



wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 20, 2019 – 10:24 AM EDT

PDB ID : 1X9F
Title : Hemoglobin Dodecamer from Lumbricus Erythrocrutorin
Authors : Strand, K.; Knapp, J.E.; Bhyravbhatla, B.; Royer Jr., W.E.
Deposited on : 2004-08-20
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Xtriage (Phenix) : 1.13
EDS : 2.3.2
buster-report : 1.1.7 (2018)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.3.2

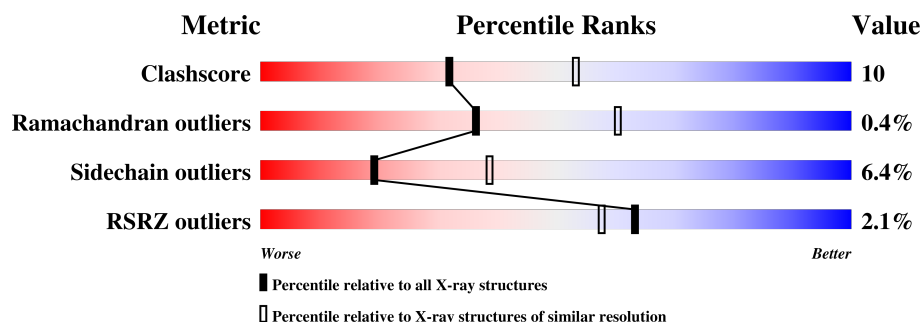
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	122126	3110 (2.60-2.60)
Ramachandran outliers	120053	3062 (2.60-2.60)
Sidechain outliers	120020	3062 (2.60-2.60)
RSRZ outliers	108989	2706 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	151	
1	E	151	
1	I	151	
2	B	145	
2	F	145	
2	J	145	
3	C	153	

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Mol	Chain	Length	Quality of chain
3	G	153	
3	K	153	
4	D	140	
4	H	140	
4	L	140	

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
6	CMO	D	1164	-	-	X	-
6	CMO	F	2162	-	-	X	-
6	CMO	H	2164	-	-	X	-
6	CMO	J	3162	-	-	X	-
6	CMO	K	3163	-	-	-	X
6	CMO	L	3164	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 14847 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 Globin IV, extracellular.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	147	Total	C	N	O	S	0	0	0
			1209	769	222	214	4			
1	E	147	Total	C	N	O	S	0	0	0
			1209	769	222	214	4			
1	I	147	Total	C	N	O	S	0	0	0
			1209	769	222	214	4			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	78	LYS	ASP	CONFLICT	UNP P13579
E	78	LYS	ASP	CONFLICT	UNP P13579
I	78	LYS	ASP	CONFLICT	UNP P13579

- Molecule 2 is a protein called Globin II, extracellular.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	145	Total	C	N	O	S	0	0	0
			1148	720	212	213	3			
2	F	145	Total	C	N	O	S	0	0	0
			1148	720	212	213	3			
2	J	145	Total	C	N	O	S	0	0	0
			1148	720	212	213	3			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	66	ASP	GLU	CONFLICT	UNP P02218
F	66	ASP	GLU	CONFLICT	UNP P02218
J	66	ASP	GLU	CONFLICT	UNP P02218

- Molecule 3 is a protein called Globin III, extracellular.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	149	Total	C	N	O	S	0	0	0
			1190	758	212	217	3			
3	G	149	Total	C	N	O	S	5	0	0
			1190	758	212	217	3			
3	K	149	Total	C	N	O	S	5	0	0
			1190	758	212	217	3			

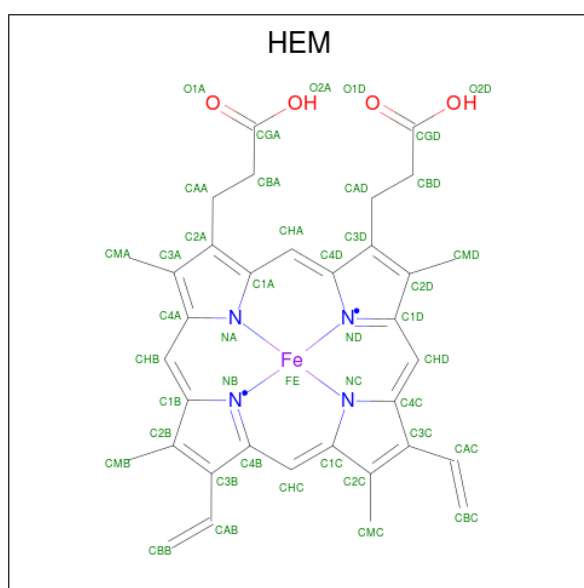
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	49	GLU	ASP	CONFLICT	UNP P11069
G	49	GLU	ASP	CONFLICT	UNP P11069
K	49	GLU	ASP	CONFLICT	UNP P11069

- Molecule 4 is a protein called hemoglobin chain d1.

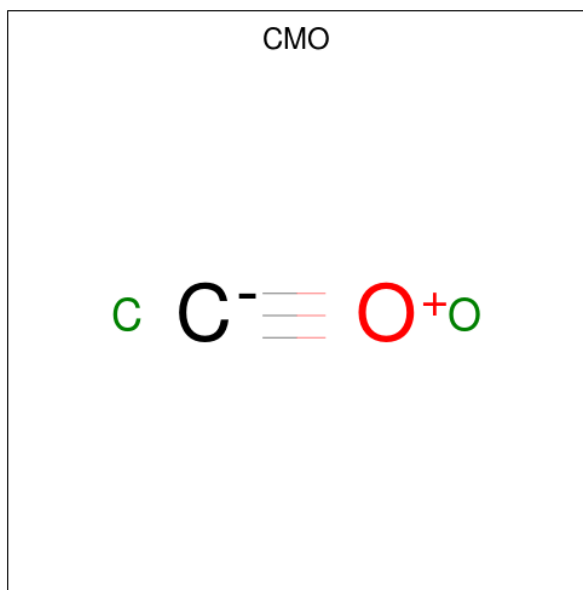
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	140	Total	C	N	O	S	0	0	0
			1129	725	198	202	4			
4	H	140	Total	C	N	O	S	0	0	0
			1129	725	198	202	4			
4	L	140	Total	C	N	O	S	0	0	0
			1129	725	198	202	4			

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



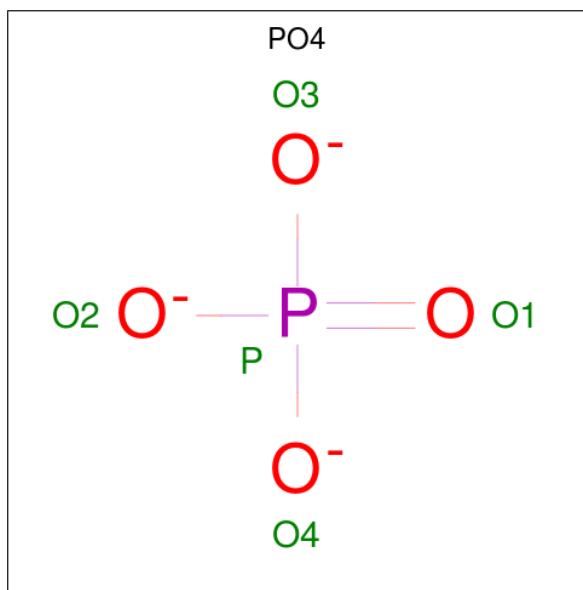
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	G	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	H	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	I	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	J	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	K	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	L	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 6 is CARBON MONOXIDE (three-letter code: CMO) (formula: CO).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 2 1 1	0	0
6	B	1	Total C O 2 1 1	0	0
6	C	1	Total C O 2 1 1	0	0
6	D	1	Total C O 2 1 1	0	0
6	E	1	Total C O 2 1 1	0	0
6	F	1	Total C O 2 1 1	0	0
6	G	1	Total C O 2 1 1	0	0
6	H	1	Total C O 2 1 1	0	0
6	I	1	Total C O 2 1 1	0	0
6	J	1	Total C O 2 1 1	0	0
6	K	1	Total C O 2 1 1	0	0
6	L	1	Total C O 2 1 1	0	0

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).

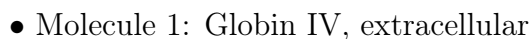


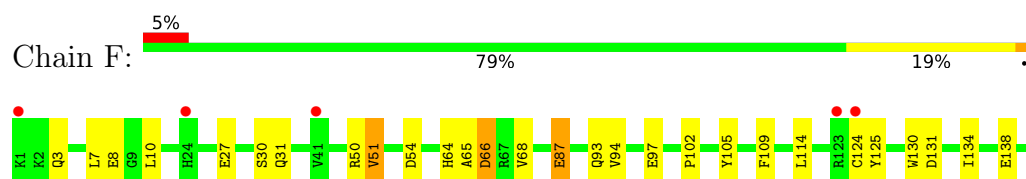
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	O	P	0	0
			5	4	1		
7	G	1	Total	O	P	0	0
			5	4	1		
7	K	1	Total	O	P	0	0
			5	4	1		

- Molecule 8 is water.

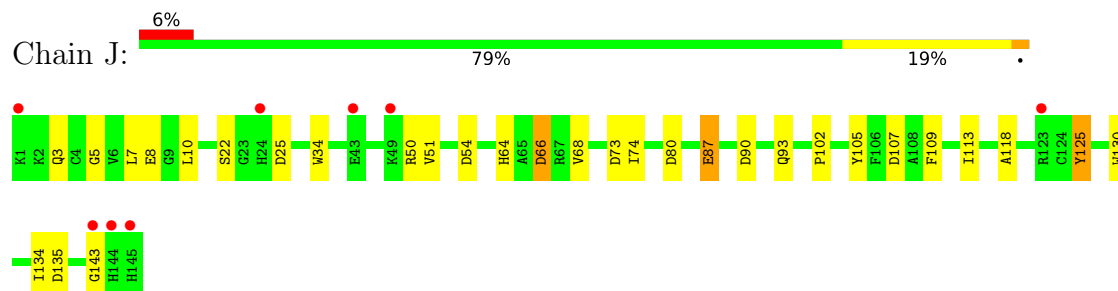
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	26	Total	O	0	0
			26	26		
8	B	31	Total	O	0	0
			31	31		
8	C	28	Total	O	0	0
			28	28		
8	D	18	Total	O	0	0
			18	18		
8	E	21	Total	O	0	0
			21	21		
8	F	23	Total	O	0	0
			23	23		
8	G	26	Total	O	0	0
			26	26		
8	H	22	Total	O	0	0
			22	22		
8	I	31	Total	O	0	0
			31	31		
8	J	13	Total	O	0	0
			13	13		
8	K	5	Total	O	0	0
			5	5		
8	L	20	Total	O	0	0
			20	20		

- Molecule 1: Globin IV, extracellular

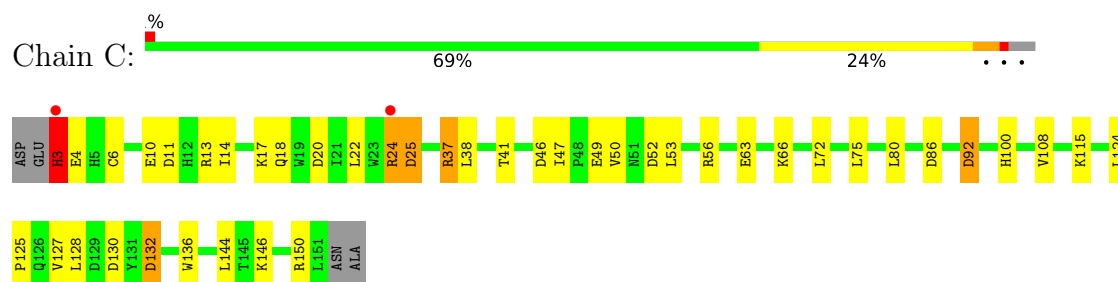




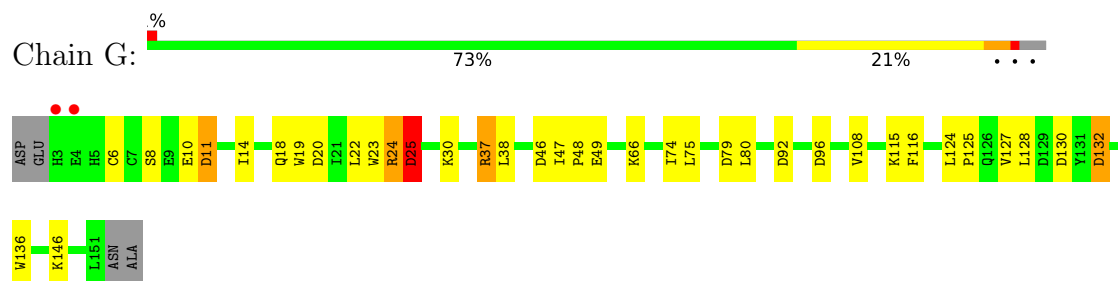
- Molecule 2: Globin II, extracellular



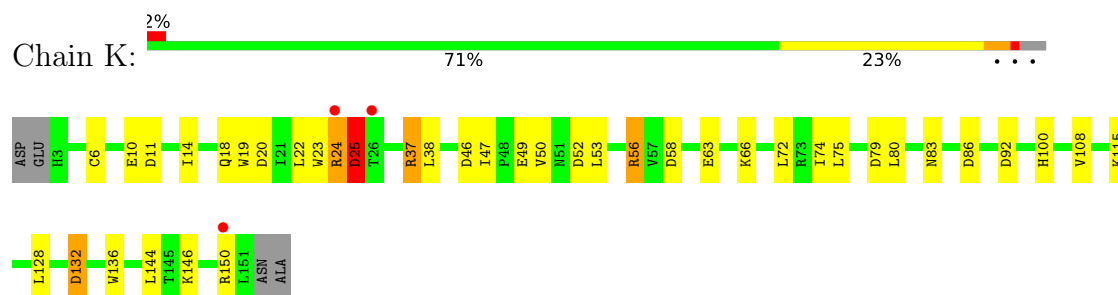
- Molecule 3: Globin III, extracellular



- Molecule 3: Globin III, extracellular

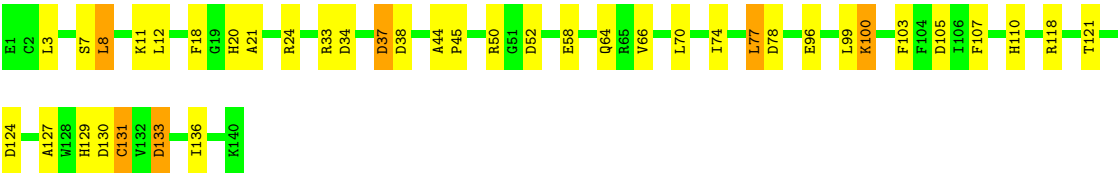


- Molecule 3: Globin III, extracellular

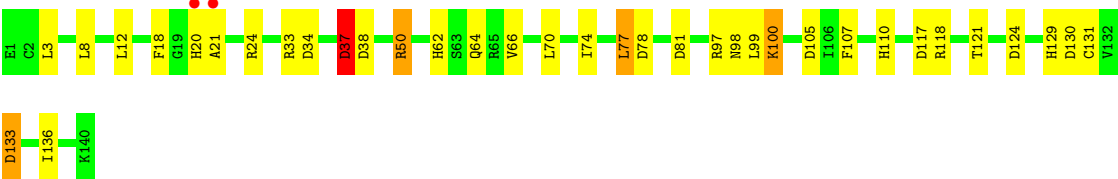


- Molecule 4: hemoglobin chain d1

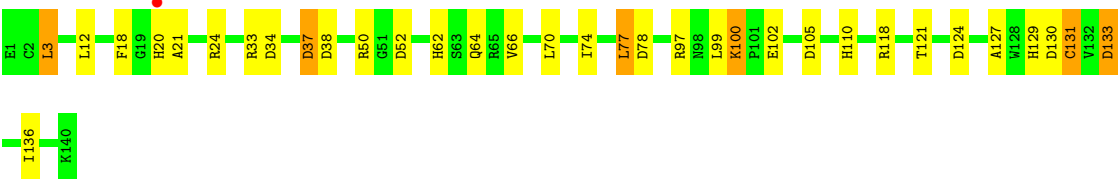
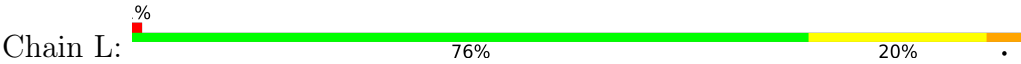




• Molecule 4: hemoglobin chain d1



• Molecule 4: hemoglobin chain d1



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	139.22Å 172.07Å 202.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	105.41 – 2.60 95.49 – 2.60	Depositor EDS
% Data completeness (in resolution range)	88.7 (105.41-2.60) 88.7 (95.49-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.10 (at 2.62Å)	Xtriage
Refinement program	REFMAC 5.2, CNS	Depositor
R, R_{free}	0.213 , 0.246 0.213 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	34.0	Xtriage
Anisotropy	0.402	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 39.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	14847	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% 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: CMO, HEM, PO4

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	0.46	0/1237	0.80	7/1670 (0.4%)
1	E	0.44	0/1237	0.79	4/1670 (0.2%)
1	I	0.46	0/1237	0.79	5/1670 (0.3%)
2	B	0.39	0/1176	0.74	3/1587 (0.2%)
2	F	0.37	0/1176	0.73	3/1587 (0.2%)
2	J	0.36	0/1176	0.74	7/1587 (0.4%)
3	C	0.46	2/1214 (0.2%)	0.93	11/1638 (0.7%)
3	G	0.36	0/1215	0.76	7/1641 (0.4%)
3	K	0.37	0/1215	0.75	8/1641 (0.5%)
4	D	0.40	0/1159	0.78	7/1568 (0.4%)
4	H	0.39	0/1159	0.79	9/1568 (0.6%)
4	L	0.39	0/1159	0.79	7/1568 (0.4%)
All	All	0.41	2/14360 (0.0%)	0.78	78/19395 (0.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3	HIS	CB-CG	7.50	1.63	1.50
3	C	3	HIS	CA-CB	6.40	1.68	1.53

The worst 5 of 78 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3	HIS	N-CA-C	-16.69	65.95	111.00
3	C	3	HIS	CA-CB-CG	10.63	131.68	113.60
3	G	11	ASP	CB-CG-OD2	6.54	124.19	118.30
3	C	11	ASP	CB-CG-OD2	6.48	124.13	118.30
1	E	85	ASP	CB-CG-OD2	6.44	124.09	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1209	0	1194	32	0
1	E	1209	0	1195	31	0
1	I	1209	0	1194	28	0
2	B	1148	0	1103	16	0
2	F	1148	0	1104	19	0
2	J	1148	0	1103	20	0
3	C	1190	0	1195	29	0
3	G	1190	0	1196	26	0
3	K	1190	0	1196	24	0
4	D	1129	0	1105	26	0
4	H	1129	0	1105	22	0
4	L	1129	0	1105	24	0
5	A	43	0	30	1	0
5	B	43	0	30	0	0
5	C	43	0	30	5	0
5	D	43	0	30	4	0
5	E	43	0	30	1	0
5	F	43	0	30	1	0
5	G	43	0	30	3	0
5	H	43	0	30	3	0
5	I	43	0	30	1	0
5	J	43	0	30	0	0
5	K	43	0	30	5	0
5	L	43	0	30	3	0
6	A	2	0	0	0	0
6	B	2	0	0	1	0
6	C	2	0	0	0	0
6	D	2	0	0	2	0
6	E	2	0	0	0	0
6	F	2	0	0	2	0
6	G	2	0	0	0	0
6	H	2	0	0	2	0
6	I	2	0	0	1	0
6	J	2	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	K	2	0	0	0	0
6	L	2	0	0	2	0
7	C	5	0	0	0	0
7	G	5	0	0	1	0
7	K	5	0	0	0	0
8	A	26	0	0	0	0
8	B	31	0	0	0	0
8	C	28	0	0	3	0
8	D	18	0	0	0	0
8	E	21	0	0	1	0
8	F	23	0	0	0	0
8	G	26	0	0	0	0
8	H	22	0	0	0	0
8	I	31	0	0	0	0
8	J	13	0	0	1	0
8	K	5	0	0	0	0
8	L	20	0	0	1	0
All	All	14847	0	14155	276	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 10.

The worst 5 of 276 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:C:3:HIS:ND1	3:C:4:GLU:HG2	1.76	0.99
4:H:50:ARG:HH11	4:H:50:ARG:HG2	1.33	0.90
1:A:110:GLU:HG3	1:A:113:ARG:HH22	1.34	0.90
3:K:108:VAL:HG13	5:K:160:HEM:HBC2	1.57	0.85
3:G:18:GLN:HE21	3:G:136:TRP:HE1	1.26	0.83

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	145/151 (96%)	138 (95%)	6 (4%)	1 (1%)	24	46
1	E	145/151 (96%)	136 (94%)	8 (6%)	1 (1%)	24	46
1	I	145/151 (96%)	139 (96%)	5 (3%)	1 (1%)	24	46
2	B	143/145 (99%)	140 (98%)	3 (2%)	0	100	100
2	F	143/145 (99%)	140 (98%)	3 (2%)	0	100	100
2	J	143/145 (99%)	137 (96%)	6 (4%)	0	100	100
3	C	146/153 (95%)	141 (97%)	5 (3%)	0	100	100
3	G	147/153 (96%)	141 (96%)	6 (4%)	0	100	100
3	K	147/153 (96%)	140 (95%)	7 (5%)	0	100	100
4	D	138/140 (99%)	134 (97%)	3 (2%)	1 (1%)	24	46
4	H	138/140 (99%)	135 (98%)	1 (1%)	2 (1%)	12	24
4	L	138/140 (99%)	132 (96%)	5 (4%)	1 (1%)	24	46
All	All	1718/1767 (97%)	1653 (96%)	58 (3%)	7 (0%)	36	60

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	25	SER
4	D	21	ALA
1	E	25	SER
4	H	21	ALA
1	I	25	SER

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	131/134 (98%)	125 (95%)	6 (5%)	29	55
1	E	131/134 (98%)	123 (94%)	8 (6%)	20	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	131/134 (98%)	124 (95%)	7 (5%)	25	48
2	B	117/117 (100%)	114 (97%)	3 (3%)	49	75
2	F	117/117 (100%)	112 (96%)	5 (4%)	32	58
2	J	117/117 (100%)	112 (96%)	5 (4%)	32	58
3	C	128/131 (98%)	117 (91%)	11 (9%)	11	22
3	G	128/131 (98%)	118 (92%)	10 (8%)	14	27
3	K	128/131 (98%)	116 (91%)	12 (9%)	9	18
4	D	121/121 (100%)	111 (92%)	10 (8%)	12	24
4	H	121/121 (100%)	111 (92%)	10 (8%)	12	24
4	L	121/121 (100%)	112 (93%)	9 (7%)	15	30
All	All	1491/1509 (99%)	1395 (94%)	96 (6%)	19	39

5 of 96 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	G	6	CYS
4	H	3	LEU
4	L	12	LEU
3	G	20	ASP
3	G	38	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	52	HIS
3	G	100	HIS
3	K	100	HIS
2	F	145	HIS
3	C	100	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

27 ligands are modelled in this entry.

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
6	CMO	A	1161	5	0,1,1	0.00	-	-		
5	HEM	A	160	1,6	27,50,50	2.08	8 (29%)	17,82,82	3.03	6 (35%)
6	CMO	B	1162	5	0,1,1	0.00	-	-		
5	HEM	B	160	2,6	27,50,50	2.05	8 (29%)	17,82,82	2.75	7 (41%)
6	CMO	C	1163	5	0,1,1	0.00	-	-		
7	PO4	C	154	-	4,4,4	0.79	0	6,6,6	0.54	0
5	HEM	C	160	3,6	27,50,50	2.08	9 (33%)	17,82,82	2.87	8 (47%)
6	CMO	D	1164	5	0,1,1	0.00	-	-		
5	HEM	D	160	4,6	27,50,50	2.13	9 (33%)	17,82,82	2.99	7 (41%)
5	HEM	E	160	1,6	27,50,50	2.06	8 (29%)	17,82,82	2.71	7 (41%)
6	CMO	E	2161	5	0,1,1	0.00	-	-		
5	HEM	F	160	2,6	27,50,50	2.03	8 (29%)	17,82,82	2.87	7 (41%)
6	CMO	F	2162	5	0,1,1	0.00	-	-		
7	PO4	G	154	-	4,4,4	0.77	0	6,6,6	0.44	0
5	HEM	G	160	3,6	27,50,50	2.05	9 (33%)	17,82,82	2.96	8 (47%)
6	CMO	G	2163	5	0,1,1	0.00	-	-		
5	HEM	H	160	4,6	27,50,50	2.06	9 (33%)	17,82,82	2.94	5 (29%)
6	CMO	H	2164	5	0,1,1	0.00	-	-		
5	HEM	I	160	1,6	27,50,50	2.12	9 (33%)	17,82,82	3.25	7 (41%)
6	CMO	I	3161	5	0,1,1	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	HEM	J	160	2,6	27,50,50	1.98	8 (29%)	17,82,82	2.77	7 (41%)
6	CMO	J	3162	5	0,1,1	0.00	-	-	-	-
7	PO4	K	154	-	4,4,4	0.76	0	6,6,6	0.46	0
5	HEM	K	160	3,6	27,50,50	2.07	8 (29%)	17,82,82	2.97	7 (41%)
6	CMO	K	3163	5	0,1,1	0.00	-	-	-	-
5	HEM	L	160	4,6	27,50,50	2.10	9 (33%)	17,82,82	2.90	5 (29%)
6	CMO	L	3164	5	0,1,1	0.00	-	-	-	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	HEM	A	160	1,6	-	0/6/54/54	-
5	HEM	B	160	2,6	-	0/6/54/54	-
5	HEM	C	160	3,6	-	0/6/54/54	-
5	HEM	D	160	4,6	-	0/6/54/54	-
5	HEM	E	160	1,6	-	0/6/54/54	-
5	HEM	F	160	2,6	-	0/6/54/54	-
5	HEM	G	160	3,6	-	0/6/54/54	-
5	HEM	H	160	4,6	-	0/6/54/54	-
5	HEM	I	160	1,6	-	0/6/54/54	-
5	HEM	J	160	2,6	-	0/6/54/54	-
5	HEM	K	160	3,6	-	0/6/54/54	-
5	HEM	L	160	4,6	-	0/6/54/54	-

The worst 5 of 102 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	160	HEM	C3B-CAB	-7.36	1.32	1.47
5	I	160	HEM	C3B-CAB	-7.18	1.33	1.47
5	L	160	HEM	C3B-CAB	-7.17	1.33	1.47
5	E	160	HEM	C3B-CAB	-7.05	1.33	1.47
5	A	160	HEM	C3B-CAB	-7.05	1.33	1.47

The worst 5 of 81 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	160	HEM	C4A-C3A-C2A	-9.39	100.46	107.00
5	G	160	HEM	C4A-C3A-C2A	-9.39	100.46	107.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	160	HEM	C4A-C3A-C2A	-9.38	100.47	107.00
5	A	160	HEM	C4A-C3A-C2A	-8.97	100.76	107.00
5	D	160	HEM	C4A-C3A-C2A	-8.88	100.81	107.00

There are no chirality outliers.

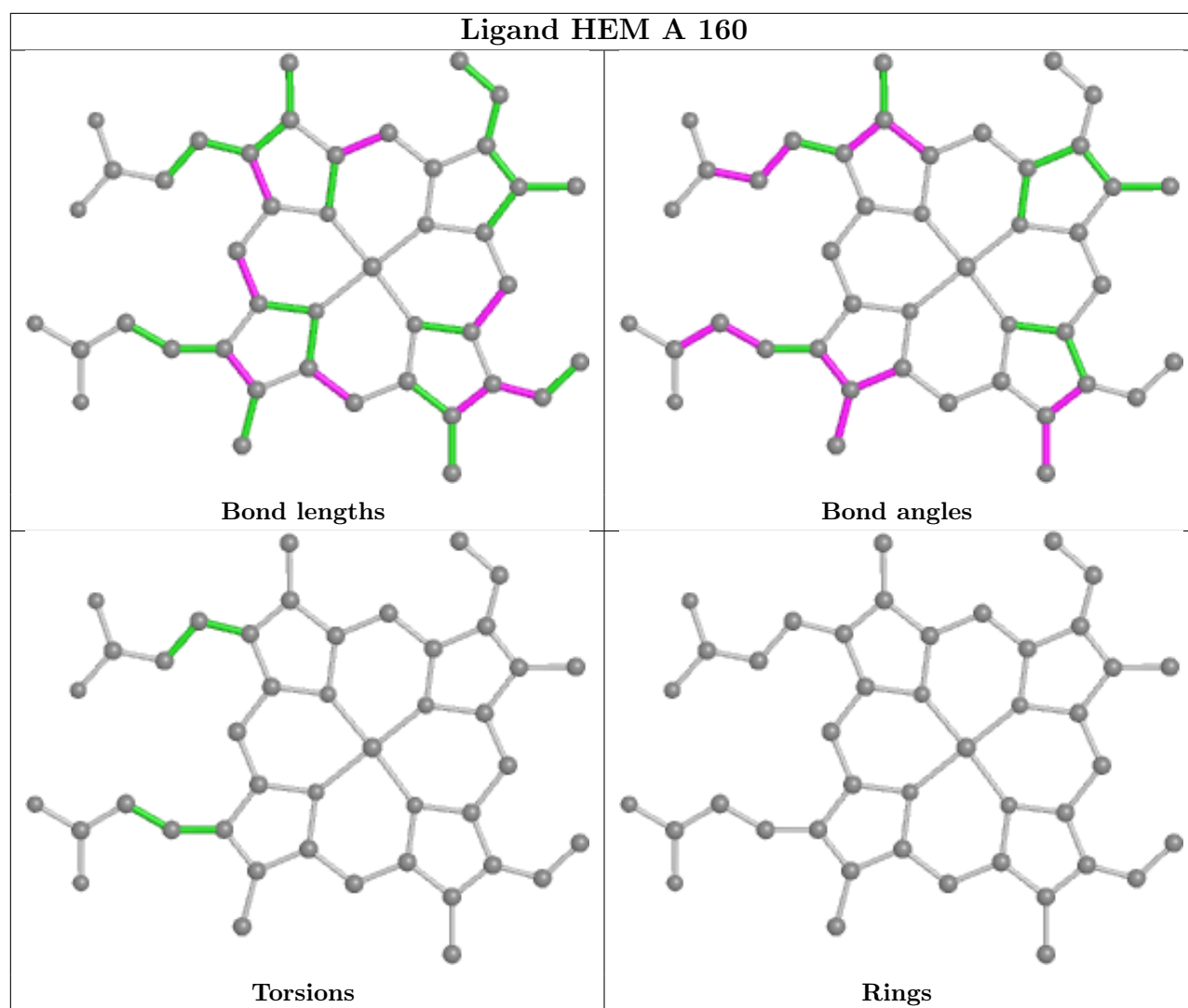
There are no torsion outliers.

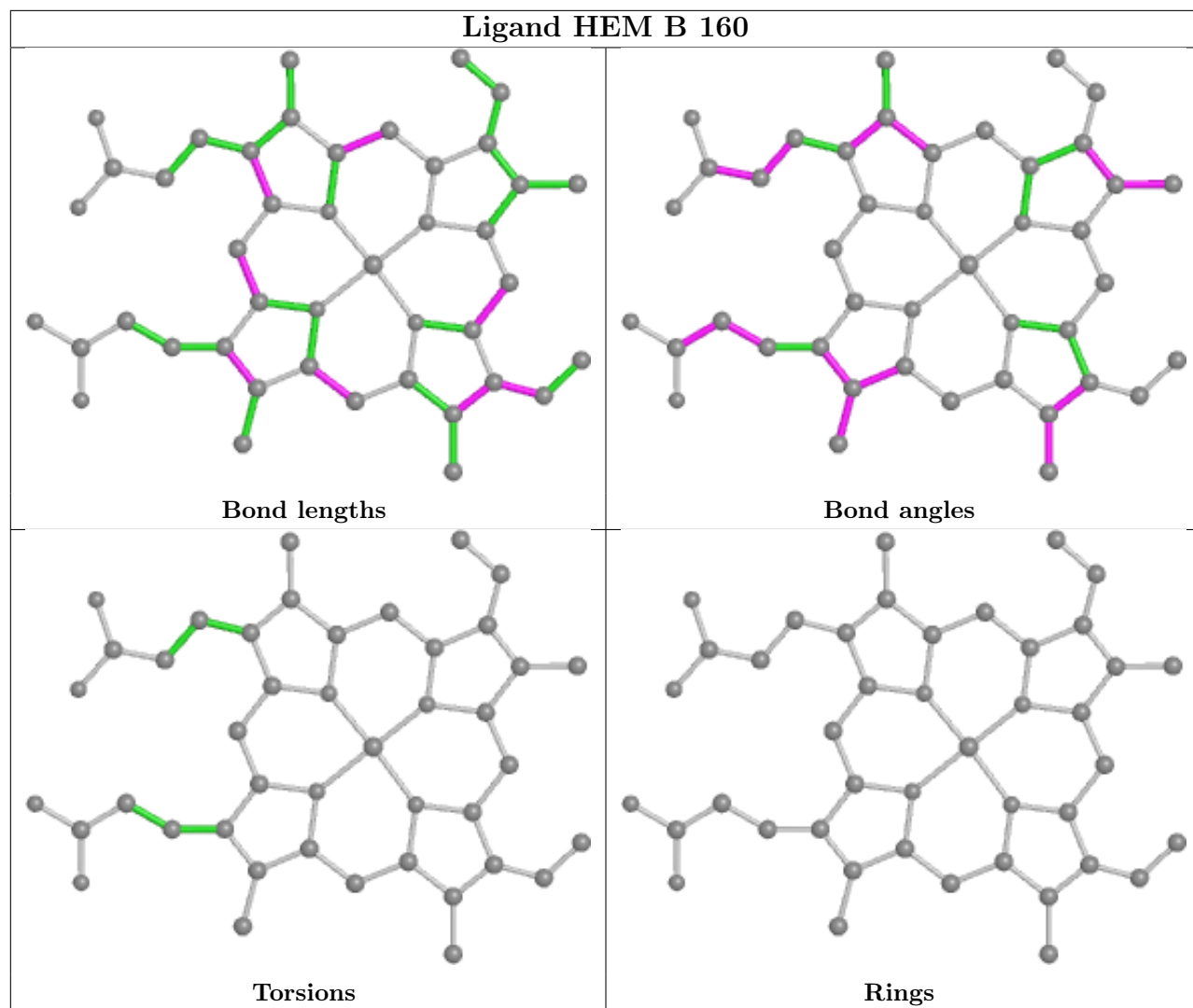
There are no ring outliers.

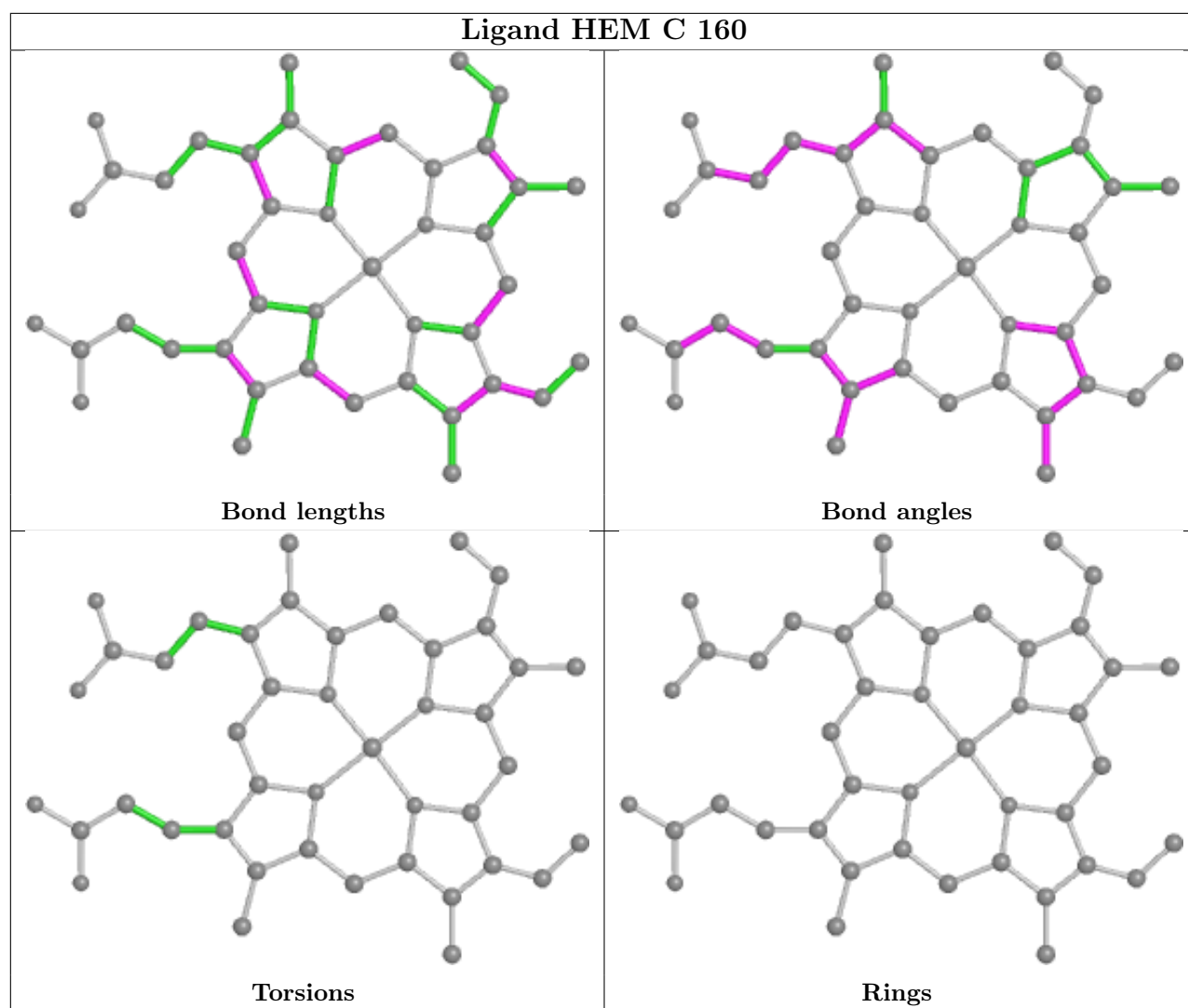
10 monomers are involved in 27 short contacts:

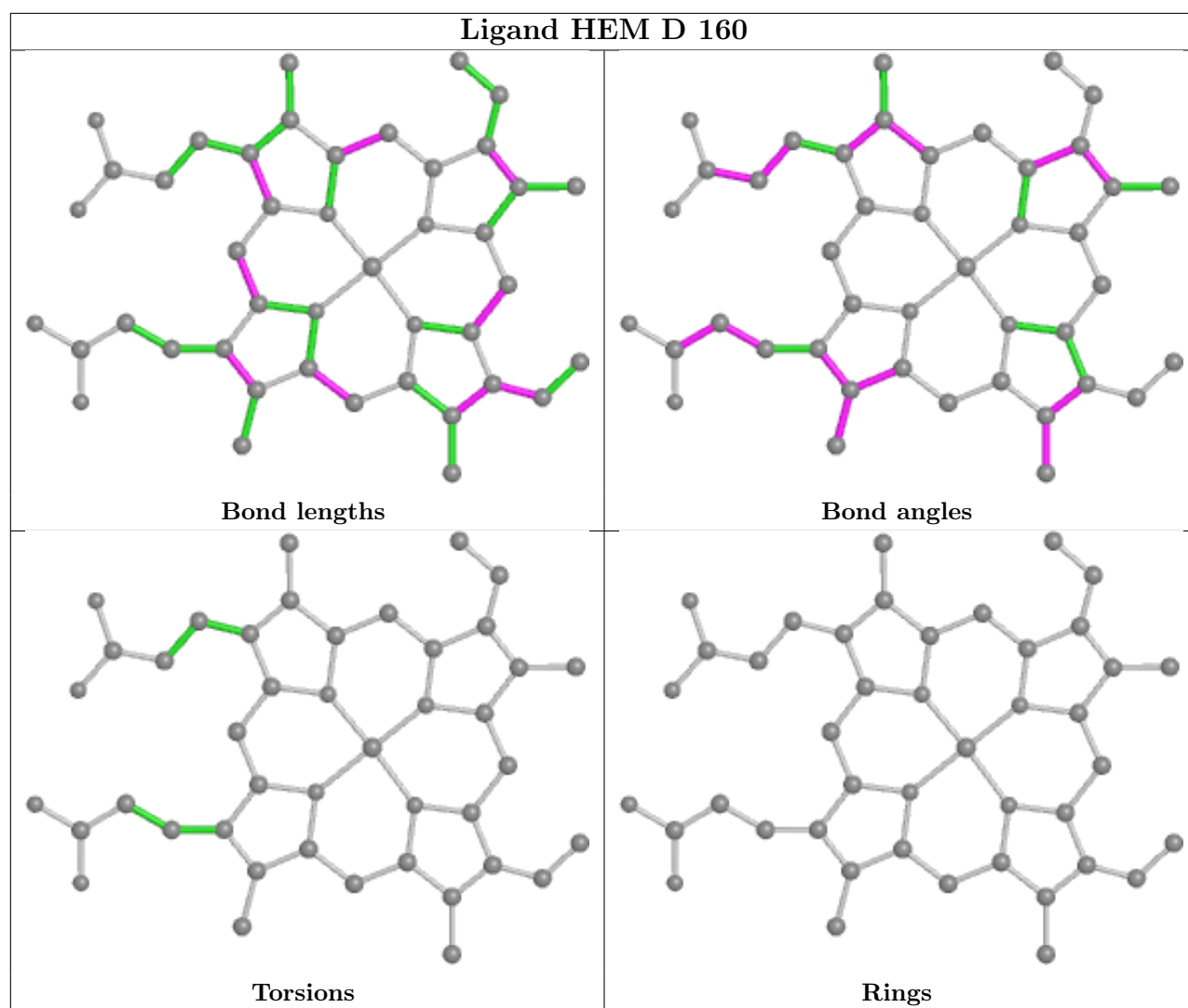
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	160	HEM	1	0
5	C	160	HEM	5	0
5	D	160	HEM	4	0
5	E	160	HEM	1	0
5	F	160	HEM	1	0
5	G	160	HEM	3	0
5	H	160	HEM	3	0
5	I	160	HEM	1	0
5	K	160	HEM	5	0
5	L	160	HEM	3	0

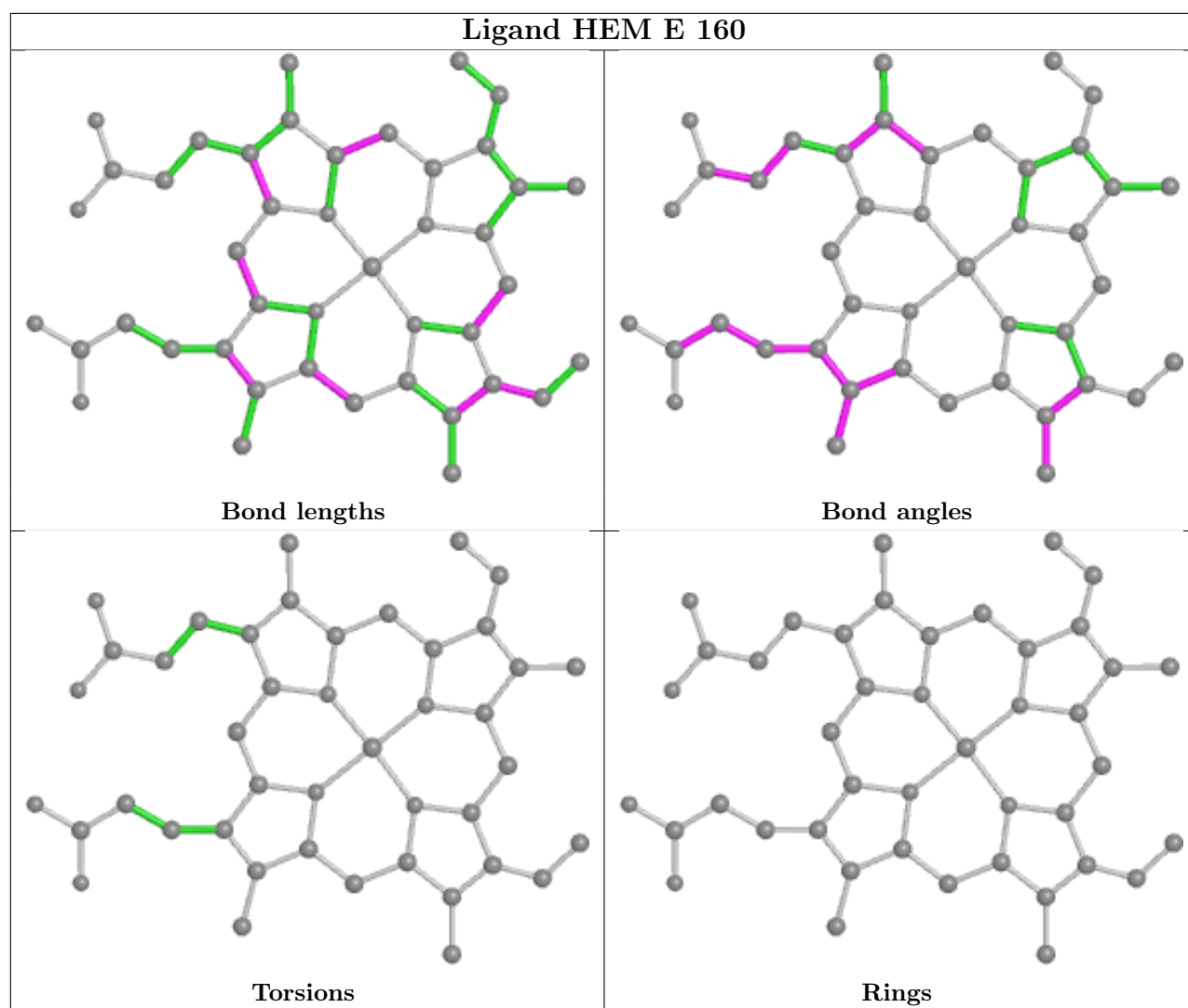
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

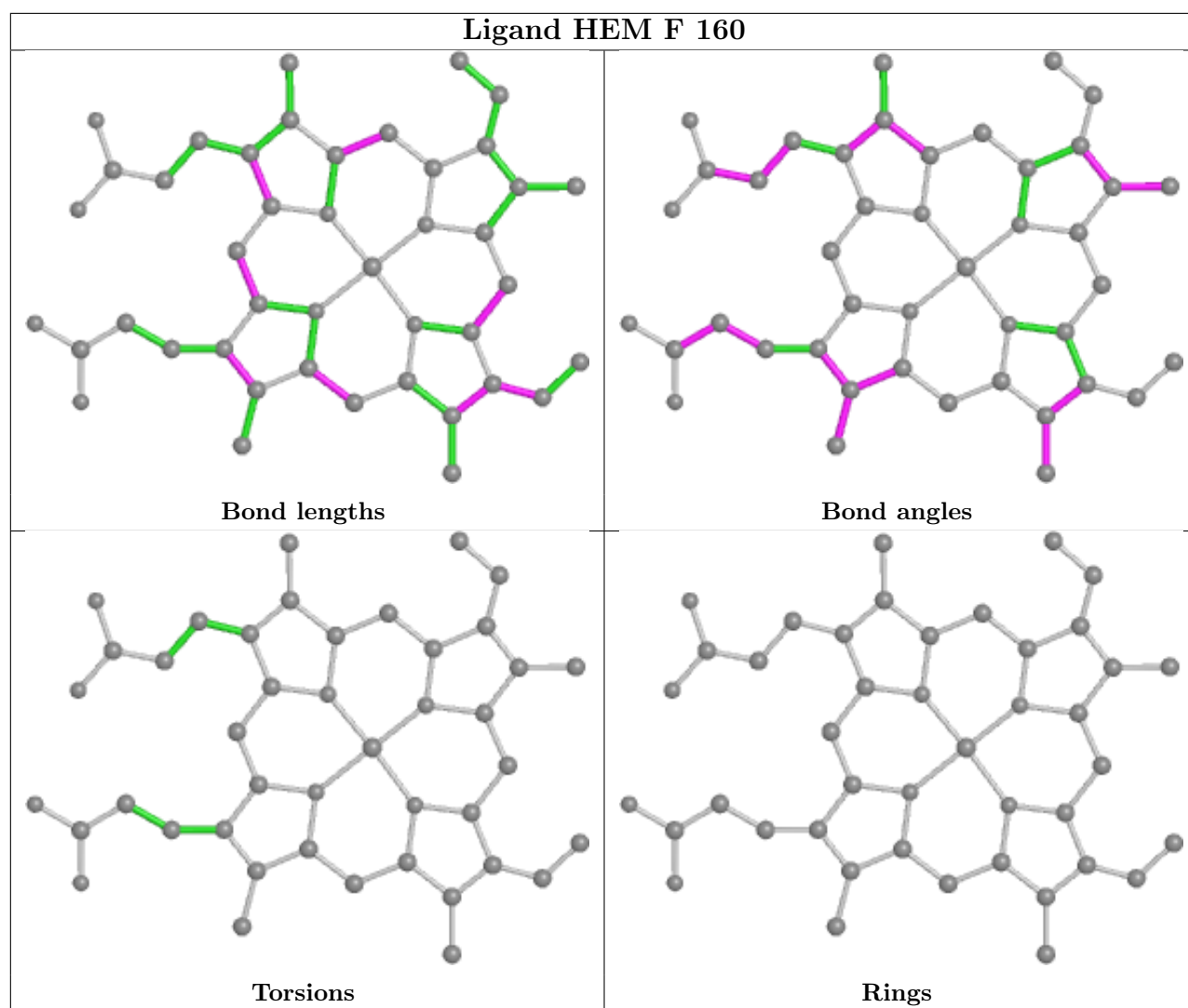


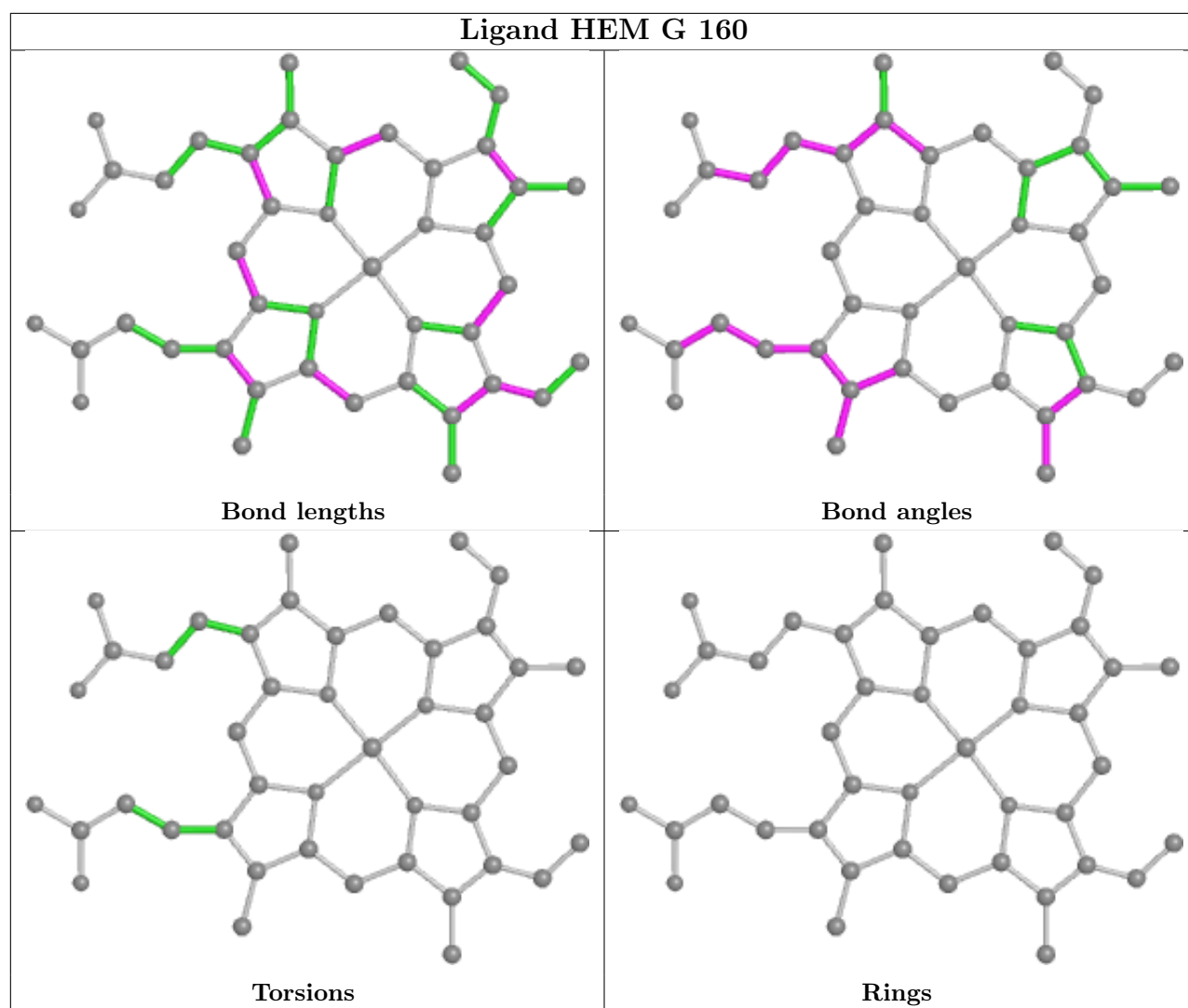


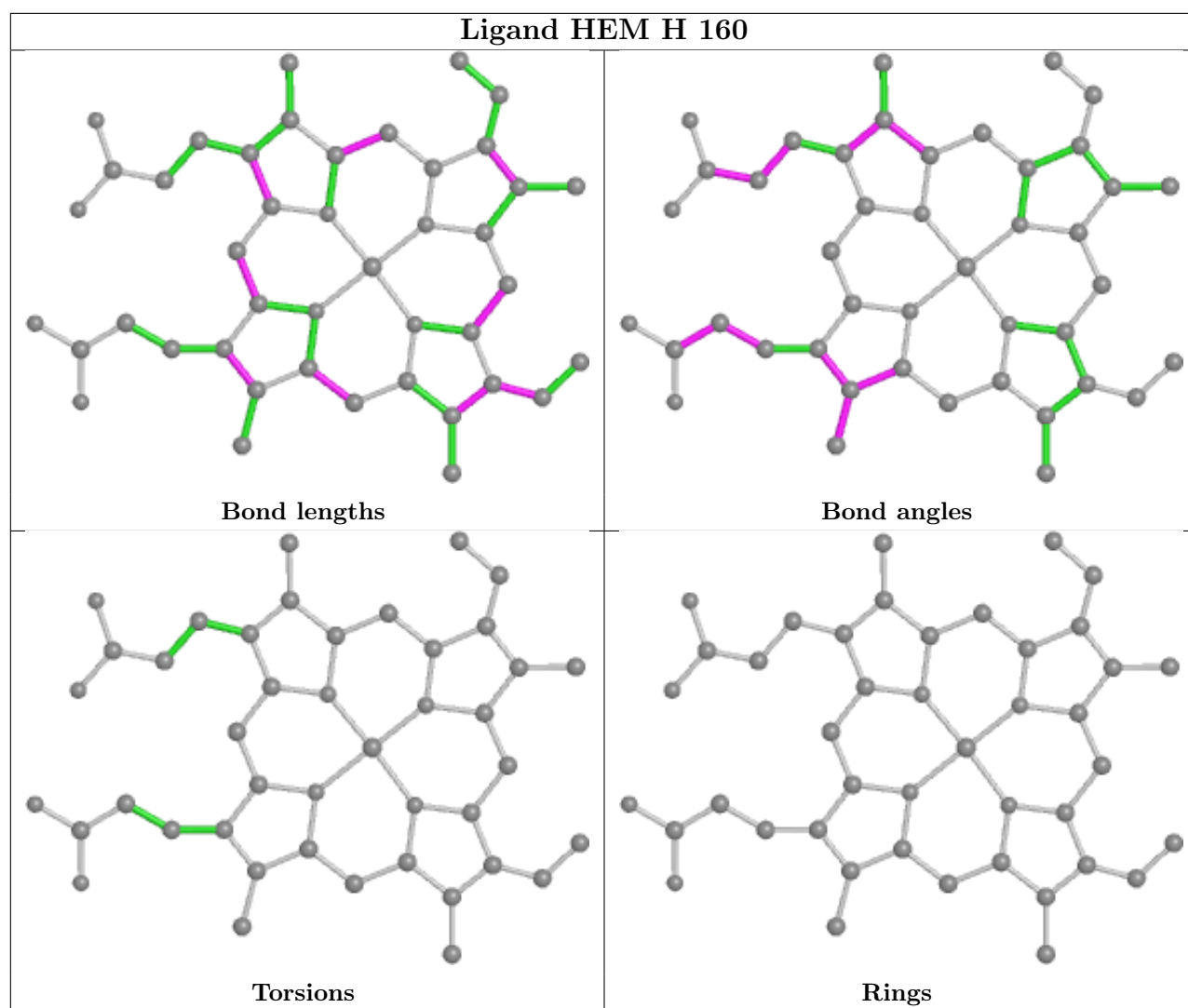




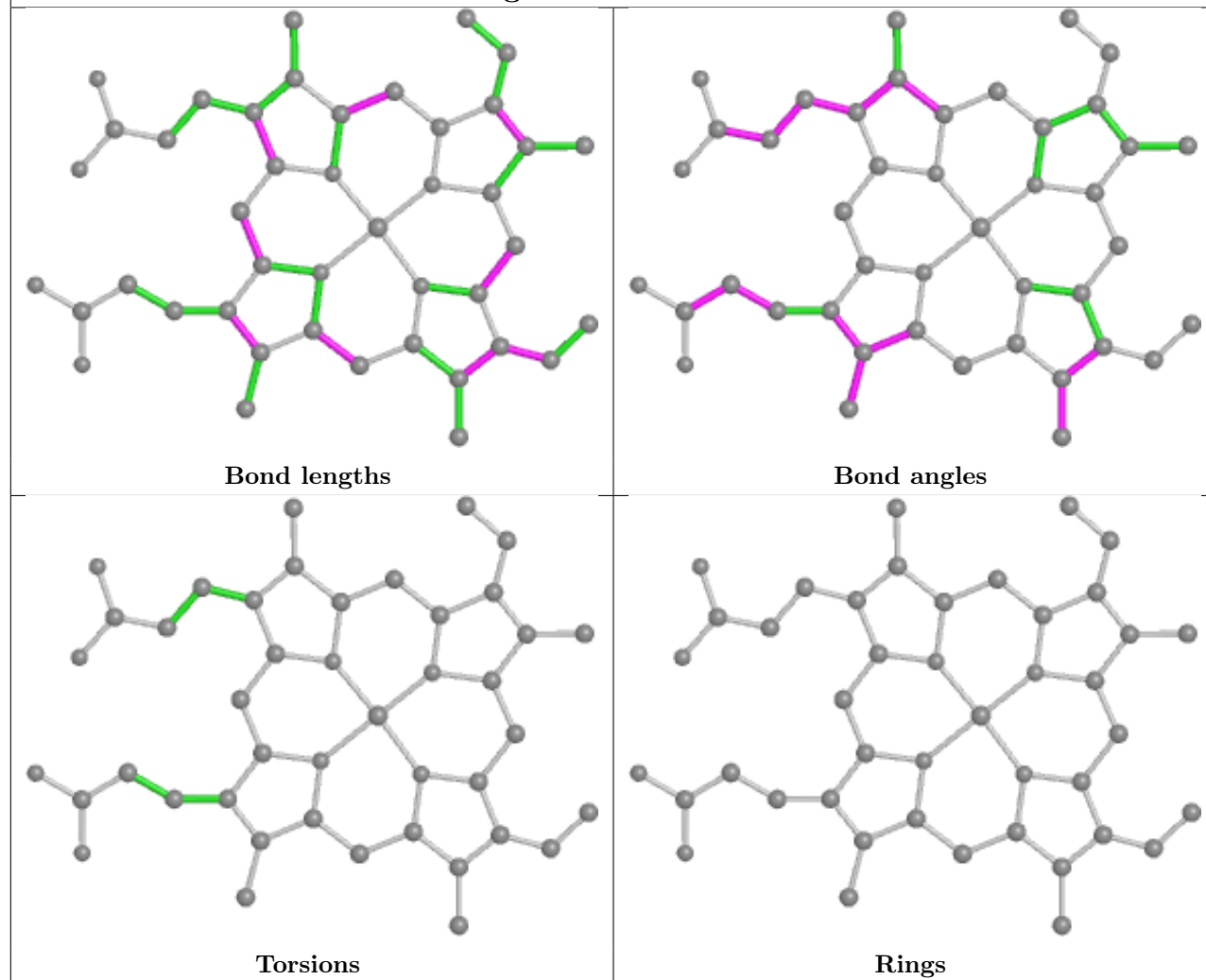


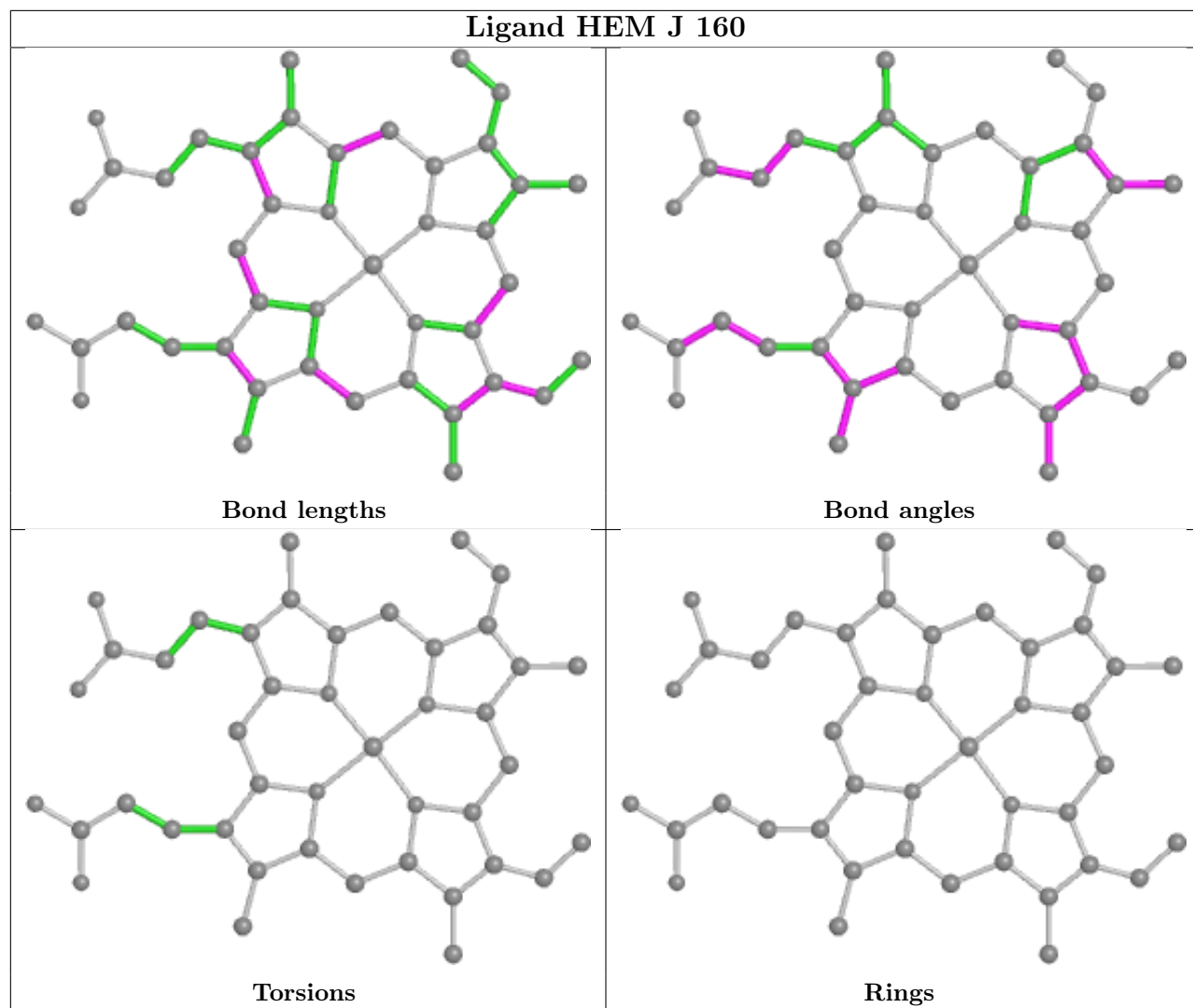


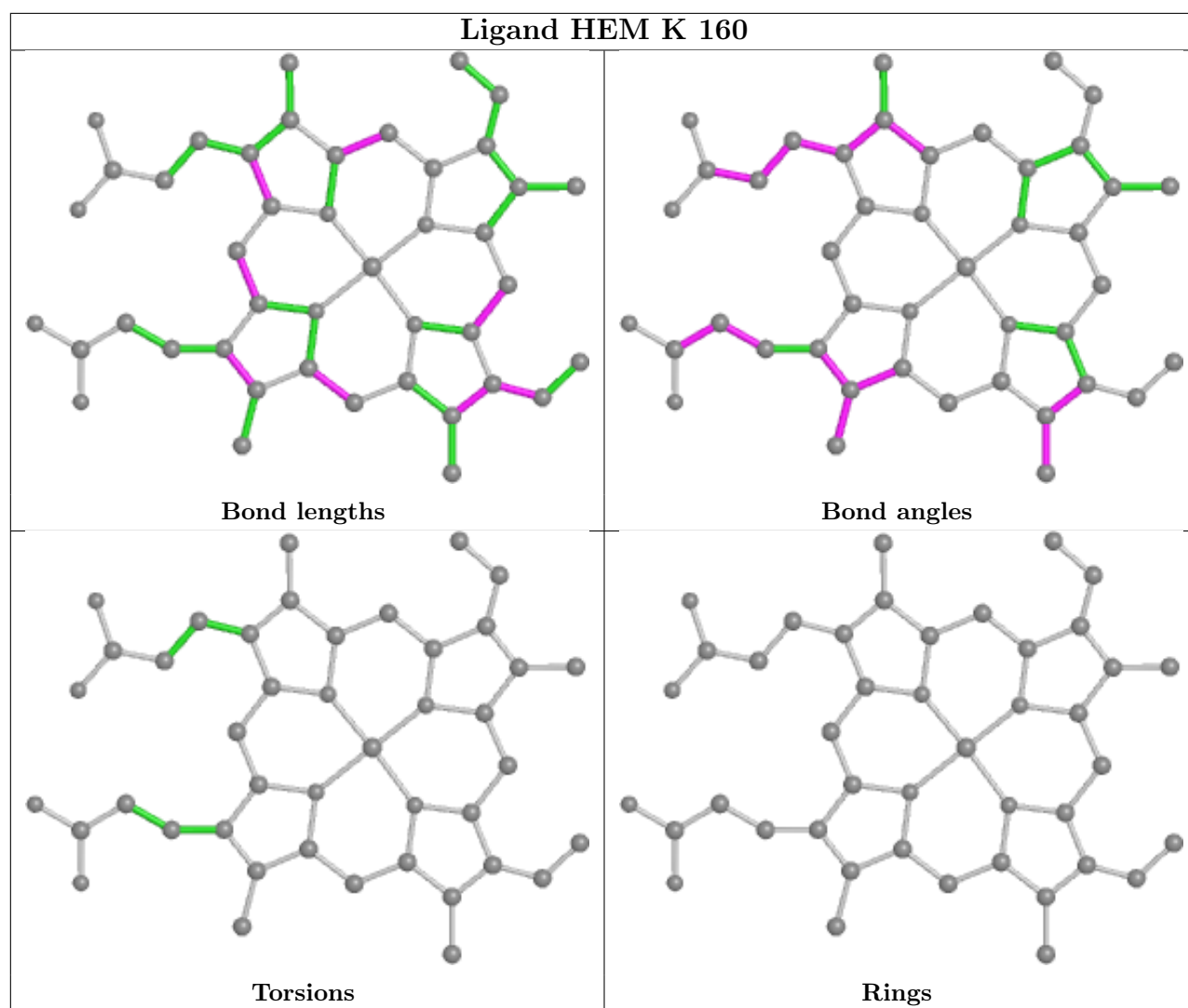


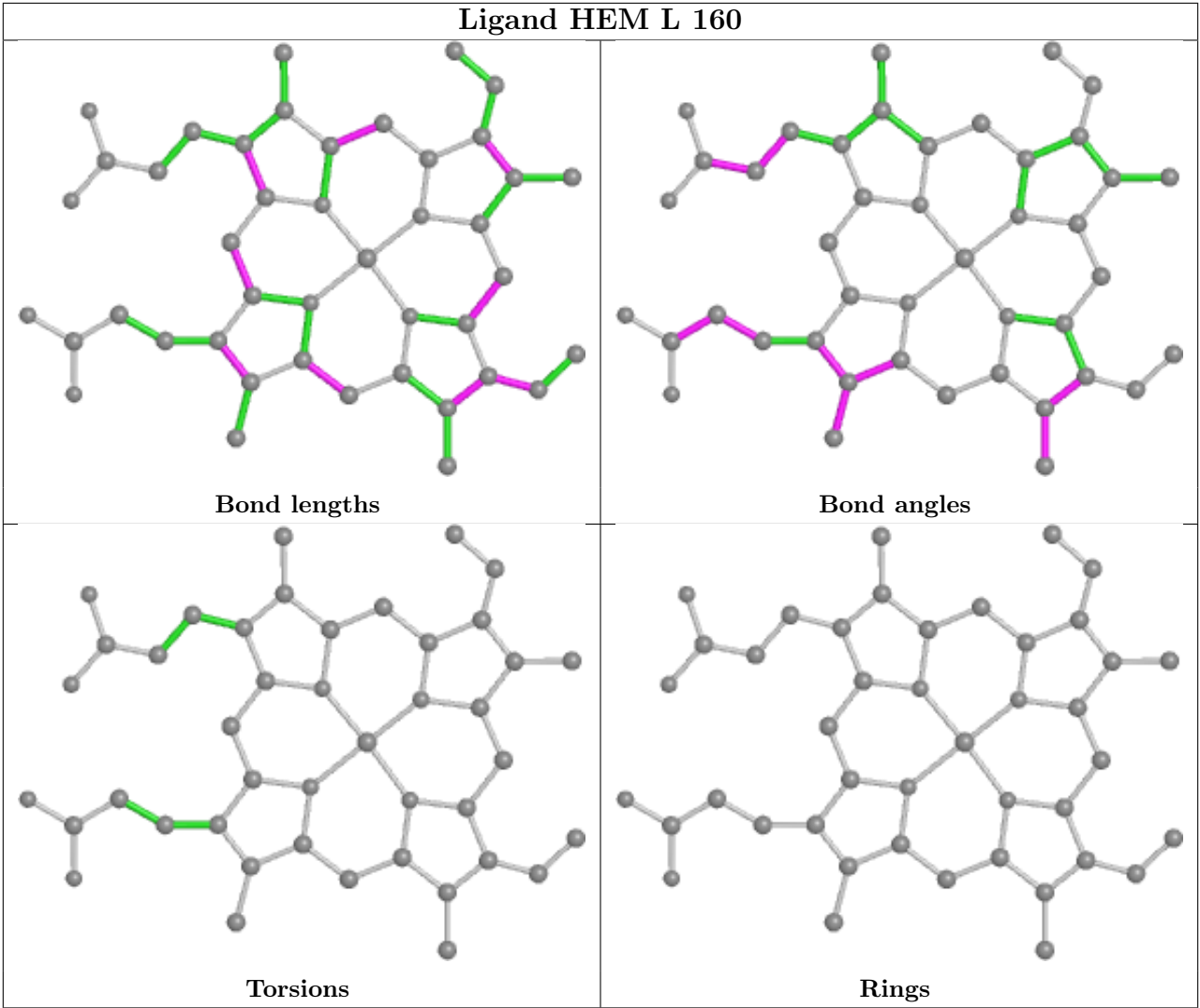


Ligand HEM I 160









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	3:HIS	C	4:GLU	N	3.51

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	147/151 (97%)	0.18	1 (0%) 87 85	15, 30, 55, 65	0
1	E	147/151 (97%)	0.18	4 (2%) 54 48	17, 31, 57, 72	0
1	I	147/151 (97%)	0.20	2 (1%) 75 71	14, 30, 56, 65	0
2	B	145/145 (100%)	0.23	5 (3%) 45 37	16, 29, 52, 87	0
2	F	145/145 (100%)	0.35	7 (4%) 30 23	16, 32, 53, 89	0
2	J	145/145 (100%)	0.46	8 (5%) 25 19	23, 35, 57, 89	0
3	C	149/153 (97%)	0.19	2 (1%) 77 73	15, 31, 52, 74	0
3	G	149/153 (97%)	0.20	2 (1%) 77 73	17, 31, 54, 69	1 (0%)
3	K	149/153 (97%)	0.21	3 (2%) 65 59	19, 37, 61, 75	1 (0%)
4	D	140/140 (100%)	0.05	0 100 100	17, 32, 54, 77	0
4	H	140/140 (100%)	0.23	2 (1%) 75 71	15, 32, 56, 78	0
4	L	140/140 (100%)	0.03	1 (0%) 87 85	17, 32, 54, 76	0
All	All	1743/1767 (98%)	0.21	37 (2%) 63 58	14, 32, 57, 89	2 (0%)

The worst 5 of 37 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	144	HIS	6.8
2	F	145	HIS	6.6
2	B	144	HIS	6.0
2	J	145	HIS	4.6
2	F	144	HIS	4.6

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

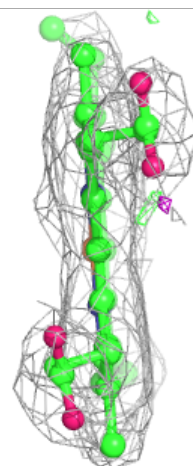
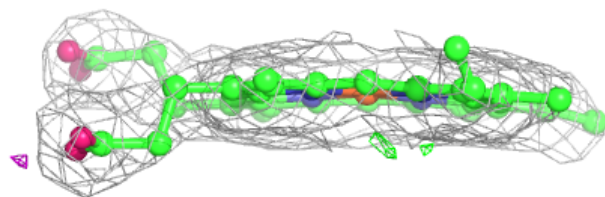
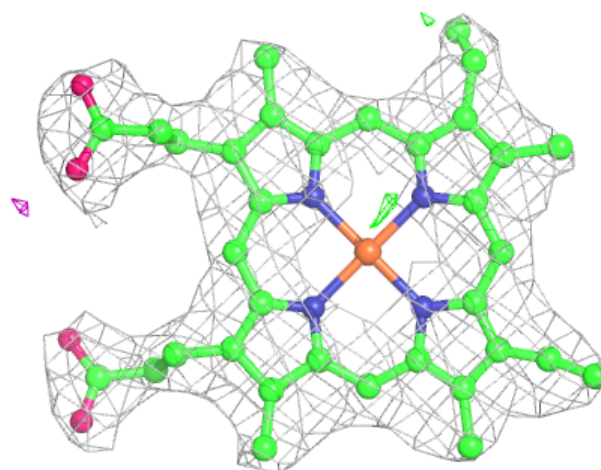
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	CMO	K	3163	2/2	0.77	0.53	40,40,40,43	0
6	CMO	L	3164	2/2	0.89	0.78	38,38,38,44	0
6	CMO	F	2162	2/2	0.91	0.55	31,31,31,36	0
6	CMO	E	2161	2/2	0.92	0.74	41,41,41,43	0
6	CMO	C	1163	2/2	0.92	0.32	30,30,30,37	0
7	PO4	K	154	5/5	0.92	0.21	26,27,28,30	0
7	PO4	C	154	5/5	0.94	0.16	23,27,28,30	0
7	PO4	G	154	5/5	0.95	0.26	23,25,27,29	0
6	CMO	J	3162	2/2	0.95	0.42	36,36,36,38	0
6	CMO	D	1164	2/2	0.95	0.45	32,32,32,37	0
6	CMO	B	1162	2/2	0.95	0.64	33,33,33,37	0
5	HEM	K	160	43/43	0.96	0.17	27,35,41,46	0
6	CMO	G	2163	2/2	0.96	0.36	33,33,33,38	0
6	CMO	H	2164	2/2	0.96	0.36	21,21,21,27	0
5	HEM	J	160	43/43	0.96	0.22	26,37,45,52	0
6	CMO	A	1161	2/2	0.96	0.61	35,35,35,35	0
5	HEM	I	160	43/43	0.97	0.18	20,26,37,42	0
5	HEM	A	160	43/43	0.97	0.18	19,26,34,39	0
5	HEM	L	160	43/43	0.97	0.17	16,24,34,42	0
5	HEM	E	160	43/43	0.97	0.17	18,25,37,43	0
5	HEM	F	160	43/43	0.98	0.17	22,26,32,34	0
5	HEM	H	160	43/43	0.98	0.17	15,21,32,38	0
5	HEM	G	160	43/43	0.98	0.18	18,26,34,42	0
5	HEM	C	160	43/43	0.98	0.17	23,28,36,38	0
5	HEM	D	160	43/43	0.98	0.19	17,24,37,40	0
5	HEM	B	160	43/43	0.98	0.18	14,19,32,38	0
6	CMO	I	3161	2/2	0.98	0.53	41,41,41,42	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.

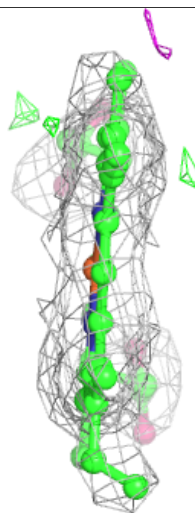
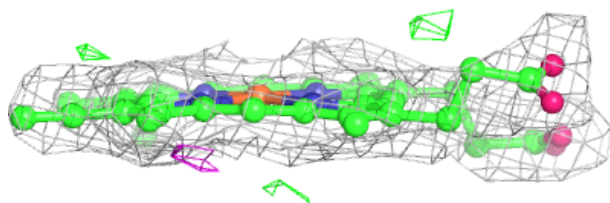
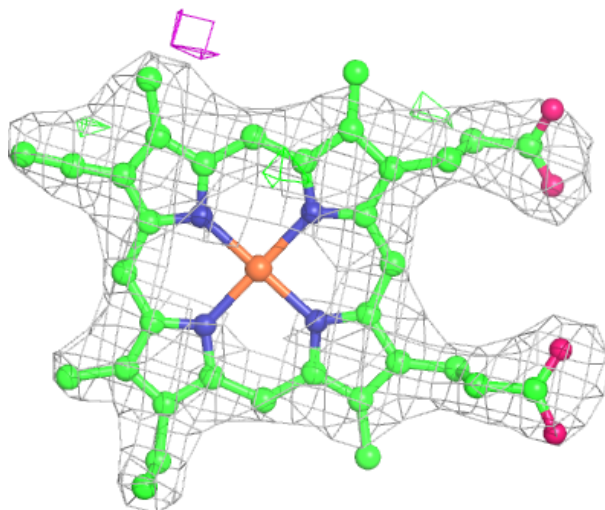
Electron density around HEM K 160:

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



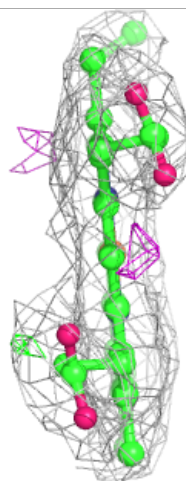
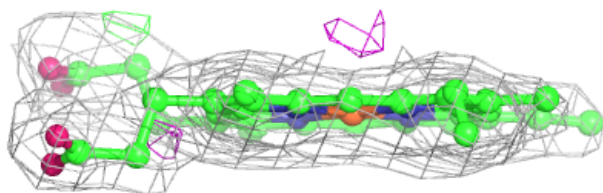
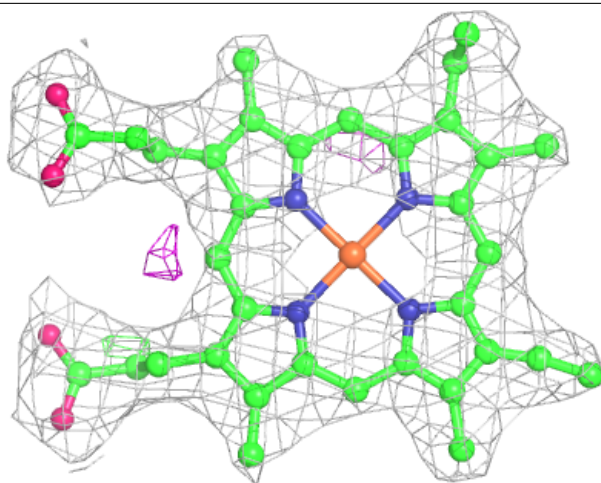
Electron density around HEM J 160:

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and green (positive)



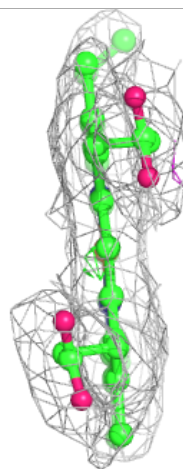
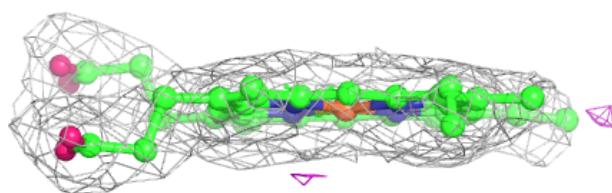
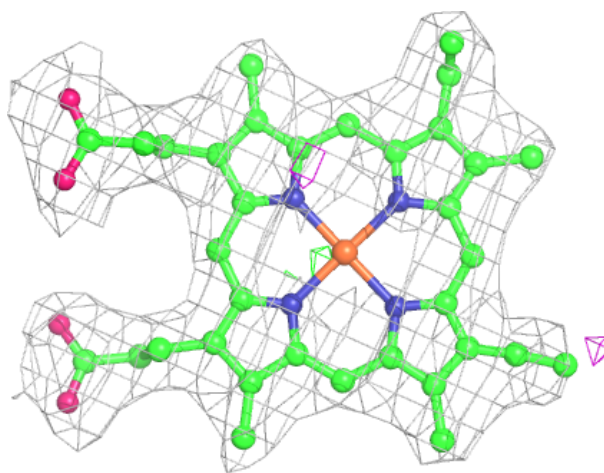
Electron density around HEM I 160:

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



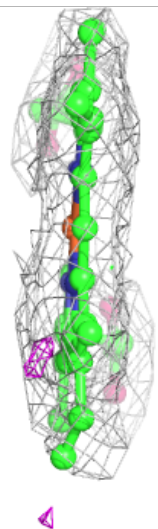
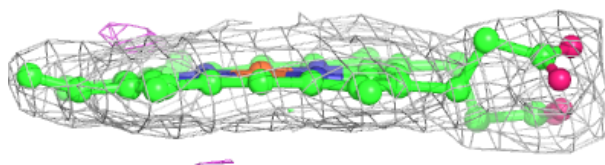
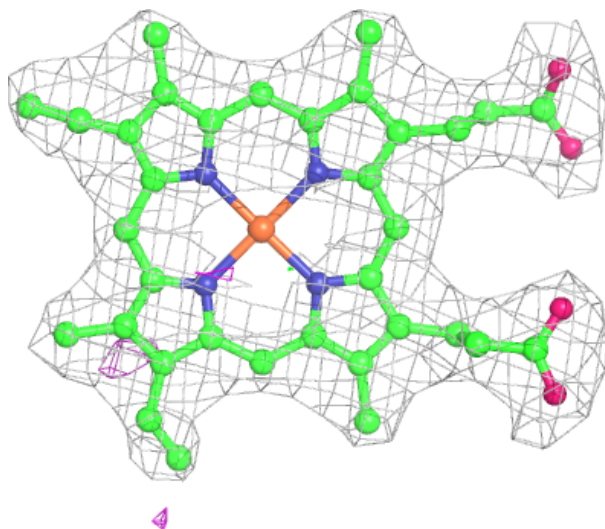
Electron density around HEM A 160:

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



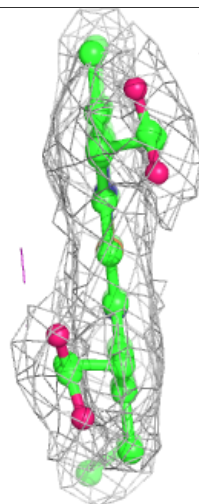
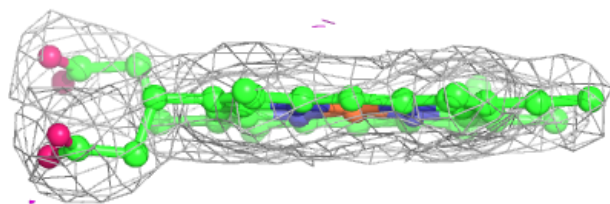
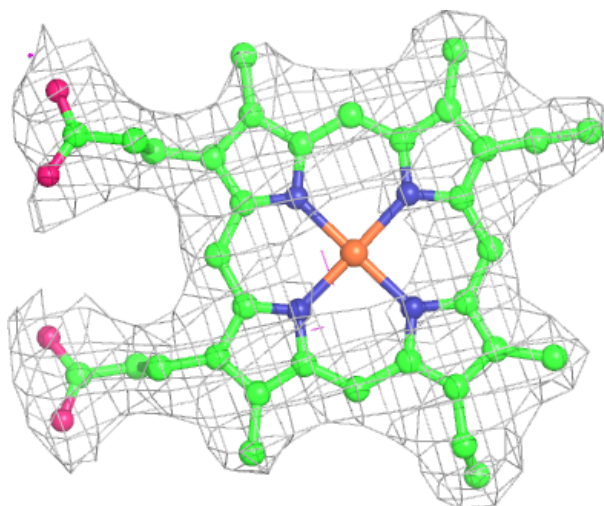
Electron density around HEM L 160:

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



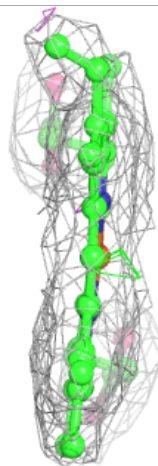
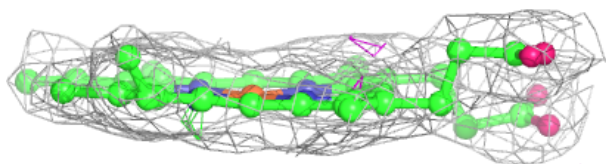
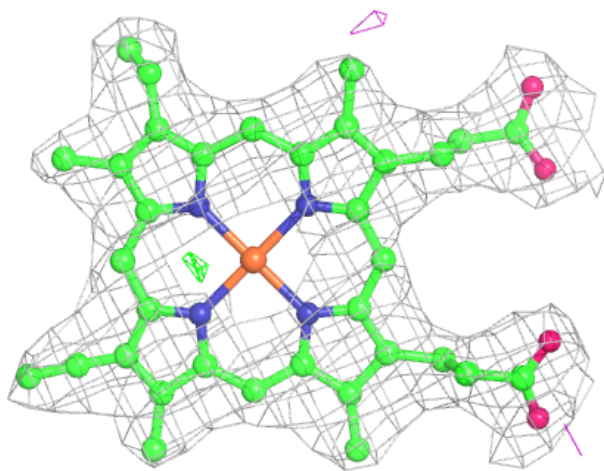
Electron density around HEM E 160:

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and green (positive)



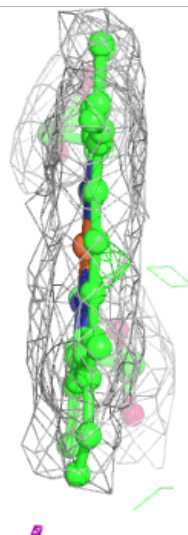
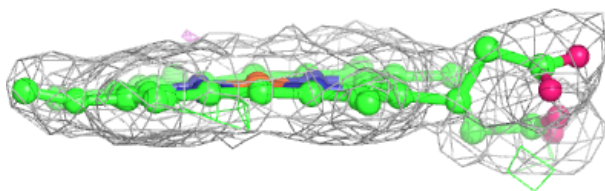
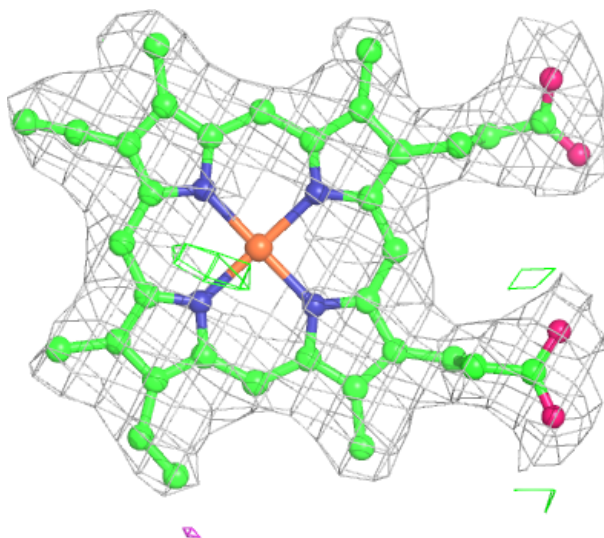
Electron density around HEM F 160:

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



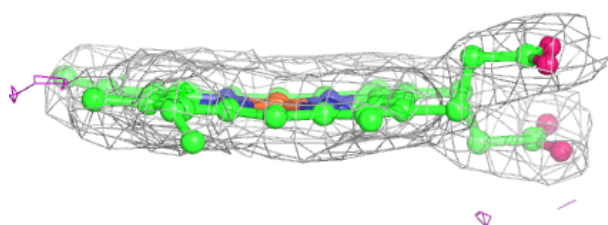
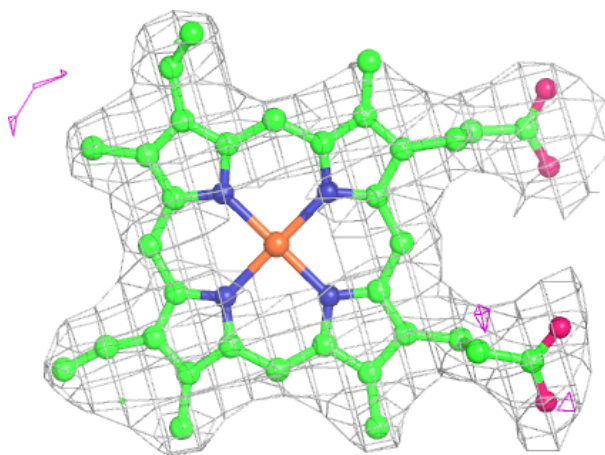
Electron density around HEM H 160:

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



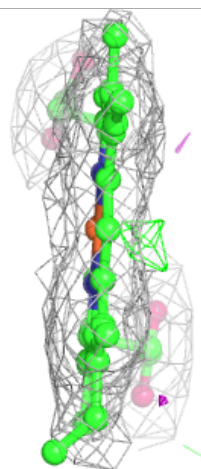
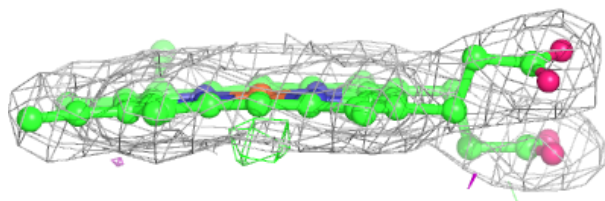
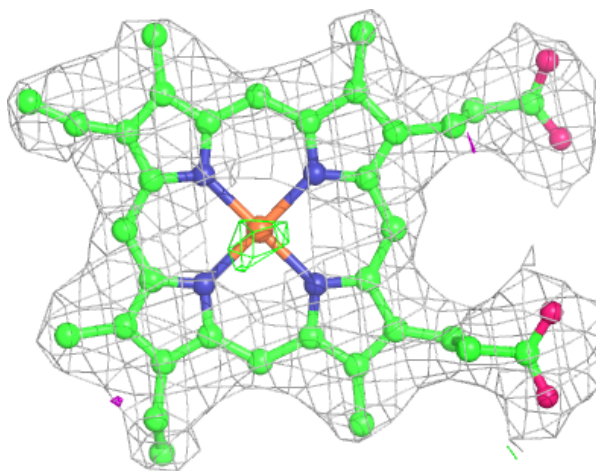
Electron density around HEM G 160:

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



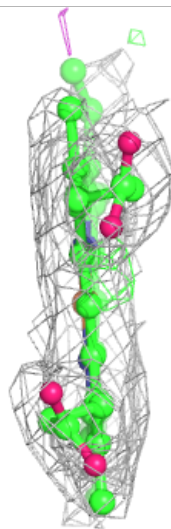
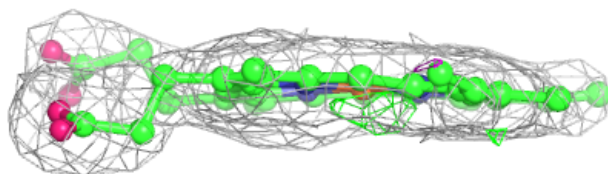
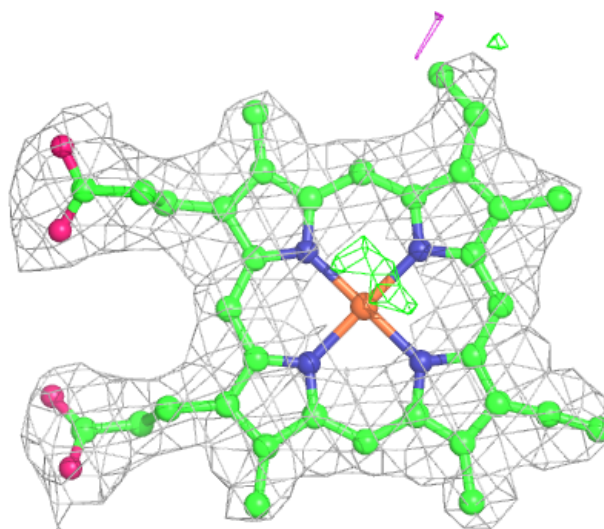
Electron density around HEM C 160:

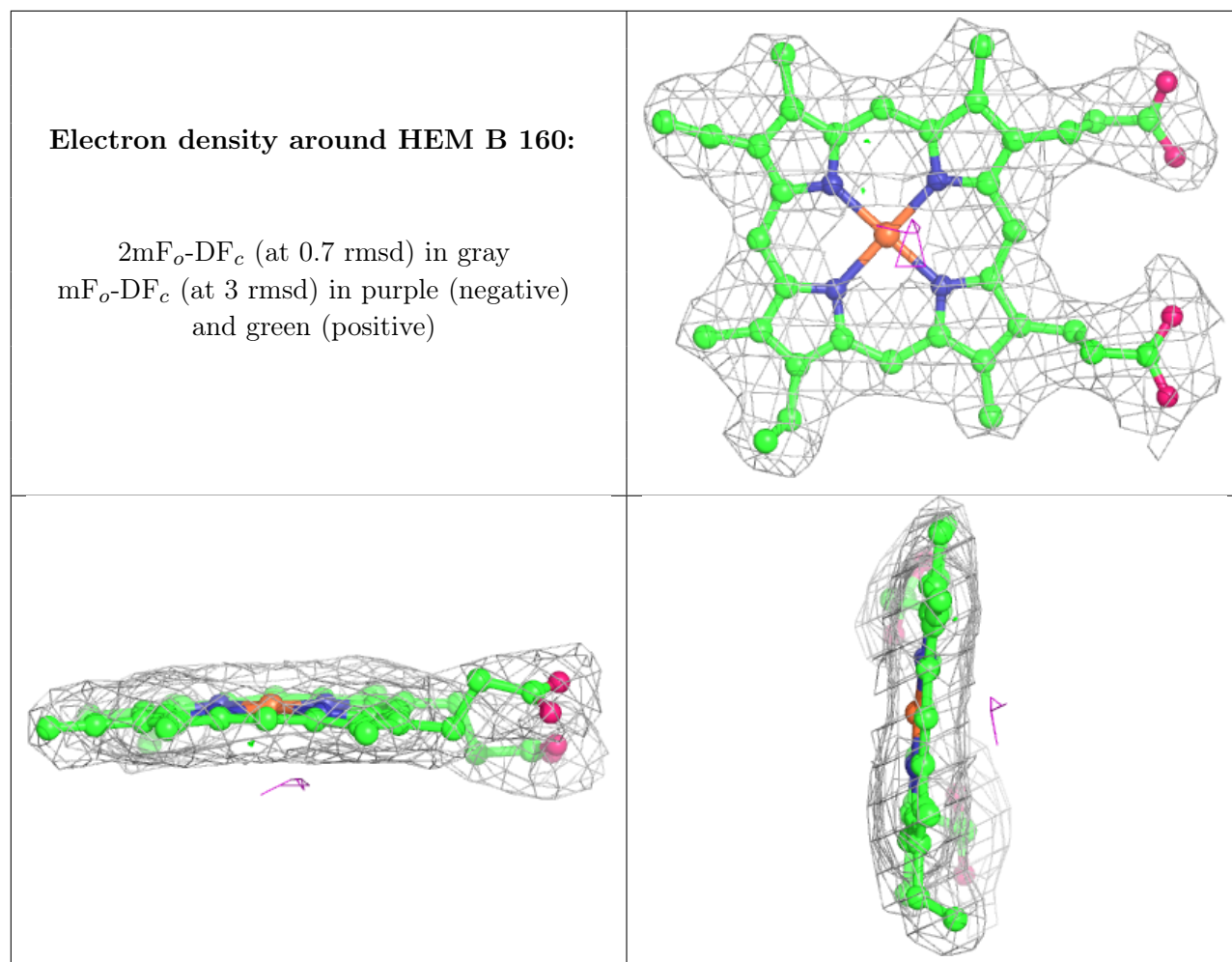
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM D 160:

$2mF_o-DF_c$ (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.