



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 8, 2020 – 02:13 AM EST

PDB ID : 7K5G  
Title : 1.95 Å resolution structure of WT BfrB from *Pseudomonas aeruginosa* in complex with a protein-protein interaction inhibitor KM-5-28  
Authors : Lovell, S.; Battaile, K.P.; Soldano, A.; Punchi-Hewage, A.; Meraz, K.; Annor-Gyamfi, J.K.; Yao, H.; Bunce, R.A.; Rivera, M.  
Deposited on : 2020-09-16  
Resolution : 1.95 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](mailto: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.

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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 : 2.15.1  
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) : 2.15.1

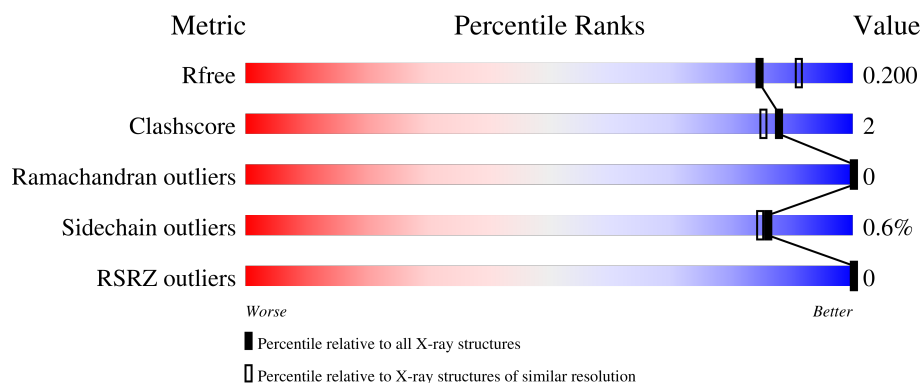
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

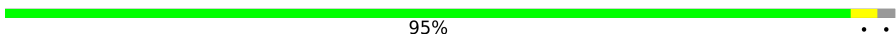
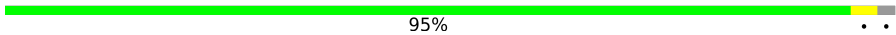
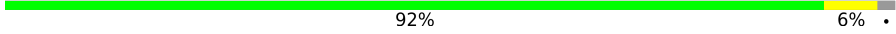
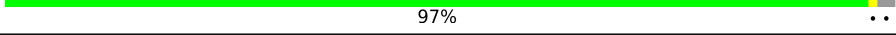
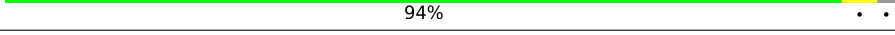
The reported resolution of this entry is 1.95 Å.

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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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  $\geq 3$ , 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	 95% ..
1	B	158	 95% ..
1	C	158	 92% 6% .
1	D	158	 97% ..
1	E	158	 94% . .

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Mol	Chain	Length	Quality of chain
1	F	158	 94% . .
1	G	158	 96% . .
1	H	158	 94% . .
1	I	158	 96% . .
1	J	158	 92% 6% .
1	K	158	 96% . .
1	L	158	 96% . .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	VXS	H	202	-	X	-	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 16458 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	155	Total	C	N	O	S	0	2	0
			1253	797	211	238	7			
1	B	155	Total	C	N	O	S	0	2	0
			1258	798	213	240	7			
1	C	155	Total	C	N	O	S	0	2	0
			1261	799	215	240	7			
1	D	155	Total	C	N	O	S	0	2	0
			1264	800	216	241	7			
1	E	155	Total	C	N	O	S	0	3	0
			1262	801	211	243	7			
1	F	155	Total	C	N	O	S	0	2	0
			1251	796	211	237	7			
1	G	155	Total	C	N	O	S	0	2	0
			1258	799	212	240	7			
1	H	155	Total	C	N	O	S	0	3	0
			1253	797	210	239	7			
1	I	155	Total	C	N	O	S	0	2	0
			1252	796	209	240	7			
1	J	155	Total	C	N	O	S	0	2	0
			1256	798	212	239	7			
1	K	155	Total	C	N	O	S	0	2	0
			1258	798	213	240	7			
1	L	156	Total	C	N	O	S	0	3	0
			1267	805	217	238	7			

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

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

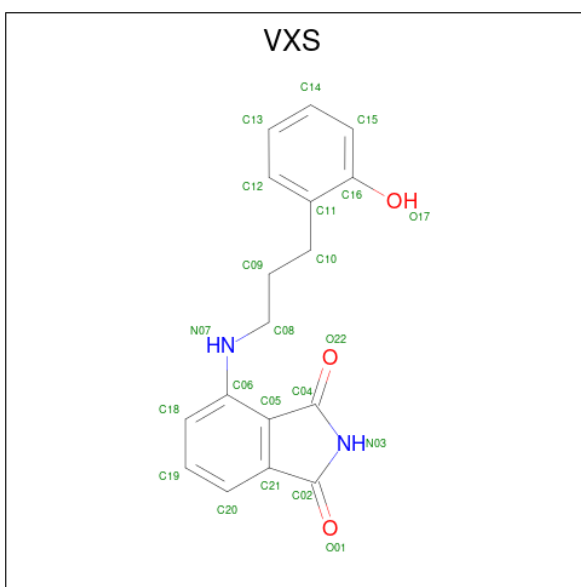
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total K 1 1	0	0

- # HEM

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

- 
- WORLD WIDE  
PDB  
PROTEIN DATA BANK



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 22	C 17	N 2	O 3	0	0
4	B	1	Total 22	C 17	N 2	O 3	0	0
4	C	1	Total 14	C 10	N 2	O 2	0	0
4	D	1	Total 44	C 34	N 4	O 6	0	1
4	E	1	Total 22	C 17	N 2	O 3	0	0
4	F	1	Total 22	C 17	N 2	O 3	0	0
4	H	1	Total 16	C 12	N 2	O 2	0	0
4	I	1	Total 22	C 17	N 2	O 3	0	0
4	J	1	Total 22	C 17	N 2	O 3	0	0
4	K	1	Total 22	C 17	N 2	O 3	0	0
4	L	1	Total 13	C 9	N 2	O 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	61	Total O 61 61	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	68	Total 68	O 68	0	0
5	C	69	Total 69	O 69	0	0
5	D	73	Total 73	O 73	0	0
5	E	70	Total 70	O 70	0	0
5	F	63	Total 63	O 63	0	0
5	G	73	Total 73	O 73	0	0
5	H	71	Total 71	O 71	0	0
5	I	71	Total 71	O 71	0	0
5	J	75	Total 75	O 75	0	0
5	K	68	Total 68	O 68	0	0
5	L	58	Total 58	O 58	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

Chain A:  95% . .



- Molecule 1: Ferroxidase

Chain B:  95% . .



- Molecule 1: Ferroxidase

Chain C:  92% 6% .



- Molecule 1: Ferroxidase

Chain D:  97% . .



- Molecule 1: Ferroxidase

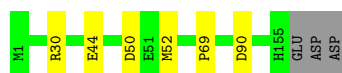
Chain E:  94% . .



- Molecule 1: Ferroxidase

Chain F:  94% . .





- Molecule 1: Ferroxidase

Chain G: 96% ..



- Molecule 1: Ferroxidase

Chain H: 94% ..



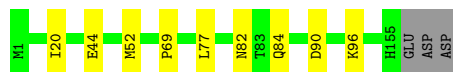
- Molecule 1: Ferroxidase

Chain I: 96% ..



- Molecule 1: Ferroxidase

Chain J: 92% 6% .



- Molecule 1: Ferroxidase

Chain K: 96% ..



- Molecule 1: Ferroxidase

Chain L: 96% ..



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	129.74Å 194.79Å 202.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.75 – 1.95 48.70 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.75-1.95) 99.9 (48.70-1.95)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.30 (at 1.95Å)	Xtriage
Refinement program	PHENIX 1.17rc2_3615	Depositor
R, $R_{free}$	0.158 , 0.193 0.168 , 0.200	Depositor DCC
$R_{free}$ test set	9224 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.2	Xtriage
Anisotropy	0.408	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 57.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	16458	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.81% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, K, VXS

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	0.47	0/1279	0.56	0/1724
1	B	0.46	0/1284	0.54	0/1731
1	C	0.47	0/1288	0.55	0/1737
1	D	0.47	0/1291	0.58	0/1741
1	E	0.50	0/1291	0.57	0/1741
1	F	0.48	0/1278	0.54	0/1725
1	G	0.46	0/1285	0.54	0/1733
1	H	0.45	0/1282	0.55	0/1730
1	I	0.46	0/1279	0.56	0/1727
1	J	0.51	0/1283	0.55	0/1731
1	K	0.45	0/1284	0.54	0/1731
1	L	0.46	0/1297	0.54	0/1749
All	All	0.47	0/15421	0.55	0/20800

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1253	0	1230	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1258	0	1232	3	0
1	C	1261	0	1233	6	0
1	D	1264	0	1237	1	0
1	E	1262	0	1233	6	0
1	F	1251	0	1214	3	0
1	G	1258	0	1228	2	0
1	H	1253	0	1220	3	0
1	I	1252	0	1207	2	0
1	J	1256	0	1223	5	0
1	K	1258	0	1232	2	0
1	L	1267	0	1241	4	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	D	1	0	0	0	0
3	A	43	0	30	2	0
3	C	43	0	30	3	0
3	D	43	0	30	2	0
3	E	43	0	30	4	0
3	H	43	0	30	5	0
3	K	43	0	30	4	0
3	L	43	0	30	4	0
4	A	22	0	0	1	0
4	B	22	0	0	1	0
4	C	14	0	0	1	0
4	D	44	0	0	0	0
4	E	22	0	0	1	0
4	F	22	0	0	1	0
4	H	16	0	0	1	0
4	I	22	0	0	1	0
4	J	22	0	0	1	0
4	K	22	0	0	1	0
4	L	13	0	0	1	0
5	A	61	0	0	2	0
5	B	68	0	0	0	0
5	C	69	0	0	2	0
5	D	73	0	0	1	0
5	E	70	0	0	2	0
5	F	63	0	0	0	0
5	G	73	0	0	1	0
5	H	71	0	0	0	0
5	I	71	0	0	0	0
5	J	75	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	K	68	0	0	0	0
5	L	58	0	0	0	0
All	All	16458	0	14940	60	0

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

All (60) 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)
3:K:201:HEM:HBC2	3:K:201:HEM:HMC1	1.57	0.87
3:E:201:HEM:HBC2	3:E:201:HEM:HMC1	1.74	0.70
3:D:202:HEM:HBC2	3:D:202:HEM:HMC2	1.72	0.69
3:K:201:HEM:HBC2	3:K:201:HEM:CMC	2.24	0.68
1:I:69:PRO:O	4:I:201:VXS:N03	2.27	0.67
1:F:69:PRO:O	4:F:201:VXS:N03	2.29	0.65
1:B:69:PRO:O	4:B:202:VXS:N03	2.29	0.65
1:J:82:ASN:OD1	1:J:84:GLN:HG2	1.97	0.64
1:K:69:PRO:O	4:K:202:VXS:N03	2.30	0.64
3:A:202:HEM:HBC2	3:A:202:HEM:HMC1	1.80	0.64
1:C:69:PRO:O	4:C:202:VXS:N03	2.32	0.63
1:E:69:PRO:O	4:E:202:VXS:N03	2.34	0.61
3:H:201:HEM:CMC	3:H:201:HEM:HBC2	2.30	0.60
3:H:201:HEM:HBC2	3:H:201:HEM:HMC2	1.83	0.60
3:E:201:HEM:CMC	3:E:201:HEM:HBC2	2.32	0.59
1:J:69:PRO:O	4:J:201:VXS:N03	2.36	0.59
3:D:202:HEM:HBC2	3:D:202:HEM:CMC	2.32	0.58
3:C:201:HEM:HMC2	3:C:201:HEM:HBC2	1.86	0.56
1:L:69:PRO:O	4:L:202:VXS:N03	2.42	0.53
3:C:201:HEM:HBB2	3:C:201:HEM:CMB	2.39	0.52
1:C:20:ILE:HD11	1:C:75:GLY:HA3	1.92	0.52
3:E:201:HEM:HBB2	3:E:201:HEM:CMB	2.40	0.52
3:C:201:HEM:HBC2	3:C:201:HEM:CMC	2.40	0.51
3:L:201:HEM:HBB2	3:L:201:HEM:CMB	2.41	0.51
3:A:202:HEM:HBC2	3:A:202:HEM:CMC	2.41	0.50
1:D:130:HIS:NE2	5:D:301:HOH:O	2.35	0.50
1:A:84:GLN:NE2	5:A:301:HOH:O	2.42	0.48
1:E:99:LYS:CD	5:E:363:HOH:O	2.61	0.48
1:C:99:LYS:CD	5:C:321:HOH:O	2.61	0.48
3:L:201:HEM:HBC2	3:L:201:HEM:HMC1	1.96	0.48
3:L:201:HEM:HBB2	3:L:201:HEM:HMB1	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:44:GLU:OE1	1:F:90:ASP:OD2	2.33	0.47
3:H:201:HEM:CMB	3:H:201:HEM:HBB2	2.45	0.47
1:L:52:MET:HB3	3:L:201:HEM:CHD	2.45	0.47
1:E:147[A]:GLU:CD	1:E:147[A]:GLU:H	2.19	0.46
1:H:69:PRO:O	4:H:202:VXS:N03	2.48	0.46
1:A:20:ILE:HD11	1:A:75:GLY:HA3	1.98	0.46
1:C:57:LYS:NZ	5:C:303:HOH:O	2.49	0.46
1:E:134:LEU:HD21	5:E:306:HOH:O	2.16	0.46
1:A:110:GLN:CG	5:A:360:HOH:O	2.64	0.46
3:H:201:HEM:CHB	1:J:52:MET:HB3	2.46	0.46
1:H:133:TYR:O	1:H:137:GLN:HG2	2.16	0.44
1:H:44:GLU:OE1	1:H:90:ASP:OD2	2.37	0.43
1:L:20:ILE:HD11	1:L:75:GLY:HA3	2.00	0.43
1:C:94:GLU:OE2	1:C:130:HIS:ND1	2.41	0.43
1:F:52:MET:HB3	3:K:201:HEM:CHD	2.49	0.42
1:G:44:GLU:OE1	1:G:90:ASP:OD2	2.38	0.42
1:E:52:MET:HB3	3:E:201:HEM:CHB	2.50	0.42
1:J:44:GLU:OE1	1:J:90:ASP:OD2	2.38	0.42
1:A:69:PRO:O	4:A:203:VXS:N03	2.53	0.42
1:G:110:GLN:CG	5:G:272:HOH:O	2.67	0.42
1:J:20:ILE:HG23	1:J:77:LEU:HD12	2.03	0.41
1:C:140:LEU:O	1:C:144:VAL:HG22	2.21	0.41
1:B:20:ILE:HD11	1:B:75:GLY:HA3	2.03	0.41
1:E:94:GLU:OE2	1:E:130:HIS:ND1	2.46	0.41
1:L:25:TYR:N	1:L:25:TYR:CD1	2.87	0.41
1:B:44:GLU:OE1	1:B:90:ASP:OD2	2.40	0.40
1:I:20:ILE:HD11	1:I:75:GLY:HA3	2.04	0.40
3:H:201:HEM:CBC	3:H:201:HEM:HMC2	2.51	0.40
1:K:52:MET:HB3	3:K:201:HEM:CHB	2.52	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	155/158 (98%)	154 (99%)	1 (1%)	0	100	100
1	B	155/158 (98%)	154 (99%)	1 (1%)	0	100	100
1	C	155/158 (98%)	155 (100%)	0	0	100	100
1	D	155/158 (98%)	153 (99%)	2 (1%)	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%)	156 (100%)	0	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%)	155 (100%)	0	0	100	100
1	L	157/158 (99%)	156 (99%)	1 (1%)	0	100	100
All	All	1864/1896 (98%)	1858 (100%)	6 (0%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	134/144 (93%)	134 (100%)	0	100	100
1	B	135/144 (94%)	135 (100%)	0	100	100
1	C	136/144 (94%)	135 (99%)	1 (1%)	84	82
1	D	137/144 (95%)	136 (99%)	1 (1%)	84	82
1	E	136/144 (94%)	136 (100%)	0	100	100
1	F	132/144 (92%)	130 (98%)	2 (2%)	65	60
1	G	135/144 (94%)	135 (100%)	0	100	100
1	H	133/144 (92%)	132 (99%)	1 (1%)	81	80
1	I	132/144 (92%)	131 (99%)	1 (1%)	81	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	134/144 (93%)	133 (99%)	1 (1%)	84	82
1	K	135/144 (94%)	133 (98%)	2 (2%)	65	60
1	L	135/144 (94%)	135 (100%)	0	100	100
All	All	1614/1728 (93%)	1605 (99%)	9 (1%)	86	85

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	121	LYS
1	D	50	ASP
1	F	30	ARG
1	F	50	ASP
1	H	30	ARG
1	I	121	LYS
1	J	96	LYS
1	K	50	ASP
1	K	96	LYS

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

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 3 are monoatomic - leaving 19 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	HEM	L	201	1	27,50,50	1.82	4 (14%)	17,82,82	1.63	5 (29%)
4	VXS	D	203[B]	-	24,24,24	1.65	6 (25%)	33,33,33	1.56	6 (18%)
4	VXS	L	202	-	14,14,24	2.28	8 (57%)	19,20,33	1.58	4 (21%)
3	HEM	H	201	1	27,50,50	2.02	4 (14%)	17,82,82	1.73	5 (29%)
4	VXS	C	202	-	15,15,24	2.23	7 (46%)	21,21,33	1.67	6 (28%)
4	VXS	J	201	-	24,24,24	2.19	11 (45%)	33,33,33	2.01	10 (30%)
3	HEM	E	201	1	27,50,50	1.75	5 (18%)	17,82,82	1.74	5 (29%)
4	VXS	E	202	-	24,24,24	2.20	9 (37%)	33,33,33	1.79	11 (33%)
4	VXS	H	202	-	17,17,24	2.86	8 (47%)	23,23,33	2.81	12 (52%)
3	HEM	C	201	1	27,50,50	1.81	6 (22%)	17,82,82	2.15	8 (47%)
3	HEM	D	202	1	27,50,50	1.85	5 (18%)	17,82,82	1.62	5 (29%)
3	HEM	A	202	1	27,50,50	1.90	4 (14%)	17,82,82	1.89	8 (47%)
4	VXS	B	202	-	24,24,24	2.07	10 (41%)	33,33,33	1.74	11 (33%)
4	VXS	F	201	-	24,24,24	1.91	8 (33%)	33,33,33	1.65	7 (21%)
4	VXS	I	201	-	24,24,24	2.25	10 (41%)	33,33,33	1.80	10 (30%)
4	VXS	D	203[A]	-	24,24,24	1.71	5 (20%)	33,33,33	1.74	7 (21%)
4	VXS	K	202	-	24,24,24	2.07	10 (41%)	33,33,33	1.73	11 (33%)
4	VXS	A	203	-	24,24,24	1.70	7 (29%)	33,33,33	1.51	7 (21%)
3	HEM	K	201	1	27,50,50	1.79	4 (14%)	17,82,82	2.05	8 (47%)

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	HEM	L	201	1	-	0/6/54/54	-
4	VXS	D	203[B]	-	-	1/7/19/19	0/3/3/3
4	VXS	L	202	-	-	0/2/14/19	0/2/2/3
3	HEM	H	201	1	-	0/6/54/54	-
4	VXS	C	202	-	-	2/3/15/19	0/2/2/3
4	VXS	J	201	-	-	2/7/19/19	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEM	E	201	1	-	0/6/54/54	-
4	VXS	E	202	-	-	4/7/19/19	0/3/3/3
4	VXS	H	202	-	-	4/5/17/19	0/2/2/3
3	HEM	C	201	1	-	0/6/54/54	-
3	HEM	D	202	1	-	0/6/54/54	-
3	HEM	A	202	1	-	0/6/54/54	-
4	VXS	B	202	-	-	5/7/19/19	0/3/3/3
4	VXS	F	201	-	-	1/7/19/19	0/3/3/3
4	VXS	I	201	-	-	2/7/19/19	0/3/3/3
4	VXS	D	203[A]	-	-	2/7/19/19	0/3/3/3
4	VXS	K	202	-	-	3/7/19/19	0/3/3/3
4	VXS	A	203	-	-	5/7/19/19	0/3/3/3
3	HEM	K	201	1	-	0/6/54/54	-

All (131) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	201	HEM	C3B-C2B	-5.87	1.32	1.40
4	H	202	VXS	C02-N03	-5.79	1.30	1.38
4	K	202	VXS	C04-N03	5.18	1.46	1.38
3	A	202	HEM	C3C-C2C	-5.07	1.33	1.40
3	H	201	HEM	C3C-C2C	-4.83	1.33	1.40
4	E	202	VXS	C04-N03	4.77	1.45	1.38
4	H	202	VXS	C20-C21	-4.73	1.32	1.39
3	K	201	HEM	C3B-C2B	-4.59	1.34	1.40
3	A	202	HEM	C3B-C2B	-4.44	1.34	1.40
4	H	202	VXS	C05-C06	-4.36	1.33	1.41
4	I	201	VXS	C04-N03	4.35	1.45	1.38
4	J	201	VXS	C10-C11	4.34	1.60	1.51
3	L	201	HEM	C3B-C2B	-4.22	1.34	1.40
3	C	201	HEM	C3C-C2C	-4.21	1.34	1.40
4	J	201	VXS	C04-N03	4.21	1.44	1.38
4	E	202	VXS	C02-N03	4.20	1.44	1.38
3	E	201	HEM	C3C-C2C	-4.15	1.34	1.40
3	D	202	HEM	C3B-C2B	-4.08	1.34	1.40
4	D	203[A]	VXS	C04-N03	4.07	1.44	1.38
3	K	201	HEM	C3C-C2C	-4.06	1.34	1.40
4	H	202	VXS	C09-C08	4.02	1.67	1.51
4	D	203[B]	VXS	C04-N03	4.01	1.44	1.38
4	F	201	VXS	C04-N03	4.00	1.44	1.38
4	L	202	VXS	C06-N07	3.91	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	201	HEM	C3C-C2C	-3.90	1.35	1.40
4	B	202	VXS	C21-C02	3.86	1.54	1.48
3	D	202	HEM	C3C-C2C	-3.84	1.35	1.40
4	A	203	VXS	C04-N03	3.83	1.44	1.38
4	I	201	VXS	C18-C06	3.76	1.46	1.39
3	L	201	HEM	C3C-CAC	3.76	1.55	1.47
4	H	202	VXS	C06-N07	3.63	1.47	1.37
4	J	201	VXS	C02-N03	3.63	1.44	1.38
4	H	202	VXS	O01-C02	-3.61	1.16	1.23
4	C	202	VXS	C21-C02	3.58	1.54	1.48
4	F	201	VXS	C18-C06	3.55	1.45	1.39
3	L	201	HEM	C3B-CAB	3.51	1.55	1.47
4	I	201	VXS	C10-C11	3.50	1.58	1.51
4	C	202	VXS	C18-C06	3.49	1.45	1.39
4	I	201	VXS	C21-C02	3.49	1.53	1.48
3	C	201	HEM	C3B-C2B	-3.48	1.35	1.40
3	H	201	HEM	C3C-CAC	3.47	1.54	1.47
4	I	201	VXS	C02-N03	3.45	1.43	1.38
4	A	203	VXS	C21-C02	3.42	1.53	1.48
4	E	202	VXS	C21-C02	3.42	1.53	1.48
3	D	202	HEM	C3B-CAB	3.40	1.54	1.47
4	D	203[A]	VXS	C02-N03	3.34	1.43	1.38
4	D	203[B]	VXS	C02-N03	3.34	1.43	1.38
3	D	202	HEM	C3C-CAC	3.34	1.54	1.47
4	A	203	VXS	C18-C06	3.33	1.45	1.39
4	E	202	VXS	C18-C06	3.32	1.45	1.39
4	L	202	VXS	C02-N03	3.29	1.43	1.38
3	E	201	HEM	C3B-C2B	-3.23	1.35	1.40
4	B	202	VXS	C16-C11	3.20	1.44	1.40
3	A	202	HEM	C3C-CAC	3.19	1.54	1.47
4	B	202	VXS	C04-N03	3.18	1.43	1.38
3	C	201	HEM	C3B-CAB	3.17	1.54	1.47
3	C	201	HEM	C3C-CAC	3.12	1.54	1.47
4	B	202	VXS	C18-C06	3.10	1.44	1.39
4	L	202	VXS	C04-N03	3.08	1.43	1.38
4	E	202	VXS	C19-C20	3.03	1.45	1.38
4	F	201	VXS	C19-C20	3.02	1.45	1.38
3	E	201	HEM	C3C-CAC	2.99	1.53	1.47
4	F	201	VXS	C02-N03	2.98	1.43	1.38
3	A	202	HEM	C3B-CAB	2.96	1.54	1.47
4	C	202	VXS	C04-N03	2.96	1.43	1.38
4	K	202	VXS	C02-N03	2.95	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	201	VXS	C18-C06	2.94	1.44	1.39
4	I	201	VXS	C16-C11	2.92	1.44	1.40
4	B	202	VXS	C19-C20	2.91	1.45	1.38
4	L	202	VXS	C18-C06	2.91	1.44	1.39
3	K	201	HEM	C3C-CAC	2.87	1.53	1.47
3	E	201	HEM	C3B-CAB	2.87	1.53	1.47
4	C	202	VXS	C02-N03	2.86	1.42	1.38
4	C	202	VXS	C19-C20	2.85	1.44	1.38
4	L	202	VXS	C19-C20	2.84	1.44	1.38
4	B	202	VXS	C10-C11	2.83	1.57	1.51
4	D	203[A]	VXS	C06-N07	2.81	1.45	1.37
4	J	201	VXS	C09-C08	2.79	1.62	1.51
4	J	201	VXS	C06-N07	2.79	1.45	1.37
4	K	202	VXS	C10-C11	2.75	1.57	1.51
4	B	202	VXS	C06-N07	2.74	1.45	1.37
3	H	201	HEM	C3B-CAB	2.74	1.53	1.47
4	K	202	VXS	C21-C02	2.71	1.52	1.48
4	K	202	VXS	C19-C20	2.70	1.44	1.38
4	E	202	VXS	C06-N07	2.69	1.44	1.37
4	E	202	VXS	C10-C11	2.64	1.56	1.51
4	I	201	VXS	C19-C20	2.63	1.44	1.38
3	K	201	HEM	C3B-CAB	2.63	1.53	1.47
4	I	201	VXS	C06-N07	2.62	1.44	1.37
4	K	202	VXS	C18-C06	2.62	1.44	1.39
4	K	202	VXS	C06-N07	2.56	1.44	1.37
4	A	203	VXS	O01-C02	-2.56	1.18	1.23
4	I	201	VXS	C09-C08	2.55	1.61	1.51
4	F	201	VXS	C06-N07	2.52	1.44	1.37
4	K	202	VXS	C16-C11	2.51	1.43	1.40
4	H	202	VXS	C21-C05	2.51	1.45	1.40
4	D	203[B]	VXS	C21-C02	2.48	1.52	1.48
4	D	203[B]	VXS	C06-N07	2.46	1.44	1.37
4	J	201	VXS	C19-C20	2.44	1.44	1.38
4	J	201	VXS	O01-C02	-2.40	1.18	1.23
4	F	201	VXS	O01-C02	-2.39	1.18	1.23
4	J	201	VXS	C21-C02	2.33	1.52	1.48
4	D	203[A]	VXS	C18-C06	2.31	1.43	1.39
4	E	202	VXS	C21-C05	2.28	1.44	1.40
4	L	202	VXS	C21-C02	2.27	1.52	1.48
4	A	203	VXS	C06-N07	2.27	1.43	1.37
4	I	201	VXS	C21-C05	2.26	1.44	1.40
4	E	202	VXS	C16-C11	2.20	1.43	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	201	VXS	C08-N07	2.19	1.50	1.45
4	B	202	VXS	C09-C08	2.19	1.60	1.51
4	C	202	VXS	C06-N07	2.19	1.43	1.37
4	K	202	VXS	C09-C08	2.18	1.60	1.51
4	H	202	VXS	C18-C06	2.18	1.43	1.39
4	A	203	VXS	C19-C20	2.17	1.43	1.38
4	F	201	VXS	C21-C02	2.17	1.51	1.48
4	B	202	VXS	O01-C02	-2.15	1.18	1.23
4	L	202	VXS	O01-C02	-2.14	1.18	1.23
3	C	201	HEM	CMB-C2B	2.13	1.56	1.51
4	D	203[B]	VXS	C18-C06	2.13	1.43	1.39
4	L	202	VXS	C08-N07	2.12	1.48	1.45
4	B	202	VXS	C02-N03	2.11	1.41	1.38
4	J	201	VXS	C16-C11	2.11	1.43	1.40
4	D	203[B]	VXS	C05-C06	-2.11	1.37	1.41
4	K	202	VXS	O01-C02	-2.10	1.19	1.23
3	D	202	HEM	CAA-C2A	2.10	1.55	1.52
4	F	201	VXS	C10-C11	2.08	1.55	1.51
4	C	202	VXS	C09-C08	2.07	1.61	1.48
3	E	201	HEM	CMB-C2B	2.05	1.56	1.51
3	C	201	HEM	CMD-C2D	2.04	1.55	1.51
4	A	203	VXS	C02-N03	2.04	1.41	1.38
4	D	203[A]	VXS	C21-C02	2.01	1.51	1.48

All (146) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	202	VXS	C04-N03-C02	7.92	119.28	112.52
4	J	201	VXS	C12-C11-C16	-5.21	112.59	118.16
4	J	201	VXS	C08-C09-C10	5.06	121.96	112.95
4	E	202	VXS	C12-C11-C16	-4.64	113.21	118.16
4	H	202	VXS	O22-C04-C05	4.55	135.32	128.55
4	I	201	VXS	C12-C11-C16	-4.55	113.30	118.16
4	F	201	VXS	C12-C11-C16	-4.35	113.51	118.16
4	K	202	VXS	C12-C11-C16	-4.21	113.67	118.16
4	D	203[A]	VXS	C12-C11-C16	-4.19	113.69	118.16
4	B	202	VXS	C12-C11-C16	-4.08	113.81	118.16
4	D	203[A]	VXS	C15-C16-C11	4.02	125.28	120.41
4	H	202	VXS	C21-C05-C06	4.00	124.66	121.91
4	H	202	VXS	C18-C06-C05	-3.79	112.75	119.10
3	C	201	HEM	CMA-C3A-C4A	-3.79	122.64	128.46
4	D	203[A]	VXS	C05-C06-N07	3.71	125.71	121.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	202	VXS	O01-C02-C21	3.61	137.15	127.67
4	D	203[B]	VXS	C05-C06-N07	3.58	125.56	121.32
4	J	201	VXS	C05-C06-N07	3.56	125.54	121.32
4	F	201	VXS	C15-C16-C11	3.53	124.68	120.41
4	B	202	VXS	C10-C11-C16	3.48	127.15	120.51
4	K	202	VXS	C10-C11-C16	3.45	127.09	120.51
3	K	201	HEM	CMA-C3A-C4A	-3.43	123.19	128.46
4	L	202	VXS	C08-N07-C06	3.36	127.72	122.44
4	A	203	VXS	C12-C11-C16	-3.34	114.59	118.16
4	H	202	VXS	C05-C06-N07	3.33	125.27	121.32
4	I	201	VXS	C10-C11-C16	3.30	126.80	120.51
4	J	201	VXS	C15-C16-C11	3.28	124.38	120.41
3	K	201	HEM	CBA-CAA-C2A	-3.28	106.44	112.49
4	C	202	VXS	C08-N07-C06	3.26	129.98	123.21
4	H	202	VXS	C08-N07-C06	3.24	131.18	123.39
4	C	202	VXS	O22-C04-C05	3.19	133.30	128.55
4	I	201	VXS	C05-C06-N07	3.16	125.07	121.32
4	D	203[B]	VXS	C12-C11-C16	-3.16	114.78	118.16
4	E	202	VXS	C10-C11-C16	3.11	126.44	120.51
4	J	201	VXS	C10-C11-C16	3.07	126.36	120.51
3	C	201	HEM	CMB-C2B-C3B	3.07	130.41	124.68
4	I	201	VXS	O22-C04-C05	3.05	133.09	128.55
3	K	201	HEM	CAD-CBD-CGD	-3.04	107.56	112.67
3	A	202	HEM	CMB-C2B-C3B	3.03	130.35	124.68
4	A	203	VXS	C15-C16-C11	3.02	124.06	120.41
4	D	203[B]	VXS	C15-C16-C11	3.00	124.04	120.41
4	E	202	VXS	O22-C04-C05	3.00	133.01	128.55
4	B	202	VXS	C08-C09-C10	2.99	118.28	112.95
4	F	201	VXS	O22-C04-C05	2.99	133.00	128.55
3	C	201	HEM	CMD-C2D-C1D	-2.99	123.87	128.46
4	E	202	VXS	C15-C16-C11	2.96	123.99	120.41
4	F	201	VXS	C08-N07-C06	2.93	130.44	123.39
4	L	202	VXS	O22-C04-C05	2.92	132.89	128.55
3	D	202	HEM	CAD-CBD-CGD	-2.90	107.81	112.67
4	A	203	VXS	C05-C06-N07	2.85	124.70	121.32
4	K	202	VXS	C05-C06-N07	2.84	124.69	121.32
3	H	201	HEM	CMD-C2D-C1D	-2.81	124.14	128.46
3	A	202	HEM	CMD-C2D-C1D	-2.74	124.25	128.46
4	B	202	VXS	C21-C05-C06	2.72	123.78	121.91
3	C	201	HEM	CMA-C3A-C2A	2.72	130.06	124.94
4	I	201	VXS	C15-C16-C11	2.71	123.69	120.41
3	C	201	HEM	CAD-CBD-CGD	-2.70	108.14	112.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	202	VXS	C09-C08-N07	2.70	118.75	111.49
4	K	202	VXS	C08-C09-C10	2.69	117.74	112.95
4	E	202	VXS	C08-N07-C06	2.69	129.86	123.39
4	D	203[A]	VXS	C10-C11-C12	2.68	125.22	119.37
4	C	202	VXS	O01-C02-C21	2.68	134.70	127.67
4	E	202	VXS	C08-C09-C10	2.68	117.72	112.95
3	H	201	HEM	CAD-CBD-CGD	-2.67	108.19	112.67
3	L	201	HEM	CMB-C2B-C3B	2.61	129.57	124.68
4	K	202	VXS	O22-C04-C05	2.61	132.43	128.55
4	B	202	VXS	O01-C02-C21	2.60	134.49	127.67
4	K	202	VXS	C15-C16-C11	2.60	123.55	120.41
4	K	202	VXS	C08-N07-C06	2.59	129.61	123.39
4	E	202	VXS	O01-C02-C21	2.57	134.42	127.67
4	I	201	VXS	O01-C02-C21	2.55	134.35	127.67
4	B	202	VXS	O22-C04-C05	2.55	132.34	128.55
3	C	201	HEM	CBA-CAA-C2A	-2.54	107.81	112.49
3	A	202	HEM	CMC-C2C-C3C	2.53	129.42	124.68
4	J	201	VXS	C09-C08-N07	2.51	118.24	111.49
3	E	201	HEM	C4C-C3C-C2C	2.50	108.65	106.90
3	C	201	HEM	CMC-C2C-C3C	2.50	129.36	124.68
3	L	201	HEM	CMC-C2C-C3C	2.50	129.36	124.68
4	J	201	VXS	C13-C12-C11	2.49	124.61	120.89
4	F	201	VXS	C10-C11-C16	2.49	125.25	120.51
4	J	201	VXS	O22-C04-C05	2.48	132.24	128.55
4	C	202	VXS	C05-C06-N07	2.47	124.25	121.32
3	A	202	HEM	CBD-CAD-C3D	-2.47	107.93	112.48
4	L	202	VXS	O01-C02-C21	2.46	134.13	127.67
3	H	201	HEM	CMA-C3A-C4A	-2.46	124.69	128.46
4	I	201	VXS	C08-N07-C06	2.45	129.29	123.39
4	B	202	VXS	C05-C06-N07	2.44	124.22	121.32
4	I	201	VXS	C18-C06-C05	-2.44	115.02	119.10
4	K	202	VXS	O01-C02-C21	2.42	134.01	127.67
3	H	201	HEM	CBA-CAA-C2A	-2.42	108.03	112.49
4	J	201	VXS	C18-C06-C05	-2.42	115.06	119.10
4	E	202	VXS	C05-C06-N07	2.41	124.18	121.32
3	H	201	HEM	CMC-C2C-C3C	2.40	129.17	124.68
4	B	202	VXS	C08-N07-C06	2.39	129.15	123.39
3	D	202	HEM	CBA-CAA-C2A	-2.37	108.11	112.49
3	E	201	HEM	CMA-C3A-C4A	-2.34	124.87	128.46
4	I	201	VXS	C13-C12-C11	2.34	124.39	120.89
3	D	202	HEM	CMC-C2C-C3C	2.33	129.04	124.68
4	K	202	VXS	C18-C06-C05	-2.33	115.20	119.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	203[A]	VXS	C18-C06-C05	-2.32	115.22	119.10
4	H	202	VXS	C21-C02-N03	-2.30	103.78	105.89
3	A	202	HEM	CMA-C3A-C4A	-2.30	124.93	128.46
3	L	201	HEM	CBA-CAA-C2A	-2.30	108.25	112.49
4	C	202	VXS	C18-C06-C05	-2.29	115.27	119.10
3	K	201	HEM	CMD-C2D-C1D	-2.28	124.96	128.46
4	E	202	VXS	C13-C12-C11	2.28	124.30	120.89
4	L	202	VXS	C18-C06-C05	-2.27	115.29	119.10
3	E	201	HEM	CBA-CAA-C2A	-2.27	108.30	112.49
4	E	202	VXS	C18-C06-C05	-2.26	115.32	119.10
4	B	202	VXS	C18-C06-C05	-2.25	115.34	119.10
4	A	203	VXS	C18-C06-C05	-2.25	115.34	119.10
3	E	201	HEM	CAD-CBD-CGD	-2.24	108.91	112.67
4	D	203[B]	VXS	O01-C02-C21	2.24	133.54	127.67
4	A	203	VXS	O01-C02-C21	2.22	133.50	127.67
3	K	201	HEM	CAA-CBA-CGA	-2.21	108.97	112.67
3	D	202	HEM	CBD-CAD-C3D	-2.21	108.41	112.48
4	F	201	VXS	O01-C02-C21	2.20	133.44	127.67
4	D	203[A]	VXS	O01-C02-C21	2.17	133.37	127.67
4	H	202	VXS	C19-C18-C06	2.17	123.14	118.62
3	E	201	HEM	C4A-C3A-C2A	2.17	108.51	107.00
4	B	202	VXS	C15-C16-C11	2.17	123.03	120.41
3	C	201	HEM	CAA-CBA-CGA	-2.17	109.03	112.67
4	B	202	VXS	C13-C12-C11	2.16	124.12	120.89
3	K	201	HEM	C4C-C3C-C2C	2.16	108.41	106.90
3	A	202	HEM	CAD-CBD-CGD	-2.15	109.07	112.67
4	D	203[B]	VXS	C18-C06-C05	-2.15	115.51	119.10
4	D	203[B]	VXS	C21-C05-C06	2.14	123.38	121.91
4	F	201	VXS	C18-C06-C05	-2.13	115.53	119.10
4	J	201	VXS	O01-C02-C21	2.13	133.25	127.67
4	H	202	VXS	O01-C02-N03	-2.11	119.07	125.56
4	K	202	VXS	C13-C12-C11	2.10	124.04	120.89
4	H	202	VXS	C19-C20-C21	-2.09	115.85	119.81
4	A	203	VXS	O22-C04-C05	2.09	131.66	128.55
4	D	203[A]	VXS	O22-C04-C05	2.09	131.66	128.55
3	A	202	HEM	CAA-CBA-CGA	-2.09	109.16	112.67
3	K	201	HEM	CBD-CAD-C3D	-2.09	108.63	112.48
3	L	201	HEM	C1D-C2D-C3D	2.08	108.44	107.00
4	C	202	VXS	C21-C05-C06	2.07	123.33	121.91
4	E	202	VXS	C21-C05-C06	2.07	123.33	121.91
4	I	201	VXS	C08-C09-C10	2.06	116.61	112.95
4	A	203	VXS	C21-C05-C06	2.05	123.32	121.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	201	HEM	CMB-C2B-C3B	2.05	128.51	124.68
4	K	202	VXS	C21-C05-C06	2.05	123.32	121.91
3	A	202	HEM	CBA-CAA-C2A	-2.04	108.72	112.49
3	L	201	HEM	CAA-CBA-CGA	-2.02	109.28	112.67
3	D	202	HEM	CMB-C2B-C3B	2.00	128.43	124.68

There are no chirality outliers.

All (31) torsion outliers are listed below:

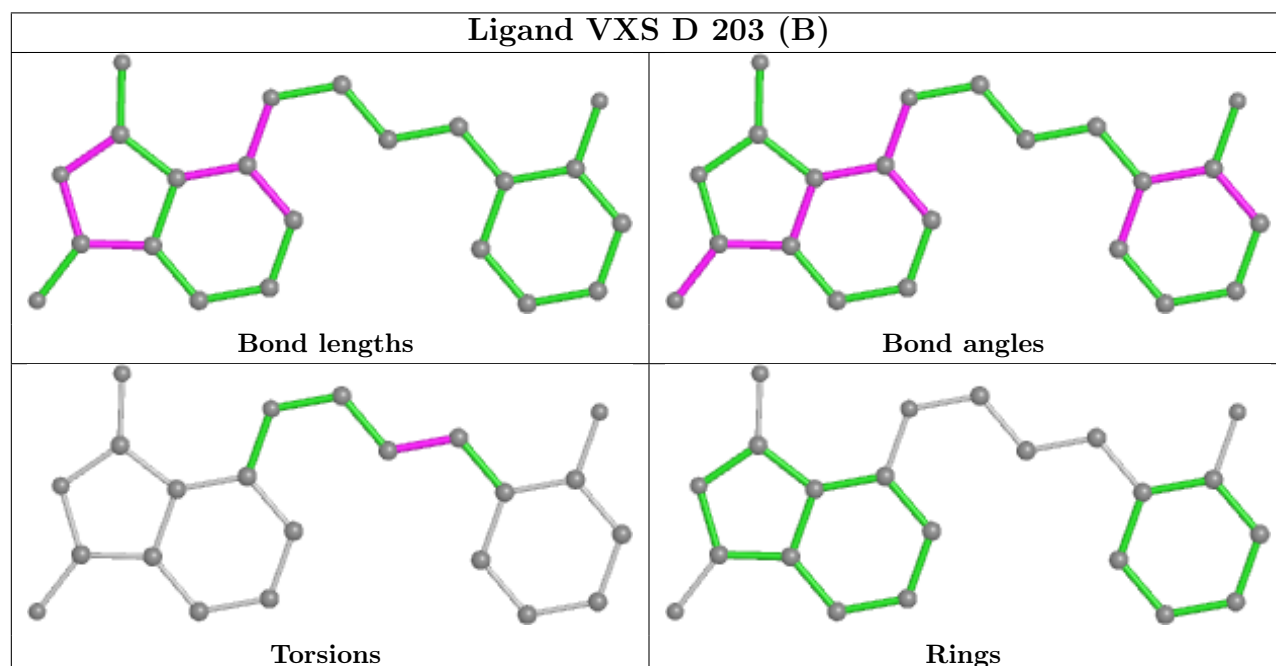
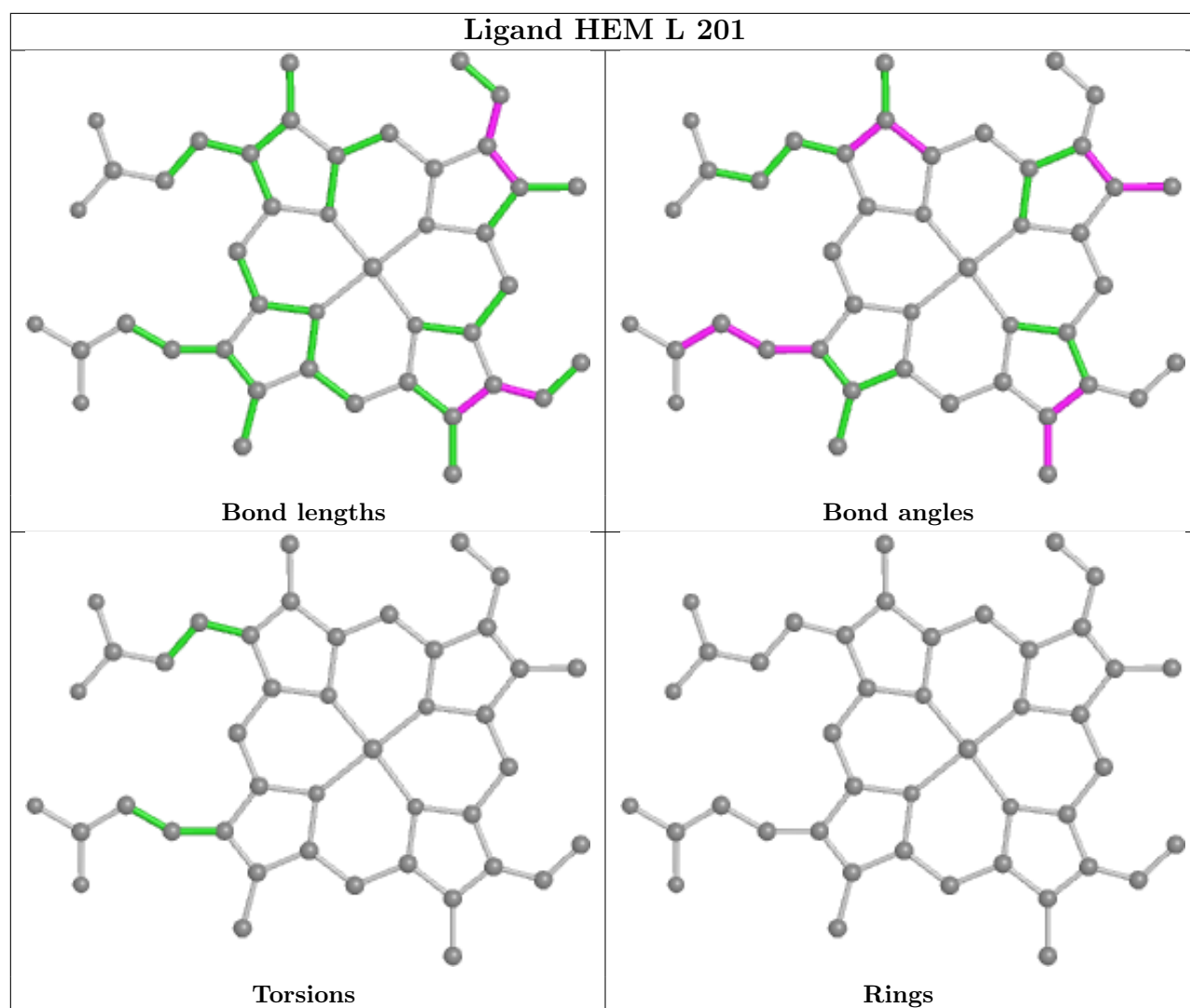
Mol	Chain	Res	Type	Atoms
4	D	203[A]	VXS	C08-C09-C10-C11
4	A	203	VXS	N07-C08-C09-C10
4	J	201	VXS	N07-C08-C09-C10
4	H	202	VXS	C08-C09-C10-C11
4	A	203	VXS	C08-C09-C10-C11
4	D	203[B]	VXS	C08-C09-C10-C11
4	B	202	VXS	C18-C06-N07-C08
4	B	202	VXS	C05-C06-N07-C08
4	H	202	VXS	C18-C06-N07-C08
4	H	202	VXS	C09-C08-N07-C06
4	A	203	VXS	C09-C08-N07-C06
4	H	202	VXS	C05-C06-N07-C08
4	D	203[A]	VXS	C09-C08-N07-C06
4	I	201	VXS	C09-C10-C11-C12
4	E	202	VXS	C09-C10-C11-C12
4	A	203	VXS	C09-C10-C11-C12
4	I	201	VXS	C09-C10-C11-C16
4	A	203	VXS	C09-C10-C11-C16
4	E	202	VXS	C09-C10-C11-C16
4	C	202	VXS	C05-C06-N07-C08
4	B	202	VXS	C09-C10-C11-C16
4	B	202	VXS	C09-C10-C11-C12
4	C	202	VXS	C18-C06-N07-C08
4	K	202	VXS	C09-C10-C11-C16
4	K	202	VXS	C05-C06-N07-C08
4	E	202	VXS	C05-C06-N07-C08
4	F	201	VXS	C09-C10-C11-C16
4	E	202	VXS	C18-C06-N07-C08
4	B	202	VXS	N07-C08-C09-C10
4	K	202	VXS	C18-C06-N07-C08
4	J	201	VXS	C09-C10-C11-C12

There are no ring outliers.

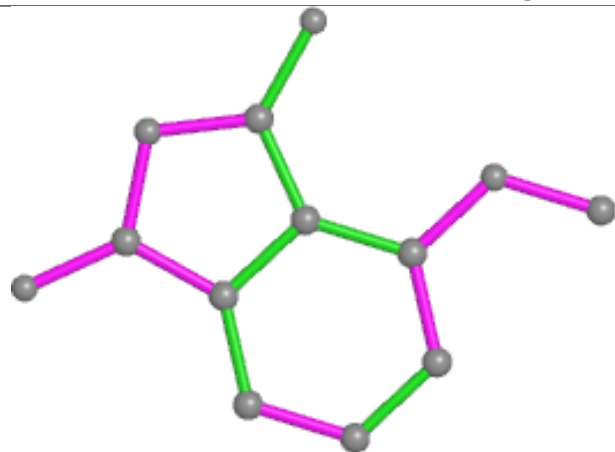
17 monomers are involved in 34 short contacts:

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

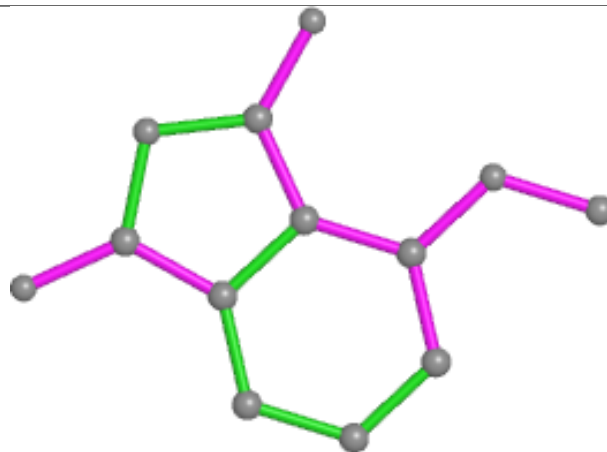
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



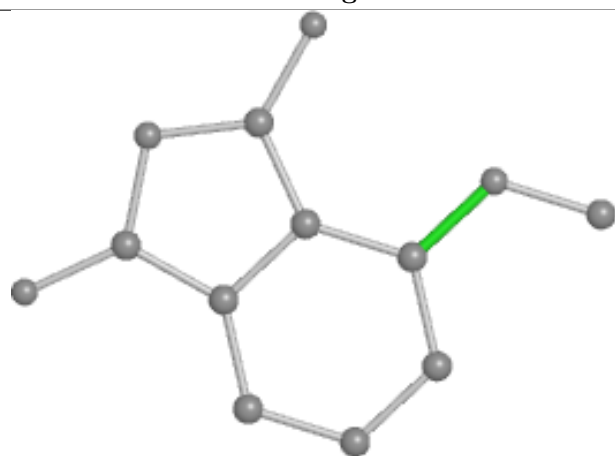
## Ligand VXS L 202



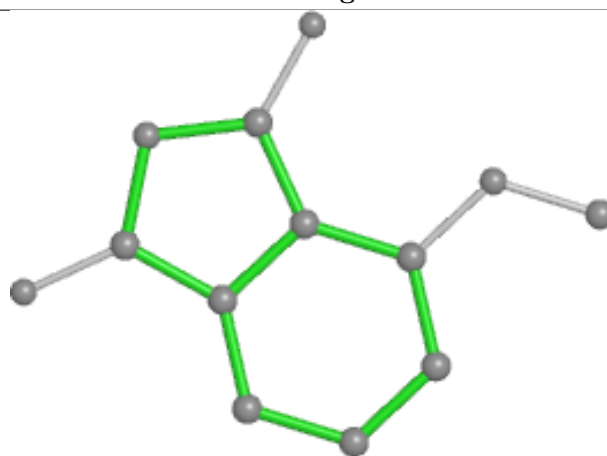
Bond lengths



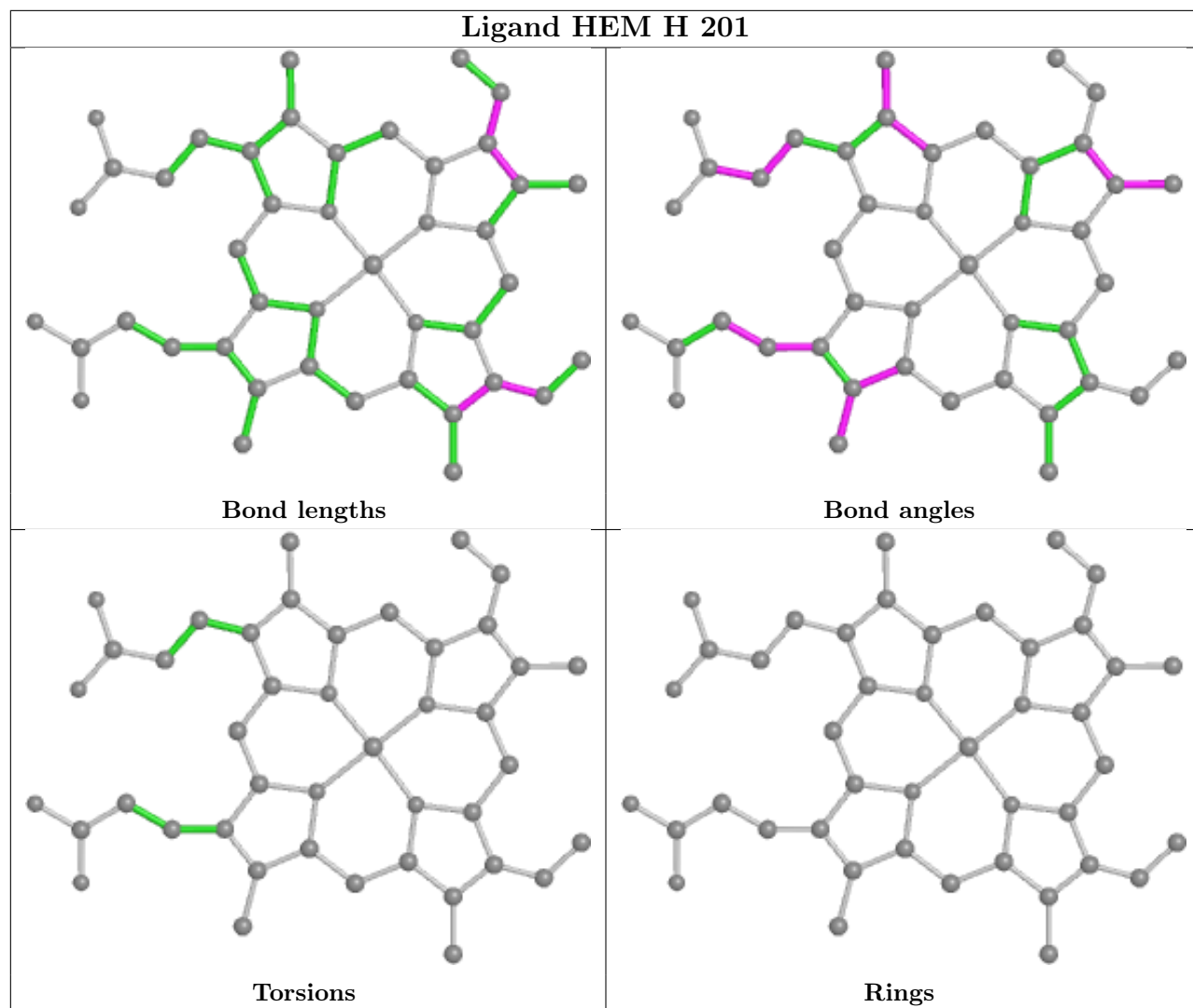
Bond angles



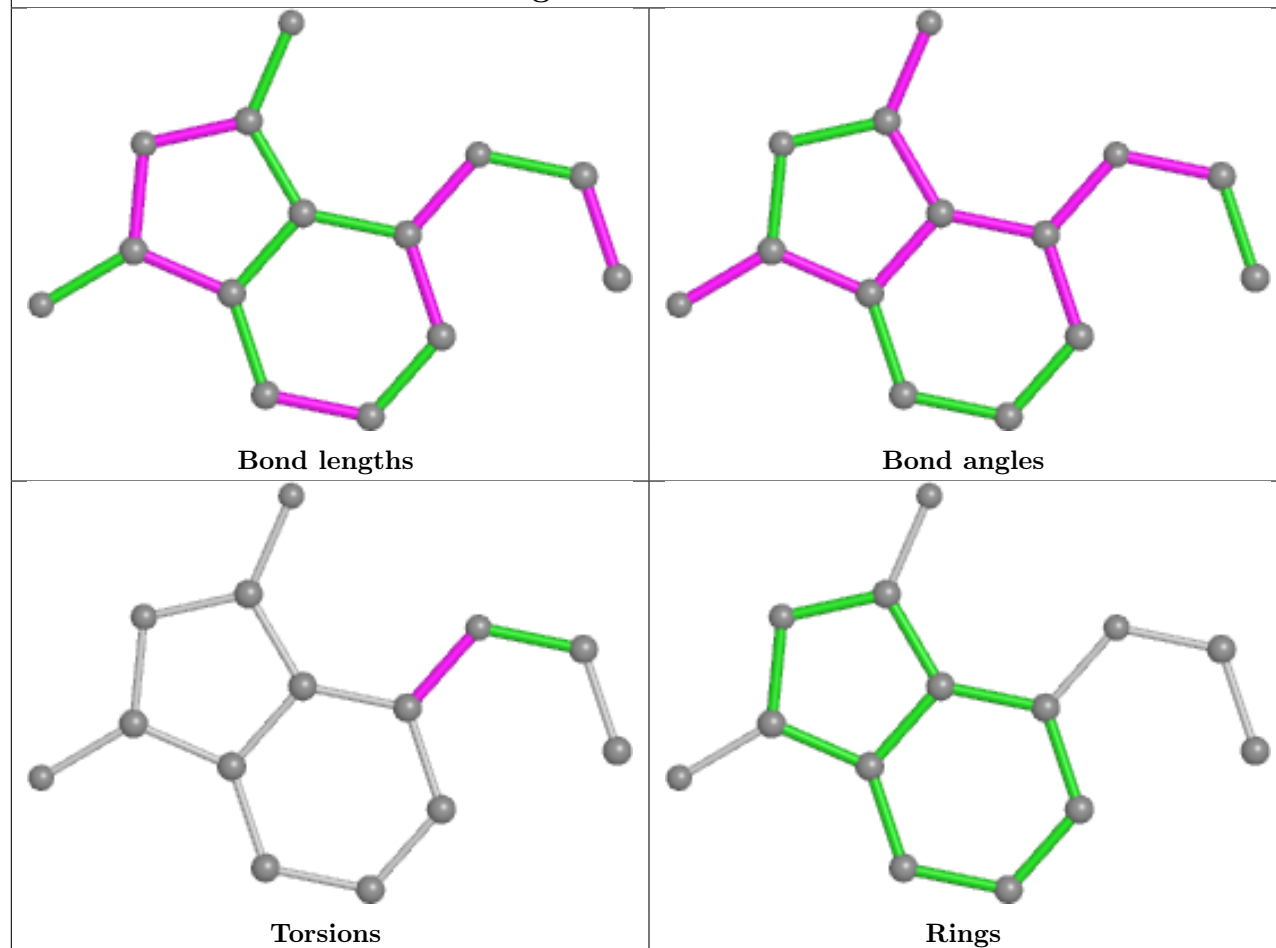
Torsions



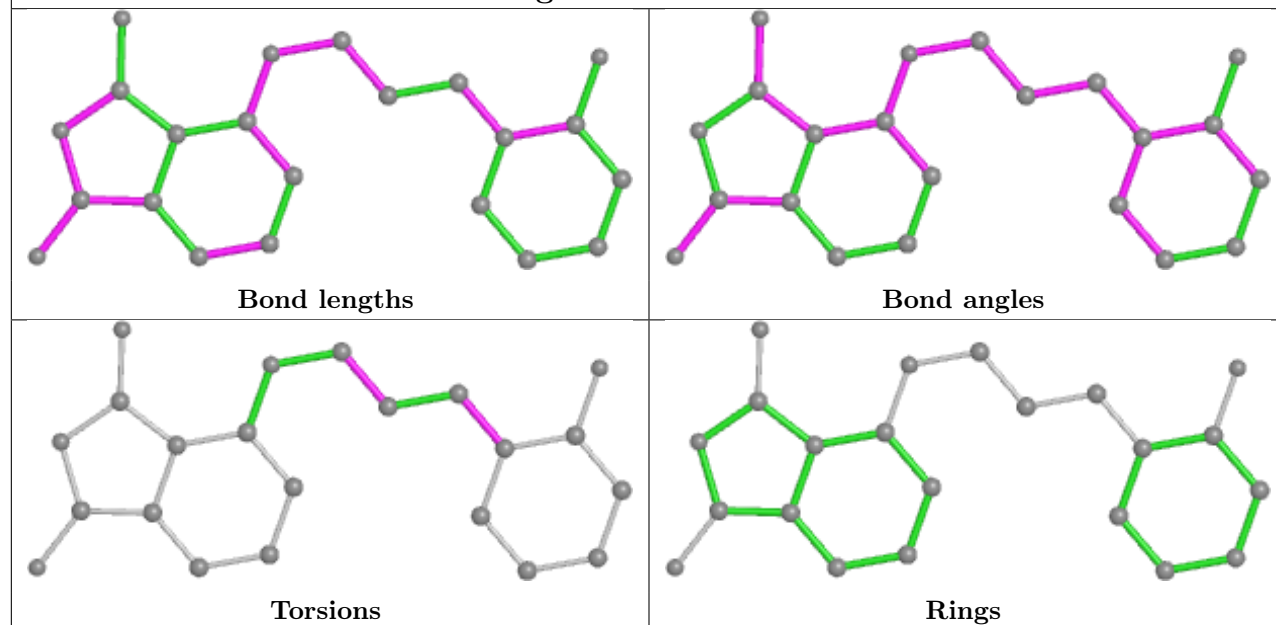
Rings

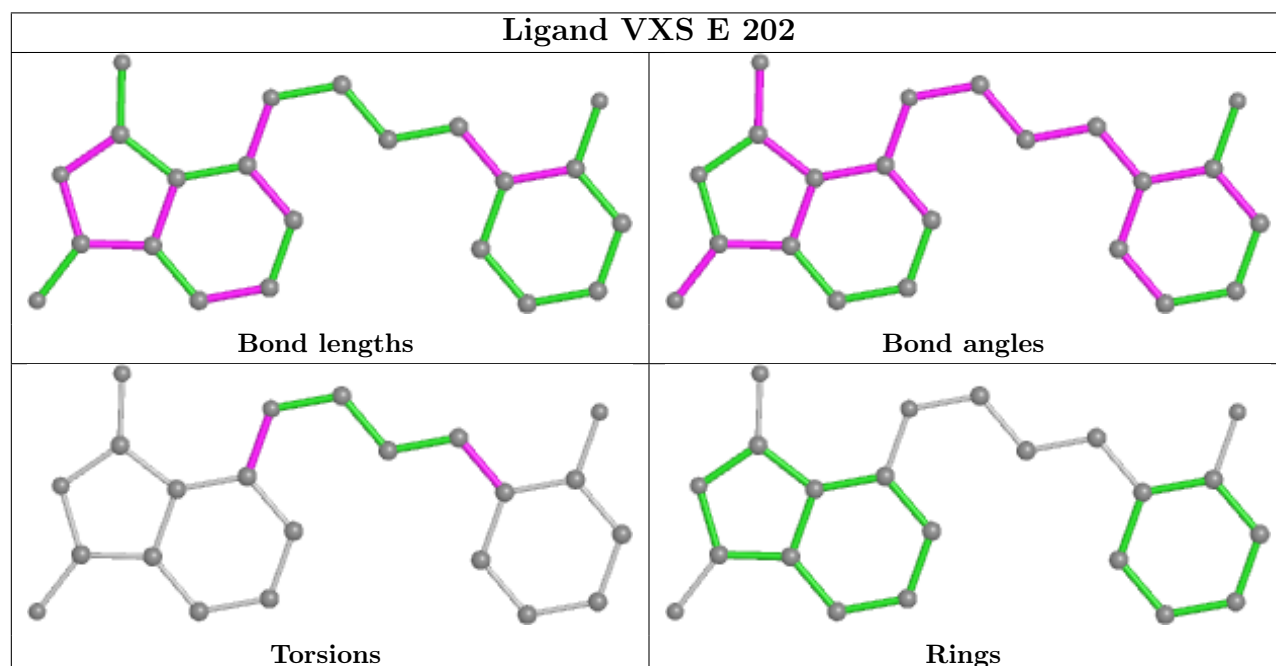
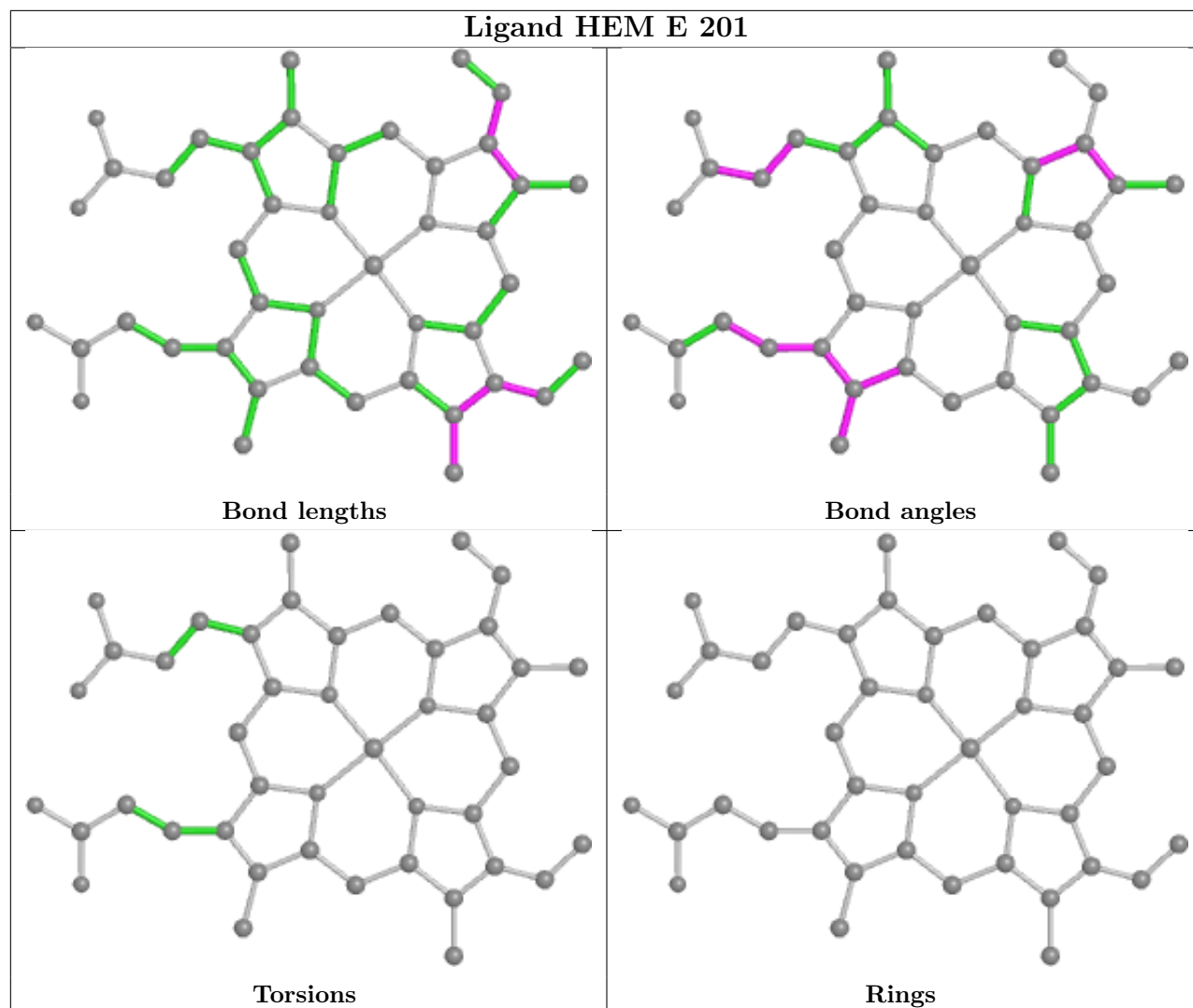


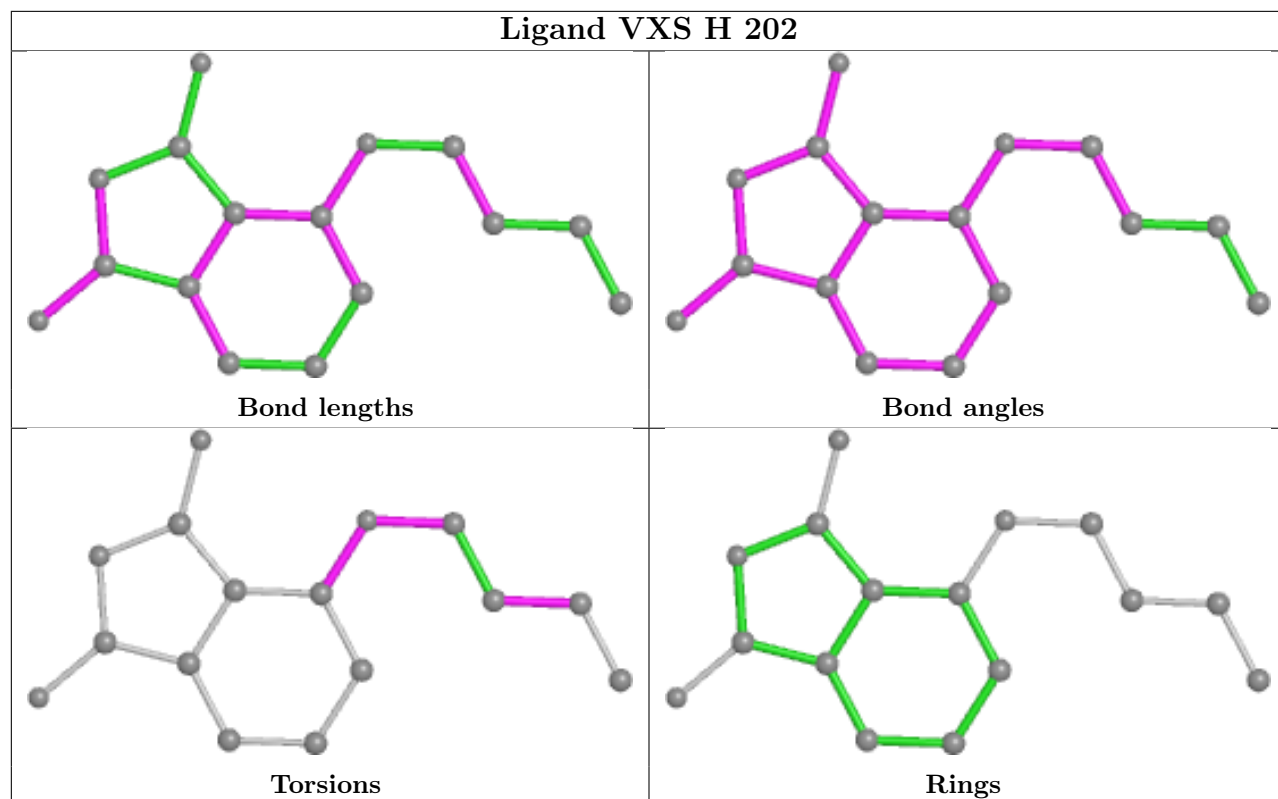
## Ligand VXS C 202



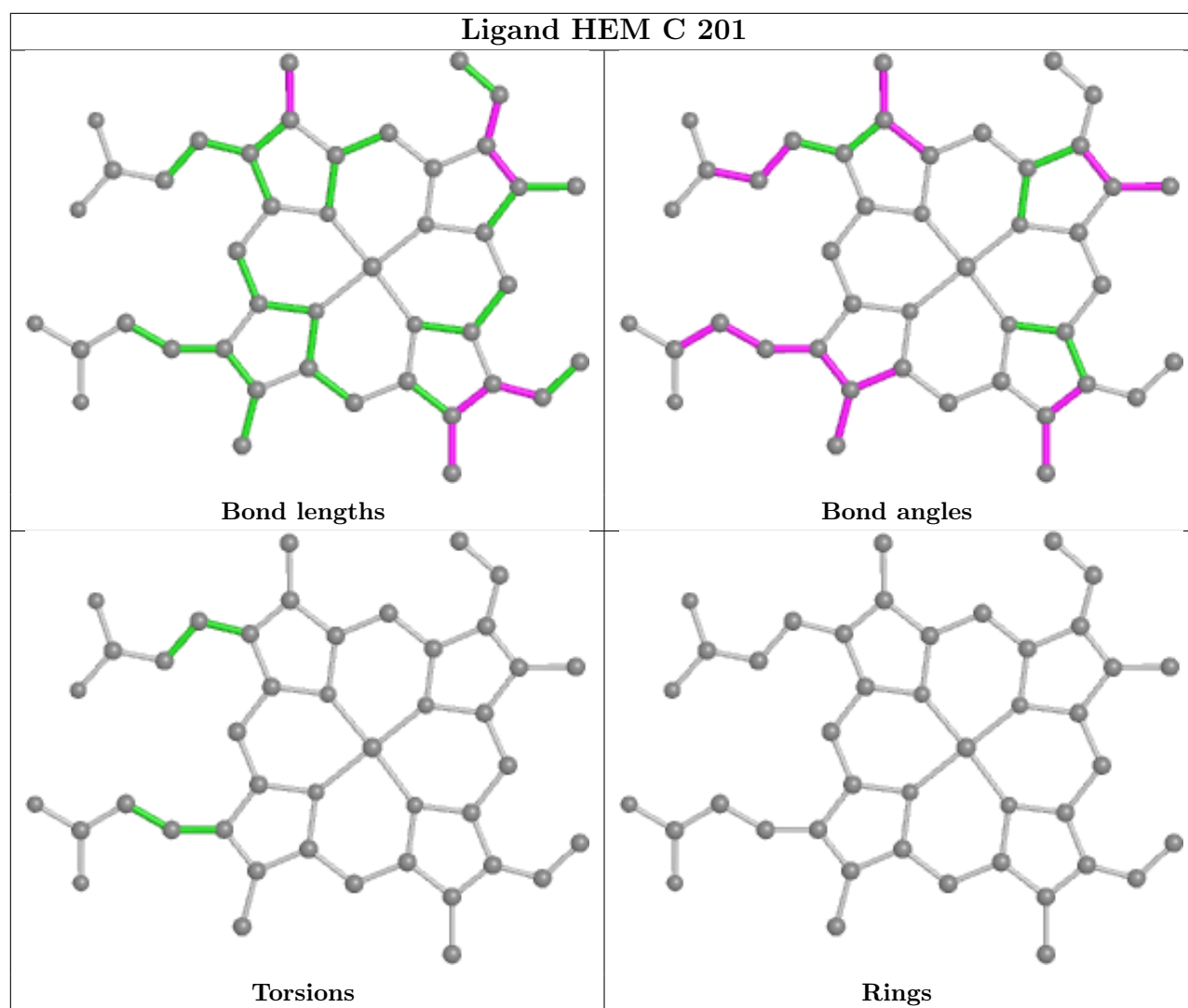
## Ligand VXS J 201

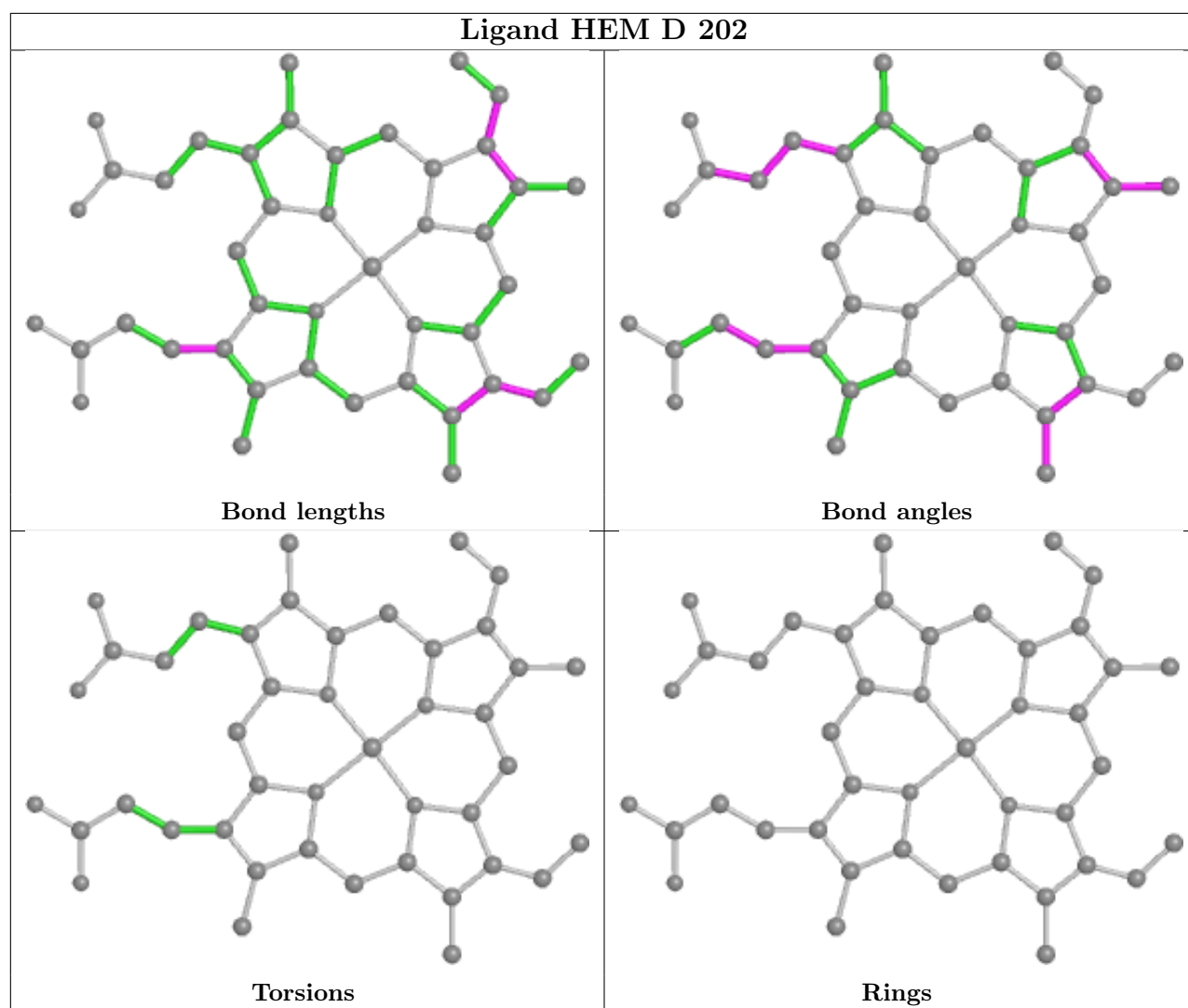


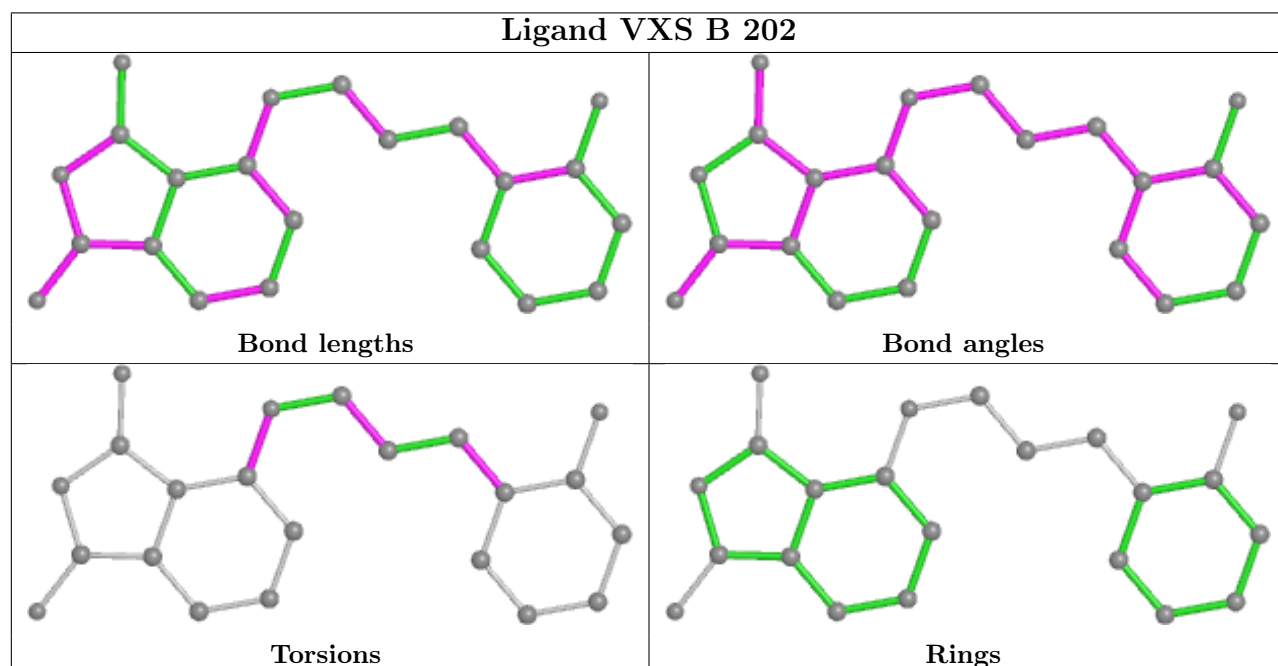
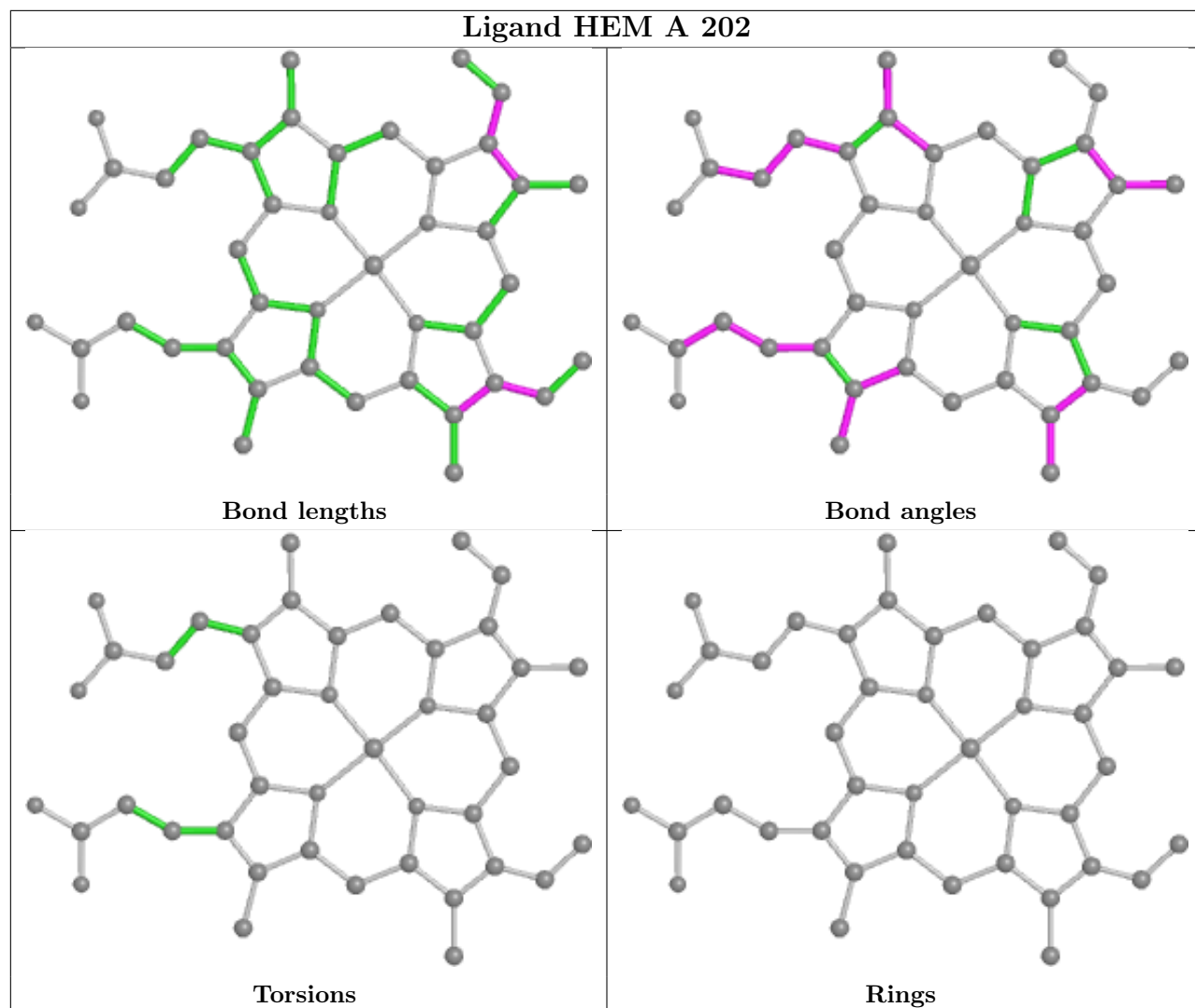




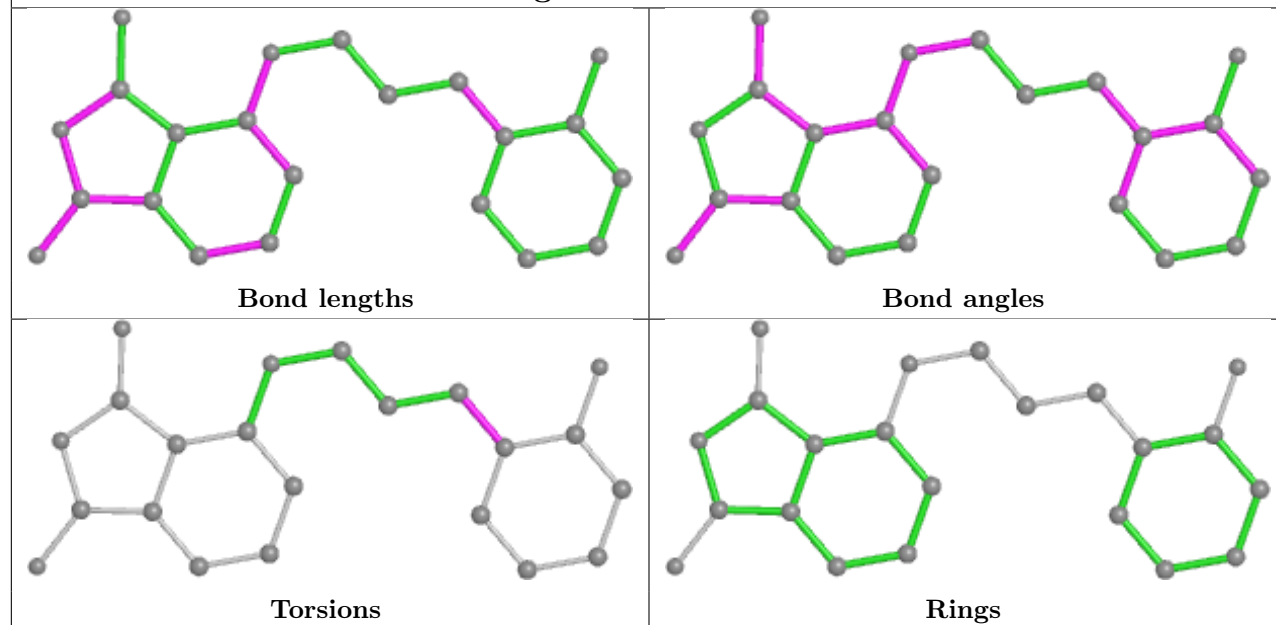




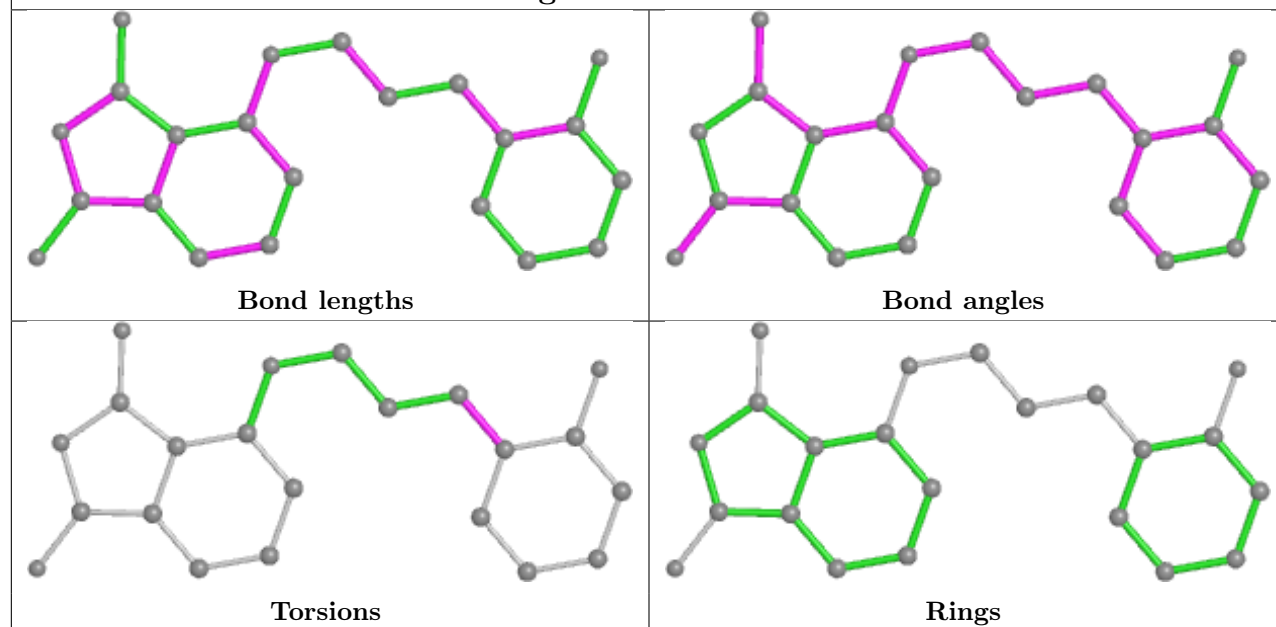




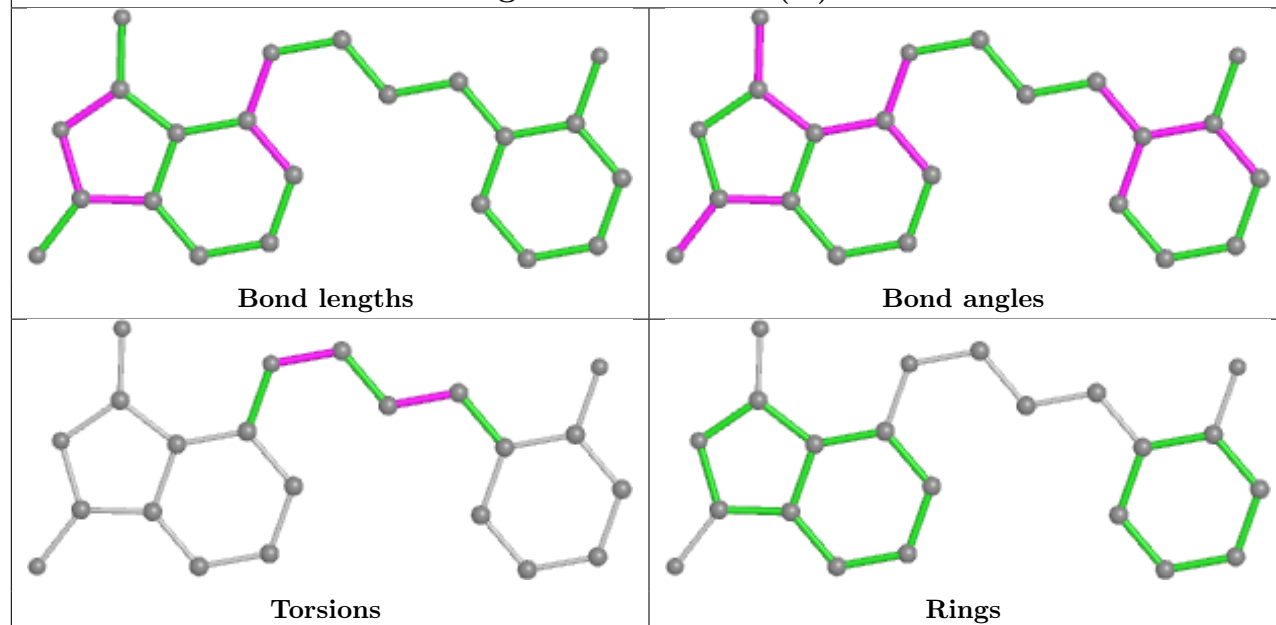
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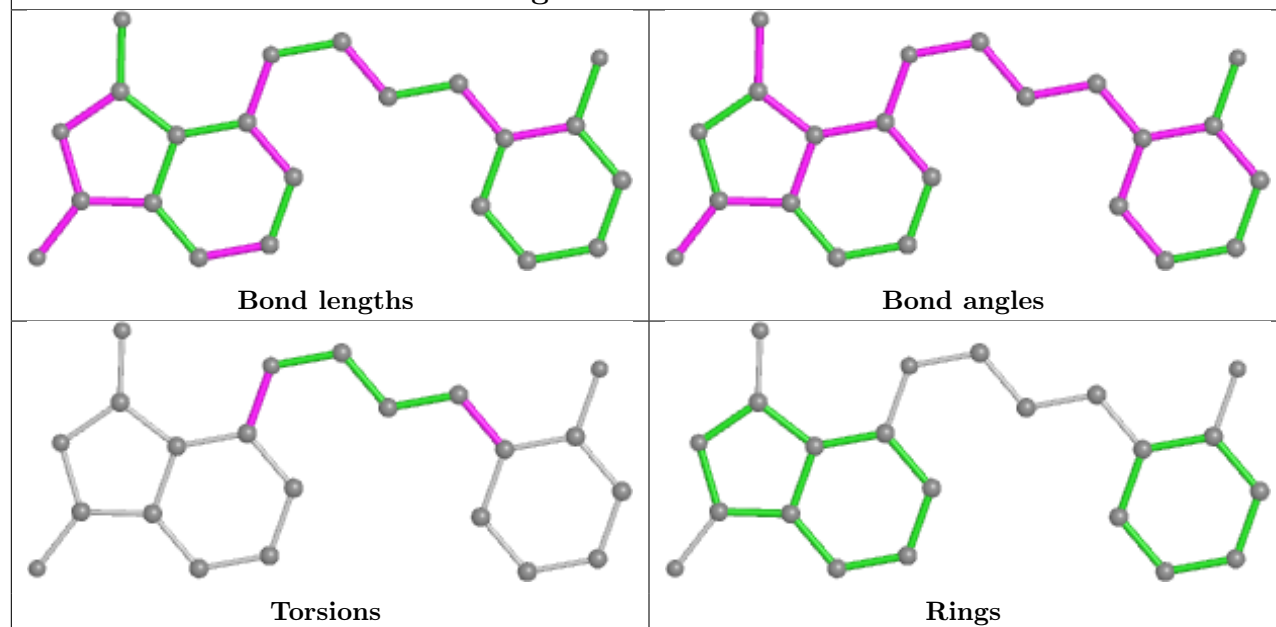
## Ligand VXS I 201



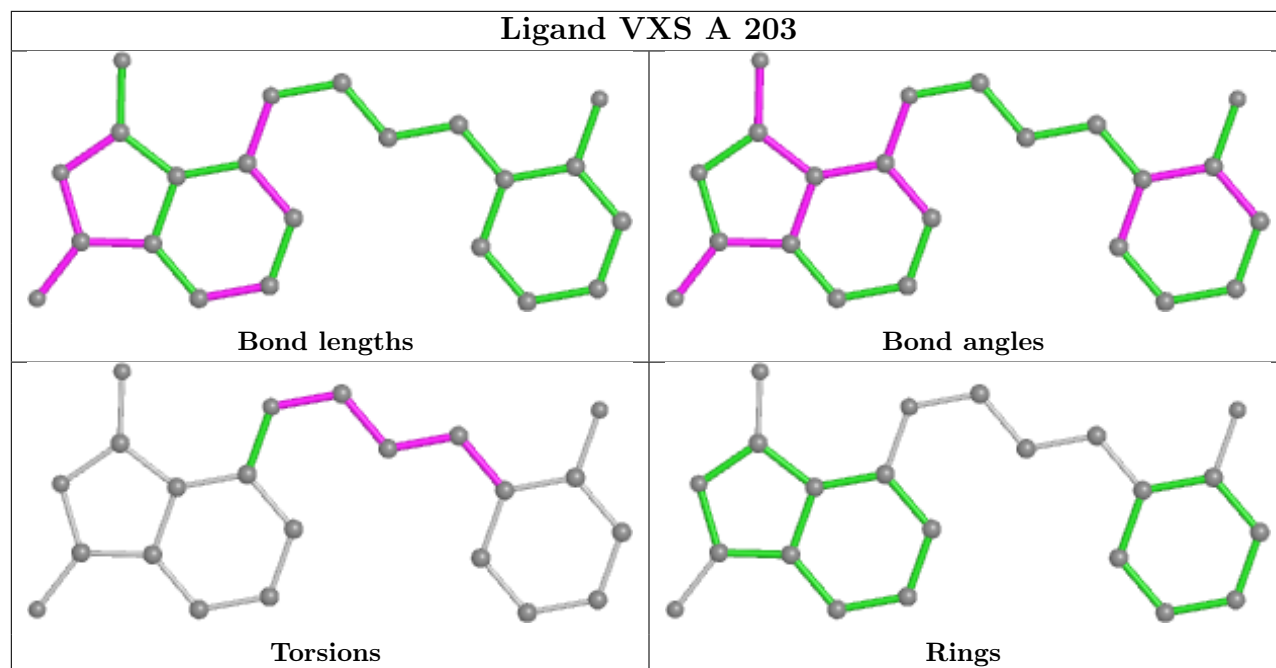
## Ligand VXS D 203 (A)



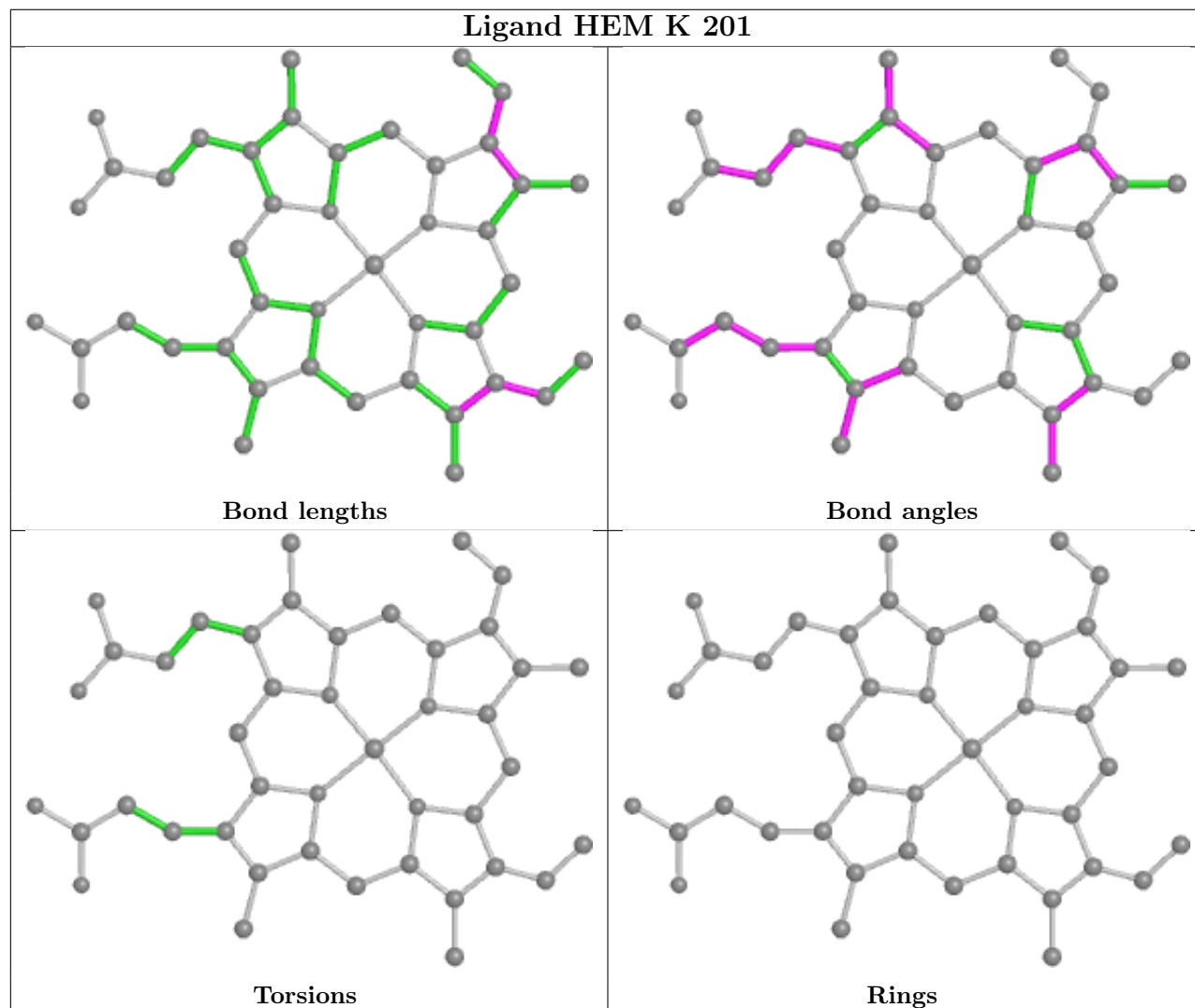
## Ligand VXS K 202



## Ligand VXS A 203



## Ligand HEM K 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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	155/158 (98%)	-0.44	0 100 100	21, 25, 35, 44	0
1	B	155/158 (98%)	-0.48	0 100 100	20, 26, 36, 45	0
1	C	155/158 (98%)	-0.43	0 100 100	20, 25, 35, 49	0
1	D	155/158 (98%)	-0.42	0 100 100	20, 25, 35, 49	0
1	E	155/158 (98%)	-0.41	0 100 100	19, 24, 33, 47	0
1	F	155/158 (98%)	-0.41	0 100 100	20, 25, 35, 49	0
1	G	155/158 (98%)	-0.46	0 100 100	20, 25, 34, 52	0
1	H	155/158 (98%)	-0.40	0 100 100	20, 25, 34, 43	0
1	I	155/158 (98%)	-0.48	0 100 100	21, 26, 35, 48	0
1	J	155/158 (98%)	-0.40	0 100 100	20, 25, 33, 51	0
1	K	155/158 (98%)	-0.44	0 100 100	21, 26, 35, 49	0
1	L	156/158 (98%)	-0.38	0 100 100	20, 26, 35, 57	0
All	All	1861/1896 (98%)	-0.43	0 100 100	19, 25, 35, 57	0

There are no RSRZ outliers to report.

### 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 [i](#)

There are no monosaccharides in this entry.



## 6.4 Ligands ⓘ

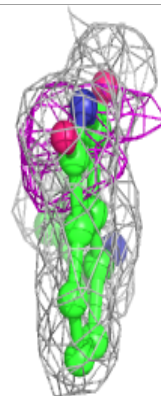
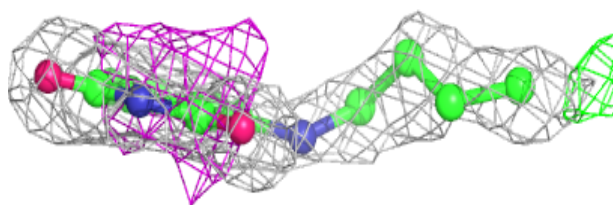
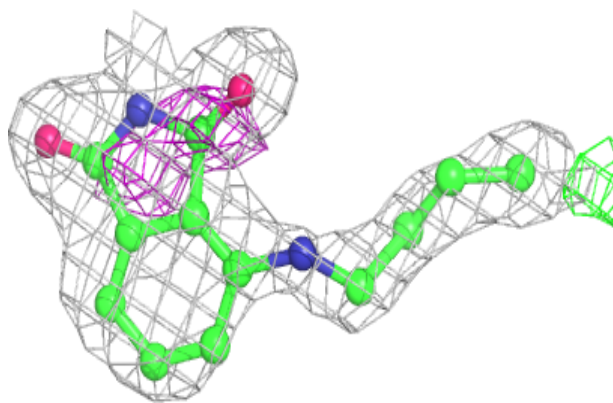
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	VXS	H	202	16/22	0.76	0.29	32,45,56,57	0
4	VXS	I	201	22/22	0.83	0.26	34,47,72,76	0
4	VXS	K	202	22/22	0.84	0.24	36,47,65,69	0
4	VXS	C	202	14/22	0.84	0.22	32,42,49,50	0
4	VXS	E	202	22/22	0.86	0.28	33,51,60,68	0
4	VXS	B	202	22/22	0.86	0.32	29,44,68,78	0
4	VXS	F	201	22/22	0.87	0.26	32,44,55,65	0
4	VXS	J	201	22/22	0.90	0.18	34,43,59,64	0
4	VXS	A	203	22/22	0.91	0.15	27,33,53,61	0
4	VXS	L	202	13/22	0.94	0.16	30,36,42,48	0
4	VXS	D	203[A]	22/22	0.95	0.14	25,33,43,46	22
4	VXS	D	203[B]	22/22	0.95	0.14	25,32,41,44	22
3	HEM	H	201	43/43	0.97	0.11	19,27,45,53	0
3	HEM	A	202	43/43	0.97	0.12	22,28,48,58	0
3	HEM	E	201	43/43	0.97	0.11	20,26,47,52	0
3	HEM	C	201	43/43	0.97	0.12	23,28,45,60	0
3	HEM	L	201	43/43	0.97	0.12	22,26,36,38	43
3	HEM	D	202	43/43	0.97	0.12	22,26,35,38	43
3	HEM	K	201	43/43	0.97	0.11	22,26,46,49	0
2	K	D	201	1/1	1.00	0.08	22,22,22,22	0
2	K	B	201	1/1	1.00	0.09	21,21,21,21	0
2	K	A	201	1/1	1.00	0.07	20,20,20,20	0

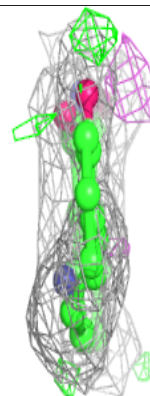
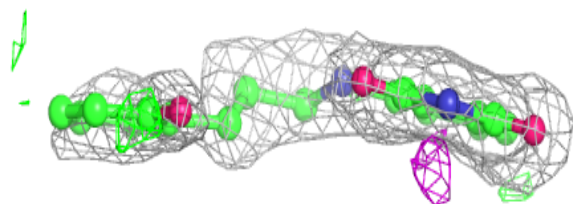
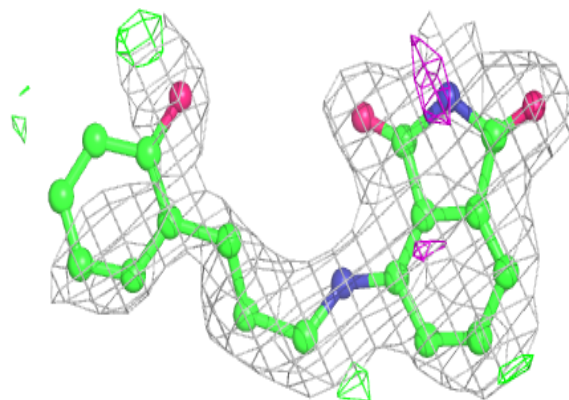
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around VXS 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)

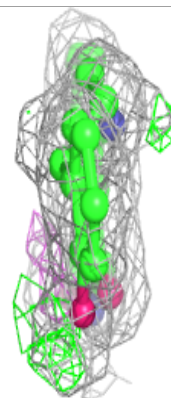
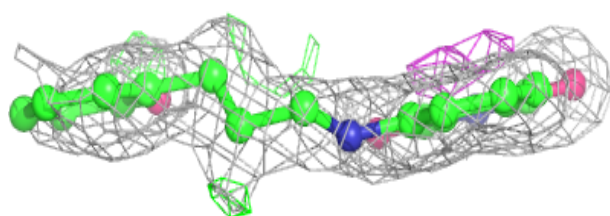
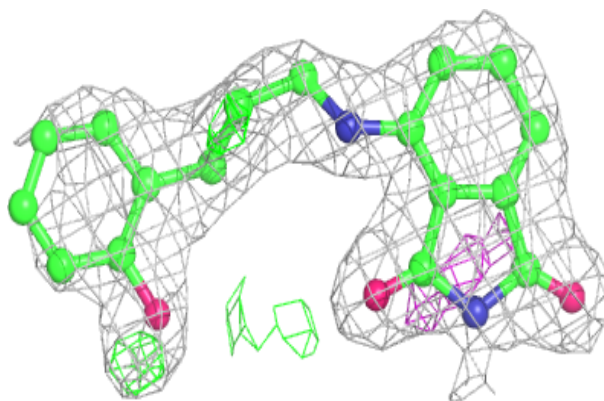
**Electron density around VXS I 201:**

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

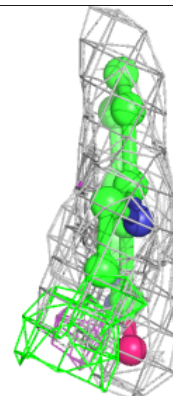
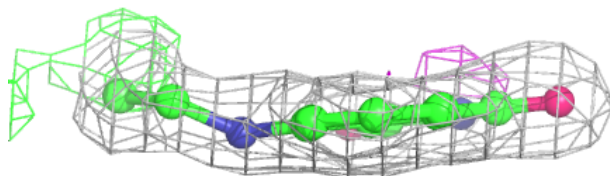
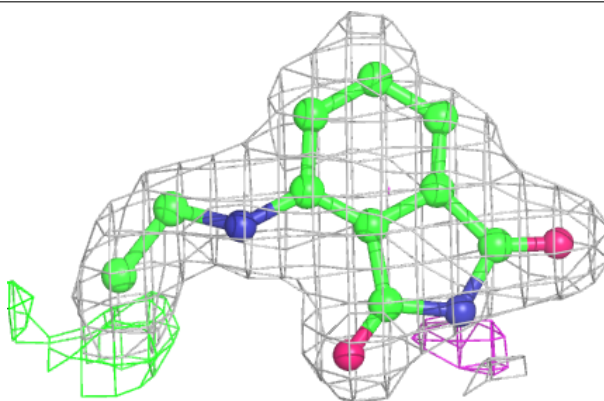


**Electron density around VXS K 202:**

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

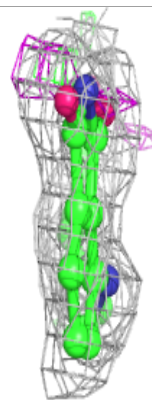
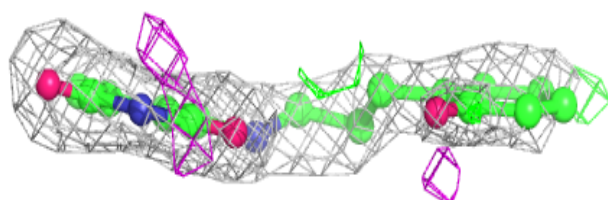
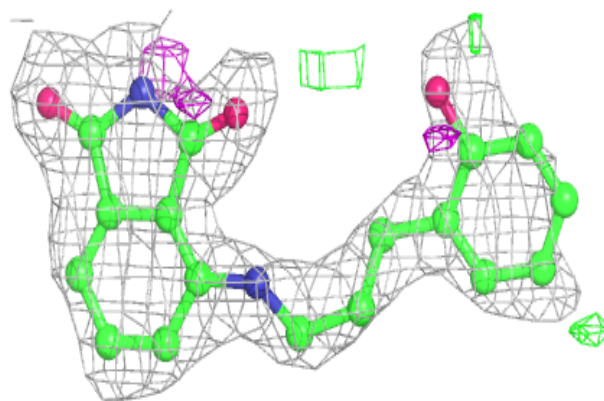
**Electron density around VXS C 202:**

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

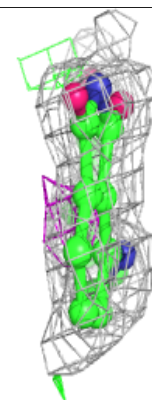
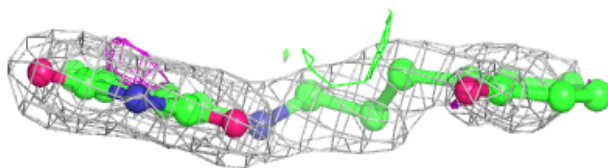
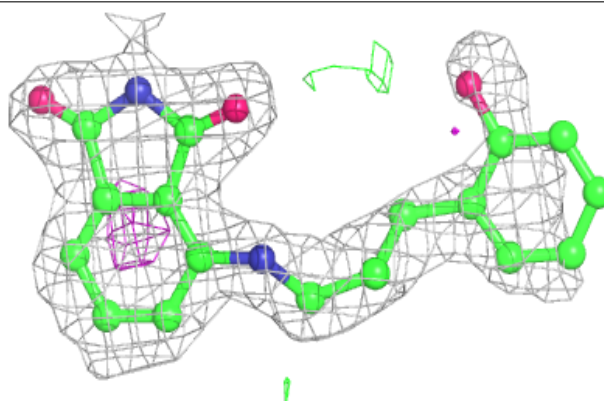


**Electron density around VXS E 202:**

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

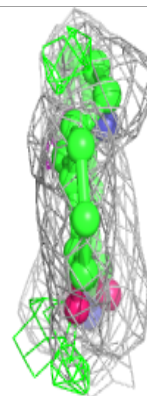
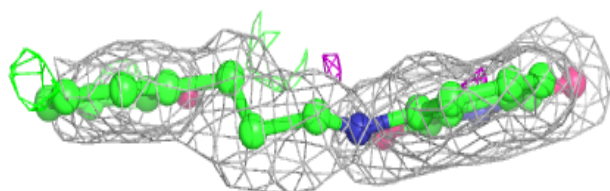
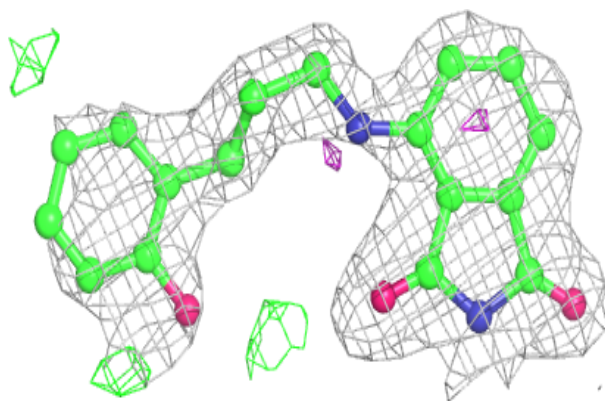
**Electron density around VXS B 202:**

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

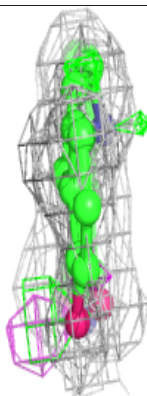
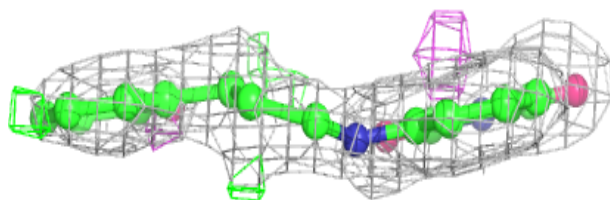
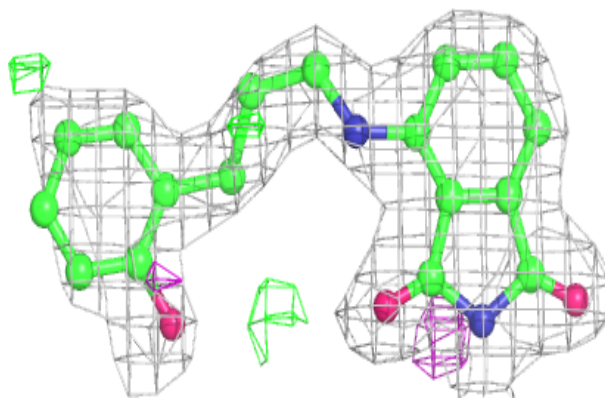


**Electron density around VXS F 201:**

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

**Electron density around VXS J 201:**

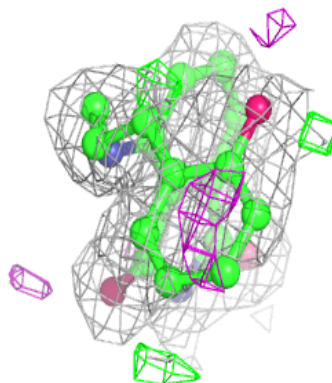
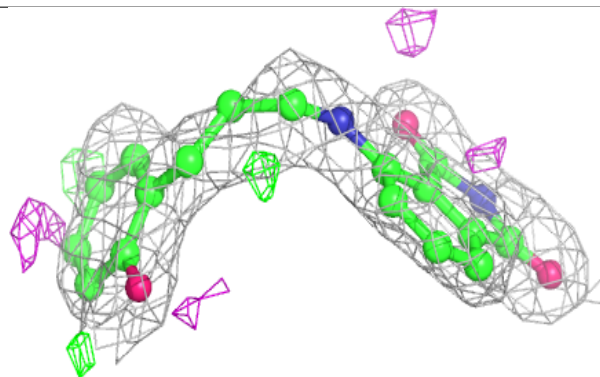
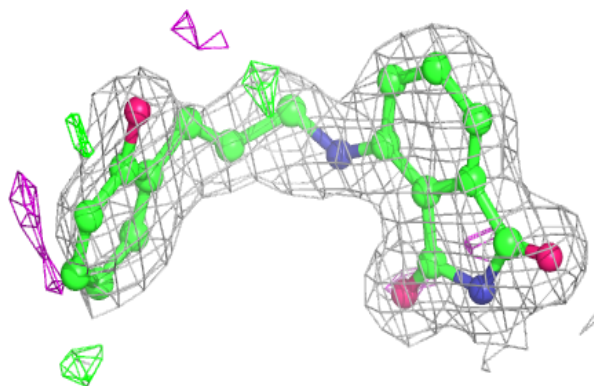
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





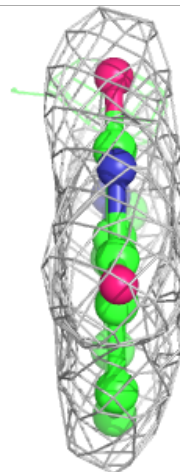
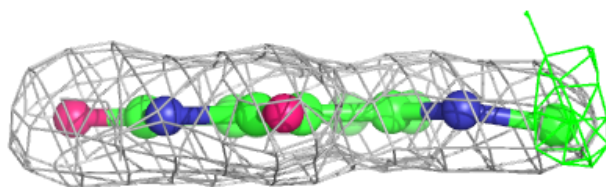
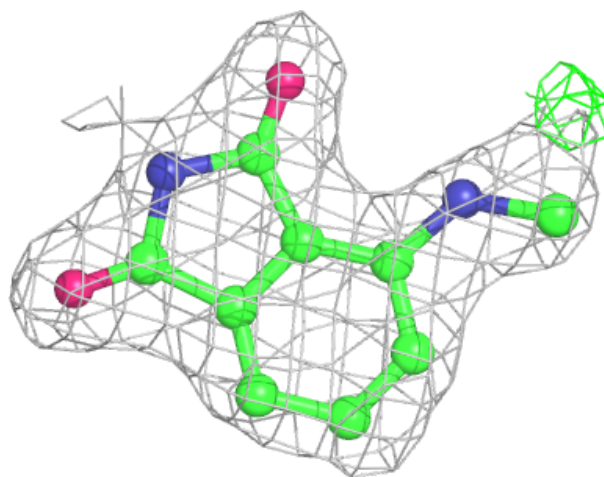
**Electron density around VXS A 203:**

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



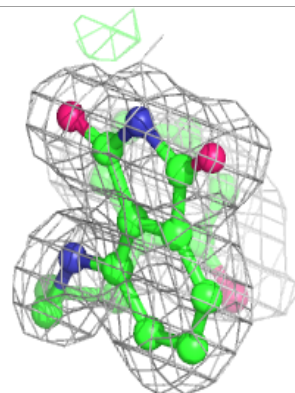
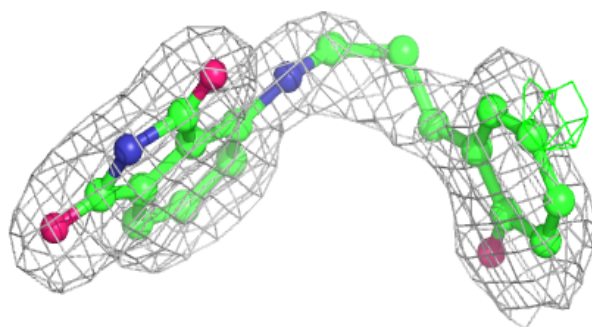
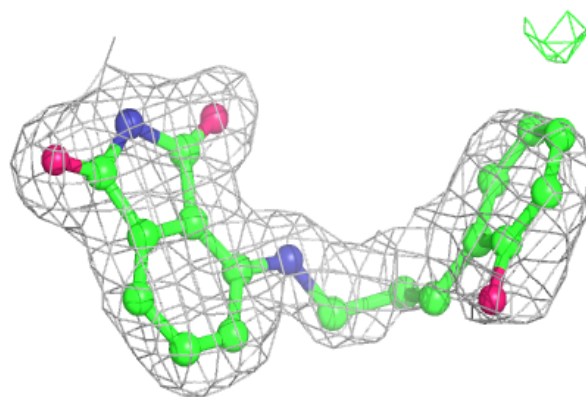
**Electron density around VXS L 202:**

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

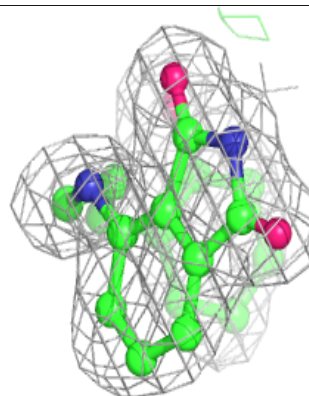
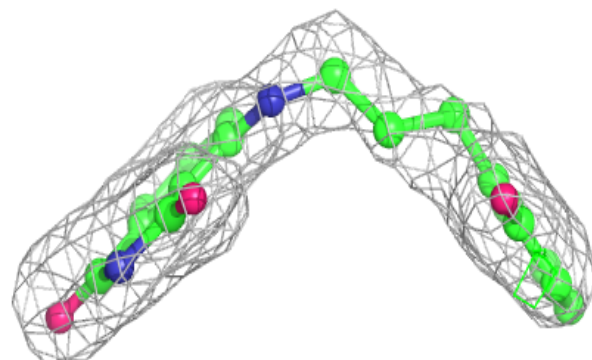
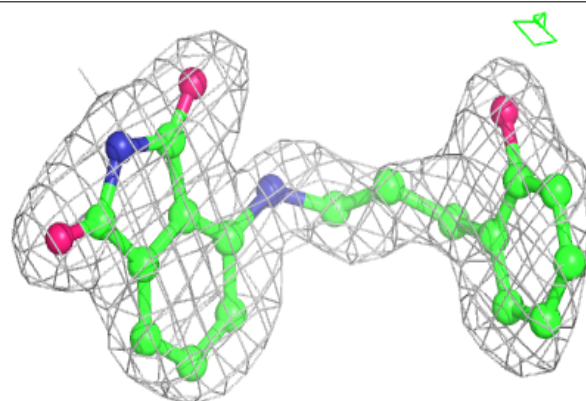


**Electron density around VXS D 203 (A):**

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

**Electron density around VXS D 203 (B):**

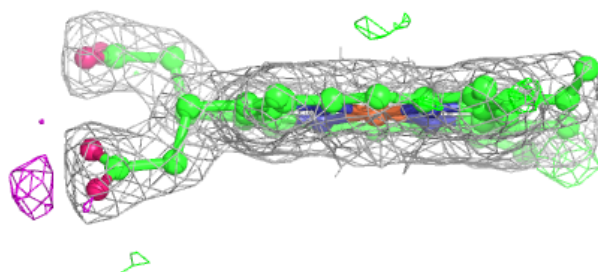
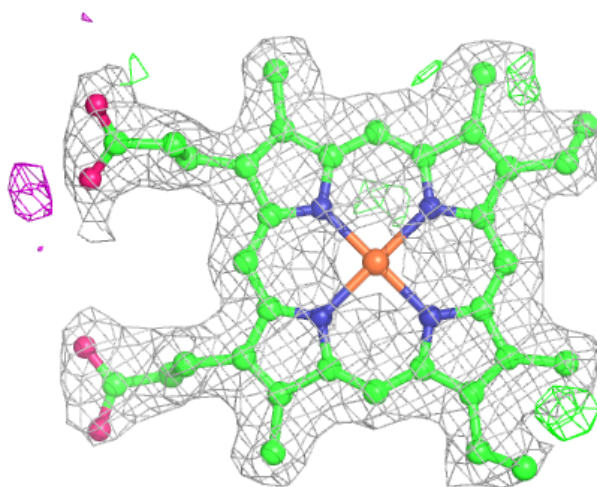
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





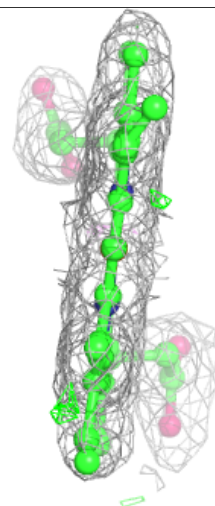
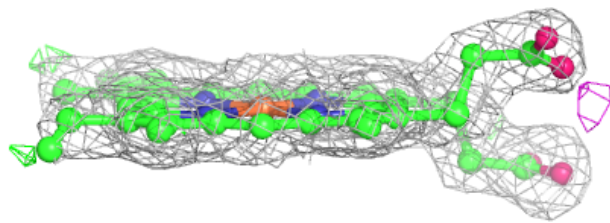
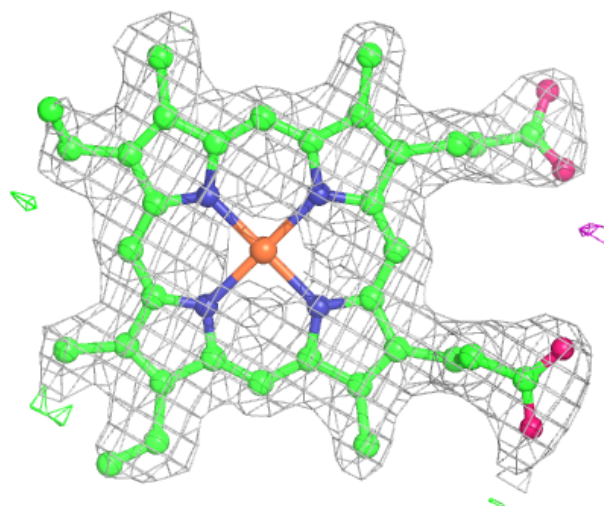
**Electron density around HEM H 201:**

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



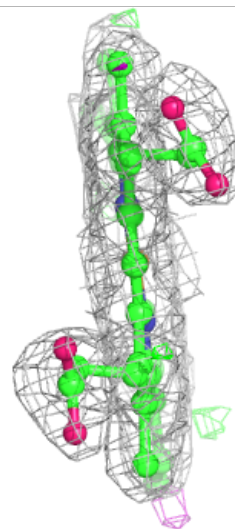
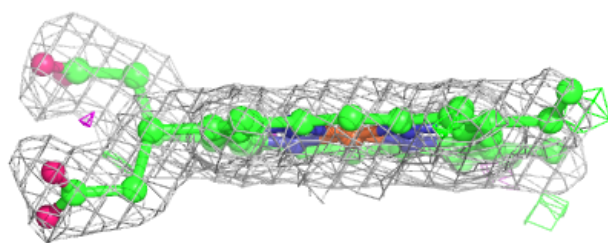
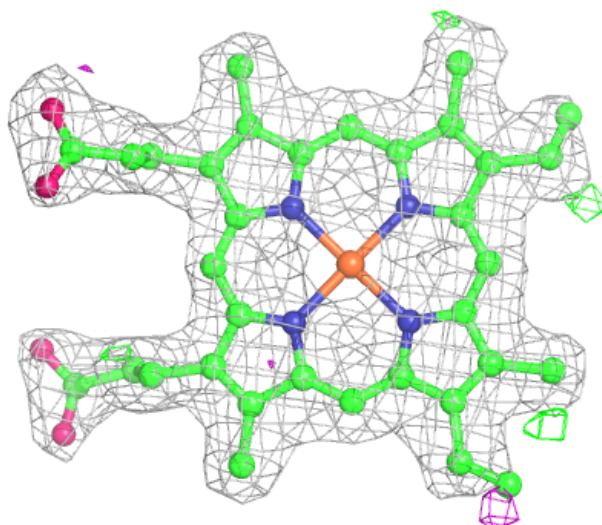
**Electron density around HEM A 202:**

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



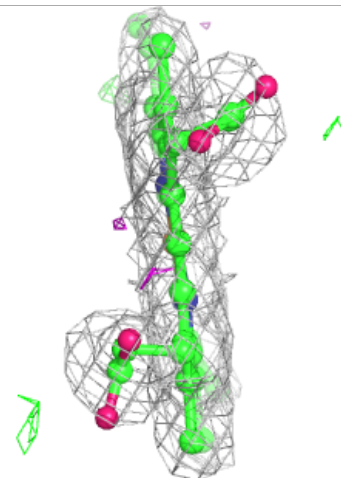
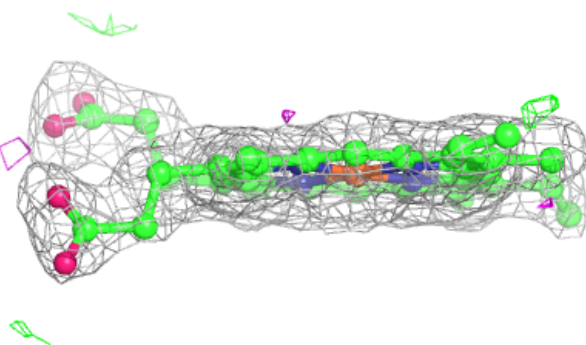
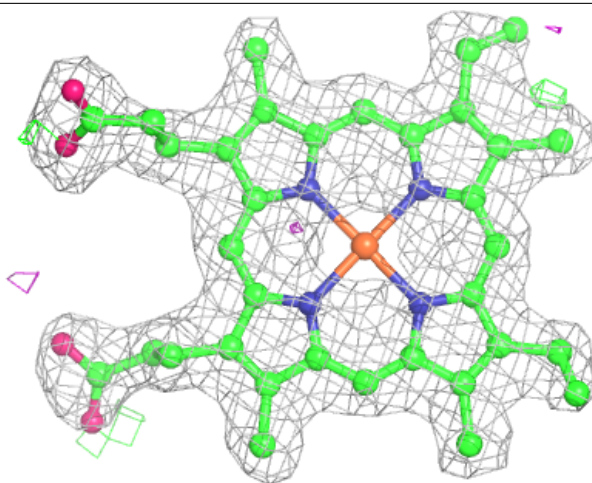
**Electron density around HEM E 201:**

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



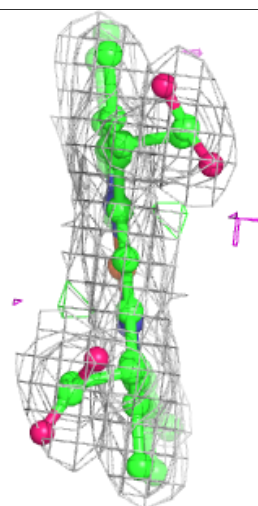
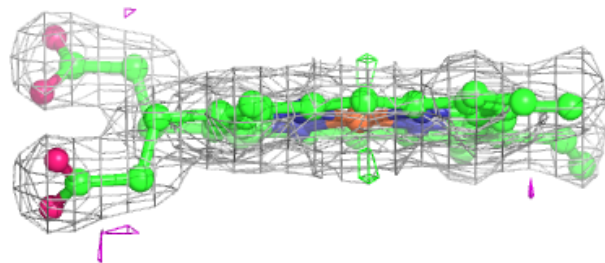
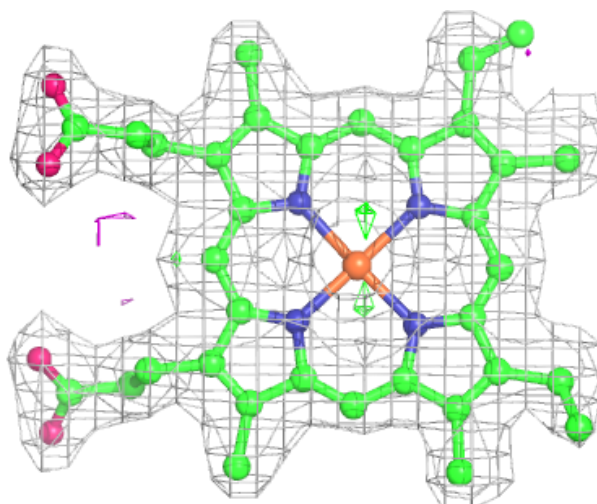
**Electron density around HEM C 201:**

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



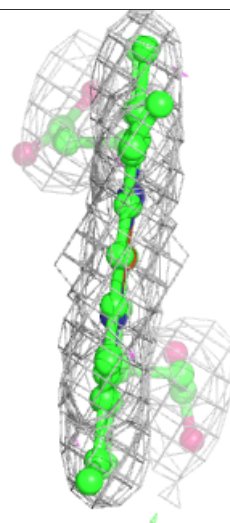
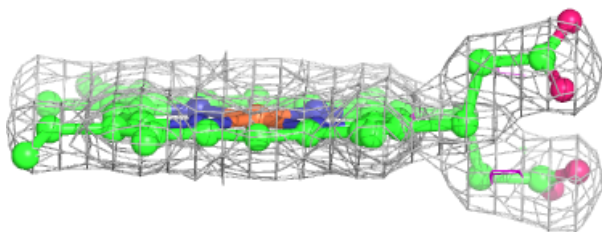
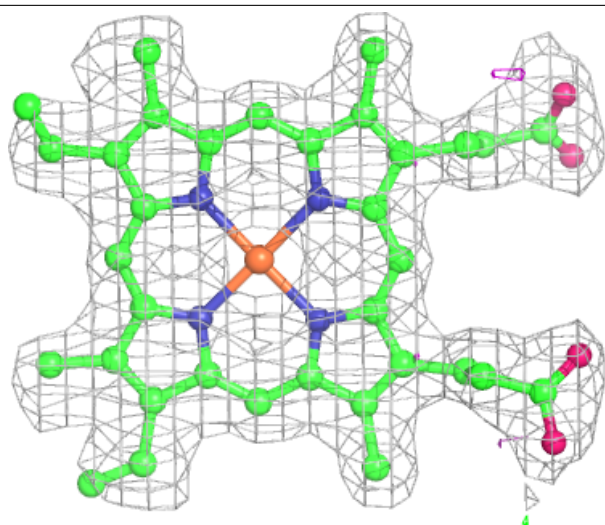
**Electron density around HEM L 201:**

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

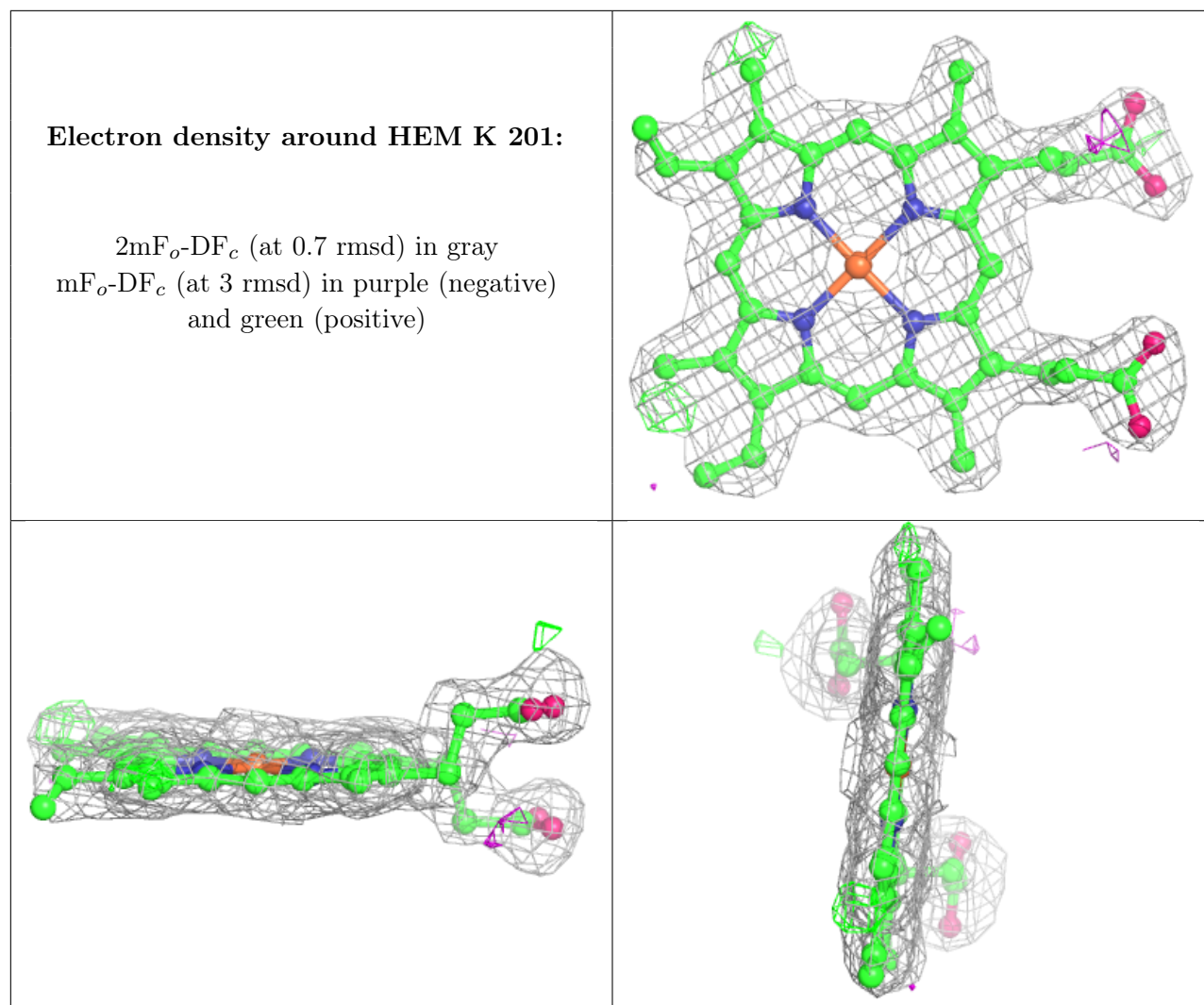


**Electron density around HEM D 202:**

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







## 6.5 Other polymers ⓘ

There are no such residues in this entry.