



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:28 PM UTC

PDB ID : 1QDB / pdb_00001qdb
Title : CYTOCHROME C NITRITE REDUCTASE
Authors : Einsle, O.; Messerschmidt, A.; Stach, P.; Huber, R.; Kroneck, P.M.H.
Deposited on : 1999-05-19
Resolution : 1.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

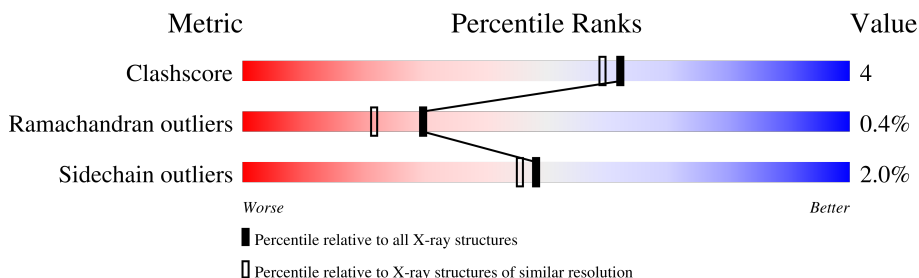
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	473	
1	B	473	
1	C	473	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13431 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

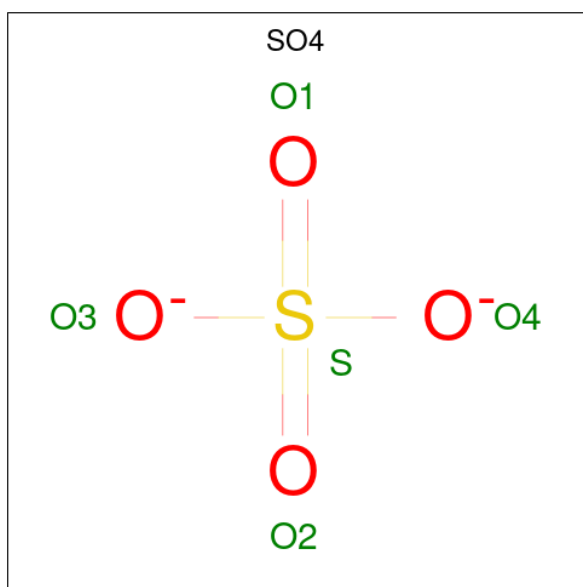
- Molecule 1 is a protein called CYTOCHROME C NITRITE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	473	Total	C	N	O	S	93	0	0
			3751	2367	654	710	20			
1	B	473	Total	C	N	O	S	14	0	0
			3751	2367	654	710	20			
1	C	473	Total	C	N	O	S	17	0	0
			3751	2367	654	710	20			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

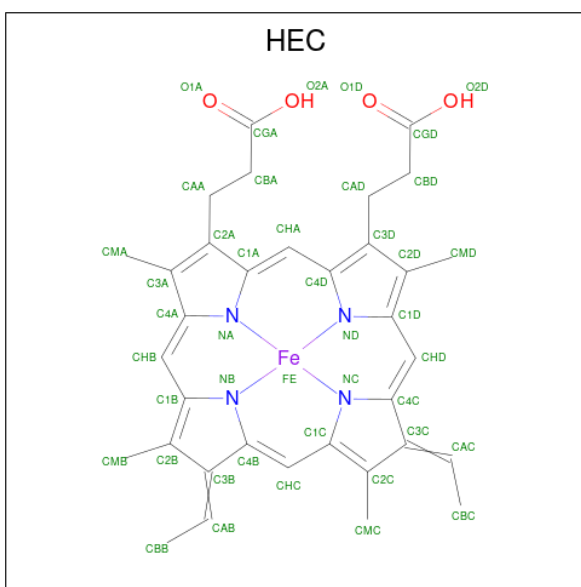
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		
2	B	1	Total	Ca	0	0
			1	1		
2	C	1	Total	Ca	0	0
			1	1		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 5 is water.

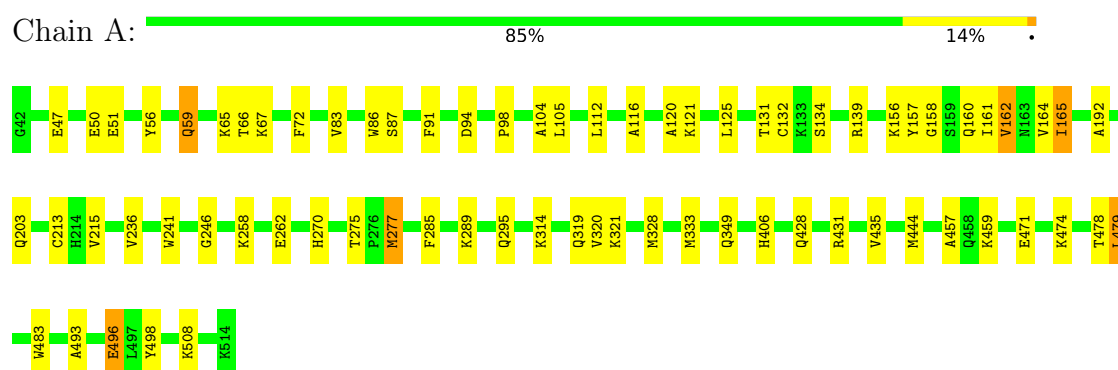
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	371	Total	O	0	0
			371	371		
5	B	505	Total	O	0	0
			505	505		
5	C	609	Total	O	0	0
			609	609		

3 Residue-property plots

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. 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. 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.

Note EDS was not executed.

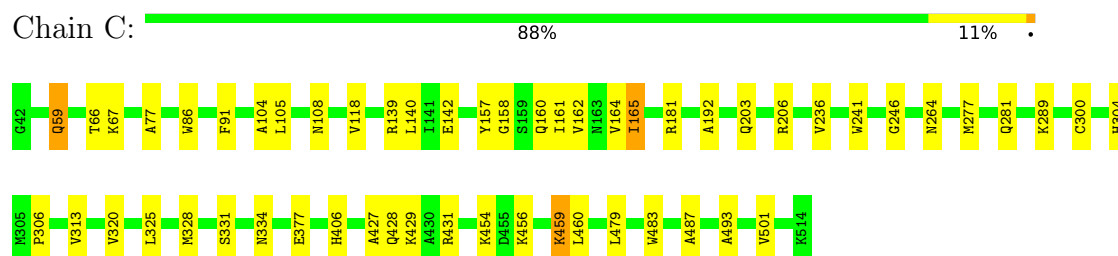
• Molecule 1: CYTOCHROME C NITRITE REDUCTASE



• Molecule 1: CYTOCHROME C NITRITE REDUCTASE



• Molecule 1: CYTOCHROME C NITRITE REDUCTASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	107.48Å 185.34Å 92.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 1.90	Depositor
% Data completeness (in resolution range)	100.0 (25.00-1.90)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.184 , 0.220	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13431	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, HEC, CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.49	0/3840	0.95	12/5173 (0.2%)
1	B	0.51	1/3840 (0.0%)	0.94	10/5173 (0.2%)
1	C	0.56	0/3840	0.95	9/5173 (0.2%)
All	All	0.52	1/11520 (0.0%)	0.95	31/15519 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	411	HIS	CD2-NE2	5.12	1.43	1.37

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	134	SER	N-CA-C	7.91	118.32	108.11
1	B	134	SER	N-CA-C	7.60	117.92	108.11
1	B	331	SER	N-CA-C	6.59	121.06	112.89
1	A	236	VAL	N-CA-C	6.54	118.24	108.23
1	C	104	ALA	N-CA-C	6.36	118.74	111.11
1	A	162	VAL	N-CA-C	6.35	119.30	113.20
1	A	277	MET	N-CA-C	6.27	120.14	110.42
1	C	501	VAL	N-CA-C	6.26	117.01	110.62
1	C	331	SER	N-CA-C	6.26	120.65	112.89
1	C	236	VAL	N-CA-C	6.13	117.41	108.58
1	C	66	THR	N-CA-C	-6.12	105.66	113.01
1	A	125	LEU	CA-C-N	5.95	127.34	120.98
1	A	125	LEU	C-N-CA	5.95	127.34	120.98
1	B	406	HIS	N-CA-C	5.84	119.23	111.75
1	A	333	MET	N-CA-C	5.81	119.84	112.87
1	B	241	TRP	N-CA-C	5.78	120.03	112.92
1	A	406	HIS	N-CA-C	5.75	118.32	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	236	VAL	N-CA-C	5.62	116.68	108.58
1	C	406	HIS	N-CA-C	5.59	118.91	111.75
1	A	131	THR	N-CA-C	5.57	122.67	110.80
1	B	66	THR	N-CA-C	-5.45	106.48	113.01
1	B	104	ALA	N-CA-C	5.40	117.59	111.11
1	A	66	THR	N-CA-C	-5.37	106.81	113.19
1	B	166	GLY	N-CA-C	5.34	119.08	111.12
1	B	277	MET	N-CA-C	5.26	118.58	110.42
1	B	131	THR	N-CA-C	5.22	121.92	110.80
1	C	277	MET	N-CA-C	5.16	118.41	110.42
1	A	125	LEU	N-CA-C	5.13	117.06	110.39
1	C	313	VAL	N-CA-C	5.12	115.46	107.99
1	A	104	ALA	N-CA-C	5.10	117.23	111.11
1	C	108	ASN	N-CA-C	-5.09	105.81	111.36

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3751	0	3658	43	0
1	B	3751	0	3658	27	0
1	C	3751	0	3658	31	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	15	0	0	0	0
3	B	15	0	0	0	0
3	C	15	0	0	1	0
4	A	215	0	150	1	0
4	B	215	0	150	1	0
4	C	215	0	150	1	0
5	A	371	0	0	3	0
5	B	505	0	0	2	0
5	C	609	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	13431	0	11424	95	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 4.

All (95) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:GLN:HE22	1:B:295:GLN:HE22	1.29	0.78
1:A:319:GLN:O	1:A:321:LYS:HD2	1.86	0.75
1:C:456:LYS:O	1:C:459:LYS:HD3	1.87	0.74
1:A:295:GLN:HE22	1:B:349:GLN:HE22	1.34	0.73
1:B:140:LEU:HD12	1:B:161:ILE:HD11	1.71	0.73
1:A:139:ARG:HH22	1:A:160:GLN:HE21	1.43	0.67
1:C:140:LEU:HD12	1:C:161:ILE:HD11	1.77	0.66
1:A:56:TYR:HB3	1:A:59:GLN:NE2	2.12	0.64
1:C:142:GLU:OE2	1:C:181:ARG:HD2	1.98	0.63
1:B:203:GLN:HE21	1:B:203:GLN:HA	1.64	0.62
1:A:428:GLN:HE21	1:A:428:GLN:HA	1.63	0.61
1:C:59:GLN:HE21	1:C:59:GLN:H	1.47	0.60
1:C:139:ARG:HH22	1:C:160:GLN:HE21	1.49	0.59
1:B:59:GLN:NE2	1:B:59:GLN:H	2.02	0.58
1:C:59:GLN:H	1:C:59:GLN:NE2	2.02	0.57
1:A:56:TYR:HB3	1:A:59:GLN:HE21	1.70	0.56
1:B:142:GLU:OE2	1:B:181:ARG:HD2	2.05	0.56
1:A:349:GLN:HE22	1:B:295:GLN:NE2	2.03	0.56
1:B:58:ARG:HH12	1:C:203:GLN:NE2	2.04	0.54
1:B:338:GLU:CD	1:B:342:LYS:HD3	2.33	0.53
1:C:428:GLN:HE21	1:C:428:GLN:HA	1.74	0.53
1:A:431:ARG:O	1:A:435:VAL:HG23	2.09	0.53
1:C:157:TYR:HB3	1:C:161:ILE:HG12	1.90	0.53
1:C:203:GLN:HE21	1:C:203:GLN:HA	1.74	0.53
1:B:289:LYS:NZ	5:B:1734:HOH:O	2.42	0.52
1:B:59:GLN:H	1:B:59:GLN:HE21	1.56	0.52
5:A:1669:HOH:O	1:B:436:LYS:HG2	2.10	0.51
1:A:203:GLN:HA	1:A:203:GLN:HE21	1.77	0.50
1:A:116:ALA:HB3	1:A:471:GLU:HG2	1.94	0.50
1:B:164:VAL:O	1:B:165:ILE:C	2.55	0.49
1:B:139:ARG:HH22	1:B:160:GLN:HE21	1.59	0.49
1:A:164:VAL:O	1:A:165:ILE:C	2.56	0.49
1:A:444:MET:HE1	1:B:439:ALA:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:86:TRP:CE3	1:C:91:PHE:HB3	2.49	0.48
1:A:428:GLN:HA	1:A:428:GLN:NE2	2.30	0.47
1:C:246:GLY:HA3	1:C:289:LYS:HB3	1.96	0.47
1:C:427:ALA:O	1:C:431:ARG:HG3	2.15	0.47
1:A:295:GLN:NE2	1:B:349:GLN:HE22	2.08	0.47
1:B:192:ALA:HB2	1:B:241:TRP:HB3	1.97	0.47
1:A:158:GLY:HA3	1:A:483:TRP:CE2	2.50	0.46
1:C:304:HIS:C	1:C:306:PRO:HD3	2.41	0.46
1:A:246:GLY:HA3	1:A:289:LYS:HB3	1.97	0.46
4:B:517:HEC:HBC3	4:B:517:HEC:HMC3	1.98	0.46
1:A:258:LYS:O	1:A:262:GLU:HG3	2.15	0.46
1:C:377:GLU:HG3	5:C:2056:HOH:O	2.16	0.46
1:B:312:SER:HB3	1:C:334:ASN:HD22	1.81	0.45
1:B:510:SER:O	1:B:513:LYS:HE3	2.16	0.45
1:C:459:LYS:NZ	5:C:2008:HOH:O	2.39	0.45
1:A:47:GLU:H	1:A:47:GLU:CD	2.25	0.45
1:B:162:VAL:HG23	1:B:493:ALA:HB2	1.97	0.45
1:A:94:ASP:HB2	1:A:112:LEU:HB2	1.98	0.45
1:B:64:LYS:HE3	5:B:1812:HOH:O	2.15	0.45
1:A:478:THR:HG22	1:A:479:LEU:N	2.31	0.45
1:B:157:TYR:HB3	1:B:161:ILE:HG12	2.00	0.45
1:C:164:VAL:O	1:C:165:ILE:C	2.60	0.44
1:A:192:ALA:HB2	1:A:241:TRP:HB3	2.00	0.44
1:A:47:GLU:CD	1:A:139:ARG:HD3	2.43	0.44
1:A:121:LYS:HA	1:A:121:LYS:HD2	1.77	0.44
1:C:281:GLN:HG2	3:C:1503:SO4:O2	2.18	0.44
1:A:428:GLN:HE22	1:A:431:ARG:HH11	1.66	0.44
1:A:508:LYS:HE2	5:A:1734:HOH:O	2.17	0.44
1:C:164:VAL:HG22	1:C:165:ILE:N	2.33	0.44
1:C:162:VAL:HG23	1:C:493:ALA:HB2	2.00	0.43
1:C:192:ALA:HB2	1:C:241:TRP:HB3	2.00	0.43
1:A:87:SER:HB3	1:A:270:HIS:CE1	2.53	0.43
1:A:120:ALA:HB1	1:A:156:LYS:HA	1.99	0.43
1:A:86:TRP:CE3	1:A:91:PHE:HB3	2.53	0.43
1:A:496:GLU:CD	1:A:496:GLU:H	2.27	0.43
1:B:135:PRO:HD2	1:B:163:ASN:O	2.19	0.43
1:C:429:LYS:HD3	5:C:1751:HOH:O	2.18	0.43
1:A:83:VAL:HB	1:A:457:ALA:HB1	2.00	0.43
1:C:158:GLY:HA3	1:C:483:TRP:CE2	2.53	0.43
1:C:203:GLN:HE22	1:C:206:ARG:HE	1.65	0.43
1:A:50:GLU:H	1:A:50:GLU:CD	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:300:CYS:HA	4:C:518:HEC:CHC	2.50	0.42
1:A:65:LYS:C	1:A:67:LYS:H	2.27	0.42
1:B:203:GLN:HE22	1:B:206:ARG:HE	1.68	0.42
1:B:94:ASP:HB2	1:B:112:LEU:HB2	2.02	0.42
1:A:157:TYR:HB3	1:A:161:ILE:HG13	2.01	0.42
1:C:77:ALA:HA	1:C:454:LYS:HB2	2.01	0.42
1:C:325:LEU:O	1:C:328:MET:HG3	2.20	0.42
1:C:428:GLN:HE22	1:C:431:ARG:HH11	1.67	0.42
1:A:215:VAL:HG12	1:A:285:PHE:HB3	2.02	0.41
1:A:162:VAL:HG23	1:A:493:ALA:HB2	2.02	0.41
1:C:162:VAL:HG11	1:C:487:ALA:HB2	2.03	0.41
1:A:72:PHE:CD1	1:A:72:PHE:C	2.98	0.41
1:A:65:LYS:C	1:A:67:LYS:N	2.79	0.41
1:A:132:CYS:HB3	1:A:213:CYS:SG	2.61	0.41
1:A:498:TYR:HB2	5:A:1718:HOH:O	2.21	0.41
1:B:275:THR:O	1:B:277:MET:HG2	2.21	0.41
1:A:275:THR:O	1:A:277:MET:HG2	2.22	0.40
1:B:98:PRO:HD3	1:B:406:HIS:CD2	2.56	0.40
1:C:459:LYS:HE2	1:C:460:LEU:HG	2.03	0.40
1:A:98:PRO:HG3	4:A:515:HEC:CGD	2.52	0.40
1:A:428:GLN:NE2	1:A:431:ARG:HD3	2.36	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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	471/473 (100%)	454 (96%)	15 (3%)	2 (0%)	30	22
1	B	471/473 (100%)	465 (99%)	4 (1%)	2 (0%)	30	22
1	C	471/473 (100%)	462 (98%)	7 (2%)	2 (0%)	30	22
All	All	1413/1419 (100%)	1381 (98%)	26 (2%)	6 (0%)	30	22

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	165	ILE
1	B	165	ILE
1	C	165	ILE
1	A	320	VAL
1	C	320	VAL
1	B	320	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	392/392 (100%)	383 (98%)	9 (2%)	44	40
1	B	392/392 (100%)	385 (98%)	7 (2%)	51	50
1	C	392/392 (100%)	385 (98%)	7 (2%)	51	50
All	All	1176/1176 (100%)	1153 (98%)	23 (2%)	48	46

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	GLU
1	A	59	GLN
1	A	105	LEU
1	A	314	LYS
1	A	328	MET
1	A	459	LYS
1	A	474	LYS
1	A	479	LEU
1	A	496	GLU
1	B	59	GLN
1	B	105	LEU
1	B	309	GLN
1	B	387	GLU
1	B	479	LEU
1	B	496	GLU

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Mol	Chain	Res	Type
1	B	508	LYS
1	C	59	GLN
1	C	67	LYS
1	C	105	LEU
1	C	118	VAL
1	C	264	ASN
1	C	459	LYS
1	C	479	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	A	160	GLN
1	A	203	GLN
1	A	295	GLN
1	A	428	GLN
1	B	59	GLN
1	B	160	GLN
1	B	203	GLN
1	B	295	GLN
1	B	309	GLN
1	B	477	GLN
1	B	512	ASN
1	C	59	GLN
1	C	160	GLN
1	C	203	GLN
1	C	212	GLN
1	C	309	GLN
1	C	428	GLN
1	C	477	GLN
1	C	512	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 27 ligands modelled in this entry, 3 are monoatomic - leaving 24 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	HEC	B	519	1	46,50,50	1.12	2 (4%)	58,82,82	1.16	2 (3%)
4	HEC	C	516	1	46,50,50	1.23	5 (10%)	58,82,82	1.05	2 (3%)
3	SO4	C	1509	-	4,4,4	0.36	0	6,6,6	0.34	0
4	HEC	B	515	3,1	46,50,50	1.09	1 (2%)	58,82,82	1.23	4 (6%)
4	HEC	C	515	3,1	46,50,50	1.27	5 (10%)	58,82,82	1.06	2 (3%)
4	HEC	A	516	1	46,50,50	1.10	2 (4%)	58,82,82	0.92	2 (3%)
3	SO4	A	1504	-	4,4,4	0.45	0	6,6,6	0.39	0
3	SO4	A	1501	4	4,4,4	0.32	0	6,6,6	0.65	0
3	SO4	C	1503	4	4,4,4	0.54	0	6,6,6	0.89	0
4	HEC	B	517	1	46,50,50	1.13	3 (6%)	58,82,82	1.00	3 (5%)
4	HEC	B	516	1	46,50,50	1.17	5 (10%)	58,82,82	1.19	5 (8%)
4	HEC	C	517	1	46,50,50	1.16	4 (8%)	58,82,82	1.18	3 (5%)
3	SO4	C	1508	-	4,4,4	0.23	0	6,6,6	0.32	0
4	HEC	C	518	1	46,50,50	1.27	5 (10%)	58,82,82	1.30	4 (6%)
4	HEC	A	515	3,1	46,50,50	1.07	1 (2%)	58,82,82	1.00	1 (1%)
3	SO4	B	1502	4	4,4,4	0.29	0	6,6,6	0.53	0
3	SO4	B	1505	-	4,4,4	0.46	0	6,6,6	0.30	0
4	HEC	A	519	1	46,50,50	1.20	4 (8%)	58,82,82	1.00	3 (5%)
4	HEC	C	519	1	46,50,50	1.27	7 (15%)	58,82,82	1.16	5 (8%)
3	SO4	A	1506	-	4,4,4	0.31	0	6,6,6	0.15	0
3	SO4	B	1507	-	4,4,4	0.43	0	6,6,6	0.26	0
4	HEC	A	517	1	46,50,50	1.08	2 (4%)	58,82,82	1.15	5 (8%)
4	HEC	B	518	1	46,50,50	1.23	3 (6%)	58,82,82	1.38	5 (8%)
4	HEC	A	518	1	46,50,50	1.19	3 (6%)	58,82,82	1.23	4 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HEC	B	519	1	-	9/14/54/54	-
4	HEC	C	516	1	-	6/14/54/54	-
4	HEC	B	515	3,1	-	6/14/54/54	-
4	HEC	B	517	1	-	5/14/54/54	-
4	HEC	B	516	1	-	6/14/54/54	-
4	HEC	C	515	3,1	-	6/14/54/54	-
4	HEC	A	519	1	-	9/14/54/54	-
4	HEC	A	517	1	-	6/14/54/54	-
4	HEC	A	516	1	-	8/14/54/54	-
4	HEC	B	518	1	-	4/14/54/54	-
4	HEC	C	518	1	-	4/14/54/54	-
4	HEC	C	519	1	-	8/14/54/54	-
4	HEC	A	518	1	-	4/14/54/54	-
4	HEC	C	517	1	-	4/14/54/54	-
4	HEC	A	515	3,1	-	6/14/54/54	-

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	519	HEC	C3B-C4B	-3.00	1.40	1.46
4	C	515	HEC	CMC-C2C	3.00	1.56	1.50
4	C	515	HEC	CAB-C3B	2.98	1.44	1.35
4	B	516	HEC	C3B-C4B	-2.97	1.40	1.46
4	C	515	HEC	CAC-C3C	2.88	1.44	1.35
4	C	518	HEC	CMD-C2D	2.78	1.56	1.50
4	B	516	HEC	CMB-C2B	2.77	1.56	1.50
4	C	519	HEC	CMD-C2D	2.76	1.56	1.50
4	B	515	HEC	C1D-ND	-2.68	1.34	1.39
4	C	517	HEC	CAB-C3B	2.65	1.43	1.35
4	A	515	HEC	CAC-C3C	2.62	1.43	1.35
4	C	516	HEC	CMD-C2D	2.57	1.56	1.50
4	A	516	HEC	CBB-CAB	-2.57	1.40	1.49
4	B	517	HEC	CAC-C3C	2.53	1.43	1.35
4	C	517	HEC	CAC-C3C	2.47	1.43	1.35
4	A	519	HEC	CBC-CAC	-2.44	1.40	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	518	HEC	CMB-C2B	2.34	1.55	1.50
4	A	516	HEC	C1B-C2B	2.34	1.48	1.43
4	C	519	HEC	CMB-C2B	2.33	1.55	1.50
4	C	516	HEC	CAC-C3C	2.33	1.42	1.35
4	C	519	HEC	CAC-C3C	2.33	1.42	1.35
4	C	518	HEC	C1B-C2B	2.32	1.48	1.43
4	A	518	HEC	C4C-NC	-2.30	1.35	1.39
4	B	517	HEC	CAB-C3B	2.28	1.42	1.35
4	B	518	HEC	C1B-NB	-2.26	1.35	1.39
4	B	518	HEC	CAC-C3C	2.26	1.42	1.35
4	A	518	HEC	CAB-C3B	2.25	1.42	1.35
4	B	516	HEC	CBC-CAC	-2.25	1.41	1.49
4	B	518	HEC	CAB-C3B	2.23	1.42	1.35
4	C	517	HEC	CHA-C1A	2.23	1.42	1.38
4	C	517	HEC	CMC-C2C	2.22	1.55	1.50
4	A	519	HEC	CAC-C3C	2.19	1.42	1.35
4	C	516	HEC	CMB-C2B	2.17	1.55	1.50
4	A	517	HEC	CAB-C3B	2.16	1.42	1.35
4	C	518	HEC	CHB-C1B	2.16	1.44	1.39
4	C	518	HEC	C1D-C2D	2.14	1.48	1.43
4	B	519	HEC	CMD-C2D	2.14	1.55	1.50
4	A	518	HEC	C4A-NA	-2.13	1.35	1.39
4	B	516	HEC	CAC-C3C	2.12	1.41	1.35
4	A	519	HEC	CMA-C3A	2.11	1.55	1.50
4	C	515	HEC	CMD-C2D	2.09	1.55	1.50
4	C	515	HEC	O2D-CGD	-2.07	1.24	1.30
4	B	519	HEC	CAC-C3C	2.06	1.41	1.35
4	C	519	HEC	CBC-CAC	-2.06	1.41	1.49
4	C	516	HEC	C1C-NC	-2.06	1.35	1.39
4	C	516	HEC	CAB-C3B	2.05	1.41	1.35
4	C	519	HEC	C1A-NA	-2.04	1.35	1.39
4	A	517	HEC	CBB-CAB	-2.03	1.42	1.49
4	B	517	HEC	C3C-C2C	-2.03	1.34	1.41
4	C	519	HEC	CAB-C3B	2.03	1.41	1.35
4	B	516	HEC	CAB-C3B	2.01	1.41	1.35
4	A	519	HEC	CAB-C3B	2.00	1.41	1.35

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	518	HEC	CBB-CAB-C3B	-5.43	116.59	127.43
4	B	515	HEC	CBB-CAB-C3B	-5.12	117.21	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	518	HEC	CBC-CAC-C3C	-4.90	117.65	127.43
4	B	516	HEC	CBB-CAB-C3B	-4.13	119.18	127.43
4	C	517	HEC	CBB-CAB-C3B	-4.04	119.36	127.43
4	C	515	HEC	CBB-CAB-C3B	-3.79	119.86	127.43
4	A	517	HEC	CBB-CAB-C3B	-3.77	119.91	127.43
4	B	517	HEC	CBB-CAB-C3B	-3.75	119.94	127.43
4	B	519	HEC	CBC-CAC-C3C	-3.73	119.98	127.43
4	A	518	HEC	CBB-CAB-C3B	-3.70	120.04	127.43
4	C	515	HEC	CBC-CAC-C3C	-3.69	120.07	127.43
4	C	516	HEC	CBB-CAB-C3B	-3.67	120.10	127.43
4	A	517	HEC	CMB-C2B-C1B	-3.46	120.15	125.42
4	C	517	HEC	CBC-CAC-C3C	-3.40	120.63	127.43
4	A	518	HEC	CBC-CAC-C3C	-3.40	120.64	127.43
4	B	518	HEC	CBC-CAC-C3C	-3.36	120.72	127.43
4	A	516	HEC	CBC-CAC-C3C	-3.27	120.89	127.43
4	C	519	HEC	CBB-CAB-C3B	-3.21	121.02	127.43
4	A	515	HEC	CBB-CAB-C3B	-3.04	121.35	127.43
4	C	518	HEC	CMC-C2C-C1C	-2.94	120.94	125.42
4	A	516	HEC	CBB-CAB-C3B	-2.93	121.57	127.43
4	C	518	HEC	CBB-CAB-C3B	-2.85	121.73	127.43
4	B	518	HEC	CBA-CAA-C2A	-2.78	104.86	112.53
4	A	519	HEC	CBC-CAC-C3C	-2.71	122.01	127.43
4	B	517	HEC	CHC-C4B-NB	-2.71	121.50	124.45
4	C	517	HEC	CMB-C2B-C1B	-2.66	121.36	125.42
4	B	515	HEC	CAD-C3D-C4D	2.65	130.11	124.94
4	B	518	HEC	CMB-C2B-C1B	-2.57	121.51	125.42
4	C	519	HEC	C4B-NB-C1B	-2.55	101.67	105.82
4	B	516	HEC	CBC-CAC-C3C	-2.47	122.49	127.43
4	B	515	HEC	CMB-C2B-C1B	-2.43	121.72	125.42
4	A	519	HEC	CMC-C2C-C1C	-2.40	121.76	125.42
4	B	518	HEC	C2A-C1A-NA	2.38	112.62	110.32
4	A	517	HEC	CAA-C2A-C3A	-2.35	123.46	127.87
4	C	518	HEC	C2A-C1A-NA	2.31	112.55	110.32
4	A	517	HEC	CAA-C2A-C1A	2.30	129.52	124.85
4	C	519	HEC	CBC-CAC-C3C	-2.29	122.86	127.43
4	C	516	HEC	CBC-CAC-C3C	-2.21	123.02	127.43
4	B	516	HEC	C3D-C4D-ND	2.20	112.59	110.15
4	C	519	HEC	CMC-C2C-C1C	-2.20	122.08	125.42
4	A	518	HEC	CAD-C3D-C4D	2.18	129.19	124.94
4	B	516	HEC	C1A-C2A-C3A	-2.17	104.25	107.11
4	A	517	HEC	CMB-C2B-C3B	2.16	131.63	126.55
4	B	519	HEC	CBB-CAB-C3B	-2.14	123.16	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	519	HEC	CBB-CAB-C3B	-2.12	123.19	127.43
4	B	515	HEC	CMB-C2B-C3B	2.12	131.53	126.55
4	B	517	HEC	CBC-CAC-C3C	-2.11	123.21	127.43
4	A	518	HEC	CAA-C2A-C1A	2.08	129.08	124.85
4	C	519	HEC	C4D-ND-C1D	-2.04	102.50	105.82
4	B	516	HEC	C2A-C1A-NA	2.04	112.29	110.32

There are no chirality outliers.

All (91) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	515	HEC	C2C-C3C-CAC-CBC
4	A	515	HEC	C4C-C3C-CAC-CBC
4	A	516	HEC	C2B-C3B-CAB-CBB
4	A	516	HEC	C4B-C3B-CAB-CBB
4	A	516	HEC	C2C-C3C-CAC-CBC
4	A	516	HEC	C4C-C3C-CAC-CBC
4	A	517	HEC	C2B-C3B-CAB-CBB
4	A	517	HEC	C4B-C3B-CAB-CBB
4	A	517	HEC	C2C-C3C-CAC-CBC
4	A	517	HEC	C4C-C3C-CAC-CBC
4	A	518	HEC	C2B-C3B-CAB-CBB
4	A	518	HEC	C4B-C3B-CAB-CBB
4	A	518	HEC	C2C-C3C-CAC-CBC
4	A	518	HEC	C4C-C3C-CAC-CBC
4	A	519	HEC	C2B-C3B-CAB-CBB
4	A	519	HEC	C4B-C3B-CAB-CBB
4	A	519	HEC	C2C-C3C-CAC-CBC
4	A	519	HEC	C4C-C3C-CAC-CBC
4	B	515	HEC	C2B-C3B-CAB-CBB
4	B	515	HEC	C2C-C3C-CAC-CBC
4	B	515	HEC	C4C-C3C-CAC-CBC
4	B	516	HEC	C2B-C3B-CAB-CBB
4	B	516	HEC	C4B-C3B-CAB-CBB
4	B	516	HEC	C2C-C3C-CAC-CBC
4	B	516	HEC	C4C-C3C-CAC-CBC
4	B	517	HEC	C2B-C3B-CAB-CBB
4	B	517	HEC	C4B-C3B-CAB-CBB
4	B	517	HEC	C2C-C3C-CAC-CBC
4	B	517	HEC	C4C-C3C-CAC-CBC
4	B	518	HEC	C2B-C3B-CAB-CBB
4	B	518	HEC	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
4	B	518	HEC	C2C-C3C-CAC-CBC
4	B	518	HEC	C4C-C3C-CAC-CBC
4	B	519	HEC	C2B-C3B-CAB-CBB
4	B	519	HEC	C4B-C3B-CAB-CBB
4	B	519	HEC	C2C-C3C-CAC-CBC
4	B	519	HEC	C4C-C3C-CAC-CBC
4	C	515	HEC	C2B-C3B-CAB-CBB
4	C	515	HEC	C2C-C3C-CAC-CBC
4	C	515	HEC	C4C-C3C-CAC-CBC
4	C	516	HEC	C2B-C3B-CAB-CBB
4	C	516	HEC	C4B-C3B-CAB-CBB
4	C	516	HEC	C2C-C3C-CAC-CBC
4	C	516	HEC	C4C-C3C-CAC-CBC
4	C	517	HEC	C2B-C3B-CAB-CBB
4	C	517	HEC	C4B-C3B-CAB-CBB
4	C	517	HEC	C2C-C3C-CAC-CBC
4	C	517	HEC	C4C-C3C-CAC-CBC
4	C	518	HEC	C2B-C3B-CAB-CBB
4	C	518	HEC	C4B-C3B-CAB-CBB
4	C	518	HEC	C2C-C3C-CAC-CBC
4	C	518	HEC	C4C-C3C-CAC-CBC
4	C	519	HEC	C2B-C3B-CAB-CBB
4	C	519	HEC	C4B-C3B-CAB-CBB
4	C	519	HEC	C2C-C3C-CAC-CBC
4	C	519	HEC	C4C-C3C-CAC-CBC
4	A	515	HEC	C4B-C3B-CAB-CBB
4	B	515	HEC	C4B-C3B-CAB-CBB
4	A	515	HEC	C2B-C3B-CAB-CBB
4	B	519	HEC	C2A-CAA-CBA-CGA
4	C	515	HEC	CAA-CBA-CGA-O1A
4	A	515	HEC	CAA-CBA-CGA-O1A
4	A	516	HEC	CAA-CBA-CGA-O1A
4	B	516	HEC	CAA-CBA-CGA-O1A
4	B	515	HEC	CAA-CBA-CGA-O1A
4	B	516	HEC	CAA-CBA-CGA-O2A
4	A	516	HEC	CAA-CBA-CGA-O2A
4	B	519	HEC	CAD-CBD-CGD-O2D
4	C	515	HEC	CAA-CBA-CGA-O2A
4	C	516	HEC	CAA-CBA-CGA-O2A
4	C	519	HEC	CAD-CBD-CGD-O1D
4	C	519	HEC	CAD-CBD-CGD-O2D
4	A	515	HEC	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
4	A	519	HEC	CAD-CBD-CGD-O2D
4	C	516	HEC	CAA-CBA-CGA-O1A
4	B	515	HEC	CAA-CBA-CGA-O2A
4	A	519	HEC	CAD-CBD-CGD-O1D
4	A	519	HEC	C2A-CAA-CBA-CGA
4	B	519	HEC	CAD-CBD-CGD-O1D
4	B	517	HEC	C1A-C2A-CAA-CBA
4	A	517	HEC	CAA-CBA-CGA-O2A
4	A	517	HEC	CAA-CBA-CGA-O1A
4	A	516	HEC	CAD-CBD-CGD-O2D
4	C	519	HEC	CAA-CBA-CGA-O1A
4	A	519	HEC	CAA-CBA-CGA-O1A
4	B	519	HEC	CAA-CBA-CGA-O1A
4	A	516	HEC	CAD-CBD-CGD-O1D
4	A	519	HEC	CAA-CBA-CGA-O2A
4	B	519	HEC	CAA-CBA-CGA-O2A
4	C	515	HEC	C4B-C3B-CAB-CBB
4	C	519	HEC	CAA-CBA-CGA-O2A

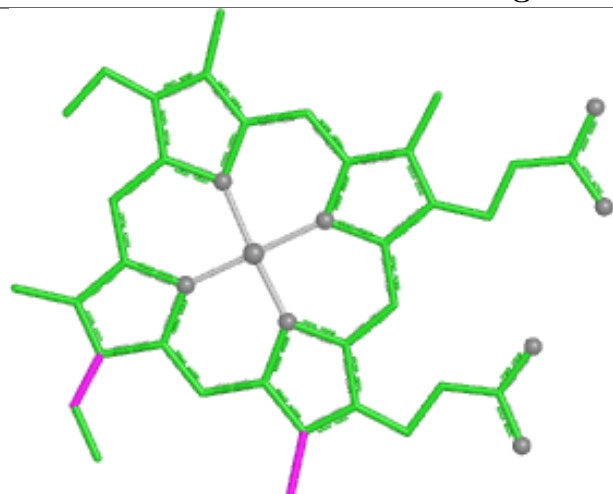
There are no ring outliers.

4 monomers are involved in 4 short contacts:

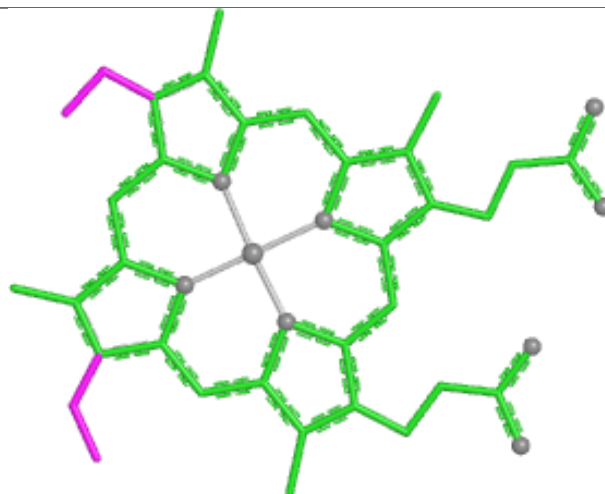
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1503	SO4	1	0
4	B	517	HEC	1	0
4	C	518	HEC	1	0
4	A	515	HEC	1	0

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

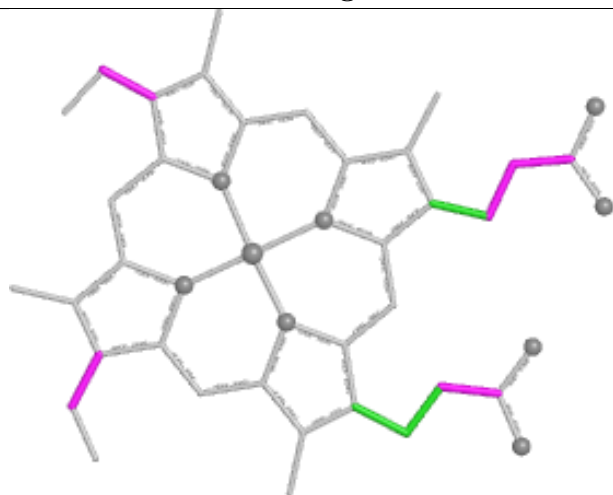
Ligand HEC B 519



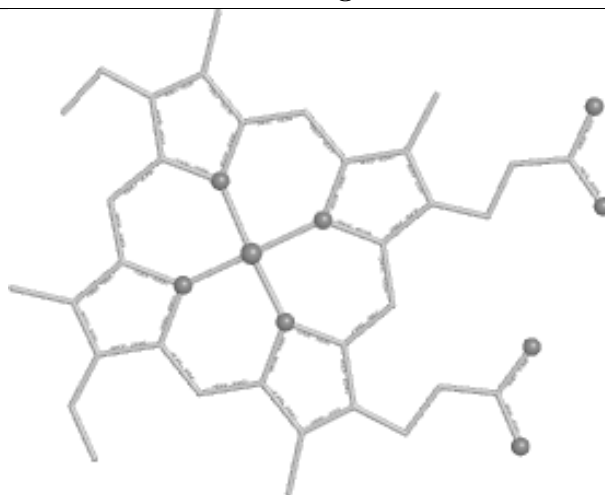
Bond lengths



Bond angles

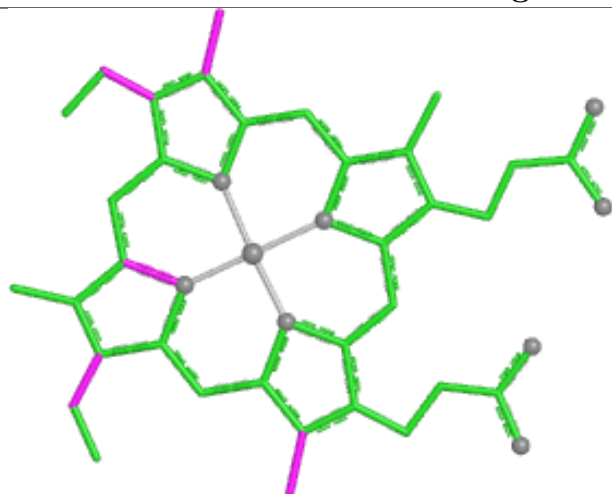


Torsions

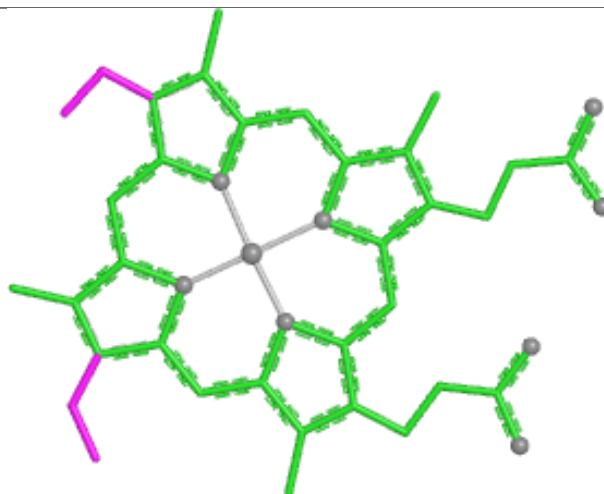


Rings

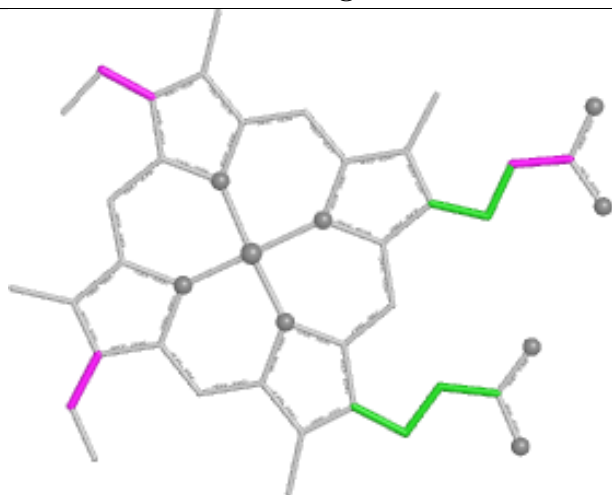
Ligand HEC C 516



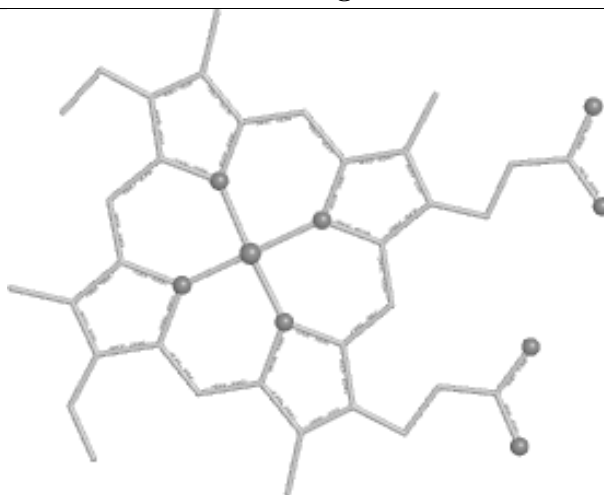
Bond lengths



Bond angles

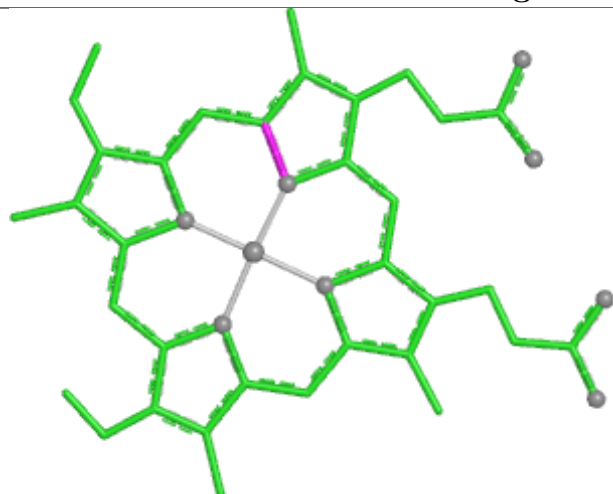


Torsions

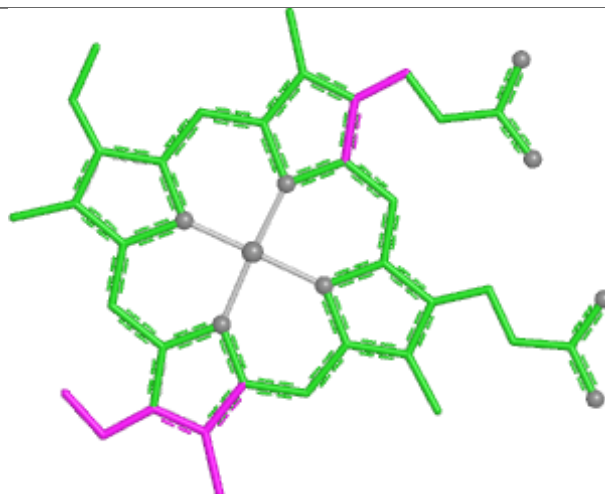


Rings

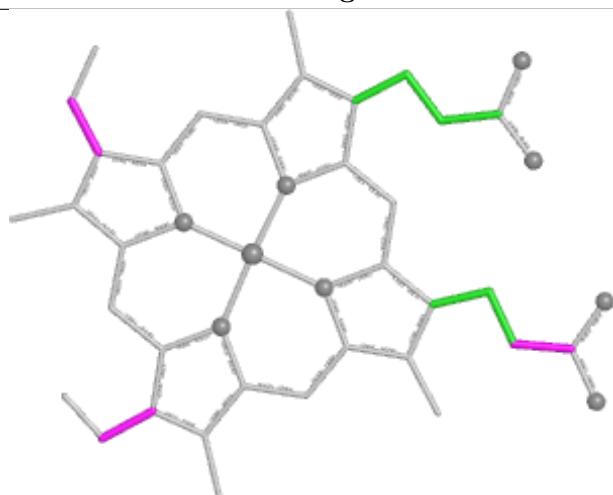
Ligand HEC B 515



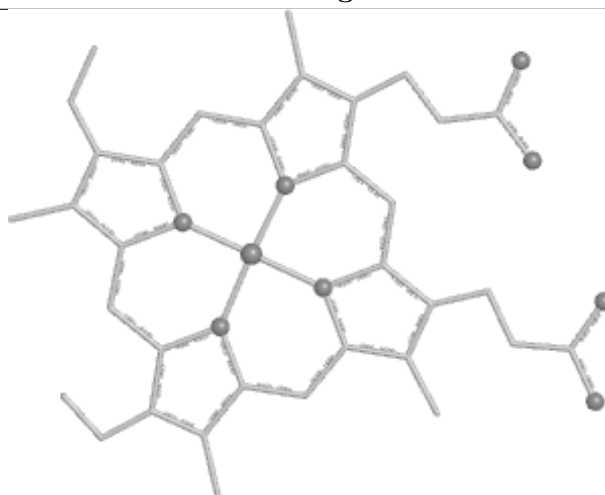
Bond lengths



Bond angles

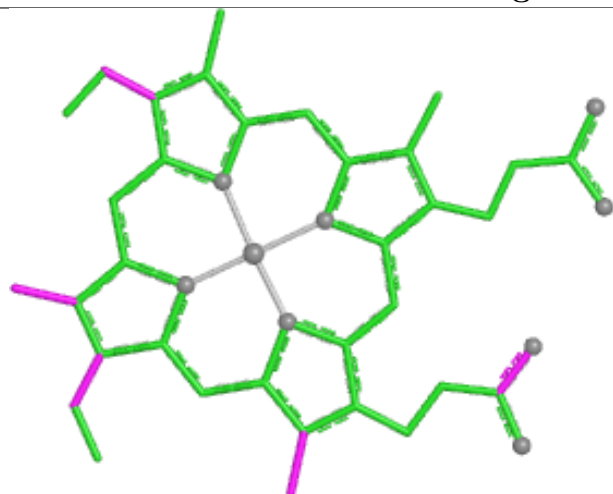


Torsions

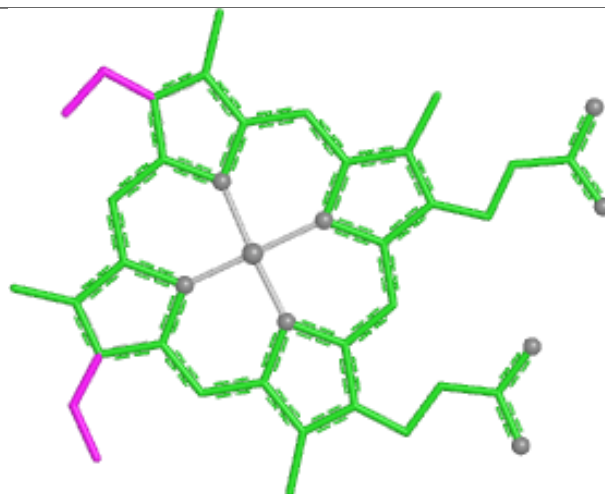


Rings

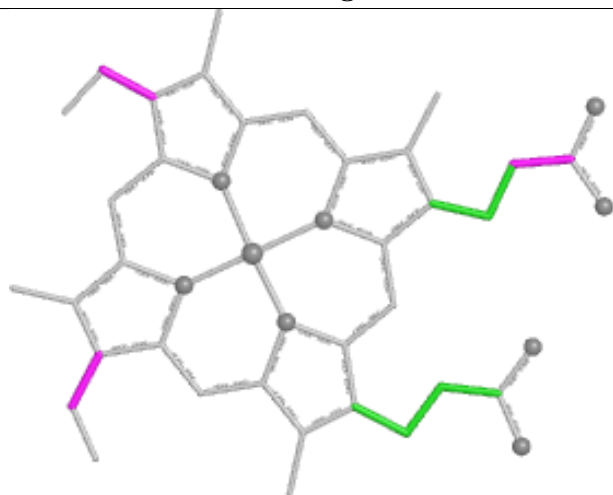
Ligand HEC C 515



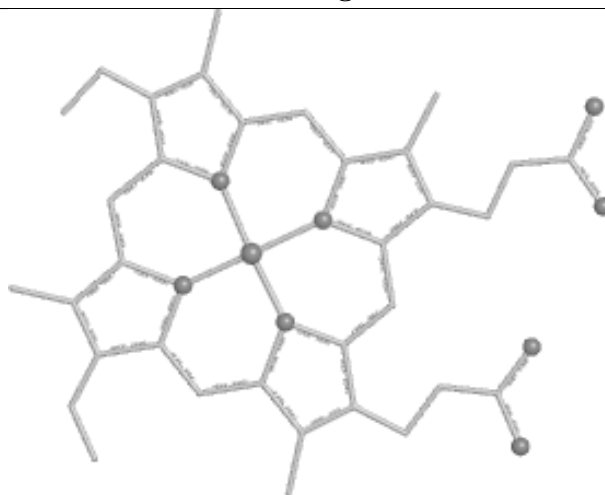
Bond lengths



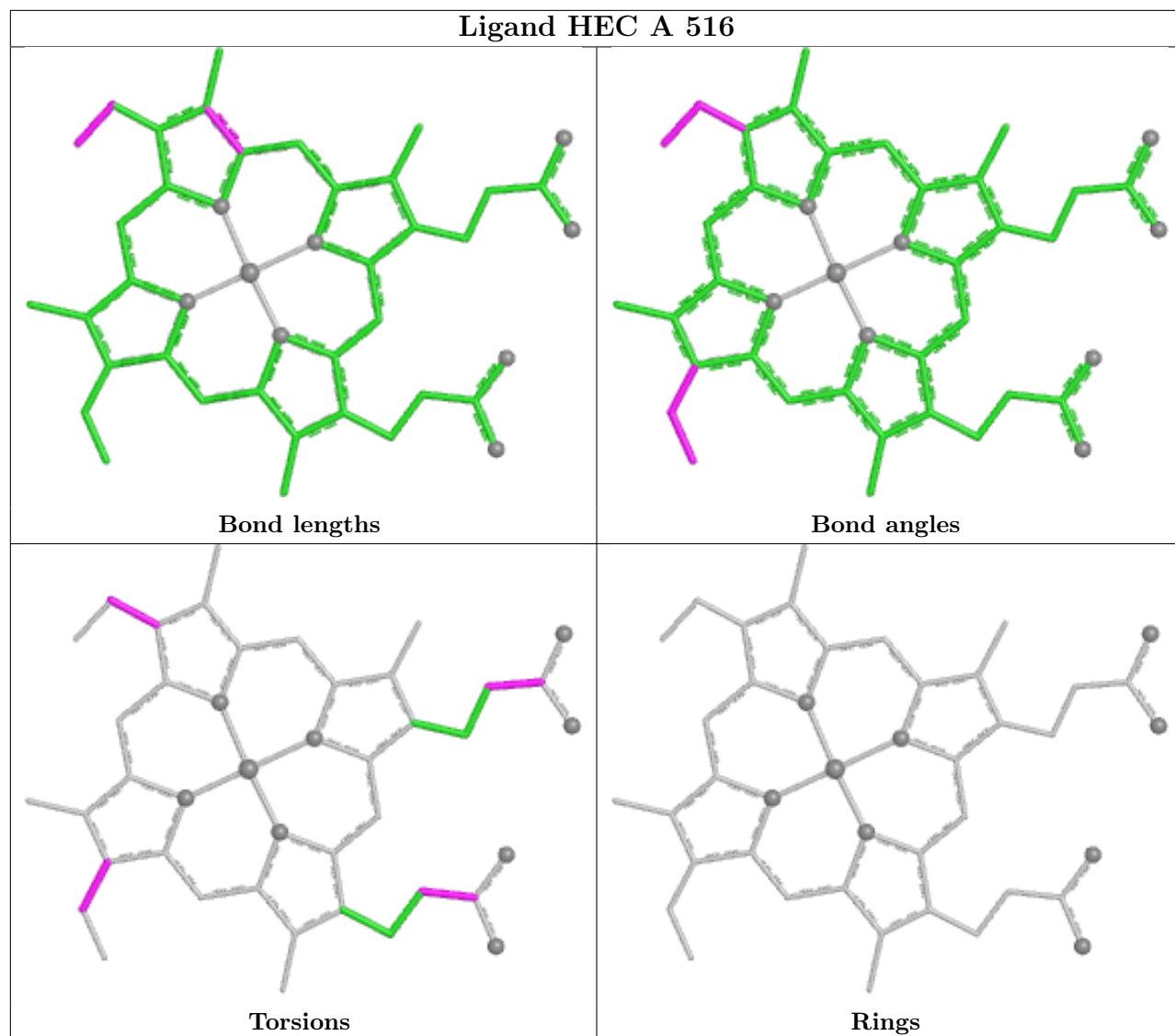
Bond angles



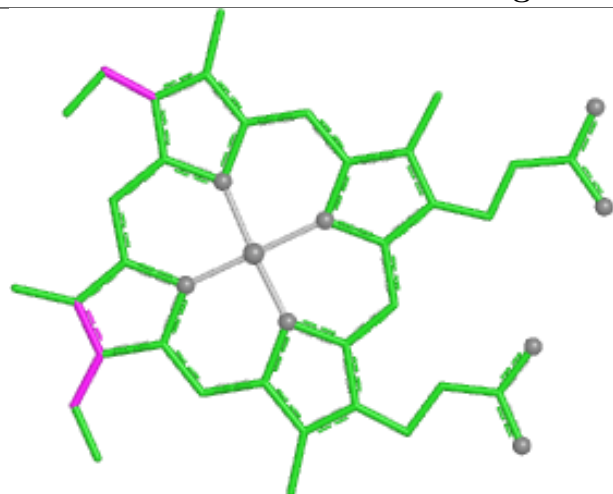
Torsions



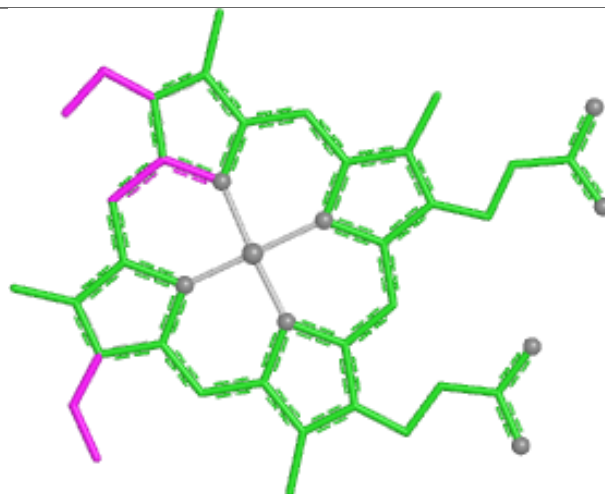
Rings



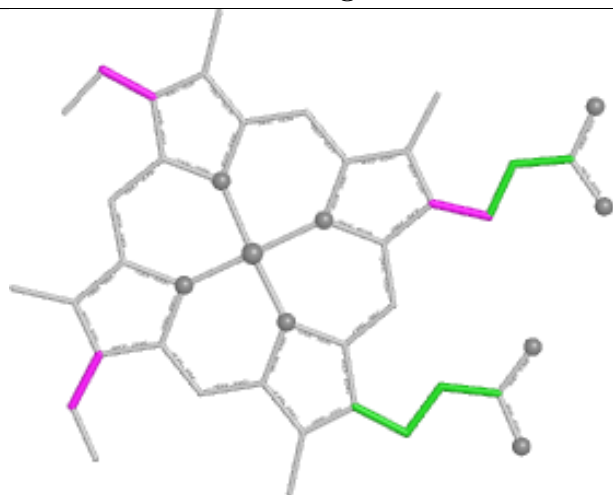
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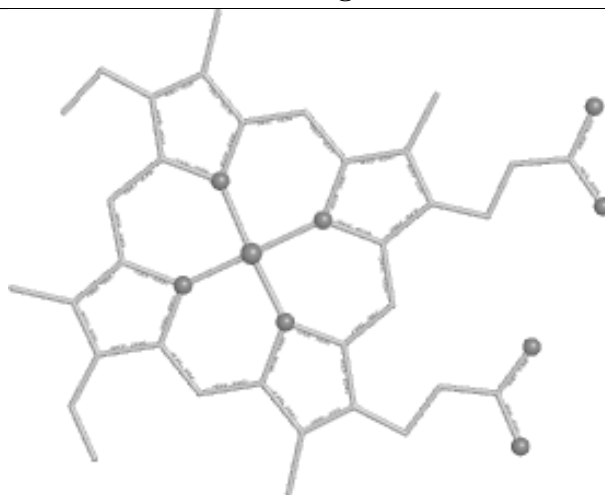
Bond lengths



Bond angles

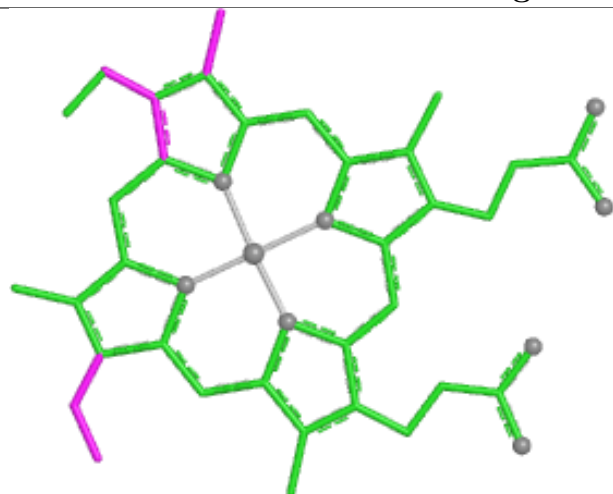


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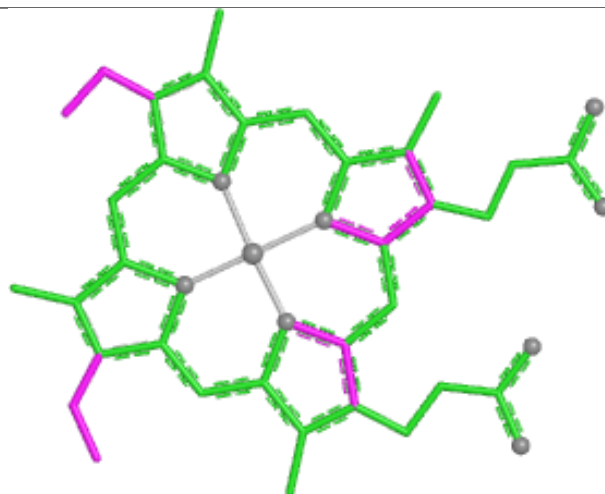


Rings

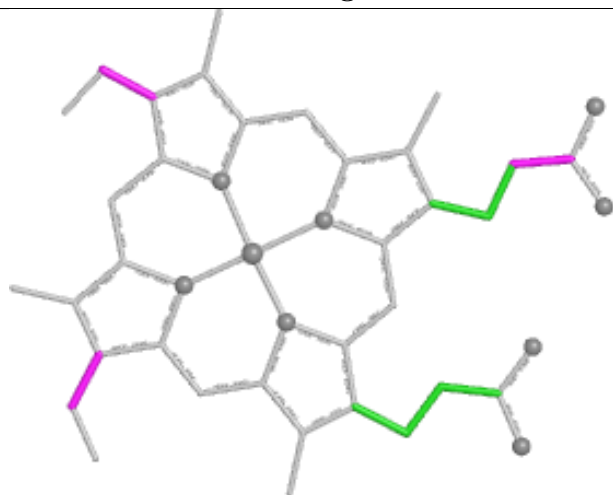
Ligand HEC B 516



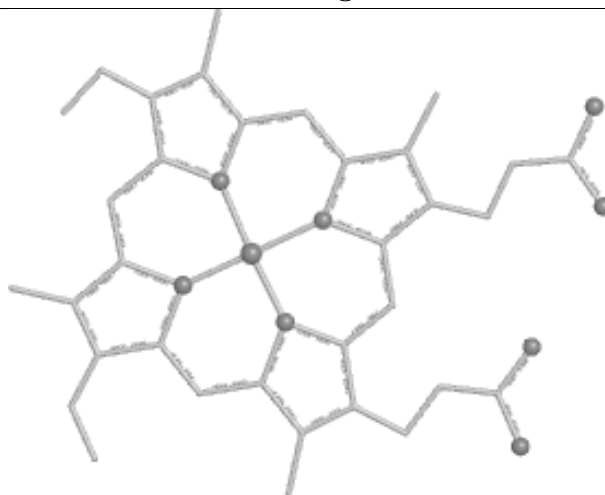
Bond lengths



Bond angles

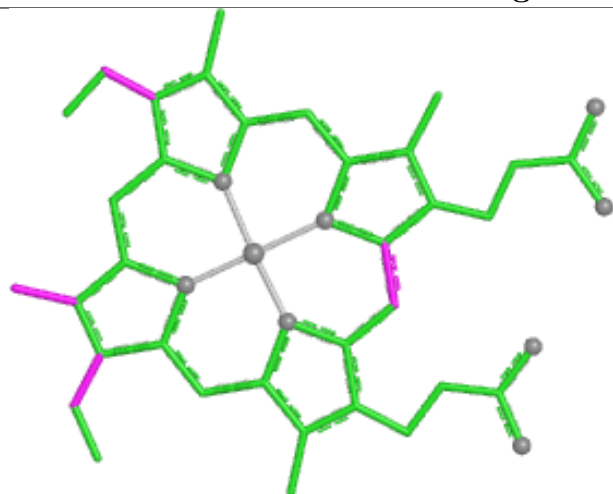


Torsions

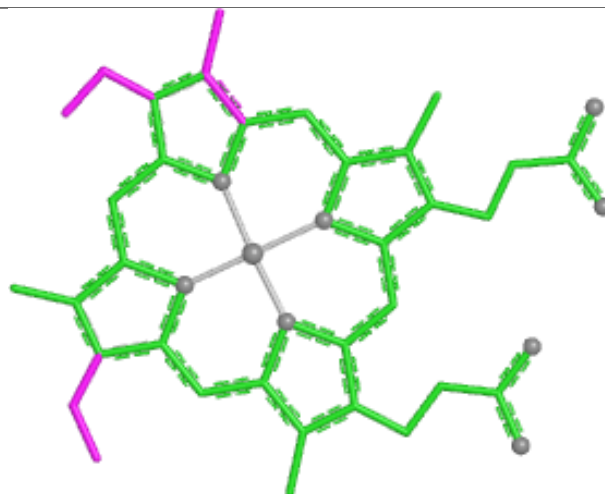


Rings

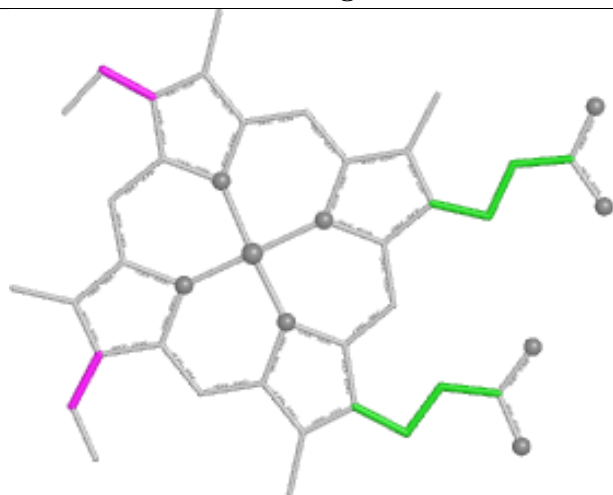
Ligand HEC C 517



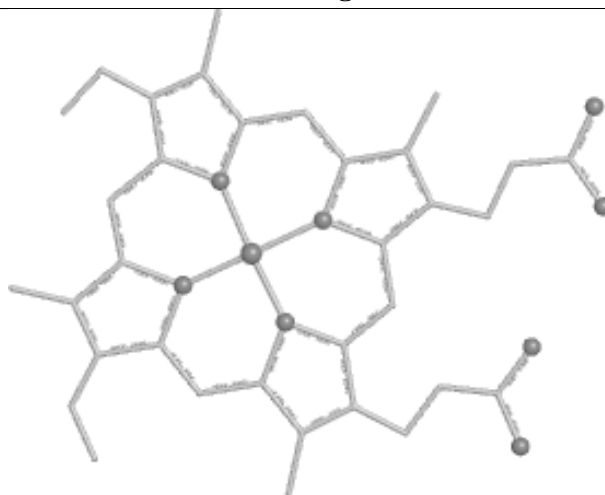
Bond lengths



Bond angles

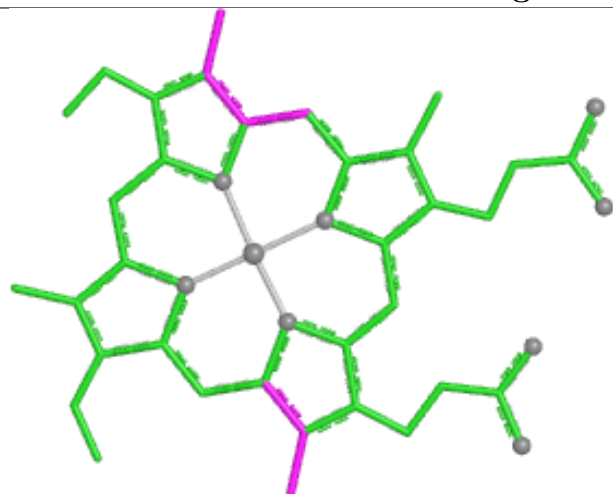


Torsions

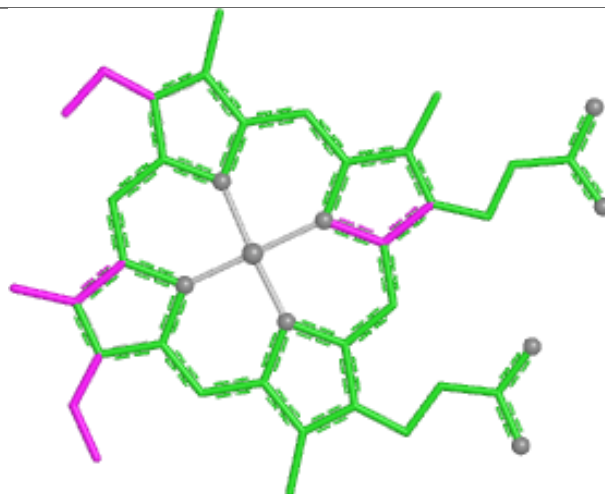


Rings

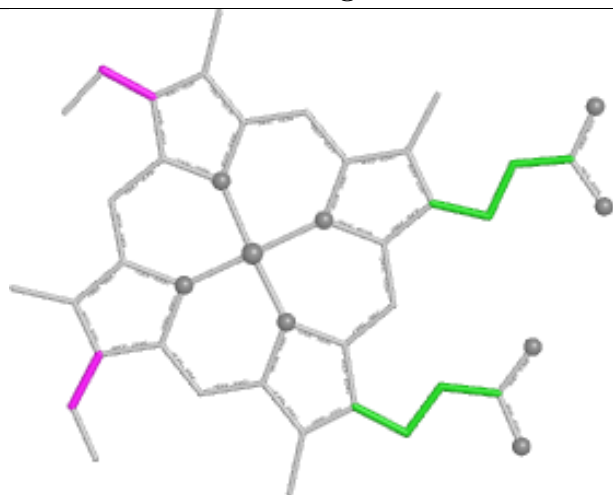
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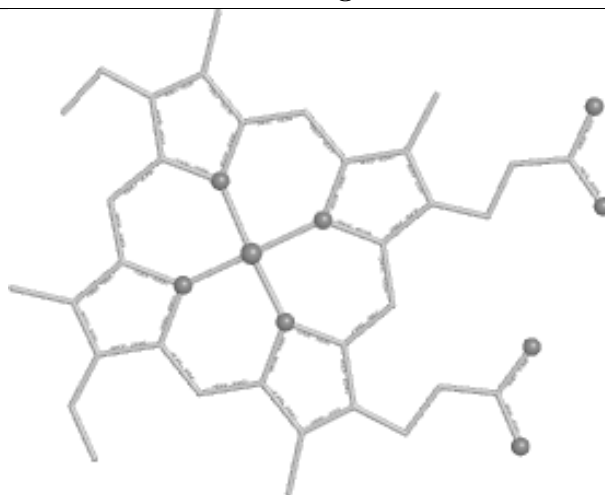
Bond lengths



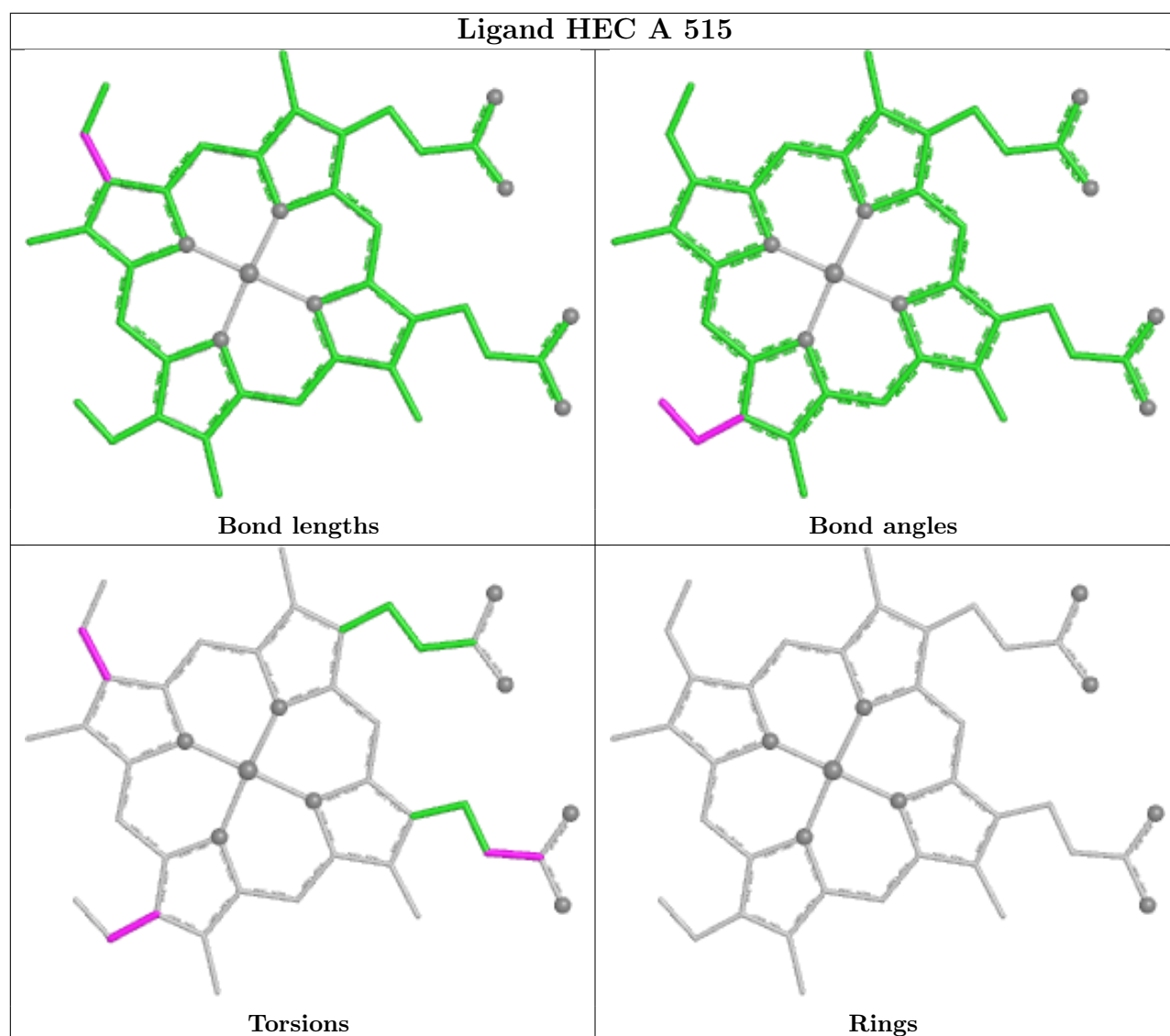
Bond angles

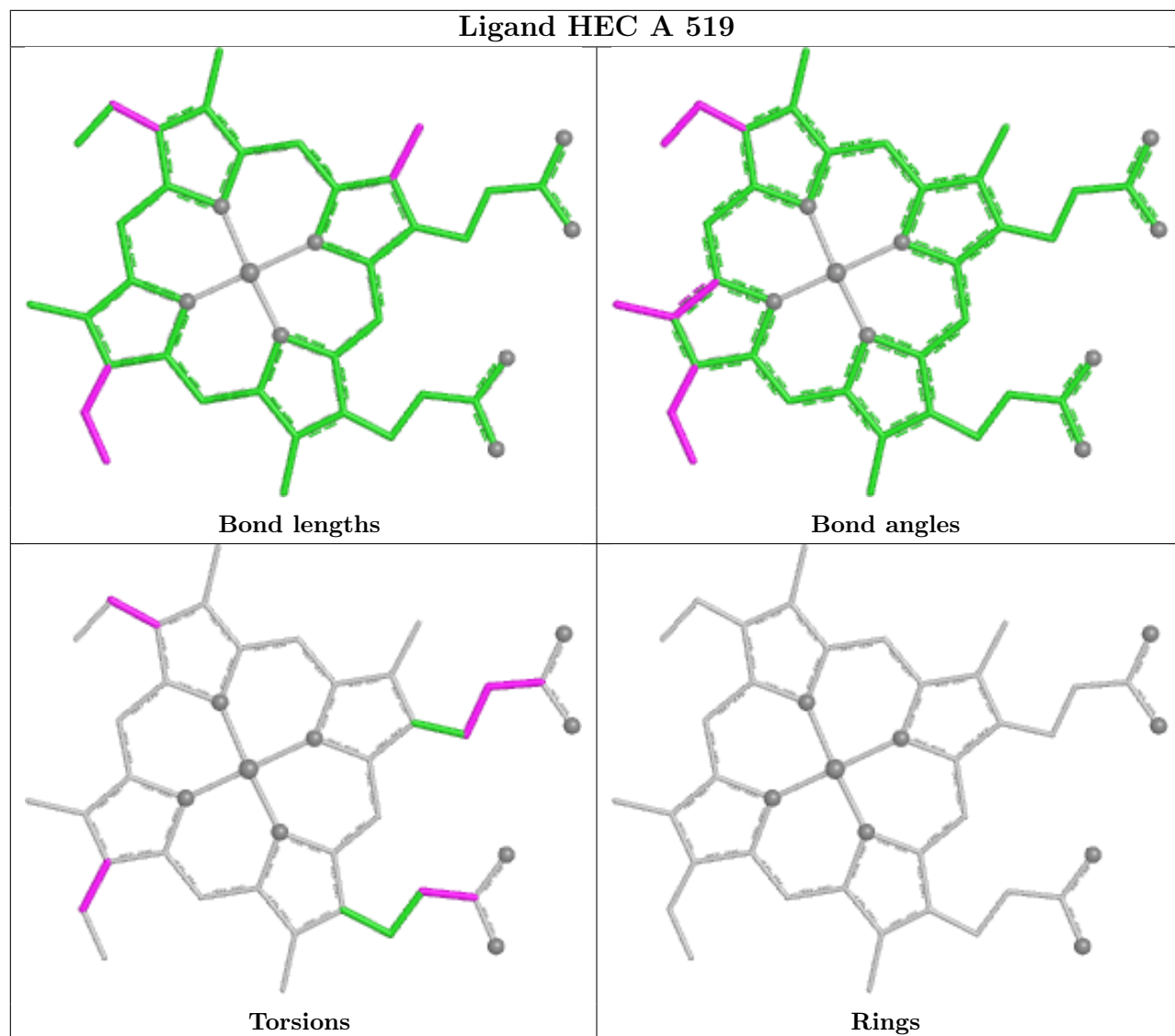


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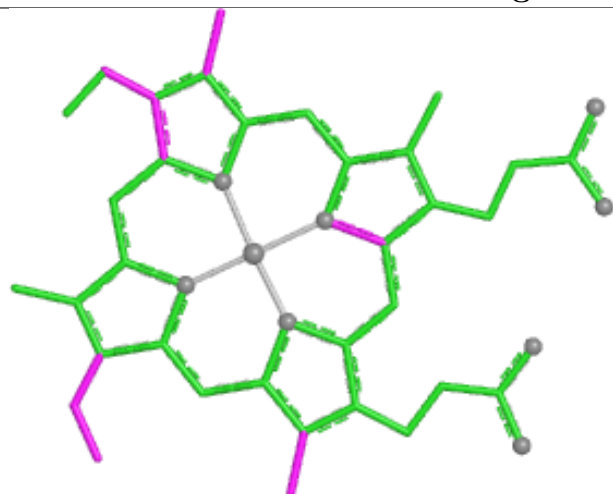


Rings

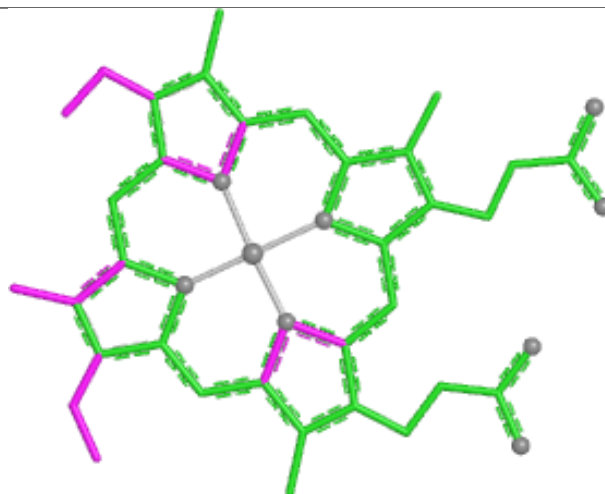




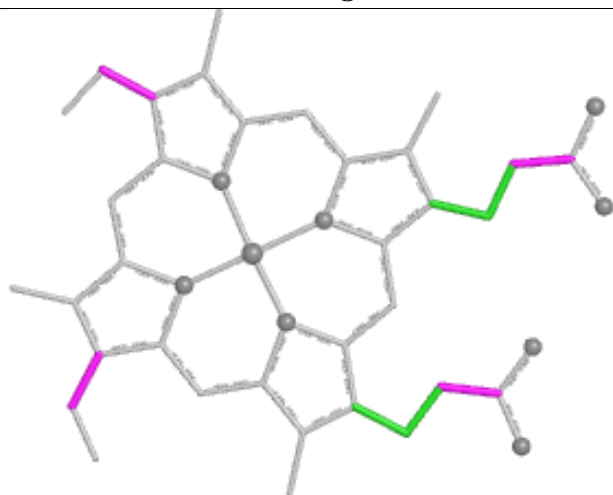
Ligand HEC C 519



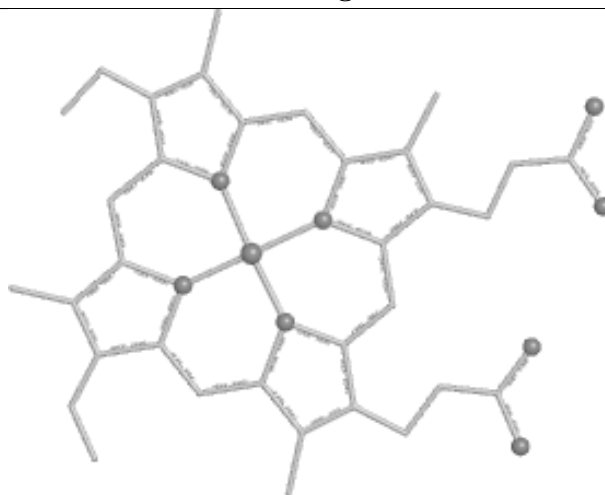
Bond lengths



Bond angles

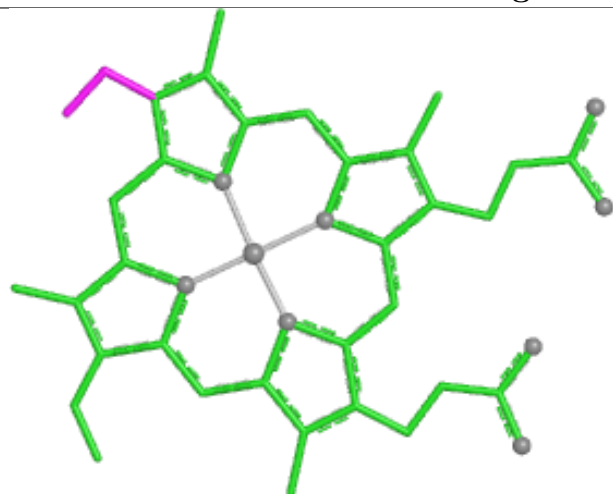


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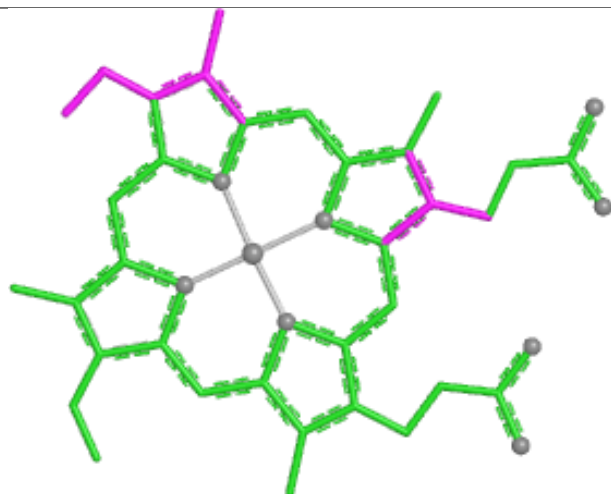


Rings

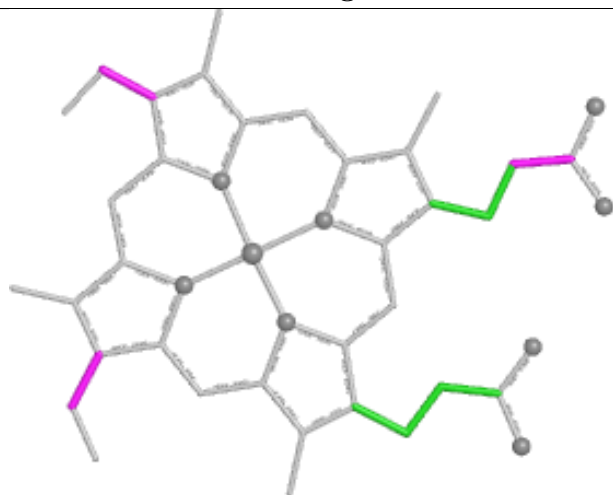
Ligand HEC A 517



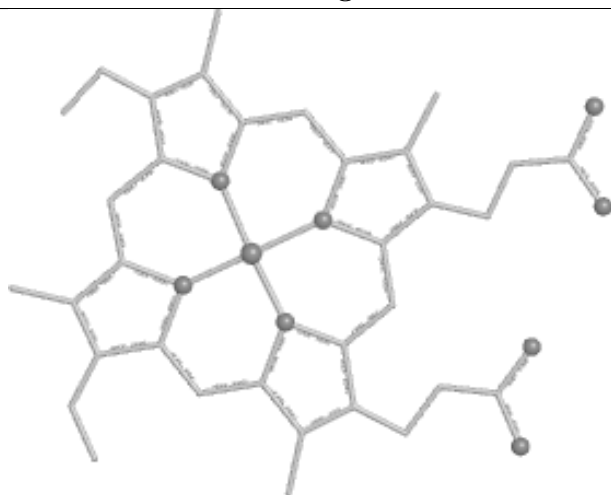
Bond lengths



Bond angles

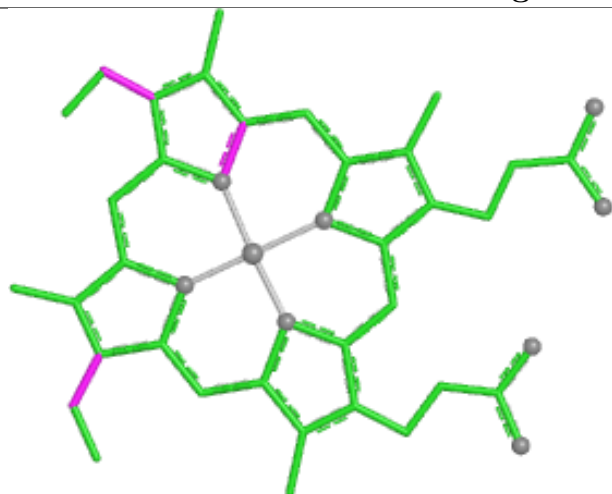


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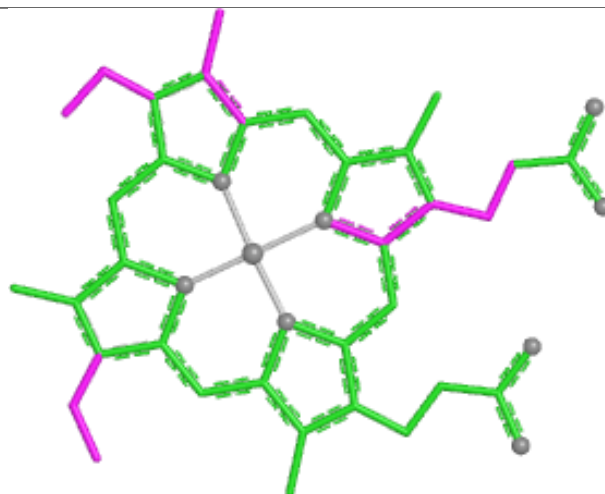


Rings

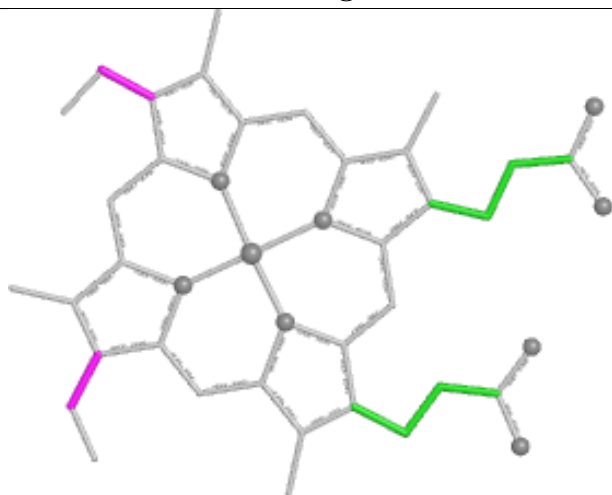
Ligand HEC B 518



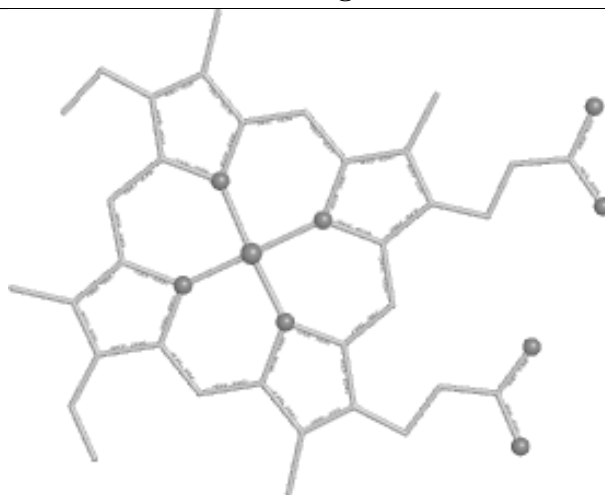
Bond lengths



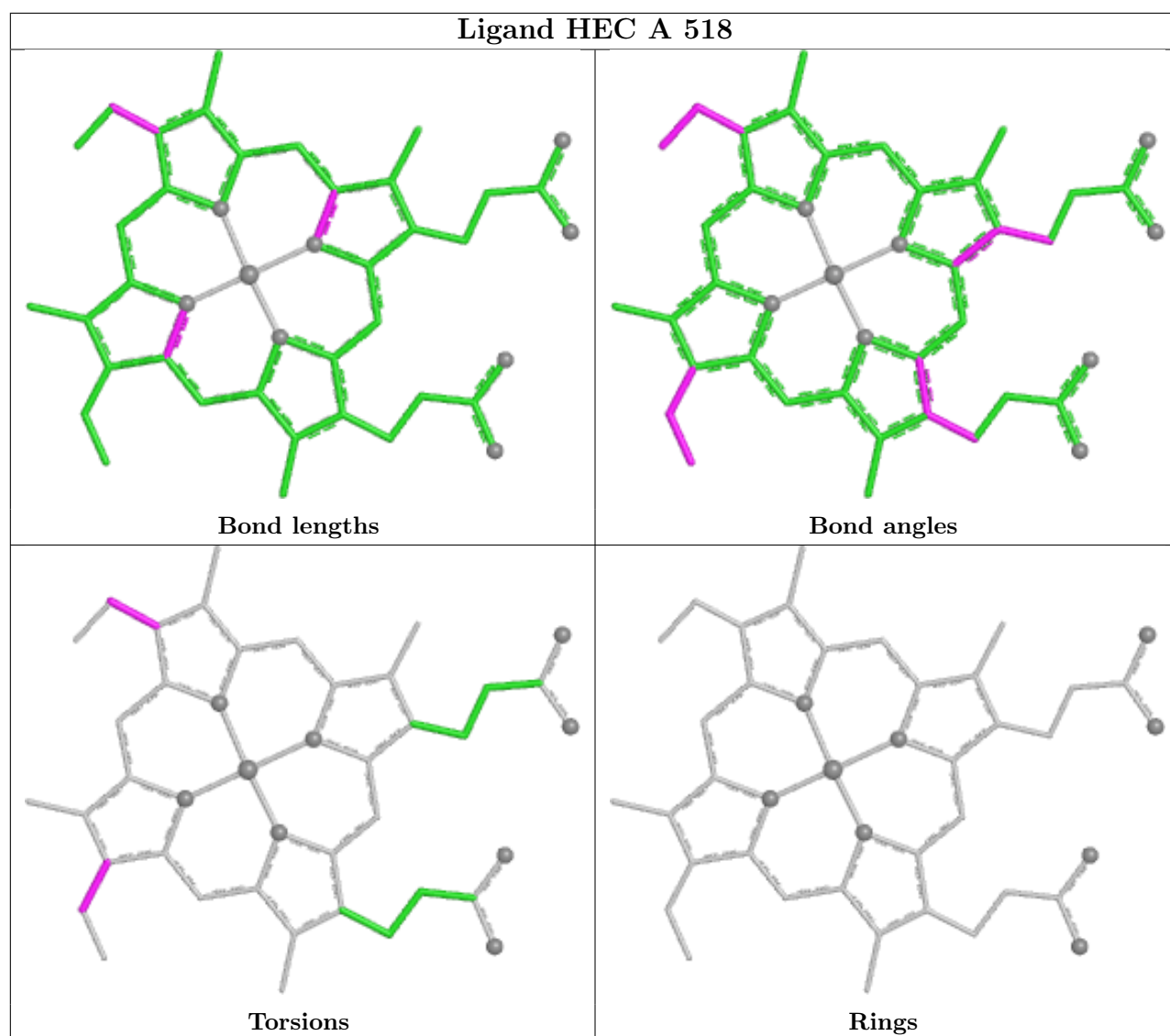
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.