



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2026 – 10:23 PM UTC

PDB ID : 7TCE / pdb_00007tce
Title : Crystal structure of delta sub IV Rhodobacter Sphaeroides bc1 with the anti-malarial drug atovaquone.
Authors : Esser, L.; Xia, D.; Zhou, F.
Deposited on : 2021-12-23
Resolution : 3.85 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

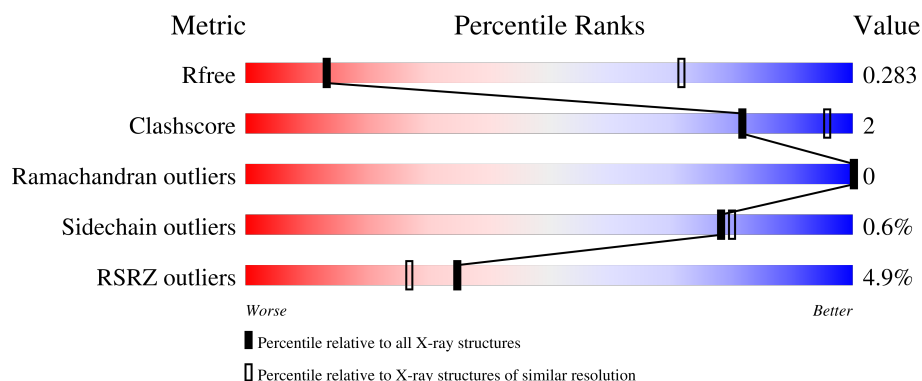
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.85 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	1165 (4.02-3.70)
Clashscore	190562	1207 (4.02-3.70)
Ramachandran outliers	187476	1149 (4.02-3.70)
Sidechain outliers	187428	1142 (4.02-3.70)
RSRZ outliers	180081	1164 (4.02-3.70)

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	6% 88% 8% .
1	E	445	5% 87% 9% .
1	K	445	4% 88% 8% .
1	O	445	6% 89% 7% .
2	B	269	4% 93% 5% .

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Mol	Chain	Length	Quality of chain
2	F	269	
2	L	269	
2	P	269	
3	C	187	
3	G	187	
3	M	187	
3	Q	187	

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 54681 atoms, of which 26895 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
			6856	2325	3411	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
			3790	1240	1837	326	374	13			
2	F	256	Total	C	H	N	O	S	0	0	0
			3790	1240	1837	326	374	13			
2	L	256	Total	C	H	N	O	S	0	0	0
			3790	1240	1837	326	374	13			
2	P	256	Total	C	H	N	O	S	0	0	0
			3790	1240	1837	326	374	13			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	264	HIS	-	expression tag	UNP A3PFR5
B	265	HIS	-	expression tag	UNP A3PFR5
B	266	HIS	-	expression tag	UNP A3PFR5
B	267	HIS	-	expression tag	UNP A3PFR5
B	268	HIS	-	expression tag	UNP A3PFR5
B	269	HIS	-	expression tag	UNP A3PFR5
F	264	HIS	-	expression tag	UNP A3PFR5
F	265	HIS	-	expression tag	UNP A3PFR5

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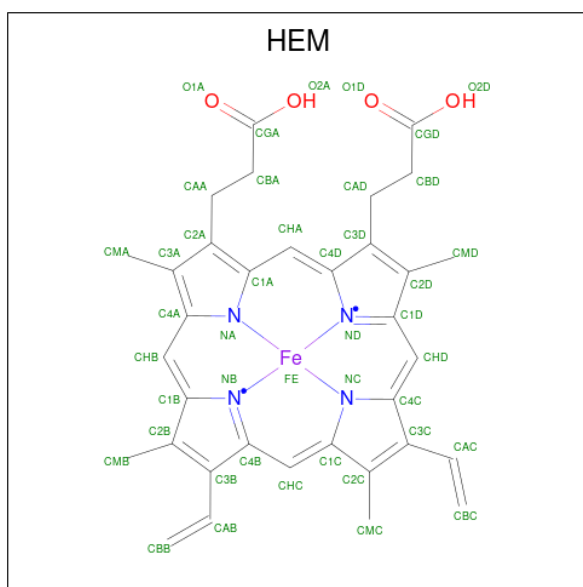
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Chain	Residue	Modelled	Actual	Comment	Reference
F	266	HIS	-	expression tag	UNP A3PFR5
F	267	HIS	-	expression tag	UNP A3PFR5
F	268	HIS	-	expression tag	UNP A3PFR5
F	269	HIS	-	expression tag	UNP A3PFR5
L	264	HIS	-	expression tag	UNP A3PFR5
L	265	HIS	-	expression tag	UNP A3PFR5
L	266	HIS	-	expression tag	UNP A3PFR5
L	267	HIS	-	expression tag	UNP A3PFR5
L	268	HIS	-	expression tag	UNP A3PFR5
L	269	HIS	-	expression tag	UNP A3PFR5
P	264	HIS	-	expression tag	UNP A3PFR5
P	265	HIS	-	expression tag	UNP A3PFR5
P	266	HIS	-	expression tag	UNP A3PFR5
P	267	HIS	-	expression tag	UNP A3PFR5
P	268	HIS	-	expression tag	UNP A3PFR5
P	269	HIS	-	expression tag	UNP A3PFR5

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

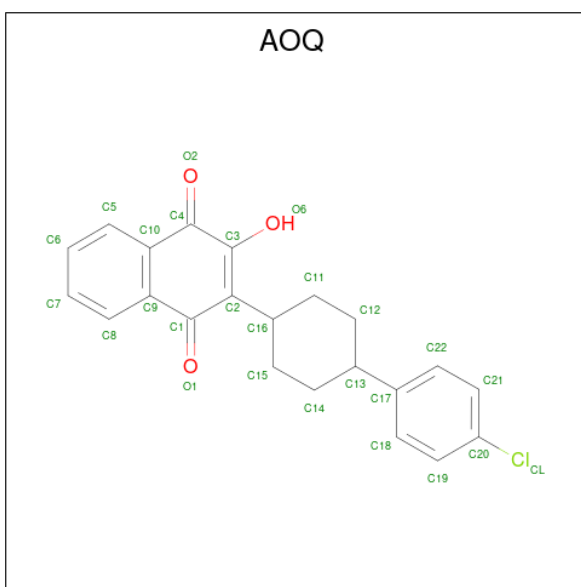
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	179	Total 2645	C 845	H 1304	N 237	O 253	S 6	0	0	0
3	G	179	Total 2645	C 845	H 1304	N 237	O 253	S 6	0	0	0
3	M	179	Total 2645	C 845	H 1304	N 237	O 253	S 6	0	0	0
3	Q	179	Total 2645	C 845	H 1304	N 237	O 253	S 6	0	0	0

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



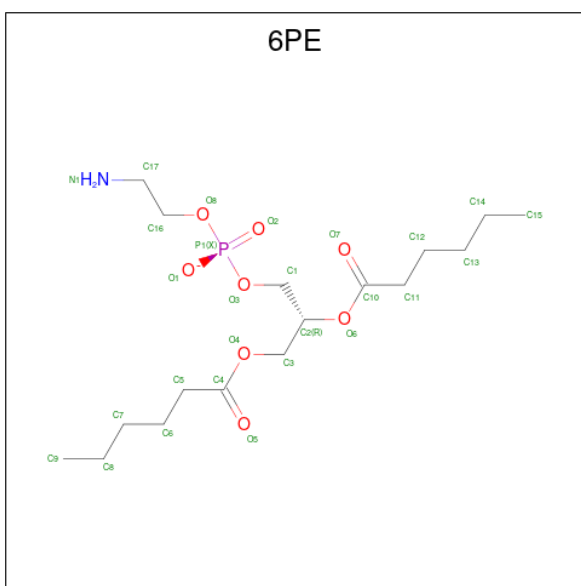
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
4	A	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
4	E	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
4	E	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
4	K	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
4	K	1	Total	C	Fe	H	N	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 2-[trans-4-(4-chlorophenyl)cyclohexyl]-3-hydroxynaphthalene-1,4-dione (CCD ID: AOQ) (formula: $C_{22}H_{19}ClO_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 44	C 22	Cl 1	H 18	O 3	0	0
5	E	1	Total 44	C 22	Cl 1	H 18	O 3	0	0
5	K	1	Total 44	C 22	Cl 1	H 18	O 3	0	0
5	O	1	Total 44	C 22	Cl 1	H 18	O 3	0	0

- Molecule 6 is 1,2-DIHEXANOYL-SN-GLYCERO-3-PHOSPHOETHANOLAMINE (CCD ID: 6PE) (formula: $C_{17}H_{33}NO_8P$).

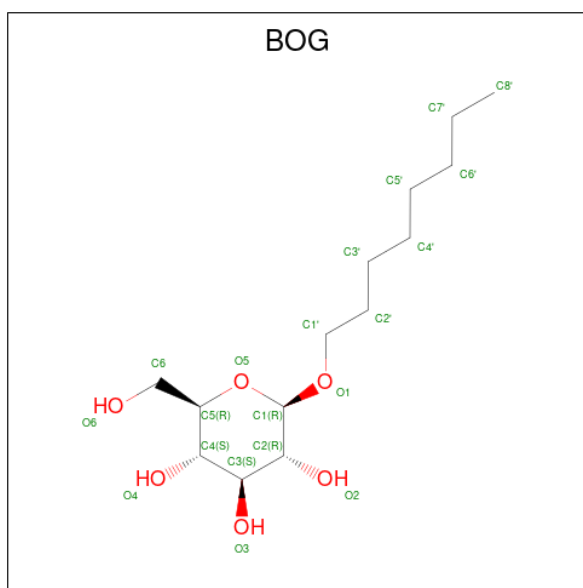


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	H	N	O	P	
			60	17	33	1	8	1	
6	E	1	Total	C	H	N	O	P	
			60	17	33	1	8	1	
6	K	1	Total	C	H	N	O	P	
			60	17	33	1	8	1	
6	O	1	Total	C	H	N	O	P	
			60	17	33	1	8	1	

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

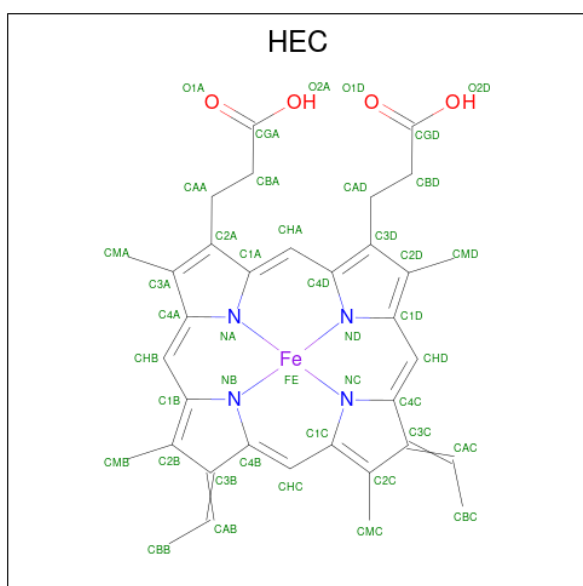
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Sr	0	0
			1	1		
7	B	1	Total	Sr	0	0
			1	1		
7	E	1	Total	Sr	0	0
			1	1		
7	F	1	Total	Sr	0	0
			1	1		
7	L	1	Total	Sr	0	0
			1	1		
7	P	1	Total	Sr	0	0
			1	1		

- Molecule 8 is octyl beta-D-glucopyranoside (CCD ID: BOG) (formula: C₁₄H₂₈O₆).



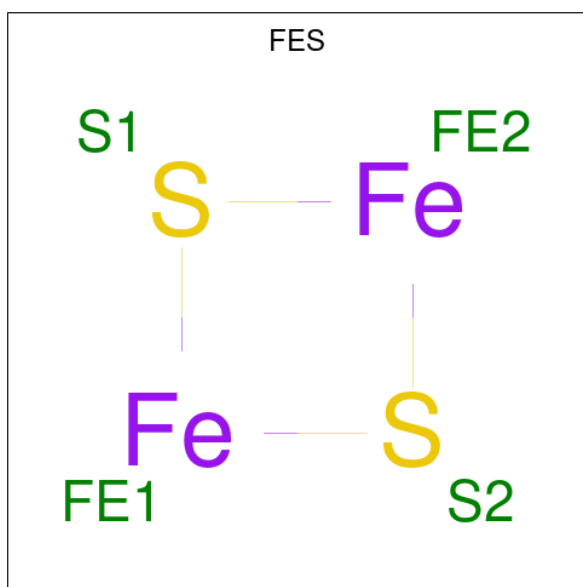
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total 48	C 14	H 28	O 6	0	0
8	E	1	Total 48	C 14	H 28	O 6	0	0
8	K	1	Total 48	C 14	H 28	O 6	0	0
8	O	1	Total 48	C 14	H 28	O 6	0	0

- Molecule 9 is HEME C (CCD ID: HEC) (formula: $\text{C}_{34}\text{H}_{34}\text{FeN}_4\text{O}_4$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
9	B	1	Total 75	C 34	Fe 1	H 32	N 4	O 4	0	0
9	F	1	Total 75	C 34	Fe 1	H 32	N 4	O 4	0	0
9	L	1	Total 75	C 34	Fe 1	H 32	N 4	O 4	0	0
9	P	1	Total 75	C 34	Fe 1	H 32	N 4	O 4	0	0

- Molecule 10 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).

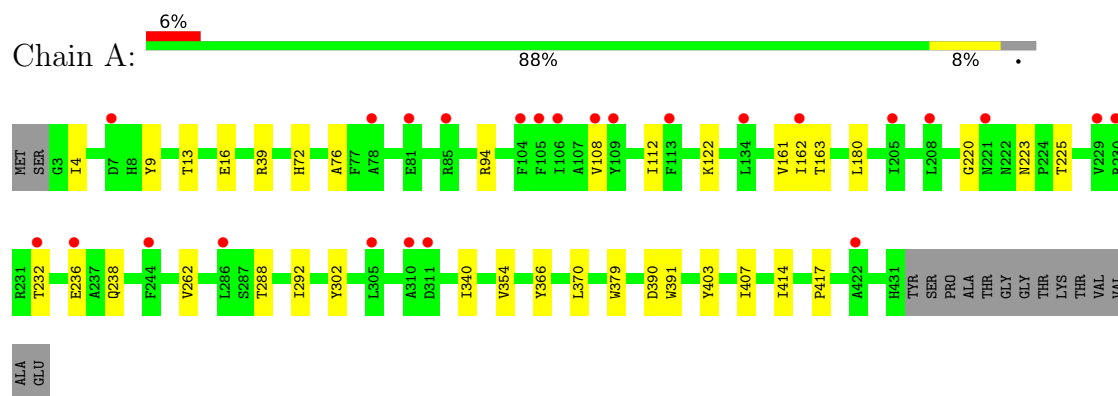


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	C	1	Total	Fe	S	0	0
			4	2	2		
10	G	1	Total	Fe	S	0	0
			4	2	2		
10	M	1	Total	Fe	S	0	0
			4	2	2		
10	Q	1	Total	Fe	S	0	0
			4	2	2		

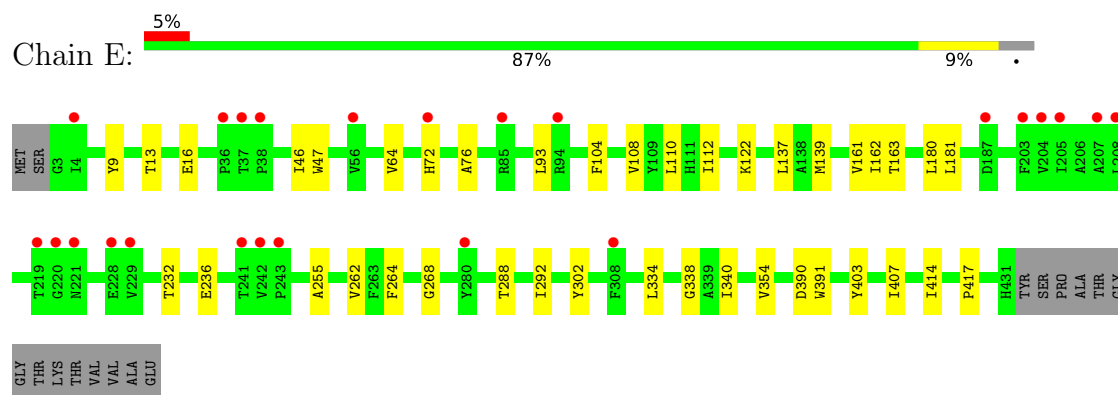
3 Residue-property plots [i](#)

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.

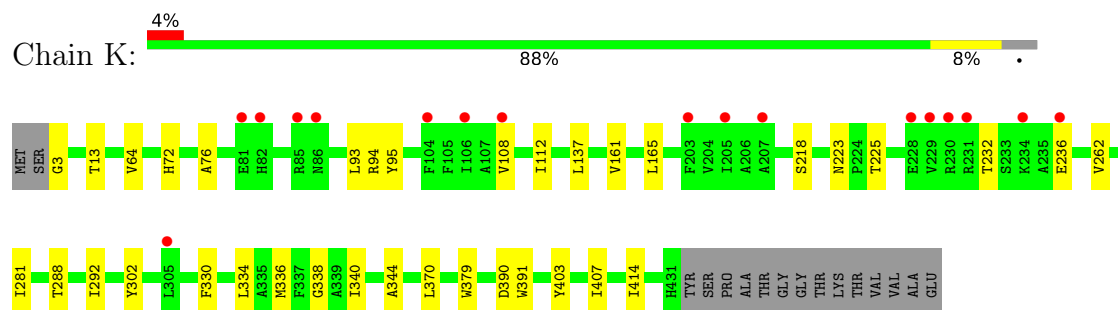
• Molecule 1: Cytochrome b



• Molecule 1: Cytochrome b

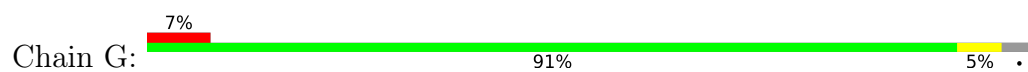


• Molecule 1: Cytochrome b

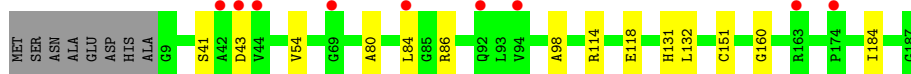
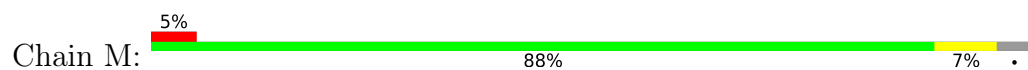


• Molecule 1: Cytochrome b

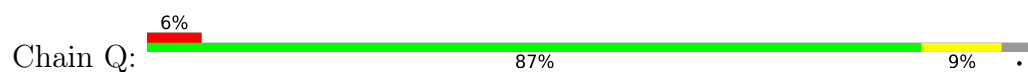




- Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	127.27Å 156.39Å 141.41Å 90.00° 96.67° 90.00°	Depositor
Resolution (Å)	39.43 – 3.85 39.43 – 3.85	Depositor EDS
% Data completeness (in resolution range)	94.6 (39.43-3.85) 81.5 (39.43-3.85)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.56 (at 3.76Å)	Xtrriage
Refinement program	PHENIX 1.20_4444	Depositor
R, R_{free}	0.241 , 0.273 0.255 , 0.283	Depositor DCC
R_{free} test set	1433 reflections (2.84%)	wwPDB-VP
Wilson B-factor (Å ²)	136.5	Xtrriage
Anisotropy	0.490	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 72.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	54681	wwPDB-VP
Average B, all atoms (Å ²)	192.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 56.24 % 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 2.8184e-05. 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: HEM, BOG, 6PE, HEC, FES, SR, AOQ

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	0.18	0/3576	0.37	0/4906
1	E	0.18	0/3576	0.37	0/4906
1	K	0.18	0/3576	0.36	0/4906
1	O	0.23	0/3576	0.48	0/4906
2	B	0.17	0/2010	0.33	0/2733
2	F	0.17	0/2010	0.34	0/2733
2	L	0.16	0/2010	0.33	0/2733
2	P	0.21	0/2010	0.45	0/2733
3	C	0.17	0/1371	0.35	0/1868
3	G	0.18	0/1371	0.37	0/1868
3	M	0.17	0/1371	0.37	0/1868
3	Q	0.22	0/1371	0.48	0/1868
All	All	0.19	0/27828	0.39	0/38028

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3445	3411	3427	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	3445	3412	3427	25	0
1	K	3445	3412	3427	23	0
1	O	3445	3412	3427	23	0
2	B	1953	1837	1848	4	0
2	F	1953	1837	1848	2	0
2	L	1953	1837	1848	5	0
2	P	1953	1837	1848	8	0
3	C	1341	1304	1307	9	0
3	G	1341	1304	1307	6	0
3	M	1341	1304	1307	9	0
3	Q	1341	1304	1307	7	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	2	0
5	A	26	18	18	1	0
5	E	26	18	18	1	0
5	K	26	18	18	0	0
5	O	26	18	18	3	0
6	A	27	33	33	0	0
6	E	27	33	33	0	0
6	K	27	33	33	0	0
6	O	27	33	33	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	E	1	0	0	0	0
7	F	1	0	0	0	0
7	L	1	0	0	0	0
7	P	1	0	0	0	0
8	A	20	28	28	1	0
8	E	20	28	28	1	0
8	K	20	28	28	1	0
8	O	20	28	28	0	0
9	B	43	32	30	0	0
9	F	43	32	30	0	0
9	L	43	32	30	0	0
9	P	43	32	30	0	0
10	C	4	0	0	1	0
10	G	4	0	0	0	0
10	M	4	0	0	0	0
10	Q	4	0	0	0	0
All	All	27786	26895	27004	135	0

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

All (135) 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:132:LEU:HD13	1:E:161:VAL:HG13	1.71	0.72
3:M:151:CYS:O	1:O:302:TYR:OH	2.07	0.72
3:C:151:CYS:O	1:E:302:TYR:OH	2.08	0.70
1:O:46:ILE:HD12	1:O:255:ALA:HB1	1.74	0.68
1:E:232:THR:OG1	1:E:236:GLU:OE1	2.12	0.67
1:K:302:TYR:OH	3:Q:151:CYS:O	2.09	0.66
1:K:161:VAL:HG13	3:Q:132:LEU:HD13	1.77	0.66
1:O:232:THR:OG1	1:O:236:GLU:OE1	2.15	0.64
1:A:161:VAL:HG13	3:G:132:LEU:HD13	1.80	0.63
3:Q:40:PRO:O	3:Q:45:GLN:NE2	2.32	0.63
1:K:3:GLY:N	1:K:218:SER:O	2.33	0.62
4:A:1001:HEM:HHD	4:A:1001:HEM:HBC2	1.82	0.61
3:C:132:LEU:HD12	3:C:152:HIS:CE1	2.36	0.61
3:G:132:LEU:HD12	3:G:152:HIS:CE1	2.36	0.61
3:M:41:SER:OG	3:M:43:ASP:OD1	2.19	0.60
3:M:86:ARG:NH2	3:M:118:GLU:O	2.34	0.60
2:P:6:VAL:HG21	2:P:109:GLY:O	2.03	0.59
1:K:137:LEU:HD21	1:K:340:ILE:HG21	1.87	0.57
4:K:1001:HEM:HBC2	4:K:1001:HEM:HHD	1.88	0.56
1:A:302:TYR:OH	3:G:151:CYS:O	2.18	0.56
1:O:288:THR:HG22	1:O:292:ILE:HD11	1.88	0.56
1:O:64:VAL:HG11	1:O:93:LEU:HD13	1.88	0.55
1:A:94:ARG:NH1	4:A:1001:HEM:O1A	2.39	0.55
4:E:1001:HEM:HBC2	4:E:1001:HEM:HMC1	1.87	0.55
4:O:1001:HEM:HMC1	4:O:1001:HEM:HBC2	1.88	0.55
1:A:122:LYS:NZ	1:A:354:VAL:O	2.36	0.55
3:C:41:SER:OG	3:C:43:ASP:OD1	2.25	0.54
2:P:65:ALA:O	2:P:68:THR:OG1	2.27	0.53
3:M:54:VAL:HG11	3:M:184:ILE:HD12	1.90	0.52
3:Q:132:LEU:HD12	3:Q:152:HIS:CE1	2.44	0.52
1:K:94:ARG:NH1	4:K:1001:HEM:O1A	2.44	0.51
1:O:292:ILE:HG21	5:O:1003:AOQ:H2	1.91	0.51
1:E:64:VAL:HG11	1:E:93:LEU:HD13	1.93	0.51
1:A:370:LEU:HD22	1:A:403:TYR:CE2	2.46	0.51
1:A:403:TYR:HA	1:A:407:ILE:HD12	1.93	0.50
1:A:366:TYR:CD1	1:A:407:ILE:HD13	2.47	0.50
1:A:232:THR:OG1	1:A:236:GLU:OE1	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:288:THR:CG2	1:E:292:ILE:HD11	2.42	0.50
3:M:132:LEU:HD22	1:O:164:GLY:C	2.37	0.50
1:K:403:TYR:HA	1:K:407:ILE:HD12	1.94	0.49
4:K:1001:HEM:HBB2	4:K:1001:HEM:HHC	1.94	0.49
2:P:46:PRO:O	2:P:49:SER:OG	2.26	0.49
3:M:114:ARG:NH2	3:M:160:GLY:O	2.45	0.49
1:O:132:GLY:O	4:O:1002:HEM:HMC3	2.12	0.49
1:E:288:THR:HG22	1:E:292:ILE:HD11	1.94	0.49
1:O:407:ILE:HG22	1:O:411:LEU:HD12	1.95	0.49
1:O:288:THR:CG2	1:O:292:ILE:HD11	2.43	0.49
1:O:403:TYR:HA	1:O:407:ILE:HD12	1.95	0.48
4:A:1001:HEM:HBB2	4:A:1001:HEM:HHC	1.95	0.48
3:C:86:ARG:NH2	3:C:118:GLU:O	2.45	0.48
1:A:354:VAL:HG21	1:A:417:PRO:HB3	1.94	0.48
2:B:132:TYR:OH	2:B:205:HIS:ND1	2.28	0.48
1:E:403:TYR:HA	1:E:407:ILE:HD12	1.95	0.48
3:Q:41:SER:OG	3:Q:43:ASP:OD1	2.31	0.48
1:K:262:VAL:HG13	8:K:1005:BOG:H8'1	1.96	0.48
1:E:390:ASP:OD1	1:E:391:TRP:N	2.46	0.48
1:A:4:ILE:HD11	1:A:220:GLY:HA3	1.95	0.48
1:A:262:VAL:HG13	8:A:1006:BOG:H8'1	1.96	0.48
1:O:81:GLU:OE1	1:O:85:ARG:NE	2.46	0.48
1:O:154:MET:HE1	5:O:1003:AOQ:H3	1.96	0.48
1:A:379:TRP:NE1	2:B:114:MET:O	2.43	0.48
1:K:165:LEU:HD13	1:K:336:MET:HE1	1.94	0.48
1:E:108:VAL:O	1:E:112:ILE:N	2.42	0.48
1:K:288:THR:CG2	1:K:292:ILE:HD11	2.43	0.48
3:G:41:SER:OG	3:G:43:ASP:OD1	2.32	0.48
1:K:288:THR:HG22	1:K:292:ILE:HD11	1.95	0.47
1:A:390:ASP:OD1	1:A:391:TRP:N	2.47	0.47
1:A:288:THR:HG22	1:A:292:ILE:HD11	1.96	0.47
1:E:9:TYR:OH	1:E:16:GLU:OE1	2.31	0.47
2:F:169:CYS:O	2:F:177:THR:OG1	2.12	0.47
1:O:354:VAL:HG21	1:O:417:PRO:HB3	1.95	0.47
1:A:39:ARG:NH2	1:A:238:GLN:O	2.48	0.47
1:K:390:ASP:OD1	1:K:391:TRP:N	2.48	0.47
3:M:98:ALA:O	3:M:114:ARG:NH1	2.46	0.47
3:M:131:HIS:O	3:M:132:LEU:HD23	2.15	0.46
2:P:19:THR:HB	2:P:224:MET:HE3	1.97	0.46
3:C:114:ARG:NH2	3:C:160:GLY:O	2.48	0.46
1:A:163:THR:HG22	1:A:180:LEU:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:163:THR:HG22	1:E:180:LEU:HB3	1.98	0.46
1:E:47:TRP:CZ2	1:E:110:LEU:HD13	2.51	0.45
1:K:108:VAL:O	1:K:112:ILE:N	2.44	0.45
3:M:80:ALA:O	3:M:84:LEU:HD13	2.16	0.45
2:B:220:GLU:OE2	2:B:226:ARG:NH1	2.49	0.45
1:E:162:ILE:HD11	5:E:1003:AOQ:H14	1.98	0.45
3:G:54:VAL:HG11	3:G:184:ILE:HD12	1.99	0.45
3:G:80:ALA:O	3:G:84:LEU:HD13	2.18	0.44
1:K:72:HIS:O	1:K:76:ALA:N	2.46	0.44
1:O:108:VAL:O	1:O:112:ILE:N	2.45	0.44
1:O:390:ASP:OD1	1:O:391:TRP:N	2.51	0.44
1:A:72:HIS:O	1:A:76:ALA:N	2.47	0.44
2:P:42:MET:HE1	2:P:214:PHE:CE2	2.53	0.44
1:E:262:VAL:HG13	8:E:1005:BOG:H8'1	2.00	0.43
1:A:288:THR:CG2	1:A:292:ILE:HD11	2.49	0.43
1:O:334:LEU:O	1:O:338:GLY:N	2.48	0.43
1:E:122:LYS:NZ	1:E:354:VAL:O	2.48	0.43
1:E:264:PHE:O	1:E:268:GLY:N	2.52	0.43
1:A:108:VAL:O	1:A:112:ILE:N	2.43	0.43
2:P:29:LEU:HD22	2:P:50:LEU:HD22	2.00	0.43
3:C:54:VAL:HG11	3:C:184:ILE:HD12	2.00	0.42
2:L:220:GLU:OE2	2:L:226:ARG:NH1	2.52	0.42
1:E:104:PHE:CE2	1:E:139:MET:HE3	2.54	0.42
3:Q:71:PRO:HG2	3:Q:135:VAL:HG22	2.01	0.42
1:A:223:ASN:OD1	1:A:225:THR:OG1	2.27	0.42
1:O:414:ILE:HG22	1:O:414:ILE:O	2.20	0.42
3:C:154:SER:OG	10:C:1001:FES:S1	2.70	0.42
1:K:223:ASN:OD1	1:K:225:THR:OG1	2.29	0.42
1:O:64:VAL:HG11	1:O:93:LEU:CD1	2.49	0.42
1:O:85:ARG:NH2	2:P:218:ALA:O	2.50	0.42
1:K:95:TYR:OH	2:L:105:LYS:NZ	2.51	0.42
3:C:58:GLU:OE1	3:C:58:GLU:N	2.52	0.42
1:O:140:MET:HE3	5:O:1003:AOQ:H16	2.01	0.42
1:O:428:PHE:CE2	2:P:255:VAL:HG12	2.55	0.42
2:L:26:GLN:HG2	2:L:58:LEU:HD21	2.02	0.41
1:O:165:LEU:HD13	1:O:336:MET:HE1	2.02	0.41
3:Q:88:VAL:HG11	3:Q:93:LEU:HD21	2.03	0.41
1:E:137:LEU:HD21	1:E:340:ILE:HG21	2.02	0.41
1:E:334:LEU:O	1:E:338:GLY:N	2.51	0.41
1:E:64:VAL:HG11	1:E:93:LEU:CD1	2.50	0.41
1:E:72:HIS:O	1:E:76:ALA:N	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:354:VAL:HG21	1:E:417:PRO:HB3	2.03	0.41
1:K:232:THR:OG1	1:K:236:GLU:OE1	2.39	0.41
1:E:163:THR:HG21	1:E:181:LEU:HD23	2.03	0.41
1:K:330:PHE:CE2	1:K:334:LEU:HD11	2.56	0.41
1:A:9:TYR:OH	1:A:16:GLU:OE1	2.37	0.41
2:B:29:LEU:HD22	2:B:50:LEU:HD22	2.02	0.41
1:E:46:ILE:HD12	1:E:255:ALA:HB1	2.02	0.41
1:E:163:THR:HG21	1:E:181:LEU:CD2	2.51	0.41
1:K:340:ILE:O	1:K:344:ALA:N	2.48	0.41
1:K:334:LEU:O	1:K:338:GLY:N	2.50	0.41
2:F:26:GLN:HG2	2:F:58:LEU:HD21	2.04	0.40
1:K:64:VAL:HG11	1:K:93:LEU:HD13	2.02	0.40
1:K:281:ILE:HD11	2:L:107:ARG:NH1	2.36	0.40
1:K:379:TRP:NE1	2:L:114:MET:O	2.52	0.40
1:A:162:ILE:HD11	5:A:1003:AOQ:H7	2.03	0.40
1:K:370:LEU:HD22	1:K:403:TYR:CE2	2.56	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%)	413 (97%)	14 (3%)	0	100	100
1	E	427/445 (96%)	414 (97%)	13 (3%)	0	100	100
1	K	427/445 (96%)	413 (97%)	14 (3%)	0	100	100
1	O	427/445 (96%)	408 (96%)	19 (4%)	0	100	100
2	B	254/269 (94%)	245 (96%)	9 (4%)	0	100	100
2	F	254/269 (94%)	245 (96%)	9 (4%)	0	100	100
2	L	254/269 (94%)	244 (96%)	10 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	P	254/269 (94%)	242 (95%)	12 (5%)	0	100	100
3	C	177/187 (95%)	166 (94%)	11 (6%)	0	100	100
3	G	177/187 (95%)	167 (94%)	10 (6%)	0	100	100
3	M	177/187 (95%)	166 (94%)	11 (6%)	0	100	100
3	Q	177/187 (95%)	164 (93%)	13 (7%)	0	100	100
All	All	3432/3604 (95%)	3287 (96%)	145 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	354/366 (97%)	351 (99%)	3 (1%)	73	77
1	E	354/366 (97%)	352 (99%)	2 (1%)	78	80
1	K	354/366 (97%)	352 (99%)	2 (1%)	78	80
1	O	354/366 (97%)	351 (99%)	3 (1%)	73	77
2	B	203/215 (94%)	203 (100%)	0	100	100
2	F	203/215 (94%)	203 (100%)	0	100	100
2	L	203/215 (94%)	203 (100%)	0	100	100
2	P	203/215 (94%)	202 (100%)	1 (0%)	81	82
3	C	138/144 (96%)	138 (100%)	0	100	100
3	G	138/144 (96%)	138 (100%)	0	100	100
3	M	138/144 (96%)	138 (100%)	0	100	100
3	Q	138/144 (96%)	133 (96%)	5 (4%)	31	54
All	All	2780/2900 (96%)	2764 (99%)	16 (1%)	78	80

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	THR
1	A	340	ILE
1	A	414	ILE
1	E	13	THR
1	E	414	ILE
1	K	13	THR
1	K	414	ILE
1	O	13	THR
1	O	178	THR
1	O	321	ILE
2	P	239	VAL
3	Q	27	THR
3	Q	31	VAL
3	Q	49	SER
3	Q	52	VAL
3	Q	65	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	HIS
1	A	72	HIS
1	A	86	ASN
1	A	188	ASN
1	A	217	HIS
2	B	200	HIS
3	C	92	GLN
1	E	86	ASN
2	F	200	HIS
3	G	39	ASN
3	G	92	GLN
1	K	72	HIS
1	K	86	ASN
1	K	188	ASN
1	K	217	HIS
2	L	200	HIS
2	L	248	ASN
1	O	86	ASN
1	O	316	GLN
2	P	161	GLN
3	Q	39	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 34 ligands modelled in this entry, 6 are monoatomic - leaving 28 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$
8	BOG	E	1005	-	20,20,20	1.02	1 (5%)	25,25,25	1.12	3 (12%)
9	HEC	L	1001	2	46,50,50	1.86	5 (10%)	58,82,82	1.62	5 (8%)
6	6PE	K	1004	-	26,26,26	0.78	1 (3%)	29,31,31	0.77	1 (3%)
9	HEC	B	1001	2	46,50,50	1.87	7 (15%)	58,82,82	1.61	5 (8%)
10	FES	C	1001	3	0,4,4	-	-	-	-	-
6	6PE	O	1004	-	26,26,26	0.74	1 (3%)	29,31,31	1.13	3 (10%)
8	BOG	K	1005	-	20,20,20	0.95	1 (5%)	25,25,25	1.17	2 (8%)
5	AOQ	K	1003	-	29,29,29	1.06	1 (3%)	41,42,42	1.92	8 (19%)
5	AOQ	O	1003	-	29,29,29	1.02	1 (3%)	41,42,42	2.05	8 (19%)
10	FES	Q	1001	3	0,4,4	-	-	-	-	-
8	BOG	O	1005	-	20,20,20	0.95	1 (5%)	25,25,25	1.19	2 (8%)
10	FES	M	1001	3	0,4,4	-	-	-	-	-
6	6PE	A	1004	-	26,26,26	0.76	1 (3%)	29,31,31	1.01	3 (10%)
4	HEM	E	1001	1	50,50,50	1.42	10 (20%)	67,82,82	1.09	4 (5%)
5	AOQ	E	1003	-	29,29,29	1.05	1 (3%)	41,42,42	1.93	10 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	HEM	O	1002	1	50,50,50	1.41	8 (16%)	67,82,82	1.08	2 (2%)
5	AOQ	A	1003	-	29,29,29	1.00	1 (3%)	41,42,42	1.70	8 (19%)
4	HEM	E	1002	1	50,50,50	1.43	8 (16%)	67,82,82	1.10	3 (4%)
4	HEM	A	1002	1	50,50,50	1.44	9 (18%)	67,82,82	1.09	4 (5%)
6	6PE	E	1004	-	26,26,26	0.77	1 (3%)	29,31,31	0.98	3 (10%)
4	HEM	A	1001	1	50,50,50	1.50	10 (20%)	67,82,82	1.32	9 (13%)
4	HEM	K	1002	1	50,50,50	1.43	8 (16%)	67,82,82	1.10	4 (5%)
4	HEM	O	1001	1	50,50,50	1.41	10 (20%)	67,82,82	1.08	4 (5%)
4	HEM	K	1001	1	50,50,50	1.52	10 (20%)	67,82,82	1.34	9 (13%)
9	HEC	F	1001	2	46,50,50	1.87	7 (15%)	58,82,82	1.63	5 (8%)
8	BOG	A	1006	-	20,20,20	0.95	1 (5%)	25,25,25	1.14	2 (8%)
9	HEC	P	1001	2	46,50,50	1.86	8 (17%)	58,82,82	1.64	5 (8%)
10	FES	G	1001	3	0,4,4	-	-	-	-	-

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
8	BOG	E	1005	-	-	4/11/31/31	0/1/1/1
9	HEC	L	1001	2	-	8/14/54/54	-
6	6PE	K	1004	-	-	13/30/30/30	-
9	HEC	B	1001	2	-	8/14/54/54	-
10	FES	C	1001	3	-	-	0/1/1/1
6	6PE	O	1004	-	-	12/30/30/30	-
8	BOG	K	1005	-	-	6/11/31/31	0/1/1/1
5	AOQ	K	1003	-	-	3/8/38/38	0/4/4/4
5	AOQ	O	1003	-	-	2/8/38/38	0/4/4/4
10	FES	Q	1001	3	-	-	0/1/1/1
8	BOG	O	1005	-	-	6/11/31/31	0/1/1/1
10	FES	M	1001	3	-	-	0/1/1/1
6	6PE	A	1004	-	-	10/30/30/30	-
4	HEM	E	1001	1	-	0/14/54/54	-
5	AOQ	E	1003	-	-	2/8/38/38	0/4/4/4
4	HEM	O	1002	1	-	3/14/54/54	-
5	AOQ	A	1003	-	-	3/8/38/38	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HEM	E	1002	1	-	3/14/54/54	-
4	HEM	A	1002	1	-	3/14/54/54	-
6	6PE	E	1004	-	-	7/30/30/30	-
4	HEM	A	1001	1	-	1/14/54/54	-
4	HEM	K	1002	1	-	3/14/54/54	-
4	HEM	O	1001	1	-	0/14/54/54	-
4	HEM	K	1001	1	-	1/14/54/54	-
9	HEC	F	1001	2	-	6/14/54/54	-
8	BOG	A	1006	-	-	6/11/31/31	0/1/1/1
9	HEC	P	1001	2	-	6/14/54/54	-
10	FES	G	1001	3	-	-	0/1/1/1

All (112) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	F	1001	HEC	CAC-C3C	6.36	1.55	1.35
9	B	1001	HEC	CAC-C3C	6.31	1.55	1.35
9	L	1001	HEC	CAC-C3C	6.30	1.55	1.35
9	B	1001	HEC	CAB-C3B	6.28	1.55	1.35
9	P	1001	HEC	CAB-C3B	6.24	1.55	1.35
9	P	1001	HEC	CAC-C3C	6.23	1.55	1.35
9	F	1001	HEC	CAB-C3B	6.22	1.55	1.35
9	L	1001	HEC	CAB-C3B	6.21	1.55	1.35
9	F	1001	HEC	C3D-C2D	5.75	1.53	1.38
9	P	1001	HEC	C3D-C2D	5.71	1.53	1.38
9	B	1001	HEC	C3D-C2D	5.68	1.53	1.38
9	L	1001	HEC	C3D-C2D	5.67	1.53	1.38
4	A	1002	HEM	FE-NB	4.36	2.08	1.94
4	K	1001	HEM	FE-NA	4.28	2.09	1.95
4	E	1002	HEM	FE-NB	4.26	2.08	1.94
4	O	1002	HEM	FE-NB	4.04	2.07	1.94
4	K	1002	HEM	FE-NB	3.99	2.07	1.94
4	A	1001	HEM	FE-NA	3.83	2.07	1.95
4	O	1002	HEM	FE-NC	3.67	2.07	1.95
4	A	1002	HEM	FE-NC	3.53	2.06	1.95
4	A	1001	HEM	FE-NB	3.51	2.05	1.94
4	E	1002	HEM	FE-NC	3.51	2.06	1.95
4	K	1002	HEM	FE-NC	3.47	2.06	1.95
5	E	1003	AOQ	C20-CL	3.42	1.82	1.74
5	K	1003	AOQ	C20-CL	3.41	1.82	1.74
4	K	1001	HEM	FE-ND	3.40	2.05	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1003	AOQ	C20-CL	3.39	1.82	1.74
5	O	1003	AOQ	C20-CL	3.39	1.82	1.74
4	E	1001	HEM	FE-ND	3.34	2.05	1.94
4	K	1001	HEM	CAC-C3C	3.32	1.56	1.47
4	O	1002	HEM	CAC-C3C	3.32	1.56	1.47
4	O	1001	HEM	FE-NB	3.31	2.05	1.94
4	K	1001	HEM	FE-NB	3.28	2.05	1.94
4	A	1001	HEM	FE-NC	3.24	2.05	1.95
4	O	1001	HEM	FE-ND	3.24	2.04	1.94
4	A	1002	HEM	CAC-C3C	3.24	1.56	1.47
4	E	1001	HEM	FE-NB	3.20	2.04	1.94
4	A	1001	HEM	CAC-C3C	3.18	1.55	1.47
4	K	1002	HEM	CAB-C3B	3.17	1.55	1.47
4	K	1002	HEM	CAC-C3C	3.17	1.55	1.47
4	A	1002	HEM	CAB-C3B	3.16	1.55	1.47
4	E	1002	HEM	CAC-C3C	3.14	1.55	1.47
4	O	1002	HEM	CAB-C3B	3.11	1.55	1.47
4	A	1001	HEM	FE-ND	3.11	2.04	1.94
4	E	1001	HEM	FE-NC	3.09	2.05	1.95
4	A	1001	HEM	CAB-C3B	3.08	1.55	1.47
4	E	1001	HEM	CAB-C3B	3.07	1.55	1.47
4	O	1001	HEM	CAB-C3B	3.07	1.55	1.47
4	E	1002	HEM	CAB-C3B	3.06	1.55	1.47
4	E	1001	HEM	CAC-C3C	3.06	1.55	1.47
4	K	1001	HEM	CAB-C3B	3.05	1.55	1.47
4	O	1001	HEM	CAC-C3C	3.01	1.55	1.47
4	O	1001	HEM	FE-NC	2.91	2.04	1.95
4	K	1001	HEM	FE-NC	2.91	2.04	1.95
4	E	1001	HEM	FE-NA	2.90	2.04	1.95
4	A	1002	HEM	FE-NA	2.58	2.03	1.95
4	E	1002	HEM	FE-NA	2.56	2.03	1.95
4	O	1001	HEM	FE-NA	2.53	2.03	1.95
8	A	1006	BOG	C4-C5	2.50	1.58	1.53
8	E	1005	BOG	C4-C5	2.48	1.58	1.53
4	K	1002	HEM	FE-NA	2.47	2.03	1.95
9	B	1001	HEC	CMC-C2C	2.44	1.55	1.50
8	K	1005	BOG	C4-C5	2.43	1.58	1.53
8	O	1005	BOG	C4-C5	2.41	1.58	1.53
9	F	1001	HEC	CMC-C2C	2.38	1.55	1.50
9	L	1001	HEC	CMC-C2C	2.37	1.55	1.50
4	O	1001	HEM	CMC-C2C	2.36	1.55	1.50
9	P	1001	HEC	CMC-C2C	2.33	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	1001	HEM	CMC-C2C	2.32	1.55	1.50
6	K	1004	6PE	P1-O3	2.29	1.68	1.59
6	E	1004	6PE	P1-O3	2.27	1.68	1.59
4	K	1002	HEM	CMC-C2C	2.26	1.55	1.50
4	E	1002	HEM	CMB-C2B	2.26	1.55	1.50
4	A	1001	HEM	CMC-C2C	2.25	1.55	1.50
6	O	1004	6PE	P1-O3	2.24	1.68	1.59
4	K	1001	HEM	CMC-C2C	2.23	1.55	1.50
6	A	1004	6PE	P1-O3	2.22	1.68	1.59
4	O	1002	HEM	CMB-C2B	2.21	1.55	1.50
4	E	1002	HEM	CMC-C2C	2.21	1.55	1.50
4	K	1002	HEM	CMB-C2B	2.21	1.55	1.50
4	A	1002	HEM	CMB-C2B	2.21	1.55	1.50
4	A	1002	HEM	CMC-C2C	2.17	1.55	1.50
4	O	1001	HEM	CMD-C2D	2.14	1.55	1.50
4	K	1001	HEM	CMA-C3A	2.13	1.55	1.50
9	L	1001	HEC	CMB-C2B	2.13	1.55	1.50
9	F	1001	HEC	CMB-C2B	2.12	1.55	1.50
4	E	1001	HEM	CMB-C2B	2.11	1.55	1.50
4	O	1001	HEM	CMA-C3A	2.10	1.55	1.50
4	E	1001	HEM	CMD-C2D	2.09	1.55	1.50
4	A	1001	HEM	CMA-C3A	2.09	1.55	1.50
9	P	1001	HEC	CMB-C2B	2.08	1.55	1.50
4	A	1001	HEM	CMB-C2B	2.08	1.55	1.50
4	E	1001	HEM	CMA-C3A	2.08	1.55	1.50
4	E	1002	HEM	CMA-C3A	2.08	1.55	1.50
9	P	1001	HEC	CMD-C2D	2.08	1.55	1.50
9	B	1001	HEC	CMB-C2B	2.08	1.55	1.50
4	K	1001	HEM	CMD-C2D	2.07	1.55	1.50
9	P	1001	HEC	CMA-C3A	2.07	1.55	1.50
4	O	1001	HEM	CMB-C2B	2.07	1.55	1.50
4	A	1002	HEM	CMA-C3A	2.05	1.55	1.50
9	P	1001	HEC	C3B-C2B	-2.05	1.34	1.41
4	K	1001	HEM	CMB-C2B	2.05	1.55	1.50
4	A	1001	HEM	CMD-C2D	2.04	1.55	1.50
9	F	1001	HEC	CMD-C2D	2.03	1.54	1.50
4	A	1002	HEM	CMD-C2D	2.02	1.54	1.50
9	B	1001	HEC	CMD-C2D	2.02	1.54	1.50
4	O	1002	HEM	CMC-C2C	2.02	1.54	1.50
4	O	1002	HEM	CMA-C3A	2.02	1.54	1.50
9	B	1001	HEC	CMA-C3A	2.01	1.54	1.50
4	O	1002	HEM	CMD-C2D	2.01	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	1002	HEM	CMA-C3A	2.00	1.54	1.50
9	F	1001	HEC	CMA-C3A	2.00	1.54	1.50

All (112) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	O	1003	AOQ	C16-C2-C1	8.44	129.58	119.11
5	K	1003	AOQ	C16-C2-C1	7.13	127.95	119.11
9	P	1001	HEC	CBB-CAB-C3B	-6.63	114.17	127.43
9	B	1001	HEC	CBB-CAB-C3B	-6.54	114.37	127.43
9	F	1001	HEC	CBC-CAC-C3C	-6.52	114.41	127.43
9	F	1001	HEC	CBB-CAB-C3B	-6.36	114.72	127.43
9	L	1001	HEC	CBC-CAC-C3C	-6.25	114.95	127.43
9	P	1001	HEC	CBC-CAC-C3C	-6.14	115.17	127.43
9	B	1001	HEC	CBC-CAC-C3C	-6.13	115.17	127.43
9	L	1001	HEC	CBB-CAB-C3B	-6.08	115.28	127.43
5	E	1003	AOQ	C11-C16-C2	5.30	125.06	113.81
5	O	1003	AOQ	C11-C12-C13	4.62	119.11	110.61
5	K	1003	AOQ	C11-C12-C13	4.55	118.98	110.61
5	E	1003	AOQ	C11-C12-C13	4.44	118.77	110.61
5	A	1003	AOQ	O6-C3-C4	-4.40	108.80	116.89
5	A	1003	AOQ	C12-C11-C16	4.14	118.47	111.18
5	E	1003	AOQ	C16-C2-C1	4.12	124.22	119.11
5	A	1003	AOQ	C11-C12-C13	3.81	117.61	110.61
9	L	1001	HEC	C4D-ND-C1D	3.62	111.73	105.82
9	F	1001	HEC	C4D-ND-C1D	3.59	111.67	105.82
9	P	1001	HEC	C4D-ND-C1D	3.55	111.61	105.82
5	E	1003	AOQ	O1-C1-C9	-3.50	115.97	121.57
9	B	1001	HEC	C4D-ND-C1D	3.47	111.48	105.82
5	O	1003	AOQ	C11-C16-C2	3.39	121.01	113.81
6	O	1004	6PE	C2-O6-C10	3.36	125.83	117.80
5	K	1003	AOQ	O1-C1-C9	-3.35	116.22	121.57
5	K	1003	AOQ	C11-C16-C2	3.31	120.83	113.81
5	E	1003	AOQ	O6-C3-C4	-3.29	110.84	116.89
5	O	1003	AOQ	O6-C3-C4	-3.17	111.06	116.89
5	A	1003	AOQ	C15-C16-C2	3.11	120.42	113.81
4	A	1001	HEM	C3B-C2B-C1B	3.05	108.70	106.41
5	A	1003	AOQ	O6-C3-C2	2.99	126.14	121.84
5	E	1003	AOQ	C12-C13-C17	2.92	119.58	112.67
4	K	1001	HEM	C3B-C4B-NB	-2.87	107.41	109.47
5	O	1003	AOQ	O1-C1-C9	-2.76	117.16	121.57
4	K	1001	HEM	C3B-C2B-C1B	2.74	108.47	106.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1001	HEM	C3B-C4B-NB	-2.74	107.50	109.47
4	O	1002	HEM	CMC-C2C-C1C	-2.73	119.91	124.73
5	K	1003	AOQ	C2-C3-C4	2.71	126.00	123.40
4	K	1001	HEM	C1B-NB-C4B	2.69	108.39	105.21
5	O	1003	AOQ	C2-C3-C4	2.69	125.98	123.40
5	K	1003	AOQ	O6-C3-C4	-2.67	111.98	116.89
8	O	1005	BOG	C1-C2-C3	-2.67	104.40	110.01
4	A	1001	HEM	C1B-NB-C4B	2.67	108.36	105.21
5	E	1003	AOQ	C15-C16-C2	-2.67	108.16	113.81
6	E	1004	6PE	C2-O6-C10	2.64	124.12	117.80
4	K	1002	HEM	CMC-C2C-C1C	-2.62	120.12	124.73
8	K	1005	BOG	C1-C2-C3	-2.62	104.51	110.01
5	A	1003	AOQ	C22-C17-C13	2.61	127.70	121.09
8	A	1006	BOG	C1-C2-C3	-2.58	104.59	110.01
4	A	1002	HEM	CMC-C2C-C1C	-2.57	120.21	124.73
5	K	1003	AOQ	C12-C11-C16	2.56	115.68	111.18
9	P	1001	HEC	C2A-C1A-NA	-2.55	107.86	110.32
5	A	1003	AOQ	C18-C17-C13	-2.54	114.66	121.09
4	K	1001	HEM	CHD-C1D-ND	2.52	127.13	124.42
6	A	1004	6PE	C2-O6-C10	2.51	123.80	117.80
6	A	1004	6PE	O1-P1-O2	2.49	124.04	112.44
4	E	1002	HEM	CMC-C2C-C1C	-2.48	120.37	124.73
4	E	1002	HEM	C4D-ND-C1D	2.47	108.13	105.21
5	K	1003	AOQ	O1-C1-C2	2.46	125.42	121.14
6	O	1004	6PE	O1-P1-O2	2.45	123.85	112.44
9	L	1001	HEC	C2A-C1A-NA	-2.44	107.97	110.32
4	K	1001	HEM	CHD-C4C-C3C	2.41	129.27	125.21
4	A	1002	HEM	C4D-ND-C1D	2.41	108.06	105.21
9	F	1001	HEC	CAA-CBA-CGA	-2.39	107.33	113.67
4	A	1001	HEM	C4D-ND-C1D	2.37	108.02	105.21
4	K	1001	HEM	C4D-ND-C1D	2.35	107.99	105.21
9	P	1001	HEC	CAA-CBA-CGA	-2.35	107.44	113.67
5	O	1003	AOQ	C14-C13-C17	-2.33	107.15	112.67
6	E	1004	6PE	O1-P1-O2	2.31	123.18	112.44
9	F	1001	HEC	C2A-C1A-NA	-2.30	108.10	110.32
6	E	1004	6PE	O6-C10-C11	-2.30	106.51	111.48
8	E	1005	BOG	O3-C3-C4	-2.30	104.96	110.38
4	K	1001	HEM	CAC-C3C-C4C	2.29	130.30	124.82
9	B	1001	HEC	C2A-C1A-NA	-2.29	108.11	110.32
5	A	1003	AOQ	O1-C1-C9	-2.28	117.92	121.57
4	E	1001	HEM	C4D-ND-C1D	2.25	107.87	105.21
9	L	1001	HEC	CAA-CBA-CGA	-2.25	107.70	113.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	1003	AOQ	C12-C11-C16	2.24	115.13	111.18
4	K	1002	HEM	C4D-ND-C1D	2.24	107.86	105.21
4	E	1001	HEM	C2A-C1A-NA	-2.24	107.66	110.15
4	E	1001	HEM	C1B-NB-C4B	2.24	107.86	105.21
4	A	1001	HEM	CHD-C1D-ND	2.23	126.82	124.42
4	K	1001	HEM	CHC-C1C-NC	2.22	126.86	124.45
6	K	1004	6PE	O1-P1-O2	2.21	122.74	112.44
4	O	1001	HEM	C2A-C1A-NA	-2.21	107.70	110.15
9	B	1001	HEC	CAA-CBA-CGA	-2.20	107.83	113.67
4	A	1001	HEM	CHD-C4C-C3C	2.20	128.91	125.21
8	E	1005	BOG	C1-C2-C3	-2.18	105.42	110.01
8	O	1005	BOG	O3-C3-C4	-2.18	105.24	110.38
5	E	1003	AOQ	O1-C1-C2	2.17	124.92	121.14
5	O	1003	AOQ	O1-C1-C2	2.16	124.91	121.14
8	K	1005	BOG	O3-C3-C4	-2.16	105.29	110.38
4	O	1001	HEM	C4D-ND-C1D	2.16	107.76	105.21
4	A	1001	HEM	CHC-C1C-NC	2.14	126.79	124.45
4	K	1002	HEM	C1B-NB-C4B	2.13	107.73	105.21
4	O	1001	HEM	C1B-NB-C4B	2.13	107.73	105.21
8	A	1006	BOG	O3-C3-C4	-2.13	105.37	110.38
4	O	1002	HEM	C4D-ND-C1D	2.12	107.72	105.21
6	A	1004	6PE	O6-C10-C11	-2.11	106.91	111.48
4	A	1001	HEM	CAC-C3C-C4C	2.10	129.84	124.82
4	O	1001	HEM	O2D-CGD-CBD	2.09	120.59	114.00
4	E	1001	HEM	C3B-C2B-C1B	2.09	107.98	106.41
5	E	1003	AOQ	C22-C17-C13	2.07	126.34	121.09
4	K	1002	HEM	CHA-C4D-ND	2.07	126.93	124.37
4	A	1002	HEM	CHA-C4D-ND	2.06	126.91	124.37
6	O	1004	6PE	O6-C2-C3	-2.05	100.98	108.34
4	A	1002	HEM	C1B-NB-C4B	2.04	107.62	105.21
8	E	1005	BOG	O2-C2-C3	-2.02	105.60	110.38
4	E	1002	HEM	C3D-C4D-ND	-2.02	107.96	110.17
4	A	1001	HEM	O2D-CGD-CBD	2.02	120.37	114.00
4	K	1001	HEM	O2D-CGD-CBD	2.01	120.36	114.00

There are no chirality outliers.

All (116) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1003	AOQ	C15-C16-C2-C1
5	A	1003	AOQ	C15-C16-C2-C3
5	K	1003	AOQ	C15-C16-C2-C1

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Mol	Chain	Res	Type	Atoms
5	K	1003	AOQ	C15-C16-C2-C3
5	O	1003	AOQ	C15-C16-C2-C1
6	A	1004	6PE	C1-O3-P1-O2
6	A	1004	6PE	C1-O3-P1-O8
6	A	1004	6PE	O8-C16-C17-N1
6	E	1004	6PE	O8-C16-C17-N1
6	K	1004	6PE	C16-O8-P1-O1
6	K	1004	6PE	O8-C16-C17-N1
6	O	1004	6PE	C1-O3-P1-O2
6	O	1004	6PE	C1-O3-P1-O8
6	O	1004	6PE	O6-C2-C3-O4
6	O	1004	6PE	C11-C10-O6-C2
6	O	1004	6PE	O8-C16-C17-N1
8	A	1006	BOG	C2'-C1'-O1-C1
8	E	1005	BOG	C2'-C1'-O1-C1
8	K	1005	BOG	C2'-C1'-O1-C1
8	O	1005	BOG	C2'-C1'-O1-C1
9	B	1001	HEC	C2B-C3B-CAB-CBB
9	B	1001	HEC	C4B-C3B-CAB-CBB
9	B	1001	HEC	C2C-C3C-CAC-CBC
9	B	1001	HEC	C4C-C3C-CAC-CBC
9	F	1001	HEC	C2B-C3B-CAB-CBB
9	F	1001	HEC	C4B-C3B-CAB-CBB
9	F	1001	HEC	C2C-C3C-CAC-CBC
9	F	1001	HEC	C4C-C3C-CAC-CBC
9	L	1001	HEC	C2B-C3B-CAB-CBB
9	L	1001	HEC	C4B-C3B-CAB-CBB
9	L	1001	HEC	C2C-C3C-CAC-CBC
9	L	1001	HEC	C4C-C3C-CAC-CBC
9	P	1001	HEC	C2B-C3B-CAB-CBB
9	P	1001	HEC	C4B-C3B-CAB-CBB
9	P	1001	HEC	C2C-C3C-CAC-CBC
9	P	1001	HEC	C4C-C3C-CAC-CBC
6	O	1004	6PE	O7-C10-O6-C2
8	A	1006	BOG	C4-C5-C6-O6
6	K	1004	6PE	O5-C4-O4-C3
8	K	1005	BOG	C4-C5-C6-O6
6	K	1004	6PE	C5-C4-O4-C3
8	A	1006	BOG	O5-C5-C6-O6
6	A	1004	6PE	C5-C4-O4-C3
6	O	1004	6PE	C5-C4-O4-C3
8	K	1005	BOG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	O	1004	6PE	O5-C4-O4-C3
6	A	1004	6PE	O6-C2-C3-O4
8	O	1005	BOG	C4-C5-C6-O6
4	O	1002	HEM	C2A-CAA-CBA-CGA
6	A	1004	6PE	O5-C4-O4-C3
4	A	1002	HEM	C2A-CAA-CBA-CGA
4	E	1002	HEM	C2A-CAA-CBA-CGA
4	K	1002	HEM	C2A-CAA-CBA-CGA
6	K	1004	6PE	C11-C10-O6-C2
8	K	1005	BOG	C2'-C3'-C4'-C5'
8	A	1006	BOG	C2'-C3'-C4'-C5'
8	E	1005	BOG	C2'-C3'-C4'-C5'
8	O	1005	BOG	C2'-C3'-C4'-C5'
6	K	1004	6PE	O7-C10-O6-C2
6	O	1004	6PE	C1-C2-C3-O4
6	E	1004	6PE	C5-C4-O4-C3
8	O	1005	BOG	O5-C5-C6-O6
6	E	1004	6PE	O5-C4-O4-C3
5	O	1003	AOQ	C15-C16-C2-C3
6	A	1004	6PE	C12-C13-C14-C15
8	E	1005	BOG	O1-C1'-C2'-C3'
8	A	1006	BOG	O1-C1'-C2'-C3'
8	K	1005	BOG	O1-C1'-C2'-C3'
8	O	1005	BOG	C4'-C5'-C6'-C7'
8	E	1005	BOG	C4'-C5'-C6'-C7'
8	A	1006	BOG	C4'-C5'-C6'-C7'
8	K	1005	BOG	C4'-C5'-C6'-C7'
6	K	1004	6PE	C12-C13-C14-C15
6	E	1004	6PE	O3-C1-C2-C3
6	O	1004	6PE	C1-C2-O6-C10
8	O	1005	BOG	O1-C1'-C2'-C3'
6	E	1004	6PE	O3-C1-C2-O6
6	A	1004	6PE	C1-C2-C3-O4
4	A	1001	HEM	C4C-C3C-CAC-CBC
4	K	1001	HEM	C4C-C3C-CAC-CBC
6	K	1004	6PE	C17-C16-O8-P1
6	K	1004	6PE	C16-O8-P1-O2
6	K	1004	6PE	C16-O8-P1-O3
6	K	1004	6PE	O6-C2-C3-O4
4	K	1002	HEM	CAA-CBA-CGA-O2A
6	K	1004	6PE	O4-C4-C5-C6
4	E	1002	HEM	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
4	A	1002	HEM	CAA-CBA-CGA-O2A
4	O	1002	HEM	CAA-CBA-CGA-O2A
9	P	1001	HEC	CAA-CBA-CGA-O2A
5	E	1003	AOQ	C14-C13-C17-C22
4	A	1002	HEM	CAA-CBA-CGA-O1A
4	K	1002	HEM	CAA-CBA-CGA-O1A
4	O	1002	HEM	CAA-CBA-CGA-O1A
9	B	1001	HEC	CAA-CBA-CGA-O2A
4	E	1002	HEM	CAA-CBA-CGA-O1A
9	F	1001	HEC	CAA-CBA-CGA-O2A
9	L	1001	HEC	CAA-CBA-CGA-O2A
6	E	1004	6PE	C11-C10-O6-C2
9	P	1001	HEC	CAA-CBA-CGA-O1A
5	E	1003	AOQ	C11-C16-C2-C1
9	B	1001	HEC	CAD-CBD-CGD-O2D
9	L	1001	HEC	CAD-CBD-CGD-O2D
9	B	1001	HEC	CAA-CBA-CGA-O1A
9	F	1001	HEC	CAA-CBA-CGA-O1A
5	K	1003	AOQ	C14-C13-C17-C22
9	L	1001	HEC	CAA-CBA-CGA-O1A
6	O	1004	6PE	O6-C10-C11-C12
9	B	1001	HEC	CAD-CBD-CGD-O1D
9	L	1001	HEC	CAD-CBD-CGD-O1D
6	A	1004	6PE	O6-C10-C11-C12
6	A	1004	6PE	O7-C10-C11-C12
6	O	1004	6PE	O7-C10-C11-C12
6	K	1004	6PE	O6-C10-C11-C12
5	A	1003	AOQ	C14-C13-C17-C22
6	E	1004	6PE	O6-C10-C11-C12

There are no ring outliers.

12 monomers are involved in 18 short contacts:

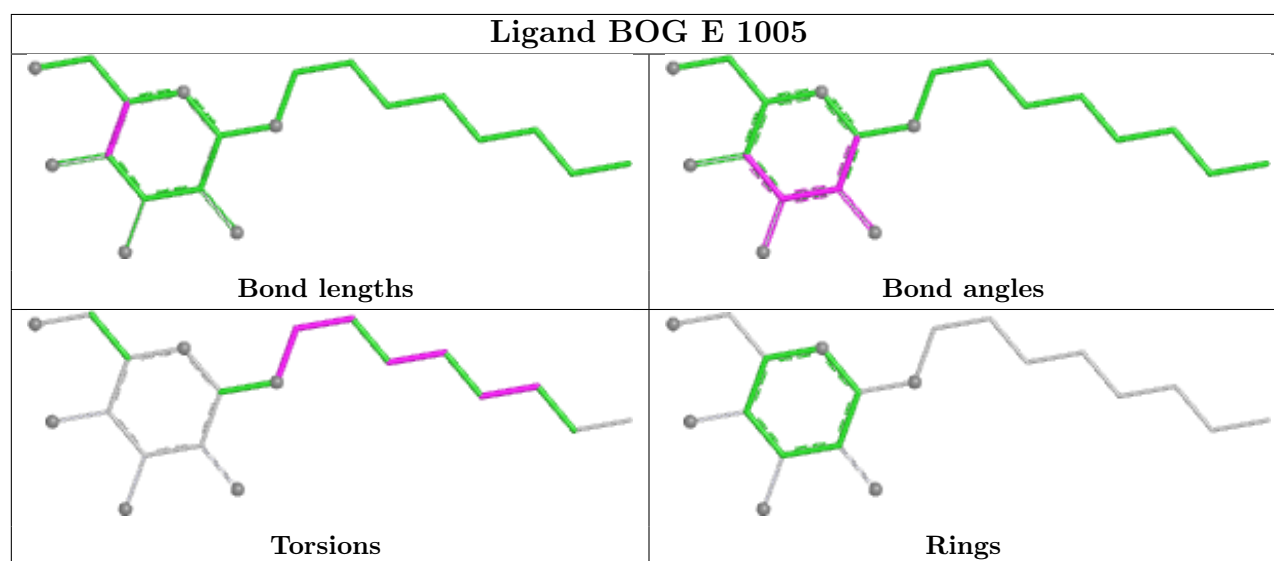
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	E	1005	BOG	1	0
10	C	1001	FES	1	0
8	K	1005	BOG	1	0
5	O	1003	AOQ	3	0
4	E	1001	HEM	1	0
5	E	1003	AOQ	1	0
4	O	1002	HEM	1	0
5	A	1003	AOQ	1	0

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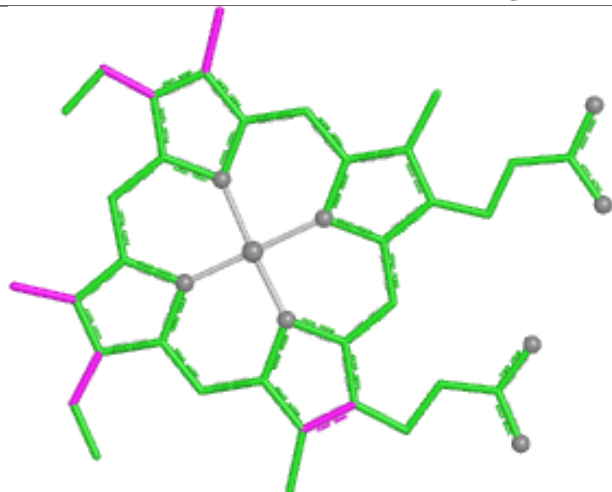
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1001	HEM	3	0
4	O	1001	HEM	1	0
4	K	1001	HEM	3	0
8	A	1006	BOG	1	0

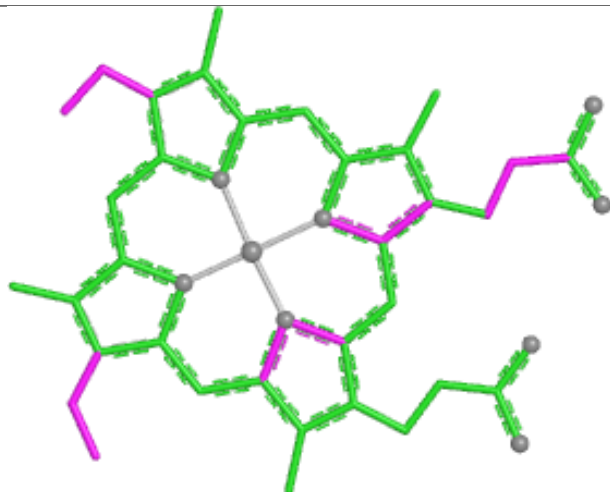
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



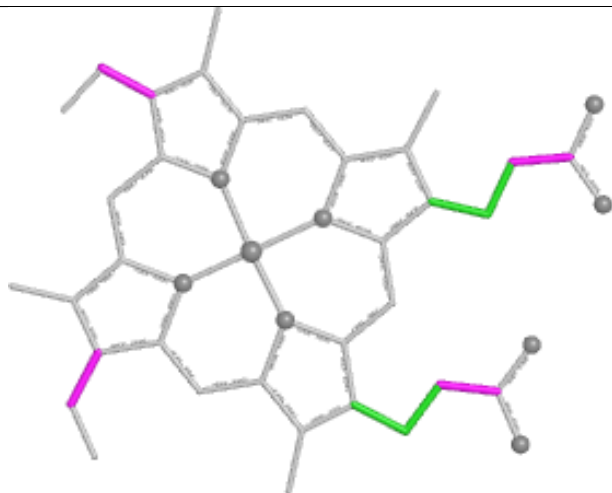
Ligand HEC L 1001



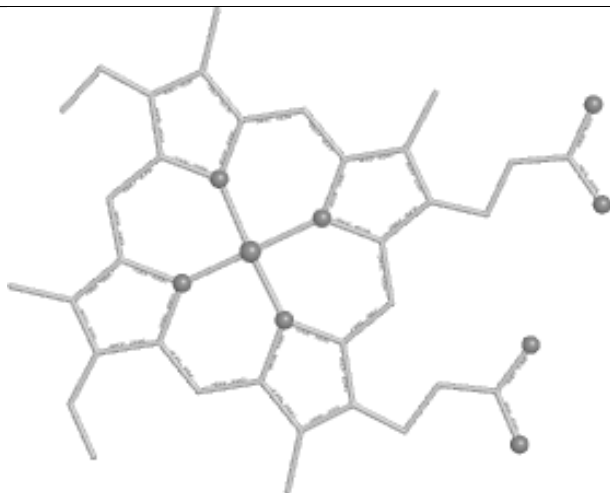
Bond lengths



Bond angles

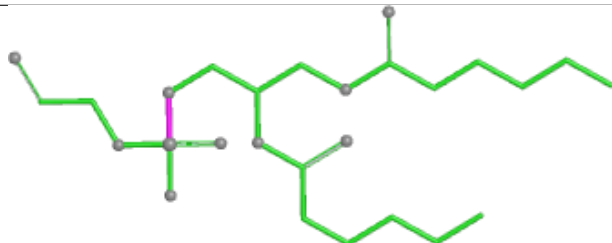


Torsions

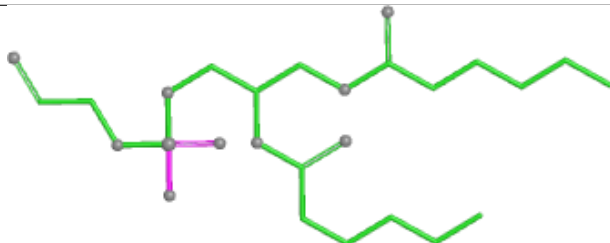


Rings

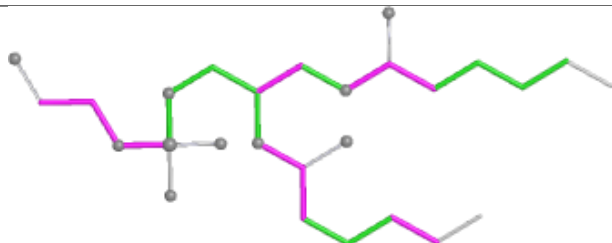
Ligand 6PE K 1004



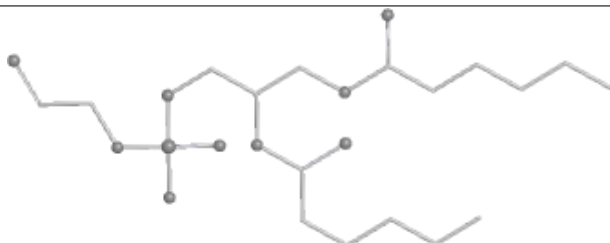
Bond lengths



Bond angles

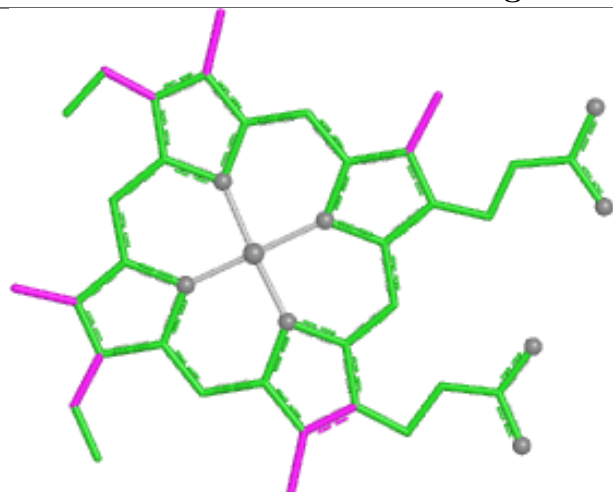


Torsions

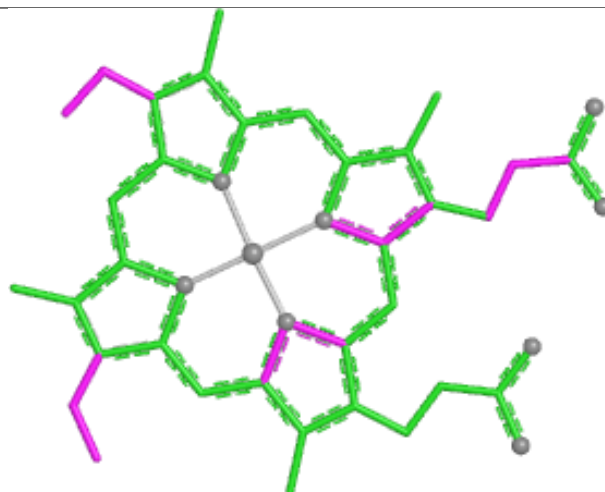


Rings

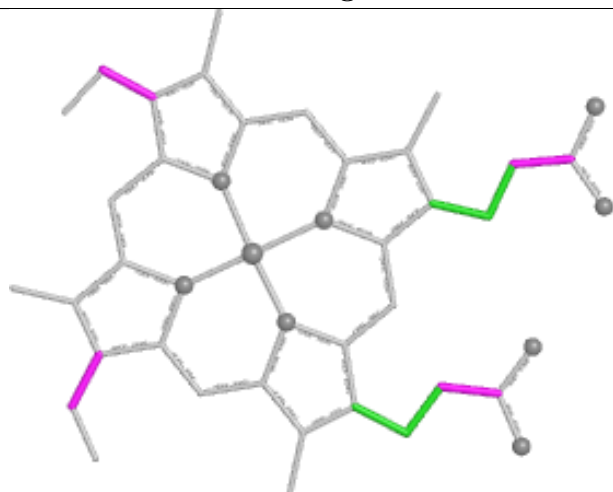
Ligand HEC B 1001



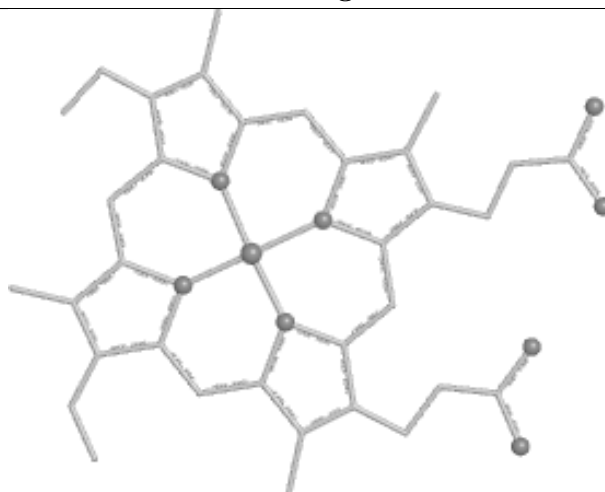
Bond lengths



Bond angles

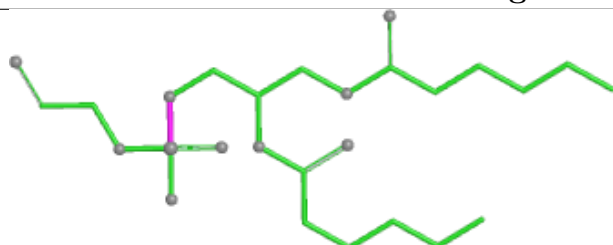


Torsions

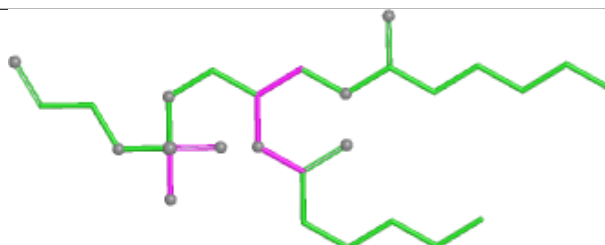


Rings

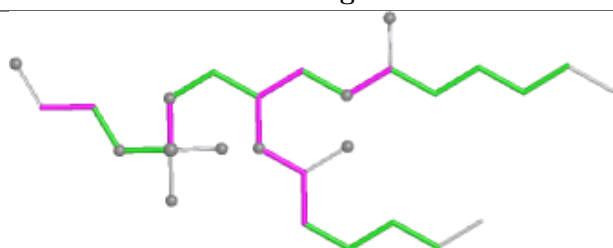
Ligand 6PE O 1004



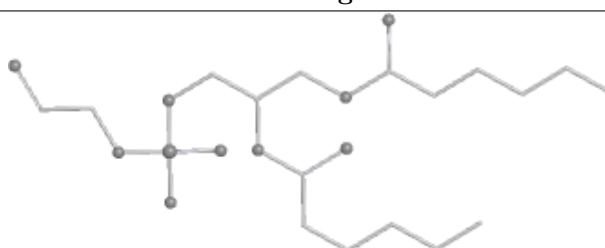
Bond lengths



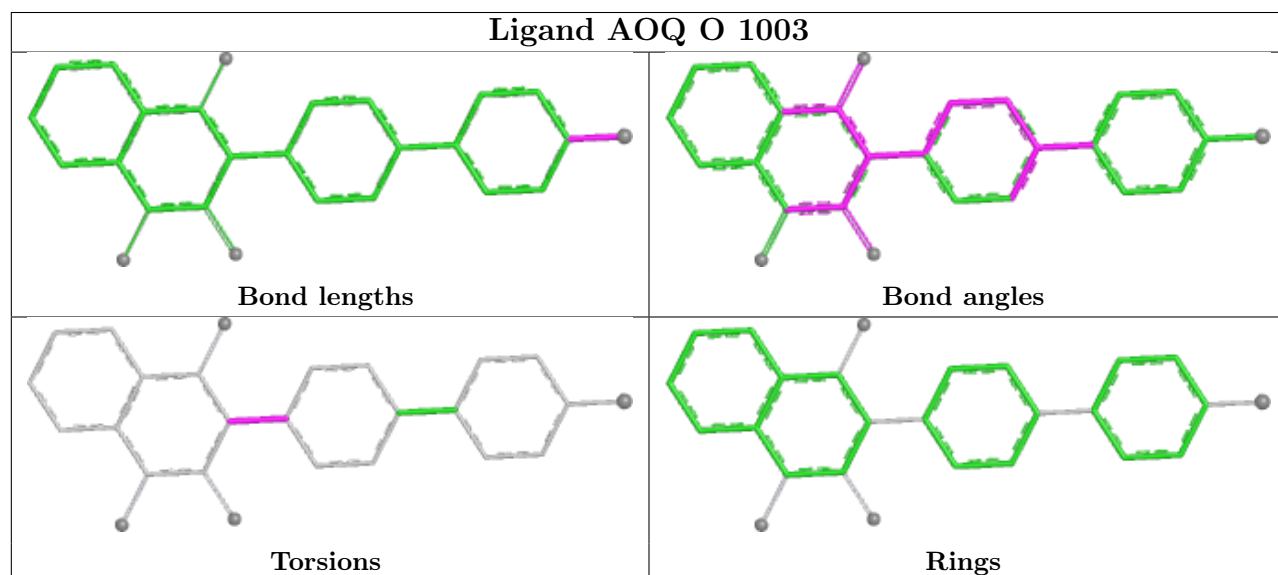
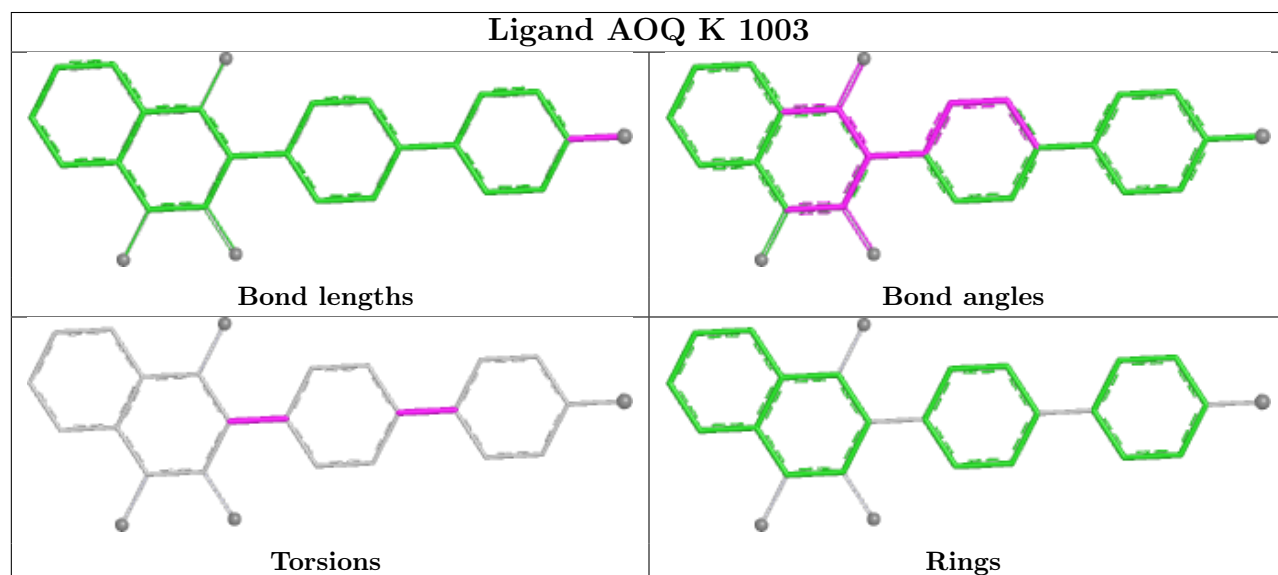
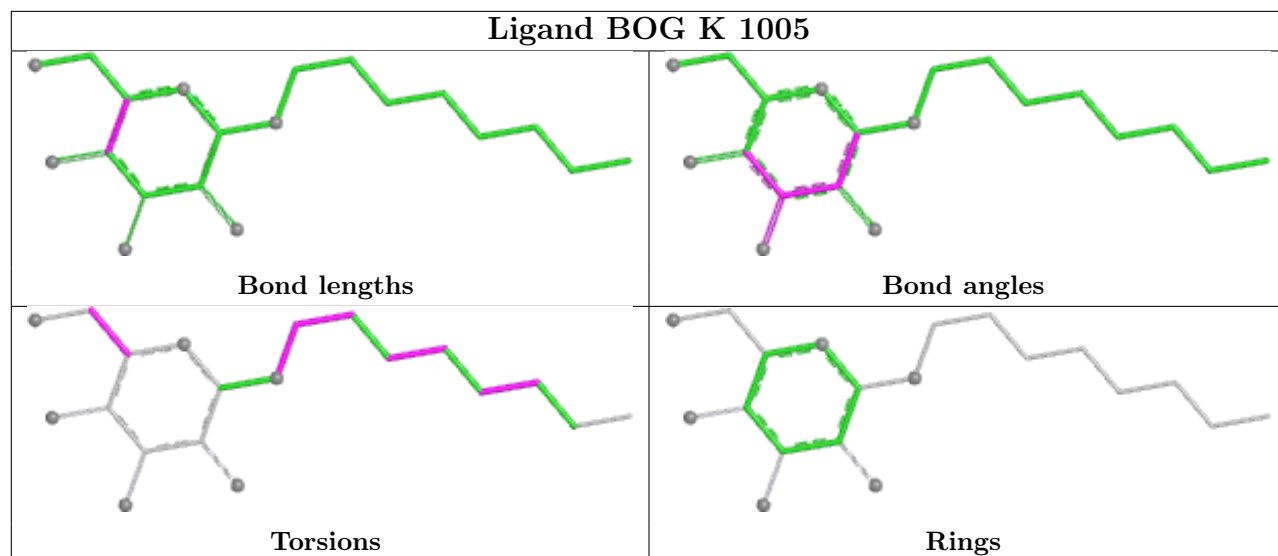
Bond angles

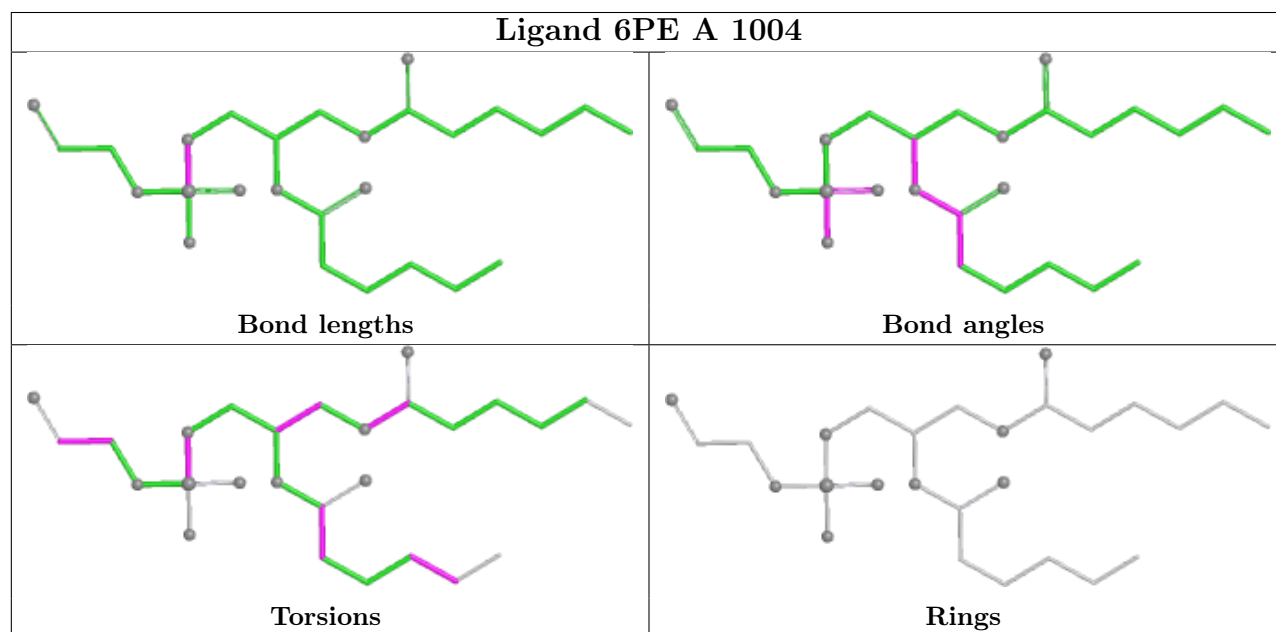
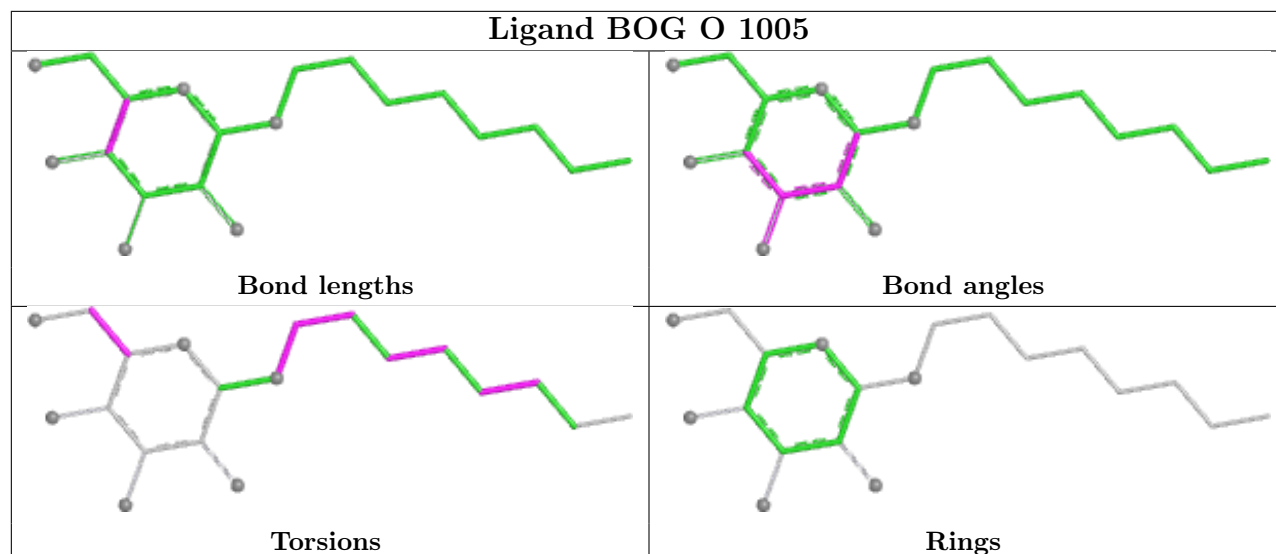


Torsions

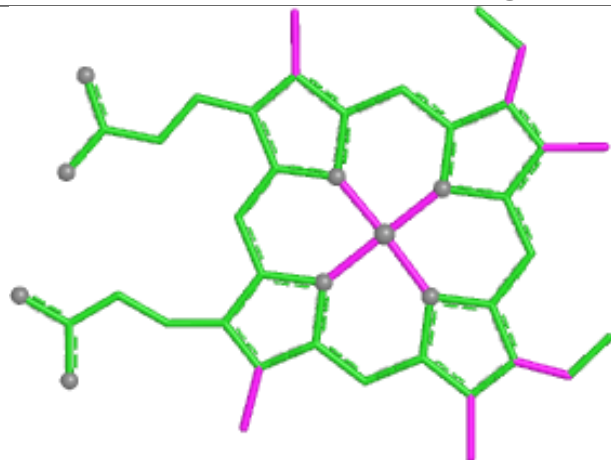


Rings

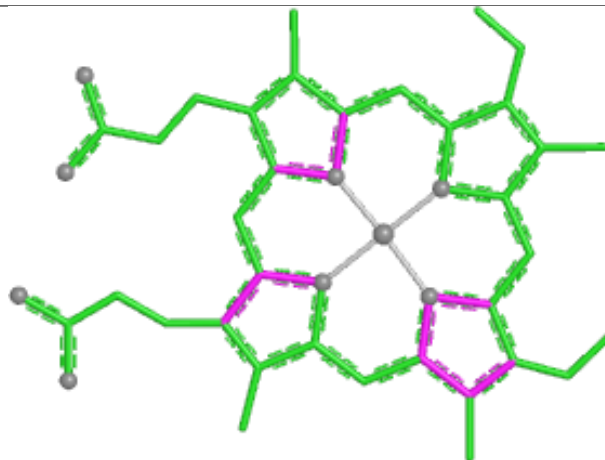




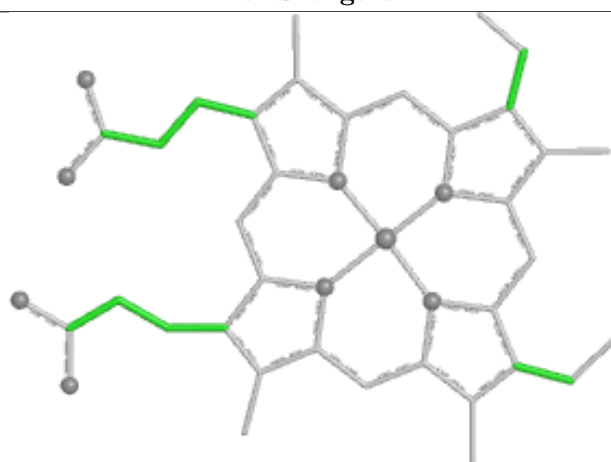
Ligand HEM E 1001



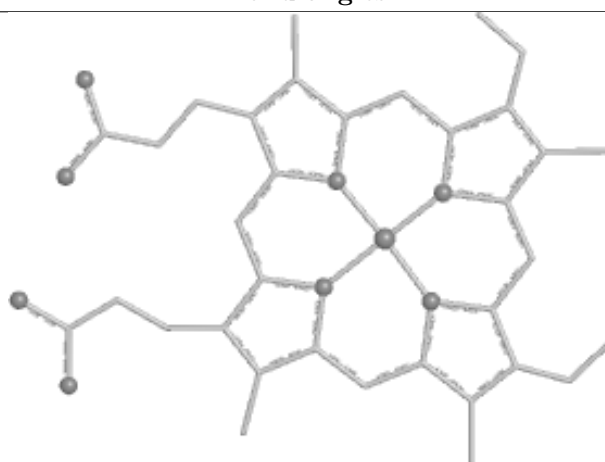
Bond lengths



Bond angles

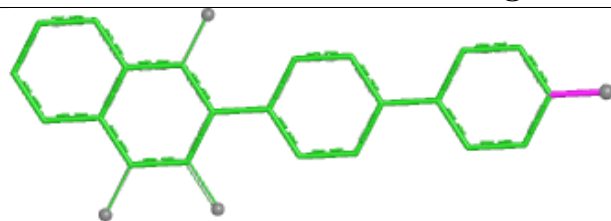


Torsions

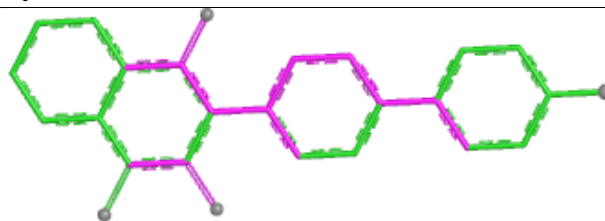


Rings

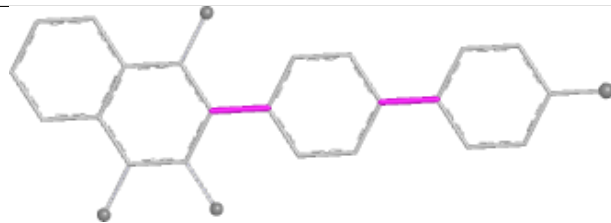
Ligand AOQ E 1003



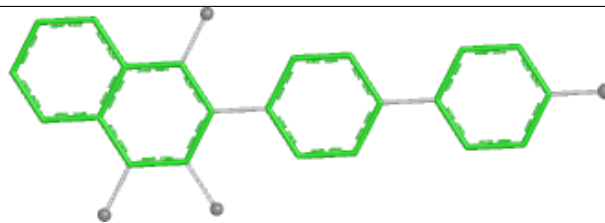
Bond lengths



Bond angles

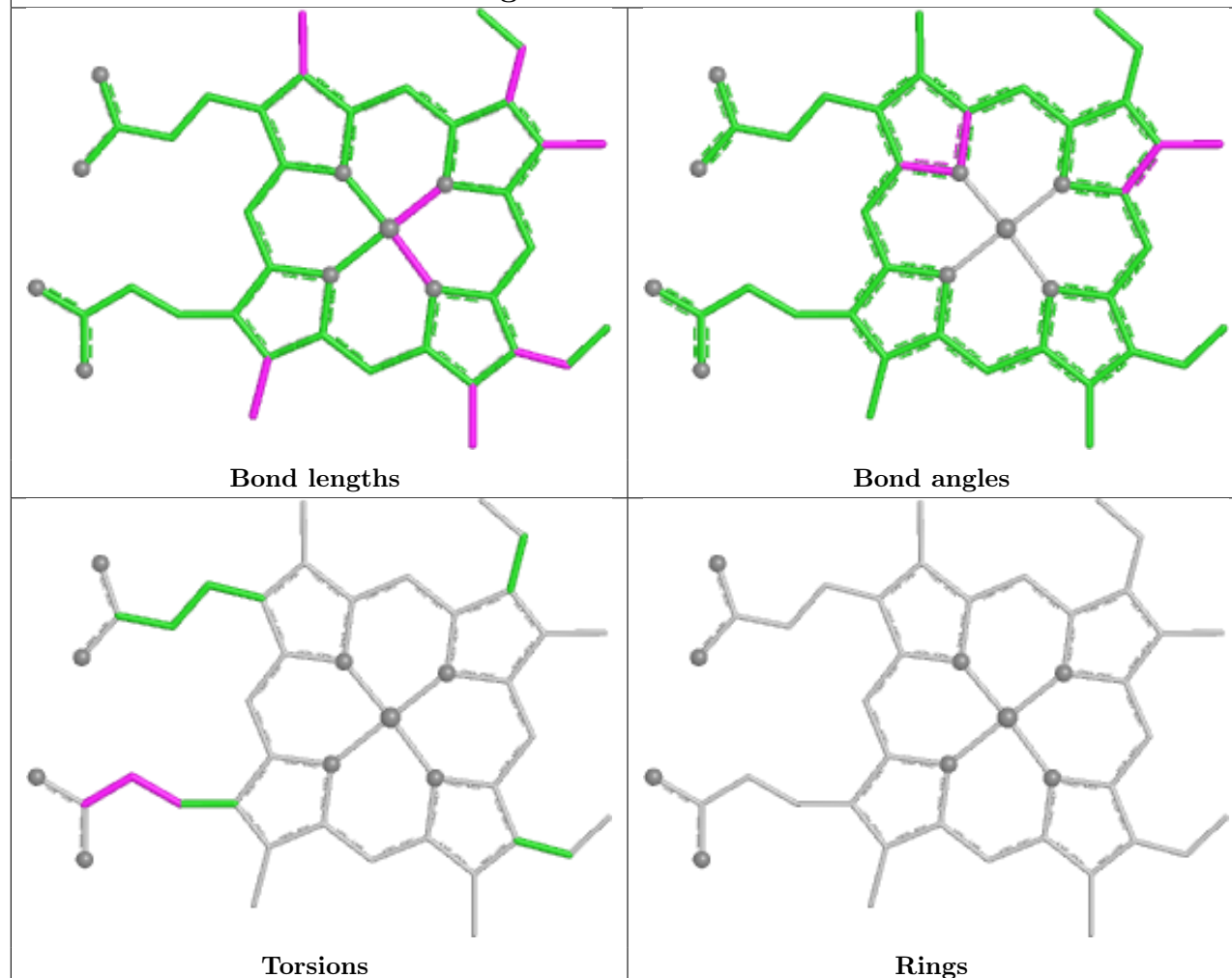


Torsions

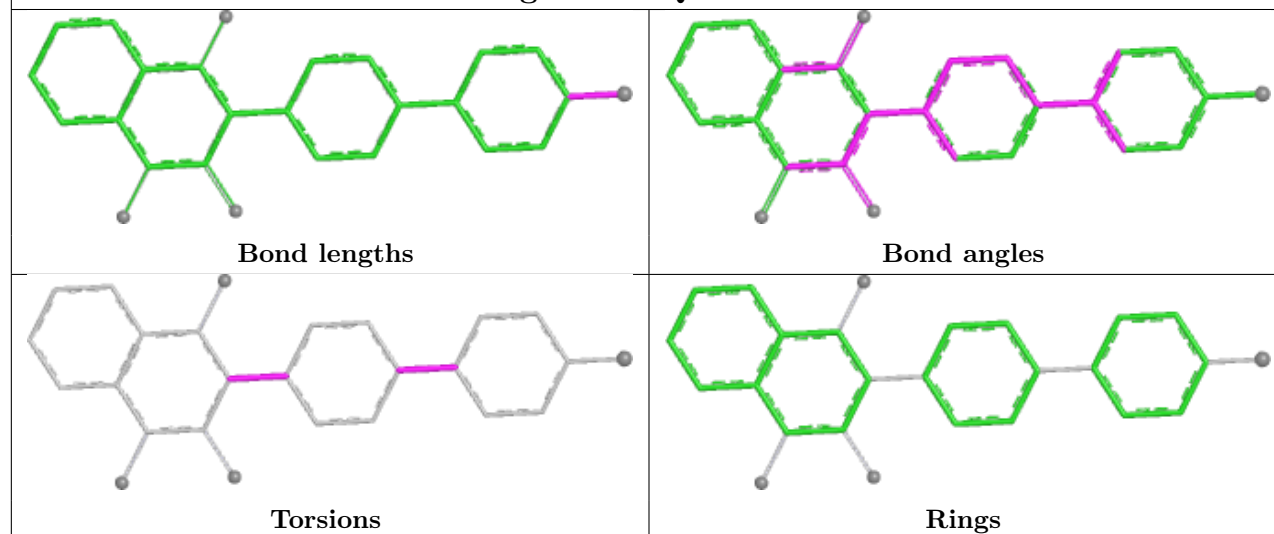


Rings

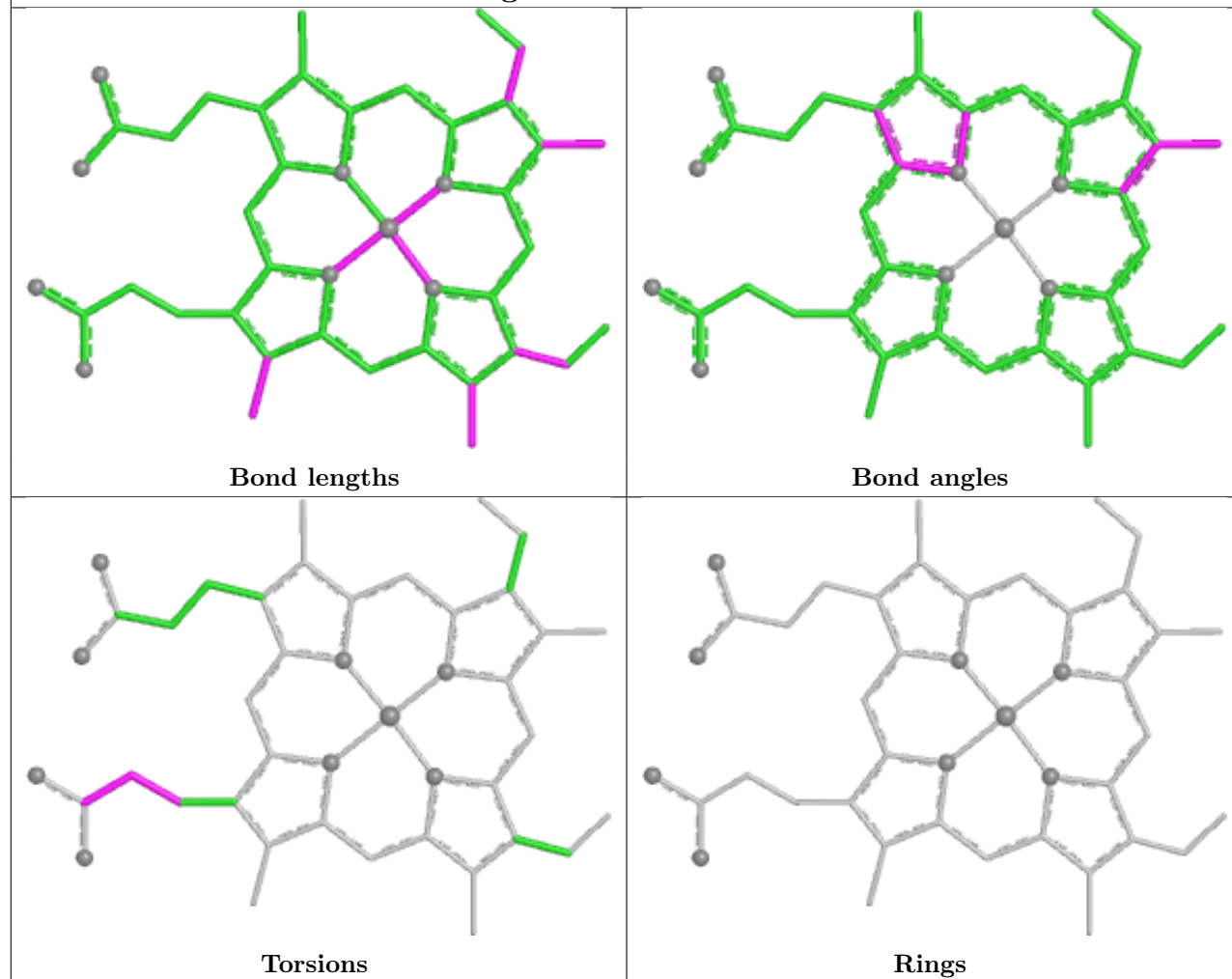
Ligand HEM O 1002



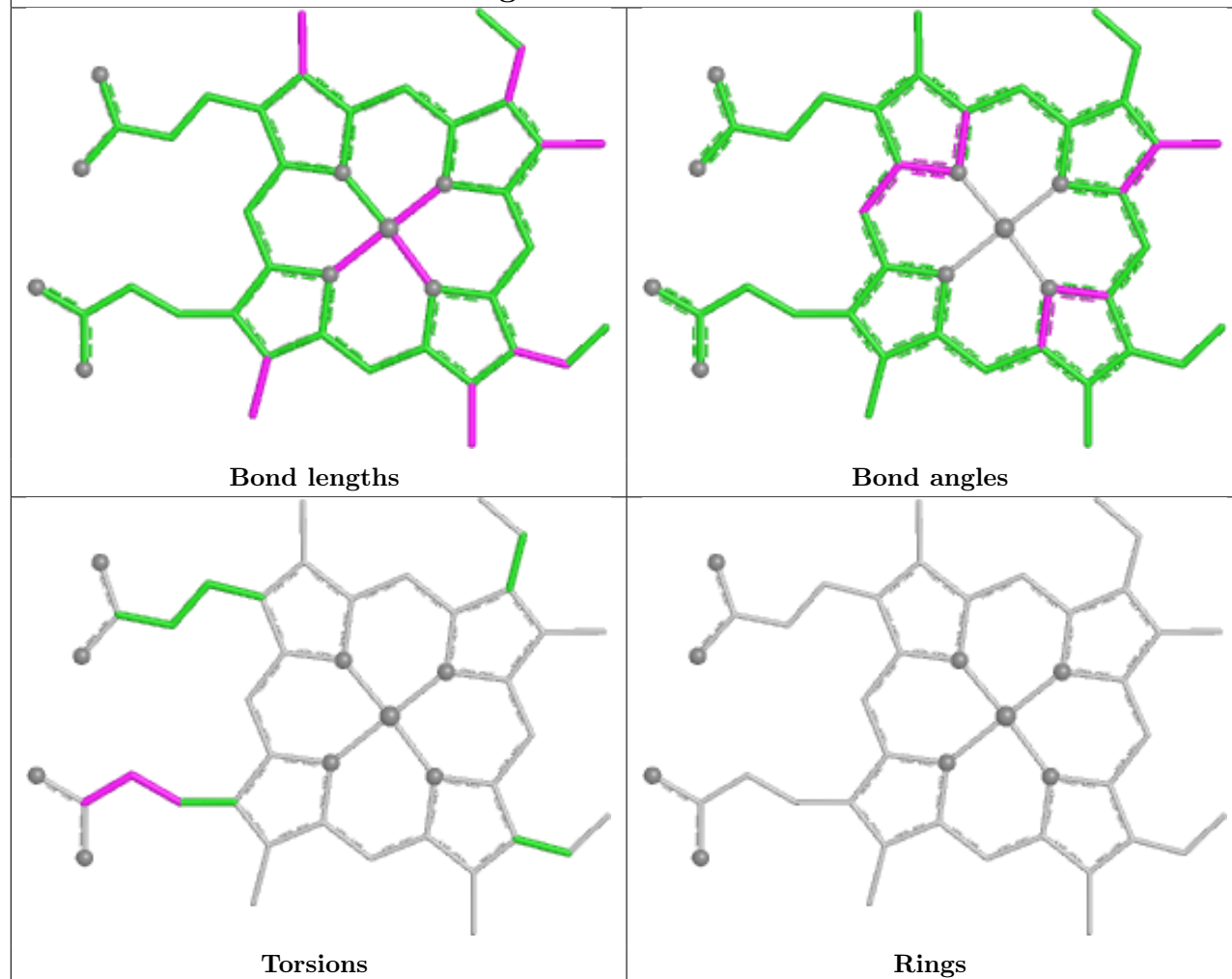
Ligand AOQ A 1003



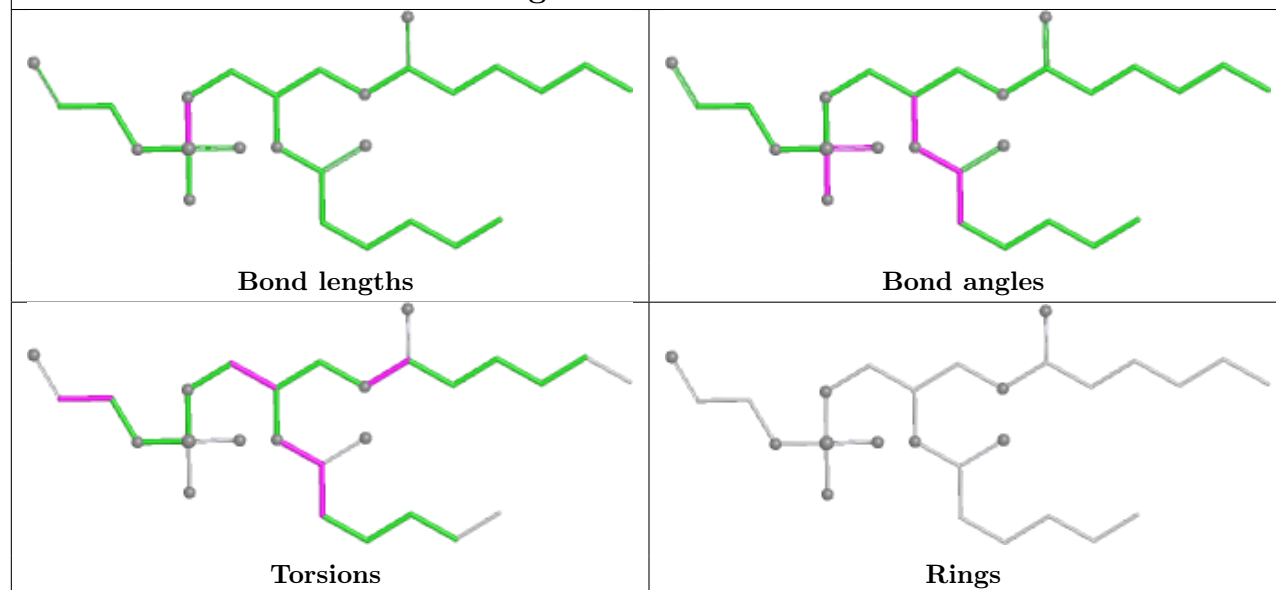
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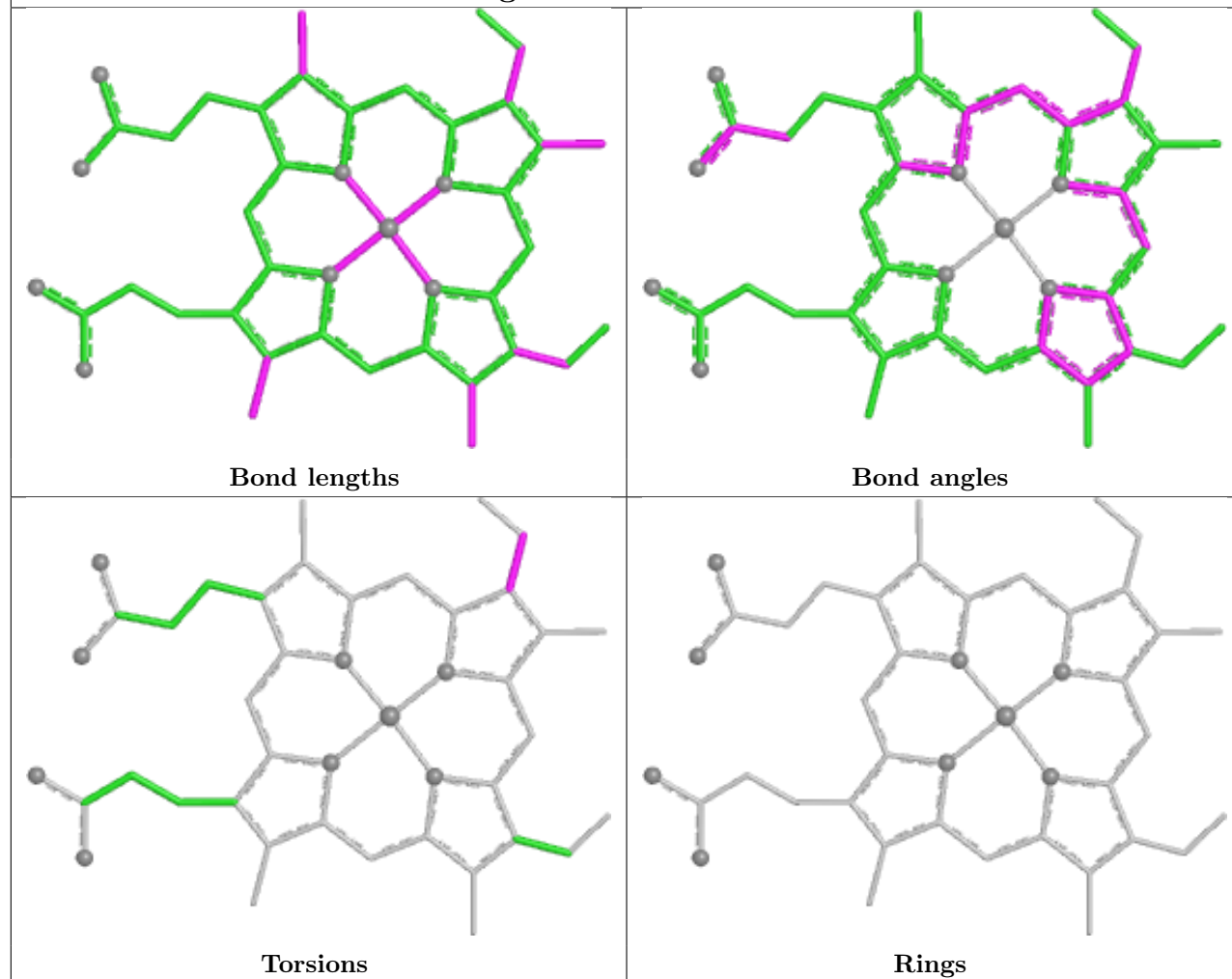
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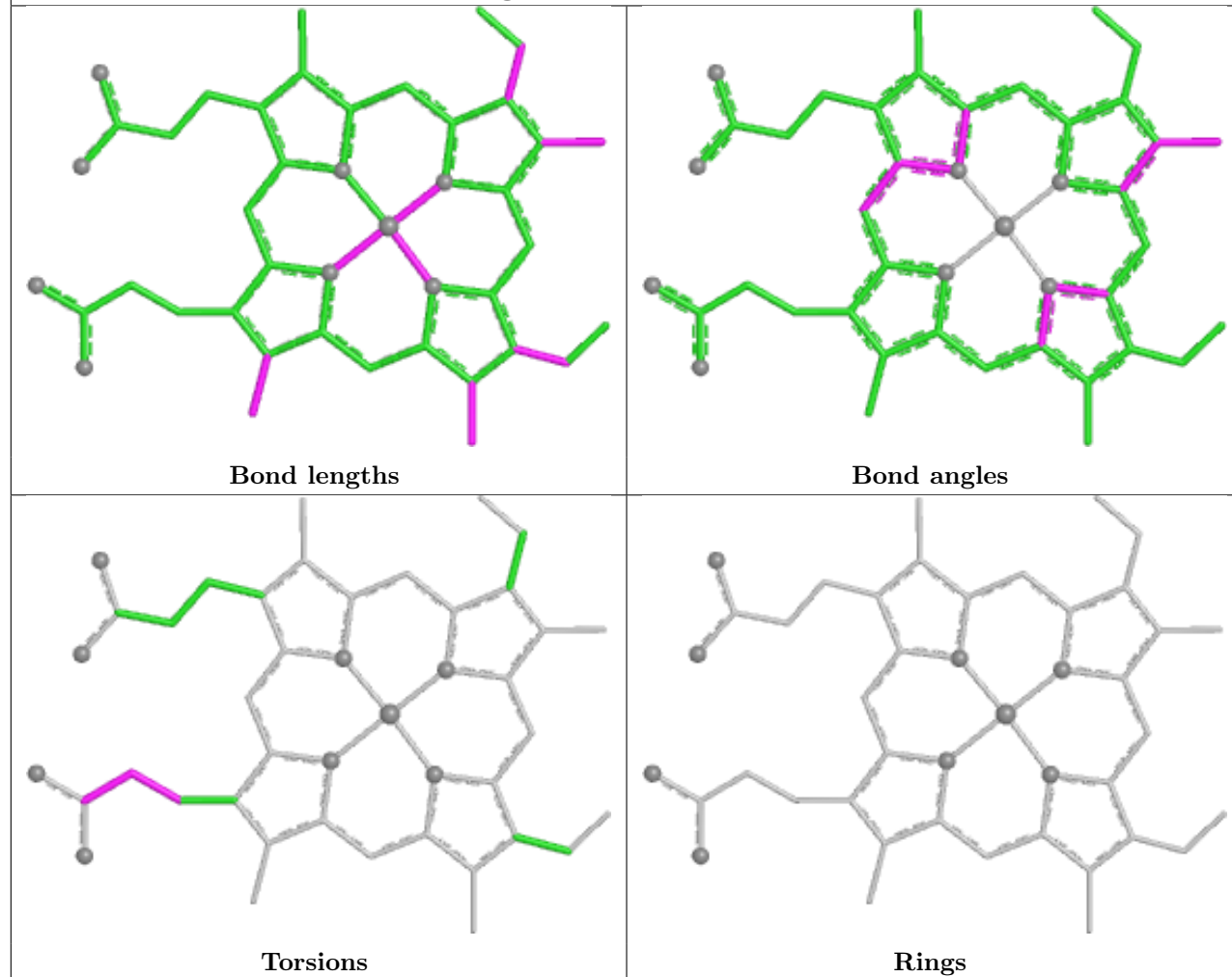
Ligand 6PE E 1004



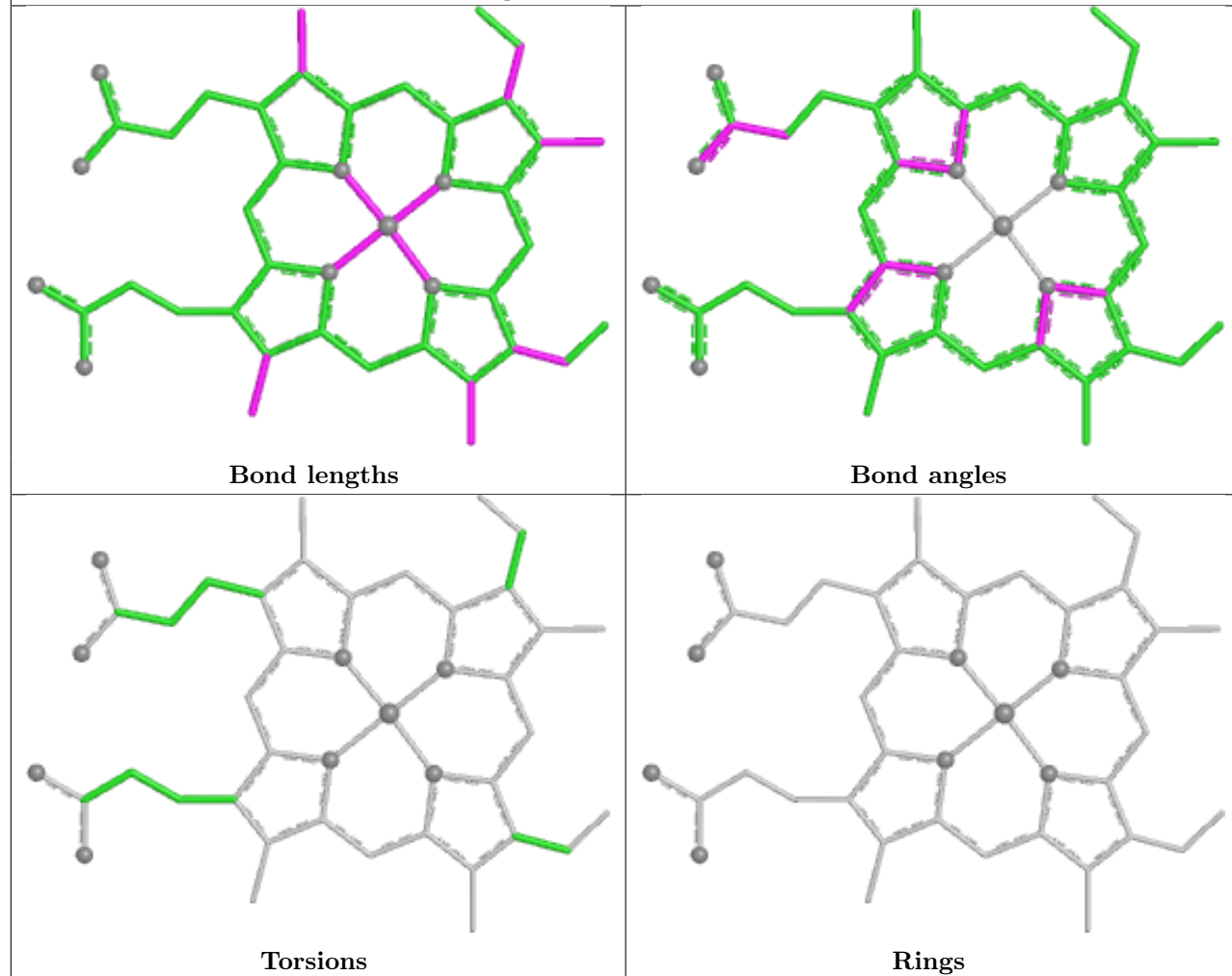
Ligand HEM A 1001



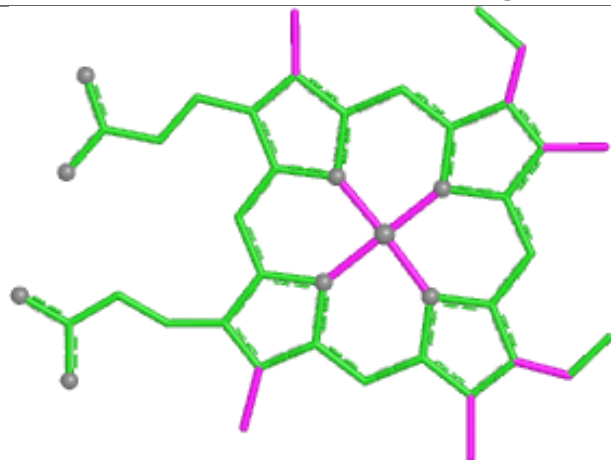
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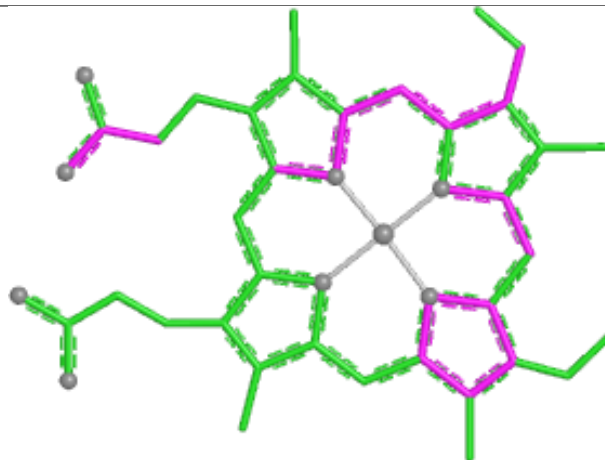
Ligand HEM O 1001



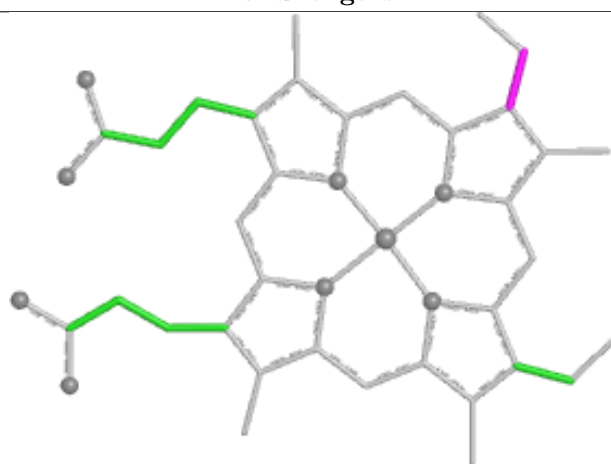
Ligand HEM K 1001



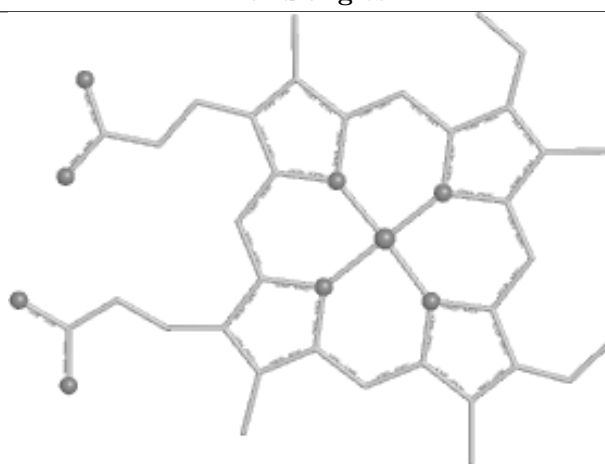
Bond lengths



Bond angles

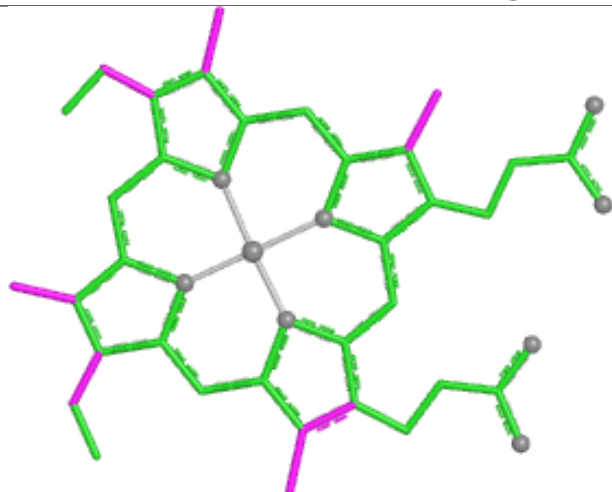


Torsions

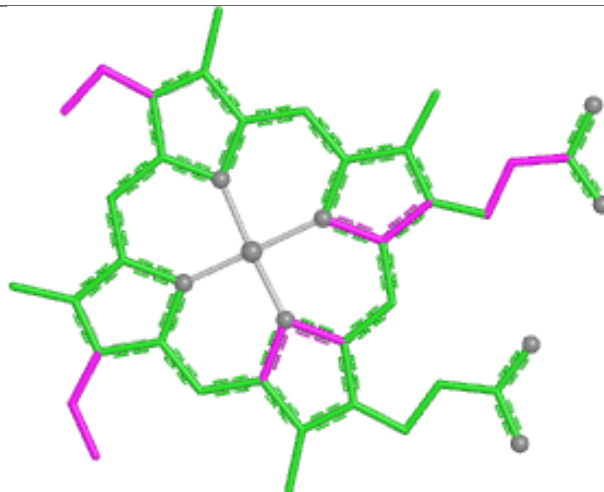


Rings

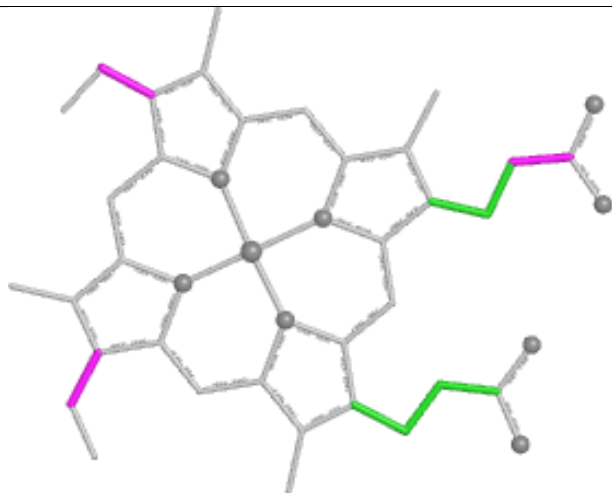
Ligand HEC F 1001



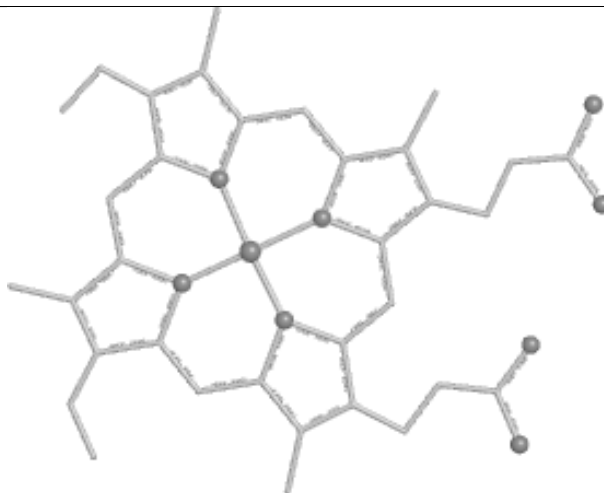
Bond lengths



Bond angles

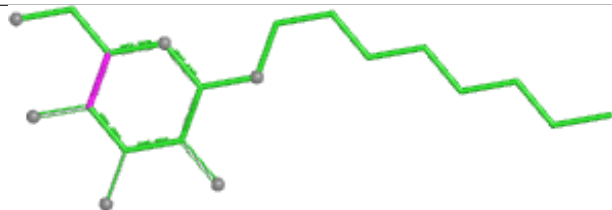


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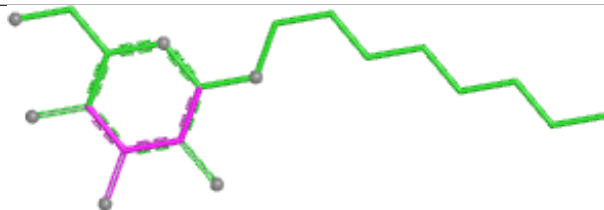


Rings

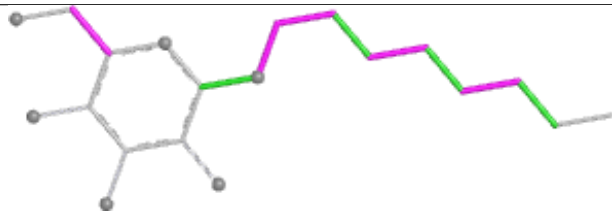
Ligand BOG A 1006



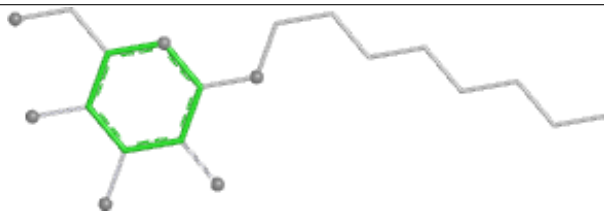
Bond lengths



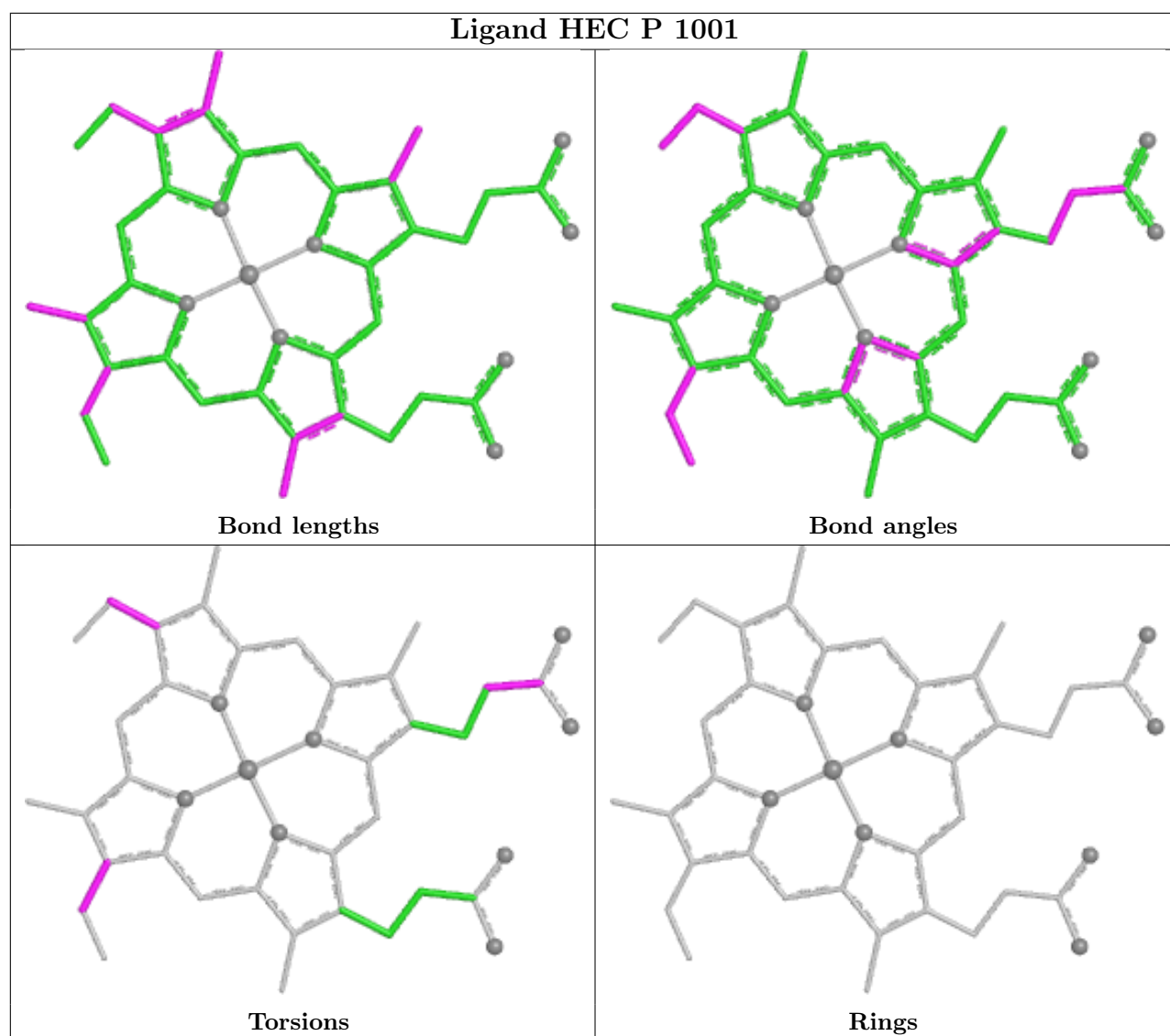
Bond angles



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%)	0.02	25 (5%)	29	23	129, 176, 232, 266	0
1	E	429/445 (96%)	0.06	24 (5%)	30	24	125, 174, 230, 291	0
1	K	429/445 (96%)	-0.02	17 (3%)	42	31	131, 171, 229, 270	0
1	O	429/445 (96%)	0.15	27 (6%)	26	22	129, 185, 250, 314	0
2	B	256/269 (95%)	-0.12	12 (4%)	36	27	150, 195, 251, 263	0
2	F	256/269 (95%)	-0.06	7 (2%)	56	38	139, 198, 244, 282	0
2	L	256/269 (95%)	-0.18	9 (3%)	47	33	144, 189, 238, 282	0
2	P	256/269 (95%)	0.03	9 (3%)	47	33	161, 211, 258, 286	0
3	C	179/187 (95%)	0.02	7 (3%)	43	31	151, 198, 242, 269	0
3	G	179/187 (95%)	0.13	13 (7%)	21	19	142, 208, 269, 300	0
3	M	179/187 (95%)	0.02	9 (5%)	34	26	168, 214, 250, 298	0
3	Q	179/187 (95%)	0.05	11 (6%)	27	22	137, 192, 254, 321	0
All	All	3456/3604 (95%)	0.01	170 (4%)	35	27	125, 189, 246, 321	0

All (170) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	38	PRO	6.6
1	E	221	ASN	6.3
1	O	36	PRO	6.3
3	C	163	ARG	6.0
3	M	43	ASP	5.6
1	K	85	ARG	5.5
1	O	37	THR	5.3
1	A	230	ARG	5.3
1	O	187	ASP	5.2
2	B	46	PRO	5.1
2	P	103	MET	4.9

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Mol	Chain	Res	Type	RSRZ
2	F	102	LEU	4.9
1	O	221	ASN	4.7
1	E	228	GLU	4.7
1	O	228	GLU	4.7
1	O	310	ALA	4.7
3	C	92	GLN	4.5
2	B	44	PHE	4.5
1	E	36	PRO	4.5
1	E	187	ASP	4.4
2	B	1	ALA	4.3
1	K	86	ASN	4.3
3	C	43	ASP	4.2
3	G	144	PHE	4.1
3	Q	144	PHE	4.1
3	G	163	ARG	4.1
1	A	85	ARG	4.0
1	E	229	VAL	4.0
3	Q	162	ILE	4.0
3	Q	163	ARG	3.9
1	E	203	PHE	3.9
2	L	193	LEU	3.9
1	O	229	VAL	3.8
3	G	165	GLY	3.7
3	M	92	GLN	3.6
3	G	167	ALA	3.6
3	Q	94	VAL	3.6
2	L	1	ALA	3.6
1	A	236	GLU	3.5
3	M	44	VAL	3.5
1	A	310	ALA	3.5
1	A	232	THR	3.5
2	P	159	ALA	3.4
1	E	38	PRO	3.4
2	B	192	ASP	3.4
3	C	44	VAL	3.4
2	B	195	GLU	3.4
2	P	102	LEU	3.4
1	O	134	LEU	3.3
1	A	422	ALA	3.3
1	O	208	LEU	3.3
2	B	152	ASP	3.3
3	Q	164	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	K	231	ARG	3.2
2	P	130	TYR	3.2
3	G	137	ILE	3.1
2	F	134	VAL	3.1
2	L	194	VAL	3.1
1	K	230	ARG	3.1
1	A	7	ASP	3.1
1	E	241	THR	3.0
1	E	308	PHE	3.0
1	K	203	PHE	3.0
1	K	229	VAL	3.0
1	O	241	THR	2.9
3	G	80	ALA	2.9
1	E	4	ILE	2.9
1	O	203	PHE	2.9
3	G	155	HIS	2.8
1	A	106	ILE	2.8
1	K	205	ILE	2.8
1	K	207	ALA	2.8
3	Q	167	ALA	2.8
2	B	45	VAL	2.8
3	G	156	TYR	2.8
1	A	81	GLU	2.8
1	A	104	PHE	2.8
1	K	82	HIS	2.8
1	O	401	PHE	2.8
1	A	244	PHE	2.8
2	B	88	HIS	2.8
1	E	243	PRO	2.8
2	L	44	PHE	2.8
3	Q	155	HIS	2.7
2	P	222	LYS	2.7
1	K	106	ILE	2.7
1	E	219	THR	2.7
1	E	208	LEU	2.7
2	L	46	PRO	2.7
3	M	163	ARG	2.7
1	A	162	ILE	2.7
2	L	102	LEU	2.6
2	F	159	ALA	2.6
3	Q	153	GLY	2.6
1	O	128	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	56	VAL	2.6
1	O	205	ILE	2.6
1	O	94	ARG	2.6
1	A	109	TYR	2.6
3	C	94	VAL	2.6
2	B	193	LEU	2.6
1	A	105	PHE	2.6
1	K	81	GLU	2.5
1	A	221	ASN	2.5
1	O	184	PRO	2.5
3	M	69	GLY	2.5
3	G	94	VAL	2.5
1	A	134	LEU	2.5
3	M	174	PRO	2.5
1	O	204	VAL	2.5
1	A	311	ASP	2.5
1	K	234	LYS	2.5
1	E	207	ALA	2.5
1	A	208	LEU	2.4
3	Q	83	GLU	2.4
1	E	220	GLY	2.4
2	B	2	GLY	2.4
2	P	160	PHE	2.4
1	O	147	TYR	2.4
1	A	113	PHE	2.4
1	O	207	ALA	2.4
1	E	205	ILE	2.3
1	K	305	LEU	2.3
1	A	108	VAL	2.3
2	P	209	GLU	2.3
3	Q	161	ARG	2.3
1	O	274	LEU	2.3
3	G	171	LEU	2.3
2	P	117	GLY	2.3
1	E	72	HIS	2.3
1	K	108	VAL	2.3
3	C	139	GLY	2.2
3	M	94	VAL	2.2
1	A	205	ILE	2.2
2	F	37	ALA	2.2
3	G	145	GLY	2.2
1	O	311	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	305	LEU	2.2
1	K	236	GLU	2.2
1	O	347	PRO	2.2
1	O	219	THR	2.2
2	L	192	ASP	2.2
1	K	228	GLU	2.2
1	A	229	VAL	2.1
1	A	286	LEU	2.1
1	K	104	PHE	2.1
2	F	20	PHE	2.1
3	G	148	PHE	2.1
3	Q	165	GLY	2.1
1	O	4	ILE	2.1
2	L	2	GLY	2.1
2	F	103	MET	2.1
2	B	219	ALA	2.1
1	E	204	VAL	2.1
1	O	280	TYR	2.1
2	B	221	PRO	2.1
1	A	78	ALA	2.1
2	P	104	ALA	2.1
3	G	162	ILE	2.1
3	C	144	PHE	2.1
1	O	35	ILE	2.1
1	E	242	VAL	2.1
1	E	85	ARG	2.0
2	L	219	ALA	2.0
1	E	94	ARG	2.0
1	E	37	THR	2.0
3	M	42	ALA	2.0
2	F	222	LYS	2.0
1	E	280	TYR	2.0
3	M	84	LEU	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.

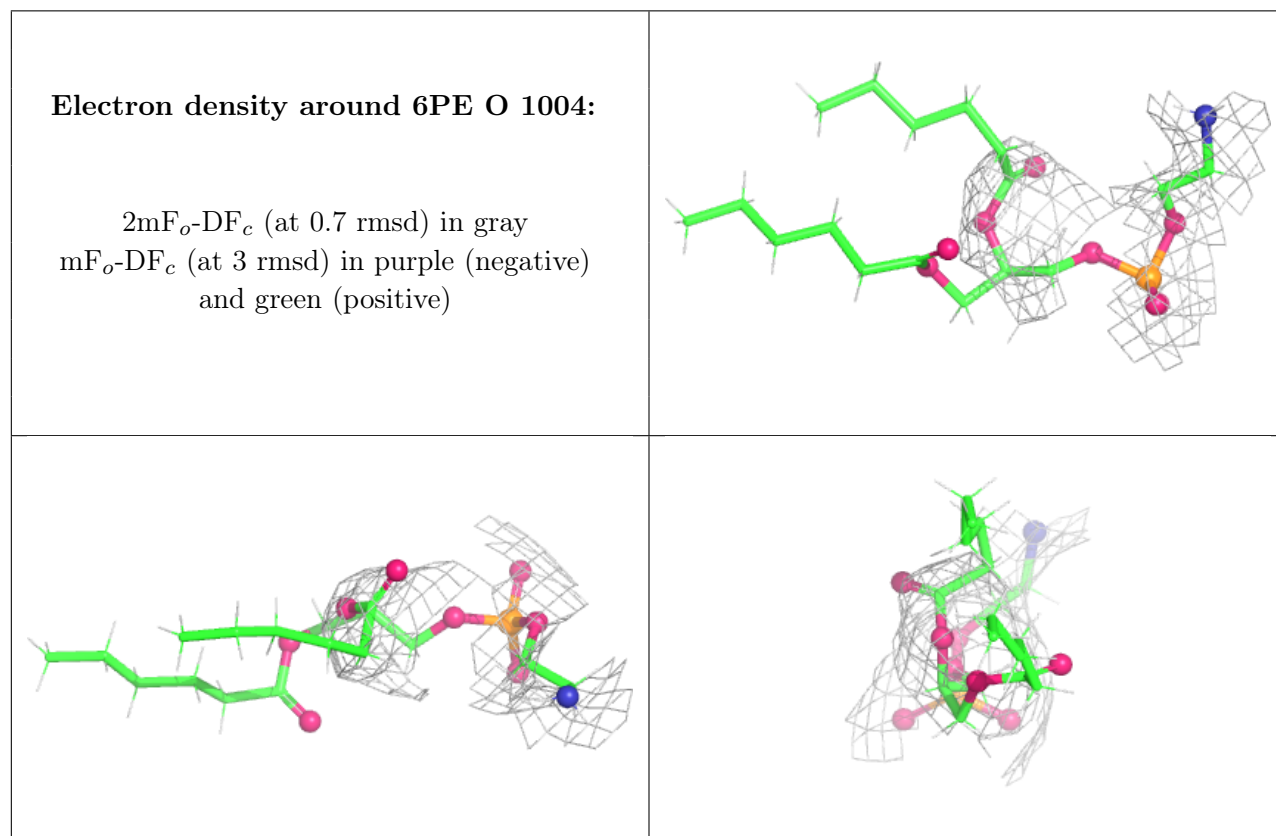
6.4 Ligands ⓘ

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	L	1002	1/1	0.70	0.07	475,475,475,475	0
7	SR	B	1002	1/1	0.76	0.07	451,451,451,451	0
6	6PE	O	1004	27/27	0.79	0.11	174,216,253,258	0
8	BOG	E	1005	20/20	0.80	0.12	181,220,230,231	0
5	AOQ	O	1003	26/26	0.85	0.21	152,185,225,229	0
6	6PE	E	1004	27/27	0.85	0.10	124,171,198,207	0
5	AOQ	A	1003	26/26	0.85	0.16	158,167,199,203	0
8	BOG	K	1005	20/20	0.85	0.13	215,261,274,274	0
5	AOQ	E	1003	26/26	0.86	0.18	138,165,203,210	0
7	SR	P	1002	1/1	0.87	0.05	434,434,434,434	0
6	6PE	A	1004	27/27	0.88	0.13	185,222,246,247	0
5	AOQ	K	1003	26/26	0.89	0.17	149,172,203,209	0
7	SR	F	1002	1/1	0.89	0.06	287,287,287,287	0
8	BOG	O	1005	20/20	0.89	0.13	186,228,251,255	0
6	6PE	K	1004	27/27	0.90	0.12	117,167,208,211	0
7	SR	A	1005	1/1	0.90	0.15	197,197,197,197	0
8	BOG	A	1006	20/20	0.90	0.10	193,233,255,258	0
7	SR	E	1006	1/1	0.92	0.05	172,172,172,172	0
9	HEC	P	1001	43/43	0.92	0.15	160,193,233,233	0
4	HEM	A	1002	43/43	0.93	0.16	161,182,219,241	0
9	HEC	F	1001	43/43	0.94	0.16	138,182,224,227	0
4	HEM	O	1002	43/43	0.94	0.17	184,204,246,261	0
4	HEM	E	1002	43/43	0.95	0.15	133,162,207,219	0
4	HEM	O	1001	43/43	0.96	0.17	148,178,221,232	0
9	HEC	L	1001	43/43	0.96	0.18	184,209,256,261	0
4	HEM	K	1002	43/43	0.96	0.13	141,165,198,211	0
4	HEM	A	1001	43/43	0.97	0.16	137,167,214,217	0
4	HEM	E	1001	43/43	0.97	0.19	151,182,228,236	0
9	HEC	B	1001	43/43	0.97	0.12	139,158,190,195	0
10	FES	G	1001	4/4	0.97	0.09	209,255,301,355	0
4	HEM	K	1001	43/43	0.98	0.15	133,170,216,228	0
10	FES	Q	1001	4/4	0.98	0.05	133,135,247,330	0
10	FES	M	1001	4/4	0.99	0.04	169,202,233,265	0
10	FES	C	1001	4/4	0.99	0.05	136,161,209,254	0

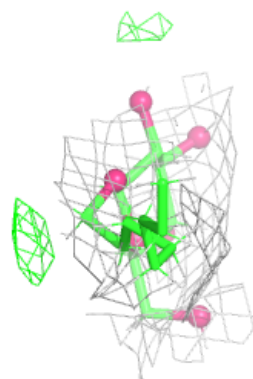
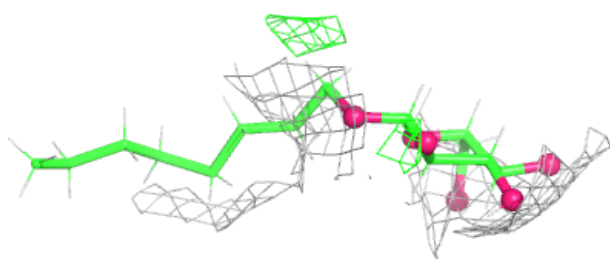
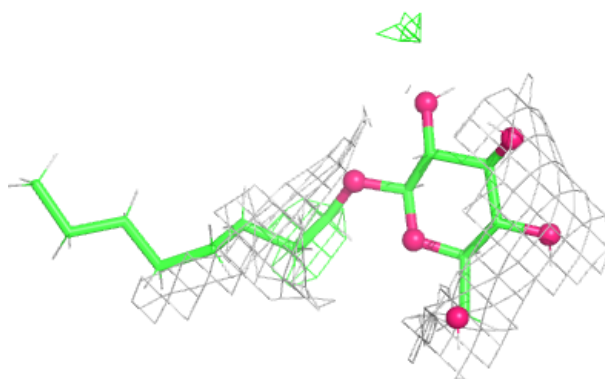
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

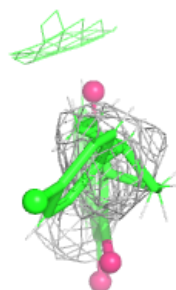
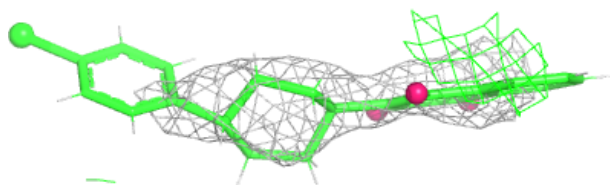
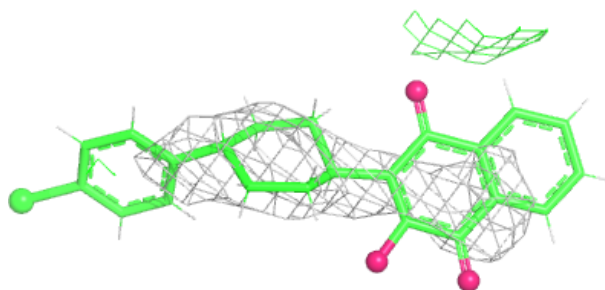


Electron density around BOG E 1005:

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

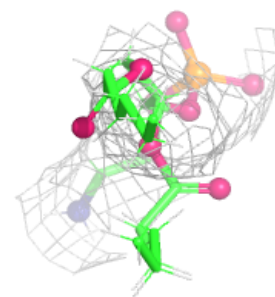
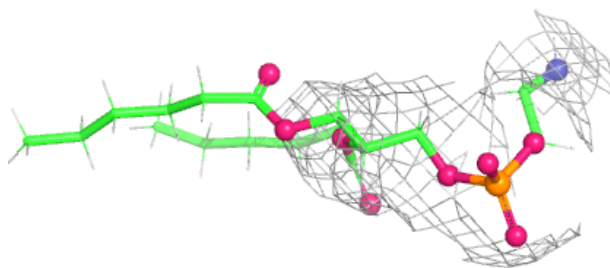
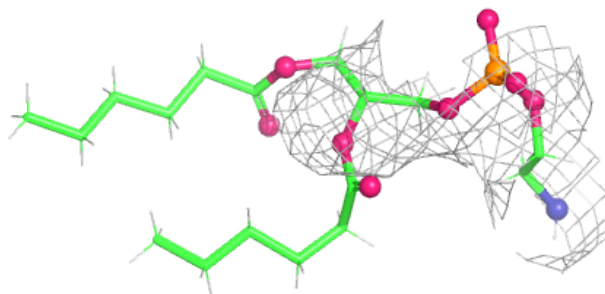
**Electron density around AOQ O 1003:**

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

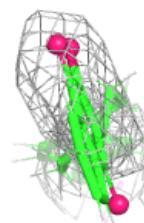
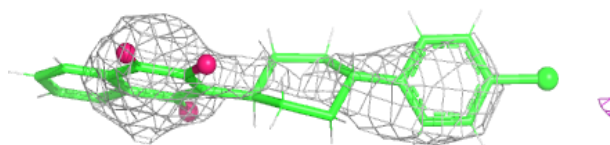
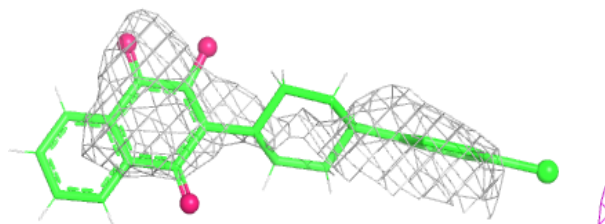


Electron density around 6PE E 1004:

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

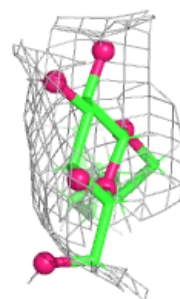
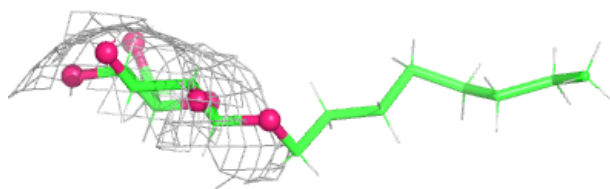
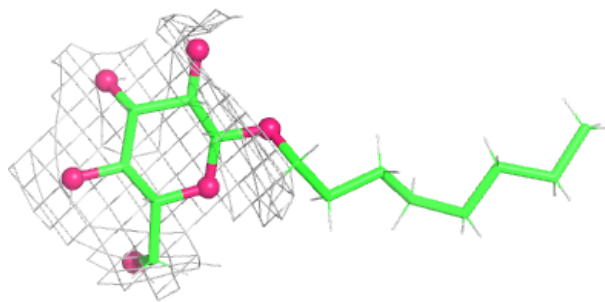
**Electron density around AOQ A 1003:**

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

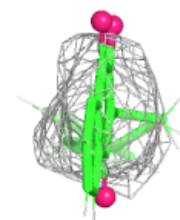
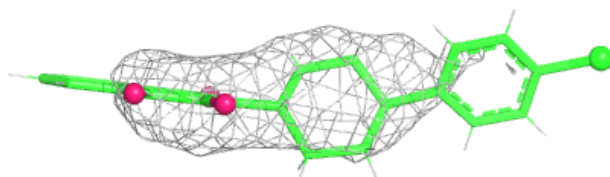
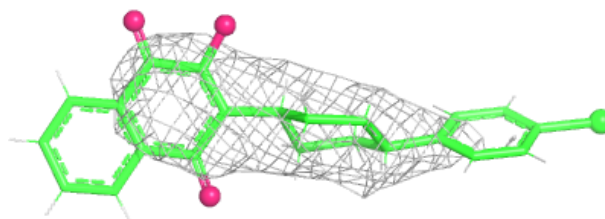


Electron density around BOG K 1005:

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

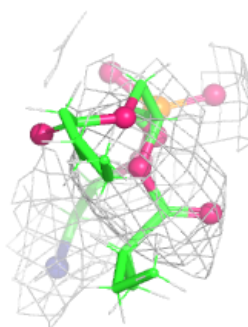
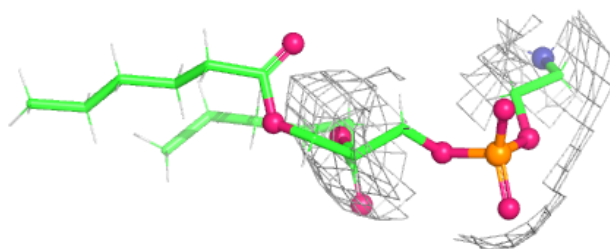
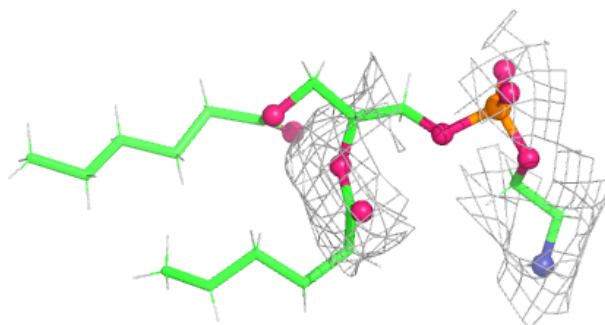
**Electron density around AOQ E 1003:**

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

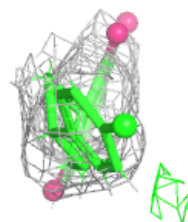
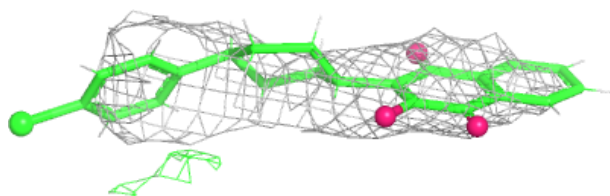
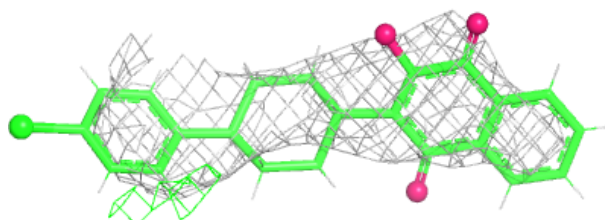


Electron density around 6PE A 1004:

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

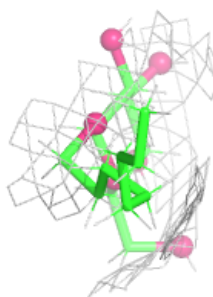
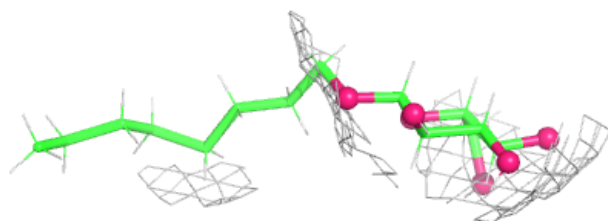
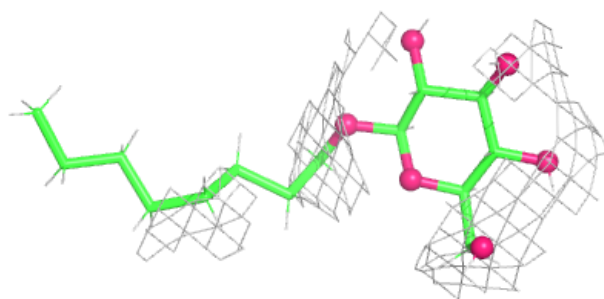
**Electron density around AOQ K 1003:**

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

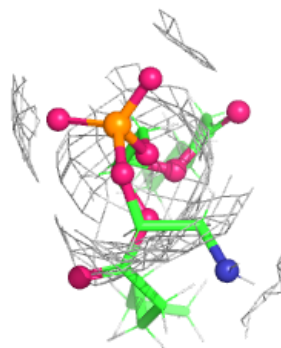
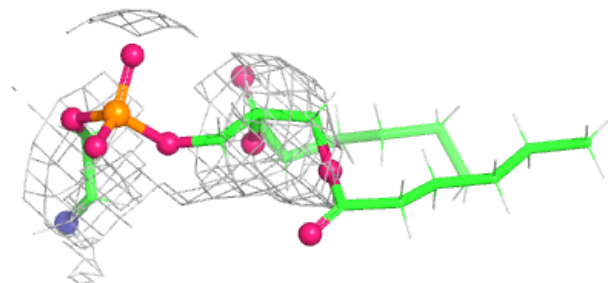
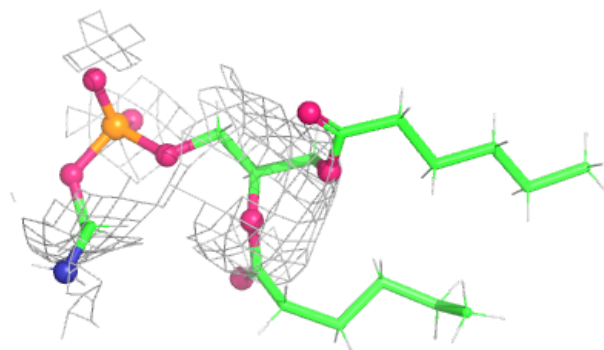


Electron density around BOG O 1005:

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

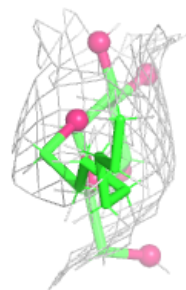
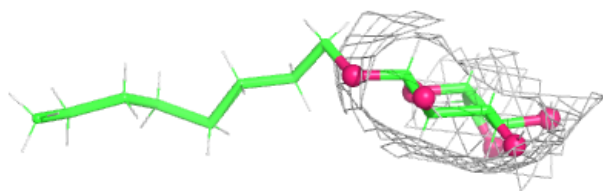
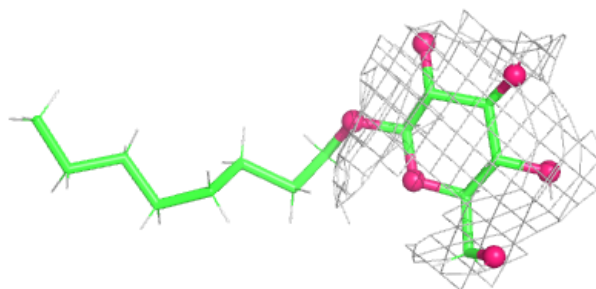
**Electron density around 6PE K 1004:**

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



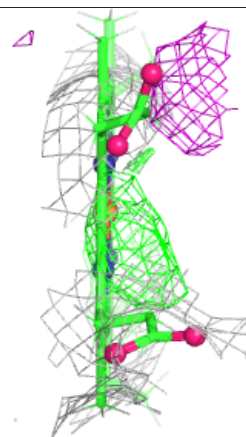
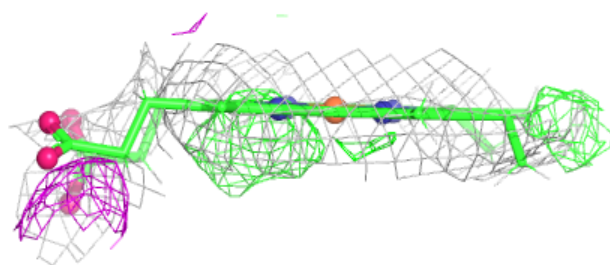
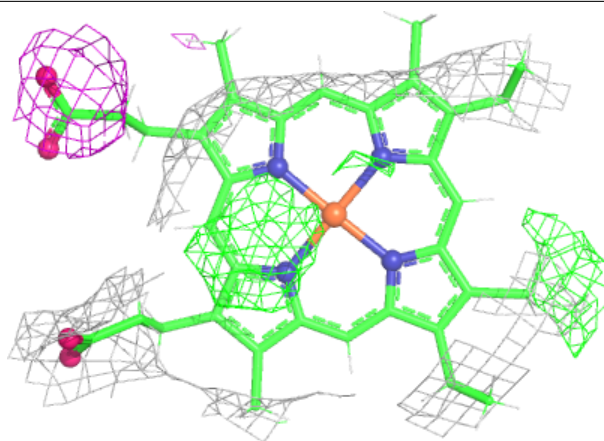
Electron density around BOG A 1006:

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



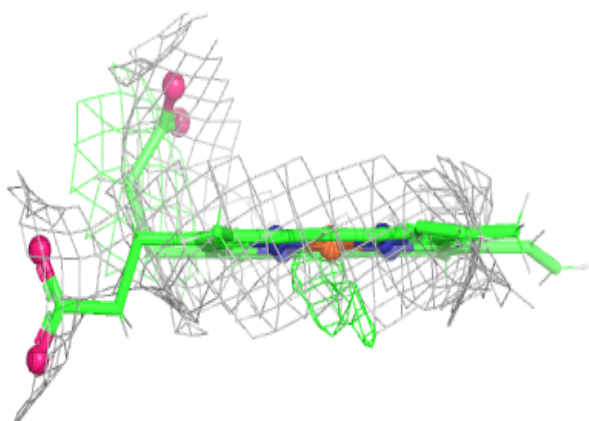
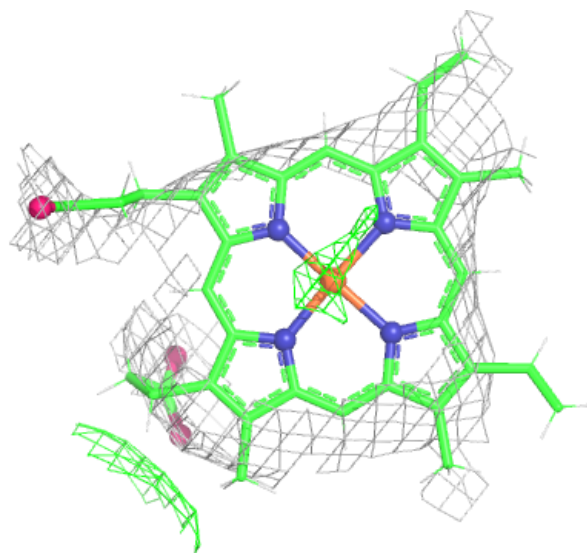
Electron density around HEC P 1001:

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



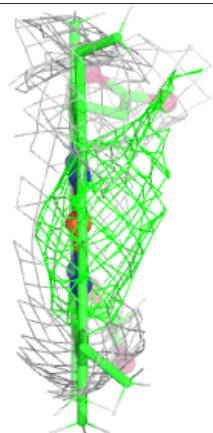
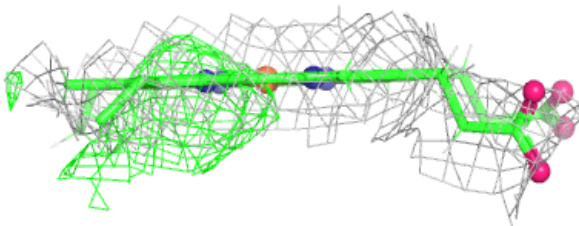
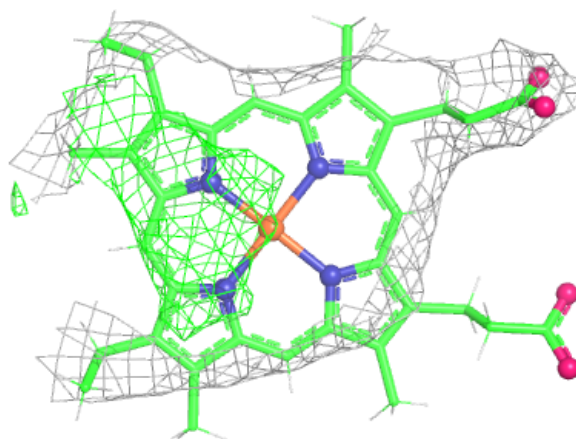
Electron density around HEM A 1002:

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



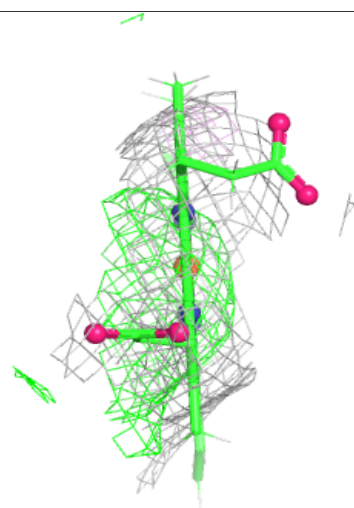
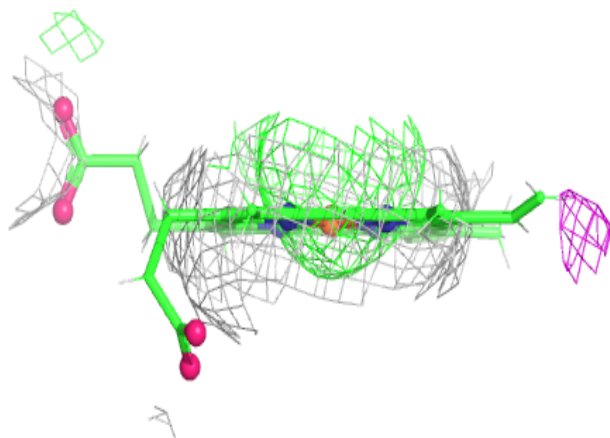
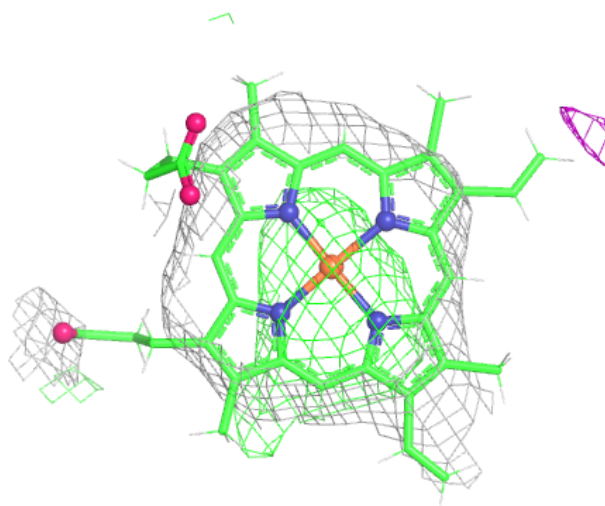
Electron density around HEC F 1001:

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



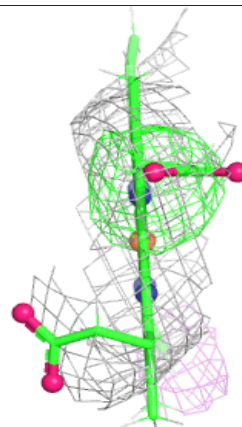
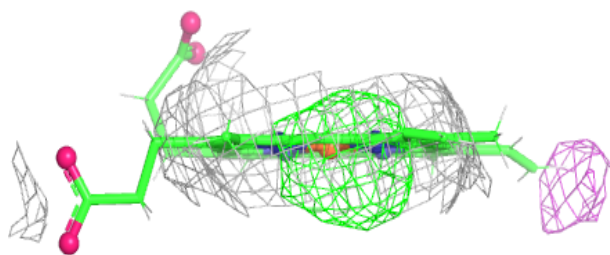
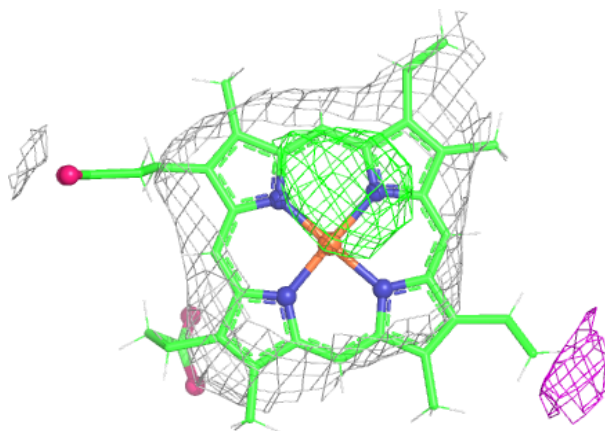
Electron density around HEM O 1002:

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



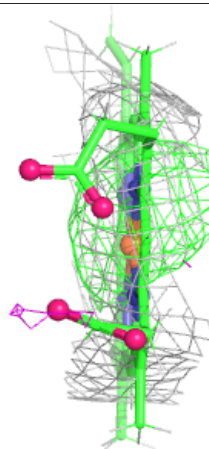
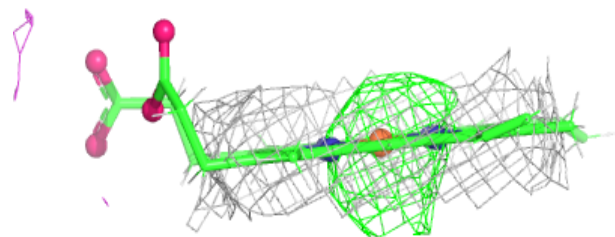
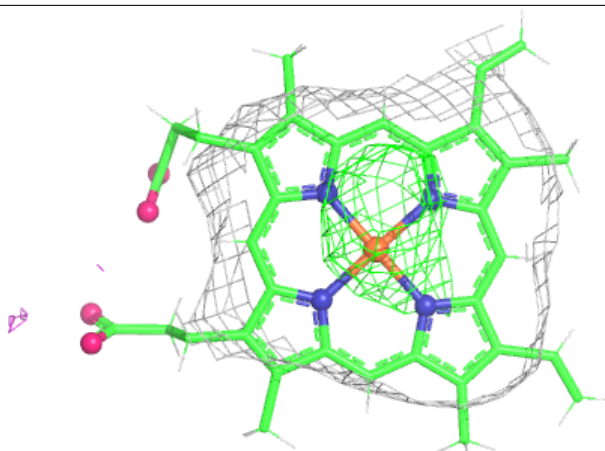
Electron density around HEM E 1002:

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



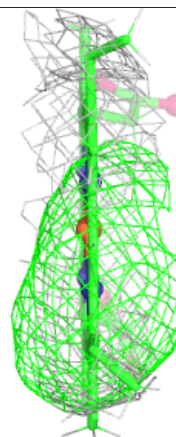
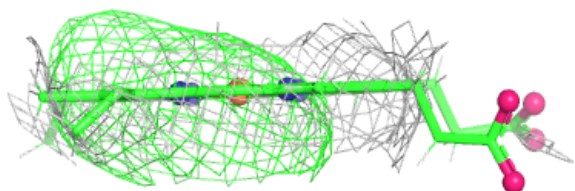
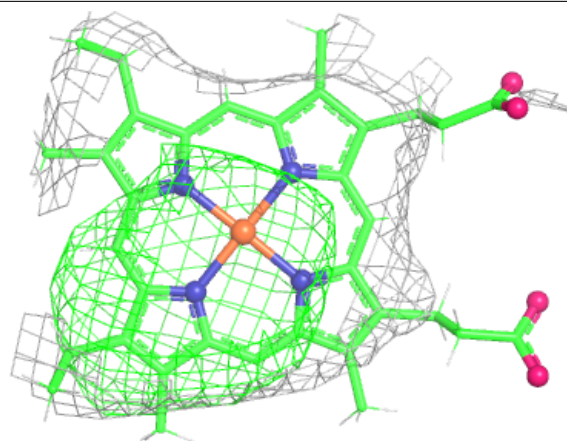
Electron density around HEM O 1001:

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



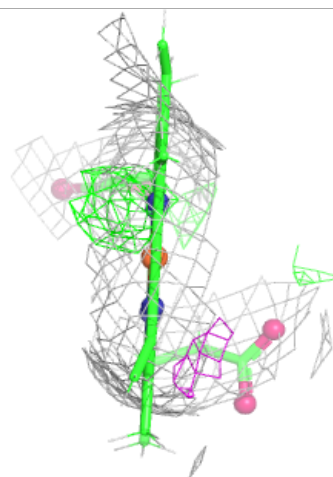
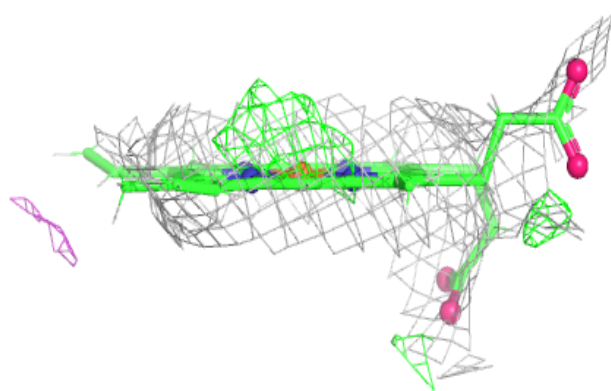
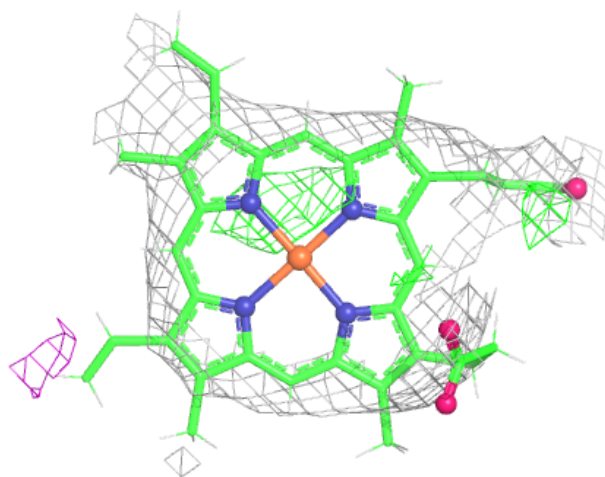
Electron density around HEC L 1001:

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



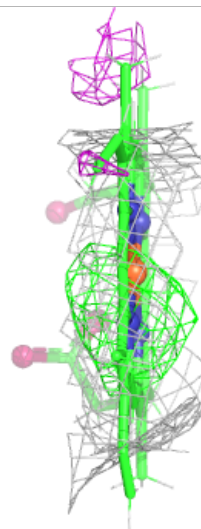
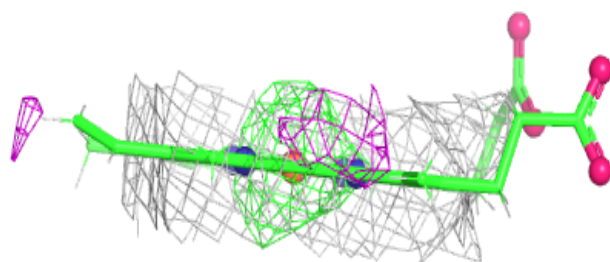
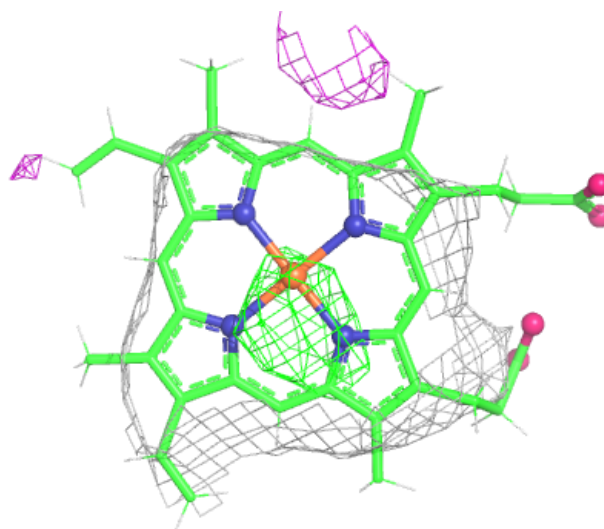
Electron density around HEM K 1002:

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



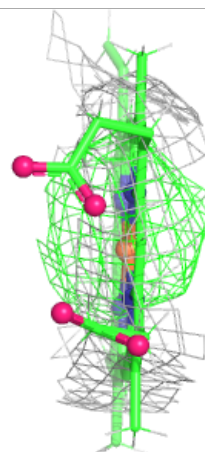
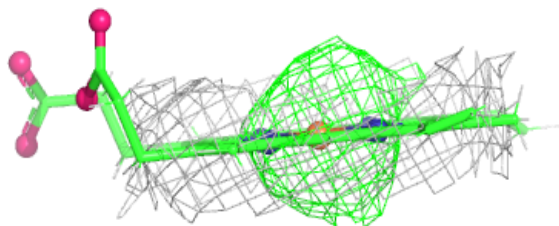
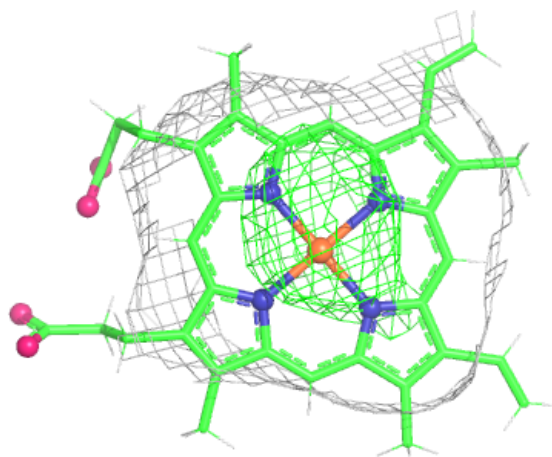
Electron density around HEM A 1001:

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



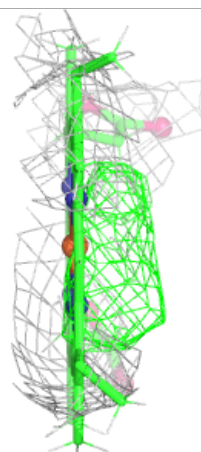
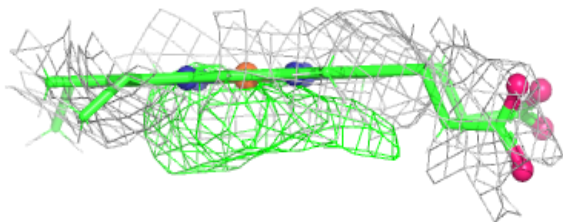
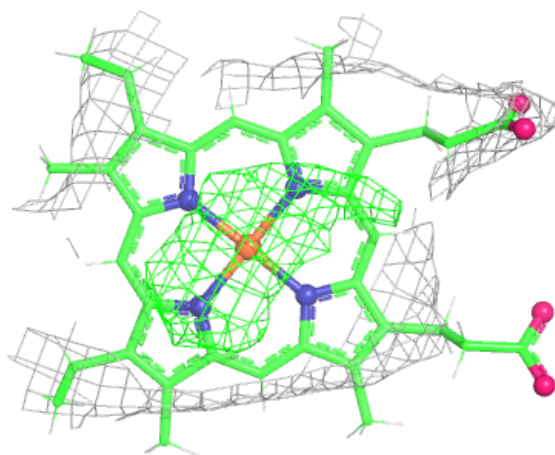
Electron density around HEM E 1001:

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



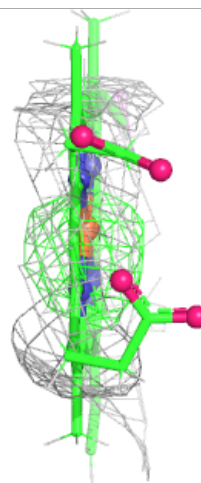
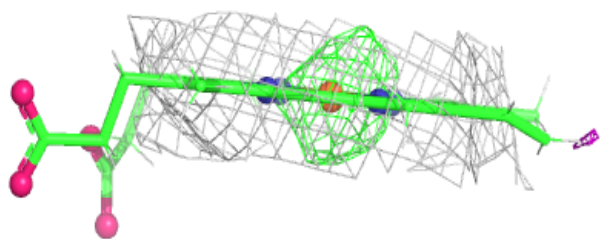
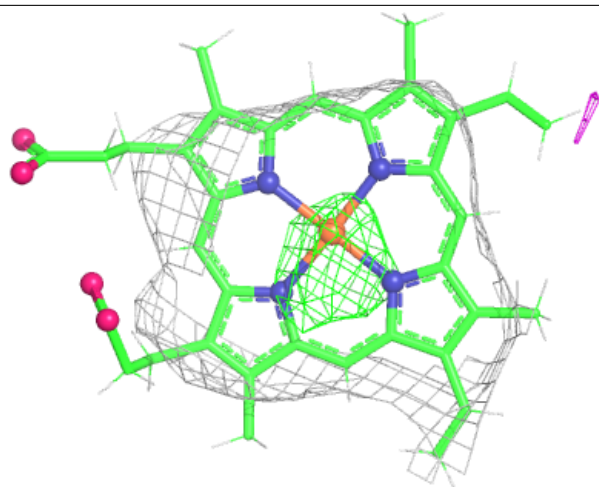
Electron density around HEC B 1001:

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



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)



6.5 Other polymers [i](#)

There are no such residues in this entry.