2		
2	H	1	Total	C	N	O	0	0
			15	11	2	2		
2	I	1	Total	C	N	O	0	0
			23	17	2	4		
2	J	1	Total	C	N	O	0	0
			23	17	2	4		
2	K	1	Total	C	N	O	0	0
			23	17	2	4		
2	L	1	Total	C	N	O	0	0
			23	17	2	4		

- Molecule 3 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	6	4		
3	A	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			11	7	4		
3	B	1	Total	C	O	0	0
			10	6	4		
3	C	1	Total	C	O	0	0
			11	7	4		
3	D	1	Total	C	O	0	0
			13	8	5		
3	D	1	Total	C	O	0	0
			8	5	3		
3	E	1	Total	C	O	0	0
			13	8	5		
3	E	1	Total	C	O	0	0
			13	8	5		
3	F	1	Total	C	O	0	0
			13	8	5		
3	F	1	Total	C	O	0	0
			8	5	3		
3	G	1	Total	C	O	0	0
			13	8	5		
3	G	1	Total	C	O	0	0
			10	6	4		
3	H	1	Total	C	O	0	0
			13	8	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	H	1	Total 13	C 8	O 5	0	0
3	H	1	Total 11	C 7	O 4	0	0
3	I	1	Total 13	C 8	O 5	0	0
3	J	1	Total 13	C 8	O 5	0	0
3	J	1	Total 10	C 6	O 4	0	0
3	K	1	Total 13	C 8	O 5	0	0
3	K	1	Total 10	C 6	O 4	0	0
3	L	1	Total 13	C 8	O 5	0	0
3	L	1	Total 13	C 8	O 5	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	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0



WORLD WIDE
PDB
PROTEIN DATA BANK

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

- Molecule 5 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	124	Total	O		
			124	124	0	0
6	B	123	Total	O		
			123	123	0	0
6	C	130	Total	O		
			130	130	0	0
6	D	133	Total	O		
			133	133	0	0
6	E	140	Total	O		
			140	140	0	0
6	F	121	Total	O		
			121	121	0	0
6	G	133	Total	O		
			133	133	0	0
6	H	131	Total	O		
			131	131	0	0
6	I	116	Total	O		
			116	116	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	J	135	Total 135	O 135	0	0
6	K	122	Total 122	O 122	0	0
6	L	115	Total 115	O 115	0	0

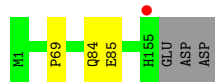
3 Residue-property plots [i](#)

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.

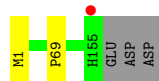
- Molecule 1: Ferroxidase



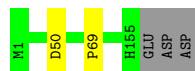
- Molecule 1: Ferroxidase



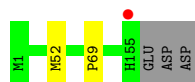
- Molecule 1: Ferroxidase



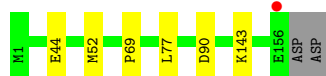
- Molecule 1: Ferroxidase



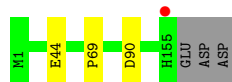
- Molecule 1: Ferroxidase



- Molecule 1: Ferroxidase



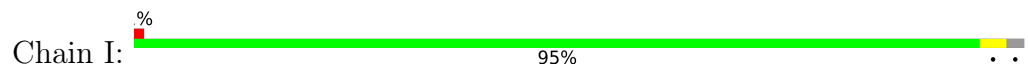
- Molecule 1: Ferroxidase



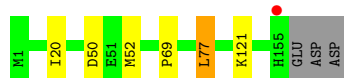
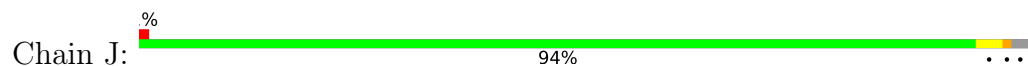
- Molecule 1: Ferroxidase



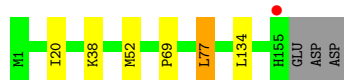
- Molecule 1: Ferroxidase



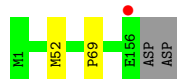
- Molecule 1: Ferroxidase



- 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	129.60Å 194.39Å 202.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.76 – 1.80 46.76 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.2 (46.76-1.80) 99.3 (46.76-1.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 1.79Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.152 , 0.179 0.163 , 0.186	Depositor DCC
R_{free} test set	11587 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	24.0	Xtriage
Anisotropy	0.418	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 39.8	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	17504	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 2.74% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: KT4, HEM, PG4, 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	0.39	0/1295	0.52	0/1744
1	B	0.38	0/1292	0.49	0/1741
1	C	0.39	0/1278	0.51	0/1724
1	D	0.37	0/1292	0.50	0/1740
1	E	0.42	0/1290	0.54	0/1738
1	F	0.40	0/1299	0.49	0/1751
1	G	0.40	0/1287	0.52	0/1736
1	H	0.39	0/1291	0.53	0/1741
1	I	0.41	0/1280	0.53	0/1727
1	J	0.42	0/1294	0.52	0/1745
1	K	0.37	0/1287	0.52	0/1736
1	L	0.38	0/1298	0.50	0/1750
All	All	0.39	0/15483	0.51	0/20873

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

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	1271	0	1249	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1265	0	1243	3	0
1	C	1254	0	1221	2	0
1	D	1268	0	1252	1	0
1	E	1266	0	1245	2	0
1	F	1272	0	1244	4	0
1	G	1260	0	1227	2	0
1	H	1264	0	1233	4	0
1	I	1256	0	1221	3	0
1	J	1267	0	1238	5	0
1	K	1260	0	1227	5	0
1	L	1271	0	1240	2	0
2	A	13	0	0	1	0
2	B	23	0	0	1	0
2	C	23	0	0	1	0
2	D	13	0	0	1	0
2	E	23	0	0	1	0
2	F	23	0	0	1	0
2	G	16	0	0	1	0
2	H	15	0	0	1	0
2	I	23	0	0	1	0
2	J	23	0	0	1	0
2	K	23	0	0	1	0
2	L	23	0	0	1	0
3	A	17	0	21	0	0
3	B	21	0	26	0	0
3	C	11	0	13	0	0
3	D	21	0	26	0	0
3	E	26	0	36	0	0
3	F	21	0	27	1	0
3	G	23	0	31	0	0
3	H	37	0	49	1	0
3	I	13	0	18	0	0
3	J	23	0	31	1	0
3	K	23	0	31	1	0
3	L	26	0	36	0	0
4	A	43	0	30	0	0
4	D	43	0	30	0	0
4	E	43	0	30	2	0
4	F	43	0	30	2	0
4	H	43	0	30	2	0
4	I	43	0	30	2	0
4	L	43	0	30	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
6	A	124	0	0	0	1
6	B	123	0	0	2	0
6	C	130	0	0	0	0
6	D	133	0	0	0	0
6	E	140	0	0	0	0
6	F	121	0	0	1	0
6	G	133	0	0	0	1
6	H	131	0	0	1	0
6	I	116	0	0	0	0
6	J	135	0	0	2	0
6	K	122	0	0	1	0
6	L	115	0	0	0	0
All	All	17504	0	15395	40	1

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 1.

The worst 5 of 40 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:J:50[A]:ASP:OD1	6:J:301:HOH:O	1.97	0.82
1:C:1:MET:SD	6:F:398:HOH:O	2.53	0.66
1:G:69:PRO:O	2:G:201:KT4:N03	2.34	0.61
1:H:69:PRO:O	2:H:201:KT4:N03	2.34	0.61
1:I:69:PRO:O	2:I:201:KT4:N03	2.34	0.61

All (1) 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:A:420:HOH:O	6:G:381:HOH:O[3_554]	2.18	0.02

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%)	155 (100%)	0	0	100	100
1	B	155/158 (98%)	154 (99%)	1 (1%)	0	100	100
1	C	154/158 (98%)	154 (100%)	0	0	100	100
1	D	154/158 (98%)	153 (99%)	1 (1%)	0	100	100
1	E	154/158 (98%)	154 (100%)	0	0	100	100
1	F	156/158 (99%)	156 (100%)	0	0	100	100
1	G	155/158 (98%)	154 (99%)	1 (1%)	0	100	100
1	H	155/158 (98%)	154 (99%)	1 (1%)	0	100	100
1	I	154/158 (98%)	154 (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	156/158 (99%)	155 (99%)	1 (1%)	0	100	100
All	All	1858/1896 (98%)	1851 (100%)	7 (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%)	136 (99%)	1 (1%)	76	73
1	B	136/144 (94%)	136 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	134/144 (93%)	134 (100%)	0	100	100
1	D	138/144 (96%)	137 (99%)	1 (1%)	76	73
1	E	137/144 (95%)	137 (100%)	0	100	100
1	F	136/144 (94%)	135 (99%)	1 (1%)	76	73
1	G	135/144 (94%)	135 (100%)	0	100	100
1	H	136/144 (94%)	135 (99%)	1 (1%)	76	73
1	I	134/144 (93%)	133 (99%)	1 (1%)	76	73
1	J	137/144 (95%)	136 (99%)	1 (1%)	76	73
1	K	135/144 (94%)	134 (99%)	1 (1%)	76	73
1	L	136/144 (94%)	136 (100%)	0	100	100
All	All	1631/1728 (94%)	1624 (100%)	7 (0%)	84	83

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

Mol	Chain	Res	Type
1	H	82	ASN
1	I	50	ASP
1	K	77	LEU
1	J	77	LEU
1	F	77	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	151	GLN
1	J	88	GLN
1	J	9	GLN
1	J	137	GLN
1	E	88	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 45 ligands modelled in this entry, 3 are monoatomic - leaving 42 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	$\# Z > 2$
2	KT4	K	201	-	25,25,25	1.80	4 (16%)	35,35,35	1.26	3 (8%)
2	KT4	B	201	-	25,25,25	1.69	6 (24%)	35,35,35	1.25	3 (8%)
4	HEM	F	204	1	50,50,50	1.35	8 (16%)	67,82,82	1.12	5 (7%)
3	PG4	H	202	-	12,12,12	0.45	0	11,11,11	0.51	0
2	KT4	I	201	-	25,25,25	1.62	4 (16%)	35,35,35	1.29	3 (8%)
3	PG4	A	202	-	9,9,12	0.51	0	8,8,11	0.26	0
3	PG4	F	203	-	7,7,12	0.43	0	6,6,11	0.30	0
3	PG4	E	203	-	12,12,12	0.44	0	11,11,11	0.36	0
3	PG4	D	202	-	12,12,12	0.53	0	11,11,11	0.46	0
3	PG4	G	203	-	9,9,12	0.47	0	8,8,11	0.54	0
3	PG4	C	202	-	10,10,12	0.45	0	9,9,11	0.35	0
3	PG4	H	203	-	12,12,12	0.39	0	11,11,11	0.59	0
3	PG4	K	202	-	12,12,12	0.38	0	11,11,11	0.57	0
4	HEM	D	204	1	50,50,50	1.41	7 (14%)	67,82,82	1.10	4 (5%)
2	KT4	C	201	-	25,25,25	1.70	5 (20%)	35,35,35	1.09	2 (5%)
4	HEM	A	204	1	50,50,50	1.46	8 (16%)	67,82,82	1.38	8 (11%)
3	PG4	D	203	-	7,7,12	0.49	0	6,6,11	0.35	0
3	PG4	K	203	-	9,9,12	0.42	0	8,8,11	0.22	0
3	PG4	A	203	-	6,6,12	0.34	0	5,5,11	0.57	0
4	HEM	I	203	1	50,50,50	1.39	9 (18%)	67,82,82	1.26	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	KT4	L	201	-	25,25,25	1.79	4 (16%)	35,35,35	1.02	3 (8%)
3	PG4	J	203	-	9,9,12	0.54	0	8,8,11	1.46	2 (25%)
2	KT4	E	201	-	25,25,25	1.73	6 (24%)	35,35,35	1.38	3 (8%)
2	KT4	F	201	-	25,25,25	1.70	4 (16%)	35,35,35	1.23	2 (5%)
3	PG4	J	202	-	12,12,12	0.43	0	11,11,11	0.49	0
3	PG4	L	202	-	12,12,12	0.55	0	11,11,11	0.24	0
3	PG4	G	202	-	12,12,12	0.49	0	11,11,11	0.63	0
2	KT4	G	201	-	17,17,25	1.85	5 (29%)	23,23,35	1.46	3 (13%)
3	PG4	B	202	-	10,10,12	0.45	0	9,9,11	0.37	0
3	PG4	F	202	-	12,12,12	0.48	0	11,11,11	0.41	0
2	KT4	H	201	-	16,16,25	1.88	5 (31%)	22,22,35	1.51	3 (13%)
2	KT4	A	201	-	14,14,25	2.54	5 (35%)	19,20,35	1.92	4 (21%)
3	PG4	H	204	-	10,10,12	0.54	0	9,9,11	0.31	0
3	PG4	E	202	-	12,12,12	0.54	0	11,11,11	0.38	0
3	PG4	I	202	-	12,12,12	0.47	0	11,11,11	0.56	0
4	HEM	L	204	1	50,50,50	1.42	7 (14%)	67,82,82	1.30	9 (13%)
2	KT4	D	201	-	14,14,25	2.52	5 (35%)	19,20,35	1.95	4 (21%)
4	HEM	E	204	1	50,50,50	1.33	7 (14%)	67,82,82	1.35	11 (16%)
3	PG4	L	203	-	12,12,12	0.52	0	11,11,11	0.32	0
3	PG4	B	203	-	9,9,12	0.45	0	8,8,11	0.44	0
2	KT4	J	201	-	25,25,25	1.74	5 (20%)	35,35,35	1.24	4 (11%)
4	HEM	H	205	1	50,50,50	1.28	7 (14%)	67,82,82	1.32	9 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	KT4	K	201	-	-	0/7/19/19	0/3/3/3
2	KT4	B	201	-	-	1/7/19/19	0/3/3/3
4	HEM	F	204	1	-	4/14/54/54	-
3	PG4	H	202	-	-	0/10/10/10	-
2	KT4	I	201	-	-	0/7/19/19	0/3/3/3
3	PG4	A	202	-	-	1/7/7/10	-
3	PG4	F	203	-	-	0/5/5/10	-
3	PG4	E	203	-	-	3/10/10/10	-
3	PG4	D	202	-	-	0/10/10/10	-
3	PG4	G	203	-	-	4/7/7/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PG4	C	202	-	-	0/8/8/10	-
3	PG4	H	203	-	-	7/10/10/10	-
3	PG4	K	202	-	-	5/10/10/10	-
4	HEM	D	204	1	-	2/14/54/54	-
2	KT4	C	201	-	-	1/7/19/19	0/3/3/3
4	HEM	A	204	1	-	4/14/54/54	-
3	PG4	D	203	-	-	0/5/5/10	-
3	PG4	K	203	-	-	1/7/7/10	-
3	PG4	A	203	-	-	1/4/4/10	-
4	HEM	I	203	1	-	4/14/54/54	-
2	KT4	L	201	-	-	0/7/19/19	0/3/3/3
3	PG4	J	203	-	-	2/7/7/10	-
2	KT4	E	201	-	-	0/7/19/19	0/3/3/3
2	KT4	F	201	-	-	0/7/19/19	0/3/3/3
3	PG4	J	202	-	-	4/10/10/10	-
3	PG4	L	202	-	-	0/10/10/10	-
3	PG4	G	202	-	-	1/10/10/10	-
2	KT4	G	201	-	-	3/5/17/19	0/2/2/3
3	PG4	B	202	-	-	0/8/8/10	-
3	PG4	F	202	-	-	0/10/10/10	-
2	KT4	H	201	-	-	2/4/16/19	0/2/2/3
2	KT4	A	201	-	-	0/2/14/19	0/2/2/3
3	PG4	H	204	-	-	2/8/8/10	-
3	PG4	E	202	-	-	0/10/10/10	-
3	PG4	I	202	-	-	4/10/10/10	-
4	HEM	L	204	1	-	4/14/54/54	-
2	KT4	D	201	-	-	0/2/14/19	0/2/2/3
4	HEM	E	204	1	-	4/14/54/54	-
3	PG4	L	203	-	-	6/10/10/10	-
3	PG4	B	203	-	-	2/7/7/10	-
2	KT4	J	201	-	-	0/7/19/19	0/3/3/3
4	HEM	H	205	1	-	4/14/54/54	-

The worst 5 of 111 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	201	KT4	C06-N07	4.81	1.46	1.37
2	C	201	KT4	C22-C02	4.75	1.55	1.48
2	A	201	KT4	C22-C02	4.63	1.55	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	204	HEM	FE-ND	4.63	2.09	1.94
2	A	201	KT4	C04-N03	4.57	1.45	1.38

The worst 5 of 91 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	201	KT4	C04-N03-C02	-5.58	107.74	112.59
2	D	201	KT4	C04-N03-C02	-5.47	107.84	112.59
2	E	201	KT4	C05-C06-N07	-4.82	115.59	121.34
2	B	201	KT4	C05-C06-N07	-4.75	115.67	121.34
2	D	201	KT4	C22-C05-C06	-4.33	119.64	121.88

There are no chirality outliers.

5 of 76 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	203	PG4	O2-C3-C4-O3
3	J	202	PG4	O1-C1-C2-O2
3	K	202	PG4	O4-C7-C8-O5
3	I	202	PG4	O1-C1-C2-O2
2	G	201	KT4	N07-C08-C09-C10

There are no ring outliers.

21 monomers are involved in 25 short contacts:

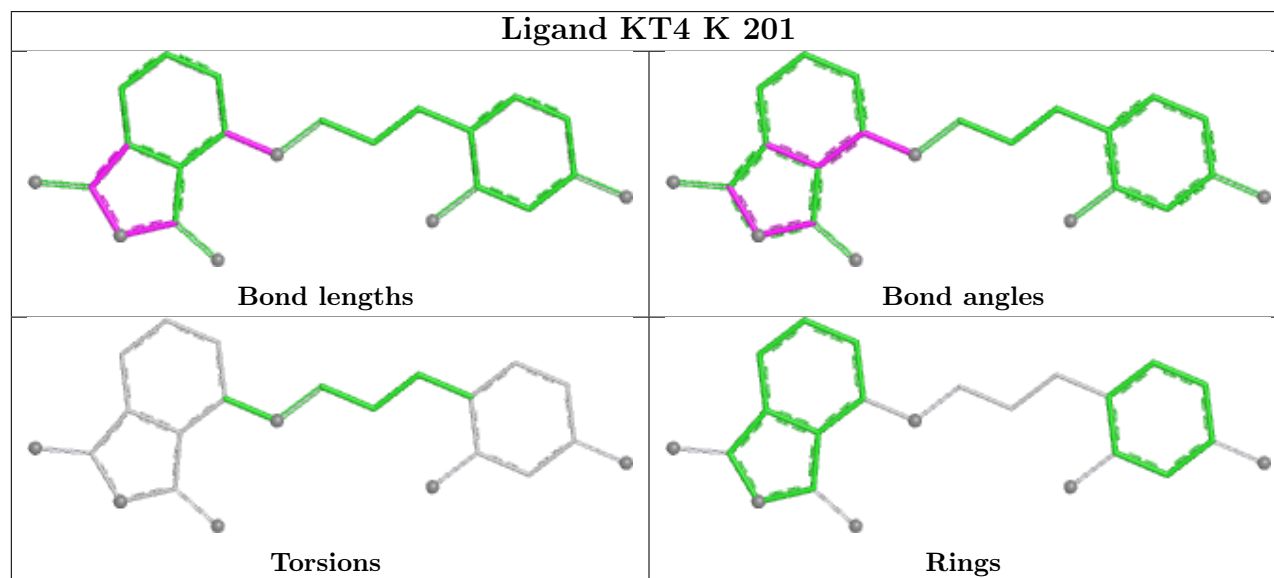
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	201	KT4	1	0
2	B	201	KT4	1	0
4	F	204	HEM	2	0
2	I	201	KT4	1	0
3	F	203	PG4	1	0
3	K	202	PG4	1	0
2	C	201	KT4	1	0
4	I	203	HEM	2	0
2	L	201	KT4	1	0
3	J	203	PG4	1	0
2	E	201	KT4	1	0
2	F	201	KT4	1	0
2	G	201	KT4	1	0
2	H	201	KT4	1	0
2	A	201	KT4	1	0

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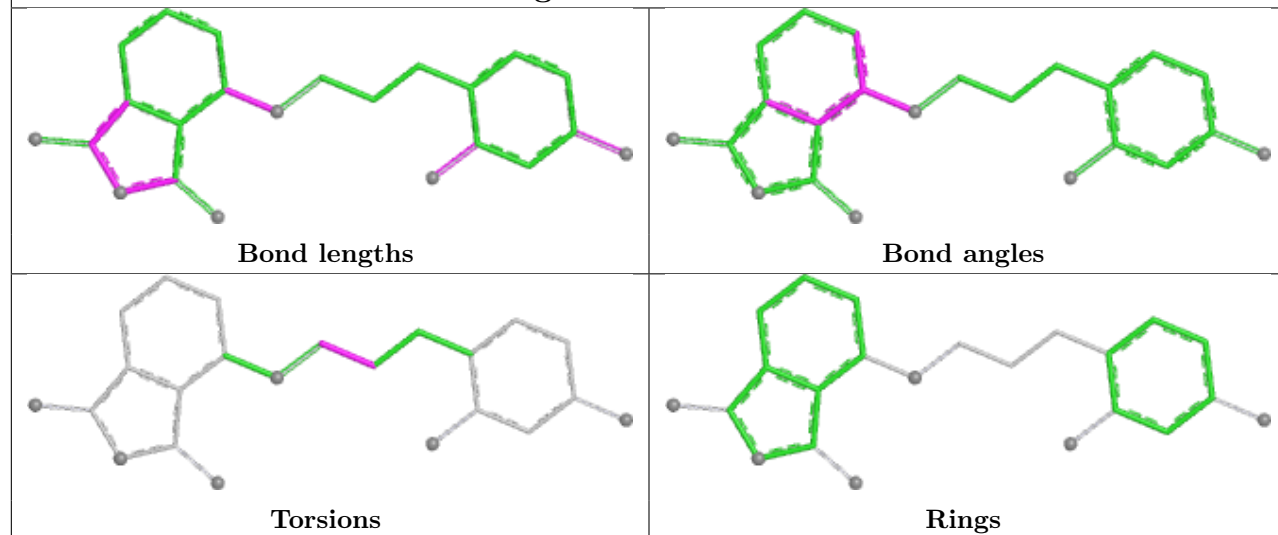
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	204	PG4	1	0
4	L	204	HEM	1	0
2	D	201	KT4	1	0
4	E	204	HEM	2	0
2	J	201	KT4	1	0
4	H	205	HEM	2	0

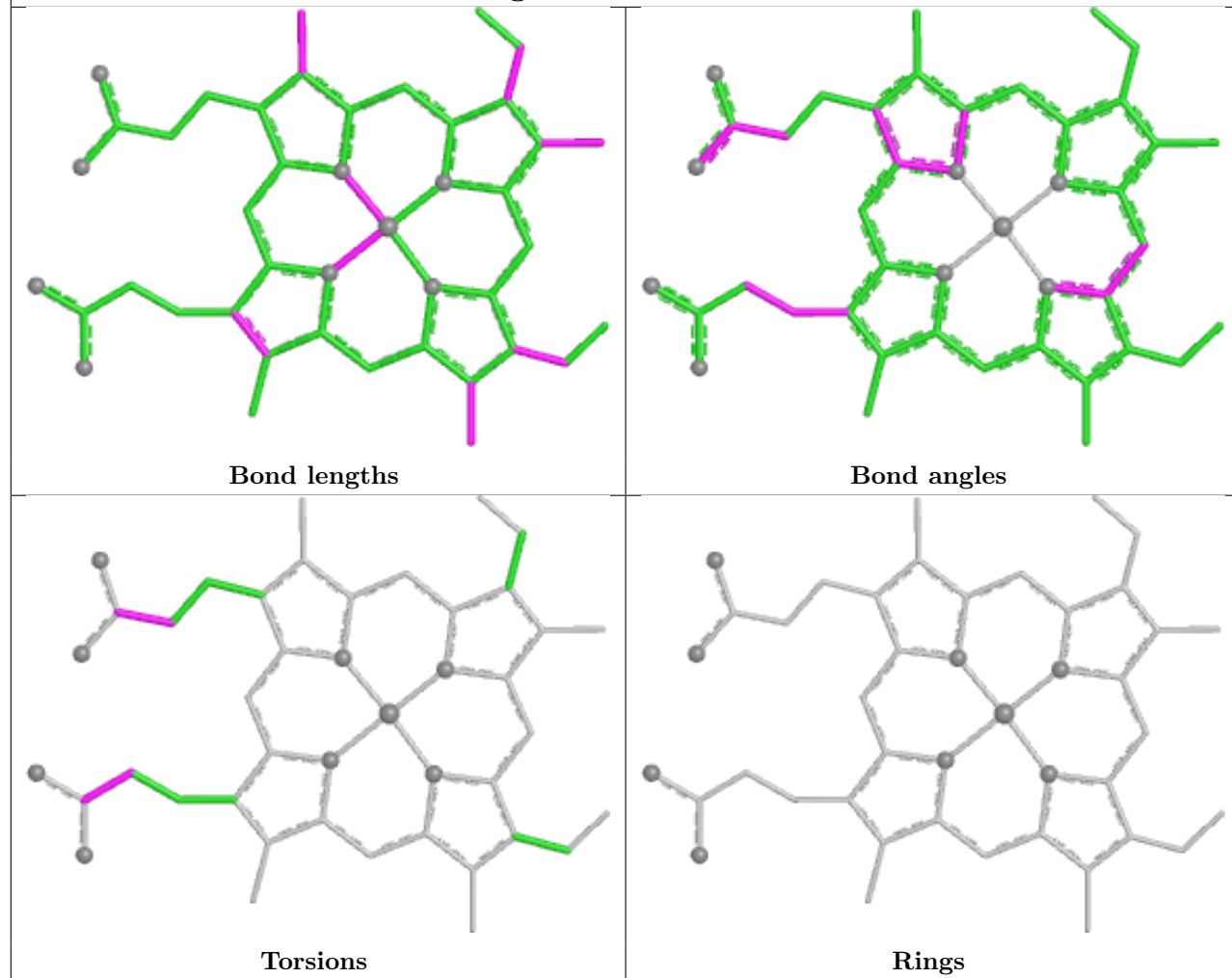
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



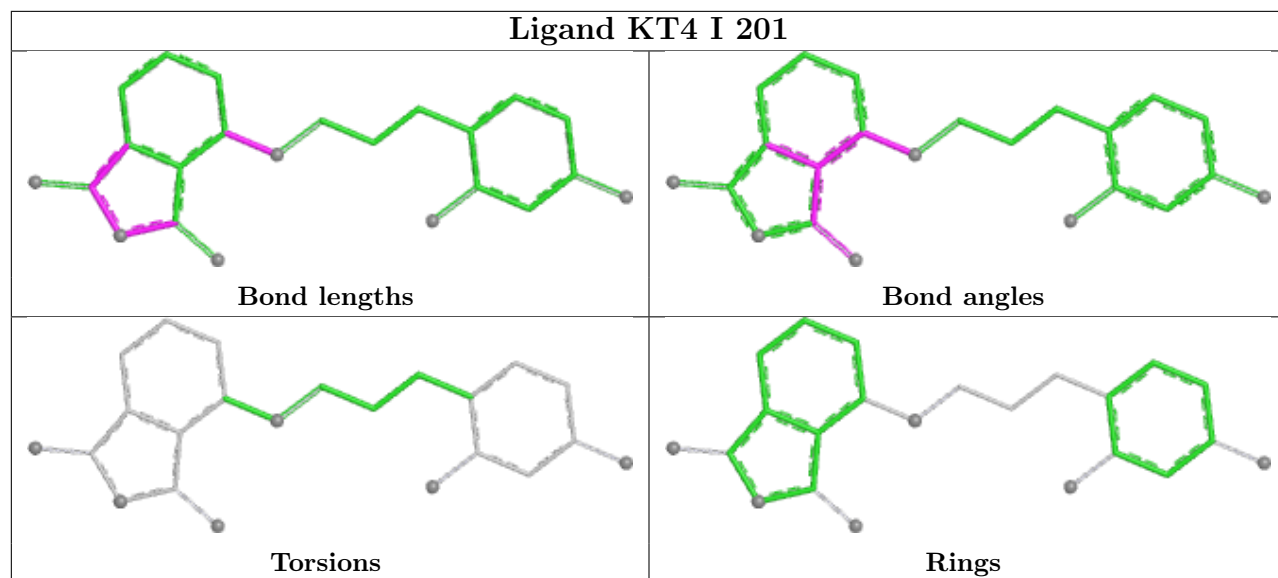
Ligand KT4 B 201



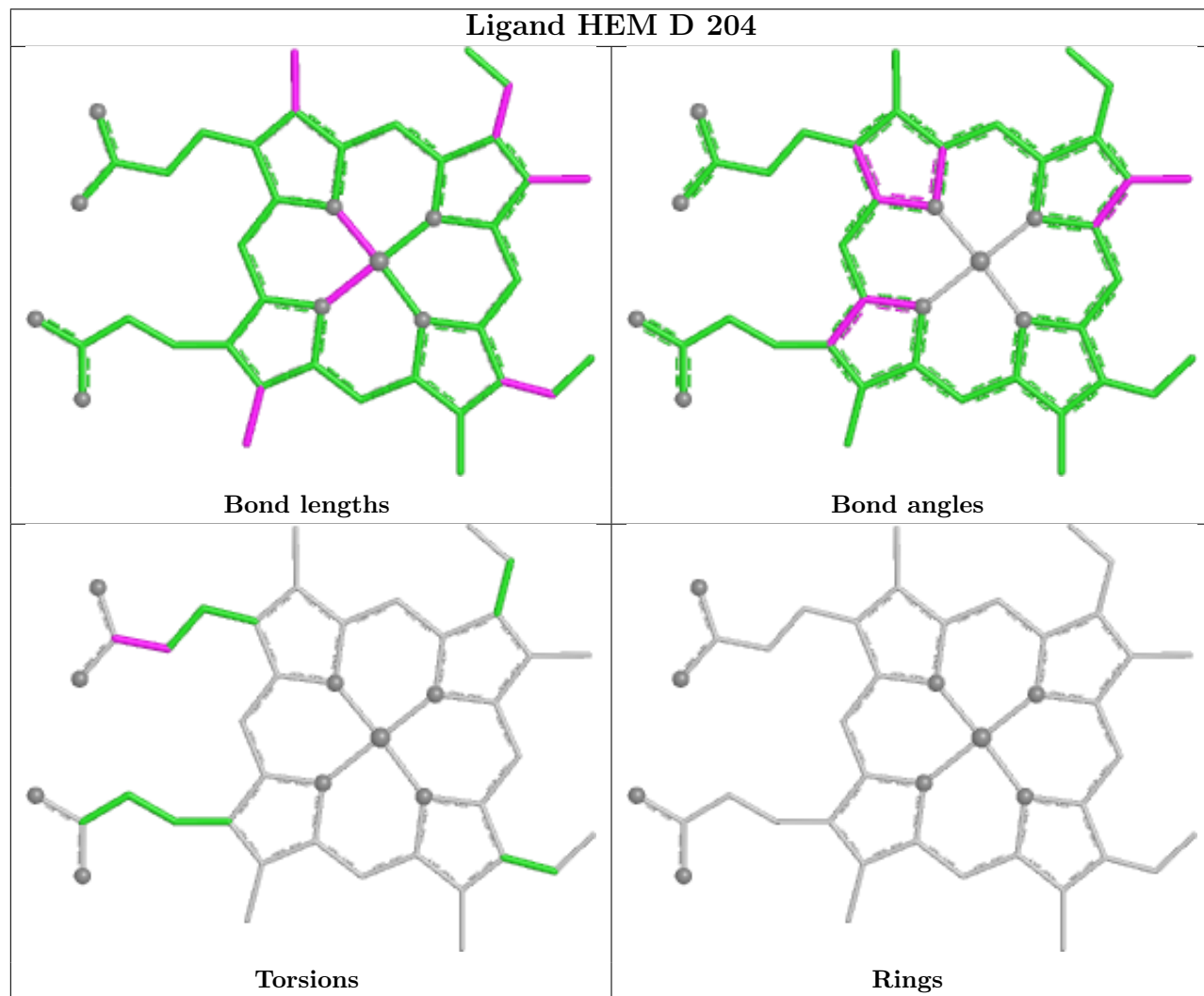
Ligand HEM F 204



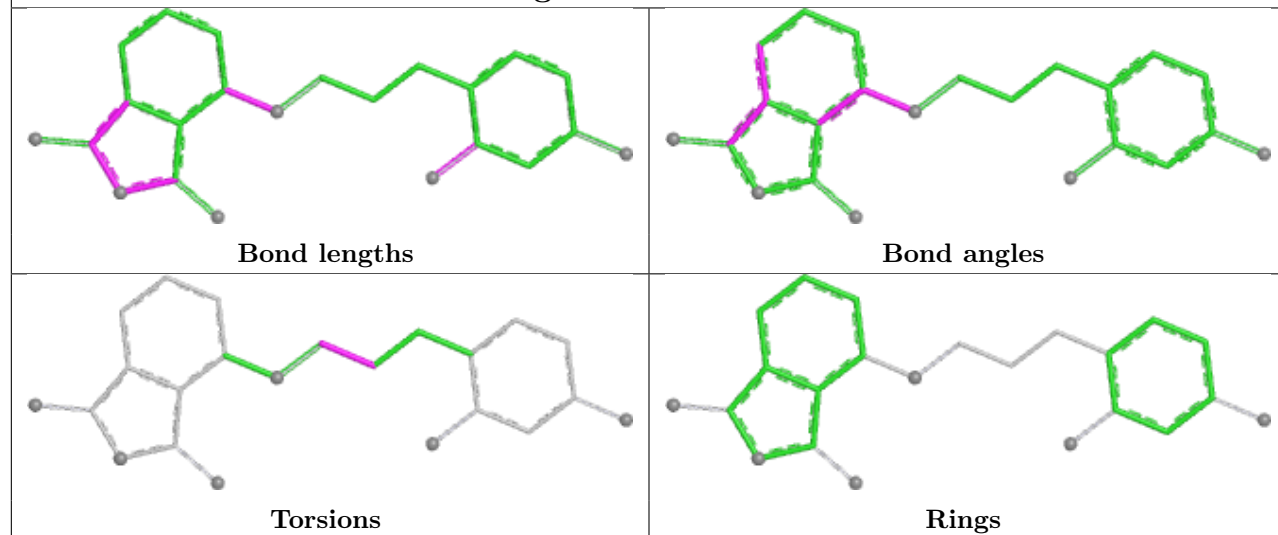
Ligand KT4 I 201



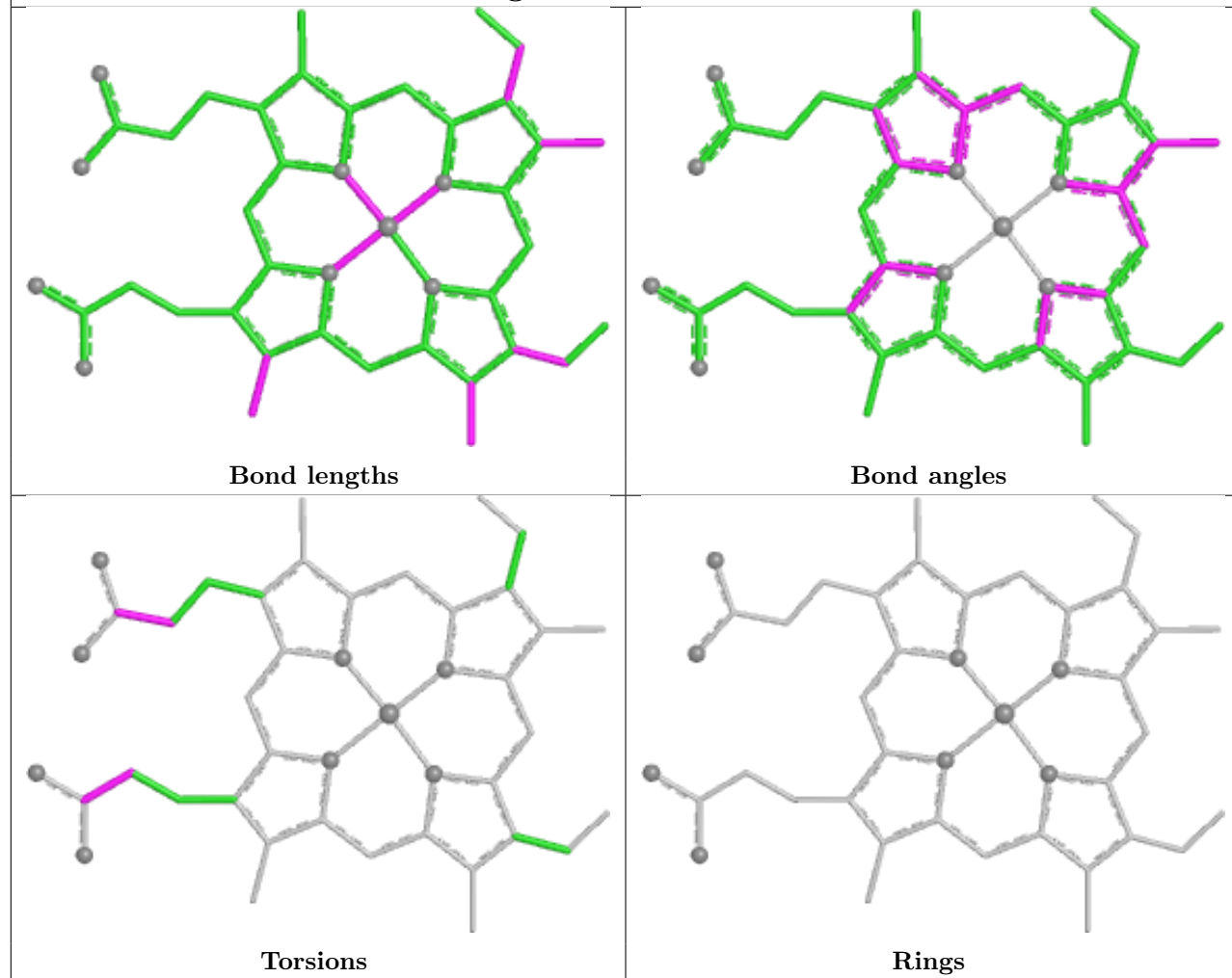
Ligand HEM D 204



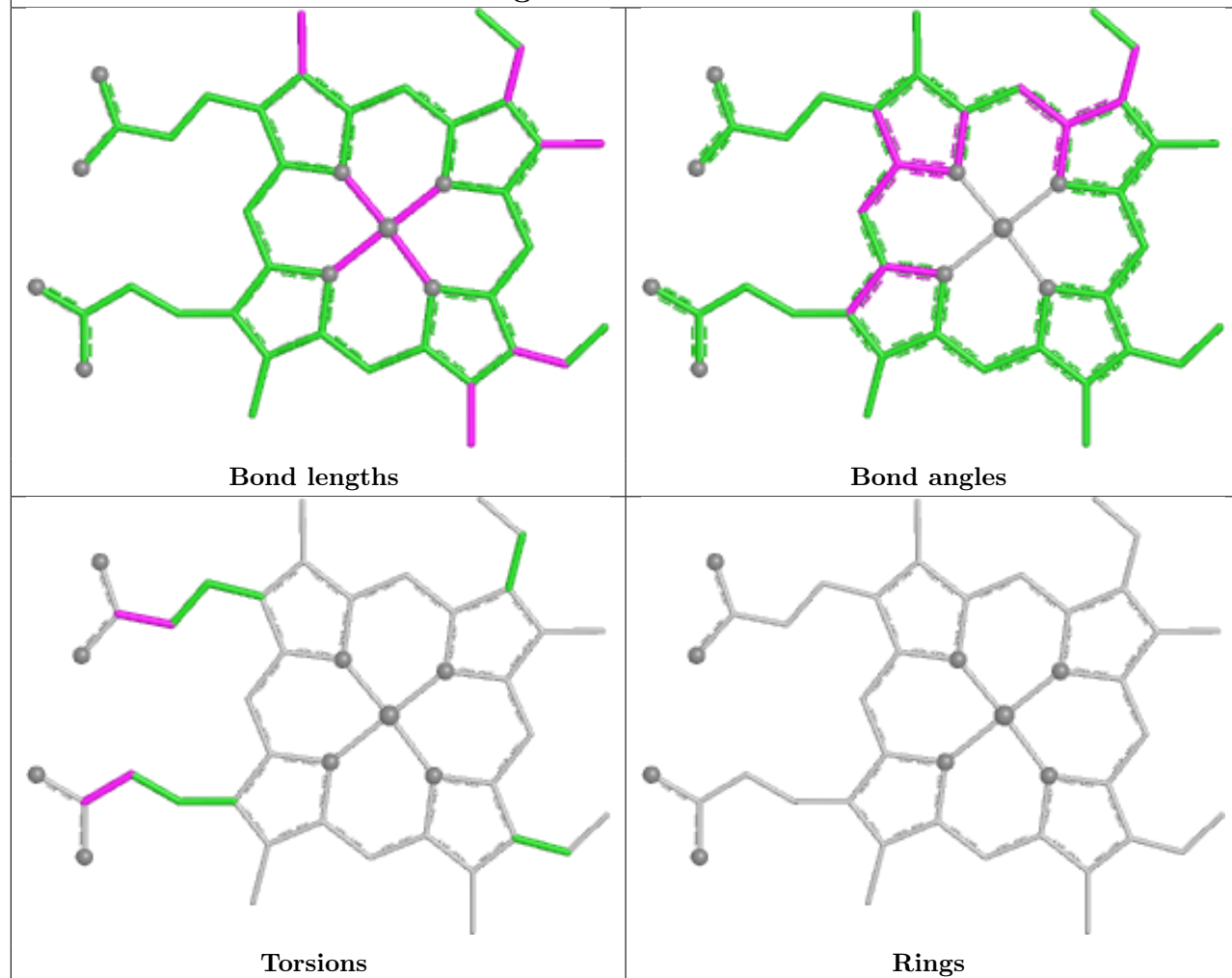
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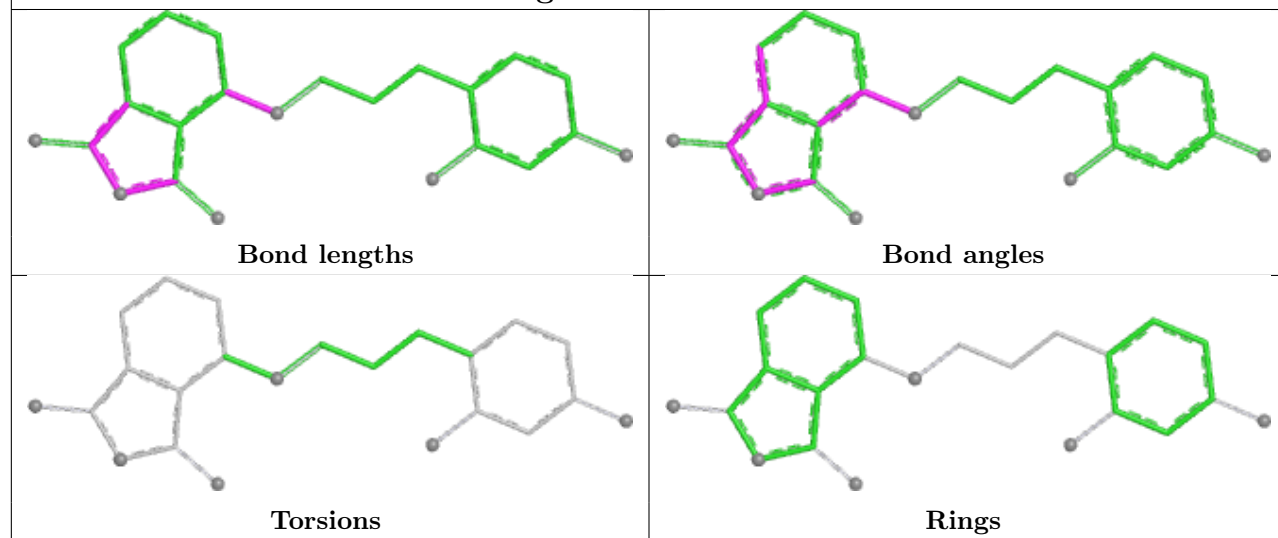
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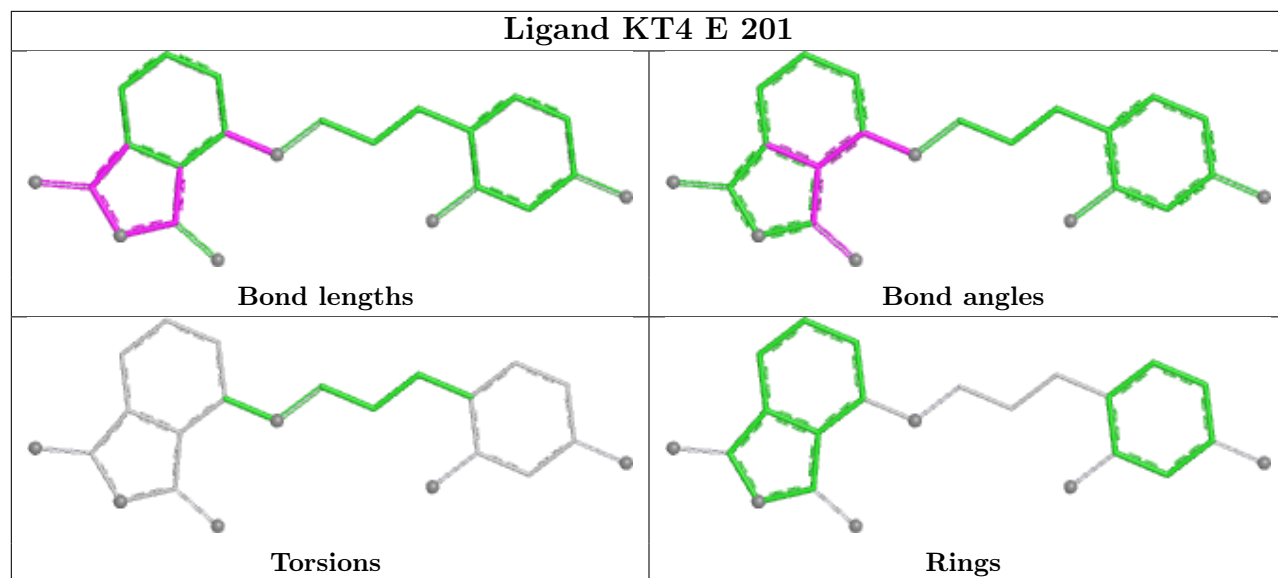
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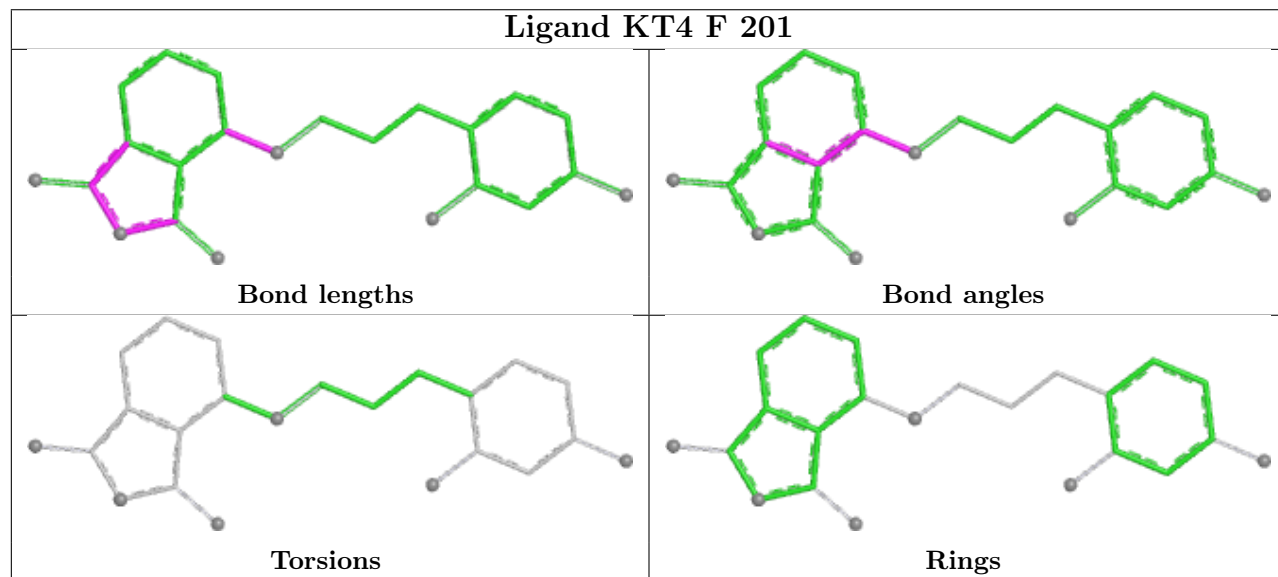
Ligand KT4 L 201



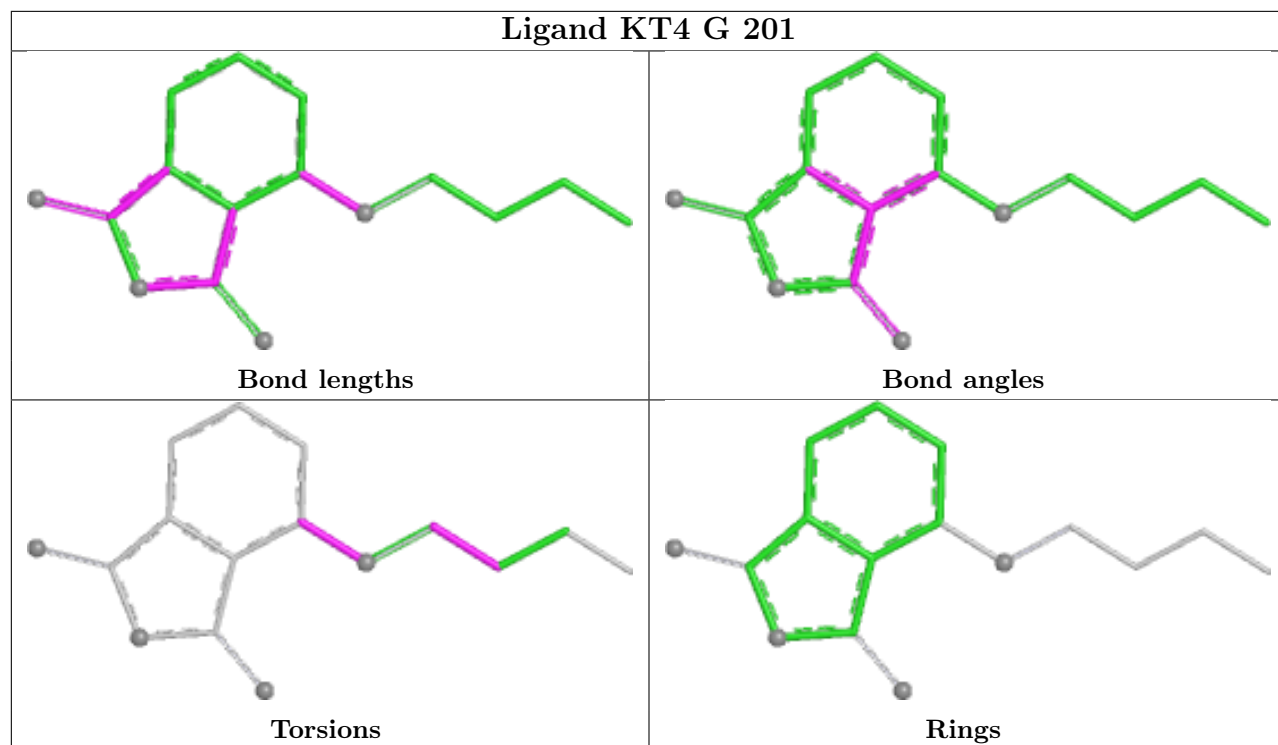
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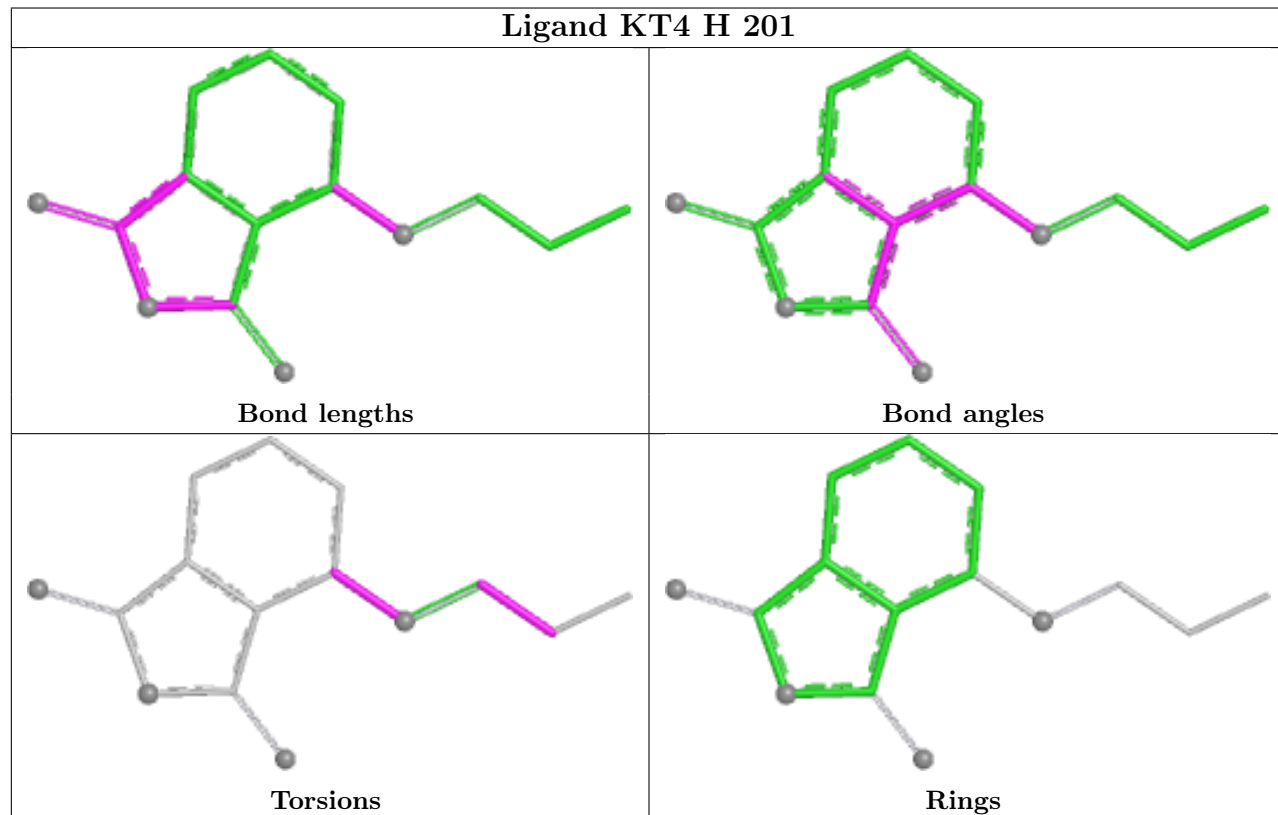
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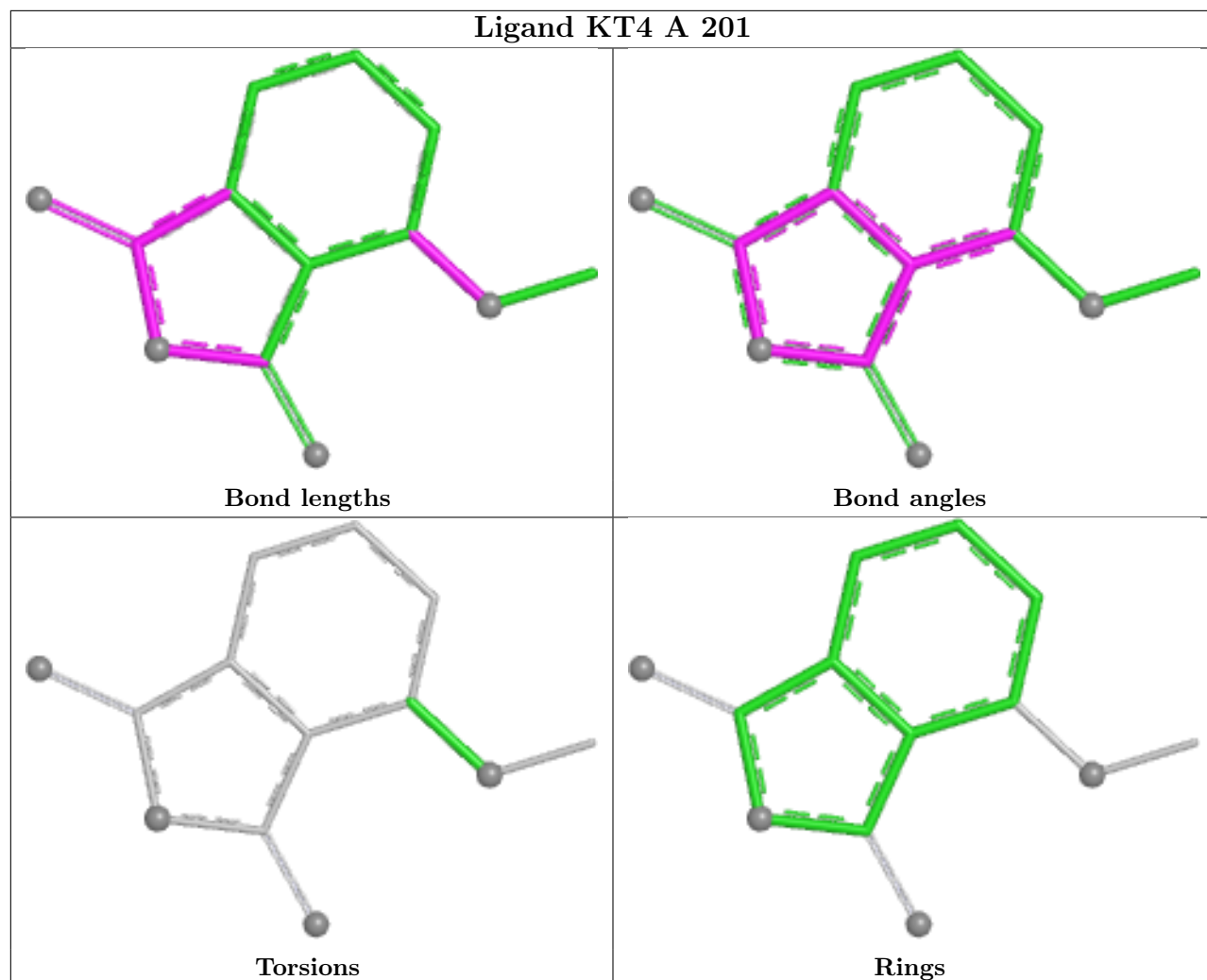
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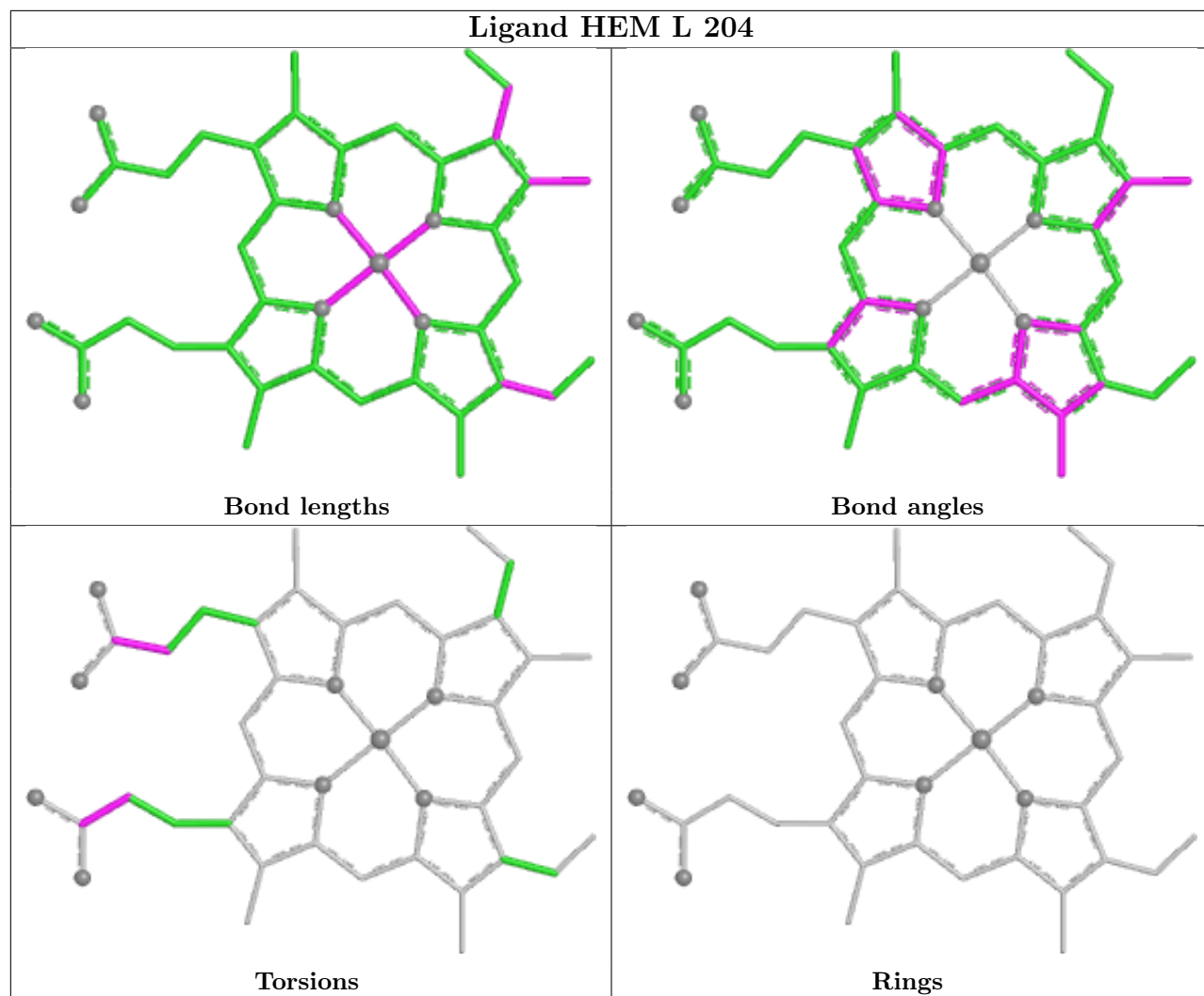


Ligand KT4 H 201

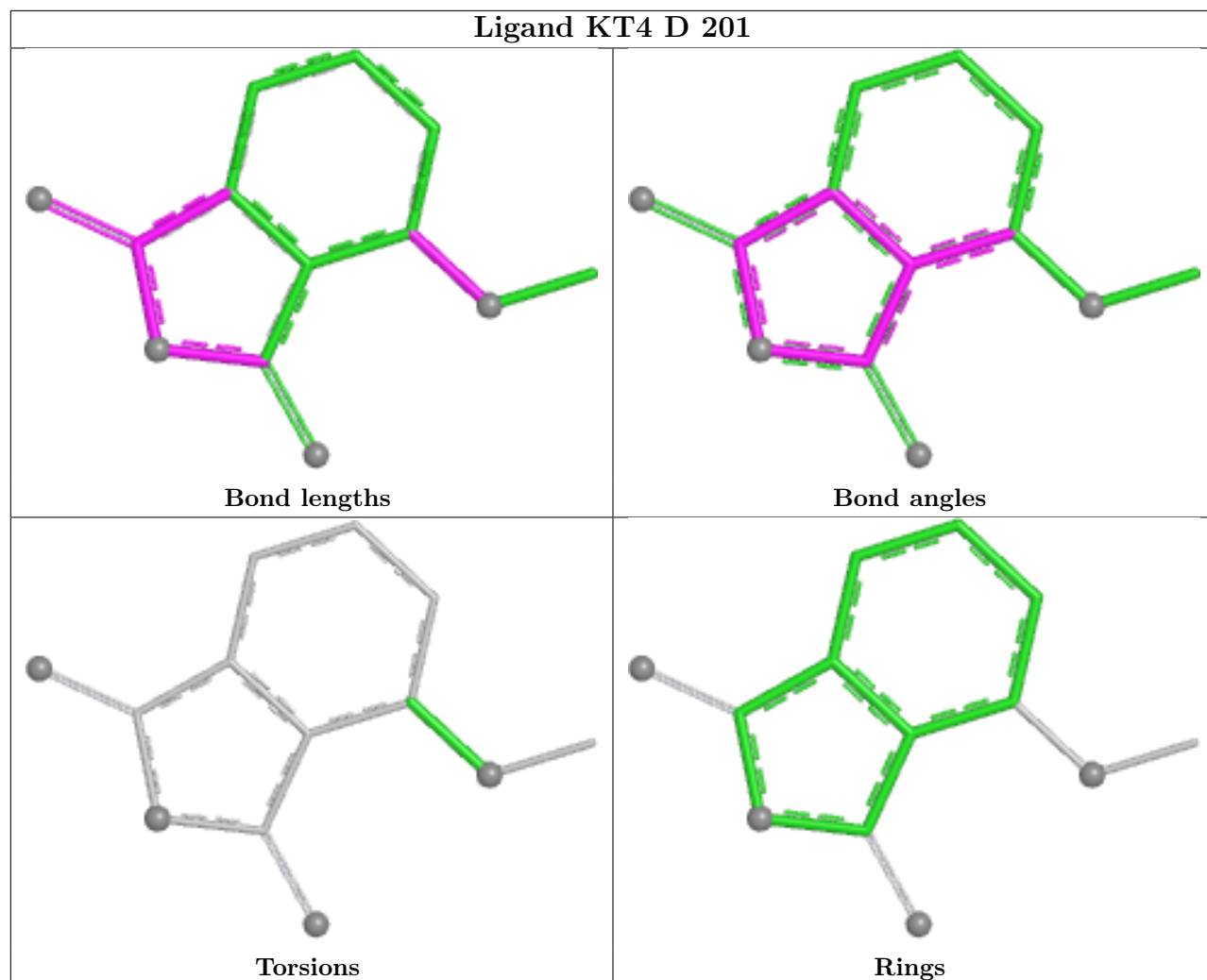


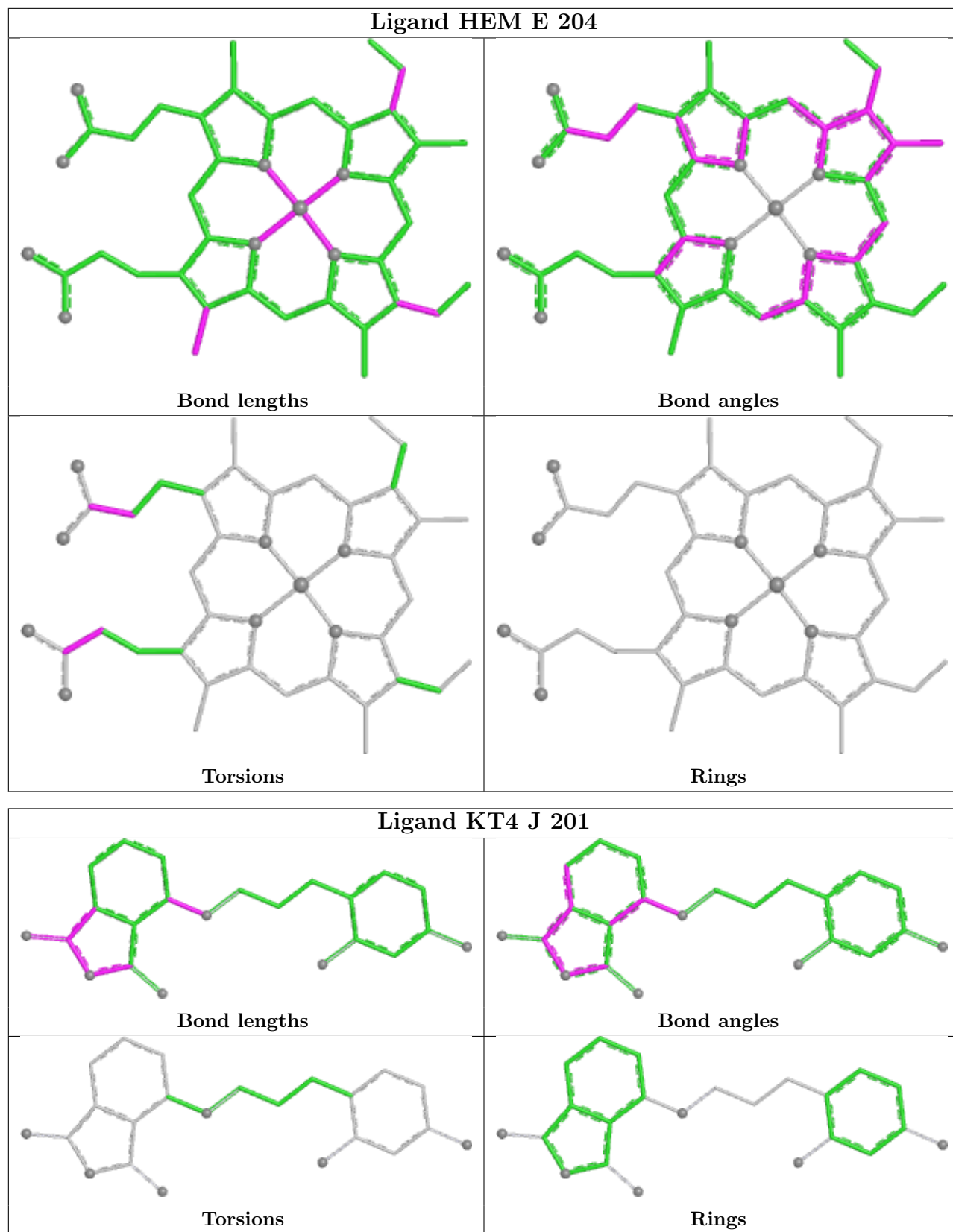
Ligand KT4 A 201

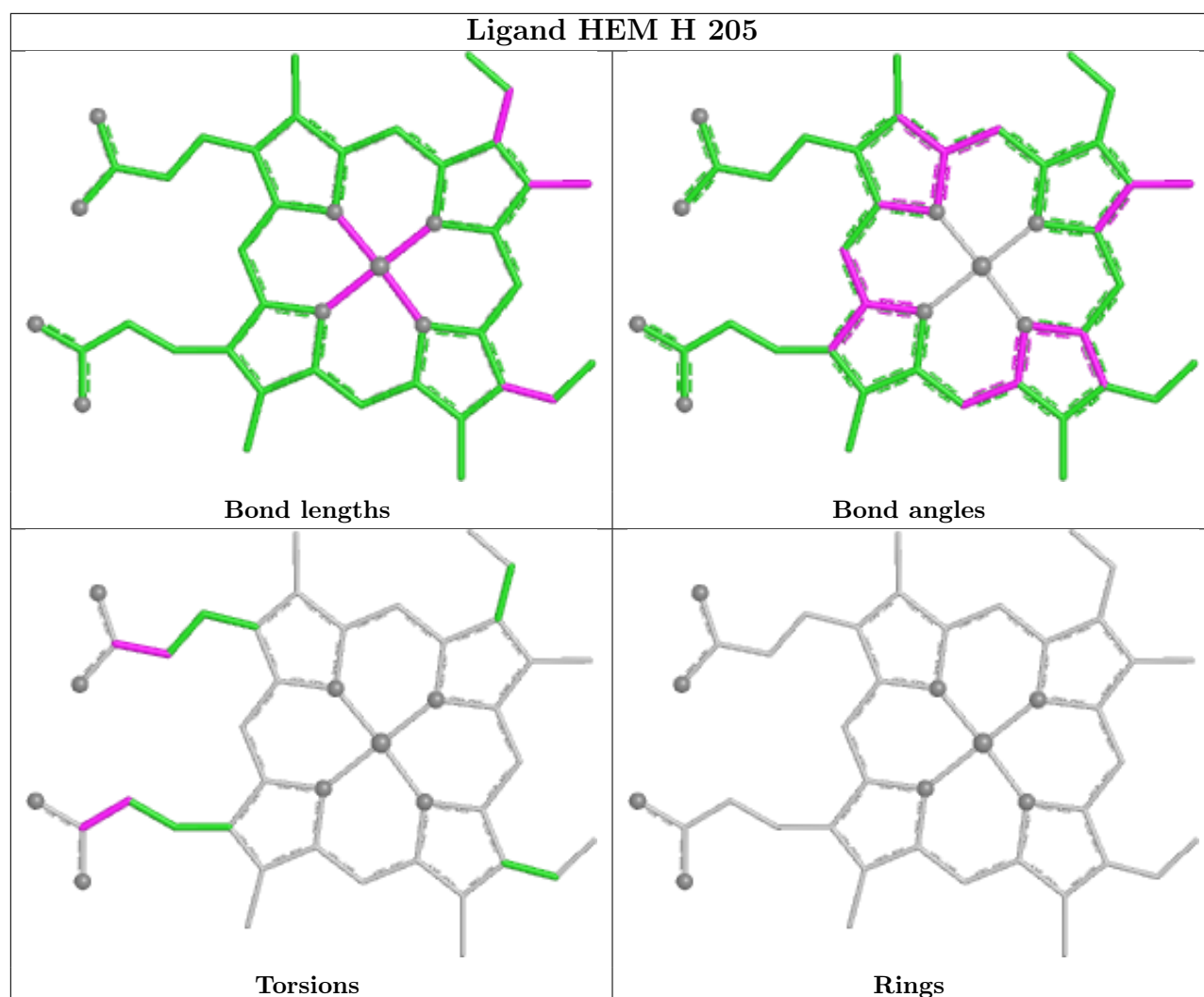




Ligand KT4 D 201







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%)	-0.33	2 (1%) 75 75	14, 23, 33, 57	1 (0%)
1	B	155/158 (98%)	-0.42	1 (0%) 85 86	14, 23, 32, 45	2 (1%)
1	C	155/158 (98%)	-0.41	1 (0%) 85 86	13, 23, 32, 46	1 (0%)
1	D	155/158 (98%)	-0.31	0 100 100	15, 24, 35, 45	1 (0%)
1	E	155/158 (98%)	-0.46	1 (0%) 85 86	14, 22, 31, 44	1 (0%)
1	F	156/158 (98%)	-0.38	1 (0%) 85 86	14, 23, 33, 59	2 (1%)
1	G	155/158 (98%)	-0.41	1 (0%) 85 86	14, 23, 31, 48	2 (1%)
1	H	155/158 (98%)	-0.34	0 100 100	15, 23, 33, 46	2 (1%)
1	I	155/158 (98%)	-0.35	1 (0%) 85 86	14, 23, 32, 46	1 (0%)
1	J	155/158 (98%)	-0.36	1 (0%) 85 86	14, 22, 30, 47	2 (1%)
1	K	155/158 (98%)	-0.36	1 (0%) 85 86	14, 23, 32, 50	2 (1%)
1	L	156/158 (98%)	-0.28	1 (0%) 85 86	15, 23, 31, 59	2 (1%)
All	All	1863/1896 (98%)	-0.37	11 (0%) 85 86	13, 23, 32, 59	19 (1%)

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	155	HIS	3.4
1	A	155	HIS	2.7
1	L	156	GLU	2.4
1	E	155	HIS	2.3
1	F	156	GLU	2.2

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PG4	H	203	13/13	0.79	0.19	41,49,55,59	0
2	KT4	H	201	15/23	0.81	0.15	29,41,44,47	0
3	PG4	D	203	8/13	0.83	0.16	37,47,53,55	0
3	PG4	A	203	7/13	0.83	0.14	33,41,45,47	0
3	PG4	H	204	11/13	0.83	0.18	42,52,81,94	0
2	KT4	C	201	23/23	0.84	0.14	29,43,54,63	0
2	KT4	A	201	13/23	0.85	0.13	28,35,42,43	0
3	PG4	F	203	8/13	0.85	0.17	42,48,53,59	0
3	PG4	L	203	13/13	0.85	0.14	41,49,64,64	0
2	KT4	I	201	23/23	0.86	0.13	29,40,51,58	0
3	PG4	J	203	10/13	0.86	0.13	29,39,47,53	0
3	PG4	E	203	13/13	0.86	0.15	40,46,57,58	0
2	KT4	G	201	16/23	0.87	0.15	30,43,54,54	0
3	PG4	H	202	13/13	0.87	0.14	35,40,51,53	0
3	PG4	B	203	10/13	0.87	0.14	35,48,56,57	0
3	PG4	C	202	11/13	0.87	0.14	31,35,47,47	0
3	PG4	J	202	13/13	0.87	0.14	37,41,50,53	0
2	KT4	B	201	23/23	0.87	0.13	28,39,55,57	0
3	PG4	K	203	10/13	0.87	0.14	35,48,60,70	0
3	PG4	L	202	13/13	0.87	0.14	36,39,45,58	0
2	KT4	E	201	23/23	0.87	0.13	28,40,53,58	0
3	PG4	G	202	13/13	0.88	0.13	35,40,48,49	0
3	PG4	G	203	10/13	0.88	0.17	39,58,77,92	0
3	PG4	E	202	13/13	0.88	0.13	27,34,45,46	0
2	KT4	F	201	23/23	0.88	0.12	28,36,52,61	0
2	KT4	D	201	13/23	0.88	0.11	30,35,42,47	0
3	PG4	I	202	13/13	0.89	0.13	37,41,45,53	0
3	PG4	D	202	13/13	0.89	0.12	36,38,51,53	0
3	PG4	B	202	11/13	0.89	0.13	34,42,45,49	0
2	KT4	K	201	23/23	0.90	0.12	28,37,46,58	0
3	PG4	K	202	13/13	0.91	0.13	34,41,51,52	0
2	KT4	L	201	23/23	0.91	0.10	28,36,43,49	0

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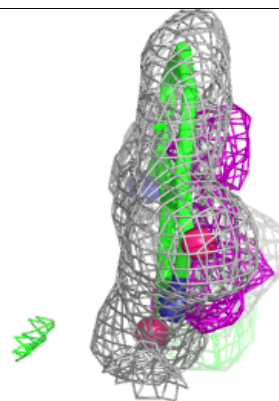
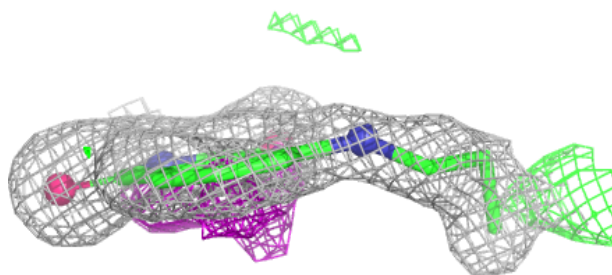
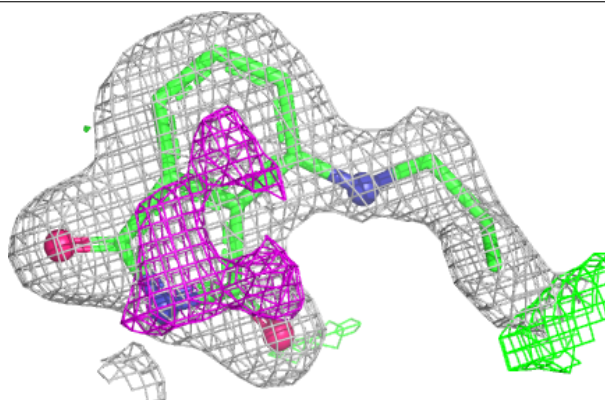
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PG4	F	202	13/13	0.92	0.11	30,36,46,49	0
3	PG4	A	202	10/13	0.92	0.11	34,40,44,52	0
2	KT4	J	201	23/23	0.93	0.09	25,33,37,43	0
4	HEM	A	204	43/43	0.97	0.08	19,24,40,44	0
4	HEM	F	204	43/43	0.97	0.08	18,22,39,43	0
4	HEM	H	205	43/43	0.97	0.09	18,23,42,45	0
4	HEM	I	203	43/43	0.97	0.09	19,23,38,41	0
4	HEM	L	204	43/43	0.97	0.09	21,23,35,39	43
4	HEM	D	204	43/43	0.98	0.07	20,24,34,36	43
4	HEM	E	204	43/43	0.98	0.07	17,21,39,46	0
5	FE2	A	205	1/1	1.00	0.01	19,19,19,19	0
5	FE2	B	204	1/1	1.00	0.01	19,19,19,19	0
5	FE2	D	205	1/1	1.00	0.01	19,19,19,19	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.

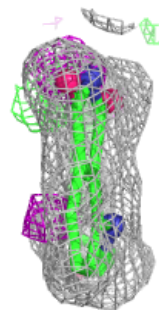
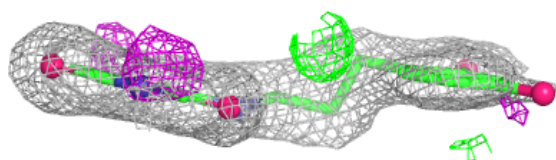
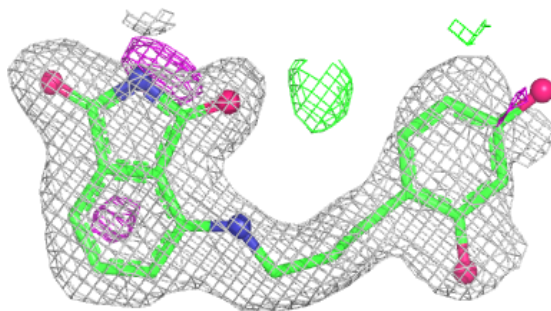
Electron density around KT4 H 201:

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



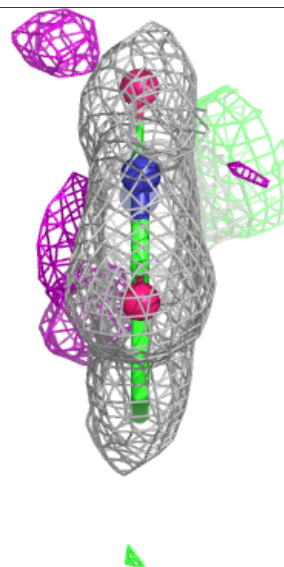
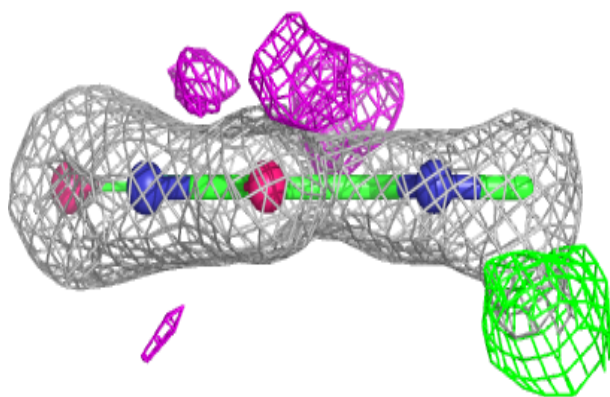
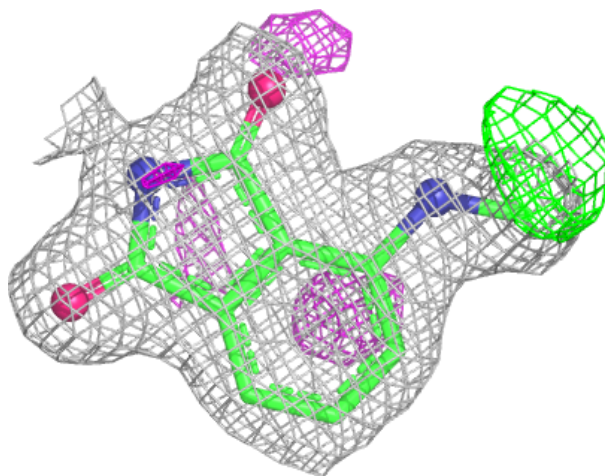
Electron density around KT4 C 201:

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



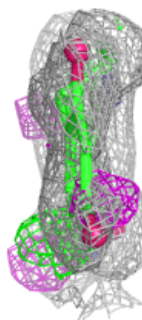
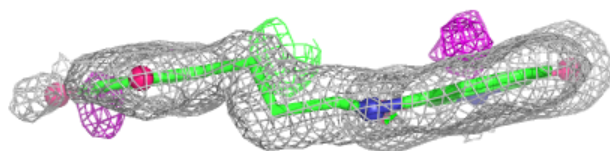
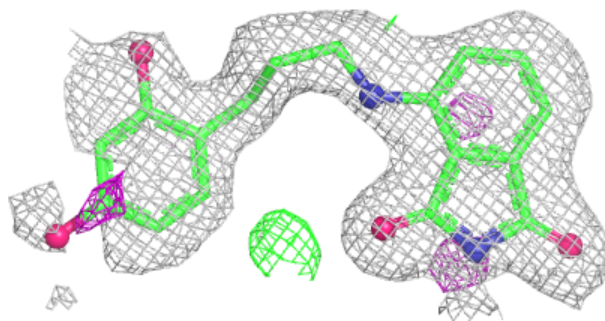
Electron density around KT4 A 201:

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

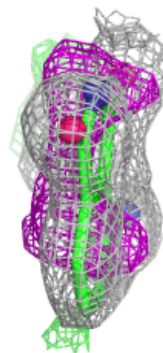
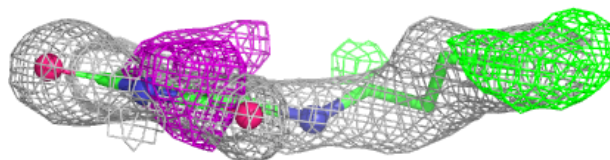
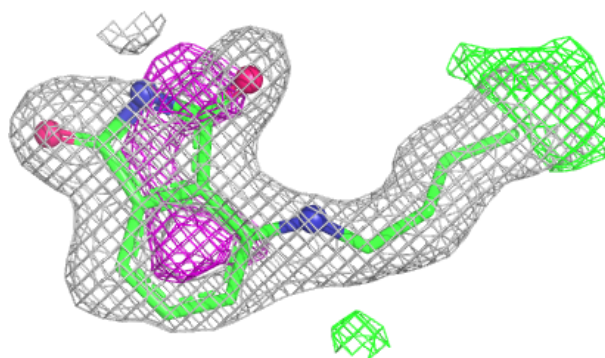


Electron density around KT4 I 201:

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

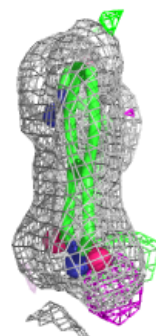
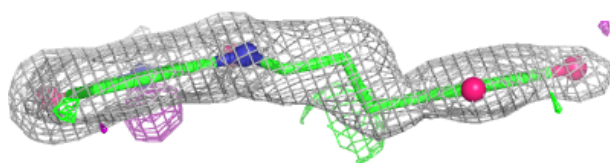
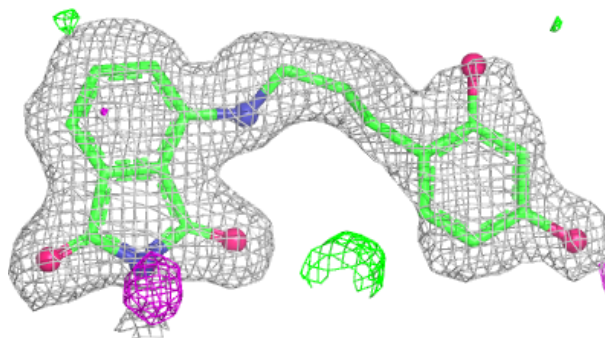
**Electron density around KT4 G 201:**

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

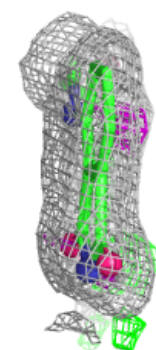
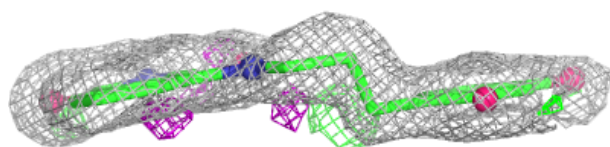
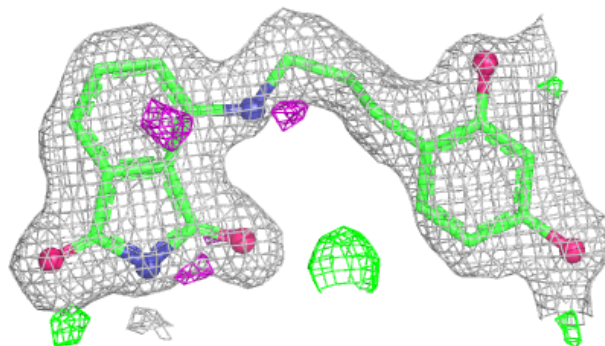


Electron density around KT4 B 201:

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

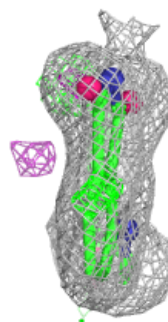
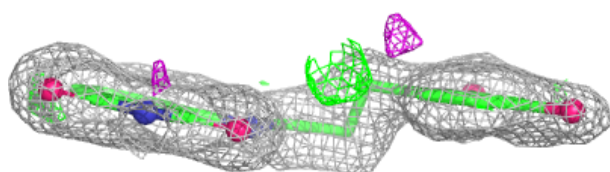
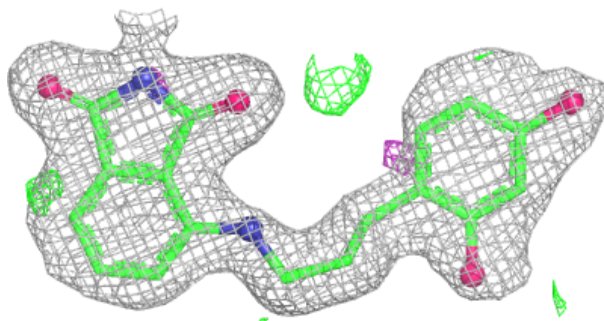
**Electron density around KT4 E 201:**

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

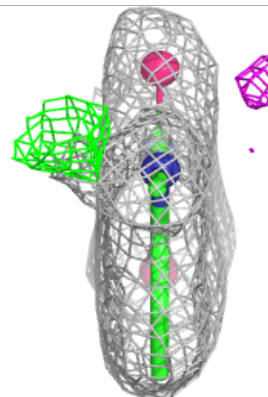
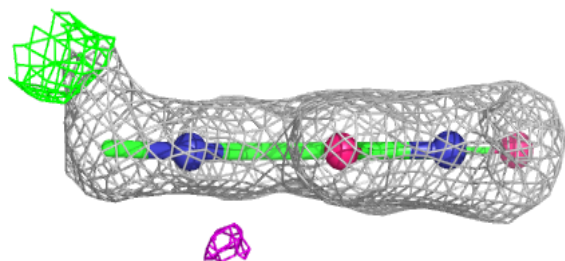
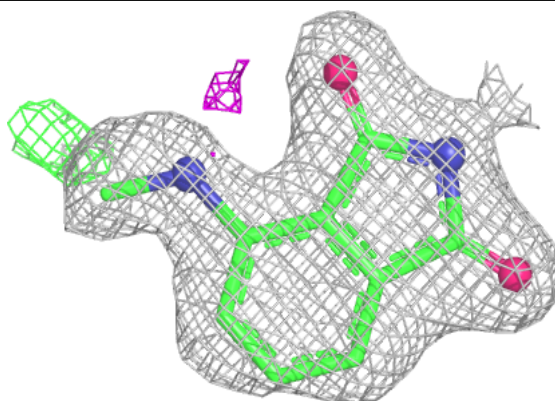


Electron density around KT4 F 201:

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

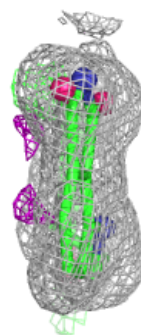
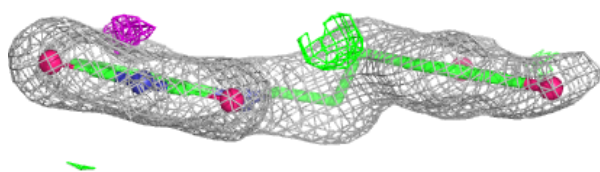
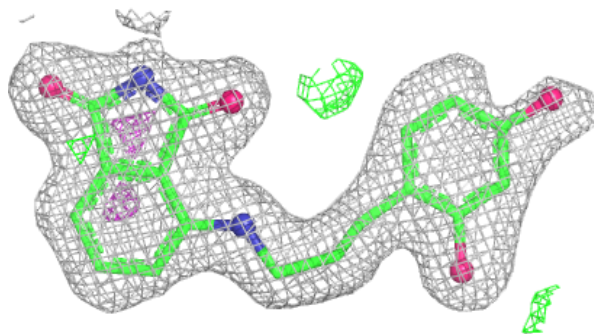
**Electron density around KT4 D 201:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
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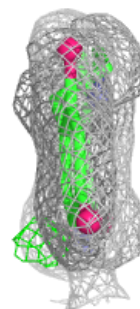
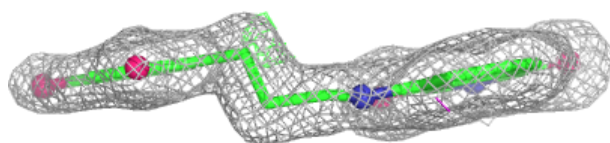
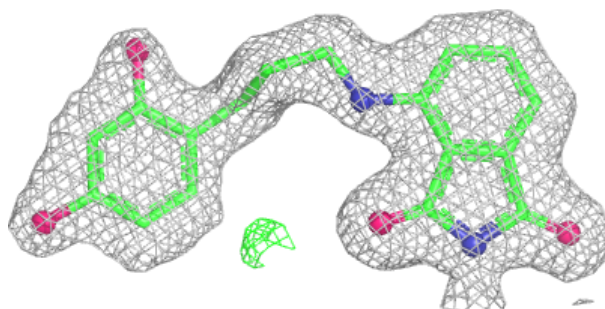


Electron density around KT4 K 201:

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

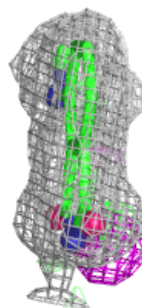
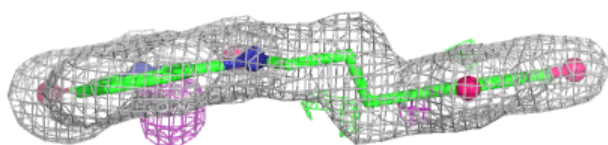
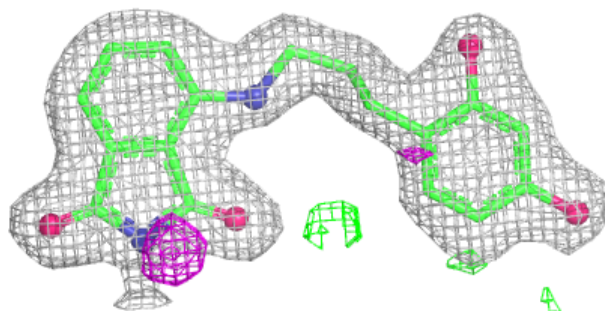
**Electron density around KT4 L 201:**

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



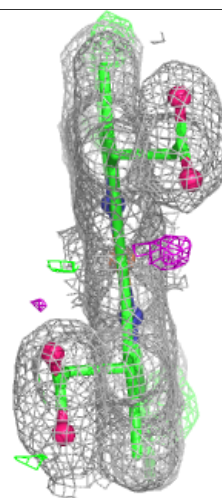
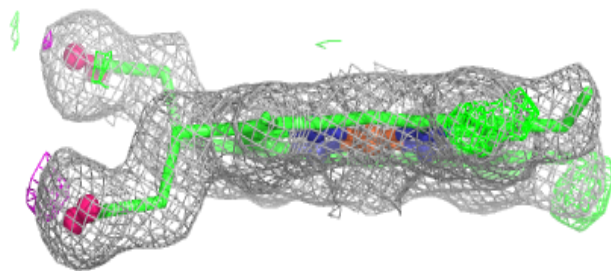
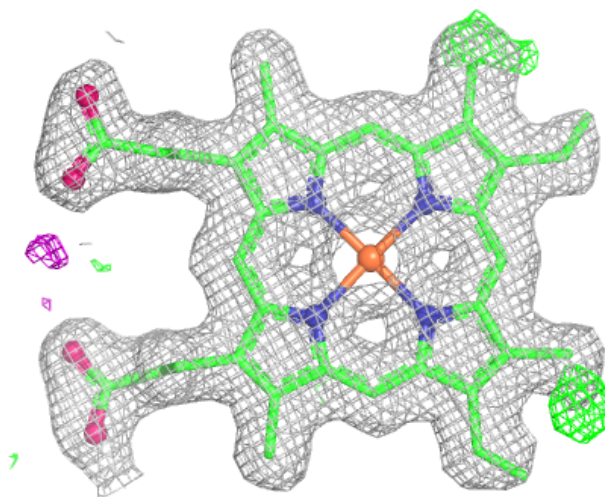
Electron density around KT4 J 201:

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



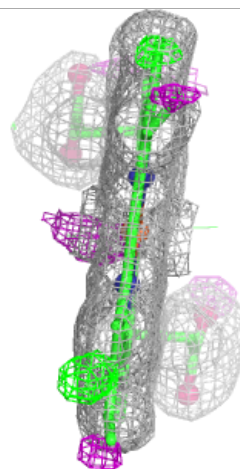
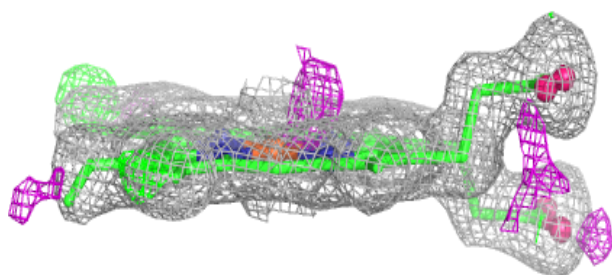
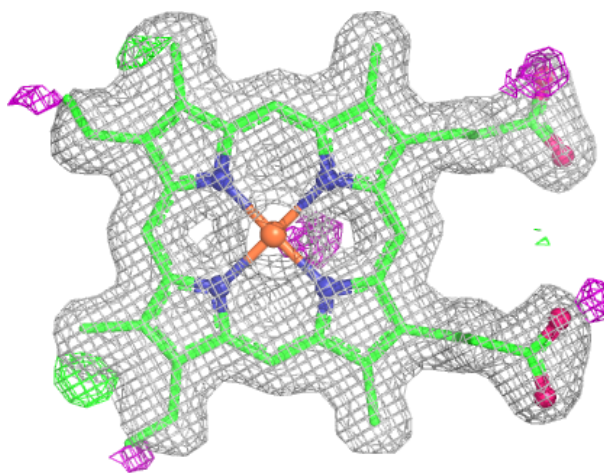
Electron density around HEM A 204:

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



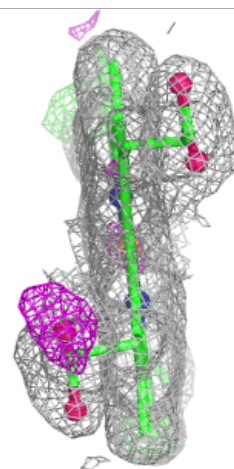
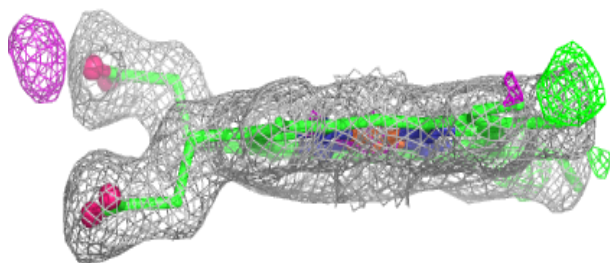
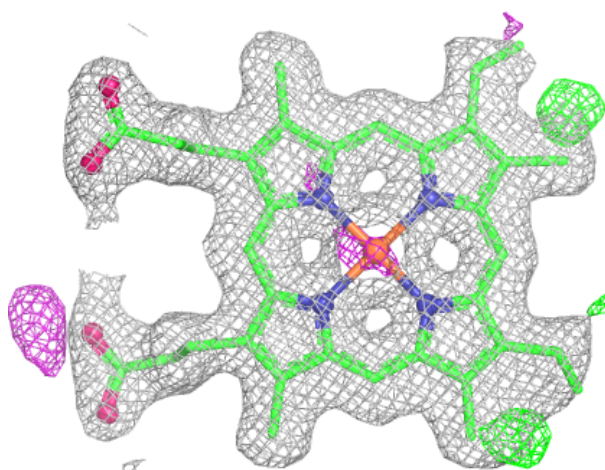
Electron density around HEM F 204:

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



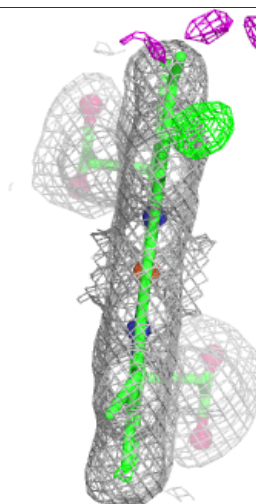
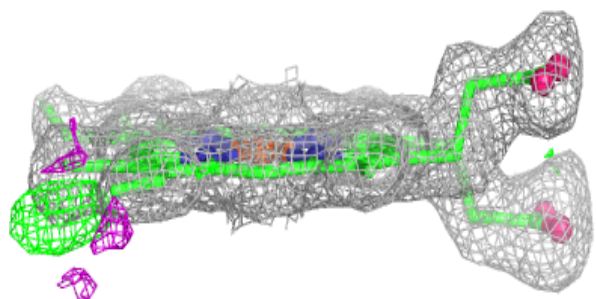
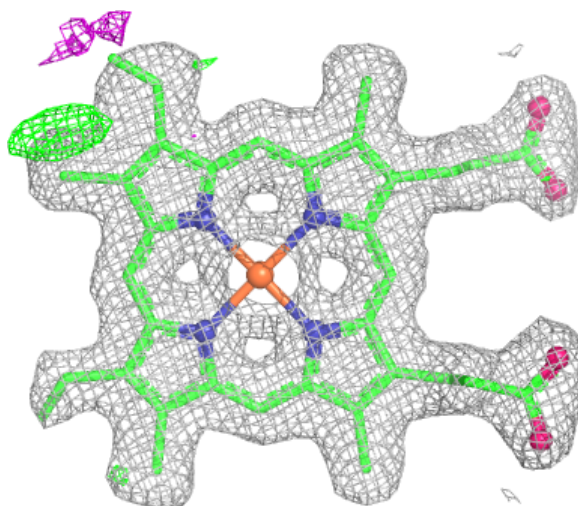
Electron density around HEM H 205:

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and green (positive)



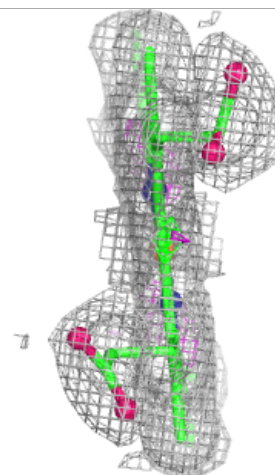
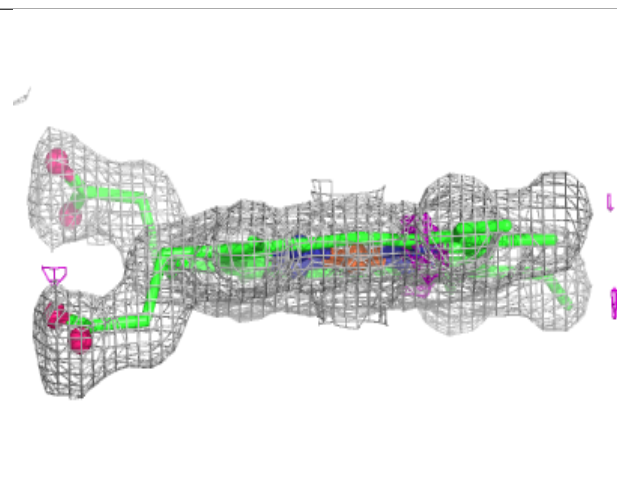
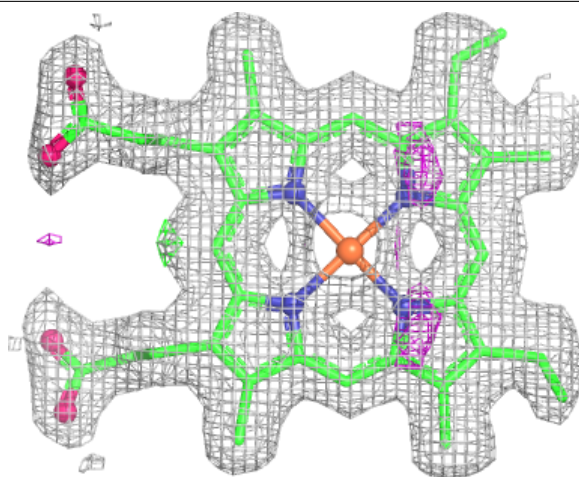
Electron density around HEM I 203:

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



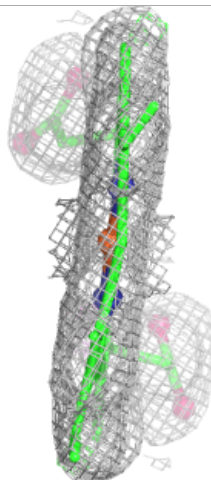
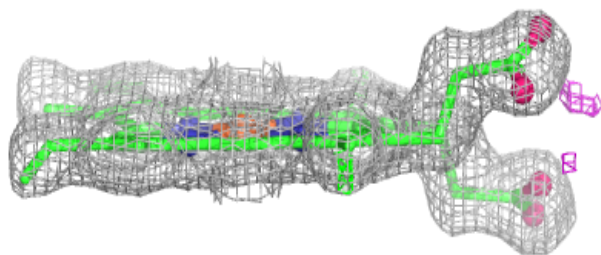
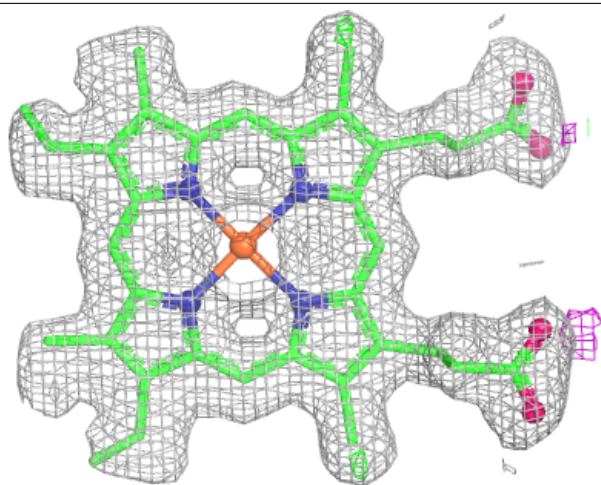
Electron density around HEM L 204:

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



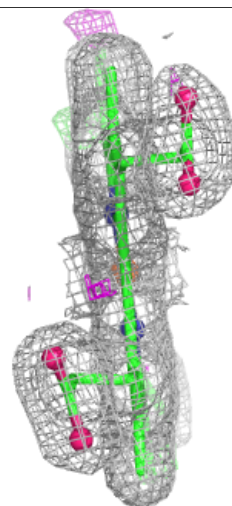
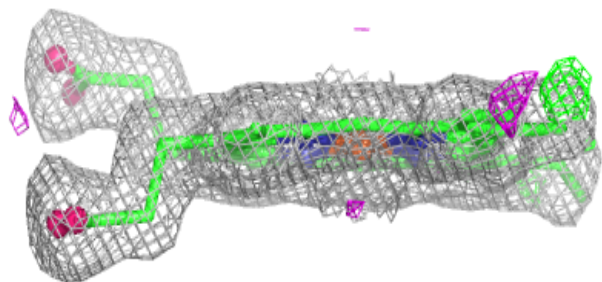
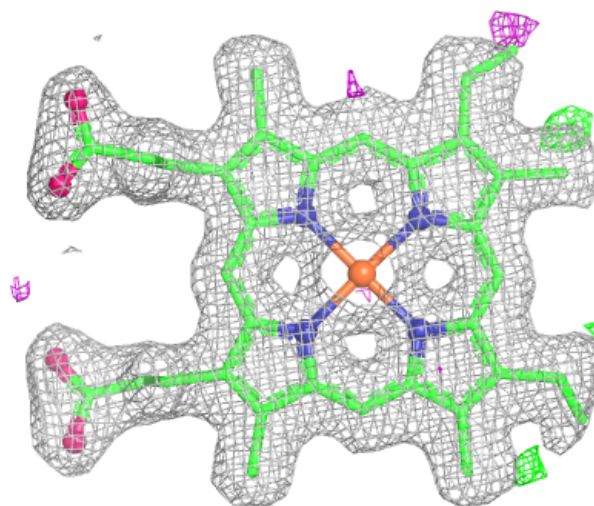
Electron density around HEM D 204:

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



Electron density around HEM E 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.