



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 05:49 PM UTC

PDB ID : 7K5E / pdb_00007k5e
Title : 1.75 Å resolution structure of WT BfrB from *Pseudomonas aeruginosa* in complex with a protein-protein interaction inhibitor JAG-5-7
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 : 1.75 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

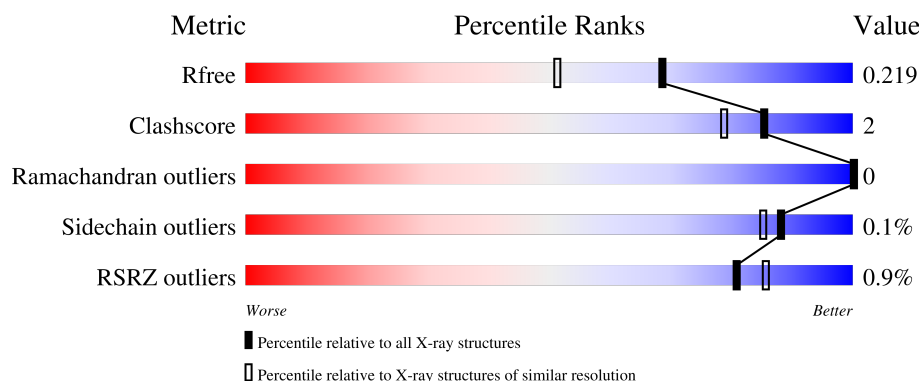
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 Å.

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



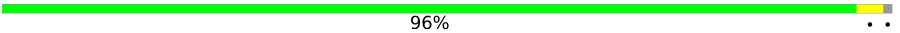
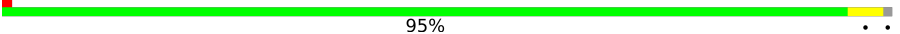
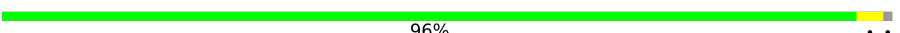
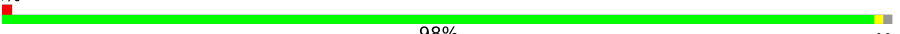
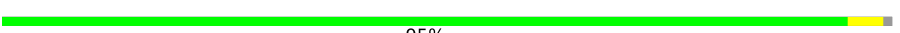
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	158	% 97% ..
1	B	158	% 95% ..
1	C	158	% 95% ..
1	D	158	% 96% ..

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Mol	Chain	Length	Quality of chain
1	E	158	 96% . .
1	F	158	 95% . .
1	G	158	 92% 6% .
1	H	158	 96% . .
1	I	158	 98% . .
1	J	158	 95% . .
1	K	158	 94% . .
1	L	158	 91% 8% .

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	VXM	C	202	-	X	-	-
4	VXM	D	203	-	X	-	-
4	VXM	E	201	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17271 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Ferroxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	156	Total	C	N	O	S	0	2	0
			1278	808	216	247	7			
1	B	156	Total	C	N	O	S	0	2	0
			1277	807	216	247	7			
1	C	156	Total	C	N	O	S	0	1	0
			1271	803	217	244	7			
1	D	156	Total	C	N	O	S	0	1	0
			1277	807	217	246	7			
1	E	156	Total	C	N	O	S	0	2	0
			1271	804	215	245	7			
1	F	156	Total	C	N	O	S	0	2	0
			1277	807	216	247	7			
1	G	156	Total	C	N	O	S	0	3	0
			1289	814	221	247	7			
1	H	156	Total	C	N	O	S	0	2	0
			1279	808	218	246	7			
1	I	156	Total	C	N	O	S	0	2	0
			1282	810	219	246	7			
1	J	156	Total	C	N	O	S	0	2	0
			1286	813	220	246	7			
1	K	156	Total	C	N	O	S	0	2	0
			1289	815	221	246	7			
1	L	156	Total	C	N	O	S	0	2	0
			1283	810	218	248	7			

- Molecule 2 is POTASSIUM ION (CCD ID: K) (formula: K).

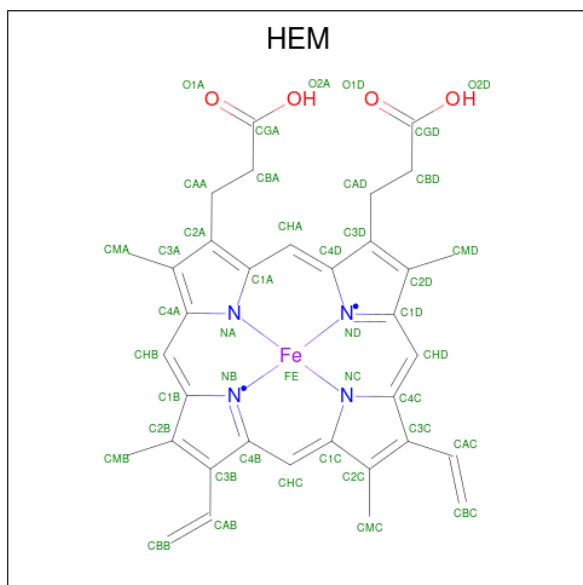
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	K	0	0
			1	1		
2	B	1	Total	K	0	0
			1	1		

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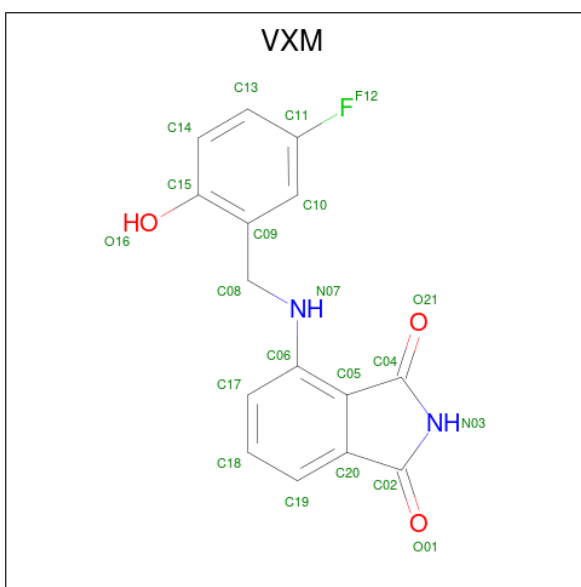
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total K 1 1	0	0

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 4 is 4-[[[(5-fluoro-2-hydroxyphenyl)methyl]amino}-1H-isoindole-1,3(2H)-dione (CCD ID: VXM) (formula: $C_{15}H_{11}FN_2O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	F	N	O	0	1
			42	30	2	4	6		
4	C	1	Total	C	N	O		0	0
			14	10	2	2			
4	D	1	Total	C	N	O		0	0
			14	10	2	2			
4	E	1	Total	C	N	O		0	0
			13	9	2	2			
4	G	1	Total	C	F	N	O	0	0
			21	15	1	2	3		
4	H	1	Total	C	F	N	O	0	1
			42	30	2	4	6		
4	I	1	Total	C	N	O		0	0
			14	10	2	2			
4	J	1	Total	C	F	N	O	0	0
			21	15	1	2	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	121	Total	O	0	0
			121	121		
5	B	100	Total	O	0	0
			100	100		
5	C	102	Total	O	0	0
			102	102		
5	D	124	Total	O	0	0
			124	124		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	123	Total 123	O 123	0	0
5	F	110	Total 110	O 110	0	0
5	G	132	Total 132	O 132	0	0
5	H	134	Total 134	O 134	0	0
5	I	132	Total 132	O 132	0	0
5	J	156	Total 156	O 156	0	0
5	K	108	Total 108	O 108	0	0
5	L	85	Total 85	O 85	0	0

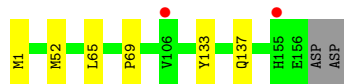
3 Residue-property plots [i](#)

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

- Molecule 1: Ferroxidase



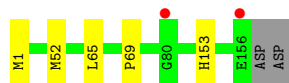
- Molecule 1: Ferroxidase



- Molecule 1: Ferroxidase



- Molecule 1: Ferroxidase



- Molecule 1: Ferroxidase



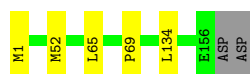
- Molecule 1: Ferroxidase



- Molecule 1: Ferroxidase



- Molecule 1: Ferroxidase



- Molecule 1: Ferroxidase



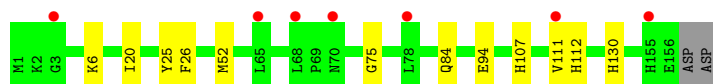
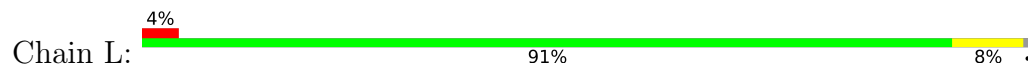
- Molecule 1: Ferroxidase



- Molecule 1: Ferroxidase



- Molecule 1: Ferroxidase



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	129.85Å 194.28Å 203.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.36 – 1.75 41.36 – 1.75	Depositor EDS
% Data completeness (in resolution range)	100.0 (41.36-1.75) 100.0 (41.36-1.75)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 1.75Å)	Xtriage
Refinement program	PHENIX 1.17rc2_3615	Depositor
R, R_{free}	0.182 , 0.213 0.192 , 0.219	Depositor DCC
R_{free} test set	12616 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	22.9	Xtriage
Anisotropy	0.756	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 37.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	17271	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.43	1/1302 (0.1%)	0.51	0/1756
1	B	0.38	0/1301	0.51	0/1755
1	C	0.46	0/1292	0.54	0/1743
1	D	0.37	0/1298	0.49	0/1750
1	E	0.42	0/1298	0.55	0/1752
1	F	0.41	0/1301	0.51	0/1755
1	G	0.38	0/1314	0.49	0/1772
1	H	0.38	0/1303	0.50	0/1757
1	I	0.40	0/1306	0.53	0/1760
1	J	0.43	0/1310	0.54	0/1764
1	K	0.39	0/1314	0.54	0/1770
1	L	0.33	0/1307	0.48	0/1762
All	All	0.40	1/15646 (0.0%)	0.52	0/21096

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	132	ASP	C-O	-6.14	1.17	1.24

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	1278	0	1236	1	0
1	B	1277	0	1234	5	0
1	C	1271	0	1230	4	0
1	D	1277	0	1238	4	0
1	E	1271	0	1228	4	0
1	F	1277	0	1234	4	0
1	G	1289	0	1249	6	0
1	H	1279	0	1243	5	0
1	I	1282	0	1252	1	0
1	J	1286	0	1263	4	0
1	K	1289	0	1261	5	0
1	L	1283	0	1247	9	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	4	0
3	B	43	0	30	5	0
3	C	43	0	30	3	0
3	D	43	0	30	1	0
3	F	43	0	30	4	0
3	H	43	0	30	5	0
3	L	43	0	30	3	0
4	B	42	0	0	2	0
4	C	14	0	0	1	0
4	D	14	0	0	1	0
4	E	13	0	0	1	0
4	G	21	0	0	1	0
4	H	42	0	0	2	0
4	I	14	0	0	1	0
4	J	21	0	0	1	0
5	A	121	0	0	0	0
5	B	100	0	0	0	0
5	C	102	0	0	0	0
5	D	124	0	0	1	0
5	E	123	0	0	1	0
5	F	110	0	0	1	0
5	G	132	0	0	1	0
5	H	134	0	0	1	0
5	I	132	0	0	0	0
5	J	156	0	0	0	0
5	K	108	0	0	1	0
5	L	85	0	0	0	0
All	All	17271	0	15125	67	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 (67) 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:H:201:HEM:HMC2	3:H:201:HEM:HBC2	1.60	0.83
3:B:202:HEM:HMC2	3:B:202:HEM:HBC2	1.71	0.72
3:H:201:HEM:HBC2	3:H:201:HEM:CMC	2.22	0.69
1:K:20:ILE:HD11	1:K:75:GLY:HA3	1.79	0.65
1:G:69:PRO:O	4:G:201:VXM:N03	2.30	0.65
1:J:69:PRO:O	4:J:201:VXM:N03	2.31	0.63
1:H:69:PRO:O	4:H:202[B]:VXM:N03	2.32	0.63
1:I:69:PRO:O	4:I:201:VXM:N03	2.32	0.62
1:C:69:PRO:O	4:C:202:VXM:N03	2.34	0.61
1:H:69:PRO:O	4:H:202[A]:VXM:N03	2.32	0.61
1:B:69:PRO:O	4:B:203[A]:VXM:N03	2.33	0.61
1:B:69:PRO:O	4:B:203[B]:VXM:N03	2.33	0.61
3:B:202:HEM:HBC2	3:B:202:HEM:CMC	2.30	0.60
1:D:69:PRO:O	4:D:203:VXM:N03	2.35	0.60
1:D:153:HIS:NE2	5:D:302:HOH:O	2.31	0.60
1:E:69:PRO:O	4:E:201:VXM:N03	2.35	0.60
3:A:202:HEM:CMB	3:A:202:HEM:HBB2	2.34	0.58
1:L:26:PHE:CD2	3:L:201:HEM:HMB3	2.39	0.57
3:C:201:HEM:HBC2	3:C:201:HEM:CMC	2.36	0.56
3:C:201:HEM:HBC2	3:C:201:HEM:HMC2	1.87	0.55
1:L:25:TYR:CZ	1:L:130:HIS:HE1	2.26	0.53
1:G:47:GLU:OE1	1:G:130[B]:HIS:CE1	2.62	0.53
3:B:202:HEM:CMB	3:B:202:HEM:HBB2	2.39	0.53
3:H:201:HEM:CMB	3:H:201:HEM:HBB2	2.40	0.52
1:E:38:LYS:NZ	5:E:305:HOH:O	2.43	0.52
1:L:25:TYR:CE2	1:L:130:HIS:HE1	2.27	0.51
3:B:202:HEM:HBB2	3:B:202:HEM:HMB1	1.94	0.50
1:H:134:LEU:HD21	5:H:314:HOH:O	2.12	0.49
3:F:201:HEM:CMB	3:F:201:HEM:HBB2	2.43	0.49
3:F:201:HEM:HMC2	3:F:201:HEM:HBC2	1.96	0.48
1:G:20:ILE:HD11	1:G:75:GLY:HA3	1.96	0.47
1:J:44:GLU:OE1	1:J:90:ASP:OD2	2.33	0.46
1:K:57:LYS:CD	5:K:267:HOH:O	2.63	0.46
1:L:25:TYR:OH	1:L:94:GLU:OE2	2.33	0.46
1:D:52:MET:HB3	3:D:202:HEM:CHD	2.47	0.45
3:A:202:HEM:HBB2	3:A:202:HEM:HMB1	1.98	0.45
1:C:1:MET:O	1:C:65:LEU:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:73:ASP:O	5:F:301:HOH:O	2.21	0.45
1:L:111:VAL:O	1:L:112:HIS:HB2	2.17	0.45
1:B:52:MET:HB3	3:B:202:HEM:CHB	2.46	0.44
1:L:20:ILE:HD11	1:L:75:GLY:HA3	1.99	0.44
3:H:201:HEM:CHB	1:J:52:MET:HB3	2.46	0.44
1:L:52:MET:HB3	3:L:201:HEM:CHD	2.48	0.44
1:K:47:GLU:OE1	1:K:130[B]:HIS:CE1	2.71	0.43
1:B:1:MET:O	1:B:65:LEU:HA	2.17	0.43
1:E:44:GLU:OE1	1:E:90:ASP:OD2	2.37	0.43
1:F:1:MET:O	1:F:65:LEU:HA	2.19	0.43
1:E:140:LEU:HD13	1:K:154:MET:HE3	2.01	0.42
1:G:134:LEU:HD21	5:G:305:HOH:O	2.18	0.42
1:L:26:PHE:CE2	3:L:201:HEM:HMB3	2.55	0.42
1:G:44:GLU:OE1	1:G:90:ASP:OD2	2.38	0.42
1:A:1:MET:O	1:A:65:LEU:HA	2.19	0.42
1:C:52:MET:HB3	3:C:201:HEM:CHD	2.50	0.42
3:A:202:HEM:HMB1	3:A:202:HEM:CBB	2.50	0.42
1:F:44:GLU:OE1	1:F:90:ASP:OD2	2.38	0.41
1:D:1:MET:O	1:D:65:LEU:HA	2.20	0.41
1:L:6:LYS:HB3	1:L:107:HIS:NE2	2.36	0.41
1:K:94:GLU:OE2	1:K:130[A]:HIS:ND1	2.51	0.41
1:F:52:MET:HB3	3:F:201:HEM:CHD	2.51	0.41
1:J:20:ILE:HD11	1:J:75:GLY:HA3	2.03	0.41
3:A:202:HEM:CMB	3:A:202:HEM:CBB	2.98	0.41
1:H:1:MET:O	1:H:65:LEU:HA	2.20	0.41
3:F:201:HEM:HBC2	3:F:201:HEM:CMC	2.51	0.40
1:B:133:TYR:O	1:B:137:GLN:HG2	2.22	0.40
1:G:1:MET:O	1:G:65:LEU:HA	2.21	0.40
1:H:52:MET:HB3	3:H:201:HEM:CHD	2.52	0.40
1:C:133:TYR:O	1:C:137:GLN:HG2	2.21	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	156/158 (99%)	155 (99%)	1 (1%)	0	100	100
1	B	156/158 (99%)	155 (99%)	1 (1%)	0	100	100
1	C	155/158 (98%)	155 (100%)	0	0	100	100
1	D	155/158 (98%)	154 (99%)	1 (1%)	0	100	100
1	E	156/158 (99%)	155 (99%)	1 (1%)	0	100	100
1	F	156/158 (99%)	156 (100%)	0	0	100	100
1	G	157/158 (99%)	157 (100%)	0	0	100	100
1	H	156/158 (99%)	155 (99%)	1 (1%)	0	100	100
1	I	156/158 (99%)	156 (100%)	0	0	100	100
1	J	156/158 (99%)	156 (100%)	0	0	100	100
1	K	156/158 (99%)	155 (99%)	1 (1%)	0	100	100
1	L	156/158 (99%)	154 (99%)	2 (1%)	0	100	100
All	All	1871/1896 (99%)	1863 (100%)	8 (0%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	137/144 (95%)	137 (100%)	0	100	100
1	B	137/144 (95%)	137 (100%)	0	100	100
1	C	136/144 (94%)	136 (100%)	0	100	100
1	D	137/144 (95%)	137 (100%)	0	100	100
1	E	136/144 (94%)	136 (100%)	0	100	100
1	F	137/144 (95%)	137 (100%)	0	100	100
1	G	139/144 (96%)	139 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	138/144 (96%)	138 (100%)	0	100	100
1	I	139/144 (96%)	139 (100%)	0	100	100
1	J	140/144 (97%)	140 (100%)	0	100	100
1	K	140/144 (97%)	140 (100%)	0	100	100
1	L	139/144 (96%)	138 (99%)	1 (1%)	76	67
All	All	1655/1728 (96%)	1654 (100%)	1 (0%)	88	85

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	84	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	9	GLN
1	B	43	HIS
1	B	84	GLN
1	B	88	GLN
1	D	88	GLN
1	D	92	ASN
1	E	88	GLN
1	E	137	GLN
1	F	137	GLN
1	G	43	HIS
1	H	88	GLN
1	H	137	GLN
1	I	84	GLN
1	I	88	GLN
1	I	137	GLN
1	J	88	GLN
1	K	88	GLN
1	K	137	GLN
1	K	155	HIS
1	L	46	HIS
1	L	112	HIS
1	L	130	HIS
1	L	137	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 20 ligands modelled in this entry, 3 are monoatomic - leaving 17 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	$\# Z > 2$
4	VXM	H	202[A]	-	23,23,23	2.65	13 (56%)	33,33,33	1.72	6 (18%)
3	HEM	H	201	1	50,50,50	1.34	6 (12%)	67,82,82	1.40	11 (16%)
4	VXM	D	203	-	15,15,23	3.31	12 (80%)	21,21,33	2.81	8 (38%)
4	VXM	J	201	-	23,23,23	2.44	12 (52%)	33,33,33	1.81	8 (24%)
3	HEM	D	202	1	50,50,50	1.46	7 (14%)	67,82,82	1.28	8 (11%)
4	VXM	B	203[B]	-	23,23,23	2.53	13 (56%)	33,33,33	1.74	6 (18%)
4	VXM	G	201	-	23,23,23	2.35	13 (56%)	33,33,33	1.89	7 (21%)
4	VXM	C	202	-	15,15,23	3.63	13 (86%)	21,21,33	2.15	7 (33%)
4	VXM	H	202[B]	-	23,23,23	2.55	12 (52%)	33,33,33	1.74	7 (21%)
3	HEM	B	202	1	50,50,50	1.44	9 (18%)	67,82,82	1.41	8 (11%)
4	VXM	I	201	-	15,15,23	3.40	9 (60%)	21,21,33	2.18	8 (38%)
3	HEM	F	201	1	50,50,50	1.40	5 (10%)	67,82,82	1.26	7 (10%)
3	HEM	L	201	1	50,50,50	1.53	8 (16%)	67,82,82	1.23	8 (11%)
3	HEM	A	202	1	50,50,50	1.44	8 (16%)	67,82,82	1.39	8 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	VXM	E	201	-	14,14,23	4.07	12 (85%)	19,20,33	2.80	7 (36%)
3	HEM	C	201	1	50,50,50	1.38	8 (16%)	67,82,82	1.33	9 (13%)
4	VXM	B	203[A]	-	23,23,23	2.55	12 (52%)	33,33,33	1.73	6 (18%)

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
4	VXM	H	202[A]	-	-	0/5/17/17	0/3/3/3
3	HEM	H	201	1	-	4/14/54/54	-
4	VXM	D	203	-	-	3/3/15/17	0/2/2/3
4	VXM	J	201	-	-	0/5/17/17	0/3/3/3
3	HEM	D	202	1	-	4/14/54/54	-
4	VXM	B	203[B]	-	-	0/5/17/17	0/3/3/3
4	VXM	G	201	-	-	2/5/17/17	0/3/3/3
4	VXM	C	202	-	-	3/3/15/17	0/2/2/3
4	VXM	H	202[B]	-	-	0/5/17/17	0/3/3/3
3	HEM	B	202	1	-	4/14/54/54	-
4	VXM	I	201	-	-	3/3/15/17	0/2/2/3
3	HEM	F	201	1	-	4/14/54/54	-
3	HEM	L	201	1	-	4/14/54/54	-
3	HEM	A	202	1	-	4/14/54/54	-
4	VXM	E	201	-	-	2/2/14/17	0/2/2/3
3	HEM	C	201	1	-	4/14/54/54	-
4	VXM	B	203[A]	-	-	0/5/17/17	0/3/3/3

All (172) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	202	VXM	C20-C02	8.56	1.60	1.48
4	I	201	VXM	C20-C02	8.24	1.60	1.48
4	E	201	VXM	C06-N07	8.21	1.52	1.37
3	L	201	HEM	FE-ND	6.01	2.13	1.94
4	E	201	VXM	C20-C02	5.99	1.57	1.48
4	E	201	VXM	C08-N07	5.76	1.54	1.45
4	H	202[A]	VXM	C20-C02	5.58	1.56	1.48
4	H	202[B]	VXM	C20-C02	5.42	1.56	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	202	VXM	C06-N07	5.38	1.51	1.37
4	D	203	VXM	C20-C02	5.26	1.56	1.48
4	D	203	VXM	C06-N07	5.23	1.51	1.37
4	I	201	VXM	C06-N07	4.72	1.49	1.37
4	B	203[B]	VXM	C20-C02	4.69	1.55	1.48
4	J	201	VXM	C20-C02	4.65	1.55	1.48
4	D	203	VXM	C04-N03	4.56	1.45	1.38
4	B	203[A]	VXM	C20-C02	4.46	1.54	1.48
4	E	201	VXM	C17-C06	4.36	1.46	1.39
3	C	201	HEM	FE-ND	4.34	2.08	1.94
3	F	201	HEM	FE-NA	4.23	2.09	1.95
4	G	201	VXM	C17-C06	4.20	1.46	1.39
3	D	202	HEM	FE-ND	4.19	2.07	1.94
4	I	201	VXM	C18-C19	4.11	1.45	1.38
3	B	202	HEM	FE-ND	4.11	2.07	1.94
4	D	203	VXM	C05-C06	4.08	1.49	1.41
4	C	202	VXM	C17-C06	4.05	1.46	1.39
3	L	201	HEM	FE-NC	4.05	2.08	1.95
4	G	201	VXM	C20-C02	3.92	1.54	1.48
4	H	202[A]	VXM	C15-C09	3.91	1.45	1.40
4	H	202[B]	VXM	C15-C09	3.90	1.45	1.40
4	I	201	VXM	C17-C06	3.87	1.46	1.39
4	D	203	VXM	C02-N03	3.85	1.44	1.38
4	J	201	VXM	C18-C19	3.83	1.45	1.38
4	E	201	VXM	C04-N03	3.82	1.44	1.38
4	B	203[B]	VXM	C02-N03	3.80	1.44	1.38
4	H	202[A]	VXM	C06-N07	3.80	1.47	1.37
4	J	201	VXM	C17-C06	3.78	1.45	1.39
4	H	202[B]	VXM	C06-N07	3.76	1.47	1.37
4	C	202	VXM	C18-C19	3.75	1.45	1.38
3	H	201	HEM	FE-ND	3.74	2.06	1.94
4	B	203[A]	VXM	C15-C09	3.72	1.45	1.40
4	B	203[A]	VXM	C02-N03	3.64	1.44	1.38
3	A	202	HEM	FE-NA	3.63	2.07	1.95
3	D	202	HEM	FE-NB	3.60	2.06	1.94
4	H	202[A]	VXM	C17-C06	3.59	1.45	1.39
4	H	202[B]	VXM	C17-C06	3.57	1.45	1.39
4	B	203[A]	VXM	C06-N07	3.56	1.46	1.37
4	G	201	VXM	C18-C19	3.54	1.45	1.38
4	H	202[A]	VXM	C18-C19	3.54	1.45	1.38
4	J	201	VXM	C15-C09	3.53	1.44	1.40
4	E	201	VXM	C18-C19	3.51	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	203[A]	VXM	C17-C06	3.51	1.45	1.39
4	H	202[B]	VXM	C18-C19	3.47	1.44	1.38
4	E	201	VXM	C05-C06	3.44	1.48	1.41
4	B	203[B]	VXM	C17-C06	3.43	1.45	1.39
4	I	201	VXM	C18-C17	3.41	1.44	1.38
3	D	202	HEM	FE-NA	3.40	2.06	1.95
4	C	202	VXM	C18-C17	3.39	1.44	1.38
4	B	203[B]	VXM	C15-C09	3.35	1.44	1.40
3	A	202	HEM	FE-ND	3.35	2.05	1.94
4	D	203	VXM	C18-C19	3.34	1.44	1.38
4	B	203[B]	VXM	C18-C19	3.33	1.44	1.38
4	B	203[B]	VXM	C06-N07	3.33	1.46	1.37
4	B	203[A]	VXM	C18-C19	3.28	1.44	1.38
4	B	203[B]	VXM	C04-N03	3.27	1.43	1.38
4	D	203	VXM	C17-C06	3.26	1.45	1.39
3	B	202	HEM	FE-NB	3.21	2.04	1.94
3	B	202	HEM	FE-NC	3.21	2.05	1.95
4	B	203[A]	VXM	C04-N03	3.20	1.43	1.38
4	G	201	VXM	C06-N07	3.15	1.45	1.37
4	E	201	VXM	C18-C17	3.10	1.44	1.38
4	D	203	VXM	C20-C05	3.06	1.46	1.40
4	J	201	VXM	C06-N07	3.03	1.45	1.37
4	J	201	VXM	C14-C13	3.01	1.43	1.38
3	F	201	HEM	FE-NB	3.01	2.04	1.94
4	B	203[B]	VXM	C14-C13	3.00	1.43	1.38
3	D	202	HEM	FE-NC	3.00	2.05	1.95
3	A	202	HEM	FE-NC	3.00	2.05	1.95
4	E	201	VXM	C02-N03	2.98	1.43	1.38
3	A	202	HEM	CAC-C3C	2.96	1.55	1.47
4	H	202[B]	VXM	C14-C13	2.93	1.43	1.38
4	G	201	VXM	C18-C17	2.93	1.43	1.38
3	L	201	HEM	CAC-C3C	2.92	1.55	1.47
4	I	201	VXM	C05-C06	2.91	1.47	1.41
4	J	201	VXM	C10-C09	2.91	1.44	1.39
3	D	202	HEM	CAB-C3B	2.90	1.55	1.47
4	H	202[B]	VXM	C08-C09	2.90	1.60	1.51
3	H	201	HEM	FE-NA	2.90	2.04	1.95
4	C	202	VXM	C09-C08	2.89	1.66	1.48
3	D	202	HEM	CAC-C3C	2.88	1.55	1.47
4	G	201	VXM	C15-C09	2.88	1.44	1.40
3	C	201	HEM	CAB-C3B	2.88	1.55	1.47
4	B	203[A]	VXM	C14-C13	2.87	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	202[A]	VXM	C14-C13	2.85	1.43	1.38
3	A	202	HEM	FE-NB	2.85	2.03	1.94
4	H	202[A]	VXM	C18-C17	2.85	1.43	1.38
4	H	202[A]	VXM	C10-C09	2.83	1.43	1.39
4	H	202[B]	VXM	C18-C17	2.82	1.43	1.38
4	C	202	VXM	C02-N03	2.82	1.42	1.38
4	H	202[A]	VXM	C08-C09	2.81	1.59	1.51
3	F	201	HEM	CAB-C3B	2.81	1.54	1.47
3	H	201	HEM	CMB-C2B	2.78	1.56	1.50
4	I	201	VXM	C20-C05	2.78	1.46	1.40
4	J	201	VXM	C18-C17	2.78	1.43	1.38
4	B	203[A]	VXM	C08-C09	2.77	1.59	1.51
3	B	202	HEM	CAB-C3B	2.73	1.54	1.47
3	L	201	HEM	CAB-C3B	2.73	1.54	1.47
3	B	202	HEM	FE-NA	2.71	2.04	1.95
3	H	201	HEM	FE-NB	2.69	2.03	1.94
4	D	203	VXM	C18-C17	2.66	1.43	1.38
4	C	202	VXM	C05-C06	2.66	1.46	1.41
4	B	203[A]	VXM	C10-C09	2.65	1.43	1.39
4	E	201	VXM	C20-C05	2.60	1.46	1.40
4	C	202	VXM	C04-N03	2.60	1.42	1.38
4	B	203[B]	VXM	F12-C11	2.59	1.42	1.36
4	B	203[B]	VXM	C10-C09	2.58	1.43	1.39
4	H	202[A]	VXM	F12-C11	2.58	1.42	1.36
3	A	202	HEM	CAB-C3B	2.58	1.54	1.47
4	C	202	VXM	C20-C05	2.57	1.45	1.40
4	G	201	VXM	C14-C13	2.57	1.43	1.38
4	B	203[A]	VXM	F12-C11	2.54	1.42	1.36
4	H	202[B]	VXM	F12-C11	2.53	1.42	1.36
4	G	201	VXM	F12-C11	2.51	1.42	1.36
3	C	201	HEM	CAC-C3C	2.50	1.54	1.47
4	G	201	VXM	C10-C09	2.49	1.43	1.39
4	E	201	VXM	C05-C04	2.49	1.57	1.49
3	F	201	HEM	CAC-C3C	2.46	1.53	1.47
4	J	201	VXM	F12-C11	2.45	1.42	1.36
4	J	201	VXM	C20-C05	2.45	1.45	1.40
3	C	201	HEM	FE-NA	2.44	2.03	1.95
4	D	203	VXM	C08-N07	2.43	1.54	1.46
3	H	201	HEM	CAC-C3C	2.42	1.53	1.47
4	I	201	VXM	C05-C04	2.41	1.56	1.49
3	A	202	HEM	CMB-C2B	2.39	1.55	1.50
4	C	202	VXM	C08-N07	2.39	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	201	HEM	FE-NC	2.37	2.03	1.95
4	E	201	VXM	C19-C20	2.37	1.43	1.39
3	H	201	HEM	CMC-C2C	2.37	1.55	1.50
4	H	202[B]	VXM	C10-C09	2.36	1.43	1.39
4	B	203[A]	VXM	C18-C17	2.32	1.42	1.38
4	H	202[A]	VXM	O16-C15	2.32	1.41	1.36
4	I	201	VXM	C09-C08	2.32	1.62	1.48
4	H	202[A]	VXM	C02-N03	2.30	1.42	1.38
4	G	201	VXM	C05-C04	2.28	1.56	1.49
4	C	202	VXM	C19-C20	2.26	1.43	1.39
3	B	202	HEM	CMD-C2D	2.26	1.55	1.50
3	L	201	HEM	CMD-C2D	2.25	1.55	1.50
4	B	203[B]	VXM	C18-C17	2.25	1.42	1.38
3	C	201	HEM	FE-NB	2.24	2.01	1.94
3	F	201	HEM	CMC-C2C	2.23	1.55	1.50
4	D	203	VXM	C05-C04	2.22	1.56	1.49
3	C	201	HEM	CMC-C2C	2.21	1.55	1.50
3	B	202	HEM	CAC-C3C	2.21	1.53	1.47
4	G	201	VXM	C20-C05	2.18	1.45	1.40
4	D	203	VXM	C09-C08	2.17	1.61	1.48
4	H	202[A]	VXM	C04-N03	2.16	1.41	1.38
3	L	201	HEM	CMA-C3A	2.15	1.55	1.50
3	B	202	HEM	CMB-C2B	2.14	1.55	1.50
4	H	202[B]	VXM	C02-N03	2.14	1.41	1.38
4	J	201	VXM	O16-C15	2.13	1.40	1.36
3	B	202	HEM	CMC-C2C	2.12	1.55	1.50
4	G	201	VXM	C10-C11	2.10	1.41	1.37
3	L	201	HEM	CMC-C2C	2.09	1.55	1.50
3	D	202	HEM	CMC-C2C	2.09	1.55	1.50
4	G	201	VXM	C08-C09	2.08	1.57	1.51
4	B	203[B]	VXM	O16-C15	2.08	1.40	1.36
4	C	202	VXM	C05-C04	2.07	1.55	1.49
4	B	203[B]	VXM	C08-C09	2.03	1.57	1.51
3	L	201	HEM	C2A-C3A	-2.03	1.33	1.38
3	A	202	HEM	CMD-C2D	2.02	1.54	1.50
3	C	201	HEM	CMA-C3A	2.02	1.54	1.50
4	J	201	VXM	C05-C04	2.01	1.55	1.49
4	H	202[B]	VXM	C04-N03	2.00	1.41	1.38

All (129) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	201	VXM	C04-N03-C02	-6.58	106.87	112.59
4	D	203	VXM	C04-N03-C02	-6.48	106.96	112.59
4	B	203[B]	VXM	C04-N03-C02	-6.32	107.10	112.59
4	B	203[A]	VXM	C04-N03-C02	-6.18	107.22	112.59
4	E	201	VXM	C20-C02-N03	5.44	110.57	105.88
4	G	201	VXM	C20-C02-N03	5.17	110.34	105.88
4	H	202[A]	VXM	C04-N03-C02	-5.17	108.09	112.59
4	C	202	VXM	C04-N03-C02	-5.04	108.21	112.59
4	H	202[B]	VXM	C04-N03-C02	-4.98	108.26	112.59
4	D	203	VXM	C06-C05-C04	4.82	134.69	129.42
4	J	201	VXM	C20-C02-N03	4.81	110.03	105.88
4	D	203	VXM	C20-C02-N03	4.78	110.00	105.88
4	D	203	VXM	C05-C06-N07	4.59	126.81	121.34
4	B	203[A]	VXM	C20-C02-N03	4.55	109.81	105.88
4	B	203[B]	VXM	C20-C02-N03	4.52	109.77	105.88
4	H	202[A]	VXM	C20-C02-N03	4.45	109.72	105.88
4	E	201	VXM	C06-C05-C04	4.44	134.28	129.42
4	H	202[B]	VXM	C20-C02-N03	4.43	109.70	105.88
4	G	201	VXM	C04-N03-C02	-4.18	108.96	112.59
4	G	201	VXM	C06-C05-C04	4.14	133.94	129.42
4	E	201	VXM	C08-N07-C06	4.02	128.72	122.37
4	J	201	VXM	C04-N03-C02	-4.00	109.11	112.59
4	I	201	VXM	C04-N03-C02	-3.93	109.17	112.59
3	A	202	HEM	C4D-ND-C1D	3.91	109.83	105.21
4	I	201	VXM	C06-C05-C04	3.89	133.67	129.42
3	B	202	HEM	C1B-NB-C4B	3.74	109.64	105.21
3	B	202	HEM	C3B-C4B-NB	-3.71	106.80	109.47
4	I	201	VXM	C20-C02-N03	3.64	109.02	105.88
4	I	201	VXM	C20-C05-C04	-3.55	104.86	108.09
4	C	202	VXM	C20-C02-N03	3.53	108.92	105.88
4	D	203	VXM	C20-C05-C04	-3.43	104.96	108.09
4	E	201	VXM	C20-C05-C04	-3.40	104.98	108.09
4	I	201	VXM	C08-N07-C06	3.37	130.30	123.22
4	C	202	VXM	C06-C05-C04	3.35	133.08	129.42
4	J	201	VXM	C06-C05-C04	3.30	133.03	129.42
4	J	201	VXM	C05-C20-C02	-3.28	105.26	108.18
3	A	202	HEM	C3D-C4D-ND	-3.17	106.69	110.17
4	C	202	VXM	C08-N07-C06	3.16	129.85	123.22
4	H	202[B]	VXM	C05-C20-C02	-3.16	105.37	108.18
4	G	201	VXM	C08-N07-C06	3.15	130.04	122.10
4	H	202[A]	VXM	C05-C20-C02	-3.11	105.41	108.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	201	HEM	C4D-ND-C1D	3.06	108.83	105.21
3	C	201	HEM	C4D-ND-C1D	3.04	108.81	105.21
3	C	201	HEM	CAA-CBA-CGA	-3.03	105.62	113.67
4	D	203	VXM	C17-C06-N07	-2.98	116.83	121.75
4	D	203	VXM	C20-C05-C06	-2.95	120.35	121.88
4	G	201	VXM	C05-C20-C02	-2.95	105.55	108.18
4	J	201	VXM	C08-N07-C06	2.93	129.50	122.10
3	A	202	HEM	C3B-C4B-NB	-2.91	107.38	109.47
3	D	202	HEM	C1B-NB-C4B	2.89	108.63	105.21
4	H	202[A]	VXM	C08-N07-C06	2.86	129.31	122.10
3	L	201	HEM	C2A-C1A-NA	-2.86	106.98	110.15
4	C	202	VXM	C20-C05-C04	-2.85	105.49	108.09
3	H	201	HEM	C4C-C3C-C2C	2.81	109.25	106.81
4	G	201	VXM	C20-C05-C06	-2.81	120.42	121.88
3	H	201	HEM	C3B-C4B-NB	-2.79	107.46	109.47
4	H	202[B]	VXM	C08-N07-C06	2.79	129.13	122.10
3	D	202	HEM	C4D-ND-C1D	2.77	108.49	105.21
4	I	201	VXM	C05-C20-C02	-2.77	105.72	108.18
3	B	202	HEM	C4D-ND-C1D	2.74	108.45	105.21
3	H	201	HEM	CHD-C4C-NC	2.71	127.41	124.45
4	G	201	VXM	C20-C05-C04	-2.71	105.62	108.09
3	F	201	HEM	C2A-C1A-NA	-2.69	107.17	110.15
3	F	201	HEM	C3D-C4D-ND	-2.67	107.25	110.17
4	C	202	VXM	C05-C20-C02	-2.67	105.81	108.18
4	D	203	VXM	C08-N07-C06	2.64	128.76	123.22
3	L	201	HEM	C4D-ND-C1D	2.63	108.32	105.21
3	B	202	HEM	C4C-C3C-C2C	2.62	109.08	106.81
3	H	201	HEM	C2A-C1A-NA	-2.61	107.25	110.15
4	B	203[B]	VXM	C05-C20-C02	-2.61	105.85	108.18
4	B	203[A]	VXM	C05-C20-C02	-2.60	105.86	108.18
3	D	202	HEM	C3B-C4B-NB	-2.56	107.63	109.47
3	C	201	HEM	C3D-C4D-ND	-2.55	107.37	110.17
4	J	201	VXM	C19-C20-C02	2.51	134.18	129.32
3	A	202	HEM	CHA-C4D-ND	2.51	127.47	124.37
4	H	202[B]	VXM	C06-C05-C04	2.50	132.16	129.42
3	H	201	HEM	CHB-C1B-NB	2.48	127.44	124.37
3	B	202	HEM	C2B-C1B-NB	-2.48	106.99	109.84
4	B	203[B]	VXM	C08-N07-C06	2.48	128.35	122.10
3	H	201	HEM	C3D-C4D-ND	-2.47	107.46	110.17
4	H	202[A]	VXM	C19-C20-C02	2.47	134.10	129.32
3	A	202	HEM	C2D-C1D-ND	-2.46	107.06	109.90
4	H	202[B]	VXM	C19-C20-C02	2.45	134.07	129.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	202	HEM	C3B-C2B-C1B	2.45	108.25	106.41
4	B	203[A]	VXM	C08-N07-C06	2.45	128.28	122.10
4	H	202[A]	VXM	C06-C05-C04	2.43	132.08	129.42
3	B	202	HEM	C3D-C4D-ND	-2.41	107.53	110.17
3	D	202	HEM	C2A-C1A-NA	-2.41	107.48	110.15
3	C	201	HEM	CHC-C4B-NB	2.38	126.98	124.42
3	C	201	HEM	C1B-NB-C4B	2.37	108.01	105.21
4	I	201	VXM	C19-C20-C02	2.37	133.90	129.32
3	A	202	HEM	C1B-NB-C4B	2.36	108.00	105.21
3	B	202	HEM	CHB-C1B-NB	2.35	127.27	124.37
3	L	201	HEM	C3D-C4D-ND	-2.35	107.60	110.17
4	H	202[B]	VXM	C08-C09-C15	2.34	123.12	119.86
3	C	201	HEM	C2A-C1A-NA	-2.34	107.56	110.15
3	H	201	HEM	CBA-CAA-C2A	-2.33	106.08	112.53
3	L	201	HEM	C1B-NB-C4B	2.32	107.96	105.21
3	D	202	HEM	C3D-C4D-ND	-2.32	107.62	110.17
3	F	201	HEM	C4D-ND-C1D	2.30	107.93	105.21
4	C	202	VXM	C19-C20-C02	2.28	133.73	129.32
3	F	201	HEM	CHC-C4B-NB	2.26	126.85	124.42
3	H	201	HEM	C4B-C3B-C2B	2.25	109.35	107.28
4	B	203[B]	VXM	C19-C20-C02	2.25	133.67	129.32
3	B	202	HEM	C2A-C1A-NA	-2.23	107.68	110.15
4	B	203[A]	VXM	C19-C20-C02	2.22	133.63	129.32
3	C	201	HEM	C2B-C1B-NB	-2.21	107.30	109.84
4	E	201	VXM	C20-C05-C06	-2.20	120.74	121.88
4	J	201	VXM	C20-C05-C06	-2.19	120.74	121.88
3	L	201	HEM	CAD-CBD-CGD	-2.18	107.89	113.67
4	B	203[B]	VXM	C06-C05-C04	2.17	131.79	129.42
4	B	203[A]	VXM	C06-C05-C04	2.16	131.78	129.42
3	A	202	HEM	CBD-CAD-C3D	-2.13	106.65	112.53
3	D	202	HEM	C2D-C1D-ND	-2.10	107.47	109.90
3	C	201	HEM	CHD-C1D-ND	2.09	126.68	124.42
3	D	202	HEM	CBD-CAD-C3D	-2.08	106.78	112.53
3	F	201	HEM	CHA-C4D-ND	2.08	126.94	124.37
3	F	201	HEM	CBA-CAA-C2A	-2.08	106.79	112.53
3	C	201	HEM	CHD-C4C-NC	2.05	126.69	124.45
4	I	201	VXM	O21-C04-N03	-2.05	119.74	125.60
4	J	201	VXM	C20-C05-C04	-2.04	106.23	108.09
4	E	201	VXM	C17-C06-N07	-2.04	118.79	121.33
3	L	201	HEM	CHC-C4B-NB	2.04	126.62	124.42
3	F	201	HEM	CHD-C4C-NC	2.02	126.66	124.45
3	A	202	HEM	CHB-C1B-NB	2.02	126.86	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	201	HEM	CHA-C1A-NA	2.02	127.52	123.86
3	L	201	HEM	C3B-C2B-C1B	2.02	107.93	106.41
3	L	201	HEM	CBA-CAA-C2A	-2.01	106.97	112.53
3	H	201	HEM	C1B-NB-C4B	2.01	107.59	105.21

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	201	VXM	C17-C06-N07-C08
4	E	201	VXM	C05-C06-N07-C08
4	D	203	VXM	C17-C06-N07-C08
4	D	203	VXM	C05-C06-N07-C08
4	C	202	VXM	C05-C06-N07-C08
4	G	201	VXM	C05-C06-N07-C08
4	I	201	VXM	C05-C06-N07-C08
4	C	202	VXM	C17-C06-N07-C08
4	G	201	VXM	C17-C06-N07-C08
4	I	201	VXM	C17-C06-N07-C08
4	I	201	VXM	C09-C08-N07-C06
4	D	203	VXM	C09-C08-N07-C06
4	C	202	VXM	C09-C08-N07-C06
3	F	201	HEM	CAA-CBA-CGA-O2A
3	A	202	HEM	CAA-CBA-CGA-O1A
3	A	202	HEM	CAD-CBD-CGD-O1D
3	C	201	HEM	CAD-CBD-CGD-O1D
3	C	201	HEM	CAD-CBD-CGD-O2D
3	H	201	HEM	CAA-CBA-CGA-O1A
3	H	201	HEM	CAD-CBD-CGD-O1D
3	F	201	HEM	CAA-CBA-CGA-O1A
3	A	202	HEM	CAA-CBA-CGA-O2A
3	A	202	HEM	CAD-CBD-CGD-O2D
3	D	202	HEM	CAD-CBD-CGD-O1D
3	D	202	HEM	CAD-CBD-CGD-O2D
3	H	201	HEM	CAA-CBA-CGA-O2A
3	C	201	HEM	CAA-CBA-CGA-O2A
3	H	201	HEM	CAD-CBD-CGD-O2D
3	B	202	HEM	CAD-CBD-CGD-O1D
3	B	202	HEM	CAD-CBD-CGD-O2D
3	C	201	HEM	CAA-CBA-CGA-O1A
3	F	201	HEM	CAD-CBD-CGD-O1D
3	F	201	HEM	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
3	L	201	HEM	CAD-CBD-CGD-O2D
3	L	201	HEM	CAD-CBD-CGD-O1D
3	D	202	HEM	CAA-CBA-CGA-O2A
3	B	202	HEM	CAA-CBA-CGA-O2A
3	D	202	HEM	CAA-CBA-CGA-O1A
3	B	202	HEM	CAA-CBA-CGA-O1A
3	L	201	HEM	CAA-CBA-CGA-O2A
3	L	201	HEM	CAA-CBA-CGA-O1A

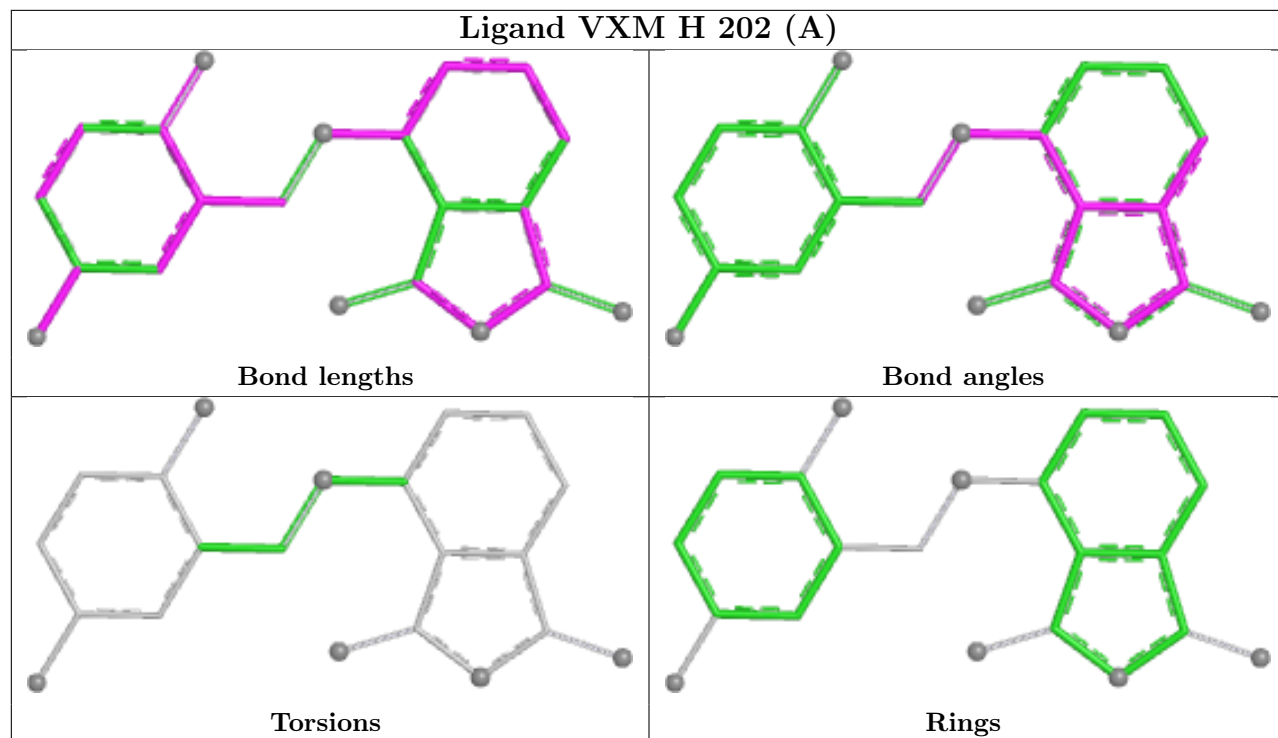
There are no ring outliers.

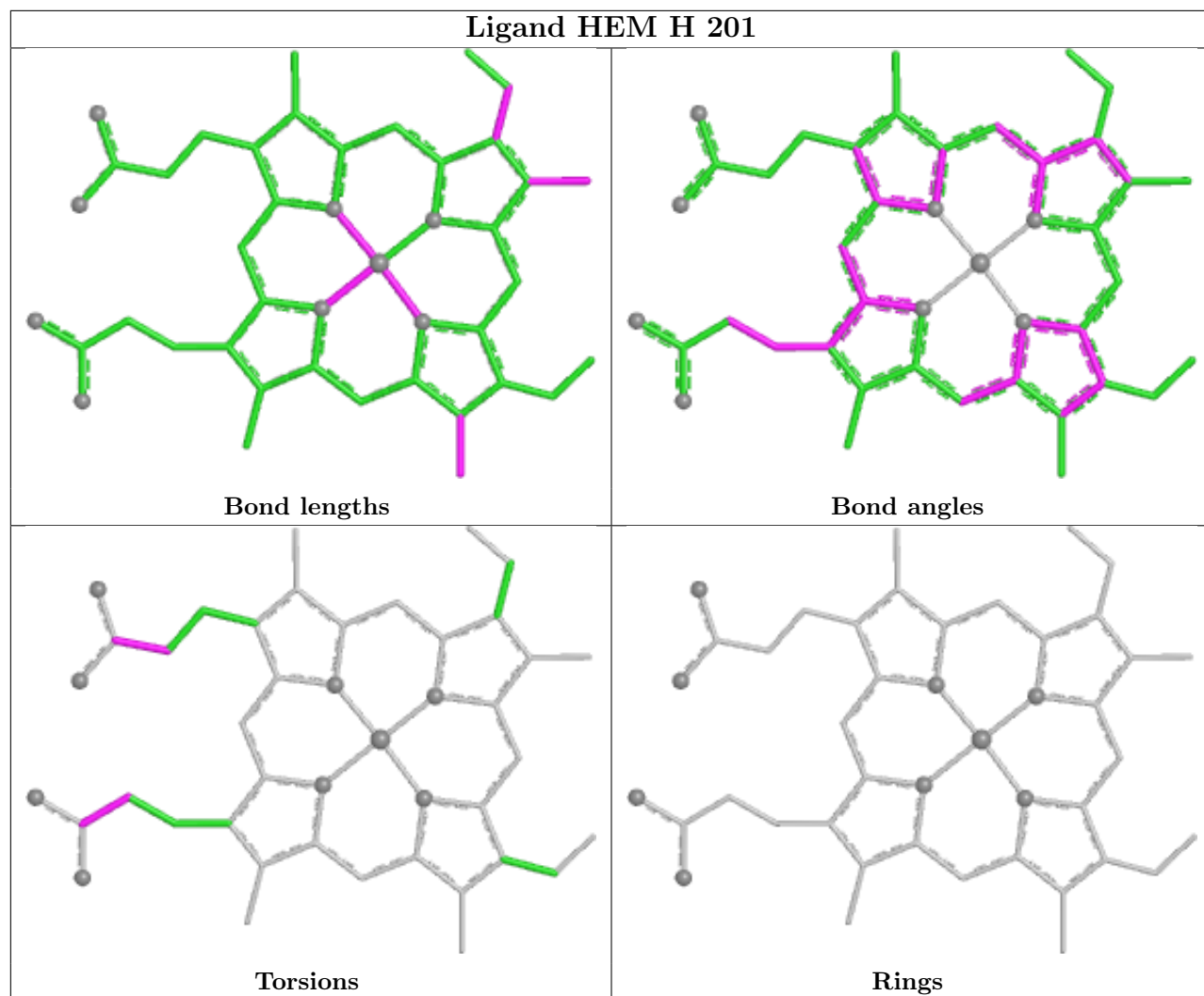
17 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	202[A]	VXM	1	0
3	H	201	HEM	5	0
4	D	203	VXM	1	0
4	J	201	VXM	1	0
3	D	202	HEM	1	0
4	B	203[B]	VXM	1	0
4	G	201	VXM	1	0
4	C	202	VXM	1	0
4	H	202[B]	VXM	1	0
3	B	202	HEM	5	0
4	I	201	VXM	1	0
3	F	201	HEM	4	0
3	L	201	HEM	3	0
3	A	202	HEM	4	0
4	E	201	VXM	1	0
3	C	201	HEM	3	0
4	B	203[A]	VXM	1	0

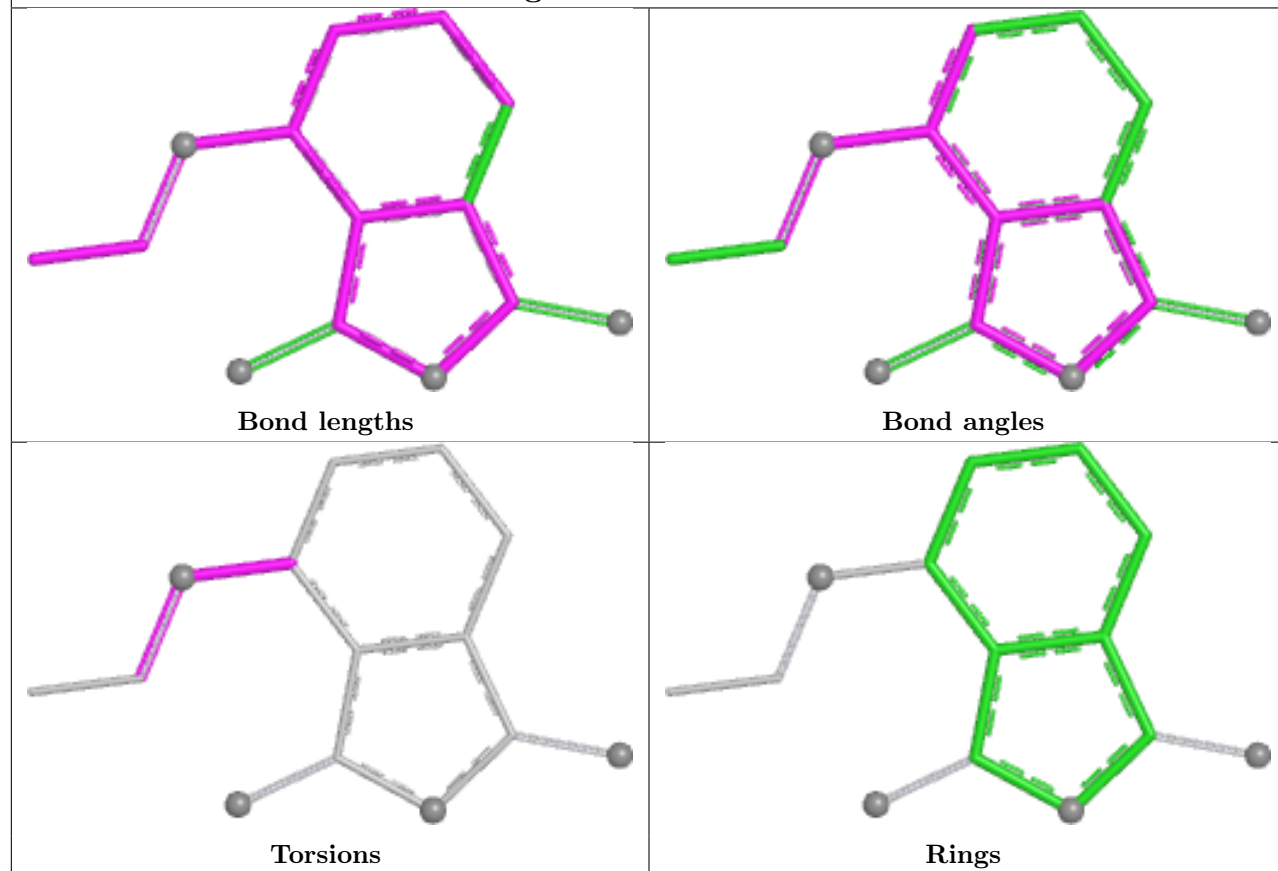
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

equivalents in the CSD to analyse the geometry.

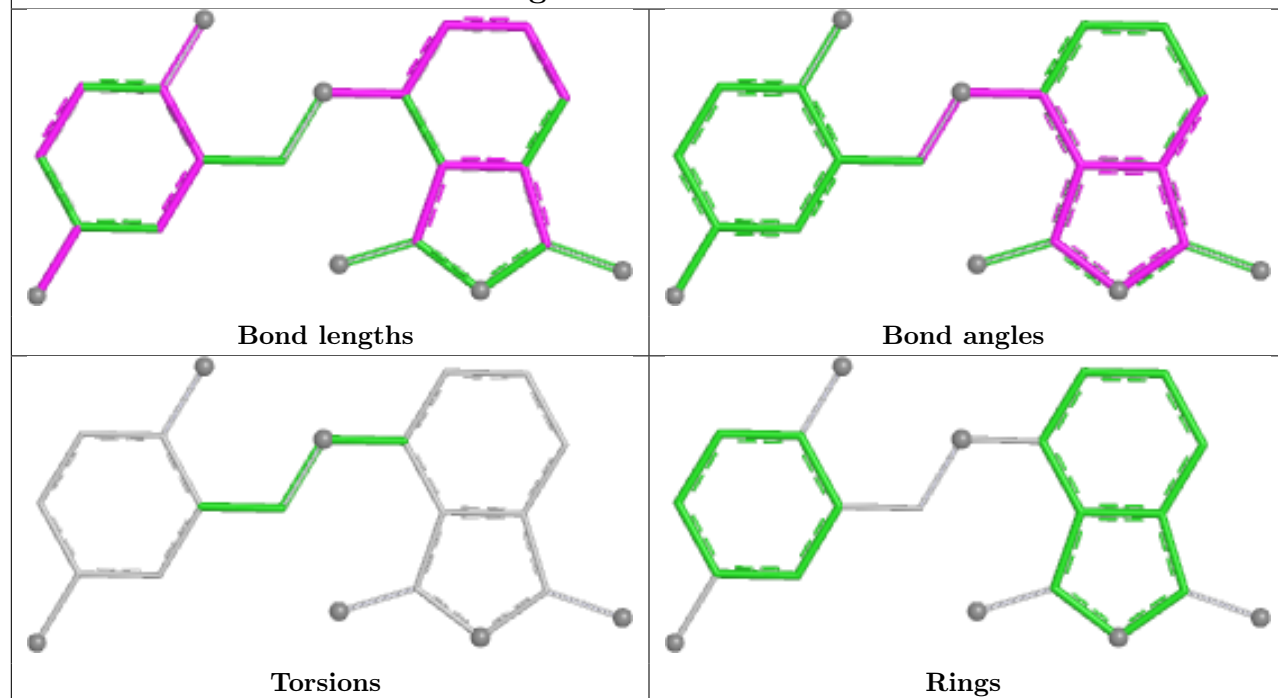


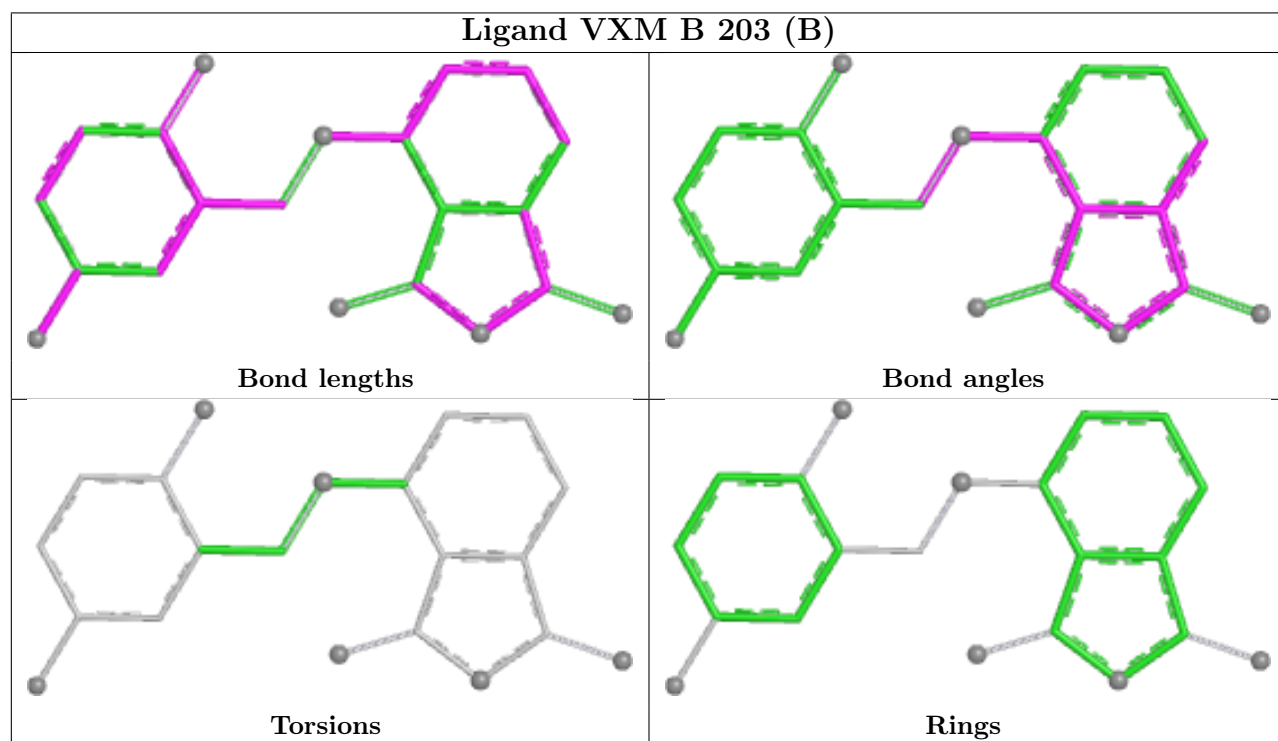
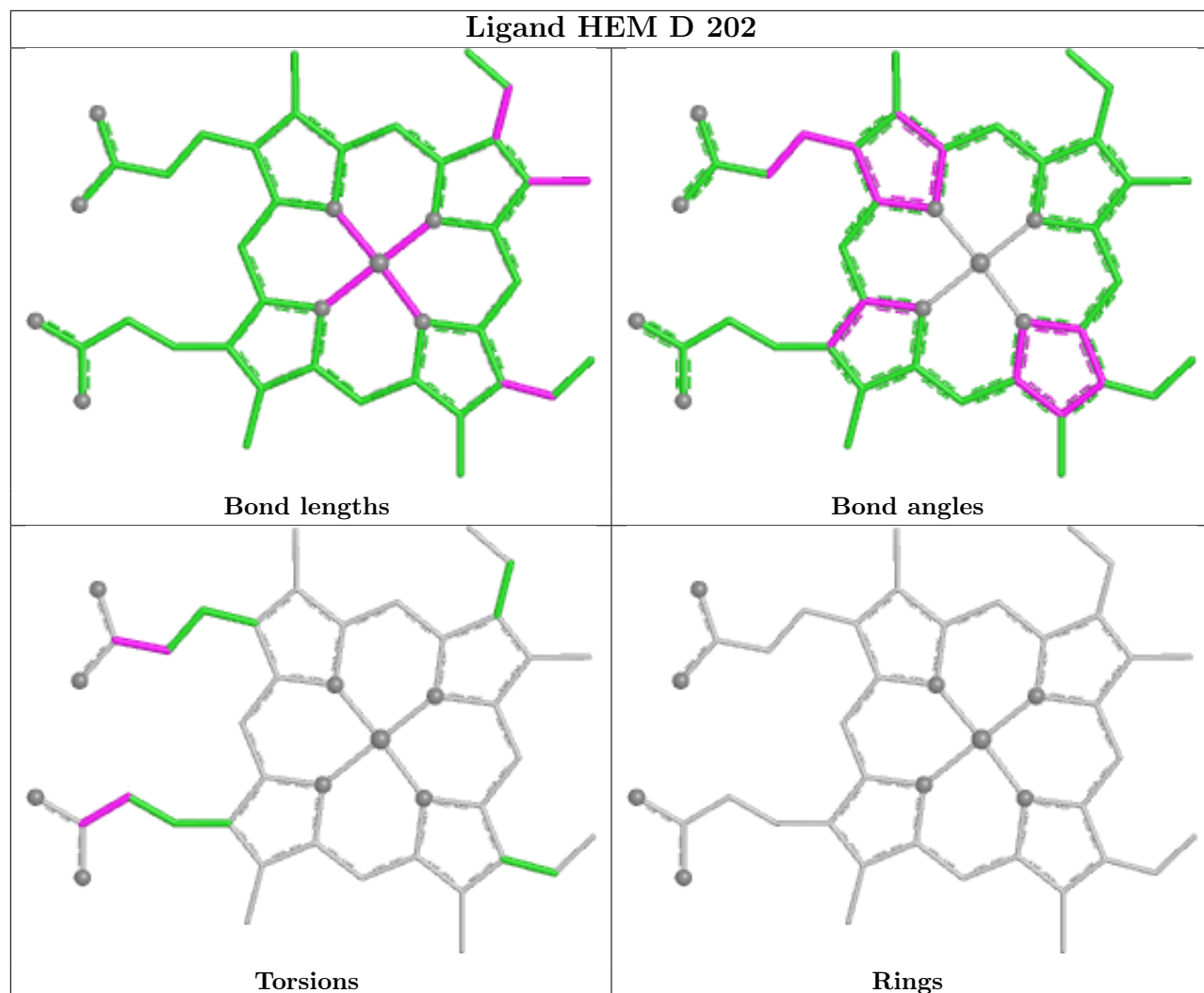


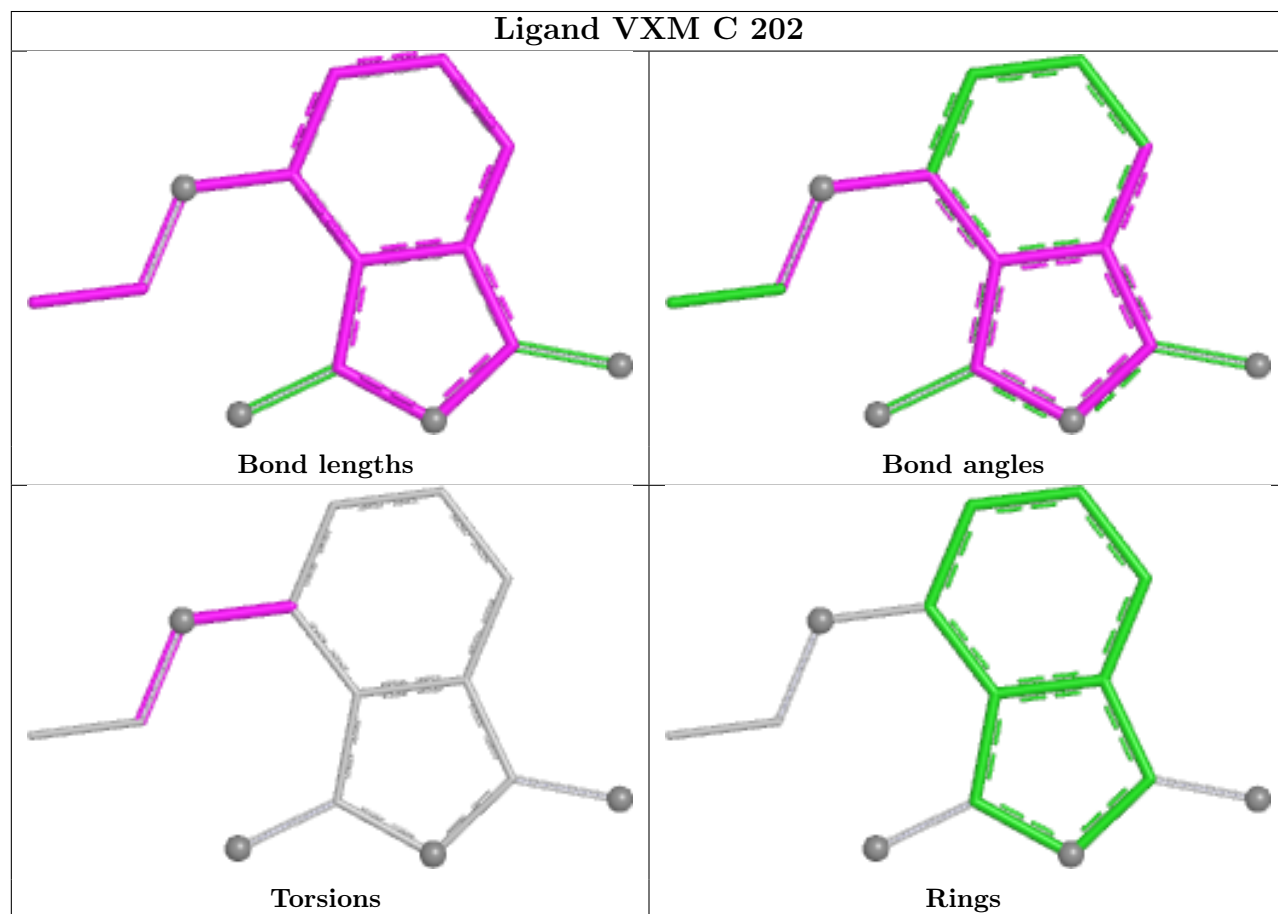
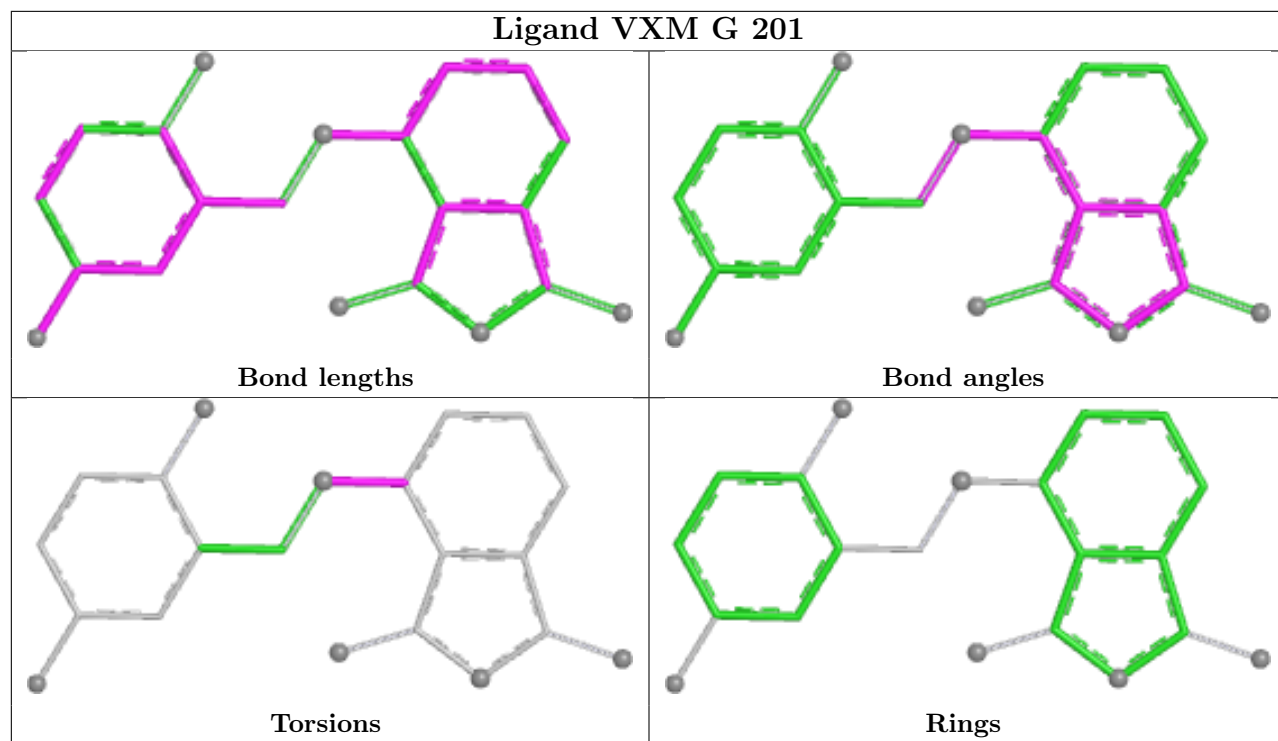
Ligand VXM D 203

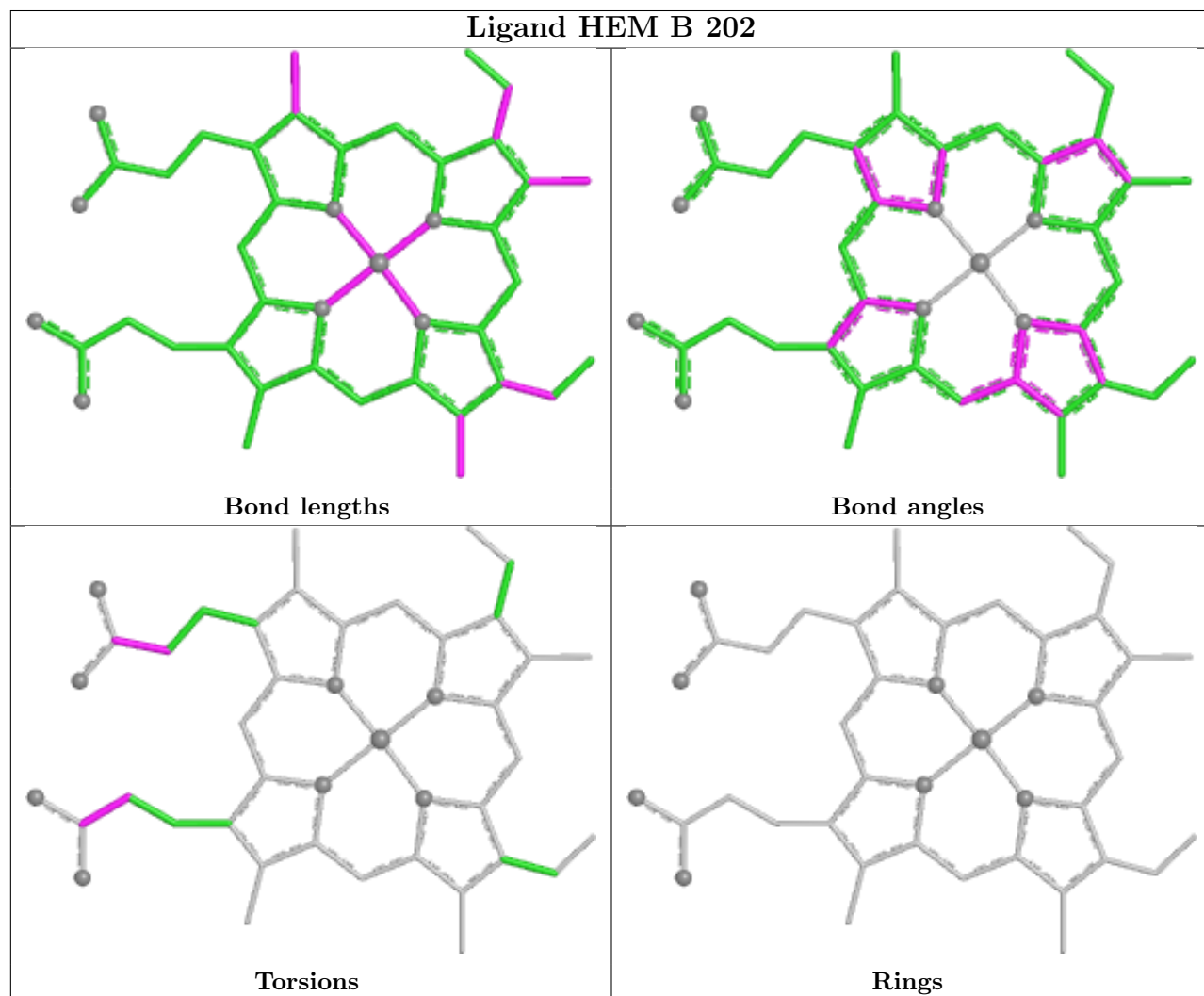
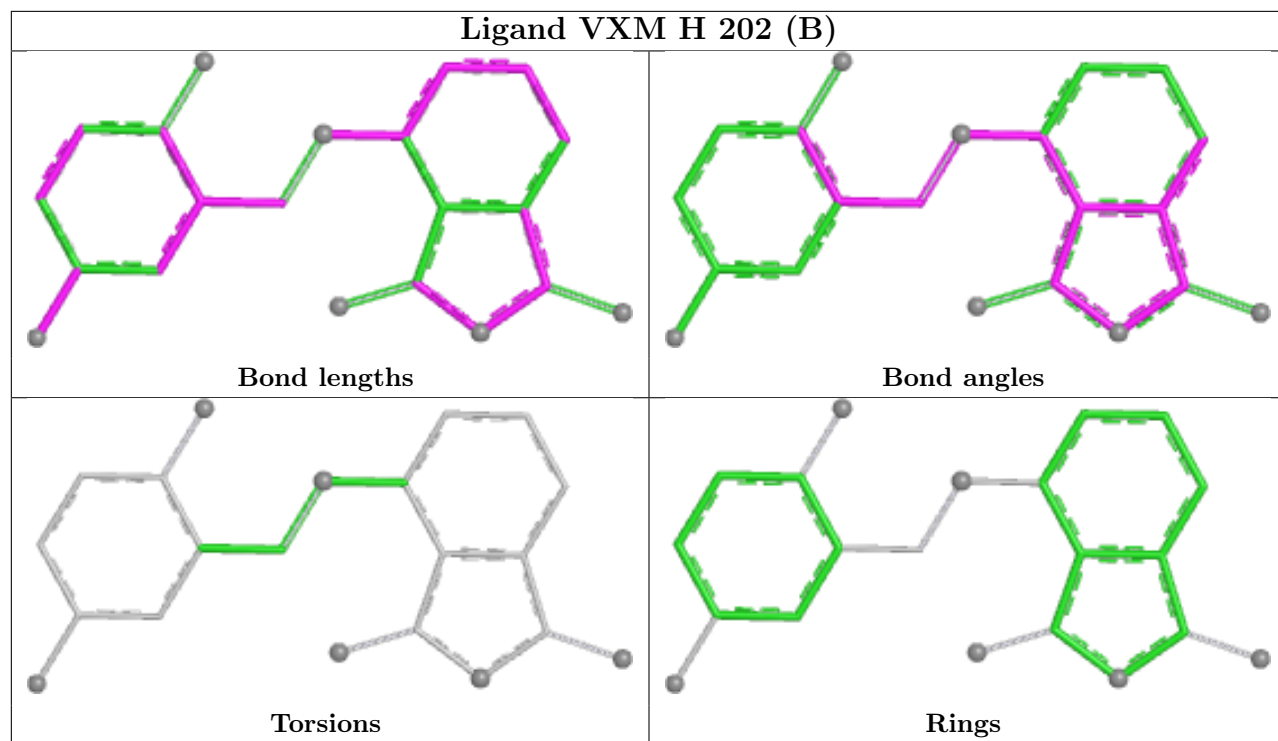


Ligand VXM J 201

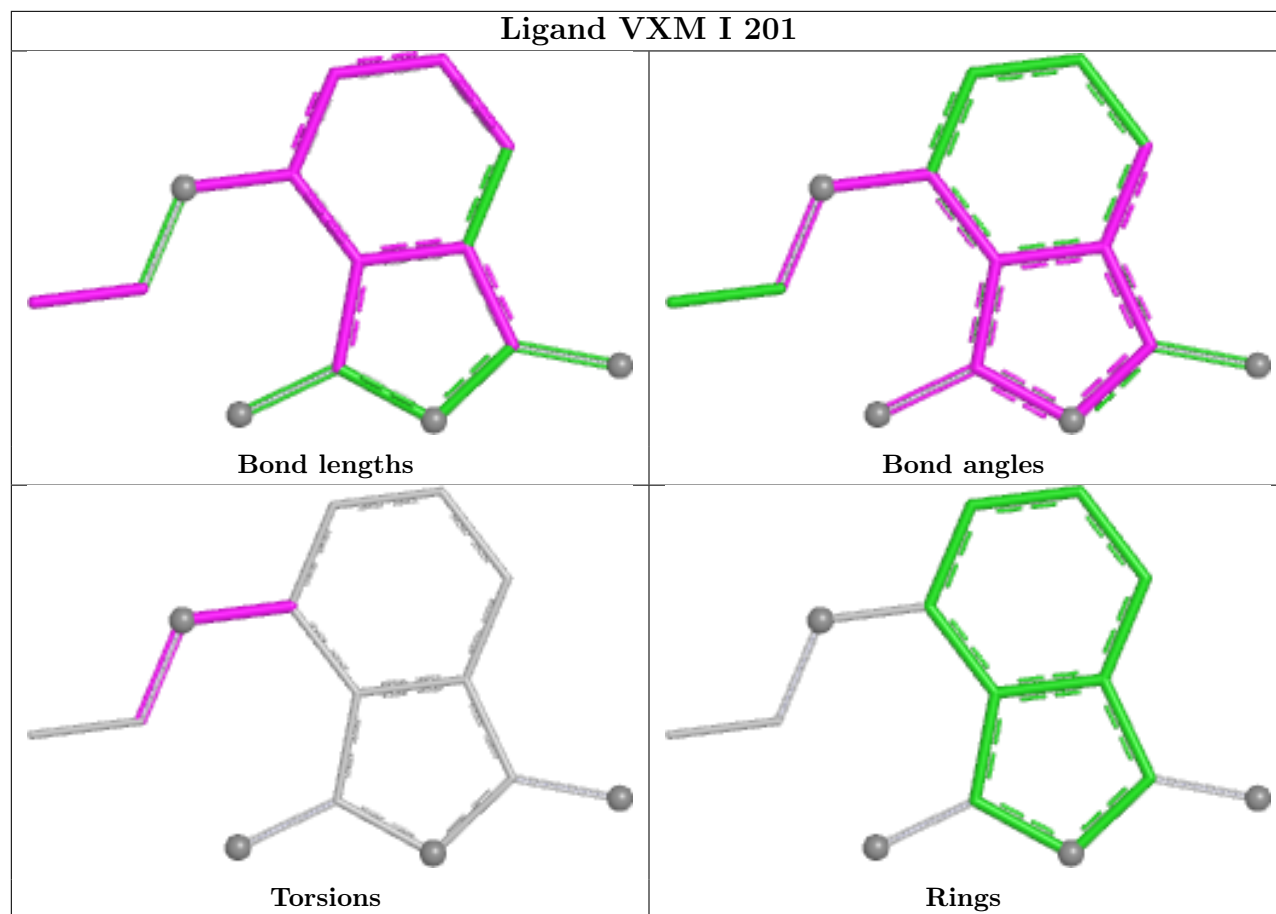


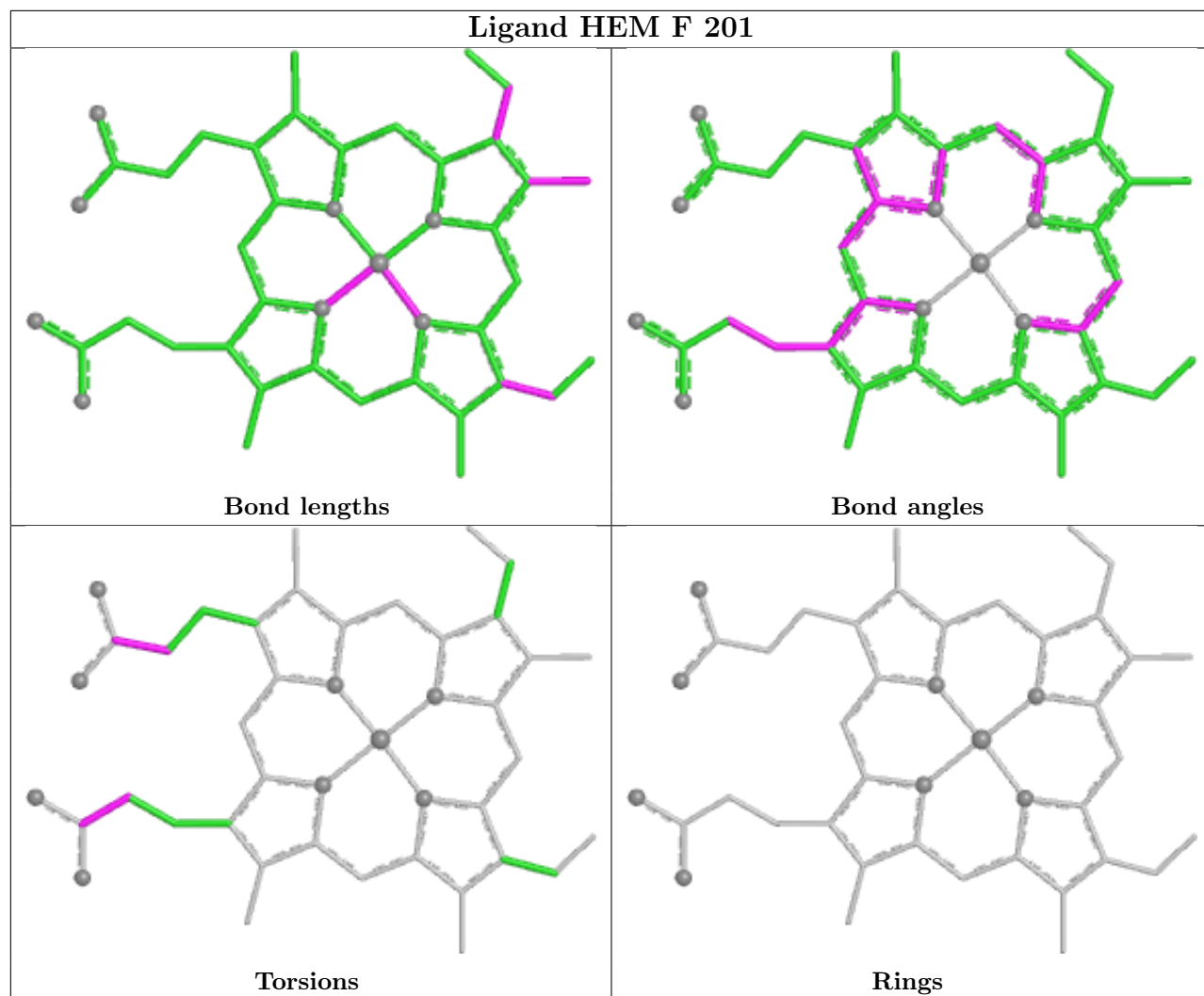


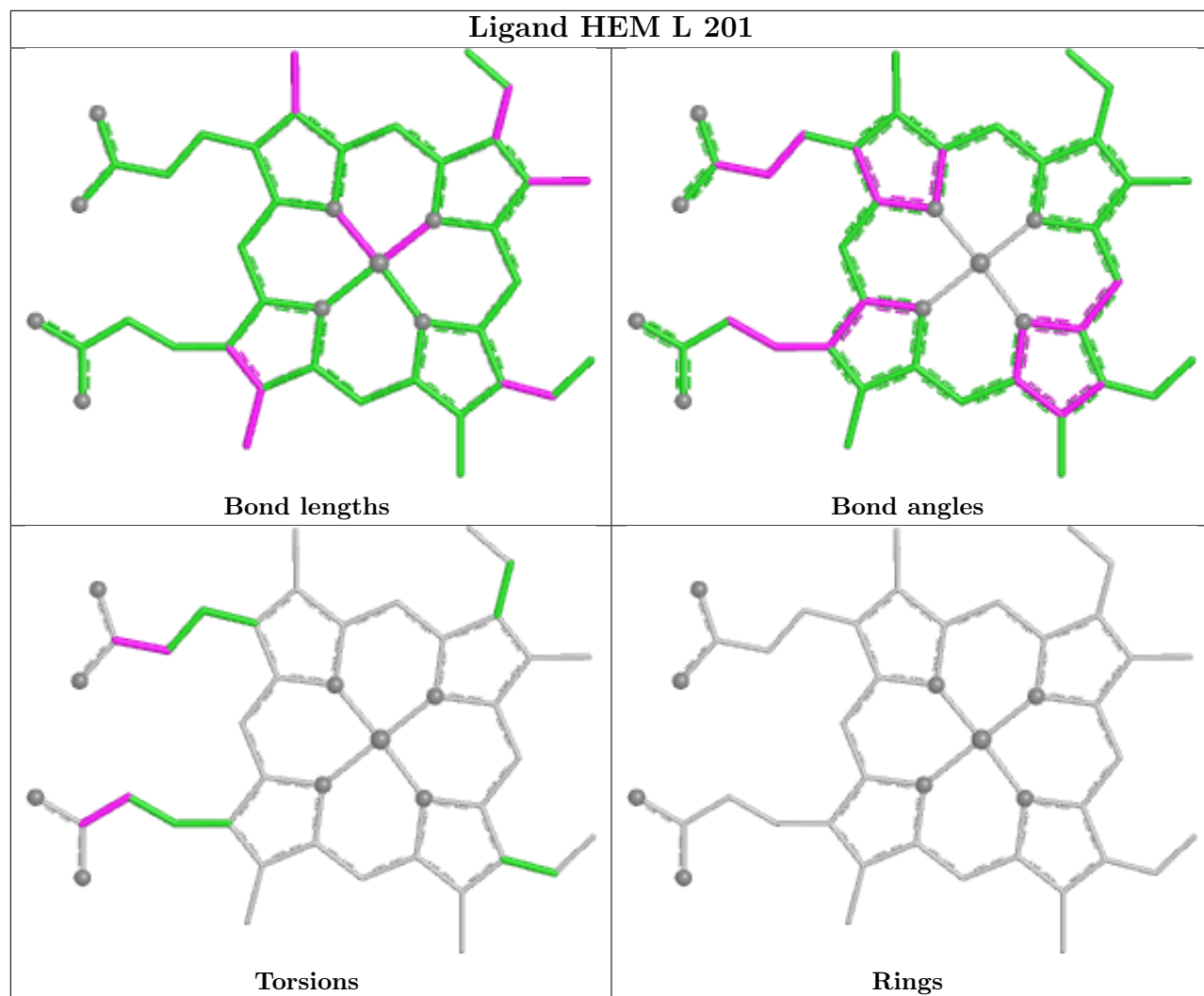


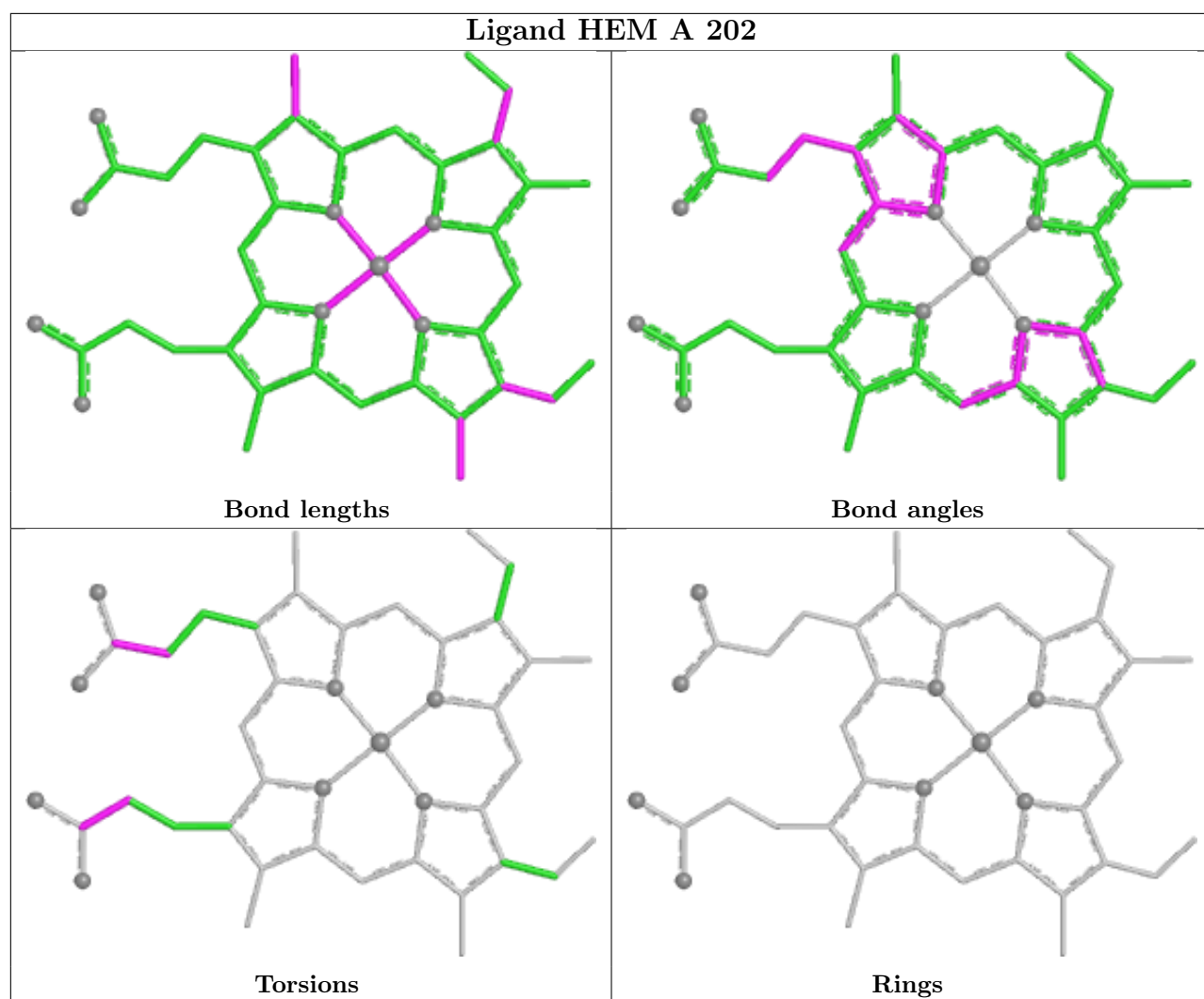


Ligand VXM I 201

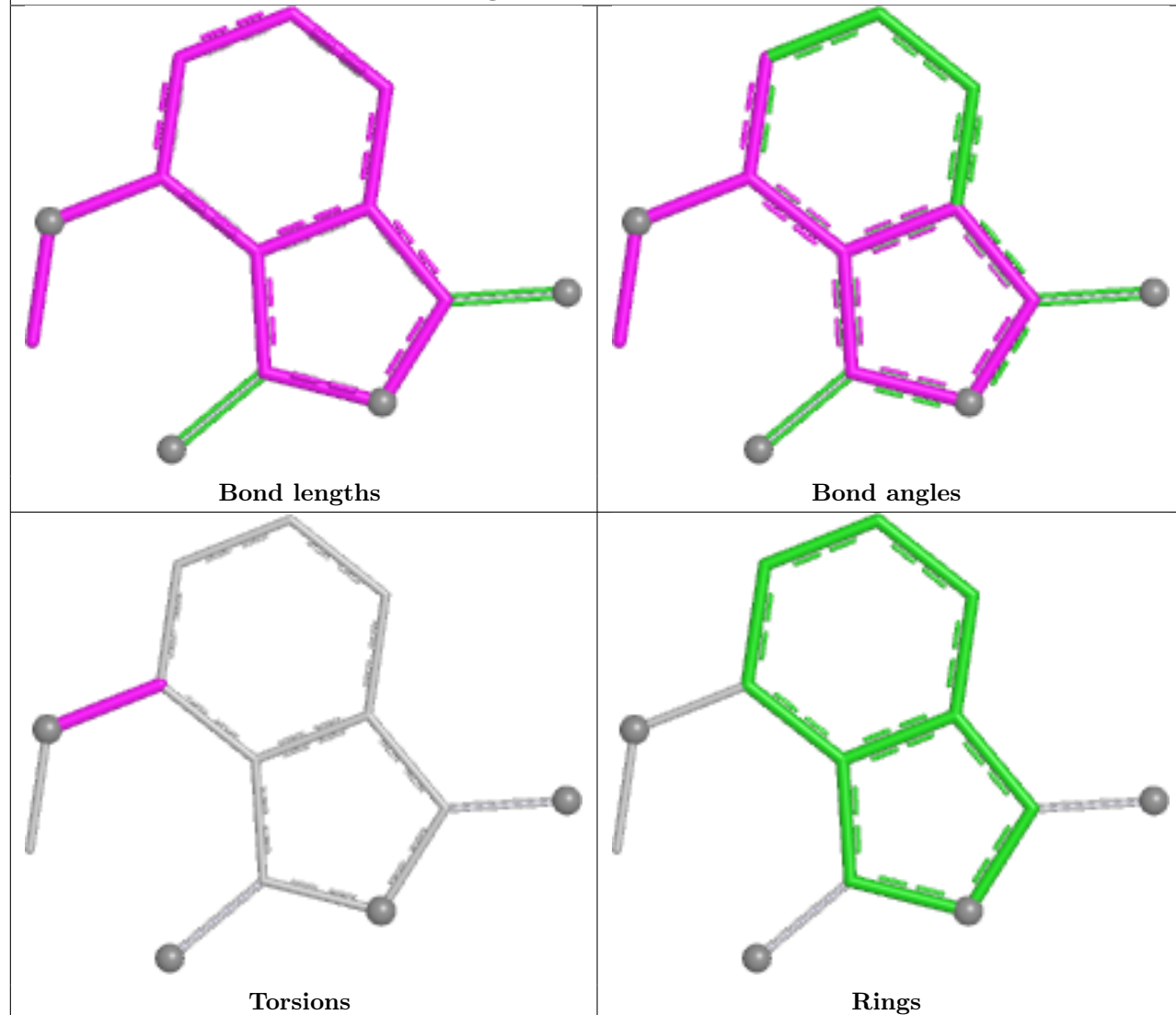


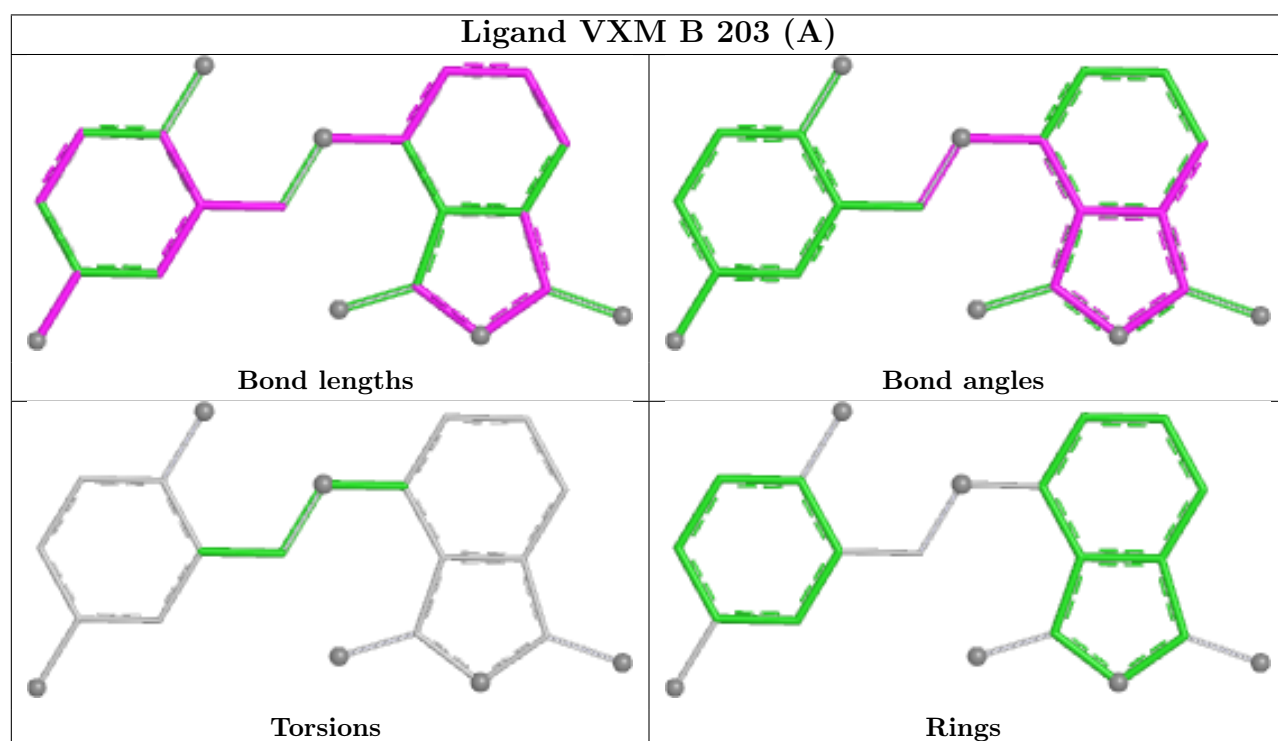
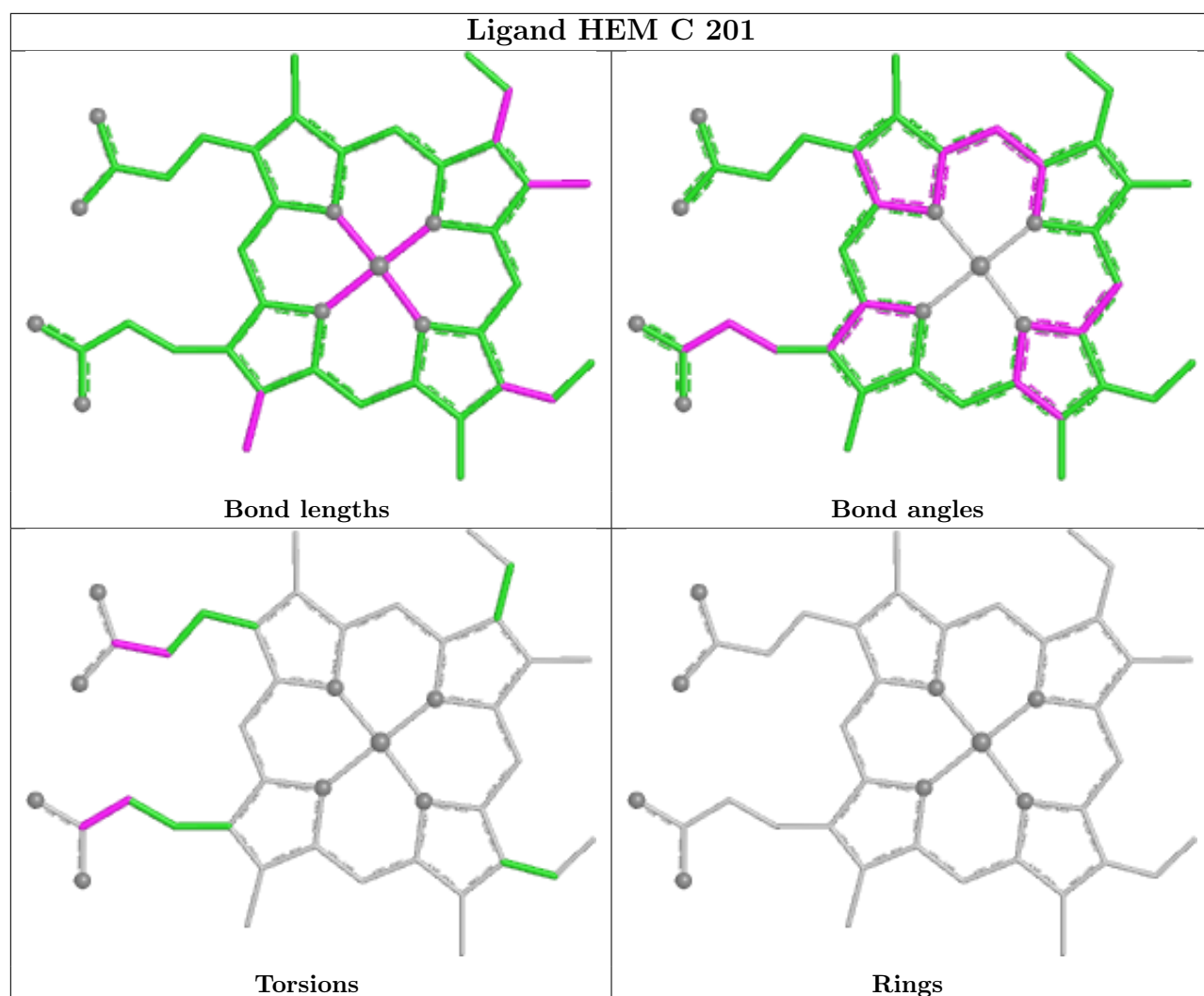






Ligand VXM E 201





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	156/158 (98%)	0.13	1 (0%) 85 89	12, 26, 37, 48	2 (1%)
1	B	156/158 (98%)	0.67	2 (1%) 75 81	13, 29, 39, 51	2 (1%)
1	C	156/158 (98%)	0.37	1 (0%) 85 89	11, 26, 37, 55	1 (0%)
1	D	156/158 (98%)	0.31	2 (1%) 75 81	12, 26, 37, 50	1 (0%)
1	E	156/158 (98%)	0.29	0 100 100	15, 25, 34, 50	2 (1%)
1	F	156/158 (98%)	0.26	1 (0%) 85 89	12, 25, 35, 52	2 (1%)
1	G	156/158 (98%)	-0.04	0 100 100	11, 25, 34, 48	3 (1%)
1	H	156/158 (98%)	-0.13	0 100 100	11, 23, 33, 48	2 (1%)
1	I	156/158 (98%)	-0.02	2 (1%) 75 81	10, 23, 33, 54	2 (1%)
1	J	156/158 (98%)	-0.32	0 100 100	10, 20, 28, 51	2 (1%)
1	K	156/158 (98%)	0.05	1 (0%) 85 89	11, 24, 37, 47	2 (1%)
1	L	156/158 (98%)	0.79	7 (4%) 38 44	14, 32, 42, 53	2 (1%)
All	All	1872/1896 (98%)	0.20	17 (0%) 81 86	10, 26, 37, 55	23 (1%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	3	GLY	3.2
1	B	106	VAL	2.6
1	L	68	LEU	2.5
1	L	65	LEU	2.5
1	I	155	HIS	2.5
1	K	155	HIS	2.4
1	L	70	ASN	2.4
1	I	156	GLU	2.4
1	B	155	HIS	2.3
1	A	7	VAL	2.3
1	D	156	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	155	HIS	2.2
1	D	80	GLY	2.1
1	C	156	GLU	2.1
1	L	78	LEU	2.1
1	L	111	VAL	2.0
1	L	155	HIS	2.0

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	VXM	B	203[A]	21/21	0.67	0.18	29,36,49,51	21
4	VXM	B	203[B]	21/21	0.67	0.18	29,36,49,50	21
4	VXM	H	202[A]	21/21	0.70	0.18	30,38,49,50	21
4	VXM	H	202[B]	21/21	0.70	0.18	30,39,49,58	21
4	VXM	C	202	14/21	0.72	0.18	32,40,49,50	0
4	VXM	I	201	14/21	0.74	0.19	33,44,56,56	0
4	VXM	E	201	13/21	0.78	0.15	35,42,46,53	0
4	VXM	G	201	21/21	0.80	0.15	33,46,58,61	0
4	VXM	J	201	21/21	0.82	0.16	28,44,63,65	0
4	VXM	D	203	14/21	0.83	0.15	32,40,48,60	0
3	HEM	B	202	43/43	0.95	0.10	21,27,42,46	0
3	HEM	A	202	43/43	0.96	0.09	20,25,39,47	0
2	K	B	201	1/1	0.96	0.06	24,24,24,24	0
3	HEM	C	201	43/43	0.96	0.09	19,27,40,44	0
3	HEM	D	202	43/43	0.96	0.09	23,26,35,38	43
3	HEM	L	201	43/43	0.96	0.09	23,29,36,39	43
3	HEM	H	201	43/43	0.97	0.08	17,22,37,39	0

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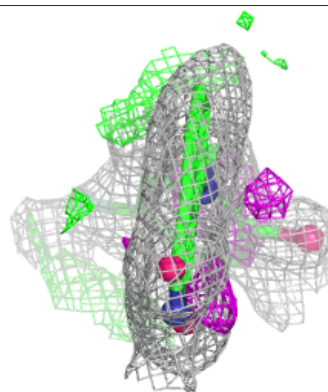
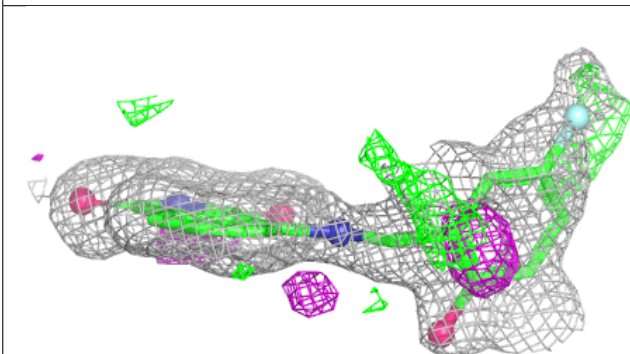
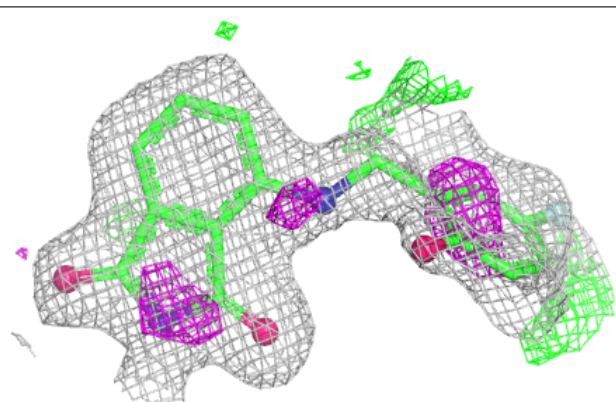
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	HEM	F	201	43/43	0.97	0.09	21,25,39,45	0
2	K	D	201	1/1	0.98	0.03	18,18,18,18	0
2	K	A	201	1/1	0.99	0.02	17,17,17,17	0

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

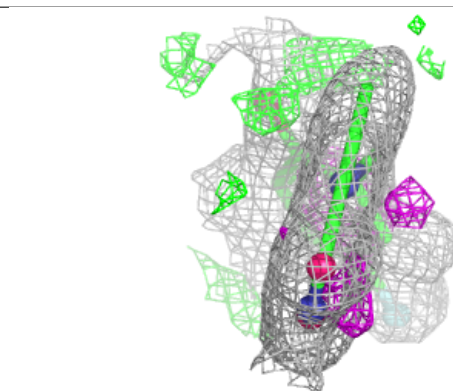
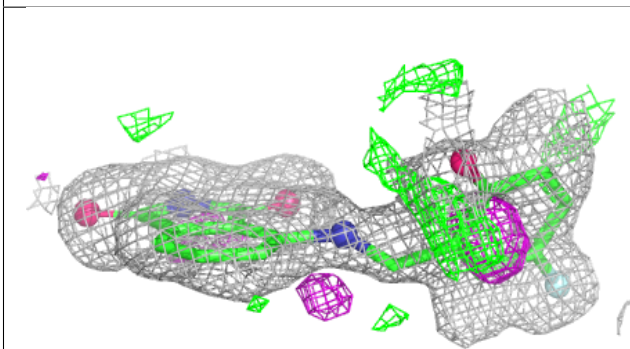
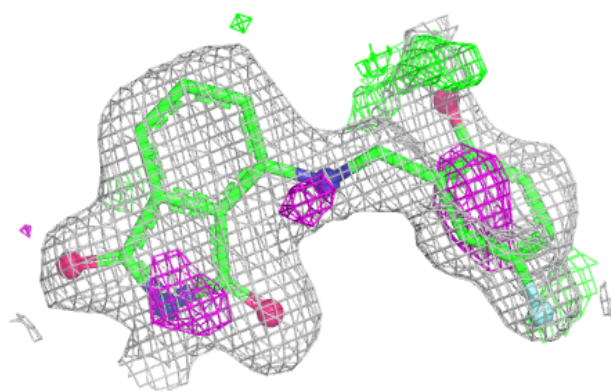
Electron density around VXM B 203 (A):

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

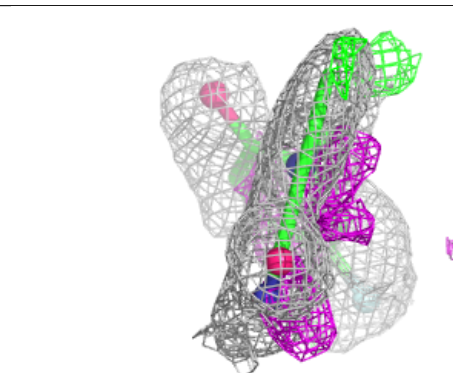
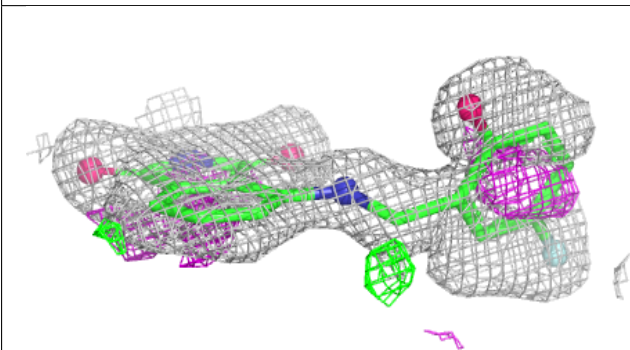
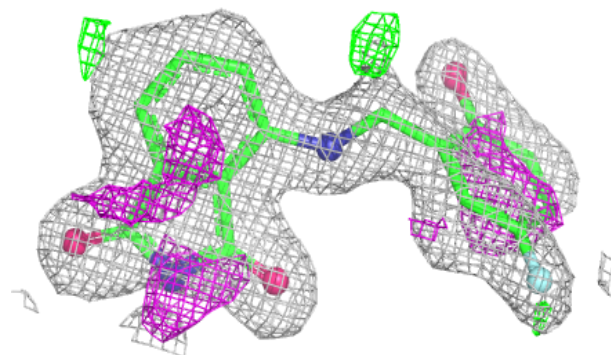


Electron density around VXM B 203 (B):

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and green (positive)

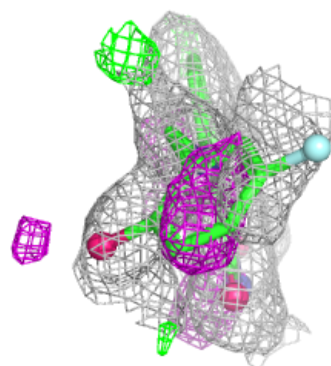
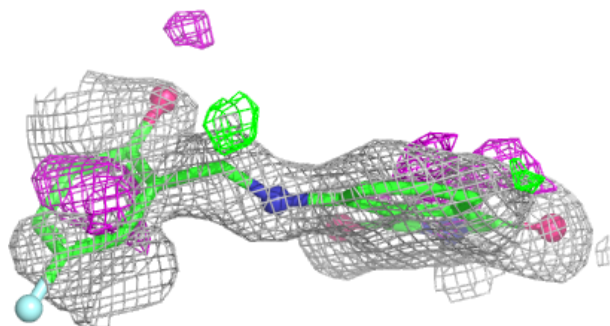
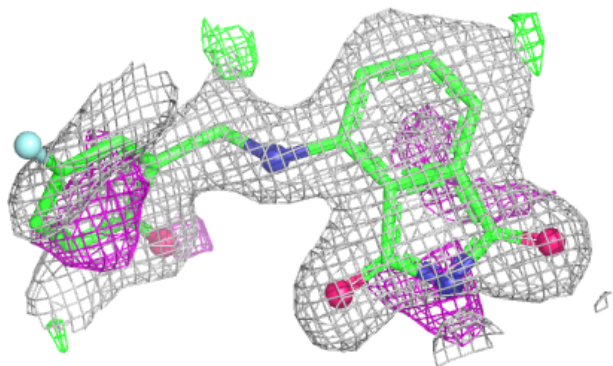
**Electron density around VXM H 202 (A):**

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

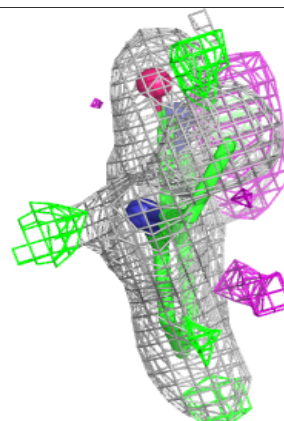
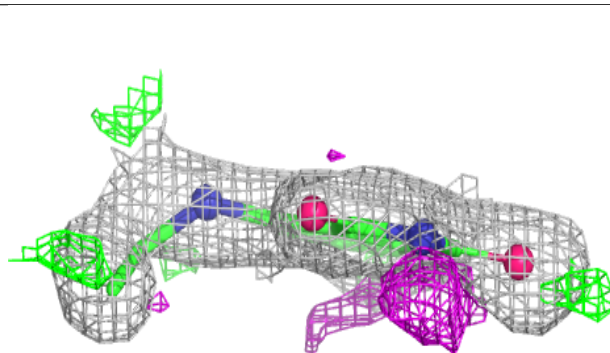
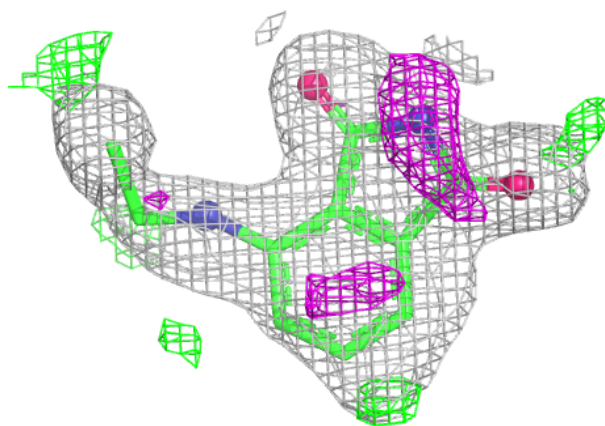


Electron density around VXM H 202 (B):

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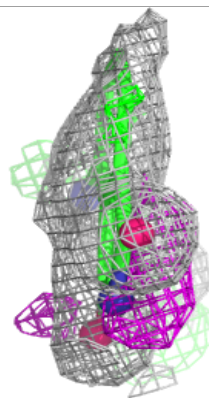
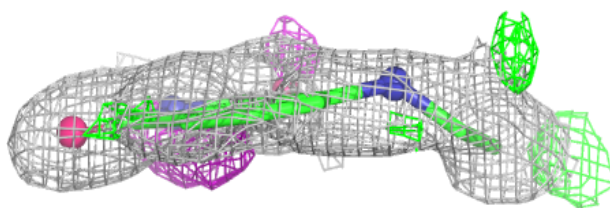
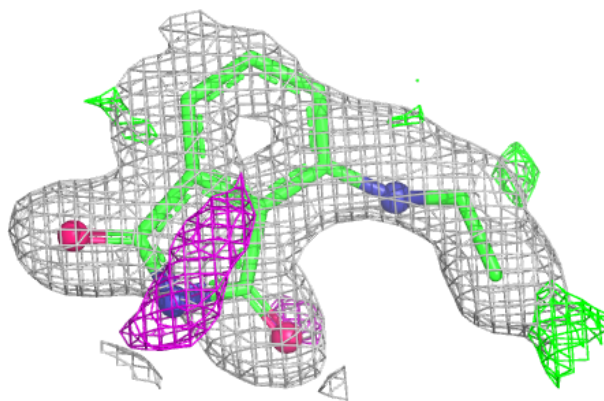
**Electron density around VXM C 202:**

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and green (positive)

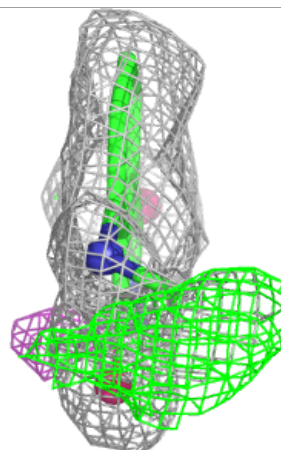
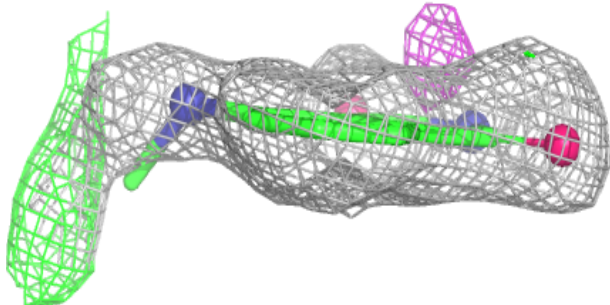
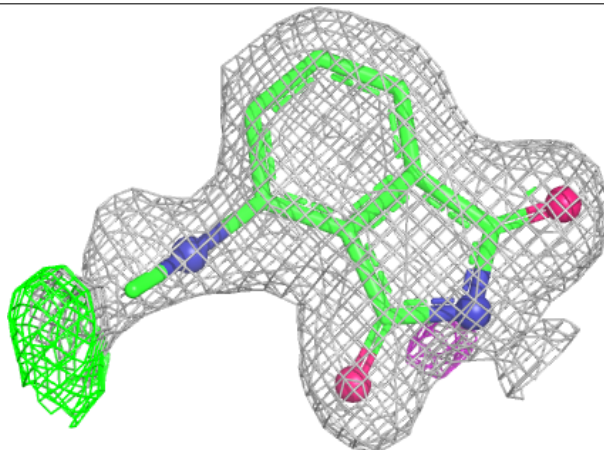


Electron density around VXM I 201:

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and green (positive)

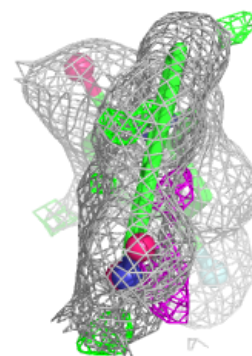
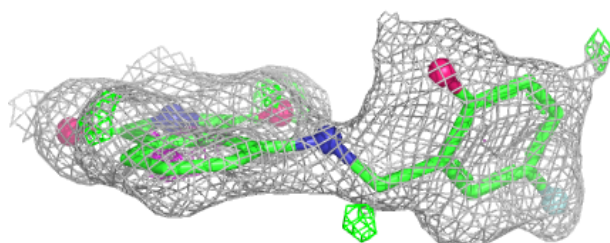
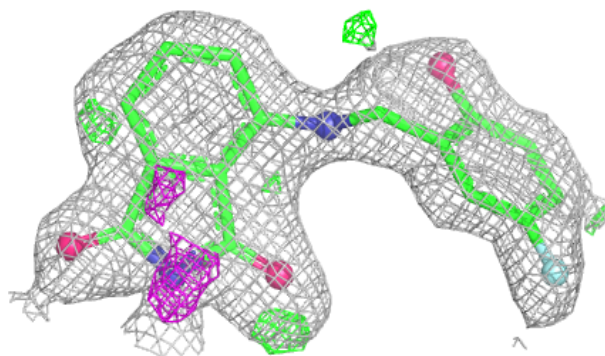
**Electron density around VXM E 201:**

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and green (positive)

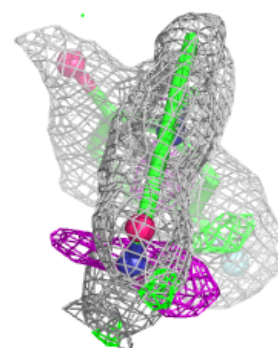
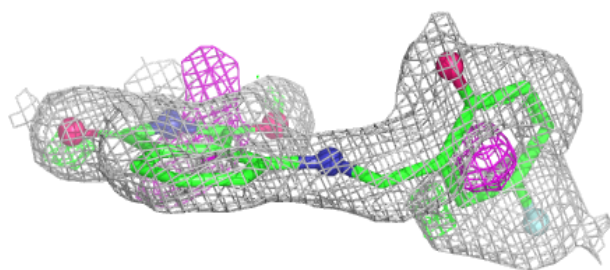
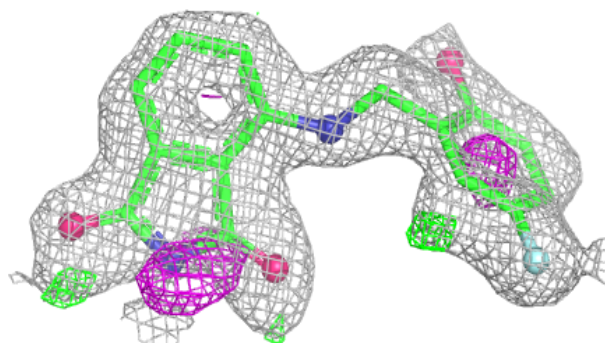


Electron density around VXM G 201:

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and green (positive)

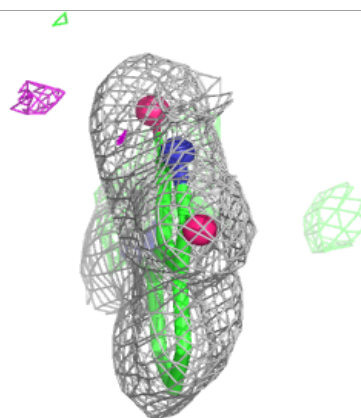
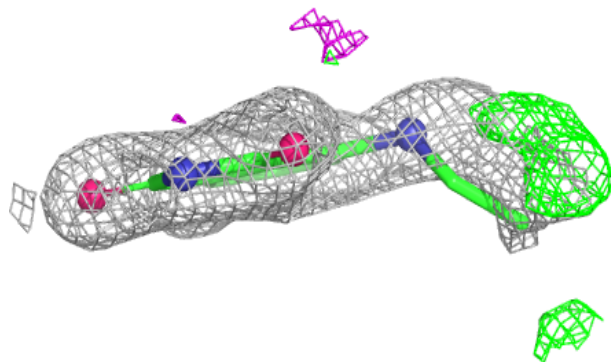
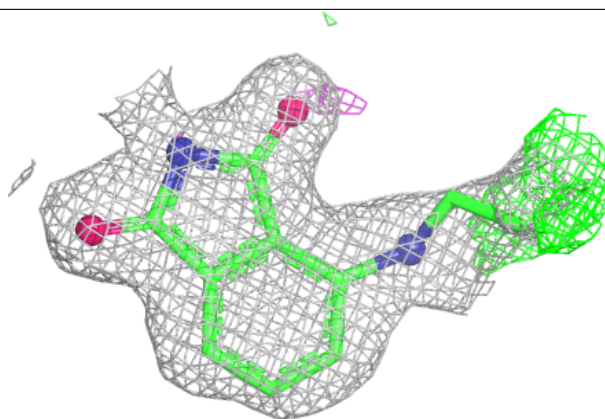
**Electron density around VXM J 201:**

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and green (positive)



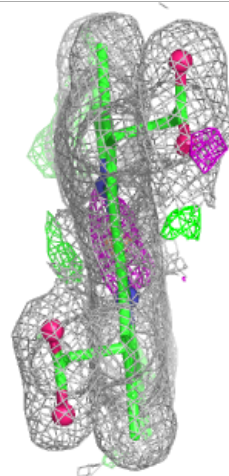
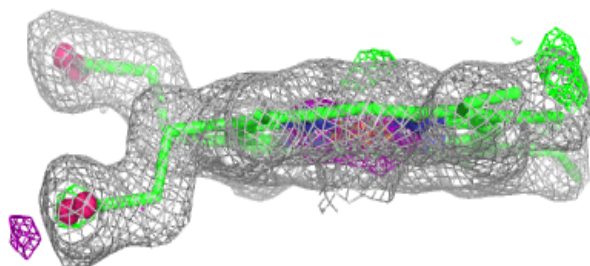
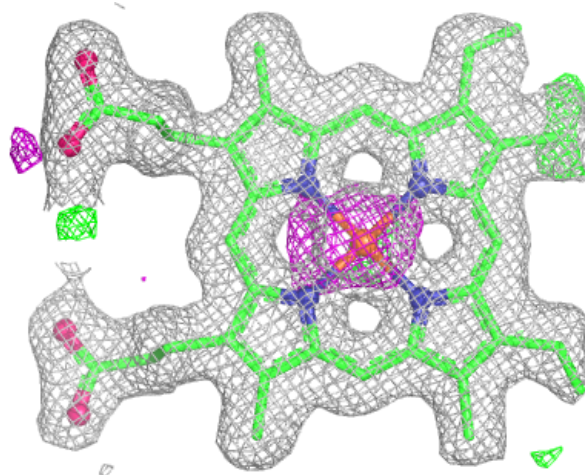
Electron density around VXM D 203:

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and green (positive)



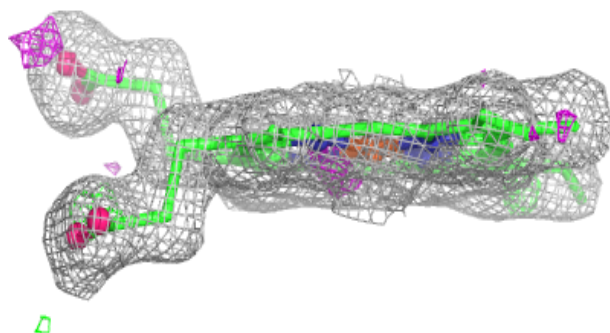
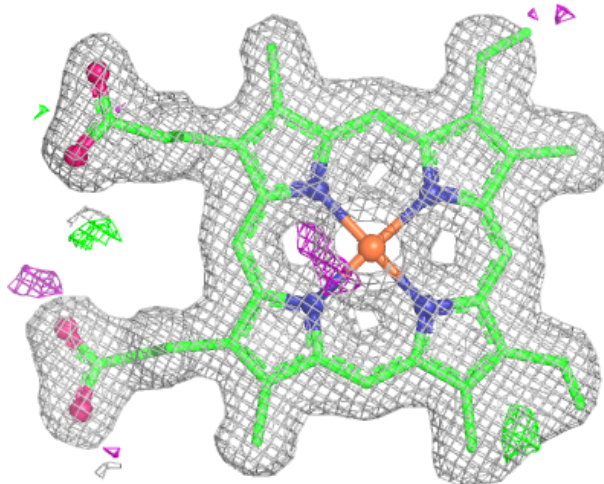
Electron density around HEM B 202:

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and green (positive)



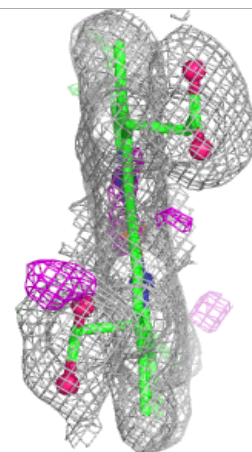
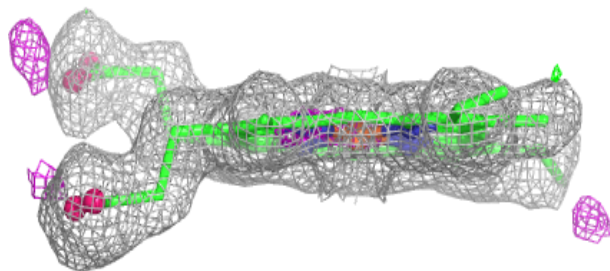
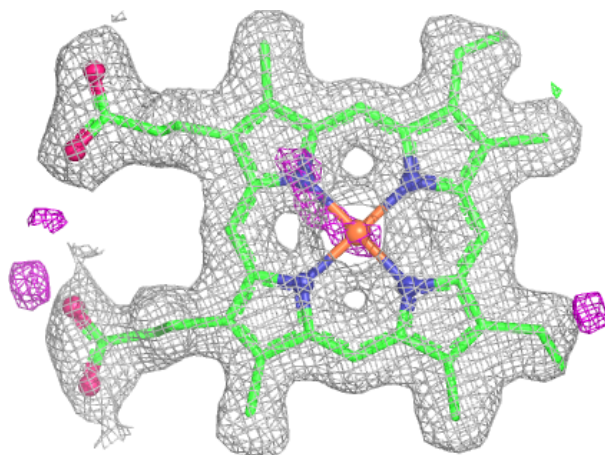
Electron density around HEM A 202:

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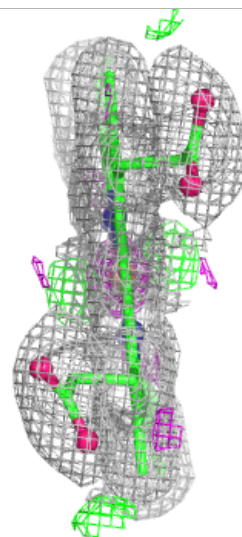
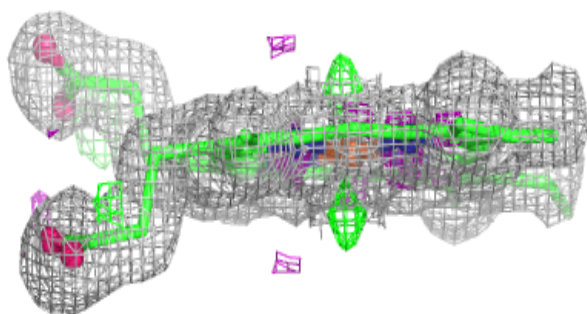
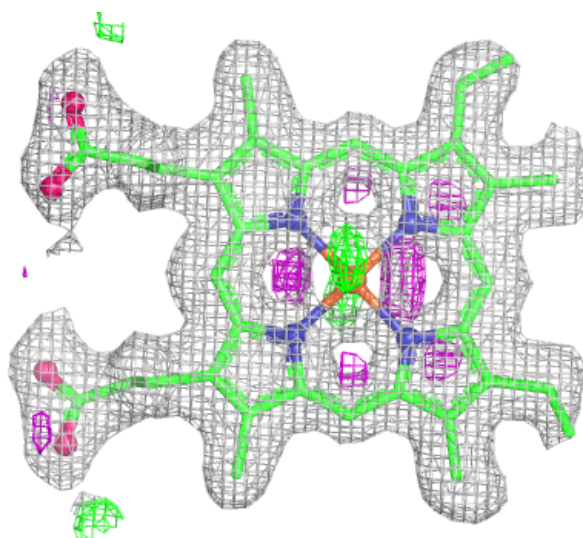
Electron density around HEM C 201:

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and green (positive)



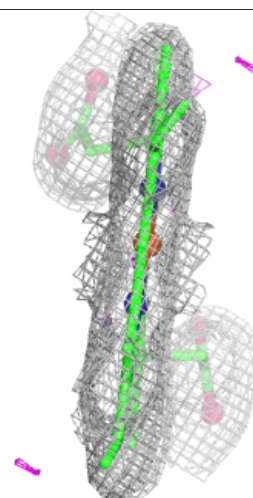
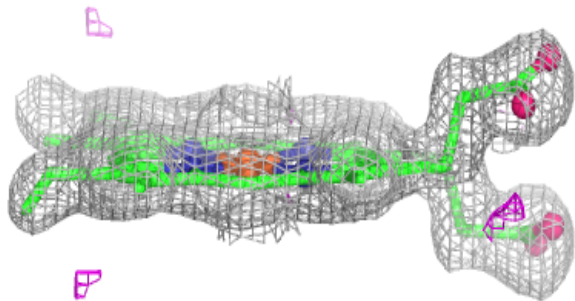
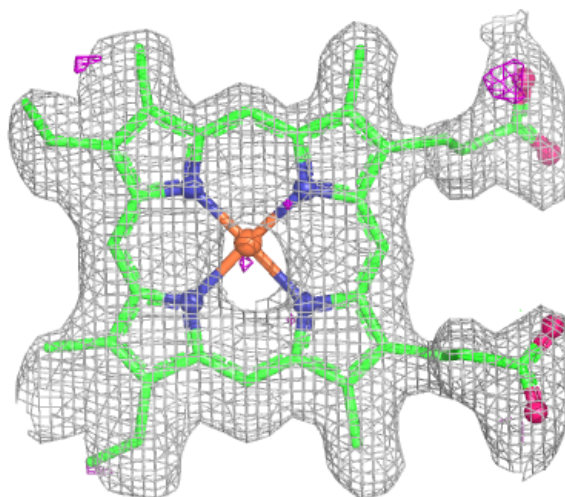
Electron density around HEM D 202:

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and green (positive)



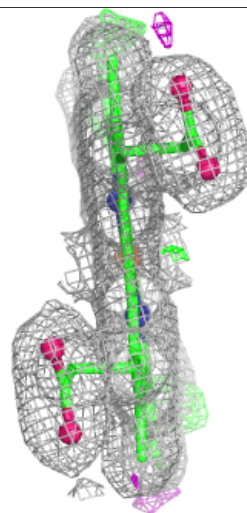
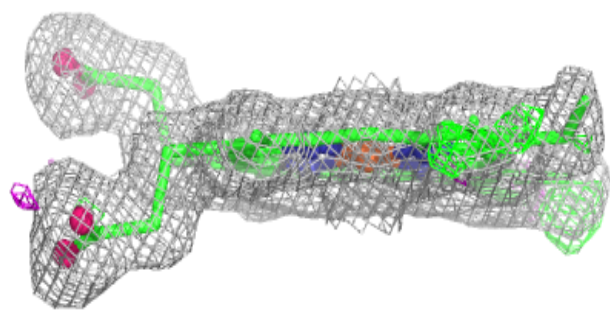
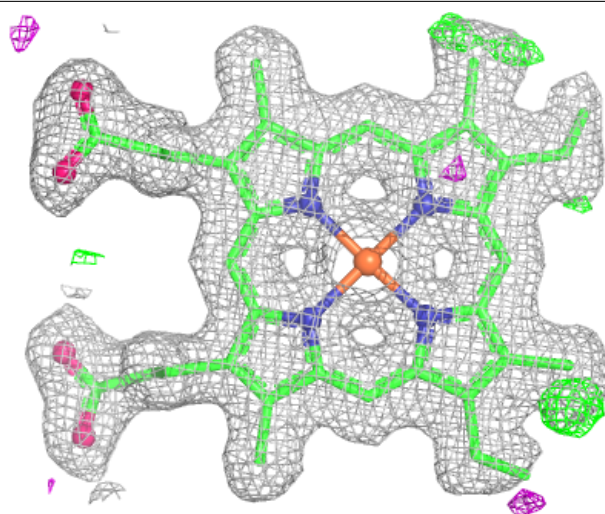
Electron density around HEM L 201:

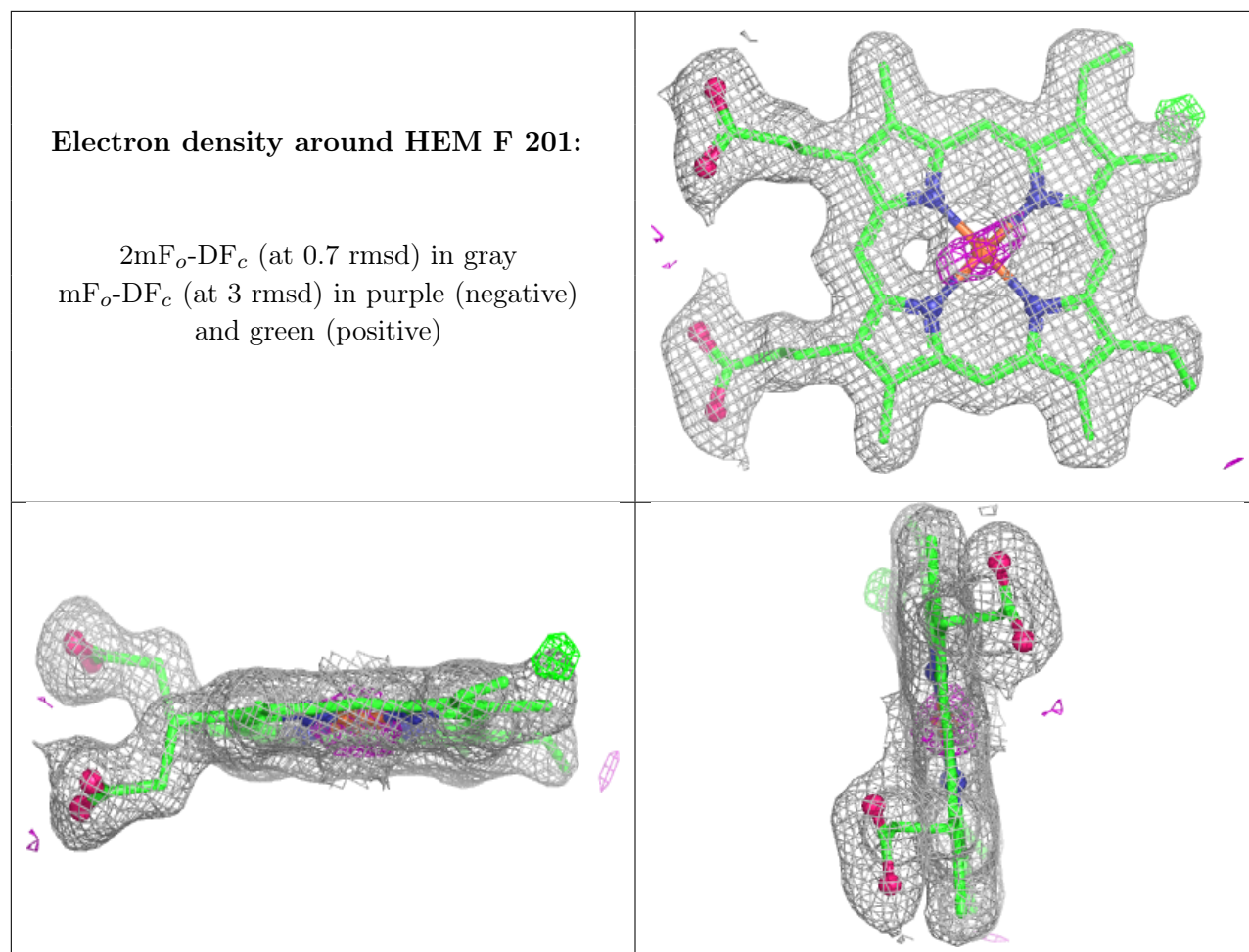
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and green (positive)



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)





6.5 Other polymers [i](#)

There are no such residues in this entry.