



Full wwPDB EM Validation Report ⓘ

Aug 31, 2026 – 02:45 PM EDT

PDB ID : 9YUQ / pdb_00009yuq
EMDB ID : EMD-73506
Title : A Bundled Antiparallel Cytochrome Nanowire Produced by *Desulfuromonas soudanensis* WTL
Authors : Petersen, H.A.; Chan, C.H.; Bond, D.R.; Wang, F.
Deposited on : 2025-10-22
Resolution : 3.11 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>
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:

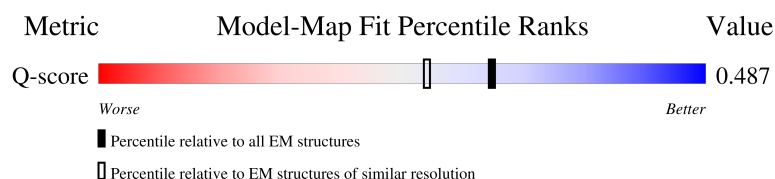
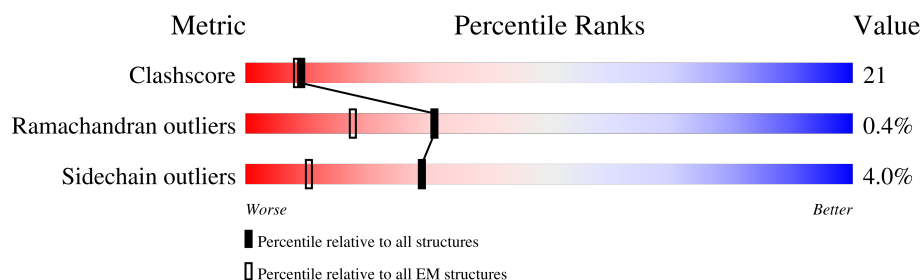
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.11 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)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14465 (2.61 - 3.61)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	C	218	 72% 17% • 9%
1	D	218	 67% 22% • 9%
1	E	218	 67% 23% • 9%
1	F	218	 70% 19% • 9%

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Mol	Chain	Length	Quality of chain
1	G	218	
1	I	218	
1	J	218	
1	K	218	
1	L	218	
1	M	218	
1	N	218	
1	P	218	
1	Q	218	
1	R	218	
1	S	218	
1	T	218	

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
2	HEC	C	301	X	-	-	-
2	HEC	C	302	X	-	-	-
2	HEC	C	303	X	-	-	-
2	HEC	C	306	X	-	-	-
2	HEC	C	307	X	-	-	-
2	HEC	C	308	X	-	-	-
2	HEC	D	301	X	-	-	-
2	HEC	D	304	X	-	-	-
2	HEC	D	305	X	-	-	-
2	HEC	E	301	X	-	-	-
2	HEC	E	302	X	-	-	-
2	HEC	E	305	X	-	-	-
2	HEC	E	306	X	-	-	-
2	HEC	F	301	X	-	-	-
2	HEC	F	302	X	-	-	-
2	HEC	F	305	X	-	-	-
2	HEC	F	306	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	HEC	G	301	X	-	-	-
2	HEC	G	302	X	-	-	-
2	HEC	G	303	X	-	-	-
2	HEC	I	301	X	-	-	-
2	HEC	I	302	X	-	-	-
2	HEC	I	303	X	-	-	-
2	HEC	J	301	X	-	-	-
2	HEC	J	302	X	-	-	-
2	HEC	J	305	X	-	-	-
2	HEC	J	306	X	-	-	-
2	HEC	K	301	X	-	-	-
2	HEC	K	302	X	-	-	-
2	HEC	K	305	X	-	-	-
2	HEC	K	306	X	-	-	-
2	HEC	L	301	X	-	-	-
2	HEC	L	302	X	-	-	-
2	HEC	L	305	X	-	-	-
2	HEC	L	306	X	-	-	-
2	HEC	M	301	X	-	-	-
2	HEC	M	302	X	-	-	-
2	HEC	M	305	X	-	-	-
2	HEC	M	306	X	-	-	-
2	HEC	N	301	X	-	-	-
2	HEC	N	302	X	-	-	-
2	HEC	N	303	X	-	-	-
2	HEC	N	306	X	-	-	-
2	HEC	N	307	X	-	-	-
2	HEC	P	301	X	-	-	-
2	HEC	P	302	X	-	-	-
2	HEC	P	303	X	-	-	-
2	HEC	P	306	X	-	-	-
2	HEC	P	307	X	-	-	-
2	HEC	P	308	X	-	-	-
2	HEC	Q	301	X	-	-	-
2	HEC	Q	304	X	-	-	-
2	HEC	Q	305	X	-	-	-
2	HEC	R	301	X	-	-	-
2	HEC	R	302	X	-	-	-
2	HEC	R	305	X	-	-	-
2	HEC	R	306	X	-	-	-
2	HEC	S	301	X	-	-	-
2	HEC	S	302	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	HEC	S	305	X	-	-	-
2	HEC	S	306	X	-	-	-
2	HEC	S	307	X	-	-	-
2	HEC	T	301	X	-	-	-
2	HEC	T	302	X	-	-	-

2 Entry composition [i](#)

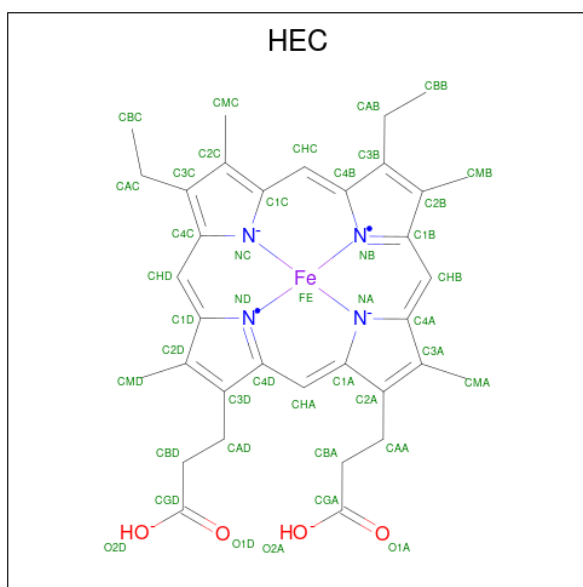
There are 3 unique types of molecules in this entry. The entry contains 24832 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Putative multiheme cytochrome c.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	N	198	Total	C	N	O	S	0	0
			1378	837	239	291	11		
1	M	198	Total	C	N	O	S	0	0
			1378	837	239	291	11		
1	L	198	Total	C	N	O	S	0	0
			1378	837	239	291	11		
1	K	198	Total	C	N	O	S	0	0
			1378	837	239	291	11		
1	J	198	Total	C	N	O	S	0	0
			1378	837	239	291	11		
1	I	198	Total	C	N	O	S	0	0
			1378	837	239	291	11		
1	C	198	Total	C	N	O	S	0	0
			1378	837	239	291	11		
1	D	198	Total	C	N	O	S	0	0
			1378	837	239	291	11		
1	E	198	Total	C	N	O	S	0	0
			1378	837	239	291	11		
1	F	198	Total	C	N	O	S	0	0
			1378	837	239	291	11		
1	G	198	Total	C	N	O	S	0	0
			1378	837	239	291	11		
1	P	198	Total	C	N	O	S	0	0
			1378	837	239	291	11		
1	Q	198	Total	C	N	O	S	0	0
			1378	837	239	291	11		
1	R	198	Total	C	N	O	S	0	0
			1378	837	239	291	11		
1	S	198	Total	C	N	O	S	0	0
			1378	837	239	291	11		
1	T	198	Total	C	N	O	S	0	0
			1378	837	239	291	11		

- Molecule 2 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



Mol	Chain	Residues	Atoms					AltConf
2	N	1	Total 43	C 34	Fe 1	N 4	O 4	0
2	N	1	Total 43	C 34	Fe 1	N 4	O 4	0
2	N	1	Total 43	C 34	Fe 1	N 4	O 4	0
2	N	1	Total 43	C 34	Fe 1	N 4	O 4	0
2	N	1	Total 43	C 34	Fe 1	N 4	O 4	0
2	M	1	Total 43	C 34	Fe 1	N 4	O 4	0
2	M	1	Total 43	C 34	Fe 1	N 4	O 4	0
2	M	1	Total 43	C 34	Fe 1	N 4	O 4	0
2	M	1	Total 43	C 34	Fe 1	N 4	O 4	0
2	L	1	Total 43	C 34	Fe 1	N 4	O 4	0
2	L	1	Total 43	C 34	Fe 1	N 4	O 4	0
2	L	1	Total 43	C 34	Fe 1	N 4	O 4	0
2	L	1	Total 43	C 34	Fe 1	N 4	O 4	0
2	K	1	Total 43	C 34	Fe 1	N 4	O 4	0

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Mol	Chain	Residues	Atoms					AltConf
2	K	1	Total 43	C 34	Fe 1	N 4	O 4	0
2	K	1	Total 43	C 34	Fe 1	N 4	O 4	0
2	K	1	Total 43	C 34	Fe 1	N 4	O 4	0
2	J	1	Total 43	C 34	Fe 1	N 4	O 4	0
2	J	1	Total 43	C 34	Fe 1	N 4	O 4	0
2	J	1	Total 43	C 34	Fe 1	N 4	O 4	0
2	J	1	Total 43	C 34	Fe 1	N 4	O 4	0
2	I	1	Total 43	C 34	Fe 1	N 4	O 4	0
2	I	1	Total 43	C 34	Fe 1	N 4	O 4	0
2	I	1	Total 43	C 34	Fe 1	N 4	O 4	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0
2	E	1	Total 43	C 34	Fe 1	N 4	O 4	0
2	E	1	Total 43	C 34	Fe 1	N 4	O 4	0

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Mol	Chain	Residues	Atoms					AltConf
2	E	1	Total 43	C 34	Fe 1	N 4	O 4	0
2	E	1	Total 43	C 34	Fe 1	N 4	O 4	0
2	F	1	Total 43	C 34	Fe 1	N 4	O 4	0
2	F	1	Total 43	C 34	Fe 1	N 4	O 4	0
2	F	1	Total 43	C 34	Fe 1	N 4	O 4	0
2	F	1	Total 43	C 34	Fe 1	N 4	O 4	0
2	G	1	Total 43	C 34	Fe 1	N 4	O 4	0
2	G	1	Total 43	C 34	Fe 1	N 4	O 4	0
2	G	1	Total 43	C 34	Fe 1	N 4	O 4	0
2	P	1	Total 43	C 34	Fe 1	N 4	O 4	0
2	P	1	Total 43	C 34	Fe 1	N 4	O 4	0
2	P	1	Total 43	C 34	Fe 1	N 4	O 4	0
2	P	1	Total 43	C 34	Fe 1	N 4	O 4	0
2	P	1	Total 43	C 34	Fe 1	N 4	O 4	0
2	P	1	Total 43	C 34	Fe 1	N 4	O 4	0
2	Q	1	Total 43	C 34	Fe 1	N 4	O 4	0
2	Q	1	Total 43	C 34	Fe 1	N 4	O 4	0
2	Q	1	Total 43	C 34	Fe 1	N 4	O 4	0
2	R	1	Total 43	C 34	Fe 1	N 4	O 4	0
2	R	1	Total 43	C 34	Fe 1	N 4	O 4	0
2	R	1	Total 43	C 34	Fe 1	N 4	O 4	0

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Mol	Chain	Residues	Atoms					AltConf
2	R	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
2	S	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
2	S	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
2	S	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
2	S	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
2	T	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
2	T	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
3	N	2	Total	Ca	0
			2	2	
3	M	2	Total	Ca	0
			2	2	
3	L	2	Total	Ca	0
			2	2	
3	K	2	Total	Ca	0
			2	2	
3	J	2	Total	Ca	0
			2	2	
3	I	2	Total	Ca	0
			2	2	
3	C	2	Total	Ca	0
			2	2	
3	D	2	Total	Ca	0
			2	2	
3	E	2	Total	Ca	0
			2	2	
3	F	2	Total	Ca	0
			2	2	
3	G	2	Total	Ca	0
			2	2	

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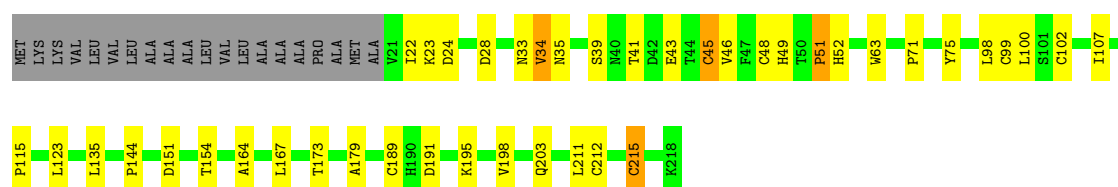
Mol	Chain	Residues	Atoms		AltConf
3	P	2	Total 2	Ca 2	0
3	Q	2	Total 2	Ca 2	0
3	R	2	Total 2	Ca 2	0
3	S	2	Total 2	Ca 2	0
3	T	2	Total 2	Ca 2	0

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

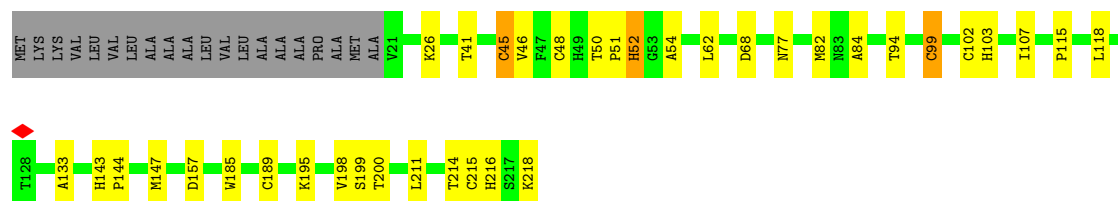
- Molecule 1: Putative multiheme cytochrome c

Chain N: 



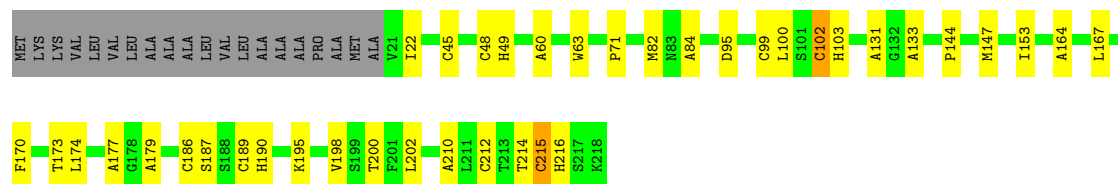
- Molecule 1: Putative multiheme cytochrome c

Chain M: 



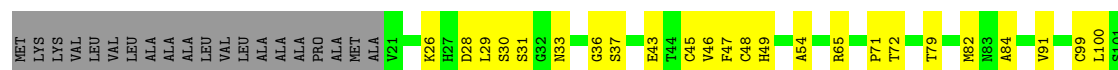
- Molecule 1: Putative multiheme cytochrome c

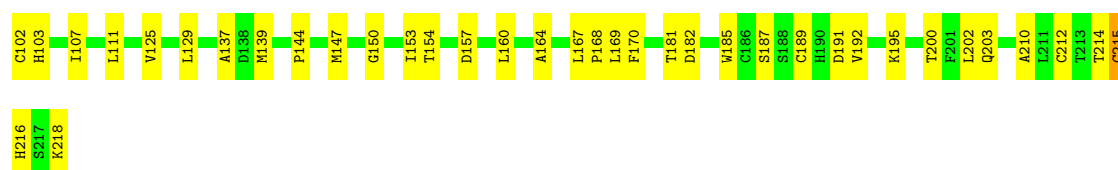
Chain L: 



- Molecule 1: Putative multiheme cytochrome c

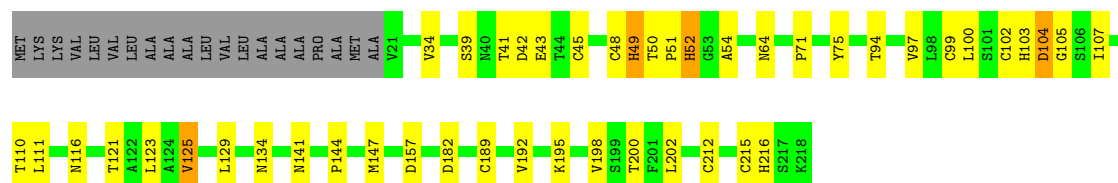
Chain K: 





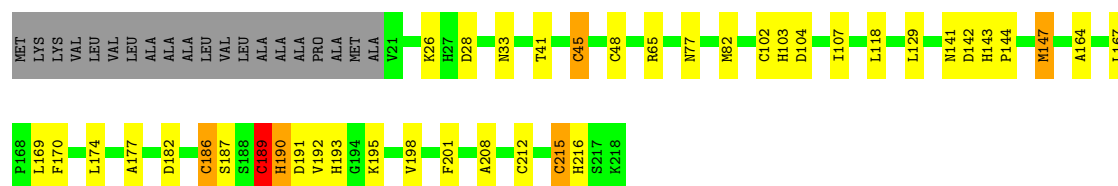
- Molecule 1: Putative multiheme cytochrome c

Chain J: 70% 19% 9%



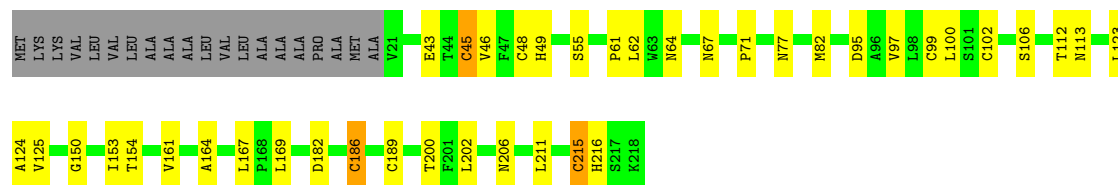
- Molecule 1: Putative multiheme cytochrome c

Chain I: 72% 16% 9%



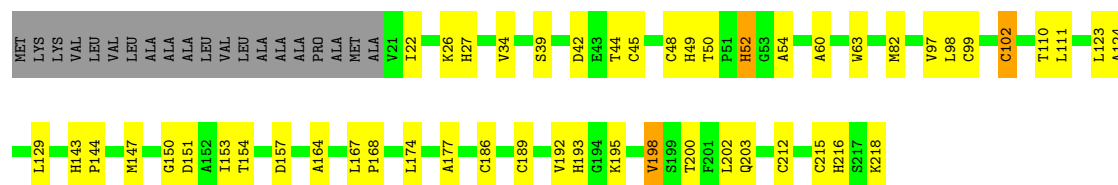
- Molecule 1: Putative multiheme cytochrome c

Chain C: 72% 17% 9%



- Molecule 1: Putative multiheme cytochrome c

Chain D: 67% 22% 9%



- Molecule 1: Putative multiheme cytochrome c

Chain E: 67% 23% 9%



- Molecule 1: Putative multiheme cytochrome c



- Molecule 1: Putative multiheme cytochrome c



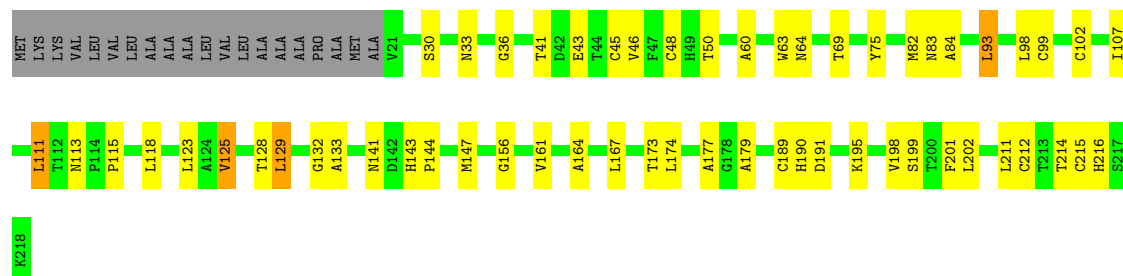
- Molecule 1: Putative multiheme cytochrome c



- Molecule 1: Putative multiheme cytochrome c



Chain R: 60% 29% 9%



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=51.44°, rise=30.75 Å, axial sym=C1	Depositor
Number of segments used	1241521	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{Å}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.195	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.038	Depositor
Recommended contour level	0.0486	Depositor
Map size (Å)	342.40002, 342.40002, 342.40002	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

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: CA, 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	C	0.17	0/1403	0.41	0/1923
1	D	0.23	0/1403	0.44	0/1923
1	E	0.22	0/1403	0.43	0/1923
1	F	0.21	0/1403	0.46	0/1923
1	G	0.13	0/1403	0.37	0/1923
1	I	0.18	0/1403	0.43	1/1923 (0.1%)
1	J	0.33	1/1403 (0.1%)	0.63	2/1923 (0.1%)
1	K	0.20	0/1403	0.44	0/1923
1	L	0.25	0/1403	0.45	0/1923
1	M	0.36	2/1403 (0.1%)	0.57	4/1923 (0.2%)
1	N	0.26	0/1403	0.50	1/1923 (0.1%)
1	P	0.25	0/1403	0.50	1/1923 (0.1%)
1	Q	0.27	0/1403	0.56	3/1923 (0.2%)
1	R	0.34	0/1403	0.67	7/1923 (0.4%)
1	S	0.29	0/1403	0.49	2/1923 (0.1%)
1	T	0.20	0/1403	0.45	0/1923
All	All	0.25	3/22448 (0.0%)	0.49	21/30768 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	I	0	1
1	N	0	1
1	Q	0	1
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	52	HIS	CG-CD2	6.68	1.43	1.35
1	M	52	HIS	CG-ND1	5.75	1.44	1.38
1	J	52	HIS	CB-CG	-5.57	1.42	1.50

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	52	HIS	CA-CB-CG	-14.72	99.08	113.80
1	J	52	HIS	N-CA-C	13.75	126.35	108.34
1	M	52	HIS	CA-CB-CG	-10.36	103.44	113.80
1	Q	52	HIS	CA-CB-CG	-7.39	106.41	113.80
1	Q	52	HIS	N-CA-C	6.92	119.44	109.14
1	J	52	HIS	CA-CB-CG	-6.90	106.90	113.80
1	R	52	HIS	N-CA-CB	6.54	122.64	110.87
1	M	52	HIS	ND1-CE1-NE2	6.38	114.78	108.40
1	R	52	HIS	CB-CA-C	-6.24	98.39	113.19
1	P	52	HIS	CB-CA-C	-6.14	101.14	114.10
1	M	51	PRO	CA-C-N	-5.93	112.00	122.20
1	M	51	PRO	C-N-CA	-5.93	112.00	122.20
1	N	45	CYS	CA-CB-SG	5.83	127.81	114.40
1	R	51	PRO	CA-C-N	-5.68	113.07	122.39
1	R	51	PRO	C-N-CA	-5.68	113.07	122.39
1	R	52	HIS	ND1-CG-CD2	-5.68	100.42	106.10
1	I	189	CYS	CA-CB-SG	5.67	127.45	114.40
1	S	52	HIS	CA-CB-CG	-5.57	108.23	113.80
1	R	189	CYS	CA-CB-SG	5.30	126.60	114.40
1	S	52	HIS	N-CA-C	5.05	121.55	110.80
1	Q	45	CYS	CA-CB-SG	5.01	125.92	114.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	I	189	CYS	Peptide
1	N	51	PRO	Peptide
1	Q	52	HIS	Peptide

5.2 Too-close contacts

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1378	0	1310	55	0
1	D	1378	0	1310	61	0
1	E	1378	0	1310	60	0
1	F	1378	0	1308	53	0
1	G	1378	0	1311	42	0
1	I	1378	0	1311	46	0
1	J	1378	0	1310	67	0
1	K	1378	0	1310	66	0
1	L	1378	0	1310	44	0
1	M	1378	0	1309	59	0
1	N	1378	0	1310	49	0
1	P	1378	0	1310	51	0
1	Q	1378	0	1310	69	0
1	R	1378	0	1310	82	0
1	S	1378	0	1308	70	0
1	T	1378	0	1310	64	0
2	C	258	0	181	60	0
2	D	129	0	87	27	0
2	E	172	0	119	42	0
2	F	172	0	119	40	0
2	G	129	0	94	22	0
2	I	129	0	93	30	0
2	J	172	0	118	43	0
2	K	172	0	119	41	0
2	L	172	0	119	32	0
2	M	172	0	119	43	0
2	N	215	0	151	42	0
2	P	258	0	181	51	0
2	Q	129	0	89	31	0
2	R	172	0	119	56	0
2	S	215	0	148	55	0
2	T	86	0	63	21	0
3	C	2	0	0	1	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	0	0
3	I	2	0	0	0	0
3	J	2	0	0	0	0
3	K	2	0	0	0	0
3	L	2	0	0	0	0
3	M	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	N	2	0	0	0	0
3	P	2	0	0	0	0
3	Q	2	0	0	0	0
3	R	2	0	0	0	0
3	S	2	0	0	0	0
3	T	2	0	0	0	0
All	All	24832	0	22876	979	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 21.

All (979) 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)
2:D:304:HEC:HAC	1:E:215:CYS:SG	1.26	1.75
1:E:48:CYS:SG	2:E:306:HEC:HAC	1.23	1.75
1:C:215:CYS:SG	2:C:301:HEC:HAC	1.19	1.74
1:R:189:CYS:SG	2:R:301:HEC:HAC	1.23	1.72
1:M:48:CYS:SG	2:M:306:HEC:HAC	1.28	1.70
1:P:102:CYS:SG	2:P:303:HEC:HAC	1.23	1.70
2:F:305:HEC:HAC	1:G:215:CYS:SG	1.28	1.70
1:K:48:CYS:SG	2:K:306:HEC:HAC	1.31	1.69
1:P:48:CYS:SG	2:P:308:HEC:HAC	1.18	1.69
1:C:48:CYS:SG	2:C:308:HEC:HAC	1.30	1.68
1:C:102:CYS:SG	2:C:303:HEC:HAC	1.26	1.68
2:S:307:HEC:HAC	1:T:215:CYS:SG	1.29	1.67
2:M:305:HEC:HAC	1:L:215:CYS:SG	1.19	1.66
1:S:48:CYS:SG	2:S:306:HEC:HAC	1.33	1.66
1:Q:48:CYS:SG	2:Q:305:HEC:HAC	1.30	1.66
2:L:305:HEC:HAC	1:K:215:CYS:SG	1.31	1.65
1:I:102:CYS:SG	2:I:303:HEC:HAC	1.25	1.63
1:N:215:CYS:SG	2:N:301:HEC:HAC	1.39	1.62
1:J:48:CYS:SG	2:J:306:HEC:HAC	1.31	1.62
1:L:48:CYS:SG	2:L:306:HEC:HAC	1.39	1.62
1:P:215:CYS:SG	2:P:301:HEC:HAC	1.37	1.60
2:J:305:HEC:HAC	1:I:215:CYS:SG	1.42	1.59
1:N:48:CYS:SG	2:N:307:HEC:HAC	1.40	1.58
1:R:48:CYS:SG	2:R:305:HEC:HAC	1.40	1.58
2:E:305:HEC:HAC	1:F:215:CYS:SG	1.44	1.58
1:D:48:CYS:SG	2:D:305:HEC:HAC	1.41	1.55
2:Q:304:HEC:HAC	1:R:215:CYS:SG	1.45	1.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:102:CYS:SG	2:S:302:HEC:HAC	1.49	1.52
1:F:48:CYS:SG	2:F:306:HEC:HAC	1.48	1.50
2:C:307:HEC:HAC	1:D:189:CYS:SG	1.49	1.50
1:T:102:CYS:SG	2:T:302:HEC:HAC	1.52	1.50
1:F:102:CYS:SG	2:F:302:HEC:HAC	1.51	1.49
1:K:102:CYS:SG	2:K:302:HEC:HAC	1.53	1.48
2:P:306:HEC:HAC	1:Q:215:CYS:SG	1.52	1.48
1:T:48:CYS:SG	2:T:301:HEC:HAC	1.52	1.47
2:P:307:HEC:HAC	1:Q:189:CYS:SG	1.58	1.43
1:K:48:CYS:SG	2:K:306:HEC:CAC	2.09	1.41
2:P:307:HEC:CAC	1:Q:189:CYS:SG	2.09	1.41
1:Q:48:CYS:SG	2:Q:305:HEC:CAC	2.09	1.41
1:J:48:CYS:SG	2:J:306:HEC:CAC	2.08	1.40
1:C:48:CYS:SG	2:C:308:HEC:CAC	2.09	1.40
1:S:48:CYS:SG	2:S:306:HEC:CAC	2.09	1.40
1:M:48:CYS:SG	2:M:306:HEC:CAC	2.09	1.40
1:I:48:CYS:SG	2:I:302:HEC:CAC	2.10	1.40
2:Q:304:HEC:CAC	1:R:215:CYS:SG	2.10	1.40
1:R:48:CYS:SG	2:R:305:HEC:CAC	2.07	1.40
1:S:102:CYS:SG	2:S:302:HEC:CAC	2.10	1.40
1:F:102:CYS:SG	2:F:302:HEC:CAC	2.08	1.40
1:P:189:CYS:SG	2:P:302:HEC:CAC	2.10	1.40
1:N:48:CYS:SG	2:N:307:HEC:CAC	2.09	1.40
1:L:102:CYS:SG	2:L:302:HEC:CAC	2.10	1.39
1:D:48:CYS:SG	2:D:305:HEC:CAC	2.09	1.39
1:R:102:CYS:SG	2:R:302:HEC:CAC	2.10	1.39
1:K:189:CYS:SG	2:K:301:HEC:CAC	2.10	1.39
1:C:189:CYS:SG	2:C:302:HEC:CAC	2.11	1.39
1:E:102:CYS:SG	2:E:302:HEC:CAC	2.10	1.39
2:F:305:HEC:CAC	1:G:215:CYS:SG	2.10	1.39
1:I:102:CYS:SG	2:I:303:HEC:CAC	2.10	1.39
1:F:48:CYS:SG	2:F:306:HEC:CAC	2.09	1.39
1:K:102:CYS:SG	2:K:302:HEC:CAC	2.10	1.39
1:P:48:CYS:SG	2:P:308:HEC:CAC	2.09	1.39
1:L:48:CYS:SG	2:L:306:HEC:CAC	2.09	1.39
2:M:305:HEC:CAC	1:L:215:CYS:SG	2.10	1.38
1:J:189:CYS:SG	2:J:301:HEC:CAC	2.10	1.38
1:G:189:CYS:SG	2:G:302:HEC:CAC	2.12	1.38
1:P:102:CYS:SG	2:P:303:HEC:CAC	2.09	1.38
2:R:306:HEC:CAC	1:S:215:CYS:SG	2.11	1.38
1:E:189:CYS:SG	2:E:301:HEC:HAC	1.63	1.38

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:306:HEC:HAC	1:S:215:CYS:SG	1.62	1.38
1:M:189:CYS:SG	2:M:301:HEC:CAC	2.11	1.38
2:K:305:HEC:CAC	1:J:215:CYS:SG	2.12	1.38
1:N:102:CYS:SG	2:N:303:HEC:CAC	2.12	1.37
1:C:102:CYS:SG	2:C:303:HEC:CAC	2.10	1.38
2:C:307:HEC:CAC	1:D:189:CYS:SG	2.11	1.37
1:E:48:CYS:SG	2:E:306:HEC:CAC	2.09	1.38
1:T:102:CYS:SG	2:T:302:HEC:CAC	2.11	1.38
1:G:102:CYS:SG	2:G:303:HEC:CAC	2.12	1.37
2:S:307:HEC:CAC	1:T:215:CYS:SG	2.11	1.37
1:T:48:CYS:SG	2:T:301:HEC:CAC	2.10	1.37
1:J:102:CYS:SG	2:J:302:HEC:CAC	2.12	1.37
1:E:102:CYS:SG	2:E:302:HEC:HAC	1.63	1.37
2:N:306:HEC:CAC	1:M:215:CYS:SG	2.13	1.37
2:L:305:HEC:CAC	1:K:215:CYS:SG	2.11	1.37
1:C:215:CYS:SG	2:C:301:HEC:CAC	2.11	1.37
2:D:304:HEC:CAC	1:E:215:CYS:SG	2.10	1.37
1:N:215:CYS:SG	2:N:301:HEC:CAC	2.11	1.36
1:P:215:CYS:SG	2:P:301:HEC:CAC	2.11	1.36
1:Q:102:CYS:SG	2:Q:301:HEC:CAC	2.13	1.36
2:C:306:HEC:CAC	1:D:215:CYS:SG	2.13	1.36
1:F:189:CYS:SG	2:F:301:HEC:CAC	2.14	1.36
1:M:102:CYS:SG	2:M:302:HEC:CAC	2.12	1.36
1:G:48:CYS:SG	2:G:301:HEC:CAC	2.11	1.36
2:P:306:HEC:CAC	1:Q:215:CYS:SG	2.13	1.36
1:N:189:CYS:SG	2:N:302:HEC:CAC	2.12	1.36
2:E:305:HEC:CAC	1:F:215:CYS:SG	2.11	1.35
1:D:102:CYS:SG	2:D:301:HEC:CAC	2.12	1.35
2:J:305:HEC:CAC	1:I:215:CYS:SG	2.12	1.35
1:E:189:CYS:SG	2:E:301:HEC:CAC	2.13	1.34
1:I:48:CYS:SG	2:I:302:HEC:HAC	1.64	1.34
2:K:305:HEC:HAC	1:J:215:CYS:SG	1.66	1.33
2:S:305:HEC:CAC	1:T:189:CYS:SG	2.16	1.33
1:K:189:CYS:SG	2:K:301:HEC:HAC	1.68	1.33
2:N:306:HEC:HAC	1:M:215:CYS:SG	1.68	1.33
1:R:189:CYS:SG	2:R:301:HEC:CAC	2.17	1.32
1:N:189:CYS:SG	2:N:302:HEC:HAC	1.68	1.32
1:R:102:CYS:SG	2:R:302:HEC:HAC	1.70	1.31
1:I:189:CYS:SG	2:I:301:HEC:CAC	2.18	1.31
1:M:189:CYS:SG	2:M:301:HEC:HAC	1.71	1.27
1:Q:102:CYS:SG	2:Q:301:HEC:HAC	1.72	1.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:102:CYS:SG	2:L:302:HEC:HAC	1.71	1.26
1:L:189:CYS:SG	2:L:301:HEC:CAC	2.22	1.26
1:J:189:CYS:SG	2:J:301:HEC:HAC	1.70	1.26
2:S:305:HEC:HAC	1:T:189:CYS:SG	1.74	1.26
1:J:102:CYS:SG	2:J:302:HEC:HAC	1.74	1.25
1:D:102:CYS:SG	2:D:301:HEC:HAC	1.72	1.25
1:S:189:CYS:SG	2:S:301:HEC:CAC	2.24	1.25
1:N:102:CYS:SG	2:N:303:HEC:HAC	1.71	1.24
1:G:102:CYS:SG	2:G:303:HEC:HAC	1.76	1.21
1:C:189:CYS:SG	2:C:302:HEC:HAC	1.74	1.20
1:M:102:CYS:SG	2:M:302:HEC:HAC	1.76	1.19
1:G:48:CYS:SG	2:G:301:HEC:HAC	1.77	1.19
1:P:189:CYS:SG	2:P:302:HEC:HAC	1.77	1.18
2:C:306:HEC:HAC	1:D:215:CYS:SG	1.77	1.17
1:L:189:CYS:SG	2:L:301:HEC:HAC	1.88	1.12
1:D:144:PRO:HB2	1:D:147:MET:HE1	1.33	1.09
1:D:45:CYS:HB2	2:D:305:HEC:HHC	1.32	1.09
1:G:189:CYS:SG	2:G:302:HEC:HAC	1.89	1.06
1:S:189:CYS:SG	2:S:301:HEC:HAC	1.92	1.05
2:C:307:HEC:HAC	1:D:189:CYS:CB	1.87	1.04
2:S:307:HEC:HAC	1:T:215:CYS:HG	1.22	1.02
2:N:306:HEC:HAC	1:M:215:CYS:HG	0.96	1.01
1:M:45:CYS:HB3	2:M:306:HEC:HHC	1.40	1.01
2:P:308:HEC:HHC	1:Q:218:LYS:HZ3	1.23	1.00
2:N:306:HEC:HBA1	2:N:306:HEC:HHA	1.40	1.00
1:F:189:CYS:SG	2:F:301:HEC:HAC	1.97	1.00
1:C:215:CYS:HG	2:C:301:HEC:HAC	1.24	0.99
1:I:189:CYS:SG	2:I:301:HEC:HAC	2.03	0.97
1:S:45:CYS:HB3	2:S:306:HEC:HHC	1.43	0.97
2:J:305:HEC:HBA1	2:J:305:HEC:HHA	1.45	0.97
1:P:45:CYS:HB3	2:P:308:HEC:HHC	1.49	0.94
1:S:102:CYS:CB	2:S:302:HEC:HAC	1.97	0.94
1:E:189:CYS:HG	2:E:301:HEC:HAC	0.80	0.94
1:S:102:CYS:CB	2:S:302:HEC:CAC	2.47	0.93
1:M:189:CYS:HG	2:M:301:HEC:HAC	1.31	0.92
1:K:189:CYS:HG	2:K:301:HEC:HAC	1.34	0.92
1:Q:45:CYS:HB2	2:Q:305:HEC:HHC	1.52	0.92
1:R:48:CYS:HG	2:R:305:HEC:HAC	1.09	0.91
1:S:48:CYS:HG	2:S:306:HEC:HAC	1.10	0.91
1:C:45:CYS:HB3	2:C:308:HEC:HHC	1.52	0.91
1:M:144:PRO:HB2	1:M:147:MET:HE1	1.52	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:102:CYS:CB	2:F:302:HEC:HAC	2.00	0.90
1:D:193:HIS:HE1	2:D:305:HEC:NC	1.69	0.90
2:C:306:HEC:HAC	1:D:215:CYS:HG	1.24	0.90
2:E:305:HEC:HAC	1:F:215:CYS:HG	1.33	0.90
2:K:305:HEC:HAC	1:J:215:CYS:HG	1.03	0.90
1:N:49:HIS:HB3	2:N:306:HEC:HHB	1.54	0.89
1:E:48:CYS:CB	2:E:306:HEC:HAC	2.01	0.89
1:E:189:CYS:HG	2:E:301:HEC:CAC	1.66	0.89
1:P:49:HIS:HB3	2:P:306:HEC:HHB	1.54	0.89
1:E:102:CYS:HG	2:E:302:HEC:HAC	1.36	0.88
1:N:189:CYS:HG	2:N:302:HEC:HAC	0.97	0.88
1:P:48:CYS:HG	2:P:308:HEC:HAC	1.36	0.88
1:L:45:CYS:HB3	2:L:306:HEC:HHC	1.53	0.88
1:J:51:PRO:HB3	2:I:301:HEC:HBC3	1.55	0.88
1:E:49:HIS:HB3	2:E:305:HEC:HHB	1.56	0.88
1:F:102:CYS:CB	2:F:302:HEC:CAC	2.51	0.88
1:D:193:HIS:HE1	2:D:305:HEC:C1C	1.88	0.86
1:L:144:PRO:HB2	1:L:147:MET:HE1	1.57	0.86
2:R:306:HEC:HAC	1:S:215:CYS:HG	0.98	0.86
2:S:305:HEC:HAC	1:T:189:CYS:HG	1.40	0.86
1:G:48:CYS:SG	2:G:301:HEC:C3C	2.63	0.85
2:E:305:HEC:ND	1:F:216:HIS:HE1	1.73	0.85
1:K:189:CYS:CB	2:K:301:HEC:HAC	2.07	0.84
1:J:41:THR:HG22	1:J:43:GLU:H	1.42	0.84
1:G:133:ALA:HA	2:G:302:HEC:HMA1	1.60	0.84
1:M:48:CYS:HG	2:M:306:HEC:HAC	1.05	0.84
1:R:189:CYS:HG	2:R:301:HEC:HAC	1.41	0.84
1:R:45:CYS:HB2	2:R:305:HEC:HHC	1.59	0.84
2:S:307:HEC:HHA	2:S:307:HEC:HBA1	1.59	0.83
1:N:48:CYS:HG	2:N:307:HEC:HAC	1.02	0.83
2:R:306:HEC:ND	1:S:216:HIS:HE1	1.76	0.82
1:L:48:CYS:HG	2:L:306:HEC:HAC	1.00	0.82
1:T:48:CYS:HG	2:T:301:HEC:HAC	1.39	0.82
1:I:144:PRO:HB2	1:I:147:MET:HE1	1.60	0.82
2:K:305:HEC:ND	1:J:216:HIS:HE1	1.78	0.82
1:T:102:CYS:CB	2:T:302:HEC:HAC	2.09	0.82
1:J:39:SER:HA	1:J:125:VAL:H	1.45	0.81
1:F:189:CYS:SG	2:F:301:HEC:CBC	2.68	0.81
1:J:144:PRO:HB2	1:J:147:MET:HE1	1.62	0.81
1:M:48:CYS:HB2	2:M:306:HEC:C3C	2.11	0.81
1:G:189:CYS:SG	2:G:302:HEC:CBC	2.69	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:307:HEC:HAD2	1:Q:200:THR:HG21	1.61	0.81
1:T:45:CYS:HB2	2:T:301:HEC:HHC	1.63	0.81
2:S:307:HEC:ND	1:T:216:HIS:HE1	1.78	0.81
2:F:305:HEC:ND	1:G:216:HIS:HE1	1.79	0.80
2:N:306:HEC:ND	1:M:216:HIS:HE1	1.79	0.80
2:L:305:HEC:ND	1:K:216:HIS:HE1	1.79	0.80
1:D:22:ILE:HD11	1:D:193:HIS:HD1	1.46	0.80
1:L:189:CYS:SG	2:L:301:HEC:CBC	2.70	0.79
2:S:305:HEC:HMA2	1:T:133:ALA:HA	1.62	0.79
2:E:305:HEC:HBA1	2:E:305:HEC:HHA	1.64	0.78
1:I:48:CYS:SG	2:I:302:HEC:C3C	2.70	0.78
2:P:308:HEC:CHC	1:Q:218:LYS:HZ3	1.96	0.78
1:J:48:CYS:HG	2:J:306:HEC:CAC	1.97	0.77
1:M:102:CYS:CB	2:M:302:HEC:CAC	2.62	0.77
1:M:103:HIS:CE1	2:M:302:HEC:C1C	2.61	0.77
1:Q:144:PRO:HB2	1:Q:147:MET:HE1	1.66	0.77
1:S:189:CYS:SG	2:S:301:HEC:CBC	2.72	0.77
2:F:305:HEC:HBA1	2:F:305:HEC:HHA	1.65	0.77
2:P:307:HEC:CAC	1:Q:189:CYS:CB	2.63	0.76
1:N:39:SER:HB3	1:N:123:LEU:HD11	1.66	0.76
2:Q:304:HEC:ND	1:R:216:HIS:HE1	1.84	0.76
1:M:48:CYS:CB	2:M:306:HEC:HAC	2.16	0.75
1:T:50:THR:HG21	1:T:113:ASN:HD22	1.50	0.75
1:P:26:LYS:HD3	2:P:303:HEC:HAD1	1.67	0.75
1:M:102:CYS:CB	2:M:302:HEC:HAC	2.15	0.75
1:K:189:CYS:HG	2:K:301:HEC:CAC	1.93	0.75
1:F:48:CYS:CB	2:F:306:HEC:HAC	2.17	0.74
1:C:216:HIS:HE1	2:C:301:HEC:ND	1.82	0.74
1:M:48:CYS:CB	2:M:306:HEC:CAC	2.66	0.74
2:I:303:HEC:HBD1	2:I:303:HEC:HHA	1.68	0.74
2:P:307:HEC:C3C	1:Q:189:CYS:HB2	2.17	0.74
1:N:45:CYS:HB2	2:N:307:HEC:HHC	1.68	0.74
1:P:189:CYS:CB	2:P:302:HEC:HAC	2.18	0.74
2:E:301:HEC:HBD2	2:E:301:HEC:HHA	1.69	0.74
1:P:103:HIS:HA	1:P:129:LEU:HD21	1.70	0.73
1:K:45:CYS:HB3	2:K:306:HEC:HHC	1.69	0.73
1:K:189:CYS:CB	2:K:301:HEC:CAC	2.65	0.73
1:I:102:CYS:HG	2:I:303:HEC:HAC	1.48	0.73
1:E:102:CYS:CB	2:E:302:HEC:CAC	2.65	0.73
2:C:307:HEC:CAC	1:D:189:CYS:CB	2.56	0.73
2:P:307:HEC:HAC	1:Q:189:CYS:CB	2.18	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:48:CYS:CB	2:F:306:HEC:CAC	2.68	0.72
1:K:48:CYS:CB	2:K:306:HEC:HAC	2.20	0.72
2:E:305:HEC:C1D	1:F:216:HIS:HE1	2.03	0.71
2:M:305:HEC:ND	1:L:216:HIS:HE1	1.85	0.71
1:Q:45:CYS:CB	2:Q:305:HEC:HHC	2.20	0.71
1:T:102:CYS:CB	2:T:302:HEC:CAC	2.67	0.71
1:P:45:CYS:HA	2:P:308:HEC:HMC2	1.71	0.71
2:R:306:HEC:CAC	1:S:215:CYS:HG	1.82	0.71
1:N:49:HIS:HD2	2:N:307:HEC:C4B	2.03	0.71
1:C:49:HIS:HB3	2:C:306:HEC:HHC	1.73	0.71
1:K:45:CYS:CB	2:K:306:HEC:HHC	2.21	0.71
1:E:102:CYS:CB	2:E:302:HEC:HAC	2.21	0.71
1:R:41:THR:HG22	1:R:43:GLU:H	1.55	0.70
1:E:49:HIS:HD2	2:E:306:HEC:C4B	2.04	0.70
1:E:48:CYS:CB	2:E:306:HEC:CAC	2.65	0.70
1:F:45:CYS:CB	2:F:306:HEC:HHC	2.21	0.70
1:K:102:CYS:CB	2:K:302:HEC:CAC	2.69	0.70
1:K:48:CYS:HB2	2:K:306:HEC:C3C	2.22	0.70
1:E:107:ILE:HG23	1:E:129:LEU:HD11	1.73	0.70
1:K:102:CYS:CB	2:K:302:HEC:HAC	2.22	0.69
1:R:48:CYS:HB2	2:R:305:HEC:C3C	2.22	0.69
1:P:215:CYS:HG	2:P:301:HEC:CAC	2.06	0.69
1:R:102:CYS:CB	2:R:302:HEC:CAC	2.70	0.69
2:D:304:HEC:HBA1	2:D:304:HEC:HHA	1.75	0.69
1:R:48:CYS:CB	2:R:305:HEC:HAC	2.23	0.69
1:N:45:CYS:CB	2:N:307:HEC:HHC	2.22	0.69
1:C:106:SER:O	3:C:304:CA:CA	1.68	0.69
1:G:144:PRO:HB2	1:G:147:MET:HE1	1.74	0.69
1:K:48:CYS:CB	2:K:306:HEC:CAC	2.71	0.68
1:J:49:HIS:HE1	2:J:306:HEC:C1B	2.05	0.68
1:J:45:CYS:CB	2:J:306:HEC:HHC	2.24	0.68
1:J:45:CYS:HB3	2:J:306:HEC:HHC	1.75	0.68
1:R:190:HIS:HB3	2:R:302:HEC:HMB1	1.75	0.68
1:N:41:THR:HG22	1:N:43:GLU:H	1.59	0.68
1:R:48:CYS:CB	2:R:305:HEC:CAC	2.72	0.68
1:F:102:CYS:HB2	2:F:302:HEC:C3C	2.24	0.68
1:J:51:PRO:HG2	2:I:301:HEC:HMD2	1.74	0.67
2:S:305:HEC:CBC	1:T:189:CYS:SG	2.83	0.67
2:C:306:HEC:ND	1:D:216:HIS:HE1	1.93	0.67
2:F:301:HEC:HBA2	2:F:301:HEC:HHA	1.77	0.67
1:E:48:CYS:HB2	2:E:306:HEC:C3C	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:102:CYS:HB2	2:S:302:HEC:C3C	2.25	0.66
2:C:306:HEC:C1D	1:D:216:HIS:HE1	2.08	0.66
1:F:48:CYS:HB2	2:F:306:HEC:C3C	2.26	0.66
1:K:103:HIS:HA	1:K:129:LEU:HD21	1.75	0.66
2:Q:304:HEC:C3C	1:R:215:CYS:SG	2.84	0.66
2:F:305:HEC:C1D	1:G:216:HIS:HE1	2.08	0.66
1:J:103:HIS:HA	1:J:129:LEU:HD21	1.78	0.66
1:P:189:CYS:CB	2:P:302:HEC:CAC	2.73	0.66
1:P:215:CYS:HG	2:P:301:HEC:HAC	1.57	0.66
1:L:45:CYS:CB	2:L:306:HEC:HHC	2.23	0.66
2:N:306:HEC:HBA2	2:N:307:HEC:C2A	2.26	0.66
1:S:102:CYS:CB	2:S:302:HEC:C3C	2.74	0.66
2:Q:304:HEC:C1D	1:R:216:HIS:HE1	2.09	0.65
1:N:33:ASN:HD22	1:N:35:ASN:HB2	1.61	0.65
1:M:94:THR:HG1	1:M:185:TRP:CD1	2.14	0.65
1:N:215:CYS:SG	2:N:301:HEC:C3C	2.85	0.65
2:D:301:HEC:HBD1	2:D:301:HEC:HHA	1.76	0.65
1:L:200:THR:HG21	2:L:301:HEC:HAD2	1.78	0.65
1:S:48:CYS:CB	2:S:306:HEC:HAC	2.27	0.65
2:P:307:HEC:C3C	1:Q:189:CYS:CB	2.74	0.65
1:S:43:GLU:OE1	1:S:115:PRO:HB3	1.97	0.65
1:M:45:CYS:HB3	2:M:306:HEC:CHC	2.22	0.64
1:D:44:THR:HG22	1:E:209:SER:HB3	1.79	0.64
1:S:48:CYS:CB	2:S:306:HEC:CAC	2.75	0.64
1:F:45:CYS:HB3	2:F:306:HEC:HHC	1.79	0.64
1:I:102:CYS:SG	2:I:303:HEC:C3C	2.85	0.64
1:I:103:HIS:HA	1:I:129:LEU:HD11	1.79	0.64
2:S:307:HEC:C1D	1:T:216:HIS:HE1	2.10	0.64
2:S:305:HEC:CMA	1:T:133:ALA:HA	2.27	0.64
2:C:307:HEC:C3C	1:D:189:CYS:HB2	2.28	0.64
2:R:306:HEC:HHA	2:R:306:HEC:HBA1	1.79	0.63
1:K:144:PRO:HB2	1:K:147:MET:HE1	1.79	0.63
2:C:303:HEC:HBD1	2:C:303:HEC:HHA	1.81	0.63
1:T:60:ALA:HB1	1:T:63:TRP:HB2	1.81	0.63
1:C:189:CYS:CB	2:C:302:HEC:HAC	2.28	0.63
1:Q:174:LEU:HD12	1:Q:177:ALA:HB3	1.81	0.63
2:L:305:HEC:C1D	1:K:216:HIS:HE1	2.12	0.63
1:D:48:CYS:CB	2:D:305:HEC:HAC	2.28	0.63
1:I:189:CYS:SG	2:I:301:HEC:CBC	2.85	0.63
1:J:189:CYS:CB	2:J:301:HEC:HAC	2.28	0.62
1:N:22:ILE:HG21	1:M:218:LYS:HZ2	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:CYS:HB2	2:C:308:HEC:C3C	2.29	0.62
1:E:49:HIS:HD2	2:E:306:HEC:NB	1.95	0.62
1:R:102:CYS:CB	2:R:302:HEC:HAC	2.29	0.62
1:L:190:HIS:CE1	2:L:302:HEC:HMA1	2.35	0.62
1:I:191:ASP:O	1:I:201:PHE:HB3	2.00	0.62
2:K:305:HEC:CAC	1:J:215:CYS:HG	1.82	0.62
1:P:189:CYS:SG	2:P:302:HEC:CBC	2.85	0.62
1:Q:50:THR:HG22	1:Q:52:HIS:H	1.64	0.62
1:E:33:ASN:HB2	1:E:37:SER:HB2	1.81	0.62
1:E:173:THR:HA	1:E:179:ALA:HA	1.82	0.62
1:Q:49:HIS:HB3	2:Q:304:HEC:HHB	1.81	0.62
1:M:133:ALA:HA	2:M:301:HEC:HMA1	1.80	0.62
1:K:200:THR:HG23	1:K:202:LEU:HG	1.82	0.62
1:G:94:THR:HB	1:G:185:TRP:CD1	2.35	0.61
1:K:49:HIS:HD2	2:K:306:HEC:C1C	2.14	0.61
1:J:110:THR:O	1:J:111:LEU:HD12	2.00	0.61
1:C:48:CYS:CB	2:C:308:HEC:CAC	2.79	0.61
1:S:45:CYS:CB	2:S:306:HEC:HHC	2.24	0.61
1:F:200:THR:HG21	2:F:301:HEC:HAD2	1.81	0.61
1:S:109:ASN:HD21	1:S:125:VAL:HB	1.65	0.61
1:N:191:ASP:HB2	1:N:203:GLN:HE21	1.65	0.61
1:R:143:HIS:HB3	2:R:301:HEC:HMC2	1.83	0.61
1:C:206:ASN:OD1	1:C:211:LEU:HB3	2.01	0.61
1:P:43:GLU:HG2	1:P:46:VAL:HB	1.83	0.61
1:F:144:PRO:HB2	1:F:147:MET:HE1	1.83	0.60
1:S:103:HIS:ND1	2:S:301:HEC:HMA1	2.15	0.60
1:T:43:GLU:HG3	1:T:46:VAL:HB	1.83	0.60
1:K:169:LEU:HB3	1:K:182:ASP:HA	1.84	0.60
1:E:107:ILE:HD11	1:E:125:VAL:HG11	1.83	0.60
1:R:22:ILE:HG21	1:S:218:LYS:HZ2	1.66	0.60
1:R:135:LEU:HD11	2:R:301:HEC:CHB	2.31	0.60
1:G:41:THR:HG22	1:G:43:GLU:H	1.67	0.60
1:E:103:HIS:HE1	2:E:302:HEC:C1B	2.14	0.60
1:R:25:THR:HG23	1:R:27:HIS:H	1.65	0.60
2:N:306:HEC:HBA1	2:N:306:HEC:CHA	2.17	0.60
1:K:33:ASN:HB3	1:K:36:GLY:O	2.02	0.60
1:E:41:THR:HG22	1:E:43:GLU:H	1.66	0.59
1:Q:103:HIS:HA	1:Q:129:LEU:HD21	1.82	0.59
1:E:63:TRP:CD2	1:E:98:LEU:HD22	2.36	0.59
1:M:48:CYS:CB	2:M:306:HEC:C3C	2.80	0.59
1:Q:200:THR:HG22	1:Q:200:THR:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:195:LYS:HB2	1:N:198:VAL:HG22	1.85	0.59
1:D:22:ILE:HD11	1:D:193:HIS:ND1	2.16	0.59
1:T:45:CYS:HB2	2:T:301:HEC:CHC	2.29	0.59
1:K:28:ASP:OD1	1:K:28:ASP:O	2.20	0.59
2:R:306:HEC:C1D	1:S:216:HIS:HE1	2.16	0.59
1:J:49:HIS:CE1	2:J:306:HEC:C1B	2.79	0.59
1:P:173:THR:HA	1:P:179:ALA:HA	1.83	0.59
1:S:189:CYS:HG	2:S:301:HEC:HAC	1.67	0.59
1:M:195:LYS:HB2	1:M:198:VAL:HG22	1.85	0.59
1:L:95:ASP:OD2	1:L:186:CYS:HB3	2.03	0.59
1:K:71:PRO:HG3	1:K:100:LEU:HD12	1.85	0.59
1:J:189:CYS:CB	2:J:301:HEC:CAC	2.81	0.59
2:E:305:HEC:HBA2	2:E:306:HEC:C2A	2.33	0.59
1:D:48:CYS:CB	2:D:305:HEC:CAC	2.81	0.59
2:E:302:HEC:HBD1	2:E:302:HEC:HHA	1.85	0.59
1:G:100:LEU:HD21	1:G:135:LEU:HB2	1.83	0.59
1:N:49:HIS:CB	2:N:306:HEC:HHB	2.29	0.58
1:L:49:HIS:HB3	2:L:305:HEC:HHB	1.85	0.58
1:F:102:CYS:CB	2:F:302:HEC:C3C	2.81	0.58
1:I:41:THR:HG22	1:I:118:LEU:HD21	1.85	0.58
1:C:189:CYS:CB	2:C:302:HEC:CAC	2.81	0.58
1:E:49:HIS:CB	2:E:305:HEC:HHB	2.30	0.58
1:R:190:HIS:HE1	2:R:302:HEC:HMA2	1.68	0.58
1:C:45:CYS:HB3	2:C:308:HEC:CHC	2.30	0.58
1:S:71:PRO:HG3	1:S:100:LEU:HD12	1.85	0.58
1:E:103:HIS:HA	1:E:129:LEU:HD22	1.83	0.58
1:C:189:CYS:HG	2:C:302:HEC:HAC	1.65	0.58
1:K:189:CYS:HB2	2:K:301:HEC:C3C	2.33	0.58
2:K:302:HEC:HBD1	2:K:302:HEC:HHA	1.86	0.58
1:C:48:CYS:CB	2:C:308:HEC:HAC	2.27	0.58
1:I:189:CYS:SG	2:I:301:HEC:C3C	2.91	0.58
2:C:308:HEC:C2B	1:D:218:LYS:HG2	2.33	0.58
1:P:60:ALA:HB1	1:P:63:TRP:HB2	1.84	0.58
1:G:133:ALA:CA	2:G:302:HEC:HMA1	2.33	0.58
1:M:218:LYS:HD2	1:M:218:LYS:C	2.29	0.58
1:K:43:GLU:HG2	1:K:46:VAL:HB	1.85	0.58
1:C:43:GLU:HG2	1:C:46:VAL:HB	1.85	0.57
2:N:306:HEC:C1D	1:M:143:HIS:HE1	2.17	0.57
2:E:305:HEC:HBA1	2:E:305:HEC:CHA	2.32	0.57
1:F:133:ALA:HA	2:F:301:HEC:HMA2	1.86	0.57
1:S:60:ALA:HB1	1:S:63:TRP:HB2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:49:HIS:HE1	2:J:306:HEC:C4A	2.18	0.57
1:R:22:ILE:O	1:R:28:ASP:HB3	2.04	0.57
1:D:144:PRO:HB2	1:D:147:MET:CE	2.21	0.57
1:D:82:MET:HE1	1:D:144:PRO:HG3	1.87	0.57
2:D:304:HEC:ND	1:E:216:HIS:HE1	1.98	0.57
1:R:111:LEU:HD13	1:R:123:LEU:HD13	1.86	0.57
1:F:150:GLY:O	1:F:154:THR:HG23	2.05	0.57
1:I:190:HIS:HE1	2:I:303:HEC:HMA2	1.69	0.57
1:F:102:CYS:SG	2:F:302:HEC:CBC	2.92	0.57
1:L:174:LEU:HD12	1:L:177:ALA:HB3	1.87	0.57
1:J:48:CYS:HB2	2:J:306:HEC:C3C	2.35	0.57
1:Q:45:CYS:HB2	2:Q:305:HEC:CHC	2.32	0.57
1:L:164:ALA:HB1	1:L:167:LEU:HB2	1.86	0.56
1:E:102:CYS:SG	2:E:302:HEC:CBC	2.91	0.56
1:C:55:SER:HB3	1:C:112:THR:HG21	1.85	0.56
1:R:102:CYS:CB	2:R:302:HEC:C3C	2.83	0.56
1:D:48:CYS:HB2	2:D:305:HEC:C3C	2.36	0.56
1:R:139:MET:HE1	2:R:301:HEC:HBB2	1.87	0.56
2:R:306:HEC:CAC	1:S:215:CYS:CB	2.83	0.56
1:T:164:ALA:HB1	1:T:167:LEU:HD12	1.86	0.56
1:L:210:ALA:O	1:L:214:THR:HG23	2.05	0.56
2:K:305:HEC:HBA1	2:K:305:HEC:HHA	1.86	0.56
1:J:48:CYS:CB	2:J:306:HEC:CAC	2.84	0.56
1:M:103:HIS:CE1	2:M:302:HEC:C4B	2.89	0.56
1:R:22:ILE:CG2	1:S:218:LYS:HZ2	2.17	0.56
1:S:103:HIS:CE1	2:S:301:HEC:HMA1	2.41	0.56
2:S:301:HEC:HBA2	2:S:301:HEC:CHA	2.36	0.56
2:N:307:HEC:C2B	1:M:218:LYS:HG2	2.36	0.56
1:M:102:CYS:CB	2:M:302:HEC:C3C	2.84	0.56
1:Q:47:PHE:HZ	1:Q:123:LEU:HD21	1.70	0.56
1:T:191:ASP:O	1:T:201:PHE:HB3	2.05	0.56
1:M:102:CYS:HB3	2:M:302:HEC:HAC	1.87	0.56
1:P:49:HIS:HD2	2:P:308:HEC:C4B	2.19	0.56
2:L:305:HEC:HHA	2:L:305:HEC:HBA1	1.86	0.56
1:C:215:CYS:CB	2:C:301:HEC:CAC	2.83	0.56
1:D:39:SER:HA	1:D:124:ALA:O	2.06	0.56
1:P:45:CYS:HB3	2:P:308:HEC:CHC	2.28	0.56
1:L:102:CYS:SG	2:L:302:HEC:CBC	2.94	0.55
1:C:216:HIS:HE1	2:C:301:HEC:C1D	2.19	0.55
2:G:302:HEC:HHA	2:G:302:HEC:HBA2	1.87	0.55
1:R:97:VAL:HG13	1:R:98:LEU:HD23	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:102:CYS:SG	2:P:303:HEC:C3C	2.91	0.55
1:S:102:CYS:HB3	2:S:302:HEC:HAC	1.86	0.55
1:C:169:LEU:HB3	1:C:182:ASP:HA	1.87	0.55
1:T:128:THR:HG22	1:T:129:LEU:H	1.72	0.55
1:F:45:CYS:HB2	2:F:306:HEC:HHC	1.88	0.55
1:J:48:CYS:CB	2:J:306:HEC:C3C	2.84	0.55
1:P:215:CYS:SG	2:P:301:HEC:C3C	2.93	0.55
1:I:26:LYS:HB2	2:I:303:HEC:HAD1	1.89	0.55
1:F:49:HIS:HD2	2:F:306:HEC:C1C	2.19	0.55
1:T:30:SER:HB2	1:T:41:THR:O	2.07	0.55
1:T:48:CYS:SG	2:T:301:HEC:C3C	2.94	0.55
2:N:306:HEC:CBC	1:M:215:CYS:SG	2.93	0.54
1:R:195:LYS:HB2	1:R:198:VAL:HG22	1.89	0.54
1:J:49:HIS:HE1	2:J:306:HEC:CHB	2.19	0.54
1:P:102:CYS:CB	2:P:303:HEC:CAC	2.85	0.54
2:P:307:HEC:C2C	1:Q:189:CYS:HB2	2.36	0.54
1:R:190:HIS:HB3	2:R:302:HEC:CMB	2.37	0.54
2:N:302:HEC:HBD2	2:N:302:HEC:HHA	1.90	0.54
1:E:43:GLU:HG3	1:E:46:VAL:H	1.72	0.54
1:F:22:ILE:HG21	1:G:218:LYS:HZ2	1.73	0.54
2:R:306:HEC:CBC	1:S:215:CYS:SG	2.91	0.54
1:D:26:LYS:HB3	2:D:301:HEC:HAD1	1.90	0.54
1:E:45:CYS:SG	2:E:306:HEC:HHC	2.48	0.54
2:E:306:HEC:C2B	1:F:218:LYS:HG2	2.38	0.54
1:G:189:CYS:HG	2:G:302:HEC:HAC	1.71	0.54
1:S:102:CYS:HB2	2:S:302:HEC:C2C	2.38	0.54
1:M:99:CYS:SG	2:M:301:HEC:HMB1	2.48	0.53
1:J:102:CYS:CB	2:J:302:HEC:CAC	2.86	0.53
1:F:49:HIS:HD2	2:F:306:HEC:NC	2.04	0.53
1:M:102:CYS:HB2	2:M:302:HEC:C3C	2.38	0.53
1:L:173:THR:HA	1:L:179:ALA:HA	1.89	0.53
1:K:150:GLY:HA2	1:K:153:ILE:HG22	1.90	0.53
1:I:169:LEU:HD23	1:I:182:ASP:HB2	1.90	0.53
1:R:21:VAL:HG22	1:R:23:LYS:H	1.73	0.53
1:T:144:PRO:HB2	1:T:147:MET:HE1	1.90	0.53
1:K:48:CYS:CB	2:K:306:HEC:C3C	2.86	0.53
1:E:48:CYS:HB2	2:E:306:HEC:CAC	2.38	0.53
1:F:129:LEU:HA	2:F:302:HEC:O2D	2.09	0.53
1:L:71:PRO:HG3	1:L:100:LEU:HD12	1.90	0.53
1:K:189:CYS:SG	2:K:301:HEC:CBC	2.93	0.53
1:C:211:LEU:O	2:C:301:HEC:HMC3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:22:ILE:HG21	1:Q:218:LYS:NZ	2.23	0.53
1:T:46:VAL:HG11	1:T:115:PRO:HG3	1.91	0.53
1:E:60:ALA:HB2	1:E:98:LEU:HD21	1.90	0.53
2:E:305:HEC:C3C	1:F:215:CYS:SG	2.94	0.53
2:N:306:HEC:C1D	1:M:216:HIS:HE1	2.21	0.53
1:C:215:CYS:HG	2:C:301:HEC:CAC	1.97	0.53
1:D:60:ALA:HB1	1:D:63:TRP:HB2	1.91	0.53
1:F:60:ALA:HB1	1:F:63:TRP:HB2	1.90	0.53
1:Q:109:ASN:ND2	1:Q:125:VAL:HG23	2.24	0.53
1:S:26:LYS:HB3	2:S:302:HEC:HAD1	1.89	0.53
1:N:51:PRO:HG2	1:N:52:HIS:HB2	1.90	0.53
1:M:26:LYS:HB3	2:M:302:HEC:HAD1	1.91	0.53
1:J:195:LYS:HB2	1:J:198:VAL:HG22	1.90	0.53
1:P:200:THR:HG23	1:P:202:LEU:HG	1.89	0.53
2:R:306:HEC:C1D	1:S:216:HIS:CE1	2.92	0.53
1:M:45:CYS:HA	2:M:306:HEC:HMC2	1.91	0.53
1:C:49:HIS:HD2	2:C:308:HEC:C4B	2.22	0.53
1:L:49:HIS:HD2	2:L:306:HEC:C1C	2.22	0.53
2:J:302:HEC:HBD1	2:J:302:HEC:HHA	1.89	0.53
1:D:200:THR:HG23	1:D:202:LEU:HG	1.90	0.53
2:E:301:HEC:HBD2	2:E:301:HEC:CHA	2.38	0.53
1:I:45:CYS:HB3	2:I:302:HEC:HHC	1.90	0.52
1:C:189:CYS:SG	2:C:302:HEC:CBC	2.94	0.52
1:D:164:ALA:HB1	1:D:167:LEU:HB2	1.90	0.52
1:T:195:LYS:HB2	1:T:198:VAL:HG22	1.91	0.52
1:J:102:CYS:SG	2:J:302:HEC:CBC	2.95	0.52
1:E:111:LEU:HD11	1:E:123:LEU:HD22	1.90	0.52
1:C:45:CYS:HA	2:C:308:HEC:HMC2	1.91	0.52
1:Q:103:HIS:HE1	2:Q:301:HEC:C1B	2.22	0.52
1:R:48:CYS:CB	2:R:305:HEC:C3C	2.87	0.52
1:S:151:ASP:HA	1:S:154:THR:HG22	1.91	0.52
1:G:130:SER:HB3	2:G:303:HEC:O1D	2.10	0.52
1:M:200:THR:HA	2:M:302:HEC:HBA1	1.91	0.52
2:K:305:HEC:C1D	1:J:216:HIS:HE1	2.22	0.52
1:D:27:HIS:CE1	1:D:192:VAL:HG13	2.45	0.52
1:L:45:CYS:HA	2:L:306:HEC:HMC2	1.92	0.52
1:Q:118:LEU:HD21	1:Q:123:LEU:HB2	1.90	0.52
2:Q:304:HEC:ND	1:R:143:HIS:HE1	2.08	0.52
1:M:77:ASN:OD1	1:M:82:MET:HB2	2.10	0.52
1:P:25:THR:HB	1:P:201:PHE:HZ	1.74	0.52
1:J:71:PRO:HG3	1:J:100:LEU:HD12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:38:GLY:HA2	1:G:126:THR:HB	1.92	0.52
1:Q:102:CYS:SG	2:Q:301:HEC:CBC	2.97	0.52
1:E:30:SER:OG	1:E:44:THR:HG22	2.10	0.52
1:N:45:CYS:HB2	2:N:307:HEC:CHC	2.39	0.51
1:E:102:CYS:CB	2:E:302:HEC:C3C	2.89	0.51
1:J:51:PRO:HG2	2:I:301:HEC:CMD	2.38	0.51
1:C:49:HIS:HD2	2:C:308:HEC:CHC	2.23	0.51
1:C:102:CYS:SG	2:C:303:HEC:C3C	2.96	0.51
1:N:75:TYR:HB3	1:N:144:PRO:HB3	1.91	0.51
1:L:103:HIS:HE1	2:L:302:HEC:C1B	2.23	0.51
1:R:79:THR:HG22	1:R:80:GLY:H	1.75	0.51
1:F:43:GLU:OE1	1:F:115:PRO:HB3	2.10	0.51
1:S:195:LYS:HB2	1:S:198:VAL:HG22	1.92	0.51
1:N:102:CYS:CB	2:N:303:HEC:CAC	2.88	0.51
2:J:305:HEC:C1D	1:I:143:HIS:HE1	2.23	0.51
1:N:22:ILE:HG21	1:M:218:LYS:NZ	2.25	0.51
1:J:49:HIS:HE1	2:J:306:HEC:NB	1.87	0.51
1:E:49:HIS:CD2	2:E:306:HEC:C4B	2.88	0.51
1:S:54:ALA:HA	1:T:141:ASN:HB2	1.92	0.51
1:N:49:HIS:HD2	2:N:307:HEC:NB	2.04	0.51
1:L:133:ALA:HA	2:L:301:HEC:HMA1	1.93	0.51
2:P:306:HEC:C4C	1:Q:143:HIS:HE1	2.24	0.51
1:R:133:ALA:HA	2:R:301:HEC:HMA2	1.93	0.51
1:C:123:LEU:HD11	1:C:125:VAL:CG1	2.41	0.51
1:R:65:ARG:HH21	2:R:302:HEC:HBC1	1.75	0.51
1:K:29:LEU:O	1:K:47:PHE:HE2	1.93	0.50
1:Q:192:VAL:HG11	2:Q:305:HEC:C2D	2.40	0.50
1:I:195:LYS:HB2	1:I:198:VAL:HG22	1.94	0.50
1:R:65:ARG:NH2	2:R:302:HEC:HBC1	2.25	0.50
1:R:218:LYS:HD2	1:R:218:LYS:C	2.36	0.50
2:C:306:HEC:C1D	1:D:143:HIS:HE1	2.24	0.50
1:D:102:CYS:CB	2:D:301:HEC:CAC	2.88	0.50
1:L:95:ASP:OD2	1:L:95:ASP:C	2.54	0.50
1:K:150:GLY:O	1:K:154:THR:HG23	2.11	0.50
1:C:200:THR:HG23	1:C:202:LEU:HG	1.93	0.50
1:D:102:CYS:SG	2:D:301:HEC:CBC	2.97	0.50
2:P:308:HEC:C2B	1:Q:218:LYS:HG2	2.41	0.50
1:Q:51:PRO:CB	2:R:301:HEC:HBC2	2.41	0.50
1:L:22:ILE:HD12	1:K:218:LYS:NZ	2.27	0.50
1:K:102:CYS:SG	2:K:302:HEC:CBC	2.96	0.50
1:E:60:ALA:HB1	1:E:63:TRP:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:51:PRO:HB3	2:R:301:HEC:HBC2	1.94	0.50
2:D:304:HEC:CAC	1:E:215:CYS:CB	2.89	0.50
1:R:193:HIS:CD2	1:S:218:LYS:HD3	2.47	0.50
2:S:307:HEC:HAD1	1:T:82:MET:HE3	1.93	0.50
1:J:200:THR:HG23	1:J:202:LEU:HG	1.93	0.50
1:E:107:ILE:CG2	1:E:129:LEU:HD11	2.41	0.50
1:G:96:ALA:O	1:G:100:LEU:HB2	2.12	0.50
1:P:164:ALA:HB1	1:P:167:LEU:HB2	1.92	0.50
2:N:306:HEC:CAC	1:M:215:CYS:HG	1.81	0.50
2:C:307:HEC:HAC	1:D:189:CYS:HB3	1.87	0.50
2:P:306:HEC:CGA	2:P:306:HEC:HHA	2.42	0.50
1:N:33:ASN:C	1:N:35:ASN:H	2.19	0.49
1:S:49:HIS:HD2	2:S:306:HEC:C1C	2.24	0.49
1:N:51:PRO:CG	1:N:52:HIS:HB2	2.42	0.49
1:J:189:CYS:SG	2:J:301:HEC:CBC	2.95	0.49
2:C:306:HEC:ND	1:D:143:HIS:HE1	2.08	0.49
1:F:48:CYS:CB	2:F:306:HEC:C3C	2.89	0.49
1:S:109:ASN:ND2	1:S:125:VAL:HB	2.26	0.49
2:S:301:HEC:HBA2	2:S:301:HEC:HHA	1.95	0.49
1:F:49:HIS:CD2	2:F:306:HEC:C1C	2.96	0.49
2:D:304:HEC:HBA1	2:D:304:HEC:CHA	2.42	0.49
1:N:173:THR:HA	1:N:179:ALA:HA	1.94	0.49
1:M:189:CYS:SG	2:M:301:HEC:CBC	2.97	0.49
1:F:71:PRO:HB3	1:F:139:MET:HG2	1.95	0.49
1:I:190:HIS:CE1	2:I:303:HEC:HMA2	2.48	0.49
2:G:301:HEC:HBA1	2:G:301:HEC:HHA	1.95	0.49
1:P:169:LEU:HB3	1:P:182:ASP:HA	1.95	0.49
1:K:91:VAL:HG11	1:K:139:MET:HG3	1.94	0.49
1:J:104:ASP:CG	1:J:105:GLY:H	2.20	0.49
1:R:191:ASP:HB2	1:R:203:GLN:HG2	1.95	0.49
1:R:100:LEU:HD22	1:R:104:ASP:HB3	1.94	0.49
1:S:48:CYS:CB	2:S:306:HEC:C3C	2.90	0.49
1:T:190:HIS:HB3	2:T:302:HEC:HMB2	1.95	0.49
2:N:306:HEC:HBA2	2:N:307:HEC:C3A	2.43	0.48
2:L:302:HEC:HBD1	2:L:302:HEC:HHA	1.95	0.48
1:I:186:CYS:O	1:I:190:HIS:HB2	2.13	0.48
1:Q:49:HIS:HD2	2:Q:305:HEC:C4B	2.26	0.48
1:Q:79:THR:HG22	1:Q:80:GLY:H	1.77	0.48
1:C:62:LEU:HB2	2:C:306:HEC:CMA	2.43	0.48
2:C:306:HEC:HHA	2:C:306:HEC:HBA1	1.93	0.48
1:R:102:CYS:SG	2:R:302:HEC:C3C	2.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:211:LEU:O	1:M:214:THR:HG22	2.14	0.48
1:K:31:SER:HA	1:K:37:SER:HB2	1.95	0.48
2:C:306:HEC:HBA2	2:C:308:HEC:C2A	2.43	0.48
1:G:77:ASN:OD1	1:G:82:MET:HB2	2.14	0.48
1:P:22:ILE:HG21	1:Q:218:LYS:HZ1	1.79	0.48
1:P:111:LEU:HD11	1:P:123:LEU:HD22	1.95	0.48
1:R:107:ILE:HD11	1:R:127:ALA:O	2.13	0.48
1:E:118:LEU:HD21	1:E:123:LEU:HD12	1.95	0.48
1:P:41:THR:HG22	1:P:118:LEU:HD21	1.95	0.48
1:P:49:HIS:CB	2:P:306:HEC:HHB	2.34	0.48
1:R:190:HIS:CE1	2:R:302:HEC:HMA2	2.48	0.48
1:S:102:CYS:HB3	2:S:302:HEC:CAC	2.40	0.48
1:M:115:PRO:HG2	1:M:118:LEU:HD13	1.96	0.48
1:F:129:LEU:HD23	2:F:302:HEC:O2D	2.14	0.48
1:S:48:CYS:HB2	2:S:306:HEC:C3C	2.43	0.48
2:F:301:HEC:HBA2	2:F:301:HEC:CHA	2.43	0.48
1:I:129:LEU:HD23	2:I:303:HEC:O2D	2.13	0.48
1:Q:195:LYS:HB2	1:Q:198:VAL:HG22	1.95	0.48
1:R:60:ALA:HB1	1:R:63:TRP:HB2	1.95	0.48
1:M:189:CYS:CB	2:M:301:HEC:HAC	2.44	0.48
1:D:49:HIS:HD2	2:D:305:HEC:C1C	2.26	0.48
1:Q:77:ASN:OD1	1:Q:82:MET:HB2	2.13	0.48
1:R:52:HIS:CD2	2:S:301:HEC:ND	2.82	0.48
1:R:62:LEU:HD12	2:R:306:HEC:C3A	2.44	0.48
1:K:28:ASP:O	1:K:30:SER:N	2.47	0.48
1:I:26:LYS:HD2	2:I:303:HEC:HBA2	1.96	0.48
1:C:48:CYS:CB	2:C:308:HEC:C3C	2.92	0.48
1:P:96:ALA:O	1:P:100:LEU:HB2	2.13	0.48
1:S:102:CYS:SG	2:S:302:HEC:CBC	2.99	0.48
1:M:102:CYS:SG	2:M:302:HEC:CBC	2.96	0.47
1:T:102:CYS:HB3	2:T:302:HEC:HAC	1.92	0.47
1:T:173:THR:HA	1:T:179:ALA:HA	1.96	0.47
1:L:22:ILE:HD12	1:K:218:LYS:HZ3	1.79	0.47
2:L:305:HEC:C1D	1:K:216:HIS:CE1	2.94	0.47
1:C:123:LEU:HD11	1:C:125:VAL:HG12	1.95	0.47
2:P:306:HEC:CAC	1:Q:215:CYS:HG	2.20	0.47
1:T:45:CYS:HA	2:T:301:HEC:HMC3	1.95	0.47
1:N:52:HIS:CD2	2:M:301:HEC:C1D	2.98	0.47
1:M:48:CYS:HG	2:M:306:HEC:CAC	1.97	0.47
1:K:170:PHE:CE2	1:K:187:SER:HB2	2.49	0.47
1:D:50:THR:HG22	1:D:52:HIS:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:41:THR:HA	1:F:118:LEU:HD11	1.95	0.47
2:M:305:HEC:HBA2	2:M:305:HEC:HHA	1.96	0.47
1:G:202:LEU:HD22	1:G:211:LEU:HD22	1.97	0.47
1:T:211:LEU:O	1:T:214:THR:HG22	2.14	0.47
1:F:31:SER:HA	1:F:37:SER:O	2.14	0.47
1:G:105:GLY:O	1:G:129:LEU:HD12	2.14	0.47
1:T:83:ASN:HB3	1:T:156:GLY:HA3	1.96	0.47
1:L:49:HIS:HD2	2:L:306:HEC:CHC	2.27	0.47
1:I:143:HIS:HB3	2:I:301:HEC:HMC2	1.97	0.47
1:P:174:LEU:HD12	1:P:177:ALA:HB3	1.97	0.47
1:R:148:SER:HB2	1:R:180:LYS:HD3	1.97	0.47
2:M:305:HEC:CAC	1:L:215:CYS:CB	2.92	0.47
2:P:306:HEC:HMC3	2:P:306:HEC:HBC3	1.97	0.47
1:R:56:ALA:HB3	1:R:60:ALA:HB3	1.97	0.47
1:S:211:LEU:O	1:S:214:THR:HG22	2.15	0.47
1:K:26:LYS:HB2	1:K:26:LYS:HE3	1.76	0.47
2:K:305:HEC:HBA2	2:K:306:HEC:C2A	2.45	0.47
1:I:104:ASP:C	1:I:104:ASP:OD1	2.57	0.47
2:E:305:HEC:HHA	2:E:305:HEC:CBA	2.40	0.47
1:F:60:ALA:HB2	1:F:98:LEU:HD11	1.97	0.47
1:F:173:THR:HA	1:F:179:ALA:HA	1.97	0.47
1:R:187:SER:HA	1:R:190:HIS:O	2.14	0.47
1:J:51:PRO:HB2	2:I:301:HEC:CHD	2.45	0.46
2:J:305:HEC:ND	1:I:216:HIS:HE1	2.10	0.46
1:T:33:ASN:HB3	1:T:36:GLY:O	2.15	0.46
1:D:195:LYS:HB2	1:D:198:VAL:HG22	1.97	0.46
1:E:75:TYR:HB3	1:E:144:PRO:HB3	1.98	0.46
1:R:143:HIS:CD2	2:R:301:HEC:HBC3	2.49	0.46
1:R:143:HIS:ND1	1:R:144:PRO:HD2	2.30	0.46
1:I:77:ASN:OD1	1:I:82:MET:HB2	2.15	0.46
1:R:135:LEU:HD12	2:R:301:HEC:HMB2	1.97	0.46
1:N:164:ALA:HB1	1:N:167:LEU:HB2	1.97	0.46
1:C:67:ASN:HD22	1:C:97:VAL:HG22	1.80	0.46
1:F:99:CYS:HA	2:F:302:HEC:HAB	1.82	0.46
2:R:306:HEC:HAC	1:S:215:CYS:CB	2.43	0.46
2:N:306:HEC:ND	1:M:143:HIS:HE1	2.07	0.46
2:J:305:HEC:HBA2	2:J:306:HEC:HMA2	1.96	0.46
1:D:144:PRO:CB	1:D:147:MET:HE1	2.24	0.46
2:P:308:HEC:CHC	1:Q:218:LYS:NZ	2.74	0.46
1:N:45:CYS:HA	2:N:307:HEC:HMC2	1.97	0.46
1:I:28:ASP:HB3	1:I:33:ASN:HD21	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:187:SER:HA	1:I:190:HIS:O	2.14	0.46
1:T:75:TYR:HD2	1:T:144:PRO:HB3	1.80	0.46
1:M:103:HIS:CE1	2:M:302:HEC:CHC	2.95	0.46
2:L:305:HEC:HBA2	2:L:306:HEC:C2A	2.45	0.46
1:J:50:THR:HB	1:J:64:ASN:CG	2.41	0.46
1:J:75:TYR:HB3	1:J:144:PRO:HB3	1.97	0.46
1:D:168:PRO:HD2	1:D:203:GLN:HE22	1.80	0.46
1:Q:62:LEU:HD22	2:Q:304:HEC:C3A	2.46	0.46
1:R:49:HIS:HD2	2:R:305:HEC:CHC	2.28	0.46
2:M:305:HEC:C1D	1:L:216:HIS:HE1	2.27	0.46
1:L:103:HIS:CE1	2:L:302:HEC:C1B	2.98	0.46
1:L:195:LYS:HB2	1:L:198:VAL:HG22	1.97	0.46
2:K:305:HEC:C1D	1:J:216:HIS:CE1	2.98	0.46
1:C:64:ASN:HD21	1:C:113:ASN:HB3	1.80	0.46
1:Q:71:PRO:HG3	1:Q:100:LEU:HD12	1.98	0.46
1:Q:170:PHE:CD2	1:Q:185:TRP:HB2	2.51	0.46
1:C:77:ASN:OD1	1:C:82:MET:HB2	2.16	0.46
1:R:109:ASN:HB3	1:R:123:LEU:O	2.16	0.46
1:T:123:LEU:HD11	1:T:125:VAL:HG23	1.98	0.46
2:N:307:HEC:HMC3	2:N:307:HEC:HBC3	1.98	0.46
1:F:26:LYS:NZ	2:F:302:HEC:HBD2	2.31	0.46
1:F:71:PRO:HG3	1:F:100:LEU:HD22	1.98	0.46
2:F:305:HEC:HBA1	2:F:305:HEC:CHA	2.40	0.46
1:M:46:VAL:HG21	1:M:115:PRO:HD3	1.98	0.45
1:P:49:HIS:CD2	2:P:308:HEC:C4B	2.99	0.45
1:R:52:HIS:HD1	1:R:53:GLY:H	1.63	0.45
1:R:103:HIS:O	1:R:134:ASN:HA	2.17	0.45
1:C:71:PRO:HG3	1:C:100:LEU:HD12	1.99	0.45
1:C:216:HIS:CE1	2:C:301:HEC:C1D	2.97	0.45
1:D:52:HIS:HD2	2:E:301:HEC:C1D	2.29	0.45
1:G:102:CYS:SG	2:G:303:HEC:C3C	2.99	0.45
2:T:302:HEC:HMD1	2:T:302:HEC:HBD1	1.96	0.45
1:L:48:CYS:HB2	2:L:306:HEC:C3C	2.47	0.45
2:G:302:HEC:HBA2	2:G:302:HEC:CHA	2.46	0.45
1:M:48:CYS:HB2	2:M:306:HEC:C2C	2.47	0.45
2:K:305:HEC:CBC	1:J:215:CYS:SG	3.00	0.45
1:P:151:ASP:HA	1:P:154:THR:HG22	1.99	0.45
2:P:306:HEC:C3C	1:Q:215:CYS:SG	2.99	0.45
1:T:50:THR:OG1	1:T:64:ASN:ND2	2.46	0.45
1:T:102:CYS:SG	2:T:302:HEC:CBC	2.98	0.45
1:K:47:PHE:HD1	1:K:111:LEU:HD21	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:45:CYS:HB2	1:F:209:SER:OG	2.17	0.45
1:S:47:PHE:CD1	1:S:111:LEU:HD11	2.52	0.45
1:S:135:LEU:HD11	2:S:301:HEC:CHB	2.46	0.45
1:C:215:CYS:CB	2:C:301:HEC:C3C	2.95	0.45
1:N:100:LEU:HD21	1:N:135:LEU:HB2	1.98	0.45
1:K:170:PHE:HE2	1:K:187:SER:HB2	1.82	0.45
1:I:164:ALA:HB1	1:I:167:LEU:HB2	1.98	0.45
1:C:49:HIS:CD2	2:C:308:HEC:C4B	2.99	0.45
1:D:193:HIS:HE1	2:D:305:HEC:CHC	2.29	0.45
1:G:60:ALA:HB1	1:G:63:TRP:HB2	1.98	0.45
2:K:305:HEC:HBA1	2:K:305:HEC:CHA	2.46	0.45
2:C:306:HEC:C3C	1:D:215:CYS:SG	2.98	0.45
2:Q:304:HEC:C1D	1:R:216:HIS:CE1	2.94	0.45
1:R:133:ALA:HA	2:R:301:HEC:CMA	2.47	0.45
1:R:186:CYS:O	1:R:190:HIS:HB2	2.17	0.45
1:T:64:ASN:HB3	1:T:111:LEU:HD13	1.99	0.45
1:K:102:CYS:CB	2:K:302:HEC:C3C	2.95	0.45
1:K:210:ALA:O	1:K:214:THR:HG23	2.17	0.45
1:C:161:VAL:HG23	1:C:161:VAL:O	2.16	0.45
2:Q:301:HEC:HBD1	2:Q:301:HEC:HHA	1.98	0.45
1:R:191:ASP:O	1:R:201:PHE:HB3	2.17	0.45
1:T:174:LEU:HD12	1:T:177:ALA:HB3	1.99	0.45
1:N:46:VAL:HG21	1:N:115:PRO:HB3	1.98	0.45
1:N:49:HIS:CD2	2:N:307:HEC:C4B	2.90	0.45
1:I:193:HIS:HE1	2:I:302:HEC:C1A	2.30	0.45
1:P:102:CYS:O	1:P:107:ILE:HG22	2.17	0.45
1:L:198:VAL:HG21	1:L:202:LEU:O	2.17	0.44
1:K:107:ILE:HD11	1:K:125:VAL:HG11	1.99	0.44
1:E:52:HIS:CE1	2:F:301:HEC:C4A	2.98	0.44
2:G:302:HEC:HBD1	2:G:302:HEC:HMD3	1.98	0.44
1:Q:102:CYS:CB	2:Q:301:HEC:CAC	2.94	0.44
1:R:43:GLU:CG	1:R:46:VAL:HB	2.47	0.44
1:T:144:PRO:HB2	1:T:147:MET:CE	2.47	0.44
1:K:192:VAL:HG11	2:K:306:HEC:C2D	2.48	0.44
2:J:305:HEC:HBA2	2:J:306:HEC:CMA	2.48	0.44
2:C:306:HEC:CBC	1:D:215:CYS:SG	3.01	0.44
1:N:33:ASN:C	1:N:35:ASN:N	2.76	0.44
1:J:48:CYS:HB2	2:J:306:HEC:C2C	2.48	0.44
1:E:211:LEU:O	1:E:214:THR:HG22	2.16	0.44
1:G:39:SER:HA	1:G:124:ALA:O	2.18	0.44
2:P:306:HEC:HHA	2:P:306:HEC:CBA	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:29:LEU:HD21	2:R:302:HEC:HMD2	1.99	0.44
2:S:305:HEC:HBA1	1:T:132:GLY:O	2.17	0.44
1:K:45:CYS:HB2	2:K:306:HEC:HHC	1.97	0.44
1:K:72:THR:HG22	1:K:137:ALA:HB1	1.98	0.44
1:G:190:HIS:HE1	2:G:302:HEC:ND	2.13	0.44
1:Q:103:HIS:CE1	2:Q:301:HEC:C1B	2.98	0.44
1:I:129:LEU:HA	2:I:303:HEC:O2D	2.17	0.44
1:M:189:CYS:CB	2:M:301:HEC:CAC	2.93	0.44
2:L:305:HEC:HBA1	2:L:305:HEC:CHA	2.47	0.44
1:K:170:PHE:HD2	1:K:185:TRP:HB2	1.83	0.44
1:G:63:TRP:CE2	1:G:98:LEU:HB3	2.53	0.44
1:L:170:PHE:HD2	1:K:79:THR:HG21	1.82	0.44
1:K:49:HIS:CD2	2:K:306:HEC:C1C	3.00	0.44
1:K:168:PRO:HD2	1:K:203:GLN:HE22	1.83	0.44
1:I:102:CYS:CB	2:I:303:HEC:CAC	2.92	0.44
1:C:189:CYS:SG	2:C:302:HEC:C3C	3.02	0.44
1:Q:200:THR:HA	2:Q:301:HEC:HBA1	2.00	0.44
1:C:49:HIS:HD2	2:C:308:HEC:C1C	2.31	0.44
1:K:26:LYS:CG	2:K:302:HEC:HAD1	2.47	0.44
1:G:102:CYS:SG	2:G:303:HEC:CBC	3.02	0.44
1:Q:49:HIS:HD2	2:Q:305:HEC:CHC	2.31	0.44
1:S:192:VAL:HG21	2:S:306:HEC:CMD	2.48	0.44
1:N:34:VAL:O	1:N:34:VAL:HG22	2.18	0.43
1:J:192:VAL:HG11	2:J:306:HEC:C2D	2.48	0.43
2:I:301:HEC:HBD1	2:I:301:HEC:HMD1	2.00	0.43
1:G:91:VAL:HG12	1:G:92:ALA:H	1.83	0.43
1:R:49:HIS:HD2	2:R:305:HEC:C1C	2.31	0.43
1:J:116:ASN:HB2	2:I:301:HEC:HBD2	2.00	0.43
1:G:170:PHE:CD1	1:G:185:TRP:HB2	2.53	0.43
1:P:189:CYS:HB2	2:P:302:HEC:C3C	2.48	0.43
1:S:49:HIS:HD2	2:S:306:HEC:NC	2.12	0.43
2:S:307:HEC:C1D	1:T:216:HIS:CE1	2.93	0.43
1:J:147:MET:HE3	1:J:147:MET:HB3	1.88	0.43
1:F:164:ALA:HB1	1:F:167:LEU:HB2	1.99	0.43
1:P:102:CYS:CB	2:P:303:HEC:C3C	2.96	0.43
1:S:86:PRO:HG3	1:S:144:PRO:HB3	1.99	0.43
1:N:151:ASP:HA	1:N:154:THR:HG22	1.99	0.43
1:D:102:CYS:HB2	2:D:301:HEC:HMC2	2.00	0.43
1:E:63:TRP:CE2	1:E:98:LEU:HD22	2.52	0.43
1:T:190:HIS:HB3	2:T:302:HEC:CMB	2.49	0.43
1:T:190:HIS:CG	2:T:302:HEC:HMB3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:123:LEU:HD12	1:J:123:LEU:HA	1.72	0.43
1:G:190:HIS:CD2	2:G:303:HEC:HMB3	2.54	0.43
1:S:75:TYR:CD1	1:S:144:PRO:HG3	2.54	0.43
1:T:143:HIS:CG	1:T:144:PRO:HD2	2.54	0.43
1:M:50:THR:HG21	1:M:54:ALA:O	2.17	0.43
1:L:82:MET:C	1:L:84:ALA:H	2.26	0.43
1:K:164:ALA:HB1	1:K:167:LEU:HB2	2.01	0.43
1:I:170:PHE:CE2	1:I:187:SER:HB2	2.53	0.43
1:Q:108:GLY:C	1:Q:109:ASN:HD22	2.27	0.43
1:Q:118:LEU:HD12	1:Q:118:LEU:HA	1.81	0.43
2:Q:304:HEC:C1D	1:R:143:HIS:HE1	2.32	0.43
1:K:157:ASP:OD1	1:K:160:LEU:HG	2.18	0.43
1:S:21:VAL:HG22	1:S:23:LYS:H	1.83	0.43
1:T:93:LEU:HD23	1:T:93:LEU:HA	1.85	0.43
1:D:52:HIS:CD2	2:E:301:HEC:C1D	3.01	0.43
1:P:103:HIS:HE1	2:P:303:HEC:C4A	2.31	0.43
1:P:148:SER:OG	1:P:151:ASP:OD2	2.32	0.43
1:R:49:HIS:HB3	2:R:306:HEC:HBB	2.01	0.43
1:N:63:TRP:CE2	1:N:98:LEU:HG	2.53	0.43
2:D:305:HEC:HMC3	2:D:305:HEC:HBC3	2.00	0.43
2:F:305:HEC:C1D	1:G:216:HIS:CE1	2.93	0.43
1:P:44:THR:HG22	1:Q:209:SER:OG	2.19	0.43
1:Q:33:ASN:O	1:Q:34:VAL:HG22	2.19	0.43
1:Q:48:CYS:HB2	2:Q:305:HEC:C3C	2.48	0.43
1:C:150:GLY:O	1:C:154:THR:HG23	2.19	0.43
1:G:170:PHE:CZ	1:G:187:SER:HB2	2.54	0.43
1:S:43:GLU:CD	1:S:115:PRO:HB3	2.43	0.43
1:S:49:HIS:CD2	2:S:306:HEC:C1C	3.02	0.43
1:J:52:HIS:ND1	1:I:142:ASP:OD1	2.46	0.42
1:I:174:LEU:HD12	1:I:177:ALA:HB3	2.01	0.42
1:D:49:HIS:HD2	2:D:305:HEC:NC	2.16	0.42
1:N:100:LEU:HD23	1:N:100:LEU:HA	1.84	0.42
1:K:49:HIS:HD2	2:K:306:HEC:CHC	2.31	0.42
1:J:189:CYS:HB2	2:J:301:HEC:C3C	2.48	0.42
1:E:102:CYS:HB2	2:E:302:HEC:C3C	2.49	0.42
1:Q:129:LEU:HD12	2:Q:301:HEC:O2D	2.19	0.42
1:N:211:LEU:O	2:N:301:HEC:HMC3	2.19	0.42
1:P:195:LYS:HB2	1:P:198:VAL:HG12	2.02	0.42
1:T:82:MET:C	1:T:84:ALA:H	2.27	0.42
1:M:41:THR:HG23	1:M:118:LEU:HD11	2.00	0.42
1:C:45:CYS:CB	2:C:308:HEC:HHC	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:306:HEC:HBA1	2:C:306:HEC:CHA	2.50	0.42
1:R:190:HIS:CE1	2:R:302:HEC:CMA	3.03	0.42
2:J:305:HEC:HBA2	2:J:306:HEC:C3A	2.49	0.42
1:E:103:HIS:CE1	2:E:302:HEC:C1B	2.94	0.42
1:Q:205:THR:HG23	1:Q:207:ALA:H	1.84	0.42
1:D:153:ILE:HD12	1:D:157:ASP:O	2.19	0.42
1:Q:100:LEU:HD21	1:Q:135:LEU:HB2	2.02	0.42
1:Q:100:LEU:HD23	1:Q:100:LEU:HA	1.87	0.42
1:R:50:THR:C	1:R:52:HIS:H	2.28	0.42
1:C:95:ASP:OD1	1:C:186:CYS:HB3	2.20	0.42
1:Q:116:ASN:HB2	2:R:301:HEC:HBD1	2.01	0.42
1:R:28:ASP:CG	1:R:33:ASN:HD22	2.27	0.42
2:R:305:HEC:HHC	1:S:218:LYS:HZ1	1.84	0.42
1:S:82:MET:HG3	1:S:84:ALA:O	2.20	0.42
2:S:307:HEC:CAC	1:T:215:CYS:HG	2.03	0.42
1:D:97:VAL:HG13	1:D:98:LEU:HD23	2.01	0.42
1:D:129:LEU:HA	2:D:301:HEC:O2D	2.20	0.42
1:E:26:LYS:HB3	1:E:201:PHE:HE2	1.85	0.42
1:Q:102:CYS:HB2	2:Q:301:HEC:HMC2	2.02	0.42
1:R:102:CYS:HB2	2:R:302:HEC:C3C	2.50	0.42
1:S:129:LEU:HA	2:S:302:HEC:O2D	2.19	0.42
2:N:306:HEC:HBA2	2:N:307:HEC:CAA	2.50	0.42
1:M:102:CYS:SG	1:M:107:ILE:HD13	2.59	0.42
1:E:100:LEU:HD23	1:E:100:LEU:HA	1.87	0.42
1:E:104:ASP:O	1:E:105:GLY:C	2.63	0.42
1:E:149:TYR:O	1:E:153:ILE:HG22	2.20	0.42
1:S:62:LEU:HB2	2:S:307:HEC:HMA2	2.02	0.42
1:S:164:ALA:HB1	1:S:167:LEU:HB2	2.01	0.42
1:L:60:ALA:HB1	1:L:63:TRP:HB2	2.02	0.42
1:J:49:HIS:ND1	2:J:305:HEC:HHB	2.35	0.42
1:J:52:HIS:CD2	2:I:301:HEC:C4D	3.03	0.42
1:J:182:ASP:OD1	1:J:182:ASP:N	2.52	0.42
2:C:302:HEC:HMC3	2:C:302:HEC:HBC3	2.02	0.42
1:P:123:LEU:HD12	1:P:123:LEU:HA	1.78	0.42
1:R:21:VAL:HA	1:S:218:LYS:O	2.19	0.42
1:K:191:ASP:OD2	1:K:195:LYS:HD3	2.20	0.41
1:J:54:ALA:HA	1:I:141:ASN:ND2	2.35	0.41
2:C:308:HEC:C3B	1:D:218:LYS:HG2	2.50	0.41
1:D:151:ASP:HA	1:D:154:THR:HG22	2.00	0.41
1:E:104:ASP:OD1	1:E:104:ASP:C	2.63	0.41
1:S:45:CYS:HA	2:S:306:HEC:HMC2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:82:MET:C	1:S:84:ALA:H	2.28	0.41
1:T:107:ILE:CD1	2:T:302:HEC:HAC	2.50	0.41
1:N:189:CYS:CB	2:N:302:HEC:CAC	2.96	0.41
2:L:306:HEC:HBC3	2:L:306:HEC:HMC3	2.02	0.41
1:J:192:VAL:HG11	2:J:306:HEC:C1D	2.50	0.41
1:D:150:GLY:HA2	1:D:153:ILE:HG22	2.02	0.41
1:P:87:LEU:HB2	1:P:90:ASP:OD1	2.19	0.41
1:Q:33:ASN:O	1:Q:33:ASN:OD1	2.38	0.41
1:E:198:VAL:HG21	1:E:202:LEU:O	2.20	0.41
1:F:135:LEU:HD11	2:F:301:HEC:CHB	2.50	0.41
1:N:23:LYS:HG3	1:N:24:ASP:OD1	2.21	0.41
1:K:144:PRO:HB2	1:K:147:MET:CE	2.47	0.41
1:J:102:CYS:HG	2:J:302:HEC:HAC	1.70	0.41
1:Q:125:VAL:HG12	1:Q:127:ALA:H	1.85	0.41
1:T:202:LEU:HD22	1:T:211:LEU:HD22	2.02	0.41
1:N:28:ASP:OD2	1:N:28:ASP:C	2.63	0.41
1:D:42:ASP:OD1	1:D:42:ASP:N	2.53	0.41
1:G:102:CYS:CB	2:G:303:HEC:CAC	2.97	0.41
1:G:198:VAL:HB	1:G:205:THR:HG22	2.03	0.41
1:P:129:LEU:HD11	1:P:133:ALA:HB1	2.02	0.41
2:Q:305:HEC:C2B	1:R:218:LYS:HG2	2.50	0.41
1:S:62:LEU:HB2	2:S:307:HEC:CMA	2.51	0.41
2:K:305:HEC:CAC	1:J:215:CYS:CB	2.97	0.41
1:J:102:CYS:CB	2:J:302:HEC:C3C	2.99	0.41
1:I:65:ARG:HH22	1:I:107:ILE:HG13	1.86	0.41
1:E:157:ASP:OD1	1:E:159:GLU:HB2	2.20	0.41
1:G:87:LEU:O	1:G:91:VAL:HG23	2.21	0.41
2:R:305:HEC:HBC3	2:R:305:HEC:HMC3	2.01	0.41
1:D:48:CYS:CB	2:D:305:HEC:C3C	2.99	0.41
1:G:63:TRP:CZ2	1:G:98:LEU:HB3	2.56	0.41
2:G:303:HEC:HHA	2:G:303:HEC:HBD1	2.03	0.41
1:Q:49:HIS:CD2	2:Q:305:HEC:C4B	3.04	0.41
1:S:52:HIS:HD2	2:S:305:HEC:C4D	2.33	0.41
1:T:147:MET:HE3	1:T:147:MET:HB3	1.88	0.41
1:D:50:THR:HG21	1:D:54:ALA:O	2.21	0.41
1:E:125:VAL:HG12	1:E:127:ALA:HB2	2.03	0.41
1:L:48:CYS:HB3	1:L:63:TRP:CZ3	2.56	0.41
1:E:95:ASP:OD1	1:E:95:ASP:N	2.54	0.41
1:F:62:LEU:HB2	2:F:305:HEC:CMA	2.51	0.41
1:P:49:HIS:HD2	2:P:308:HEC:CHC	2.34	0.41
1:R:68:ASP:OD2	1:R:69:THR:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:193:HIS:HD2	1:S:218:LYS:HD3	1.86	0.41
1:R:198:VAL:HG21	1:R:202:LEU:O	2.20	0.41
2:R:302:HEC:HHA	2:R:302:HEC:HBD1	2.01	0.41
1:T:107:ILE:HD11	2:T:302:HEC:HAC	2.02	0.41
1:T:191:ASP:N	1:T:201:PHE:O	2.54	0.41
1:N:49:HIS:HD2	2:N:307:HEC:CHC	2.32	0.41
1:J:94:THR:O	1:J:97:VAL:HG12	2.21	0.41
1:T:45:CYS:CB	2:T:301:HEC:HHC	2.43	0.41
1:T:107:ILE:HG22	1:T:125:VAL:HG11	2.02	0.41
2:M:305:HEC:C1D	1:L:216:HIS:CE1	3.01	0.40
1:J:45:CYS:HB2	2:J:306:HEC:HHC	2.00	0.40
1:J:107:ILE:HD11	2:J:302:HEC:CMD	2.51	0.40
2:J:305:HEC:CHD	1:I:143:HIS:HE1	2.34	0.40
1:I:82:MET:HE1	1:I:144:PRO:HG3	2.02	0.40
1:C:164:ALA:HB1	1:C:167:LEU:HB2	2.02	0.40
2:C:308:HEC:HBA1	2:C:308:HEC:HHA	2.03	0.40
1:R:62:LEU:HB2	2:R:306:HEC:CMA	2.50	0.40
1:R:133:ALA:O	2:R:301:HEC:HMA2	2.21	0.40
1:L:48:CYS:SG	2:L:306:HEC:C3C	3.03	0.40
1:F:210:ALA:O	1:F:214:THR:HG23	2.21	0.40
2:P:307:HEC:C3C	1:Q:189:CYS:SG	3.01	0.40
1:R:164:ALA:HB1	1:R:167:LEU:HB2	2.03	0.40
1:S:63:TRP:CE2	1:S:98:LEU:HB3	2.56	0.40
1:N:71:PRO:HG3	1:N:100:LEU:HD12	2.04	0.40
1:M:62:LEU:HB2	2:M:305:HEC:CMA	2.52	0.40
1:J:42:ASP:O	1:I:208:ALA:N	2.52	0.40
1:J:102:CYS:HB2	2:J:302:HEC:HMC2	2.03	0.40
1:J:102:CYS:HB3	2:J:302:HEC:C3C	2.52	0.40
1:C:123:LEU:HD12	1:C:124:ALA:N	2.36	0.40
1:C:150:GLY:HA2	1:C:153:ILE:HG22	2.04	0.40
1:C:189:CYS:HB2	2:C:302:HEC:C3C	2.51	0.40
1:F:218:LYS:HD2	1:F:218:LYS:C	2.46	0.40
1:T:102:CYS:CB	2:T:302:HEC:C3C	2.99	0.40
1:N:102:CYS:SG	2:N:303:HEC:CBC	3.02	0.40
1:M:82:MET:C	1:M:84:ALA:H	2.29	0.40
1:M:102:CYS:HB2	2:M:302:HEC:C2C	2.51	0.40
1:K:82:MET:C	1:K:84:ALA:H	2.29	0.40
1:K:218:LYS:C	1:K:218:LYS:HD2	2.47	0.40
1:I:45:CYS:HB3	2:I:302:HEC:CHC	2.50	0.40
1:D:111:LEU:HD23	1:D:111:LEU:HA	1.92	0.40
1:D:174:LEU:HD12	1:D:177:ALA:HB3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:147:MET:HE2	1:G:147:MET:HB3	1.95	0.40
2:P:308:HEC:HHA	2:P:308:HEC:HBA1	2.03	0.40
1:Q:170:PHE:HD2	1:Q:185:TRP:HB2	1.87	0.40
1:T:115:PRO:HD2	1:T:118:LEU:HD21	2.03	0.40
1:K:54:ALA:HB3	1:J:141:ASN:HB2	2.03	0.40
1:E:151:ASP:HA	1:E:154:THR:HG22	2.04	0.40
1:F:64:ASN:OD1	1:F:111:LEU:HB3	2.22	0.40
1:Q:75:TYR:HB3	1:Q:144:PRO:HB3	2.02	0.40
1:Q:82:MET:C	1:Q:84:ALA:H	2.30	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	C	196/218 (90%)	180 (92%)	15 (8%)	1 (0%)	24	55
1	D	196/218 (90%)	174 (89%)	21 (11%)	1 (0%)	24	55
1	E	196/218 (90%)	174 (89%)	21 (11%)	1 (0%)	24	55
1	F	196/218 (90%)	174 (89%)	21 (11%)	1 (0%)	24	55
1	G	196/218 (90%)	171 (87%)	25 (13%)	0	100	100
1	I	196/218 (90%)	176 (90%)	20 (10%)	0	100	100
1	J	196/218 (90%)	175 (89%)	18 (9%)	3 (2%)	8	30
1	K	196/218 (90%)	173 (88%)	23 (12%)	0	100	100
1	L	196/218 (90%)	174 (89%)	21 (11%)	1 (0%)	24	55
1	M	196/218 (90%)	180 (92%)	16 (8%)	0	100	100
1	N	196/218 (90%)	175 (89%)	20 (10%)	1 (0%)	24	55
1	P	196/218 (90%)	164 (84%)	31 (16%)	1 (0%)	24	55
1	Q	196/218 (90%)	177 (90%)	17 (9%)	2 (1%)	12	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	R	196/218 (90%)	173 (88%)	23 (12%)	0	100	100
1	S	196/218 (90%)	170 (87%)	26 (13%)	0	100	100
1	T	196/218 (90%)	169 (86%)	26 (13%)	1 (0%)	24	55
All	All	3136/3488 (90%)	2779 (89%)	344 (11%)	13 (0%)	31	60

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	125	VAL
1	J	104	ASP
1	E	122	ALA
1	T	125	VAL
1	N	34	VAL
1	J	34	VAL
1	L	131	ALA
1	P	131	ALA
1	Q	34	VAL
1	D	34	VAL
1	Q	61	PRO
1	C	61	PRO
1	F	61	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 PDB entries followed by that with respect to all EM entries.

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	C	152/164 (93%)	148 (97%)	4 (3%)	40	66
1	D	152/164 (93%)	144 (95%)	8 (5%)	20	49
1	E	152/164 (93%)	144 (95%)	8 (5%)	20	49
1	F	152/164 (93%)	145 (95%)	7 (5%)	24	53
1	G	152/164 (93%)	148 (97%)	4 (3%)	40	66
1	I	152/164 (93%)	145 (95%)	7 (5%)	24	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	152/164 (93%)	146 (96%)	6 (4%)	28	58
1	K	152/164 (93%)	147 (97%)	5 (3%)	33	61
1	L	152/164 (93%)	146 (96%)	6 (4%)	28	58
1	M	152/164 (93%)	146 (96%)	6 (4%)	28	58
1	N	152/164 (93%)	148 (97%)	4 (3%)	40	66
1	P	152/164 (93%)	147 (97%)	5 (3%)	33	61
1	Q	152/164 (93%)	146 (96%)	6 (4%)	28	58
1	R	152/164 (93%)	143 (94%)	9 (6%)	18	45
1	S	152/164 (93%)	148 (97%)	4 (3%)	40	66
1	T	152/164 (93%)	143 (94%)	9 (6%)	18	45
All	All	2432/2624 (93%)	2334 (96%)	98 (4%)	29	57

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	99	CYS
1	N	107	ILE
1	N	212	CYS
1	N	215	CYS
1	M	45	CYS
1	M	52	HIS
1	M	68	ASP
1	M	99	CYS
1	M	157	ASP
1	M	199	SER
1	L	99	CYS
1	L	102	CYS
1	L	153	ILE
1	L	187	SER
1	L	212	CYS
1	L	215	CYS
1	K	65	ARG
1	K	99	CYS
1	K	181	THR
1	K	212	CYS
1	K	215	CYS
1	J	49	HIS
1	J	99	CYS

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Mol	Chain	Res	Type
1	J	121	THR
1	J	134	ASN
1	J	157	ASP
1	J	212	CYS
1	I	45	CYS
1	I	147	MET
1	I	186	CYS
1	I	190	HIS
1	I	192	VAL
1	I	212	CYS
1	I	215	CYS
1	C	45	CYS
1	C	99	CYS
1	C	186	CYS
1	C	215	CYS
1	D	52	HIS
1	D	99	CYS
1	D	102	CYS
1	D	110	THR
1	D	123	LEU
1	D	186	CYS
1	D	198	VAL
1	D	212	CYS
1	E	45	CYS
1	E	52	HIS
1	E	97	VAL
1	E	99	CYS
1	E	129	LEU
1	E	142	ASP
1	E	158	THR
1	E	212	CYS
1	F	52	HIS
1	F	87	LEU
1	F	99	CYS
1	F	107	ILE
1	F	209	SER
1	F	215	CYS
1	F	218	LYS
1	G	34	VAL
1	G	46	VAL
1	G	126	THR
1	G	212	CYS

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Mol	Chain	Res	Type
1	P	29	LEU
1	P	45	CYS
1	P	77	ASN
1	P	99	CYS
1	P	148	SER
1	Q	41	THR
1	Q	52	HIS
1	Q	102	CYS
1	Q	157	ASP
1	Q	212	CYS
1	Q	215	CYS
1	R	25	THR
1	R	52	HIS
1	R	87	LEU
1	R	99	CYS
1	R	126	THR
1	R	186	CYS
1	R	189	CYS
1	R	192	VAL
1	R	212	CYS
1	S	52	HIS
1	S	74	THR
1	S	85	VAL
1	S	215	CYS
1	T	69	THR
1	T	93	LEU
1	T	98	LEU
1	T	99	CYS
1	T	111	LEU
1	T	129	LEU
1	T	161	VAL
1	T	199	SER
1	T	212	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	N	203	GLN
1	M	103	HIS
1	K	203	GLN
1	I	83	ASN
1	C	64	ASN

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Mol	Chain	Res	Type
1	D	203	GLN
1	E	83	ASN
1	G	35	ASN
1	P	83	ASN
1	Q	109	ASN
1	R	83	ASN
1	S	141	ASN
1	T	35	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 96 ligands modelled in this entry, 32 are monoatomic - leaving 64 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	$\# Z > 2$
2	HEC	R	301	1,3	50,50,50	1.63	8 (16%)	68,82,82	2.67	30 (44%)
2	HEC	Q	301	1	50,50,50	1.58	2 (4%)	68,82,82	1.46	10 (14%)
2	HEC	F	302	1	50,50,50	1.54	2 (4%)	68,82,82	1.23	6 (8%)
2	HEC	D	305	1	50,50,50	1.66	5 (10%)	68,82,82	1.23	7 (10%)
2	HEC	L	305	1	50,50,50	1.53	5 (10%)	68,82,82	1.16	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEC	L	306	1	50,50,50	1.59	5 (10%)	68,82,82	1.18	3 (4%)
2	HEC	N	301	1	50,50,50	1.53	3 (6%)	68,82,82	1.07	2 (2%)
2	HEC	J	306	1	50,50,50	1.77	6 (12%)	68,82,82	1.69	13 (19%)
2	HEC	G	301	1	50,50,50	1.54	3 (6%)	68,82,82	1.05	3 (4%)
2	HEC	I	303	1	50,50,50	1.55	2 (4%)	68,82,82	1.19	5 (7%)
2	HEC	S	302	1	50,50,50	1.54	3 (6%)	68,82,82	1.28	6 (8%)
2	HEC	P	302	1	50,50,50	1.54	3 (6%)	68,82,82	1.11	3 (4%)
2	HEC	T	302	1	50,50,50	1.64	4 (8%)	68,82,82	1.59	15 (22%)
2	HEC	F	301	1,3	50,50,50	1.59	5 (10%)	68,82,82	1.83	20 (29%)
2	HEC	P	308	1	50,50,50	1.66	5 (10%)	68,82,82	1.63	15 (22%)
2	HEC	S	307	1	50,50,50	1.62	6 (12%)	68,82,82	1.21	7 (10%)
2	HEC	F	305	1	50,50,50	1.52	4 (8%)	68,82,82	1.26	6 (8%)
2	HEC	M	302	1	50,50,50	1.53	3 (6%)	68,82,82	1.55	10 (14%)
2	HEC	E	305	1	50,50,50	1.97	8 (16%)	68,82,82	1.98	19 (27%)
2	HEC	C	307	1,3	50,50,50	1.54	3 (6%)	68,82,82	1.15	5 (7%)
2	HEC	K	306	1	50,50,50	1.62	5 (10%)	68,82,82	1.21	6 (8%)
2	HEC	J	302	1	50,50,50	1.54	3 (6%)	68,82,82	1.58	11 (16%)
2	HEC	J	301	1	50,50,50	1.53	3 (6%)	68,82,82	1.09	3 (4%)
2	HEC	P	301	1	50,50,50	1.53	3 (6%)	68,82,82	1.11	3 (4%)
2	HEC	D	304	1	50,50,50	1.53	3 (6%)	68,82,82	1.25	6 (8%)
2	HEC	P	307	1	50,50,50	1.57	4 (8%)	68,82,82	1.46	10 (14%)
2	HEC	T	301	1	50,50,50	1.60	5 (10%)	68,82,82	1.25	4 (5%)
2	HEC	N	307	1	50,50,50	1.57	5 (10%)	68,82,82	1.32	7 (10%)
2	HEC	L	301	1,3	50,50,50	1.97	10 (20%)	68,82,82	3.58	35 (51%)
2	HEC	M	306	1	50,50,50	1.67	3 (6%)	68,82,82	1.39	8 (11%)
2	HEC	D	301	1	50,50,50	1.61	3 (6%)	68,82,82	1.69	12 (17%)
2	HEC	C	301	1	50,50,50	1.56	4 (8%)	68,82,82	1.12	5 (7%)
2	HEC	R	306	1	50,50,50	1.55	5 (10%)	68,82,82	1.20	5 (7%)
2	HEC	I	301	1,3	50,50,50	1.85	9 (18%)	68,82,82	2.72	23 (33%)
2	HEC	S	305	1,3	50,50,50	1.66	6 (12%)	68,82,82	2.57	29 (42%)
2	HEC	P	306	1	50,50,50	1.60	5 (10%)	68,82,82	1.29	6 (8%)
2	HEC	Q	304	1	50,50,50	1.78	5 (10%)	68,82,82	1.89	18 (26%)
2	HEC	P	303	1	50,50,50	1.55	2 (4%)	68,82,82	1.36	7 (10%)
2	HEC	I	302	1	50,50,50	1.55	4 (8%)	68,82,82	1.05	4 (5%)
2	HEC	C	306	1	50,50,50	1.63	5 (10%)	68,82,82	1.61	14 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEC	E	302	1	50,50,50	1.55	4 (8%)	68,82,82	1.37	9 (13%)
2	HEC	R	305	1	50,50,50	1.56	4 (8%)	68,82,82	1.15	3 (4%)
2	HEC	K	305	1	50,50,50	1.53	4 (8%)	68,82,82	1.24	6 (8%)
2	HEC	C	303	1	50,50,50	1.54	4 (8%)	68,82,82	1.30	7 (10%)
2	HEC	S	306	1	50,50,50	1.62	5 (10%)	68,82,82	1.17	4 (5%)
2	HEC	J	305	1	50,50,50	1.63	5 (10%)	68,82,82	1.64	13 (19%)
2	HEC	C	308	1	50,50,50	1.62	4 (8%)	68,82,82	1.49	8 (11%)
2	HEC	N	306	1	50,50,50	1.73	7 (14%)	68,82,82	1.70	16 (23%)
2	HEC	G	303	1	50,50,50	1.55	2 (4%)	68,82,82	1.57	13 (19%)
2	HEC	L	302	1	50,50,50	1.59	5 (10%)	68,82,82	1.66	15 (22%)
2	HEC	Q	305	1	50,50,50	1.59	4 (8%)	68,82,82	1.49	11 (16%)
2	HEC	N	303	1	50,50,50	1.55	2 (4%)	68,82,82	1.55	10 (14%)
2	HEC	N	302	1	50,50,50	1.56	3 (6%)	68,82,82	1.07	3 (4%)
2	HEC	K	301	1	50,50,50	1.54	3 (6%)	68,82,82	1.13	3 (4%)
2	HEC	M	305	1	50,50,50	1.54	5 (10%)	68,82,82	1.36	10 (14%)
2	HEC	C	302	1	50,50,50	1.54	3 (6%)	68,82,82	1.19	4 (5%)
2	HEC	E	301	1,3	50,50,50	1.54	2 (4%)	68,82,82	1.30	8 (11%)
2	HEC	F	306	1	50,50,50	1.67	6 (12%)	68,82,82	1.34	8 (11%)
2	HEC	R	302	1	50,50,50	1.54	3 (6%)	68,82,82	1.54	10 (14%)
2	HEC	S	301	1	50,50,50	1.96	10 (20%)	68,82,82	4.13	41 (60%)
2	HEC	G	302	1,3	50,50,50	1.67	4 (8%)	68,82,82	1.88	22 (32%)
2	HEC	E	306	1	50,50,50	1.50	3 (6%)	68,82,82	1.25	8 (11%)
2	HEC	M	301	1,3	50,50,50	1.56	4 (8%)	68,82,82	1.91	16 (23%)
2	HEC	K	302	1	50,50,50	1.56	3 (6%)	68,82,82	1.38	8 (11%)

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
2	HEC	R	301	1,3	1/1/3/7	8/14/54/54	-
2	HEC	Q	301	1	1/1/3/7	7/14/54/54	-
2	HEC	F	302	1	1/1/3/7	7/14/54/54	-
2	HEC	D	305	1	1/1/3/7	4/14/54/54	-
2	HEC	L	305	1	1/1/3/7	8/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEC	L	306	1	1/1/3/7	6/14/54/54	-
2	HEC	N	301	1	1/1/3/7	7/14/54/54	-
2	HEC	J	306	1	1/1/3/7	6/14/54/54	-
2	HEC	G	301	1	1/1/3/7	8/14/54/54	-
2	HEC	I	303	1	1/1/3/7	7/14/54/54	-
2	HEC	S	302	1	1/1/3/7	4/14/54/54	-
2	HEC	P	302	1	1/1/3/7	8/14/54/54	-
2	HEC	T	302	1	1/1/3/7	7/14/54/54	-
2	HEC	F	301	1,3	1/1/3/7	7/14/54/54	-
2	HEC	P	308	1	1/1/3/7	7/14/54/54	-
2	HEC	S	307	1	1/1/3/7	11/14/54/54	-
2	HEC	F	305	1	1/1/3/7	9/14/54/54	-
2	HEC	M	302	1	1/1/3/7	5/14/54/54	-
2	HEC	E	305	1	1/1/3/7	8/14/54/54	-
2	HEC	C	307	1,3	1/1/3/7	7/14/54/54	-
2	HEC	K	306	1	1/1/3/7	4/14/54/54	-
2	HEC	J	302	1	1/1/3/7	6/14/54/54	-
2	HEC	J	301	1	1/1/3/7	5/14/54/54	-
2	HEC	P	301	1	1/1/3/7	6/14/54/54	-
2	HEC	D	304	1	1/1/3/7	8/14/54/54	-
2	HEC	P	307	1	1/1/3/7	7/14/54/54	-
2	HEC	T	301	1	1/1/3/7	9/14/54/54	-
2	HEC	N	307	1	1/1/3/7	5/14/54/54	-
2	HEC	L	301	1,3	1/1/3/7	7/14/54/54	-
2	HEC	M	306	1	1/1/3/7	4/14/54/54	-
2	HEC	D	301	1	1/1/3/7	6/14/54/54	-
2	HEC	C	301	1	1/1/3/7	7/14/54/54	-
2	HEC	R	306	1	1/1/3/7	10/14/54/54	-
2	HEC	I	301	1,3	1/1/3/7	10/14/54/54	-
2	HEC	S	305	1,3	1/1/3/7	9/14/54/54	-
2	HEC	P	306	1	1/1/3/7	10/14/54/54	-
2	HEC	Q	304	1	1/1/3/7	10/14/54/54	-
2	HEC	P	303	1	1/1/3/7	2/14/54/54	-
2	HEC	I	302	1	1/1/3/7	9/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEC	C	306	1	1/1/3/7	8/14/54/54	-
2	HEC	E	302	1	1/1/3/7	8/14/54/54	-
2	HEC	R	305	1	1/1/3/7	5/14/54/54	-
2	HEC	K	305	1	1/1/3/7	8/14/54/54	-
2	HEC	C	303	1	1/1/3/7	6/14/54/54	-
2	HEC	S	306	1	1/1/3/7	5/14/54/54	-
2	HEC	J	305	1	1/1/3/7	7/14/54/54	-
2	HEC	C	308	1	1/1/3/7	9/14/54/54	-
2	HEC	N	306	1	1/1/3/7	8/14/54/54	-
2	HEC	G	303	1	1/1/3/7	7/14/54/54	-
2	HEC	L	302	1	1/1/3/7	6/14/54/54	-
2	HEC	Q	305	1	1/1/3/7	5/14/54/54	-
2	HEC	N	303	1	1/1/3/7	6/14/54/54	-
2	HEC	N	302	1	1/1/3/7	7/14/54/54	-
2	HEC	K	301	1	1/1/3/7	7/14/54/54	-
2	HEC	M	305	1	1/1/3/7	9/14/54/54	-
2	HEC	C	302	1	1/1/3/7	6/14/54/54	-
2	HEC	E	301	1,3	1/1/3/7	9/14/54/54	-
2	HEC	F	306	1	1/1/3/7	5/14/54/54	-
2	HEC	R	302	1	1/1/3/7	4/14/54/54	-
2	HEC	S	301	1	1/1/3/7	9/14/54/54	-
2	HEC	G	302	1,3	1/1/3/7	12/14/54/54	-
2	HEC	E	306	1	1/1/3/7	1/14/54/54	-
2	HEC	M	301	1,3	1/1/3/7	10/14/54/54	-
2	HEC	K	302	1	1/1/3/7	7/14/54/54	-

All (276) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	301	HEC	C3D-C2D	8.92	1.56	1.36
2	Q	304	HEC	C3D-C2D	8.56	1.55	1.36
2	T	302	HEC	C3D-C2D	8.17	1.54	1.36
2	C	306	HEC	C3D-C2D	7.90	1.53	1.36
2	D	301	HEC	C3D-C2D	7.88	1.53	1.36
2	T	301	HEC	C3D-C2D	7.81	1.53	1.36
2	E	305	HEC	C3D-C2D	7.80	1.53	1.36
2	G	302	HEC	C3D-C2D	7.79	1.53	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	302	HEC	C3D-C2D	7.78	1.53	1.36
2	P	303	HEC	C3D-C2D	7.74	1.53	1.36
2	D	305	HEC	C3D-C2D	7.72	1.53	1.36
2	Q	301	HEC	C3D-C2D	7.71	1.53	1.36
2	S	302	HEC	C3D-C2D	7.65	1.53	1.36
2	K	302	HEC	C3D-C2D	7.65	1.53	1.36
2	C	301	HEC	C3D-C2D	7.64	1.53	1.36
2	N	302	HEC	C3D-C2D	7.62	1.53	1.36
2	C	302	HEC	C3D-C2D	7.61	1.53	1.36
2	F	302	HEC	C3D-C2D	7.61	1.53	1.36
2	N	306	HEC	C3D-C2D	7.60	1.53	1.36
2	P	306	HEC	C3D-C2D	7.59	1.53	1.36
2	P	302	HEC	C3D-C2D	7.58	1.53	1.36
2	R	302	HEC	C3D-C2D	7.56	1.53	1.36
2	M	302	HEC	C3D-C2D	7.56	1.53	1.36
2	E	302	HEC	C3D-C2D	7.56	1.53	1.36
2	P	301	HEC	C3D-C2D	7.55	1.53	1.36
2	N	303	HEC	C3D-C2D	7.55	1.53	1.36
2	C	303	HEC	C3D-C2D	7.55	1.53	1.36
2	S	307	HEC	C3D-C2D	7.55	1.53	1.36
2	R	305	HEC	C3D-C2D	7.54	1.53	1.36
2	I	303	HEC	C3D-C2D	7.54	1.53	1.36
2	R	306	HEC	C3D-C2D	7.53	1.53	1.36
2	G	303	HEC	C3D-C2D	7.51	1.53	1.36
2	G	301	HEC	C3D-C2D	7.51	1.53	1.36
2	I	302	HEC	C3D-C2D	7.50	1.52	1.36
2	F	306	HEC	C3D-C2D	7.48	1.52	1.36
2	J	301	HEC	C3D-C2D	7.48	1.52	1.36
2	N	301	HEC	C3D-C2D	7.47	1.52	1.36
2	K	301	HEC	C3D-C2D	7.46	1.52	1.36
2	C	308	HEC	C3D-C2D	7.46	1.52	1.36
2	S	306	HEC	C3D-C2D	7.44	1.52	1.36
2	J	302	HEC	C3D-C2D	7.42	1.52	1.36
2	C	307	HEC	C3D-C2D	7.42	1.52	1.36
2	J	305	HEC	C3D-C2D	7.40	1.52	1.36
2	K	306	HEC	C3D-C2D	7.40	1.52	1.36
2	L	305	HEC	C3D-C2D	7.39	1.52	1.36
2	D	304	HEC	C3D-C2D	7.37	1.52	1.36
2	P	307	HEC	C3D-C2D	7.36	1.52	1.36
2	M	306	HEC	C3D-C2D	7.35	1.52	1.36
2	M	305	HEC	C3D-C2D	7.33	1.52	1.36
2	K	305	HEC	C3D-C2D	7.33	1.52	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	306	HEC	C3D-C2D	7.24	1.52	1.36
2	J	306	HEC	C3D-C2D	7.22	1.52	1.36
2	F	305	HEC	C3D-C2D	7.19	1.52	1.36
2	E	301	HEC	C3D-C2D	7.16	1.52	1.36
2	F	301	HEC	C3D-C2D	7.16	1.52	1.36
2	P	308	HEC	C3D-C2D	7.16	1.52	1.36
2	E	305	HEC	CMA-C3A	7.08	1.65	1.50
2	N	307	HEC	C3D-C2D	7.07	1.52	1.36
2	E	306	HEC	C3D-C2D	7.05	1.52	1.36
2	Q	305	HEC	C3D-C2D	6.97	1.51	1.36
2	S	305	HEC	C3D-C2D	6.67	1.51	1.36
2	M	301	HEC	C3D-C2D	6.66	1.51	1.36
2	L	301	HEC	C3D-C2D	6.48	1.50	1.36
2	S	301	HEC	C3D-C2D	6.07	1.49	1.36
2	R	301	HEC	C3D-C2D	5.98	1.49	1.36
2	J	306	HEC	CMB-C2B	5.71	1.62	1.50
2	L	301	HEC	CHD-C4C	-4.91	1.28	1.39
2	L	301	HEC	CHD-C1D	-4.88	1.28	1.38
2	M	306	HEC	CMB-C2B	4.68	1.60	1.50
2	F	306	HEC	CMB-C2B	4.59	1.60	1.50
2	S	301	HEC	CHD-C1D	-4.39	1.29	1.38
2	S	301	HEC	CHD-C4C	-4.32	1.29	1.39
2	N	306	HEC	CMA-C3A	4.32	1.59	1.50
2	D	305	HEC	CMB-C2B	4.27	1.59	1.50
2	Q	304	HEC	CMA-C3A	4.08	1.59	1.50
2	K	306	HEC	CMB-C2B	3.93	1.58	1.50
2	C	308	HEC	CMB-C2B	3.87	1.58	1.50
2	S	306	HEC	CMB-C2B	3.75	1.58	1.50
2	P	308	HEC	CMB-C2B	3.75	1.58	1.50
2	S	301	HEC	CAC-C3C	3.75	1.60	1.51
2	L	306	HEC	CMB-C2B	3.61	1.58	1.50
2	L	301	HEC	CAC-C3C	3.57	1.60	1.51
2	L	301	HEC	C3C-C2C	-3.37	1.30	1.38
2	P	306	HEC	CMA-C3A	3.34	1.57	1.50
2	Q	305	HEC	CMB-C2B	3.33	1.57	1.50
2	S	301	HEC	C3C-C2C	-3.33	1.30	1.38
2	L	301	HEC	CMC-C2C	3.30	1.57	1.50
2	S	301	HEC	CMC-C2C	3.17	1.57	1.50
2	S	301	HEC	C1A-NA	-3.10	1.33	1.39
2	R	301	HEC	C3C-C2C	-3.07	1.30	1.38
2	E	305	HEC	C1A-C2A	3.06	1.50	1.45
2	S	301	HEC	CMD-C2D	3.02	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	307	HEC	CMB-C2B	3.00	1.56	1.50
2	L	301	HEC	CMD-C2D	2.99	1.56	1.50
2	R	305	HEC	CMB-C2B	2.93	1.56	1.50
2	S	305	HEC	C3C-C2C	-2.85	1.31	1.38
2	S	305	HEC	CHD-C4C	-2.79	1.33	1.39
2	R	301	HEC	CHD-C4C	-2.70	1.33	1.39
2	C	306	HEC	CMA-C3A	2.69	1.56	1.50
2	I	301	HEC	CHC-C1C	-2.63	1.33	1.39
2	I	301	HEC	C3C-C2C	-2.63	1.32	1.38
2	I	301	HEC	CHC-C4B	-2.59	1.33	1.38
2	C	308	HEC	CAB-C3B	2.58	1.57	1.51
2	J	306	HEC	CAB-C3B	2.55	1.57	1.51
2	S	306	HEC	CAB-C3B	2.55	1.57	1.51
2	F	301	HEC	C3C-C2C	-2.55	1.32	1.38
2	I	301	HEC	C4C-C3C	2.55	1.49	1.44
2	K	306	HEC	CAB-C3B	2.46	1.57	1.51
2	T	302	HEC	C3C-C2C	-2.45	1.32	1.38
2	L	301	HEC	CHC-C1C	-2.45	1.33	1.39
2	Q	304	HEC	CMC-C2C	2.45	1.55	1.50
2	N	306	HEC	C3C-C2C	-2.43	1.32	1.38
2	G	302	HEC	C3C-C2C	-2.43	1.32	1.38
2	F	306	HEC	CAB-C3B	2.39	1.57	1.51
2	J	305	HEC	CMA-C3A	2.37	1.55	1.50
2	R	301	HEC	CHC-C1C	-2.36	1.34	1.39
2	M	305	HEC	C3C-C2C	-2.35	1.32	1.38
2	J	305	HEC	C3C-C2C	-2.34	1.32	1.38
2	N	307	HEC	C3C-C2C	-2.33	1.32	1.38
2	S	307	HEC	O1D-CGD	2.32	1.29	1.22
2	G	302	HEC	CHC-C1C	-2.32	1.34	1.39
2	M	306	HEC	CAB-C3B	2.30	1.57	1.51
2	T	301	HEC	CMC-C2C	2.30	1.55	1.50
2	S	305	HEC	CHC-C1C	-2.29	1.34	1.39
2	R	301	HEC	C4B-C3B	-2.29	1.41	1.45
2	P	303	HEC	C3C-C2C	-2.28	1.33	1.38
2	D	304	HEC	C3C-C2C	-2.27	1.33	1.38
2	T	301	HEC	CAB-C3B	2.27	1.56	1.51
2	L	302	HEC	CMC-C2C	2.27	1.55	1.50
2	I	301	HEC	CMB-C2B	2.26	1.55	1.50
2	R	302	HEC	C2A-C3A	-2.26	1.31	1.36
2	K	305	HEC	C3C-C2C	-2.26	1.33	1.38
2	E	305	HEC	CAA-C2A	2.24	1.57	1.51
2	N	307	HEC	CAB-C3B	2.23	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	301	HEC	CMB-C2B	2.23	1.55	1.50
2	M	301	HEC	C3C-C2C	-2.23	1.33	1.38
2	L	306	HEC	CAB-C3B	2.23	1.56	1.51
2	C	306	HEC	CMC-C2C	2.22	1.55	1.50
2	E	305	HEC	CMC-C2C	2.22	1.55	1.50
2	N	303	HEC	CMC-C2C	2.22	1.55	1.50
2	Q	304	HEC	CHB-C4A	-2.22	1.34	1.38
2	D	301	HEC	CMC-C2C	2.21	1.55	1.50
2	R	301	HEC	C1B-C2B	2.21	1.49	1.44
2	P	307	HEC	CMB-C2B	2.21	1.55	1.50
2	E	306	HEC	CMB-C2B	2.20	1.55	1.50
2	J	302	HEC	CMC-C2C	2.20	1.55	1.50
2	E	301	HEC	C3C-C2C	-2.20	1.33	1.38
2	Q	301	HEC	CMC-C2C	2.19	1.55	1.50
2	N	306	HEC	CAC-C3C	2.19	1.56	1.51
2	N	306	HEC	C1A-C2A	2.19	1.49	1.45
2	F	305	HEC	C3C-C2C	-2.19	1.33	1.38
2	R	302	HEC	CMC-C2C	2.19	1.55	1.50
2	G	303	HEC	CMC-C2C	2.18	1.55	1.50
2	M	301	HEC	C4B-NB	-2.18	1.36	1.40
2	E	305	HEC	C3C-C2C	-2.18	1.33	1.38
2	S	301	HEC	CHB-C4A	2.18	1.42	1.38
2	E	306	HEC	C3C-C2C	-2.17	1.33	1.38
2	M	305	HEC	CMA-C3A	2.17	1.55	1.50
2	P	308	HEC	CAB-C3B	2.16	1.56	1.51
2	I	301	HEC	CAB-C3B	2.16	1.56	1.51
2	N	302	HEC	CMB-C2B	2.16	1.55	1.50
2	Q	305	HEC	C3C-C2C	-2.15	1.33	1.38
2	C	301	HEC	C3C-C2C	-2.15	1.33	1.38
2	G	301	HEC	CMC-C2C	2.15	1.55	1.50
2	T	301	HEC	C3C-C2C	-2.15	1.33	1.38
2	E	305	HEC	CMD-C2D	2.15	1.55	1.50
2	P	307	HEC	C2A-C3A	-2.14	1.32	1.36
2	S	307	HEC	CAD-C3D	2.14	1.56	1.51
2	K	306	HEC	CMA-C3A	2.14	1.55	1.50
2	S	301	HEC	CHC-C1C	-2.14	1.34	1.39
2	G	302	HEC	CMD-C2D	2.13	1.55	1.50
2	J	301	HEC	CMB-C2B	2.13	1.55	1.50
2	S	302	HEC	CMC-C2C	2.13	1.55	1.50
2	K	306	HEC	C3C-C2C	-2.13	1.33	1.38
2	K	305	HEC	CMA-C3A	2.13	1.55	1.50
2	C	308	HEC	C3C-C2C	-2.13	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	305	HEC	C4A-C3A	2.12	1.49	1.45
2	J	305	HEC	CMD-C2D	2.12	1.55	1.50
2	S	305	HEC	CHD-C1D	-2.12	1.34	1.38
2	L	306	HEC	C3C-C2C	-2.12	1.33	1.38
2	C	303	HEC	C3C-C2C	-2.12	1.33	1.38
2	I	302	HEC	CMC-C2C	2.12	1.55	1.50
2	P	301	HEC	CMB-C2B	2.11	1.55	1.50
2	J	306	HEC	C4B-C3B	2.11	1.48	1.45
2	I	303	HEC	C3C-C2C	-2.10	1.33	1.38
2	K	302	HEC	CMC-C2C	2.10	1.55	1.50
2	C	307	HEC	CMB-C2B	2.10	1.55	1.50
2	L	305	HEC	C3C-C2C	-2.10	1.33	1.38
2	P	301	HEC	CMC-C2C	2.10	1.55	1.50
2	P	302	HEC	CMB-C2B	2.10	1.55	1.50
2	P	308	HEC	C3C-C2C	-2.10	1.33	1.38
2	T	301	HEC	CMB-C2B	2.10	1.55	1.50
2	R	306	HEC	C3C-C2C	-2.10	1.33	1.38
2	D	301	HEC	CMB-C2B	2.10	1.55	1.50
2	L	305	HEC	CMB-C2B	2.09	1.55	1.50
2	R	305	HEC	C3C-C2C	-2.09	1.33	1.38
2	R	306	HEC	CMA-C3A	2.09	1.55	1.50
2	S	306	HEC	C3C-C2C	-2.09	1.33	1.38
2	L	302	HEC	C3C-C2C	-2.09	1.33	1.38
2	T	302	HEC	CMC-C2C	2.09	1.55	1.50
2	S	307	HEC	C3C-C2C	-2.09	1.33	1.38
2	I	302	HEC	CAB-C3B	2.09	1.56	1.51
2	N	306	HEC	CAA-C2A	2.09	1.56	1.51
2	J	301	HEC	CMC-C2C	2.09	1.55	1.50
2	S	305	HEC	CAC-C3C	2.09	1.56	1.51
2	C	302	HEC	CMC-C2C	2.09	1.55	1.50
2	M	302	HEC	CAB-C3B	2.09	1.56	1.51
2	F	301	HEC	CHC-C1C	-2.09	1.34	1.39
2	Q	305	HEC	CAB-C3B	2.09	1.56	1.51
2	N	302	HEC	CMC-C2C	2.08	1.55	1.50
2	L	305	HEC	CMA-C3A	2.08	1.55	1.50
2	E	302	HEC	CMB-C2B	2.08	1.55	1.50
2	E	302	HEC	CMC-C2C	2.08	1.55	1.50
2	P	306	HEC	CMC-C2C	2.08	1.55	1.50
2	L	301	HEC	C1A-NA	-2.08	1.35	1.39
2	C	307	HEC	C3C-C2C	-2.08	1.33	1.38
2	J	302	HEC	CMB-C2B	2.08	1.55	1.50
2	L	302	HEC	CAB-C3B	2.08	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	301	HEC	C3C-C2C	-2.07	1.33	1.38
2	F	301	HEC	CHD-C4C	-2.07	1.34	1.39
2	I	302	HEC	CMB-C2B	2.07	1.55	1.50
2	G	301	HEC	CMB-C2B	2.07	1.55	1.50
2	D	304	HEC	CMA-C3A	2.07	1.55	1.50
2	P	308	HEC	C2A-C3A	-2.06	1.32	1.36
2	L	306	HEC	CMA-C3A	2.06	1.55	1.50
2	K	305	HEC	CMB-C2B	2.06	1.55	1.50
2	Q	304	HEC	C3B-C2B	-2.06	1.32	1.36
2	E	302	HEC	CAB-C3B	2.05	1.56	1.51
2	J	305	HEC	CMC-C2C	2.05	1.55	1.50
2	J	306	HEC	CMA-C3A	2.05	1.55	1.50
2	L	301	HEC	CHB-C4A	2.05	1.42	1.38
2	D	305	HEC	CMA-C3A	2.05	1.55	1.50
2	S	307	HEC	CMD-C2D	2.05	1.55	1.50
2	R	301	HEC	CHC-C4B	-2.04	1.34	1.38
2	F	305	HEC	CMC-C2C	2.04	1.55	1.50
2	C	306	HEC	CMD-C2D	2.04	1.55	1.50
2	K	301	HEC	CMC-C2C	2.04	1.55	1.50
2	L	302	HEC	CHC-C1C	-2.04	1.34	1.39
2	N	301	HEC	CMB-C2B	2.04	1.54	1.50
2	D	305	HEC	C3C-C2C	-2.04	1.33	1.38
2	C	301	HEC	CMB-C2B	2.03	1.54	1.50
2	P	306	HEC	C3C-C2C	-2.03	1.33	1.38
2	P	302	HEC	CMC-C2C	2.03	1.54	1.50
2	R	306	HEC	CMB-C2B	2.03	1.54	1.50
2	F	302	HEC	CMC-C2C	2.03	1.54	1.50
2	D	305	HEC	CAB-C3B	2.03	1.56	1.51
2	S	302	HEC	C3C-C2C	-2.03	1.33	1.38
2	C	302	HEC	CMB-C2B	2.03	1.54	1.50
2	I	301	HEC	CAC-C3C	2.03	1.56	1.51
2	C	303	HEC	CMC-C2C	2.03	1.54	1.50
2	S	306	HEC	CMA-C3A	2.03	1.54	1.50
2	K	302	HEC	CMB-C2B	2.02	1.54	1.50
2	M	302	HEC	C3C-C2C	-2.02	1.33	1.38
2	R	306	HEC	CMC-C2C	2.02	1.54	1.50
2	I	301	HEC	CMC-C2C	2.02	1.54	1.50
2	S	307	HEC	CMA-C3A	2.02	1.54	1.50
2	M	305	HEC	CMC-C2C	2.02	1.54	1.50
2	C	306	HEC	CMB-C2B	2.02	1.54	1.50
2	P	306	HEC	CMB-C2B	2.02	1.54	1.50
2	L	305	HEC	CMC-C2C	2.02	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	303	HEC	CMA-C3A	2.01	1.54	1.50
2	F	306	HEC	CMA-C3A	2.01	1.54	1.50
2	R	305	HEC	CMA-C3A	2.01	1.54	1.50
2	J	306	HEC	CMD-C2D	2.01	1.54	1.50
2	N	306	HEC	CMD-C2D	2.01	1.54	1.50
2	M	305	HEC	CMD-C2D	2.01	1.54	1.50
2	F	306	HEC	C3C-C2C	-2.01	1.33	1.38
2	N	307	HEC	CMA-C3A	2.01	1.54	1.50
2	C	301	HEC	CMD-C2D	2.01	1.54	1.50
2	T	302	HEC	CMD-C2D	2.01	1.54	1.50
2	F	301	HEC	CAC-C3C	2.00	1.56	1.51
2	M	301	HEC	CMD-C2D	2.00	1.54	1.50
2	R	301	HEC	CMB-C2B	2.00	1.54	1.50
2	F	305	HEC	CMB-C2B	2.00	1.54	1.50
2	P	307	HEC	CMC-C2C	2.00	1.54	1.50
2	F	306	HEC	CMD-C2D	2.00	1.54	1.50

All (664) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	301	HEC	CAC-C3C-C4C	10.16	138.89	124.91
2	S	301	HEC	C2A-C1A-NA	-9.93	100.74	110.32
2	S	301	HEC	C4A-NA-C1A	9.86	121.90	105.82
2	S	301	HEC	C3C-C4C-NC	9.28	120.45	110.15
2	S	301	HEC	C4C-NC-C1C	-9.11	90.97	105.82
2	L	301	HEC	C2A-C1A-NA	-8.94	101.69	110.32
2	I	301	HEC	CAC-C3C-C2C	-8.59	113.29	126.89
2	L	301	HEC	C4A-NA-C1A	8.37	119.46	105.82
2	L	301	HEC	C3C-C4C-NC	8.31	119.37	110.15
2	I	301	HEC	C1D-ND-C4D	8.30	115.04	105.21
2	S	301	HEC	CHA-C1A-C2A	8.14	137.72	124.86
2	Q	304	HEC	C1D-ND-C4D	7.72	114.35	105.21
2	L	301	HEC	C4C-NC-C1C	-7.66	93.34	105.82
2	S	305	HEC	CAD-C3D-C4D	6.87	136.66	124.70
2	S	301	HEC	C3A-C4A-NA	-6.82	97.02	109.64
2	L	301	HEC	CHA-C1A-C2A	6.69	135.43	124.86
2	R	301	HEC	CAD-C3D-C4D	6.67	136.32	124.70
2	S	301	HEC	CAB-C3B-C4B	-6.57	116.24	124.79
2	E	305	HEC	CHB-C4A-NA	-6.43	117.45	124.45
2	S	301	HEC	C4A-CHB-C1B	6.30	139.41	126.02
2	R	301	HEC	CAB-C3B-C4B	-5.91	117.10	124.79
2	L	301	HEC	C3A-C4A-NA	-5.87	98.78	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	301	HEC	CHC-C1C-C2C	-5.82	110.52	127.43
2	S	301	HEC	C2C-C1C-NC	5.82	119.47	110.14
2	R	301	HEC	CAD-C3D-C2D	-5.72	117.15	127.87
2	M	301	HEC	C4B-NB-C1B	5.72	111.98	105.21
2	D	301	HEC	C1D-ND-C4D	5.72	111.98	105.21
2	S	305	HEC	CAD-C3D-C2D	-5.63	117.33	127.87
2	S	305	HEC	CHD-C1D-ND	5.57	131.26	124.37
2	S	301	HEC	CAB-C3B-C2B	5.55	137.75	127.56
2	G	303	HEC	CAD-CBD-CGD	-5.53	99.00	113.67
2	L	301	HEC	CBC-CAC-C3C	5.49	127.31	112.42
2	R	301	HEC	CHD-C1D-ND	5.48	131.15	124.37
2	S	301	HEC	CHA-C4D-ND	5.47	130.31	124.42
2	S	301	HEC	CAD-C3D-C4D	5.39	134.09	124.70
2	R	301	HEC	CAD-CBD-CGD	-5.32	99.54	113.67
2	S	301	HEC	CHA-C4D-C3D	-5.27	117.08	124.77
2	L	302	HEC	C1D-ND-C4D	5.25	111.43	105.21
2	L	301	HEC	C2B-C1B-NB	-5.19	103.90	109.90
2	S	301	HEC	C2B-C1B-NB	-5.11	103.99	109.90
2	L	301	HEC	C4A-CHB-C1B	5.09	136.85	126.02
2	J	302	HEC	C1D-ND-C4D	5.05	111.19	105.21
2	S	305	HEC	C2A-C1A-NA	-5.03	105.47	110.32
2	N	303	HEC	C1D-ND-C4D	5.02	111.16	105.21
2	G	303	HEC	C1D-ND-C4D	4.97	111.09	105.21
2	C	306	HEC	CAD-CBD-CGD	-4.97	100.49	113.67
2	S	301	HEC	CHB-C1B-C2B	4.97	132.87	125.03
2	L	301	HEC	CHC-C1C-C2C	-4.95	113.06	127.43
2	R	301	HEC	CAB-C3B-C2B	4.95	136.65	127.56
2	M	301	HEC	CAB-C3B-C4B	-4.93	118.37	124.79
2	C	306	HEC	C1D-ND-C4D	4.92	111.04	105.21
2	N	306	HEC	C1D-ND-C4D	4.91	111.02	105.21
2	S	301	HEC	C1C-CHC-C4B	-4.91	114.71	126.25
2	S	305	HEC	CHB-C4A-NA	4.89	129.78	124.45
2	T	301	HEC	C1D-ND-C4D	4.87	110.97	105.21
2	S	301	HEC	C2D-C1D-ND	4.86	115.43	109.84
2	L	301	HEC	CAB-C3B-C4B	-4.85	118.47	124.79
2	I	301	HEC	CHC-C4B-C3B	-4.82	116.34	125.23
2	I	301	HEC	CBC-CAC-C3C	4.82	125.48	112.42
2	E	305	HEC	C1D-ND-C4D	4.81	110.91	105.21
2	S	301	HEC	CAC-C3C-C4C	4.80	131.51	124.91
2	L	301	HEC	C2D-C1D-ND	4.78	115.33	109.84
2	L	301	HEC	CAB-C3B-C2B	4.77	136.33	127.56
2	L	301	HEC	CHB-C4A-C3A	4.74	135.36	125.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	302	HEC	C1D-ND-C4D	4.68	110.75	105.21
2	L	301	HEC	CAD-C3D-C4D	4.67	132.83	124.70
2	Q	301	HEC	C1D-ND-C4D	4.64	110.71	105.21
2	F	306	HEC	CAD-CBD-CGD	-4.64	101.36	113.67
2	P	303	HEC	C1D-ND-C4D	4.64	110.70	105.21
2	L	301	HEC	CBA-CAA-C2A	-4.64	99.71	112.53
2	I	301	HEC	C3B-C4B-NB	4.62	115.23	110.17
2	R	301	HEC	CHB-C1B-C2B	4.59	132.27	125.03
2	L	301	HEC	C2C-C1C-NC	4.54	117.42	110.14
2	L	301	HEC	CHA-C4D-ND	4.53	129.30	124.42
2	S	301	HEC	CHB-C4A-NA	4.53	129.39	124.45
2	J	306	HEC	C1B-C2B-C3B	-4.52	102.22	106.98
2	J	306	HEC	C2B-C1B-NB	4.51	115.12	109.90
2	J	305	HEC	CHA-C1A-C2A	4.49	131.96	124.86
2	S	301	HEC	CBC-CAC-C3C	4.47	124.53	112.42
2	L	301	HEC	C1C-CHC-C4B	-4.46	115.76	126.25
2	C	308	HEC	C1D-ND-C4D	4.45	110.48	105.21
2	S	305	HEC	C4A-NA-C1A	4.44	113.06	105.82
2	G	302	HEC	C2A-C1A-NA	-4.43	106.05	110.32
2	L	301	HEC	CHD-C4C-C3C	-4.42	115.62	125.30
2	F	302	HEC	C1D-ND-C4D	4.35	110.35	105.21
2	K	302	HEC	C1D-ND-C4D	4.32	110.33	105.21
2	Q	305	HEC	CAB-C3B-C4B	-4.32	119.17	124.79
2	S	302	HEC	C1D-ND-C4D	4.31	110.31	105.21
2	R	302	HEC	C1D-ND-C4D	4.30	110.30	105.21
2	M	301	HEC	C2B-C1B-NB	-4.29	104.95	109.90
2	S	301	HEC	CMD-C2D-C1D	4.28	131.72	125.03
2	J	306	HEC	CAB-C3B-C4B	-4.19	119.34	124.79
2	C	308	HEC	CAB-C3B-C4B	-4.18	119.35	124.79
2	J	305	HEC	C2A-C1A-NA	-4.17	106.30	110.32
2	G	302	HEC	CAB-C3B-C4B	-4.16	119.38	124.79
2	R	305	HEC	CAD-CBD-CGD	-4.14	102.67	113.67
2	E	305	HEC	C4A-C3A-C2A	-4.13	100.84	106.97
2	D	301	HEC	CAB-C3B-C4B	-4.13	119.42	124.79
2	K	302	HEC	CAD-C3D-C4D	4.12	131.87	124.70
2	P	306	HEC	C1D-ND-C4D	4.11	110.07	105.21
2	S	305	HEC	CHD-C1D-C2D	-4.10	115.28	126.95
2	M	301	HEC	CAD-C3D-C4D	4.10	131.85	124.70
2	F	301	HEC	CAB-C3B-C4B	-4.08	119.47	124.79
2	S	305	HEC	C3C-C4C-NC	4.07	114.67	110.15
2	P	302	HEC	C1D-ND-C4D	4.06	110.01	105.21
2	E	302	HEC	C1D-ND-C4D	4.05	110.00	105.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	302	HEC	C1D-ND-C4D	4.03	109.98	105.21
2	L	301	HEC	C1D-C2D-C3D	-4.03	102.75	106.98
2	R	301	HEC	C2B-C1B-NB	-4.01	105.27	109.90
2	S	301	HEC	CHD-C1D-C2D	-4.01	115.56	126.95
2	E	301	HEC	CAD-C3D-C4D	3.99	131.65	124.70
2	M	302	HEC	CAB-C3B-C4B	-3.98	119.61	124.79
2	I	301	HEC	CAB-C3B-C2B	3.95	134.82	127.56
2	L	301	HEC	C4B-NB-C1B	3.95	109.89	105.21
2	L	302	HEC	CAB-C3B-C4B	-3.95	119.65	124.79
2	M	306	HEC	CAD-CBD-CGD	-3.93	103.23	113.67
2	R	301	HEC	C4A-NA-C1A	3.92	112.22	105.82
2	R	301	HEC	CHD-C1D-C2D	-3.92	115.81	126.95
2	K	306	HEC	CAD-CBD-CGD	-3.92	103.27	113.67
2	N	303	HEC	CAD-CBD-CGD	-3.92	103.27	113.67
2	J	305	HEC	CMA-C3A-C4A	-3.91	117.84	124.73
2	L	301	HEC	C1B-C2B-C3B	3.91	111.09	106.98
2	I	301	HEC	C4B-NB-C1B	-3.91	100.58	105.21
2	S	301	HEC	CHB-C4A-C3A	3.90	133.59	125.49
2	E	302	HEC	CAD-C3D-C4D	3.89	131.47	124.70
2	G	302	HEC	CAB-C3B-C2B	3.89	134.70	127.56
2	R	301	HEC	CAC-C3C-C4C	3.88	130.25	124.91
2	P	303	HEC	CAB-C3B-C4B	-3.88	119.74	124.79
2	S	301	HEC	CHD-C4C-C3C	-3.87	116.84	125.30
2	F	301	HEC	CAB-C3B-C2B	3.86	134.65	127.56
2	S	305	HEC	CMA-C3A-C4A	-3.84	117.97	124.73
2	N	307	HEC	CAB-C3B-C4B	-3.81	119.83	124.79
2	P	308	HEC	CAB-C3B-C4B	-3.81	119.83	124.79
2	I	303	HEC	CAD-C3D-C4D	3.81	131.34	124.70
2	S	301	HEC	C4B-NB-C1B	3.81	109.72	105.21
2	E	306	HEC	CAD-CBD-CGD	-3.79	103.60	113.67
2	L	302	HEC	CAB-C3B-C2B	3.79	134.53	127.56
2	I	301	HEC	CAB-C3B-C4B	-3.79	119.85	124.79
2	K	302	HEC	CAB-C3B-C4B	-3.79	119.86	124.79
2	P	308	HEC	C1C-CHC-C4B	3.78	135.14	126.25
2	F	301	HEC	C2A-C1A-NA	-3.78	106.68	110.32
2	S	305	HEC	CAB-C3B-C4B	-3.77	119.88	124.79
2	S	301	HEC	C1B-C2B-C3B	3.76	110.94	106.98
2	C	301	HEC	C1D-ND-C4D	3.76	109.66	105.21
2	S	301	HEC	CHD-C1D-ND	3.76	129.01	124.37
2	S	301	HEC	C1D-C2D-C3D	-3.74	103.05	106.98
2	E	302	HEC	CAB-C3B-C4B	-3.74	119.93	124.79
2	S	305	HEC	C4C-NC-C1C	-3.73	99.73	105.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	301	HEC	CHB-C4A-NA	3.72	128.51	124.45
2	J	301	HEC	C1D-ND-C4D	3.72	109.61	105.21
2	C	303	HEC	CAD-C3D-C4D	3.72	131.18	124.70
2	N	306	HEC	C1A-CHA-C4D	3.71	133.91	126.02
2	M	302	HEC	CAB-C3B-C2B	3.70	134.35	127.56
2	C	307	HEC	CAD-C3D-C4D	3.69	131.13	124.70
2	S	301	HEC	CAD-C3D-C2D	-3.69	120.96	127.87
2	R	301	HEC	C4C-NC-C1C	-3.68	99.82	105.82
2	N	302	HEC	C1D-ND-C4D	3.68	109.56	105.21
2	Q	301	HEC	CAD-CBD-CGD	-3.68	103.91	113.67
2	C	306	HEC	CAA-C2A-C3A	-3.68	120.98	127.87
2	M	305	HEC	CAD-CBD-CGD	-3.66	103.95	113.67
2	N	303	HEC	CAB-C3B-C4B	-3.66	120.03	124.79
2	M	302	HEC	CAD-CBD-CGD	-3.66	103.96	113.67
2	J	302	HEC	CAD-C3D-C4D	3.65	131.06	124.70
2	C	303	HEC	C1D-ND-C4D	3.65	109.53	105.21
2	Q	301	HEC	CAB-C3B-C4B	-3.65	120.04	124.79
2	L	301	HEC	CHA-C4D-C3D	-3.64	119.46	124.77
2	R	305	HEC	C1D-ND-C4D	3.61	109.48	105.21
2	D	301	HEC	CAB-C3B-C2B	3.59	134.15	127.56
2	R	301	HEC	C2A-C1A-NA	-3.58	106.86	110.32
2	L	306	HEC	CAD-CBD-CGD	-3.58	104.17	113.67
2	P	301	HEC	C1D-ND-C4D	3.57	109.43	105.21
2	M	301	HEC	C2D-C1D-ND	3.56	113.93	109.84
2	Q	304	HEC	CAA-C2A-C3A	-3.56	121.20	127.87
2	S	305	HEC	CHB-C1B-C2B	3.55	130.63	125.03
2	P	307	HEC	CAD-C3D-C4D	3.55	130.88	124.70
2	S	302	HEC	CAB-C3B-C4B	-3.54	120.18	124.79
2	L	301	HEC	CMD-C2D-C1D	3.54	130.57	125.03
2	D	305	HEC	C1D-ND-C4D	3.54	109.40	105.21
2	N	301	HEC	C1D-ND-C4D	3.51	109.36	105.21
2	D	305	HEC	CAD-CBD-CGD	-3.49	104.40	113.67
2	R	301	HEC	C3C-C4C-NC	3.48	114.02	110.15
2	G	302	HEC	C1D-ND-C4D	3.47	109.32	105.21
2	L	301	HEC	CAD-C3D-C2D	-3.47	121.36	127.87
2	G	301	HEC	C1D-ND-C4D	3.47	109.32	105.21
2	E	305	HEC	C1A-CHA-C4D	3.46	133.37	126.02
2	C	306	HEC	CHA-C4D-ND	3.45	128.14	124.42
2	I	301	HEC	C2D-C1D-ND	-3.44	105.88	109.84
2	J	302	HEC	CAB-C3B-C4B	-3.44	120.31	124.79
2	N	303	HEC	CAB-C3B-C2B	3.43	133.86	127.56
2	L	301	HEC	CHB-C1B-C2B	3.43	130.44	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	301	HEC	C4A-C3A-C2A	3.42	112.05	106.97
2	T	302	HEC	CAB-C3B-C2B	3.41	133.83	127.56
2	R	301	HEC	C3A-C4A-NA	-3.40	103.34	109.64
2	T	302	HEC	C1D-ND-C4D	3.40	109.23	105.21
2	Q	304	HEC	CHB-C1B-NB	3.39	128.07	124.42
2	R	302	HEC	CMA-C3A-C4A	3.39	130.70	124.73
2	S	301	HEC	CHC-C1C-NC	3.39	130.00	123.86
2	M	301	HEC	C3B-C4B-NB	-3.38	106.46	110.17
2	D	301	HEC	CAD-C3D-C4D	3.38	130.59	124.70
2	I	301	HEC	CBB-CAB-C3B	3.38	121.57	112.42
2	S	305	HEC	C3A-C4A-NA	-3.37	103.39	109.64
2	Q	304	HEC	CHB-C1B-C2B	-3.34	119.76	125.03
2	R	306	HEC	C1D-ND-C4D	3.34	109.16	105.21
2	G	303	HEC	CAD-C3D-C4D	3.33	130.51	124.70
2	J	306	HEC	CAD-CBD-CGD	-3.32	104.87	113.67
2	G	302	HEC	C4A-NA-C1A	3.31	111.22	105.82
2	N	306	HEC	C3D-C4D-ND	-3.30	107.16	110.35
2	S	305	HEC	CHA-C1A-C2A	3.30	130.08	124.86
2	I	302	HEC	C1D-ND-C4D	3.30	109.11	105.21
2	Q	301	HEC	CAD-C3D-C4D	3.30	130.45	124.70
2	S	307	HEC	CAD-C3D-C4D	3.29	130.43	124.70
2	S	301	HEC	CBA-CAA-C2A	-3.29	103.44	112.53
2	I	301	HEC	CHC-C4B-NB	3.28	128.43	124.37
2	F	301	HEC	CAD-C3D-C4D	3.28	130.41	124.70
2	R	302	HEC	CAB-C3B-C4B	-3.27	120.53	124.79
2	R	302	HEC	CAB-C3B-C2B	3.26	133.55	127.56
2	I	303	HEC	CAB-C3B-C4B	-3.25	120.55	124.79
2	R	306	HEC	CAA-C2A-C3A	-3.25	121.78	127.87
2	E	305	HEC	C1A-C2A-C3A	3.25	111.39	107.11
2	Q	301	HEC	CAB-C3B-C2B	3.25	133.53	127.56
2	P	303	HEC	CAB-C3B-C2B	3.25	133.52	127.56
2	E	302	HEC	CAB-C3B-C2B	3.24	133.50	127.56
2	Q	304	HEC	C3D-C4D-ND	-3.23	107.23	110.35
2	E	305	HEC	C3D-C4D-ND	-3.23	107.23	110.35
2	M	301	HEC	CHB-C1B-C2B	3.21	130.10	125.03
2	M	301	HEC	CAB-C3B-C2B	3.20	133.44	127.56
2	M	305	HEC	C2A-C1A-NA	-3.20	107.24	110.32
2	F	301	HEC	C4C-NC-C1C	-3.20	100.61	105.82
2	S	305	HEC	CAB-C3B-C2B	3.20	133.43	127.56
2	R	302	HEC	CAA-CBA-CGA	-3.20	105.19	113.67
2	K	302	HEC	CAB-C3B-C2B	3.19	133.43	127.56
2	G	303	HEC	CAB-C3B-C4B	-3.19	120.64	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	301	HEC	CAC-C3C-C4C	3.19	129.30	124.91
2	M	306	HEC	CAB-C3B-C4B	-3.19	120.64	124.79
2	M	306	HEC	C2B-C1B-NB	3.19	113.59	109.90
2	J	302	HEC	CAD-CBD-CGD	-3.18	105.22	113.67
2	J	306	HEC	CMB-C2B-C3B	3.18	134.76	126.15
2	J	302	HEC	CAB-C3B-C2B	3.18	133.40	127.56
2	D	304	HEC	CAD-CBD-CGD	-3.18	105.23	113.67
2	K	301	HEC	C1D-ND-C4D	3.18	108.97	105.21
2	F	301	HEC	C4A-NA-C1A	3.18	111.00	105.82
2	R	301	HEC	C4A-C3A-C2A	3.17	111.68	106.97
2	R	301	HEC	C4B-NB-C1B	3.17	108.96	105.21
2	L	301	HEC	CHD-C1D-C2D	-3.17	117.95	126.95
2	P	308	HEC	CHA-C4D-C3D	-3.16	120.16	124.77
2	C	303	HEC	CAB-C3B-C4B	-3.16	120.67	124.79
2	M	302	HEC	CAA-CBA-CGA	-3.16	105.29	113.67
2	S	305	HEC	C2D-C1D-ND	3.15	113.46	109.84
2	C	308	HEC	CAB-C3B-C2B	3.13	133.32	127.56
2	E	301	HEC	CAB-C3B-C4B	-3.13	120.71	124.79
2	N	303	HEC	CAD-C3D-C4D	3.13	130.15	124.70
2	F	302	HEC	CAB-C3B-C4B	-3.13	120.72	124.79
2	D	301	HEC	CAD-CBD-CGD	-3.13	105.37	113.67
2	L	301	HEC	CHC-C1C-NC	3.12	129.52	123.86
2	C	302	HEC	CAB-C3B-C4B	-3.11	120.74	124.79
2	S	305	HEC	C4A-C3A-C2A	3.10	111.58	106.97
2	M	305	HEC	C1D-ND-C4D	3.09	108.87	105.21
2	I	301	HEC	CAD-C3D-C2D	3.08	133.63	127.87
2	J	305	HEC	C1D-ND-C4D	3.08	108.85	105.21
2	T	302	HEC	CAB-C3B-C4B	-3.08	120.78	124.79
2	S	306	HEC	CAD-CBD-CGD	-3.08	105.51	113.67
2	T	302	HEC	CHC-C4B-NB	3.07	128.16	124.37
2	E	305	HEC	C3A-C4A-NA	3.06	115.31	109.64
2	M	306	HEC	C1B-C2B-C3B	-3.06	103.76	106.98
2	S	302	HEC	CAB-C3B-C2B	3.06	133.18	127.56
2	S	306	HEC	C1D-ND-C4D	3.05	108.82	105.21
2	L	305	HEC	C1D-ND-C4D	3.05	108.81	105.21
2	M	302	HEC	CAD-C3D-C4D	3.04	130.00	124.70
2	F	301	HEC	C3C-C4C-NC	3.04	113.53	110.15
2	E	305	HEC	CMA-C3A-C4A	3.04	130.08	124.73
2	N	301	HEC	CAD-C3D-C4D	3.03	129.99	124.70
2	R	301	HEC	CBC-CAC-C3C	3.03	120.63	112.42
2	G	302	HEC	CHA-C1A-C2A	3.02	129.64	124.86
2	P	307	HEC	CAB-C3B-C4B	-3.02	120.86	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	301	HEC	C3D-C4D-ND	3.02	113.27	110.35
2	D	304	HEC	C1D-ND-C4D	3.02	108.78	105.21
2	T	302	HEC	C1B-C2B-C3B	3.01	110.14	106.98
2	E	305	HEC	C1D-C2D-C3D	-3.00	103.83	106.98
2	J	305	HEC	CMA-C3A-C2A	2.99	134.23	126.15
2	S	307	HEC	CAA-C2A-C3A	-2.98	122.28	127.87
2	F	301	HEC	CHD-C1D-ND	2.98	128.05	124.37
2	K	306	HEC	C1D-ND-C4D	2.97	108.73	105.21
2	S	305	HEC	CAD-CBD-CGD	-2.97	105.79	113.67
2	G	303	HEC	CAB-C3B-C2B	2.97	133.01	127.56
2	C	308	HEC	CAD-CBD-CGD	-2.96	105.81	113.67
2	N	306	HEC	CAD-C3D-C4D	2.96	129.85	124.70
2	D	301	HEC	CAA-CBA-CGA	-2.96	105.82	113.67
2	J	306	HEC	CHB-C4A-NA	2.95	127.67	124.45
2	M	305	HEC	CAD-C3D-C4D	2.95	129.84	124.70
2	S	305	HEC	C2B-C1B-NB	-2.95	106.49	109.90
2	I	301	HEC	C3D-C4D-ND	-2.94	107.51	110.35
2	L	302	HEC	CAD-CBD-CGD	-2.94	105.86	113.67
2	C	303	HEC	CAB-C3B-C2B	2.94	132.96	127.56
2	J	305	HEC	C1D-C2D-C3D	-2.94	103.89	106.98
2	Q	304	HEC	C4A-CHB-C1B	-2.93	119.80	126.02
2	F	306	HEC	C2B-C1B-NB	2.93	113.28	109.90
2	N	306	HEC	C4C-NC-C1C	-2.92	101.06	105.82
2	P	303	HEC	CAA-CBA-CGA	-2.92	105.92	113.67
2	K	301	HEC	CAB-C3B-C4B	-2.92	120.99	124.79
2	M	301	HEC	CHD-C1D-C2D	-2.91	118.67	126.95
2	K	305	HEC	C1D-ND-C4D	2.91	108.65	105.21
2	P	308	HEC	CHA-C4D-ND	2.89	127.53	124.42
2	M	301	HEC	CHA-C4D-C3D	-2.89	120.56	124.77
2	P	308	HEC	CAD-CBD-CGD	-2.89	106.00	113.67
2	N	307	HEC	CAD-CBD-CGD	-2.89	106.01	113.67
2	P	307	HEC	CAA-C2A-C1A	2.86	130.67	124.85
2	J	306	HEC	CHB-C1B-NB	-2.86	121.34	124.42
2	R	301	HEC	CHA-C1A-C2A	2.85	129.36	124.86
2	Q	304	HEC	C3A-C4A-NA	2.85	114.91	109.64
2	L	306	HEC	CAD-C3D-C4D	2.85	129.66	124.70
2	R	306	HEC	CAA-C2A-C1A	2.85	130.64	124.85
2	S	305	HEC	CBA-CAA-C2A	-2.83	104.71	112.53
2	J	302	HEC	CAA-CBA-CGA	-2.83	106.17	113.67
2	L	302	HEC	CHC-C4B-C3B	-2.83	120.02	125.23
2	Q	305	HEC	CAD-CBD-CGD	-2.83	106.17	113.67
2	L	301	HEC	C4A-C3A-C2A	2.82	111.16	106.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	302	HEC	CHB-C4A-NA	2.81	127.52	124.45
2	C	306	HEC	CAA-CBA-CGA	-2.81	106.21	113.67
2	R	302	HEC	CHA-C1A-NA	2.81	127.51	124.45
2	S	301	HEC	C4C-C3C-C2C	-2.80	102.53	106.87
2	I	303	HEC	CAB-C3B-C2B	2.80	132.71	127.56
2	F	302	HEC	CAB-C3B-C2B	2.80	132.70	127.56
2	C	308	HEC	CMB-C2B-C1B	-2.80	120.66	125.03
2	Q	305	HEC	CMB-C2B-C1B	-2.80	120.66	125.03
2	J	302	HEC	CMD-C2D-C1D	2.79	129.40	125.03
2	G	302	HEC	CHD-C1D-ND	2.79	127.82	124.37
2	S	305	HEC	CHC-C4B-NB	2.79	127.82	124.37
2	K	305	HEC	CAD-C3D-C4D	2.79	129.56	124.70
2	E	305	HEC	C4C-NC-C1C	-2.79	101.27	105.82
2	R	301	HEC	C2D-C1D-ND	2.78	113.04	109.84
2	G	302	HEC	C1D-C2D-C3D	-2.78	104.05	106.98
2	E	305	HEC	CHB-C1B-NB	2.78	127.42	124.42
2	T	302	HEC	CAD-C3D-C2D	2.78	133.07	127.87
2	K	301	HEC	CAD-C3D-C4D	2.77	129.53	124.70
2	S	305	HEC	CBC-CAC-C3C	2.77	119.93	112.42
2	S	302	HEC	CAD-CBD-CGD	-2.77	106.33	113.67
2	N	306	HEC	C1D-C2D-C3D	-2.76	104.07	106.98
2	M	306	HEC	CMB-C2B-C3B	2.76	133.61	126.15
2	J	301	HEC	CAB-C3B-C4B	-2.76	121.20	124.79
2	P	308	HEC	C4A-CHB-C1B	-2.75	120.17	126.02
2	I	301	HEC	CHC-C1C-C2C	-2.75	119.45	127.43
2	S	305	HEC	CHA-C4D-C3D	2.75	128.78	124.77
2	N	302	HEC	CAD-C3D-C4D	2.74	129.48	124.70
2	T	302	HEC	CAA-CBA-CGA	-2.74	106.39	113.67
2	T	301	HEC	C2A-C1A-NA	-2.74	107.68	110.32
2	C	301	HEC	CAA-CBA-CGA	-2.74	106.41	113.67
2	S	307	HEC	CAA-C2A-C1A	2.74	130.41	124.85
2	F	306	HEC	C1D-ND-C4D	2.73	108.44	105.21
2	E	305	HEC	CHC-C4B-NB	2.73	127.75	124.37
2	J	305	HEC	CAD-CBD-CGD	-2.73	106.42	113.67
2	F	306	HEC	C1B-C2B-C3B	-2.73	104.11	106.98
2	L	306	HEC	C1D-ND-C4D	2.72	108.43	105.21
2	L	302	HEC	CBB-CAB-C3B	2.72	119.79	112.42
2	P	301	HEC	CAA-CBA-CGA	-2.72	106.46	113.67
2	G	302	HEC	CHC-C4B-C3B	-2.71	120.22	125.23
2	Q	304	HEC	CHC-C4B-NB	2.71	127.72	124.37
2	N	306	HEC	CHB-C4A-NA	-2.71	121.50	124.45
2	D	305	HEC	C2B-C1B-NB	2.71	113.03	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	304	HEC	C4A-C3A-C2A	-2.70	102.97	106.97
2	R	301	HEC	CHC-C1C-C2C	-2.70	119.59	127.43
2	F	305	HEC	C1D-C2D-C3D	-2.70	104.14	106.98
2	G	302	HEC	C4C-NC-C1C	-2.70	101.43	105.82
2	I	302	HEC	CAD-CBD-CGD	-2.69	106.54	113.67
2	J	305	HEC	C4A-NA-C1A	2.68	110.19	105.82
2	M	306	HEC	C1D-ND-C4D	2.68	108.38	105.21
2	I	303	HEC	C1D-ND-C4D	2.68	108.38	105.21
2	R	302	HEC	CBB-CAB-C3B	2.68	119.67	112.42
2	S	301	HEC	CHA-C1A-NA	-2.67	121.54	124.45
2	C	307	HEC	C1D-ND-C4D	2.67	108.37	105.21
2	J	305	HEC	CHB-C4A-NA	2.67	127.36	124.45
2	F	301	HEC	CHA-C1A-C2A	2.67	129.08	124.86
2	P	308	HEC	CMB-C2B-C3B	2.67	133.37	126.15
2	F	301	HEC	C2B-C1B-NB	-2.67	106.82	109.90
2	T	302	HEC	CAC-C3C-C4C	2.67	128.58	124.91
2	C	308	HEC	CMB-C2B-C3B	2.66	133.34	126.15
2	Q	305	HEC	CAB-C3B-C2B	2.64	132.41	127.56
2	D	304	HEC	C1D-C2D-C3D	-2.64	104.20	106.98
2	L	302	HEC	CAA-CBA-CGA	-2.63	106.68	113.67
2	P	303	HEC	CBD-CAD-C3D	-2.63	105.26	112.53
2	N	306	HEC	C3C-C4C-NC	2.63	113.07	110.15
2	S	301	HEC	CAD-CBD-CGD	-2.63	106.70	113.67
2	N	306	HEC	CHA-C1A-C2A	2.62	129.01	124.86
2	Q	305	HEC	CMB-C2B-C3B	2.62	133.23	126.15
2	E	301	HEC	C4B-NB-C1B	2.62	108.31	105.21
2	J	305	HEC	C4C-NC-C1C	-2.61	101.56	105.82
2	E	305	HEC	CAD-C3D-C4D	2.61	129.25	124.70
2	D	304	HEC	C2A-C1A-NA	-2.61	107.81	110.32
2	E	302	HEC	CAA-CBA-CGA	-2.61	106.75	113.67
2	T	302	HEC	C2B-C1B-NB	-2.60	106.89	109.90
2	G	302	HEC	CHC-C4B-NB	2.60	127.58	124.37
2	N	306	HEC	CAD-C3D-C2D	-2.60	123.00	127.87
2	N	306	HEC	CHC-C4B-NB	2.59	127.57	124.37
2	J	305	HEC	CAD-C3D-C4D	2.58	129.20	124.70
2	N	307	HEC	CAB-C3B-C2B	2.58	132.30	127.56
2	G	302	HEC	CBA-CAA-C2A	-2.57	105.42	112.53
2	R	301	HEC	CMD-C2D-C1D	2.57	129.04	125.03
2	N	307	HEC	C1D-C2D-C3D	-2.56	104.28	106.98
2	R	302	HEC	CBC-CAC-C3C	-2.56	105.47	112.42
2	R	301	HEC	C4A-CHB-C1B	2.56	131.46	126.02
2	C	307	HEC	CAB-C3B-C4B	-2.56	121.46	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	305	HEC	CMC-C2C-C1C	2.56	129.31	125.42
2	Q	305	HEC	C1D-C2D-C3D	-2.55	104.30	106.98
2	Q	304	HEC	C1A-C2A-C3A	2.55	110.46	107.11
2	G	302	HEC	C1C-CHC-C4B	-2.54	120.27	126.25
2	L	301	HEC	CAA-C2A-C1A	-2.54	119.68	124.85
2	D	301	HEC	CBB-CAB-C3B	2.54	119.31	112.42
2	F	301	HEC	CBC-CAC-C3C	2.53	119.29	112.42
2	T	302	HEC	CBB-CAB-C3B	2.53	119.28	112.42
2	F	301	HEC	C1D-ND-C4D	2.53	108.20	105.21
2	L	301	HEC	CMC-C2C-C1C	2.53	129.26	125.42
2	E	302	HEC	CBB-CAB-C3B	2.52	119.27	112.42
2	P	302	HEC	CAB-C3B-C4B	-2.51	121.52	124.79
2	E	305	HEC	C3C-C4C-NC	2.51	112.94	110.15
2	L	302	HEC	C2A-C1A-NA	-2.51	107.90	110.32
2	E	305	HEC	CAB-C3B-C4B	-2.51	121.53	124.79
2	P	307	HEC	CAA-C2A-C3A	-2.51	123.17	127.87
2	R	302	HEC	CAD-C3D-C4D	2.50	129.06	124.70
2	S	305	HEC	C1D-C2D-C3D	-2.50	104.35	106.98
2	P	307	HEC	C3C-C4C-NC	-2.50	107.38	110.15
2	N	306	HEC	CAA-CBA-CGA	2.50	120.29	113.67
2	N	307	HEC	CMC-C2C-C1C	2.50	129.22	125.42
2	J	305	HEC	CHA-C1A-NA	-2.49	121.74	124.45
2	F	301	HEC	CHD-C1D-C2D	-2.49	119.87	126.95
2	K	302	HEC	CBB-CAB-C3B	2.49	119.16	112.42
2	I	301	HEC	CHA-C4D-ND	2.49	127.10	124.42
2	P	307	HEC	C4D-C3D-C2D	-2.48	103.28	106.89
2	I	301	HEC	CHC-C1C-NC	2.48	128.36	123.86
2	C	306	HEC	C2A-C1A-NA	-2.48	107.93	110.32
2	F	306	HEC	CAB-C3B-C4B	-2.48	121.56	124.79
2	K	305	HEC	CAD-CBD-CGD	-2.48	107.09	113.67
2	N	306	HEC	C4C-CHD-C1D	-2.47	120.45	126.25
2	T	302	HEC	CHA-C1A-NA	2.47	127.14	124.45
2	G	302	HEC	O2D-CGD-CBD	2.46	121.78	114.00
2	K	305	HEC	C1D-C2D-C3D	-2.46	104.39	106.98
2	Q	304	HEC	C2D-C1D-ND	-2.46	107.02	109.84
2	E	301	HEC	CAB-C3B-C2B	2.45	132.07	127.56
2	M	301	HEC	CHD-C1D-ND	2.45	127.40	124.37
2	S	301	HEC	CMA-C3A-C4A	-2.45	120.41	124.73
2	L	302	HEC	CAD-C3D-C4D	2.45	128.96	124.70
2	S	305	HEC	C1C-CHC-C4B	-2.44	120.50	126.25
2	D	305	HEC	C1B-C2B-C3B	-2.44	104.41	106.98
2	D	305	HEC	CAB-C3B-C4B	-2.44	121.61	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	305	HEC	CBB-CAB-C3B	2.44	119.03	112.42
2	T	302	HEC	CHC-C4B-C3B	-2.44	120.73	125.23
2	G	303	HEC	CMC-C2C-C3C	2.44	130.79	125.62
2	F	301	HEC	C1D-C2D-C3D	-2.43	104.42	106.98
2	P	303	HEC	CBB-CAB-C3B	2.43	119.00	112.42
2	F	305	HEC	C1D-ND-C4D	2.43	108.08	105.21
2	F	305	HEC	CAD-C3D-C4D	2.42	128.91	124.70
2	M	305	HEC	C1D-C2D-C3D	-2.41	104.44	106.98
2	E	306	HEC	C1D-C2D-C3D	-2.41	104.45	106.98
2	I	301	HEC	O1D-CGD-CBD	-2.40	115.47	123.09
2	J	302	HEC	CMC-C2C-C3C	2.40	130.71	125.62
2	R	306	HEC	CAD-C3D-C4D	2.40	128.87	124.70
2	Q	304	HEC	CMA-C3A-C4A	2.39	128.94	124.73
2	T	301	HEC	C1D-C2D-C3D	-2.38	104.47	106.98
2	L	302	HEC	CHC-C1C-C2C	-2.38	120.51	127.43
2	K	306	HEC	CAB-C3B-C4B	-2.38	121.69	124.79
2	I	301	HEC	O2D-CGD-CBD	2.38	121.50	114.00
2	K	305	HEC	C2A-C1A-NA	-2.37	108.03	110.32
2	S	307	HEC	C2A-C1A-NA	-2.37	108.03	110.32
2	F	305	HEC	C2A-C1A-NA	-2.37	108.03	110.32
2	L	305	HEC	C1D-C2D-C3D	-2.37	104.48	106.98
2	F	302	HEC	CAD-C3D-C4D	2.37	128.83	124.70
2	C	308	HEC	C1D-C2D-C3D	-2.37	104.49	106.98
2	I	301	HEC	CHD-C4C-C3C	2.37	130.49	125.30
2	Q	304	HEC	C4B-NB-C1B	-2.37	102.40	105.21
2	D	301	HEC	CMC-C2C-C3C	2.37	130.64	125.62
2	M	305	HEC	CAA-CBA-CGA	-2.36	107.40	113.67
2	C	306	HEC	CAA-C2A-C1A	2.36	129.65	124.85
2	N	306	HEC	CBD-CAD-C3D	-2.36	106.01	112.53
2	K	302	HEC	CAD-C3D-C2D	-2.36	123.45	127.87
2	C	301	HEC	CAD-C3D-C4D	2.36	128.81	124.70
2	P	306	HEC	CAD-C3D-C4D	2.36	128.81	124.70
2	G	302	HEC	CHD-C1D-C2D	-2.35	120.26	126.95
2	F	306	HEC	CMB-C2B-C3B	2.35	132.49	126.15
2	C	306	HEC	CHB-C1B-NB	2.34	126.94	124.42
2	L	302	HEC	CHC-C4B-NB	2.34	127.26	124.37
2	J	302	HEC	CMC-C2C-C1C	-2.34	121.86	125.42
2	P	308	HEC	C1B-C2B-C3B	-2.34	104.52	106.98
2	M	302	HEC	CBB-CAB-C3B	2.33	118.75	112.42
2	S	301	HEC	C3D-C4D-ND	2.33	112.61	110.35
2	S	302	HEC	CBB-CAB-C3B	2.33	118.73	112.42
2	L	302	HEC	C3B-C4B-NB	2.33	112.72	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	306	HEC	C1D-C2D-C3D	-2.32	104.54	106.98
2	P	306	HEC	CAA-C2A-C3A	-2.32	123.52	127.87
2	R	302	HEC	CAD-CBD-CGD	-2.32	107.52	113.67
2	R	301	HEC	C1C-CHC-C4B	-2.32	120.80	126.25
2	M	305	HEC	CHA-C1A-C2A	2.31	128.52	124.86
2	I	301	HEC	CAD-C3D-C4D	-2.31	120.67	124.70
2	N	303	HEC	CMC-C2C-C3C	2.31	130.53	125.62
2	E	305	HEC	CHA-C1A-C2A	2.31	128.51	124.86
2	E	306	HEC	C4B-NB-C1B	2.31	107.94	105.21
2	P	302	HEC	CAD-C3D-C4D	2.30	128.71	124.70
2	L	305	HEC	CAA-C2A-C3A	-2.30	123.55	127.87
2	P	307	HEC	C4C-NC-C1C	2.30	109.57	105.82
2	P	308	HEC	CHB-C4A-NA	2.30	126.96	124.45
2	J	306	HEC	C2C-C1C-NC	-2.30	106.46	110.14
2	E	305	HEC	CAD-C3D-C2D	-2.30	123.57	127.87
2	P	303	HEC	CMB-C2B-C1B	-2.29	121.45	125.03
2	Q	304	HEC	C4A-NA-C1A	-2.29	102.09	105.82
2	K	302	HEC	CHD-C1D-ND	2.29	127.20	124.37
2	P	308	HEC	CHB-C1B-NB	-2.29	121.96	124.42
2	G	303	HEC	CHC-C4B-NB	2.29	127.20	124.37
2	G	303	HEC	CMC-C2C-C1C	-2.29	121.94	125.42
2	F	306	HEC	CHB-C4A-NA	2.28	126.94	124.45
2	M	306	HEC	C1D-C2D-C3D	-2.28	104.58	106.98
2	D	305	HEC	CMB-C2B-C3B	2.28	132.32	126.15
2	T	302	HEC	CAC-C3C-C2C	-2.28	123.28	126.89
2	S	306	HEC	CMB-C2B-C3B	2.28	132.31	126.15
2	R	301	HEC	CHC-C4B-NB	2.27	127.18	124.37
2	E	306	HEC	CAB-C3B-C4B	-2.27	121.84	124.79
2	F	301	HEC	C3A-C4A-NA	-2.26	105.45	109.64
2	F	301	HEC	CHC-C1C-C2C	-2.26	120.87	127.43
2	F	301	HEC	C1C-CHC-C4B	-2.26	120.94	126.25
2	J	306	HEC	C1D-C2D-C3D	-2.26	104.61	106.98
2	R	301	HEC	O1D-CGD-CBD	-2.25	115.94	123.09
2	L	302	HEC	CHA-C4D-ND	2.25	126.85	124.42
2	E	305	HEC	CHA-C1A-NA	-2.25	122.00	124.45
2	E	302	HEC	CAD-C3D-C2D	-2.25	123.66	127.87
2	C	302	HEC	CAB-C3B-C2B	2.25	131.69	127.56
2	K	306	HEC	C1D-C2D-C3D	-2.25	104.62	106.98
2	J	306	HEC	C4B-NB-C1B	-2.25	102.55	105.21
2	F	305	HEC	CAA-C2A-C3A	-2.24	123.66	127.87
2	L	301	HEC	CMB-C2B-C1B	-2.24	121.53	125.03
2	M	301	HEC	CHC-C4B-NB	2.24	127.14	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	304	HEC	C3C-C4C-NC	-2.24	107.67	110.15
2	J	301	HEC	CAD-C3D-C4D	2.23	128.59	124.70
2	J	306	HEC	CAD-C3D-C4D	2.23	128.59	124.70
2	L	305	HEC	CAD-C3D-C4D	2.23	128.58	124.70
2	C	302	HEC	CHC-C4B-NB	2.23	127.12	124.37
2	P	306	HEC	CHC-C4B-NB	2.22	127.12	124.37
2	E	301	HEC	C2B-C1B-NB	-2.22	107.33	109.90
2	J	305	HEC	C3C-C4C-NC	2.22	112.62	110.15
2	E	301	HEC	CAD-C3D-C2D	-2.22	123.70	127.87
2	E	306	HEC	CAD-C3D-C4D	2.22	128.57	124.70
2	C	308	HEC	C2B-C1B-NB	2.22	112.47	109.90
2	C	303	HEC	CHD-C1D-ND	2.22	127.11	124.37
2	S	307	HEC	CAA-CBA-CGA	-2.22	107.78	113.67
2	Q	304	HEC	CHC-C4B-C3B	-2.22	121.14	125.23
2	Q	305	HEC	C2D-C1D-ND	2.21	112.38	109.84
2	C	307	HEC	CHD-C1D-ND	2.21	127.10	124.37
2	P	306	HEC	CMA-C3A-C4A	2.21	128.62	124.73
2	M	302	HEC	CHC-C4B-C3B	-2.21	121.16	125.23
2	J	306	HEC	CMC-C2C-C1C	2.21	128.78	125.42
2	R	301	HEC	C1D-C2D-C3D	-2.20	104.66	106.98
2	R	301	HEC	CMA-C3A-C4A	-2.20	120.85	124.73
2	G	303	HEC	CAD-C3D-C2D	-2.20	123.75	127.87
2	T	302	HEC	CMA-C3A-C4A	2.19	128.59	124.73
2	Q	305	HEC	CHA-C4D-C3D	-2.19	121.58	124.77
2	C	306	HEC	C1D-C2D-C3D	-2.19	104.68	106.98
2	P	308	HEC	CHA-C1A-NA	2.19	126.84	124.45
2	S	302	HEC	CAA-CBA-CGA	-2.19	107.86	113.67
2	Q	304	HEC	CAD-CBD-CGD	-2.19	107.86	113.67
2	M	301	HEC	CMD-C2D-C1D	2.18	128.44	125.03
2	G	302	HEC	C3C-C4C-NC	2.18	112.57	110.15
2	G	303	HEC	CHC-C4B-C3B	-2.18	121.21	125.23
2	C	307	HEC	CAB-C3B-C2B	2.18	131.56	127.56
2	C	306	HEC	O1A-CGA-CBA	-2.17	116.20	123.09
2	C	306	HEC	CHA-C1A-C2A	2.17	128.29	124.86
2	M	306	HEC	CHB-C4A-NA	2.17	126.81	124.45
2	I	301	HEC	C3C-C4C-NC	-2.16	107.75	110.15
2	M	302	HEC	C2A-C1A-NA	-2.16	108.24	110.32
2	P	307	HEC	CAC-C3C-C4C	-2.16	121.94	124.91
2	C	301	HEC	CAA-C2A-C3A	-2.16	123.82	127.87
2	N	302	HEC	CAB-C3B-C4B	-2.16	121.98	124.79
2	M	305	HEC	CAA-C2A-C3A	-2.16	123.83	127.87
2	F	302	HEC	CAA-CBA-CGA	-2.16	107.94	113.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	302	HEC	CHD-C1D-ND	2.16	127.03	124.37
2	Q	305	HEC	CAC-C3C-C2C	2.16	130.30	126.89
2	J	302	HEC	CHC-C1C-NC	2.15	127.77	123.86
2	K	302	HEC	CAA-CBA-CGA	-2.15	107.96	113.67
2	G	301	HEC	CAA-C2A-C3A	-2.15	123.84	127.87
2	F	302	HEC	CAD-CBD-CGD	-2.15	107.97	113.67
2	R	301	HEC	CBB-CAB-C3B	2.15	118.24	112.42
2	M	305	HEC	CHB-C4A-NA	2.15	126.79	124.45
2	L	302	HEC	CHC-C1C-NC	2.15	127.75	123.86
2	I	301	HEC	C1C-CHC-C4B	-2.14	121.20	126.25
2	Q	301	HEC	CHC-C4B-C3B	-2.14	121.28	125.23
2	D	301	HEC	CMC-C2C-C1C	-2.14	122.16	125.42
2	G	301	HEC	CAA-CBA-CGA	-2.14	107.99	113.67
2	S	305	HEC	CHC-C1C-C2C	-2.14	121.22	127.43
2	P	301	HEC	CAD-C3D-C4D	2.13	128.41	124.70
2	N	307	HEC	C2D-C1D-ND	2.13	112.29	109.84
2	P	308	HEC	C4C-CHD-C1D	-2.13	121.24	126.25
2	L	301	HEC	C4C-C3C-C2C	-2.13	103.58	106.87
2	G	302	HEC	C3A-C4A-NA	-2.13	105.70	109.64
2	D	304	HEC	CAA-C2A-C3A	-2.13	123.88	127.87
2	N	303	HEC	CAA-CBA-CGA	-2.13	108.03	113.67
2	R	305	HEC	C1D-C2D-C3D	-2.13	104.74	106.98
2	M	301	HEC	CAD-C3D-C2D	-2.12	123.89	127.87
2	N	306	HEC	CHC-C1C-C2C	-2.12	121.26	127.43
2	M	301	HEC	C1D-C2D-C3D	-2.12	104.75	106.98
2	F	305	HEC	CAA-C2A-C1A	2.12	129.16	124.85
2	J	302	HEC	CBB-CAB-C3B	2.11	118.15	112.42
2	S	306	HEC	C2B-C1B-NB	2.11	112.34	109.90
2	Q	301	HEC	CAA-CBA-CGA	-2.11	108.07	113.67
2	E	301	HEC	CHD-C1D-ND	2.11	126.97	124.37
2	K	306	HEC	CMB-C2B-C3B	2.11	131.85	126.15
2	I	303	HEC	CHD-C1D-ND	2.10	126.97	124.37
2	F	301	HEC	C1B-C2B-C3B	2.10	109.19	106.98
2	E	306	HEC	C3B-C4B-NB	-2.09	107.88	110.17
2	D	301	HEC	CHC-C4B-C3B	-2.09	121.38	125.23
2	G	303	HEC	CHD-C1D-ND	2.09	126.95	124.37
2	P	308	HEC	C2C-C1C-NC	-2.09	106.80	110.14
2	G	302	HEC	CAD-C3D-C4D	2.09	128.34	124.70
2	S	307	HEC	CHA-C1A-C2A	2.09	128.16	124.86
2	C	306	HEC	CHC-C1C-NC	2.09	127.64	123.86
2	N	306	HEC	CAC-C3C-C4C	2.08	127.78	124.91
2	G	302	HEC	CMD-C2D-C3D	2.08	131.79	126.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	306	HEC	C2A-C1A-NA	-2.08	108.31	110.32
2	E	301	HEC	CHD-C1D-C2D	-2.08	121.03	126.95
2	E	305	HEC	C4C-CHD-C1D	-2.08	121.36	126.25
2	N	307	HEC	CHD-C1D-C2D	-2.08	121.05	126.95
2	S	305	HEC	CHD-C4C-C3C	-2.07	120.77	125.30
2	M	305	HEC	CAD-C3D-C2D	-2.07	123.99	127.87
2	F	301	HEC	CHC-C4B-NB	2.07	126.93	124.37
2	Q	301	HEC	CHC-C4B-NB	2.07	126.93	124.37
2	E	306	HEC	CHD-C1D-C2D	-2.07	121.08	126.95
2	C	303	HEC	CAD-C3D-C2D	-2.07	124.00	127.87
2	F	301	HEC	CAD-C3D-C2D	-2.06	124.00	127.87
2	N	303	HEC	CHC-C4B-C3B	-2.06	121.42	125.23
2	Q	304	HEC	CMC-C2C-C3C	2.06	129.99	125.62
2	P	307	HEC	C1D-ND-C4D	2.06	107.64	105.21
2	L	305	HEC	CAB-C3B-C4B	-2.06	122.11	124.79
2	S	305	HEC	CHC-C4B-C3B	-2.05	121.44	125.23
2	C	303	HEC	CAA-CBA-CGA	-2.05	108.22	113.67
2	Q	305	HEC	CHD-C1D-C2D	-2.05	121.12	126.95
2	G	303	HEC	CHC-C1C-NC	2.05	127.58	123.86
2	G	302	HEC	CMA-C3A-C4A	-2.05	121.12	124.73
2	L	305	HEC	C2A-C1A-NA	-2.05	108.35	110.32
2	G	302	HEC	CHC-C1C-C2C	-2.04	121.50	127.43
2	T	302	HEC	C4D-C3D-C2D	-2.04	103.92	106.89
2	G	303	HEC	CHC-C1C-C2C	-2.04	121.50	127.43
2	S	301	HEC	CAA-C2A-C1A	-2.04	120.71	124.85
2	P	308	HEC	CAB-C3B-C2B	2.04	131.30	127.56
2	Q	301	HEC	CHD-C1D-ND	2.03	126.88	124.37
2	D	304	HEC	CHA-C1A-C2A	2.03	128.08	124.86
2	M	302	HEC	CMC-C2C-C3C	2.03	129.94	125.62
2	C	306	HEC	CHC-C1C-C2C	-2.03	121.52	127.43
2	L	302	HEC	CAC-C3C-C4C	2.03	127.71	124.91
2	E	306	HEC	CHD-C1D-ND	2.03	126.88	124.37
2	C	301	HEC	CHB-C1B-NB	2.03	126.61	124.42
2	D	301	HEC	C4B-NB-C1B	-2.03	102.81	105.21
2	Q	301	HEC	CMC-C2C-C3C	2.03	129.92	125.62
2	K	305	HEC	CAA-C2A-C3A	-2.03	124.07	127.87
2	T	301	HEC	CAD-CBD-CGD	-2.02	108.30	113.67
2	P	308	HEC	C3D-C4D-ND	2.02	112.31	110.35
2	S	301	HEC	CMB-C2B-C1B	-2.02	121.88	125.03
2	D	301	HEC	CHC-C1C-NC	2.02	127.52	123.86
2	F	306	HEC	C1D-C2D-C3D	-2.02	104.86	106.98
2	I	302	HEC	CHA-C4D-ND	2.02	126.60	124.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	301	HEC	O1D-CGD-CBD	-2.02	116.69	123.09
2	C	306	HEC	C4A-CHB-C1B	-2.02	121.73	126.02
2	J	306	HEC	C1D-ND-C4D	2.02	107.59	105.21
2	D	305	HEC	CHB-C4A-NA	2.02	126.65	124.45
2	S	307	HEC	CHB-C4A-NA	2.01	126.64	124.45
2	N	303	HEC	CHD-C1D-ND	2.01	126.86	124.37
2	K	306	HEC	C2B-C1B-NB	2.01	112.23	109.90
2	N	303	HEC	CMC-C2C-C1C	-2.01	122.36	125.42
2	P	307	HEC	CHB-C4A-NA	2.01	126.64	124.45
2	E	302	HEC	CMB-C2B-C1B	-2.01	121.90	125.03
2	I	302	HEC	C1D-C2D-C3D	-2.01	104.87	106.98
2	L	305	HEC	CHA-C4D-ND	2.00	126.58	124.42

All (64) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	N	301	HEC	NA
2	N	302	HEC	NA
2	N	303	HEC	NA
2	N	306	HEC	NA
2	N	307	HEC	NA
2	M	301	HEC	NA
2	M	302	HEC	NA
2	M	305	HEC	NA
2	M	306	HEC	NA
2	L	301	HEC	NA
2	L	302	HEC	NA
2	L	305	HEC	NA
2	L	306	HEC	NA
2	K	301	HEC	NA
2	K	302	HEC	NA
2	K	305	HEC	NA
2	K	306	HEC	NA
2	J	301	HEC	NA
2	J	302	HEC	NA
2	J	305	HEC	NA
2	J	306	HEC	NA
2	I	301	HEC	NA
2	I	302	HEC	NA
2	I	303	HEC	NA
2	C	301	HEC	NA
2	C	302	HEC	NA

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Mol	Chain	Res	Type	Atom
2	C	303	HEC	NA
2	C	306	HEC	NA
2	C	307	HEC	NA
2	C	308	HEC	NA
2	D	301	HEC	NA
2	D	304	HEC	NA
2	D	305	HEC	NA
2	E	301	HEC	NA
2	E	302	HEC	NA
2	E	305	HEC	NA
2	E	306	HEC	NA
2	F	301	HEC	NA
2	F	302	HEC	NA
2	F	305	HEC	NA
2	F	306	HEC	NA
2	G	301	HEC	NA
2	G	302	HEC	NA
2	G	303	HEC	NA
2	P	301	HEC	NA
2	P	302	HEC	NA
2	P	303	HEC	NA
2	P	306	HEC	NA
2	P	307	HEC	NA
2	P	308	HEC	NA
2	Q	301	HEC	NA
2	Q	304	HEC	NA
2	Q	305	HEC	NA
2	R	301	HEC	NA
2	R	302	HEC	NA
2	R	305	HEC	NA
2	R	306	HEC	NA
2	S	301	HEC	NA
2	S	302	HEC	NA
2	S	305	HEC	NA
2	S	306	HEC	NA
2	S	307	HEC	NA
2	T	301	HEC	NA
2	T	302	HEC	NA

All (449) torsion outliers are listed below:

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Mol	Chain	Res	Type	Atoms
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Mol	Chain	Res	Type	Atoms
2	N	306	HEC	C1A-C2A-CAA-CBA
2	N	306	HEC	C3A-C2A-CAA-CBA
2	M	301	HEC	C3D-CAD-CBD-CGD
2	J	305	HEC	C1A-C2A-CAA-CBA
2	J	305	HEC	C3A-C2A-CAA-CBA
2	I	301	HEC	C2D-C3D-CAD-CBD
2	C	306	HEC	C2A-CAA-CBA-CGA
2	G	302	HEC	C2D-C3D-CAD-CBD
2	P	307	HEC	C3D-CAD-CBD-CGD
2	R	306	HEC	C1A-C2A-CAA-CBA
2	R	306	HEC	C3A-C2A-CAA-CBA
2	S	305	HEC	C2D-C3D-CAD-CBD
2	S	305	HEC	C4D-C3D-CAD-CBD
2	S	307	HEC	C1A-C2A-CAA-CBA
2	S	307	HEC	C3A-C2A-CAA-CBA
2	T	302	HEC	C4D-C3D-CAD-CBD
2	N	303	HEC	C4B-C3B-CAB-CBB
2	I	301	HEC	C4B-C3B-CAB-CBB
2	C	303	HEC	C4B-C3B-CAB-CBB
2	C	308	HEC	C4B-C3B-CAB-CBB
2	F	302	HEC	C4B-C3B-CAB-CBB
2	Q	301	HEC	C4B-C3B-CAB-CBB
2	R	301	HEC	C4B-C3B-CAB-CBB
2	T	302	HEC	C4B-C3B-CAB-CBB
2	I	303	HEC	C4B-C3B-CAB-CBB
2	G	303	HEC	C4B-C3B-CAB-CBB
2	M	302	HEC	C2B-C3B-CAB-CBB
2	J	302	HEC	C2B-C3B-CAB-CBB
2	I	301	HEC	C2B-C3B-CAB-CBB
2	Q	301	HEC	C2B-C3B-CAB-CBB
2	M	302	HEC	C4B-C3B-CAB-CBB
2	J	302	HEC	C4B-C3B-CAB-CBB
2	C	307	HEC	C4B-C3B-CAB-CBB
2	F	301	HEC	C4B-C3B-CAB-CBB
2	G	302	HEC	C4B-C3B-CAB-CBB
2	N	303	HEC	C2B-C3B-CAB-CBB
2	L	302	HEC	C2B-C3B-CAB-CBB
2	C	303	HEC	C2B-C3B-CAB-CBB
2	E	302	HEC	C2B-C3B-CAB-CBB
2	F	302	HEC	C2B-C3B-CAB-CBB
2	G	303	HEC	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
2	T	302	HEC	C2B-C3B-CAB-CBB
2	I	301	HEC	C2C-C3C-CAC-CBC
2	L	302	HEC	C4B-C3B-CAB-CBB
2	S	301	HEC	C4B-C3B-CAB-CBB
2	K	302	HEC	C2B-C3B-CAB-CBB
2	I	303	HEC	C2B-C3B-CAB-CBB
2	R	302	HEC	C2B-C3B-CAB-CBB
2	S	302	HEC	C2B-C3B-CAB-CBB
2	S	301	HEC	C4C-C3C-CAC-CBC
2	E	302	HEC	C4B-C3B-CAB-CBB
2	P	303	HEC	C4B-C3B-CAB-CBB
2	P	307	HEC	C4B-C3B-CAB-CBB
2	S	302	HEC	C4B-C3B-CAB-CBB
2	F	301	HEC	C2B-C3B-CAB-CBB
2	G	302	HEC	C2B-C3B-CAB-CBB
2	R	301	HEC	C2B-C3B-CAB-CBB
2	D	301	HEC	C2B-C3B-CAB-CBB
2	K	302	HEC	C4B-C3B-CAB-CBB
2	D	301	HEC	C4B-C3B-CAB-CBB
2	R	302	HEC	C4B-C3B-CAB-CBB
2	C	307	HEC	C2B-C3B-CAB-CBB
2	C	308	HEC	C2B-C3B-CAB-CBB
2	P	303	HEC	C2B-C3B-CAB-CBB
2	P	307	HEC	C2B-C3B-CAB-CBB
2	I	301	HEC	C4C-C3C-CAC-CBC
2	F	301	HEC	C4C-C3C-CAC-CBC
2	N	302	HEC	C2B-C3B-CAB-CBB
2	K	301	HEC	C2B-C3B-CAB-CBB
2	J	301	HEC	C2B-C3B-CAB-CBB
2	C	302	HEC	C2B-C3B-CAB-CBB
2	S	301	HEC	C2B-C3B-CAB-CBB
2	C	302	HEC	C4B-C3B-CAB-CBB
2	K	302	HEC	C2D-C3D-CAD-CBD
2	I	303	HEC	C2D-C3D-CAD-CBD
2	E	305	HEC	C3A-C2A-CAA-CBA
2	F	305	HEC	C3A-C2A-CAA-CBA
2	L	301	HEC	C2B-C3B-CAB-CBB
2	P	302	HEC	C2B-C3B-CAB-CBB
2	L	305	HEC	C1A-C2A-CAA-CBA
2	K	302	HEC	C4D-C3D-CAD-CBD
2	I	301	HEC	C4D-C3D-CAD-CBD
2	I	303	HEC	C4D-C3D-CAD-CBD

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Mol	Chain	Res	Type	Atoms
2	C	303	HEC	C4D-C3D-CAD-CBD
2	C	306	HEC	C1A-C2A-CAA-CBA
2	D	301	HEC	C4D-C3D-CAD-CBD
2	D	304	HEC	C1A-C2A-CAA-CBA
2	E	301	HEC	C4D-C3D-CAD-CBD
2	E	302	HEC	C4D-C3D-CAD-CBD
2	E	305	HEC	C1A-C2A-CAA-CBA
2	F	305	HEC	C1A-C2A-CAA-CBA
2	G	303	HEC	C4D-C3D-CAD-CBD
2	P	306	HEC	C1A-C2A-CAA-CBA
2	Q	304	HEC	C1A-C2A-CAA-CBA
2	M	301	HEC	C2B-C3B-CAB-CBB
2	E	301	HEC	C2B-C3B-CAB-CBB
2	F	301	HEC	C2C-C3C-CAC-CBC
2	L	301	HEC	C4B-C3B-CAB-CBB
2	G	302	HEC	C2C-C3C-CAC-CBC
2	N	302	HEC	C4B-C3B-CAB-CBB
2	J	301	HEC	C4B-C3B-CAB-CBB
2	T	302	HEC	C2D-C3D-CAD-CBD
2	N	301	HEC	C3D-CAD-CBD-CGD
2	L	305	HEC	C2A-CAA-CBA-CGA
2	L	305	HEC	C3D-CAD-CBD-CGD
2	J	301	HEC	C3D-CAD-CBD-CGD
2	J	305	HEC	C3D-CAD-CBD-CGD
2	C	301	HEC	C3D-CAD-CBD-CGD
2	C	306	HEC	C3D-CAD-CBD-CGD
2	D	304	HEC	C3D-CAD-CBD-CGD
2	F	301	HEC	C3D-CAD-CBD-CGD
2	P	306	HEC	C3D-CAD-CBD-CGD
2	S	301	HEC	C3D-CAD-CBD-CGD
2	G	302	HEC	C4C-C3C-CAC-CBC
2	E	305	HEC	C2B-C3B-CAB-CBB
2	Q	304	HEC	C2B-C3B-CAB-CBB
2	E	305	HEC	C2C-C3C-CAC-CBC
2	S	301	HEC	C2C-C3C-CAC-CBC
2	K	305	HEC	C1A-C2A-CAA-CBA
2	G	302	HEC	C4D-C3D-CAD-CBD
2	N	307	HEC	C2B-C3B-CAB-CBB
2	N	307	HEC	C4B-C3B-CAB-CBB
2	P	302	HEC	C4B-C3B-CAB-CBB
2	D	301	HEC	C2D-C3D-CAD-CBD
2	P	306	HEC	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
2	K	301	HEC	C4B-C3B-CAB-CBB
2	L	301	HEC	C4C-C3C-CAC-CBC
2	P	306	HEC	C2C-C3C-CAC-CBC
2	C	306	HEC	C2B-C3B-CAB-CBB
2	E	305	HEC	C4C-C3C-CAC-CBC
2	L	305	HEC	C2B-C3B-CAB-CBB
2	P	306	HEC	C4C-C3C-CAC-CBC
2	M	305	HEC	C2B-C3B-CAB-CBB
2	P	301	HEC	C2B-C3B-CAB-CBB
2	S	306	HEC	C2B-C3B-CAB-CBB
2	N	306	HEC	C3D-CAD-CBD-CGD
2	L	301	HEC	C3D-CAD-CBD-CGD
2	K	302	HEC	C3D-CAD-CBD-CGD
2	C	307	HEC	C3D-CAD-CBD-CGD
2	E	305	HEC	C2A-CAA-CBA-CGA
2	E	305	HEC	C3D-CAD-CBD-CGD
2	G	303	HEC	C3D-CAD-CBD-CGD
2	P	308	HEC	C3D-CAD-CBD-CGD
2	Q	304	HEC	C2A-CAA-CBA-CGA
2	Q	305	HEC	C3D-CAD-CBD-CGD
2	R	306	HEC	C2A-CAA-CBA-CGA
2	R	306	HEC	C3D-CAD-CBD-CGD
2	S	307	HEC	C3D-CAD-CBD-CGD
2	K	305	HEC	C2B-C3B-CAB-CBB
2	L	305	HEC	C3A-C2A-CAA-CBA
2	C	303	HEC	C2D-C3D-CAD-CBD
2	C	306	HEC	C3A-C2A-CAA-CBA
2	D	304	HEC	C3A-C2A-CAA-CBA
2	E	301	HEC	C2D-C3D-CAD-CBD
2	G	303	HEC	C2D-C3D-CAD-CBD
2	N	301	HEC	C4D-C3D-CAD-CBD
2	E	301	HEC	C4B-C3B-CAB-CBB
2	Q	304	HEC	C4B-C3B-CAB-CBB
2	K	305	HEC	C3A-C2A-CAA-CBA
2	J	302	HEC	C2D-C3D-CAD-CBD
2	E	302	HEC	C2D-C3D-CAD-CBD
2	Q	304	HEC	C3A-C2A-CAA-CBA
2	R	301	HEC	C2D-C3D-CAD-CBD
2	I	302	HEC	C3D-CAD-CBD-CGD
2	P	302	HEC	C3D-CAD-CBD-CGD
2	P	306	HEC	C2A-CAA-CBA-CGA
2	G	301	HEC	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
2	T	301	HEC	C2B-C3B-CAB-CBB
2	N	301	HEC	C2D-C3D-CAD-CBD
2	N	303	HEC	C2D-C3D-CAD-CBD
2	Q	301	HEC	C2D-C3D-CAD-CBD
2	E	305	HEC	C4B-C3B-CAB-CBB
2	M	301	HEC	C4B-C3B-CAB-CBB
2	J	302	HEC	C4D-C3D-CAD-CBD
2	I	302	HEC	C2C-C3C-CAC-CBC
2	Q	304	HEC	C2C-C3C-CAC-CBC
2	S	306	HEC	C4B-C3B-CAB-CBB
2	N	307	HEC	C3D-CAD-CBD-CGD
2	K	305	HEC	C2A-CAA-CBA-CGA
2	C	308	HEC	C3D-CAD-CBD-CGD
2	R	301	HEC	C2A-CAA-CBA-CGA
2	N	302	HEC	C4D-C3D-CAD-CBD
2	N	303	HEC	C4D-C3D-CAD-CBD
2	M	305	HEC	C1A-C2A-CAA-CBA
2	F	301	HEC	C1A-C2A-CAA-CBA
2	F	302	HEC	C4D-C3D-CAD-CBD
2	P	307	HEC	C1A-C2A-CAA-CBA
2	Q	301	HEC	C4D-C3D-CAD-CBD
2	R	301	HEC	C4D-C3D-CAD-CBD
2	G	301	HEC	C4C-C3C-CAC-CBC
2	P	306	HEC	C2B-C3B-CAB-CBB
2	M	305	HEC	C3A-C2A-CAA-CBA
2	M	306	HEC	C2B-C3B-CAB-CBB
2	M	305	HEC	C4B-C3B-CAB-CBB
2	C	306	HEC	C4B-C3B-CAB-CBB
2	P	302	HEC	C2C-C3C-CAC-CBC
2	T	301	HEC	C4B-C3B-CAB-CBB
2	G	301	HEC	C1A-C2A-CAA-CBA
2	M	306	HEC	C3D-CAD-CBD-CGD
2	K	305	HEC	C3D-CAD-CBD-CGD
2	K	306	HEC	C3D-CAD-CBD-CGD
2	I	302	HEC	C2A-CAA-CBA-CGA
2	F	302	HEC	C3D-CAD-CBD-CGD
2	Q	304	HEC	C3D-CAD-CBD-CGD
2	Q	304	HEC	C4C-C3C-CAC-CBC
2	P	301	HEC	C4B-C3B-CAB-CBB
2	M	306	HEC	C4B-C3B-CAB-CBB
2	Q	305	HEC	C4B-C3B-CAB-CBB
2	S	305	HEC	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
2	N	302	HEC	C2D-C3D-CAD-CBD
2	P	307	HEC	C3A-C2A-CAA-CBA
2	L	305	HEC	C4B-C3B-CAB-CBB
2	M	301	HEC	C4D-C3D-CAD-CBD
2	M	302	HEC	C4D-C3D-CAD-CBD
2	L	302	HEC	C4D-C3D-CAD-CBD
2	C	301	HEC	C4D-C3D-CAD-CBD
2	C	307	HEC	C4D-C3D-CAD-CBD
2	P	307	HEC	C4D-C3D-CAD-CBD
2	S	301	HEC	C1A-C2A-CAA-CBA
2	F	305	HEC	C2B-C3B-CAB-CBB
2	S	307	HEC	C2B-C3B-CAB-CBB
2	K	305	HEC	C4B-C3B-CAB-CBB
2	N	303	HEC	C3D-CAD-CBD-CGD
2	Q	305	HEC	C2B-C3B-CAB-CBB
2	I	302	HEC	C4C-C3C-CAC-CBC
2	P	302	HEC	C4C-C3C-CAC-CBC
2	G	302	HEC	C1A-C2A-CAA-CBA
2	L	301	HEC	C2C-C3C-CAC-CBC
2	T	301	HEC	C2C-C3C-CAC-CBC
2	R	306	HEC	C2B-C3B-CAB-CBB
2	J	305	HEC	C2C-C3C-CAC-CBC
2	D	305	HEC	C4D-C3D-CAD-CBD
2	R	302	HEC	C4D-C3D-CAD-CBD
2	M	302	HEC	C2D-C3D-CAD-CBD
2	L	302	HEC	C2D-C3D-CAD-CBD
2	F	302	HEC	C2D-C3D-CAD-CBD
2	G	301	HEC	C3A-C2A-CAA-CBA
2	J	306	HEC	C3D-CAD-CBD-CGD
2	G	301	HEC	C3D-CAD-CBD-CGD
2	T	301	HEC	C3D-CAD-CBD-CGD
2	K	306	HEC	C2B-C3B-CAB-CBB
2	K	306	HEC	C4B-C3B-CAB-CBB
2	S	305	HEC	C2B-C3B-CAB-CBB
2	C	307	HEC	C2D-C3D-CAD-CBD
2	F	301	HEC	C3A-C2A-CAA-CBA
2	M	302	HEC	C3D-CAD-CBD-CGD
2	E	306	HEC	C3D-CAD-CBD-CGD
2	N	306	HEC	C4C-C3C-CAC-CBC
2	J	305	HEC	C4C-C3C-CAC-CBC
2	F	306	HEC	C2B-C3B-CAB-CBB
2	K	301	HEC	C4D-C3D-CAD-CBD

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Mol	Chain	Res	Type	Atoms
2	R	302	HEC	C2D-C3D-CAD-CBD
2	N	302	HEC	C3D-CAD-CBD-CGD
2	N	306	HEC	C2A-CAA-CBA-CGA
2	E	301	HEC	C3D-CAD-CBD-CGD
2	T	301	HEC	C2A-CAA-CBA-CGA
2	N	306	HEC	C2C-C3C-CAC-CBC
2	F	306	HEC	C4B-C3B-CAB-CBB
2	R	306	HEC	C4B-C3B-CAB-CBB
2	T	301	HEC	C4C-C3C-CAC-CBC
2	F	305	HEC	C2C-C3C-CAC-CBC
2	S	307	HEC	C2C-C3C-CAC-CBC
2	S	307	HEC	C4B-C3B-CAB-CBB
2	C	308	HEC	C1A-C2A-CAA-CBA
2	P	306	HEC	C4B-C3B-CAB-CBB
2	J	301	HEC	C2C-C3C-CAC-CBC
2	C	302	HEC	C4C-C3C-CAC-CBC
2	S	307	HEC	C4C-C3C-CAC-CBC
2	C	302	HEC	C2C-C3C-CAC-CBC
2	N	306	HEC	C2B-C3B-CAB-CBB
2	N	301	HEC	C2C-C3C-CAC-CBC
2	F	305	HEC	C4C-C3C-CAC-CBC
2	L	305	HEC	C2C-C3C-CAC-CBC
2	F	305	HEC	C4B-C3B-CAB-CBB
2	L	306	HEC	C4B-C3B-CAB-CBB
2	N	301	HEC	C4C-C3C-CAC-CBC
2	J	301	HEC	C4C-C3C-CAC-CBC
2	C	301	HEC	C2D-C3D-CAD-CBD
2	P	301	HEC	C3D-CAD-CBD-CGD
2	S	307	HEC	C2A-CAA-CBA-CGA
2	C	302	HEC	C1A-C2A-CAA-CBA
2	L	306	HEC	C2B-C3B-CAB-CBB
2	M	305	HEC	C3D-CAD-CBD-CGD
2	I	303	HEC	C3D-CAD-CBD-CGD
2	F	305	HEC	C3D-CAD-CBD-CGD
2	S	306	HEC	C3D-CAD-CBD-CGD
2	S	305	HEC	C2C-C3C-CAC-CBC
2	M	301	HEC	C2D-C3D-CAD-CBD
2	P	307	HEC	C2D-C3D-CAD-CBD
2	F	306	HEC	C4D-C3D-CAD-CBD
2	L	305	HEC	C4C-C3C-CAC-CBC
2	G	301	HEC	C2B-C3B-CAB-CBB
2	C	301	HEC	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
2	N	301	HEC	C2B-C3B-CAB-CBB
2	D	305	HEC	C2D-C3D-CAD-CBD
2	Q	305	HEC	C1A-C2A-CAA-CBA
2	S	305	HEC	C4B-C3B-CAB-CBB
2	K	301	HEC	C2D-C3D-CAD-CBD
2	G	301	HEC	C4B-C3B-CAB-CBB
2	P	301	HEC	C2C-C3C-CAC-CBC
2	D	304	HEC	C2A-CAA-CBA-CGA
2	Q	301	HEC	C3D-CAD-CBD-CGD
2	R	305	HEC	C3D-CAD-CBD-CGD
2	J	306	HEC	C4B-C3B-CAB-CBB
2	L	302	HEC	CAD-CBD-CGD-O2D
2	J	302	HEC	CAD-CBD-CGD-O1D
2	G	302	HEC	C3A-C2A-CAA-CBA
2	P	301	HEC	C4C-C3C-CAC-CBC
2	K	302	HEC	CAD-CBD-CGD-O1D
2	T	301	HEC	C1A-C2A-CAA-CBA
2	C	308	HEC	C2C-C3C-CAC-CBC
2	J	302	HEC	CAD-CBD-CGD-O2D
2	L	302	HEC	CAD-CBD-CGD-O1D
2	T	302	HEC	C3D-CAD-CBD-CGD
2	C	301	HEC	C2B-C3B-CAB-CBB
2	Q	301	HEC	CAD-CBD-CGD-O2D
2	T	302	HEC	CAD-CBD-CGD-O1D
2	M	305	HEC	CAA-CBA-CGA-O1A
2	I	301	HEC	CAD-CBD-CGD-O1D
2	D	301	HEC	CAD-CBD-CGD-O1D
2	N	306	HEC	C4B-C3B-CAB-CBB
2	S	302	HEC	CAD-CBD-CGD-O1D
2	C	301	HEC	C3A-C2A-CAA-CBA
2	C	302	HEC	C3A-C2A-CAA-CBA
2	Q	301	HEC	CAD-CBD-CGD-O1D
2	Q	304	HEC	CAD-CBD-CGD-O2D
2	T	302	HEC	CAD-CBD-CGD-O2D
2	R	305	HEC	C4D-C3D-CAD-CBD
2	J	305	HEC	C2B-C3B-CAB-CBB
2	I	301	HEC	CAD-CBD-CGD-O2D
2	S	302	HEC	CAD-CBD-CGD-O2D
2	G	303	HEC	CAD-CBD-CGD-O1D
2	N	301	HEC	C4B-C3B-CAB-CBB
2	E	301	HEC	CAA-CBA-CGA-O2A
2	S	305	HEC	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
2	S	301	HEC	C3A-C2A-CAA-CBA
2	P	302	HEC	C4D-C3D-CAD-CBD
2	D	301	HEC	CAD-CBD-CGD-O2D
2	P	302	HEC	CAD-CBD-CGD-O2D
2	M	305	HEC	CAA-CBA-CGA-O2A
2	K	302	HEC	CAD-CBD-CGD-O2D
2	I	302	HEC	CAA-CBA-CGA-O2A
2	I	302	HEC	CAD-CBD-CGD-O2D
2	M	301	HEC	CAA-CBA-CGA-O2A
2	Q	304	HEC	CAD-CBD-CGD-O1D
2	C	308	HEC	C3A-C2A-CAA-CBA
2	I	301	HEC	C2A-CAA-CBA-CGA
2	C	308	HEC	C4C-C3C-CAC-CBC
2	M	305	HEC	CAD-CBD-CGD-O2D
2	E	301	HEC	CAA-CBA-CGA-O1A
2	S	305	HEC	CAA-CBA-CGA-O1A
2	K	305	HEC	C4C-C3C-CAC-CBC
2	T	301	HEC	CAA-CBA-CGA-O2A
2	C	307	HEC	C1A-C2A-CAA-CBA
2	K	305	HEC	C2C-C3C-CAC-CBC
2	D	304	HEC	C2C-C3C-CAC-CBC
2	I	303	HEC	C2C-C3C-CAC-CBC
2	C	303	HEC	CAD-CBD-CGD-O1D
2	R	305	HEC	C2C-C3C-CAC-CBC
2	I	302	HEC	CAA-CBA-CGA-O1A
2	M	306	HEC	C4D-C3D-CAD-CBD
2	D	304	HEC	C2B-C3B-CAB-CBB
2	P	302	HEC	CAD-CBD-CGD-O1D
2	C	301	HEC	C4B-C3B-CAB-CBB
2	M	301	HEC	CAA-CBA-CGA-O1A
2	C	306	HEC	C4C-C3C-CAC-CBC
2	F	302	HEC	C2C-C3C-CAC-CBC
2	S	307	HEC	CAA-CBA-CGA-O2A
2	D	304	HEC	C4C-C3C-CAC-CBC
2	K	306	HEC	C1A-C2A-CAA-CBA
2	P	308	HEC	C1A-C2A-CAA-CBA
2	P	308	HEC	C4D-C3D-CAD-CBD
2	M	305	HEC	CAD-CBD-CGD-O1D
2	I	303	HEC	C4C-C3C-CAC-CBC
2	I	302	HEC	CAD-CBD-CGD-O1D
2	R	306	HEC	C2C-C3C-CAC-CBC
2	G	302	HEC	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
2	G	302	HEC	CAD-CBD-CGD-O1D
2	L	306	HEC	CAD-CBD-CGD-O1D
2	L	306	HEC	CAD-CBD-CGD-O2D
2	R	306	HEC	CAD-CBD-CGD-O1D
2	L	301	HEC	CAA-CBA-CGA-O2A
2	E	302	HEC	CAD-CBD-CGD-O1D
2	R	301	HEC	CAD-CBD-CGD-O1D
2	D	305	HEC	C2C-C3C-CAC-CBC
2	R	306	HEC	C4C-C3C-CAC-CBC
2	K	301	HEC	C2C-C3C-CAC-CBC
2	N	302	HEC	CAD-CBD-CGD-O2D
2	T	301	HEC	CAA-CBA-CGA-O1A
2	F	305	HEC	C4D-C3D-CAD-CBD
2	E	301	HEC	CAD-CBD-CGD-O2D
2	E	302	HEC	CAD-CBD-CGD-O2D
2	J	306	HEC	C2B-C3B-CAB-CBB
2	S	307	HEC	CAA-CBA-CGA-O1A
2	M	301	HEC	C4C-C3C-CAC-CBC
2	N	307	HEC	CAA-CBA-CGA-O1A
2	C	303	HEC	CAD-CBD-CGD-O2D
2	P	308	HEC	CAA-CBA-CGA-O1A
2	S	301	HEC	CAD-CBD-CGD-O1D
2	L	306	HEC	CAA-CBA-CGA-O1A
2	I	302	HEC	C4B-C3B-CAB-CBB
2	G	302	HEC	CAA-CBA-CGA-O1A
2	R	305	HEC	CAA-CBA-CGA-O1A
2	G	302	HEC	CAD-CBD-CGD-O2D
2	G	303	HEC	CAD-CBD-CGD-O2D
2	R	306	HEC	CAD-CBD-CGD-O2D
2	E	302	HEC	C2C-C3C-CAC-CBC
2	C	307	HEC	CAD-CBD-CGD-O2D
2	I	301	HEC	CAA-CBA-CGA-O2A
2	C	306	HEC	CAD-CBD-CGD-O2D
2	F	306	HEC	CAD-CBD-CGD-O2D
2	N	303	HEC	CAD-CBD-CGD-O2D
2	M	301	HEC	CAD-CBD-CGD-O2D
2	L	301	HEC	CAA-CBA-CGA-O1A
2	D	305	HEC	CAD-CBD-CGD-O2D
2	F	306	HEC	C2D-C3D-CAD-CBD
2	J	305	HEC	C4B-C3B-CAB-CBB
2	P	301	HEC	C4D-C3D-CAD-CBD
2	R	301	HEC	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
2	N	302	HEC	CAD-CBD-CGD-O1D
2	C	308	HEC	CAA-CBA-CGA-O2A
2	E	301	HEC	CAD-CBD-CGD-O1D
2	F	302	HEC	CAD-CBD-CGD-O2D
2	P	308	HEC	CAD-CBD-CGD-O2D
2	S	306	HEC	CAA-CBA-CGA-O2A
2	P	306	HEC	CAD-CBD-CGD-O1D
2	P	306	HEC	CAD-CBD-CGD-O2D
2	P	308	HEC	CAD-CBD-CGD-O1D
2	C	308	HEC	CAA-CBA-CGA-O1A
2	E	302	HEC	C4C-C3C-CAC-CBC
2	M	301	HEC	CAD-CBD-CGD-O1D
2	K	301	HEC	CAD-CBD-CGD-O2D
2	F	305	HEC	CAD-CBD-CGD-O2D
2	Q	305	HEC	CAA-CBA-CGA-O2A
2	S	301	HEC	CAD-CBD-CGD-O2D
2	S	307	HEC	CAD-CBD-CGD-O2D
2	N	307	HEC	CAA-CBA-CGA-O2A
2	L	306	HEC	CAA-CBA-CGA-O2A
2	G	301	HEC	CAA-CBA-CGA-O2A
2	P	308	HEC	CAA-CBA-CGA-O2A
2	R	301	HEC	CAD-CBD-CGD-O2D
2	R	305	HEC	CAA-CBA-CGA-O2A
2	S	305	HEC	CAD-CBD-CGD-O2D
2	D	304	HEC	C4B-C3B-CAB-CBB
2	J	306	HEC	CAA-CBA-CGA-O2A
2	J	306	HEC	CAD-CBD-CGD-O1D
2	J	306	HEC	CAD-CBD-CGD-O2D
2	S	306	HEC	CAA-CBA-CGA-O1A
2	K	301	HEC	C4C-C3C-CAC-CBC

There are no ring outliers.

64 monomers are involved in 636 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	R	301	HEC	14	0
2	Q	301	HEC	10	0
2	F	302	HEC	11	0
2	D	305	HEC	13	0
2	L	305	HEC	9	0
2	L	306	HEC	12	0
2	N	301	HEC	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	306	HEC	20	0
2	G	301	HEC	4	0
2	I	303	HEC	12	0
2	S	302	HEC	12	0
2	P	302	HEC	6	0
2	T	302	HEC	13	0
2	F	301	HEC	9	0
2	P	308	HEC	14	0
2	S	307	HEC	11	0
2	F	305	HEC	8	0
2	M	302	HEC	14	0
2	E	305	HEC	12	0
2	C	307	HEC	6	0
2	K	306	HEC	14	0
2	J	302	HEC	10	0
2	J	301	HEC	6	0
2	P	301	HEC	5	0
2	D	304	HEC	6	0
2	P	307	HEC	9	0
2	T	301	HEC	8	0
2	N	307	HEC	16	0
2	L	301	HEC	5	0
2	M	306	HEC	12	0
2	D	301	HEC	8	0
2	C	301	HEC	10	0
2	R	306	HEC	14	0
2	I	301	HEC	12	0
2	S	305	HEC	8	0
2	P	306	HEC	10	0
2	Q	304	HEC	10	0
2	P	303	HEC	7	0
2	I	302	HEC	6	0
2	C	306	HEC	14	0
2	E	302	HEC	11	0
2	R	305	HEC	12	0
2	K	305	HEC	12	0
2	C	303	HEC	4	0
2	S	306	HEC	14	0
2	J	305	HEC	10	0
2	C	308	HEC	18	0
2	N	306	HEC	16	0
2	G	303	HEC	8	0

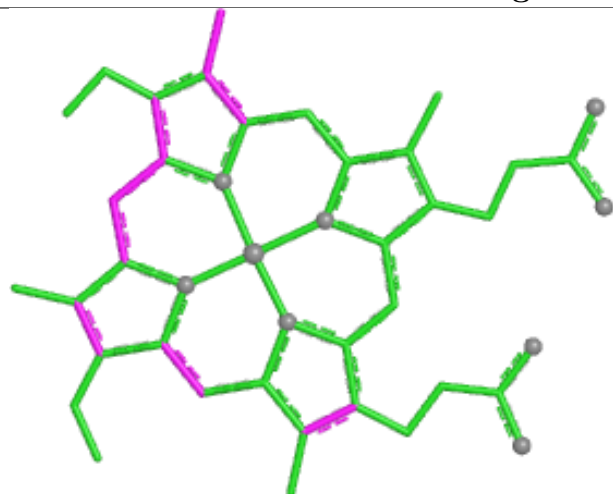
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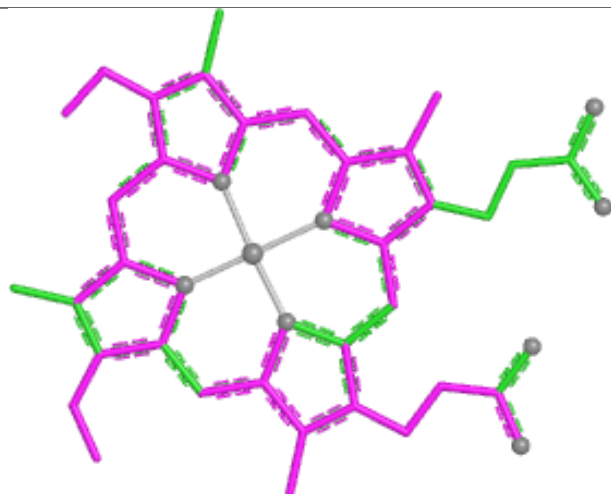
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	302	HEC	7	0
2	Q	305	HEC	11	0
2	N	303	HEC	4	0
2	N	302	HEC	5	0
2	K	301	HEC	8	0
2	M	305	HEC	8	0
2	C	302	HEC	9	0
2	E	301	HEC	8	0
2	F	306	HEC	12	0
2	R	302	HEC	16	0
2	S	301	HEC	10	0
2	G	302	HEC	10	0
2	E	306	HEC	12	0
2	M	301	HEC	9	0
2	K	302	HEC	8	0

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.

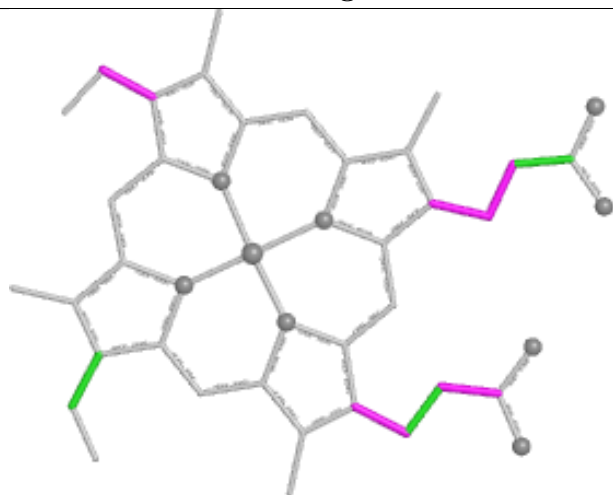
Ligand HEC R 301



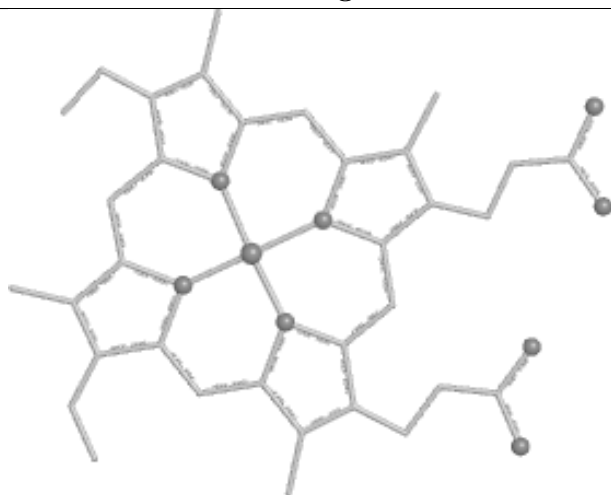
Bond lengths



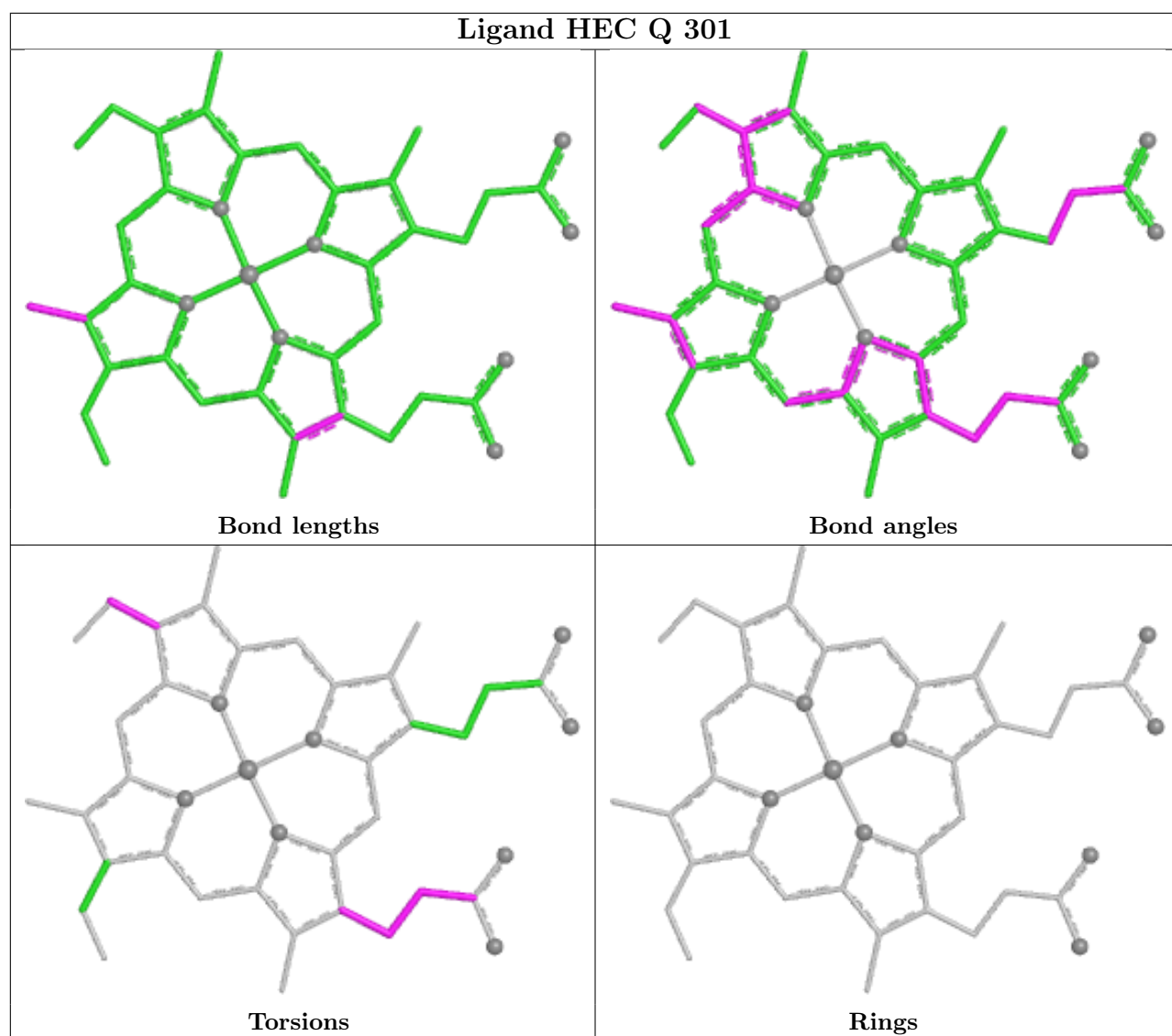
Bond angles



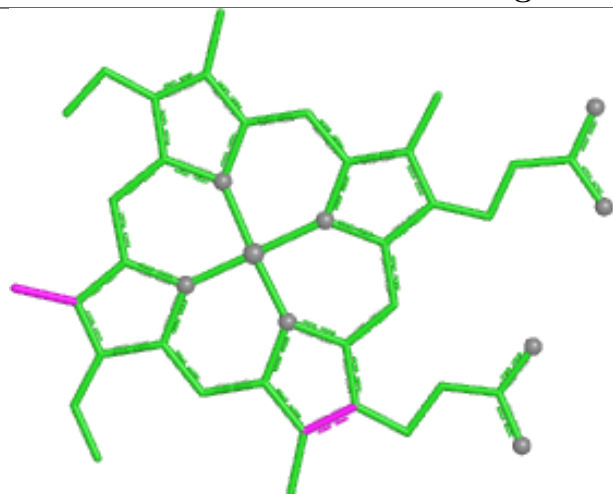
Torsions



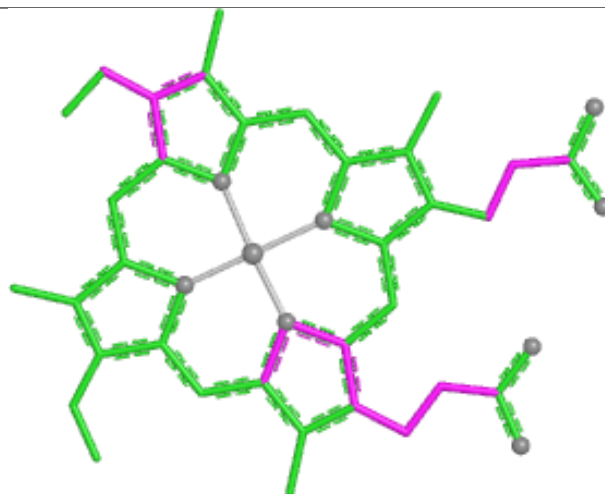
Rings



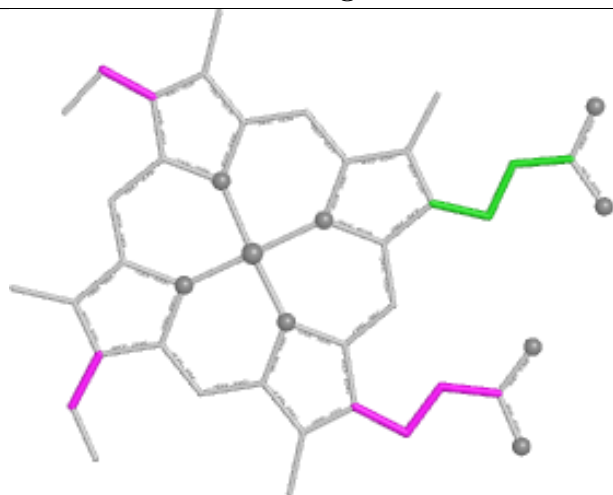
Ligand HEC F 302



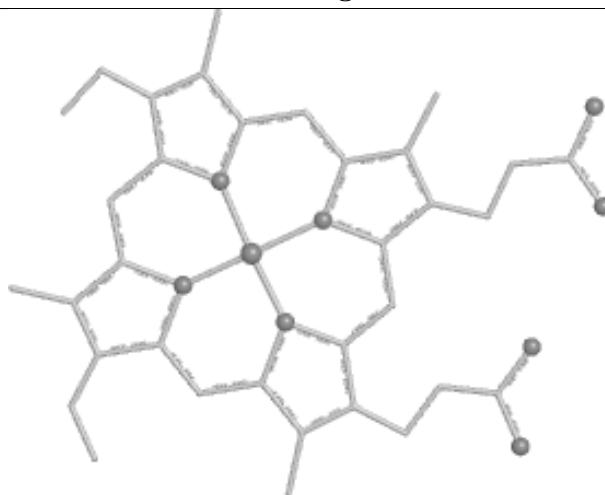
Bond lengths



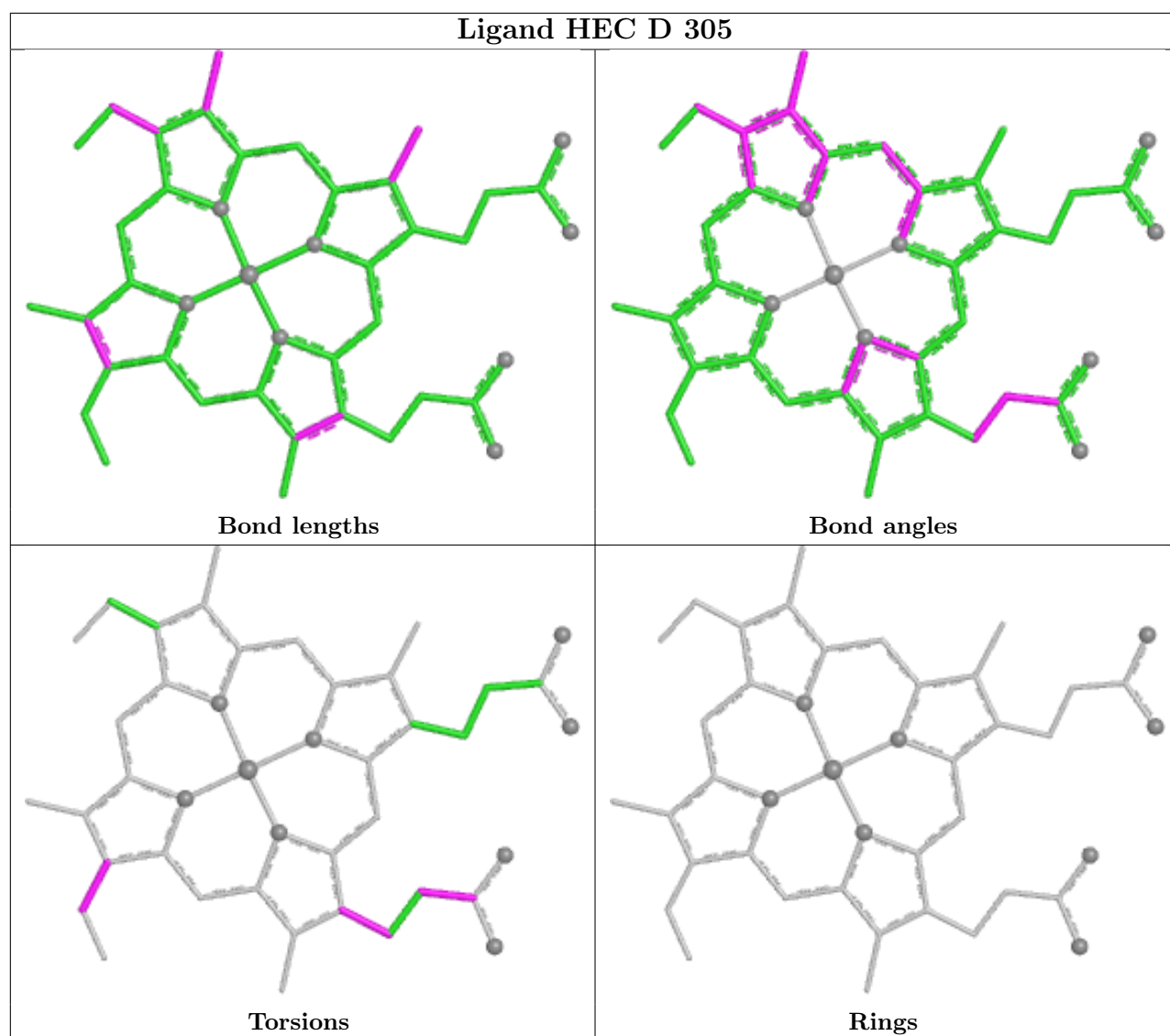
Bond angles



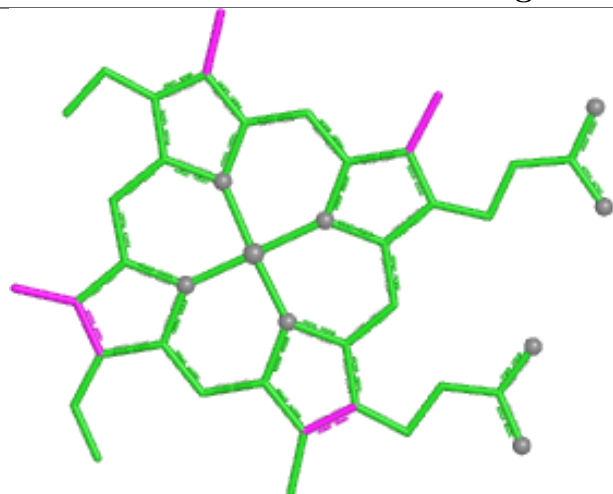
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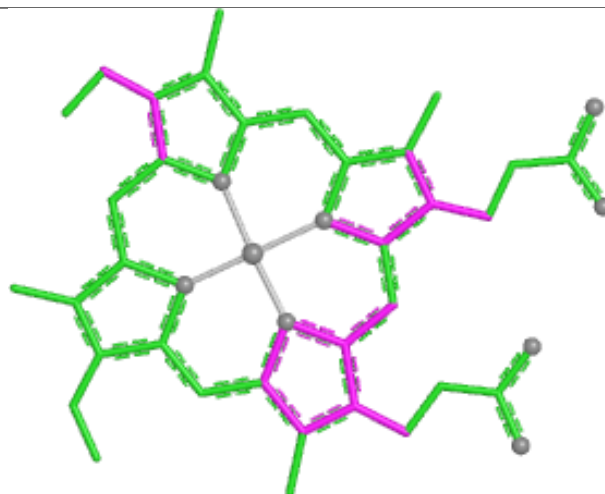
Rings



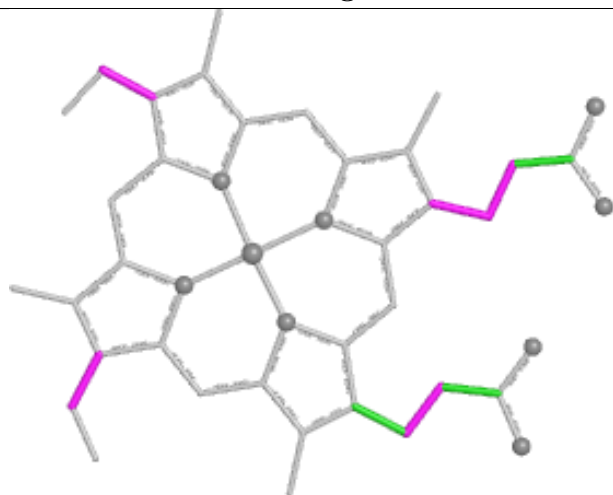
Ligand HEC L 305



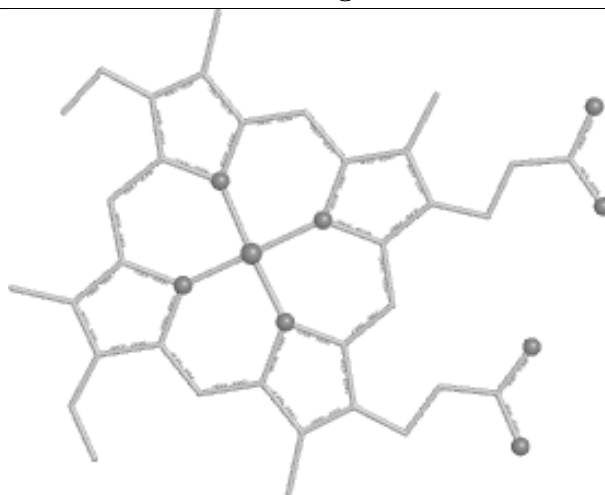
Bond lengths



Bond angles

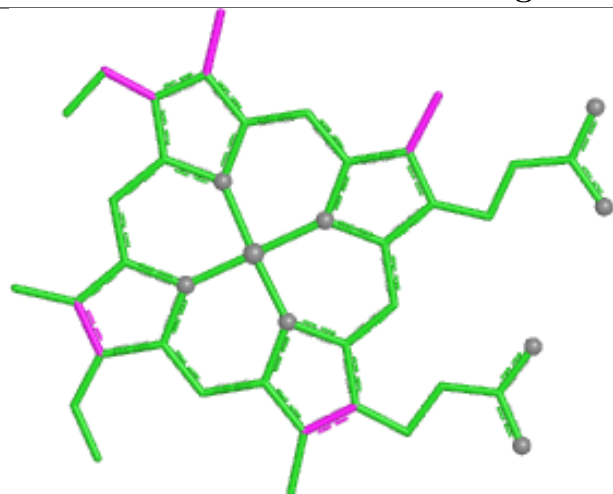


Torsions

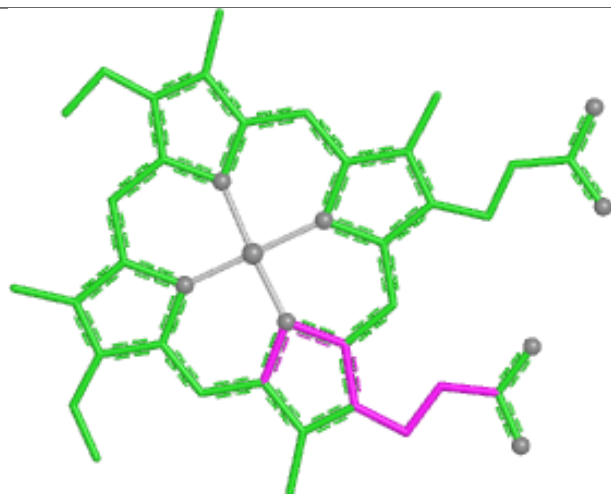


Rings

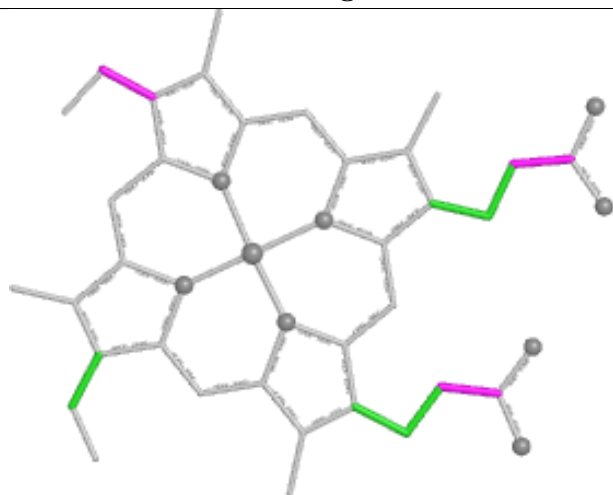
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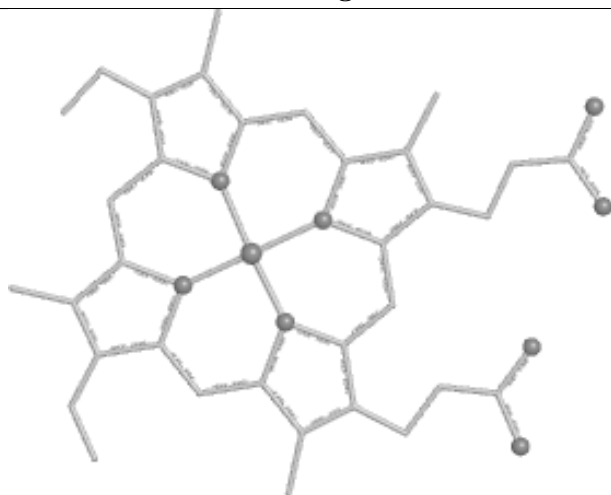
Bond lengths



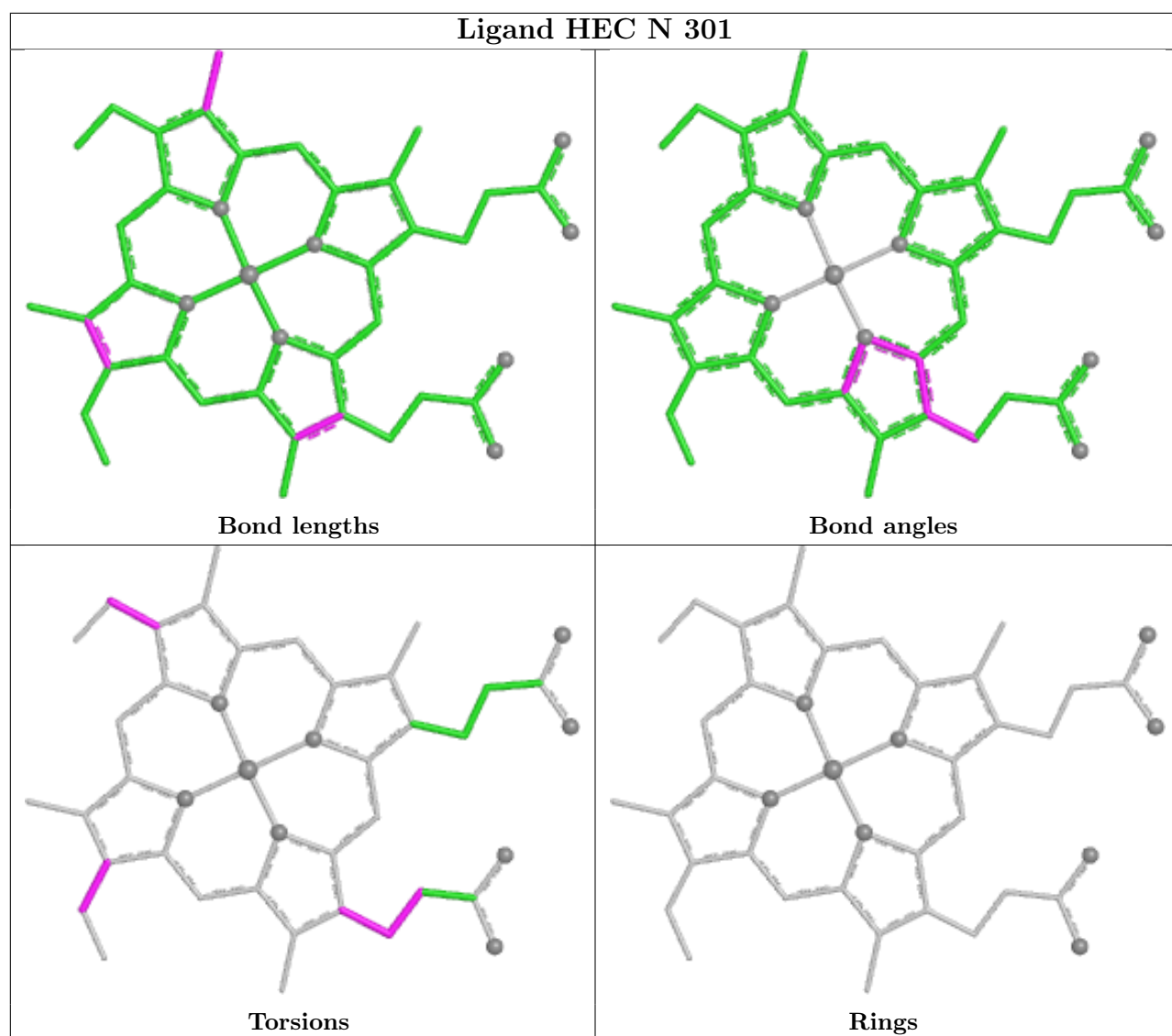
Bond angles



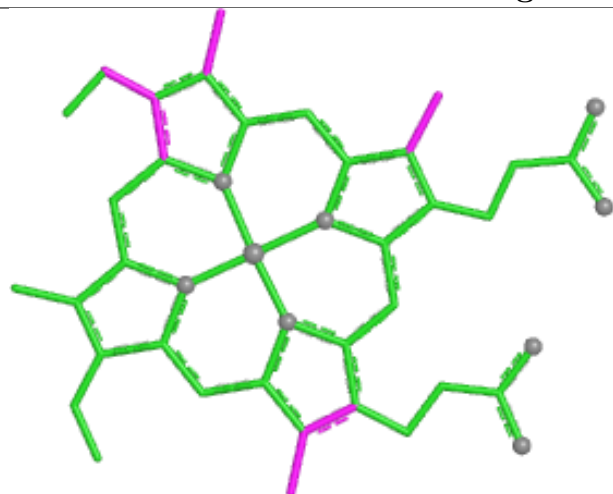
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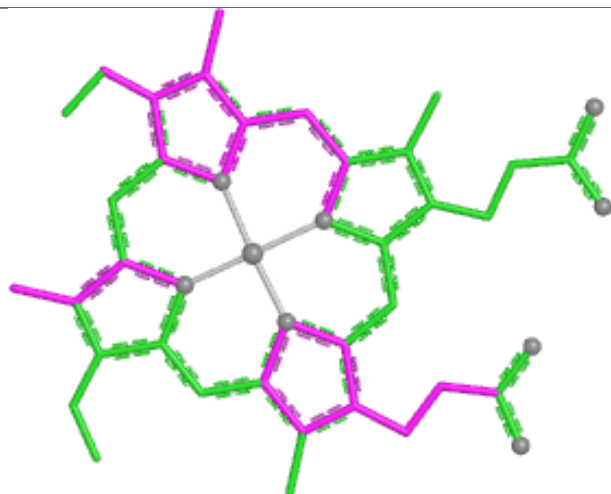
Rings



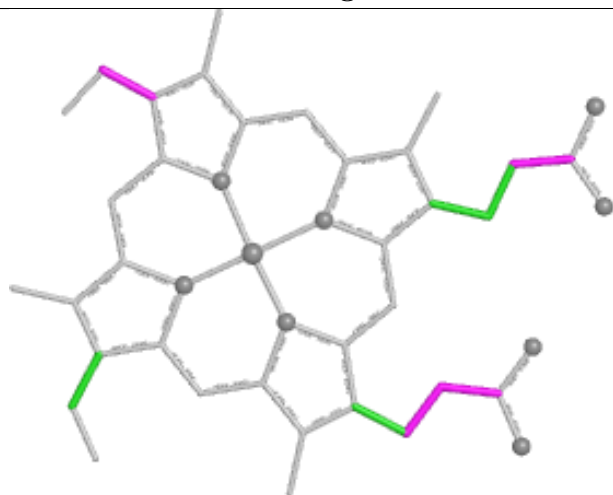
Ligand HEC J 306



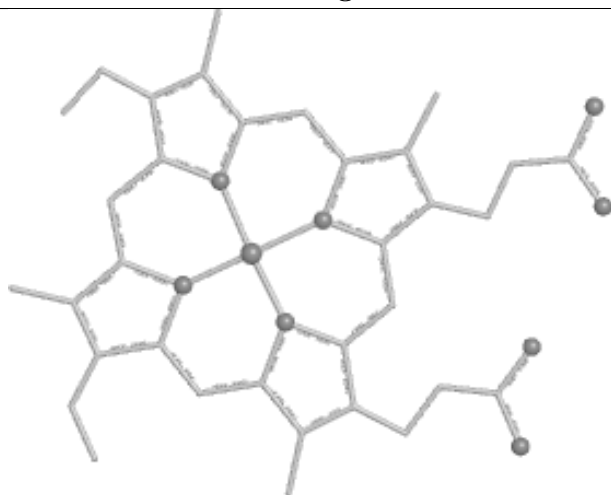
Bond lengths



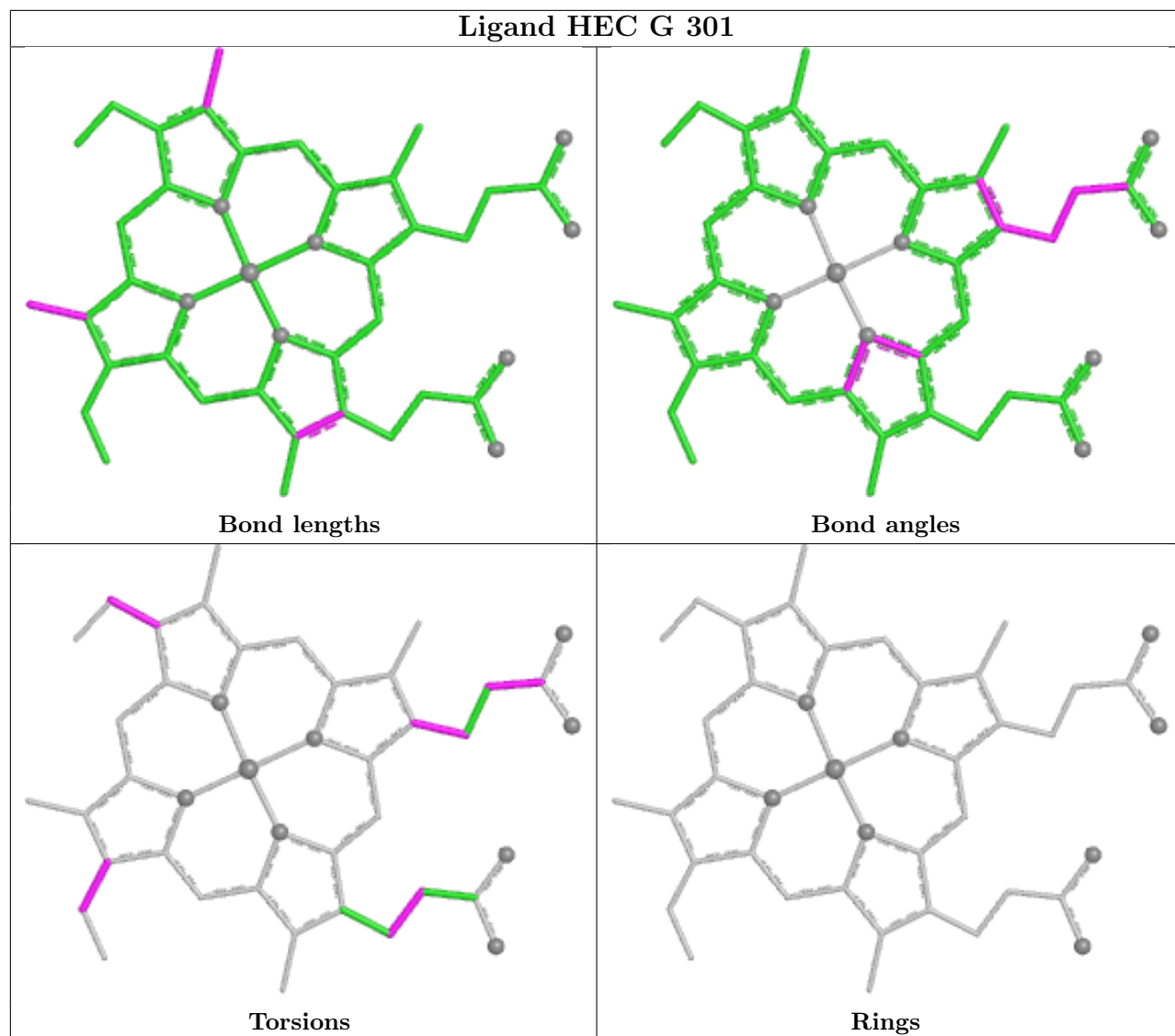
Bond angles



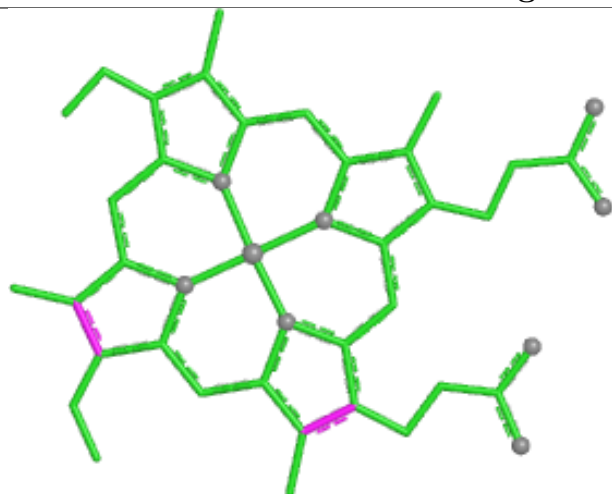
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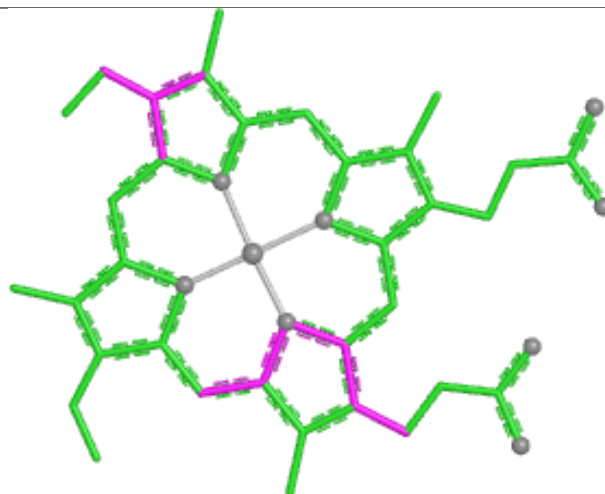
Rings



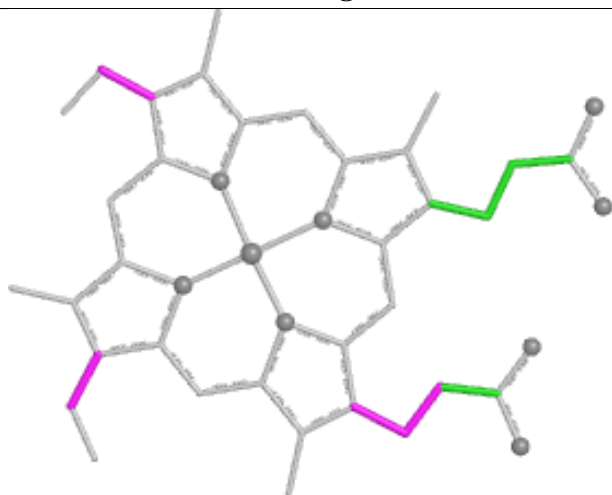
Ligand HEC I 303



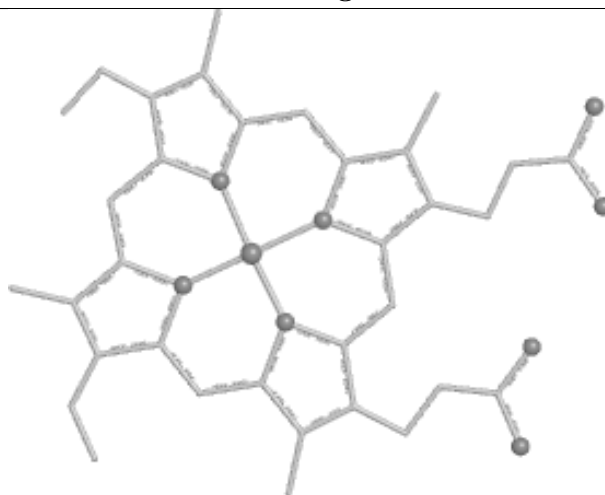
Bond lengths



Bond angles

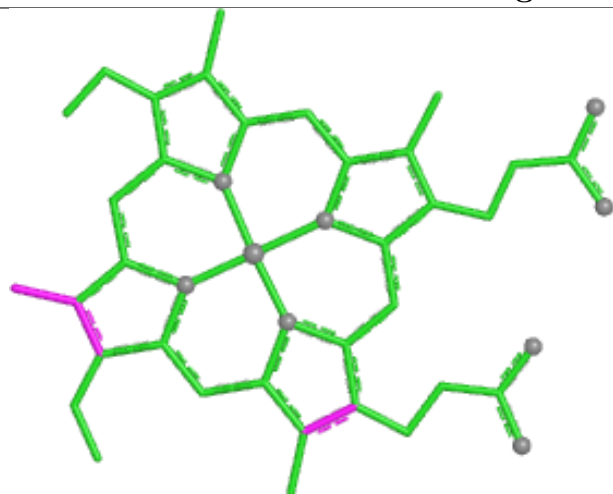


Torsions

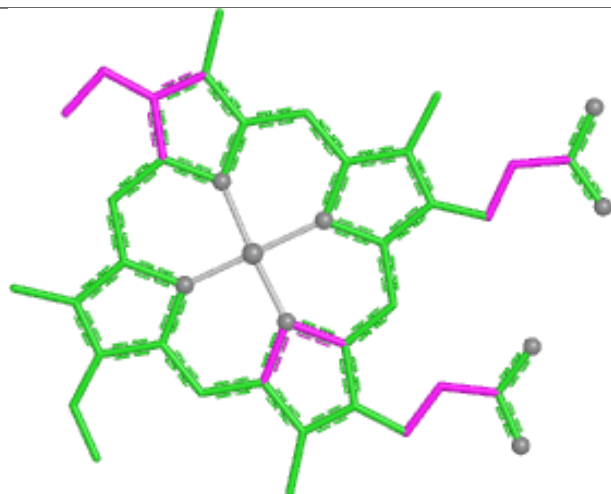


Rings

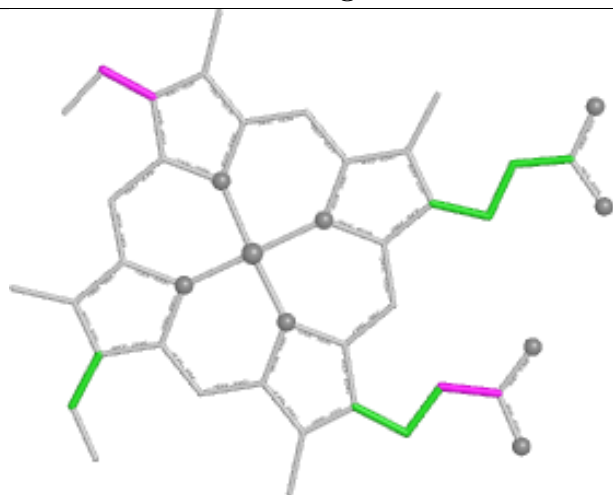
Ligand HEC S 302



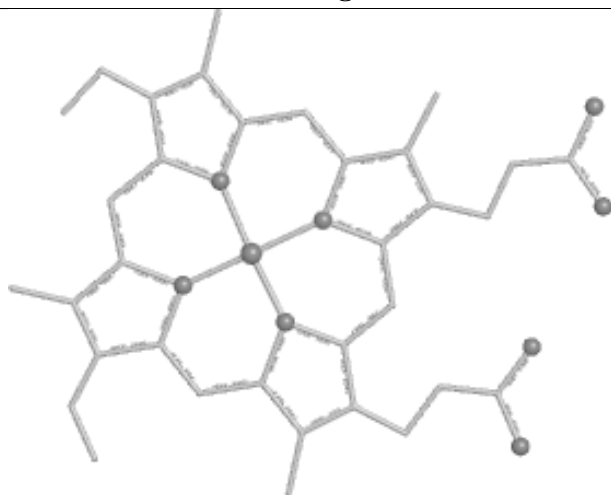
Bond lengths



Bond angles

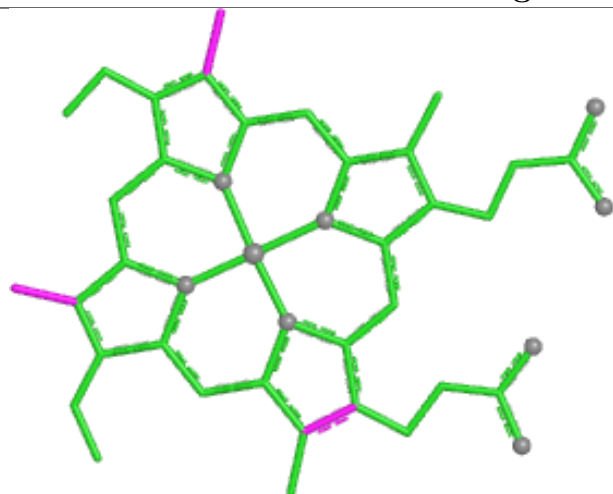


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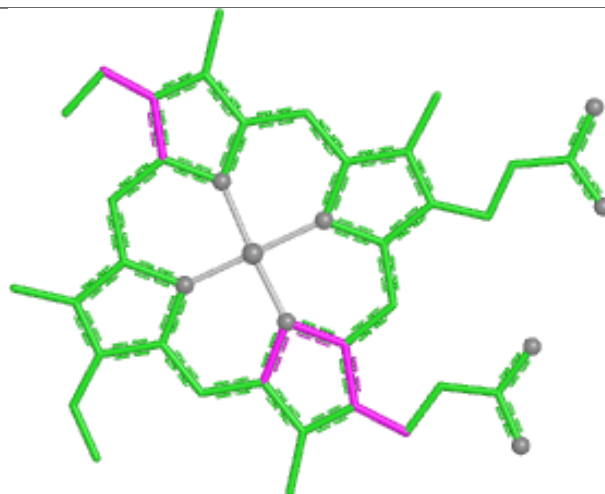


Rings

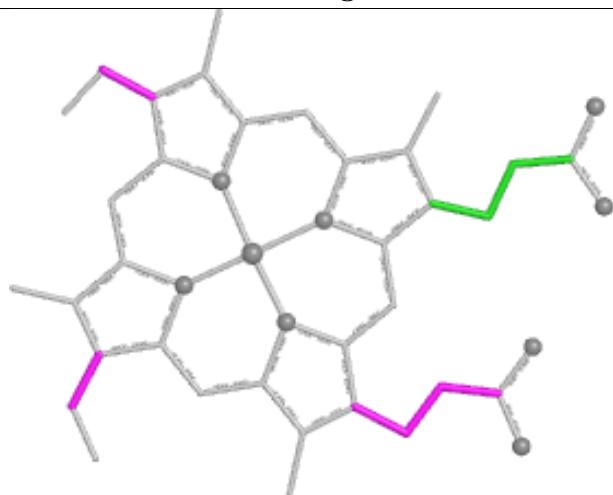
Ligand HEC P 302



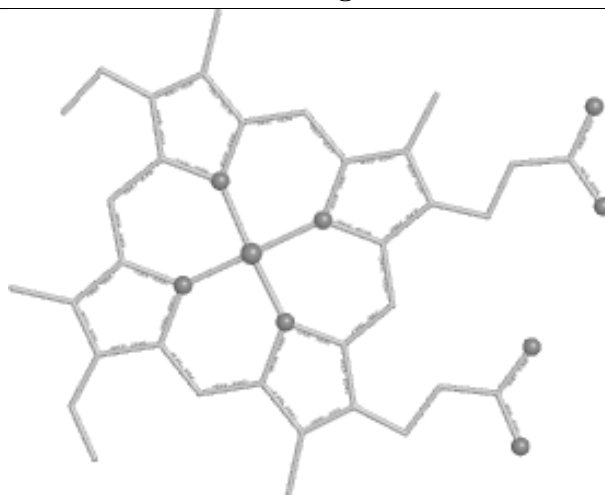
Bond lengths



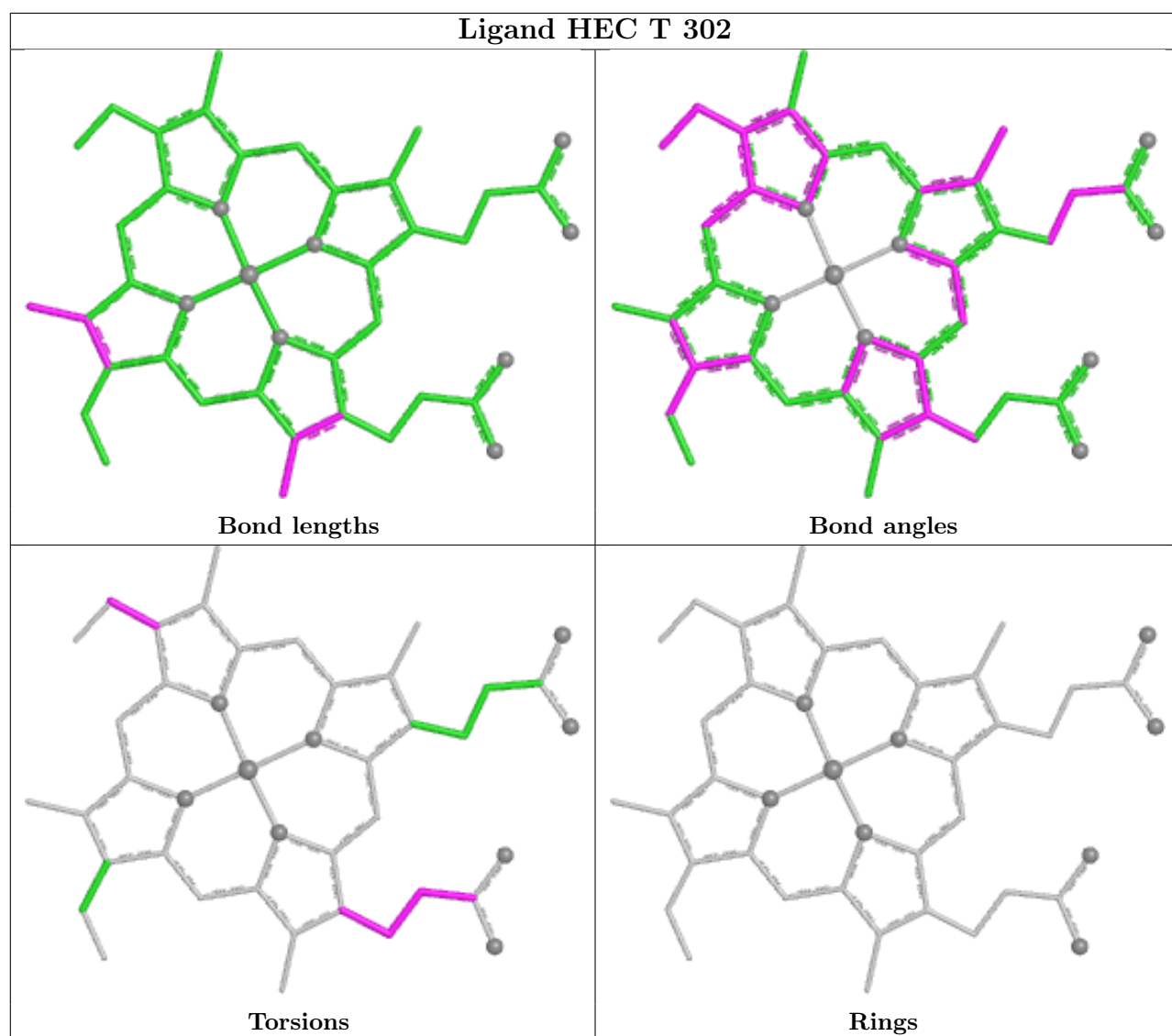
Bond angles



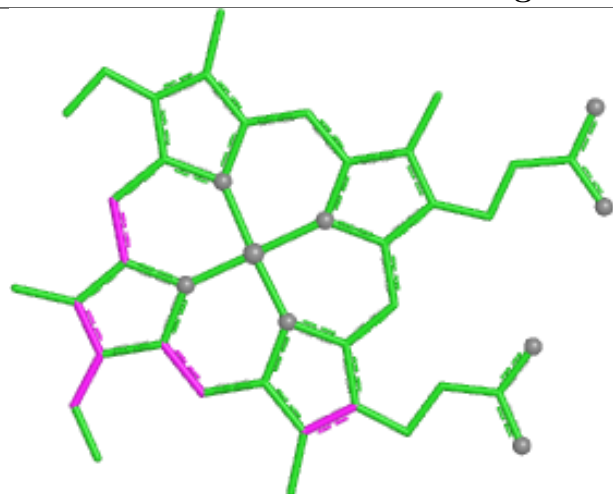
Torsions



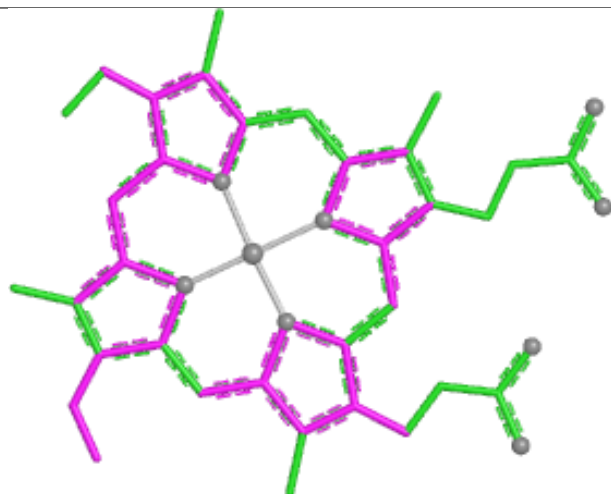
Rings



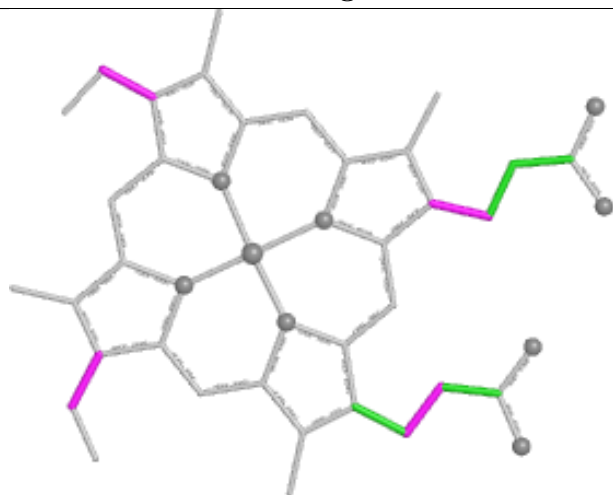
Ligand HEC F 301



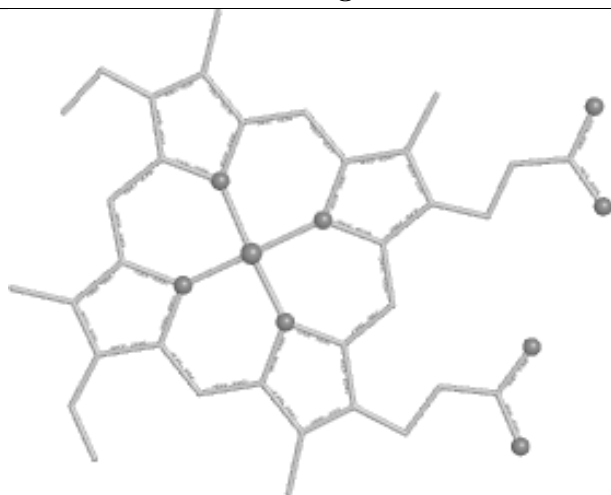
Bond lengths



Bond angles

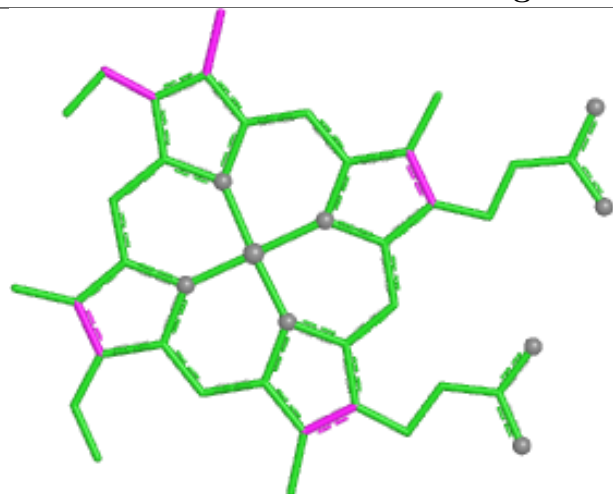


Torsions

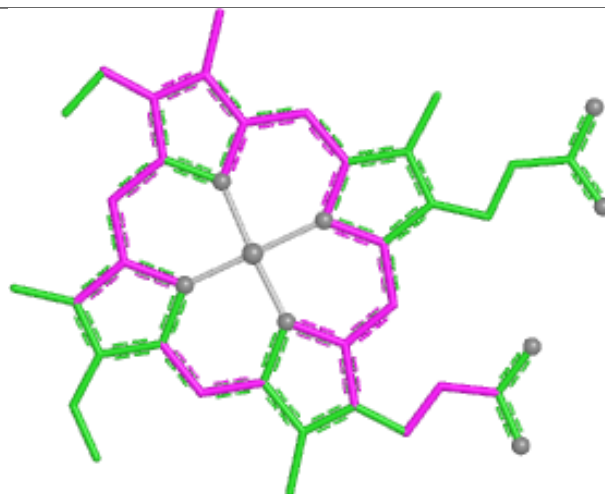


Rings

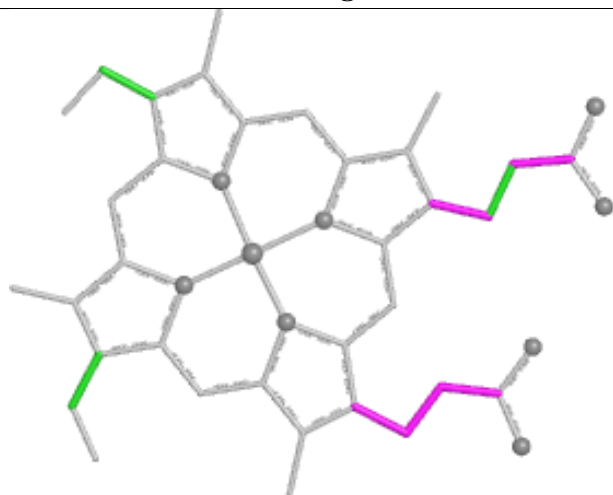
Ligand HEC P 308



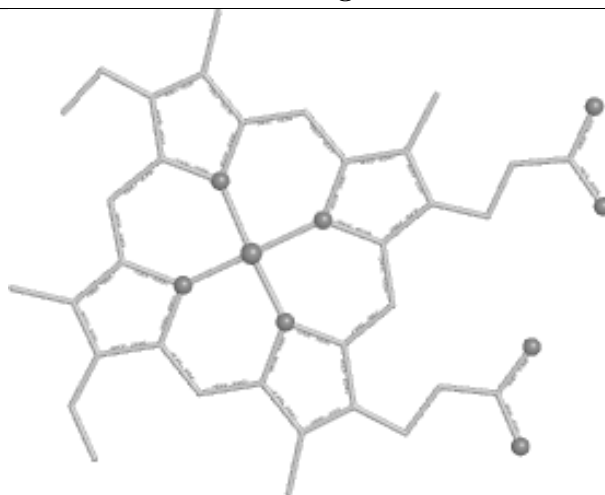
Bond lengths



Bond angles

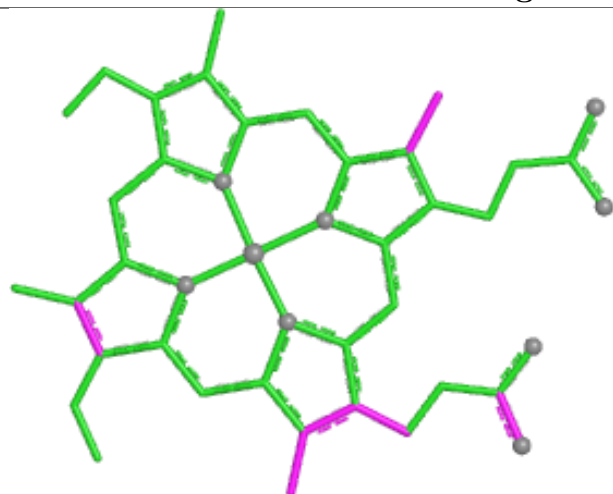


Torsions

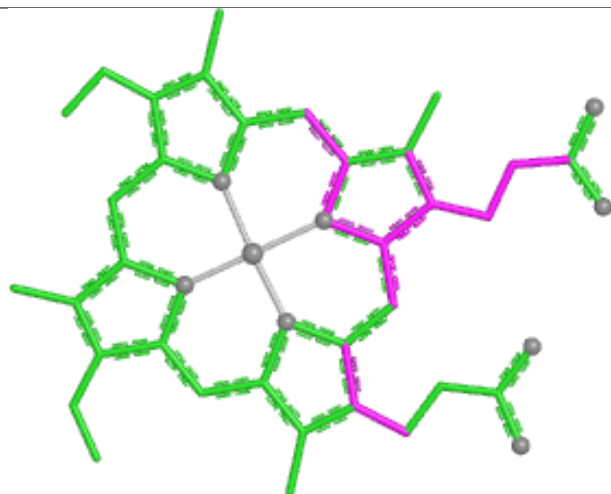


Rings

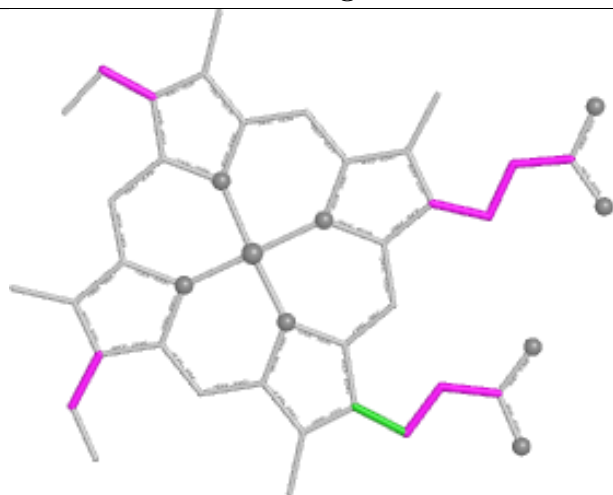
Ligand HEC S 307



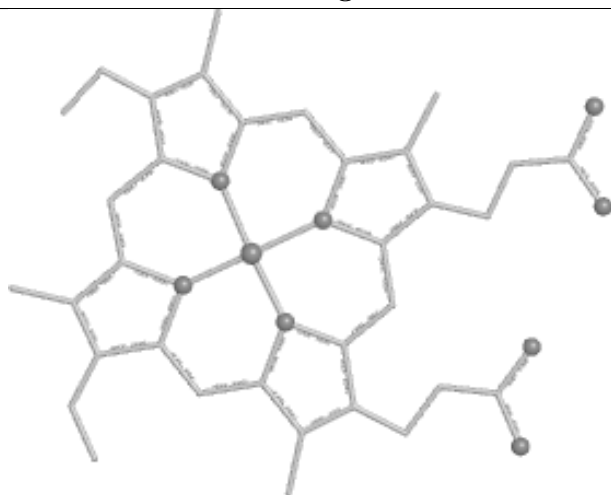
Bond lengths



Bond angles

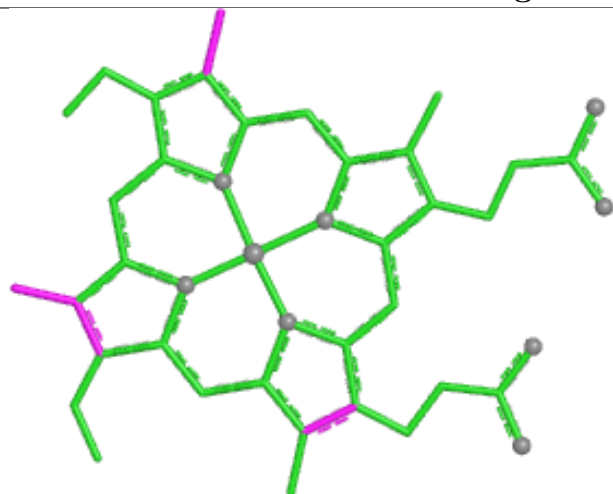


Torsions

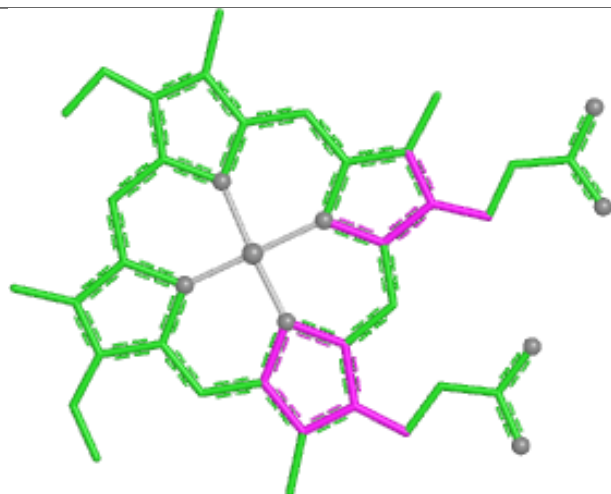


Rings

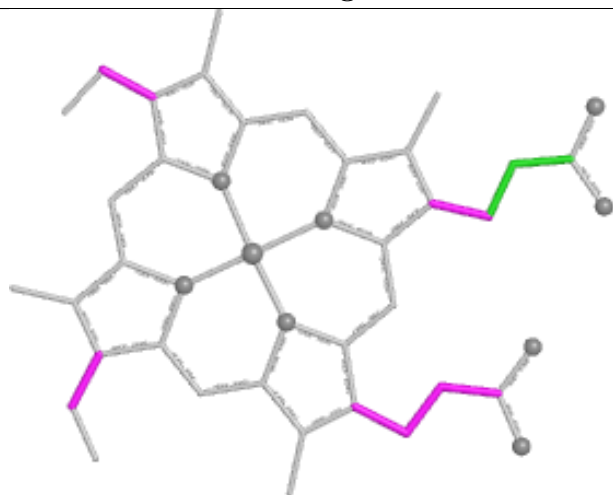
Ligand HEC F 305



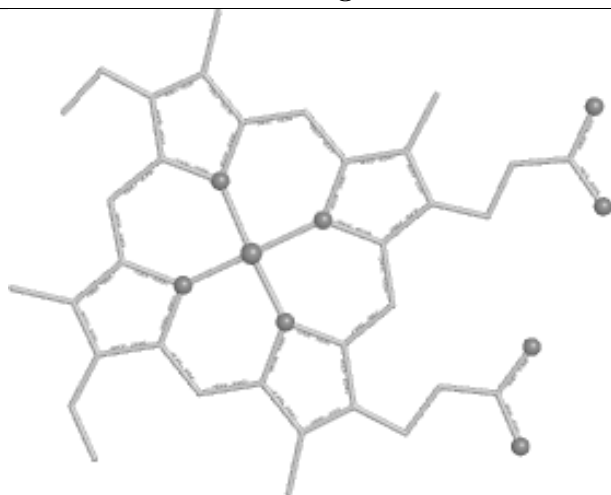
Bond lengths



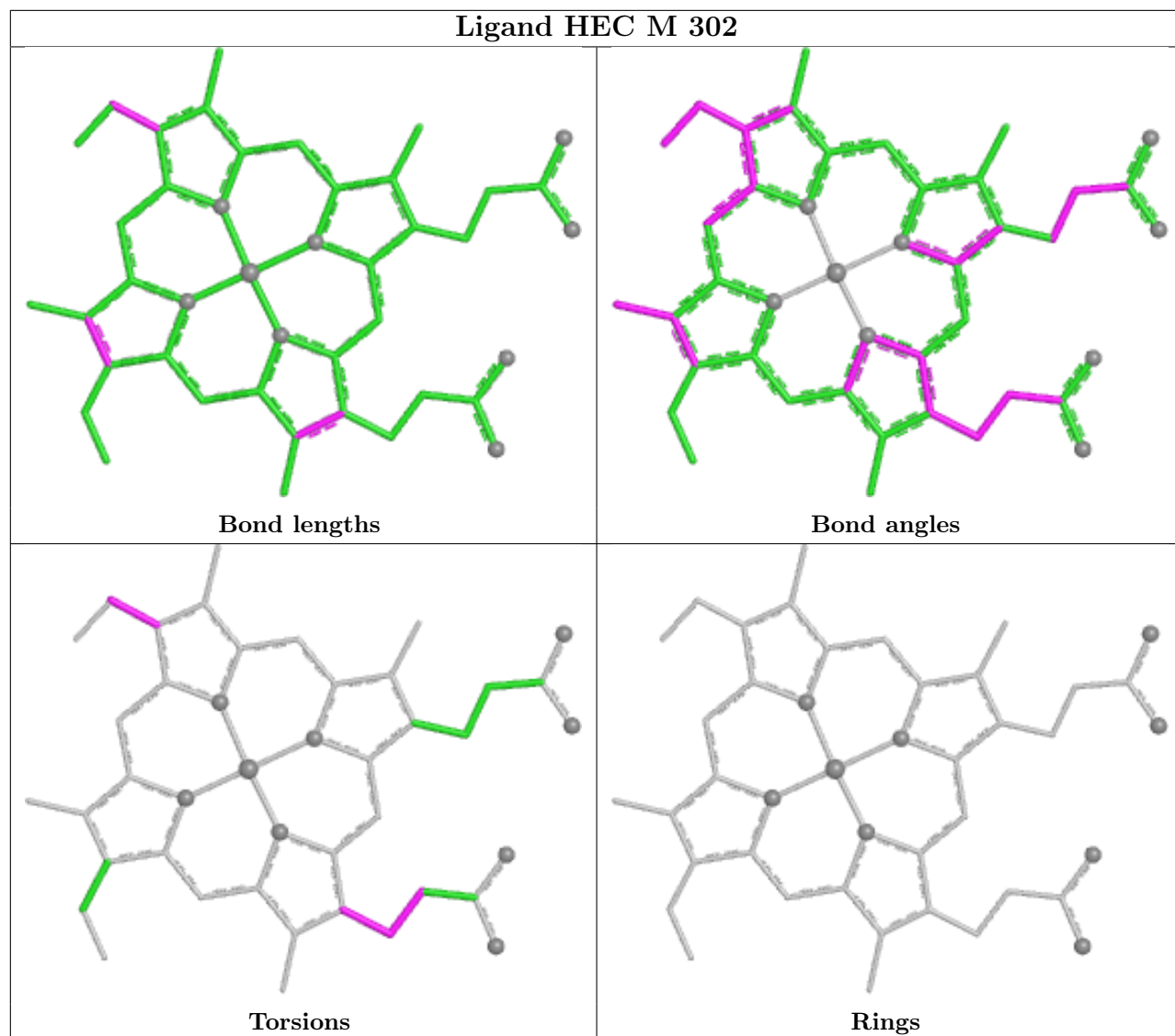
Bond angles



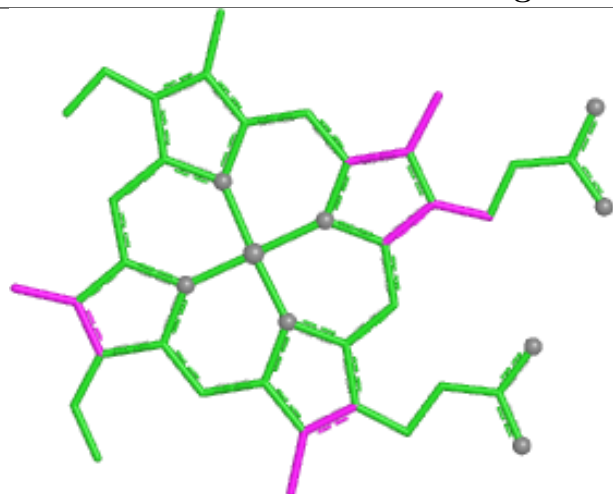
Torsions



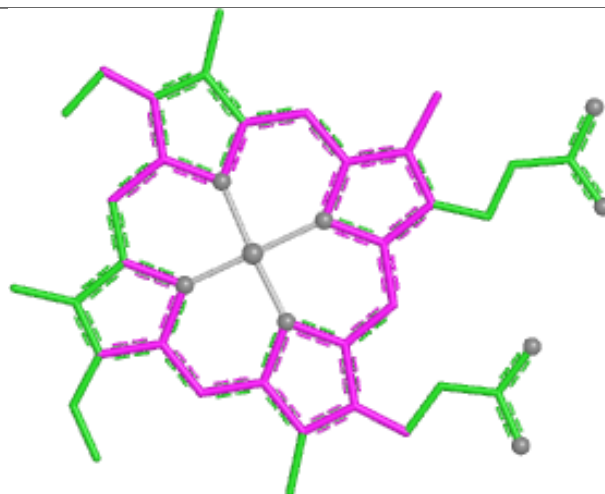
Rings



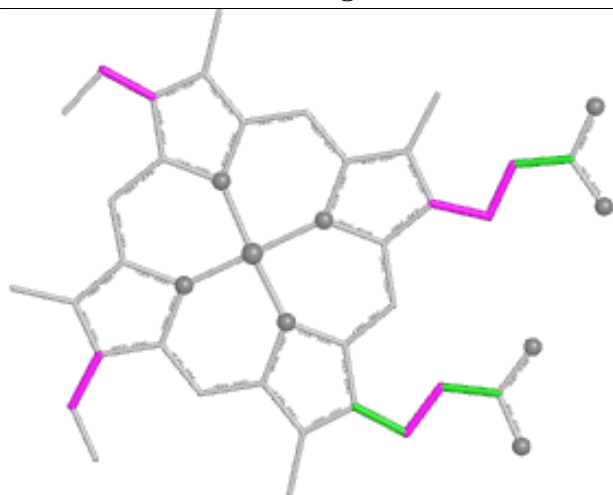
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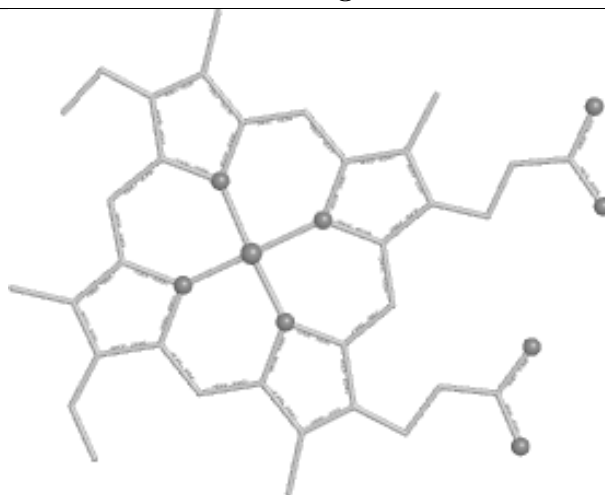
Bond lengths



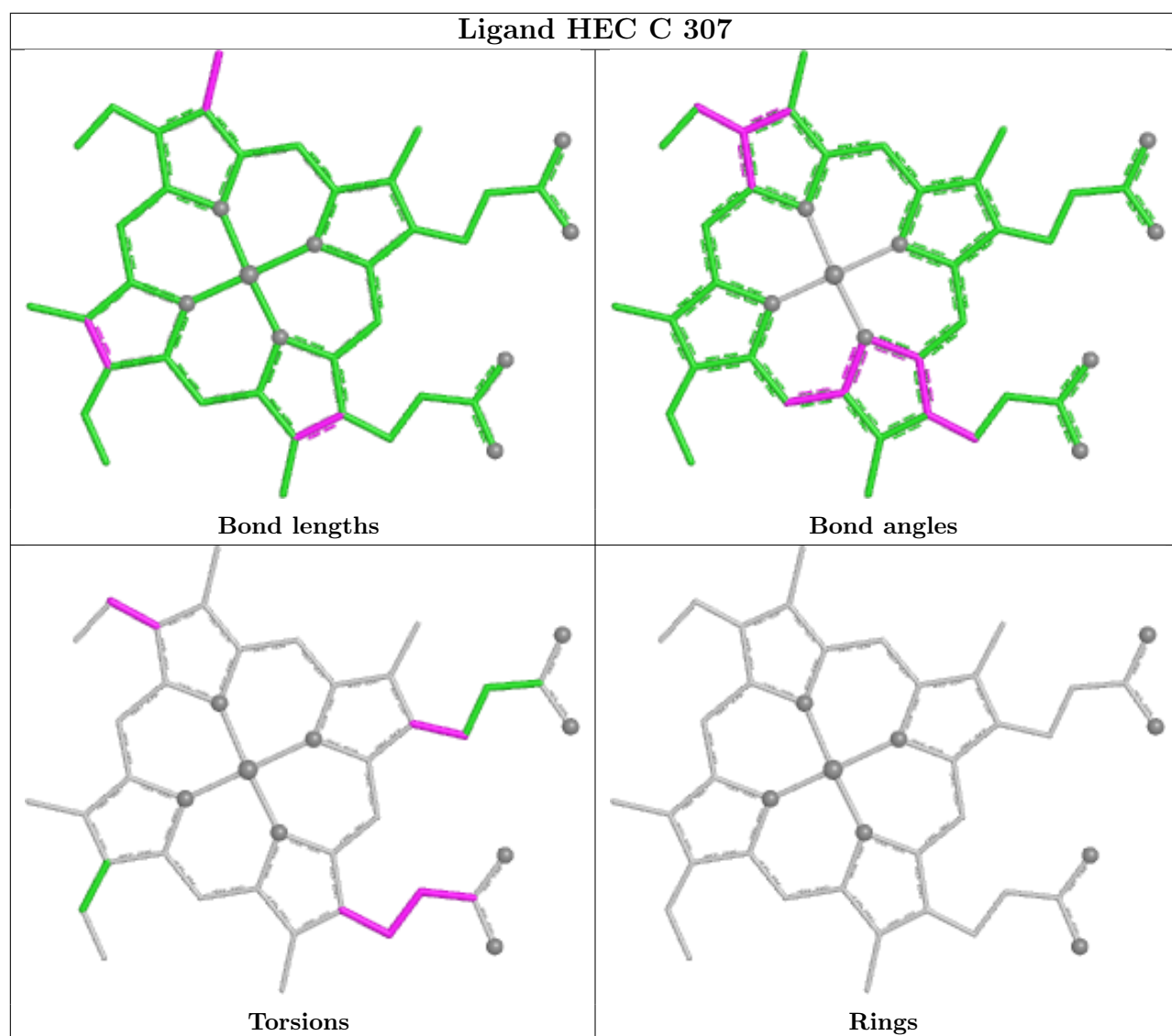
Bond angles

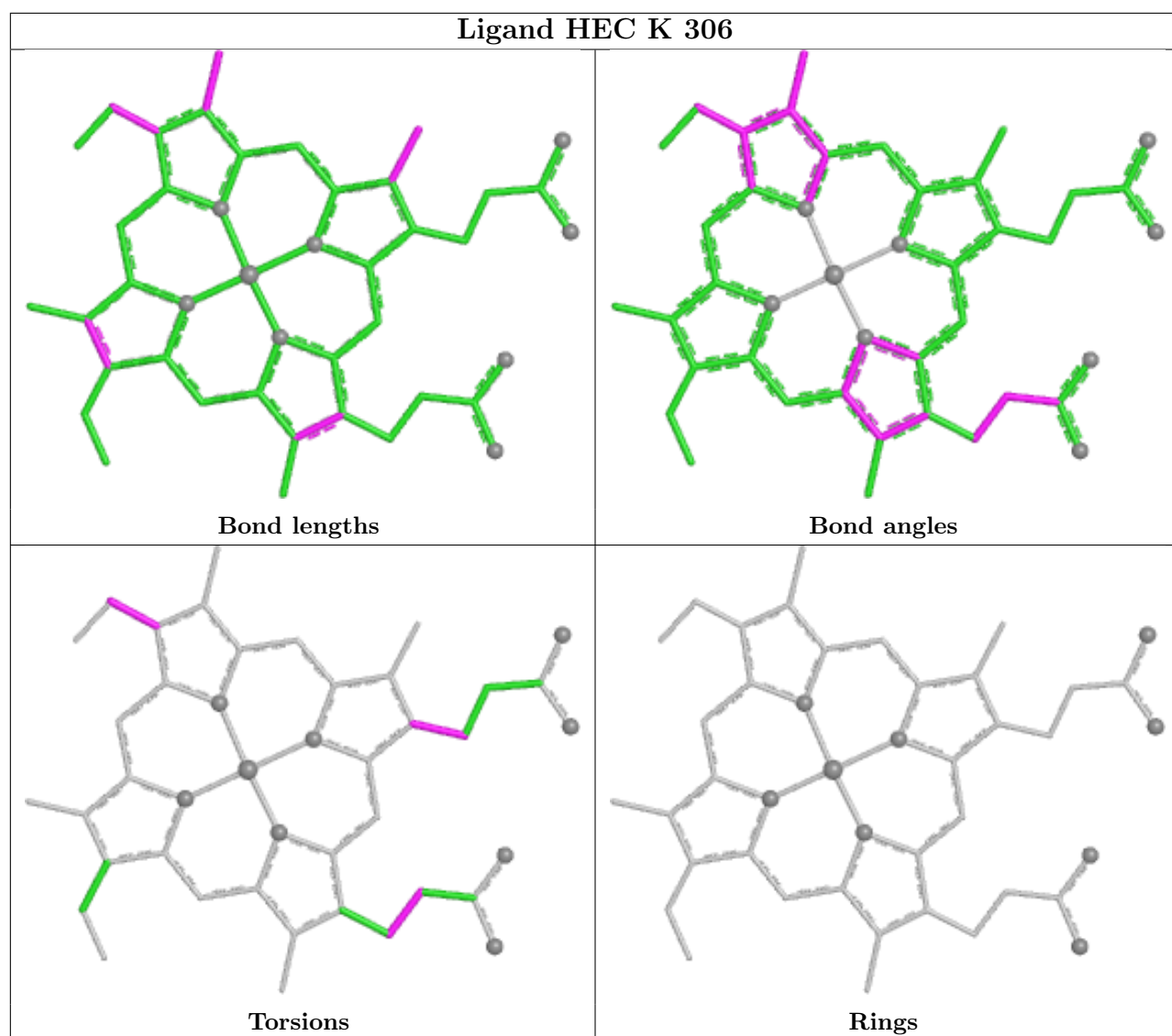


Torsions

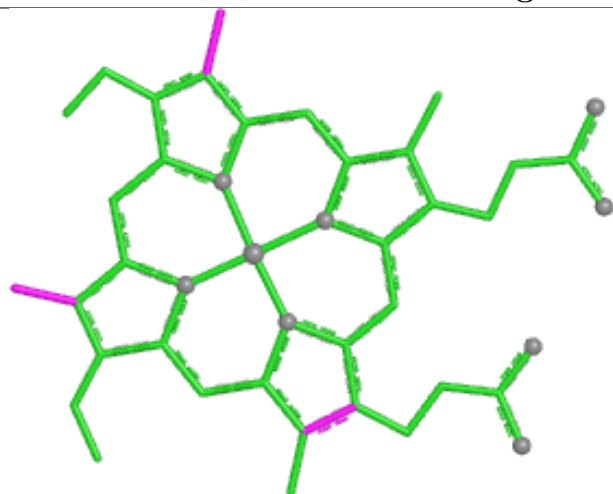


Rings

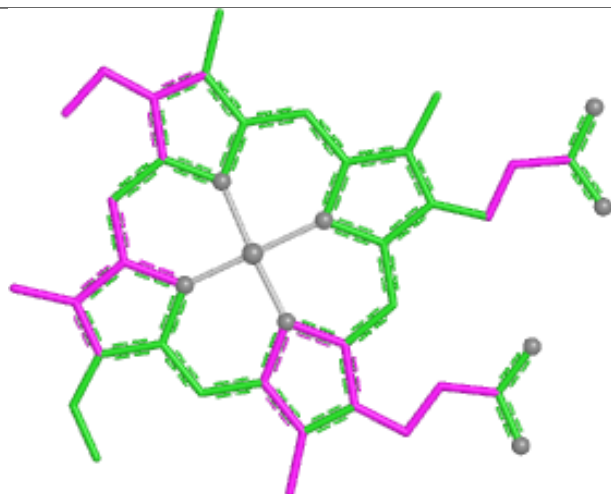




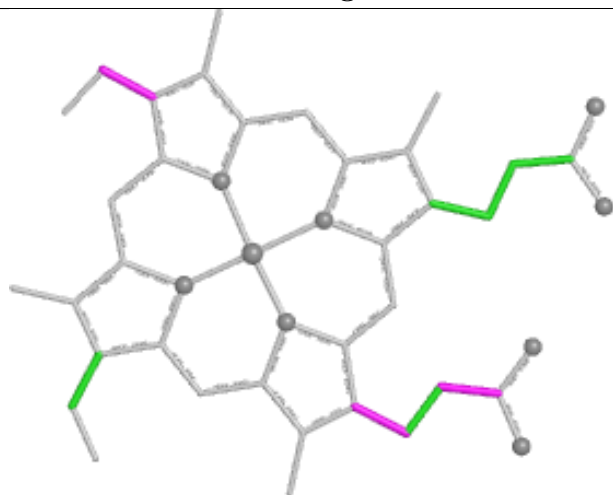
Ligand HEC J 302



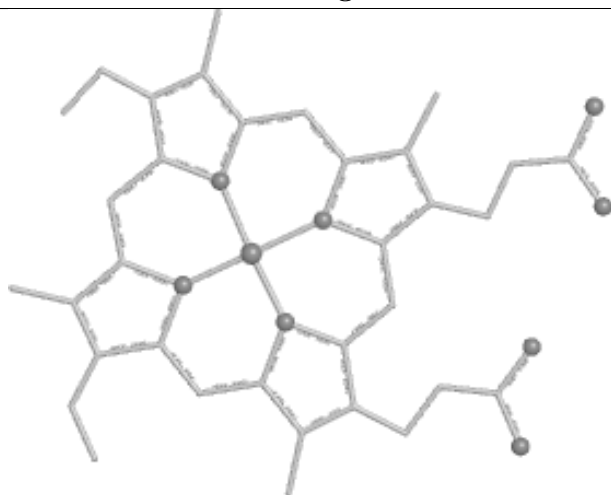
Bond lengths



Bond angles

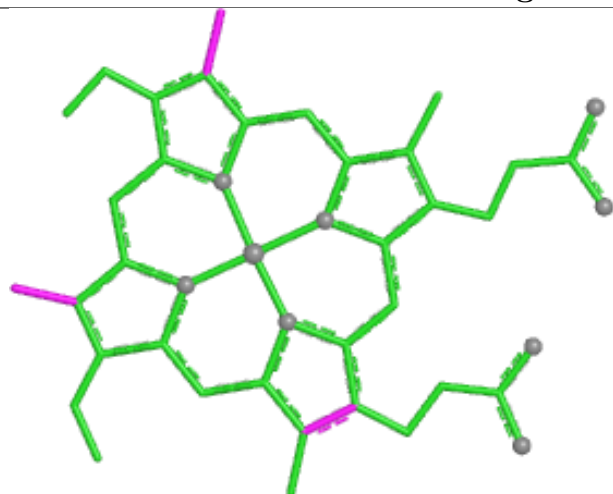


Torsions

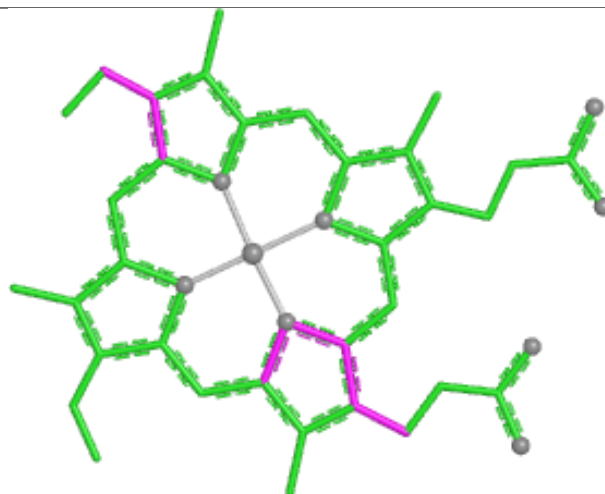


Rings

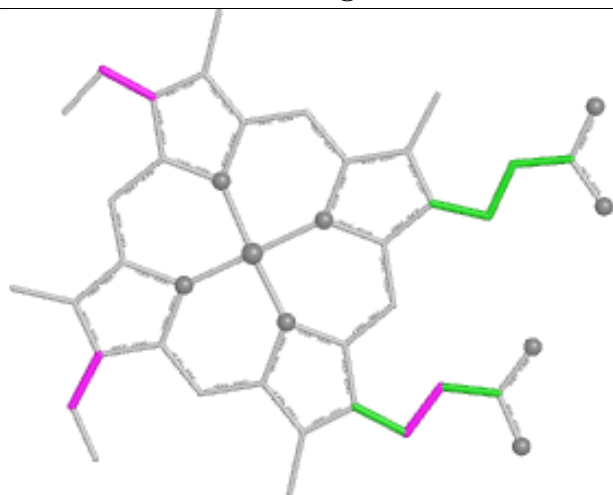
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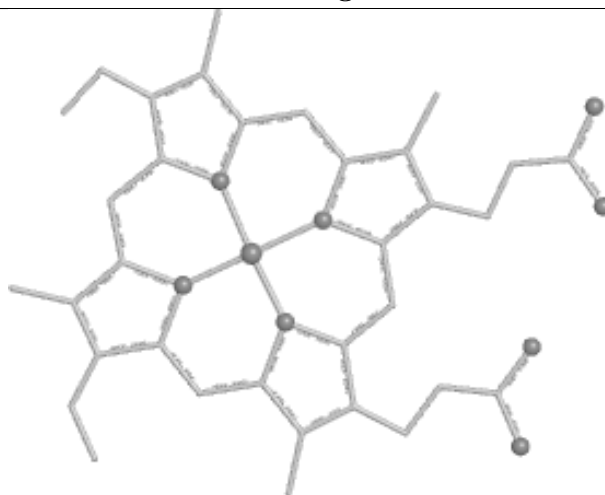
Bond lengths



Bond angles

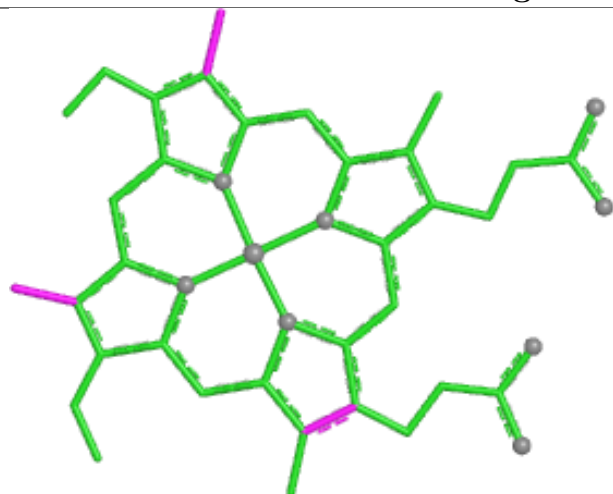


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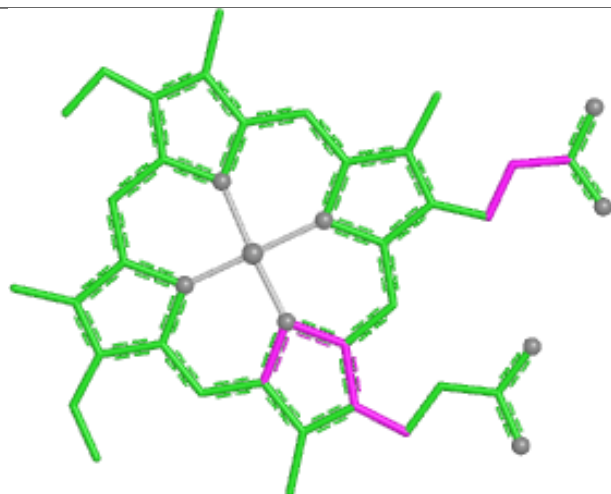


Rings

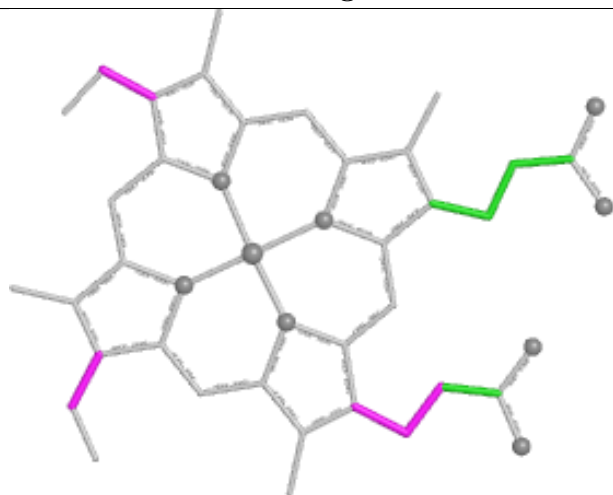
Ligand HEC P 301



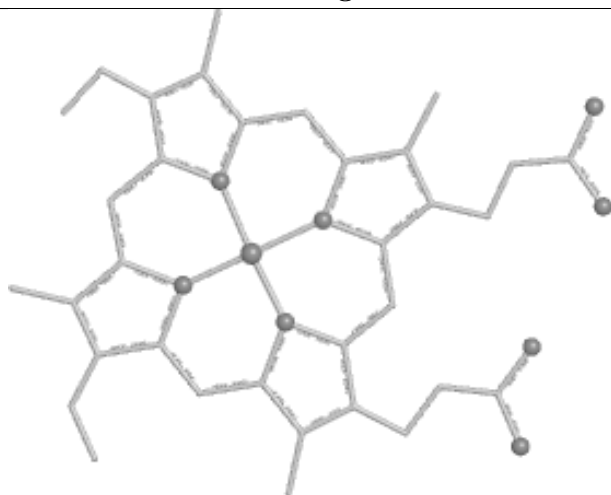
Bond lengths



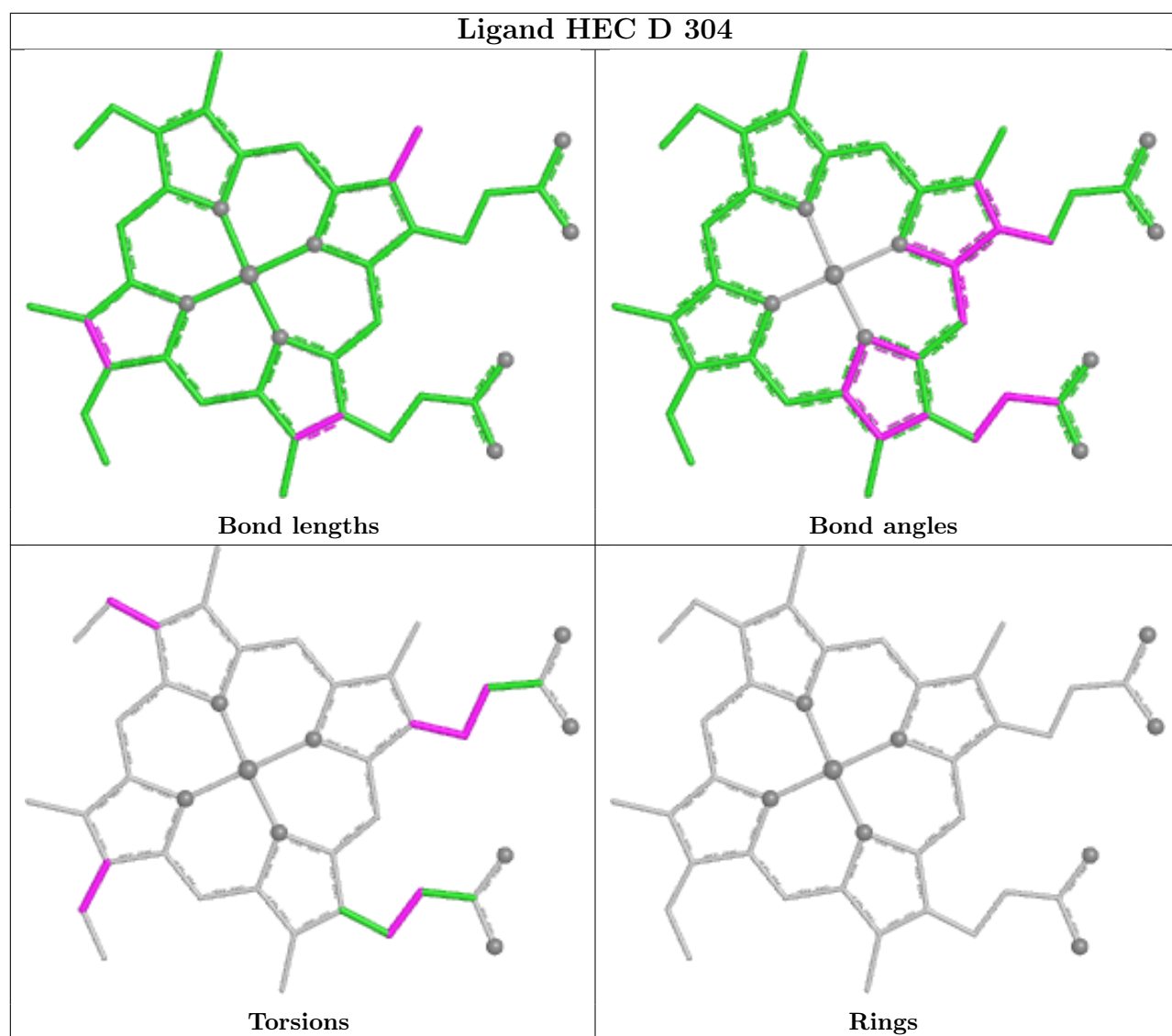
Bond angles



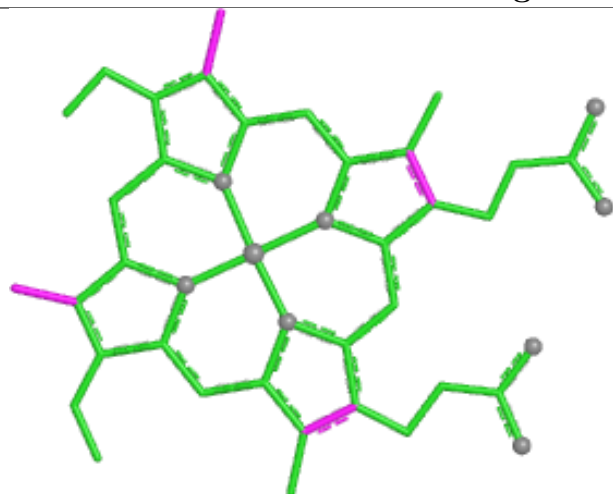
Torsions



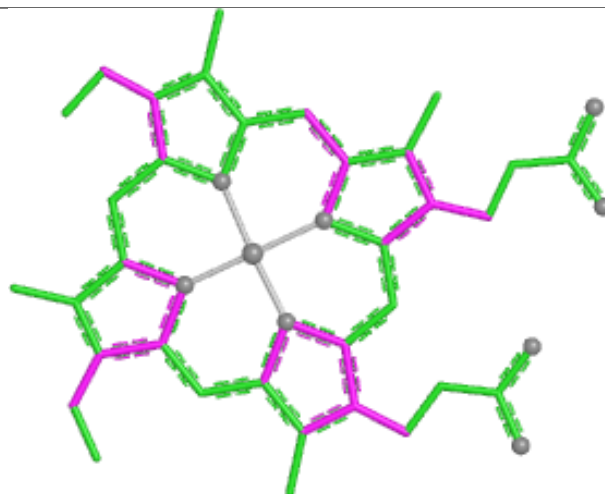
Rings



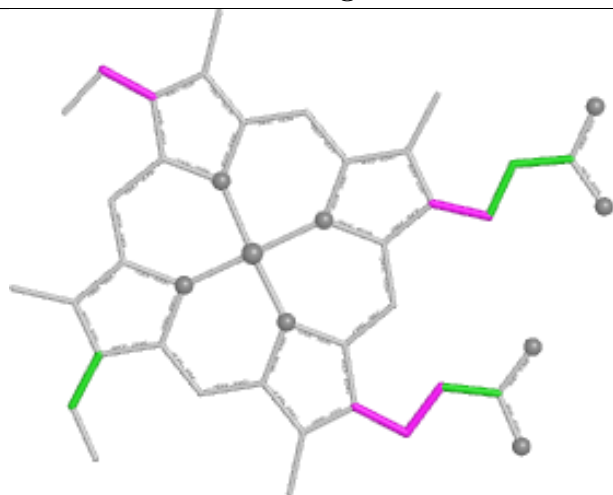
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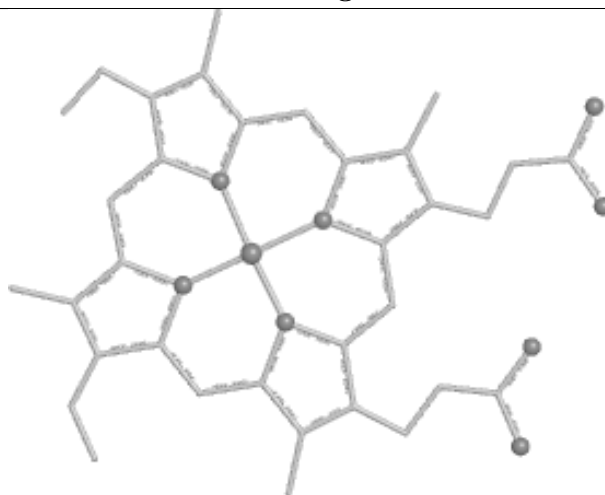
Bond lengths



Bond angles

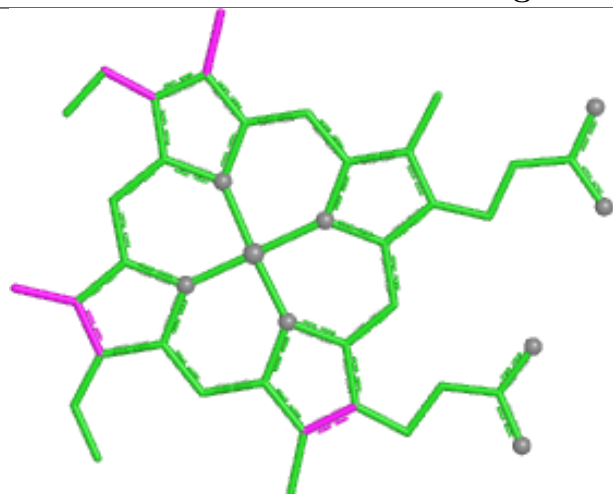


Torsions

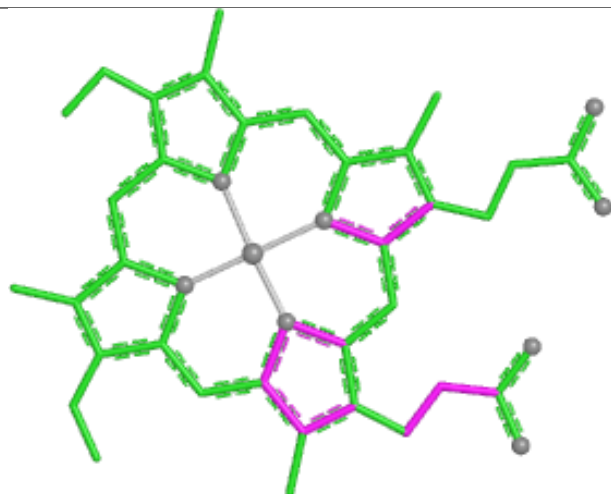


Rings

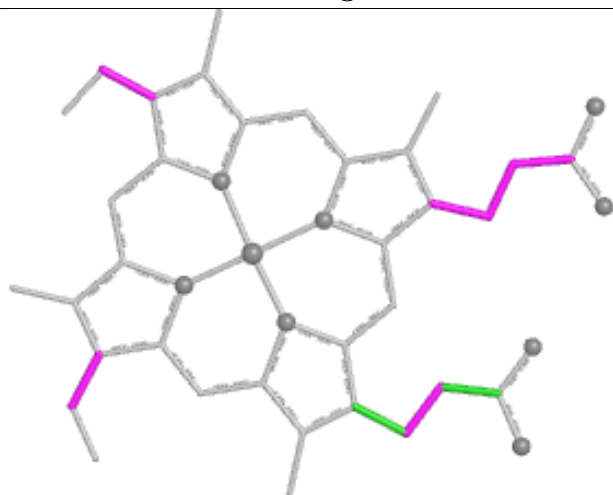
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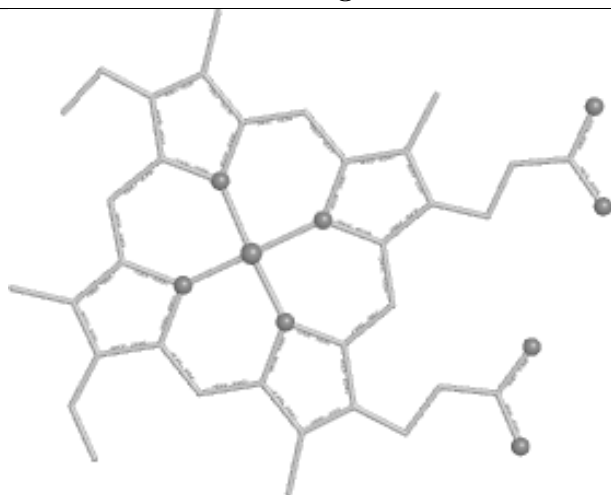
Bond lengths



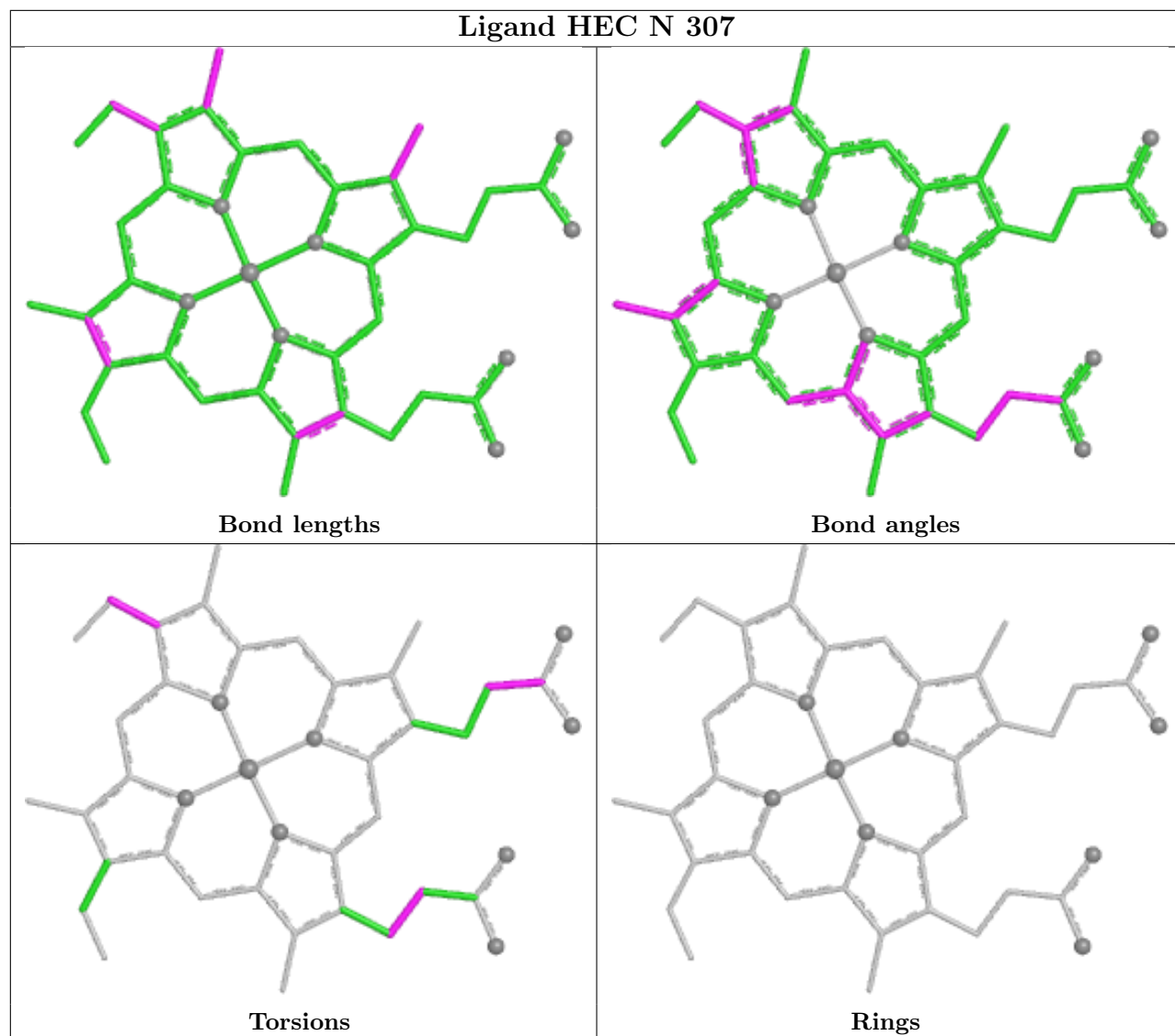
Bond angles



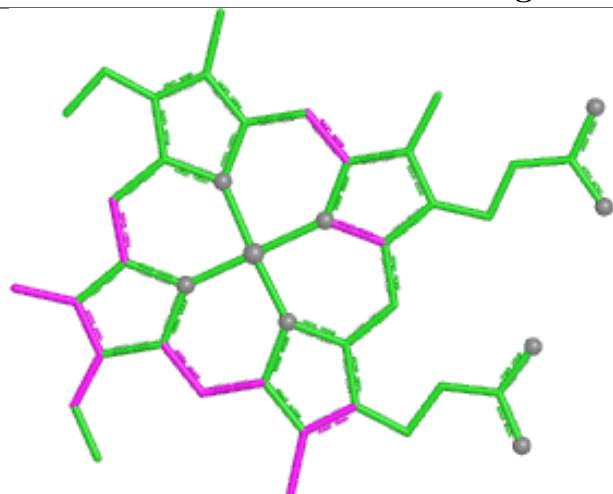
Torsions



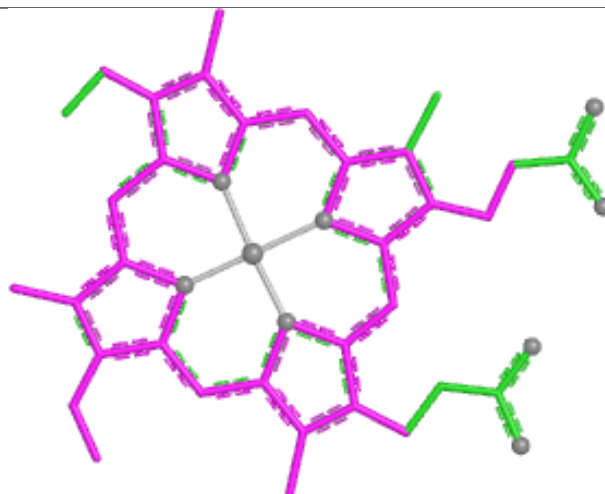
Rings



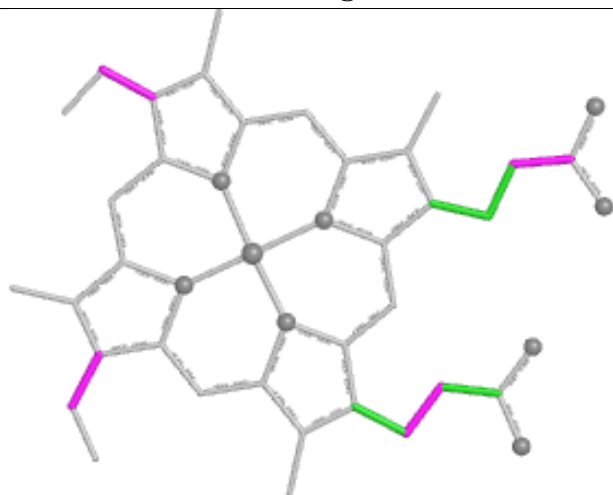
Ligand HEC L 301



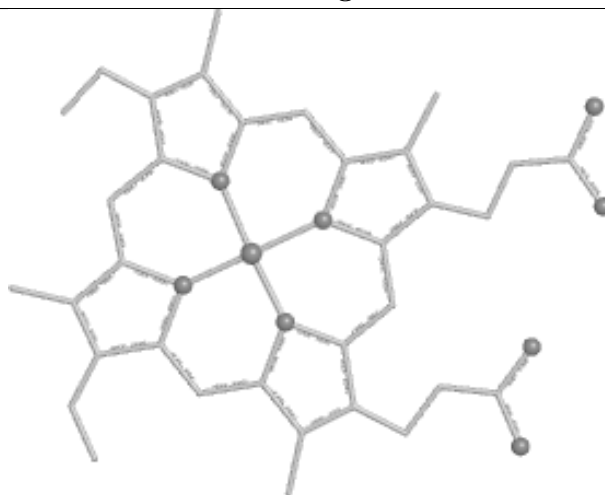
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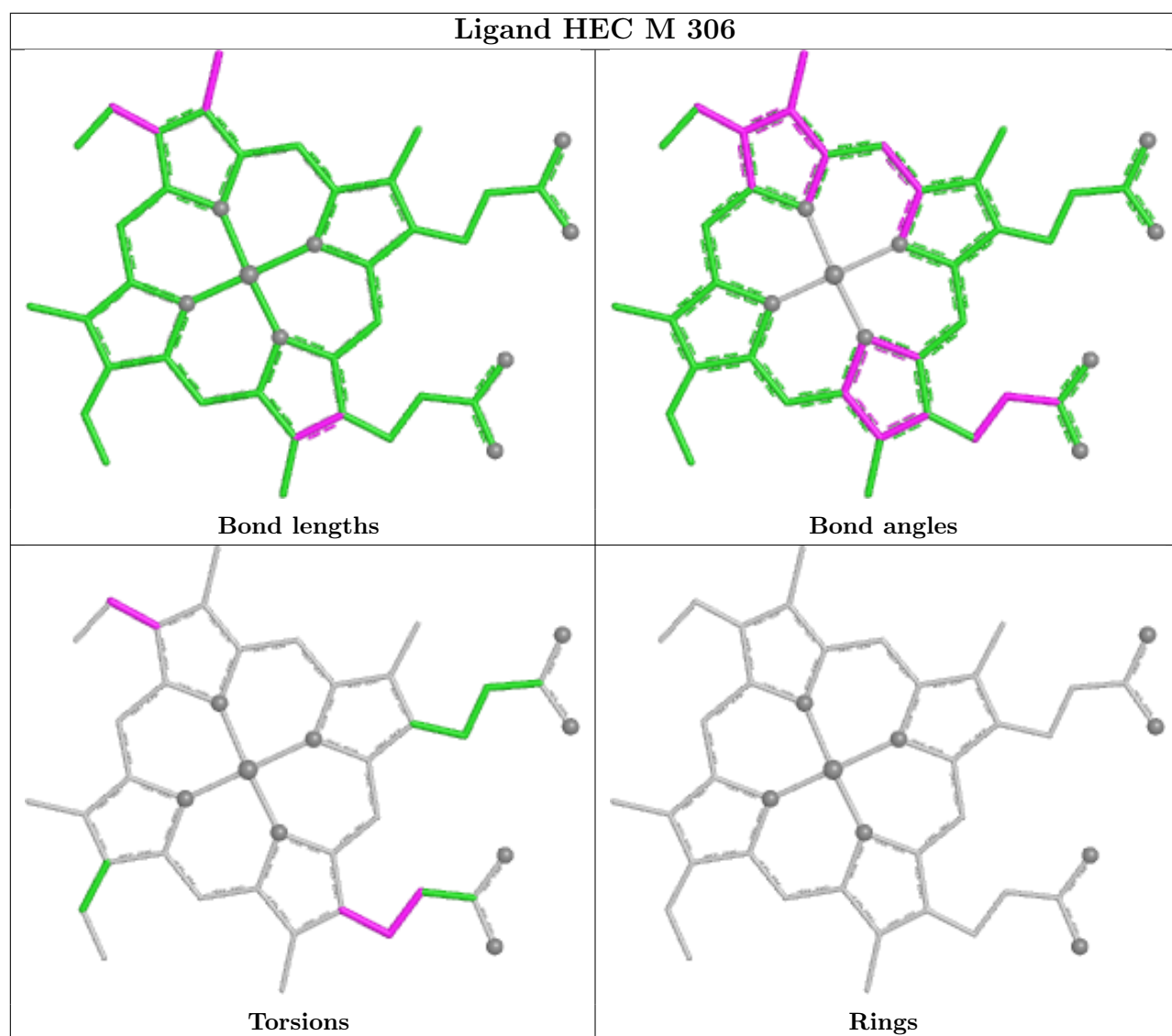
Bond angles

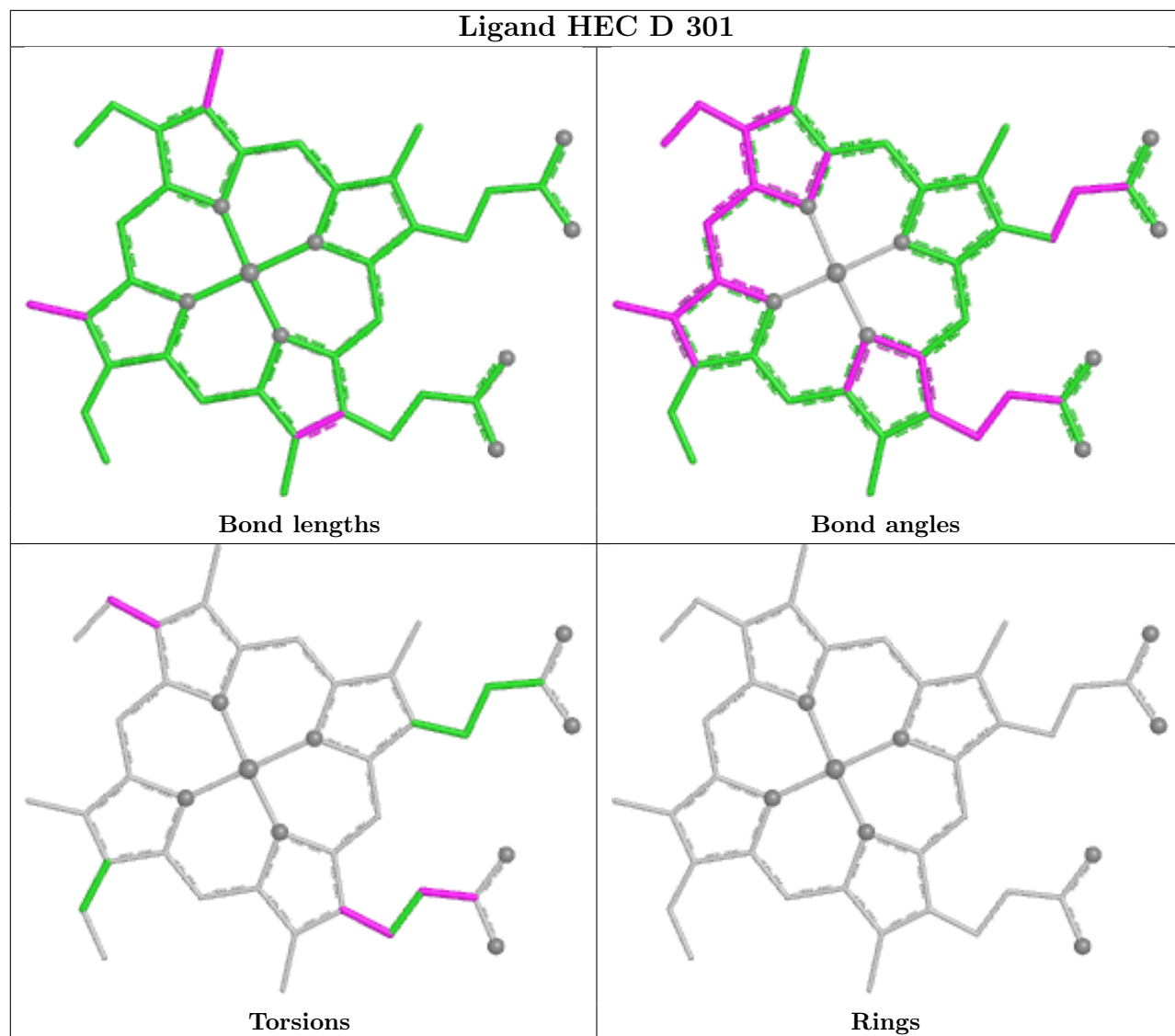


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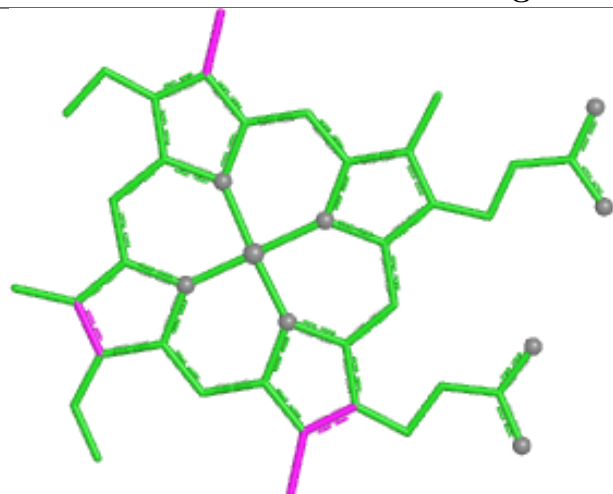


Rings

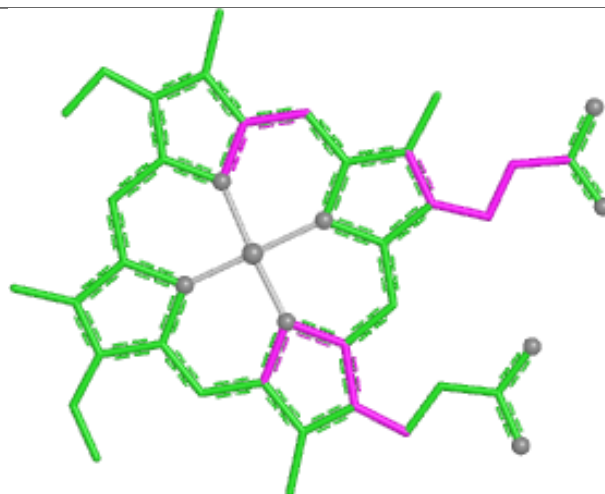




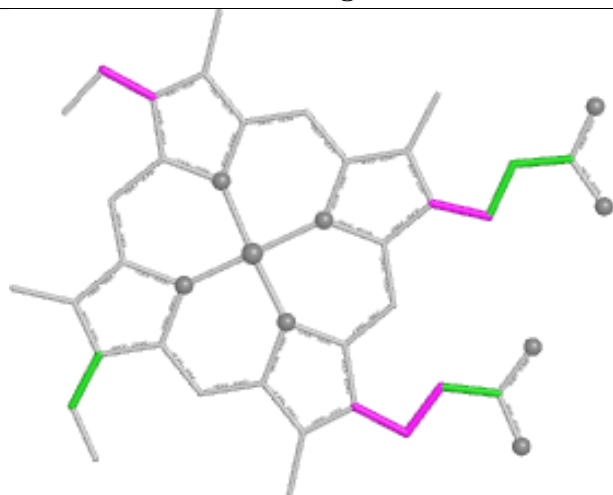
Ligand HEC C 301



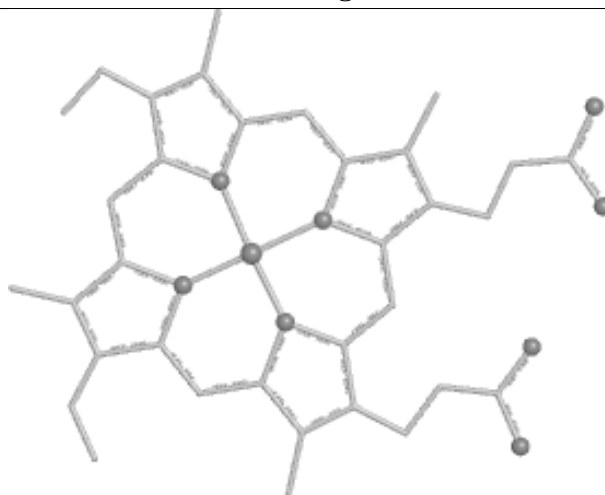
Bond lengths



Bond angles

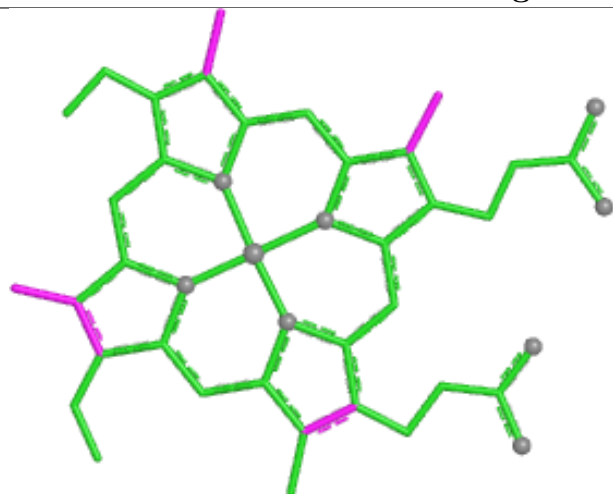


Torsions

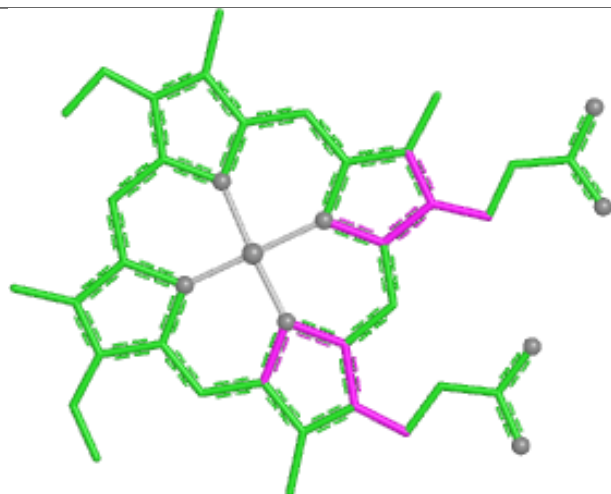


Rings

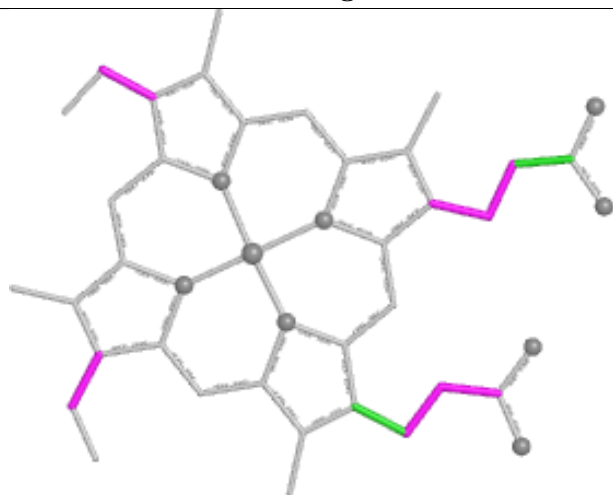
Ligand HEC R 306



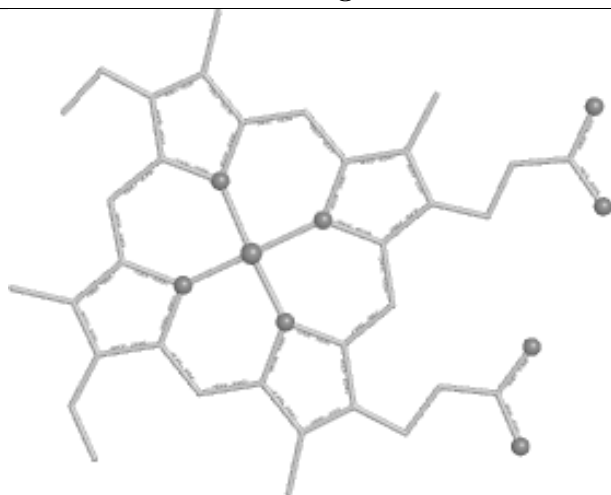
Bond lengths



Bond angles

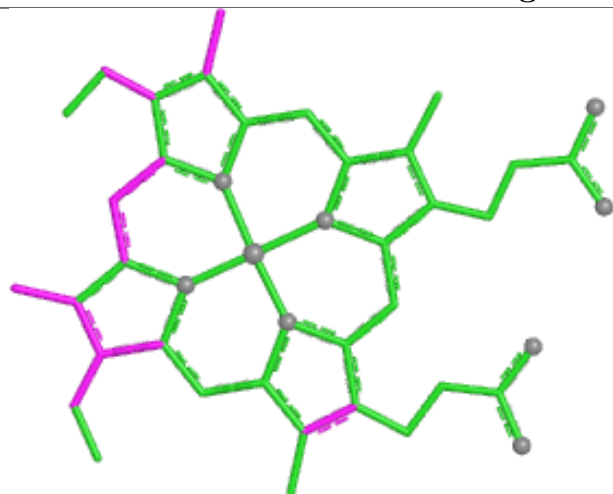


Torsions

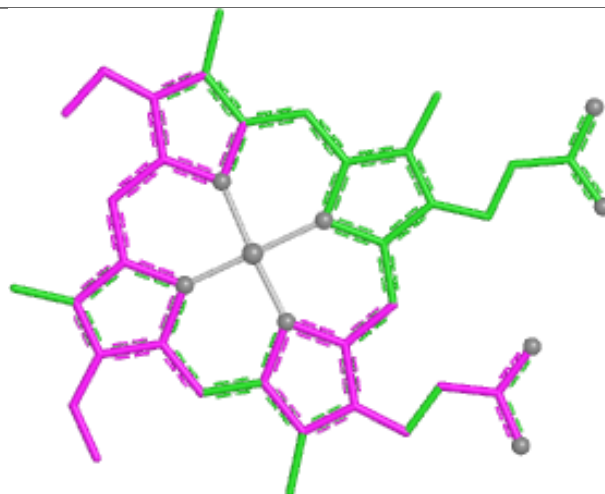


Rings

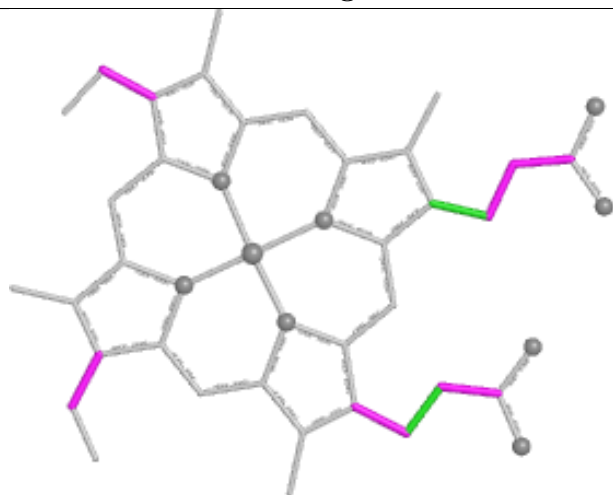
Ligand HEC I 301



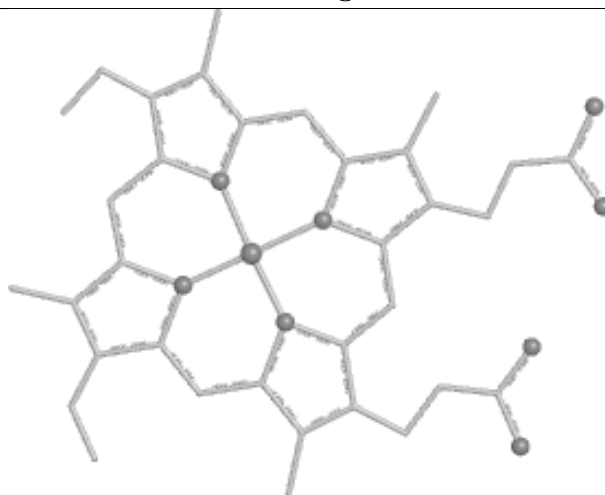
Bond lengths



Bond angles

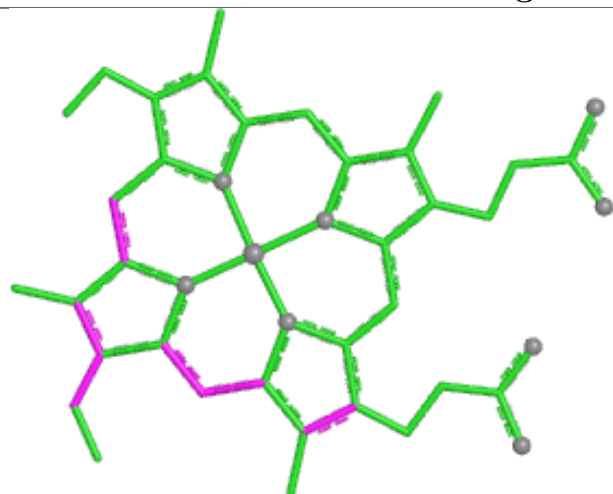


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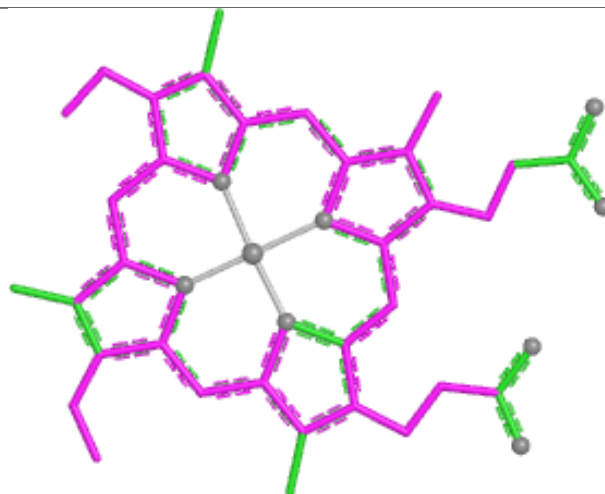


Rings

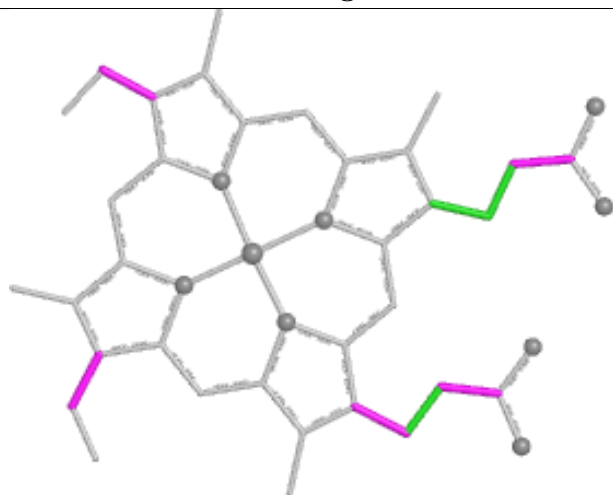
Ligand HEC S 305



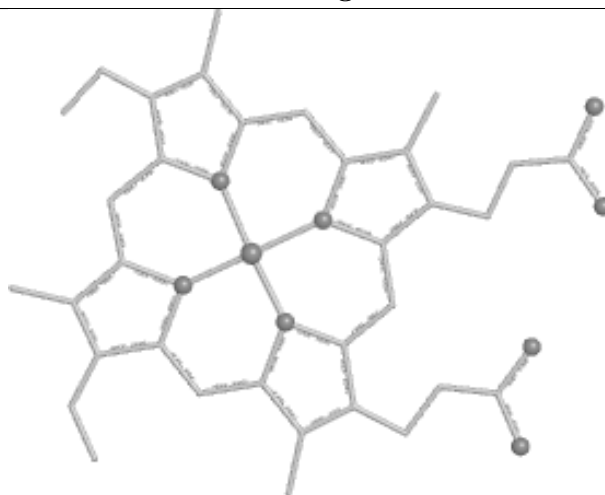
Bond lengths



Bond angles

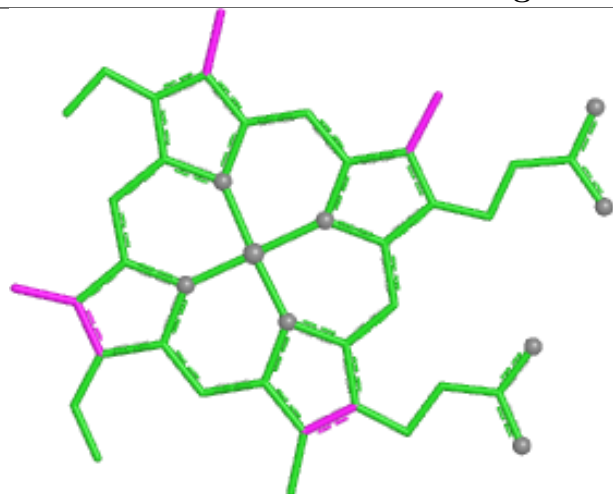


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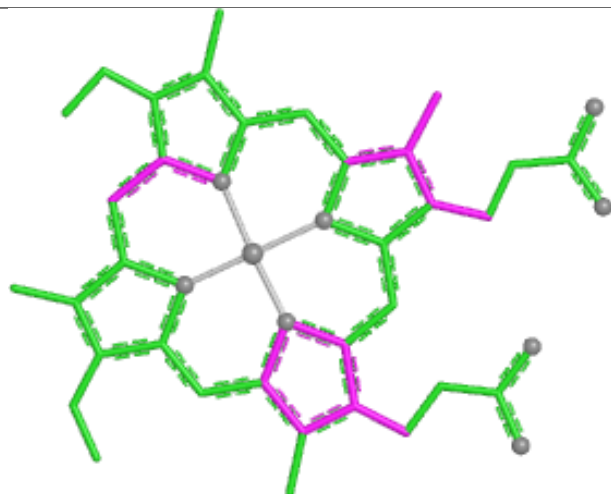


Rings

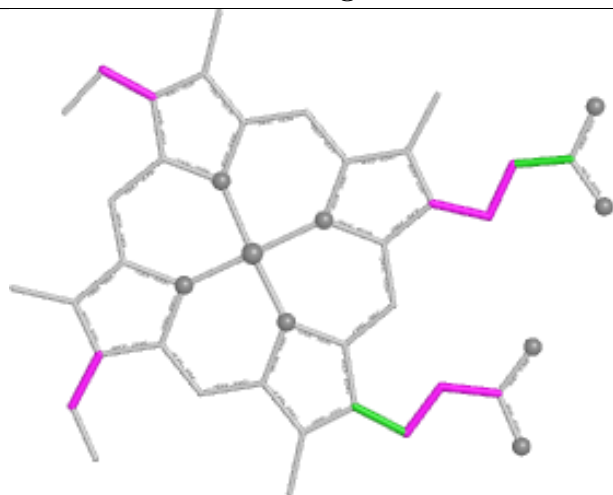
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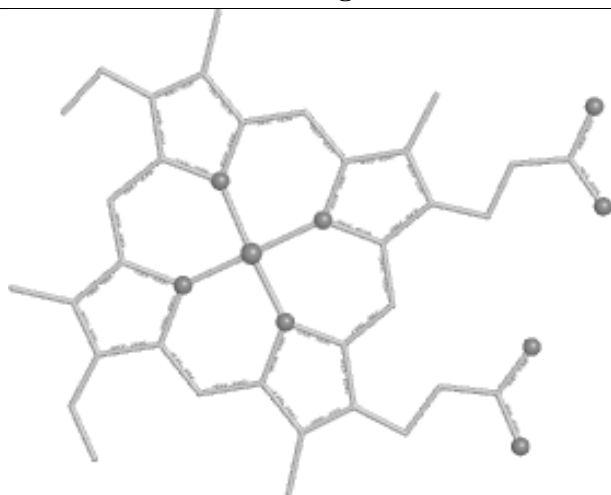
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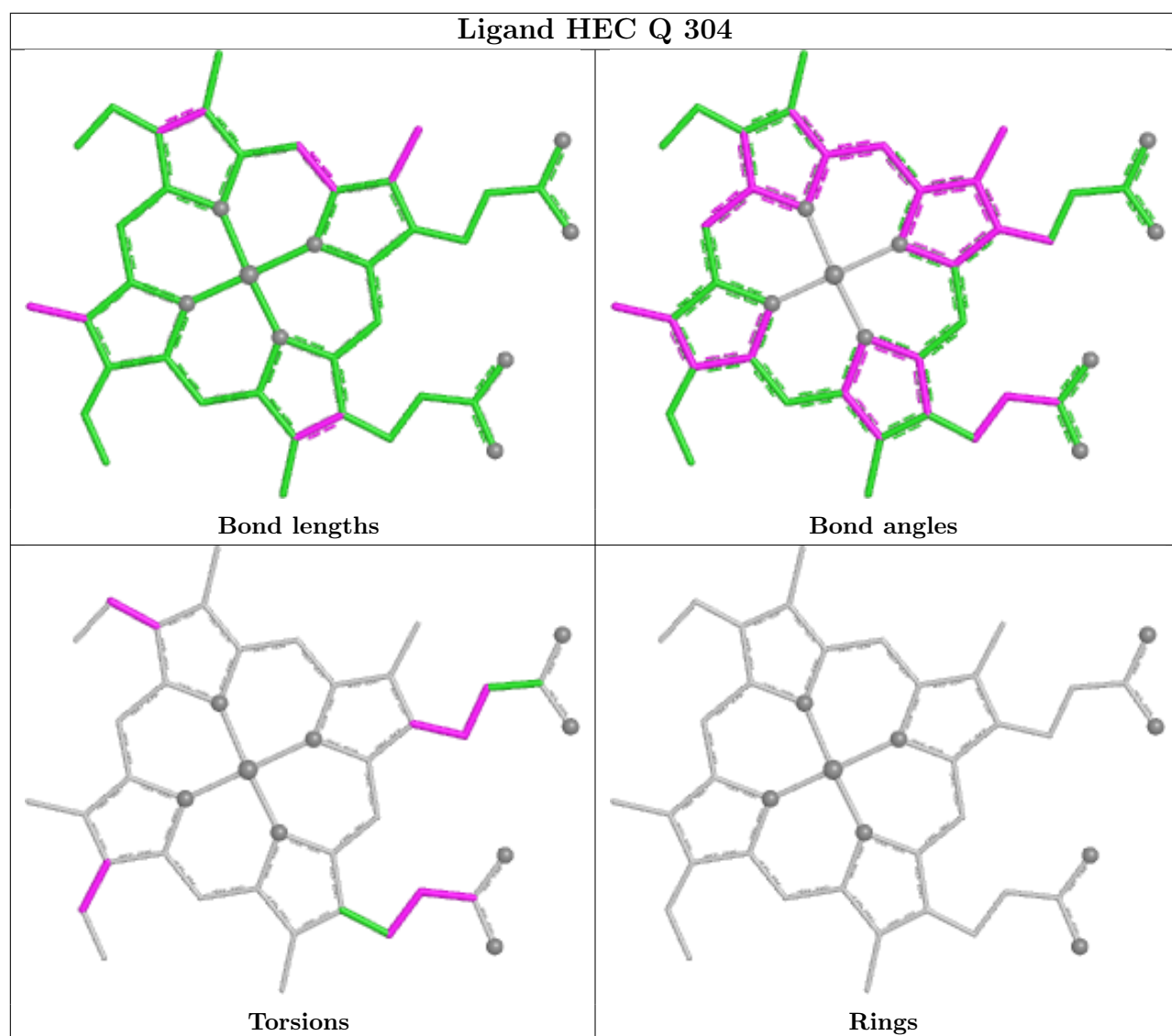
Bond angles



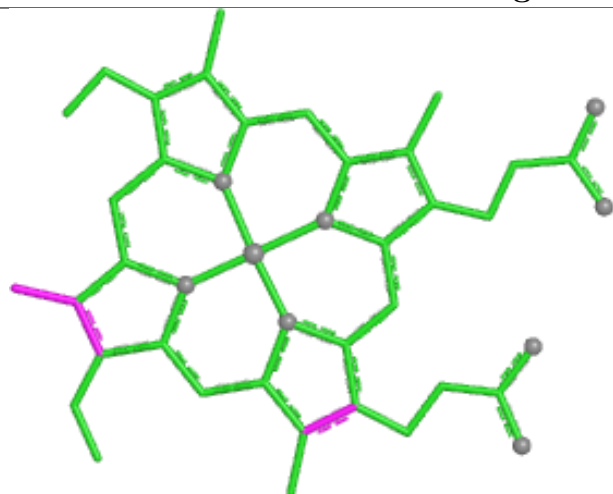
Torsions



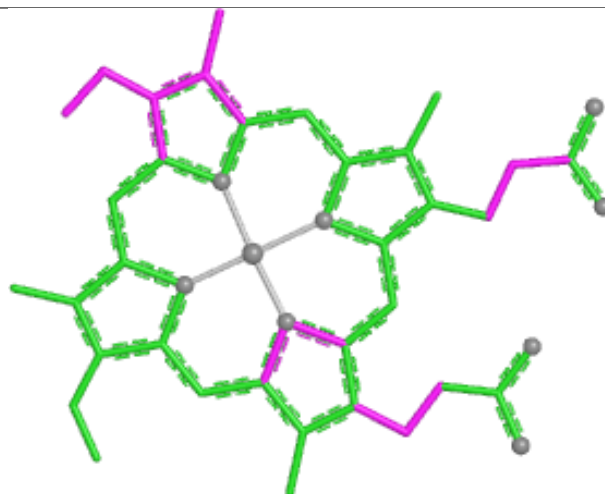
Rings



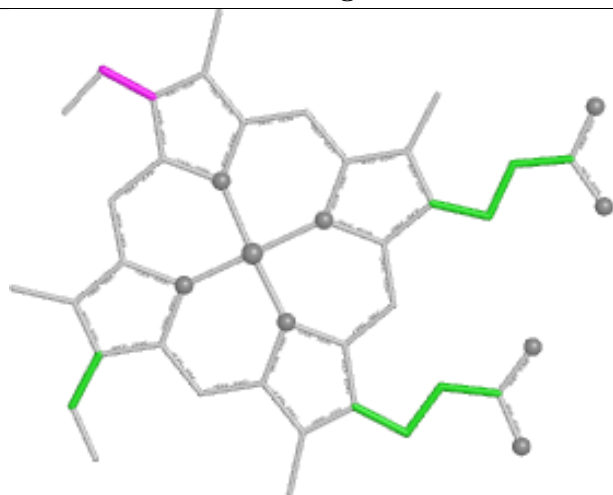
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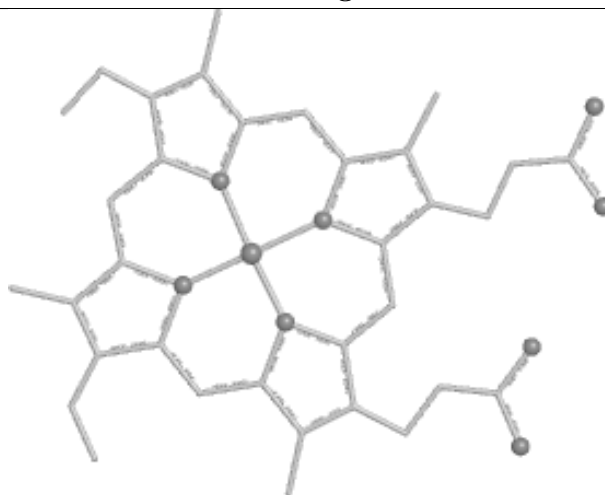
Bond lengths



Bond angles

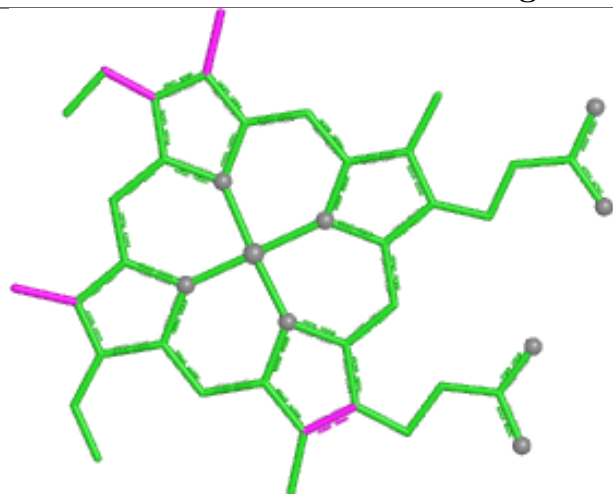


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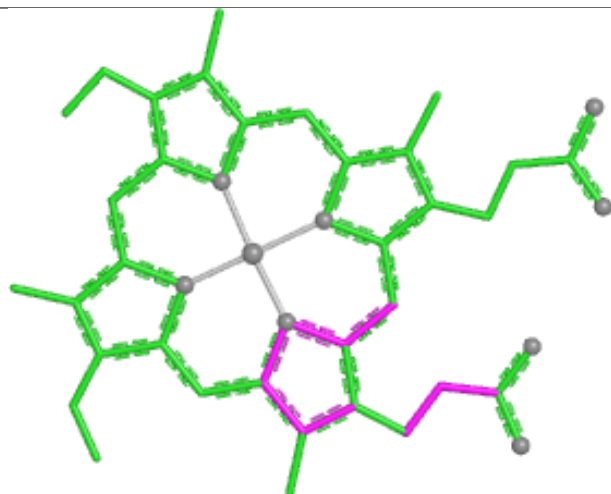


Rings

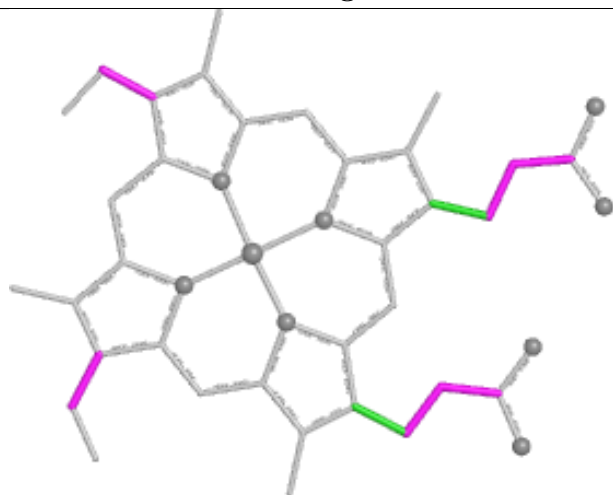
Ligand HEC I 302



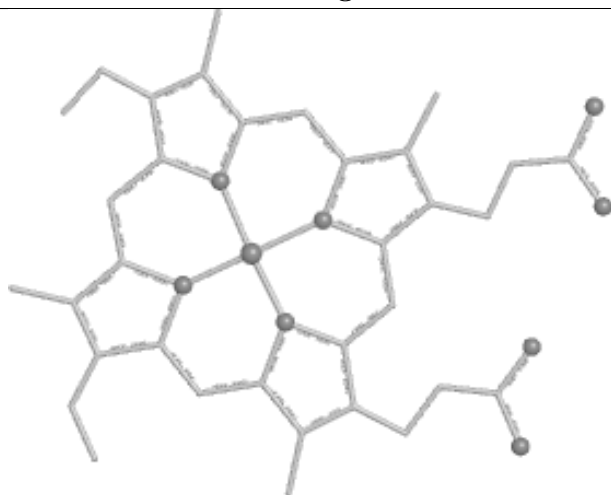
Bond lengths



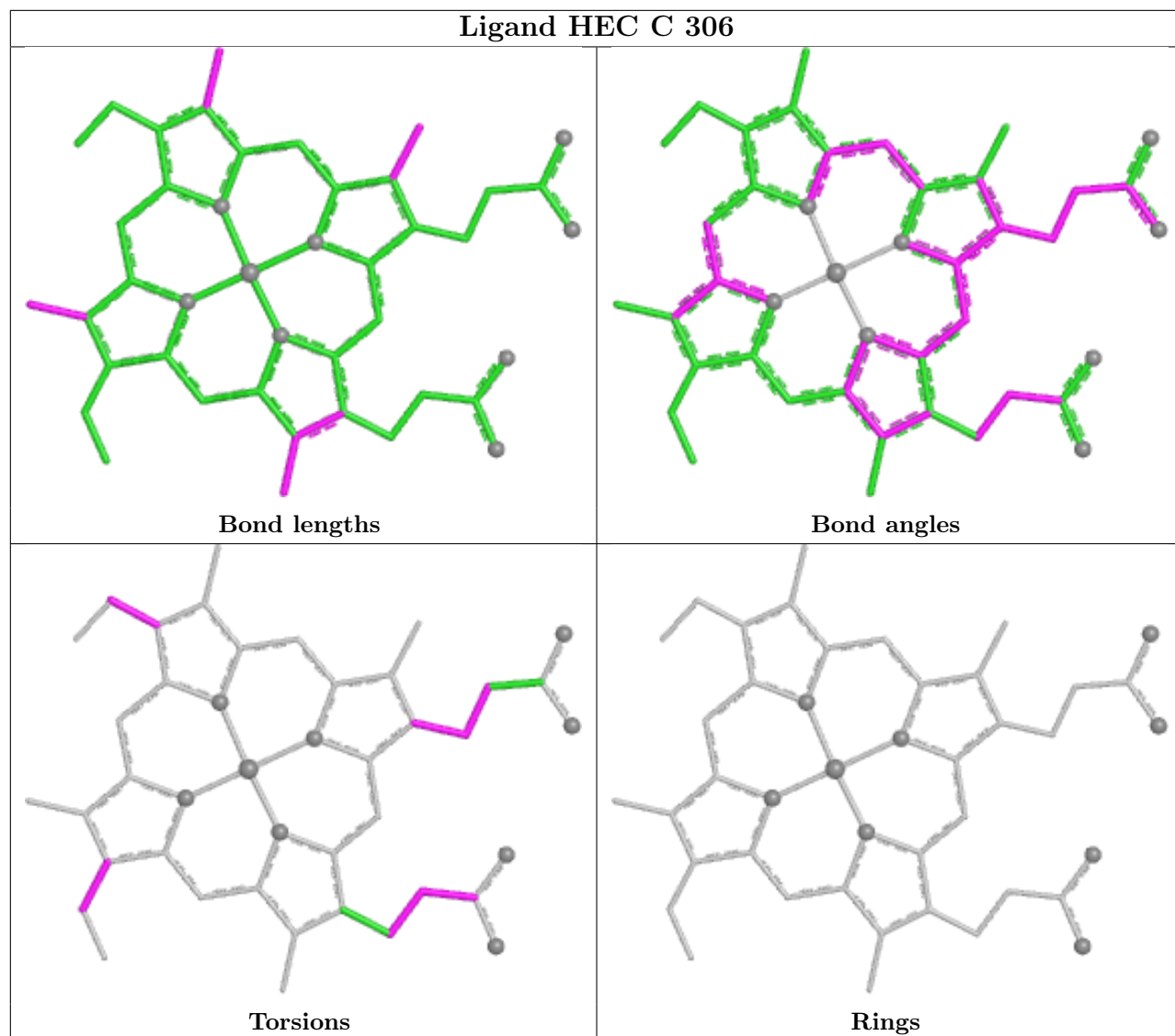
Bond angles



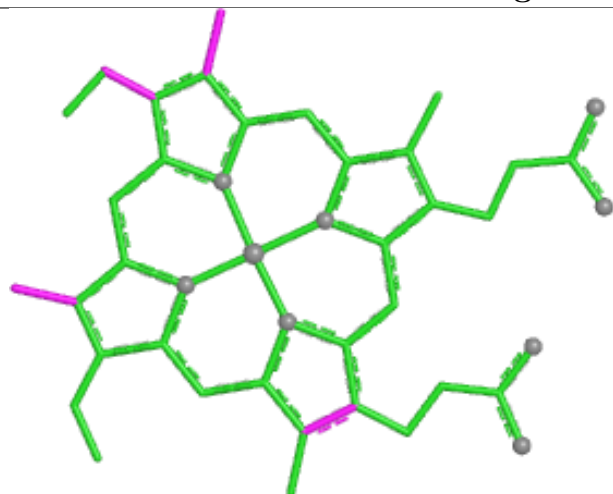
Torsions



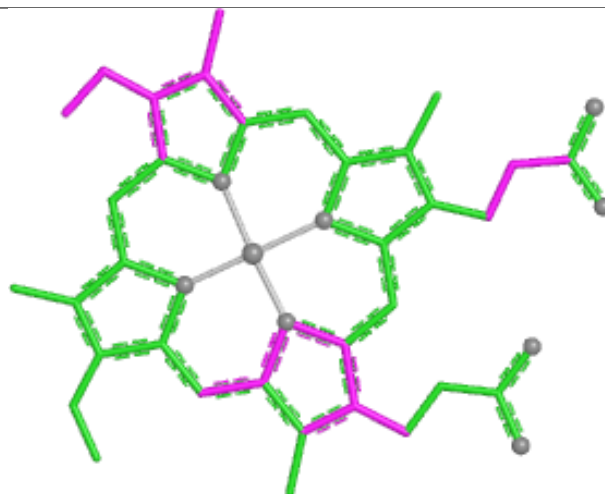
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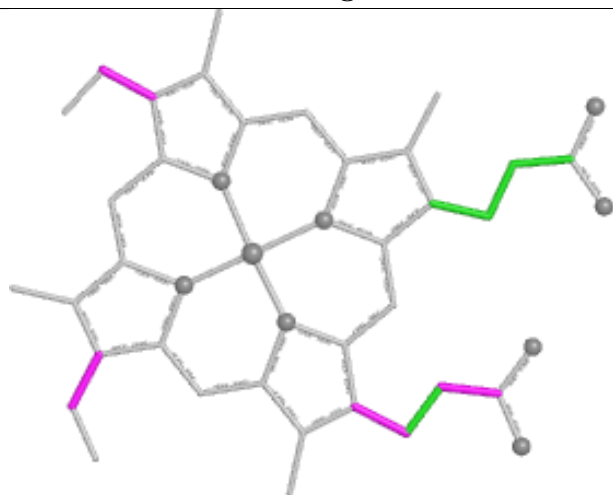
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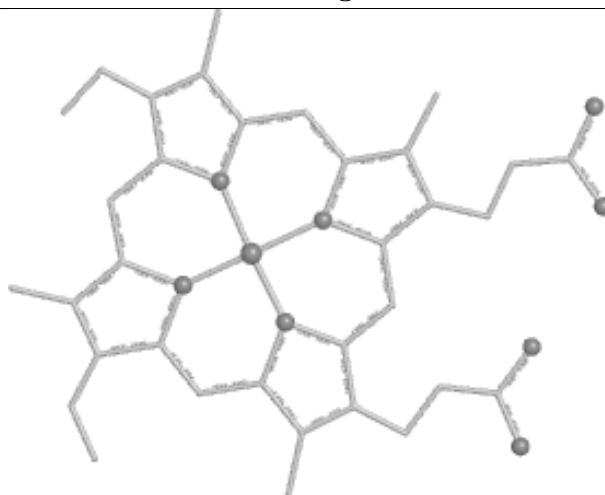
Bond lengths



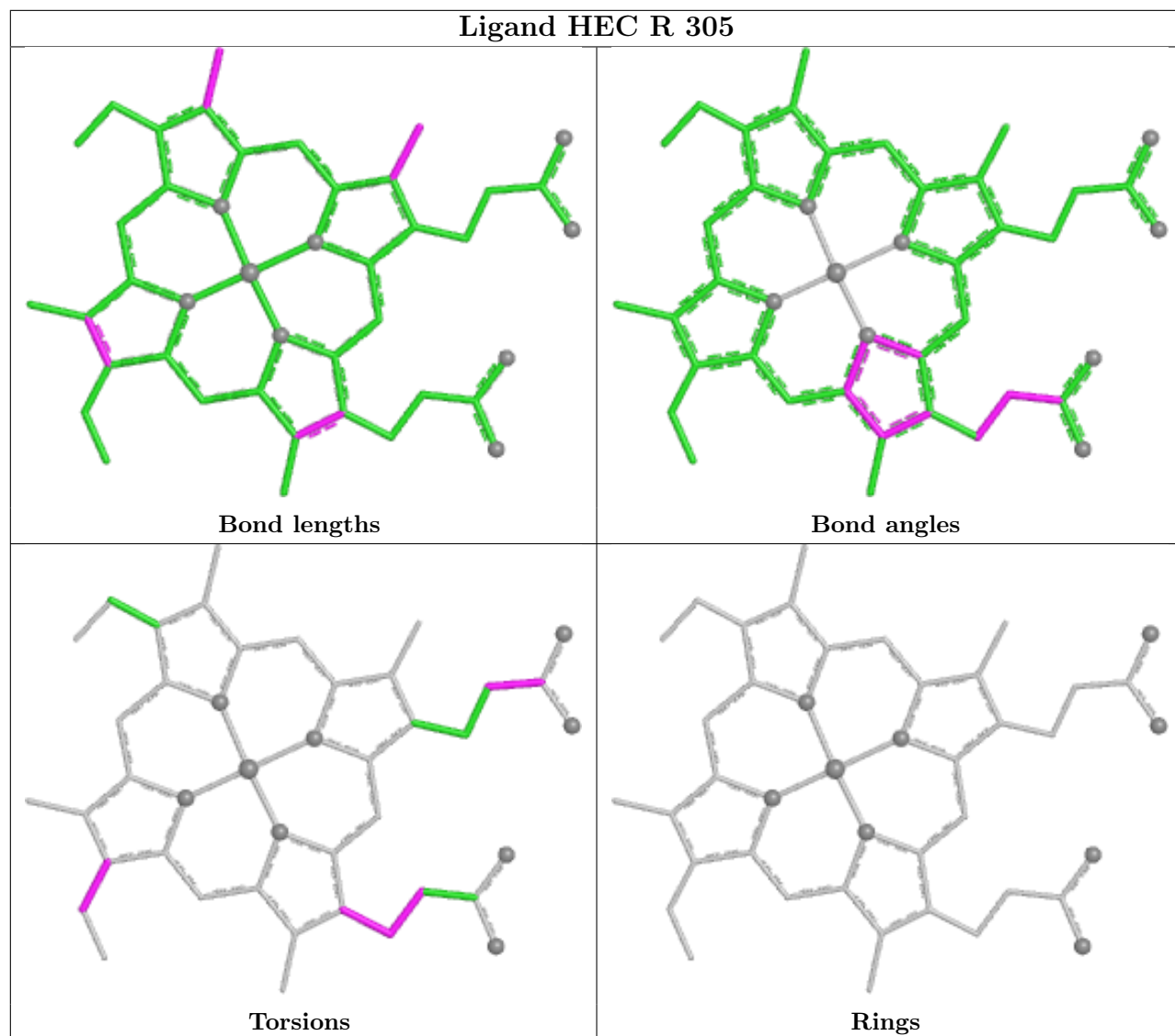
Bond angles

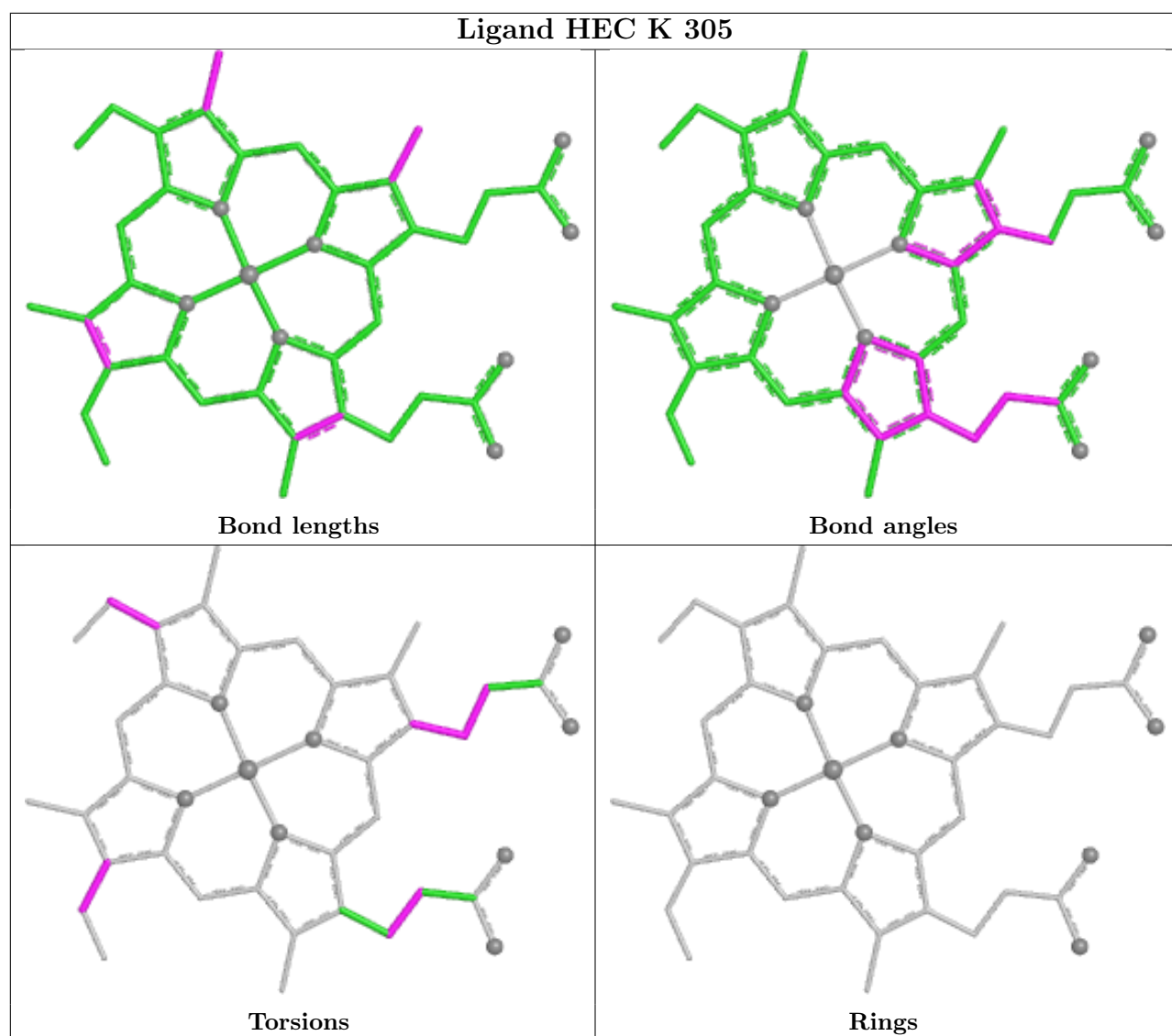


Torsions

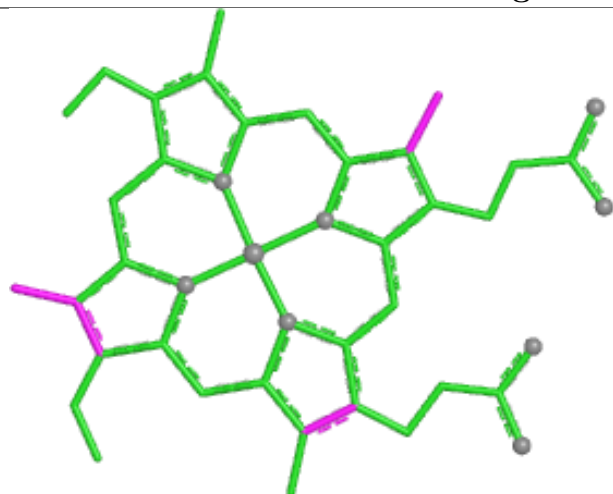


Rings

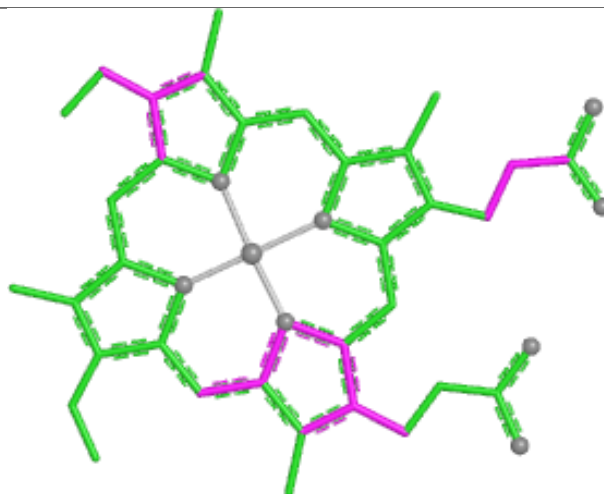




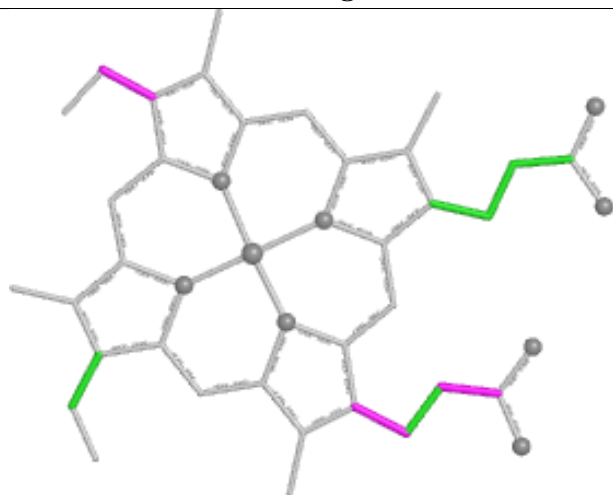
Ligand HEC C 303



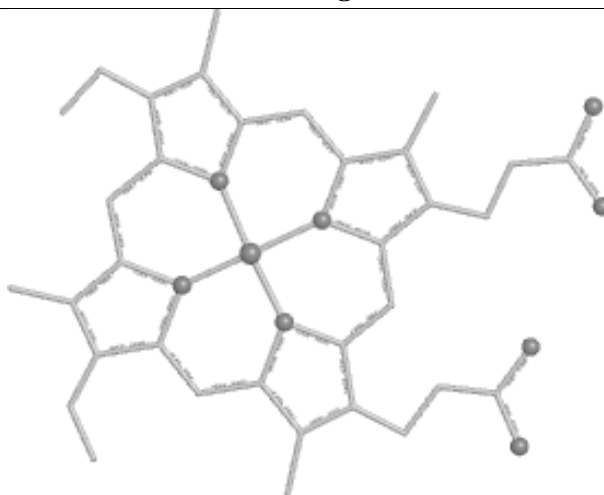
Bond lengths



Bond angles

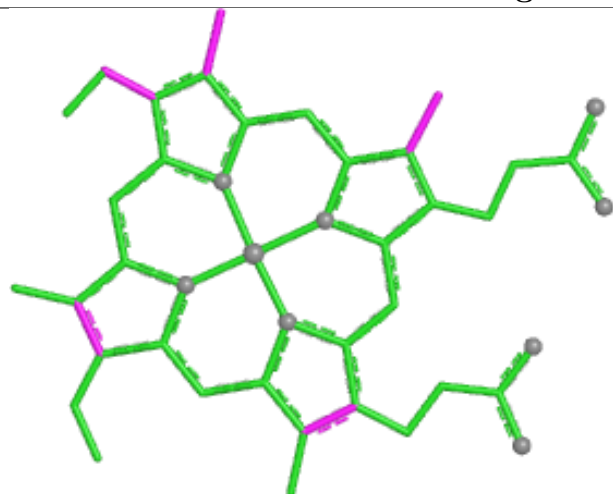


Torsions

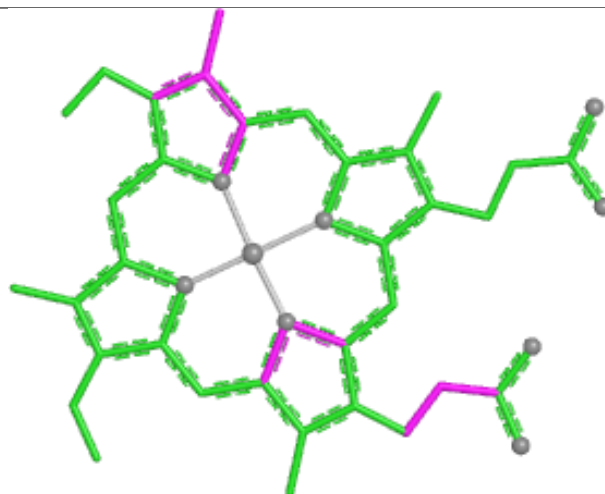


Rings

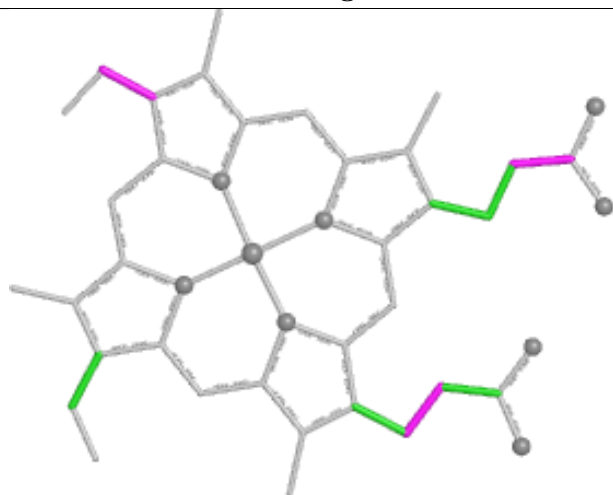
Ligand HEC S 306



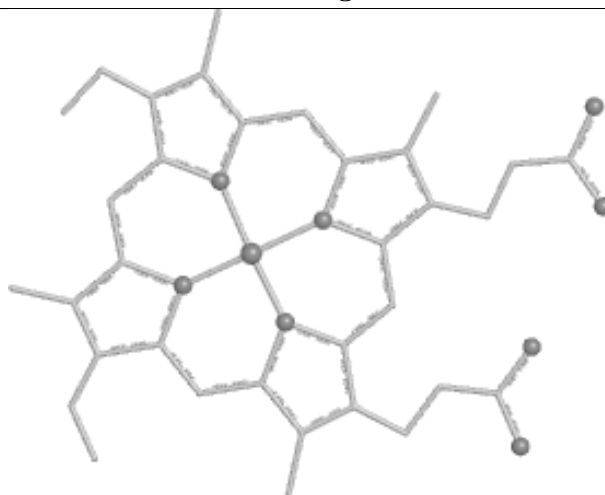
Bond lengths



Bond angles

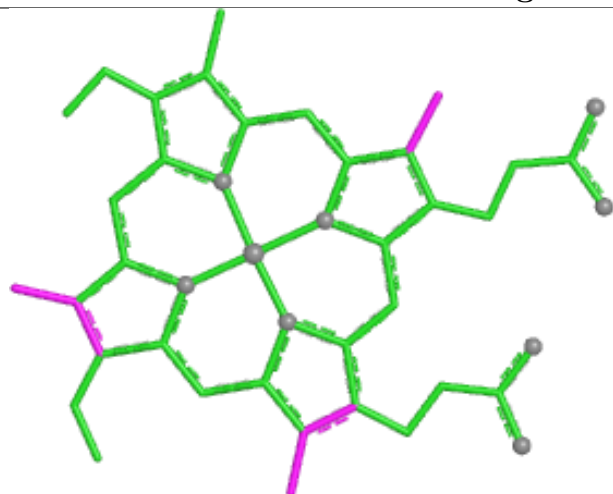


Torsions

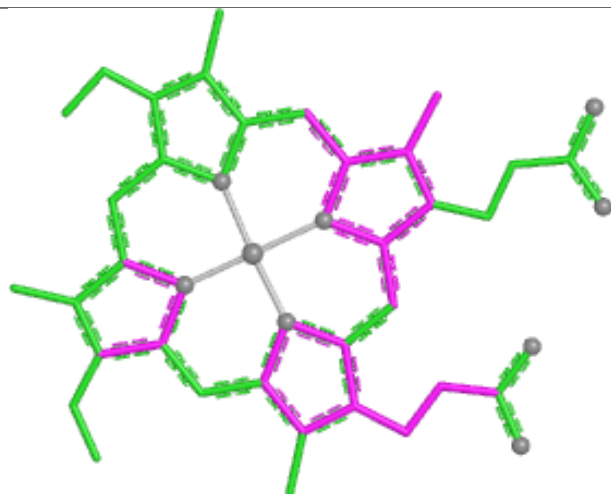


Rings

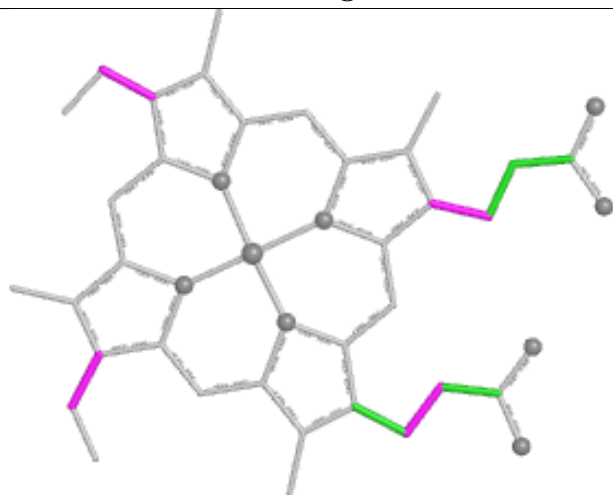
Ligand HEC J 305



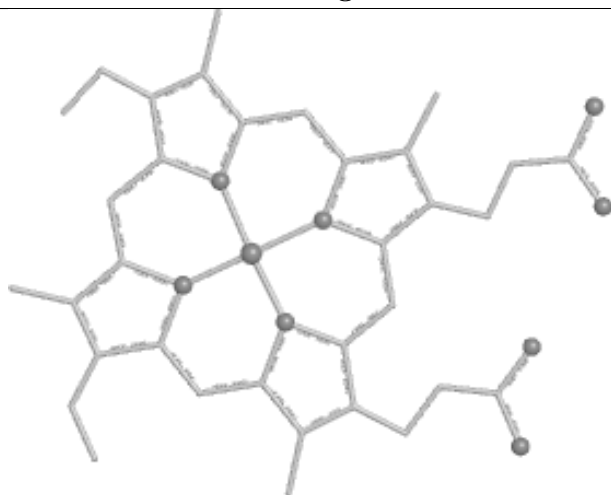
Bond lengths



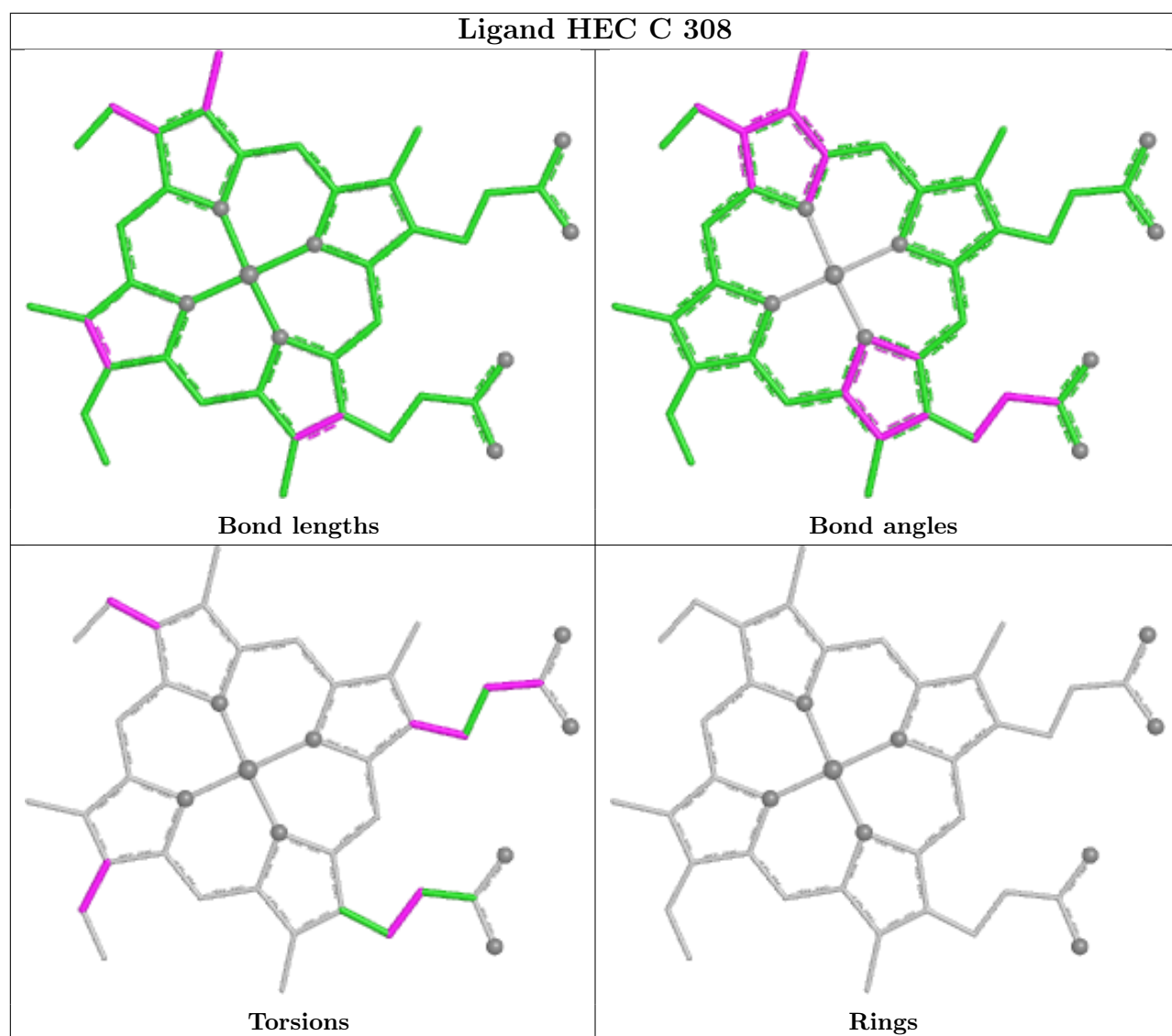
Bond angles

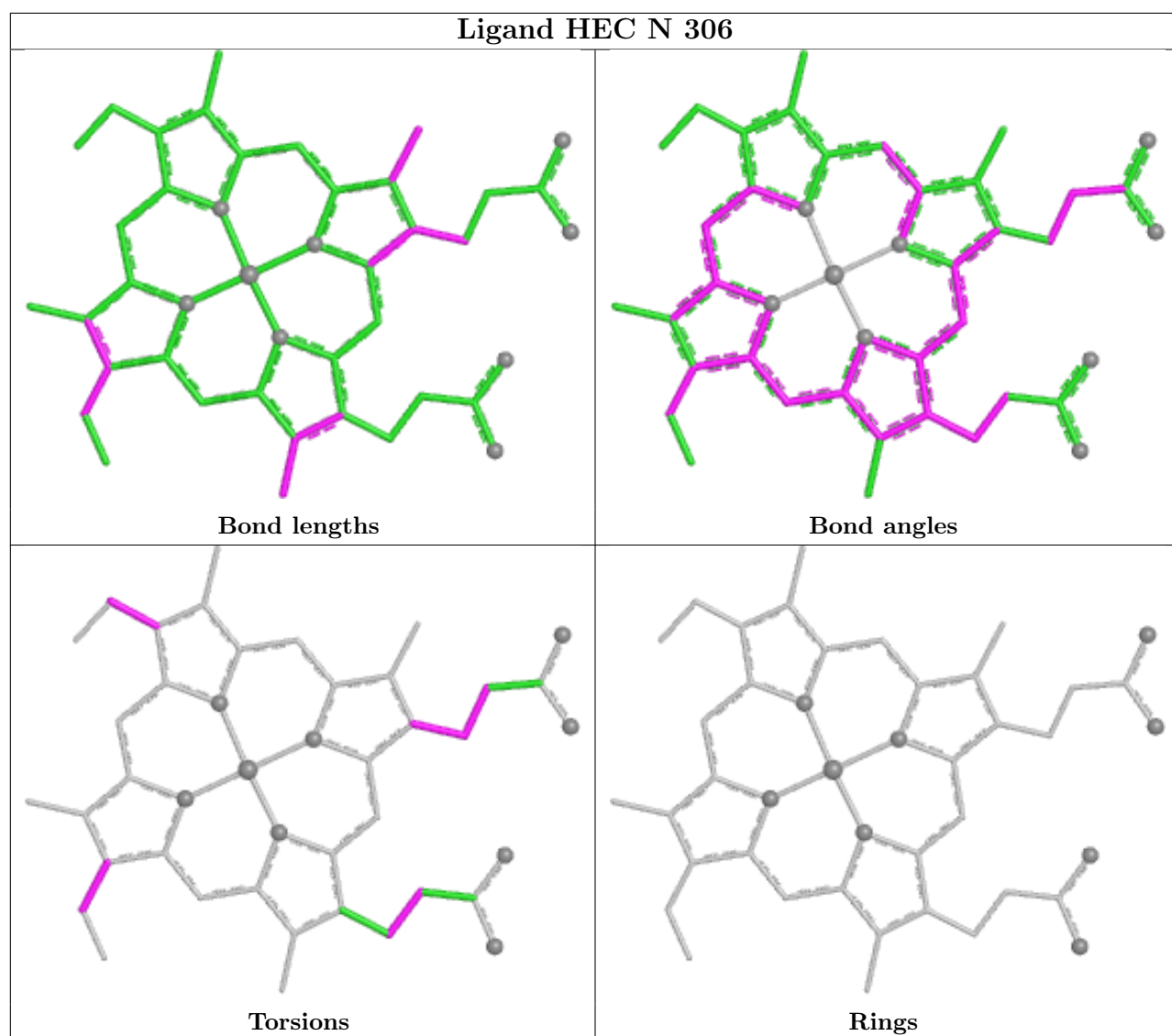


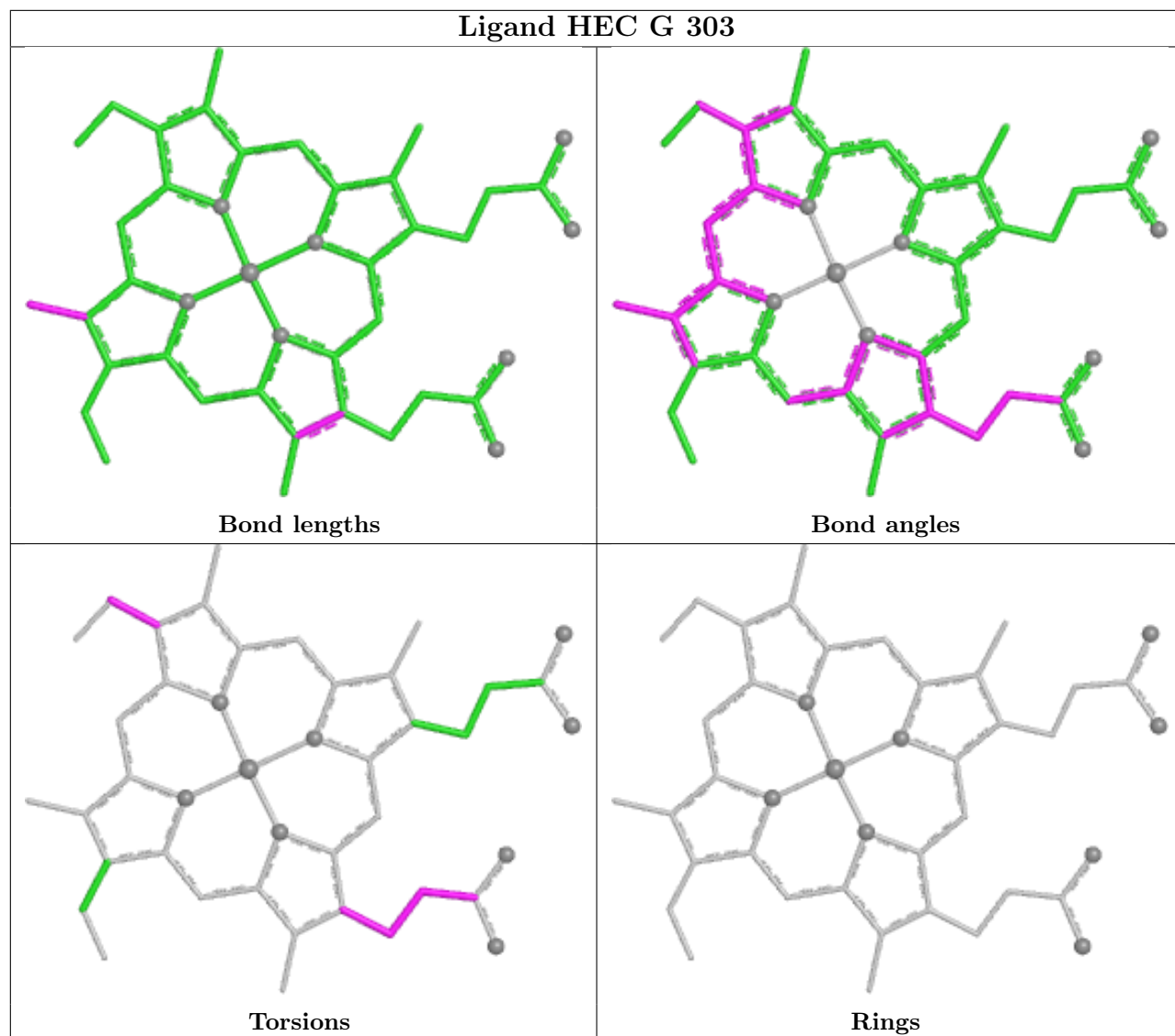
Torsions



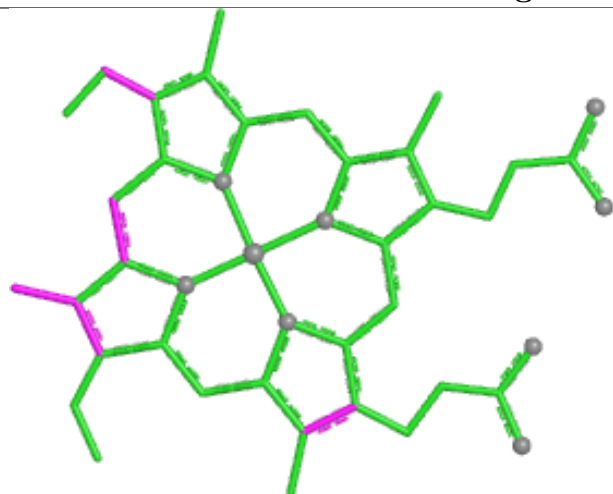
Rings



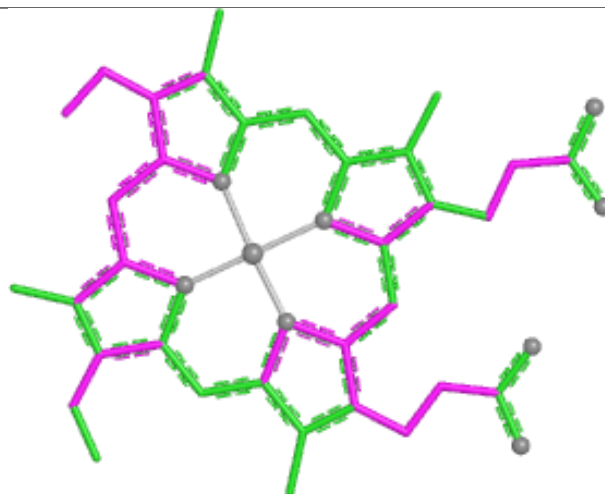




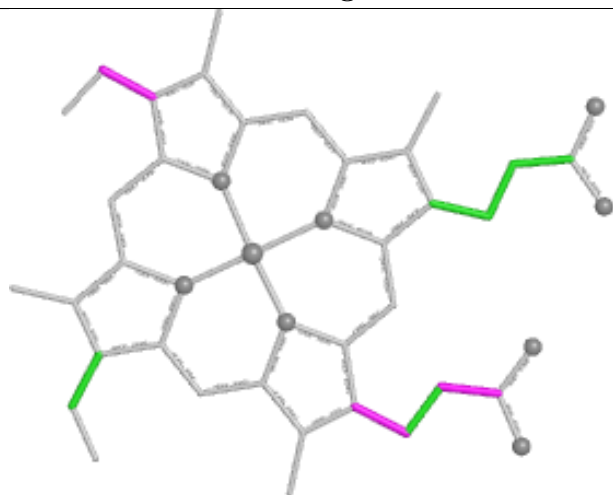
Ligand HEC L 302



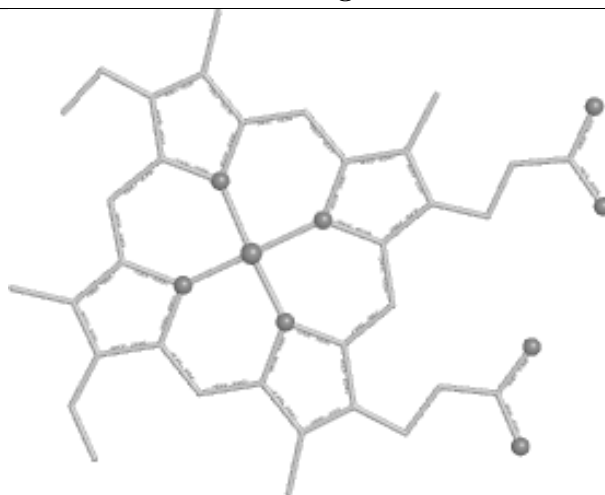
Bond lengths



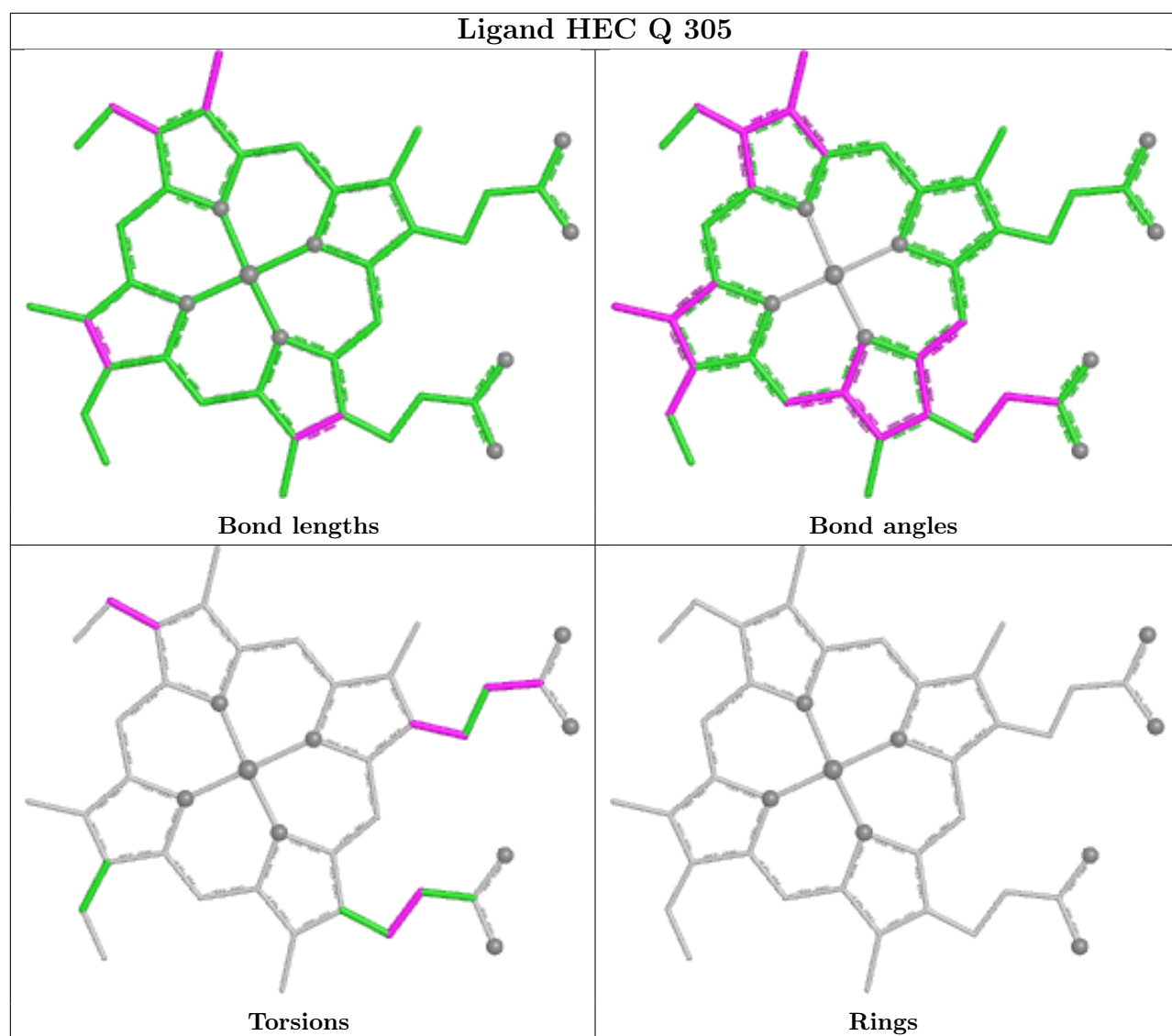
Bond angles

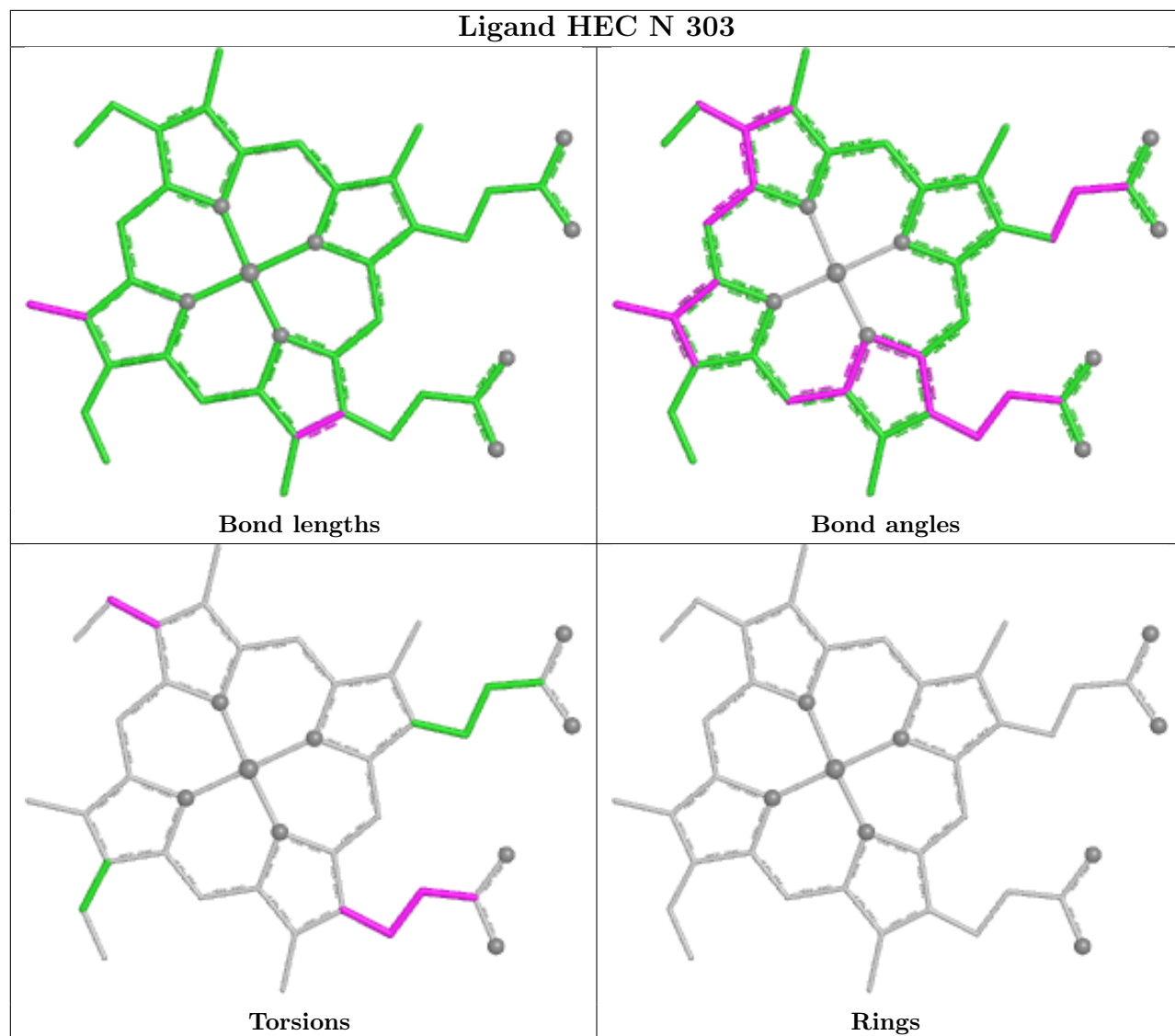


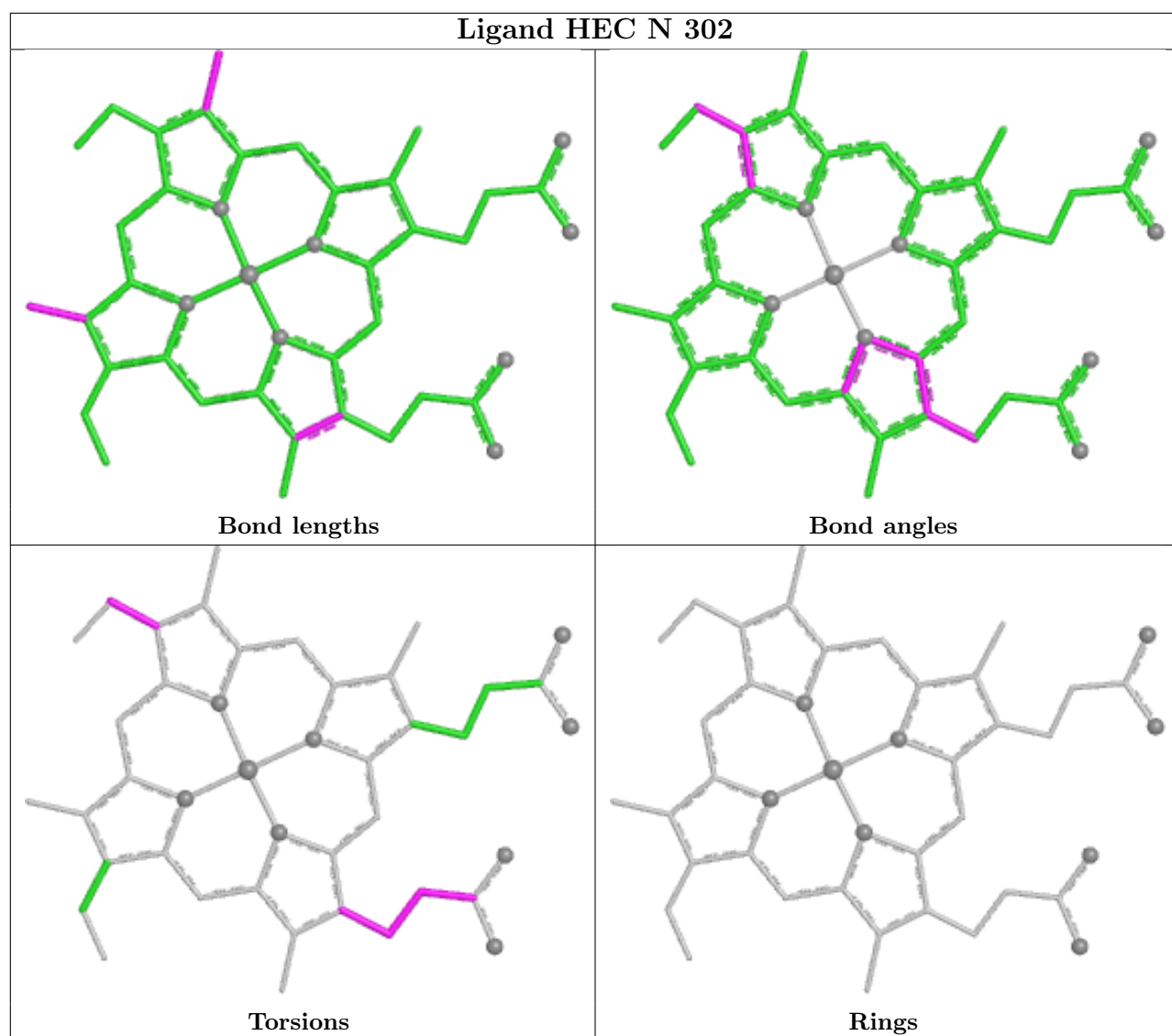
Torsions

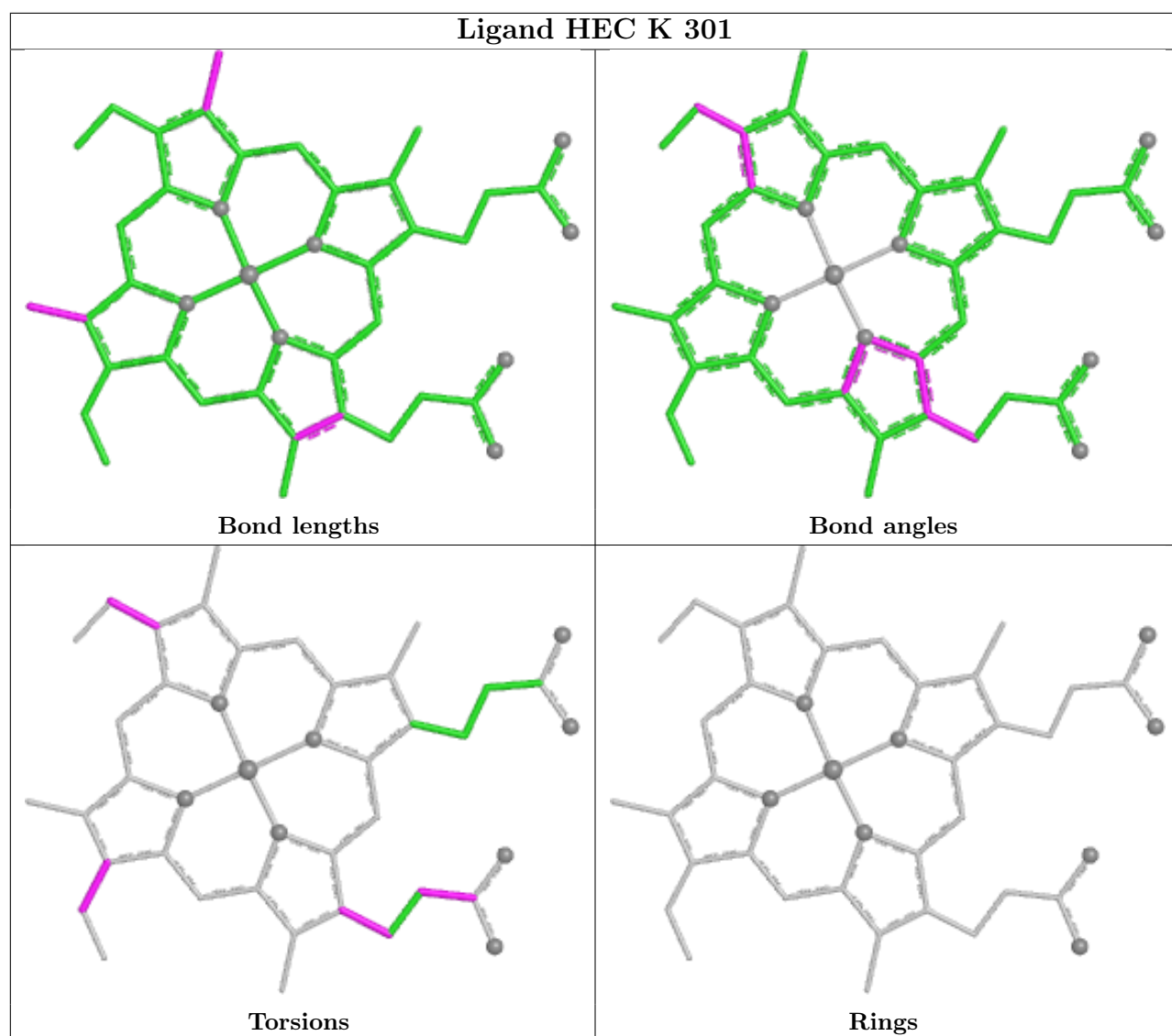


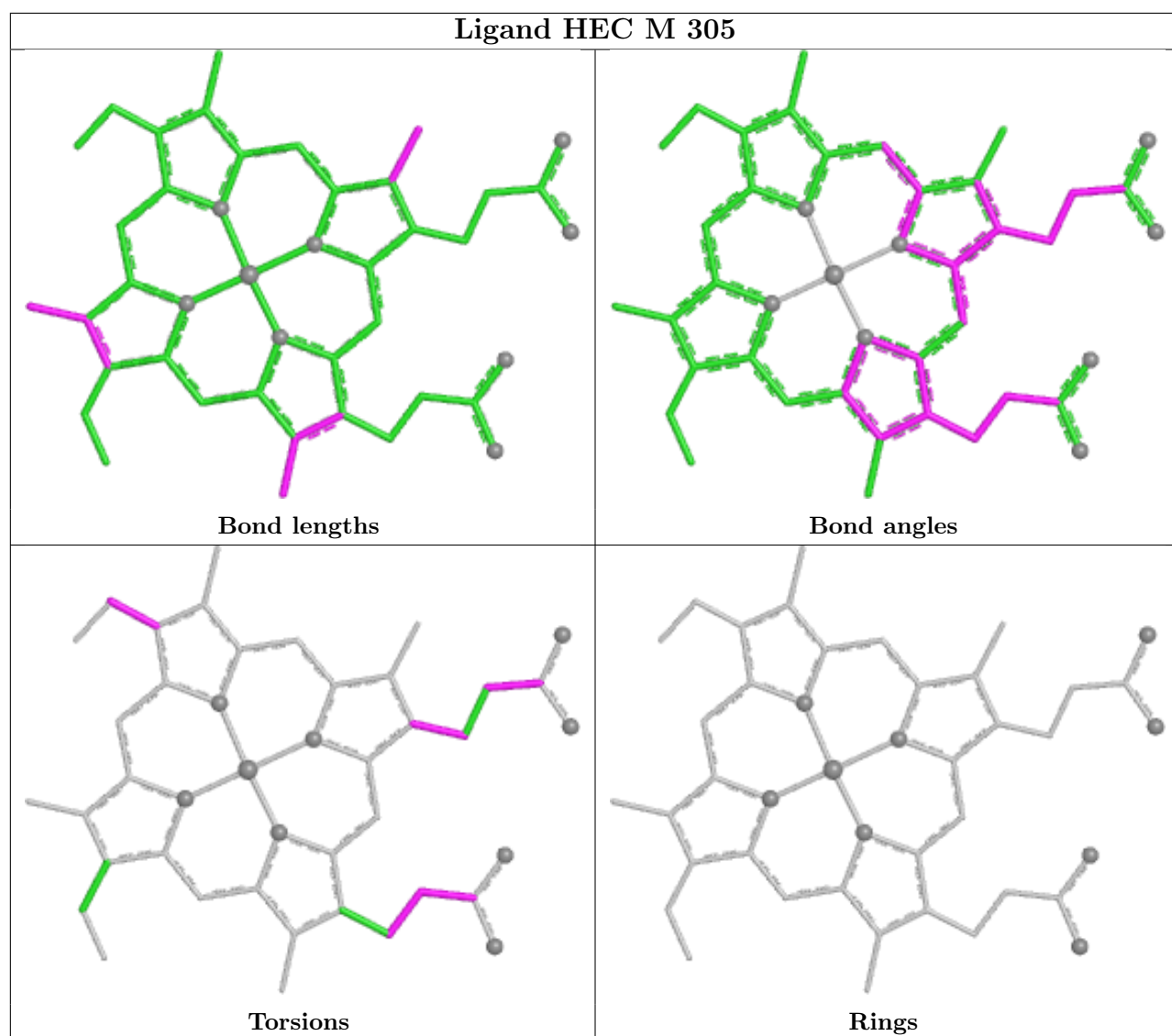
Rings

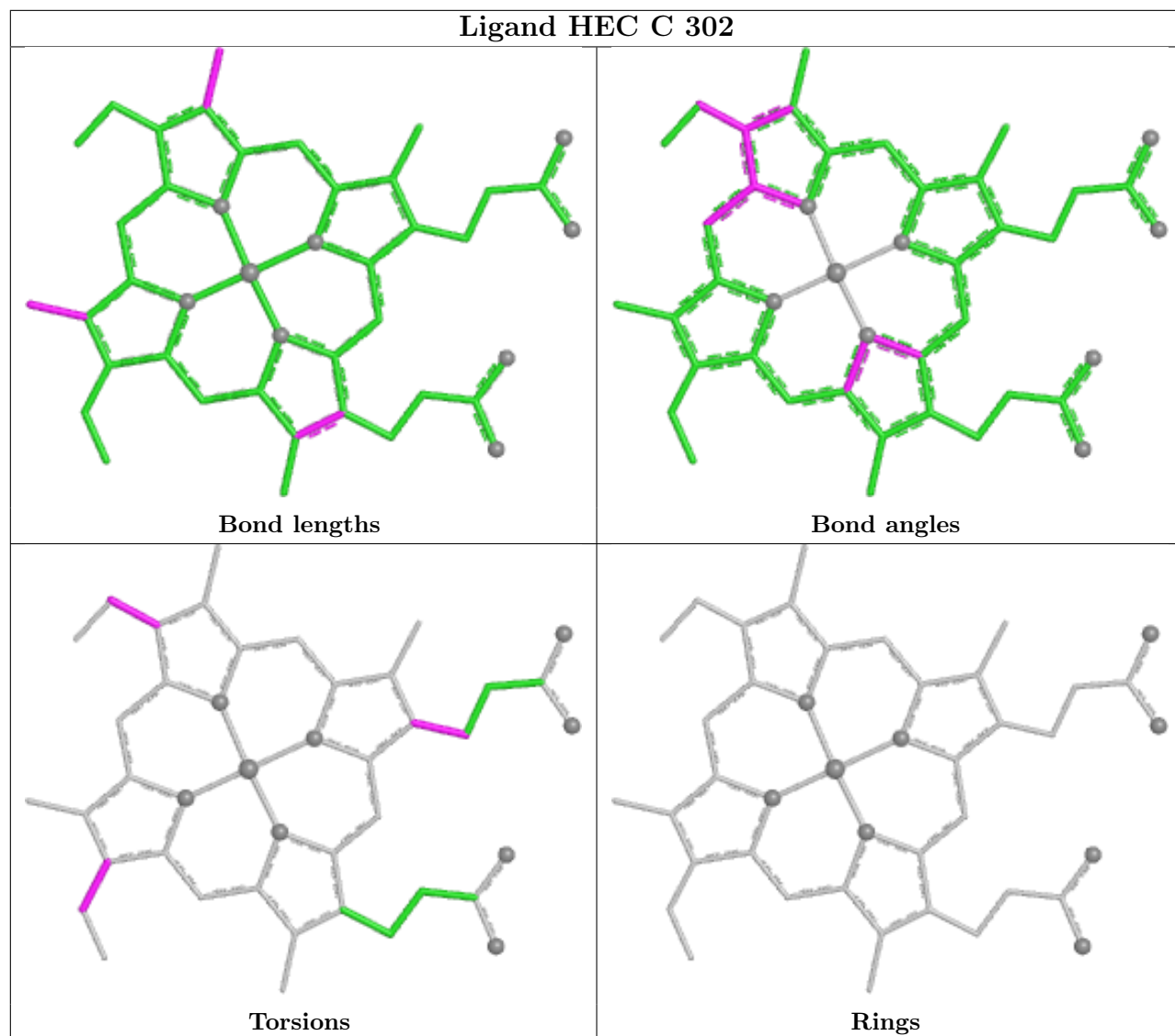




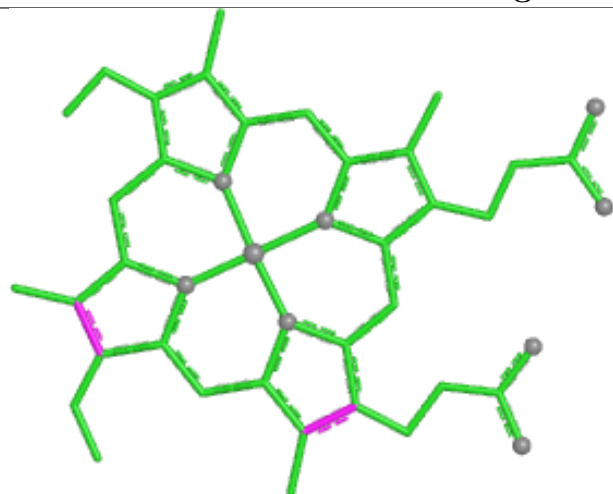




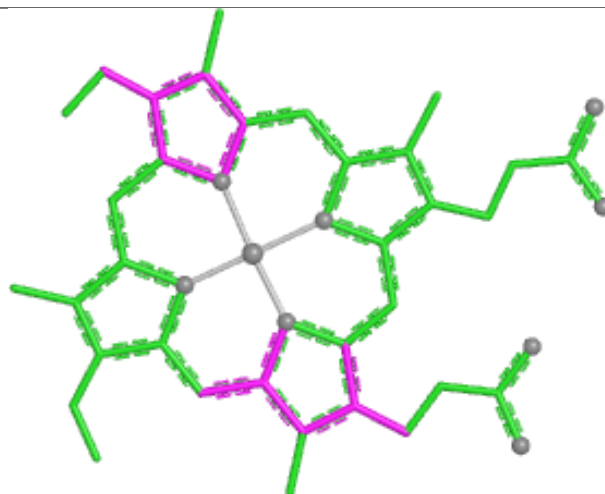




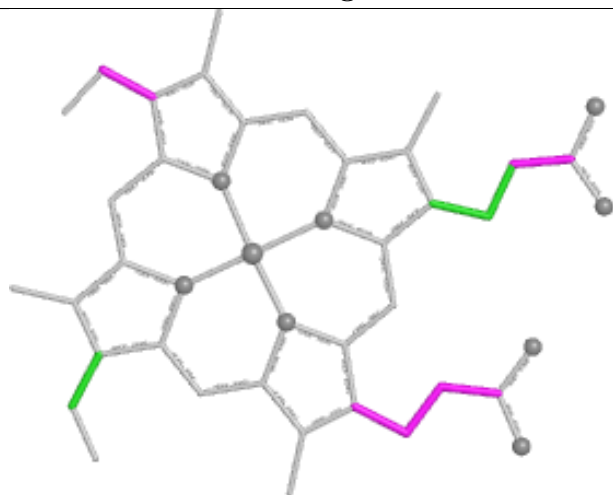
Ligand HEC E 301



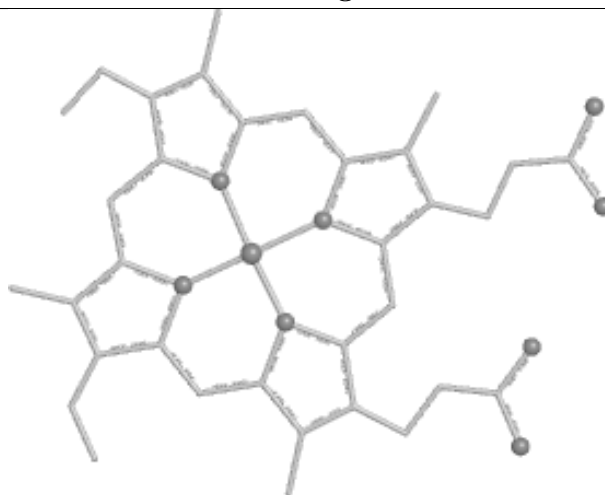
Bond lengths



Bond angles

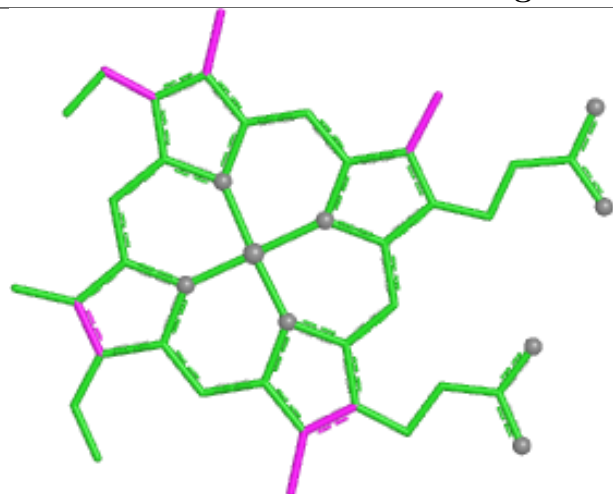


Torsions

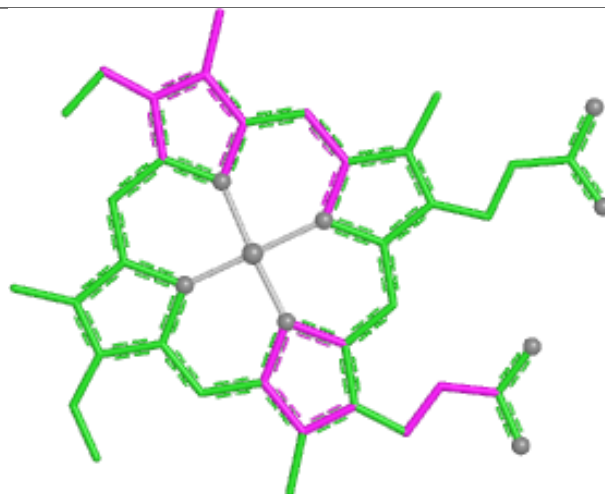


Rings

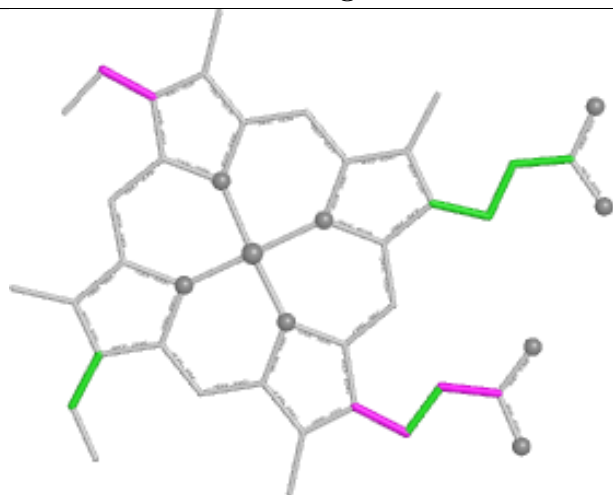
Ligand HEC F 306



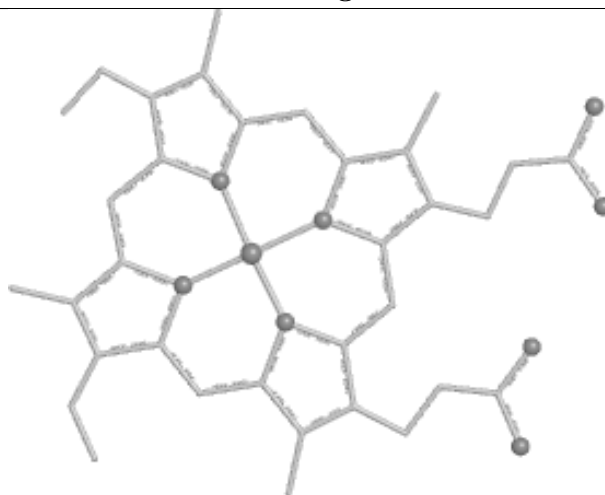
Bond lengths



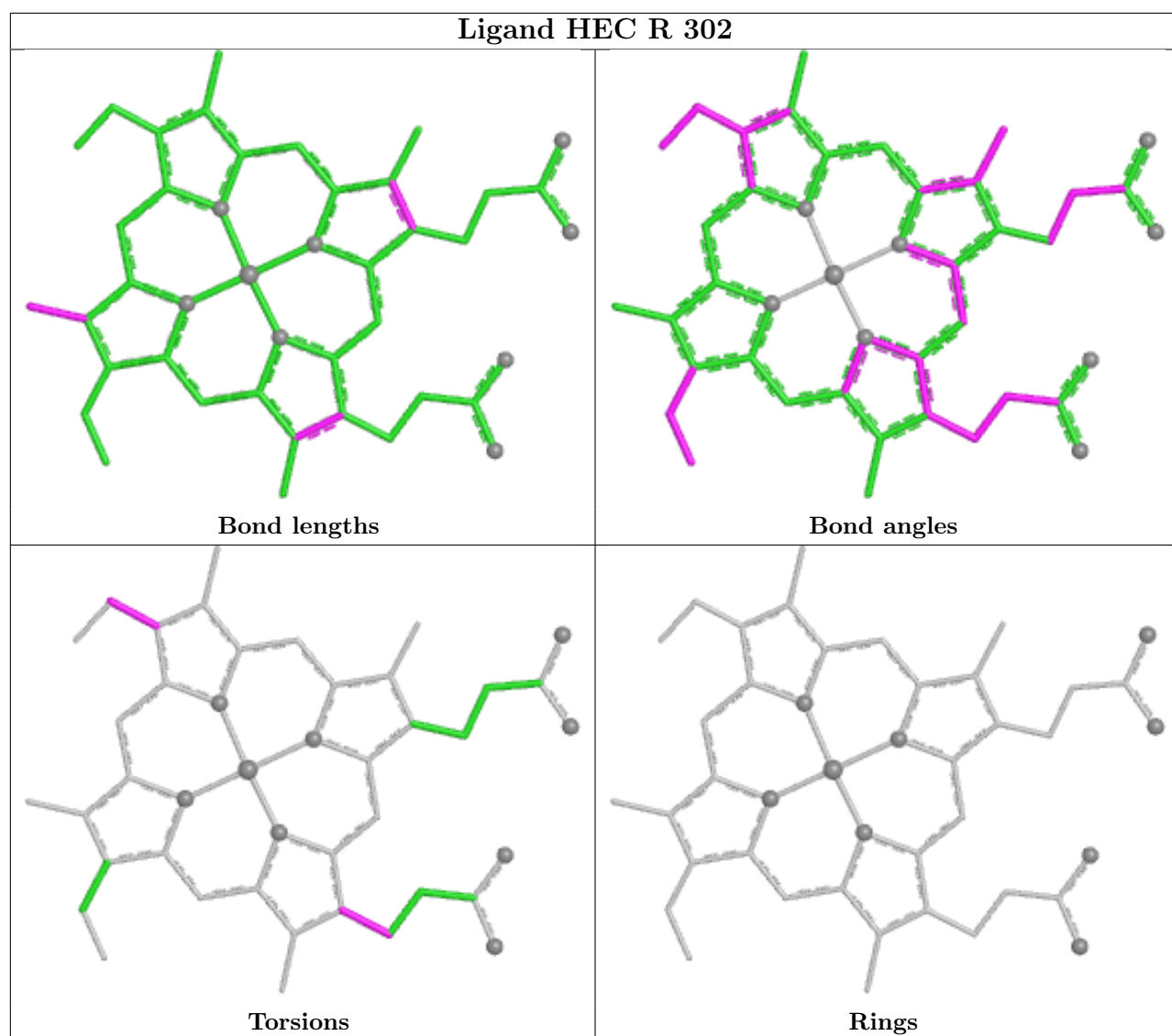
Bond angles



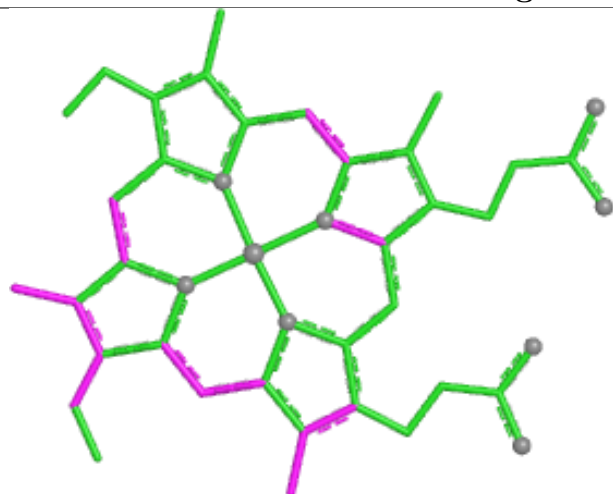
Torsions



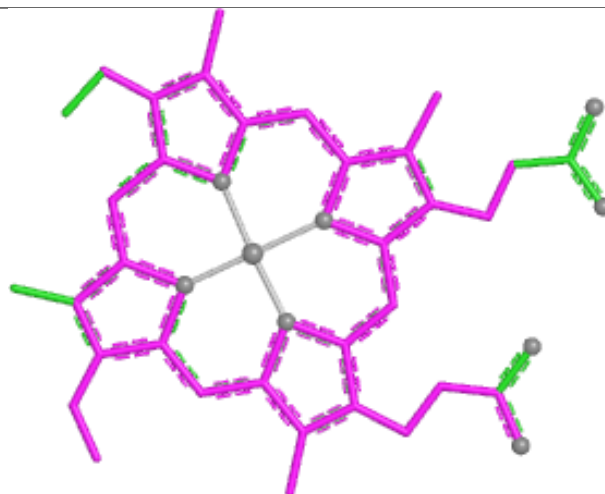
Rings



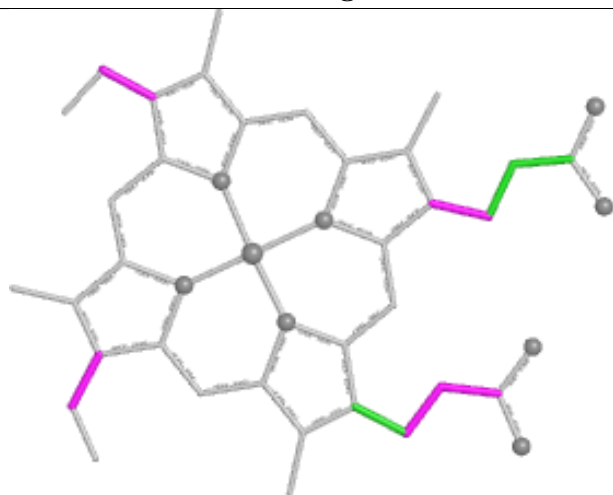
Ligand HEC S 301



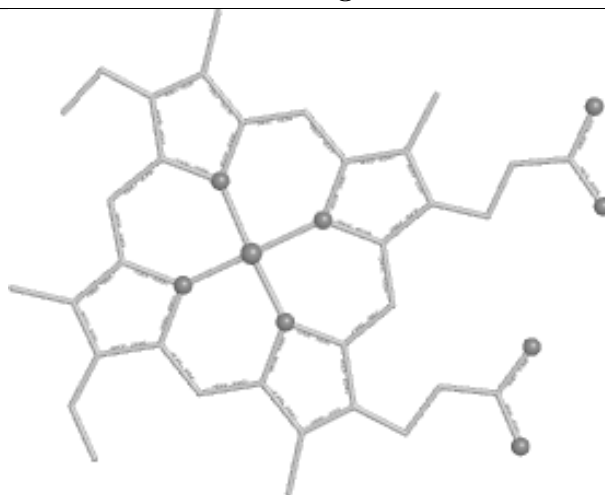
Bond lengths



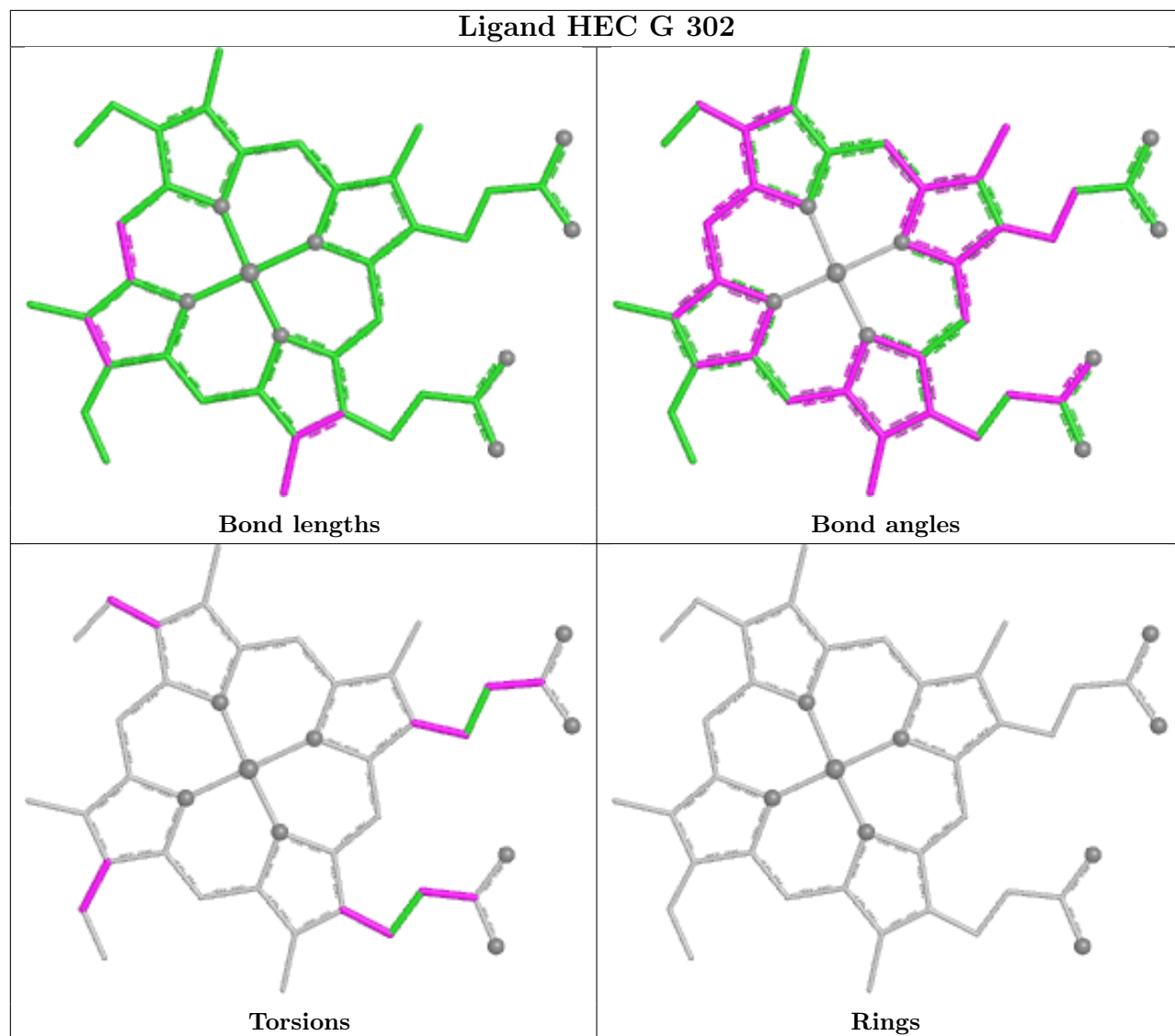
Bond angles



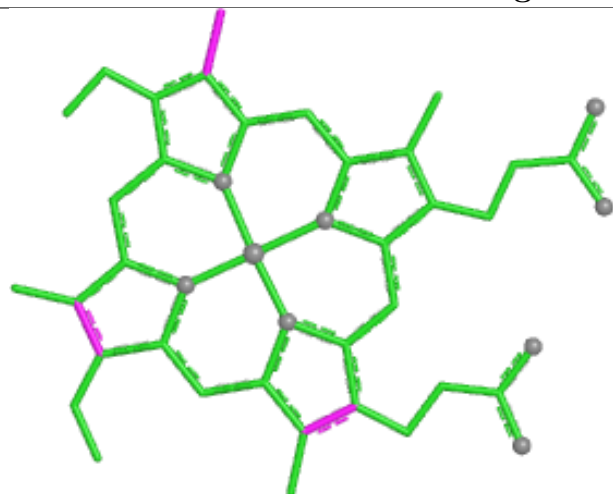
Torsions



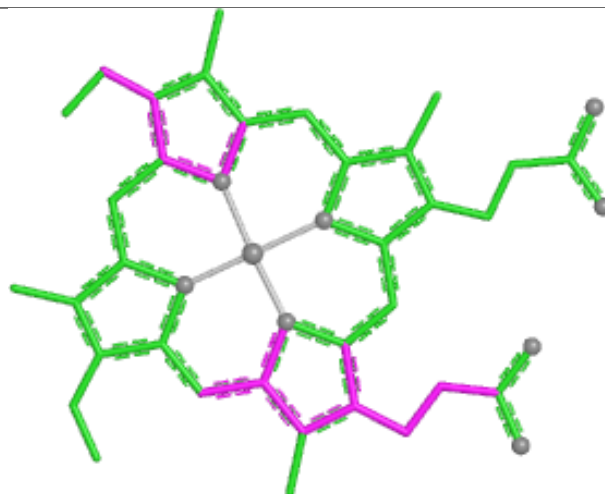
Rings



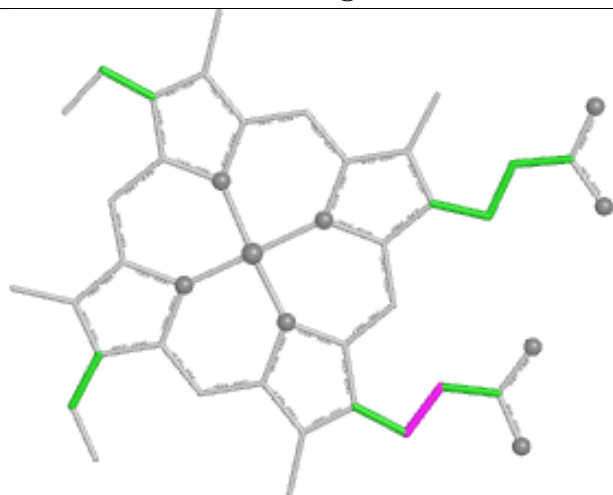
Ligand HEC E 306



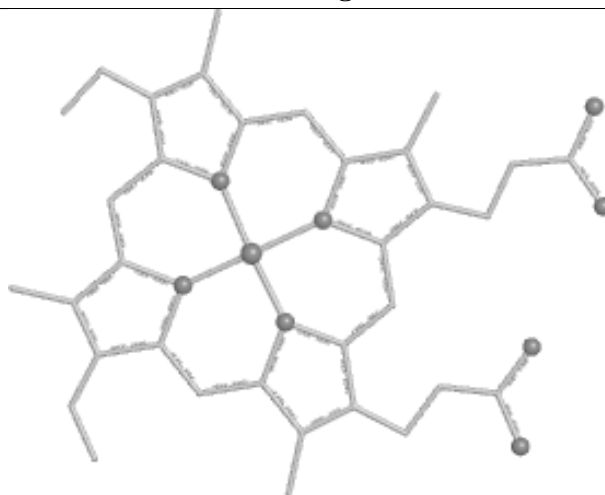
Bond lengths



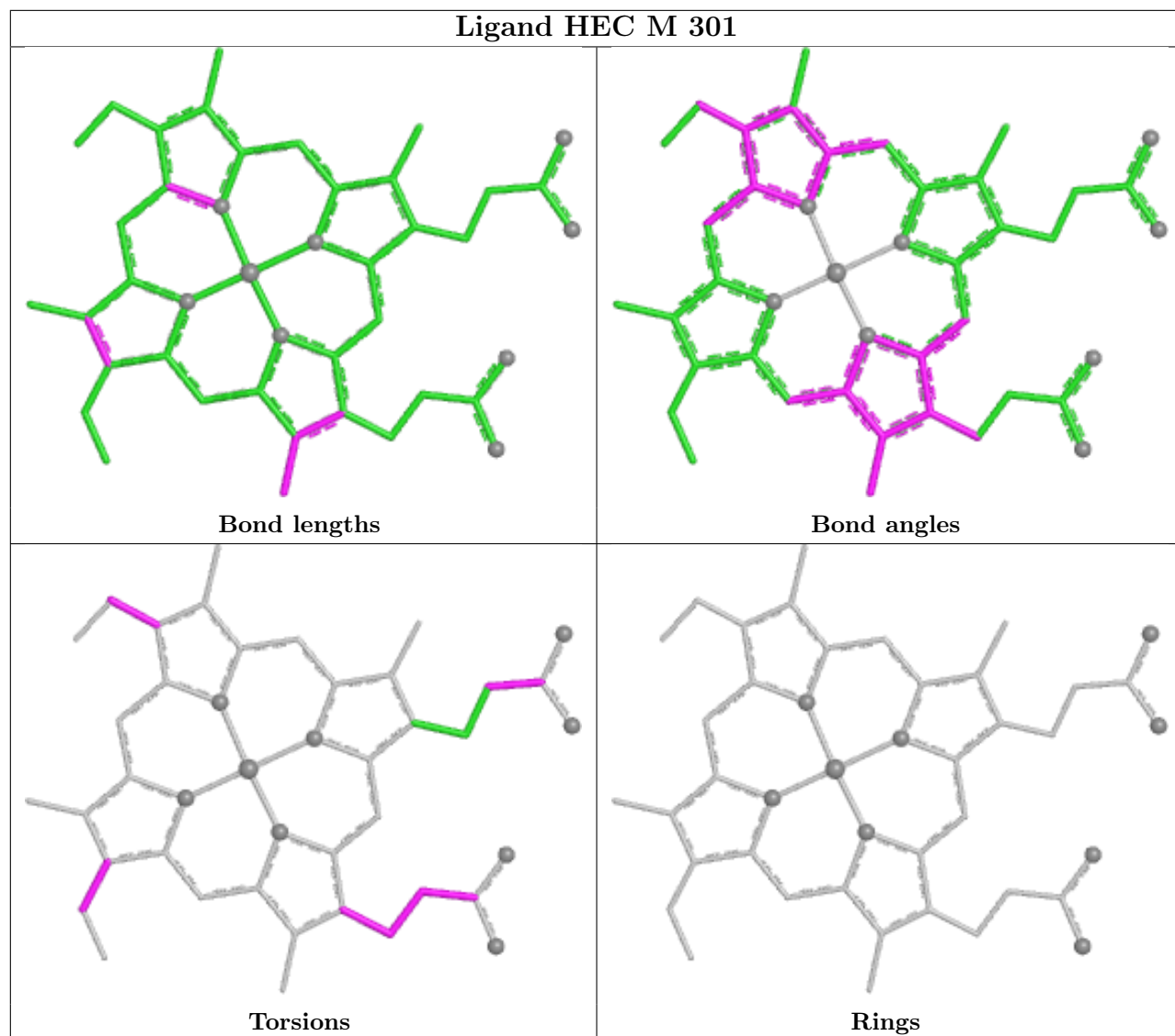
Bond angles

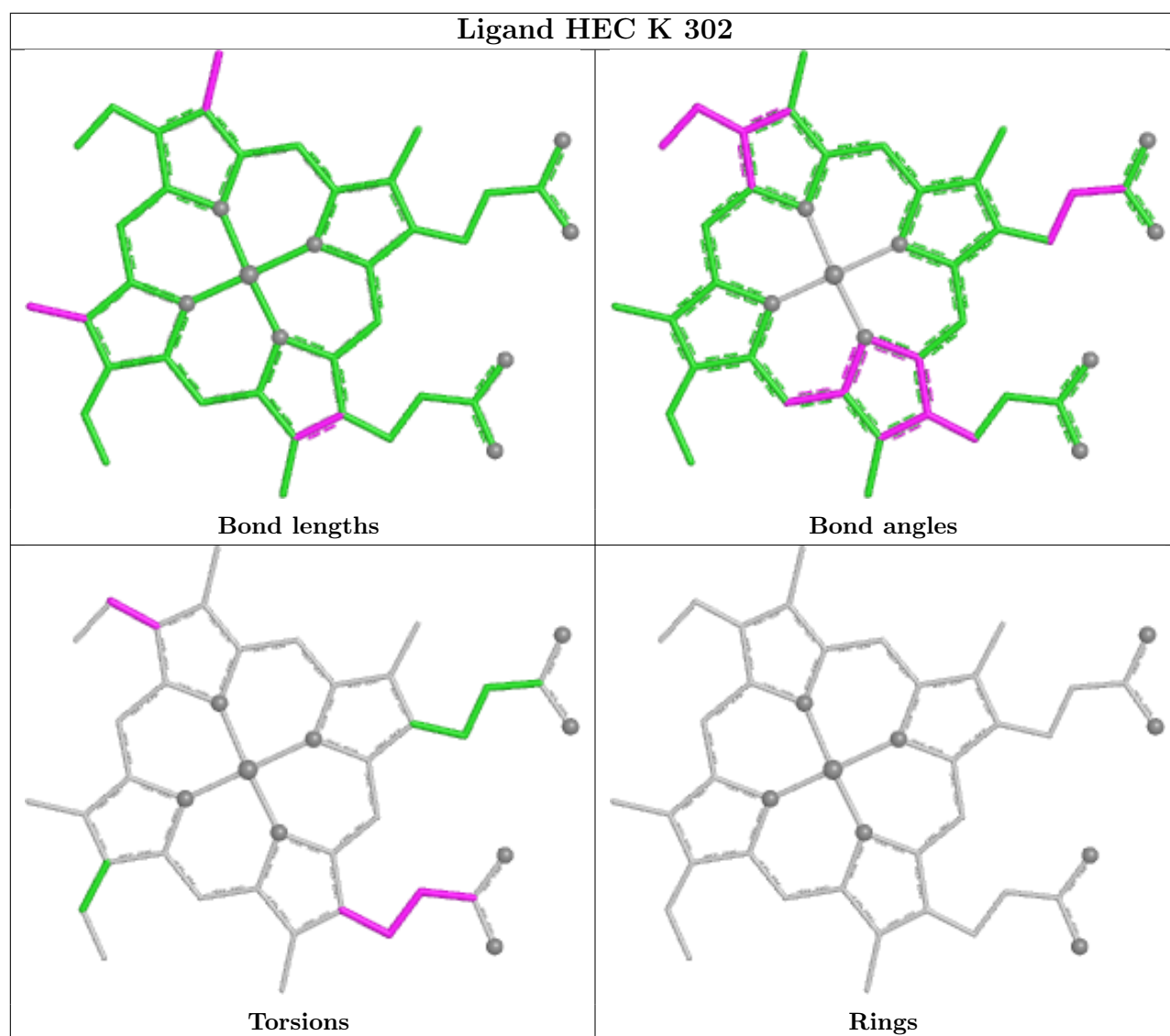


Torsions



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.

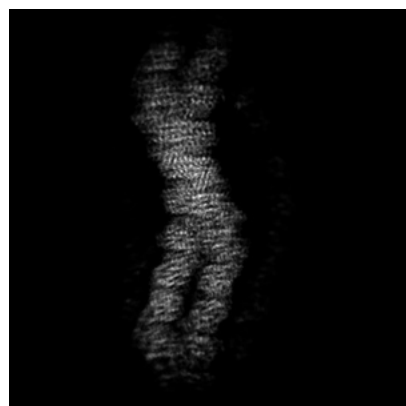
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-73506. These allow visual inspection of the internal detail of the map and identification of artifacts.

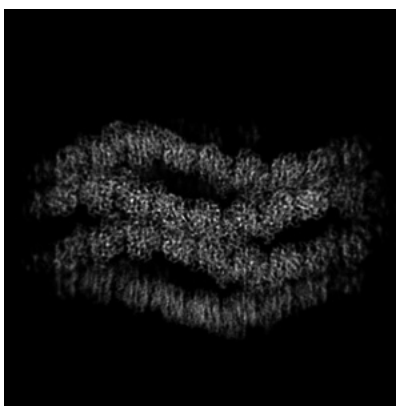
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

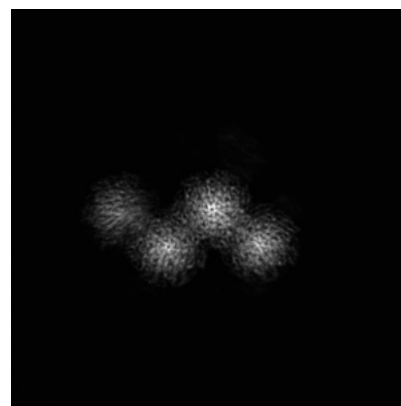
6.1.1 Primary map



X

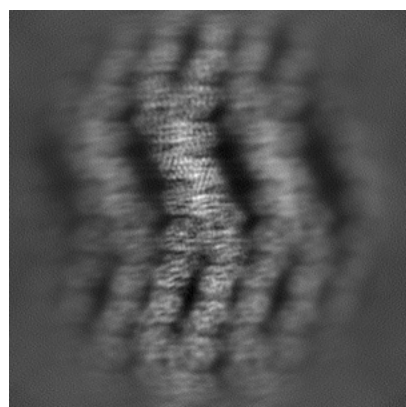


Y

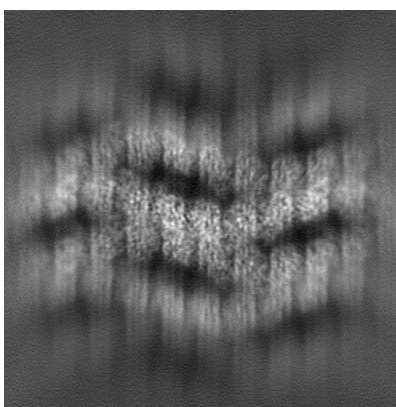


Z

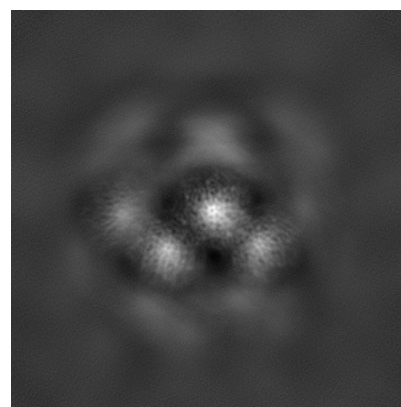
6.1.2 Raw map



X



Y



Z

The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

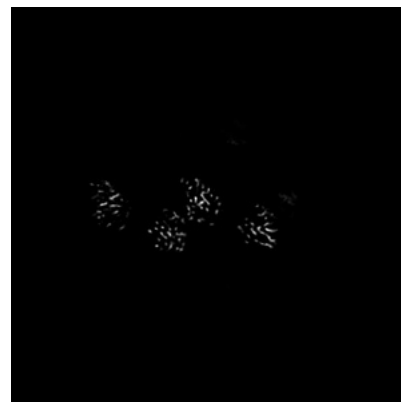
6.2.1 Primary map



X Index: 160

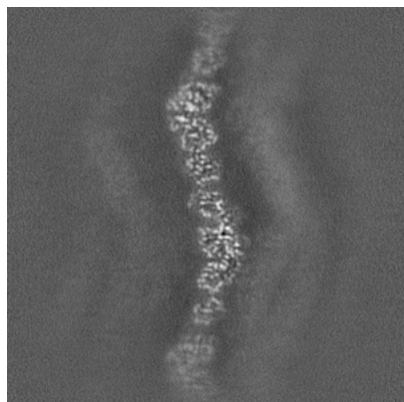


Y Index: 160

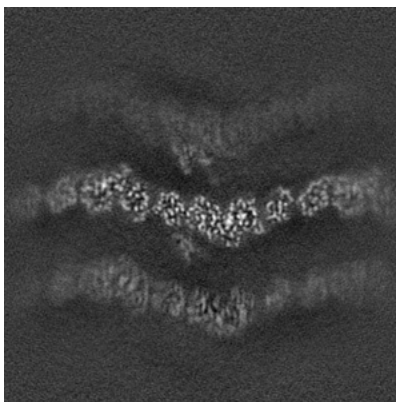


Z Index: 160

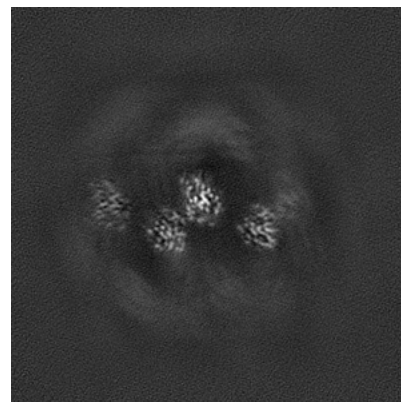
6.2.2 Raw map



X Index: 160



Y Index: 160



Z Index: 160

The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

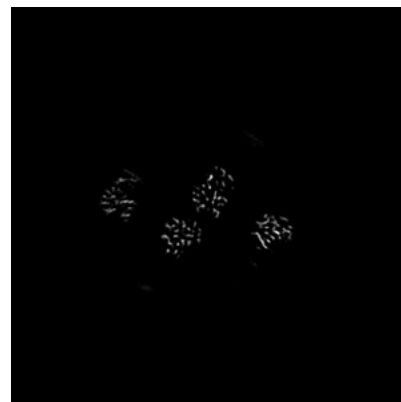
6.3.1 Primary map



X Index: 158

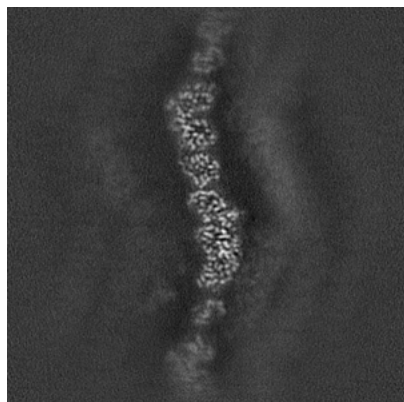


Y Index: 131

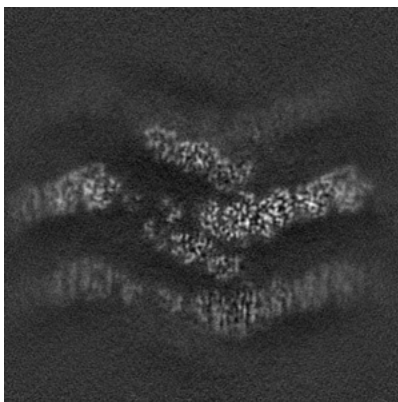


Z Index: 129

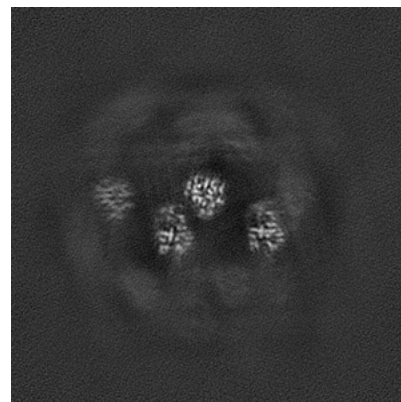
6.3.2 Raw map



X Index: 158



Y Index: 151



Z Index: 141

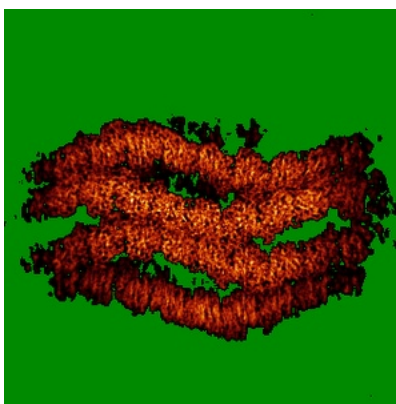
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

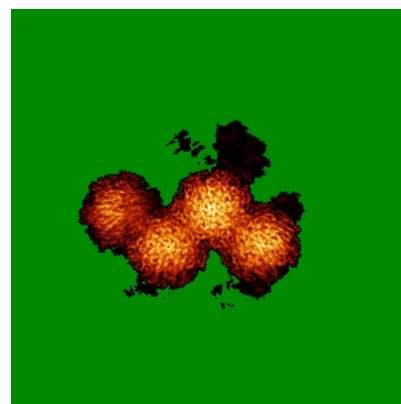
6.4.1 Primary map



X

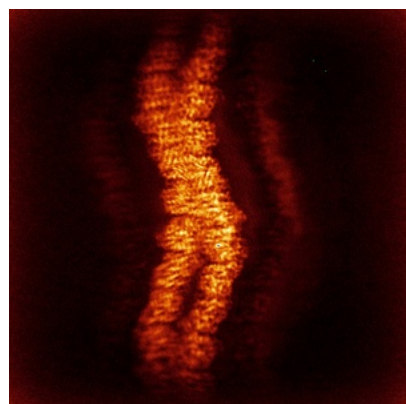


Y

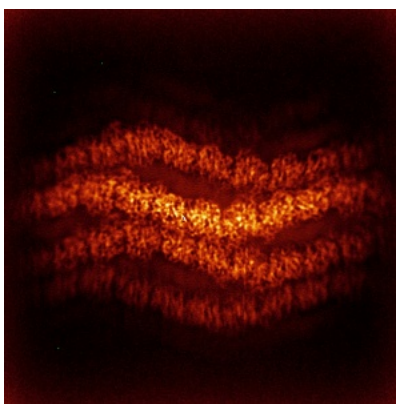


Z

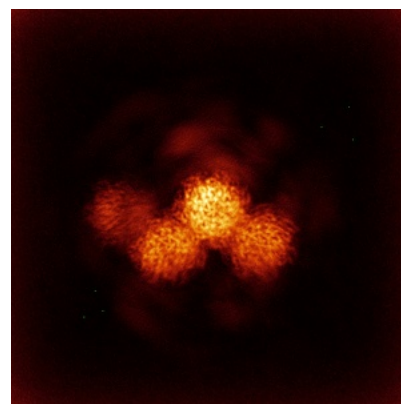
6.4.2 Raw map



X



Y

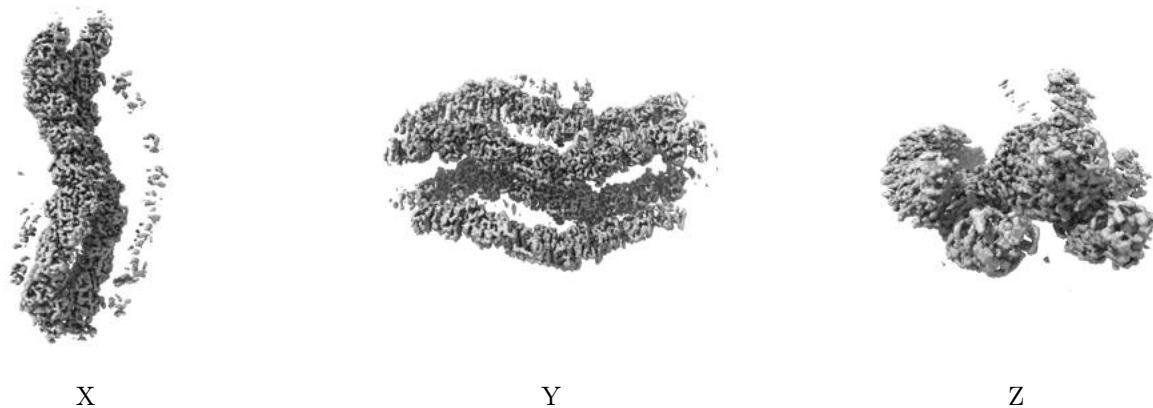


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

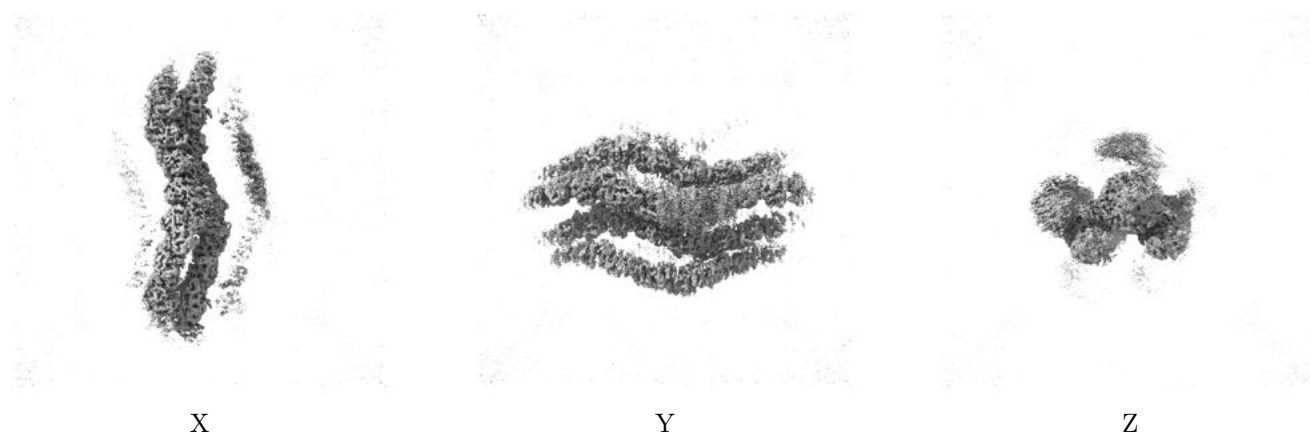
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0486. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

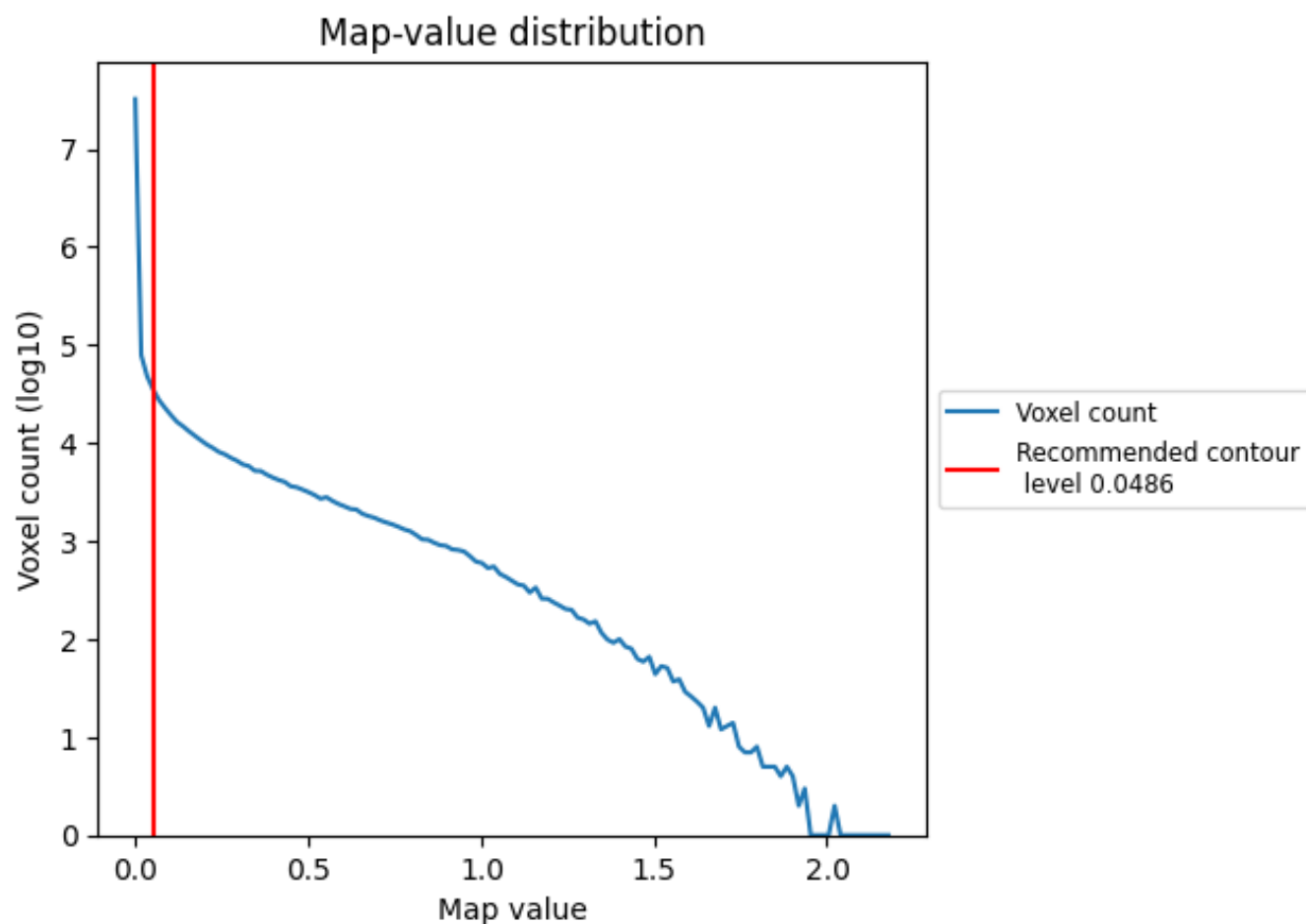
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

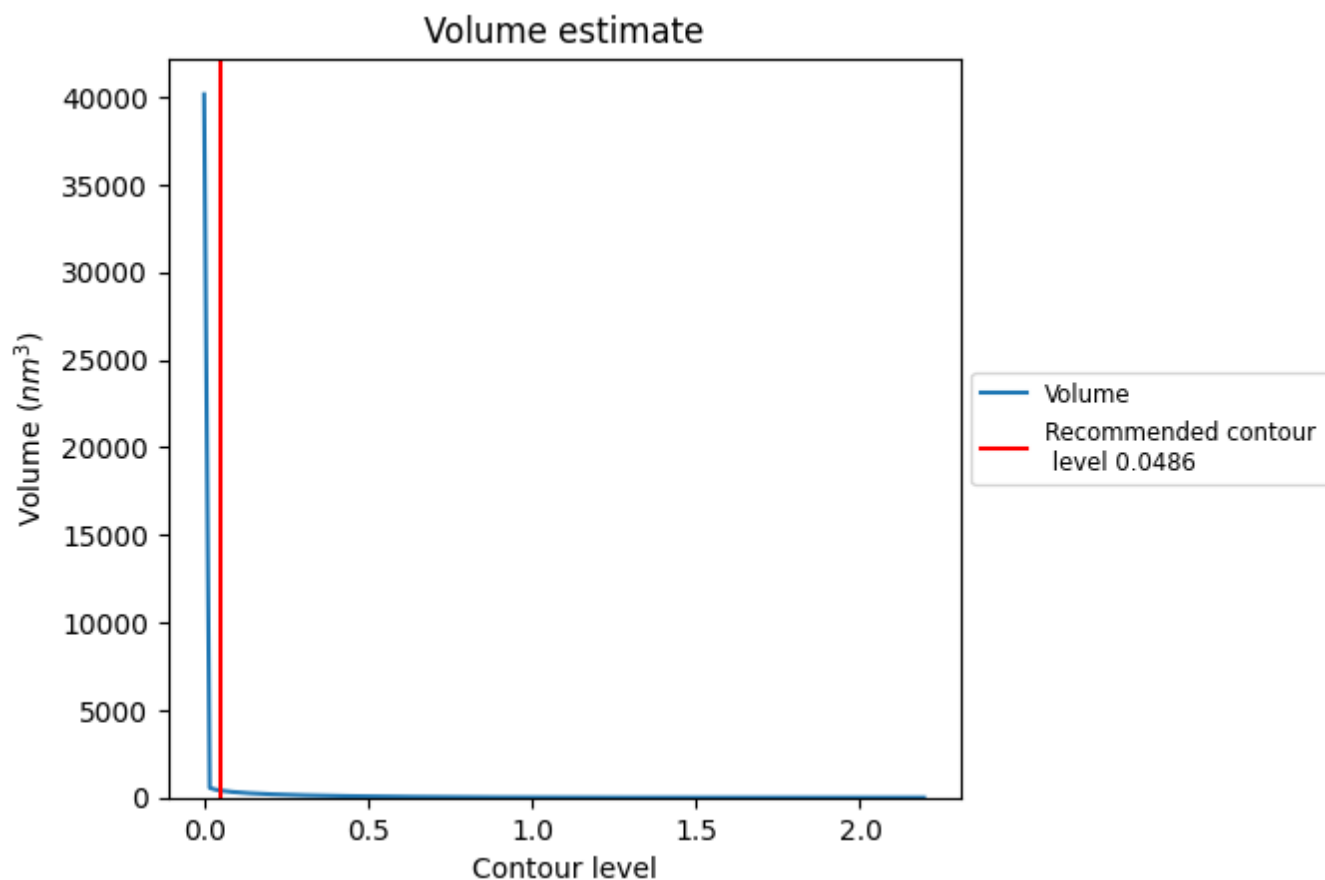
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

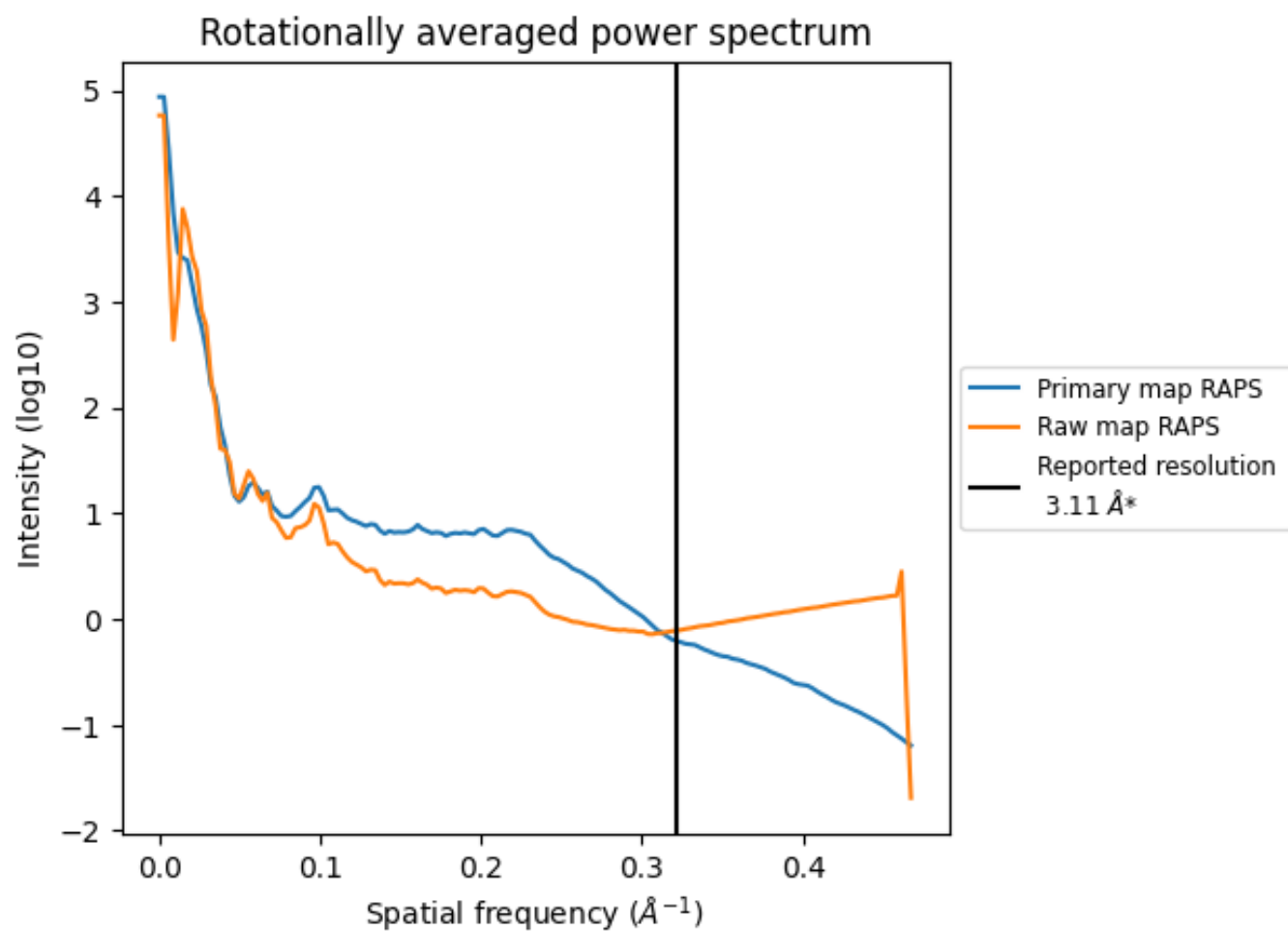
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 402 nm³; this corresponds to an approximate mass of 363 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

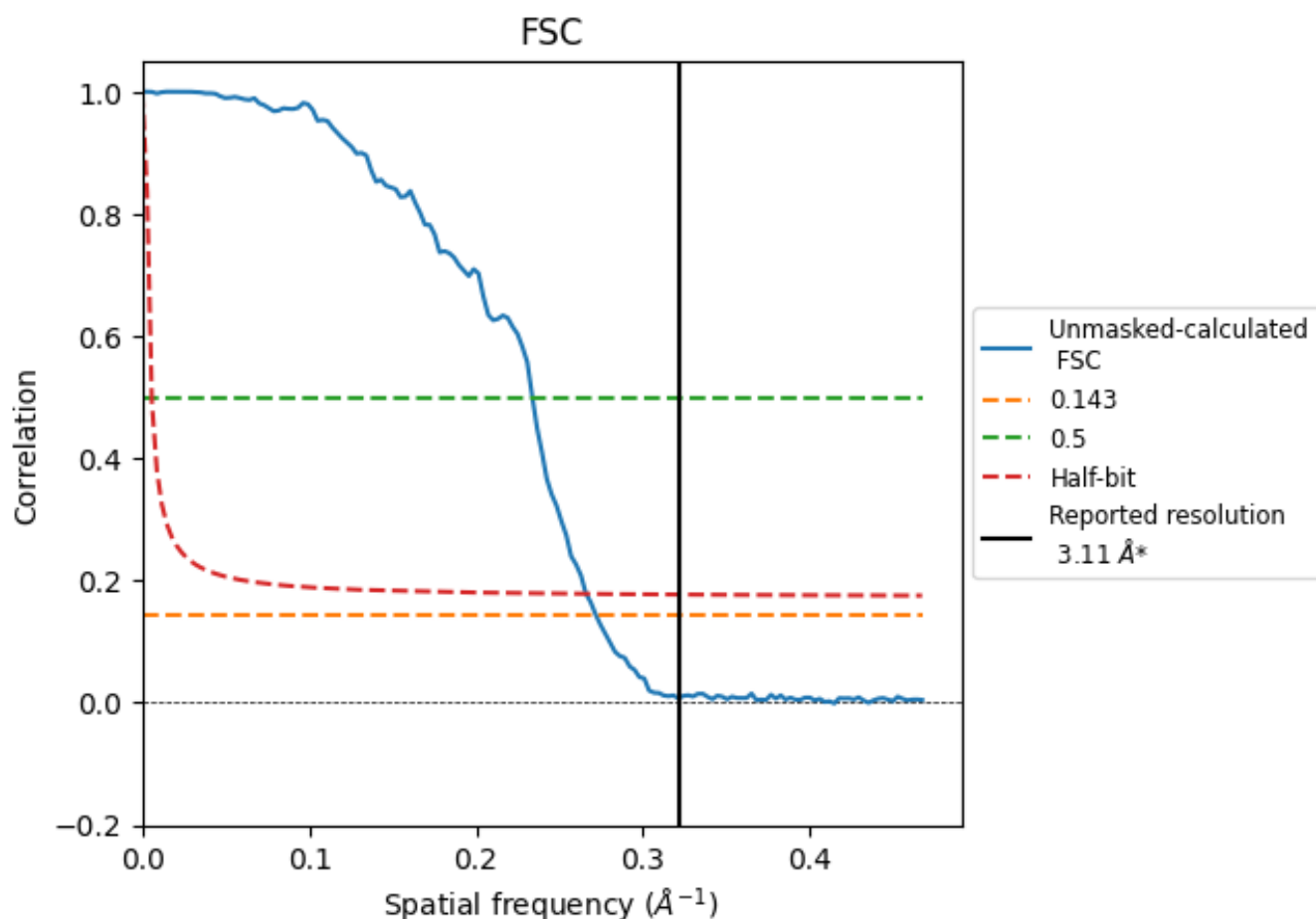


*Reported resolution corresponds to spatial frequency of 0.322 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.322 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.11	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.68	4.28	3.76

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.68 differs from the reported value 3.11 by more than 10 %

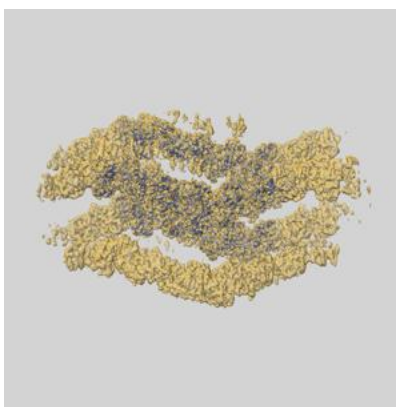
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-73506 and PDB model 9YUQ. Per-residue inclusion information can be found in section [3](#) on page [12](#).

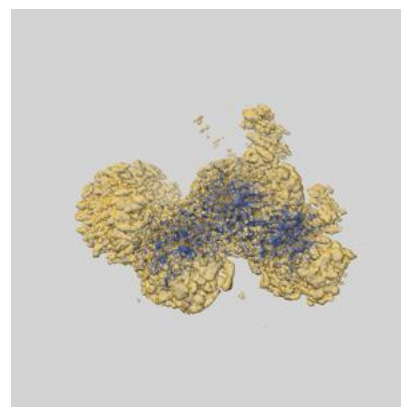
9.1 Map-model overlay [i](#)



X



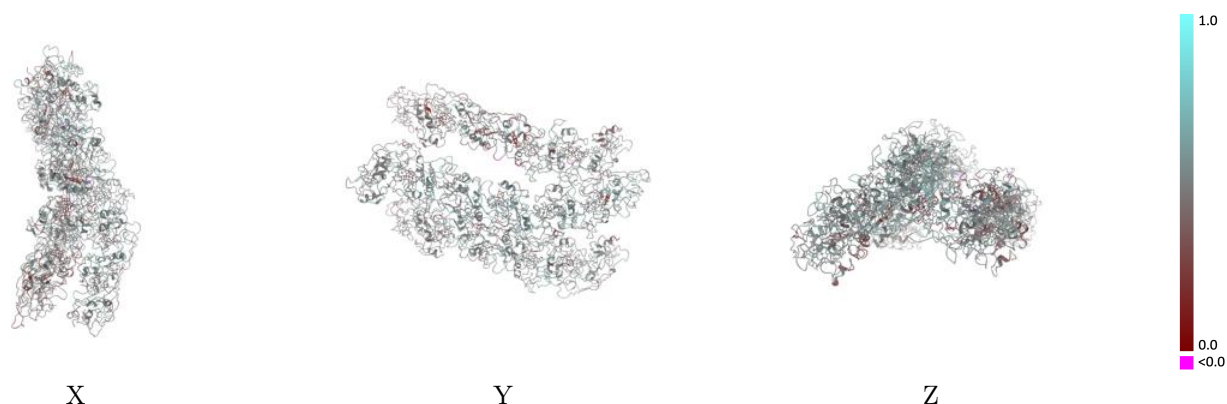
Y



Z

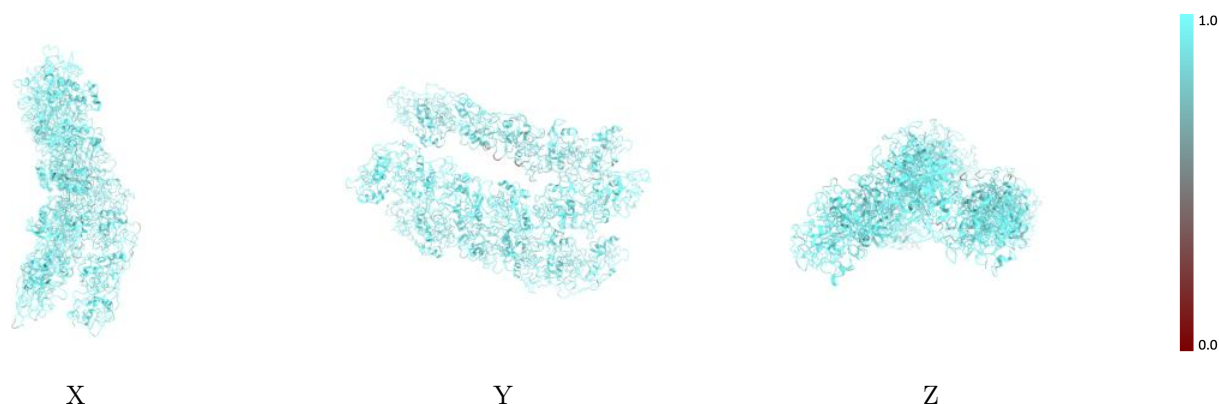
The images above show the 3D surface view of the map at the recommended contour level 0.0486 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



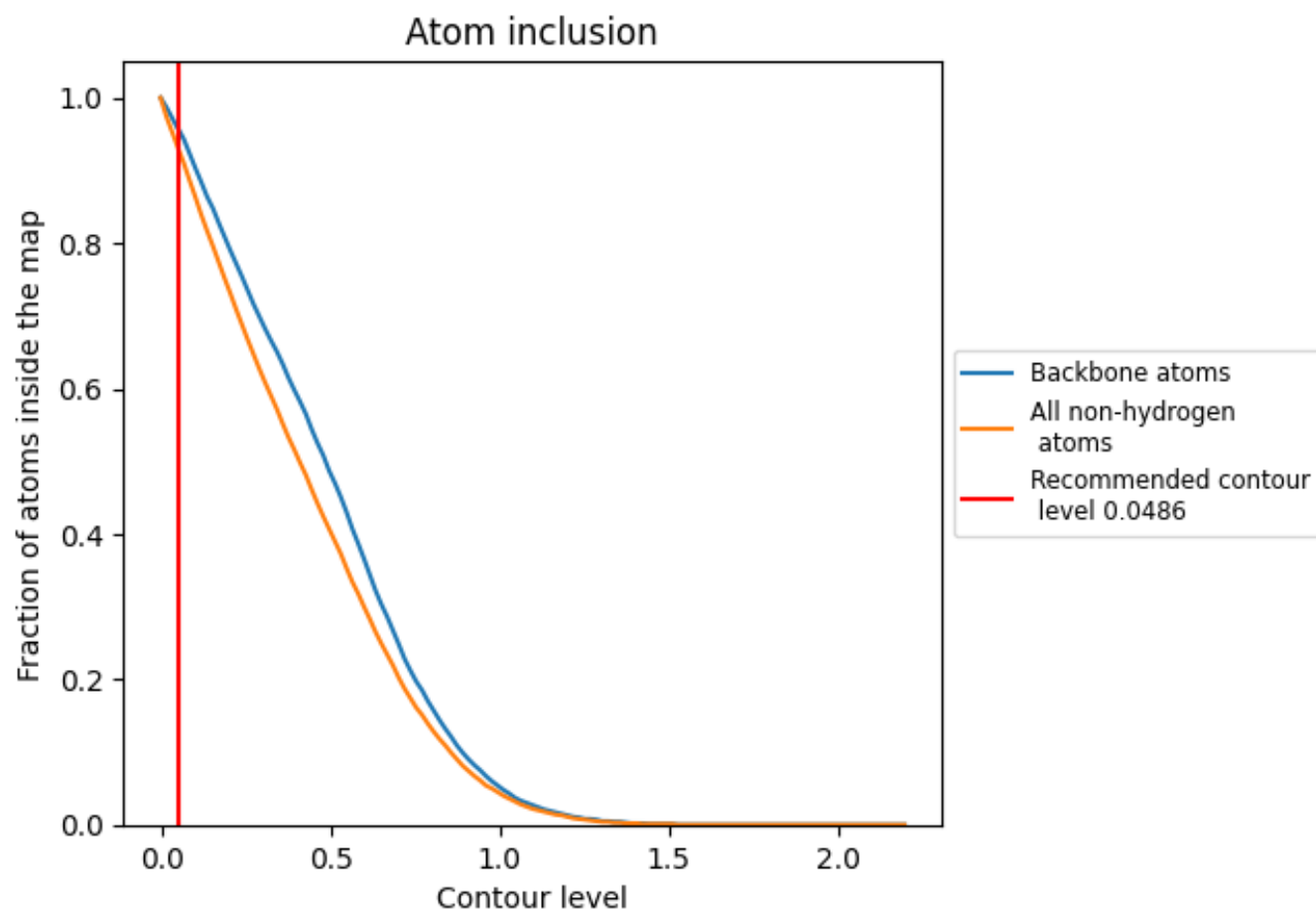
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0486).

9.4 Atom inclusion ⓘ



At the recommended contour level, 96% of all backbone atoms, 93% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0486) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9320	 0.4870
C	 0.9280	 0.4700
D	 0.9420	 0.5060
E	 0.9310	 0.4960
F	 0.9250	 0.4970
G	 0.9120	 0.4610
I	 0.9600	 0.5080
J	 0.9650	 0.5320
K	 0.9560	 0.5330
L	 0.9480	 0.5230
M	 0.9550	 0.5130
N	 0.9430	 0.4890
P	 0.9090	 0.4610
Q	 0.9130	 0.4840
R	 0.8860	 0.4320
S	 0.9260	 0.4540
T	 0.9170	 0.4420

