



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 2, 2026 – 10:52 PM EDT

PDB ID : 5KKZ / pdb_00005kkz
Title : Rhodobacter sphaeroides bc1 with famoxadone
Authors : Xia, D.; Esser, L.; Zhou, F.; Tang, W.K.; Yu, C.A.
Deposited on : 2016-06-23
Resolution : 2.97 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 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

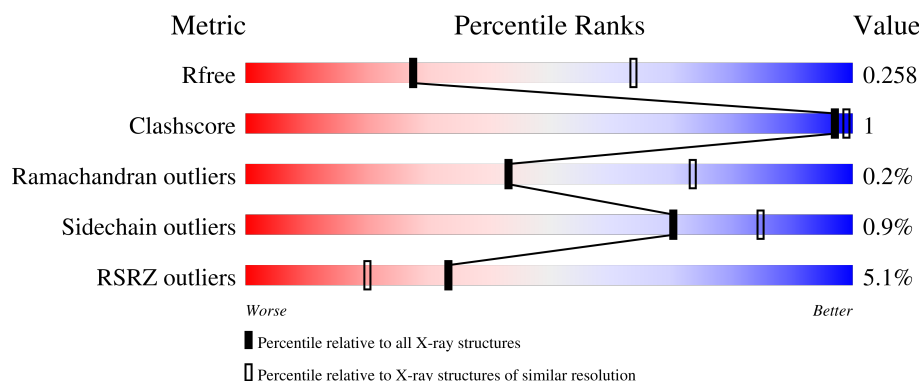
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.97 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	3580 (3.00-2.96)
Clashscore	190562	3904 (3.00-2.96)
Ramachandran outliers	187476	3761 (3.00-2.96)
Sidechain outliers	187428	3764 (3.00-2.96)
RSRZ outliers	180081	3579 (3.00-2.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	445	0% 93% • •
1	E	445	3% 92% • •
1	K	445	2% 93% • •
1	O	445	2% 93% • •
2	B	272	5% 93% • 6%

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Mol	Chain	Length	Quality of chain
2	F	272	
2	L	272	
2	P	272	
3	C	187	
3	G	187	
3	M	187	
3	Q	187	

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
9	HEC	B	1001	X	-	-	-
9	HEC	F	1001	X	-	-	-
9	HEC	L	1001	X	-	-	-
9	HEC	P	1001	X	-	-	-

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 54985 atoms, of which 27067 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 Cytochrome b.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	429	Total	C	H	N	O	S	0	0	0
			6857	2325	3412	548	557	15			
1	E	429	Total	C	H	N	O	S	0	0	0
			6857	2325	3412	548	557	15			
1	K	429	Total	C	H	N	O	S	0	0	0
			6857	2325	3412	548	557	15			
1	O	429	Total	C	H	N	O	S	0	0	0
			6857	2325	3412	548	557	15			

- Molecule 2 is a protein called Cytochrome c1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	256	Total	C	H	N	O	S	0	0	0
			3792	1240	1839	326	374	13			
2	F	256	Total	C	H	N	O	S	0	0	0
			3792	1240	1839	326	374	13			
2	L	256	Total	C	H	N	O	S	0	0	0
			3792	1240	1839	326	374	13			
2	P	256	Total	C	H	N	O	S	0	0	0
			3792	1240	1839	326	374	13			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	98	PRO	ALA	variant	UNP Q02760
B	264	GLY	-	expression tag	UNP Q02760
B	265	THR	-	expression tag	UNP Q02760
B	266	GLY	-	expression tag	UNP Q02760
B	267	HIS	-	expression tag	UNP Q02760
B	268	HIS	-	expression tag	UNP Q02760
B	269	HIS	-	expression tag	UNP Q02760
B	270	HIS	-	expression tag	UNP Q02760

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Chain	Residue	Modelled	Actual	Comment	Reference
B	271	HIS	-	expression tag	UNP Q02760
B	272	HIS	-	expression tag	UNP Q02760
F	98	PRO	ALA	variant	UNP Q02760
F	264	GLY	-	expression tag	UNP Q02760
F	265	THR	-	expression tag	UNP Q02760
F	266	GLY	-	expression tag	UNP Q02760
F	267	HIS	-	expression tag	UNP Q02760
F	268	HIS	-	expression tag	UNP Q02760
F	269	HIS	-	expression tag	UNP Q02760
F	270	HIS	-	expression tag	UNP Q02760
F	271	HIS	-	expression tag	UNP Q02760
F	272	HIS	-	expression tag	UNP Q02760
L	98	PRO	ALA	variant	UNP Q02760
L	264	GLY	-	expression tag	UNP Q02760
L	265	THR	-	expression tag	UNP Q02760
L	266	GLY	-	expression tag	UNP Q02760
L	267	HIS	-	expression tag	UNP Q02760
L	268	HIS	-	expression tag	UNP Q02760
L	269	HIS	-	expression tag	UNP Q02760
L	270	HIS	-	expression tag	UNP Q02760
L	271	HIS	-	expression tag	UNP Q02760
L	272	HIS	-	expression tag	UNP Q02760
P	98	PRO	ALA	variant	UNP Q02760
P	264	GLY	-	expression tag	UNP Q02760
P	265	THR	-	expression tag	UNP Q02760
P	266	GLY	-	expression tag	UNP Q02760
P	267	HIS	-	expression tag	UNP Q02760
P	268	HIS	-	expression tag	UNP Q02760
P	269	HIS	-	expression tag	UNP Q02760
P	270	HIS	-	expression tag	UNP Q02760
P	271	HIS	-	expression tag	UNP Q02760
P	272	HIS	-	expression tag	UNP Q02760

- Molecule 3 is a protein called Ubiquinol-cytochrome c reductase iron-sulfur subunit.

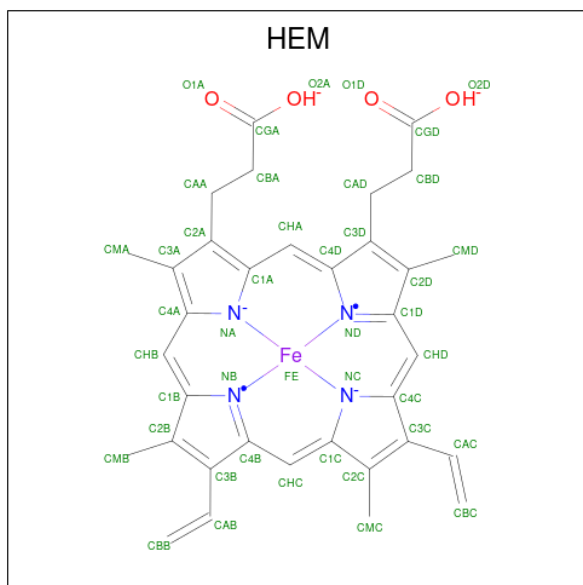
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	179	Total	C	H	N	O	S	0	0	0
			2645	845	1304	237	253	6			
3	G	179	Total	C	H	N	O	S	0	0	0
			2645	845	1304	237	253	6			
3	M	179	Total	C	H	N	O	S	0	0	0
			2645	845	1304	237	253	6			

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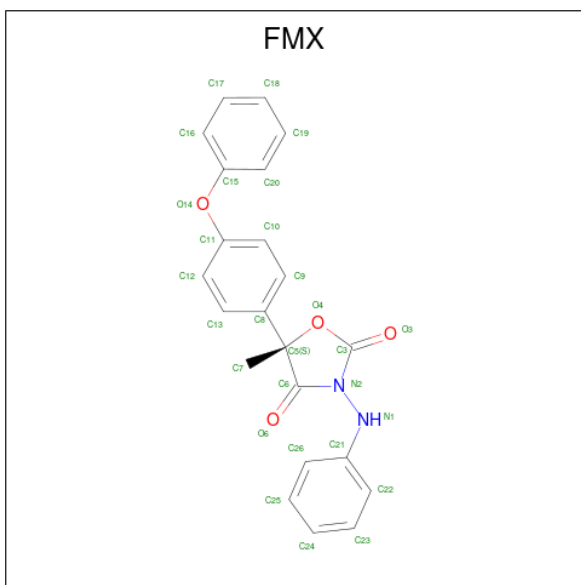
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	Q	179	Total	C	H	N	O	S	0	0	0
			2645	845	1304	237	253	6			

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



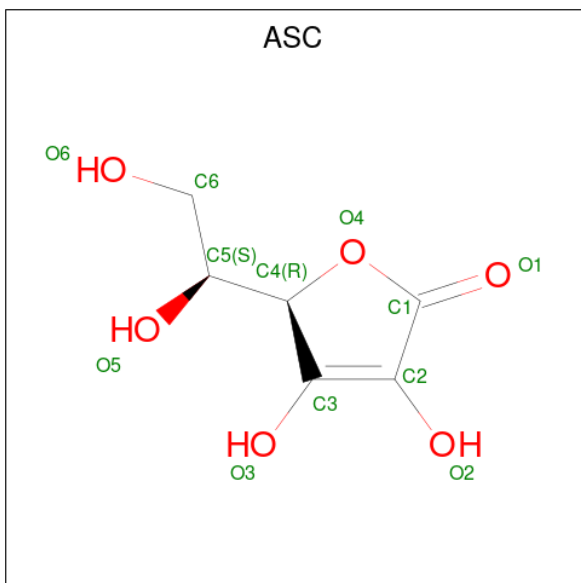
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
4	A	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
4	E	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
4	E	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
4	K	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
4	K	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
4	O	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
4	O	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

- Molecule 5 is FAMOXADONE (CCD ID: FMX) (formula: $C_{22}H_{18}N_2O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	0	0
			46	22	18	2	4		
5	E	1	Total	C	H	N	O	0	0
			46	22	18	2	4		
5	K	1	Total	C	H	N	O	0	0
			46	22	18	2	4		
5	O	1	Total	C	H	N	O	0	0
			46	22	18	2	4		

- Molecule 6 is ASCORBIC ACID (CCD ID: ASC) (formula: $C_6H_8O_6$).

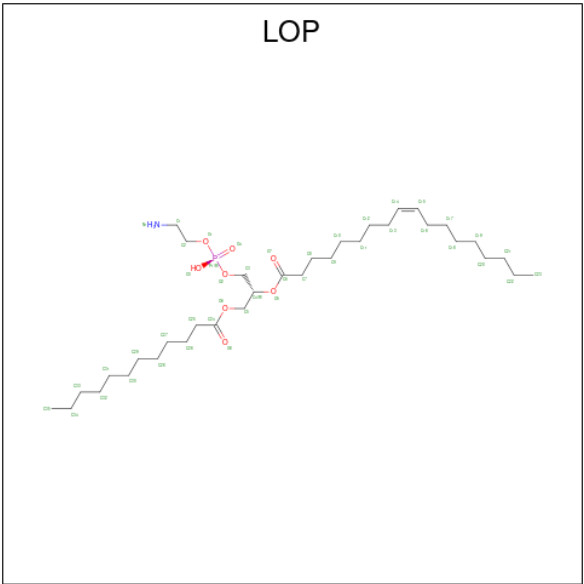


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			19	6	7	6		
6	E	1	Total	C	H	O	0	0
			19	6	7	6		
6	K	1	Total	C	H	O	0	0
			19	6	7	6		
6	O	1	Total	C	H	O	0	0
			19	6	7	6		

- Molecule 7 is STRONTIUM ION (CCD ID: SR) (formula: Sr).

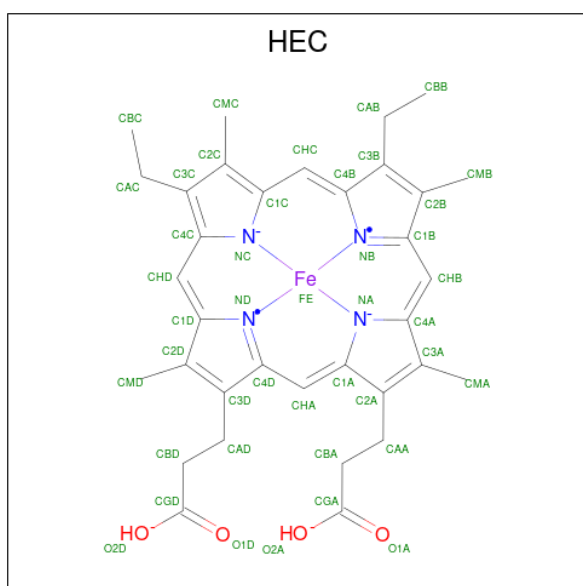
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Sr	0	0
			1	1		
7	B	1	Total	Sr	0	0
			1	1		
7	F	1	Total	Sr	0	0
			1	1		
7	K	1	Total	Sr	0	0
			1	1		
7	L	1	Total	Sr	0	0
			1	1		
7	P	1	Total	Sr	0	0
			1	1		

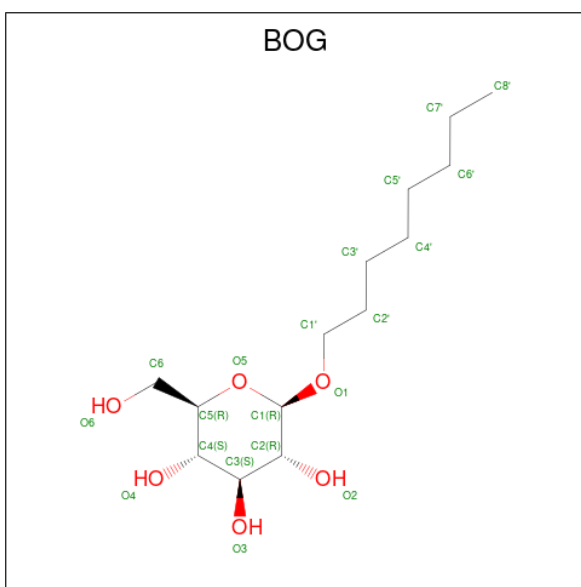
- Molecule 8 is (1R)-2-{[(R)-(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(DODECANOYLOXY)METHYL]ETHYL (9Z)-OCTADEC-9-ENOATE (CCD ID: LOP) (formula: C₃₅H₆₈NO₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	H	N	O	P	
			112	35	67	1	8	1	
8	E	1	Total	C	H	N	O	P	
			112	35	67	1	8	1	
8	K	1	Total	C	H	N	O	P	
			112	35	67	1	8	1	
8	O	1	Total	C	H	N	O	P	
			112	35	67	1	8	1	

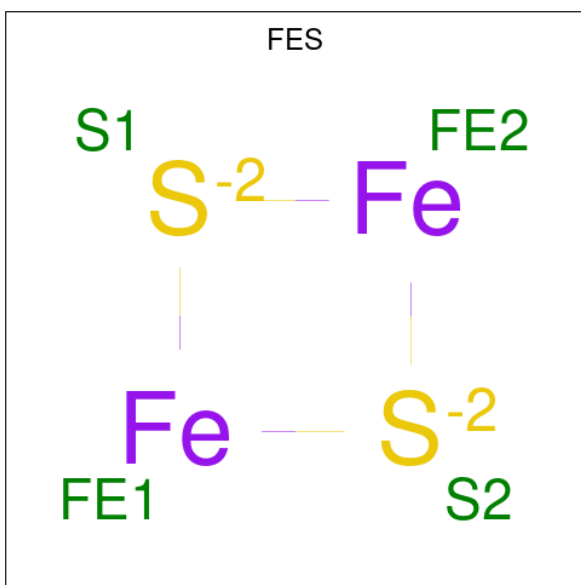
- Molecule 9 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	B	1	Total	C	H	O	0	0
			48	14	28	6		
10	F	1	Total	C	H	O	0	0
			47	14	27	6		
10	K	1	Total	C	H	O	0	0
			48	14	28	6		
10	P	1	Total	C	H	O	0	0
			48	14	28	6		

- Molecule 11 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	C	1	Total Fe S 4 2 2	0	0
11	G	1	Total Fe S 4 2 2	0	0
11	M	1	Total Fe S 4 2 2	0	0
11	Q	1	Total Fe S 4 2 2	0	0

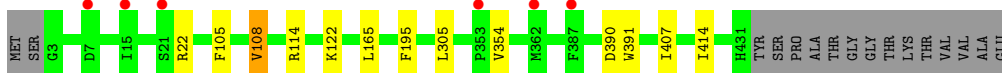
- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	1	Total O 1 1	0	0
12	E	1	Total O 1 1	0	0
12	K	1	Total O 1 1	0	0
12	O	1	Total O 1 1	0	0

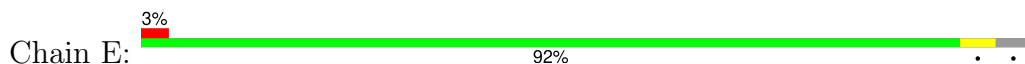
3 Residue-property plots [i](#)

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: Cytochrome b



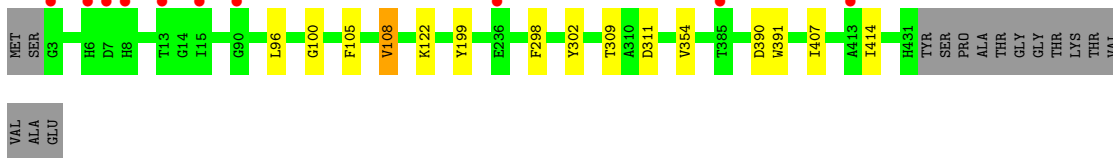
- Molecule 1: Cytochrome b



- Molecule 1: Cytochrome b

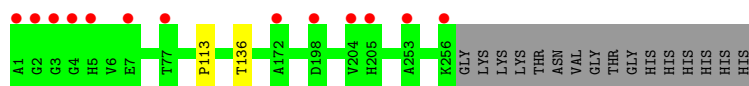


- Molecule 1: Cytochrome b

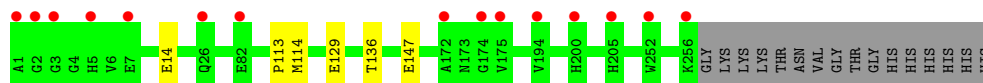


- Molecule 2: Cytochrome c1

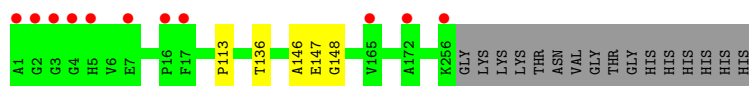




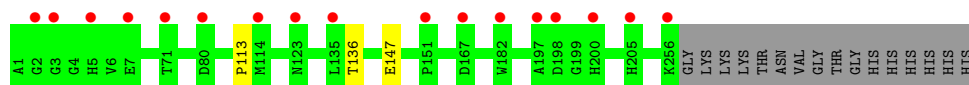
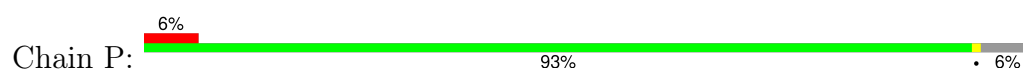
- Molecule 2: Cytochrome c1



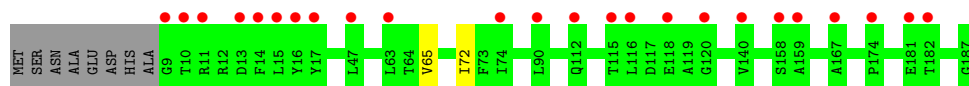
- Molecule 2: Cytochrome c1



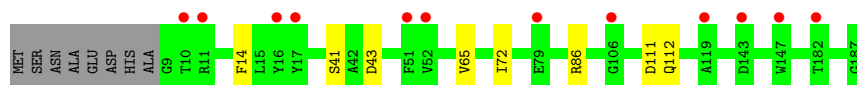
- Molecule 2: Cytochrome c1



- Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit



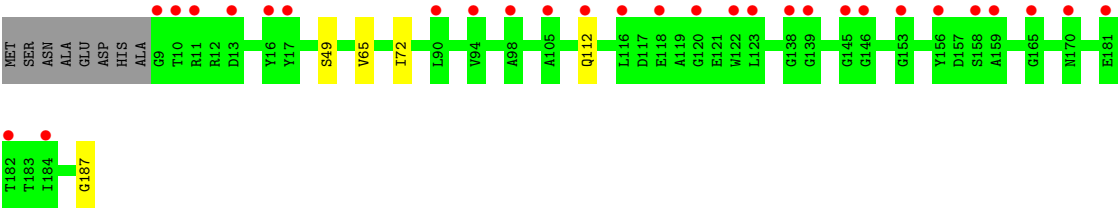
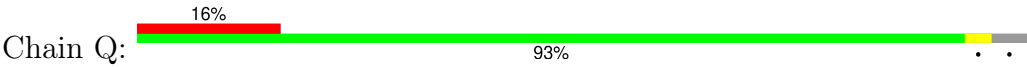
- Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit



- Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit



- Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	120.77Å 128.28Å 128.28Å 63.92° 88.63° 63.38°	Depositor
Resolution (Å)	29.98 – 2.97 29.98 – 2.97	Depositor EDS
% Data completeness (in resolution range)	96.7 (29.98-2.97) 77.6 (29.98-2.97)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.91 (at 2.95Å)	Xtriage
Refinement program	PHENIX (1.11rc1_2513: ???)	Depositor
R, R_{free}	0.215 , 0.258 0.219 , 0.258	Depositor DCC
R_{free} test set	2014 reflections (1.65%)	wwPDB-VP
Wilson B-factor (Å ²)	47.3	Xtriage
Anisotropy	0.256	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 50.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.015 for h,h-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	54985	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 63.55 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.4951e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: LOP, ASC, SR, FMX, BOG, HEM, FES, HEC

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	0.60	0/3576	0.72	0/4906
1	E	0.52	0/3576	0.70	0/4906
1	K	0.61	0/3576	0.75	0/4906
1	O	0.56	0/3576	0.72	0/4906
2	B	0.53	0/2010	0.71	0/2733
2	F	0.45	0/2010	0.63	0/2733
2	L	0.56	0/2010	0.72	0/2733
2	P	0.43	0/2010	0.65	0/2733
3	C	0.44	0/1371	0.68	0/1868
3	G	0.45	0/1371	0.65	1/1868 (0.1%)
3	M	0.49	0/1371	0.67	1/1868 (0.1%)
3	Q	0.44	0/1371	0.66	0/1868
All	All	0.53	0/27828	0.70	2/38028 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	14	PHE	N-CA-C	5.11	117.75	111.82
3	M	14	PHE	N-CA-C	5.05	117.68	111.82

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	3445	3412	3427	7	0
1	E	3445	3412	3427	10	0
1	K	3445	3412	3427	8	0
1	O	3445	3412	3427	7	0
2	B	1953	1839	1848	0	0
2	F	1953	1839	1848	2	0
2	L	1953	1839	1848	1	0
2	P	1953	1839	1848	0	0
3	C	1341	1304	1307	0	0
3	G	1341	1304	1307	3	0
3	M	1341	1304	1307	2	0
3	Q	1341	1304	1307	2	0
4	A	86	60	60	3	0
4	E	86	60	60	1	0
4	K	86	60	60	3	0
4	O	86	60	60	3	0
5	A	28	18	18	0	0
5	E	28	18	18	0	0
5	K	28	18	18	0	0
5	O	28	18	18	0	0
6	A	12	7	7	0	0
6	E	12	7	7	1	0
6	K	12	7	7	1	0
6	O	12	7	7	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	F	1	0	0	0	0
7	K	1	0	0	0	0
7	L	1	0	0	0	0
7	P	1	0	0	0	0
8	A	45	67	67	0	0
8	E	45	67	67	0	0
8	K	45	67	67	1	0
8	O	45	67	67	0	0
9	B	43	32	30	0	0
9	F	43	32	30	1	0
9	L	43	32	30	1	0
9	P	43	32	30	1	0
10	B	20	28	28	0	0
10	F	20	27	28	0	0
10	K	20	28	28	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	P	20	28	28	0	0
11	C	4	0	0	0	0
11	G	4	0	0	0	0
11	M	4	0	0	0	0
11	Q	4	0	0	0	0
12	A	1	0	0	0	0
12	E	1	0	0	0	0
12	K	1	0	0	0	0
12	O	1	0	0	0	0
All	All	27918	27067	27168	49	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 1.

All (49) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:291:HIS:ND1	6:K:1004:ASC:O1	2.18	0.77
1:A:122:LYS:NZ	1:A:354:VAL:O	2.26	0.68
9:P:1001:HEC:HBB3	9:P:1001:HEC:HMB3	1.79	0.64
9:L:1001:HEC:HBB3	9:L:1001:HEC:HMB3	1.83	0.61
3:Q:49:SER:OG	3:Q:187:GLY:O	2.21	0.59
1:O:122:LYS:NZ	1:O:354:VAL:O	2.34	0.58
9:F:1001:HEC:HMB3	9:F:1001:HEC:HBB3	1.87	0.55
1:E:291:HIS:ND1	6:E:1004:ASC:O1	2.40	0.54
4:A:1001:HEM:HHD	4:A:1001:HEM:HBC2	1.88	0.54
4:O:1001:HEM:HBB2	4:O:1001:HEM:HHC	1.90	0.54
1:E:309:THR:OG1	1:E:311:ASP:OD1	2.22	0.53
1:A:114:ARG:NH1	4:A:1002:HEM:O2A	2.38	0.53
4:K:1001:HEM:HBB2	4:K:1001:HEM:HHC	1.90	0.53
1:K:309:THR:OG1	1:K:311:ASP:OD1	2.24	0.52
1:K:122:LYS:NZ	1:K:354:VAL:O	2.33	0.51
3:M:41:SER:OG	3:M:43:ASP:OD1	2.24	0.49
4:K:1001:HEM:HBC2	4:K:1001:HEM:HHD	1.95	0.48
1:K:358:ARG:NH2	8:K:1006:LOP:O1	2.47	0.47
1:O:390:ASP:OD1	1:O:391:TRP:N	2.46	0.47
4:A:1001:HEM:HBB2	4:A:1001:HEM:HHC	1.98	0.46
1:A:390:ASP:OD1	1:A:391:TRP:N	2.49	0.46
1:A:22:ARG:NE	1:E:126:GLU:OE1	2.47	0.46
1:E:122:LYS:NZ	1:E:354:VAL:O	2.42	0.45
1:E:379:TRP:NE1	2:F:114:MET:O	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:1001:HEM:HBD2	4:K:1001:HEM:HHA	1.98	0.44
1:E:425:GLU:O	1:E:429:ASN:ND2	2.42	0.44
3:Q:112:GLN:OE1	3:Q:112:GLN:N	2.50	0.43
1:A:105:PHE:HA	1:A:108:VAL:HG22	2.00	0.43
2:F:14:GLU:OE2	2:F:129:GLU:OE2	2.36	0.43
4:O:1001:HEM:HBD2	4:O:1001:HEM:HHA	1.98	0.43
1:K:422:ALA:N	1:K:426:GLU:OE1	2.46	0.43
1:E:165:LEU:HD22	1:E:305:LEU:HD11	2.01	0.42
1:E:292:ILE:O	1:E:292:ILE:HG13	2.19	0.42
3:G:41:SER:OG	3:G:43:ASP:OD1	2.31	0.42
1:O:309:THR:OG1	1:O:311:ASP:OD1	2.31	0.42
1:O:298:PHE:CE2	1:O:302:TYR:HB2	2.55	0.42
1:A:195:PHE:HE2	1:E:195:PHE:HE2	1.66	0.42
1:O:96:LEU:O	1:O:100:GLY:N	2.48	0.41
1:O:199:TYR:CZ	4:O:1001:HEM:HBC1	2.55	0.41
3:G:112:GLN:OE1	3:G:112:GLN:N	2.50	0.41
3:G:86:ARG:HG2	3:G:111:ASP:HB3	2.02	0.41
3:M:112:GLN:OE1	3:M:112:GLN:N	2.48	0.41
1:A:165:LEU:HD22	1:A:305:LEU:HD11	2.03	0.41
1:K:292:ILE:O	1:K:292:ILE:HG13	2.21	0.41
1:E:199:TYR:CE2	4:E:1001:HEM:HBC1	2.55	0.41
2:L:146:ALA:O	2:L:148:GLY:N	2.54	0.40
1:K:54:CYS:SG	1:K:103:LEU:HG	2.61	0.40
1:K:359:TYR:CZ	1:K:421:PRO:HD3	2.56	0.40
1:O:105:PHE:HA	1:O:108:VAL:HG22	2.03	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	427/445 (96%)	422 (99%)	5 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	427/445 (96%)	422 (99%)	5 (1%)	0	100	100
1	K	427/445 (96%)	422 (99%)	5 (1%)	0	100	100
1	O	427/445 (96%)	422 (99%)	5 (1%)	0	100	100
2	B	254/272 (93%)	244 (96%)	9 (4%)	1 (0%)	30	62
2	F	254/272 (93%)	244 (96%)	8 (3%)	2 (1%)	16	47
2	L	254/272 (93%)	244 (96%)	8 (3%)	2 (1%)	16	47
2	P	254/272 (93%)	244 (96%)	8 (3%)	2 (1%)	16	47
3	C	177/187 (95%)	168 (95%)	9 (5%)	0	100	100
3	G	177/187 (95%)	169 (96%)	8 (4%)	0	100	100
3	M	177/187 (95%)	170 (96%)	7 (4%)	0	100	100
3	Q	177/187 (95%)	169 (96%)	8 (4%)	0	100	100
All	All	3432/3616 (95%)	3340 (97%)	85 (2%)	7 (0%)	43	73

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	113	PRO
2	B	113	PRO
2	L	113	PRO
2	P	147	GLU
2	F	147	GLU
2	L	147	GLU
2	P	113	PRO

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	354/366 (97%)	351 (99%)	3 (1%)	73	86
1	E	354/366 (97%)	350 (99%)	4 (1%)	65	82
1	K	354/366 (97%)	350 (99%)	4 (1%)	65	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	O	354/366 (97%)	351 (99%)	3 (1%)	73	86
2	B	203/216 (94%)	202 (100%)	1 (0%)	81	89
2	F	203/216 (94%)	202 (100%)	1 (0%)	81	89
2	L	203/216 (94%)	202 (100%)	1 (0%)	81	89
2	P	203/216 (94%)	202 (100%)	1 (0%)	81	89
3	C	138/144 (96%)	136 (99%)	2 (1%)	59	80
3	G	138/144 (96%)	136 (99%)	2 (1%)	59	80
3	M	138/144 (96%)	136 (99%)	2 (1%)	59	80
3	Q	138/144 (96%)	136 (99%)	2 (1%)	59	80
All	All	2780/2904 (96%)	2754 (99%)	26 (1%)	70	85

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	VAL
1	A	407	ILE
1	A	414	ILE
2	B	136	THR
3	C	65	VAL
3	C	72	ILE
1	E	108	VAL
1	E	385	THR
1	E	407	ILE
1	E	414	ILE
2	F	136	THR
3	G	65	VAL
3	G	72	ILE
1	K	6	HIS
1	K	108	VAL
1	K	407	ILE
1	K	414	ILE
2	L	136	THR
3	M	65	VAL
3	M	72	ILE
1	O	108	VAL
1	O	407	ILE
1	O	414	ILE
2	P	136	THR
3	Q	65	VAL

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Mol	Chain	Res	Type
3	Q	72	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	192	ASN
1	A	316	GLN
1	A	319	ASN
2	B	22	GLN
2	B	26	GLN
2	B	30	GLN
2	B	111	HIS
1	E	20	HIS
1	E	86	ASN
1	E	192	ASN
1	E	316	GLN
2	F	22	GLN
2	F	200	HIS
1	K	20	HIS
1	K	192	ASN
1	K	319	ASN
2	L	22	GLN
2	L	200	HIS
1	O	192	ASN
1	O	319	ASN
2	P	22	GLN
2	P	111	HIS
3	Q	37	GLN
3	Q	185	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 38 ligands modelled in this entry, 6 are monoatomic - leaving 32 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	HEM	K	1001	1	50,50,50	1.44	8 (16%)	67,82,82	1.34	12 (17%)
5	FMX	E	1003	-	30,31,31	0.92	3 (10%)	36,44,44	1.21	4 (11%)
11	FES	G	1001	3	0,4,4	-	-	-		
5	FMX	K	1003	-	30,31,31	0.85	1 (3%)	36,44,44	1.37	7 (19%)
8	LOP	E	1005	-	44,44,44	1.07	2 (4%)	47,49,49	1.32	8 (17%)
4	HEM	A	1002	1	50,50,50	1.65	8 (16%)	67,82,82	1.16	7 (10%)
9	HEC	F	1001	2	50,50,50	1.66	6 (12%)	68,82,82	1.50	14 (20%)
6	ASC	A	1004	-	12,12,12	0.89	0	17,17,17	2.56	5 (29%)
4	HEM	A	1001	1	50,50,50	1.57	10 (20%)	67,82,82	1.22	8 (11%)
4	HEM	O	1001	1	50,50,50	1.46	8 (16%)	67,82,82	1.46	13 (19%)
4	HEM	E	1002	1	50,50,50	1.59	7 (14%)	67,82,82	1.18	8 (11%)
11	FES	M	1001	3	0,4,4	-	-	-		
5	FMX	A	1003	-	30,31,31	0.97	2 (6%)	36,44,44	1.67	7 (19%)
11	FES	C	1001	3	0,4,4	-	-	-		
4	HEM	O	1002	1	50,50,50	1.55	7 (14%)	67,82,82	1.18	5 (7%)
10	BOG	B	1003	-	20,20,20	1.01	1 (5%)	25,25,25	1.25	3 (12%)
10	BOG	P	1003	-	20,20,20	1.00	1 (5%)	25,25,25	1.02	2 (8%)
11	FES	Q	1001	3	0,4,4	-	-	-		
10	BOG	K	1007	-	20,20,20	1.11	2 (10%)	25,25,25	1.01	1 (4%)
8	LOP	K	1006	-	44,44,44	1.14	2 (4%)	47,49,49	1.10	6 (12%)
6	ASC	E	1004	-	12,12,12	0.88	0	17,17,17	2.46	8 (47%)
10	BOG	F	1003	-	20,20,20	1.08	1 (5%)	25,25,25	1.19	3 (12%)
4	HEM	K	1002	1	50,50,50	1.78	8 (16%)	67,82,82	1.21	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	FMX	O	1003	-	30,31,31	1.07	3 (10%)	36,44,44	1.54	5 (13%)
8	LOP	A	1006	-	44,44,44	1.02	1 (2%)	47,49,49	1.45	6 (12%)
9	HEC	P	1001	2	50,50,50	1.78	6 (12%)	68,82,82	1.27	6 (8%)
8	LOP	O	1005	-	44,44,44	1.15	2 (4%)	47,49,49	1.18	5 (10%)
9	HEC	L	1001	2	50,50,50	1.66	8 (16%)	68,82,82	1.39	10 (14%)
6	ASC	O	1004	-	12,12,12	1.06	0	17,17,17	2.71	6 (35%)
9	HEC	B	1001	2	50,50,50	1.72	7 (14%)	68,82,82	1.41	12 (17%)
4	HEM	E	1001	1	50,50,50	1.38	7 (14%)	67,82,82	1.19	11 (16%)
6	ASC	K	1004	-	12,12,12	0.94	0	17,17,17	2.35	7 (41%)

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	HEM	K	1001	1	-	6/14/54/54	-
5	FMX	E	1003	-	-	0/14/33/33	0/4/4/4
11	FES	G	1001	3	-	-	0/1/1/1
5	FMX	K	1003	-	-	0/14/33/33	0/4/4/4
8	LOP	E	1005	-	-	23/48/48/48	-
4	HEM	A	1002	1	-	5/14/54/54	-
9	HEC	F	1001	2	1/1/7/7	6/14/54/54	-
6	ASC	A	1004	-	-	2/6/22/22	0/1/1/1
4	HEM	A	1001	1	-	6/14/54/54	-
4	HEM	O	1001	1	-	5/14/54/54	-
4	HEM	E	1002	1	-	2/14/54/54	-
11	FES	M	1001	3	-	-	0/1/1/1
5	FMX	A	1003	-	-	0/14/33/33	0/4/4/4
11	FES	C	1001	3	-	-	0/1/1/1
4	HEM	O	1002	1	-	2/14/54/54	-
10	BOG	B	1003	-	-	5/11/31/31	0/1/1/1
10	BOG	P	1003	-	-	6/11/31/31	0/1/1/1
11	FES	Q	1001	3	-	-	0/1/1/1
10	BOG	K	1007	-	-	6/11/31/31	0/1/1/1
8	LOP	K	1006	-	-	18/48/48/48	-
6	ASC	E	1004	-	-	4/6/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	BOG	F	1003	-	-	4/11/31/31	0/1/1/1
4	HEM	K	1002	1	-	2/14/54/54	-
5	FMX	O	1003	-	-	0/14/33/33	0/4/4/4
8	LOP	A	1006	-	-	22/48/48/48	-
9	HEC	P	1001	2	1/1/7/7	6/14/54/54	-
8	LOP	O	1005	-	-	14/48/48/48	-
9	HEC	L	1001	2	1/1/7/7	5/14/54/54	-
6	ASC	O	1004	-	-	3/6/22/22	0/1/1/1
9	HEC	B	1001	2	1/1/7/7	7/14/54/54	-
4	HEM	E	1001	1	-	5/14/54/54	-
6	ASC	K	1004	-	-	4/6/22/22	0/1/1/1

All (111) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	F	1001	HEC	C3D-C2D	6.92	1.51	1.36
4	K	1002	HEM	FE-NA	6.83	2.17	1.95
9	B	1001	HEC	C3D-C2D	6.64	1.51	1.36
9	L	1001	HEC	C3D-C2D	6.63	1.51	1.36
9	P	1001	HEC	C3D-C2D	6.50	1.50	1.36
9	P	1001	HEC	FE-ND	6.24	2.14	1.94
4	A	1002	HEM	FE-NC	6.09	2.15	1.95
9	F	1001	HEC	FE-NB	5.20	2.10	1.94
4	E	1002	HEM	FE-NA	5.15	2.12	1.95
4	K	1002	HEM	FE-NB	5.06	2.10	1.94
4	O	1002	HEM	FE-NC	4.99	2.11	1.95
4	A	1001	HEM	FE-NB	4.91	2.10	1.94
4	E	1002	HEM	FE-NB	4.36	2.08	1.94
9	B	1001	HEC	FE-ND	3.93	2.07	1.94
4	O	1001	HEM	CMC-C2C	3.87	1.58	1.50
9	L	1001	HEC	FE-NC	3.86	2.07	1.95
4	O	1002	HEM	FE-ND	3.83	2.06	1.94
4	O	1001	HEM	FE-NB	3.72	2.06	1.94
9	L	1001	HEC	FE-NB	3.72	2.06	1.94
4	K	1002	HEM	CMB-C2B	3.61	1.58	1.50
4	K	1002	HEM	CAC-C3C	3.54	1.56	1.47
4	E	1002	HEM	CAB-C3B	3.43	1.56	1.47
9	P	1001	HEC	FE-NC	3.42	2.06	1.95
4	K	1002	HEM	CAB-C3B	3.37	1.56	1.47
4	A	1001	HEM	CMC-C2C	3.34	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	1002	HEM	CAC-C3C	3.33	1.56	1.47
4	E	1001	HEM	CMB-C2B	3.32	1.57	1.50
10	P	1003	BOG	O5-C1	3.32	1.50	1.41
4	K	1001	HEM	CAC-C3C	3.28	1.56	1.47
4	A	1002	HEM	FE-ND	3.25	2.04	1.94
10	B	1003	BOG	O5-C1	3.23	1.50	1.41
10	F	1003	BOG	O5-C1	3.22	1.50	1.41
4	E	1002	HEM	CMC-C2C	3.11	1.57	1.50
8	K	1006	LOP	C25-C24	3.11	1.59	1.50
4	A	1002	HEM	CAB-C3B	3.10	1.55	1.47
5	K	1003	FMX	C21-N1	3.09	1.46	1.41
4	A	1001	HEM	C3B-C2B	-3.06	1.31	1.37
10	K	1007	BOG	O5-C1	3.00	1.49	1.41
9	B	1001	HEC	FE-NA	2.97	2.04	1.95
4	O	1002	HEM	CAC-C3C	2.96	1.55	1.47
5	O	1003	FMX	C21-N1	2.95	1.45	1.41
4	E	1001	HEM	CAC-C3C	2.93	1.55	1.47
4	O	1001	HEM	CAC-C3C	2.93	1.55	1.47
4	K	1001	HEM	CMC-C2C	2.90	1.56	1.50
8	E	1005	LOP	C7-C6	2.90	1.59	1.50
4	E	1002	HEM	CMB-C2B	2.90	1.56	1.50
4	O	1002	HEM	CAB-C3B	2.87	1.55	1.47
4	K	1001	HEM	CMB-C2B	2.86	1.56	1.50
4	O	1001	HEM	CMD-C2D	2.86	1.56	1.50
4	O	1002	HEM	CMB-C2B	2.84	1.56	1.50
9	B	1001	HEC	CMB-C2B	2.84	1.56	1.50
8	O	1005	LOP	C7-C6	2.82	1.58	1.50
4	O	1001	HEM	CMB-C2B	2.81	1.56	1.50
4	E	1001	HEM	CMA-C3A	2.79	1.56	1.50
4	A	1001	HEM	CAC-C3C	2.77	1.54	1.47
4	K	1001	HEM	FE-ND	2.74	2.03	1.94
4	E	1001	HEM	FE-ND	2.72	2.03	1.94
9	F	1001	HEC	FE-ND	2.71	2.03	1.94
8	K	1006	LOP	C7-C6	2.71	1.58	1.50
4	A	1002	HEM	C3C-C2C	-2.66	1.31	1.37
4	O	1001	HEM	CMA-C3A	2.66	1.56	1.50
4	O	1002	HEM	CMA-C3A	2.66	1.56	1.50
9	P	1001	HEC	CMC-C2C	2.65	1.56	1.50
9	B	1001	HEC	CMC-C2C	2.64	1.56	1.50
4	A	1001	HEM	CMA-C3A	2.63	1.56	1.50
5	O	1003	FMX	O6-C6	-2.63	1.18	1.22
8	A	1006	LOP	C7-C6	2.60	1.58	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	1001	HEC	FE-NC	2.57	2.03	1.95
4	A	1002	HEM	CMB-C2B	2.55	1.56	1.50
8	O	1005	LOP	C25-C24	2.49	1.57	1.50
9	P	1001	HEC	CMB-C2B	2.48	1.55	1.50
4	K	1001	HEM	CAB-C3B	2.47	1.54	1.47
5	E	1003	FMX	C21-N1	2.46	1.45	1.41
4	K	1002	HEM	CMC-C2C	2.45	1.55	1.50
10	K	1007	BOG	O3-C3	2.45	1.49	1.43
4	E	1001	HEM	CMC-C2C	2.44	1.55	1.50
4	A	1001	HEM	CMD-C2D	2.38	1.55	1.50
5	E	1003	FMX	O6-C6	-2.38	1.18	1.22
4	A	1002	HEM	CAC-C3C	2.37	1.53	1.47
4	K	1001	HEM	CMD-C2D	2.36	1.55	1.50
4	K	1001	HEM	C2A-C3A	-2.35	1.32	1.38
4	K	1002	HEM	C1B-C2B	2.34	1.49	1.44
4	K	1001	HEM	CMA-C3A	2.33	1.55	1.50
5	A	1003	FMX	C3-N2	-2.32	1.38	1.43
9	F	1001	HEC	FE-NA	2.31	2.02	1.95
9	F	1001	HEC	CMC-C2C	2.31	1.55	1.50
4	A	1001	HEM	CAB-C3B	2.27	1.53	1.47
9	P	1001	HEC	FE-NA	2.26	2.02	1.95
9	L	1001	HEC	CMB-C2B	2.26	1.55	1.50
4	A	1002	HEM	CMA-C3A	2.26	1.55	1.50
4	O	1001	HEM	C2A-C3A	-2.26	1.33	1.38
9	F	1001	HEC	FE-NC	2.21	2.02	1.95
4	A	1001	HEM	CMB-C2B	2.19	1.55	1.50
8	E	1005	LOP	C25-C24	2.18	1.57	1.50
9	L	1001	HEC	CMC-C2C	2.18	1.55	1.50
4	A	1002	HEM	CAA-C2A	2.18	1.56	1.51
4	A	1001	HEM	C2A-C3A	-2.18	1.33	1.38
5	E	1003	FMX	C3-N2	-2.17	1.38	1.43
4	E	1001	HEM	FE-NB	2.15	2.01	1.94
5	O	1003	FMX	C3-N2	-2.12	1.38	1.43
4	E	1001	HEM	C2A-C3A	-2.12	1.33	1.38
5	A	1003	FMX	C21-N1	2.11	1.44	1.41
4	O	1002	HEM	CMC-C2C	2.07	1.55	1.50
9	L	1001	HEC	FE-ND	2.06	2.01	1.94
9	L	1001	HEC	CMD-C2D	2.05	1.55	1.50
9	L	1001	HEC	CAC-C3C	2.05	1.56	1.51
4	O	1001	HEM	C3B-C2B	-2.03	1.33	1.37
4	K	1002	HEM	C2A-C3A	-2.02	1.33	1.38
4	E	1002	HEM	CMA-C3A	2.02	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	1001	HEC	C4B-NB	-2.02	1.36	1.40
4	A	1001	HEM	FE-ND	-2.01	1.88	1.94

All (196) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	O	1004	ASC	C4-O4-C1	-7.49	101.06	109.27
6	A	1004	ASC	O5-C5-C4	-5.59	100.15	110.74
5	A	1003	FMX	O4-C3-O3	5.57	129.24	122.54
6	A	1004	ASC	C4-O4-C1	-5.37	103.38	109.27
6	O	1004	ASC	O5-C5-C4	-5.13	101.01	110.74
9	F	1001	HEC	C1D-ND-C4D	5.01	111.14	105.21
9	B	1001	HEC	CAA-CBA-CGA	-4.70	101.21	113.67
5	O	1003	FMX	O6-C6-N2	4.48	130.81	124.43
8	A	1006	LOP	O6-C24-C25	4.46	125.44	111.83
9	P	1001	HEC	C1D-ND-C4D	4.42	110.45	105.21
6	E	1004	ASC	C4-O4-C1	-4.38	104.47	109.27
6	K	1004	ASC	C4-O4-C1	-4.35	104.50	109.27
6	A	1004	ASC	O4-C1-C2	-4.30	106.06	109.86
6	K	1004	ASC	O4-C1-O1	4.17	126.76	121.27
6	A	1004	ASC	O4-C4-C3	-4.14	99.61	103.76
4	O	1001	HEM	CAD-C3D-C4D	4.09	131.83	124.70
8	A	1006	LOP	O6-C5-C4	4.09	120.18	108.40
9	L	1001	HEC	CMD-C2D-C1D	4.07	131.39	125.03
6	K	1004	ASC	C6-C5-C4	-4.03	105.08	111.86
6	E	1004	ASC	O6-C6-C5	-3.98	102.80	111.16
5	K	1003	FMX	O4-C5-C7	3.93	111.71	106.54
6	E	1004	ASC	O4-C1-C2	-3.88	106.43	109.86
8	A	1006	LOP	O5-C6-C7	3.83	119.77	111.48
5	O	1003	FMX	O4-C3-O3	3.81	127.13	122.54
8	E	1005	LOP	O6-C5-C4	3.76	119.23	108.40
4	A	1002	HEM	CMC-C2C-C1C	-3.72	118.17	124.73
9	L	1001	HEC	C1D-ND-C4D	3.72	109.61	105.21
6	K	1004	ASC	O5-C5-C4	-3.72	103.69	110.74
9	B	1001	HEC	C1D-ND-C4D	3.70	109.59	105.21
6	E	1004	ASC	C5-C4-C3	-3.69	107.94	114.71
9	F	1001	HEC	CAA-CBA-CGA	-3.59	104.15	113.67
9	P	1001	HEC	CAA-CBA-CGA	-3.54	104.28	113.67
5	O	1003	FMX	C21-N1-N2	3.50	122.68	116.20
5	A	1003	FMX	O4-C5-C7	3.48	111.12	106.54
9	L	1001	HEC	CBD-CAD-C3D	-3.45	102.99	112.53
6	E	1004	ASC	O5-C5-C4	-3.44	104.22	110.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	O	1001	HEM	C3C-C2C-C1C	-3.37	103.85	107.05
8	O	1005	LOP	O6-C24-O8	-3.36	115.22	123.63
9	L	1001	HEC	C1D-C2D-C3D	-3.36	103.45	106.98
9	L	1001	HEC	CAC-C3C-C4C	-3.33	120.33	124.91
6	O	1004	ASC	O4-C1-C2	-3.32	106.92	109.86
8	E	1005	LOP	O6-C24-C25	3.32	121.95	111.83
6	O	1004	ASC	O4-C1-O1	3.31	125.64	121.27
4	K	1001	HEM	CBA-CAA-C2A	-3.31	103.39	112.53
5	K	1003	FMX	C9-C8-C5	3.30	126.18	120.71
9	F	1001	HEC	C2A-C1A-NA	-3.29	107.15	110.32
4	A	1001	HEM	C4C-C3C-C2C	3.23	109.61	106.81
9	B	1001	HEC	CAC-C3C-C4C	-3.22	120.48	124.91
8	O	1005	LOP	O6-C24-C25	3.22	121.64	111.83
6	E	1004	ASC	O4-C1-O1	3.21	125.50	121.27
4	O	1002	HEM	CMB-C2B-C1B	-3.20	120.03	125.03
5	E	1003	FMX	O4-C3-O3	3.15	126.33	122.54
9	P	1001	HEC	CMD-C2D-C1D	3.12	129.91	125.03
6	A	1004	ASC	O4-C1-O1	3.10	125.36	121.27
9	L	1001	HEC	CAC-C3C-C2C	3.10	131.79	126.89
4	K	1002	HEM	C3D-C4D-ND	-3.07	106.81	110.17
4	K	1002	HEM	C4D-ND-C1D	3.06	108.83	105.21
4	O	1001	HEM	C3B-C4B-NB	-3.06	107.27	109.47
4	K	1001	HEM	O2D-CGD-CBD	3.05	123.65	114.00
9	L	1001	HEC	CMC-C2C-C1C	-3.02	120.82	125.42
10	B	1003	BOG	O1-C1-C2	2.99	112.82	108.27
5	K	1003	FMX	O6-C6-N2	2.95	128.63	124.43
8	O	1005	LOP	C5-C4-C3	2.95	118.66	111.78
9	L	1001	HEC	CAA-CBA-CGA	-2.93	105.89	113.67
8	A	1006	LOP	C5-C4-C3	2.93	118.61	111.78
6	O	1004	ASC	O5-C5-C6	2.87	115.56	109.03
8	E	1005	LOP	C5-C4-C3	2.87	118.48	111.78
5	A	1003	FMX	C13-C8-C5	-2.87	115.97	120.71
4	O	1002	HEM	CMC-C2C-C1C	-2.86	119.69	124.73
5	E	1003	FMX	O4-C5-C7	2.84	110.28	106.54
9	F	1001	HEC	CAC-C3C-C4C	-2.84	121.01	124.91
5	K	1003	FMX	C13-C8-C5	-2.83	116.02	120.71
5	A	1003	FMX	O6-C6-N2	2.82	128.44	124.43
4	O	1001	HEM	CBA-CAA-C2A	-2.82	104.75	112.53
8	K	1006	LOP	O6-C24-O8	-2.79	116.65	123.63
4	A	1001	HEM	CHD-C4C-NC	-2.78	121.42	124.45
4	A	1002	HEM	CMB-C2B-C1B	-2.77	120.70	125.03
5	E	1003	FMX	C21-N1-N2	2.76	121.31	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	1001	HEC	CAC-C3C-C2C	2.75	131.23	126.89
9	F	1001	HEC	CMD-C2D-C1D	2.75	129.32	125.03
4	E	1002	HEM	CMB-C2B-C1B	-2.73	120.76	125.03
4	O	1001	HEM	CAD-C3D-C2D	-2.71	122.79	127.87
8	E	1005	LOP	O5-C6-C7	2.71	117.35	111.48
5	A	1003	FMX	C9-C8-C5	2.70	125.19	120.71
4	E	1001	HEM	C4C-C3C-C2C	2.70	109.16	106.81
8	K	1006	LOP	C5-C4-C3	2.68	118.02	111.78
10	F	1003	BOG	C6-C5-C4	-2.66	106.49	113.02
5	K	1003	FMX	O4-C3-O3	2.65	125.73	122.54
4	A	1002	HEM	CAA-CBA-CGA	-2.64	106.67	113.67
6	K	1004	ASC	O1-C1-C2	-2.61	125.42	129.33
4	E	1001	HEM	CHD-C4C-NC	2.61	127.29	124.45
4	O	1001	HEM	CHA-C4D-ND	-2.60	121.15	124.37
4	O	1001	HEM	C4B-C3B-C2B	2.57	109.64	107.28
4	K	1001	HEM	CAC-C3C-C4C	2.57	130.95	124.82
9	P	1001	HEC	CAD-C3D-C4D	2.57	129.17	124.70
4	K	1001	HEM	CHD-C4C-NC	-2.55	121.67	124.45
8	K	1006	LOP	O6-C24-C25	2.55	119.61	111.83
8	O	1005	LOP	O5-C6-O7	-2.55	117.75	123.70
4	E	1002	HEM	CHD-C4C-NC	-2.52	121.70	124.45
5	A	1003	FMX	C9-C10-C11	-2.49	116.88	119.73
4	A	1001	HEM	CAC-C3C-C2C	-2.48	120.37	128.43
6	K	1004	ASC	O4-C1-C2	-2.47	107.67	109.86
9	F	1001	HEC	CAD-C3D-C4D	2.46	128.98	124.70
8	O	1005	LOP	O6-C5-C4	2.45	115.47	108.40
8	A	1006	LOP	O5-C6-O7	-2.44	117.99	123.70
10	F	1003	BOG	O1-C1-C2	2.43	111.97	108.27
4	O	1002	HEM	C3D-C4D-ND	-2.42	107.51	110.17
5	K	1003	FMX	O3-C3-N2	2.41	128.18	119.95
4	E	1002	HEM	C3D-C4D-ND	-2.41	107.53	110.17
4	O	1001	HEM	O1A-CGA-CBA	-2.40	115.47	123.09
8	K	1006	LOP	C5-O6-C24	2.40	125.91	117.12
4	E	1001	HEM	CAC-C3C-C4C	-2.39	119.11	124.82
9	B	1001	HEC	CAD-C3D-C4D	2.39	128.87	124.70
6	K	1004	ASC	C5-C4-C3	-2.39	110.33	114.71
10	K	1007	BOG	C3-C4-C5	2.39	114.56	110.23
9	F	1001	HEC	O1D-CGD-CBD	-2.38	115.53	123.09
4	K	1002	HEM	O2D-CGD-O1D	2.38	129.46	123.33
10	F	1003	BOG	O5-C5-C4	2.38	113.98	109.70
4	A	1001	HEM	CHD-C4C-C3C	2.37	129.21	125.21
4	O	1001	HEM	CHC-C4B-C3B	2.37	129.80	125.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1001	HEM	CBA-CAA-C2A	-2.36	106.02	112.53
5	A	1003	FMX	C21-N1-N2	2.35	120.54	116.20
5	O	1003	FMX	O4-C5-C7	2.34	109.62	106.54
9	L	1001	HEC	CAD-C3D-C4D	2.33	128.76	124.70
4	E	1002	HEM	C2A-C1A-NA	-2.33	107.57	110.15
4	K	1001	HEM	CAC-C3C-C2C	-2.32	120.88	128.43
4	K	1002	HEM	CMC-C2C-C1C	-2.32	120.64	124.73
9	B	1001	HEC	CHB-C4A-NA	-2.32	121.93	124.45
4	E	1001	HEM	CMB-C2B-C1B	-2.31	121.42	125.03
9	F	1001	HEC	CBD-CAD-C3D	-2.31	106.16	112.53
8	A	1006	LOP	O6-C24-O8	-2.31	117.86	123.63
10	P	1003	BOG	O1-C1-C2	2.30	111.77	108.27
9	F	1001	HEC	CMC-C2C-C1C	-2.28	121.94	125.42
8	E	1005	LOP	O6-C24-O8	-2.28	117.93	123.63
8	E	1005	LOP	O5-C6-O7	-2.26	118.42	123.70
6	O	1004	ASC	O4-C4-C3	-2.25	101.50	103.76
5	E	1003	FMX	O3-C3-N2	2.24	127.61	119.95
4	E	1001	HEM	CMB-C2B-C3B	2.24	133.84	128.43
4	K	1001	HEM	CHD-C4C-C3C	2.23	128.98	125.21
5	O	1003	FMX	C13-C8-C5	-2.23	117.01	120.71
9	F	1001	HEC	CHB-C4A-NA	2.23	126.89	124.45
4	E	1001	HEM	C3B-C2B-C1B	-2.23	104.73	106.41
4	A	1001	HEM	C3C-C2C-C1C	-2.23	104.93	107.05
4	O	1001	HEM	C4C-C3C-C2C	2.22	108.74	106.81
4	E	1002	HEM	O2A-CGA-CBA	2.22	121.01	114.00
4	K	1002	HEM	O1A-CGA-CBA	-2.22	116.07	123.09
4	O	1002	HEM	C4D-ND-C1D	2.21	107.83	105.21
9	B	1001	HEC	CMC-C2C-C1C	-2.21	122.06	125.42
9	F	1001	HEC	CAC-C3C-C2C	2.20	130.37	126.89
6	E	1004	ASC	O4-C4-C5	2.20	116.92	110.07
4	K	1001	HEM	CHA-C4D-ND	-2.19	121.66	124.37
4	A	1001	HEM	CHD-C1D-ND	2.18	126.77	124.42
4	A	1001	HEM	CAC-C3C-C4C	2.17	130.00	124.82
9	F	1001	HEC	O2D-CGD-CBD	2.16	120.84	114.00
4	O	1001	HEM	O2D-CGD-CBD	2.16	120.83	114.00
4	E	1001	HEM	CBA-CAA-C2A	-2.15	106.59	112.53
4	O	1002	HEM	C2A-C1A-NA	-2.14	107.78	110.15
9	B	1001	HEC	C4D-C3D-C2D	-2.13	103.78	106.89
10	B	1003	BOG	C4-C3-C2	2.13	114.58	110.83
4	K	1001	HEM	CAB-C3B-C2B	-2.12	121.53	128.43
4	E	1002	HEM	C4D-ND-C1D	2.12	107.72	105.21
9	P	1001	HEC	O1A-CGA-CBA	-2.12	116.37	123.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	K	1006	LOP	O5-C6-C7	2.11	116.05	111.48
5	K	1003	FMX	C21-N1-N2	2.10	120.09	116.20
9	L	1001	HEC	CMC-C2C-C3C	2.10	130.08	125.62
4	K	1001	HEM	CHA-C1A-C2A	-2.10	120.70	125.30
9	F	1001	HEC	C3C-C4C-NC	-2.10	107.82	110.15
4	E	1001	HEM	C4B-C3B-C2B	2.10	109.21	107.28
4	K	1002	HEM	CAD-CBD-CGD	-2.09	108.13	113.67
4	K	1001	HEM	O1D-CGD-CBD	-2.08	116.48	123.09
4	K	1001	HEM	CHA-C1A-NA	2.08	127.64	123.86
4	A	1002	HEM	CAD-CBD-CGD	-2.08	108.14	113.67
4	A	1002	HEM	CMC-C2C-C3C	2.08	133.45	128.43
10	P	1003	BOG	O5-C5-C4	2.07	113.44	109.70
4	A	1002	HEM	CAA-C2A-C1A	2.07	128.98	124.94
9	P	1001	HEC	C3C-C4C-NC	-2.06	107.87	110.15
4	K	1001	HEM	C4A-NA-C1A	-2.06	102.47	105.82
4	E	1001	HEM	CHA-C1A-NA	2.06	127.59	123.86
4	E	1001	HEM	CBD-CAD-C3D	-2.06	106.84	112.53
4	A	1002	HEM	C4D-ND-C1D	2.06	107.64	105.21
6	E	1004	ASC	C6-C5-C4	-2.05	108.40	111.86
9	B	1001	HEC	C1A-CHA-C4D	2.05	130.38	126.02
4	O	1001	HEM	CAC-C3C-C4C	-2.04	119.95	124.82
10	B	1003	BOG	C3-C4-C5	2.04	113.93	110.23
9	B	1001	HEC	CHA-C1A-NA	2.04	126.67	124.45
4	K	1002	HEM	CAC-C3C-C4C	-2.03	119.98	124.82
9	B	1001	HEC	O1A-CGA-CBA	-2.02	116.67	123.09
9	F	1001	HEC	CMC-C2C-C3C	2.02	129.91	125.62
4	E	1001	HEM	C3C-C2C-C1C	-2.02	105.13	107.05
8	E	1005	LOP	O5-C4-C3	2.02	115.57	108.34
8	K	1006	LOP	O5-C4-C3	2.01	115.55	108.34
4	O	1001	HEM	CBD-CAD-C3D	2.01	118.08	112.53
9	B	1001	HEC	CMD-C2D-C1D	2.00	128.16	125.03
4	E	1002	HEM	CHD-C1D-ND	2.00	126.58	124.42
4	E	1002	HEM	CMD-C2D-C1D	-2.00	121.91	125.03
8	E	1005	LOP	O8-C24-C25	-2.00	115.96	123.78

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	B	1001	HEC	NA
9	F	1001	HEC	NA
9	L	1001	HEC	NA
9	P	1001	HEC	NA

All (168) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1002	HEM	C1A-C2A-CAA-CBA
4	O	1001	HEM	C2D-C3D-CAD-CBD
4	O	1001	HEM	C4D-C3D-CAD-CBD
6	E	1004	ASC	C3-C4-C5-C6
6	E	1004	ASC	C3-C4-C5-O5
6	E	1004	ASC	O4-C4-C5-C6
6	E	1004	ASC	O4-C4-C5-O5
6	K	1004	ASC	C3-C4-C5-C6
6	K	1004	ASC	C3-C4-C5-O5
6	K	1004	ASC	O4-C4-C5-C6
6	K	1004	ASC	O4-C4-C5-O5
6	O	1004	ASC	C4-C5-C6-O6
6	O	1004	ASC	O5-C5-C6-O6
8	A	1006	LOP	C3-O2-P1-O1
8	A	1006	LOP	C3-O2-P1-O4
8	E	1005	LOP	C2-O1-P1-O2
8	E	1005	LOP	C2-O1-P1-O4
8	O	1005	LOP	C2-O1-P1-O2
9	B	1001	HEC	C4C-C3C-CAC-CBC
9	F	1001	HEC	C4C-C3C-CAC-CBC
9	L	1001	HEC	C4C-C3C-CAC-CBC
9	P	1001	HEC	C2C-C3C-CAC-CBC
9	P	1001	HEC	C4C-C3C-CAC-CBC
9	B	1001	HEC	C2C-C3C-CAC-CBC
4	K	1001	HEM	C4D-C3D-CAD-CBD
9	F	1001	HEC	C2C-C3C-CAC-CBC
9	L	1001	HEC	C2B-C3B-CAB-CBB
10	P	1003	BOG	O5-C5-C6-O6
9	L	1001	HEC	C2C-C3C-CAC-CBC
9	P	1001	HEC	C2B-C3B-CAB-CBB
10	B	1003	BOG	O5-C5-C6-O6
9	B	1001	HEC	C2B-C3B-CAB-CBB
10	P	1003	BOG	C4-C5-C6-O6
4	A	1002	HEM	C2A-CAA-CBA-CGA
8	E	1005	LOP	C6-C7-C8-C9
4	A	1002	HEM	C3A-C2A-CAA-CBA
9	F	1001	HEC	C2B-C3B-CAB-CBB
8	E	1005	LOP	O7-C6-O5-C4
4	K	1001	HEM	C2D-C3D-CAD-CBD
8	A	1006	LOP	O7-C6-O5-C4
8	K	1006	LOP	O7-C6-O5-C4
10	K	1007	BOG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
8	A	1006	LOP	C13-C14-C15-C16
8	O	1005	LOP	C13-C14-C15-C16
9	L	1001	HEC	C4B-C3B-CAB-CBB
8	O	1005	LOP	C16-C17-C18-C19
8	O	1005	LOP	C17-C18-C19-C20
8	E	1005	LOP	C17-C18-C19-C20
10	K	1007	BOG	C4-C5-C6-O6
10	F	1003	BOG	C3'-C4'-C5'-C6'
9	P	1001	HEC	C4B-C3B-CAB-CBB
8	E	1005	LOP	C7-C6-O5-C4
8	E	1005	LOP	C9-C10-C11-C12
8	A	1006	LOP	C11-C12-C13-C14
8	O	1005	LOP	C11-C12-C13-C14
8	A	1006	LOP	C9-C10-C11-C12
4	O	1001	HEM	C4B-C3B-CAB-CBB
8	A	1006	LOP	C24-C25-C26-C27
8	E	1005	LOP	C11-C12-C13-C14
8	K	1006	LOP	C11-C12-C13-C14
10	B	1003	BOG	C4-C5-C6-O6
8	A	1006	LOP	C7-C6-O5-C4
8	O	1005	LOP	O7-C6-O5-C4
8	O	1005	LOP	C30-C31-C32-C33
10	K	1007	BOG	C2'-C3'-C4'-C5'
10	K	1007	BOG	C1'-C2'-C3'-C4'
8	A	1006	LOP	C15-C16-C17-C18
8	K	1006	LOP	C15-C16-C17-C18
8	K	1006	LOP	C13-C14-C15-C16
8	K	1006	LOP	C9-C10-C11-C12
9	F	1001	HEC	C4B-C3B-CAB-CBB
8	O	1005	LOP	C15-C16-C17-C18
9	B	1001	HEC	C4B-C3B-CAB-CBB
8	O	1005	LOP	C9-C10-C11-C12
8	A	1006	LOP	O2-C3-C4-C5
8	K	1006	LOP	O2-C3-C4-C5
8	E	1005	LOP	C30-C31-C32-C33
10	K	1007	BOG	C3'-C4'-C5'-C6'
8	E	1005	LOP	C16-C17-C18-C19
8	E	1005	LOP	C3-C4-C5-O6
8	E	1005	LOP	O8-C24-O6-C5
10	P	1003	BOG	C2'-C3'-C4'-C5'
10	B	1003	BOG	C2'-C3'-C4'-C5'
10	P	1003	BOG	C3'-C4'-C5'-C6'

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Mol	Chain	Res	Type	Atoms
8	A	1006	LOP	O2-C3-C4-O5
8	K	1006	LOP	C7-C6-O5-C4
4	A	1001	HEM	C4C-C3C-CAC-CBC
4	K	1001	HEM	C4B-C3B-CAB-CBB
4	K	1001	HEM	C4C-C3C-CAC-CBC
8	E	1005	LOP	O5-C4-C5-O6
8	K	1006	LOP	C18-C19-C20-C21
8	A	1006	LOP	C25-C26-C27-C28
10	F	1003	BOG	C2'-C3'-C4'-C5'
8	E	1005	LOP	C28-C29-C30-C31
8	A	1006	LOP	O5-C4-C5-O6
10	F	1003	BOG	C1'-C2'-C3'-C4'
8	A	1006	LOP	C3-C4-C5-O6
8	A	1006	LOP	C2-O1-P1-O2
8	A	1006	LOP	C2-O1-P1-O3
8	A	1006	LOP	C2-O1-P1-O4
8	E	1005	LOP	N1-C1-C2-O1
8	E	1005	LOP	C2-O1-P1-O3
8	K	1006	LOP	C3-O2-P1-O4
8	K	1006	LOP	C29-C30-C31-C32
4	E	1001	HEM	C3D-CAD-CBD-CGD
8	A	1006	LOP	C12-C13-C14-C15
8	E	1005	LOP	C18-C19-C20-C21
8	K	1006	LOP	C28-C29-C30-C31
8	K	1006	LOP	C32-C33-C34-C35
8	K	1006	LOP	O2-C3-C4-O5
8	E	1005	LOP	C14-C15-C16-C17
10	K	1007	BOG	C5'-C6'-C7'-C8'
8	O	1005	LOP	C26-C27-C28-C29
4	A	1001	HEM	C3D-CAD-CBD-CGD
10	B	1003	BOG	C3'-C4'-C5'-C6'
4	E	1001	HEM	CAD-CBD-CGD-O1D
4	A	1001	HEM	CAA-CBA-CGA-O2A
10	B	1003	BOG	C1'-C2'-C3'-C4'
8	O	1005	LOP	C28-C29-C30-C31
4	A	1001	HEM	CAA-CBA-CGA-O1A
8	A	1006	LOP	C32-C33-C34-C35
4	O	1002	HEM	CAA-CBA-CGA-O1A
4	K	1001	HEM	CAA-CBA-CGA-O2A
4	K	1002	HEM	CAA-CBA-CGA-O1A
4	E	1002	HEM	CAA-CBA-CGA-O1A
4	K	1001	HEM	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
4	K	1002	HEM	CAA-CBA-CGA-O2A
9	P	1001	HEC	CAA-CBA-CGA-O2A
9	F	1001	HEC	CAA-CBA-CGA-O2A
4	E	1001	HEM	CAD-CBD-CGD-O2D
4	O	1002	HEM	CAA-CBA-CGA-O2A
4	E	1002	HEM	CAA-CBA-CGA-O2A
10	P	1003	BOG	C1'-C2'-C3'-C4'
9	P	1001	HEC	CAA-CBA-CGA-O1A
8	E	1005	LOP	O2-C3-C4-C5
8	E	1005	LOP	C12-C13-C14-C15
4	O	1001	HEM	CAA-CBA-CGA-O2A
9	B	1001	HEC	CAA-CBA-CGA-O2A
4	A	1002	HEM	CAA-CBA-CGA-O2A
9	F	1001	HEC	CAA-CBA-CGA-O1A
8	K	1006	LOP	C14-C15-C16-C17
4	O	1001	HEM	CAA-CBA-CGA-O1A
8	O	1005	LOP	O2-C3-C4-O5
10	P	1003	BOG	C5'-C6'-C7'-C8'
4	E	1001	HEM	CAA-CBA-CGA-O1A
8	K	1006	LOP	C12-C13-C14-C15
4	A	1002	HEM	CAA-CBA-CGA-O1A
6	A	1004	ASC	O4-C4-C5-C6
8	O	1005	LOP	C12-C13-C14-C15
6	A	1004	ASC	C3-C4-C5-C6
6	O	1004	ASC	C3-C4-C5-C6
8	A	1006	LOP	O6-C24-C25-C26
4	A	1001	HEM	CAD-CBD-CGD-O1D
4	A	1001	HEM	CAD-CBD-CGD-O2D
8	K	1006	LOP	O6-C24-C25-C26
8	O	1005	LOP	O8-C24-O6-C5
8	K	1006	LOP	C19-C20-C21-C22
10	F	1003	BOG	C5'-C6'-C7'-C8'
9	B	1001	HEC	CAA-CBA-CGA-O1A
8	E	1005	LOP	C7-C8-C9-C10
8	E	1005	LOP	O8-C24-C25-C26
4	E	1001	HEM	CAA-CBA-CGA-O2A
8	E	1005	LOP	C26-C27-C28-C29
8	K	1006	LOP	O7-C6-C7-C8
8	A	1006	LOP	O7-C6-C7-C8
8	A	1006	LOP	O8-C24-C25-C26
9	L	1001	HEC	CAD-CBD-CGD-O1D
9	B	1001	HEC	CAD-CBD-CGD-O2D

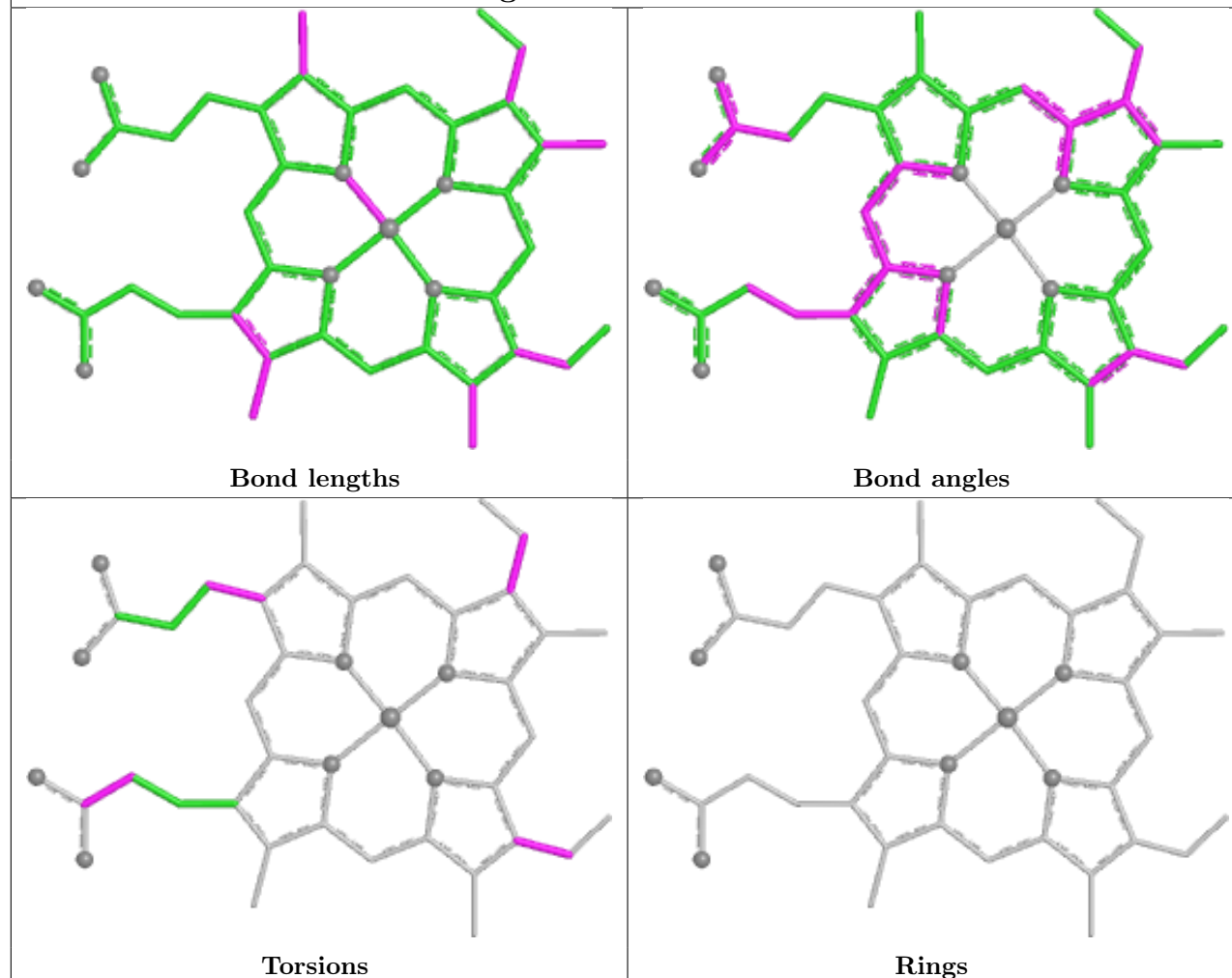
There are no ring outliers.

11 monomers are involved in 16 short contacts:

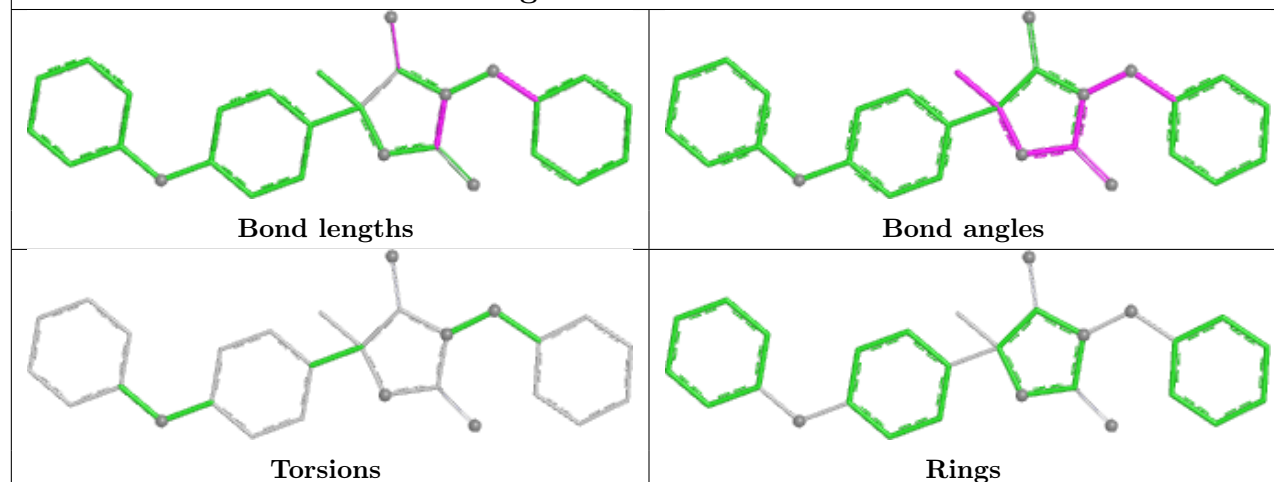
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	K	1001	HEM	3	0
4	A	1002	HEM	1	0
9	F	1001	HEC	1	0
4	A	1001	HEM	2	0
4	O	1001	HEM	3	0
8	K	1006	LOP	1	0
6	E	1004	ASC	1	0
9	P	1001	HEC	1	0
9	L	1001	HEC	1	0
4	E	1001	HEM	1	0
6	K	1004	ASC	1	0

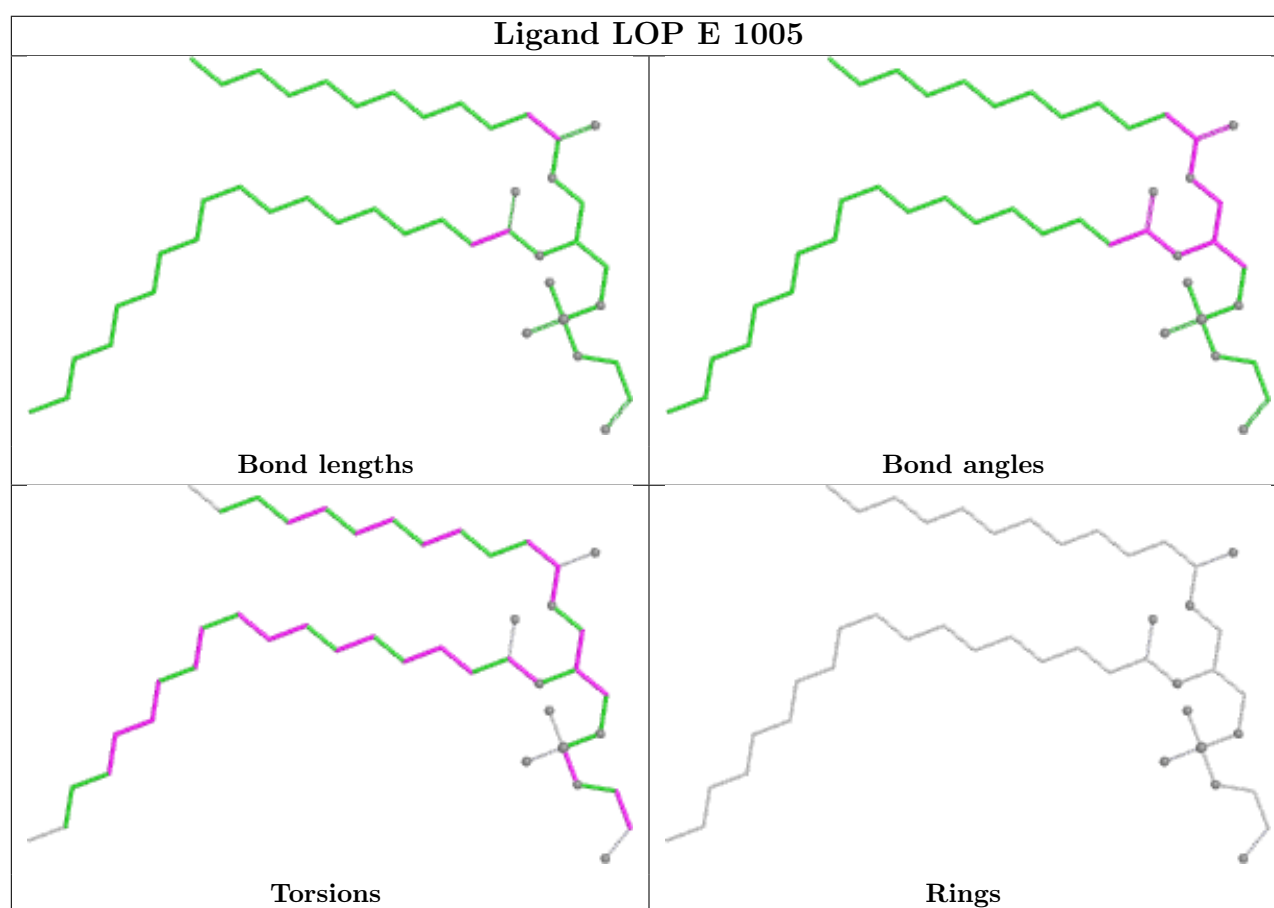
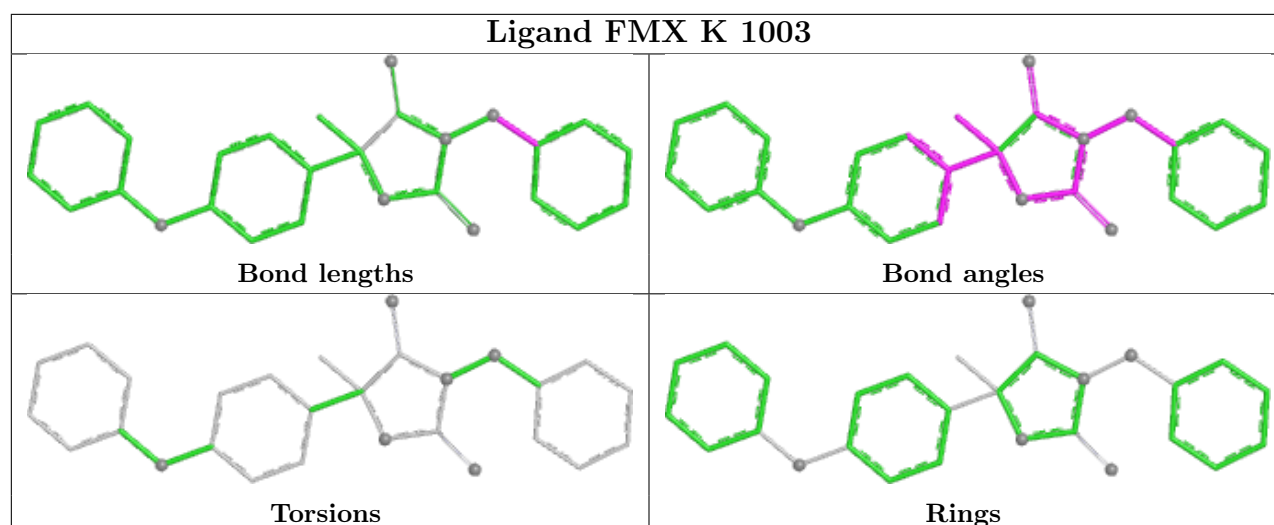
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 HEM K 1001

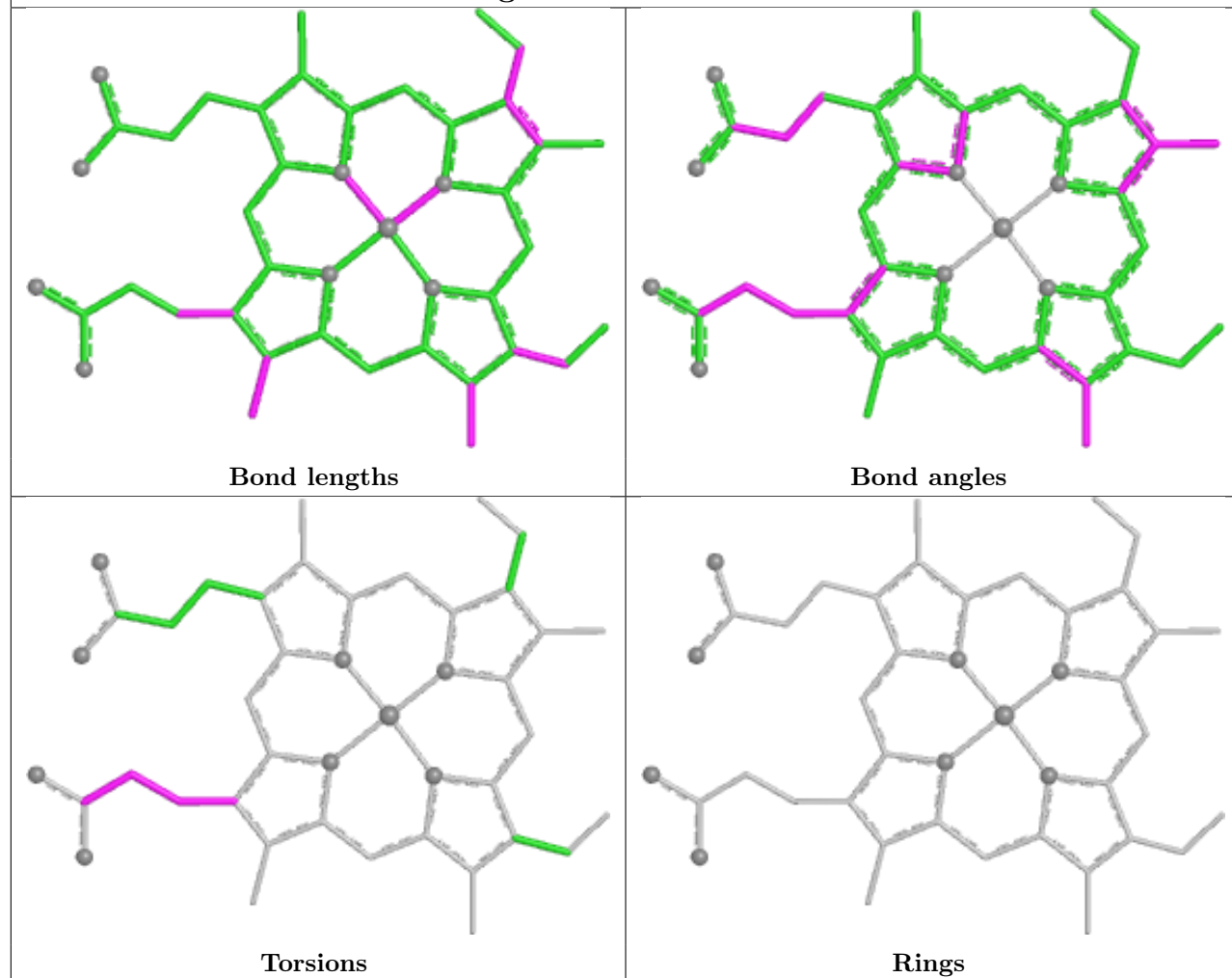


Ligand FMX E 1003

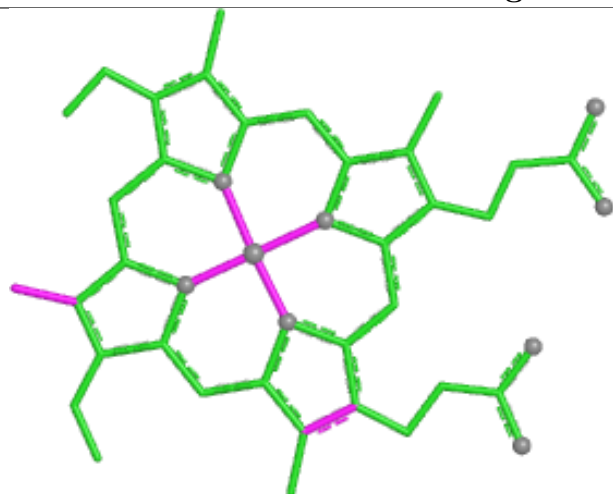




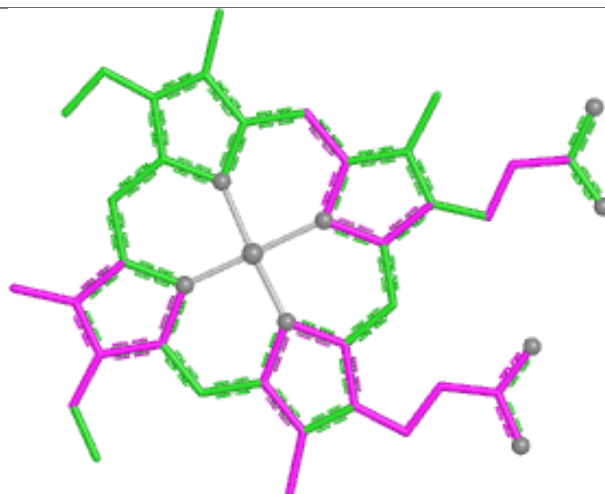
Ligand HEM A 1002



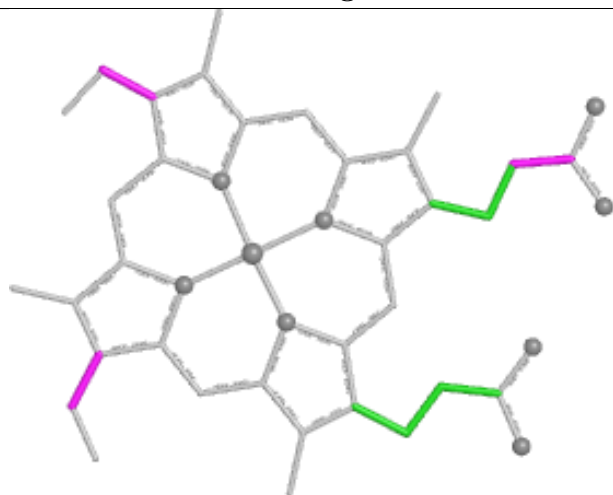
Ligand HEC F 1001



Bond lengths



Bond angles

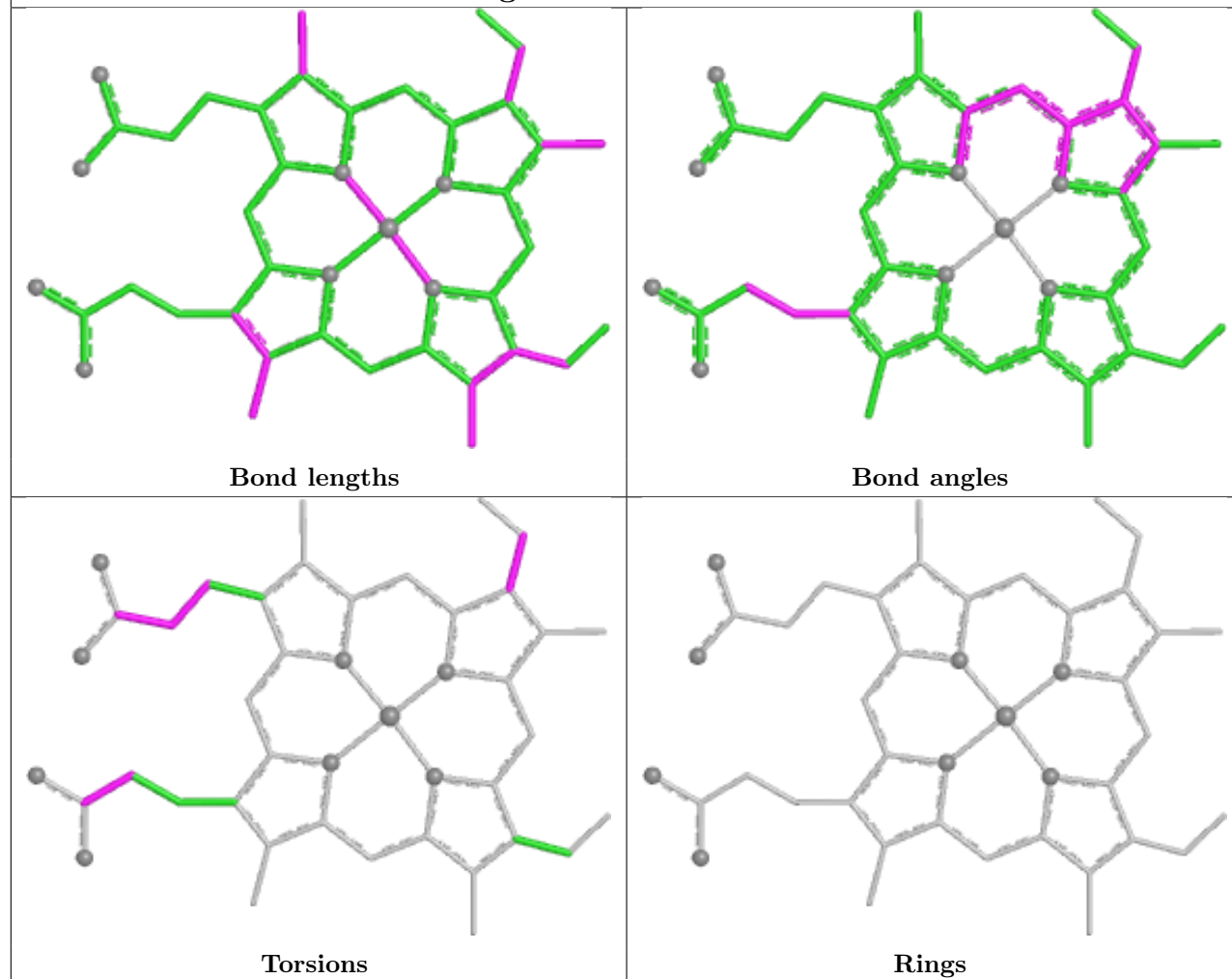


Torsions

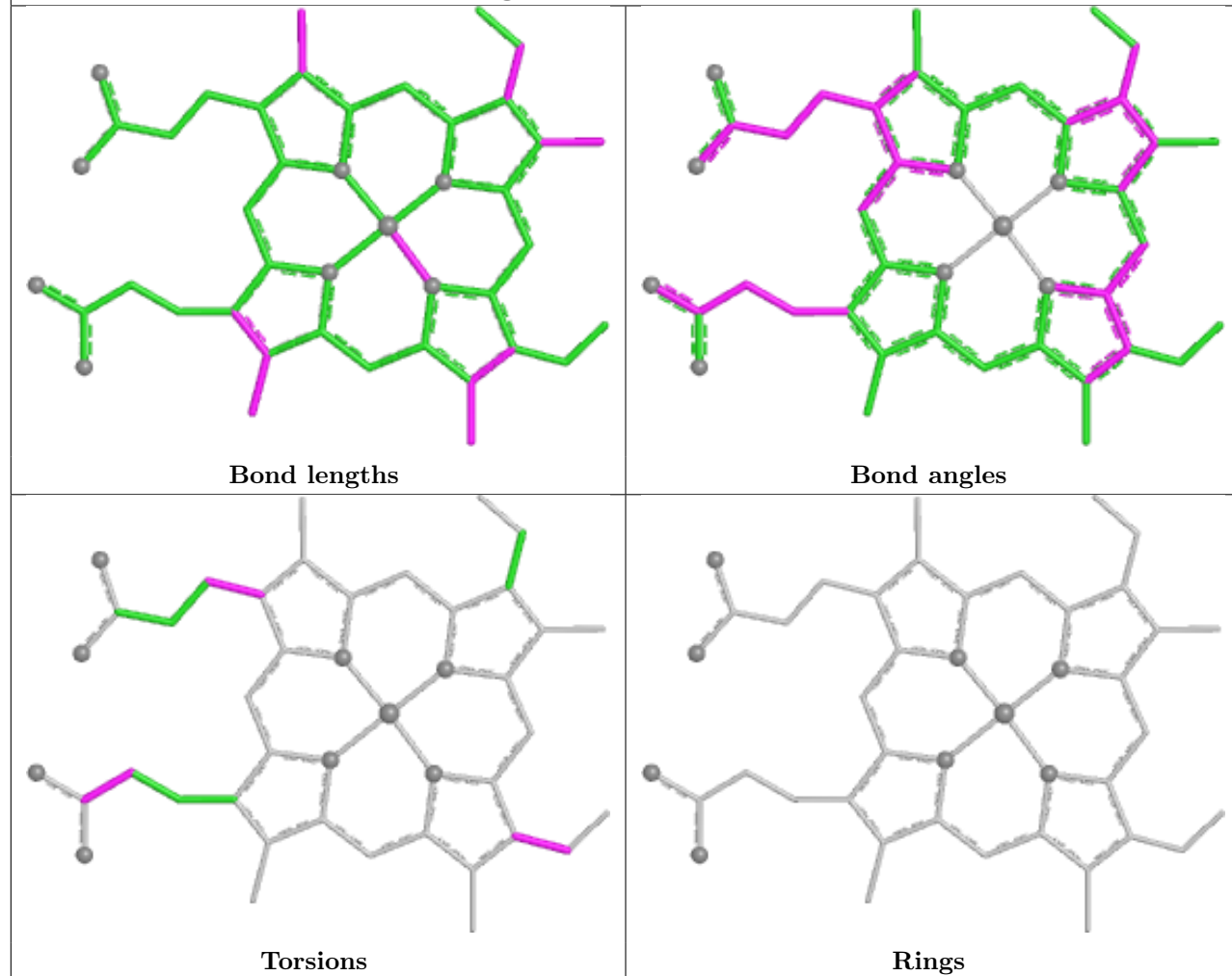


Rings

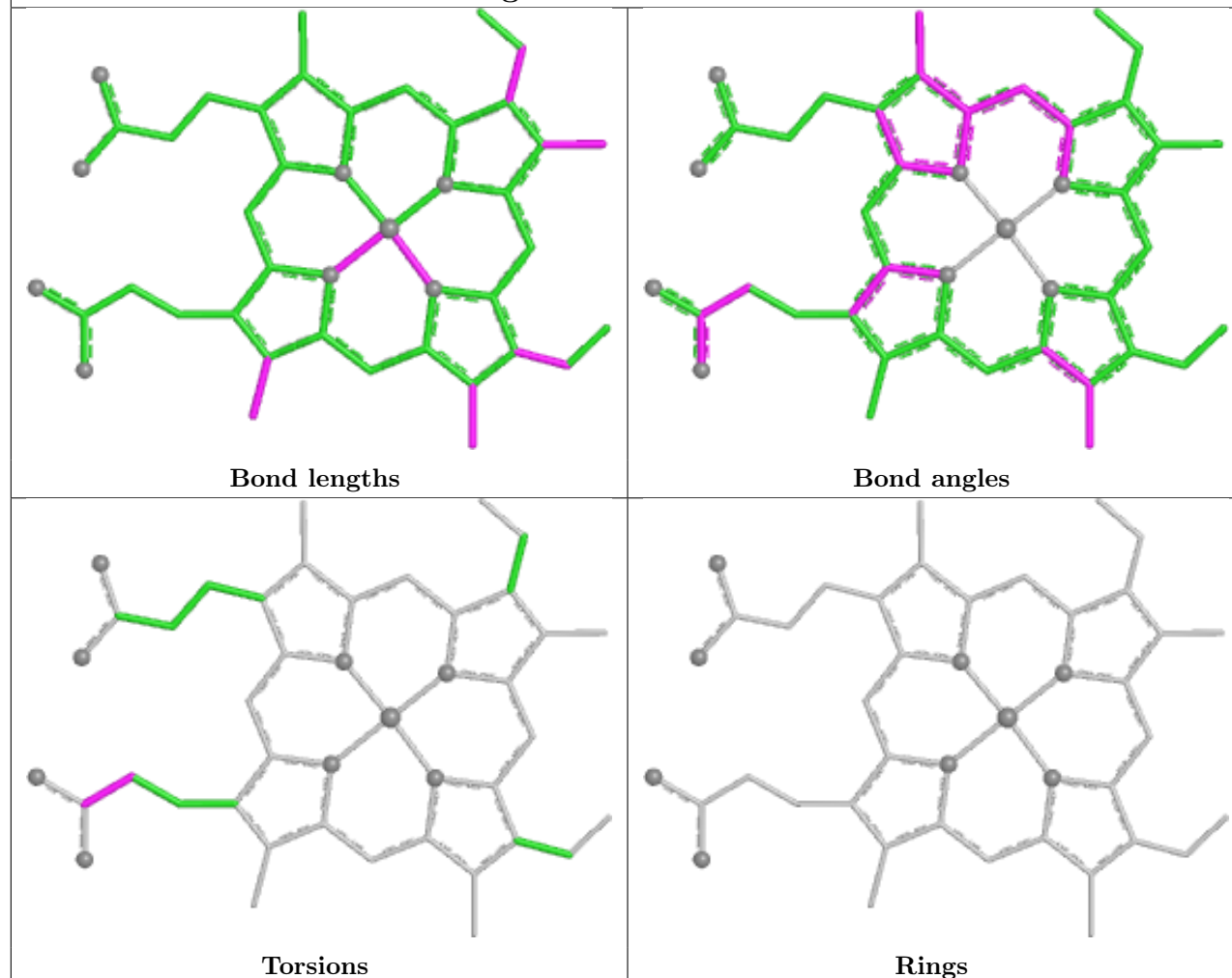
Ligand HEM A 1001



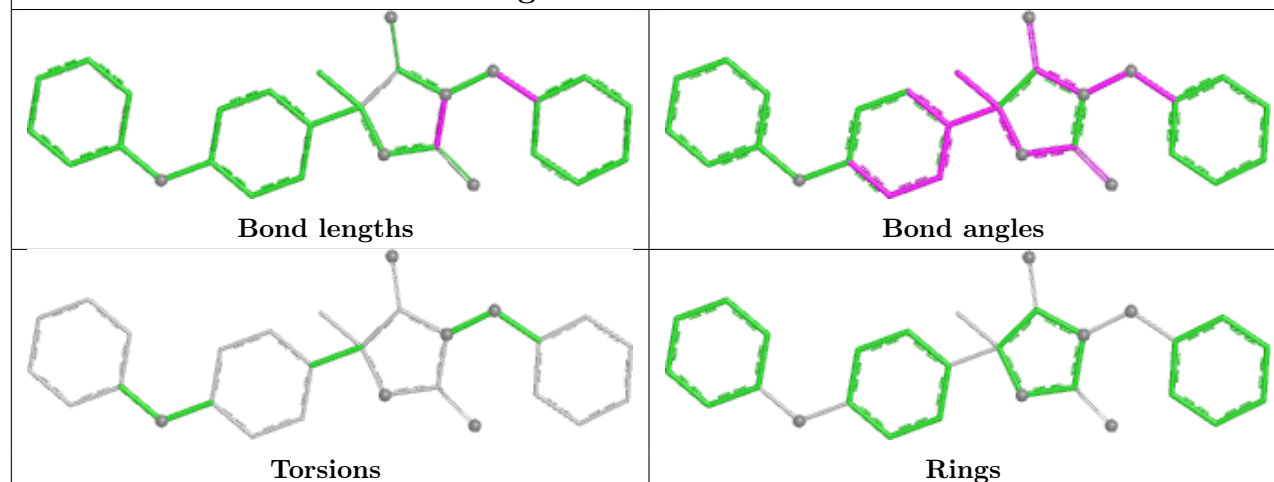
Ligand HEM O 1001



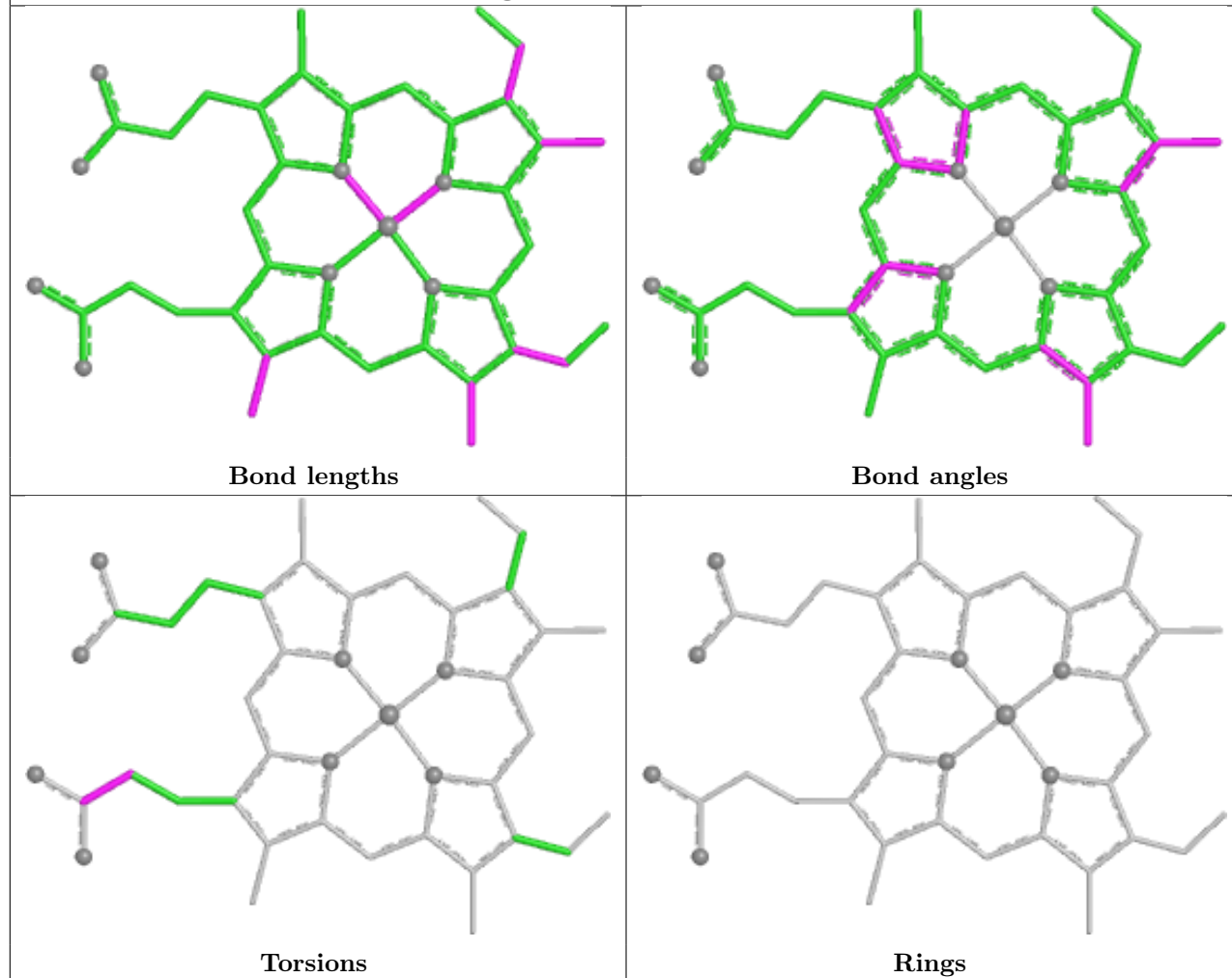
Ligand HEM E 1002



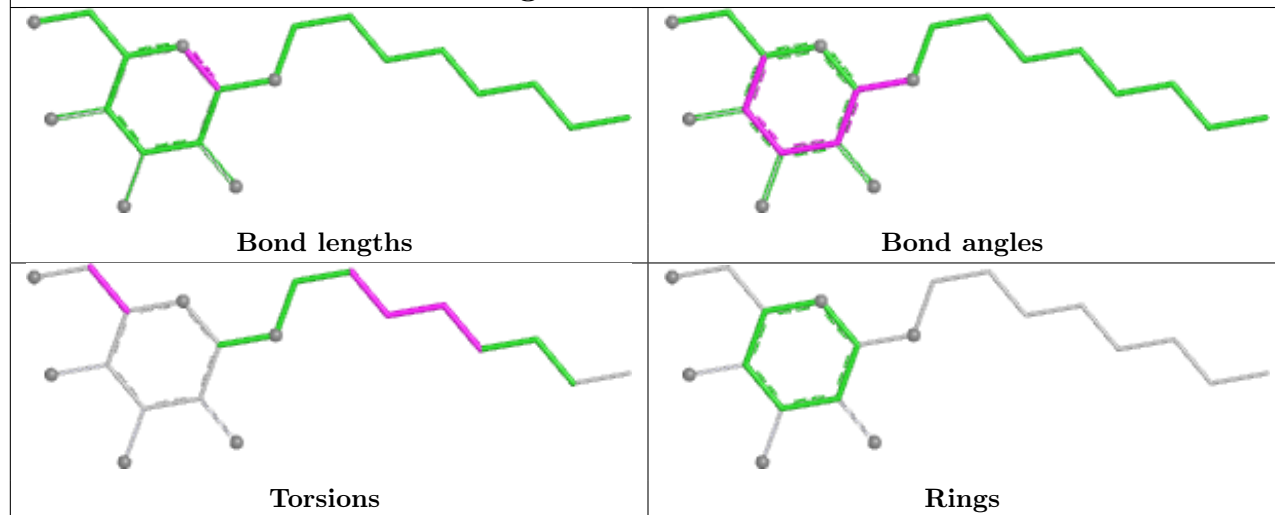
Ligand FMX A 1003

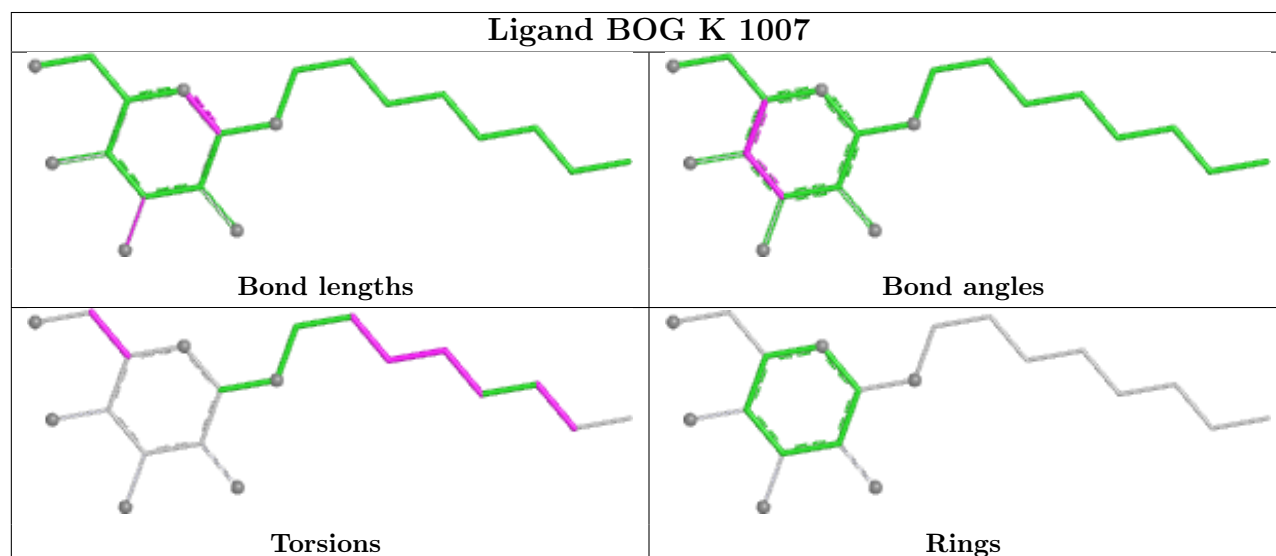
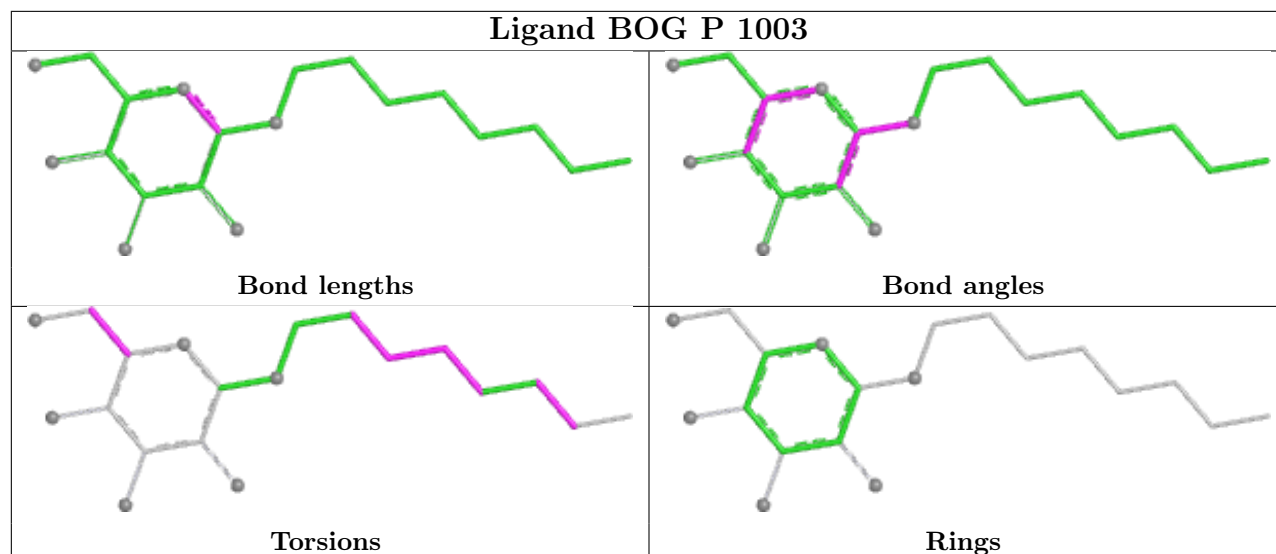


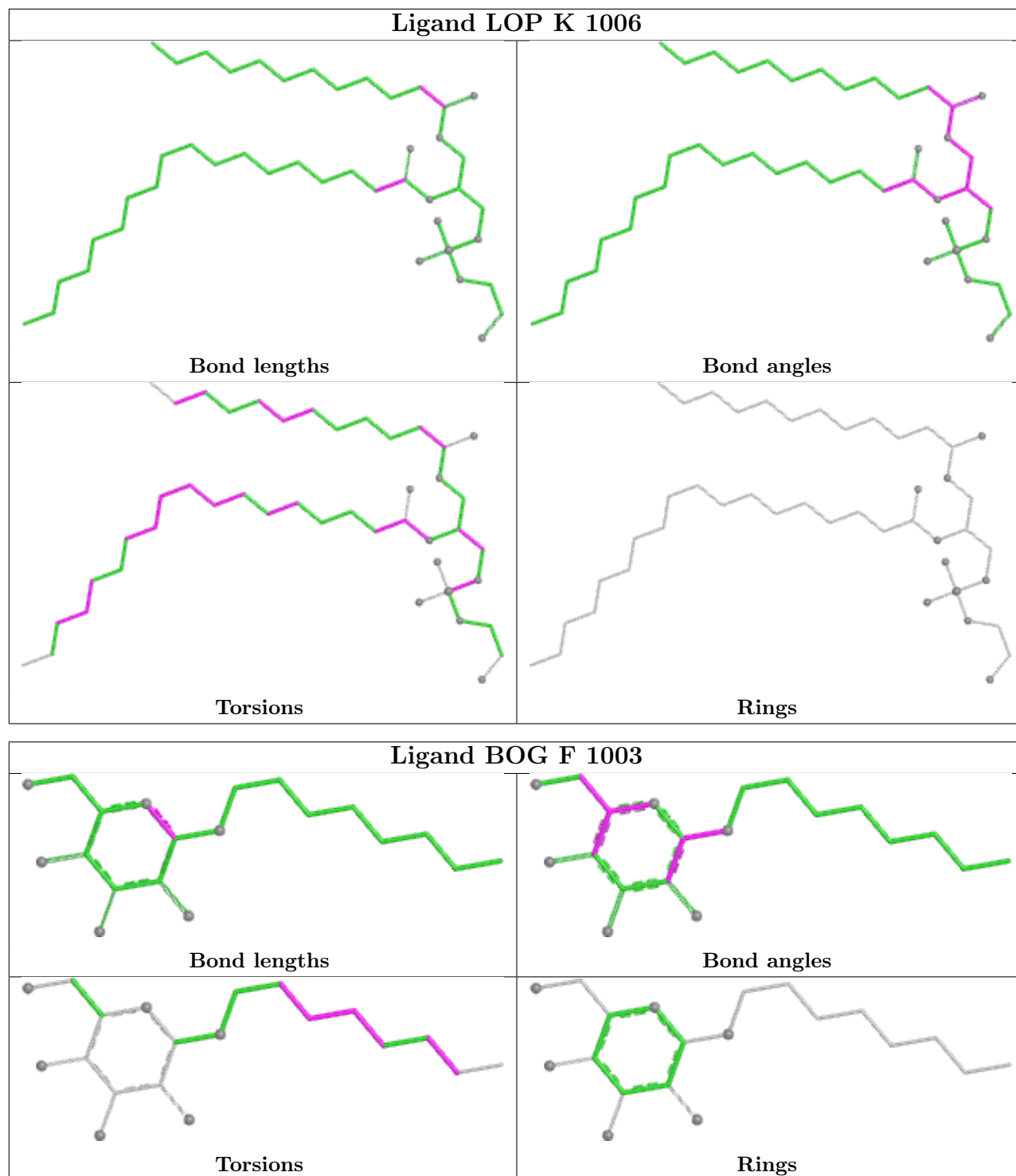
Ligand HEM O 1002



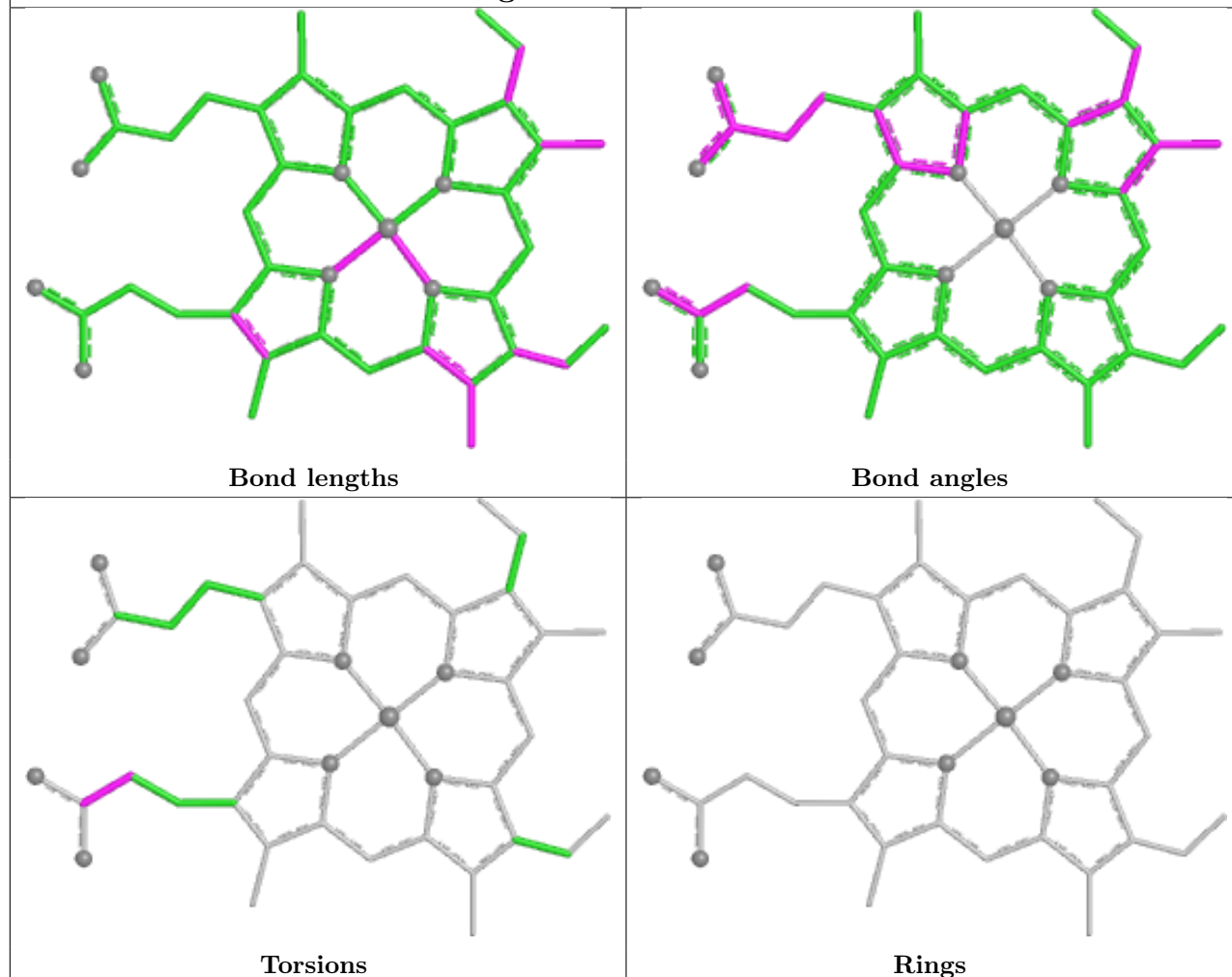
Ligand BOG B 1003



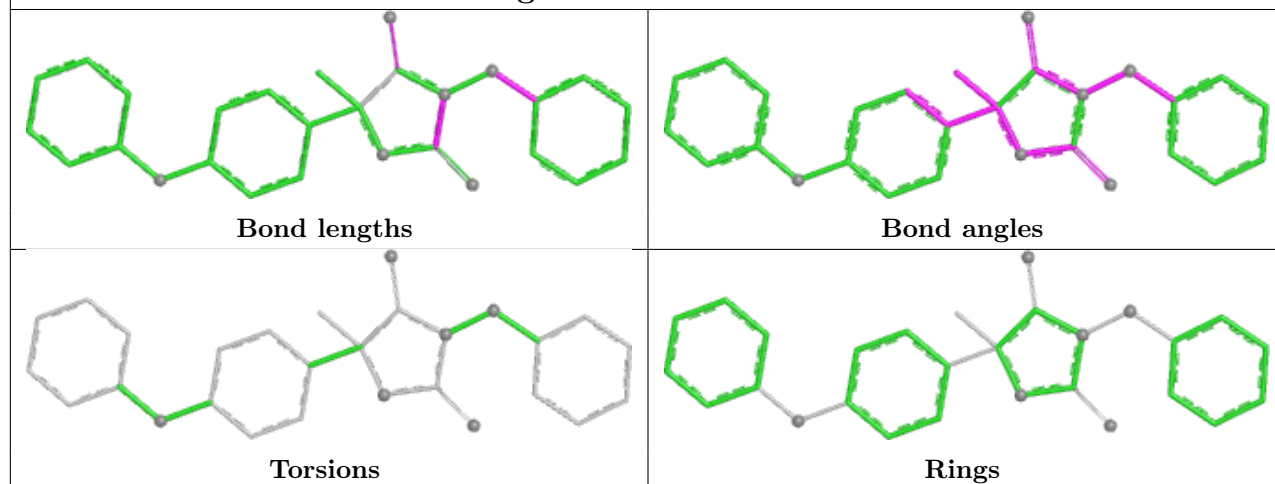


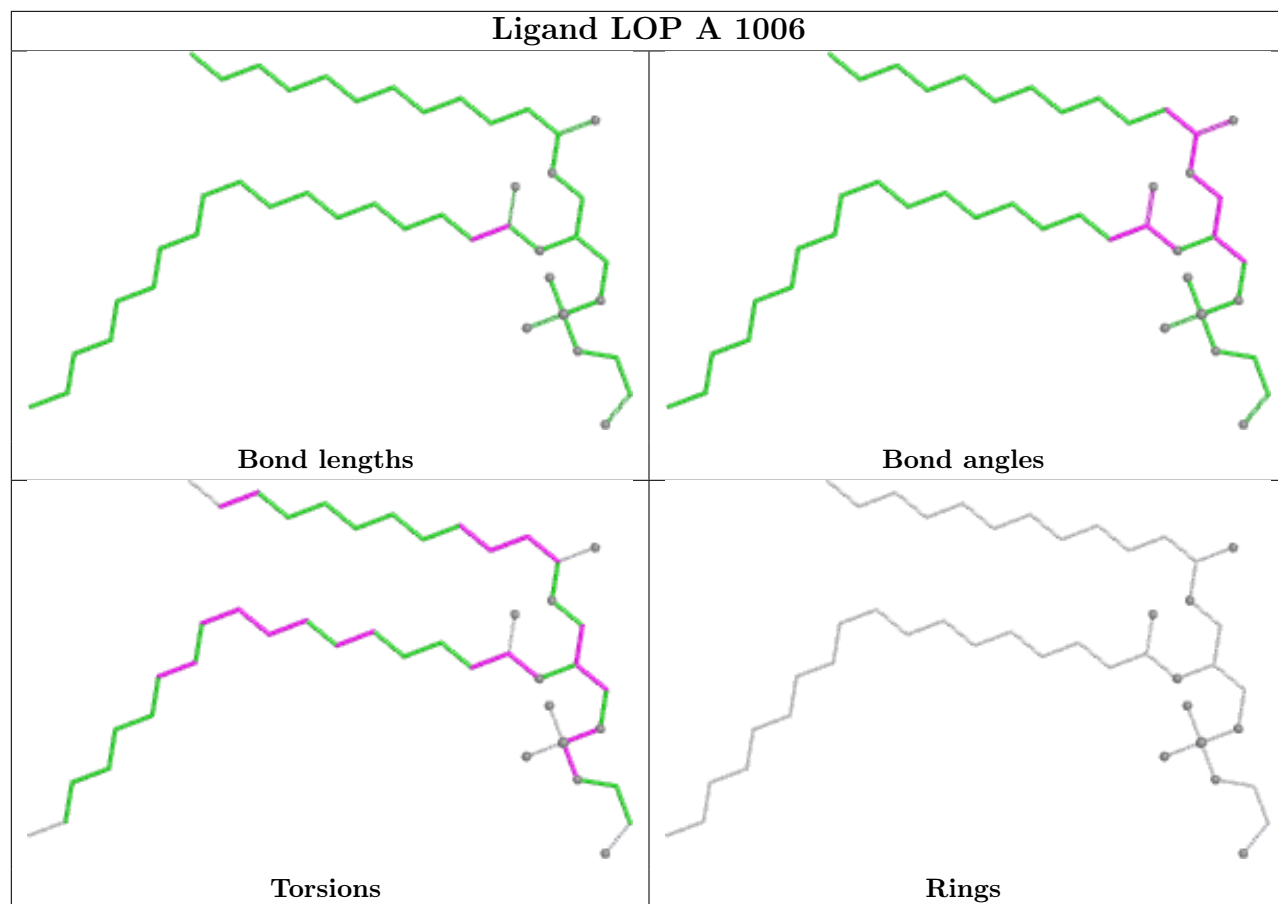


Ligand HEM K 1002

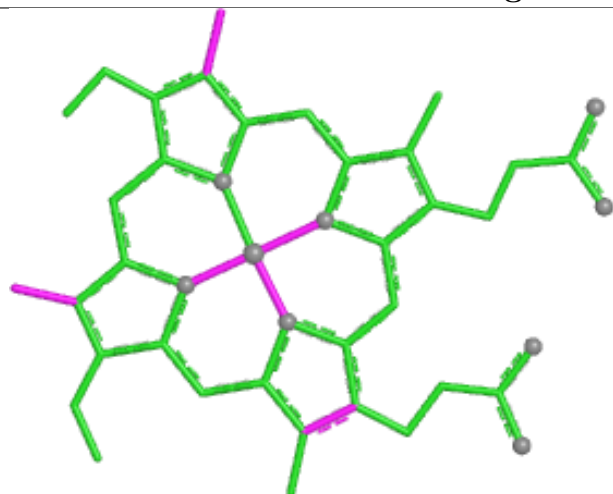


Ligand FMX O 1003

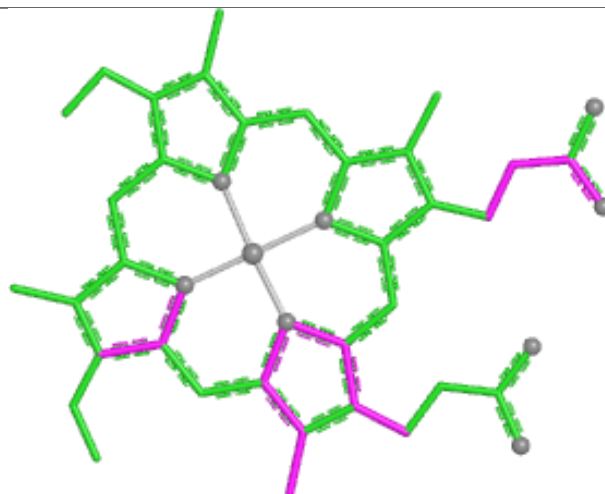




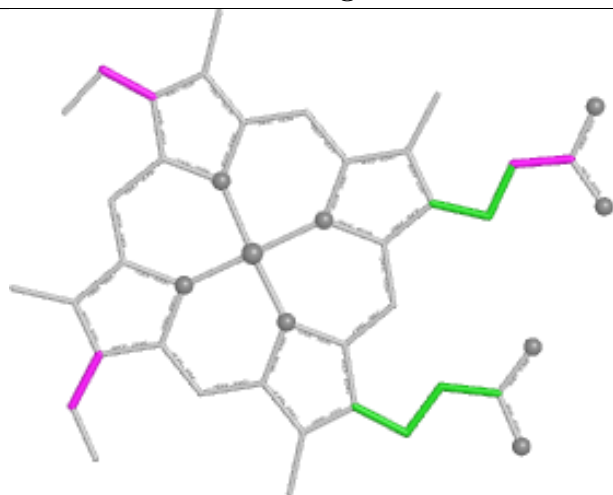
Ligand HEC P 1001



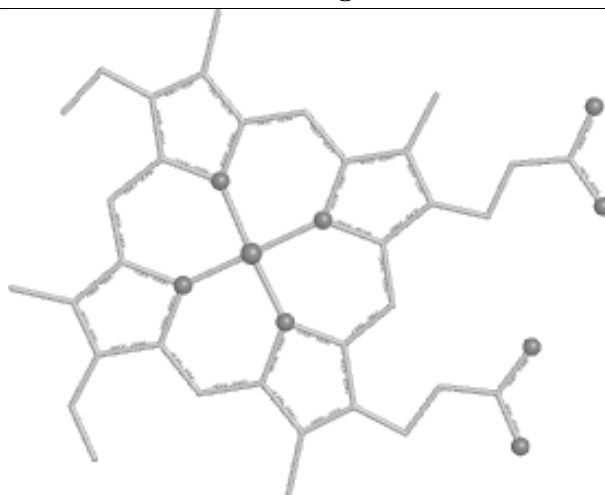
Bond lengths



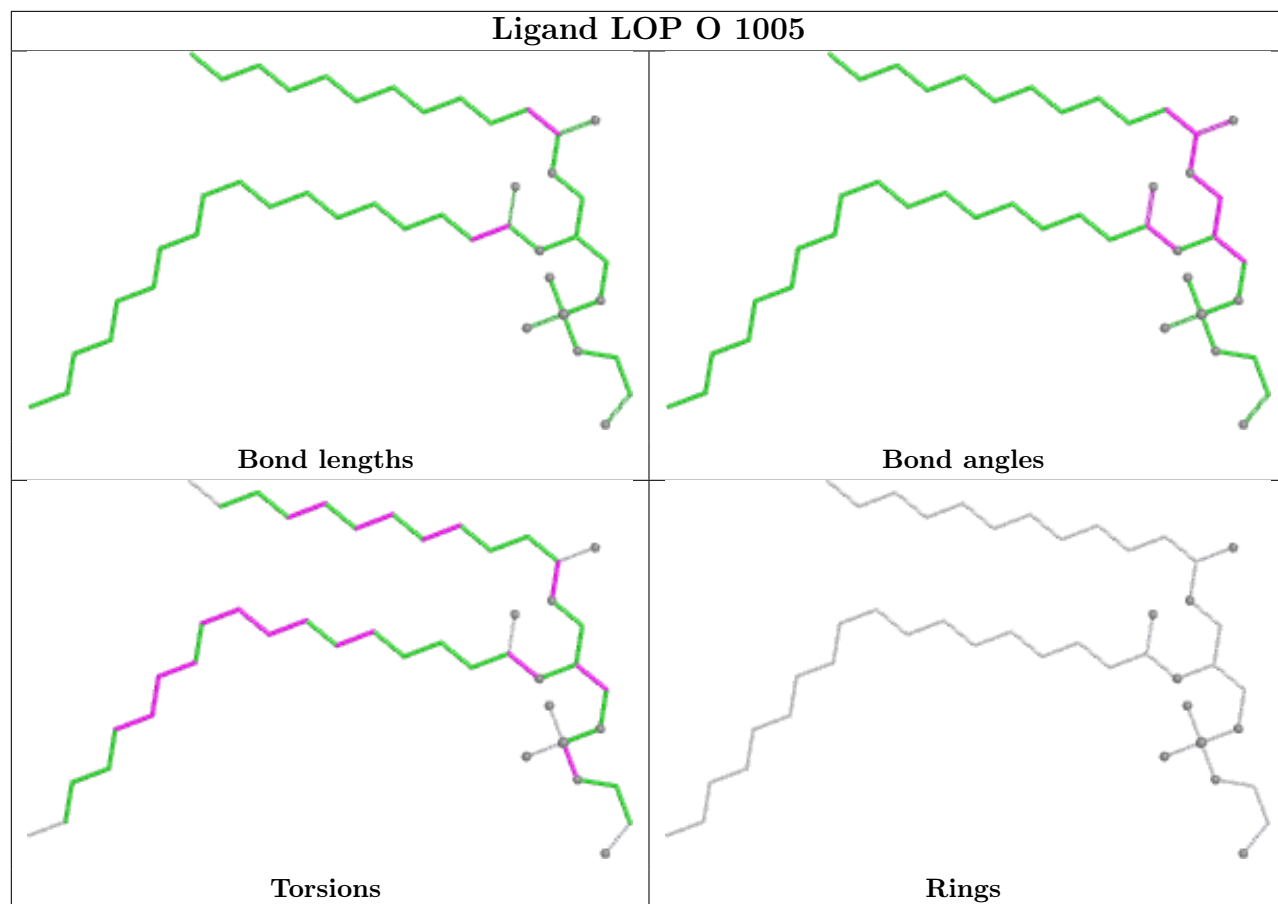
Bond angles



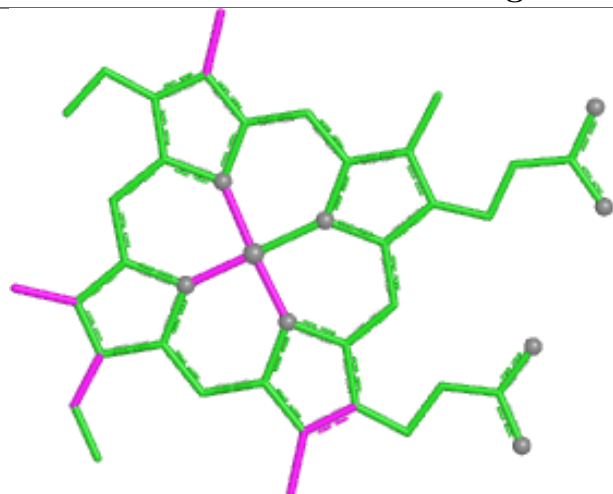
Torsions



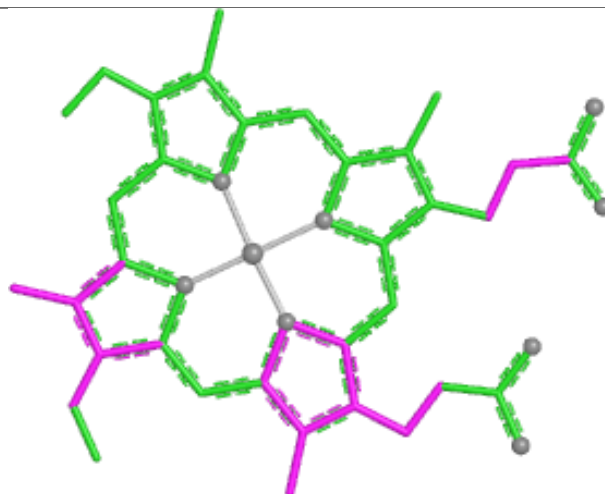
Rings



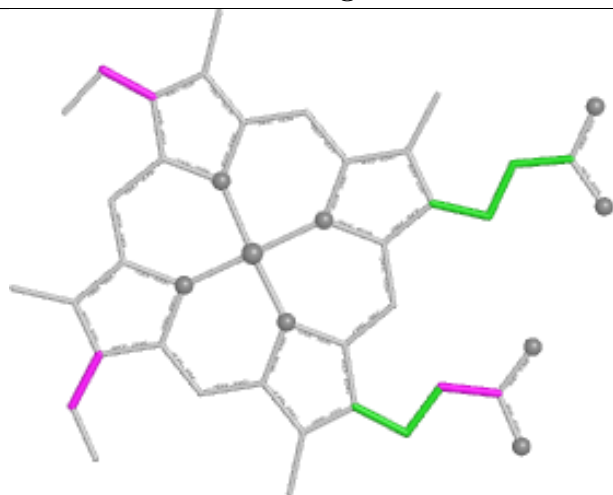
Ligand HEC L 1001



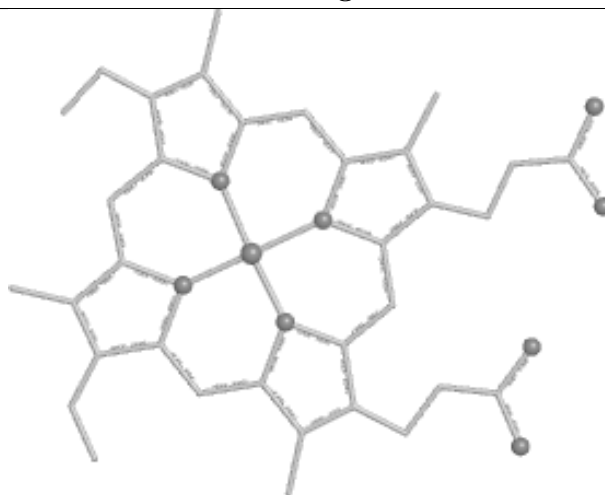
Bond lengths



Bond angles

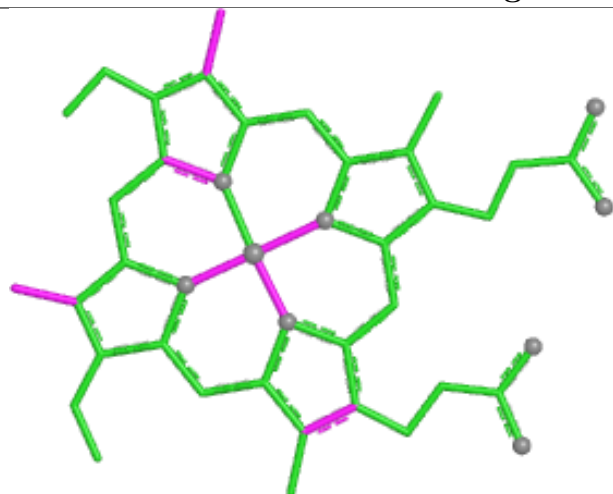


Torsions

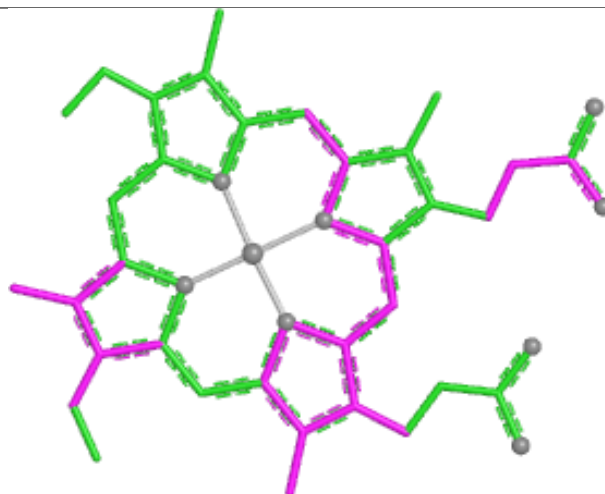


Rings

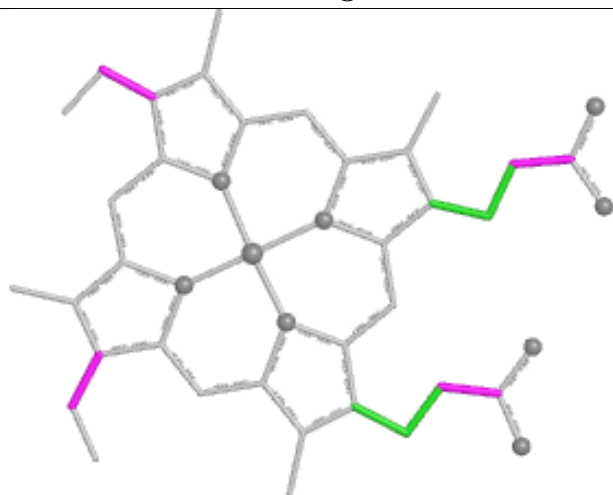
Ligand HEC B 1001



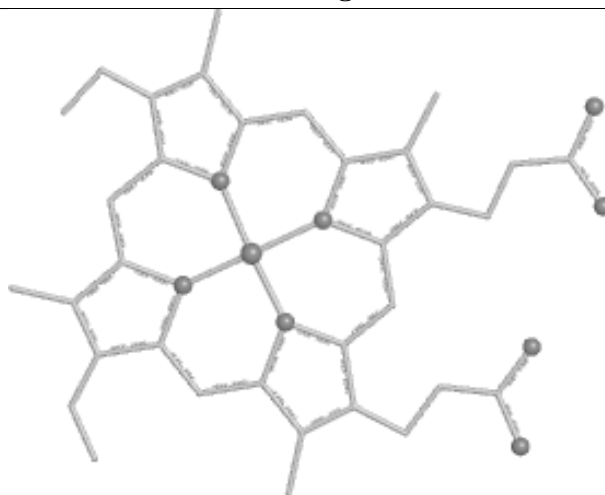
Bond lengths



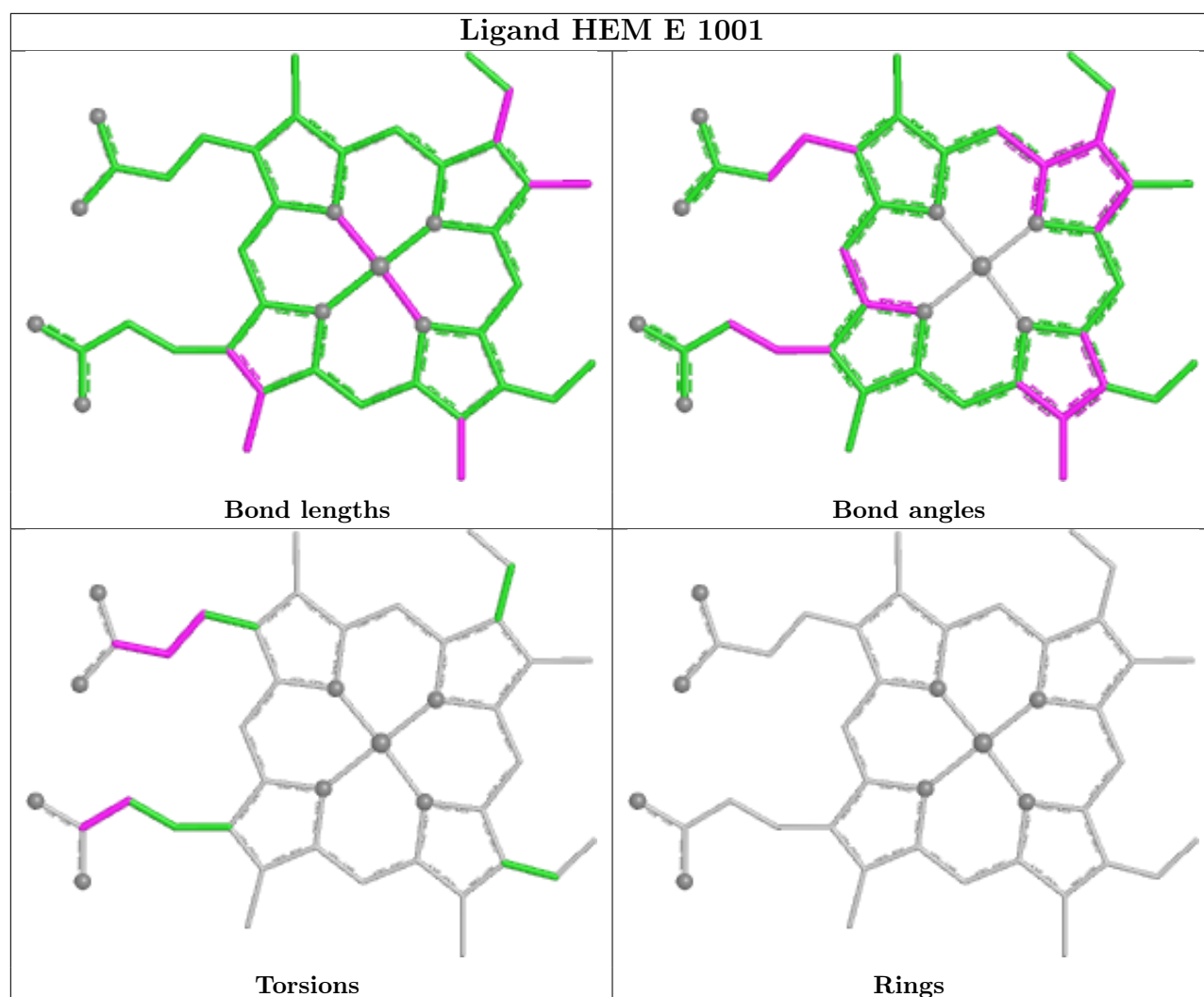
Bond angles



Torsions



Rings



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	429/445 (96%)	0.19	6 (1%) 73 55	54, 65, 102, 196	0
1	E	429/445 (96%)	0.27	12 (2%) 55 36	39, 68, 110, 167	0
1	K	429/445 (96%)	0.04	9 (2%) 63 44	21, 54, 97, 160	0
1	O	429/445 (96%)	0.21	10 (2%) 61 42	29, 68, 105, 179	0
2	B	256/272 (94%)	0.44	13 (5%) 33 20	52, 74, 123, 189	0
2	F	256/272 (94%)	0.54	15 (5%) 28 17	49, 83, 140, 178	0
2	L	256/272 (94%)	0.25	11 (4%) 40 24	38, 66, 122, 157	0
2	P	256/272 (94%)	0.63	17 (6%) 24 15	46, 90, 136, 184	0
3	C	179/187 (95%)	1.08	24 (13%) 7 5	66, 106, 163, 230	0
3	G	179/187 (95%)	0.64	12 (6%) 24 14	50, 94, 143, 186	0
3	M	179/187 (95%)	0.75	17 (9%) 14 9	45, 93, 140, 170	0
3	Q	179/187 (95%)	0.97	29 (16%) 4 3	58, 104, 151, 184	0
All	All	3456/3616 (95%)	0.41	175 (5%) 33 20	21, 74, 131, 230	0

All (175) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Q	10	THR	4.9
2	P	205	HIS	4.4
2	F	2	GLY	4.1
2	F	1	ALA	4.0
3	C	120	GLY	3.9
1	E	311	ASP	3.9
2	B	256	LYS	3.8
2	F	3	GLY	3.8
1	E	7	ASP	3.8
2	L	172	ALA	3.8
2	F	172	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
2	F	5	HIS	3.7
1	O	90	GLY	3.7
3	G	10	THR	3.7
3	M	10	THR	3.7
2	P	3	GLY	3.7
1	O	7	ASP	3.6
2	B	3	GLY	3.6
2	L	1	ALA	3.6
3	M	84	LEU	3.6
2	L	3	GLY	3.6
1	E	414	ILE	3.5
2	B	7	GLU	3.5
3	M	9	GLY	3.4
3	C	115	THR	3.4
2	L	2	GLY	3.3
3	C	118	GLU	3.3
1	E	8	HIS	3.3
2	F	205	HIS	3.3
2	F	175	VAL	3.3
1	O	6	HIS	3.2
3	M	52	VAL	3.2
3	G	182	THR	3.2
3	C	116	LEU	3.2
3	M	152	HIS	3.2
3	C	16	TYR	3.2
3	Q	158	SER	3.2
2	F	82	GLU	3.2
2	L	256	LYS	3.2
3	M	98	ALA	3.1
1	K	7	ASP	3.1
2	B	5	HIS	3.1
2	B	2	GLY	3.1
3	Q	159	ALA	3.1
3	Q	9	GLY	3.0
3	Q	123	LEU	3.0
1	E	431	HIS	3.0
2	P	123	ASN	3.0
2	L	4	GLY	3.0
3	Q	94	VAL	2.9
2	P	5	HIS	2.9
1	E	116	LEU	2.9
3	M	17	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
3	Q	116	LEU	2.8
2	P	114	MET	2.8
3	C	158	SER	2.8
1	O	3	GLY	2.8
3	C	11	ARG	2.7
2	P	197	ALA	2.7
3	Q	16	TYR	2.7
1	K	8	HIS	2.7
3	M	165	GLY	2.7
3	G	11	ARG	2.7
2	F	256	LYS	2.7
1	K	3	GLY	2.7
3	Q	146	GLY	2.7
3	C	159	ALA	2.6
1	O	8	HIS	2.6
1	A	7	ASP	2.6
2	P	256	LYS	2.6
3	G	52	VAL	2.6
3	Q	90	LEU	2.6
1	A	387	PHE	2.6
3	Q	98	ALA	2.6
3	M	16	TYR	2.6
2	P	2	GLY	2.6
3	M	11	ARG	2.6
3	C	9	GLY	2.6
3	Q	120	GLY	2.6
2	B	205	HIS	2.6
3	M	153	GLY	2.6
1	K	414	ILE	2.6
1	O	236	GLU	2.6
1	E	310	ALA	2.6
3	C	17	TYR	2.5
1	O	13	THR	2.5
3	Q	182	THR	2.5
1	E	413	ALA	2.5
2	L	5	HIS	2.5
2	B	198	ASP	2.5
2	P	80	ASP	2.5
1	E	362	MET	2.5
3	C	10	THR	2.5
3	Q	17	TYR	2.5
2	L	17	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
3	G	79	GLU	2.4
3	Q	181	GLU	2.4
2	B	253	ALA	2.4
3	G	17	TYR	2.4
2	P	71	THR	2.4
3	C	90	LEU	2.4
1	O	15	ILE	2.4
3	G	119	ALA	2.4
2	F	26	GLN	2.4
3	C	63	LEU	2.4
1	A	15	ILE	2.4
2	B	172	ALA	2.4
3	Q	122	TRP	2.4
2	F	174	GLY	2.3
3	Q	145	GLY	2.3
3	C	13	ASP	2.3
3	M	145	GLY	2.3
3	M	176	ALA	2.3
3	Q	138	GLY	2.3
2	F	7	GLU	2.3
3	Q	118	GLU	2.3
1	K	6	HIS	2.3
3	Q	156	TYR	2.3
3	Q	139	GLY	2.3
3	C	14	PHE	2.3
3	C	167	ALA	2.3
2	P	200	HIS	2.3
2	F	194	VAL	2.3
2	L	165	VAL	2.3
2	P	151	PRO	2.3
3	C	174	PRO	2.3
3	G	16	TYR	2.2
2	P	7	GLU	2.2
3	M	93	LEU	2.2
1	K	314	VAL	2.2
2	P	182	TRP	2.2
3	C	47	LEU	2.2
1	A	353	PRO	2.2
2	L	16	PRO	2.2
1	O	385	THR	2.2
2	L	7	GLU	2.2
3	Q	105	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	427	ASP	2.2
3	Q	13	ASP	2.2
3	C	74	ILE	2.1
3	C	140	VAL	2.1
1	A	362	MET	2.1
1	K	362	MET	2.1
2	B	1	ALA	2.1
2	B	204	VAL	2.1
2	P	167	ASP	2.1
3	C	182	THR	2.1
3	C	15	LEU	2.1
2	F	252	TRP	2.1
1	A	21	SER	2.1
3	G	106	GLY	2.1
3	Q	153	GLY	2.1
3	Q	165	GLY	2.1
2	B	77	THR	2.1
3	G	51	PHE	2.1
3	Q	112	GLN	2.1
3	M	135	VAL	2.1
3	Q	170	ASN	2.1
2	P	135	LEU	2.1
2	B	4	GLY	2.1
1	E	12	ARG	2.1
2	P	198	ASP	2.1
1	O	413	ALA	2.1
3	Q	184	ILE	2.1
3	M	112	GLN	2.0
1	K	89	GLY	2.0
1	K	382	ALA	2.0
3	G	143	ASP	2.0
3	C	181	GLU	2.0
3	G	147	TRP	2.0
1	E	9	TYR	2.0
2	F	200	HIS	2.0
3	C	112	GLN	2.0
3	Q	11	ARG	2.0
3	M	133	GLY	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides 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.

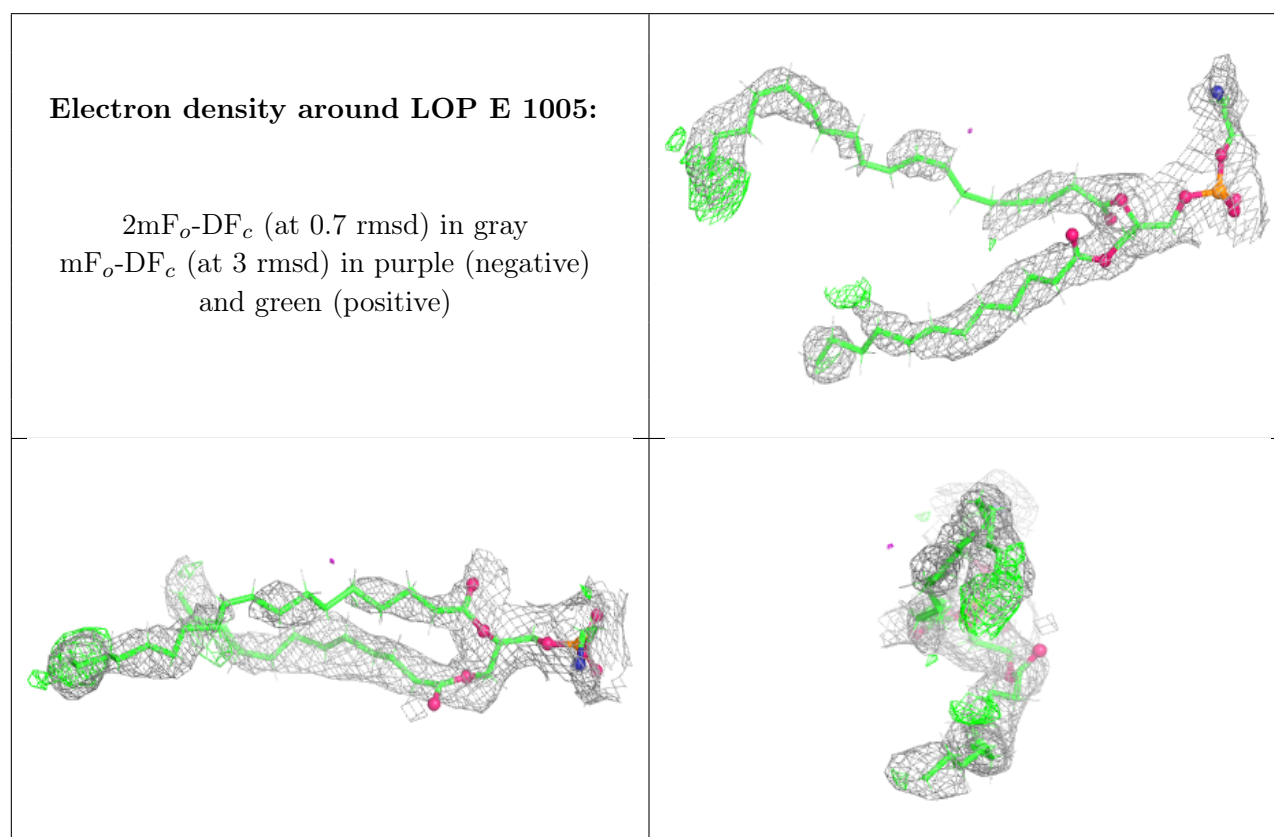
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	SR	A	1005	1/1	0.77	0.09	148,148,148,148	0
8	LOP	E	1005	45/45	0.80	0.19	71,92,108,113	0
8	LOP	A	1006	45/45	0.84	0.16	56,76,90,94	0
8	LOP	O	1005	45/45	0.84	0.16	51,84,107,118	0
10	BOG	P	1003	20/20	0.84	0.13	50,67,85,90	0
10	BOG	B	1003	20/20	0.86	0.13	50,63,70,73	0
8	LOP	K	1006	45/45	0.88	0.14	49,71,92,103	0
6	ASC	A	1004	12/12	0.88	0.14	35,46,56,62	0
6	ASC	O	1004	12/12	0.89	0.19	25,43,59,63	0
10	BOG	F	1003	20/20	0.89	0.12	48,65,80,81	0
6	ASC	K	1004	12/12	0.89	0.14	39,48,57,60	0
7	SR	F	1002	1/1	0.91	0.07	111,111,111,111	0
6	ASC	E	1004	12/12	0.92	0.15	52,56,71,76	0
5	FMX	O	1003	28/28	0.93	0.12	52,64,75,81	0
10	BOG	K	1007	20/20	0.93	0.11	39,60,75,75	0
5	FMX	A	1003	28/28	0.93	0.11	52,62,72,77	0
5	FMX	E	1003	28/28	0.94	0.11	53,67,77,79	0
7	SR	P	1002	1/1	0.94	0.05	109,109,109,109	0
5	FMX	K	1003	28/28	0.95	0.11	47,58,69,78	0
9	HEC	P	1001	43/43	0.95	0.12	63,71,89,95	0
7	SR	K	1005	1/1	0.95	0.08	110,110,110,110	0
9	HEC	F	1001	43/43	0.96	0.11	61,69,82,90	0
4	HEM	E	1001	43/43	0.96	0.13	46,52,69,82	0
4	HEM	E	1002	43/43	0.96	0.13	53,64,77,77	0
4	HEM	K	1002	43/43	0.96	0.10	30,49,74,78	0
4	HEM	O	1002	43/43	0.96	0.11	46,56,70,73	0
4	HEM	A	1001	43/43	0.96	0.13	51,52,62,62	0
9	HEC	L	1001	43/43	0.97	0.10	34,52,66,72	0
4	HEM	A	1002	43/43	0.97	0.11	54,58,70,70	0
4	HEM	O	1001	43/43	0.97	0.12	33,50,66,72	0
4	HEM	K	1001	43/43	0.97	0.12	40,49,65,71	0
9	HEC	B	1001	43/43	0.97	0.09	53,57,69,70	0

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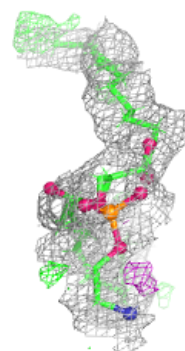
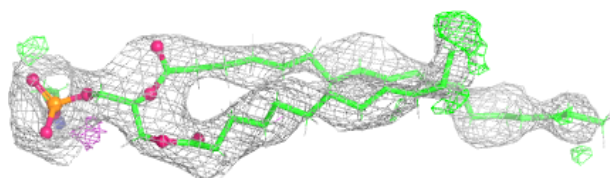
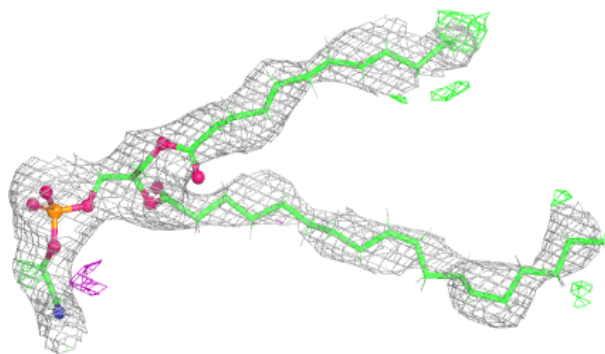
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	SR	B	1002	1/1	0.97	0.04	96,96,96,96	0
11	FES	M	1001	4/4	0.97	0.06	64,65,65,65	0
11	FES	C	1001	4/4	0.98	0.05	82,82,83,87	0
11	FES	G	1001	4/4	0.98	0.05	59,63,65,65	0
7	SR	L	1002	1/1	0.98	0.03	88,88,88,88	0
11	FES	Q	1001	4/4	0.98	0.05	67,70,72,73	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.

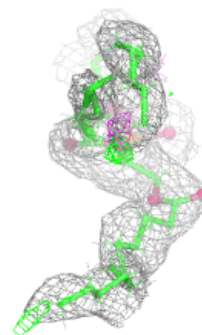
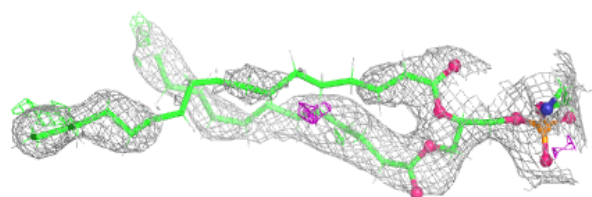
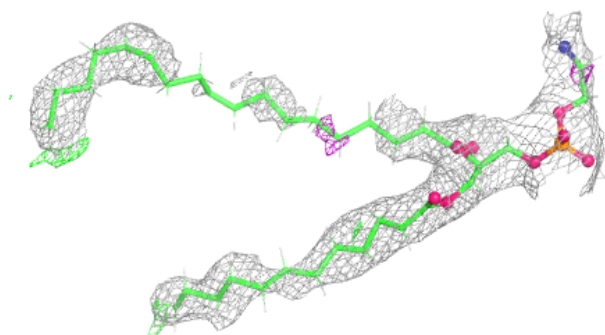


Electron density around LOP A 1006:

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

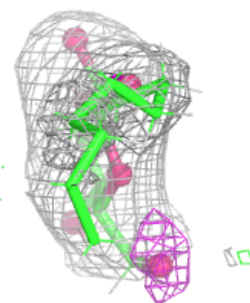
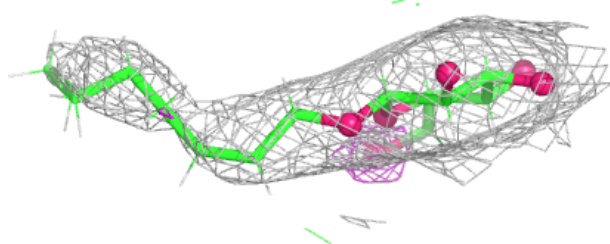
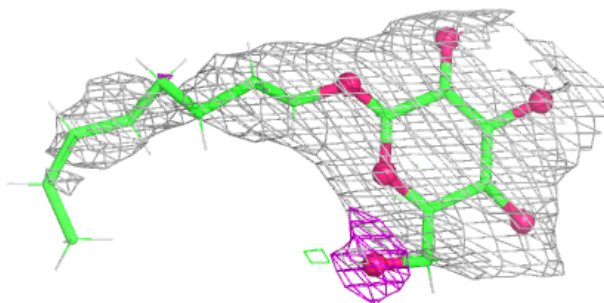
**Electron density around LOP O 1005:**

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

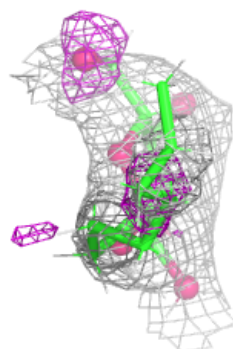
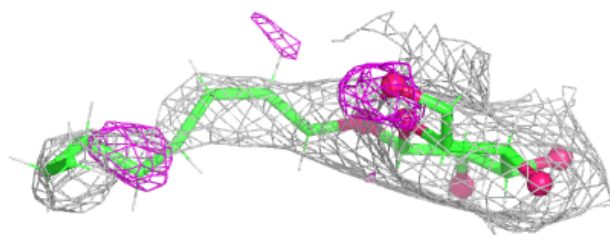
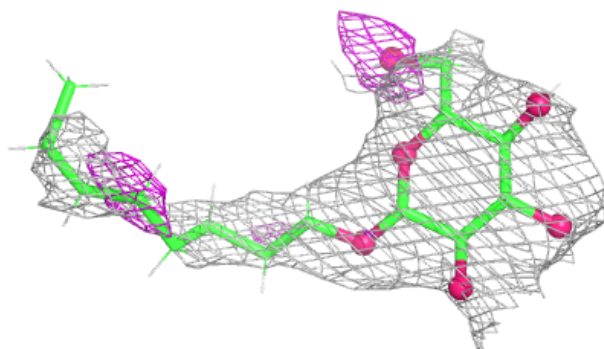


Electron density around BOG P 1003:

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

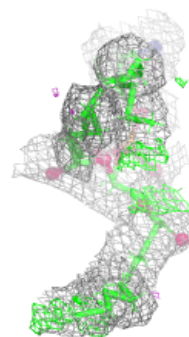
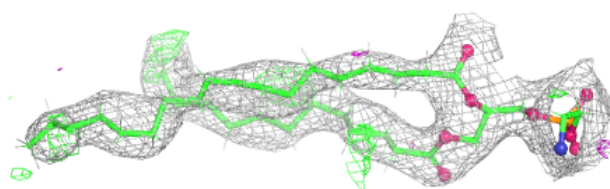
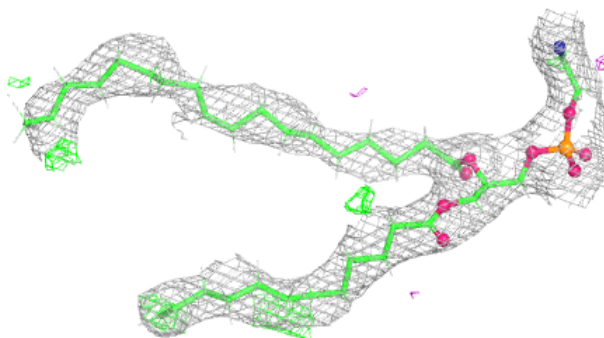
**Electron density around BOG B 1003:**

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

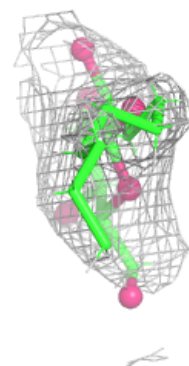
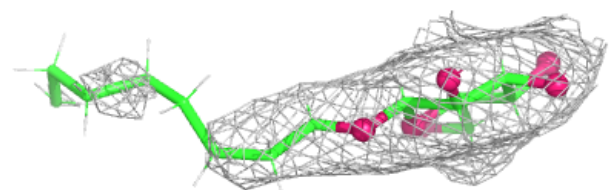
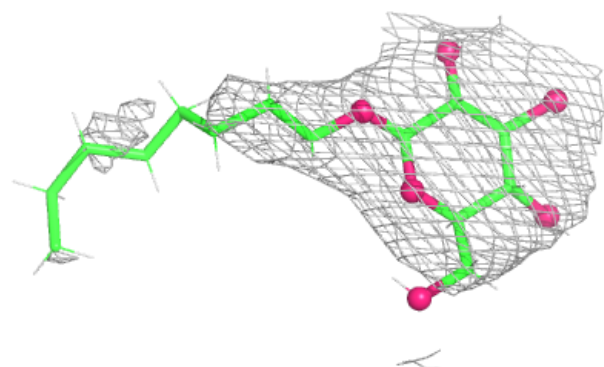


Electron density around LOP K 1006:

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

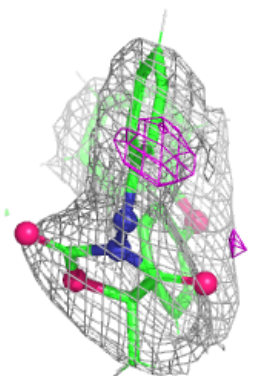
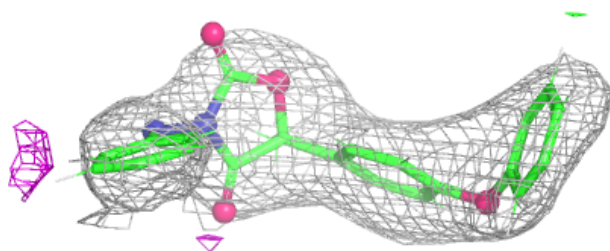
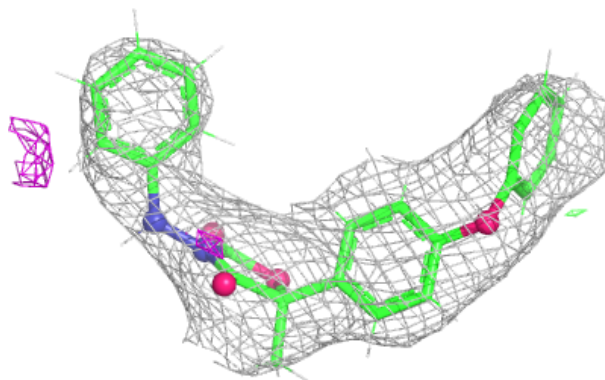
**Electron density around BOG F 1003:**

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

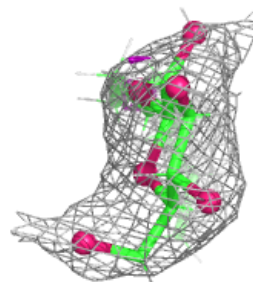
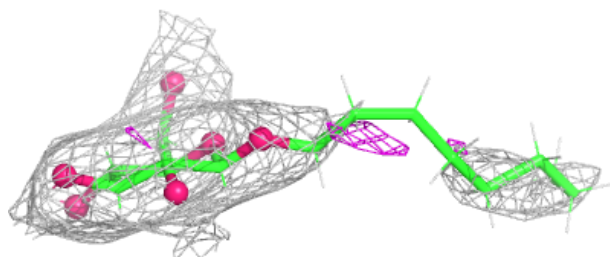
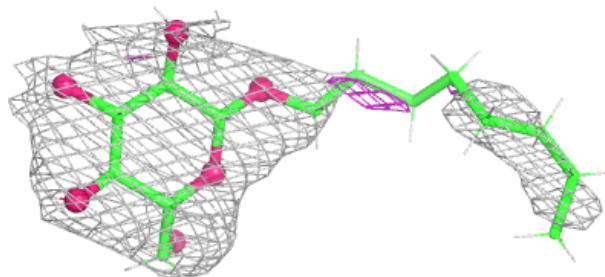


Electron density around FMX O 1003:

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

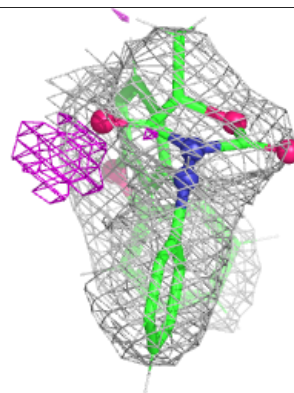
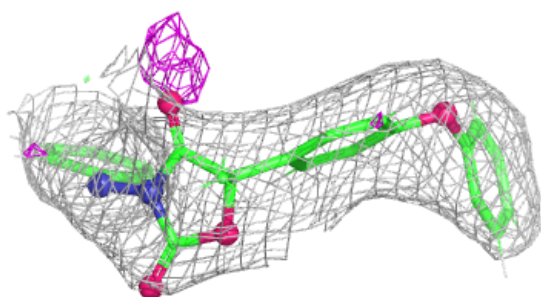
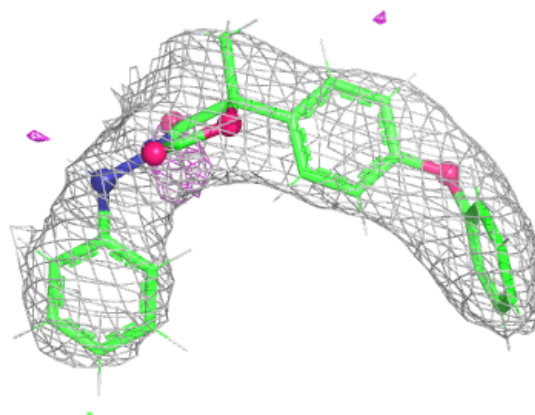
**Electron density around BOG K 1007:**

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

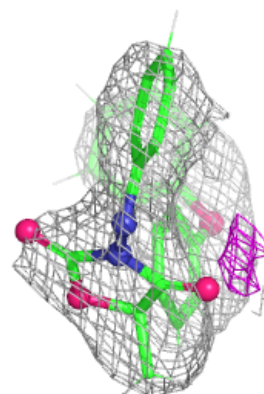
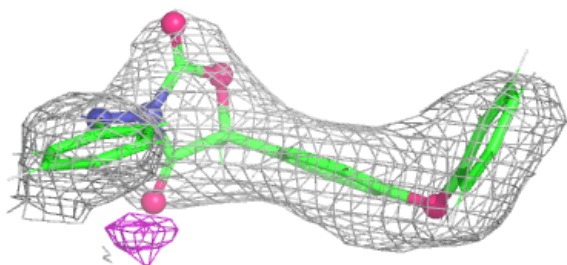
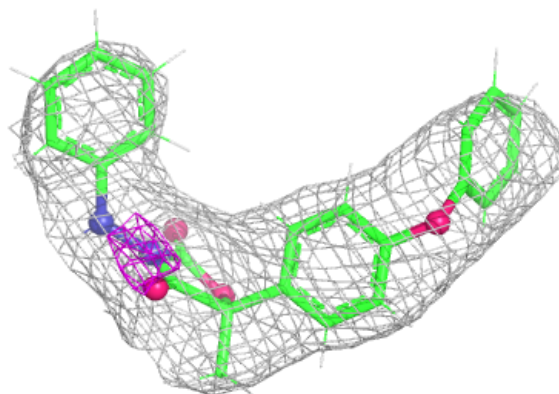


Electron density around FMX A 1003:

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

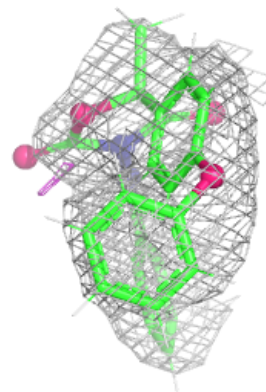
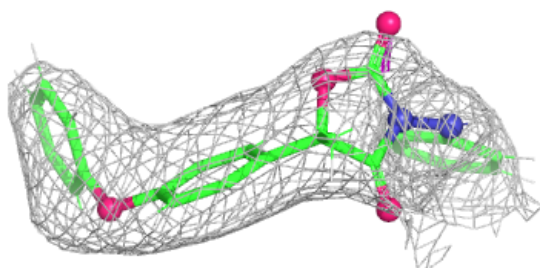
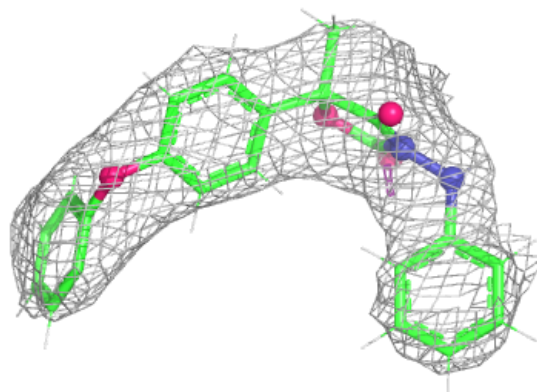
**Electron density around FMX E 1003:**

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



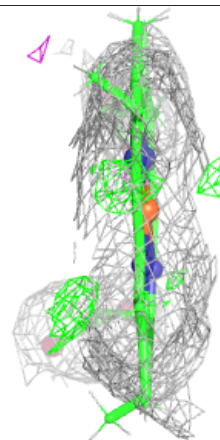
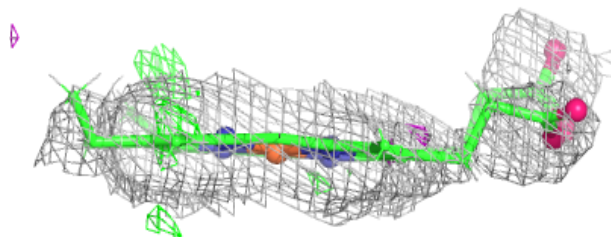
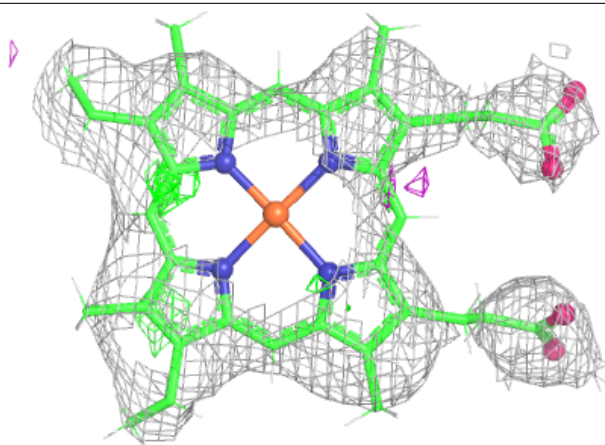
Electron density around FMX K 1003:

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and green (positive)



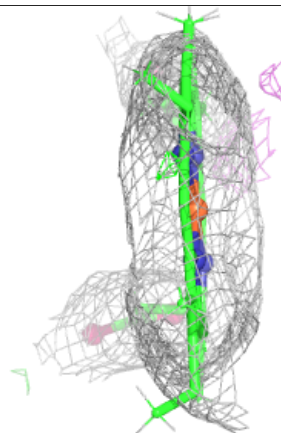
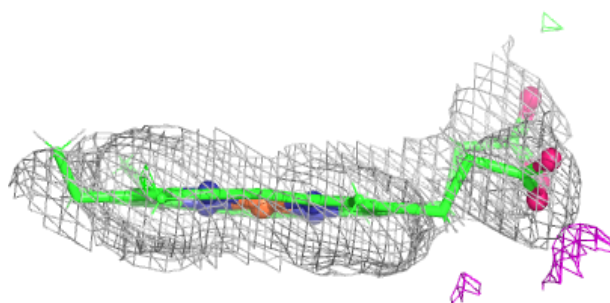
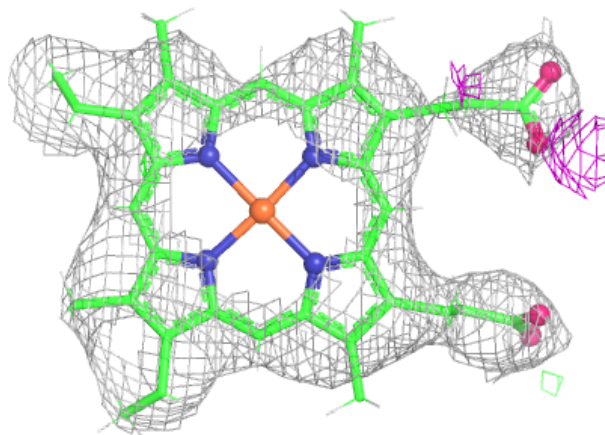
Electron density around HEC P 1001:

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



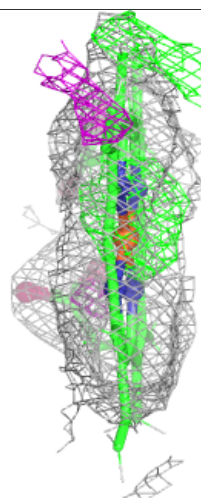
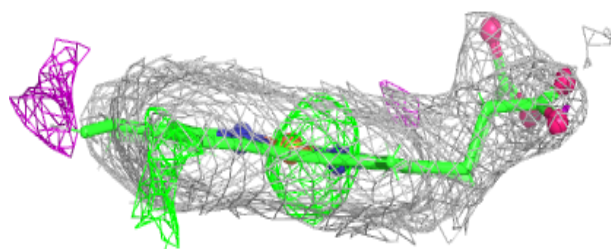
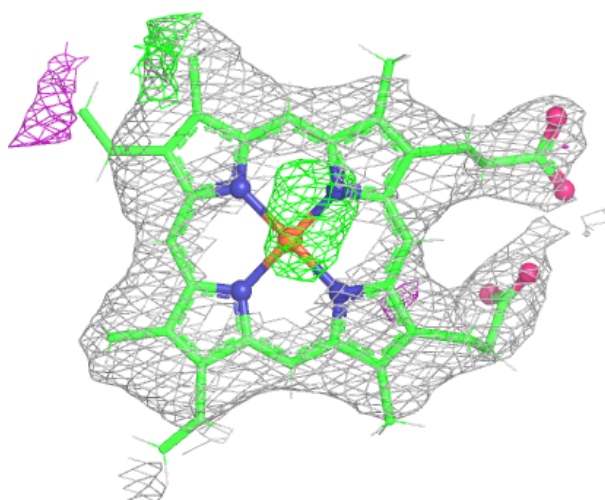
Electron density around HEC F 1001:

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



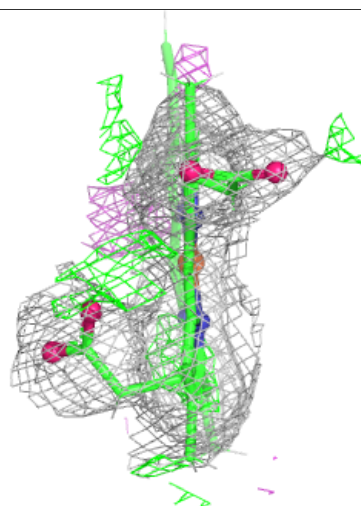
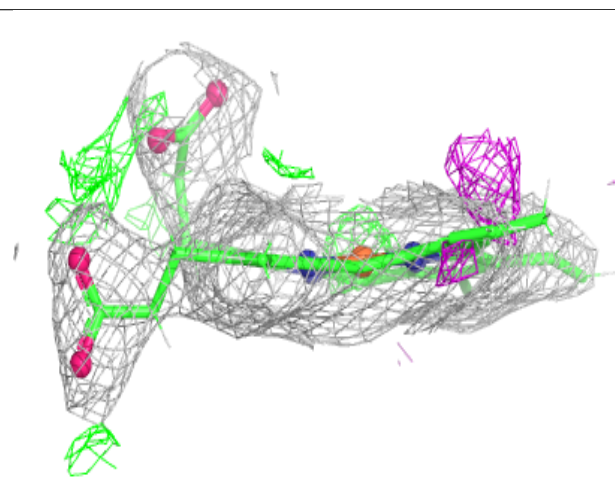
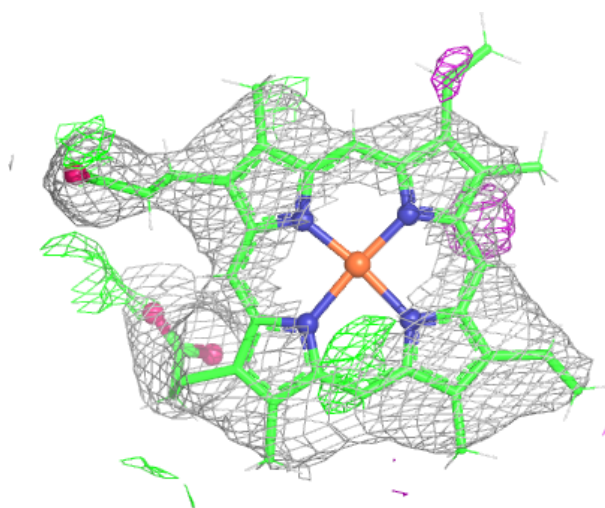
Electron density around HEM E 1001:

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



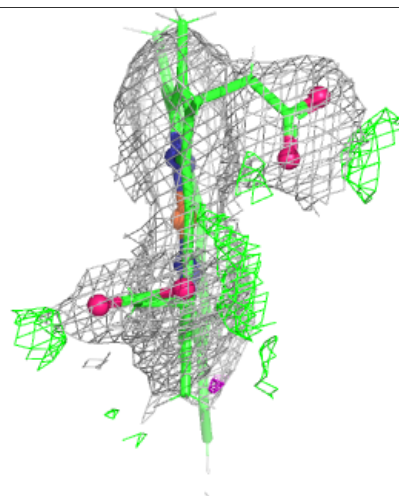
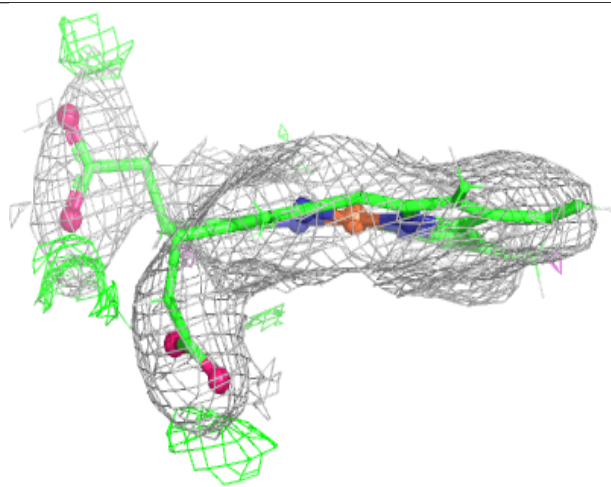
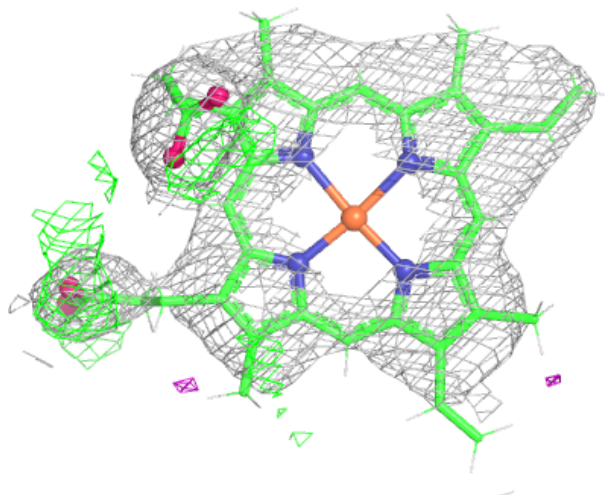
Electron density around HEM E 1002:

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



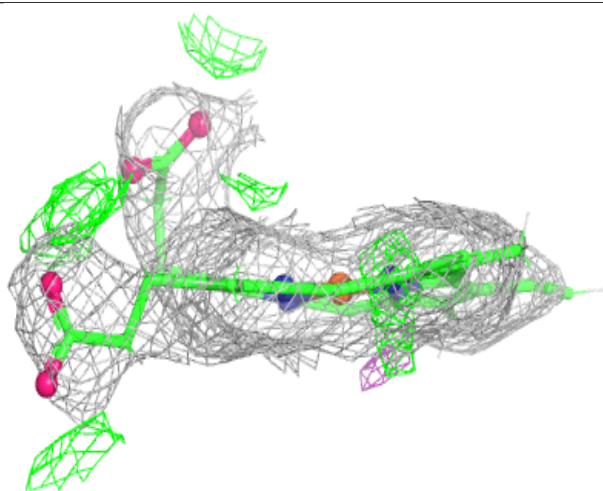
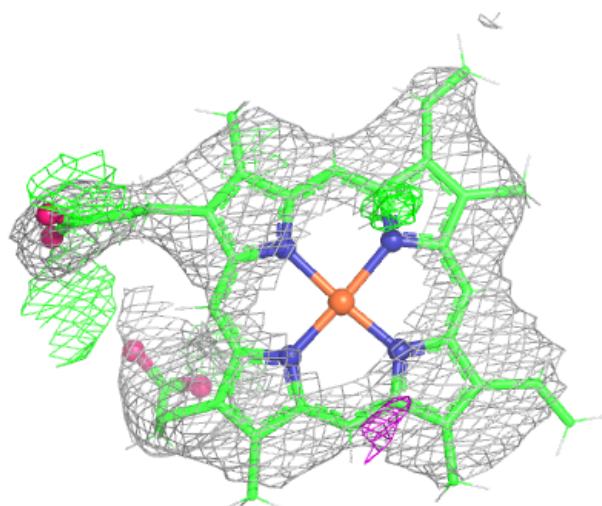
Electron density around HEM K 1002:

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



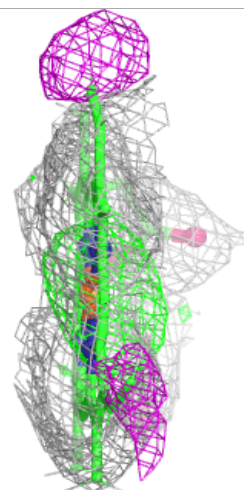
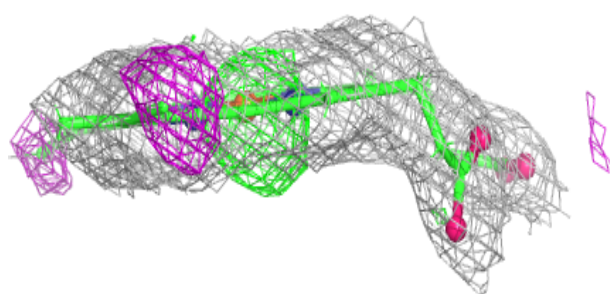
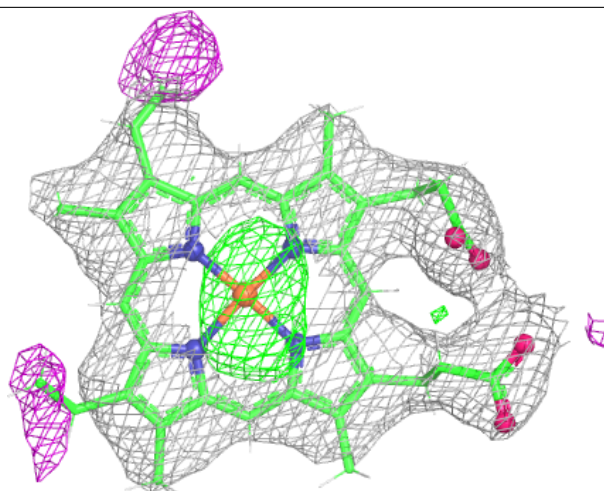
Electron density around HEM O 1002:

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



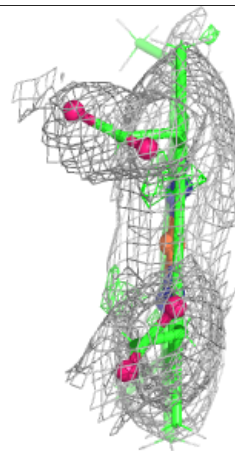
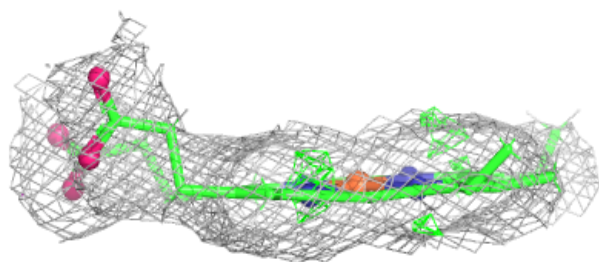
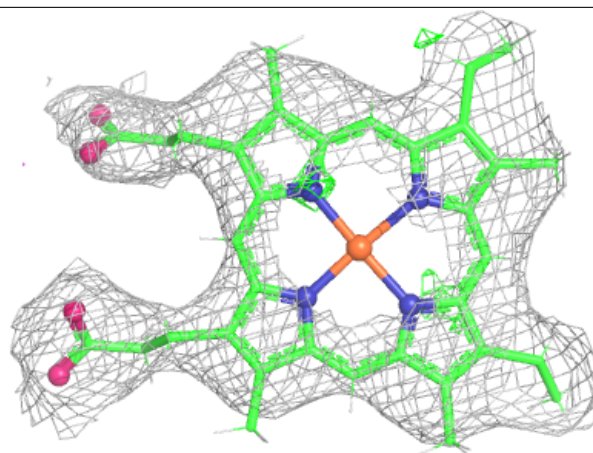
Electron density around HEM A 1001:

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



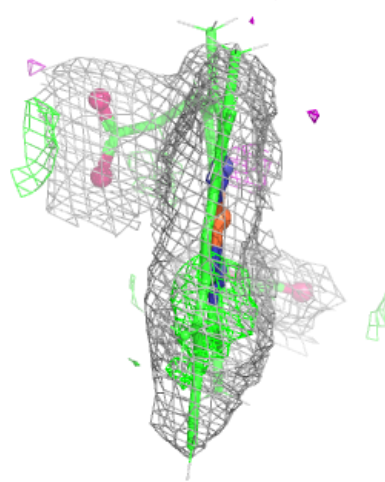
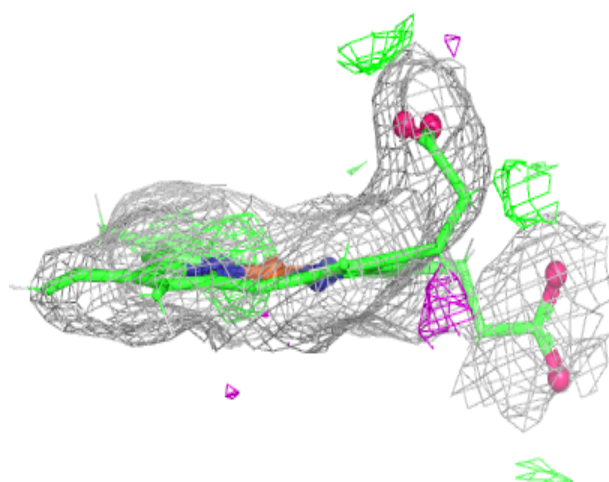
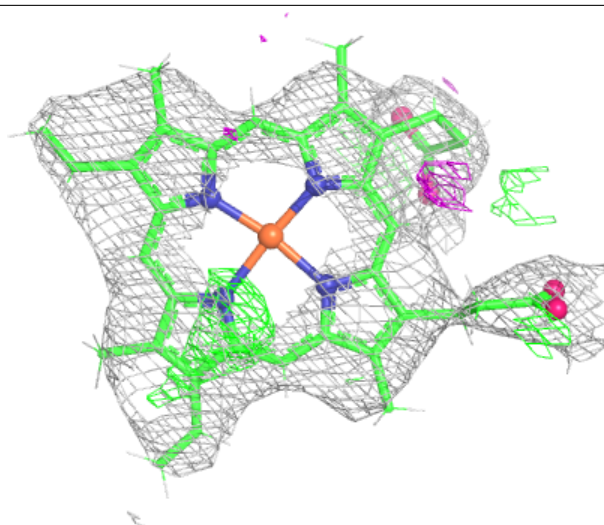
Electron density around HEC L 1001:

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



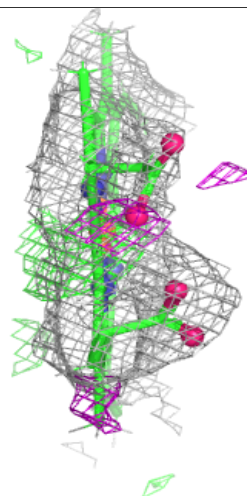
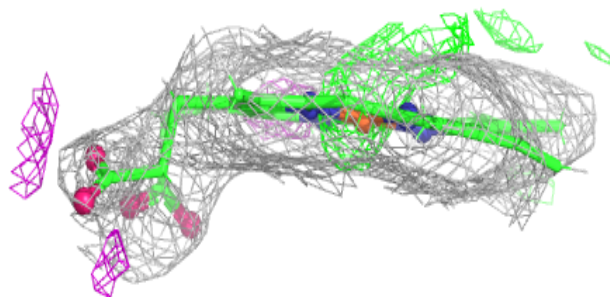
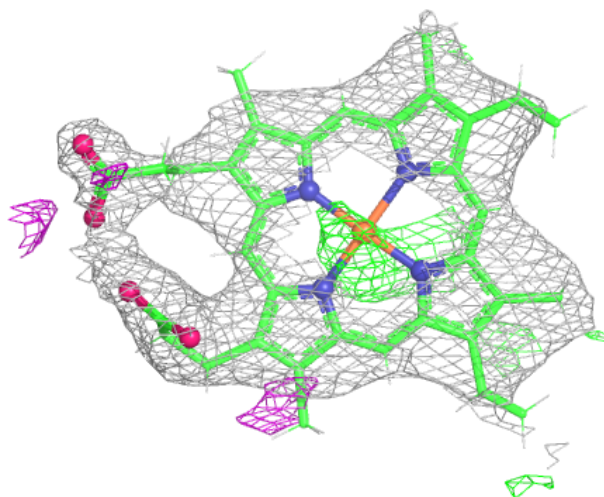
Electron density around HEM A 1002:

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



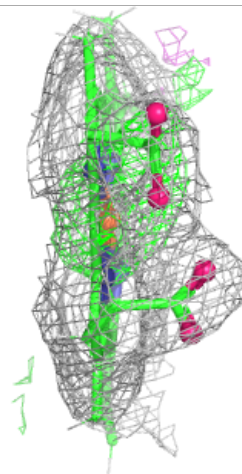
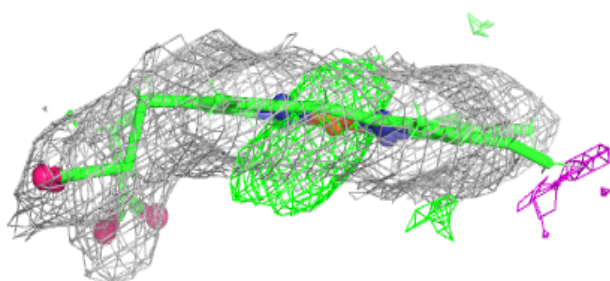
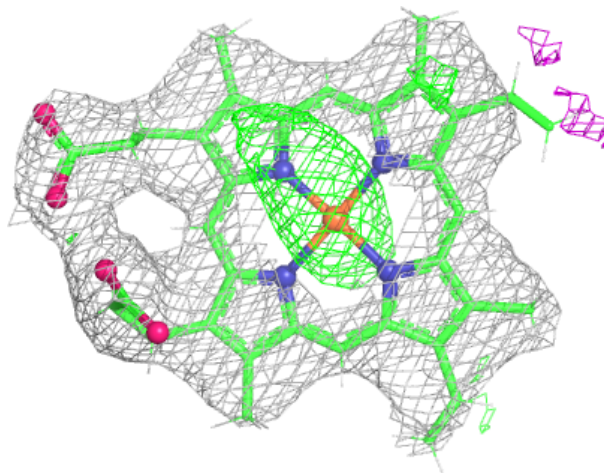
Electron density around HEM O 1001:

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



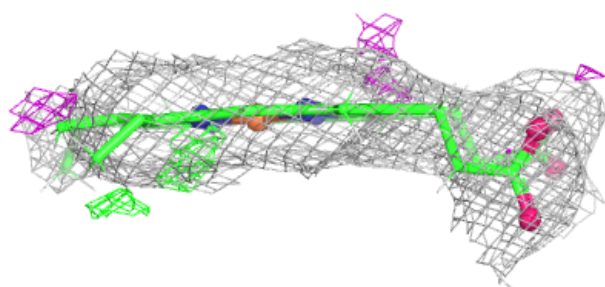
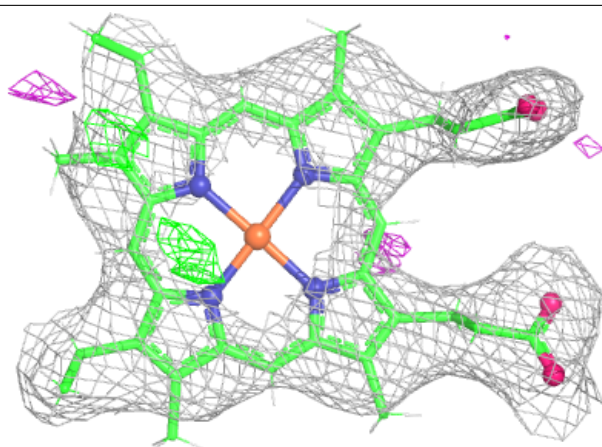
Electron density around HEM K 1001:

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



Electron density around HEC B 1001:

$2mF_o-DF_c$ (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.