



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 01:14 am BST

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

This is a Full wwPDB X-ray Structure Validation 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

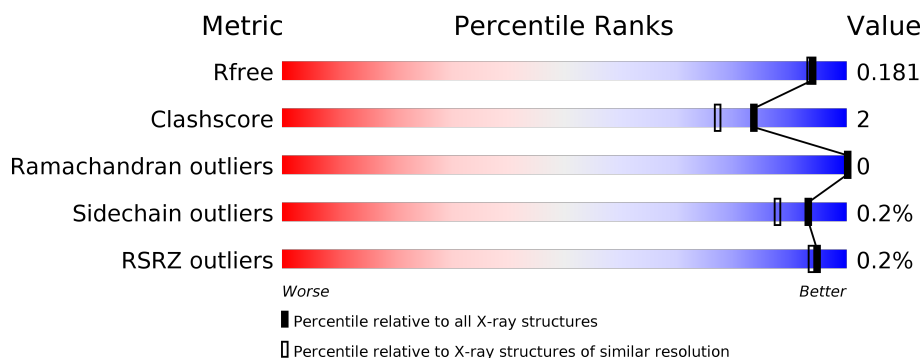
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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>%</div> <div> <div></div> <div>96%</div> <div></div> </div> <div>..</div> </div>
1	B	158	<div> <div>%</div> <div> <div></div> <div>95%</div> <div></div> </div> <div>..</div> </div>
1	C	158	<div> <div></div> <div>96%</div> <div></div> </div> <div>..</div>
1	D	158	<div> <div></div> <div>96%</div> <div></div> </div> <div>..</div>
1	E	158	<div> <div></div> <div>96%</div> <div></div> </div> <div>..</div>
1	F	158	<div> <div></div> <div>97%</div> <div></div> </div> <div>..</div>

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Mol	Chain	Length	Quality of chain
1	G	158	<div><div></div><div>96%</div><div></div></div> <div>..</div>
1	H	158	<div><div></div><div>97%</div><div></div></div> <div>..</div>
1	I	158	<div><div></div><div>96%</div><div></div></div> <div>..</div>
1	J	158	<div><div></div><div>97%</div><div></div></div> <div>..</div>
1	K	158	<div><div>%</div><div></div><div></div></div> <div>94%</div> <div>..</div>
1	L	158	<div><div></div><div></div><div></div></div> <div>94%</div> <div>5% .</div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17890 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Ferroxidase.

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

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

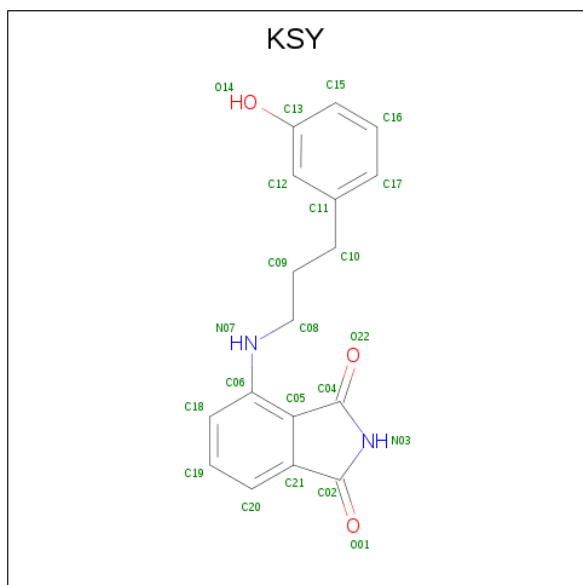
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Fe	0	0
			1	1		
2	A	1	Total	Fe	0	0
			1	1		

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

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



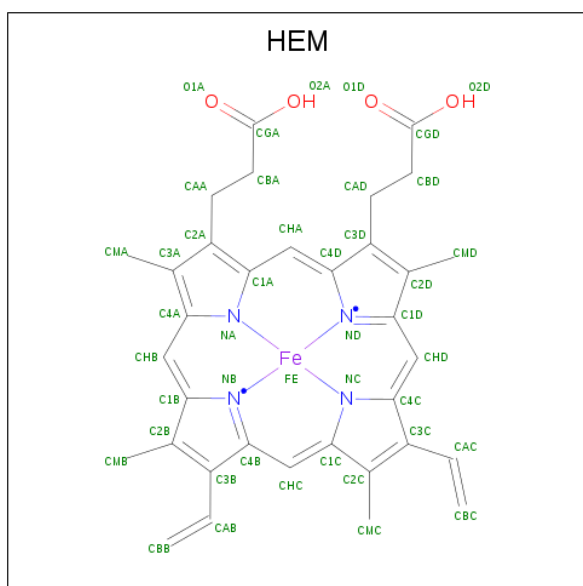
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			22	17	2	3		
3	A	1	Total	C	N	O	0	0
			22	17	2	3		
3	B	1	Total	C	N	O	0	0
			22	17	2	3		
3	C	1	Total	C	N	O	0	0
			22	17	2	3		
3	D	1	Total	C	N	O	0	0
			22	17	2	3		
3	E	1	Total	C	N	O	0	0
			22	17	2	3		
3	F	1	Total	C	N	O	0	0
			22	17	2	3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

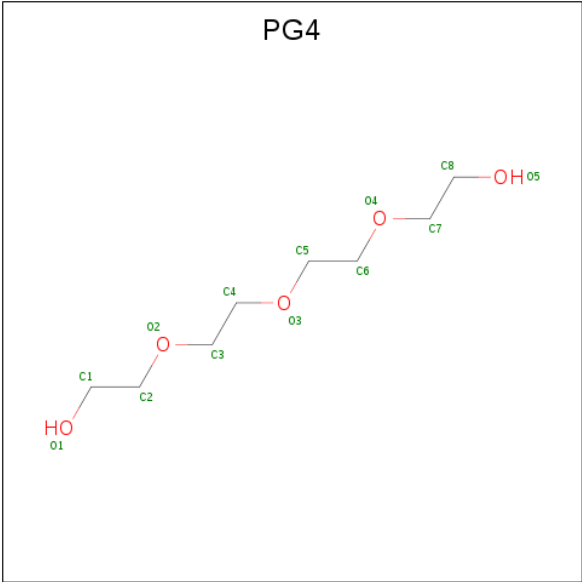
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	J	1	Total	C	N	O	0	0
			22	17	2	3		
3	K	1	Total	C	N	O	0	0
			15	11	2	2		
3	L	1	Total	C	N	O	0	0
			14	10	2	2		

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).





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

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

- Molecule 6 is water.

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

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

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA 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: 



• Molecule 1: Ferroxidase

Chain B: 



• Molecule 1: Ferroxidase

Chain C: 



• Molecule 1: Ferroxidase

Chain D: 



• Molecule 1: Ferroxidase

Chain E: 



• Molecule 1: Ferroxidase

Chain F: 



- Molecule 1: Ferroxidase

Chain G: 96% ..



- Molecule 1: Ferroxidase

Chain H: 97% ..



- Molecule 1: Ferroxidase

Chain I: 96% ..



- Molecule 1: Ferroxidase

Chain J: 97% ..



- Molecule 1: Ferroxidase

Chain K: 94% ..



- Molecule 1: Ferroxidase

Chain L: 94% 5% ..



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	129.91Å 194.88Å 203.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.72 – 1.60 48.72 – 1.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.72-1.60) 100.0 (48.72-1.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 1.60Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.147 , 0.169 0.160 , 0.181	Depositor DCC
R_{free} test set	16763 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	18.2	Xtriage
Anisotropy	0.316	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 48.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	17890	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, PG4, KSY, 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	0.40	0/1296	0.55	0/1745
1	B	0.39	0/1296	0.54	0/1747
1	C	0.40	0/1299	0.55	0/1750
1	D	0.41	0/1305	0.54	0/1757
1	E	0.49	0/1305	0.58	0/1758
1	F	0.40	0/1288	0.56	0/1737
1	G	0.40	0/1293	0.52	0/1743
1	H	0.41	0/1294	0.53	0/1745
1	I	0.40	0/1291	0.53	0/1741
1	J	0.44	0/1292	0.54	0/1742
1	K	0.39	0/1293	0.54	0/1743
1	L	0.39	0/1290	0.51	0/1739
All	All	0.41	0/15542	0.54	0/20947

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

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

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	J	26	0	36	0	0
5	K	29	0	35	1	0
5	L	13	0	18	2	0
6	A	159	0	0	2	0
6	B	147	0	0	0	0
6	C	159	0	0	3	0
6	D	154	0	0	3	2
6	E	152	0	0	1	0
6	F	156	0	0	2	0
6	G	144	0	0	3	1
6	H	152	0	0	1	0
6	I	129	0	0	3	0
6	J	154	0	0	2	0
6	K	154	0	0	4	0
6	L	136	0	0	5	0
All	All	17890	0	15476	77	2

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

All (77) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:204:HEM:HBC2	4:A:204:HEM:HMC2	1.72	0.70
1:K:126[A]:SER:OG	6:K:301:HOH:O	2.09	0.69
4:B:203:HEM:HBC2	4:B:203:HEM:HMC1	1.75	0.69
4:F:202:HEM:HBC2	4:F:202:HEM:HMC1	1.77	0.66
4:L:202:HEM:O1D	6:L:301:HOH:O	2.13	0.65
1:A:143:LYS:HE3	5:A:206:PG4:H22	1.81	0.63
4:C:202:HEM:HBC2	4:C:202:HEM:HMC1	1.82	0.62
4:L:202:HEM:HBB2	4:L:202:HEM:HMB1	1.82	0.62
4:H:202:HEM:HBC2	4:H:202:HEM:HMC2	1.82	0.61
4:B:203:HEM:CMC	4:B:203:HEM:HBC2	2.30	0.61
1:G:69:PRO:O	3:G:201:KSY:N03	2.34	0.60
1:B:69:PRO:O	3:B:202:KSY:N03	2.35	0.60
1:I:69:PRO:O	3:I:201:KSY:N03	2.34	0.60
1:H:69:PRO:O	3:H:201:KSY:N03	2.35	0.60
1:E:69:PRO:O	3:E:201:KSY:N03	2.35	0.60
1:K:69:PRO:O	3:K:201:KSY:N03	2.35	0.60
1:F:69:PRO:O	3:F:201:KSY:N03	2.35	0.59
1:C:69:PRO:O	3:C:201:KSY:N03	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:69:PRO:O	3:L:201:KSY:N03	2.36	0.59
1:A:69:PRO:O	3:A:202:KSY:N03	2.36	0.59
1:D:69:PRO:O	3:D:202:KSY:N03	2.36	0.58
1:J:69:PRO:O	3:J:201:KSY:N03	2.35	0.58
1:D:34:ASP:OD1	6:D:301:HOH:O	2.17	0.57
4:F:202:HEM:CMC	4:F:202:HEM:HBC2	2.34	0.56
3:A:203:KSY:O01	6:A:301:HOH:O	2.18	0.55
1:E:147[A]:GLU:CD	1:E:147[A]:GLU:H	2.09	0.55
4:H:202:HEM:CMC	4:H:202:HEM:HBC2	2.37	0.54
4:D:203:HEM:HMC1	4:D:203:HEM:HBC2	1.90	0.54
4:D:203:HEM:CMC	4:D:203:HEM:HBC2	2.39	0.53
4:C:202:HEM:HBC2	4:C:202:HEM:CMC	2.39	0.53
4:L:202:HEM:CMB	4:L:202:HEM:HBB2	2.39	0.53
4:L:202:HEM:HMC1	4:L:202:HEM:HBC2	1.91	0.52
1:J:103:GLU:CG	6:J:451:HOH:O	2.58	0.52
4:A:204:HEM:HBC2	4:A:204:HEM:CMC	2.38	0.50
1:L:110:GLN:CG	6:L:433:HOH:O	2.60	0.49
5:G:203:PG4:H82	1:L:136:THR:HG21	1.94	0.49
4:B:203:HEM:CHB	1:E:52:MET:HB3	2.43	0.49
1:H:103:GLU:CG	6:H:450:HOH:O	2.61	0.48
4:C:202:HEM:HBB2	4:C:202:HEM:CMB	2.43	0.48
5:L:203:PG4:H81	6:L:312:HOH:O	2.14	0.48
1:L:52:MET:HB3	4:L:202:HEM:CHD	2.44	0.48
1:G:110:GLN:CG	6:G:440:HOH:O	2.63	0.47
4:B:203:HEM:CMB	4:B:203:HEM:HBB2	2.45	0.47
1:L:126[A]:SER:OG	6:L:302:HOH:O	2.20	0.47
5:I:202:PG4:H42	6:I:370:HOH:O	2.15	0.46
5:F:205:PG4:C6	6:F:429:HOH:O	2.63	0.46
1:D:50:ASP:HB3	6:D:304:HOH:O	2.15	0.46
4:C:202:HEM:CHB	1:I:52:MET:HB3	2.46	0.45
1:G:1:MET:O	1:G:65:LEU:HA	2.17	0.45
4:L:202:HEM:CMC	4:L:202:HEM:HBC2	2.47	0.45
6:C:384:HOH:O	5:F:203:PG4:H61	2.17	0.44
6:C:378:HOH:O	5:F:203:PG4:C1	2.65	0.44
1:K:110:GLN:CG	6:K:450:HOH:O	2.66	0.44
1:K:110:GLN:CG	6:K:448:HOH:O	2.66	0.43
5:L:203:PG4:C8	6:L:312:HOH:O	2.65	0.43
1:E:99:LYS:CD	6:E:387:HOH:O	2.66	0.43
1:F:52:MET:HB3	4:F:202:HEM:CHD	2.48	0.43
1:L:1:MET:O	1:L:65:LEU:HA	2.18	0.43
1:K:84:GLN:HG3	6:K:409:HOH:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:134:LEU:HD21	6:G:307:HOH:O	2.19	0.43
1:I:1:MET:O	1:I:65:LEU:HA	2.19	0.43
1:F:134:LEU:HD21	6:F:309:HOH:O	2.19	0.42
5:I:202:PG4:C4	6:I:370:HOH:O	2.67	0.42
6:D:342:HOH:O	5:K:203:PG4:C8	2.67	0.42
1:C:20:ILE:HD11	1:C:75:GLY:HA3	2.02	0.42
5:I:202:PG4:H71	6:I:370:HOH:O	2.19	0.42
1:D:143:LYS:HZ1	5:D:206:PG4:C7	2.32	0.42
5:C:203:PG4:C6	6:C:358:HOH:O	2.68	0.42
1:B:1:MET:O	1:B:65:LEU:HA	2.20	0.42
1:H:52:MET:HB3	4:H:202:HEM:CHD	2.49	0.42
1:C:52:MET:HB3	4:C:202:HEM:CHD	2.51	0.41
1:A:123:ILE:O	1:A:127:GLU:HG2	2.21	0.41
1:B:106:VAL:O	1:B:110:GLN:HG3	2.21	0.41
1:A:134:LEU:HD21	6:A:310:HOH:O	2.21	0.40
1:J:112:HIS:HE1	6:J:435:HOH:O	2.04	0.40
1:K:1:MET:O	1:K:65:LEU:HA	2.20	0.40
5:G:202:PG4:H72	6:G:352:HOH:O	2.22	0.40

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

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

5.3 Torsion angles [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	155/158 (98%)	154 (99%)	1 (1%)	0	100 100

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

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	137/144 (95%)	137 (100%)	0	100	100
1	B	137/144 (95%)	136 (99%)	1 (1%)	84	73
1	C	138/144 (96%)	138 (100%)	0	100	100
1	D	140/144 (97%)	140 (100%)	0	100	100
1	E	138/144 (96%)	138 (100%)	0	100	100
1	F	134/144 (93%)	134 (100%)	0	100	100
1	G	136/144 (94%)	136 (100%)	0	100	100
1	H	135/144 (94%)	135 (100%)	0	100	100
1	I	135/144 (94%)	134 (99%)	1 (1%)	84	73
1	J	136/144 (94%)	136 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	136/144 (94%)	135 (99%)	1 (1%)	84	73
1	L	135/144 (94%)	134 (99%)	1 (1%)	84	73
All	All	1637/1728 (95%)	1633 (100%)	4 (0%)	93	88

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	121	LYS
1	I	121	LYS
1	K	121	LYS
1	L	121	LYS

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	KSY	D	202	-	24,24,24	1.80	5 (20%)	33,33,33	1.71	6 (18%)
5	PG4	F	205	-	8,8,12	0.45	0	7,7,11	0.46	0
5	PG4	I	204	-	7,7,12	0.38	0	6,6,11	0.45	0
5	PG4	C	203	-	12,12,12	0.51	0	11,11,11	0.59	0
5	PG4	B	205	-	5,5,12	0.51	0	4,4,11	0.14	0
3	KSY	I	201	-	24,24,24	1.62	5 (20%)	33,33,33	1.37	3 (9%)
4	HEM	H	202	1	27,50,50	1.99	5 (18%)	17,82,82	1.87	5 (29%)
3	KSY	E	201	-	24,24,24	1.64	5 (20%)	33,33,33	1.21	3 (9%)
5	PG4	F	203	-	12,12,12	0.49	0	11,11,11	0.53	0
5	PG4	J	203	-	12,12,12	0.43	0	11,11,11	0.49	0
4	HEM	C	202	1	27,50,50	1.86	4 (14%)	17,82,82	2.19	9 (52%)
5	PG4	B	204	-	7,7,12	0.57	0	6,6,11	0.22	0
5	PG4	K	202	-	7,7,12	0.49	0	6,6,11	0.22	0
5	PG4	D	204	-	12,12,12	0.49	0	11,11,11	0.45	0
5	PG4	C	204	-	7,7,12	0.51	0	6,6,11	0.25	0
5	PG4	E	204	-	7,7,12	0.49	0	6,6,11	0.34	0
4	HEM	A	204	1	27,50,50	1.86	4 (14%)	17,82,82	2.00	8 (47%)
5	PG4	A	206	-	9,9,12	0.44	0	8,8,11	0.59	0
5	PG4	L	203	-	12,12,12	0.40	0	11,11,11	0.57	0
3	KSY	L	201	-	15,15,24	2.28	6 (40%)	21,21,33	1.90	4 (19%)
3	KSY	J	201	-	24,24,24	1.71	5 (20%)	33,33,33	1.72	4 (12%)
3	KSY	K	201	-	16,16,24	2.01	5 (31%)	22,22,33	1.28	2 (9%)
3	KSY	H	201	-	17,17,24	1.94	5 (29%)	23,23,33	1.91	7 (30%)
5	PG4	F	204	-	9,9,12	0.55	0	8,8,11	0.31	0
3	KSY	G	201	-	24,24,24	1.64	5 (20%)	33,33,33	1.12	3 (9%)
5	PG4	E	203	-	9,9,12	0.54	0	8,8,11	0.29	0
5	PG4	K	204	-	7,7,12	0.50	0	6,6,11	0.39	0
5	PG4	D	206	-	7,7,12	0.41	0	6,6,11	0.32	0
5	PG4	G	203	-	9,9,12	0.51	0	8,8,11	0.16	0
5	PG4	G	202	-	12,12,12	0.52	0	11,11,11	0.41	0
3	KSY	A	203	-	24,24,24	1.77	5 (20%)	33,33,33	1.25	4 (12%)
5	PG4	E	202	-	12,12,12	0.51	0	11,11,11	0.43	0
5	PG4	A	205	-	12,12,12	0.46	0	11,11,11	0.42	0
5	PG4	J	202	-	12,12,12	0.51	0	11,11,11	0.44	0
4	HEM	L	202	1	27,50,50	1.84	4 (14%)	17,82,82	1.60	4 (23%)
3	KSY	C	201	-	24,24,24	1.65	5 (20%)	33,33,33	1.28	4 (12%)
3	KSY	B	202	-	24,24,24	1.54	5 (20%)	33,33,33	1.30	3 (9%)
5	PG4	D	205	-	9,9,12	0.53	0	8,8,11	0.25	0
5	PG4	I	203	-	7,7,12	0.56	0	6,6,11	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PG4	K	203	-	12,12,12	0.49	0	11,11,11	0.31	0
4	HEM	F	202	1	27,50,50	1.89	4 (14%)	17,82,82	1.85	6 (35%)
4	HEM	B	203	1	27,50,50	1.90	5 (18%)	17,82,82	1.72	5 (29%)
5	PG4	I	202	-	9,9,12	0.37	0	8,8,11	0.59	0
4	HEM	D	203	1	27,50,50	1.86	4 (14%)	17,82,82	1.72	4 (23%)
3	KSY	A	202	-	24,24,24	1.92	6 (25%)	33,33,33	2.05	6 (18%)
3	KSY	F	201	-	24,24,24	1.57	5 (20%)	33,33,33	1.33	3 (9%)
5	PG4	H	203	-	7,7,12	0.51	0	6,6,11	0.28	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	KSY	D	202	-	-	3/7/19/19	0/3/3/3
5	PG4	F	205	-	-	2/6/6/10	-
5	PG4	I	204	-	-	0/5/5/10	-
5	PG4	C	203	-	-	7/10/10/10	-
5	PG4	B	205	-	-	0/3/3/10	-
3	KSY	I	201	-	-	0/7/19/19	0/3/3/3
4	HEM	H	202	1	-	0/6/54/54	-
3	KSY	E	201	-	-	2/7/19/19	0/3/3/3
5	PG4	F	203	-	-	5/10/10/10	-
5	PG4	J	203	-	-	0/10/10/10	-
4	HEM	C	202	1	-	0/6/54/54	-
5	PG4	B	204	-	-	1/5/5/10	-
5	PG4	K	202	-	-	2/5/5/10	-
5	PG4	D	204	-	-	2/10/10/10	-
5	PG4	C	204	-	-	0/5/5/10	-
5	PG4	E	204	-	-	0/5/5/10	-
4	HEM	A	204	1	-	0/6/54/54	-
5	PG4	A	206	-	-	4/7/7/10	-
5	PG4	L	203	-	-	3/10/10/10	-
3	KSY	L	201	-	-	0/3/15/19	0/2/2/3
3	KSY	J	201	-	-	0/7/19/19	0/3/3/3
3	KSY	K	201	-	-	0/4/16/19	0/2/2/3
3	KSY	H	201	-	-	4/5/17/19	0/2/2/3
5	PG4	F	204	-	-	0/7/7/10	-

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

All (97) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	202	HEM	C3C-C2C	-5.39	1.32	1.40
3	A	202	KSY	C04-N03	5.26	1.46	1.38
4	F	202	HEM	C3C-C2C	-4.88	1.33	1.40
4	C	202	HEM	C3B-C2B	-4.75	1.33	1.40
4	H	202	HEM	C3B-C2B	-4.74	1.33	1.40
4	B	203	HEM	C3C-C2C	-4.71	1.33	1.40
4	A	204	HEM	C3B-C2B	-4.69	1.33	1.40
4	F	202	HEM	C3B-C2B	-4.66	1.33	1.40
3	D	202	KSY	C04-N03	4.63	1.45	1.38
3	A	203	KSY	C02-N03	4.58	1.45	1.38
3	A	202	KSY	C21-C02	4.41	1.55	1.48
4	A	204	HEM	C3C-C2C	-4.41	1.34	1.40
3	C	201	KSY	C21-C02	4.38	1.55	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	203	HEM	C3B-C2B	-4.38	1.34	1.40
3	L	201	KSY	C21-C02	4.34	1.55	1.48
4	D	203	HEM	C3C-C2C	-4.31	1.34	1.40
4	D	203	HEM	C3B-C2B	-4.31	1.34	1.40
4	L	202	HEM	C3B-C2B	-4.27	1.34	1.40
3	L	201	KSY	C02-N03	4.23	1.44	1.38
3	A	203	KSY	C04-N03	4.23	1.44	1.38
3	L	201	KSY	C04-N03	4.18	1.44	1.38
3	D	202	KSY	C02-N03	4.17	1.44	1.38
3	I	201	KSY	C21-C02	4.14	1.54	1.48
3	K	201	KSY	C21-C02	4.02	1.54	1.48
3	J	201	KSY	C02-N03	3.87	1.44	1.38
3	H	201	KSY	C21-C02	3.86	1.54	1.48
3	D	202	KSY	C21-C02	3.83	1.54	1.48
3	G	201	KSY	C21-C02	3.83	1.54	1.48
3	E	201	KSY	C04-N03	3.79	1.44	1.38
4	C	202	HEM	C3C-C2C	-3.79	1.35	1.40
3	A	202	KSY	C02-N03	3.79	1.44	1.38
4	L	202	HEM	C3C-C2C	-3.78	1.35	1.40
3	J	201	KSY	C04-N03	3.76	1.44	1.38
3	H	201	KSY	C04-N03	3.69	1.44	1.38
4	L	202	HEM	C3C-CAC	3.66	1.55	1.47
3	E	201	KSY	C21-C02	3.65	1.54	1.48
3	K	201	KSY	C04-N03	3.61	1.43	1.38
3	E	201	KSY	C02-N03	3.56	1.43	1.38
4	H	202	HEM	C3C-CAC	3.52	1.55	1.47
3	G	201	KSY	C06-N07	3.49	1.47	1.37
3	H	201	KSY	C06-N07	3.49	1.47	1.37
4	D	203	HEM	C3C-CAC	3.46	1.54	1.47
3	A	203	KSY	C21-C02	3.43	1.53	1.48
3	F	201	KSY	C04-N03	3.40	1.43	1.38
3	J	201	KSY	C06-N07	3.38	1.46	1.37
4	L	202	HEM	C3B-CAB	3.36	1.54	1.47
4	A	204	HEM	C3B-CAB	3.35	1.54	1.47
3	K	201	KSY	C06-N07	3.35	1.46	1.37
3	F	201	KSY	C02-N03	3.32	1.43	1.38
4	C	202	HEM	C3C-CAC	3.30	1.54	1.47
3	I	201	KSY	C04-N03	3.30	1.43	1.38
4	C	202	HEM	C3B-CAB	3.29	1.54	1.47
3	B	202	KSY	C21-C02	3.28	1.53	1.48
3	I	201	KSY	C02-N03	3.23	1.43	1.38
3	J	201	KSY	C21-C02	3.23	1.53	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	202	KSY	C06-N07	3.20	1.46	1.37
4	D	203	HEM	C3B-CAB	3.19	1.54	1.47
3	C	201	KSY	C06-N07	3.19	1.46	1.37
3	C	201	KSY	C04-N03	3.18	1.43	1.38
3	F	201	KSY	C06-N07	3.17	1.46	1.37
4	F	202	HEM	C3C-CAC	3.14	1.54	1.47
3	K	201	KSY	C02-N03	3.11	1.43	1.38
3	G	201	KSY	C04-N03	3.11	1.43	1.38
4	H	202	HEM	C3B-CAB	3.11	1.54	1.47
3	F	201	KSY	C21-C02	3.11	1.53	1.48
3	B	202	KSY	C04-N03	3.03	1.43	1.38
3	I	201	KSY	C06-N07	2.98	1.45	1.37
4	F	202	HEM	C3B-CAB	2.97	1.54	1.47
4	B	203	HEM	C3C-CAC	2.96	1.53	1.47
3	A	203	KSY	C06-N07	2.95	1.45	1.37
3	H	201	KSY	C02-N03	2.93	1.43	1.38
4	B	203	HEM	C3B-CAB	2.91	1.53	1.47
3	D	202	KSY	C06-N07	2.91	1.45	1.37
3	L	201	KSY	C06-N07	2.83	1.45	1.37
4	A	204	HEM	C3C-CAC	2.83	1.53	1.47
3	A	202	KSY	C06-N07	2.81	1.45	1.37
3	B	202	KSY	C02-N03	2.80	1.42	1.38
3	G	201	KSY	O01-C02	-2.79	1.17	1.23
3	E	201	KSY	C06-N07	2.74	1.45	1.37
3	C	201	KSY	C02-N03	2.62	1.42	1.38
3	C	201	KSY	O01-C02	-2.53	1.18	1.23
3	G	201	KSY	C02-N03	2.50	1.42	1.38
3	J	201	KSY	O01-C02	-2.49	1.18	1.23
3	B	202	KSY	O01-C02	-2.45	1.18	1.23
3	I	201	KSY	O01-C02	-2.44	1.18	1.23
3	E	201	KSY	O01-C02	-2.42	1.18	1.23
3	K	201	KSY	O01-C02	-2.42	1.18	1.23
4	H	202	HEM	CAA-C2A	2.41	1.55	1.52
3	A	202	KSY	O01-C02	-2.41	1.18	1.23
3	D	202	KSY	O01-C02	-2.40	1.18	1.23
3	H	201	KSY	O01-C02	-2.40	1.18	1.23
3	L	201	KSY	O01-C02	-2.38	1.18	1.23
3	A	203	KSY	O22-C04	-2.20	1.18	1.23
3	L	201	KSY	O22-C04	-2.19	1.18	1.23
3	F	201	KSY	O01-C02	-2.10	1.19	1.23
4	B	203	HEM	CAA-C2A	2.08	1.55	1.52
3	A	202	KSY	O22-C04	-2.01	1.19	1.23

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	202	KSY	C04-N03-C02	-8.24	105.49	112.52
3	D	202	KSY	C04-N03-C02	-7.02	106.53	112.52
3	L	201	KSY	C04-N03-C02	-5.97	107.43	112.52
3	J	201	KSY	C05-C06-N07	-5.52	114.77	121.32
3	H	201	KSY	C21-C05-C06	-5.52	118.11	121.91
3	J	201	KSY	C04-N03-C02	-5.48	107.85	112.52
3	A	202	KSY	C21-C02-N03	4.68	110.19	105.89
3	A	203	KSY	C04-N03-C02	-4.56	108.64	112.52
3	I	201	KSY	C21-C05-C06	-3.99	119.16	121.91
3	I	201	KSY	C05-C06-N07	-3.99	116.60	121.32
3	A	202	KSY	C05-C06-N07	-3.95	116.64	121.32
4	C	202	HEM	CMD-C2D-C1D	-3.90	122.47	128.46
3	C	201	KSY	C05-C06-N07	-3.83	116.78	121.32
3	B	202	KSY	C21-C05-C06	-3.79	119.30	121.91
3	F	201	KSY	C05-C06-N07	-3.70	116.94	121.32
3	H	201	KSY	C06-C05-C04	3.66	134.37	129.21
3	B	202	KSY	C05-C06-N07	-3.66	116.99	121.32
4	D	203	HEM	CBA-CAA-C2A	-3.66	105.74	112.49
3	L	201	KSY	C05-C06-N07	-3.61	117.04	121.32
3	D	202	KSY	C21-C02-N03	3.51	109.12	105.89
3	G	201	KSY	C05-C06-N07	-3.48	117.20	121.32
3	J	201	KSY	C21-C02-N03	3.40	109.01	105.89
3	A	202	KSY	C21-C05-C06	-3.22	119.69	121.91
4	H	202	HEM	CMA-C3A-C4A	-3.22	123.52	128.46
3	K	201	KSY	C05-C06-N07	-3.21	117.51	121.32
3	F	201	KSY	C21-C05-C06	-3.18	119.72	121.91
3	C	201	KSY	C21-C05-C06	-3.15	119.74	121.91
3	E	201	KSY	C21-C05-C06	-3.08	119.79	121.91
3	L	201	KSY	C21-C02-N03	3.05	108.69	105.89
4	A	204	HEM	CBD-CAD-C3D	-3.04	106.87	112.48
4	F	202	HEM	CMA-C3A-C4A	-3.04	123.79	128.46
3	H	201	KSY	C05-C06-N07	3.04	124.92	121.32
4	C	202	HEM	CMC-C2C-C3C	3.03	130.34	124.68
3	E	201	KSY	C05-C06-N07	-2.99	117.78	121.32
4	C	202	HEM	CBD-CAD-C3D	-2.92	107.10	112.48
4	A	204	HEM	CMB-C2B-C3B	2.89	130.09	124.68
4	C	202	HEM	C1D-C2D-C3D	2.88	109.00	107.00
3	B	202	KSY	O22-C04-C05	2.88	132.83	128.55
3	H	201	KSY	C18-C06-N07	-2.86	116.92	121.80
4	B	203	HEM	CBA-CAA-C2A	-2.86	107.21	112.49
4	A	204	HEM	CMA-C3A-C4A	-2.83	124.12	128.46
3	G	201	KSY	O22-C04-C05	2.82	132.75	128.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	202	HEM	CMD-C2D-C1D	-2.77	124.20	128.46
3	E	201	KSY	C04-N03-C02	-2.76	110.17	112.52
4	C	202	HEM	CAD-CBD-CGD	-2.73	108.08	112.67
3	J	201	KSY	C18-C06-N07	2.73	126.45	121.80
4	F	202	HEM	C4C-C3C-C2C	2.65	108.75	106.90
4	H	202	HEM	C4C-C3C-C2C	2.65	108.75	106.90
4	F	202	HEM	CAD-CBD-CGD	-2.64	108.25	112.67
4	B	203	HEM	CBD-CAD-C3D	-2.62	107.64	112.48
4	A	204	HEM	CBA-CAA-C2A	-2.62	107.66	112.49
4	B	203	HEM	C4C-C3C-C2C	2.61	108.72	106.90
4	A	204	HEM	CMC-C2C-C3C	2.60	129.55	124.68
4	L	202	HEM	CMC-C2C-C3C	2.58	129.50	124.68
4	C	202	HEM	CMA-C3A-C4A	-2.57	124.52	128.46
3	K	201	KSY	C21-C05-C06	-2.55	120.16	121.91
4	L	202	HEM	CMD-C2D-C1D	-2.53	124.58	128.46
4	F	202	HEM	CMD-C2D-C1D	-2.48	124.65	128.46
4	A	204	HEM	C4C-C3C-C2C	2.46	108.62	106.90
4	L	202	HEM	CMA-C3A-C4A	-2.43	124.73	128.46
3	H	201	KSY	C04-N03-C02	-2.41	110.47	112.52
3	D	202	KSY	C21-C05-C06	-2.39	120.26	121.91
3	A	202	KSY	C06-C05-C04	2.38	132.56	129.21
4	D	203	HEM	CBD-CAD-C3D	-2.36	108.12	112.48
3	D	202	KSY	C05-C06-N07	-2.36	118.52	121.32
4	C	202	HEM	C4C-C3C-C2C	2.31	108.51	106.90
4	H	202	HEM	C4A-C3A-C2A	2.29	108.59	107.00
4	A	204	HEM	CMD-C2D-C1D	-2.28	124.95	128.46
4	C	202	HEM	C4A-C3A-C2A	2.28	108.58	107.00
3	D	202	KSY	O22-C04-C05	-2.26	125.18	128.55
3	L	201	KSY	C21-C05-C06	-2.26	120.36	121.91
4	D	203	HEM	CMC-C2C-C3C	2.25	128.89	124.68
3	I	201	KSY	O22-C04-C05	2.24	131.88	128.55
3	A	202	KSY	O22-C04-C05	-2.21	125.26	128.55
3	H	201	KSY	O22-C04-C05	2.20	131.82	128.55
4	A	204	HEM	C4A-C3A-C2A	2.19	108.52	107.00
3	G	201	KSY	C21-C05-C06	-2.19	120.40	121.91
3	A	203	KSY	C08-N07-C06	-2.19	118.12	123.39
3	A	203	KSY	O22-C04-C05	-2.17	125.32	128.55
3	F	201	KSY	O22-C04-C05	2.17	131.78	128.55
4	B	203	HEM	CMA-C3A-C4A	-2.16	125.14	128.46
3	H	201	KSY	C19-C18-C06	2.16	123.10	118.62
4	F	202	HEM	CBD-CAD-C3D	-2.13	108.56	112.48
4	H	202	HEM	CBA-CAA-C2A	-2.09	108.63	112.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	202	HEM	CBA-CAA-C2A	-2.07	108.66	112.49
3	A	203	KSY	C21-C05-C06	-2.06	120.49	121.91
3	D	202	KSY	C06-C05-C04	2.06	132.11	129.21
4	F	202	HEM	C1D-C2D-C3D	2.05	108.42	107.00
4	B	203	HEM	CAD-CBD-CGD	-2.04	109.25	112.67
4	D	203	HEM	CMB-C2B-C3B	2.02	128.47	124.68
3	C	201	KSY	C04-N03-C02	-2.02	110.80	112.52
4	C	202	HEM	CMB-C2B-C3B	2.02	128.45	124.68
3	C	201	KSY	O22-C04-C05	2.01	131.53	128.55

There are no chirality outliers.

All (61) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	201	KSY	C18-C06-N07-C08
3	H	201	KSY	C05-C06-N07-C08
5	I	202	PG4	O4-C7-C8-O5
3	H	201	KSY	N07-C08-C09-C10
5	I	202	PG4	O3-C5-C6-O4
5	A	206	PG4	O2-C3-C4-O3
5	K	204	PG4	O2-C3-C4-O3
5	F	203	PG4	O2-C3-C4-O3
5	F	203	PG4	O3-C5-C6-O4
5	C	203	PG4	O3-C5-C6-O4
3	D	202	KSY	N07-C08-C09-C10
5	C	203	PG4	O2-C3-C4-O3
5	C	203	PG4	O4-C7-C8-O5
5	D	204	PG4	O4-C7-C8-O5
5	F	203	PG4	O1-C1-C2-O2
5	A	206	PG4	O1-C1-C2-O2
5	F	205	PG4	O2-C3-C4-O3
5	E	202	PG4	O3-C5-C6-O4
3	H	201	KSY	C08-C09-C10-C11
3	A	202	KSY	N07-C08-C09-C10
5	L	203	PG4	O4-C7-C8-O5
5	G	202	PG4	O4-C7-C8-O5
5	K	202	PG4	O4-C7-C8-O5
5	K	203	PG4	O3-C5-C6-O4
5	K	202	PG4	O3-C5-C6-O4
5	D	204	PG4	O3-C5-C6-O4
5	K	203	PG4	O1-C1-C2-O2
5	L	203	PG4	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	I	202	PG4	C5-C6-O4-C7
5	A	206	PG4	C3-C4-O3-C5
5	A	206	PG4	C6-C5-O3-C4
5	J	202	PG4	O1-C1-C2-O2
5	G	202	PG4	O3-C5-C6-O4
5	G	202	PG4	C8-C7-O4-C6
5	J	202	PG4	O3-C5-C6-O4
5	B	204	PG4	O4-C7-C8-O5
5	C	203	PG4	C8-C7-O4-C6
5	K	203	PG4	C1-C2-O2-C3
5	F	205	PG4	C3-C4-O3-C5
5	A	205	PG4	O3-C5-C6-O4
5	I	202	PG4	C3-C4-O3-C5
5	C	203	PG4	C1-C2-O2-C3
5	F	203	PG4	C8-C7-O4-C6
5	C	203	PG4	C6-C5-O3-C4
5	C	203	PG4	C5-C6-O4-C7
3	A	202	KSY	C09-C10-C11-C12
3	E	201	KSY	C09-C10-C11-C17
3	B	202	KSY	C09-C10-C11-C17
3	A	202	KSY	C09-C10-C11-C17
3	E	201	KSY	C09-C10-C11-C12
3	B	202	KSY	C09-C10-C11-C12
3	D	202	KSY	C09-C10-C11-C12
5	K	204	PG4	C4-C3-O2-C2
3	C	201	KSY	C09-C10-C11-C17
3	C	201	KSY	C09-C10-C11-C12
5	K	203	PG4	O2-C3-C4-O3
3	D	202	KSY	C09-C10-C11-C17
5	L	203	PG4	O2-C3-C4-O3
3	A	202	KSY	C08-C09-C10-C11
5	G	203	PG4	C8-C7-O4-C6
5	F	203	PG4	O4-C7-C8-O5

There are no ring outliers.

30 monomers are involved in 52 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	202	KSY	1	0
5	F	205	PG4	1	0
5	C	203	PG4	1	0
3	I	201	KSY	1	0

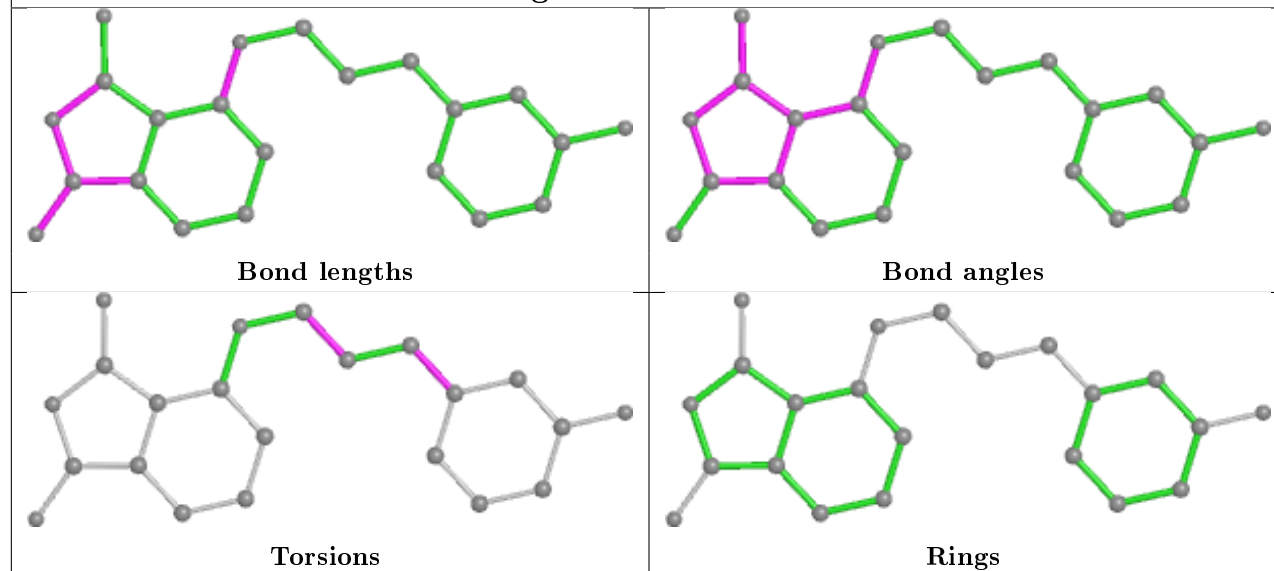
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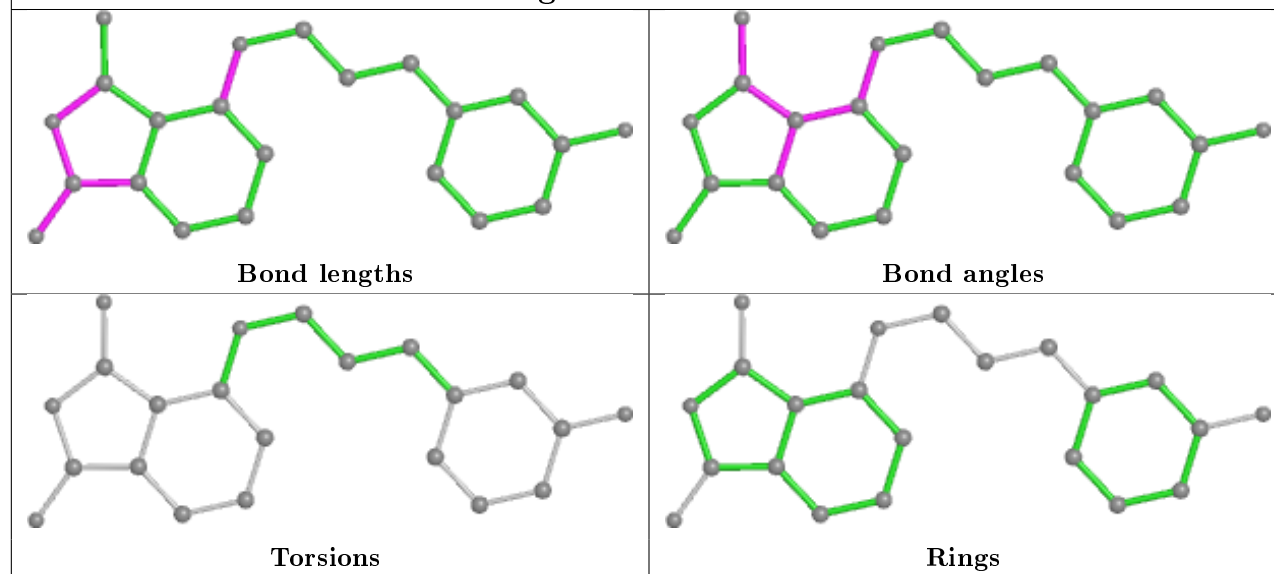
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	202	HEM	3	0
3	E	201	KSY	1	0
5	F	203	PG4	2	0
4	C	202	HEM	5	0
4	A	204	HEM	2	0
5	A	206	PG4	1	0
5	L	203	PG4	2	0
3	L	201	KSY	1	0
3	J	201	KSY	1	0
3	K	201	KSY	1	0
3	H	201	KSY	1	0
3	G	201	KSY	1	0
5	D	206	PG4	1	0
5	G	203	PG4	1	0
5	G	202	PG4	1	0
3	A	203	KSY	1	0
4	L	202	HEM	6	0
3	C	201	KSY	1	0
3	B	202	KSY	1	0
5	K	203	PG4	1	0
4	F	202	HEM	3	0
4	B	203	HEM	4	0
5	I	202	PG4	3	0
4	D	203	HEM	2	0
3	A	202	KSY	1	0
3	F	201	KSY	1	0

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

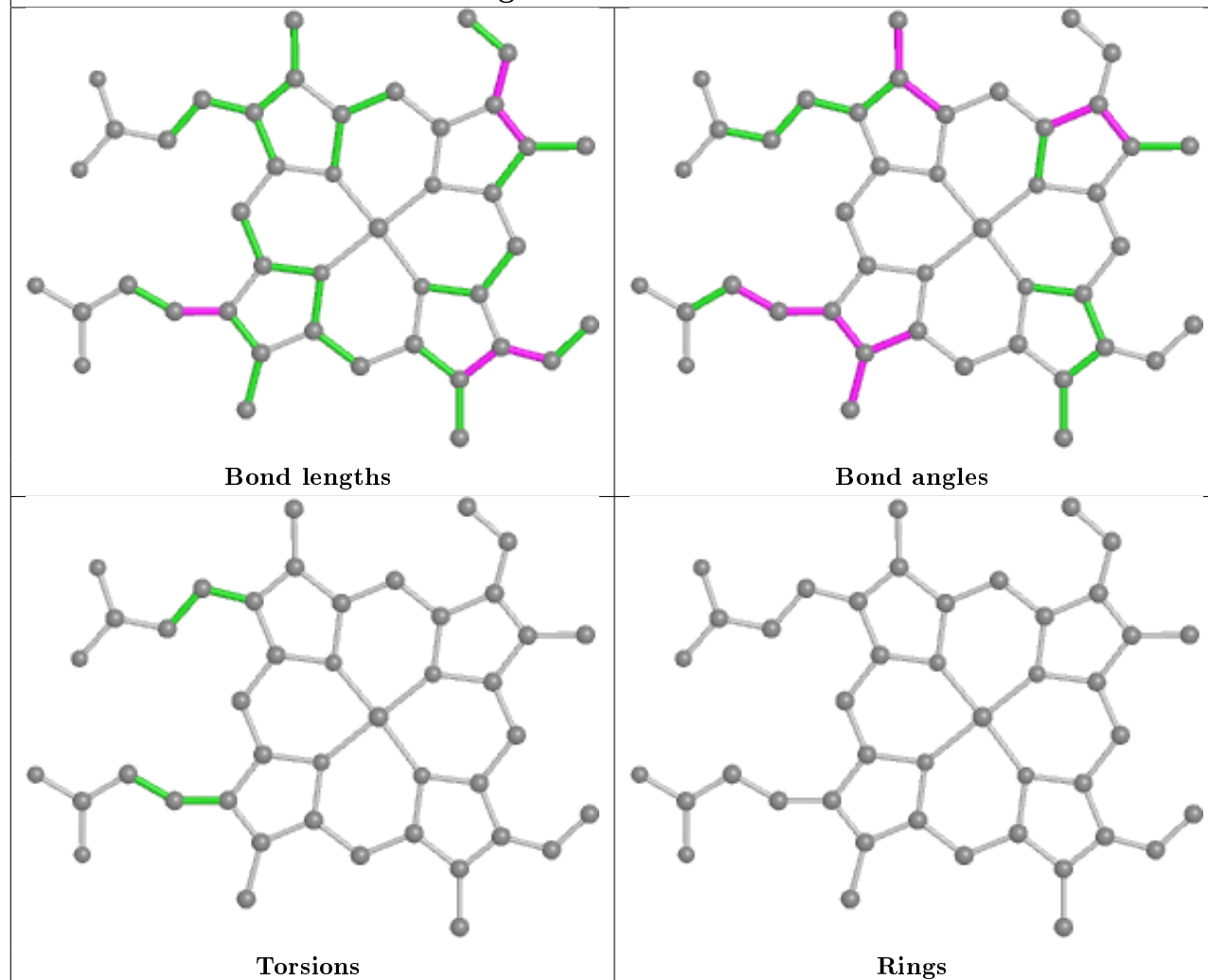
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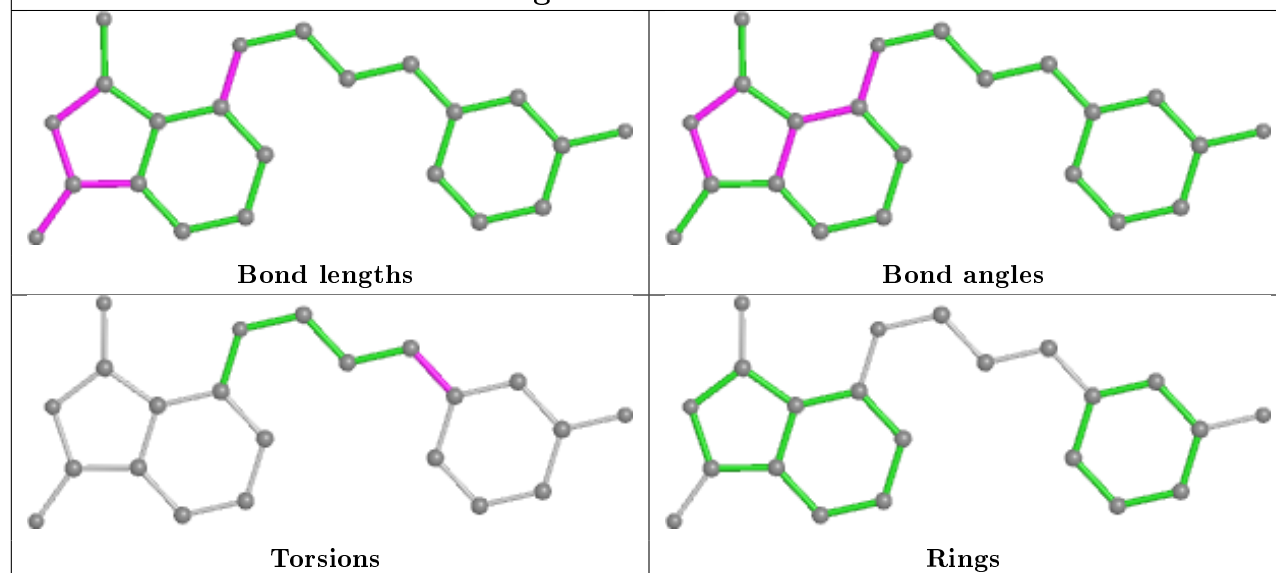
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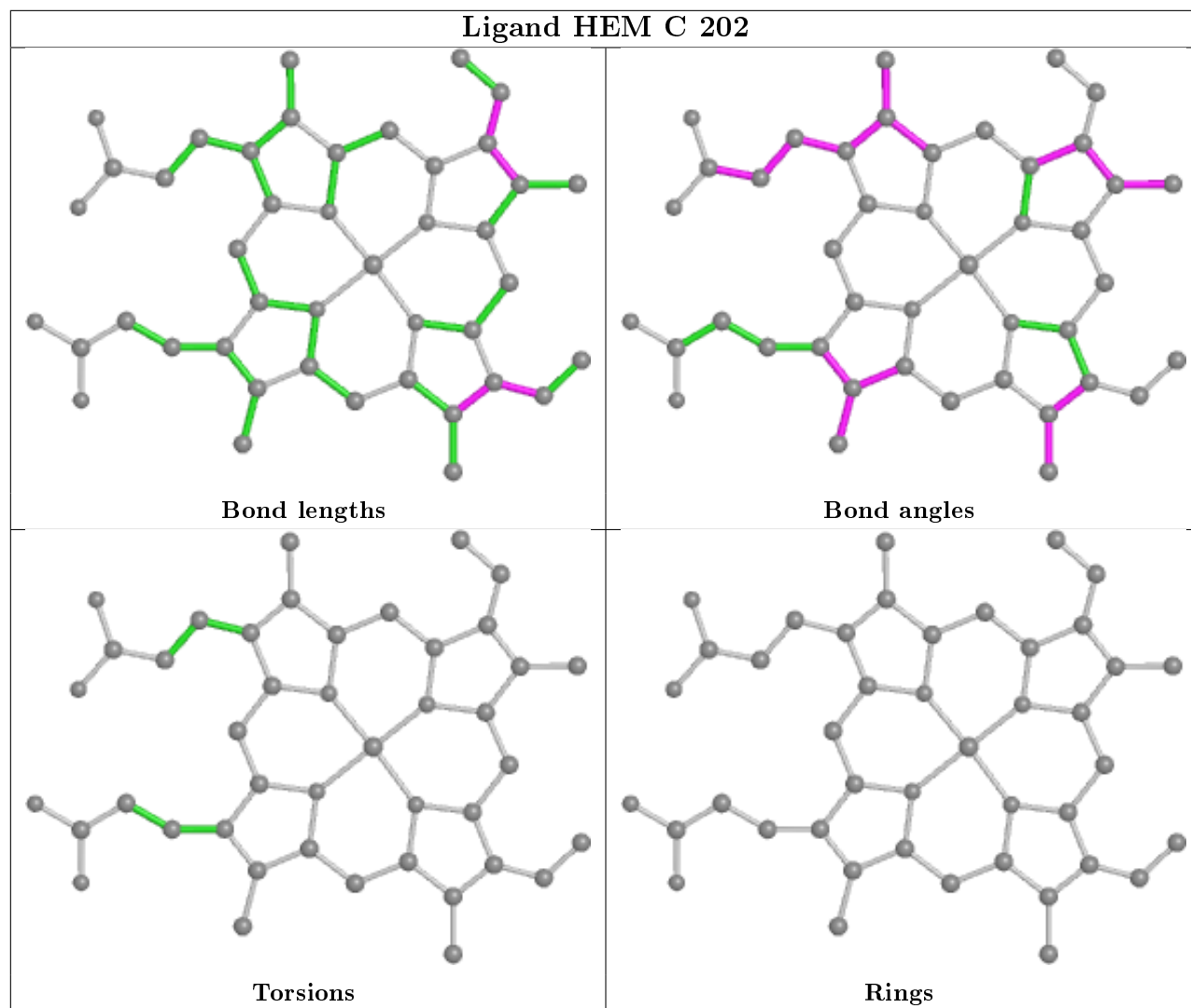


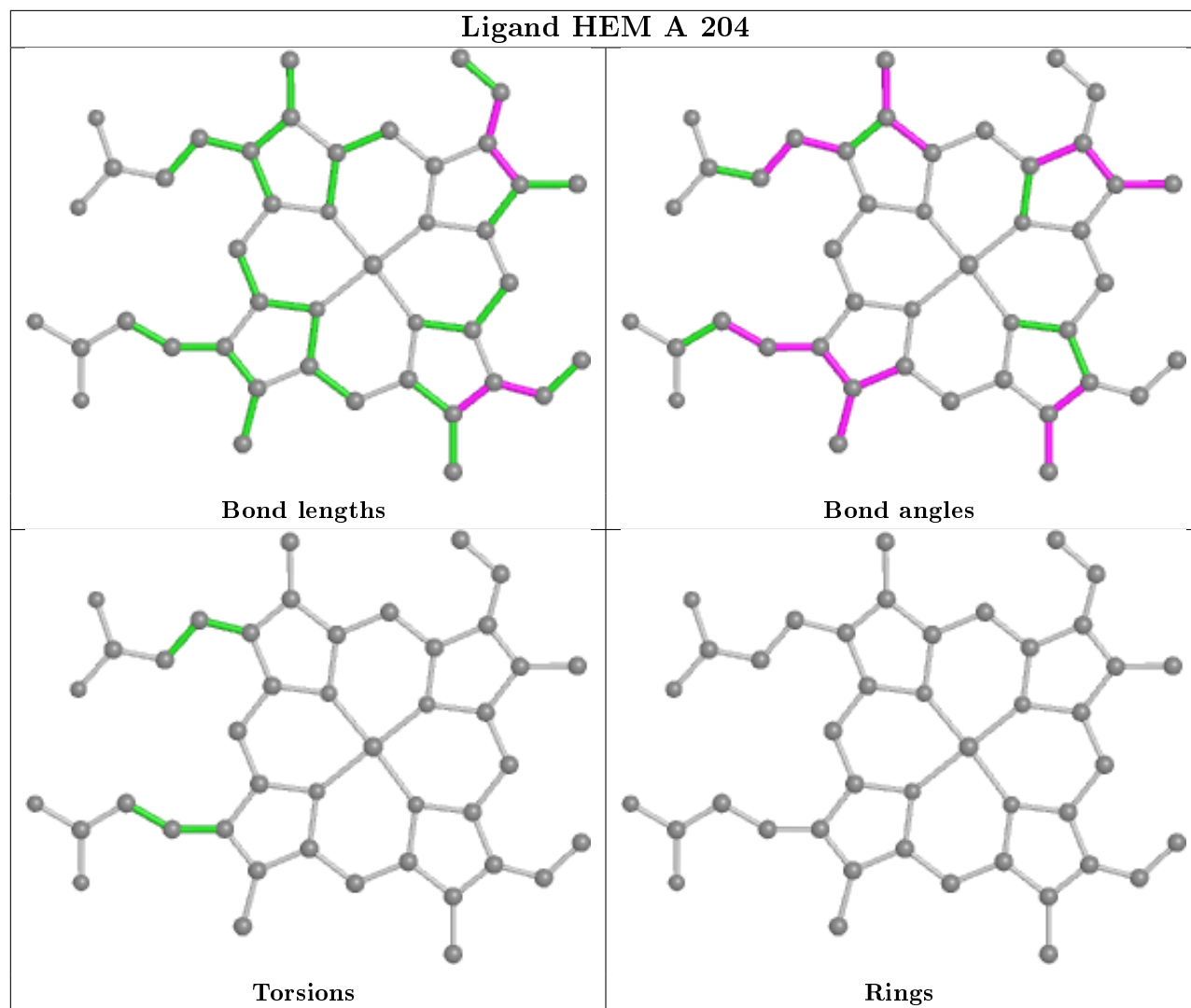
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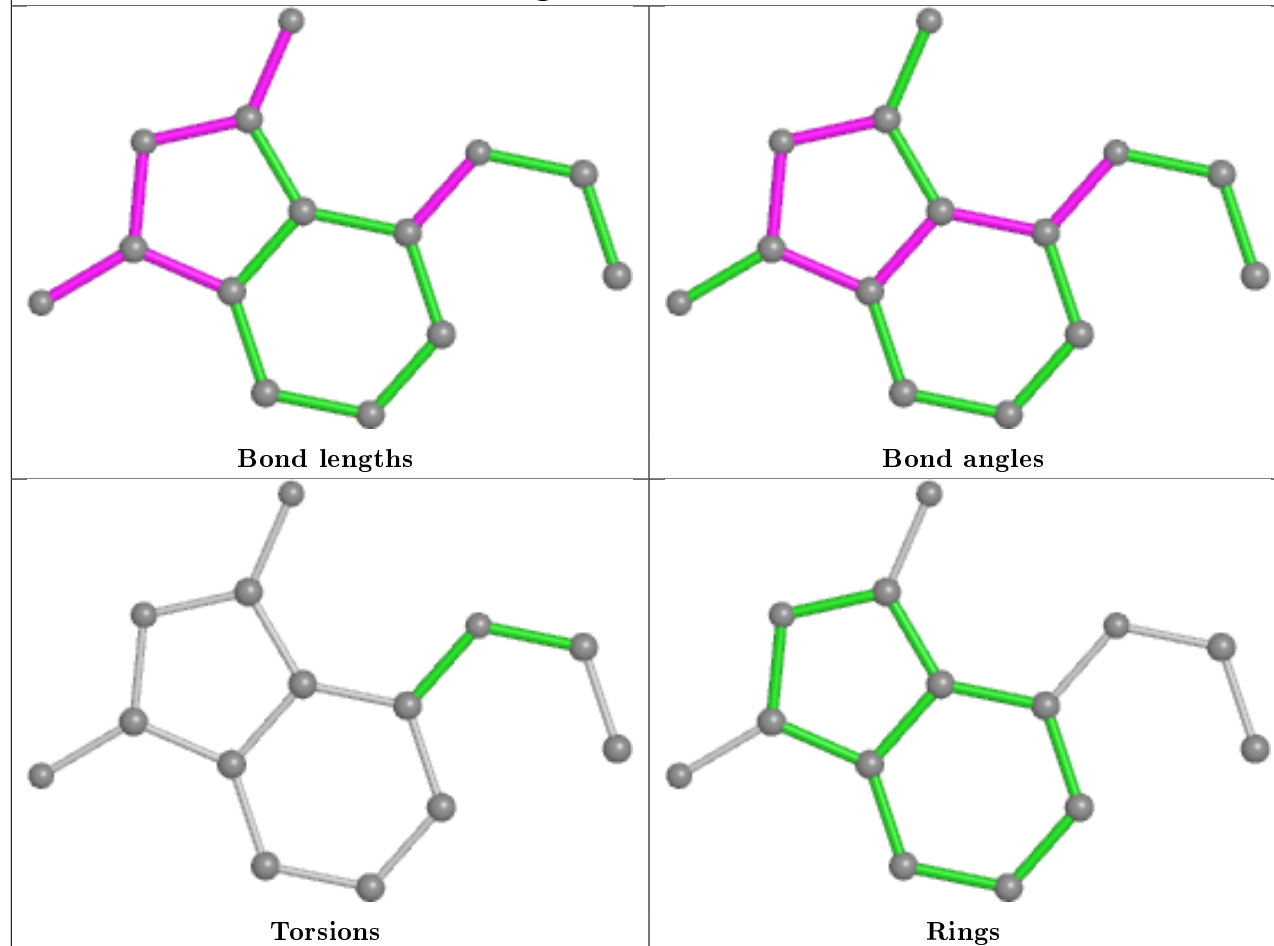
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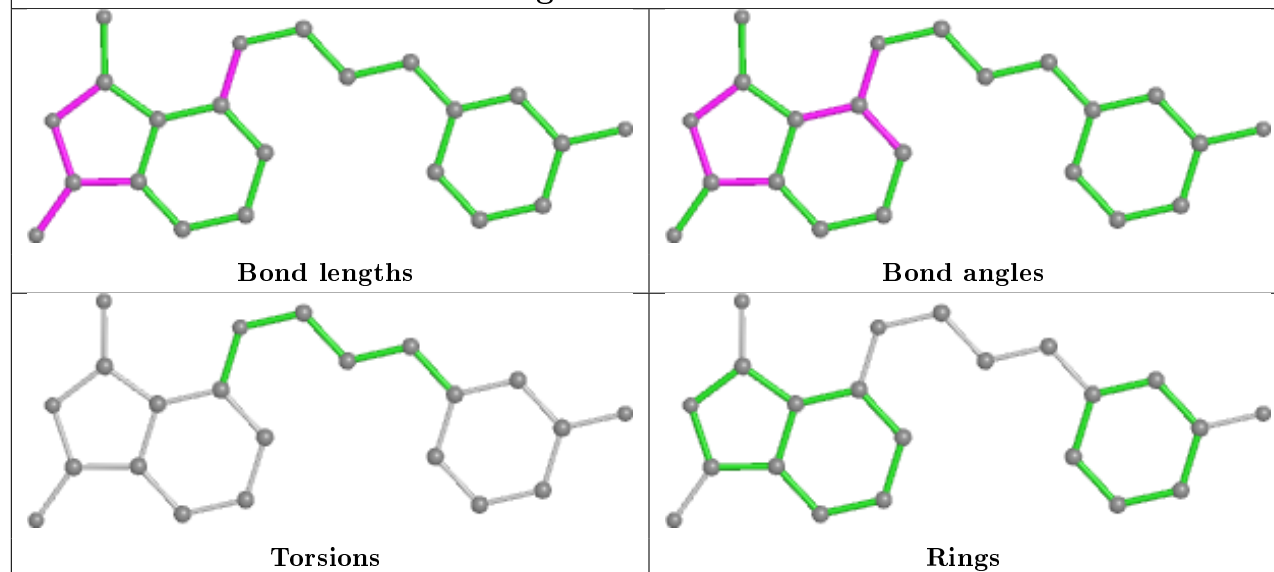




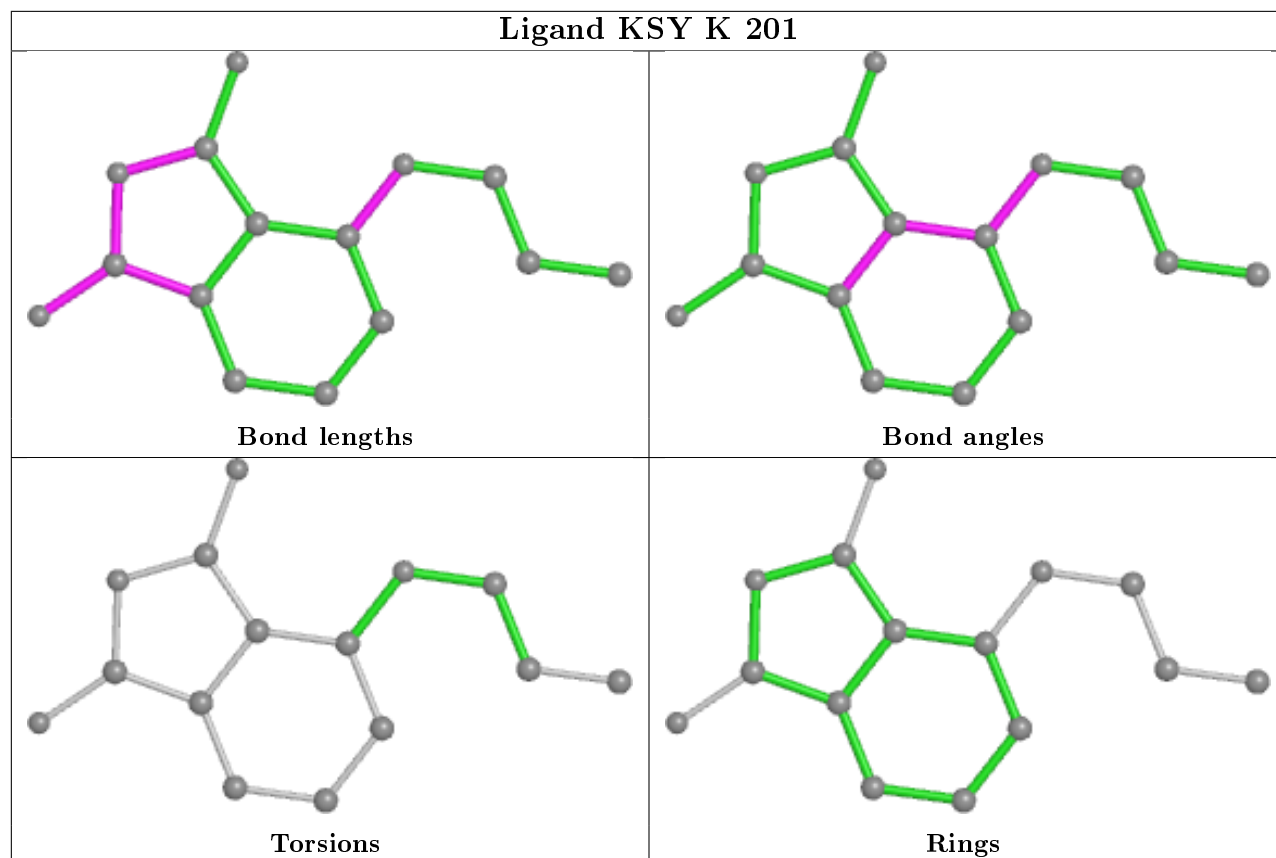
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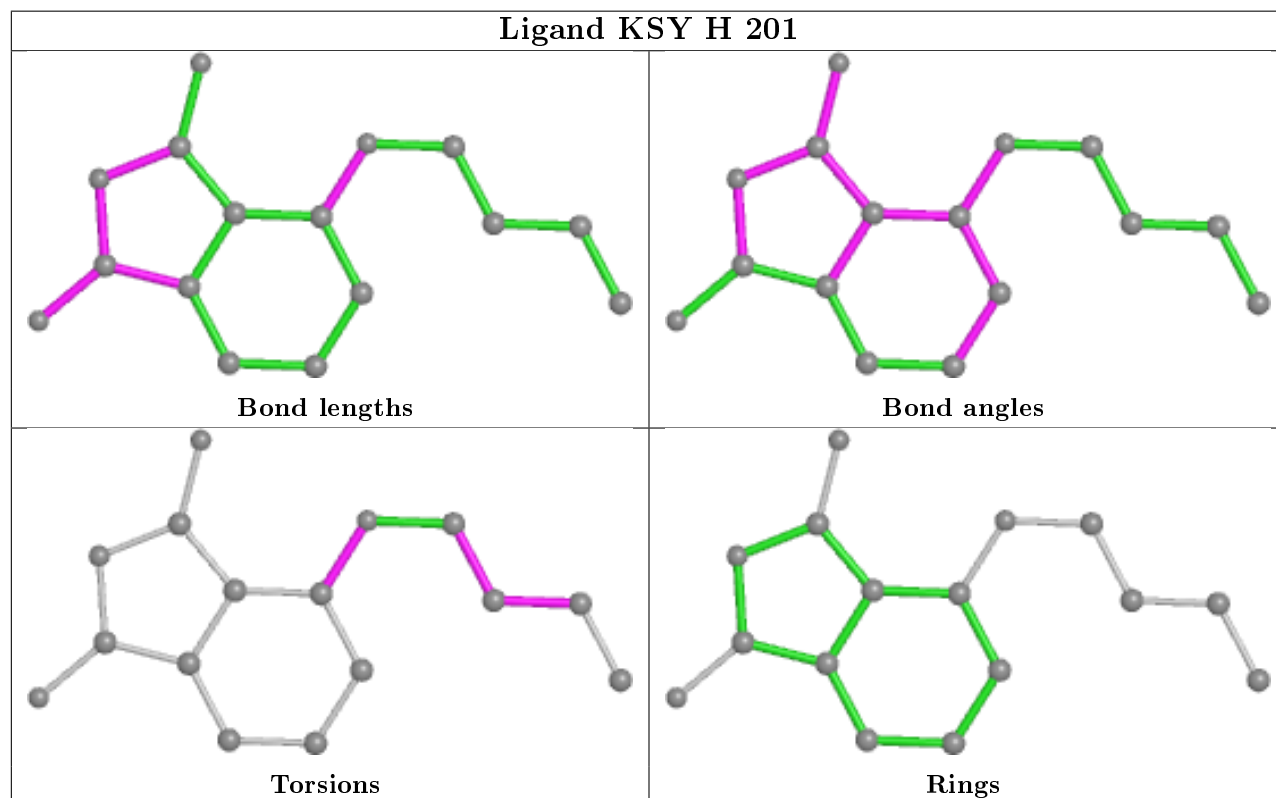
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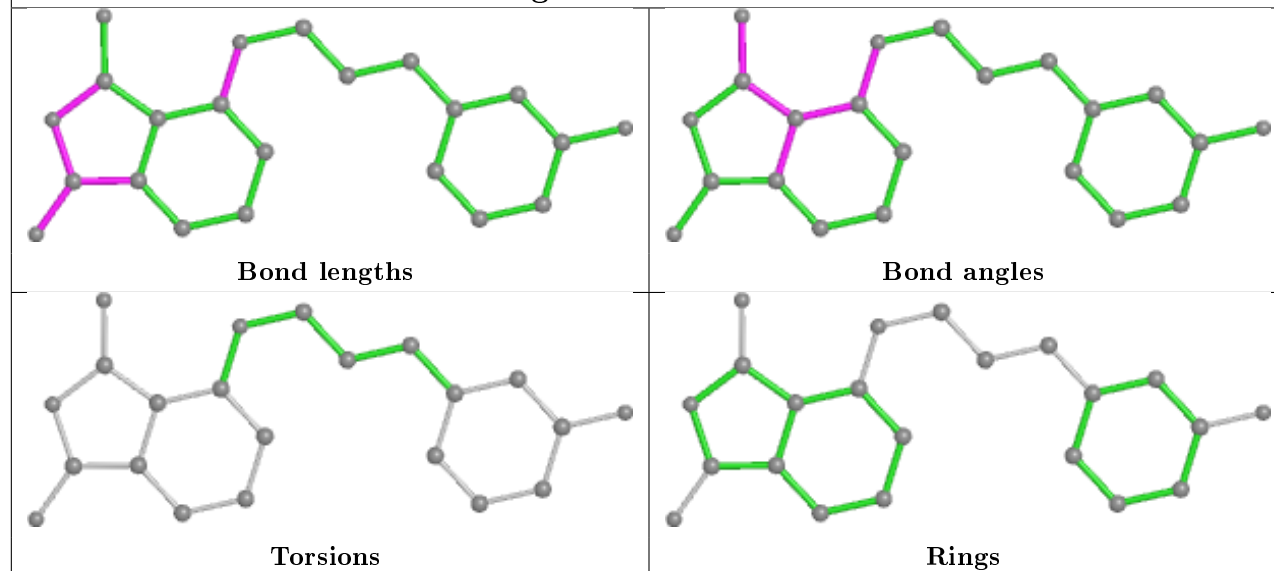
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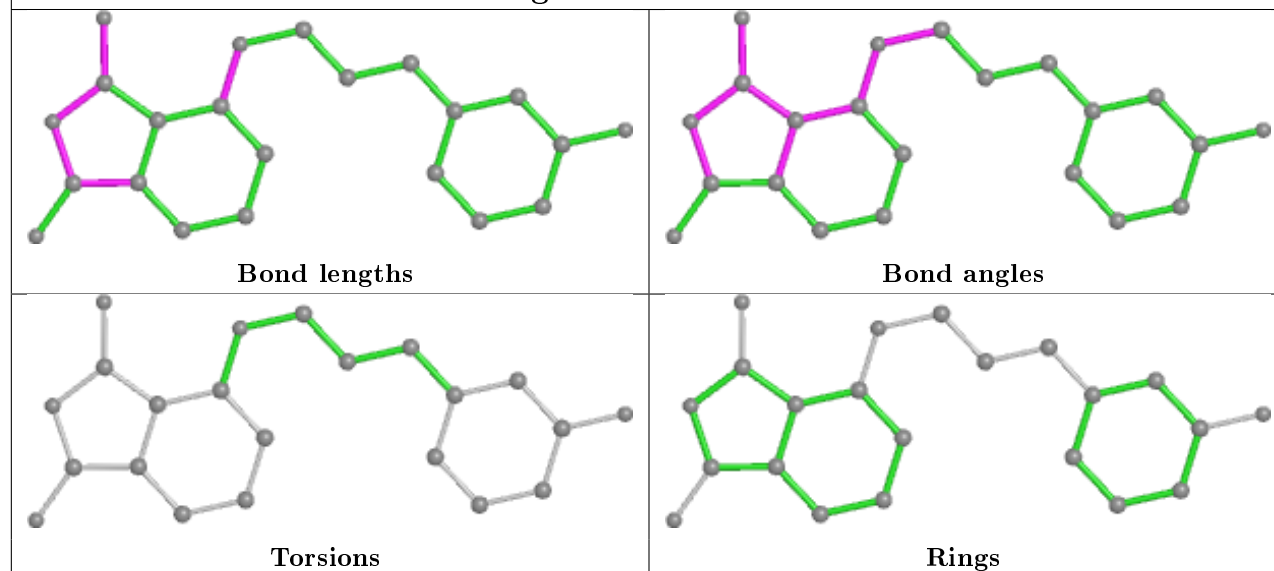
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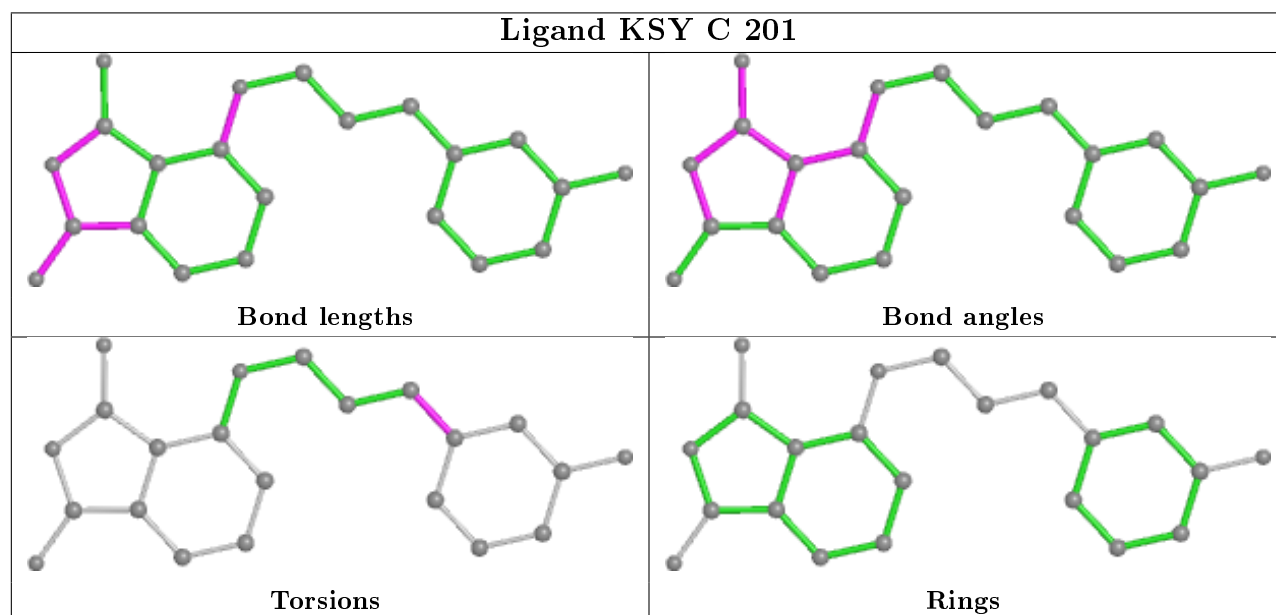
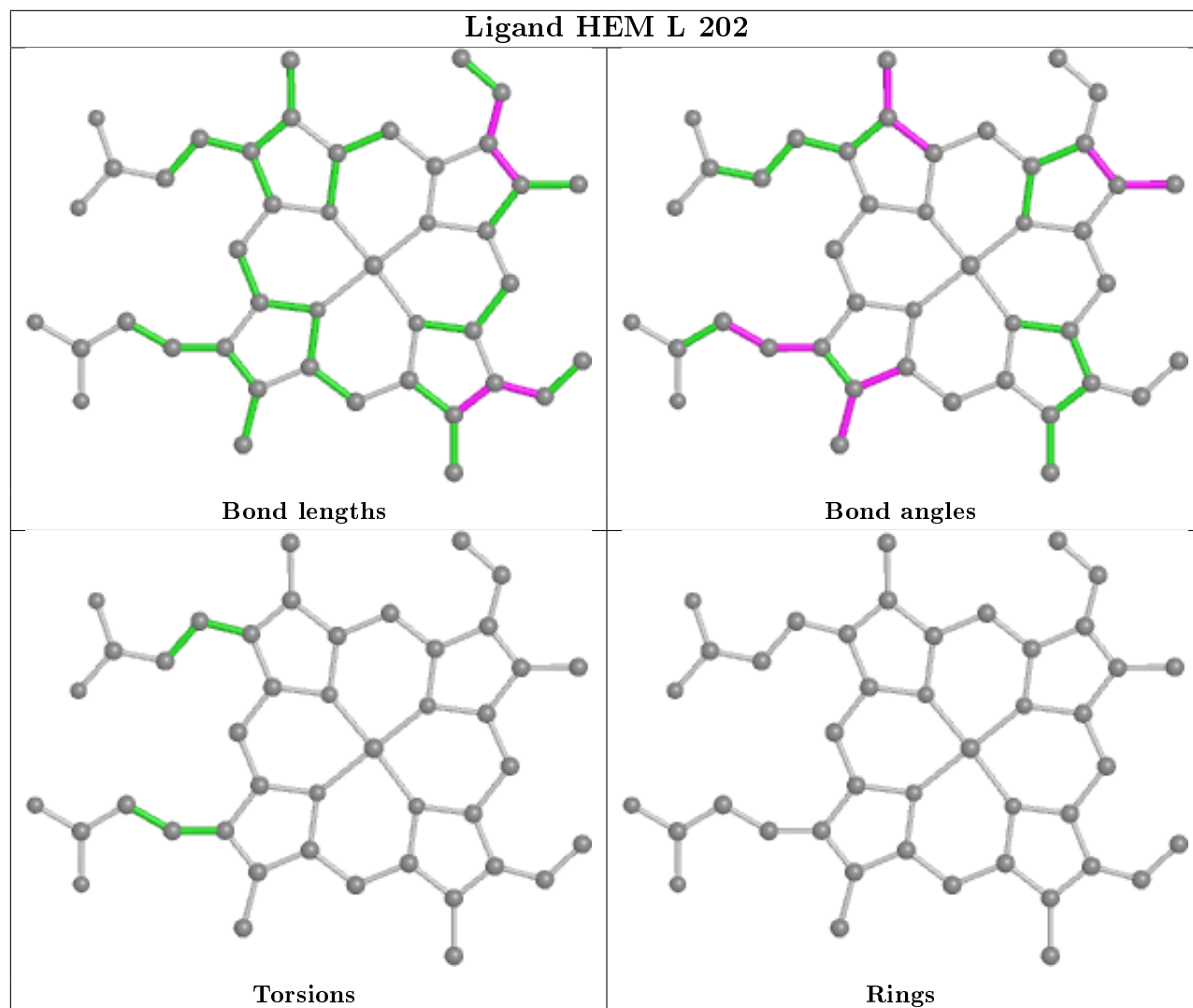


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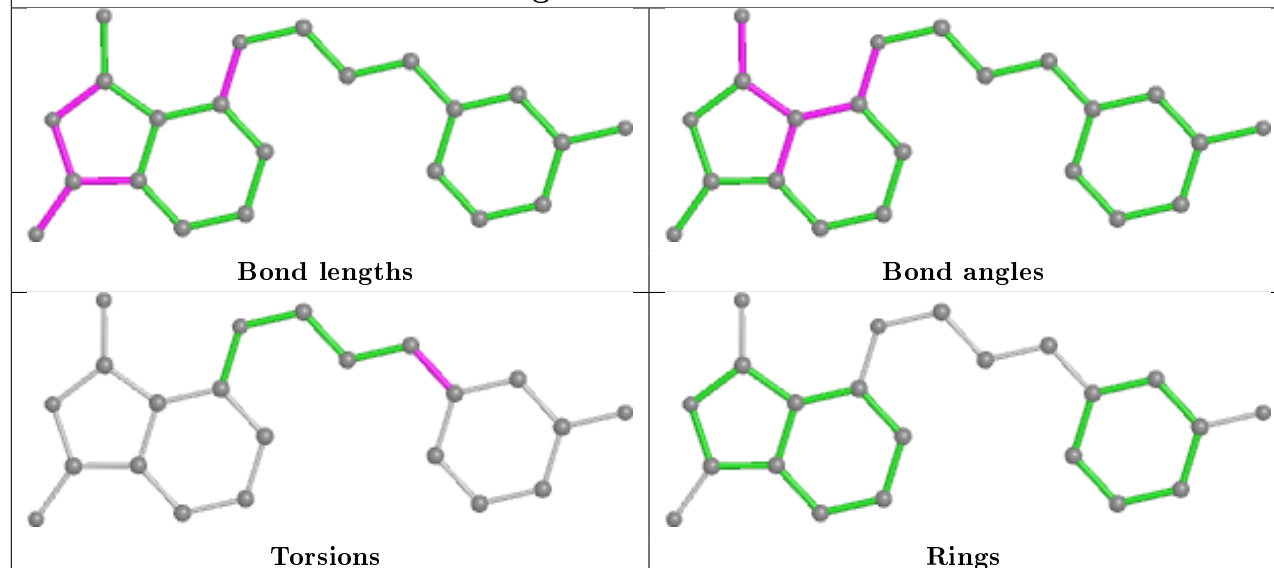


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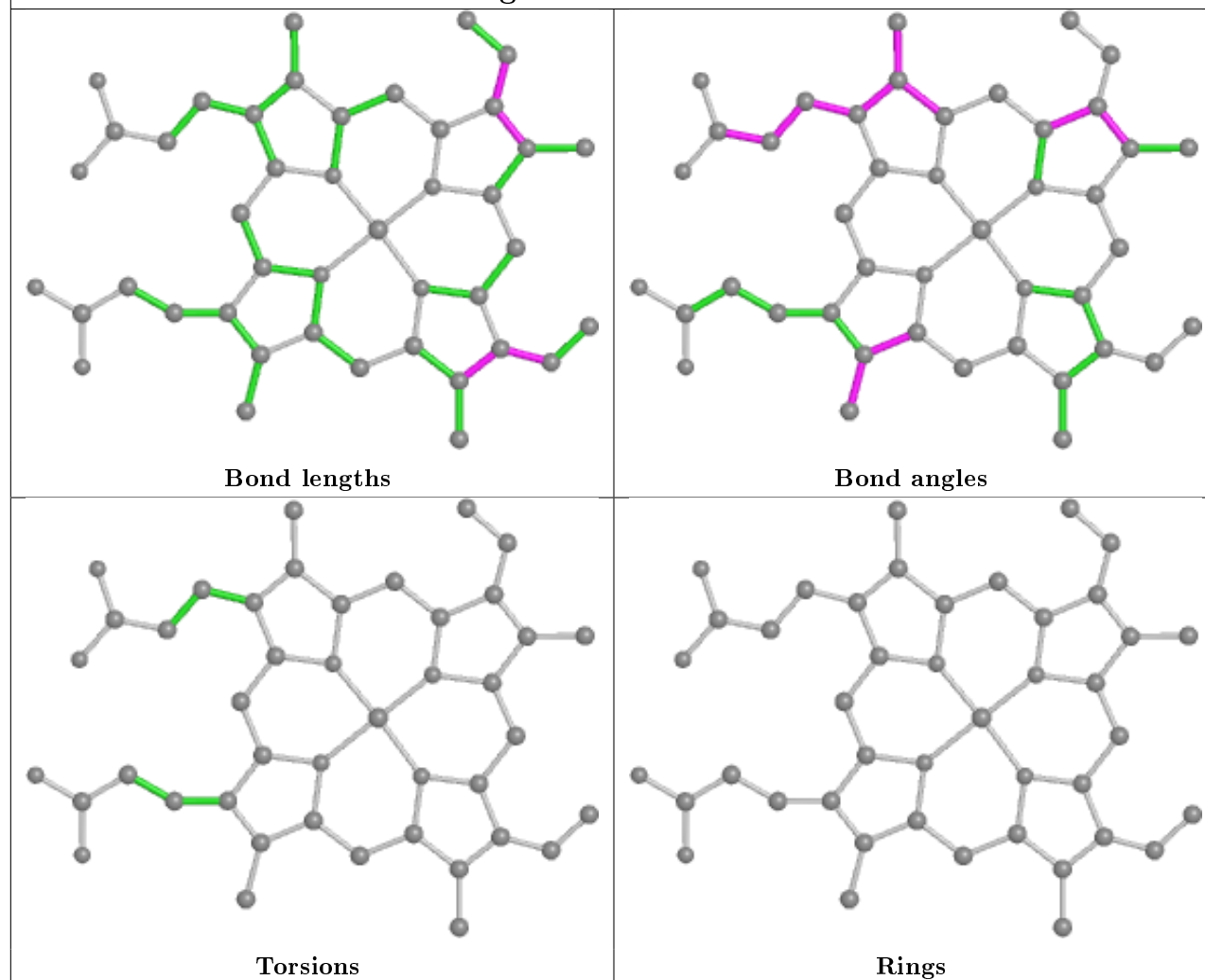


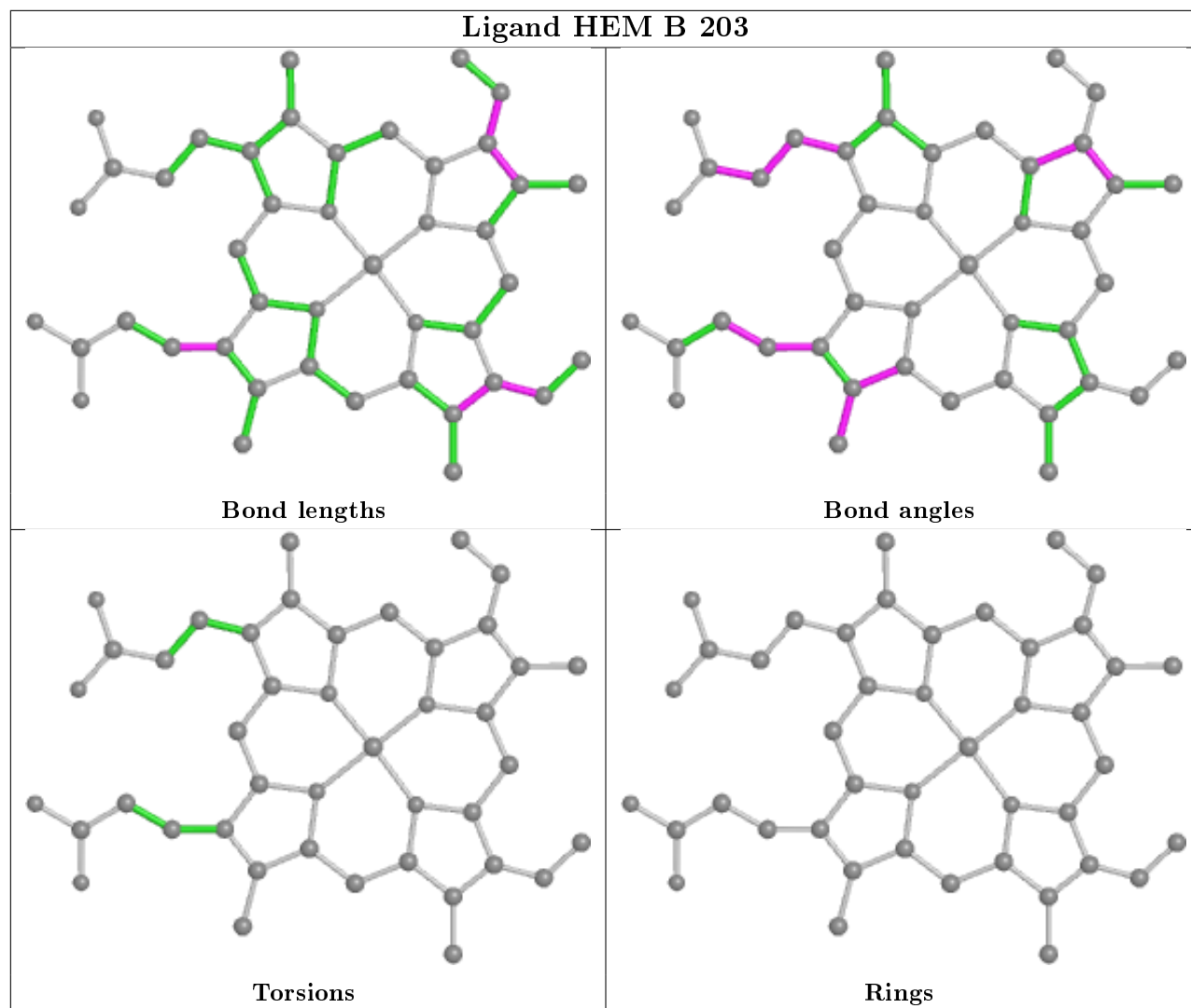


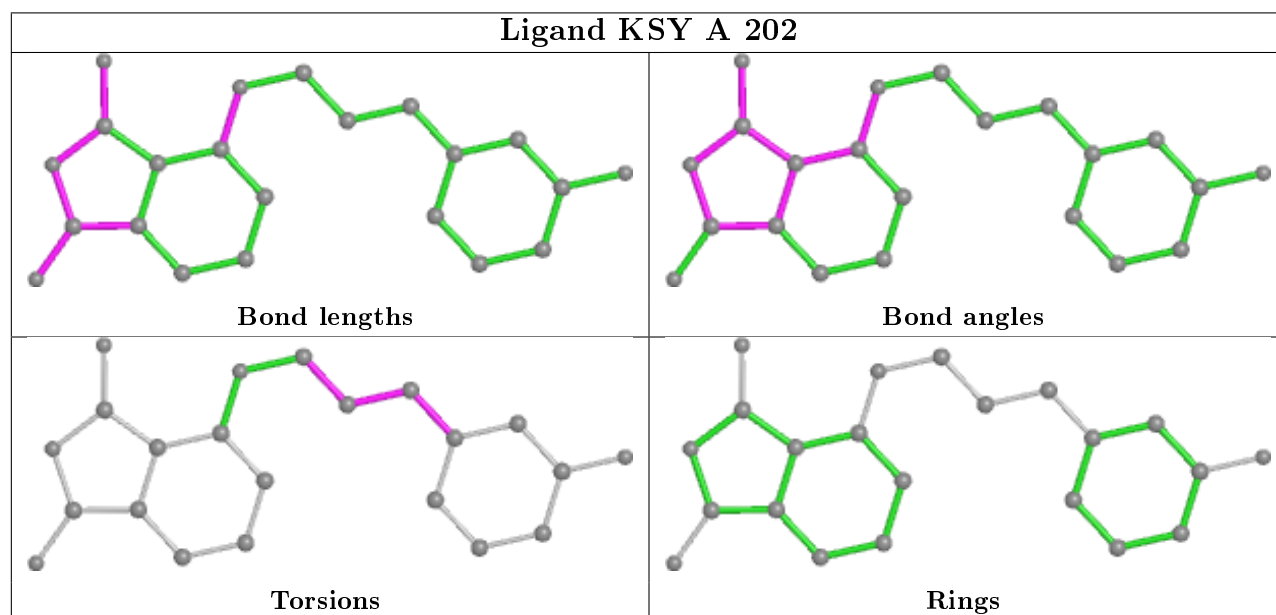
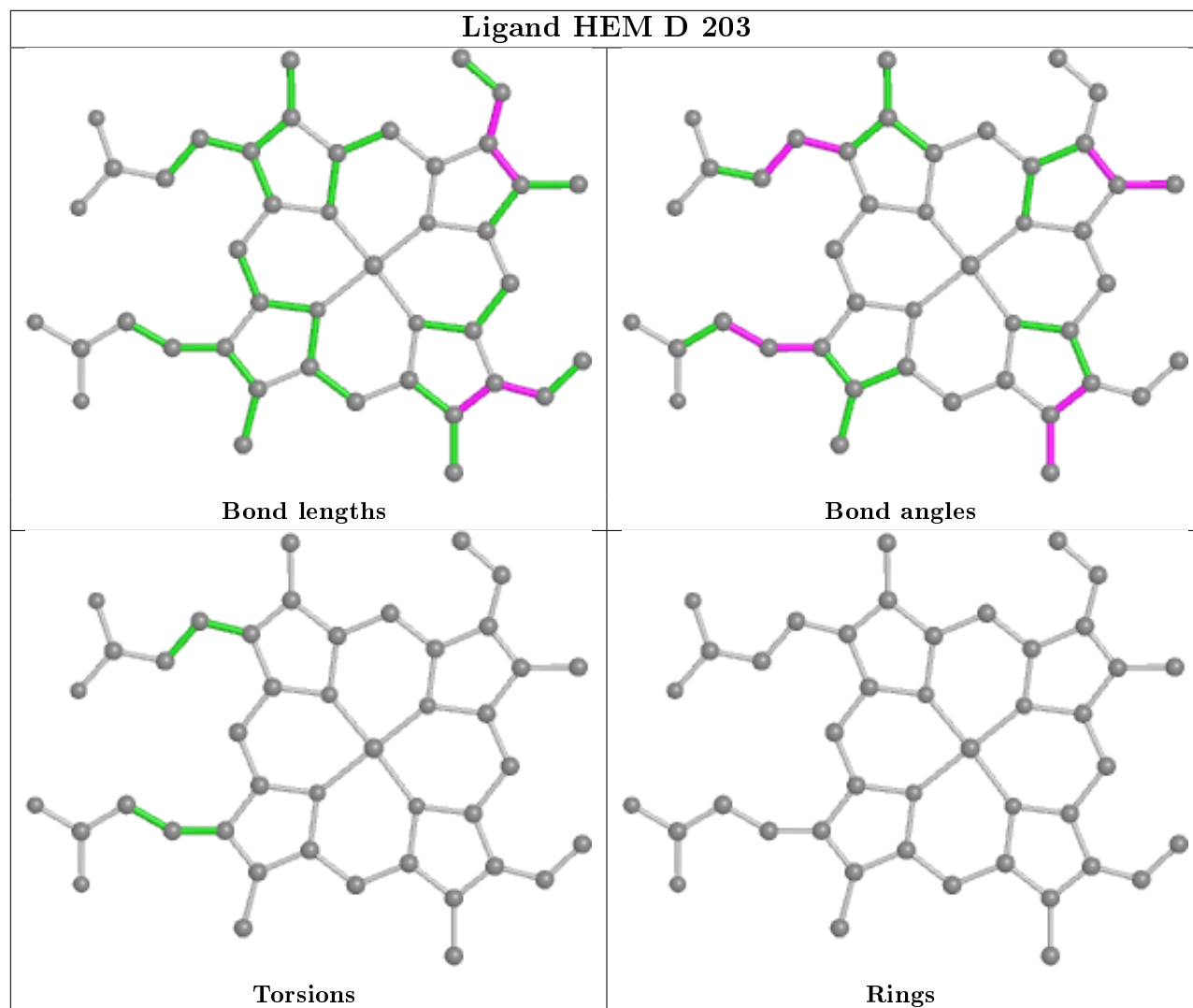
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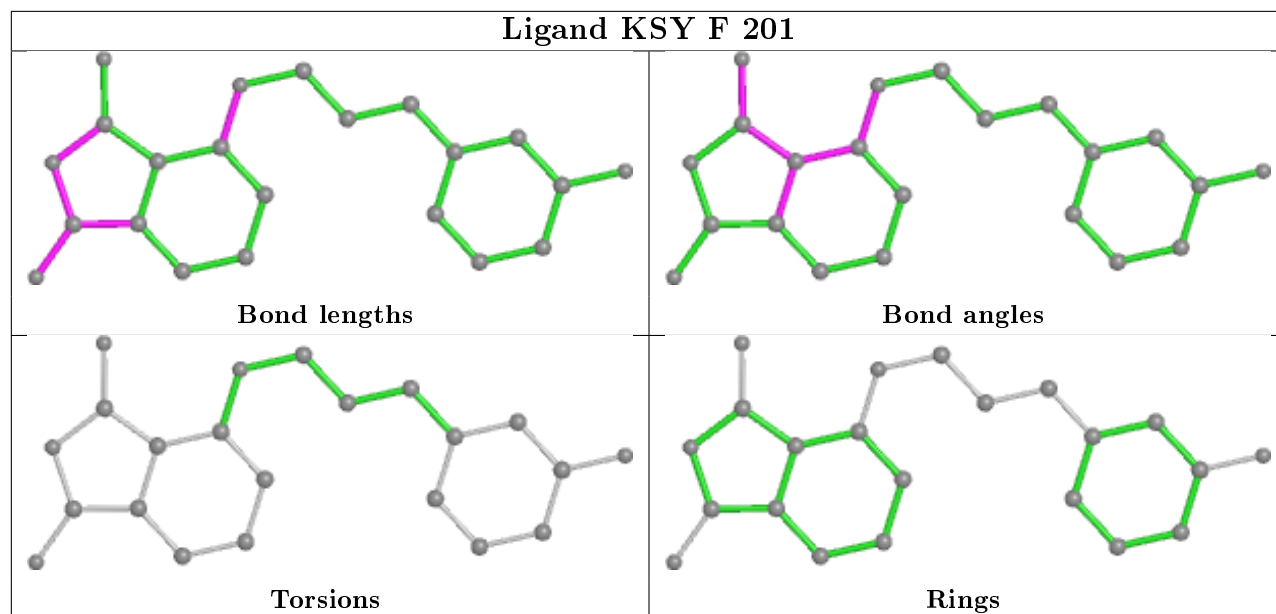


Ligand HEM F 202









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	156/158 (98%)	-0.23	1 (0%) 89 89	14, 18, 27, 45	0
1	B	156/158 (98%)	-0.27	1 (0%) 89 89	14, 18, 27, 47	0
1	C	156/158 (98%)	-0.25	0 100 100	14, 18, 27, 52	0
1	D	156/158 (98%)	-0.23	0 100 100	14, 18, 28, 49	0
1	E	156/158 (98%)	-0.26	0 100 100	13, 16, 25, 45	0
1	F	156/158 (98%)	-0.23	0 100 100	13, 17, 25, 48	0
1	G	156/158 (98%)	-0.27	0 100 100	15, 19, 27, 47	0
1	H	156/158 (98%)	-0.23	0 100 100	14, 18, 27, 43	0
1	I	156/158 (98%)	-0.29	0 100 100	15, 19, 28, 46	0
1	J	156/158 (98%)	-0.21	0 100 100	14, 18, 27, 46	0
1	K	156/158 (98%)	-0.23	1 (0%) 89 89	14, 18, 27, 47	0
1	L	156/158 (98%)	-0.23	0 100 100	15, 19, 28, 47	0
All	All	1872/1896 (98%)	-0.24	3 (0%) 95 94	13, 18, 27, 52	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	156	GLU	3.1
1	K	156	GLU	2.8
1	A	156	GLU	2.4

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

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

6.3 Carbohydrates ⓘ

There are no 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	0.54	0.20	32,38,44,45	0
5	PG4	E	203	10/13	0.67	0.21	32,37,44,49	0
5	PG4	B	204	8/13	0.68	0.22	33,38,41,43	0
3	KSY	G	201	22/22	0.68	0.28	26,35,47,49	0
5	PG4	K	204	8/13	0.72	0.20	33,43,46,47	0
5	PG4	G	203	10/13	0.74	0.24	31,41,47,55	0
5	PG4	J	202	13/13	0.74	0.17	26,38,43,46	0
3	KSY	H	201	16/22	0.74	0.24	24,30,42,43	0
5	PG4	D	204	13/13	0.75	0.17	28,40,45,48	0
3	KSY	K	201	15/22	0.77	0.18	26,30,40,43	0
5	PG4	E	202	13/13	0.77	0.18	28,33,41,42	0
5	PG4	F	204	10/13	0.77	0.18	33,38,41,50	0
5	PG4	C	203	13/13	0.77	0.22	24,39,46,48	0
5	PG4	G	202	13/13	0.78	0.17	29,37,41,44	0
5	PG4	D	205	10/13	0.78	0.19	32,36,48,48	0
3	KSY	I	201	22/22	0.78	0.30	26,35,51,57	0
5	PG4	H	203	8/13	0.78	0.18	36,38,43,45	0
5	PG4	K	203	13/13	0.79	0.20	27,36,46,48	0
3	KSY	C	201	22/22	0.79	0.25	25,34,55,57	0
3	KSY	A	203	22/22	0.80	0.23	33,42,48,51	0
5	PG4	I	204	8/13	0.81	0.18	35,41,45,48	0
5	PG4	L	203	13/13	0.81	0.17	32,37,45,46	0
5	PG4	C	204	8/13	0.82	0.16	32,36,42,47	0
5	PG4	A	205	13/13	0.82	0.15	29,37,47,48	0
5	PG4	F	203	13/13	0.82	0.17	28,38,47,50	0
3	KSY	E	201	22/22	0.82	0.25	24,33,53,56	0
3	KSY	F	201	22/22	0.83	0.25	23,30,47,50	0
3	KSY	B	202	22/22	0.84	0.24	23,34,52,57	0
5	PG4	F	205	9/13	0.84	0.19	40,44,48,51	0
5	PG4	B	205	6/13	0.84	0.18	30,40,41,42	0
5	PG4	D	206	8/13	0.85	0.15	36,43,48,48	0
5	PG4	A	206	10/13	0.85	0.19	38,41,51,54	0

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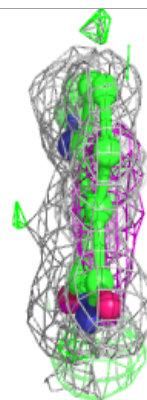
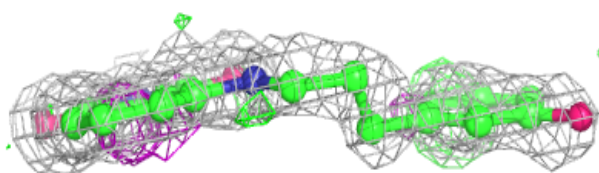
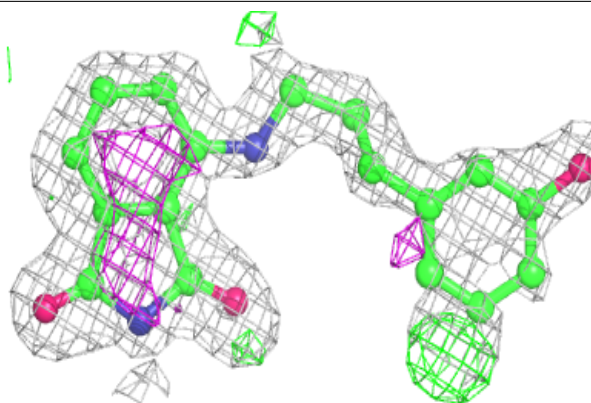
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	PG4	E	204	8/13	0.87	0.18	32,39,42,43	0
5	PG4	I	202	10/13	0.87	0.13	29,39,42,48	0
3	KSY	J	201	22/22	0.88	0.17	20,30,49,52	0
5	PG4	K	202	8/13	0.89	0.15	28,35,40,42	0
3	KSY	L	201	14/22	0.91	0.10	22,27,35,40	0
5	PG4	J	203	13/13	0.92	0.10	23,26,35,37	0
3	KSY	A	202	22/22	0.92	0.11	17,25,38,44	0
3	KSY	D	202	22/22	0.94	0.09	19,22,35,42	0
4	HEM	H	202	43/43	0.95	0.11	14,18,33,36	0
4	HEM	L	202	43/43	0.95	0.12	16,18,26,31	43
4	HEM	F	202	43/43	0.95	0.12	15,18,32,37	0
4	HEM	B	203	43/43	0.95	0.11	14,17,31,35	0
4	HEM	A	204	43/43	0.96	0.10	15,18,34,36	0
4	HEM	C	202	43/43	0.96	0.11	15,18,33,34	0
4	HEM	D	203	43/43	0.96	0.10	13,16,26,29	43
2	FE2	D	201	1/1	1.00	0.09	15,15,15,15	0
2	FE2	A	201	1/1	1.00	0.09	14,14,14,14	0
2	FE2	B	201	1/1	1.00	0.09	15,15,15,15	0

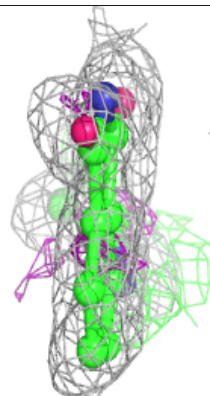
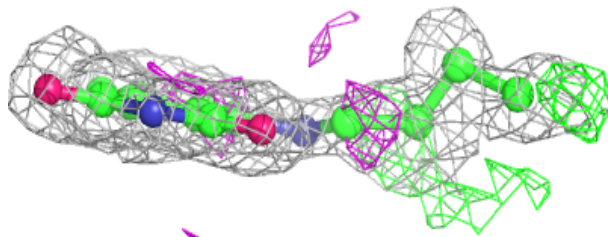
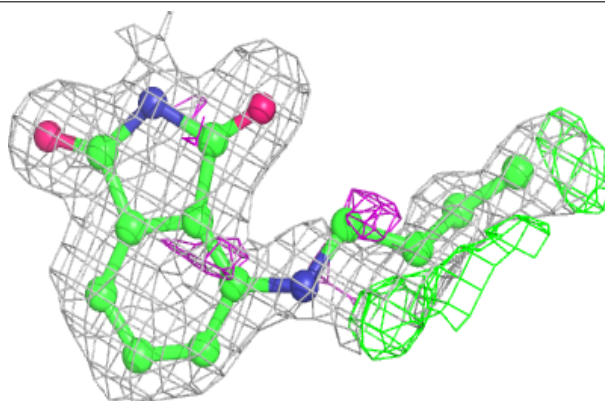
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around KSY G 201:

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

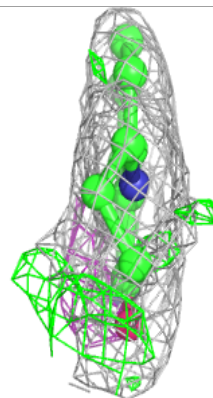
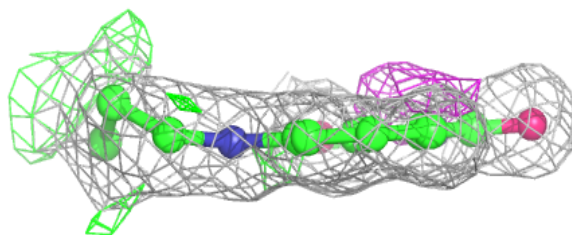
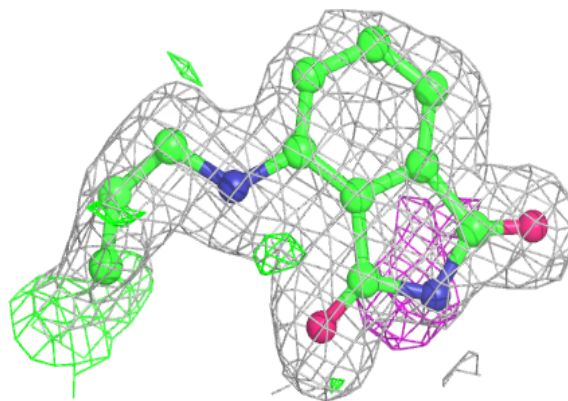
**Electron density around KSY H 201:**

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

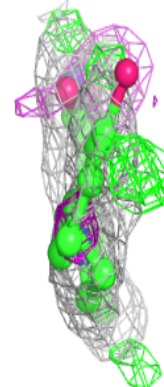
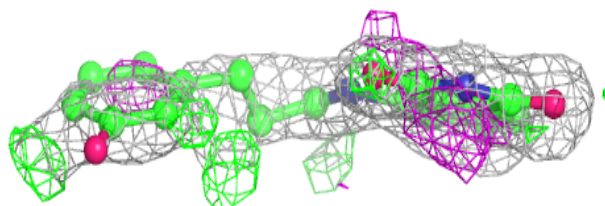
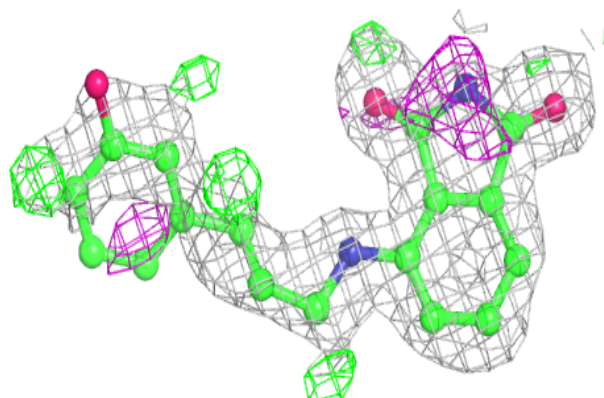


Electron density around KSY K 201:

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

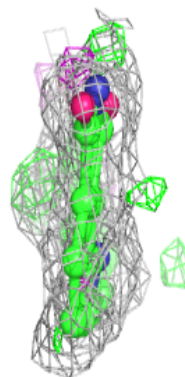
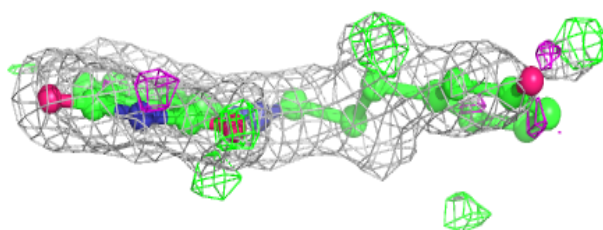
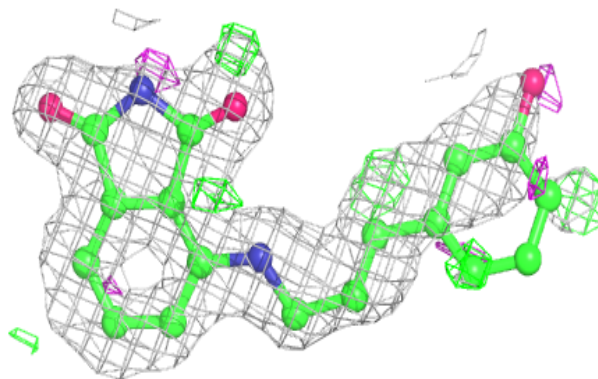
**Electron density around KSY I 201:**

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

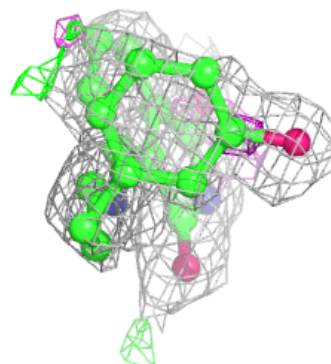
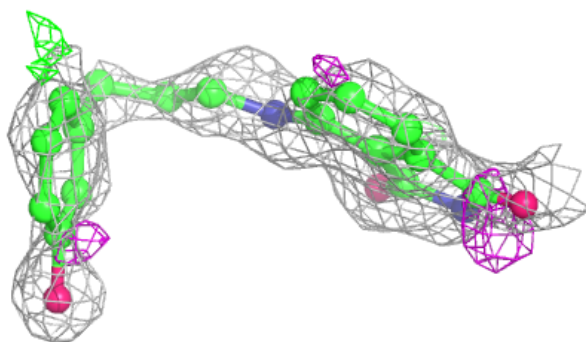
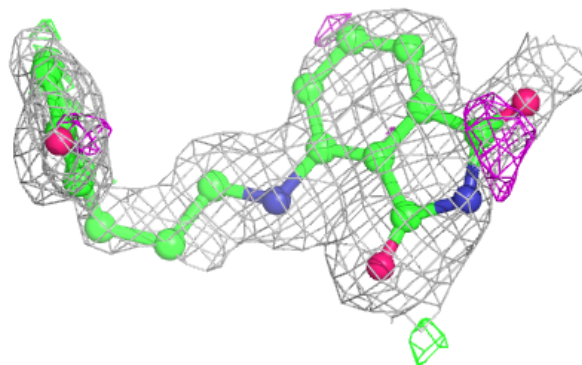


Electron density around KSY C 201:

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

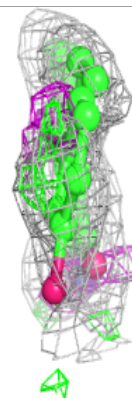
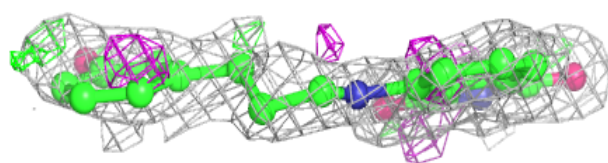
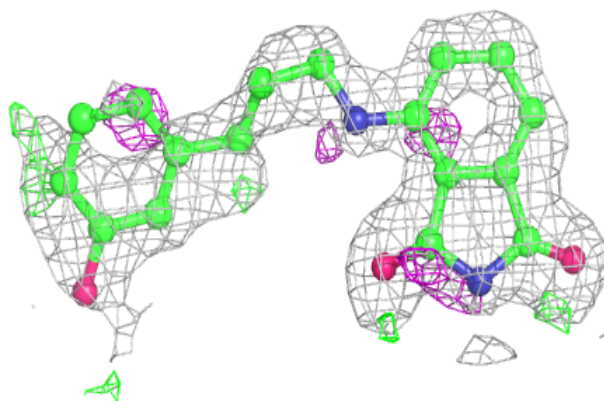
**Electron density around KSY A 203:**

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

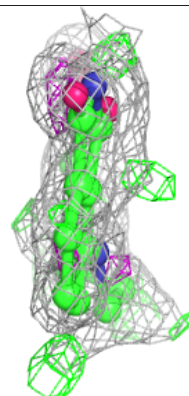
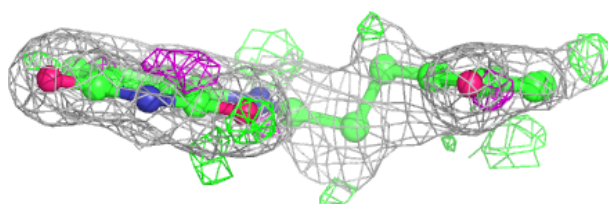
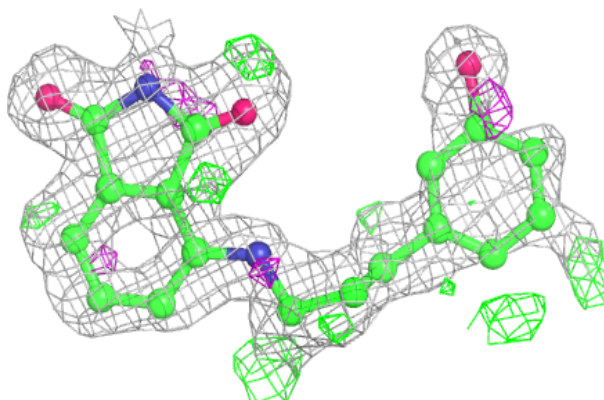


Electron density around KSY E 201:

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and green (positive)

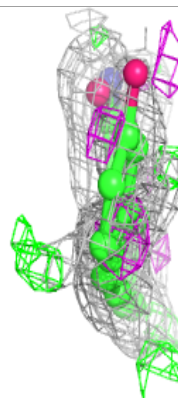
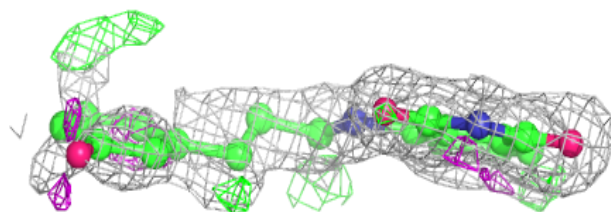
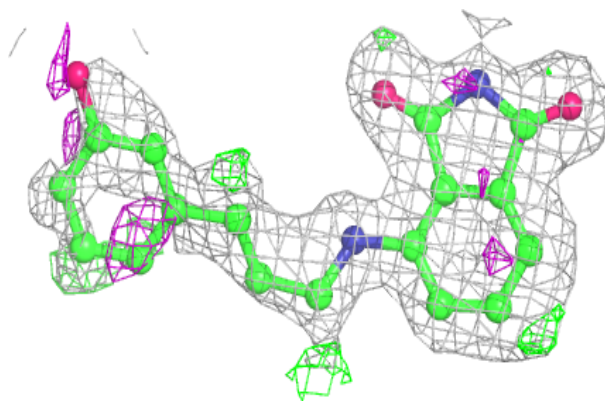
**Electron density around KSY F 201:**

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

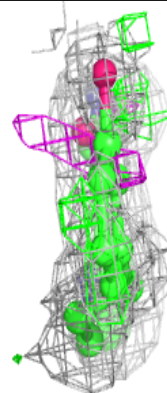
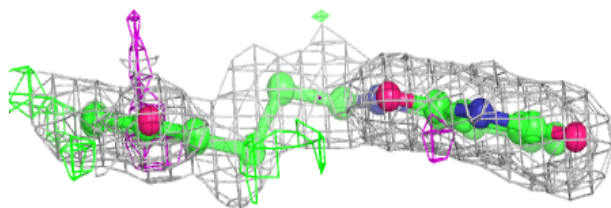
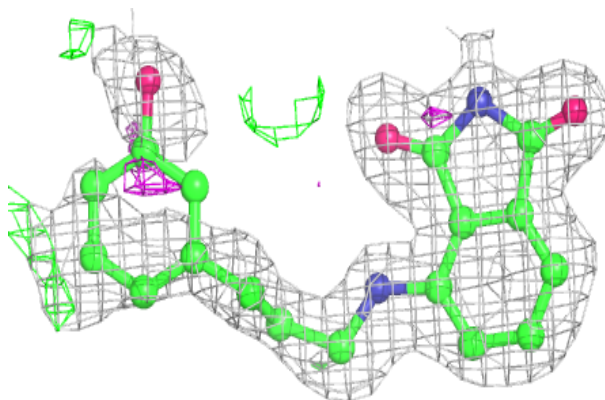


Electron density around KSY B 202:

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

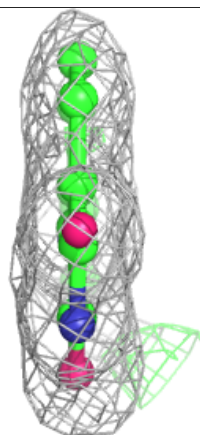
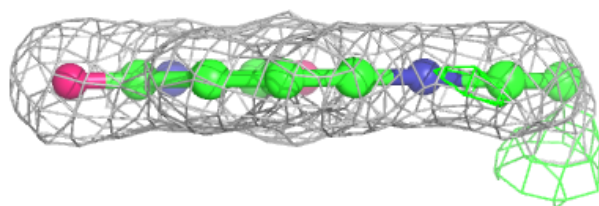
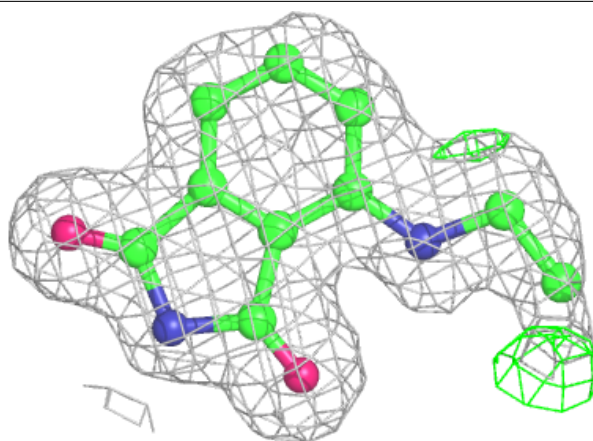
**Electron density around KSY J 201:**

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

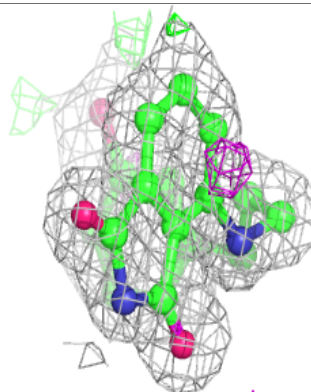
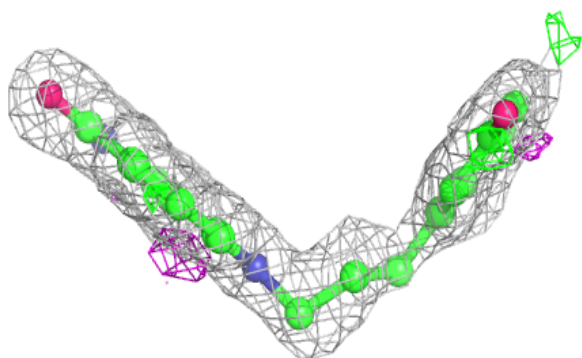
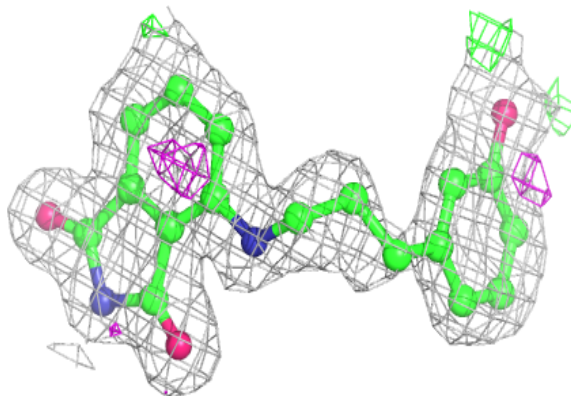


Electron density around KSY L 201:

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

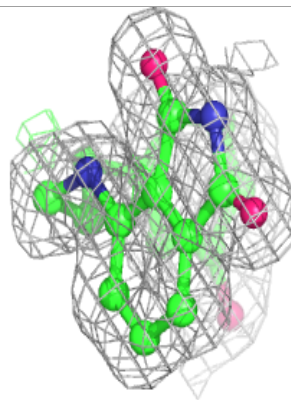
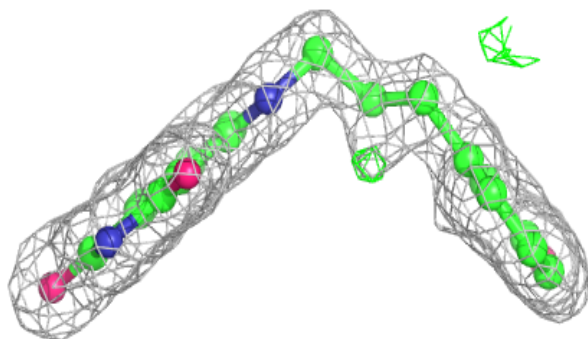
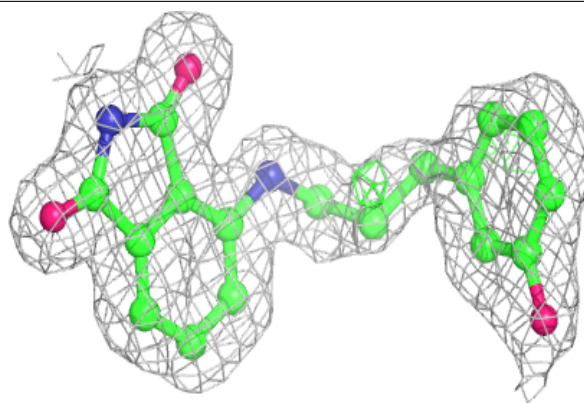
**Electron density around KSY A 202:**

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



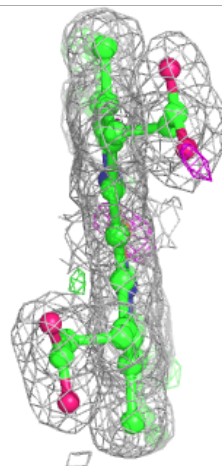
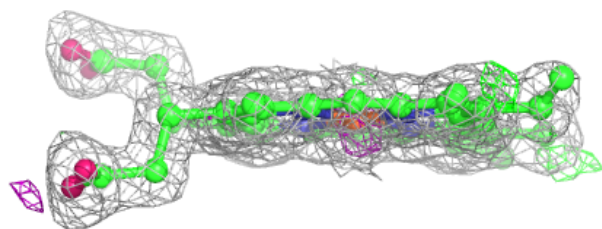
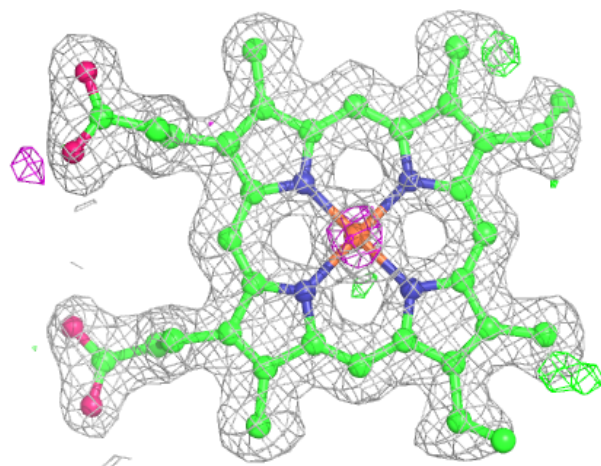
Electron density around KSY D 202:

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



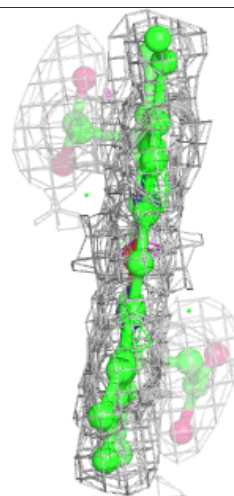
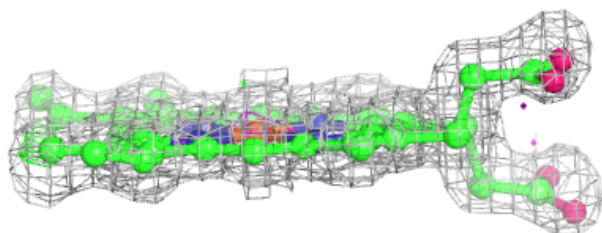
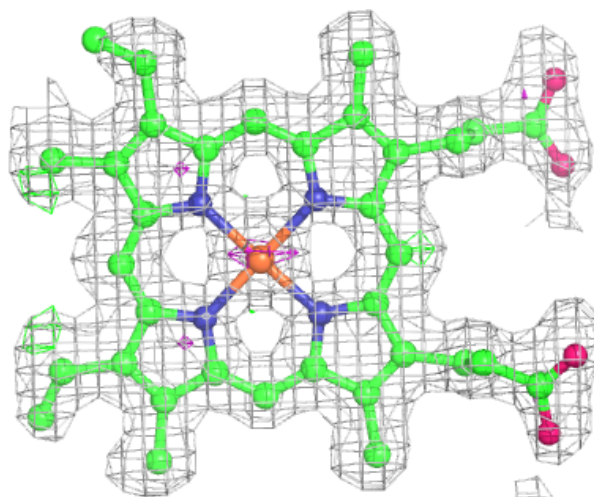
Electron density around HEM H 202:

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



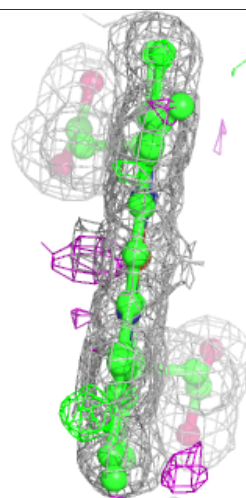
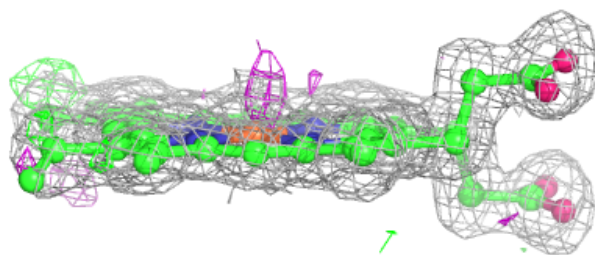
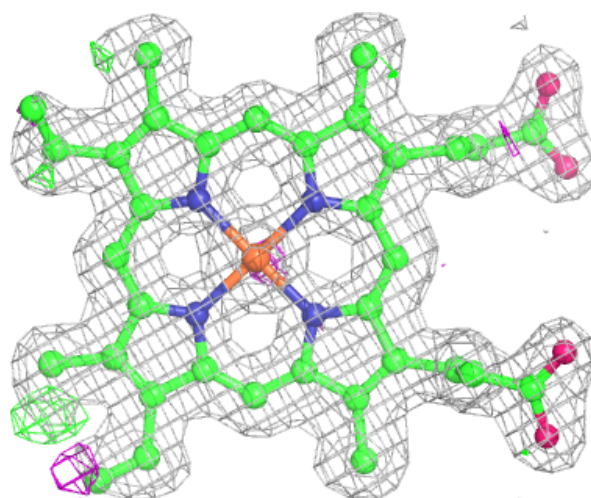
Electron density around HEM L 202:

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



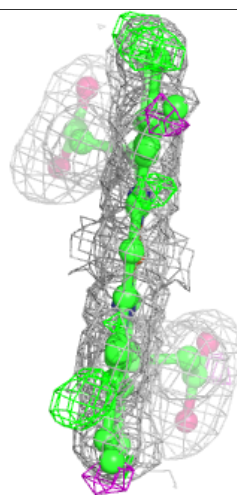
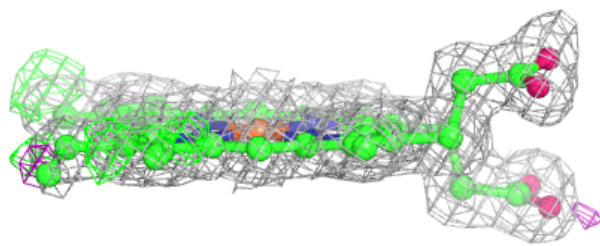
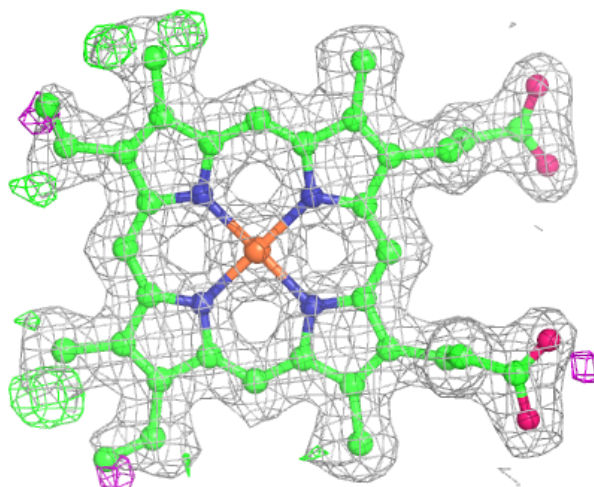
Electron density around HEM F 202:

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



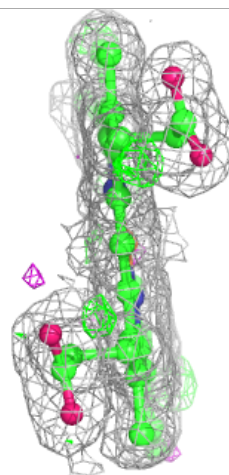
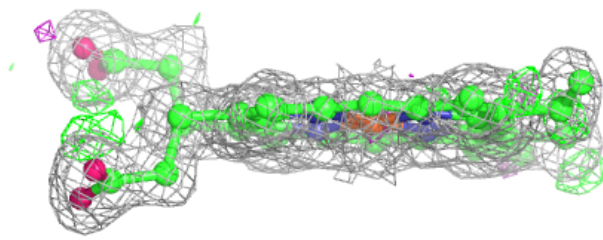
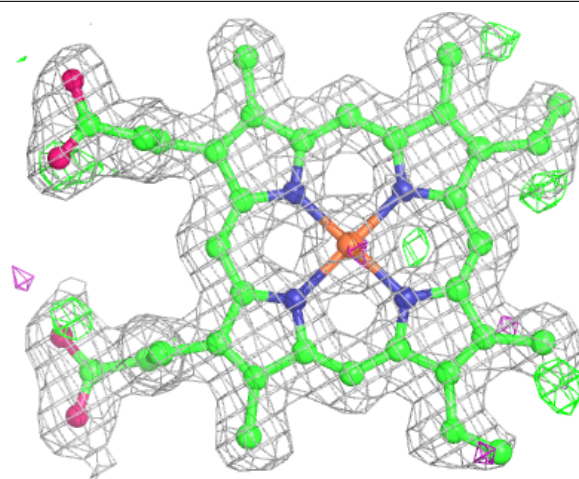
Electron density around HEM B 203:

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



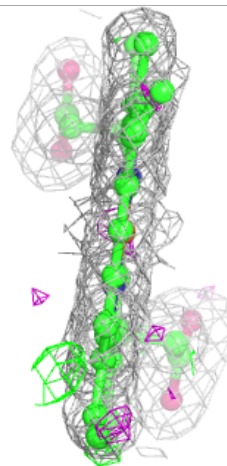
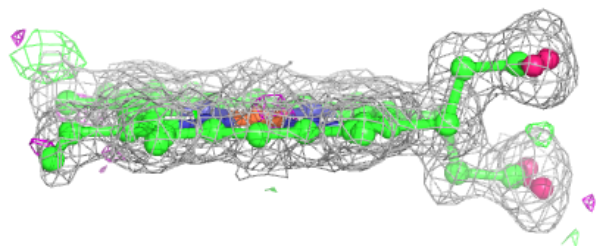
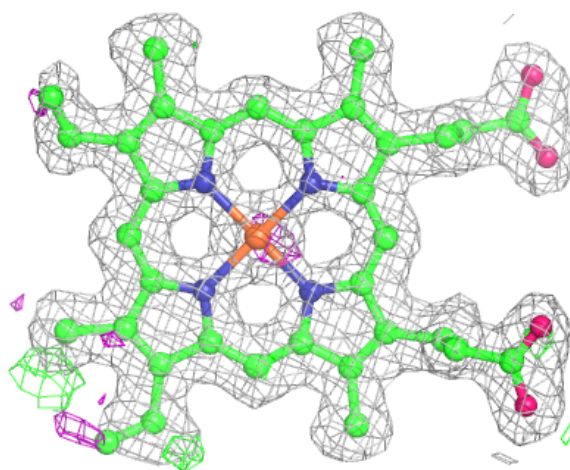
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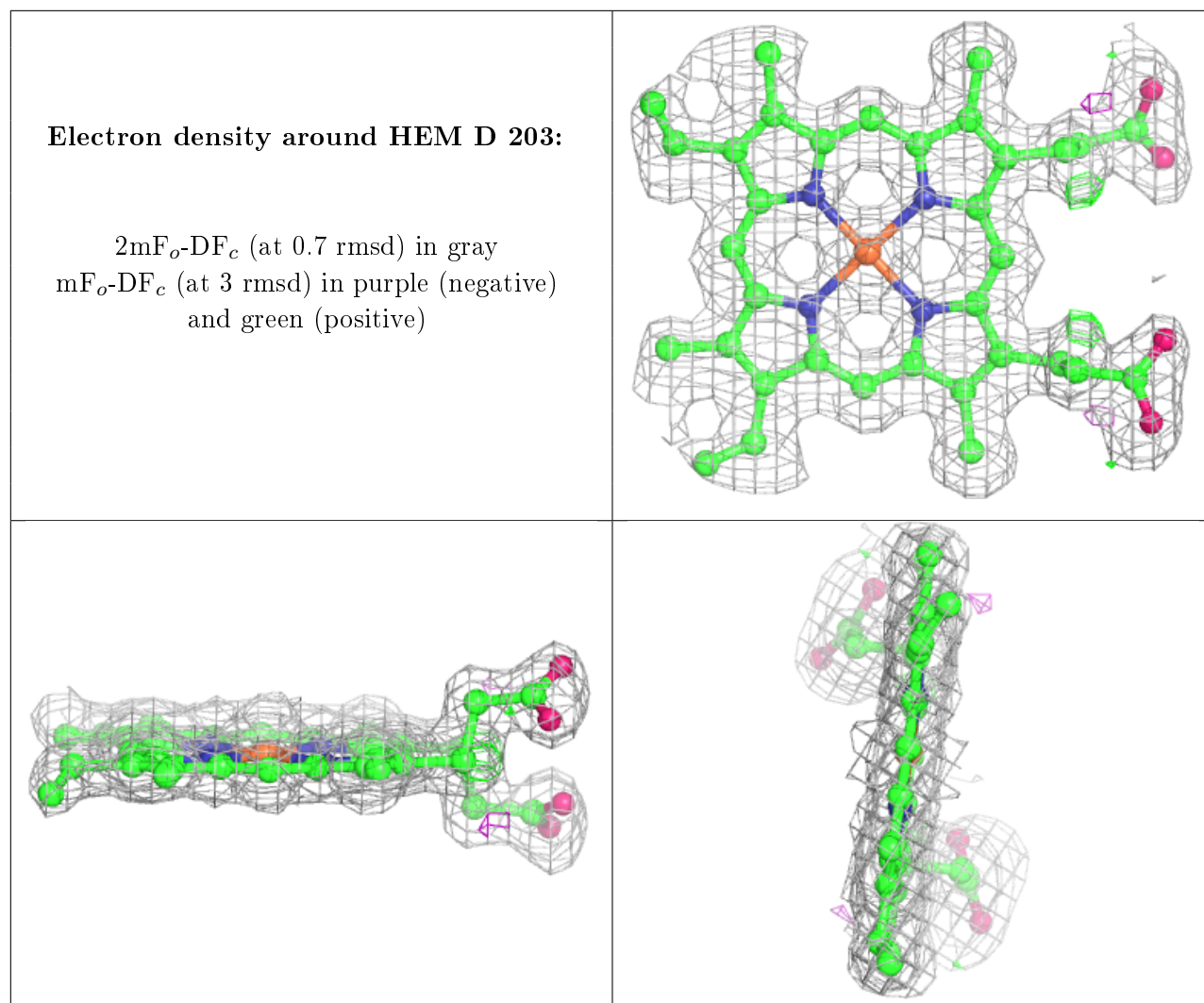
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.5 Other polymers ⓘ

There are no such residues in this entry.