



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 04:55 AM UTC

PDB ID : 6V0A / pdb_00006v0a
Title : Crystal structure of cytochrome c nitrite reductase from the bacterium *Geobacter lovleyi* with bound sulfate
Authors : Satyanarayana, L.; Campecino, J.; Hegg, L.H.; Hu, J.
Deposited on : 2019-11-18
Resolution : 2.55 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

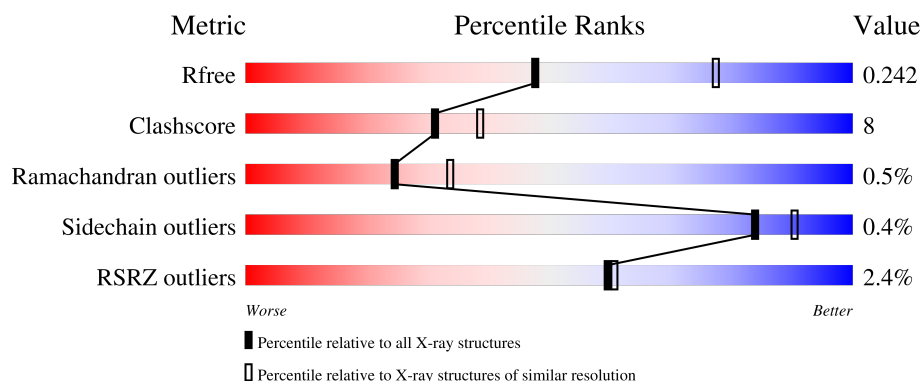
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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

Mol	Chain	Length	Quality of chain
1	A	482	 78% 13% 8%
1	B	482	 80% 12% 8%
1	C	482	 73% 18% 8%
1	D	482	 72% 20% 8%
1	E	482	 74% 18% 8%

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Mol	Chain	Length	Quality of chain
1	F	482	

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
3	SO4	A	506	-	-	X	-
3	SO4	C	506	-	-	X	-

2 Entry composition [i](#)

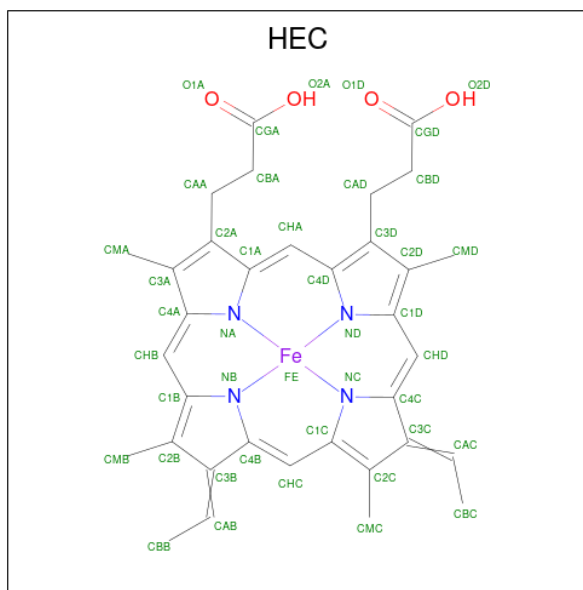
There are 4 unique types of molecules in this entry. The entry contains 23376 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Nitrite reductase (cytochrome; ammonia-forming).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	443	Total	C	N	O	S	0	0	0
			3525	2237	600	661	27			
1	B	444	Total	C	N	O	S	0	0	0
			3538	2245	604	662	27			
1	C	442	Total	C	N	O	S	0	0	0
			3525	2237	601	660	27			
1	D	444	Total	C	N	O	S	0	0	0
			3534	2243	602	662	27			
1	E	443	Total	C	N	O	S	0	0	0
			3525	2237	600	661	27			
1	F	441	Total	C	N	O	S	0	0	0
			3514	2230	598	659	27			

- Molecule 2 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



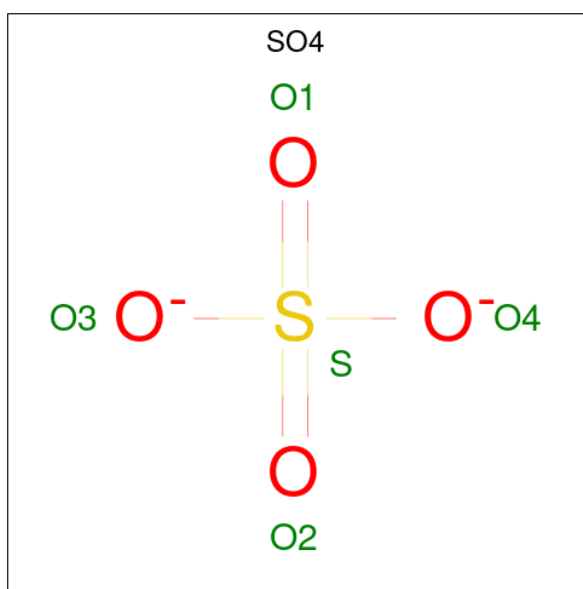
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	E	1	Total	C	Fe	N	O	
			43	34	1	4	4	
2	E	1	Total	C	Fe	N	O	
			43	34	1	4	4	
2	E	1	Total	C	Fe	N	O	
			43	34	1	4	4	
2	F	1	Total	C	Fe	N	O	
			43	34	1	4	4	
2	F	1	Total	C	Fe	N	O	
			43	34	1	4	4	
2	F	1	Total	C	Fe	N	O	
			43	34	1	4	4	
2	F	1	Total	C	Fe	N	O	
			43	34	1	4	4	

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S) (labeled as "Ligand of Interest" by depositor).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		

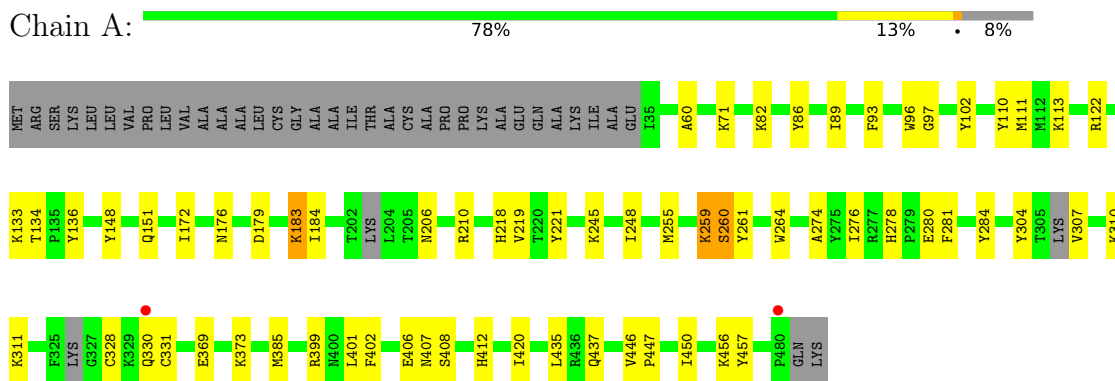
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	215	Total	O	0	0
			215	215		
4	B	236	Total	O	0	0
			236	236		
4	C	148	Total	O	0	0
			148	148		
4	D	134	Total	O	0	0
			134	134		
4	E	92	Total	O	0	0
			92	92		
4	F	70	Total	O	0	0
			70	70		

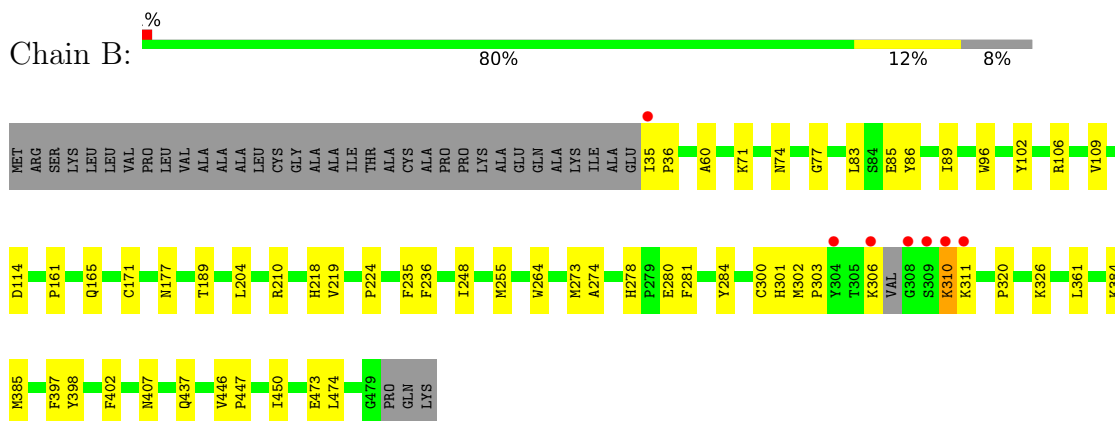
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

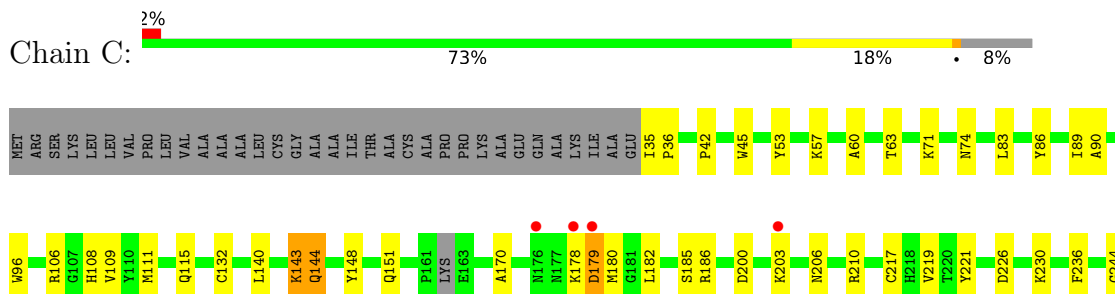
- Molecule 1: Nitrite reductase (cytochrome; ammonia-forming)

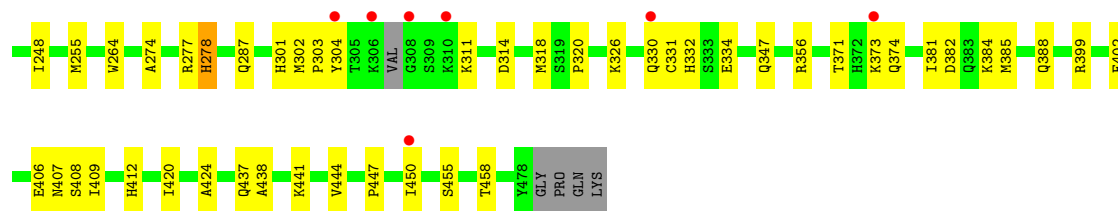


- Molecule 1: Nitrite reductase (cytochrome; ammonia-forming)

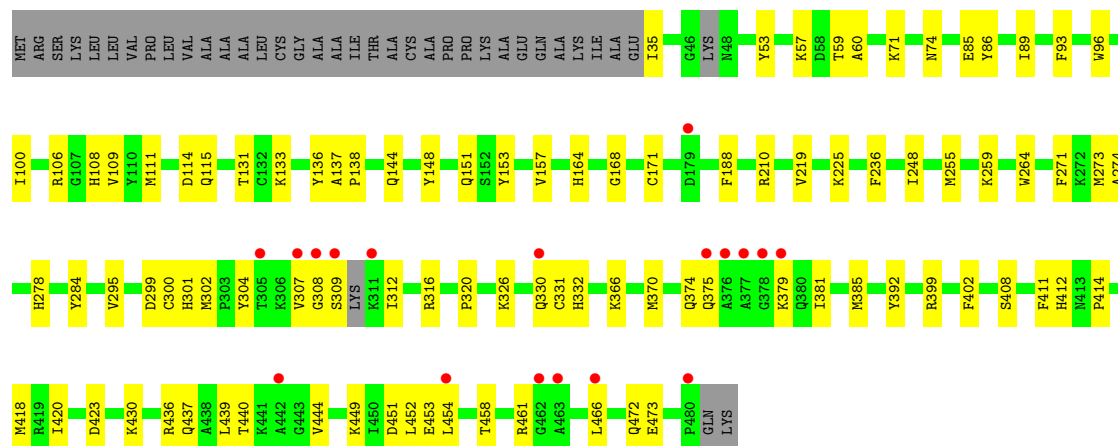


- Molecule 1: Nitrite reductase (cytochrome; ammonia-forming)

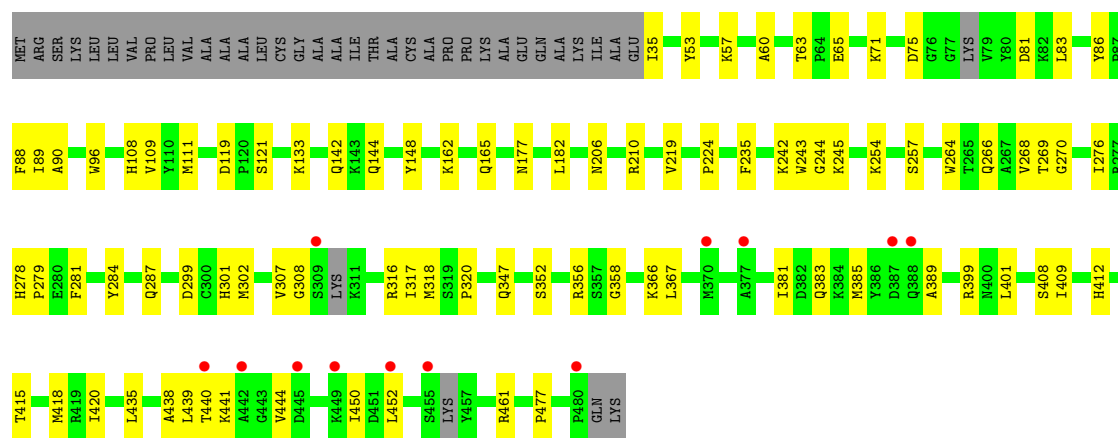
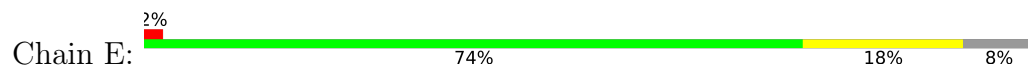




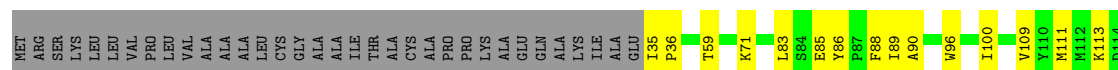
- Molecule 1: Nitrite reductase (cytochrome; ammonia-forming)

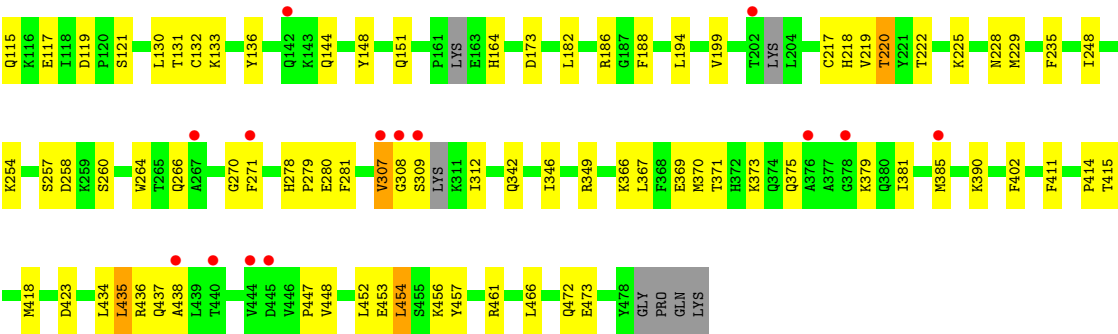


- Molecule 1: Nitrite reductase (cytochrome; ammonia-forming)



- Molecule 1: Nitrite reductase (cytochrome; ammonia-forming)





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	110.86Å 144.62Å 234.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.66 – 2.55 29.66 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.0 (29.66-2.55) 98.9 (29.66-2.55)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 2.54Å)	Xtriage
Refinement program	PHENIX 1.15.1_3469	Depositor
R, R_{free}	0.188 , 0.242 0.190 , 0.242	Depositor DCC
R_{free} test set	6077 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	33.7	Xtriage
Anisotropy	0.322	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	23376	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.45	1/3610 (0.0%)	0.62	1/4861 (0.0%)
1	B	0.45	1/3624 (0.0%)	0.64	2/4878 (0.0%)
1	C	0.43	0/3610	0.66	2/4859 (0.0%)
1	D	0.39	0/3620	0.59	0/4875
1	E	0.41	1/3610 (0.0%)	0.58	0/4861
1	F	0.36	0/3598	0.57	0/4844
All	All	0.42	3/21672 (0.0%)	0.61	5/29178 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	279	PRO	CA-CB	-9.85	1.47	1.53
1	A	446	VAL	CA-C	8.08	1.59	1.53
1	B	446	VAL	CA-C	-7.77	1.46	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	446	VAL	O-C-N	6.14	126.25	121.46
1	B	446	VAL	O-C-N	-5.23	117.38	121.46
1	C	373	LYS	CG-CD-CE	-5.22	99.28	111.30
1	C	226	ASP	CA-CB-CG	5.15	117.75	112.60
1	B	310	LYS	CG-CD-CE	-5.07	99.64	111.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3525	0	3433	47	0
1	B	3538	0	3457	36	0
1	C	3525	0	3440	58	0
1	D	3534	0	3448	73	0
1	E	3525	0	3432	66	0
1	F	3514	0	3422	67	0
2	A	215	0	151	13	0
2	B	215	0	150	10	0
2	C	215	0	150	4	0
2	D	215	0	151	14	0
2	E	215	0	150	10	0
2	F	215	0	150	8	0
3	A	5	0	0	2	0
3	B	5	0	0	0	0
3	C	5	0	0	2	0
3	D	5	0	0	0	0
3	E	5	0	0	0	0
3	F	5	0	0	0	0
4	A	215	0	0	3	0
4	B	236	0	0	0	0
4	C	148	0	0	1	0
4	D	134	0	0	4	0
4	E	92	0	0	4	0
4	F	70	0	0	3	0
All	All	23376	0	21534	359	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 8.

All (359) 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:331:CYS:SG	2:A:505:HEC:CAC	2.30	1.19
1:D:331:CYS:SG	2:D:505:HEC:CAC	2.41	1.07
1:A:331:CYS:SG	2:A:505:HEC:HAC	2.09	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:242:LYS:HD2	1:E:243:TRP:H	1.41	0.84
2:E:505:HEC:HBA2	2:F:505:HEC:HBA2	1.60	0.82
1:F:194:LEU:HB3	1:F:199:VAL:HG11	1.61	0.80
1:E:111:MET:HG2	1:E:133:LYS:HG2	1.65	0.76
1:F:136:TYR:HH	1:F:164:HIS:HD1	1.33	0.76
1:F:111:MET:HE2	1:F:133:LYS:HA	1.67	0.75
1:C:330:GLN:OE1	1:C:331:CYS:SG	2.45	0.75
1:A:122:ARG:NH2	3:A:506:SO4:O1	2.20	0.74
1:D:300:CYS:SG	2:D:504:HEC:CAC	2.76	0.74
1:C:230:LYS:NZ	4:C:601:HOH:O	2.20	0.73
1:C:384:LYS:O	1:C:384:LYS:HG2	1.82	0.73
1:A:331:CYS:SG	2:A:505:HEC:CBC	2.77	0.72
2:A:505:HEC:HBA2	2:B:505:HEC:HBA2	1.71	0.70
1:F:35:ILE:N	4:F:601:HOH:O	2.24	0.70
1:E:383:GLN:NE2	4:E:601:HOH:O	2.24	0.70
1:D:461:ARG:HB2	1:D:466:LEU:HB2	1.75	0.69
1:F:85:GLU:HA	1:F:473:GLU:HA	1.74	0.69
1:C:437:GLN:HG3	1:D:440:THR:HG21	1.75	0.68
1:C:385:MET:HE3	1:C:438:ALA:HB2	1.75	0.68
1:A:245:LYS:NZ	4:A:601:HOH:O	2.27	0.68
1:E:53:TYR:O	1:E:57:LYS:HG3	1.93	0.68
1:D:210:ARG:NH1	1:D:299:ASP:OD1	2.27	0.68
1:D:385:MET:HE1	1:D:437:GLN:HB3	1.76	0.68
1:D:53:TYR:CE2	1:D:57:LYS:HE2	2.29	0.67
1:B:35:ILE:O	1:B:177:ASN:ND2	2.28	0.66
1:C:45:TRP:CZ3	1:C:180:MET:HE1	2.30	0.66
1:D:35:ILE:N	4:D:603:HOH:O	2.28	0.66
1:D:106:ARG:HD3	1:D:114:ASP:OD2	1.96	0.65
1:F:228:ASN:ND2	4:F:602:HOH:O	2.30	0.65
1:E:302:MET:HE2	1:E:317:ILE:HD11	1.80	0.64
1:E:144:GLN:HB2	1:E:148:TYR:HB2	1.80	0.63
1:E:65:GLU:HG2	1:E:75:ASP:HB3	1.80	0.63
1:C:83:LEU:HD23	1:C:90:ALA:HA	1.79	0.63
1:E:441:LYS:O	1:E:441:LYS:HG2	1.97	0.62
1:C:455:SER:HA	1:C:458:THR:HG22	1.80	0.62
1:E:385:MET:HE2	1:E:438:ALA:HB2	1.82	0.62
1:B:60:ALA:HB2	1:B:109:VAL:HG21	1.82	0.61
1:E:367:LEU:HD11	1:E:450:ILE:HG12	1.81	0.61
1:D:331:CYS:O	1:D:332:HIS:ND1	2.33	0.61
1:D:86:TYR:O	1:D:89:ILE:HG12	2.01	0.60
1:E:415:THR:HG21	1:F:346:ILE:HG12	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:306:LYS:HD2	1:B:311:LYS:HD3	1.82	0.60
1:E:366:LYS:NZ	1:E:452:LEU:O	2.34	0.60
1:D:106:ARG:O	2:D:503:HEC:HBA2	2.02	0.60
1:C:406:GLU:OE1	1:C:408:SER:HB3	2.02	0.60
1:D:331:CYS:SG	2:D:505:HEC:HAC	2.36	0.60
1:F:218:HIS:HB3	1:F:280:GLU:HB2	1.84	0.59
1:C:182:LEU:HD11	2:C:502:HEC:HBD1	1.83	0.59
1:F:381:ILE:HG23	1:F:438:ALA:HB1	1.83	0.59
1:F:436:ARG:NH2	1:F:447:PRO:O	2.35	0.58
2:F:504:HEC:HMB3	2:F:504:HEC:HBB3	1.85	0.58
1:C:221:TYR:OH	3:C:506:SO4:O2	2.20	0.58
1:E:35:ILE:N	4:E:604:HOH:O	2.36	0.58
1:C:303:PRO:HD2	1:C:314:ASP:HB3	1.86	0.58
1:C:356:ARG:NH1	1:D:423:ASP:OD1	2.37	0.57
1:A:276:ILE:H	1:A:401:LEU:HD21	1.70	0.57
1:A:210:ARG:NH2	4:A:606:HOH:O	2.38	0.57
1:D:330:GLN:O	1:D:330:GLN:HG2	2.04	0.56
1:A:113:LYS:NZ	4:A:605:HOH:O	2.38	0.56
1:F:366:LYS:HD2	1:F:452:LEU:HA	1.87	0.56
1:C:132:CYS:HB3	1:C:217:CYS:HB3	1.87	0.56
1:D:85:GLU:HA	1:D:473:GLU:HA	1.88	0.56
1:B:385:MET:HE1	1:B:437:GLN:HG2	1.88	0.55
1:E:352:SER:HB2	1:E:477:PRO:HD2	1.88	0.55
1:F:436:ARG:NH2	1:F:448:VAL:HA	2.21	0.55
1:D:111:MET:HG3	1:D:133:LYS:HD3	1.88	0.55
1:D:331:CYS:SG	2:D:505:HEC:C3C	2.95	0.54
1:E:83:LEU:HD23	1:E:89:ILE:HG13	1.90	0.54
1:E:381:ILE:HG23	1:E:438:ALA:HB1	1.90	0.54
1:F:222:THR:HB	1:F:235:PHE:CE1	2.42	0.54
1:D:304:TYR:O	1:D:326:LYS:NZ	2.41	0.54
1:D:451:ASP:OD2	1:D:453:GLU:HG2	2.06	0.54
2:A:503:HEC:HBC3	2:A:503:HEC:HMC3	1.89	0.54
1:C:332:HIS:HB3	1:C:334:GLU:OE2	2.07	0.54
1:F:461:ARG:HB2	1:F:466:LEU:HB2	1.90	0.54
1:C:63:THR:HG22	1:C:318:MET:CE	2.37	0.54
1:D:331:CYS:SG	2:D:505:HEC:CBC	2.96	0.53
2:E:505:HEC:CBA	2:F:505:HEC:HBA2	2.37	0.53
1:F:258:ASP:OD1	1:F:260:SER:OG	2.20	0.53
1:A:96:TRP:CE3	1:A:264:TRP:HB3	2.44	0.53
1:C:255:MET:HE3	1:C:274:ALA:HB3	1.90	0.53
1:B:96:TRP:CE3	1:B:264:TRP:HB3	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:182:LEU:HD11	2:E:502:HEC:HBD1	1.91	0.52
1:C:408:SER:HB2	1:C:412:HIS:CE1	2.45	0.52
1:D:411:PHE:CD2	2:D:504:HEC:HMD2	2.44	0.52
1:E:96:TRP:CE3	1:E:264:TRP:HB3	2.45	0.52
1:E:302:MET:CE	2:E:503:HEC:HBB2	2.39	0.52
1:C:115:GLN:HE21	2:C:501:HEC:C1B	2.23	0.52
1:C:347:GLN:HG2	1:C:409:ILE:HB	1.91	0.52
1:C:371:THR:HG23	1:C:381:ILE:HD13	1.91	0.52
1:D:375:GLN:NE2	4:D:614:HOH:O	2.43	0.51
2:A:505:HEC:HBA2	2:B:505:HEC:CBA	2.38	0.51
1:B:407:ASN:HB3	2:B:504:HEC:CAA	2.41	0.51
1:A:385:MET:HE1	1:A:437:GLN:HB3	1.92	0.51
1:C:140:LEU:O	1:C:144:GLN:HB2	2.11	0.51
1:E:268:VAL:HG23	1:E:269:THR:HG23	1.93	0.51
1:D:259:LYS:H	1:D:259:LYS:HD2	1.74	0.51
1:C:45:TRP:CE3	1:C:180:MET:HE1	2.44	0.51
1:E:86:TYR:O	1:E:89:ILE:HG12	2.10	0.51
1:A:259:LYS:O	1:A:261:TYR:N	2.44	0.50
1:C:74:ASN:HB2	1:C:106:ARG:HG3	1.93	0.50
1:F:385:MET:HE1	1:F:437:GLN:HG2	1.93	0.50
1:B:85:GLU:HA	1:B:473:GLU:HA	1.93	0.50
1:B:361:LEU:HD13	1:B:397:PHE:HA	1.93	0.50
1:D:53:TYR:O	1:D:57:LYS:HG3	2.12	0.50
1:D:307:VAL:O	1:D:309:SER:N	2.44	0.50
1:F:436:ARG:HH22	1:F:448:VAL:HA	1.76	0.50
1:A:86:TYR:O	1:A:89:ILE:HG12	2.11	0.49
1:F:136:TYR:OH	1:F:164:HIS:ND1	2.26	0.49
2:A:505:HEC:HMC3	2:A:505:HEC:HBC3	1.94	0.49
1:D:225:LYS:NZ	4:D:609:HOH:O	2.38	0.49
1:E:347:GLN:HG2	1:E:409:ILE:HB	1.94	0.49
1:C:86:TYR:O	1:C:89:ILE:HG12	2.13	0.49
1:C:304:TYR:CD2	1:C:311:LYS:HE3	2.47	0.49
1:A:447:PRO:HG2	1:A:450:ILE:HD13	1.94	0.49
1:A:221:TYR:OH	3:A:506:SO4:O4	2.21	0.49
1:D:379:LYS:HE3	1:D:444:VAL:HG22	1.95	0.49
1:F:194:LEU:HB3	1:F:199:VAL:CG1	2.38	0.49
1:F:367:LEU:HB3	1:F:435:LEU:CD2	2.42	0.49
1:D:144:GLN:HB2	1:D:148:TYR:HB2	1.95	0.49
1:E:63:THR:HG22	1:E:318:MET:HE2	1.93	0.49
1:F:367:LEU:HB3	1:F:435:LEU:HD23	1.93	0.49
1:E:242:LYS:NZ	1:E:243:TRP:HB3	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:306:LYS:HE3	1:B:310:LYS:C	2.38	0.48
1:B:86:TYR:O	1:B:89:ILE:HG12	2.12	0.48
1:E:301:HIS:CE1	1:E:320:PRO:HD3	2.48	0.48
1:D:100:ILE:O	1:D:466:LEU:HD12	2.12	0.48
1:E:244:GLY:O	1:E:287:GLN:NE2	2.36	0.48
1:A:176:ASN:ND2	1:A:179:ASP:OD1	2.37	0.48
1:A:97:GLY:HA3	1:A:122:ARG:HG3	1.96	0.48
1:A:331:CYS:HG	2:A:505:HEC:CAC	2.23	0.48
1:B:302:MET:HE2	2:B:503:HEC:HBB2	1.95	0.48
1:C:60:ALA:HB2	1:C:109:VAL:HG21	1.96	0.48
1:E:177:ASN:OD1	1:E:177:ASN:N	2.47	0.48
1:B:284:TYR:CZ	2:B:504:HEC:HMC2	2.49	0.48
1:A:134:THR:HG22	1:A:136:TYR:H	1.78	0.48
1:E:219:VAL:HG12	1:E:281:PHE:HB3	1.96	0.47
1:A:219:VAL:HG12	1:A:281:PHE:HB3	1.97	0.47
1:B:301:HIS:CE1	1:B:320:PRO:HD3	2.49	0.47
1:E:367:LEU:HB3	1:E:435:LEU:HD23	1.95	0.47
2:B:504:HEC:HBC1	2:B:505:HEC:CHC	2.45	0.47
1:E:81:ASP:OD2	1:E:461:ARG:NH2	2.44	0.47
1:E:367:LEU:HB3	1:E:435:LEU:CD2	2.44	0.47
1:A:399:ARG:HG2	1:A:420:ILE:HG23	1.95	0.47
1:B:218:HIS:HB3	1:B:280:GLU:HB2	1.95	0.47
1:C:302:MET:HG2	1:C:314:ASP:O	2.14	0.47
1:D:375:GLN:HG3	1:D:381:ILE:HD13	1.97	0.47
1:E:307:VAL:HG12	1:E:307:VAL:O	2.15	0.47
1:F:83:LEU:HD23	1:F:90:ALA:HA	1.97	0.47
1:A:89:ILE:HB	1:A:93:PHE:CE2	2.49	0.47
1:A:304:TYR:HB2	1:A:311:LYS:HG3	1.97	0.47
1:D:148:TYR:HA	1:D:151:GLN:HE21	1.78	0.47
1:A:456:LYS:HE3	1:A:457:TYR:CZ	2.50	0.47
2:E:501:HEC:C4D	2:E:503:HEC:HMD2	2.45	0.47
1:C:96:TRP:CE3	1:C:264:TRP:HB3	2.49	0.47
1:A:71:LYS:HA	1:A:71:LYS:HD2	1.65	0.47
1:C:248:ILE:HD13	1:C:402:PHE:CD1	2.50	0.47
1:D:436:ARG:O	1:D:440:THR:HG23	2.15	0.47
1:C:301:HIS:CE1	1:C:320:PRO:HD3	2.49	0.47
1:D:153:TYR:O	1:D:157:VAL:HG23	2.15	0.47
1:D:259:LYS:HD2	1:D:259:LYS:N	2.29	0.47
1:D:414:PRO:O	1:D:418:MET:HG2	2.15	0.47
1:E:284:TYR:CZ	2:E:504:HEC:HMC2	2.49	0.46
1:F:144:GLN:HB2	1:F:148:TYR:HB2	1.95	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:454:LEU:HA	1:F:457:TYR:HD1	1.81	0.46
1:A:71:LYS:HE2	1:A:407:ASN:O	2.15	0.46
1:D:284:TYR:CZ	2:D:504:HEC:HMC1	2.50	0.46
1:C:206:ASN:O	1:C:210:ARG:HG3	2.16	0.46
1:E:242:LYS:HZ2	1:E:243:TRP:HB3	1.78	0.46
1:C:382:ASP:HB2	1:C:441:LYS:HZ3	1.79	0.46
1:F:182:LEU:HD11	2:F:502:HEC:HBD1	1.98	0.46
1:F:271:PHE:CZ	1:F:390:LYS:HD2	2.50	0.46
1:A:111:MET:HG3	1:A:133:LYS:HD3	1.98	0.46
1:C:42:PRO:HG3	1:C:170:ALA:HB1	1.98	0.46
1:C:374:GLN:HG3	1:C:444:VAL:HG21	1.98	0.46
1:A:259:LYS:O	1:A:260:SER:C	2.58	0.46
1:F:86:TYR:HB3	1:F:88:PHE:CZ	2.51	0.46
1:F:115:GLN:HE21	2:F:501:HEC:C1B	2.28	0.46
1:C:185:SER:OG	1:C:186:ARG:NH1	2.46	0.45
1:D:60:ALA:HB2	1:D:109:VAL:HG21	1.98	0.45
1:D:96:TRP:O	1:D:100:ILE:HD12	2.16	0.45
1:D:271:PHE:HB3	1:D:273:MET:HE3	1.98	0.45
1:F:119:ASP:OD1	1:F:121:SER:OG	2.25	0.45
1:A:259:LYS:HA	1:A:259:LYS:HD3	1.54	0.45
1:D:399:ARG:HG2	1:D:420:ILE:HG23	1.98	0.45
1:E:415:THR:HB	1:F:349:ARG:HD2	1.99	0.45
1:A:111:MET:CG	1:A:133:LYS:HD3	2.46	0.45
1:A:307:VAL:O	1:A:310:LYS:HG2	2.17	0.45
1:E:440:THR:HG21	1:F:437:GLN:HG3	1.98	0.45
1:F:96:TRP:CE3	1:F:264:TRP:HB3	2.52	0.45
1:F:248:ILE:HD13	1:F:402:PHE:CD2	2.51	0.45
1:A:172:ILE:O	1:A:183:LYS:NZ	2.49	0.45
1:D:366:LYS:HG3	1:D:452:LEU:HD23	1.98	0.45
1:E:367:LEU:HD11	1:E:450:ILE:CG1	2.47	0.45
1:F:370:MET:HA	1:F:373:LYS:HB2	1.98	0.45
1:E:439:LEU:HB3	1:E:444:VAL:HB	1.97	0.45
1:B:224:PRO:HG3	1:B:235:PHE:HE2	1.81	0.45
1:D:374:GLN:HG3	1:D:444:VAL:HG21	1.99	0.45
1:D:71:LYS:HA	1:D:71:LYS:HD2	1.68	0.45
1:D:302:MET:HE2	2:D:503:HEC:HBB2	1.99	0.45
1:E:162:LYS:HA	1:E:165:GLN:NE2	2.31	0.45
1:D:255:MET:HE3	1:D:274:ALA:HB3	1.98	0.45
1:D:330:GLN:O	1:D:330:GLN:CG	2.65	0.45
2:D:505:HEC:HMC1	2:D:505:HEC:HBC3	1.99	0.45
1:E:35:ILE:N	4:E:610:HOH:O	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:210:ARG:NH1	1:E:299:ASP:OD1	2.50	0.45
1:C:382:ASP:HB2	1:C:441:LYS:NZ	2.31	0.45
1:E:53:TYR:CE2	1:E:57:LYS:HE3	2.52	0.45
1:F:130:LEU:HD23	1:F:130:LEU:HA	1.80	0.45
1:A:82:LYS:HD3	1:A:102:TYR:CE2	2.52	0.45
2:C:501:HEC:C4D	2:C:503:HEC:HMD2	2.47	0.45
1:D:108:HIS:O	1:D:111:MET:HE3	2.17	0.45
1:F:113:LYS:HD2	1:F:117:GLU:HG3	1.98	0.45
1:F:307:VAL:O	1:F:309:SER:N	2.50	0.45
1:F:342:GLN:HG2	4:F:646:HOH:O	2.15	0.45
1:C:200:ASP:HB3	1:C:203:LYS:HG2	1.99	0.44
1:D:53:TYR:CD2	1:D:57:LYS:HE2	2.52	0.44
1:D:454:LEU:O	1:D:458:THR:HG23	2.18	0.44
1:F:219:VAL:O	1:F:279:PRO:HA	2.17	0.44
1:E:254:LYS:O	1:E:257:SER:OG	2.34	0.44
1:F:225:LYS:HB3	1:F:229:MET:HA	2.00	0.44
1:A:248:ILE:HD13	1:A:402:PHE:CD2	2.52	0.44
1:C:179:ASP:O	1:C:180:MET:HB2	2.17	0.44
1:D:96:TRP:CE3	1:D:264:TRP:HB3	2.52	0.44
1:F:85:GLU:HG2	1:F:472:GLN:O	2.17	0.44
2:A:505:HEC:CBA	2:B:505:HEC:HBA2	2.44	0.44
1:C:63:THR:HG22	1:C:318:MET:HE3	1.98	0.44
1:E:88:PHE:CE2	1:E:358:GLY:HA3	2.53	0.44
1:E:244:GLY:O	1:E:245:LYS:HG2	2.17	0.44
1:C:108:HIS:O	1:C:111:MET:HE3	2.17	0.44
1:D:248:ILE:HD13	1:D:402:PHE:CD2	2.52	0.44
1:D:301:HIS:CE1	1:D:320:PRO:HD3	2.52	0.44
1:D:439:LEU:HD12	1:D:439:LEU:HA	1.82	0.44
1:F:434:LEU:HD23	1:F:434:LEU:HA	1.83	0.44
1:A:184:ILE:O	1:A:184:ILE:HG22	2.18	0.44
1:E:206:ASN:O	1:E:210:ARG:HG3	2.18	0.44
1:C:326:LYS:HB3	1:C:326:LYS:HE3	1.68	0.44
1:D:370:MET:O	1:D:374:GLN:HG2	2.16	0.44
1:D:449:LYS:HE3	1:D:449:LYS:HB3	1.86	0.44
1:E:242:LYS:HD2	1:E:243:TRP:N	2.21	0.44
2:E:501:HEC:HHC	2:E:501:HEC:HBB2	1.99	0.44
1:F:385:MET:HE2	1:F:438:ALA:HB2	2.00	0.44
1:A:111:MET:HE3	1:A:111:MET:HB2	1.77	0.44
1:C:384:LYS:O	1:C:388:GLN:HG3	2.18	0.43
1:D:89:ILE:HB	1:D:93:PHE:CE2	2.53	0.43
1:F:173:ASP:OD1	1:F:186:ARG:NH1	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:371:THR:O	1:F:375:GLN:HG2	2.18	0.43
2:A:505:HEC:CHA	2:A:505:HEC:HBA1	2.48	0.43
1:E:88:PHE:CD2	1:E:358:GLY:HA3	2.53	0.43
1:A:259:LYS:C	1:A:261:TYR:N	2.77	0.43
1:C:278:HIS:NE2	3:C:506:SO4:O1	2.51	0.43
1:C:447:PRO:HD2	1:C:450:ILE:HD13	1.99	0.43
1:F:71:LYS:HA	1:F:71:LYS:HD2	1.66	0.43
1:F:133:LYS:HZ3	1:F:133:LYS:HG2	1.52	0.43
1:F:148:TYR:HA	1:F:151:GLN:NE2	2.33	0.43
1:C:408:SER:OG	1:C:412:HIS:N	2.49	0.43
1:D:85:GLU:HG2	1:D:472:GLN:O	2.19	0.43
1:C:53:TYR:CE2	1:C:57:LYS:HE2	2.54	0.43
1:F:366:LYS:NZ	1:F:369:GLU:OE1	2.40	0.43
1:A:328:CYS:C	1:A:330:GLN:H	2.27	0.43
1:A:408:SER:HB3	1:A:412:HIS:CE1	2.54	0.43
1:B:74:ASN:OD1	1:B:77:GLY:HA2	2.18	0.43
1:C:143:LYS:O	1:C:144:GLN:HG3	2.19	0.43
1:D:307:VAL:HG13	1:D:312:ILE:HD13	2.00	0.43
1:B:255:MET:HE3	1:B:274:ALA:HB3	2.00	0.43
1:F:132:CYS:HB3	1:F:217:CYS:HB3	2.01	0.43
1:F:266:GLN:O	1:F:270:GLY:N	2.49	0.43
1:B:303:PRO:HB3	1:B:326:LYS:HG3	2.01	0.42
1:C:71:LYS:HA	1:C:71:LYS:HD3	1.69	0.42
1:A:255:MET:HE3	1:A:274:ALA:HB3	2.00	0.42
2:A:505:HEC:HBA2	2:B:505:HEC:CAA	2.49	0.42
1:E:142:GLN:O	1:E:142:GLN:HG2	2.18	0.42
1:B:189:THR:HB	1:B:236:PHE:CZ	2.54	0.42
1:B:447:PRO:HG2	1:B:450:ILE:HD13	2.00	0.42
1:D:59:THR:HG22	1:D:316:ARG:HA	2.02	0.42
1:D:133:LYS:O	1:D:168:GLY:HA2	2.20	0.42
1:E:108:HIS:O	1:E:111:MET:HB2	2.19	0.42
1:A:435:LEU:HD23	1:A:435:LEU:HA	1.88	0.42
1:C:399:ARG:HG2	1:C:420:ILE:HG23	1.99	0.42
1:E:60:ALA:HB2	1:E:109:VAL:HG21	2.01	0.42
1:F:86:TYR:O	1:F:89:ILE:HG12	2.19	0.42
1:A:206:ASN:O	1:A:210:ARG:HG3	2.20	0.42
1:B:219:VAL:HG12	1:B:281:PHE:HB3	2.01	0.42
1:C:35:ILE:HA	1:C:36:PRO:HD3	1.85	0.42
1:F:219:VAL:O	1:F:220:THR:HB	2.20	0.42
1:F:254:LYS:O	1:F:257:SER:OG	2.28	0.42
1:F:414:PRO:O	1:F:418:MET:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:HIS:HB3	1:A:280:GLU:HB2	2.01	0.42
1:B:248:ILE:HD13	1:B:402:PHE:CD2	2.54	0.42
1:B:273:MET:HE2	1:B:398:TYR:OH	2.20	0.42
1:B:306:LYS:NZ	1:B:311:LYS:HB2	2.35	0.42
1:B:83:LEU:CD1	1:B:102:TYR:HB3	2.50	0.42
1:B:204:LEU:HD23	1:B:204:LEU:HA	1.86	0.42
1:D:136:TYR:OH	1:D:164:HIS:ND1	2.37	0.42
1:D:302:MET:CE	2:D:503:HEC:HBB2	2.49	0.42
1:E:119:ASP:OD1	1:E:121:SER:OG	2.27	0.42
1:F:35:ILE:HA	1:F:36:PRO:HD3	1.89	0.42
1:C:399:ARG:HB3	1:C:424:ALA:HB2	2.00	0.42
2:D:504:HEC:HBC3	2:D:504:HEC:HMC3	2.01	0.42
1:E:111:MET:HE2	2:E:503:HEC:C1D	2.50	0.42
2:E:505:HEC:HBA2	2:F:505:HEC:CBA	2.42	0.42
1:F:86:TYR:HB3	1:F:88:PHE:CE1	2.55	0.42
1:F:100:ILE:O	1:F:461:ARG:NH1	2.44	0.42
1:B:74:ASN:HB2	1:B:106:ARG:HG2	2.02	0.42
1:C:148:TYR:HA	1:C:151:GLN:NE2	2.35	0.42
1:D:375:GLN:CG	1:D:381:ILE:HD13	2.50	0.42
1:D:392:TYR:CZ	1:D:430:LYS:HE3	2.54	0.42
1:F:59:THR:OG1	1:F:109:VAL:HG13	2.20	0.42
1:A:284:TYR:CZ	2:A:504:HEC:HMC2	2.55	0.41
1:B:71:LYS:HD2	1:B:71:LYS:HA	1.73	0.41
1:E:83:LEU:HD22	1:E:90:ALA:HA	2.01	0.41
1:F:375:GLN:HA	1:F:379:LYS:O	2.20	0.41
1:A:148:TYR:HA	1:A:151:GLN:NE2	2.35	0.41
1:B:106:ARG:NH2	1:B:114:ASP:OD1	2.43	0.41
1:B:161:PRO:O	1:B:165:GLN:HG3	2.19	0.41
1:B:407:ASN:HB3	2:B:504:HEC:HAA2	2.03	0.41
1:A:406:GLU:OE2	1:A:412:HIS:ND1	2.41	0.41
1:C:219:VAL:HG21	1:C:236:PHE:CZ	2.55	0.41
1:E:71:LYS:HD2	1:E:71:LYS:HA	1.79	0.41
1:F:219:VAL:HG12	1:F:281:PHE:HB3	2.02	0.41
1:D:137:ALA:HB3	1:D:138:PRO:HD3	2.02	0.41
1:D:148:TYR:HA	1:D:151:GLN:NE2	2.35	0.41
1:D:131:THR:HG23	1:D:188:PHE:CZ	2.55	0.41
1:B:35:ILE:HG13	1:B:36:PRO:HD3	2.02	0.41
1:E:302:MET:HE3	2:E:503:HEC:CBB	2.51	0.41
1:E:389:ALA:HB1	1:E:435:LEU:CD1	2.50	0.41
1:E:399:ARG:HG2	1:E:420:ILE:HG23	2.03	0.41
2:A:505:HEC:HBA1	2:A:505:HEC:HHA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:300:CYS:SG	2:B:505:HEC:HHC	2.61	0.41
1:B:385:MET:HE1	1:B:437:GLN:CG	2.50	0.41
1:D:115:GLN:HE21	2:D:501:HEC:C1B	2.34	0.41
1:E:224:PRO:HG3	1:E:235:PHE:HE1	1.86	0.41
1:E:408:SER:HB3	1:E:412:HIS:CE1	2.56	0.41
1:E:418:MET:HE3	1:F:415:THR:HG22	2.03	0.41
1:F:131:THR:HG23	1:F:188:PHE:CZ	2.56	0.41
1:E:266:GLN:O	1:E:270:GLY:N	2.45	0.41
2:F:501:HEC:HHC	2:F:501:HEC:HBB2	2.02	0.41
1:A:60:ALA:HA	1:A:110:TYR:CE2	2.56	0.40
1:B:85:GLU:HB3	1:B:474:LEU:HD12	2.02	0.40
1:C:221:TYR:O	1:C:277:ARG:NH1	2.54	0.40
1:C:244:GLY:O	1:C:287:GLN:NE2	2.40	0.40
1:C:407:ASN:HB3	2:C:504:HEC:CAA	2.51	0.40
1:D:219:VAL:HG21	1:D:236:PHE:CE2	2.56	0.40
1:F:307:VAL:HG22	1:F:312:ILE:HG12	2.04	0.40
1:B:210:ARG:HH11	1:B:210:ARG:HD3	1.76	0.40
1:C:140:LEU:HD23	1:C:140:LEU:HA	1.85	0.40
1:E:316:ARG:NE	4:E:605:HOH:O	2.38	0.40
1:A:369:GLU:HG2	1:A:373:LYS:HE3	2.03	0.40
1:D:74:ASN:ND2	4:D:613:HOH:O	2.41	0.40
1:D:295:VAL:HG22	2:D:505:HEC:HBC2	2.03	0.40
1:E:53:TYR:CZ	1:E:57:LYS:HE3	2.56	0.40
1:E:276:ILE:HB	1:E:401:LEU:HG	2.03	0.40
1:F:453:GLU:O	1:F:456:LYS:HB2	2.20	0.40
1:D:408:SER:HB3	1:D:412:HIS:CE1	2.56	0.40
1:E:356:ARG:NH1	1:F:423:ASP:OD1	2.53	0.40
1:F:411:PHE:CD2	2:F:504:HEC:HMD2	2.57	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	435/482 (90%)	419 (96%)	14 (3%)	2 (0%)	24	34
1	B	440/482 (91%)	426 (97%)	13 (3%)	1 (0%)	43	56
1	C	436/482 (90%)	419 (96%)	14 (3%)	3 (1%)	18	25
1	D	438/482 (91%)	421 (96%)	15 (3%)	2 (0%)	24	34
1	E	435/482 (90%)	415 (95%)	18 (4%)	2 (0%)	24	34
1	F	433/482 (90%)	410 (95%)	19 (4%)	4 (1%)	14	20
All	All	2617/2892 (90%)	2510 (96%)	93 (4%)	14 (0%)	24	34

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	143	LYS
1	F	220	THR
1	A	260	SER
1	D	308	GLY
1	F	308	GLY
1	C	144	GLN
1	B	278	HIS
1	D	278	HIS
1	E	278	HIS
1	F	278	HIS
1	C	278	HIS
1	E	308	GLY
1	A	278	HIS
1	F	307	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	376/404 (93%)	374 (100%)	2 (0%)	81	88
1	B	377/404 (93%)	375 (100%)	2 (0%)	81	88
1	C	376/404 (93%)	374 (100%)	2 (0%)	81	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	377/404 (93%)	376 (100%)	1 (0%)	86	92
1	E	376/404 (93%)	376 (100%)	0	100	100
1	F	375/404 (93%)	373 (100%)	2 (0%)	81	88
All	All	2257/2424 (93%)	2248 (100%)	9 (0%)	84	90

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	183	LYS
1	A	259	LYS
1	B	171	CYS
1	B	384	LYS
1	C	178	LYS
1	C	179	ASP
1	D	171	CYS
1	F	435	LEU
1	F	454	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	ASN
1	A	144	GLN
1	A	151	GLN
1	A	228	ASN
1	A	380	GLN
1	B	115	GLN
1	B	144	GLN
1	B	151	GLN
1	B	158	ASN
1	B	218	HIS
1	B	400	ASN
1	B	460	ASN
1	C	115	GLN
1	C	144	GLN
1	C	151	GLN
1	C	232	GLN
1	D	94	ASN
1	D	115	GLN
1	D	151	GLN

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Mol	Chain	Res	Type
1	D	177	ASN
1	D	232	GLN
1	D	353	GLN
1	D	400	ASN
1	D	460	ASN
1	E	103	ASN
1	E	115	GLN
1	E	330	GLN
1	E	342	GLN
1	E	380	GLN
1	E	388	GLN
1	E	460	ASN
1	F	115	GLN
1	F	144	GLN
1	F	151	GLN
1	F	287	GLN
1	F	341	ASN
1	F	342	GLN
1	F	460	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

36 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	SO4	F	506	2	4,4,4	0.30	0	6,6,6	0.22	0
2	HEC	A	502	1	46,50,50	1.89	7 (15%)	58,82,82	1.28	5 (8%)
2	HEC	B	505	1	46,50,50	1.90	8 (17%)	58,82,82	1.84	14 (24%)
2	HEC	F	503	1	46,50,50	1.92	8 (17%)	58,82,82	1.56	12 (20%)
3	SO4	D	506	2	4,4,4	0.34	0	6,6,6	0.41	0
2	HEC	E	501	3,1	46,50,50	1.86	7 (15%)	58,82,82	1.44	8 (13%)
2	HEC	C	504	1	46,50,50	1.87	5 (10%)	58,82,82	1.22	6 (10%)
2	HEC	D	505	1	46,50,50	1.93	8 (17%)	58,82,82	1.44	7 (12%)
2	HEC	D	504	1	46,50,50	1.81	6 (13%)	58,82,82	1.28	7 (12%)
2	HEC	A	501	3,1	46,50,50	1.83	8 (17%)	58,82,82	1.33	5 (8%)
2	HEC	F	505	1	46,50,50	1.93	7 (15%)	58,82,82	1.23	6 (10%)
2	HEC	C	501	3,1	46,50,50	1.90	6 (13%)	58,82,82	1.34	8 (13%)
2	HEC	A	504	1	46,50,50	1.84	5 (10%)	58,82,82	1.29	4 (6%)
2	HEC	F	502	1	46,50,50	1.72	6 (13%)	58,82,82	1.26	4 (6%)
2	HEC	D	501	3,1	46,50,50	1.87	7 (15%)	58,82,82	1.10	2 (3%)
3	SO4	A	506	2	4,4,4	0.25	0	6,6,6	0.61	0
2	HEC	F	501	3,1	46,50,50	1.71	5 (10%)	58,82,82	1.20	5 (8%)
2	HEC	C	505	1	46,50,50	1.85	7 (15%)	58,82,82	1.75	13 (22%)
2	HEC	E	503	1	46,50,50	1.91	7 (15%)	58,82,82	1.21	6 (10%)
2	HEC	E	502	1	46,50,50	1.84	6 (13%)	58,82,82	1.36	4 (6%)
2	HEC	F	504	1	46,50,50	1.91	7 (15%)	58,82,82	1.30	7 (12%)
2	HEC	C	502	1	46,50,50	1.80	5 (10%)	58,82,82	1.30	3 (5%)
2	HEC	D	503	1	46,50,50	1.99	5 (10%)	58,82,82	1.36	4 (6%)
3	SO4	B	506	2	4,4,4	0.22	0	6,6,6	0.48	0
2	HEC	A	503	1	46,50,50	1.85	7 (15%)	58,82,82	1.66	7 (12%)
2	HEC	B	503	1	46,50,50	1.98	7 (15%)	58,82,82	1.80	8 (13%)
2	HEC	B	504	1	46,50,50	2.05	5 (10%)	58,82,82	1.34	6 (10%)
3	SO4	E	506	2	4,4,4	0.31	0	6,6,6	0.38	0
2	HEC	B	502	1	46,50,50	1.88	7 (15%)	58,82,82	1.48	5 (8%)
2	HEC	E	505	1	46,50,50	1.89	6 (13%)	58,82,82	1.54	9 (15%)
2	HEC	A	505	1	46,50,50	1.98	5 (10%)	58,82,82	1.58	10 (17%)
2	HEC	C	503	1	46,50,50	1.85	5 (10%)	58,82,82	1.37	8 (13%)
2	HEC	D	502	1	46,50,50	1.91	7 (15%)	58,82,82	1.32	6 (10%)
2	HEC	B	501	3,1	46,50,50	1.88	5 (10%)	58,82,82	1.49	9 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	C	506	2	4,4,4	0.20	0	6,6,6	0.54	0
2	HEC	E	504	1	46,50,50	1.83	6 (13%)	58,82,82	1.36	7 (12%)

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	A	502	1	-	6/14/54/54	-
2	HEC	B	505	1	-	10/14/54/54	-
2	HEC	F	503	1	-	4/14/54/54	-
2	HEC	E	501	3,1	-	6/14/54/54	-
2	HEC	C	504	1	-	6/14/54/54	-
2	HEC	D	505	1	-	7/14/54/54	-
2	HEC	D	504	1	-	5/14/54/54	-
2	HEC	A	501	3,1	-	6/14/54/54	-
2	HEC	F	505	1	-	7/14/54/54	-
2	HEC	C	501	3,1	-	5/14/54/54	-
2	HEC	A	504	1	-	4/14/54/54	-
2	HEC	F	502	1	-	6/14/54/54	-
2	HEC	D	501	3,1	-	5/14/54/54	-
2	HEC	F	501	3,1	-	6/14/54/54	-
2	HEC	C	505	1	-	11/14/54/54	-
2	HEC	E	503	1	-	4/14/54/54	-
2	HEC	E	502	1	-	6/14/54/54	-
2	HEC	F	504	1	-	6/14/54/54	-
2	HEC	C	502	1	-	6/14/54/54	-
2	HEC	D	503	1	-	7/14/54/54	-
2	HEC	A	503	1	-	4/14/54/54	-
2	HEC	B	503	1	-	5/14/54/54	-
2	HEC	B	504	1	-	4/14/54/54	-
2	HEC	B	502	1	-	6/14/54/54	-
2	HEC	E	505	1	-	7/14/54/54	-
2	HEC	A	505	1	-	10/14/54/54	-
2	HEC	C	503	1	-	4/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEC	D	502	1	-	6/14/54/54	-
2	HEC	B	501	3,1	-	5/14/54/54	-
2	HEC	E	504	1	-	6/14/54/54	-

All (190) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	504	HEC	CAB-C3B	7.62	1.59	1.35
2	A	505	HEC	CAC-C3C	7.25	1.58	1.35
2	B	503	HEC	CAB-C3B	6.99	1.57	1.35
2	D	503	HEC	CAC-C3C	6.84	1.57	1.35
2	F	505	HEC	CAC-C3C	6.78	1.57	1.35
2	A	505	HEC	CAB-C3B	6.76	1.57	1.35
2	D	502	HEC	CAC-C3C	6.74	1.56	1.35
2	B	502	HEC	CAC-C3C	6.73	1.56	1.35
2	F	504	HEC	CAB-C3B	6.72	1.56	1.35
2	C	501	HEC	CAB-C3B	6.70	1.56	1.35
2	A	502	HEC	CAC-C3C	6.68	1.56	1.35
2	B	505	HEC	CAC-C3C	6.66	1.56	1.35
2	E	504	HEC	CAC-C3C	6.62	1.56	1.35
2	B	504	HEC	CAC-C3C	6.59	1.56	1.35
2	C	503	HEC	CAC-C3C	6.59	1.56	1.35
2	E	505	HEC	CAC-C3C	6.58	1.56	1.35
2	D	502	HEC	CAB-C3B	6.54	1.56	1.35
2	D	503	HEC	CAB-C3B	6.45	1.55	1.35
2	D	501	HEC	CAC-C3C	6.44	1.55	1.35
2	B	501	HEC	CAB-C3B	6.44	1.55	1.35
2	D	504	HEC	CAC-C3C	6.44	1.55	1.35
2	C	505	HEC	CAC-C3C	6.38	1.55	1.35
2	C	501	HEC	CAC-C3C	6.38	1.55	1.35
2	E	501	HEC	CAC-C3C	6.37	1.55	1.35
2	F	505	HEC	CAB-C3B	6.37	1.55	1.35
2	B	505	HEC	CAB-C3B	6.36	1.55	1.35
2	A	503	HEC	CAC-C3C	6.36	1.55	1.35
2	A	504	HEC	CAC-C3C	6.33	1.55	1.35
2	F	503	HEC	CAB-C3B	6.33	1.55	1.35
2	A	501	HEC	CAC-C3C	6.33	1.55	1.35
2	E	505	HEC	CAB-C3B	6.33	1.55	1.35
2	F	504	HEC	CAC-C3C	6.31	1.55	1.35
2	E	503	HEC	CAB-C3B	6.29	1.55	1.35
2	D	505	HEC	CAB-C3B	6.28	1.55	1.35
2	C	504	HEC	CAC-C3C	6.28	1.55	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	502	HEC	CAB-C3B	6.25	1.55	1.35
2	B	501	HEC	CAC-C3C	6.21	1.55	1.35
2	F	503	HEC	CAC-C3C	6.21	1.55	1.35
2	C	504	HEC	CAB-C3B	6.21	1.55	1.35
2	C	503	HEC	CAB-C3B	6.20	1.55	1.35
2	F	501	HEC	CAC-C3C	6.20	1.55	1.35
2	D	501	HEC	CAB-C3B	6.19	1.55	1.35
2	A	504	HEC	CAB-C3B	6.15	1.55	1.35
2	A	502	HEC	CAB-C3B	6.14	1.54	1.35
2	E	503	HEC	CAC-C3C	6.10	1.54	1.35
2	C	505	HEC	CAB-C3B	6.08	1.54	1.35
2	E	502	HEC	CAC-C3C	6.05	1.54	1.35
2	D	505	HEC	CAC-C3C	6.04	1.54	1.35
2	E	501	HEC	CAB-C3B	6.03	1.54	1.35
2	C	502	HEC	CAC-C3C	6.00	1.54	1.35
2	B	503	HEC	CAC-C3C	5.91	1.54	1.35
2	C	502	HEC	CAB-C3B	5.90	1.54	1.35
2	F	502	HEC	CAC-C3C	5.88	1.54	1.35
2	E	504	HEC	CAB-C3B	5.81	1.53	1.35
2	B	502	HEC	CAB-C3B	5.65	1.53	1.35
2	A	501	HEC	CAB-C3B	5.53	1.53	1.35
2	D	504	HEC	CAB-C3B	5.47	1.52	1.35
2	F	501	HEC	CAB-C3B	5.43	1.52	1.35
2	A	503	HEC	CAB-C3B	5.38	1.52	1.35
2	F	502	HEC	CAB-C3B	4.71	1.50	1.35
2	B	503	HEC	CBB-CAB	-4.67	1.32	1.49
2	D	503	HEC	CBB-CAB	-4.62	1.32	1.49
2	B	504	HEC	CBC-CAC	-4.50	1.32	1.49
2	D	503	HEC	CBC-CAC	-4.44	1.33	1.49
2	F	503	HEC	CBC-CAC	-4.42	1.33	1.49
2	E	503	HEC	CBB-CAB	-4.35	1.33	1.49
2	B	502	HEC	CBC-CAC	-4.32	1.33	1.49
2	D	505	HEC	CBC-CAC	-4.29	1.33	1.49
2	E	501	HEC	CBB-CAB	-4.27	1.33	1.49
2	E	505	HEC	CBC-CAC	-4.26	1.33	1.49
2	F	503	HEC	CBB-CAB	-4.25	1.33	1.49
2	C	504	HEC	CBB-CAB	-4.24	1.33	1.49
2	E	503	HEC	CBC-CAC	-4.23	1.33	1.49
2	D	505	HEC	CBB-CAB	-4.21	1.33	1.49
2	F	504	HEC	CBB-CAB	-4.21	1.33	1.49
2	B	501	HEC	CBB-CAB	-4.21	1.33	1.49
2	C	501	HEC	CBB-CAB	-4.16	1.34	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	504	HEC	CBC-CAC	-4.15	1.34	1.49
2	E	502	HEC	CBC-CAC	-4.15	1.34	1.49
2	B	503	HEC	CBC-CAC	-4.15	1.34	1.49
2	B	501	HEC	CBC-CAC	-4.13	1.34	1.49
2	A	502	HEC	CBB-CAB	-4.13	1.34	1.49
2	C	501	HEC	CBC-CAC	-4.13	1.34	1.49
2	F	502	HEC	CBB-CAB	-4.11	1.34	1.49
2	D	501	HEC	CBB-CAB	-4.10	1.34	1.49
2	A	501	HEC	CBB-CAB	-4.08	1.34	1.49
2	C	504	HEC	CBC-CAC	-4.08	1.34	1.49
2	D	502	HEC	CBB-CAB	-4.08	1.34	1.49
2	F	502	HEC	CBC-CAC	-4.08	1.34	1.49
2	B	502	HEC	CBB-CAB	-4.08	1.34	1.49
2	A	503	HEC	CBB-CAB	-4.07	1.34	1.49
2	A	502	HEC	CBC-CAC	-4.06	1.34	1.49
2	C	503	HEC	CBB-CAB	-4.05	1.34	1.49
2	E	502	HEC	CBB-CAB	-4.04	1.34	1.49
2	C	505	HEC	CBB-CAB	-4.03	1.34	1.49
2	D	502	HEC	CBC-CAC	-4.03	1.34	1.49
2	B	505	HEC	CBB-CAB	-4.02	1.34	1.49
2	B	504	HEC	CBB-CAB	-4.02	1.34	1.49
2	A	505	HEC	CBC-CAC	-4.01	1.34	1.49
2	A	501	HEC	CBC-CAC	-4.01	1.34	1.49
2	C	503	HEC	CBC-CAC	-3.99	1.34	1.49
2	F	505	HEC	CBB-CAB	-3.96	1.34	1.49
2	A	503	HEC	CBC-CAC	-3.95	1.34	1.49
2	F	505	HEC	CBC-CAC	-3.95	1.34	1.49
2	D	504	HEC	CBB-CAB	-3.95	1.34	1.49
2	E	505	HEC	CBB-CAB	-3.93	1.34	1.49
2	C	505	HEC	CBC-CAC	-3.93	1.34	1.49
2	A	504	HEC	CBC-CAC	-3.92	1.35	1.49
2	A	505	HEC	CBB-CAB	-3.89	1.35	1.49
2	F	501	HEC	CBC-CAC	-3.89	1.35	1.49
2	C	502	HEC	CBB-CAB	-3.88	1.35	1.49
2	F	501	HEC	CBB-CAB	-3.88	1.35	1.49
2	C	502	HEC	CBC-CAC	-3.88	1.35	1.49
2	E	504	HEC	CBC-CAC	-3.88	1.35	1.49
2	E	501	HEC	CBC-CAC	-3.84	1.35	1.49
2	E	504	HEC	CBB-CAB	-3.84	1.35	1.49
2	D	501	HEC	CBC-CAC	-3.84	1.35	1.49
2	D	504	HEC	CBC-CAC	-3.83	1.35	1.49
2	A	504	HEC	CBB-CAB	-3.79	1.35	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	505	HEC	CBC-CAC	-3.70	1.35	1.49
2	F	502	HEC	CMB-C2B	3.04	1.57	1.50
2	A	503	HEC	CMA-C3A	2.81	1.56	1.50
2	B	503	HEC	CMC-C2C	2.60	1.56	1.50
2	B	502	HEC	CMB-C2B	2.47	1.55	1.50
2	B	505	HEC	C2A-C3A	-2.47	1.31	1.36
2	C	505	HEC	CMC-C2C	2.47	1.55	1.50
2	E	502	HEC	CMB-C2B	2.46	1.55	1.50
2	B	504	HEC	CMD-C2D	2.45	1.55	1.50
2	A	503	HEC	CMB-C2B	2.42	1.55	1.50
2	C	505	HEC	CMA-C3A	2.42	1.55	1.50
2	C	502	HEC	CMB-C2B	2.41	1.55	1.50
2	A	501	HEC	CMB-C2B	2.39	1.55	1.50
2	E	503	HEC	CMC-C2C	2.39	1.55	1.50
2	B	505	HEC	CMC-C2C	2.37	1.55	1.50
2	B	502	HEC	CMD-C2D	2.34	1.55	1.50
2	A	501	HEC	CMD-C2D	2.34	1.55	1.50
2	A	502	HEC	CMB-C2B	2.33	1.55	1.50
2	F	505	HEC	CMC-C2C	2.32	1.55	1.50
2	D	504	HEC	CMB-C2B	2.32	1.55	1.50
2	D	505	HEC	CMC-C2C	2.28	1.55	1.50
2	A	503	HEC	C3D-C2D	-2.28	1.33	1.38
2	F	503	HEC	CMB-C2B	2.27	1.55	1.50
2	F	505	HEC	CMA-C3A	2.27	1.55	1.50
2	E	504	HEC	CMB-C2B	2.27	1.55	1.50
2	F	503	HEC	CMC-C2C	2.26	1.55	1.50
2	C	505	HEC	CMB-C2B	2.26	1.55	1.50
2	E	501	HEC	CMC-C2C	2.26	1.55	1.50
2	E	503	HEC	CMB-C2B	2.25	1.55	1.50
2	D	505	HEC	C3B-C2B	-2.24	1.33	1.41
2	F	505	HEC	CMD-C2D	2.24	1.55	1.50
2	E	503	HEC	CMA-C3A	2.24	1.55	1.50
2	E	504	HEC	CMD-C2D	2.23	1.55	1.50
2	C	503	HEC	CMB-C2B	2.23	1.55	1.50
2	B	503	HEC	CMD-C2D	2.18	1.55	1.50
2	B	505	HEC	CMD-C2D	2.17	1.55	1.50
2	D	505	HEC	C3D-C2D	-2.17	1.33	1.38
2	E	501	HEC	C3B-C2B	-2.17	1.33	1.41
2	D	501	HEC	CMD-C2D	2.15	1.55	1.50
2	F	501	HEC	CMB-C2B	2.15	1.55	1.50
2	F	504	HEC	CMC-C2C	2.15	1.55	1.50
2	D	502	HEC	CMA-C3A	2.15	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	503	HEC	CMD-C2D	2.14	1.55	1.50
2	A	505	HEC	CMD-C2D	2.14	1.55	1.50
2	B	502	HEC	C3D-C2D	-2.13	1.33	1.38
2	E	501	HEC	CMB-C2B	2.13	1.55	1.50
2	A	504	HEC	C3B-C2B	-2.12	1.34	1.41
2	E	502	HEC	CMD-C2D	2.12	1.55	1.50
2	F	502	HEC	CMC-C2C	2.12	1.55	1.50
2	D	502	HEC	CMD-C2D	2.12	1.55	1.50
2	D	501	HEC	CMA-C3A	2.12	1.55	1.50
2	D	502	HEC	CMB-C2B	2.12	1.55	1.50
2	A	501	HEC	C3B-C2B	-2.11	1.34	1.41
2	A	502	HEC	CMC-C2C	2.09	1.55	1.50
2	A	501	HEC	CMC-C2C	2.09	1.55	1.50
2	B	501	HEC	CMD-C2D	2.09	1.55	1.50
2	B	505	HEC	CAD-C3D	2.08	1.56	1.51
2	E	505	HEC	CMB-C2B	2.07	1.55	1.50
2	C	501	HEC	CMD-C2D	2.07	1.55	1.50
2	D	501	HEC	CMB-C2B	2.07	1.55	1.50
2	B	503	HEC	C3B-C2B	-2.07	1.34	1.41
2	F	503	HEC	CMA-C3A	2.06	1.55	1.50
2	D	504	HEC	CMA-C3A	2.06	1.55	1.50
2	C	501	HEC	C3B-C2B	-2.04	1.34	1.41
2	D	503	HEC	CMC-C2C	2.04	1.55	1.50
2	F	504	HEC	CMD-C2D	2.04	1.54	1.50
2	E	505	HEC	CMD-C2D	2.03	1.54	1.50
2	A	502	HEC	CMD-C2D	2.03	1.54	1.50
2	D	505	HEC	CMD-C2D	2.01	1.54	1.50
2	C	504	HEC	C3B-C2B	-2.01	1.34	1.41
2	F	504	HEC	C3B-C2B	-2.01	1.34	1.41

All (205) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	503	HEC	CBA-CAA-C2A	8.78	136.81	112.53
2	B	505	HEC	CBB-CAB-C3B	-6.32	114.79	127.43
2	B	502	HEC	CBB-CAB-C3B	-6.14	115.17	127.43
2	A	503	HEC	CBB-CAB-C3B	-5.94	115.55	127.43
2	C	505	HEC	CBB-CAB-C3B	-5.89	115.66	127.43
2	A	503	HEC	CBC-CAC-C3C	-5.53	116.38	127.43
2	C	502	HEC	CBB-CAB-C3B	-5.51	116.41	127.43
2	E	502	HEC	CBC-CAC-C3C	-5.22	116.99	127.43
2	F	503	HEC	CBC-CAC-C3C	-5.00	117.44	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	502	HEC	CBB-CAB-C3B	-4.92	117.61	127.43
2	B	505	HEC	C2A-C1A-NA	-4.88	105.62	110.32
2	D	505	HEC	CBB-CAB-C3B	-4.75	117.94	127.43
2	D	503	HEC	CBB-CAB-C3B	-4.51	118.42	127.43
2	E	503	HEC	CBC-CAC-C3C	-4.47	118.50	127.43
2	B	501	HEC	CBB-CAB-C3B	-4.47	118.51	127.43
2	E	501	HEC	CBB-CAB-C3B	-4.40	118.63	127.43
2	F	504	HEC	CBB-CAB-C3B	-4.39	118.66	127.43
2	F	503	HEC	CBB-CAB-C3B	-4.36	118.72	127.43
2	E	504	HEC	CBB-CAB-C3B	-4.35	118.74	127.43
2	E	505	HEC	CBB-CAB-C3B	-4.34	118.76	127.43
2	A	501	HEC	CBB-CAB-C3B	-4.30	118.84	127.43
2	A	501	HEC	CBC-CAC-C3C	-4.28	118.87	127.43
2	A	504	HEC	CBB-CAB-C3B	-4.27	118.90	127.43
2	B	503	HEC	CBB-CAB-C3B	-4.24	118.95	127.43
2	C	502	HEC	CBC-CAC-C3C	-4.15	119.15	127.43
2	C	505	HEC	C2A-C1A-NA	-4.10	106.36	110.32
2	D	504	HEC	CBB-CAB-C3B	-4.08	119.28	127.43
2	C	504	HEC	CBB-CAB-C3B	-4.07	119.29	127.43
2	B	503	HEC	CBC-CAC-C3C	-4.07	119.30	127.43
2	C	505	HEC	CBC-CAC-C3C	-4.03	119.37	127.43
2	A	505	HEC	CBA-CAA-C2A	-4.00	101.47	112.53
2	A	505	HEC	CAD-CBD-CGD	-3.94	103.23	113.67
2	F	502	HEC	CBB-CAB-C3B	-3.92	119.59	127.43
2	C	501	HEC	CBB-CAB-C3B	-3.90	119.64	127.43
2	D	502	HEC	CBB-CAB-C3B	-3.84	119.77	127.43
2	D	502	HEC	CBC-CAC-C3C	-3.76	119.92	127.43
2	C	503	HEC	CBB-CAB-C3B	-3.74	119.95	127.43
2	F	501	HEC	CBB-CAB-C3B	-3.73	119.98	127.43
2	D	505	HEC	C2A-C1A-NA	-3.68	106.77	110.32
2	A	505	HEC	C2A-C1A-NA	-3.67	106.78	110.32
2	B	504	HEC	CBB-CAB-C3B	-3.60	120.24	127.43
2	C	503	HEC	CBC-CAC-C3C	-3.58	120.28	127.43
2	E	502	HEC	CBB-CAB-C3B	-3.53	120.37	127.43
2	B	505	HEC	CAA-C2A-C3A	-3.48	121.35	127.87
2	F	505	HEC	CBB-CAB-C3B	-3.45	120.54	127.43
2	E	505	HEC	CAD-CBD-CGD	-3.44	104.55	113.67
2	A	505	HEC	CBB-CAB-C3B	-3.41	120.63	127.43
2	A	503	HEC	C2A-C1A-NA	-3.37	107.08	110.32
2	B	504	HEC	CBC-CAC-C3C	-3.32	120.79	127.43
2	D	505	HEC	CBA-CAA-C2A	-3.31	103.37	112.53
2	B	505	HEC	CBC-CAC-C3C	-3.31	120.82	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	504	HEC	CBC-CAC-C3C	-3.31	120.83	127.43
2	F	503	HEC	C2A-C1A-NA	-3.28	107.16	110.32
2	B	501	HEC	CBC-CAC-C3C	-3.21	121.01	127.43
2	B	503	HEC	CHC-C4B-NB	3.21	127.95	124.45
2	E	505	HEC	CAA-C2A-C3A	-3.19	121.88	127.87
2	D	503	HEC	C2A-C1A-NA	-3.19	107.25	110.32
2	B	505	HEC	CMA-C3A-C4A	3.14	130.26	124.73
2	E	504	HEC	CBC-CAC-C3C	-3.12	121.20	127.43
2	E	501	HEC	C2A-C1A-NA	-3.05	107.38	110.32
2	D	503	HEC	CBC-CAC-C3C	-3.04	121.37	127.43
2	C	504	HEC	CBC-CAC-C3C	-3.01	121.41	127.43
2	B	504	HEC	C3D-C4D-ND	-3.00	106.82	110.15
2	A	502	HEC	CBC-CAC-C3C	-2.97	121.50	127.43
2	A	503	HEC	C3D-C4D-ND	-2.95	106.88	110.15
2	B	501	HEC	CBA-CAA-C2A	-2.93	104.42	112.53
2	D	505	HEC	CBC-CAC-C3C	-2.92	121.60	127.43
2	B	501	HEC	C2A-C1A-NA	-2.89	107.53	110.32
2	C	501	HEC	CBC-CAC-C3C	-2.89	121.65	127.43
2	D	503	HEC	C3D-C4D-ND	-2.87	106.97	110.15
2	B	505	HEC	C3D-C4D-ND	-2.85	106.99	110.15
2	C	503	HEC	C2A-C1A-NA	-2.84	107.59	110.32
2	E	505	HEC	C2A-C1A-NA	-2.83	107.60	110.32
2	D	501	HEC	CBC-CAC-C3C	-2.80	121.84	127.43
2	C	503	HEC	C3D-C4D-ND	-2.80	107.05	110.15
2	A	502	HEC	CBD-CAD-C3D	-2.78	104.83	112.53
2	F	505	HEC	C2A-C1A-NA	-2.75	107.67	110.32
2	E	501	HEC	CBC-CAC-C3C	-2.75	121.93	127.43
2	B	504	HEC	C2A-C1A-NA	-2.75	107.67	110.32
2	A	505	HEC	CAA-C2A-C3A	-2.73	122.75	127.87
2	E	504	HEC	C2A-C1A-NA	-2.73	107.69	110.32
2	E	501	HEC	CBA-CAA-C2A	-2.72	105.00	112.53
2	D	505	HEC	CHD-C4C-NC	2.72	127.42	124.45
2	B	502	HEC	C2A-C1A-NA	-2.70	107.72	110.32
2	E	505	HEC	CBC-CAC-C3C	-2.68	122.07	127.43
2	B	503	HEC	C3D-C4D-ND	-2.64	107.22	110.15
2	F	502	HEC	CHB-C4A-NA	2.64	127.33	124.45
2	C	505	HEC	CHA-C1A-C2A	2.60	128.96	124.86
2	E	503	HEC	CBB-CAB-C3B	-2.57	122.29	127.43
2	D	504	HEC	CBC-CAC-C3C	-2.57	122.31	127.43
2	E	505	HEC	CBA-CAA-C2A	-2.56	105.47	112.53
2	B	505	HEC	C1A-C2A-C3A	2.55	110.47	107.11
2	F	505	HEC	CBC-CAC-C3C	-2.54	122.35	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	505	HEC	C3D-C4D-ND	-2.53	107.34	110.15
2	C	505	HEC	CMC-C2C-C1C	-2.52	121.58	125.42
2	A	503	HEC	CHA-C1A-C2A	2.51	128.83	124.86
2	D	502	HEC	CAA-CBA-CGA	-2.51	107.02	113.67
2	B	505	HEC	C4D-ND-C1D	2.50	109.89	105.82
2	B	505	HEC	CHA-C1A-C2A	2.48	128.78	124.86
2	F	505	HEC	C3D-C4D-ND	-2.47	107.41	110.15
2	F	503	HEC	O2A-CGA-CBA	2.46	121.78	114.00
2	A	505	HEC	CBC-CAC-C3C	-2.46	122.52	127.43
2	D	505	HEC	CAD-CBD-CGD	-2.45	107.16	113.67
2	A	504	HEC	CAA-C2A-C1A	2.45	129.82	124.85
2	A	501	HEC	C2A-C1A-NA	-2.44	107.97	110.32
2	C	503	HEC	CBA-CAA-C2A	-2.44	105.80	112.53
2	E	505	HEC	CAA-C2A-C1A	2.44	129.81	124.85
2	B	504	HEC	CBA-CAA-C2A	-2.43	105.81	112.53
2	D	502	HEC	CBD-CAD-C3D	-2.43	105.83	112.53
2	B	501	HEC	C4B-NB-C1B	2.41	109.76	105.82
2	A	502	HEC	O2A-CGA-CBA	2.40	121.59	114.00
2	A	505	HEC	CMB-C2B-C1B	-2.40	121.76	125.42
2	E	501	HEC	CHB-C4A-NA	2.40	127.07	124.45
2	B	501	HEC	C2C-C1C-NC	-2.40	106.30	110.14
2	E	502	HEC	CHB-C4A-NA	2.39	127.06	124.45
2	F	505	HEC	CAD-CBD-CGD	-2.39	107.33	113.67
2	D	501	HEC	C2A-C1A-NA	-2.38	108.03	110.32
2	D	504	HEC	CHD-C4C-NC	2.37	127.03	124.45
2	E	505	HEC	CMB-C2B-C1B	-2.36	121.83	125.42
2	C	503	HEC	CHA-C1A-C2A	2.33	128.55	124.86
2	F	503	HEC	O1A-CGA-CBA	-2.33	115.71	123.09
2	B	505	HEC	CBD-CAD-C3D	-2.32	106.12	112.53
2	C	505	HEC	CHD-C4C-C3C	2.32	129.12	125.21
2	F	503	HEC	C3D-C4D-ND	-2.31	107.58	110.15
2	F	504	HEC	CBC-CAC-C3C	-2.31	122.81	127.43
2	C	501	HEC	CMD-C2D-C1D	-2.31	121.90	125.42
2	B	501	HEC	C4C-NC-C1C	2.31	109.58	105.82
2	C	501	HEC	C2A-C1A-NA	-2.30	108.10	110.32
2	A	504	HEC	O2A-CGA-CBA	2.30	121.28	114.00
2	C	505	HEC	CAD-CBD-CGD	-2.30	107.57	113.67
2	F	501	HEC	C2D-C1D-ND	-2.30	106.46	110.14
2	C	505	HEC	CAA-C2A-C3A	-2.28	123.61	127.87
2	E	503	HEC	O2A-CGA-CBA	2.27	121.16	114.00
2	C	505	HEC	CBD-CAD-C3D	-2.26	106.27	112.53
2	F	504	HEC	CHC-C4B-NB	2.24	126.90	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	503	HEC	C2D-C1D-ND	-2.24	106.55	110.14
2	C	504	HEC	CBA-CAA-C2A	-2.24	106.34	112.53
2	D	504	HEC	CMA-C3A-C4A	2.23	128.66	124.73
2	B	502	HEC	CBD-CAD-C3D	-2.22	106.39	112.53
2	D	502	HEC	C2D-C1D-ND	-2.22	106.59	110.14
2	A	505	HEC	C4C-NC-C1C	2.21	109.43	105.82
2	C	505	HEC	C4C-NC-C1C	2.21	109.43	105.82
2	C	504	HEC	C2A-C1A-NA	-2.21	108.19	110.32
2	C	501	HEC	C2C-C1C-NC	-2.21	106.60	110.14
2	A	501	HEC	C3D-C4D-ND	-2.21	107.70	110.15
2	F	505	HEC	CHA-C1A-C2A	2.20	128.34	124.86
2	C	503	HEC	C4D-ND-C1D	2.20	109.40	105.82
2	B	502	HEC	C3D-C4D-ND	-2.19	107.72	110.15
2	B	505	HEC	C2D-C1D-ND	-2.19	106.63	110.14
2	F	503	HEC	C2D-C1D-ND	-2.17	106.66	110.14
2	E	501	HEC	C2D-C1D-ND	-2.17	106.67	110.14
2	F	503	HEC	C4D-ND-C1D	2.17	109.35	105.82
2	F	503	HEC	C4A-NA-C1A	2.16	109.34	105.82
2	E	505	HEC	CBD-CAD-C3D	-2.16	106.57	112.53
2	B	503	HEC	C2A-C1A-NA	-2.15	108.25	110.32
2	A	505	HEC	CHC-C4B-C3B	2.15	128.84	125.21
2	C	505	HEC	C2D-C1D-ND	-2.15	106.70	110.14
2	D	504	HEC	O1A-CGA-CBA	-2.14	116.29	123.09
2	B	502	HEC	CBC-CAC-C3C	-2.14	123.16	127.43
2	C	504	HEC	C3D-C4D-ND	-2.13	107.79	110.15
2	E	503	HEC	C1D-C2D-C3D	2.13	109.25	106.82
2	E	503	HEC	O1A-CGA-CBA	-2.11	116.39	123.09
2	F	503	HEC	CHA-C1A-C2A	2.11	128.20	124.86
2	E	504	HEC	C3D-C4D-ND	-2.11	107.81	110.15
2	A	502	HEC	O1A-CGA-CBA	-2.11	116.41	123.09
2	C	505	HEC	C4D-ND-C1D	2.11	109.25	105.82
2	C	501	HEC	C4B-NB-C1B	2.10	109.25	105.82
2	C	504	HEC	C2D-C1D-ND	-2.10	106.78	110.14
2	A	503	HEC	CHD-C1D-ND	2.09	127.66	123.86
2	B	501	HEC	C2D-C1D-ND	-2.09	106.79	110.14
2	F	501	HEC	C3D-C4D-ND	-2.09	107.84	110.15
2	B	505	HEC	C4C-NC-C1C	2.09	109.22	105.82
2	A	505	HEC	C2D-C1D-ND	-2.08	106.80	110.14
2	F	504	HEC	O2D-CGD-CBD	2.08	120.57	114.00
2	B	503	HEC	O1A-CGA-CBA	-2.07	116.51	123.09
2	D	504	HEC	C2A-C1A-NA	-2.07	108.32	110.32
2	F	502	HEC	C2A-C1A-NA	-2.07	108.32	110.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	503	HEC	C2D-C1D-ND	-2.07	106.82	110.14
2	F	501	HEC	C2A-C1A-NA	-2.07	108.33	110.32
2	F	503	HEC	C4C-NC-C1C	2.06	109.19	105.82
2	E	504	HEC	C4A-NA-C1A	2.06	109.18	105.82
2	E	504	HEC	CHA-C1A-C2A	2.06	128.11	124.86
2	A	503	HEC	CBD-CAD-C3D	-2.05	106.86	112.53
2	B	505	HEC	CBA-CAA-C2A	-2.05	106.86	112.53
2	B	504	HEC	C4D-ND-C1D	2.05	109.16	105.82
2	D	505	HEC	C1A-C2A-C3A	2.05	109.80	107.11
2	C	502	HEC	CBD-CAD-C3D	-2.04	106.90	112.53
2	B	505	HEC	CAD-CBD-CGD	-2.03	108.27	113.67
2	F	502	HEC	CHD-C4C-NC	2.03	126.67	124.45
2	C	501	HEC	CMC-C2C-C1C	-2.03	122.33	125.42
2	E	501	HEC	C1D-C2D-C3D	2.03	109.14	106.82
2	F	501	HEC	C4D-ND-C1D	2.03	109.13	105.82
2	E	502	HEC	CAD-CBD-CGD	-2.03	108.29	113.67
2	D	502	HEC	O1A-CGA-CBA	-2.03	116.67	123.09
2	C	501	HEC	CMD-C2D-C3D	2.02	129.92	125.62
2	E	501	HEC	C3D-C4D-ND	-2.02	107.91	110.15
2	F	504	HEC	CAD-CBD-CGD	-2.02	108.31	113.67
2	A	501	HEC	CAA-CBA-CGA	-2.02	108.31	113.67
2	F	503	HEC	C4B-NB-C1B	2.02	109.11	105.82
2	F	504	HEC	C2C-C1C-NC	-2.02	106.91	110.14
2	B	501	HEC	C2B-C1B-NB	-2.01	106.91	110.14
2	E	504	HEC	C4C-NC-C1C	2.01	109.10	105.82
2	F	504	HEC	C4B-NB-C1B	2.01	109.09	105.82
2	B	503	HEC	CBD-CAD-C3D	-2.00	106.99	112.53
2	D	504	HEC	O2A-CGA-CBA	2.00	120.33	114.00

There are no chirality outliers.

All (180) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	HEC	C2C-C3C-CAC-CBC
2	A	501	HEC	C4C-C3C-CAC-CBC
2	A	502	HEC	C2B-C3B-CAB-CBB
2	A	502	HEC	C4B-C3B-CAB-CBB
2	A	502	HEC	C2C-C3C-CAC-CBC
2	A	502	HEC	C4C-C3C-CAC-CBC
2	A	503	HEC	C2B-C3B-CAB-CBB
2	A	503	HEC	C4B-C3B-CAB-CBB
2	A	503	HEC	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
2	A	503	HEC	C4C-C3C-CAC-CBC
2	A	504	HEC	C2B-C3B-CAB-CBB
2	A	504	HEC	C4B-C3B-CAB-CBB
2	A	504	HEC	C2C-C3C-CAC-CBC
2	A	504	HEC	C4C-C3C-CAC-CBC
2	A	505	HEC	C2B-C3B-CAB-CBB
2	A	505	HEC	C4B-C3B-CAB-CBB
2	A	505	HEC	C2C-C3C-CAC-CBC
2	A	505	HEC	C4C-C3C-CAC-CBC
2	B	501	HEC	C2C-C3C-CAC-CBC
2	B	501	HEC	C4C-C3C-CAC-CBC
2	B	502	HEC	C2B-C3B-CAB-CBB
2	B	502	HEC	C4B-C3B-CAB-CBB
2	B	502	HEC	C2C-C3C-CAC-CBC
2	B	502	HEC	C4C-C3C-CAC-CBC
2	B	503	HEC	C2B-C3B-CAB-CBB
2	B	503	HEC	C4B-C3B-CAB-CBB
2	B	503	HEC	C2C-C3C-CAC-CBC
2	B	503	HEC	C4C-C3C-CAC-CBC
2	B	504	HEC	C2B-C3B-CAB-CBB
2	B	504	HEC	C4B-C3B-CAB-CBB
2	B	504	HEC	C2C-C3C-CAC-CBC
2	B	504	HEC	C4C-C3C-CAC-CBC
2	B	505	HEC	C2B-C3B-CAB-CBB
2	B	505	HEC	C4B-C3B-CAB-CBB
2	B	505	HEC	C2C-C3C-CAC-CBC
2	B	505	HEC	C4C-C3C-CAC-CBC
2	C	501	HEC	C2C-C3C-CAC-CBC
2	C	501	HEC	C4C-C3C-CAC-CBC
2	C	502	HEC	C2B-C3B-CAB-CBB
2	C	502	HEC	C4B-C3B-CAB-CBB
2	C	502	HEC	C2C-C3C-CAC-CBC
2	C	502	HEC	C4C-C3C-CAC-CBC
2	C	503	HEC	C2B-C3B-CAB-CBB
2	C	503	HEC	C4B-C3B-CAB-CBB
2	C	503	HEC	C2C-C3C-CAC-CBC
2	C	503	HEC	C4C-C3C-CAC-CBC
2	C	504	HEC	C2B-C3B-CAB-CBB
2	C	504	HEC	C4B-C3B-CAB-CBB
2	C	504	HEC	C2C-C3C-CAC-CBC
2	C	504	HEC	C4C-C3C-CAC-CBC
2	C	505	HEC	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
2	C	505	HEC	C4B-C3B-CAB-CBB
2	C	505	HEC	C2C-C3C-CAC-CBC
2	C	505	HEC	C4C-C3C-CAC-CBC
2	D	501	HEC	C2C-C3C-CAC-CBC
2	D	501	HEC	C4C-C3C-CAC-CBC
2	D	502	HEC	C2B-C3B-CAB-CBB
2	D	502	HEC	C4B-C3B-CAB-CBB
2	D	502	HEC	C2C-C3C-CAC-CBC
2	D	502	HEC	C4C-C3C-CAC-CBC
2	D	503	HEC	C2B-C3B-CAB-CBB
2	D	503	HEC	C4B-C3B-CAB-CBB
2	D	503	HEC	C2C-C3C-CAC-CBC
2	D	503	HEC	C4C-C3C-CAC-CBC
2	D	504	HEC	C2B-C3B-CAB-CBB
2	D	504	HEC	C4B-C3B-CAB-CBB
2	D	504	HEC	C2C-C3C-CAC-CBC
2	D	504	HEC	C4C-C3C-CAC-CBC
2	D	505	HEC	C2B-C3B-CAB-CBB
2	D	505	HEC	C4B-C3B-CAB-CBB
2	D	505	HEC	C2C-C3C-CAC-CBC
2	D	505	HEC	C4C-C3C-CAC-CBC
2	E	501	HEC	C2B-C3B-CAB-CBB
2	E	501	HEC	C4B-C3B-CAB-CBB
2	E	501	HEC	C2C-C3C-CAC-CBC
2	E	501	HEC	C4C-C3C-CAC-CBC
2	E	502	HEC	C2B-C3B-CAB-CBB
2	E	502	HEC	C4B-C3B-CAB-CBB
2	E	502	HEC	C2C-C3C-CAC-CBC
2	E	502	HEC	C4C-C3C-CAC-CBC
2	E	503	HEC	C2B-C3B-CAB-CBB
2	E	503	HEC	C4B-C3B-CAB-CBB
2	E	503	HEC	C2C-C3C-CAC-CBC
2	E	503	HEC	C4C-C3C-CAC-CBC
2	E	504	HEC	C2B-C3B-CAB-CBB
2	E	504	HEC	C4B-C3B-CAB-CBB
2	E	504	HEC	C2C-C3C-CAC-CBC
2	E	504	HEC	C4C-C3C-CAC-CBC
2	E	505	HEC	C2B-C3B-CAB-CBB
2	E	505	HEC	C4B-C3B-CAB-CBB
2	E	505	HEC	C2C-C3C-CAC-CBC
2	E	505	HEC	C4C-C3C-CAC-CBC
2	F	501	HEC	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
2	F	501	HEC	C4B-C3B-CAB-CBB
2	F	501	HEC	C2C-C3C-CAC-CBC
2	F	501	HEC	C4C-C3C-CAC-CBC
2	F	502	HEC	C2B-C3B-CAB-CBB
2	F	502	HEC	C4B-C3B-CAB-CBB
2	F	502	HEC	C2C-C3C-CAC-CBC
2	F	502	HEC	C4C-C3C-CAC-CBC
2	F	503	HEC	C2B-C3B-CAB-CBB
2	F	503	HEC	C4B-C3B-CAB-CBB
2	F	503	HEC	C2C-C3C-CAC-CBC
2	F	503	HEC	C4C-C3C-CAC-CBC
2	F	504	HEC	C2B-C3B-CAB-CBB
2	F	504	HEC	C4B-C3B-CAB-CBB
2	F	504	HEC	C2C-C3C-CAC-CBC
2	F	504	HEC	C4C-C3C-CAC-CBC
2	F	505	HEC	C2B-C3B-CAB-CBB
2	F	505	HEC	C4B-C3B-CAB-CBB
2	F	505	HEC	C2C-C3C-CAC-CBC
2	F	505	HEC	C4C-C3C-CAC-CBC
2	B	503	HEC	C2A-CAA-CBA-CGA
2	B	505	HEC	C2A-CAA-CBA-CGA
2	C	505	HEC	C2A-CAA-CBA-CGA
2	D	505	HEC	C2A-CAA-CBA-CGA
2	A	505	HEC	C2A-CAA-CBA-CGA
2	A	501	HEC	C2B-C3B-CAB-CBB
2	C	505	HEC	C1A-C2A-CAA-CBA
2	D	501	HEC	CAA-CBA-CGA-O2A
2	D	503	HEC	C2A-CAA-CBA-CGA
2	F	501	HEC	CAA-CBA-CGA-O2A
2	B	501	HEC	CAA-CBA-CGA-O1A
2	E	501	HEC	CAA-CBA-CGA-O2A
2	F	502	HEC	CAA-CBA-CGA-O1A
2	F	502	HEC	CAA-CBA-CGA-O2A
2	C	502	HEC	CAA-CBA-CGA-O2A
2	D	502	HEC	CAA-CBA-CGA-O1A
2	B	501	HEC	CAA-CBA-CGA-O2A
2	C	501	HEC	CAA-CBA-CGA-O2A
2	D	501	HEC	CAA-CBA-CGA-O1A
2	C	502	HEC	CAA-CBA-CGA-O1A
2	B	502	HEC	CAA-CBA-CGA-O2A
2	B	505	HEC	CAA-CBA-CGA-O2A
2	A	502	HEC	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
2	B	502	HEC	CAA-CBA-CGA-O1A
2	D	502	HEC	CAA-CBA-CGA-O2A
2	F	501	HEC	CAA-CBA-CGA-O1A
2	E	501	HEC	CAA-CBA-CGA-O1A
2	A	502	HEC	CAA-CBA-CGA-O1A
2	E	502	HEC	CAA-CBA-CGA-O1A
2	C	501	HEC	CAA-CBA-CGA-O1A
2	A	505	HEC	C1A-C2A-CAA-CBA
2	A	501	HEC	CAA-CBA-CGA-O2A
2	B	505	HEC	CAA-CBA-CGA-O1A
2	B	505	HEC	C1A-C2A-CAA-CBA
2	C	505	HEC	CAA-CBA-CGA-O1A
2	C	505	HEC	CAD-CBD-CGD-O2D
2	E	502	HEC	CAA-CBA-CGA-O2A
2	D	503	HEC	CAA-CBA-CGA-O2A
2	E	505	HEC	C1A-C2A-CAA-CBA
2	A	505	HEC	CAD-CBD-CGD-O2D
2	B	505	HEC	CAD-CBD-CGD-O2D
2	D	505	HEC	CAD-CBD-CGD-O2D
2	A	501	HEC	CAA-CBA-CGA-O1A
2	B	505	HEC	CAD-CBD-CGD-O1D
2	C	505	HEC	CAD-CBD-CGD-O1D
2	D	503	HEC	CAA-CBA-CGA-O1A
2	E	504	HEC	CAA-CBA-CGA-O2A
2	E	505	HEC	CAD-CBD-CGD-O2D
2	F	505	HEC	CAD-CBD-CGD-O2D
2	D	505	HEC	CAD-CBD-CGD-O1D
2	A	505	HEC	CAD-CBD-CGD-O1D
2	E	505	HEC	CAD-CBD-CGD-O1D
2	F	504	HEC	CAA-CBA-CGA-O2A
2	F	504	HEC	CAA-CBA-CGA-O1A
2	A	505	HEC	CAA-CBA-CGA-O1A
2	F	505	HEC	C2A-CAA-CBA-CGA
2	F	505	HEC	CAD-CBD-CGD-O1D
2	C	505	HEC	CAA-CBA-CGA-O2A
2	E	504	HEC	CAA-CBA-CGA-O1A
2	A	505	HEC	CAA-CBA-CGA-O2A
2	C	504	HEC	CAA-CBA-CGA-O2A
2	A	501	HEC	C4B-C3B-CAB-CBB
2	B	501	HEC	C4B-C3B-CAB-CBB
2	C	501	HEC	C4B-C3B-CAB-CBB
2	D	501	HEC	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
2	C	504	HEC	CAA-CBA-CGA-O1A
2	C	505	HEC	C3A-C2A-CAA-CBA
2	D	504	HEC	CAA-CBA-CGA-O2A

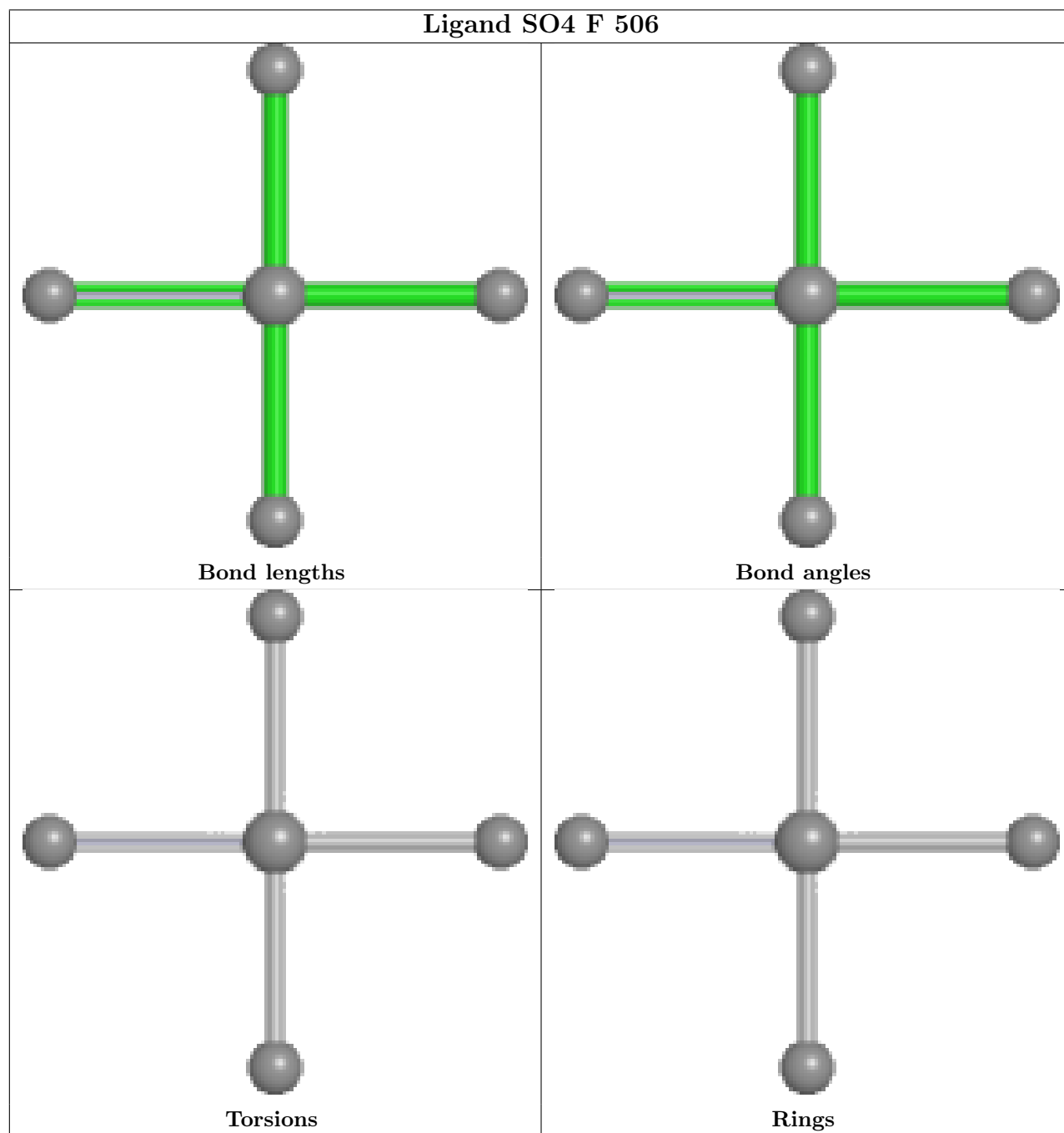
There are no ring outliers.

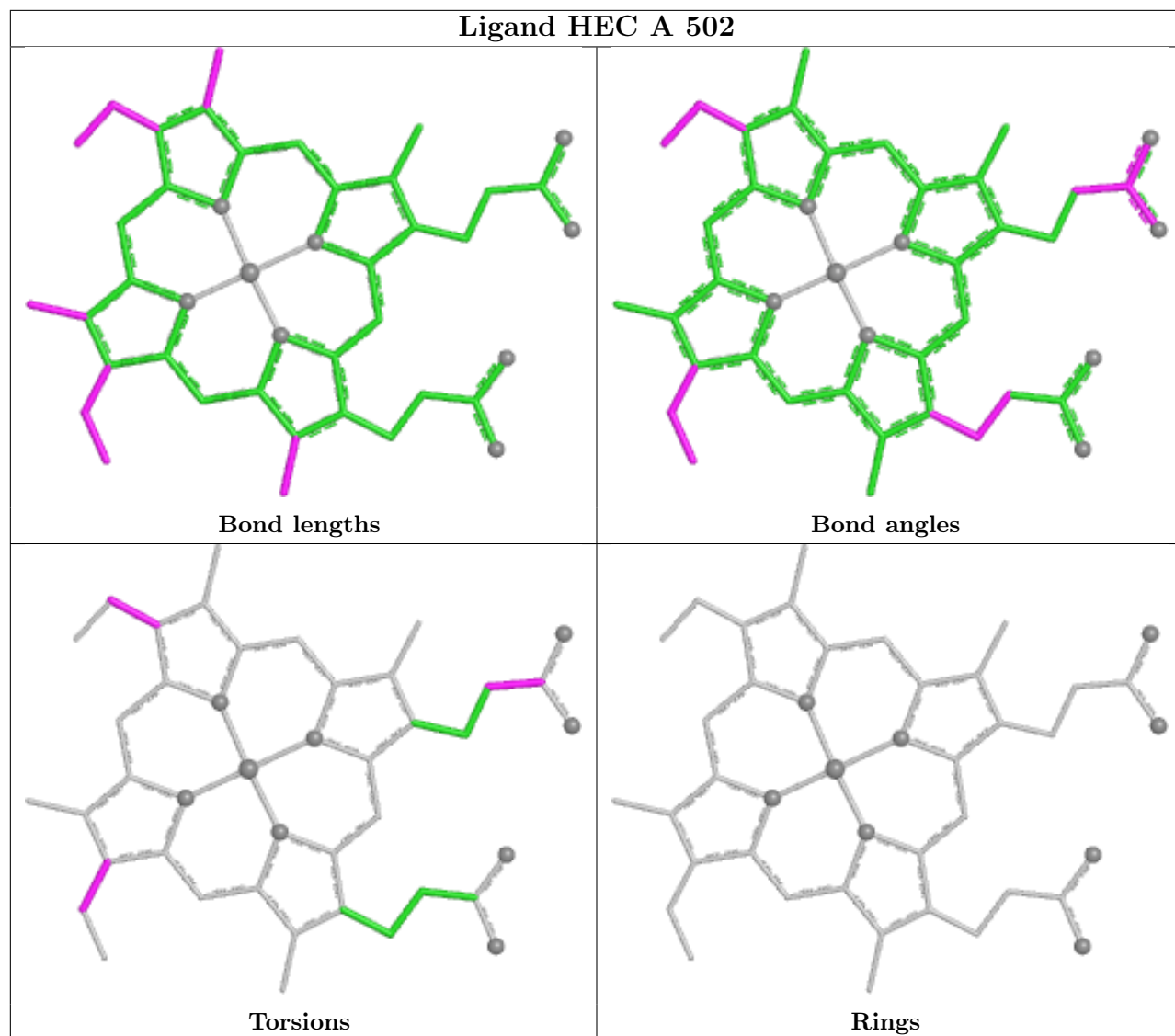
25 monomers are involved in 56 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	505	HEC	6	0
2	E	501	HEC	2	0
2	C	504	HEC	1	0
2	D	505	HEC	6	0
2	D	504	HEC	4	0
2	F	505	HEC	3	0
2	C	501	HEC	2	0
2	A	504	HEC	1	0
2	F	502	HEC	1	0
2	D	501	HEC	1	0
3	A	506	SO4	2	0
2	F	501	HEC	2	0
2	E	503	HEC	4	0
2	E	502	HEC	1	0
2	F	504	HEC	2	0
2	C	502	HEC	1	0
2	D	503	HEC	3	0
2	A	503	HEC	1	0
2	B	503	HEC	1	0
2	B	504	HEC	4	0
2	E	505	HEC	3	0
2	A	505	HEC	11	0
2	C	503	HEC	1	0
3	C	506	SO4	2	0
2	E	504	HEC	1	0

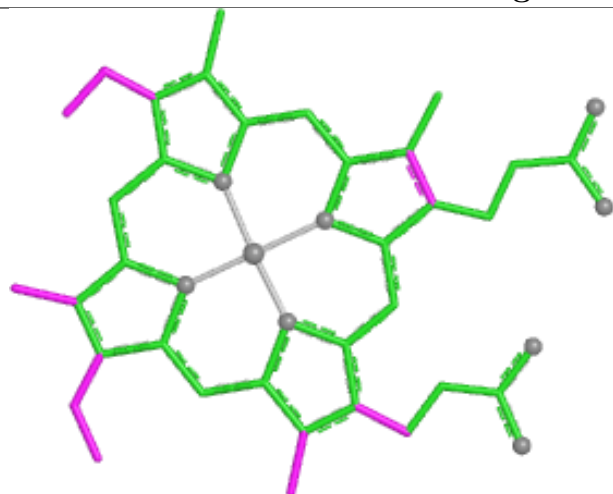
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

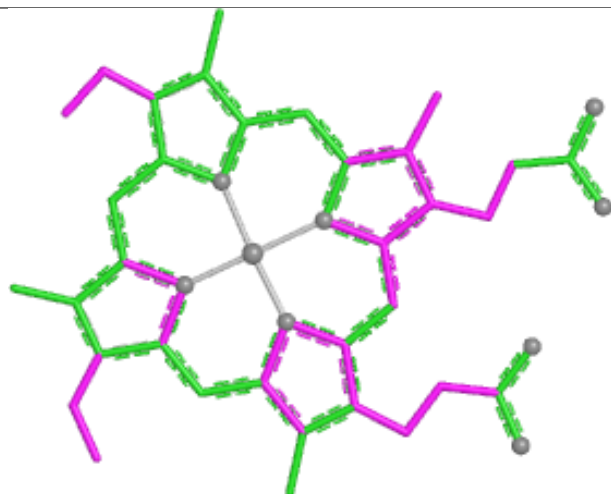




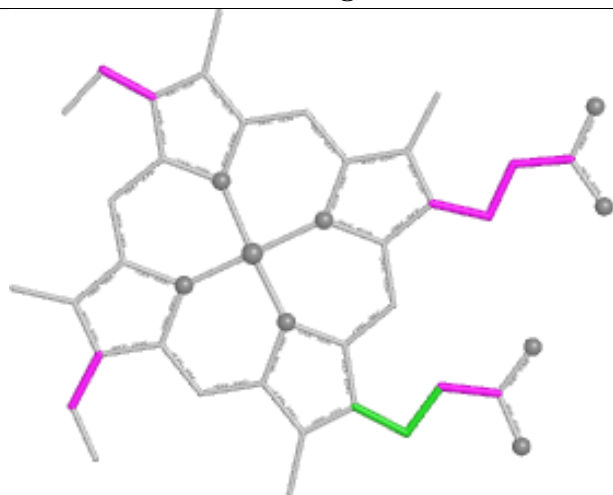
Ligand HEC B 505



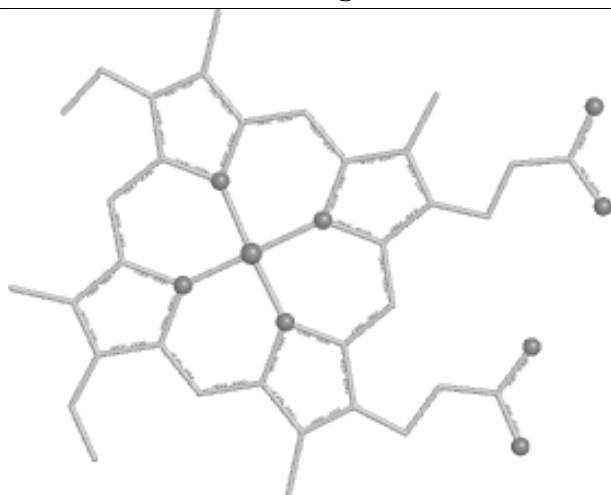
Bond lengths



Bond angles

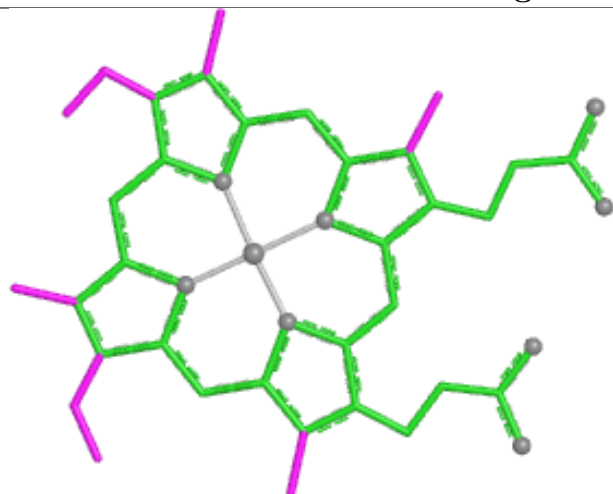


Torsions

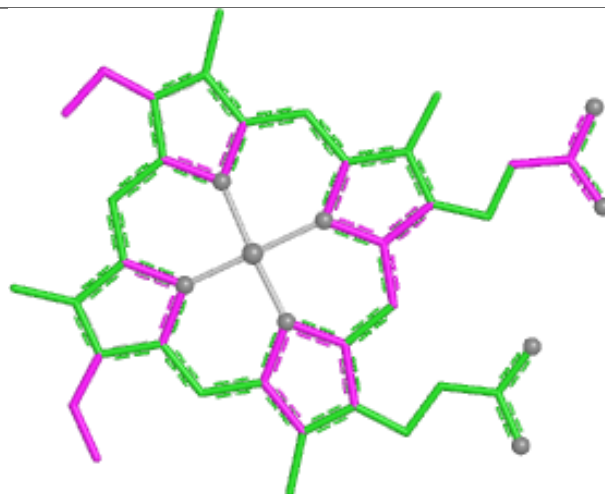


Rings

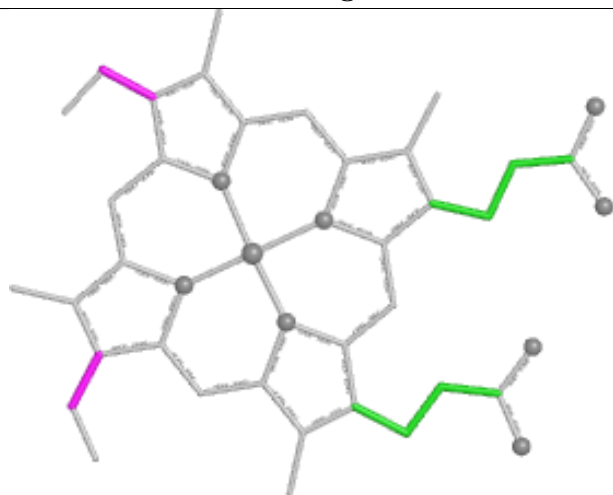
Ligand HEC F 503



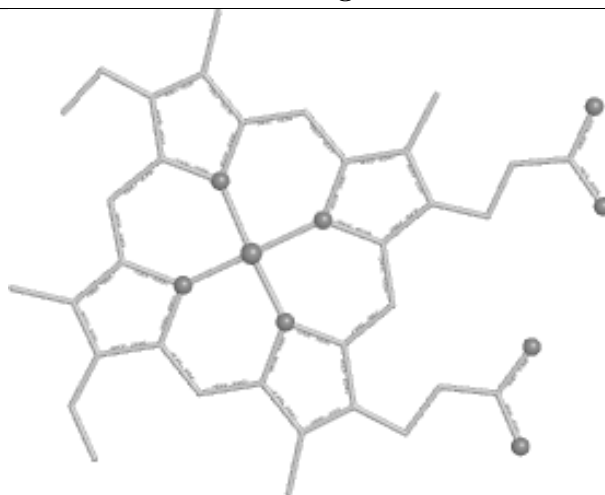
Bond lengths



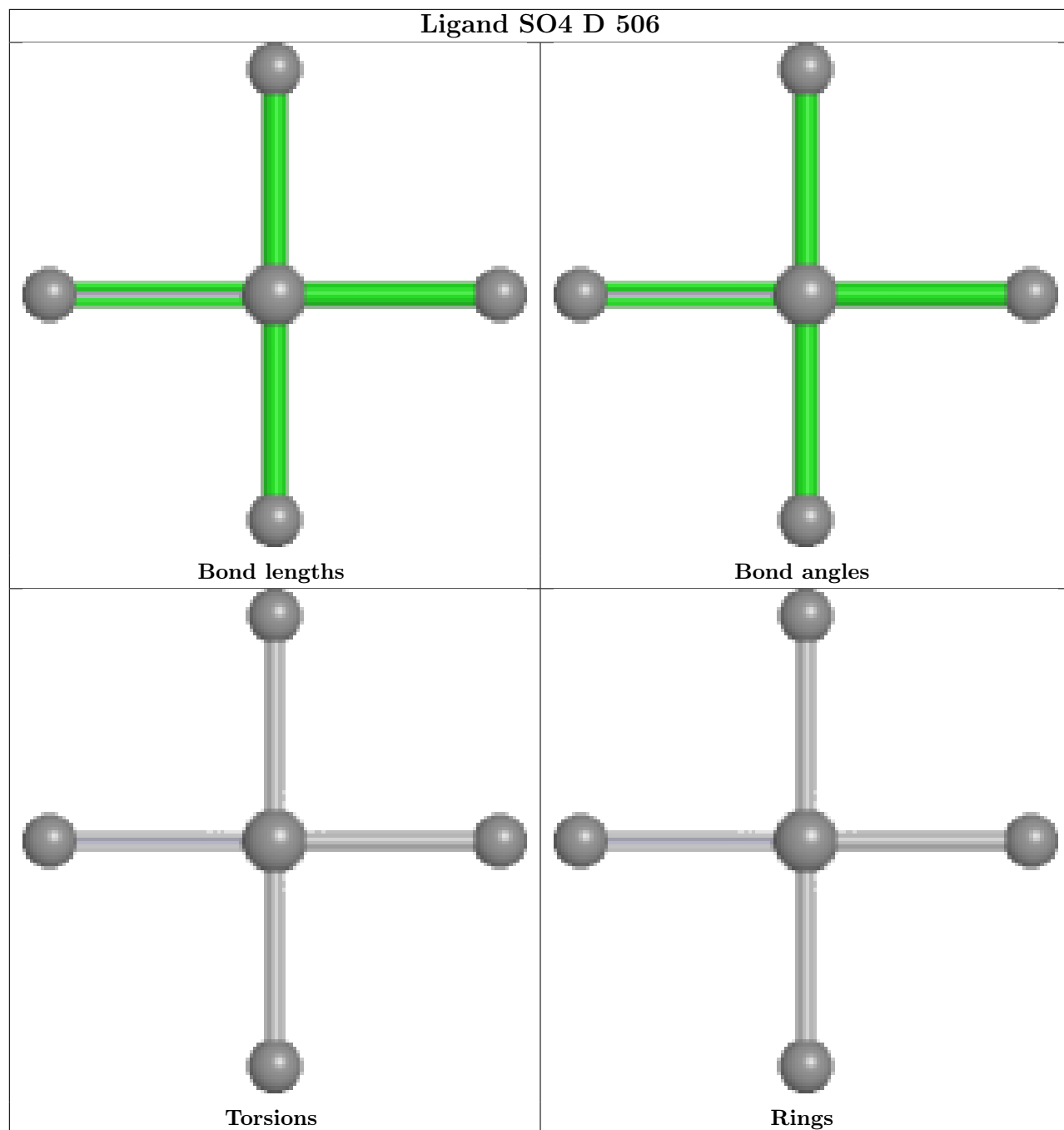
Bond angles



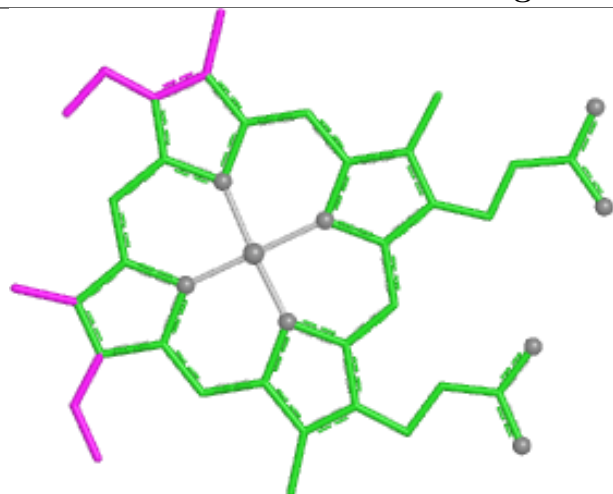
Torsions



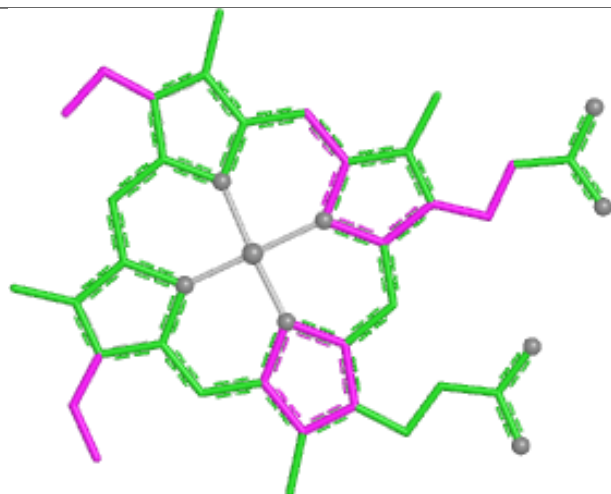
Rings



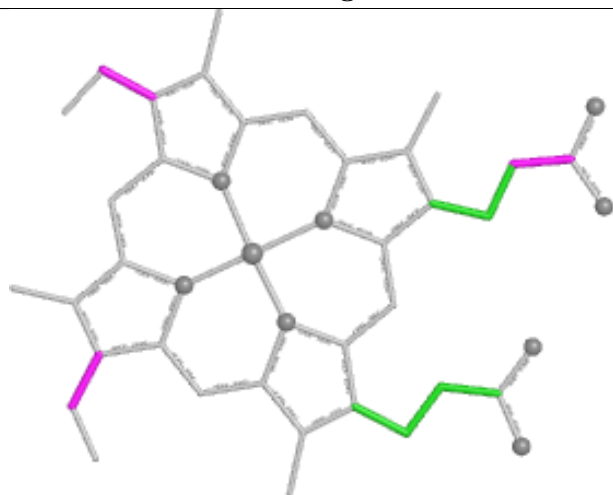
Ligand HEC E 501



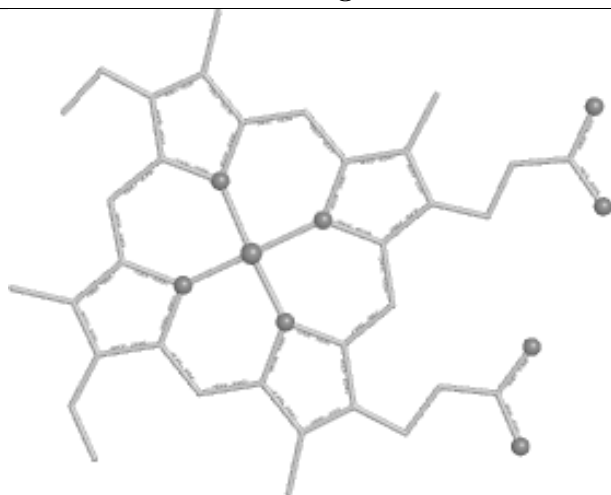
Bond lengths



Bond angles

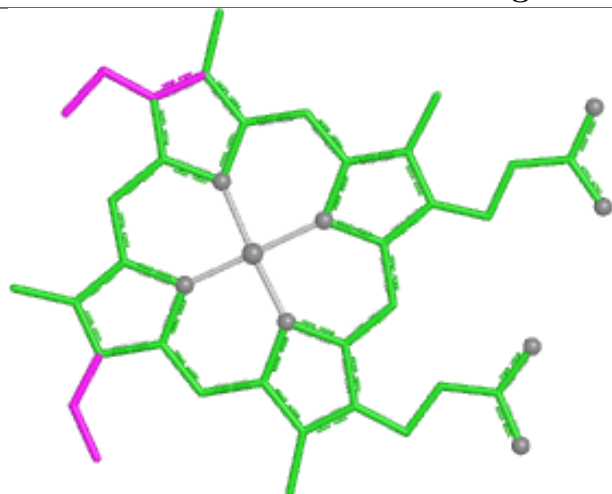


Torsions

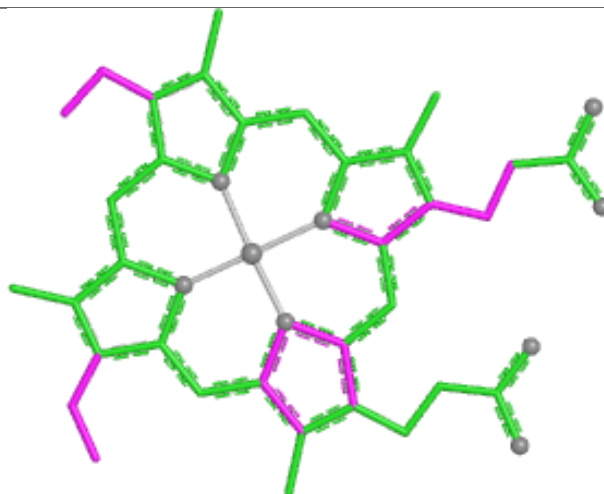


Rings

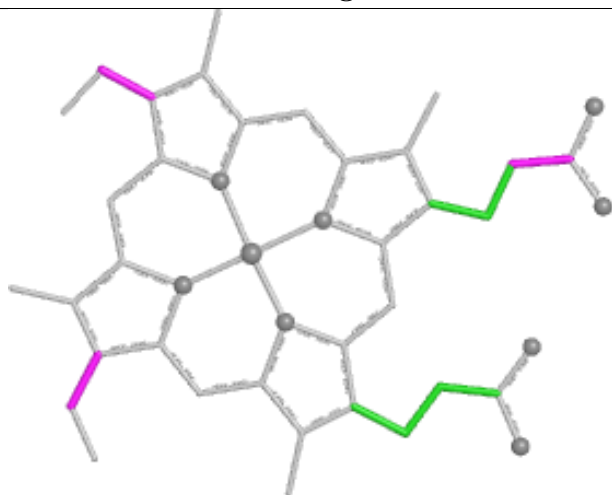
Ligand HEC C 504



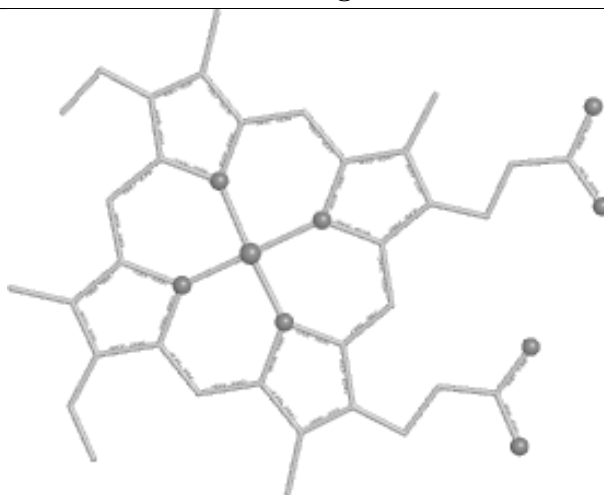
Bond lengths



Bond angles

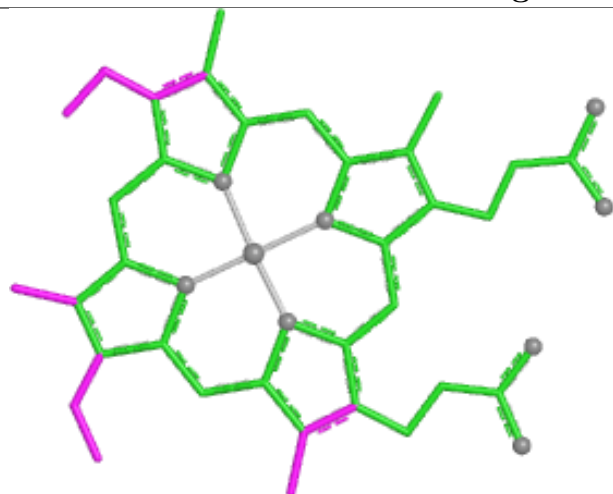


Torsions

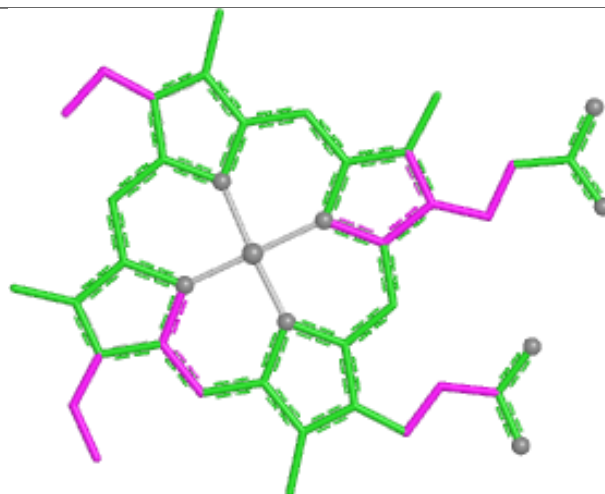


Rings

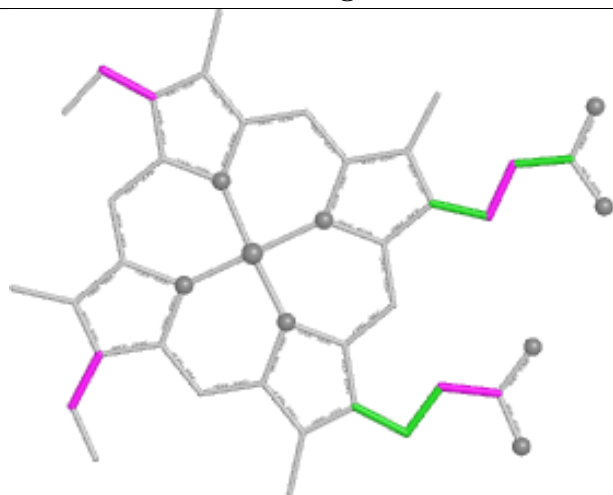
Ligand HEC D 505



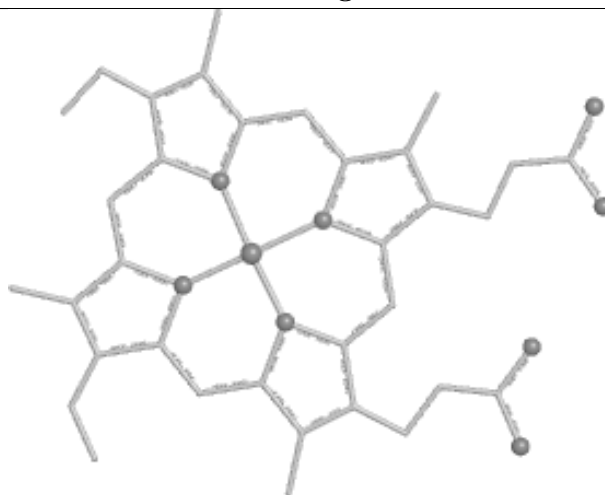
Bond lengths



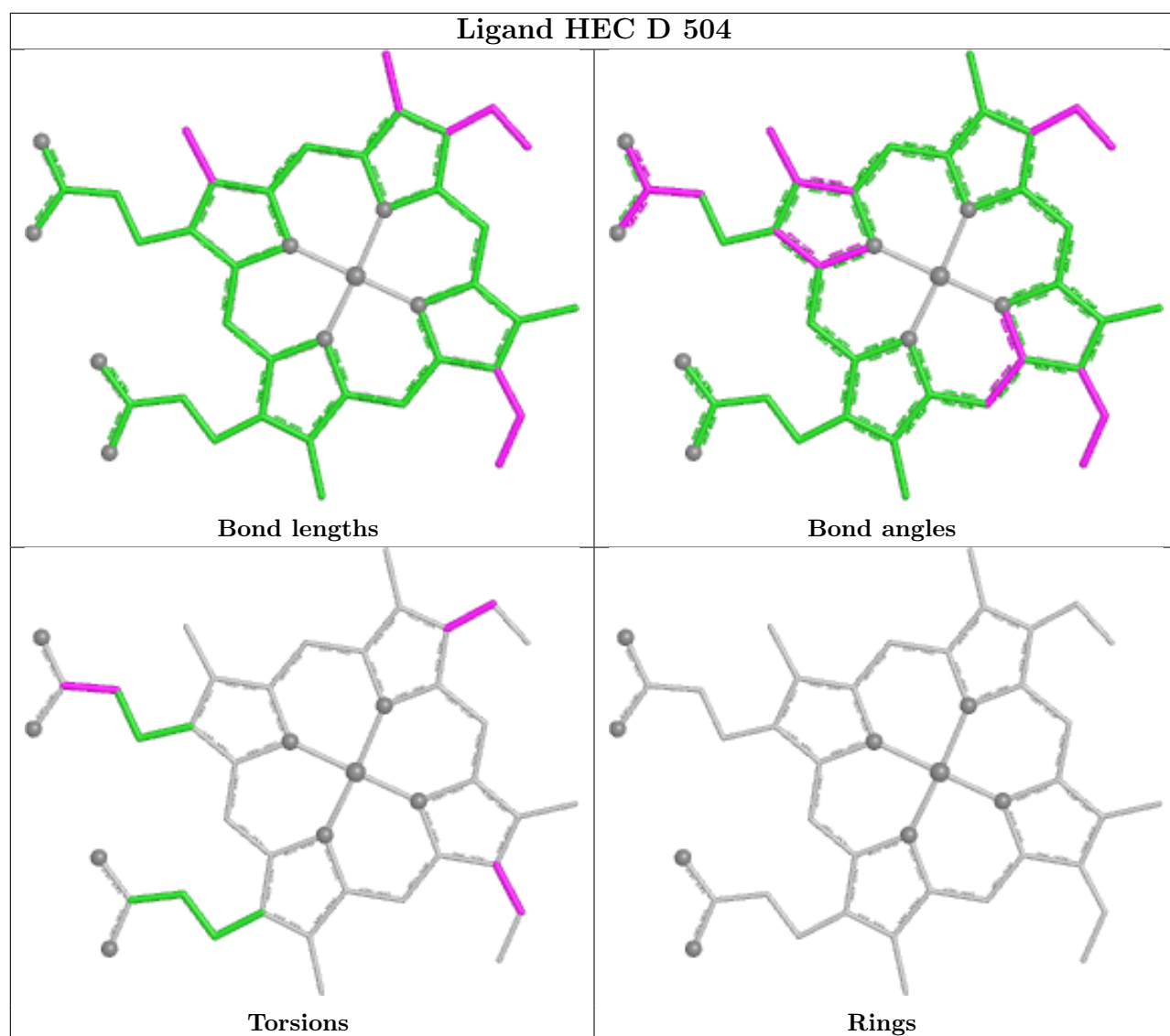
Bond angles



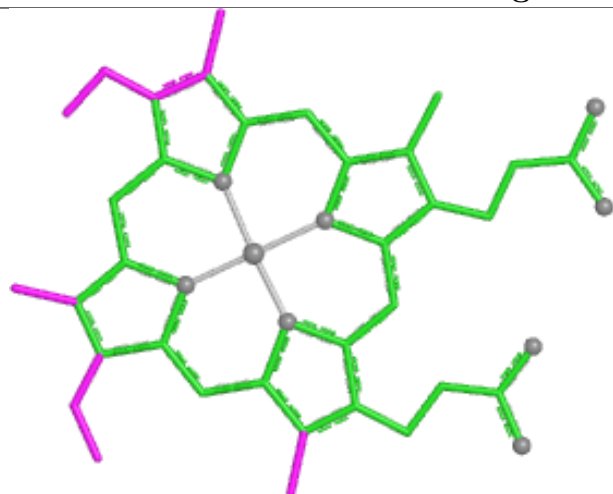
Torsions



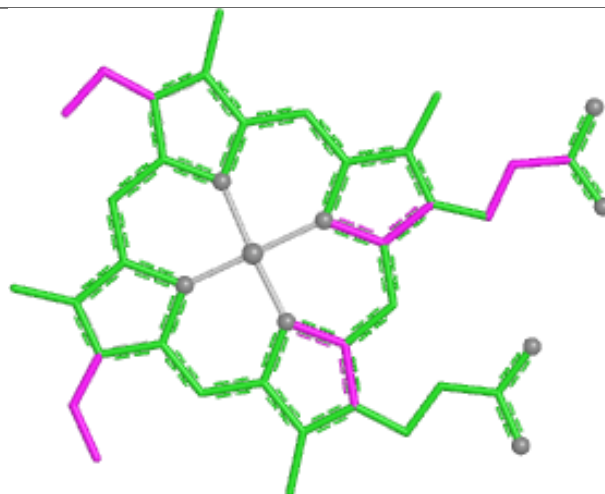
Rings



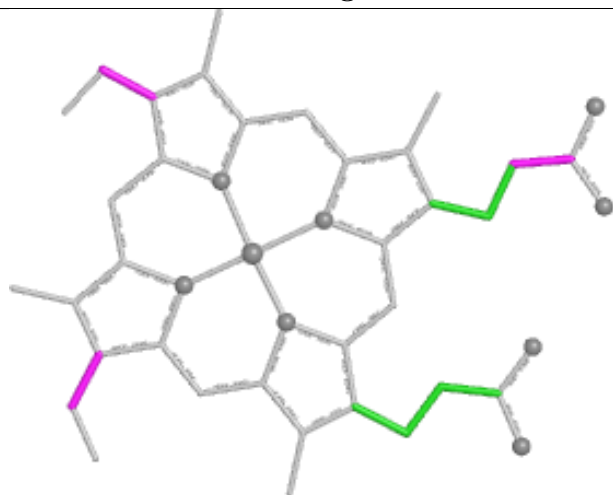
Ligand HEC A 501



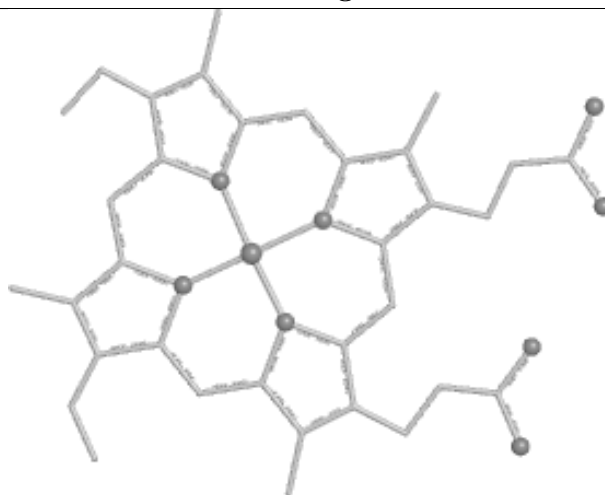
Bond lengths



Bond angles

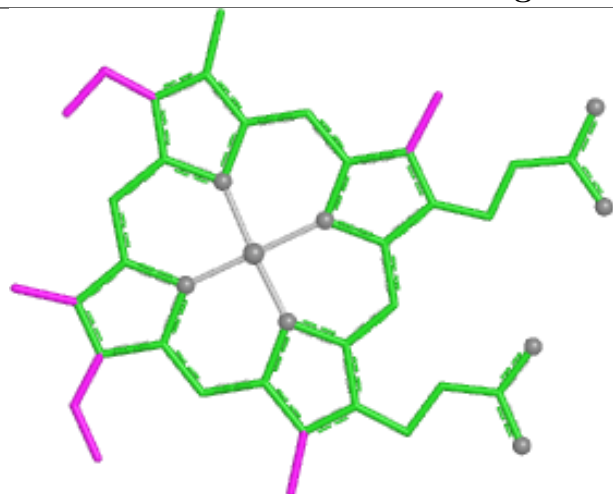


Torsions

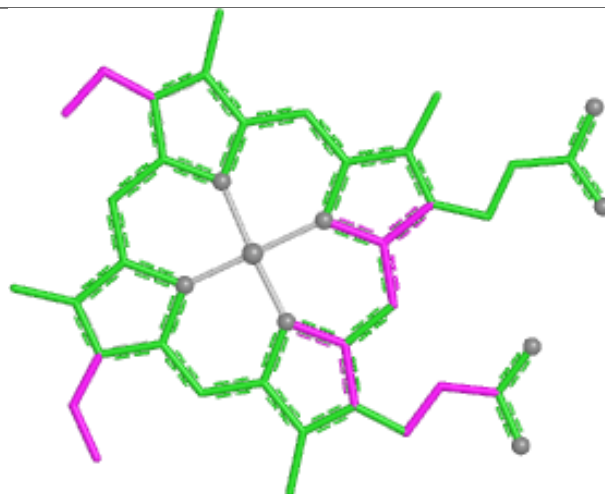


Rings

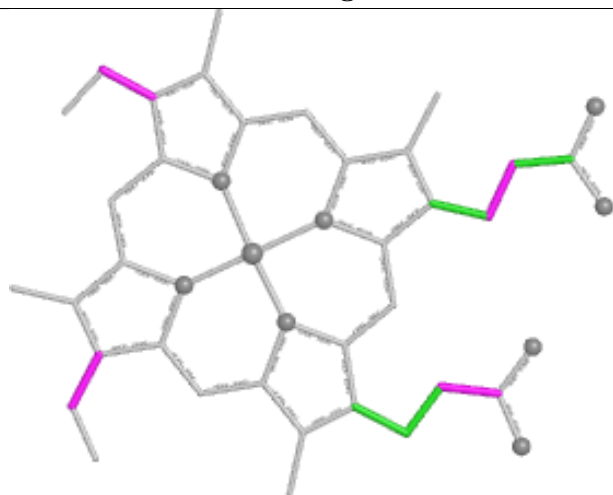
Ligand HEC F 505



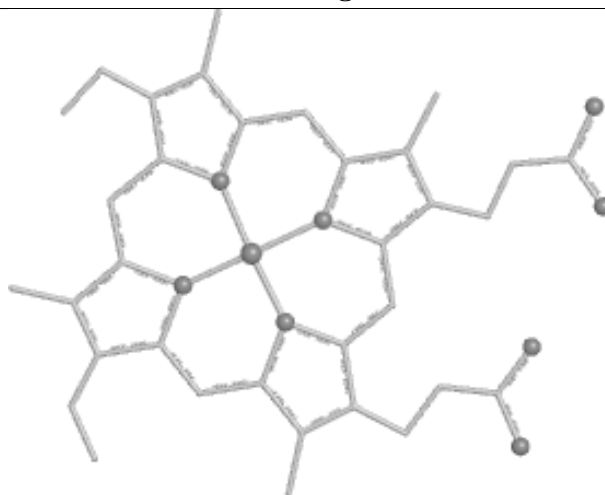
Bond lengths



Bond angles

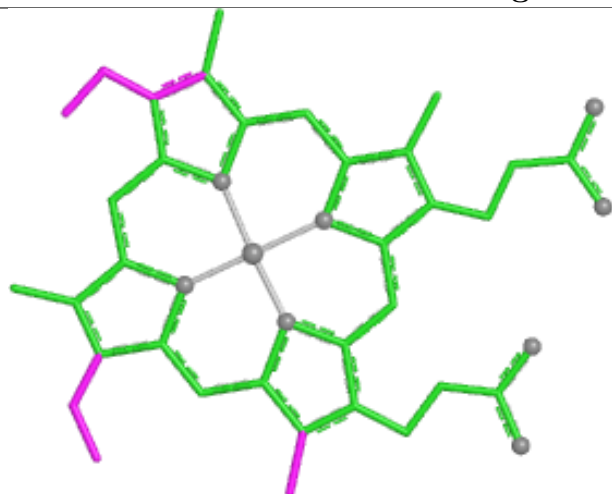


Torsions

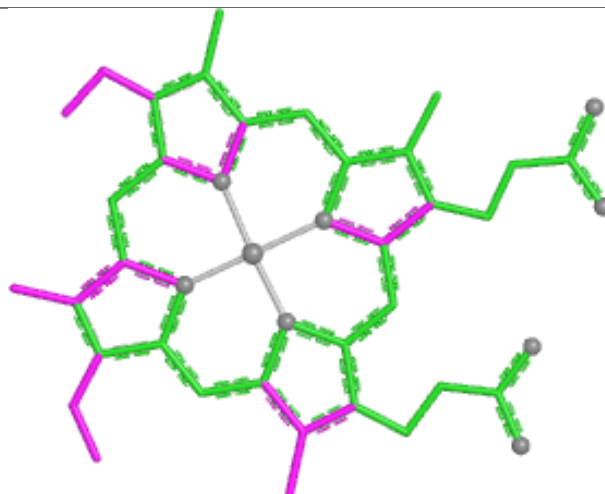


Rings

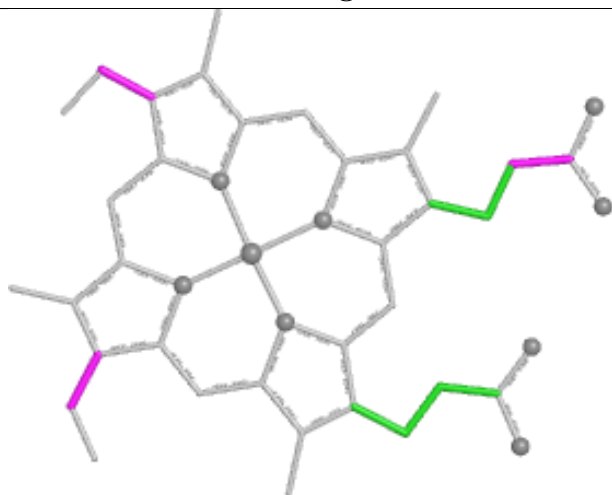
Ligand HEC C 501



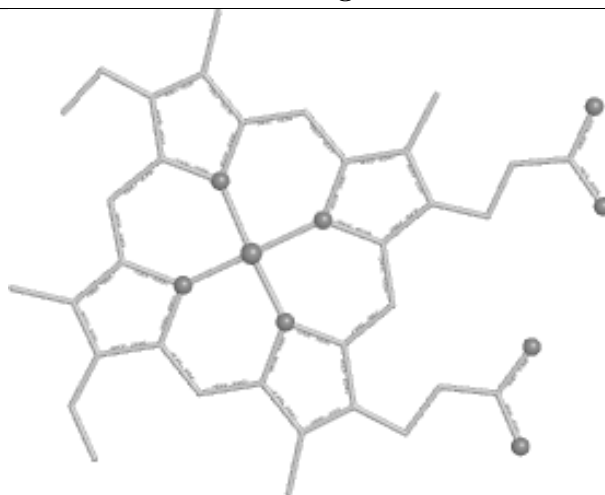
Bond lengths



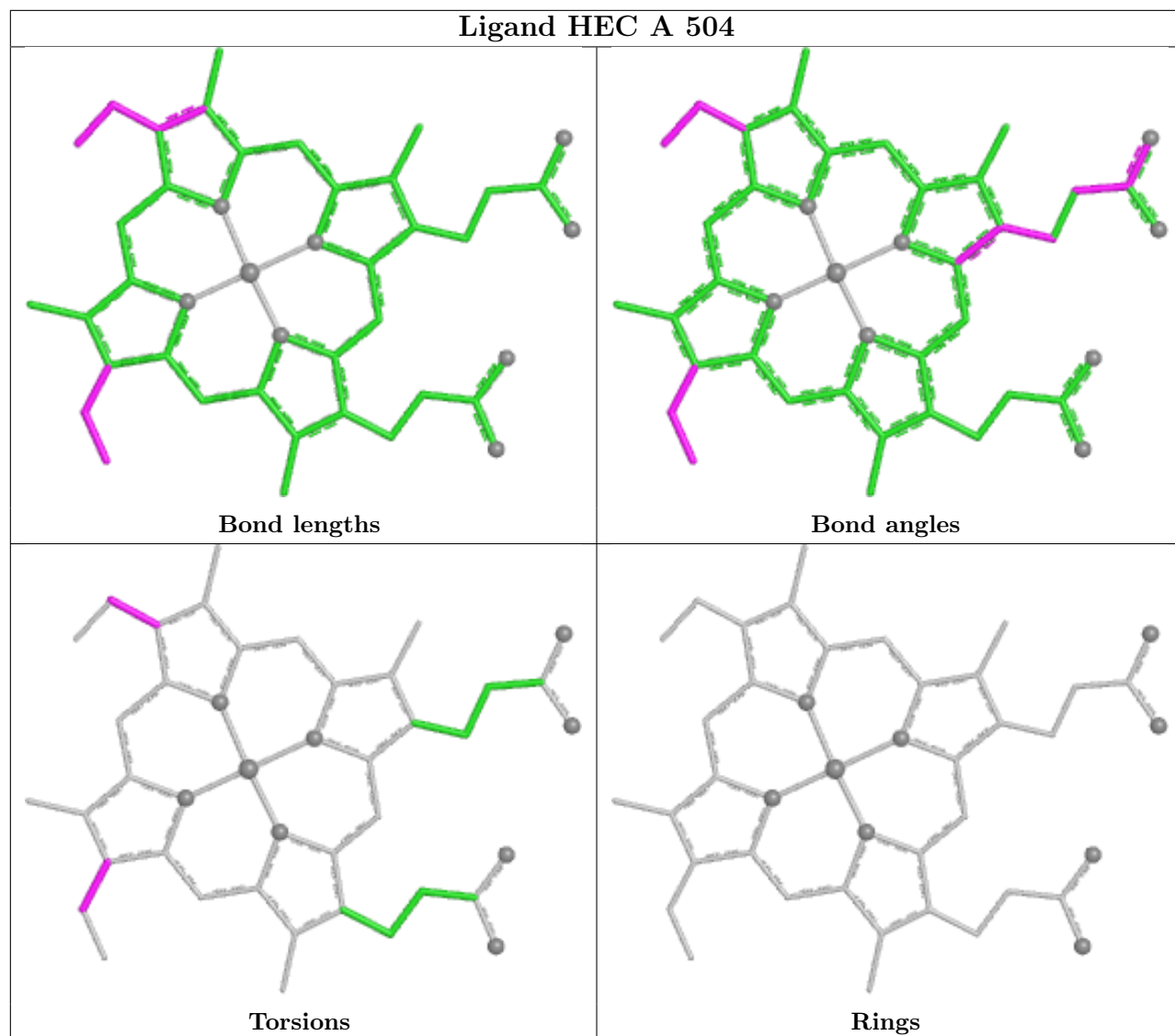
Bond angles



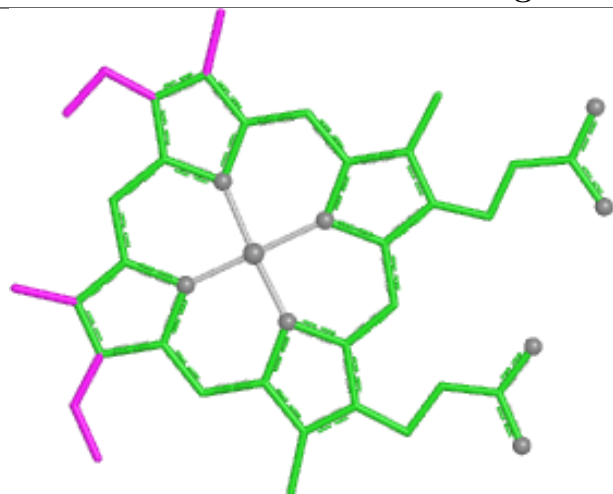
Torsions



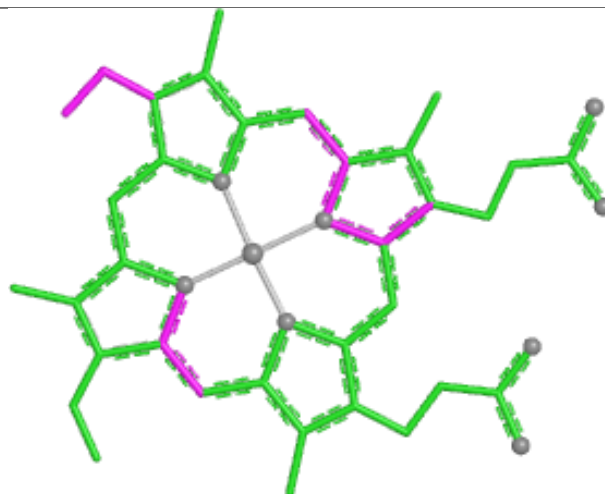
Rings



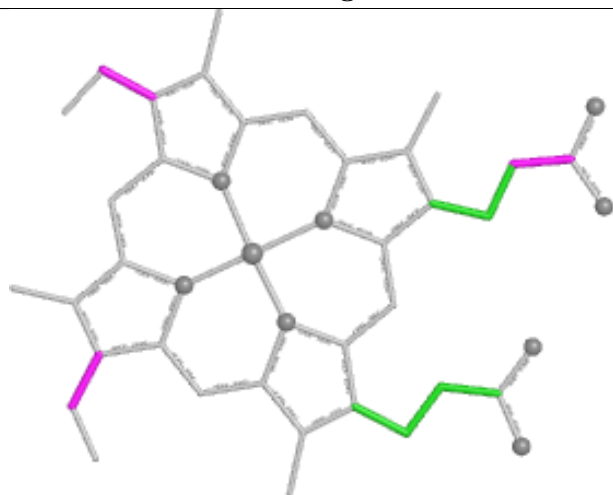
Ligand HEC F 502



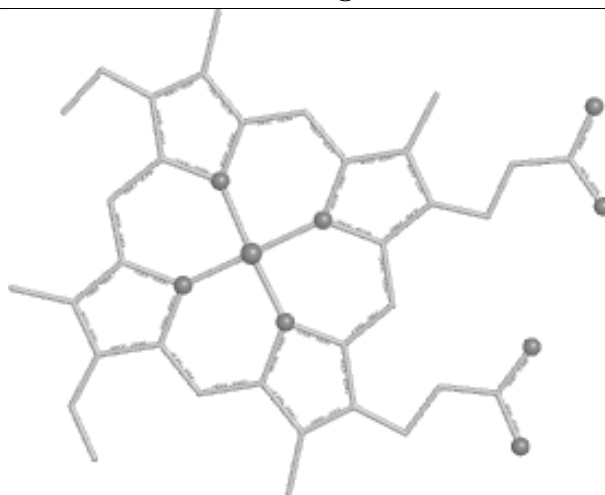
Bond lengths



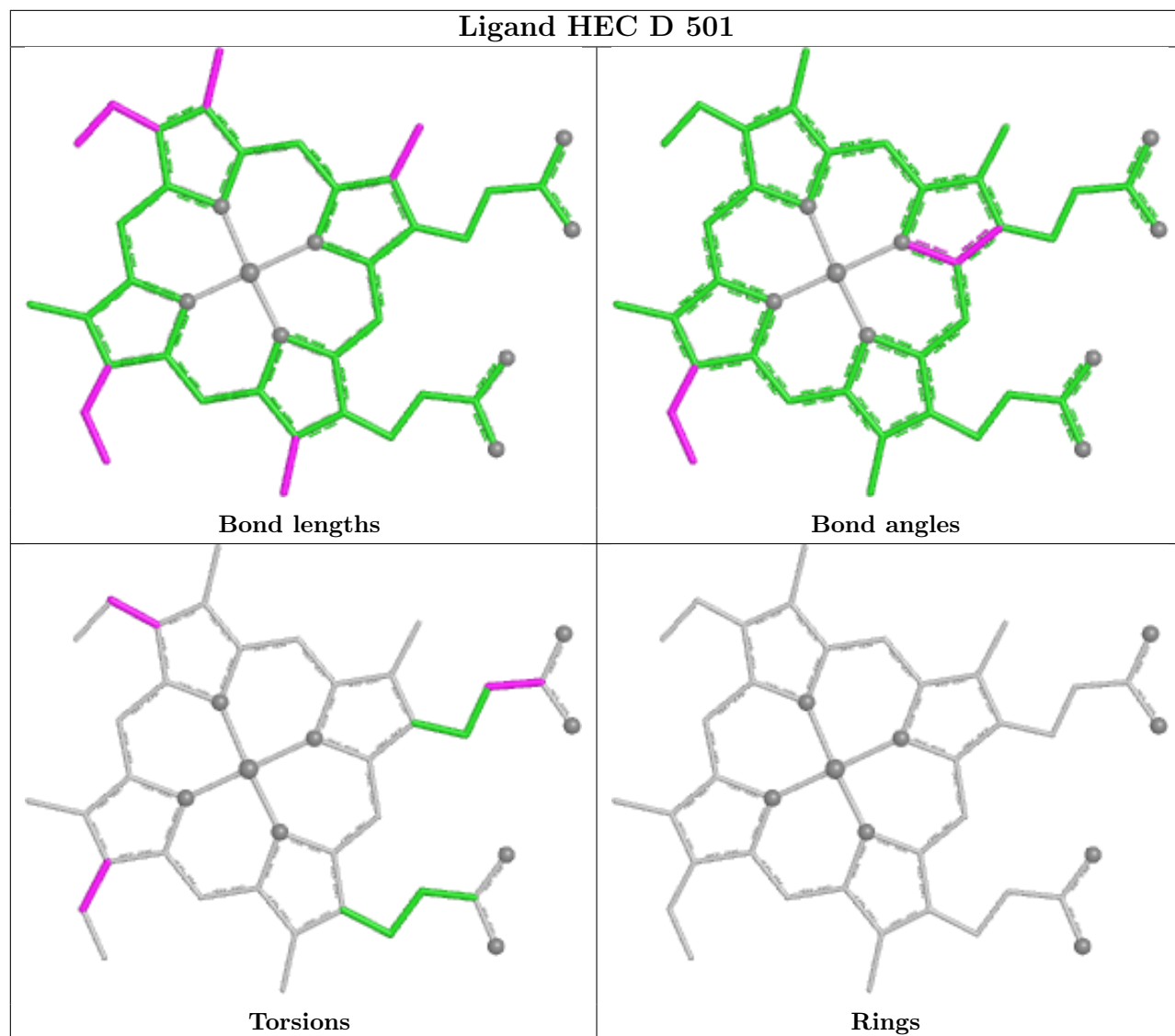
Bond angles

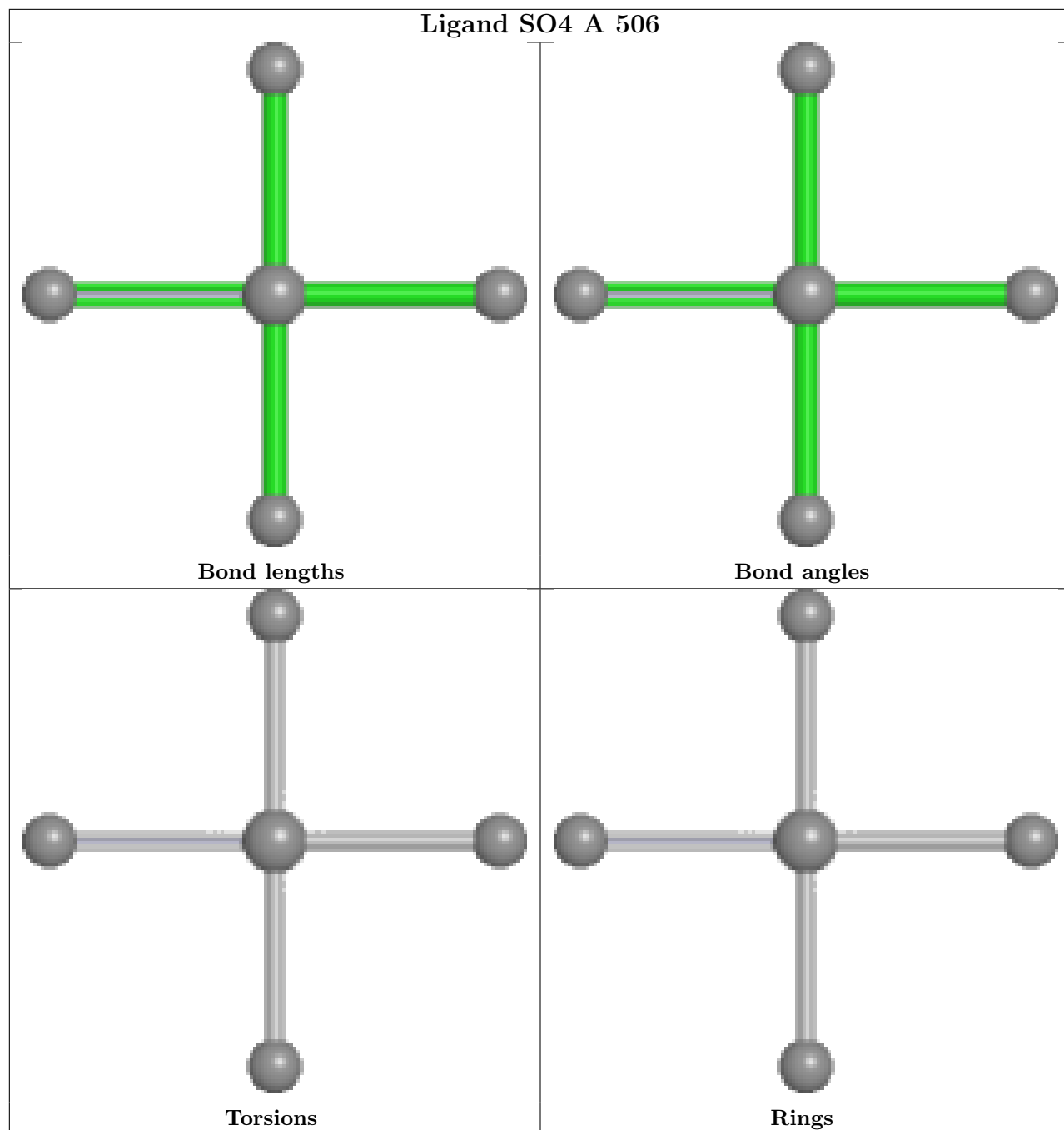


Torsions

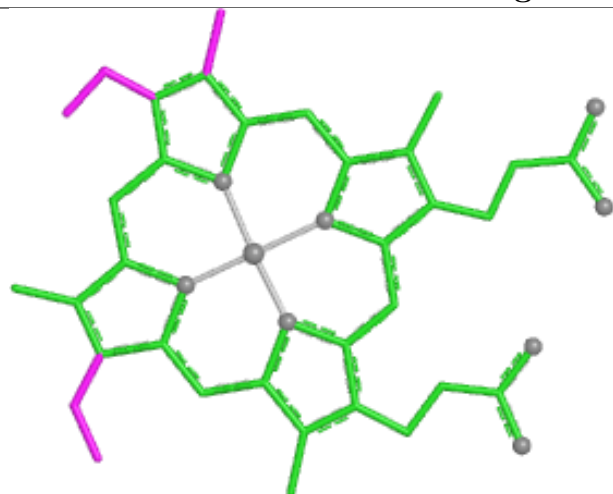


Rings

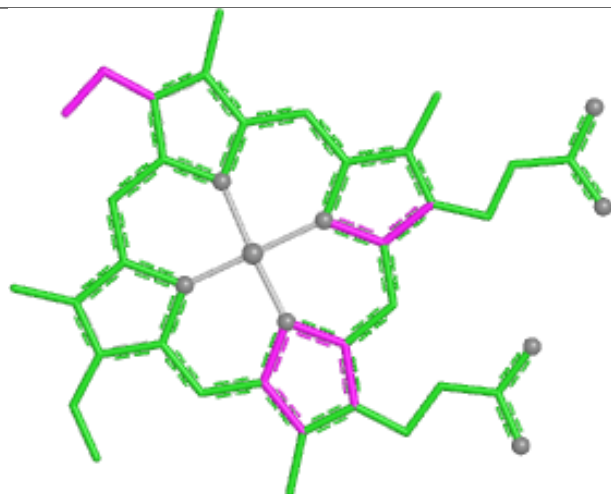




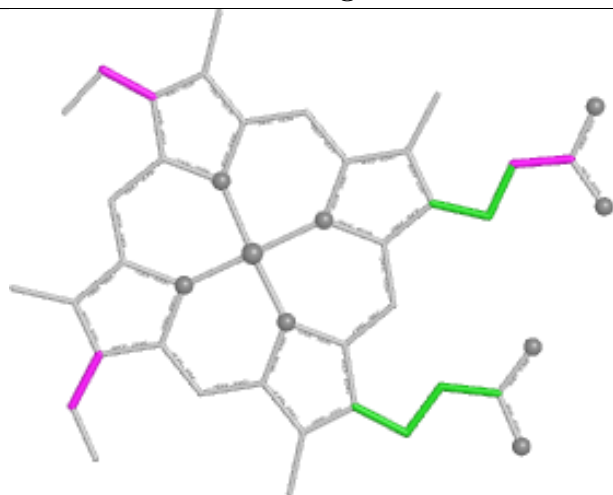
Ligand HEC F 501



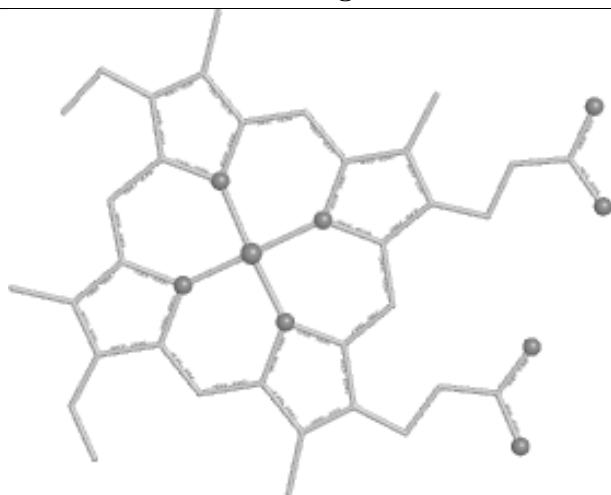
Bond lengths



Bond angles

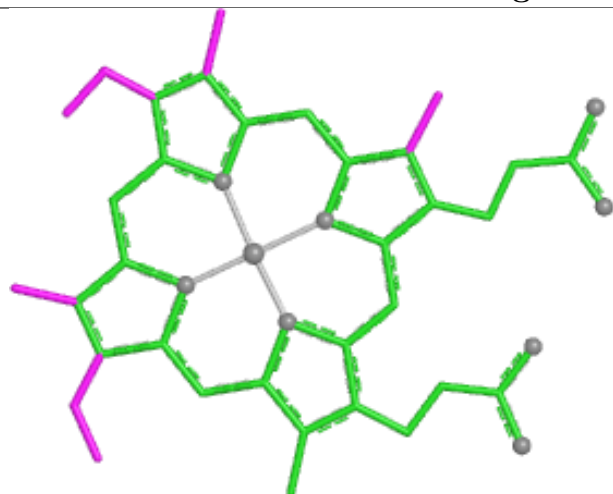


Torsions

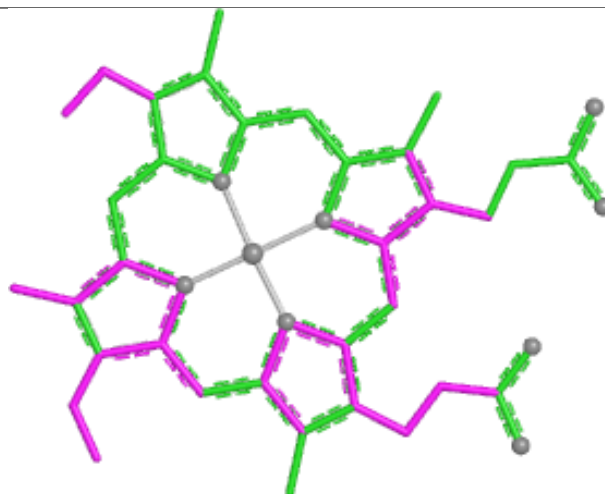


Rings

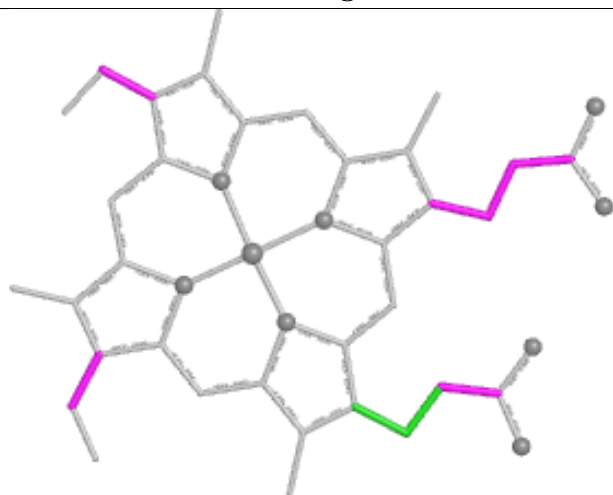
Ligand HEC C 505



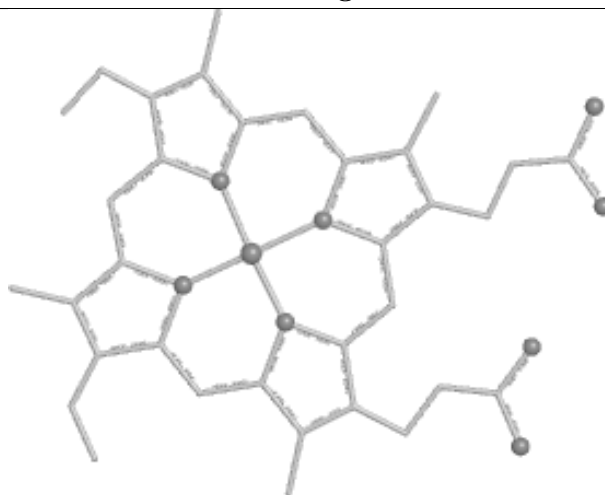
Bond lengths



Bond angles

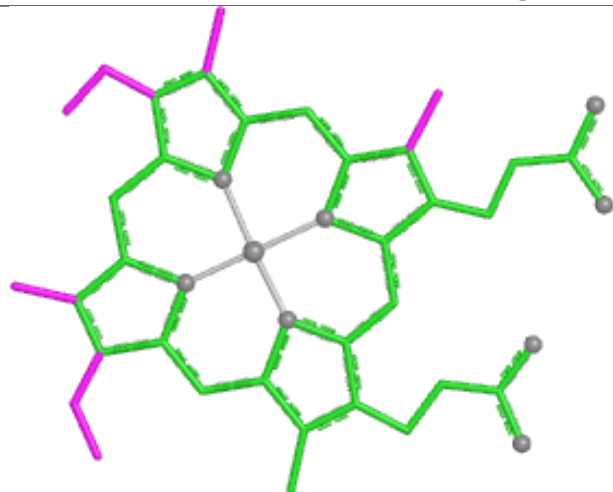


Torsions

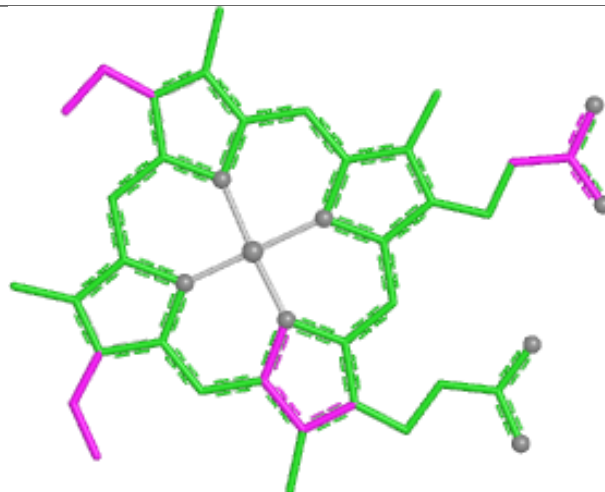


Rings

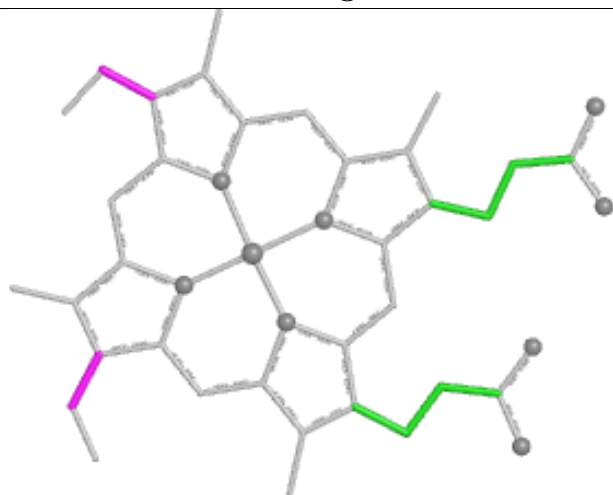
Ligand HEC E 503



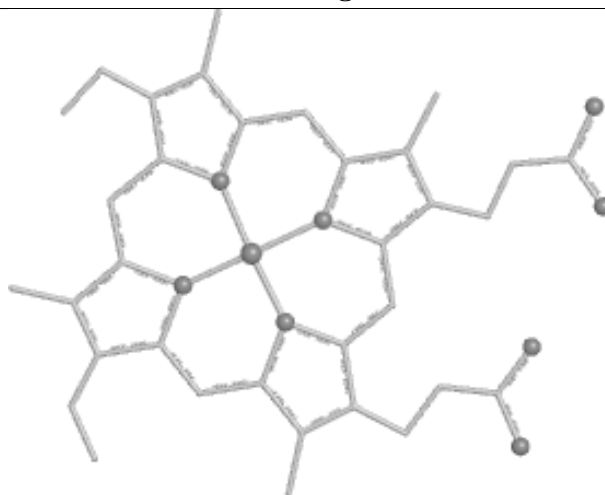
Bond lengths



Bond angles

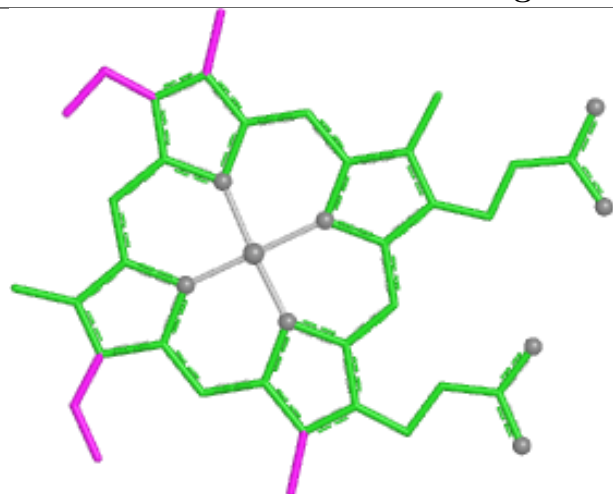


Torsions

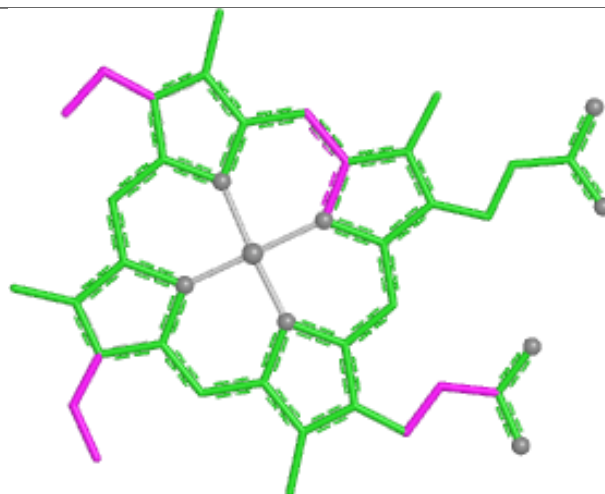


Rings

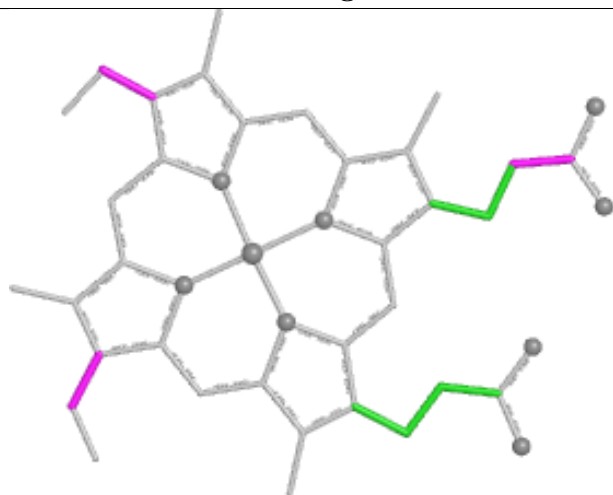
Ligand HEC E 502



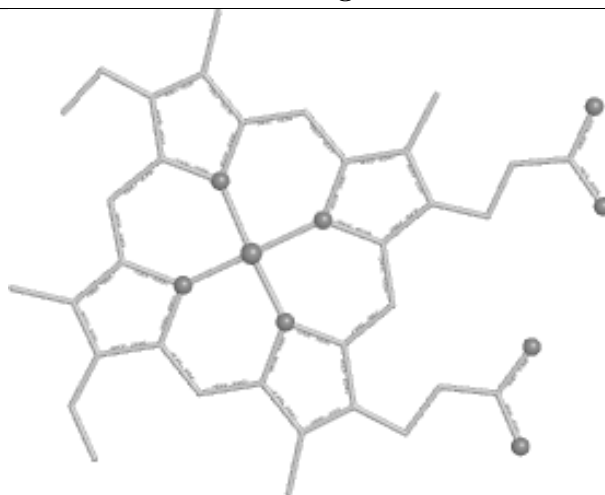
Bond lengths



Bond angles

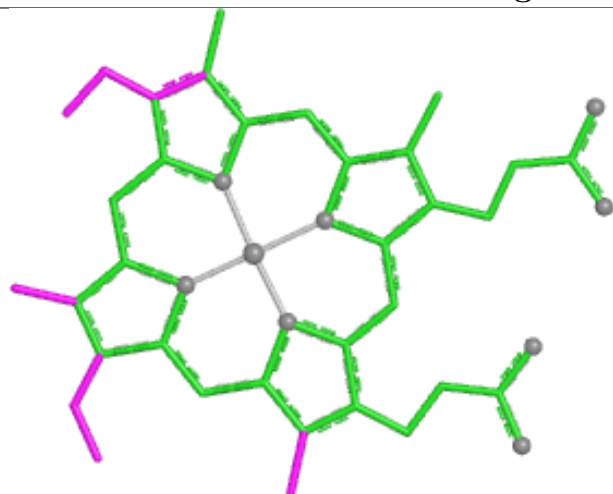


Torsions

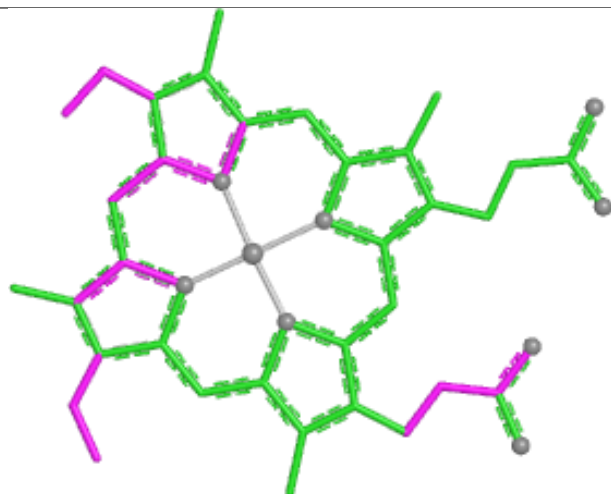


Rings

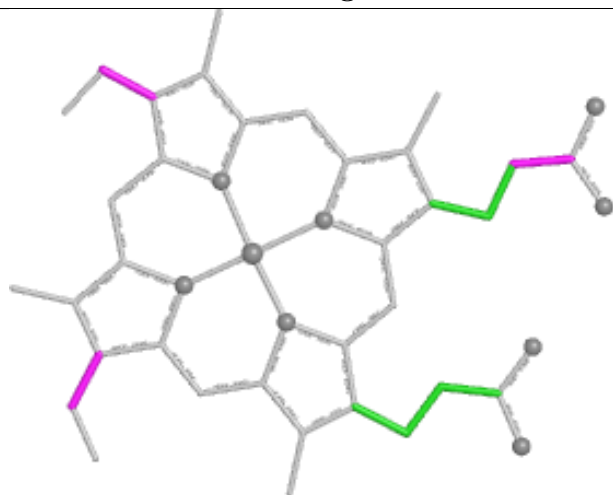
Ligand HEC F 504



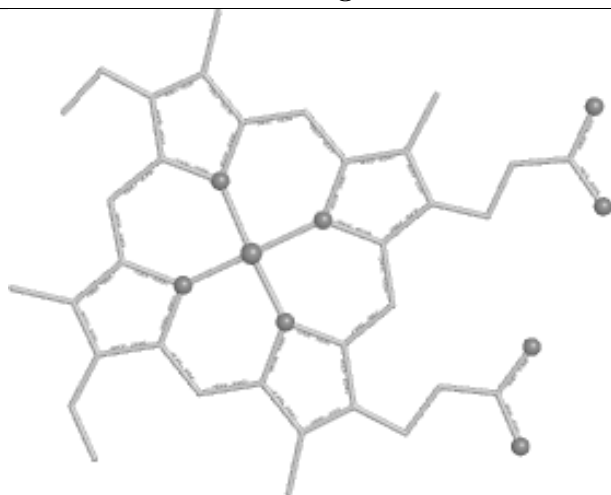
Bond lengths



Bond angles

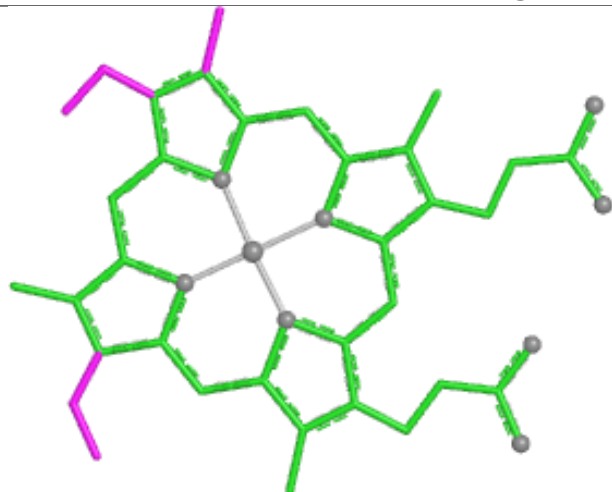


Torsions

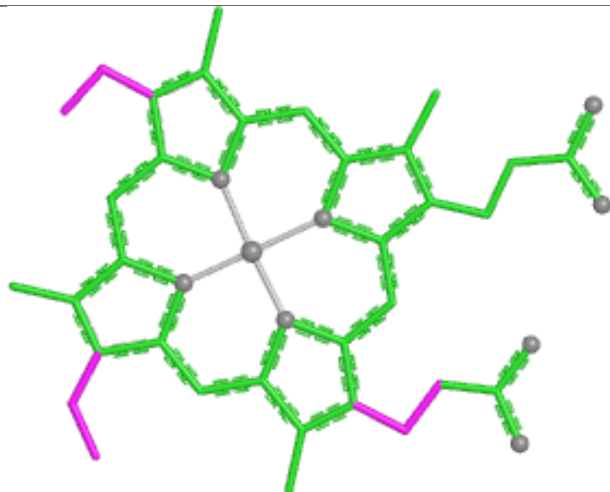


Rings

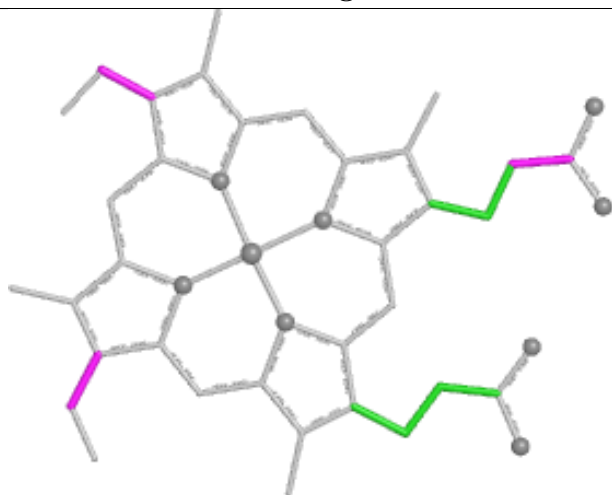
Ligand HEC C 502



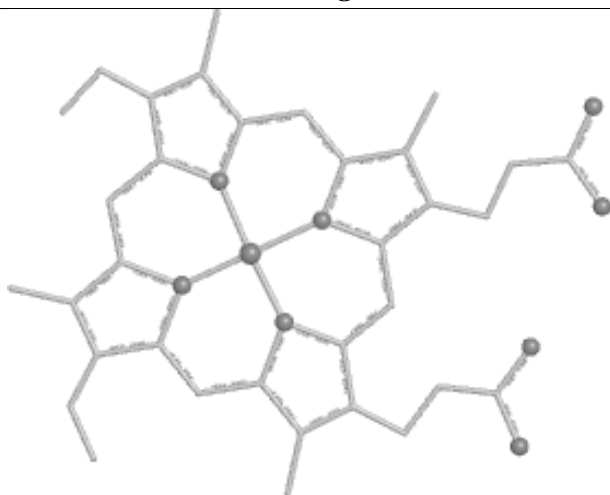
Bond lengths



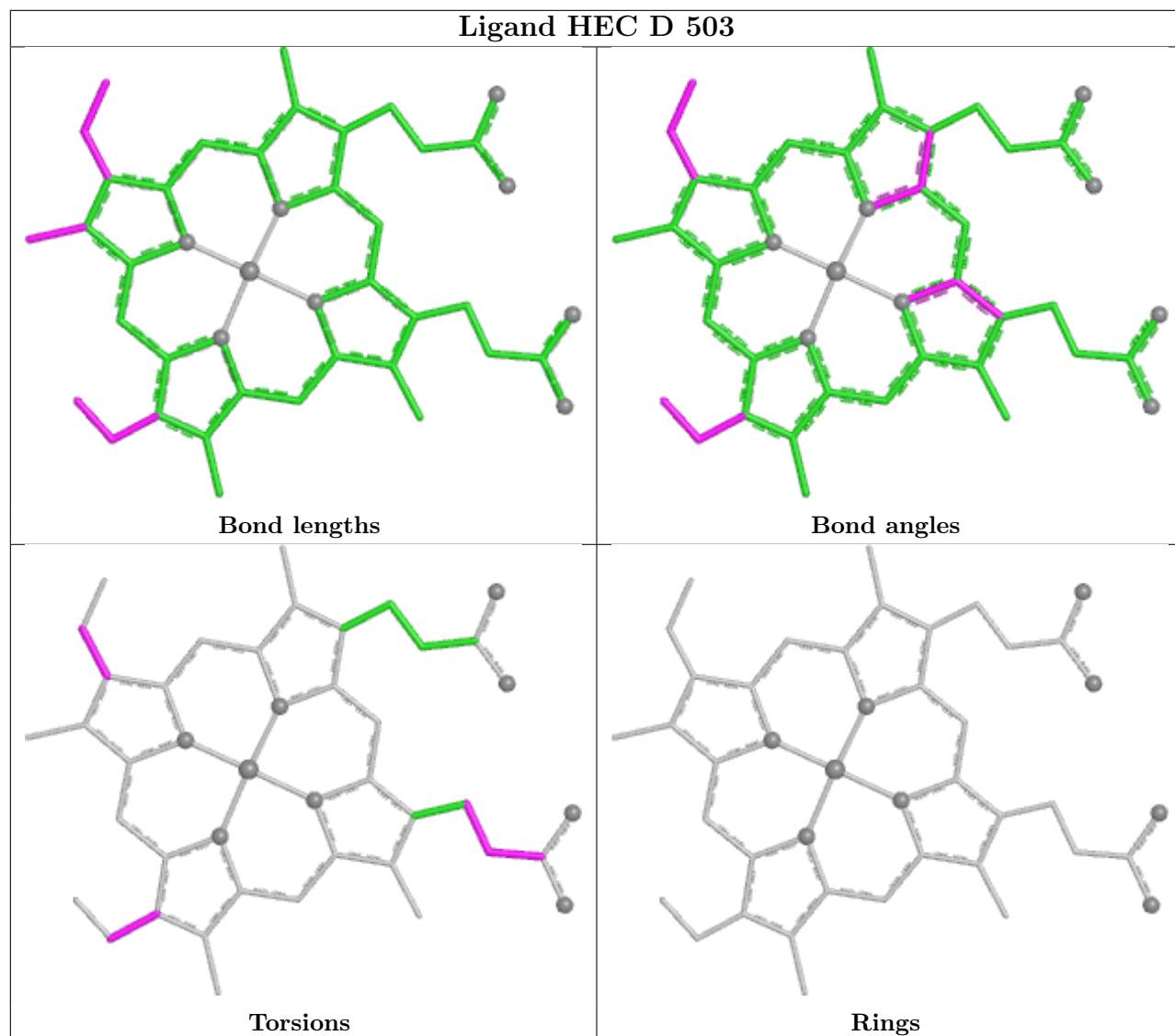
Bond angles

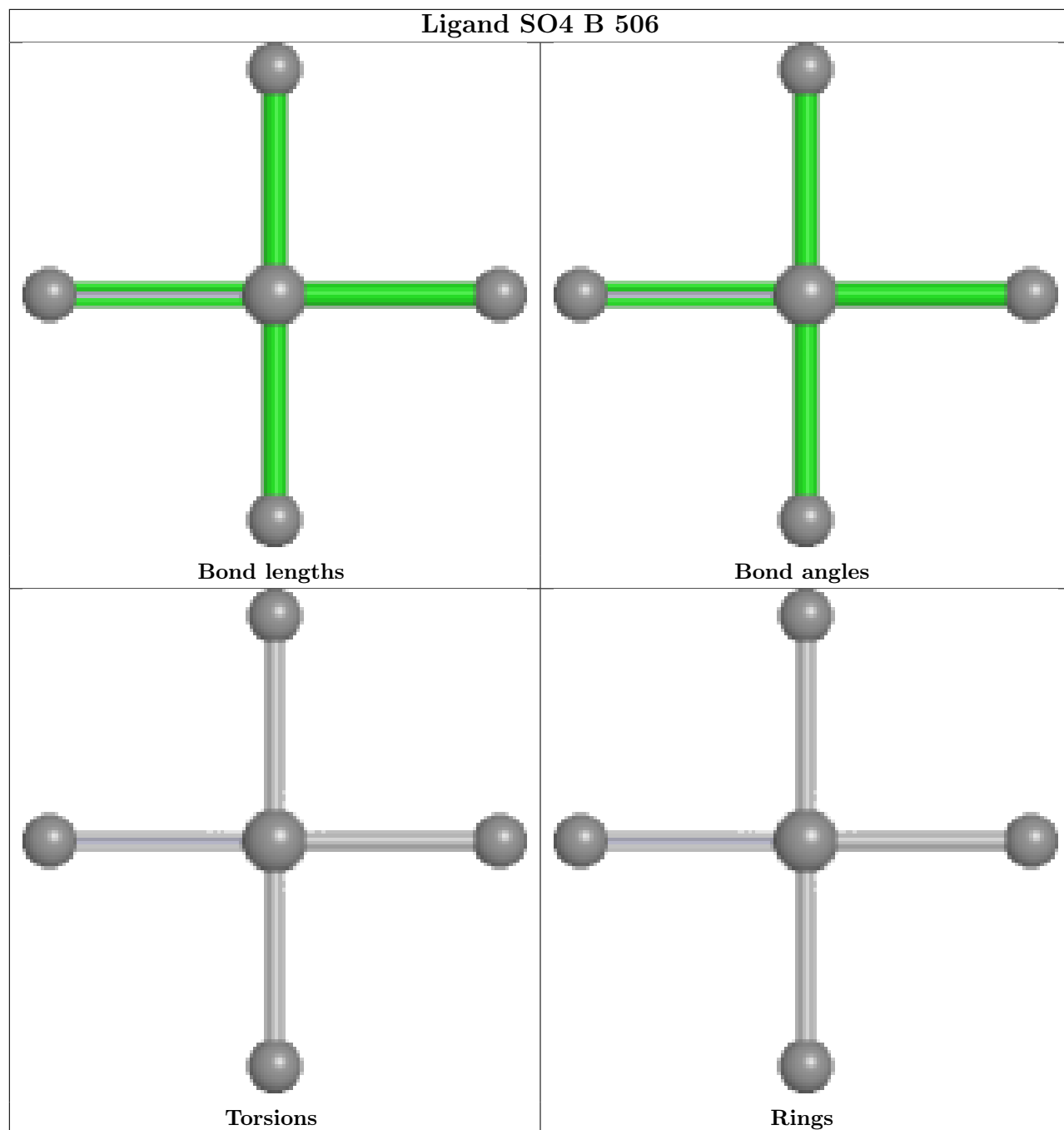


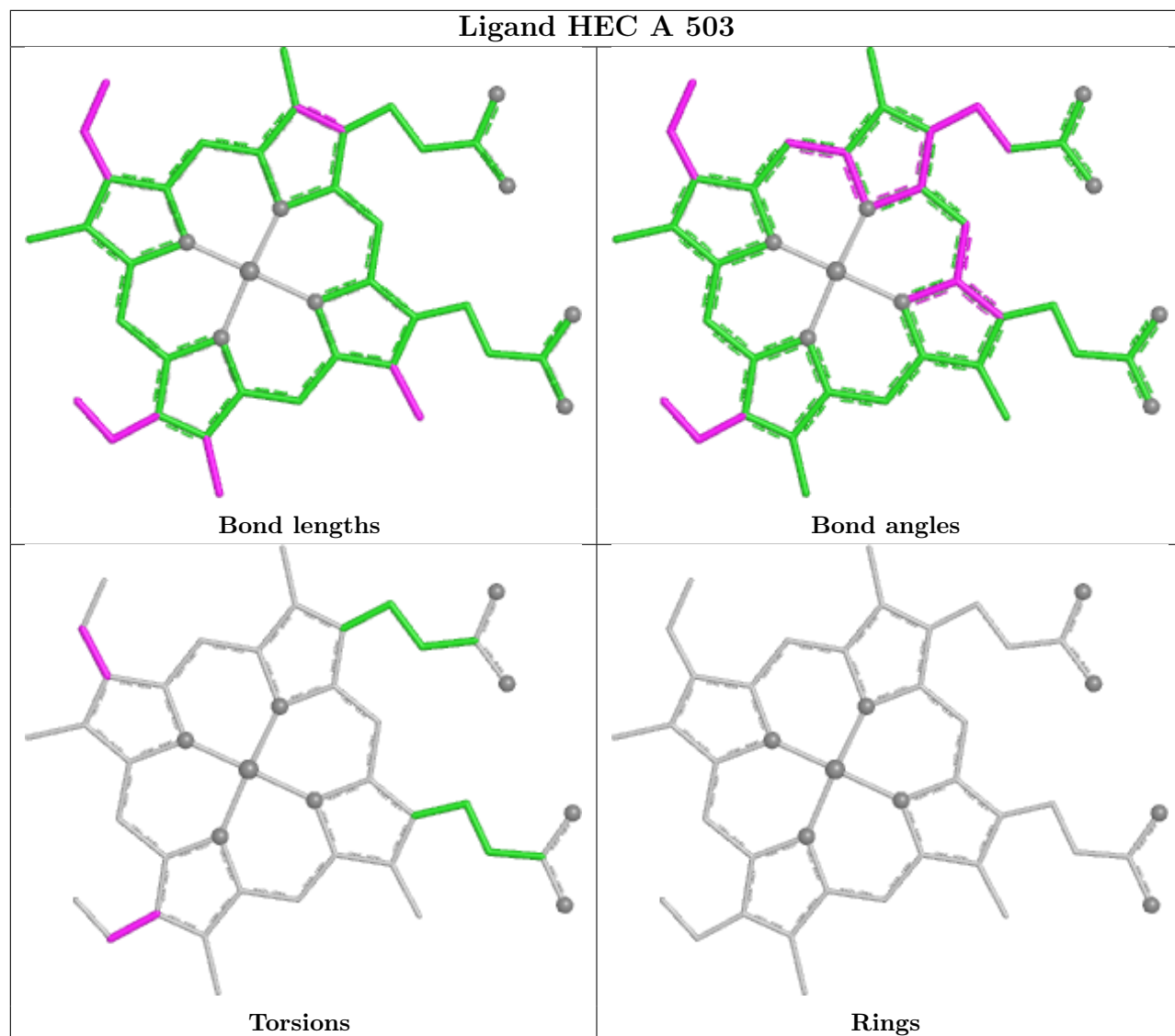
Torsions



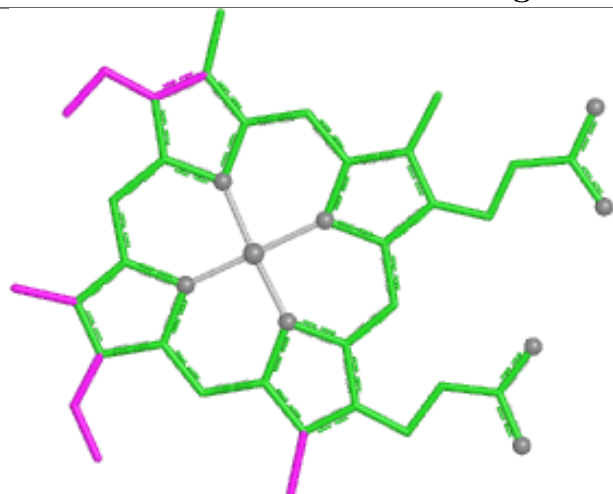
Rings



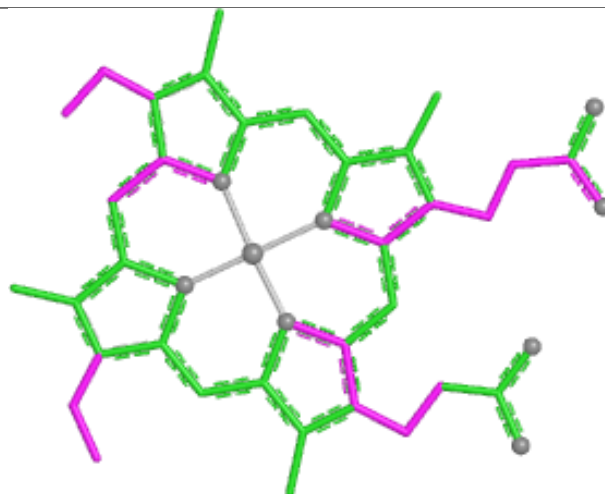




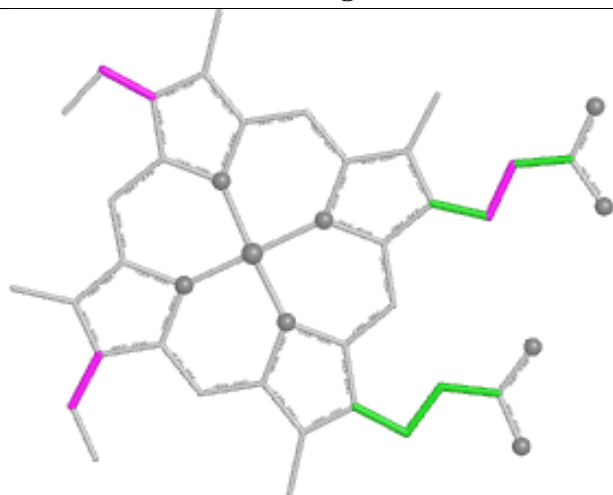
Ligand HEC B 503



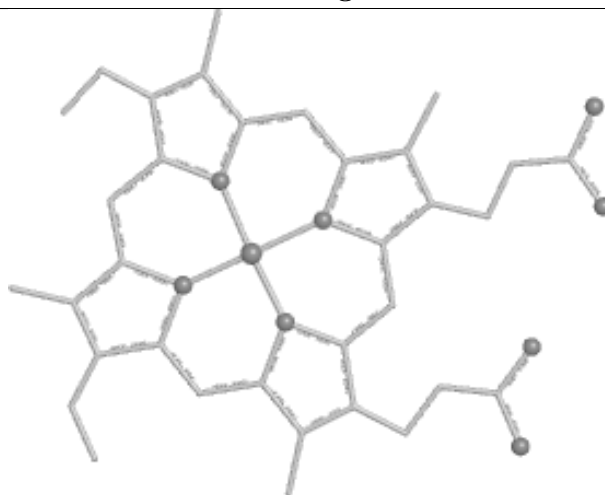
Bond lengths



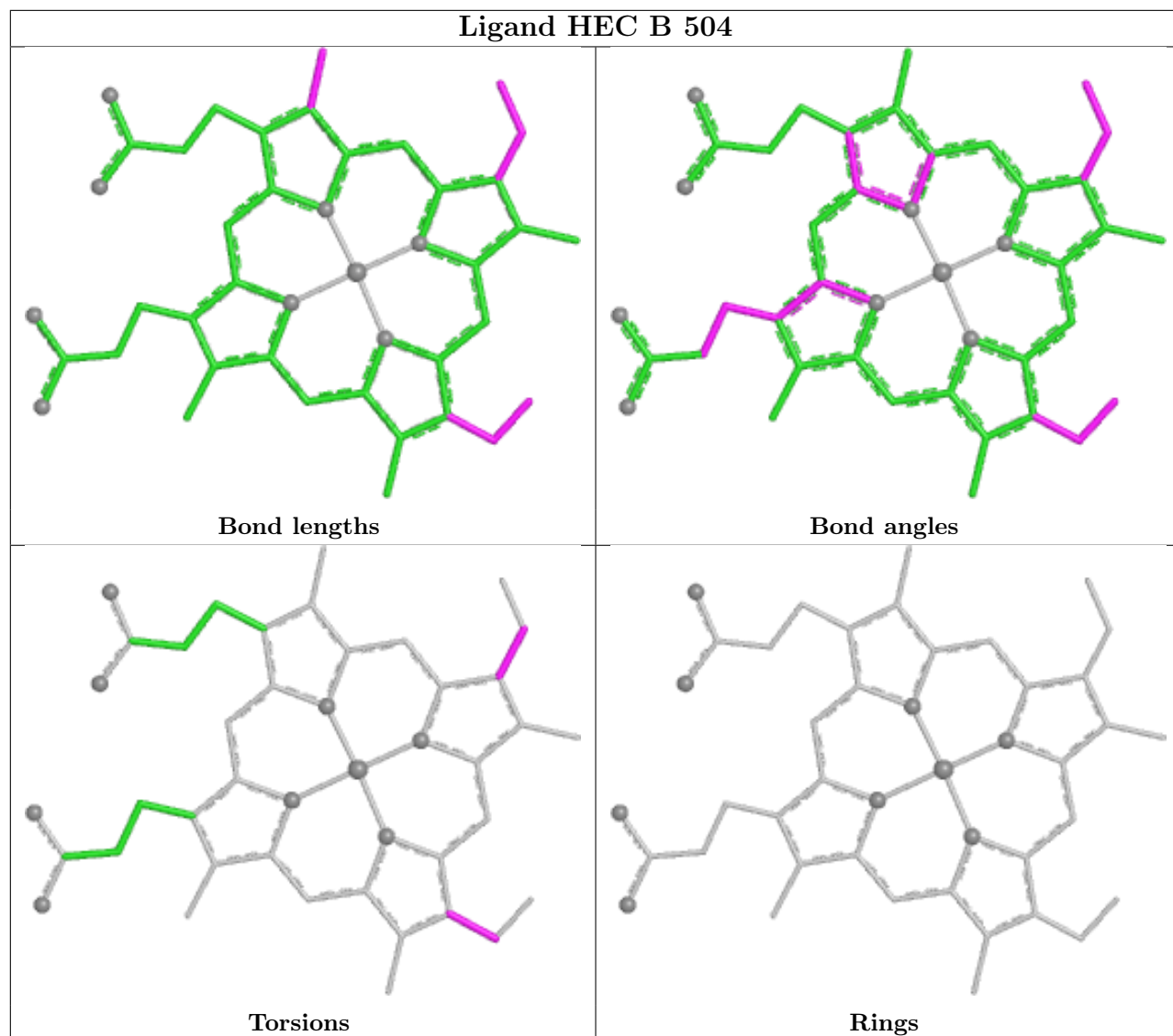
Bond angles

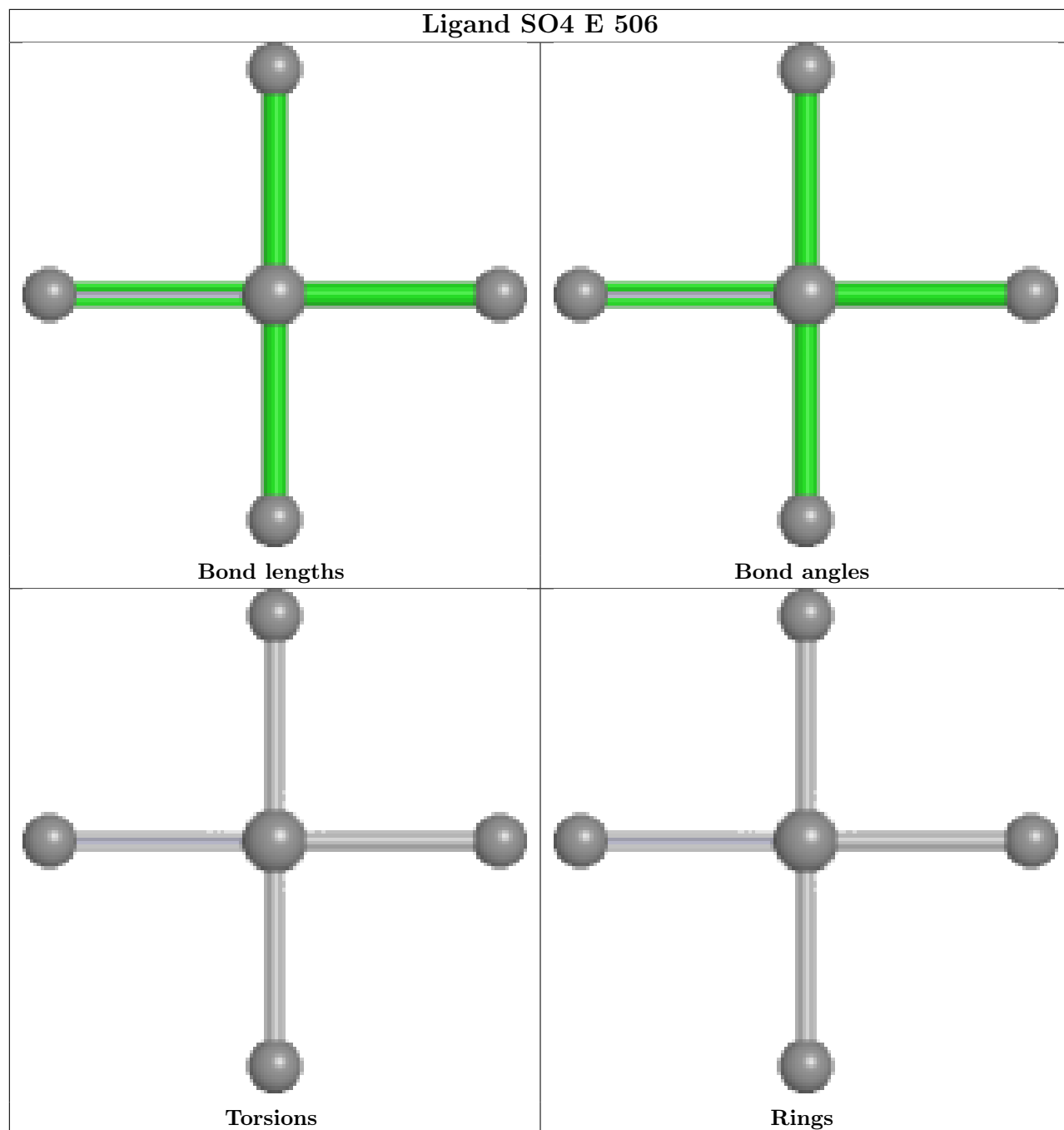


Torsions

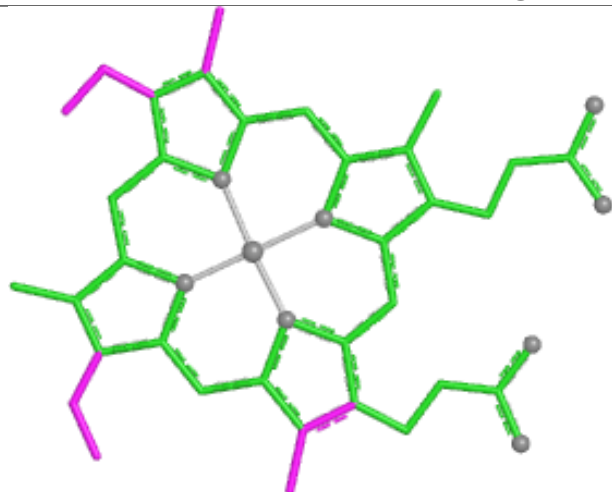


Rings

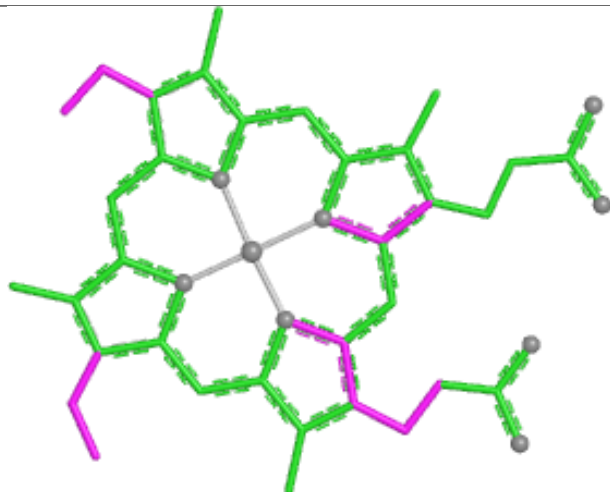




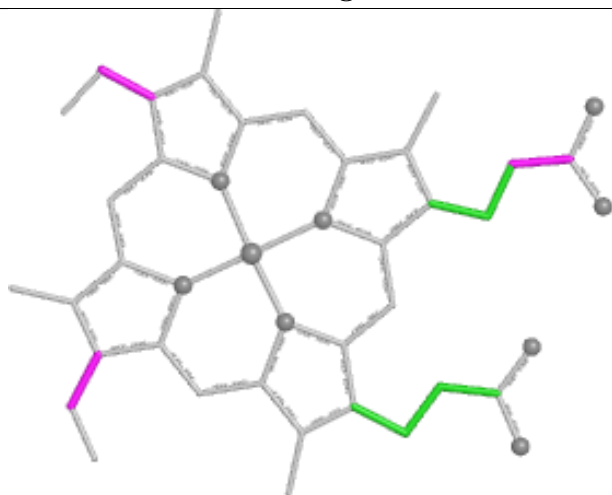
Ligand HEC B 502



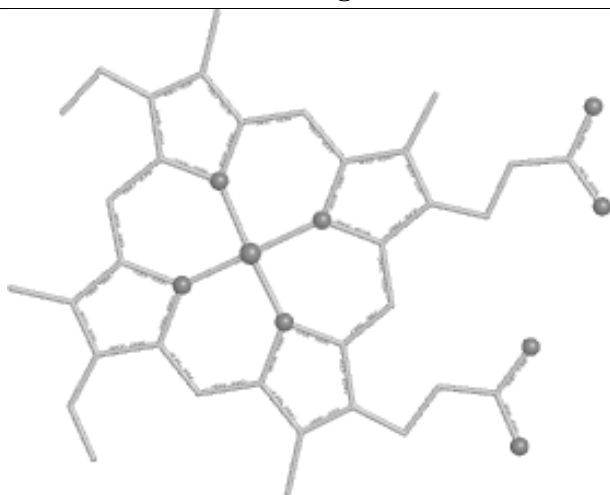
Bond lengths



Bond angles

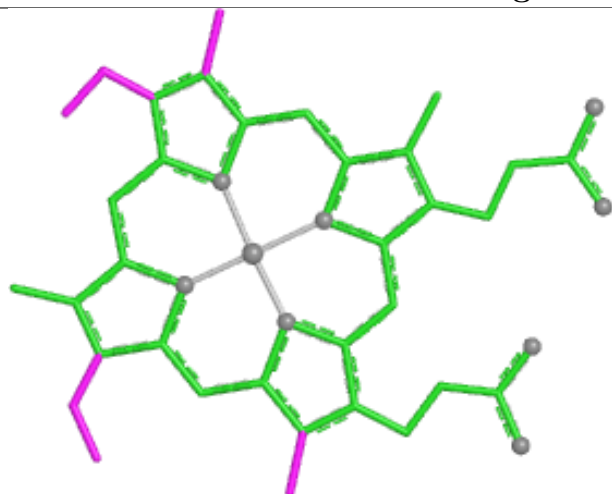


Torsions

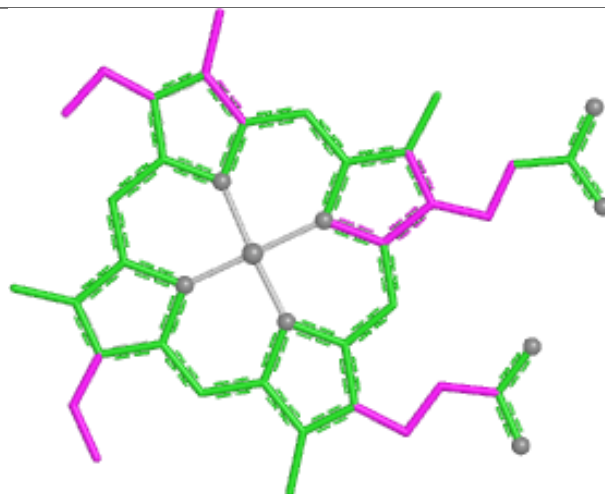


Rings

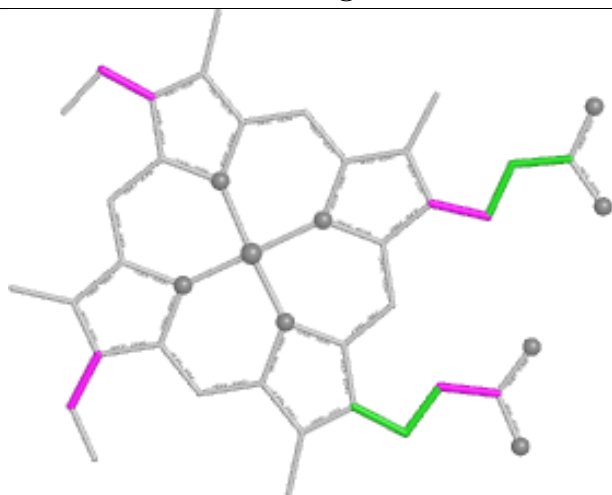
Ligand HEC E 505



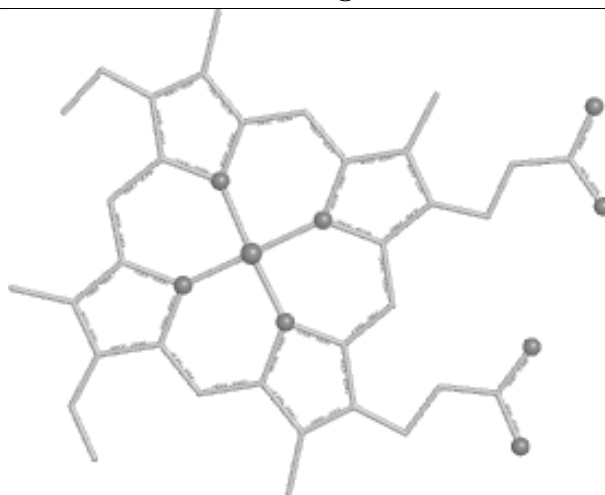
Bond lengths



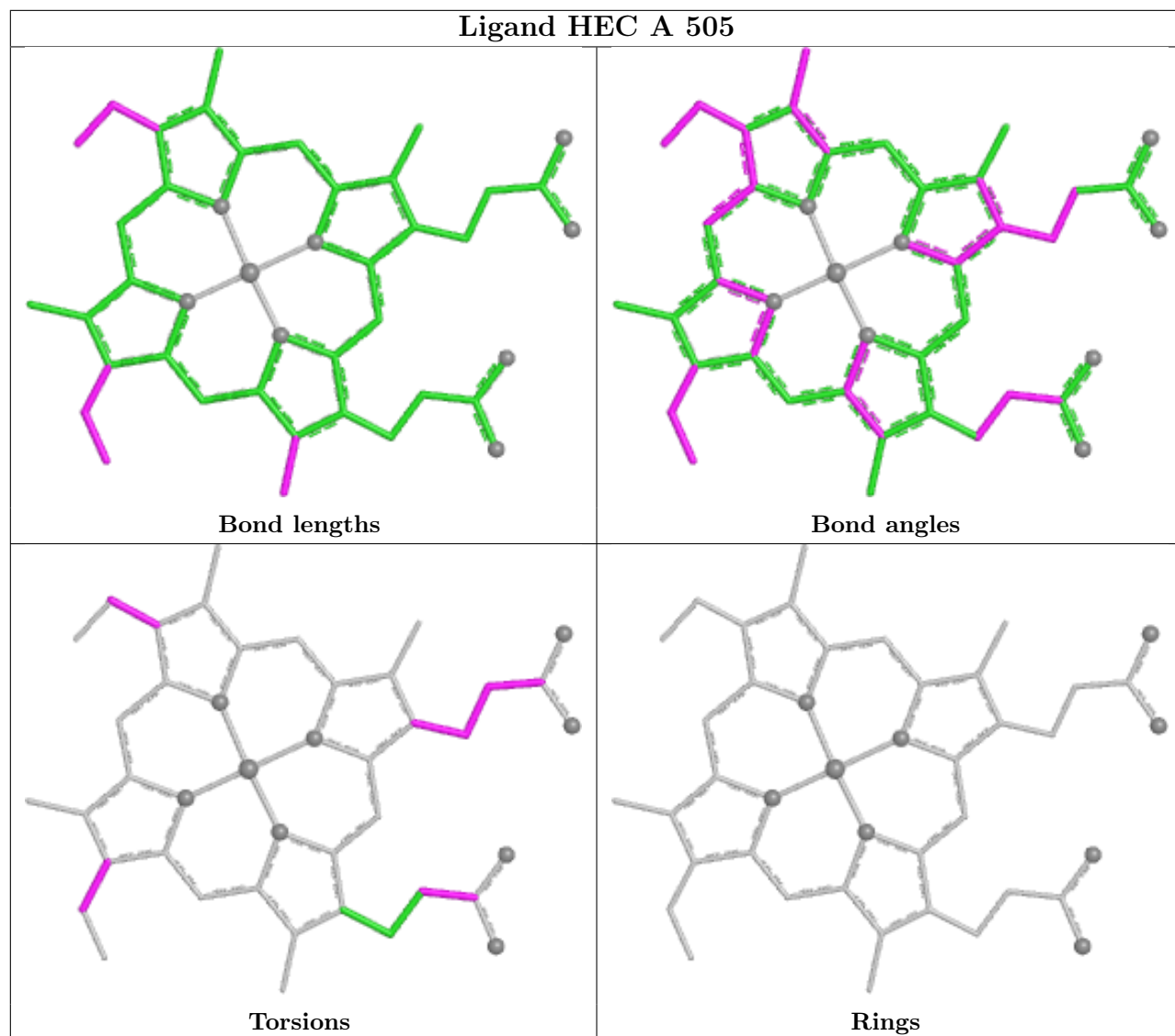
Bond angles



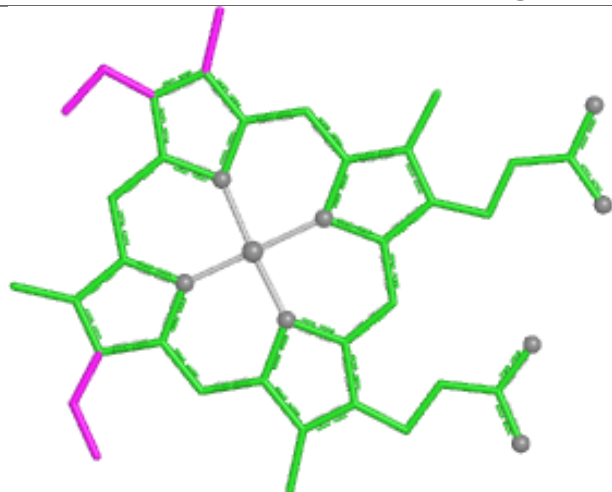
Torsions



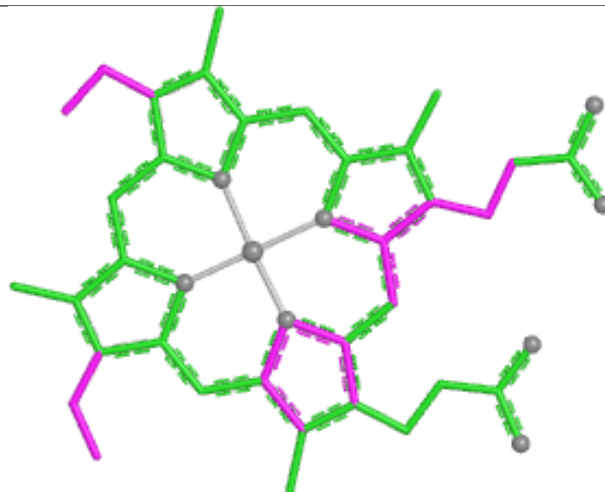
Rings



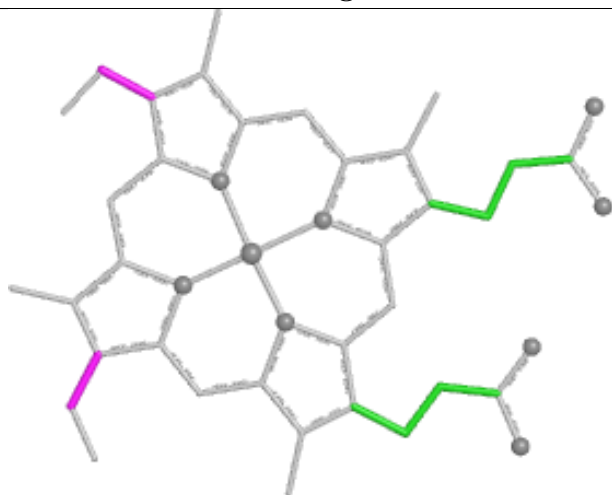
Ligand HEC C 503



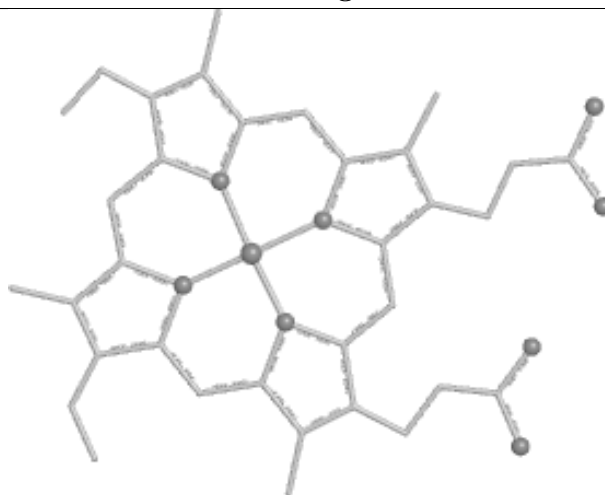
Bond lengths



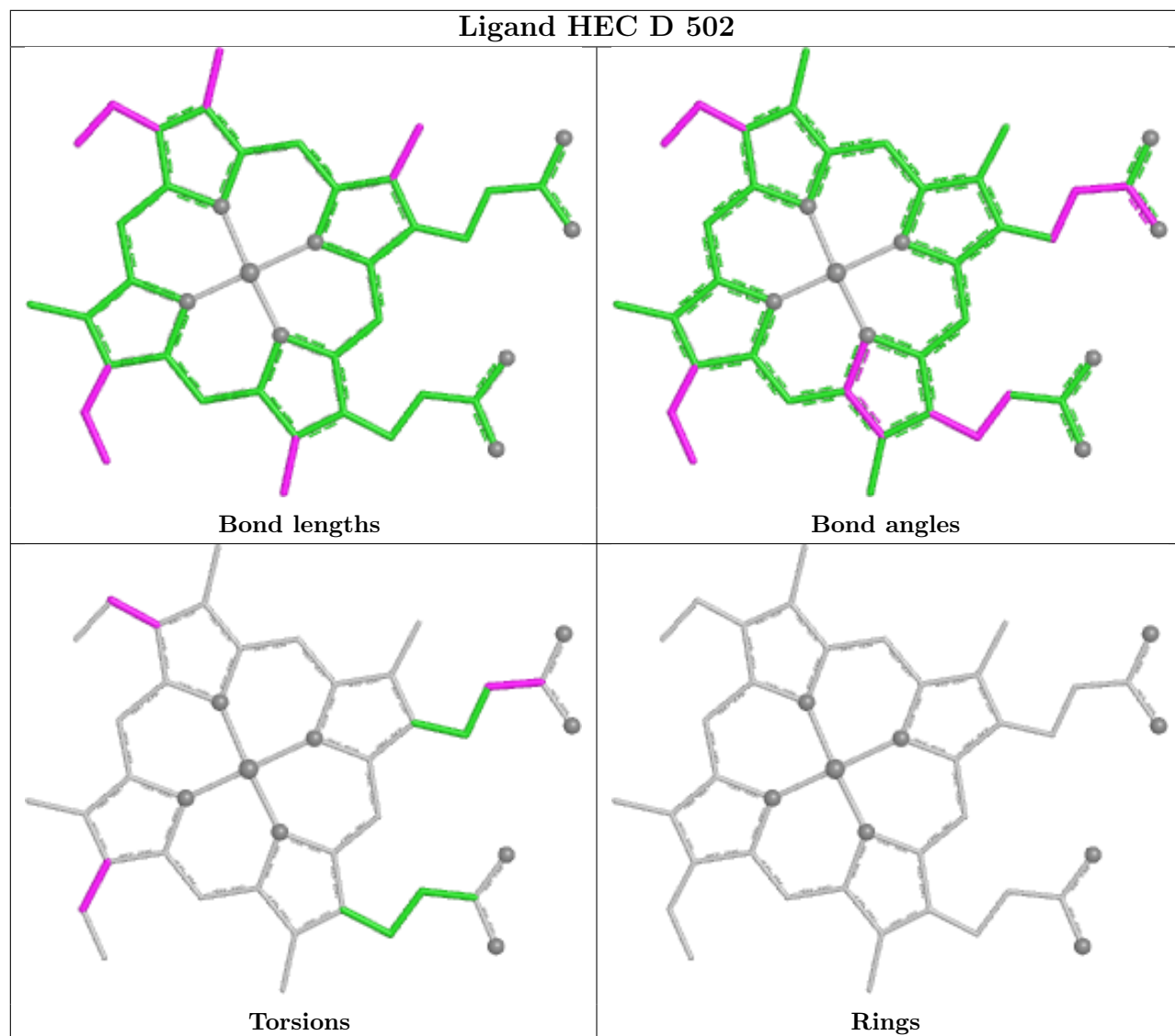
Bond angles



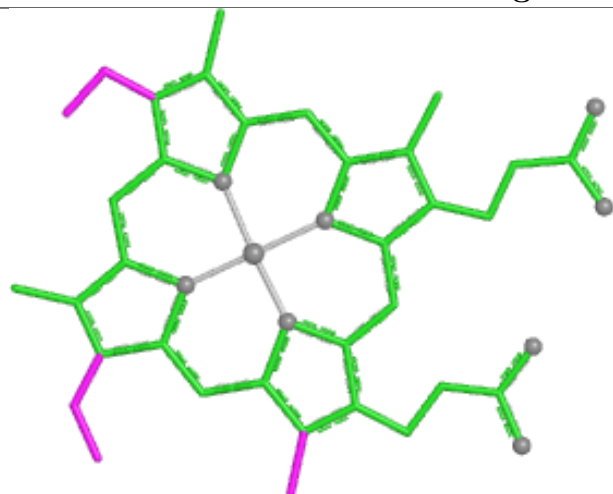
Torsions



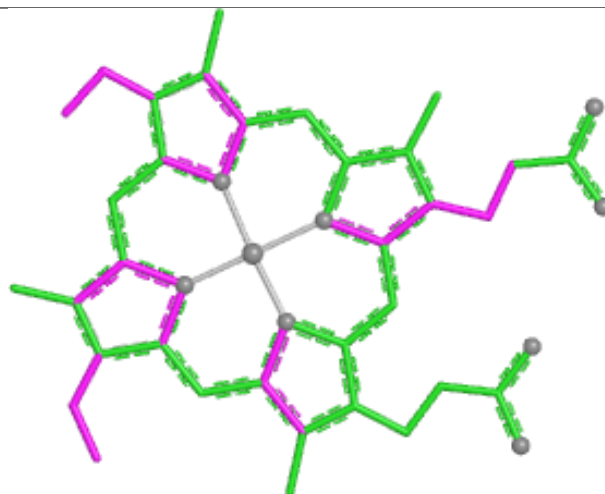
Rings



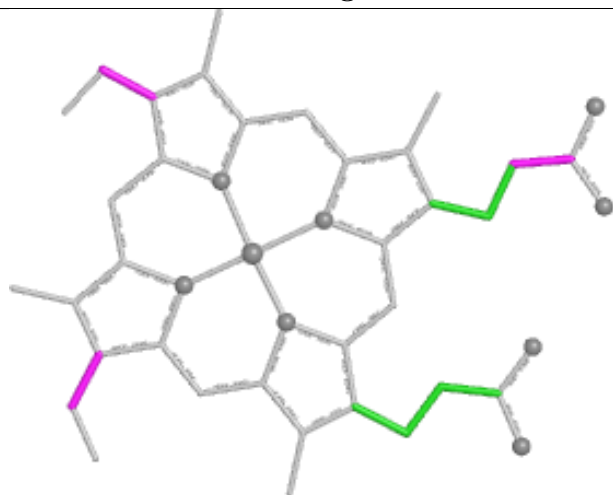
Ligand HEC B 501



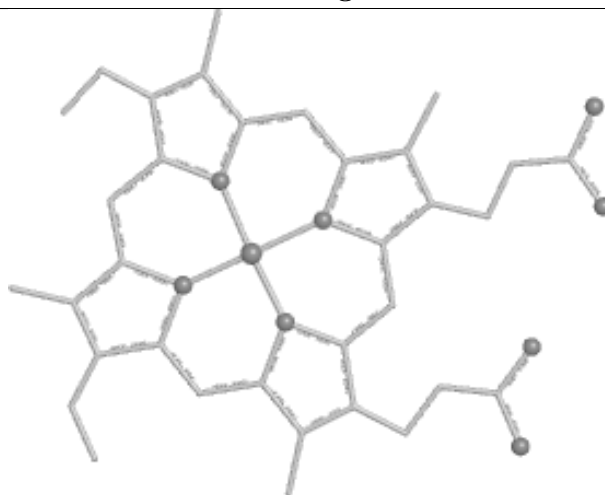
Bond lengths



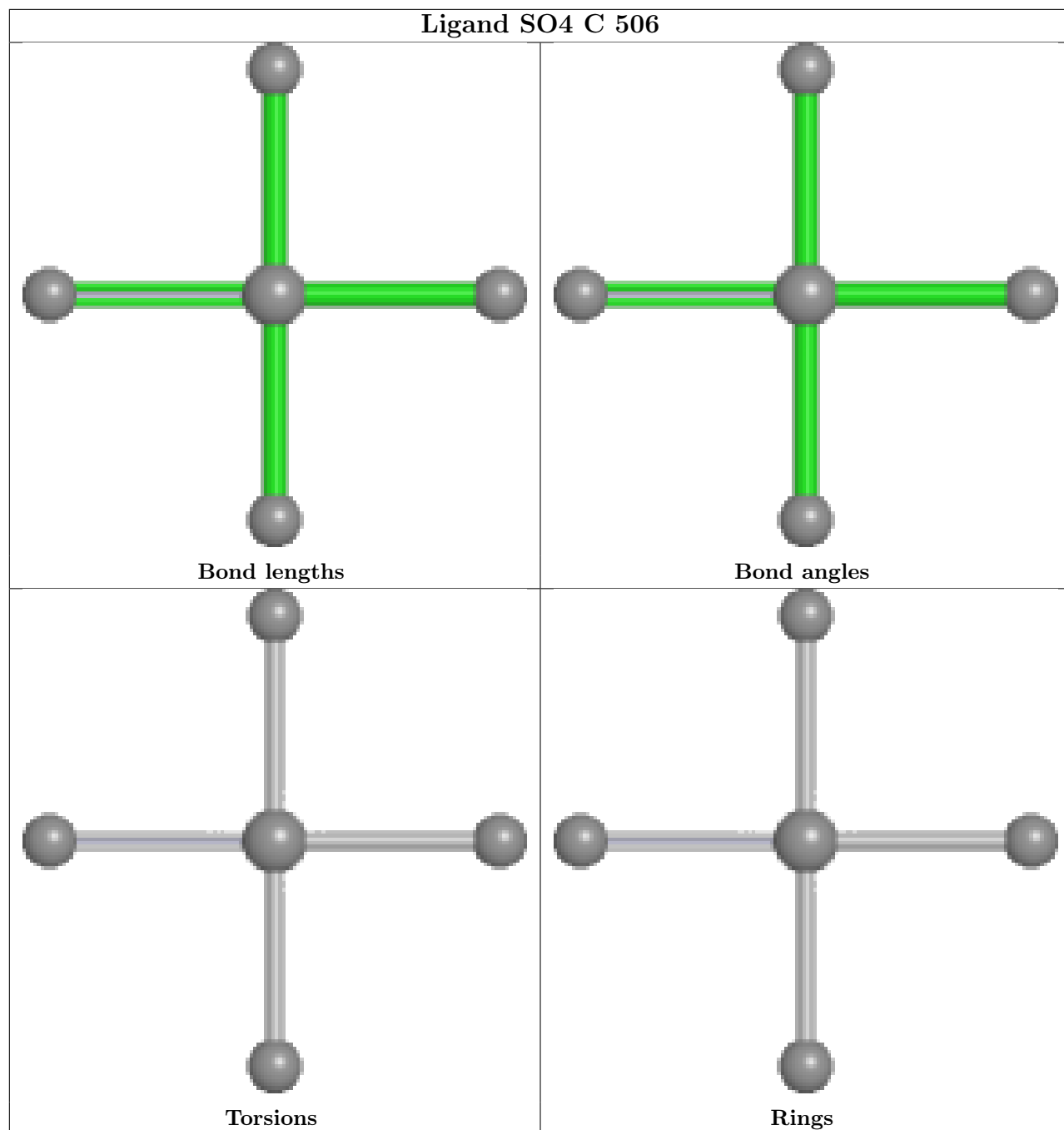
Bond angles

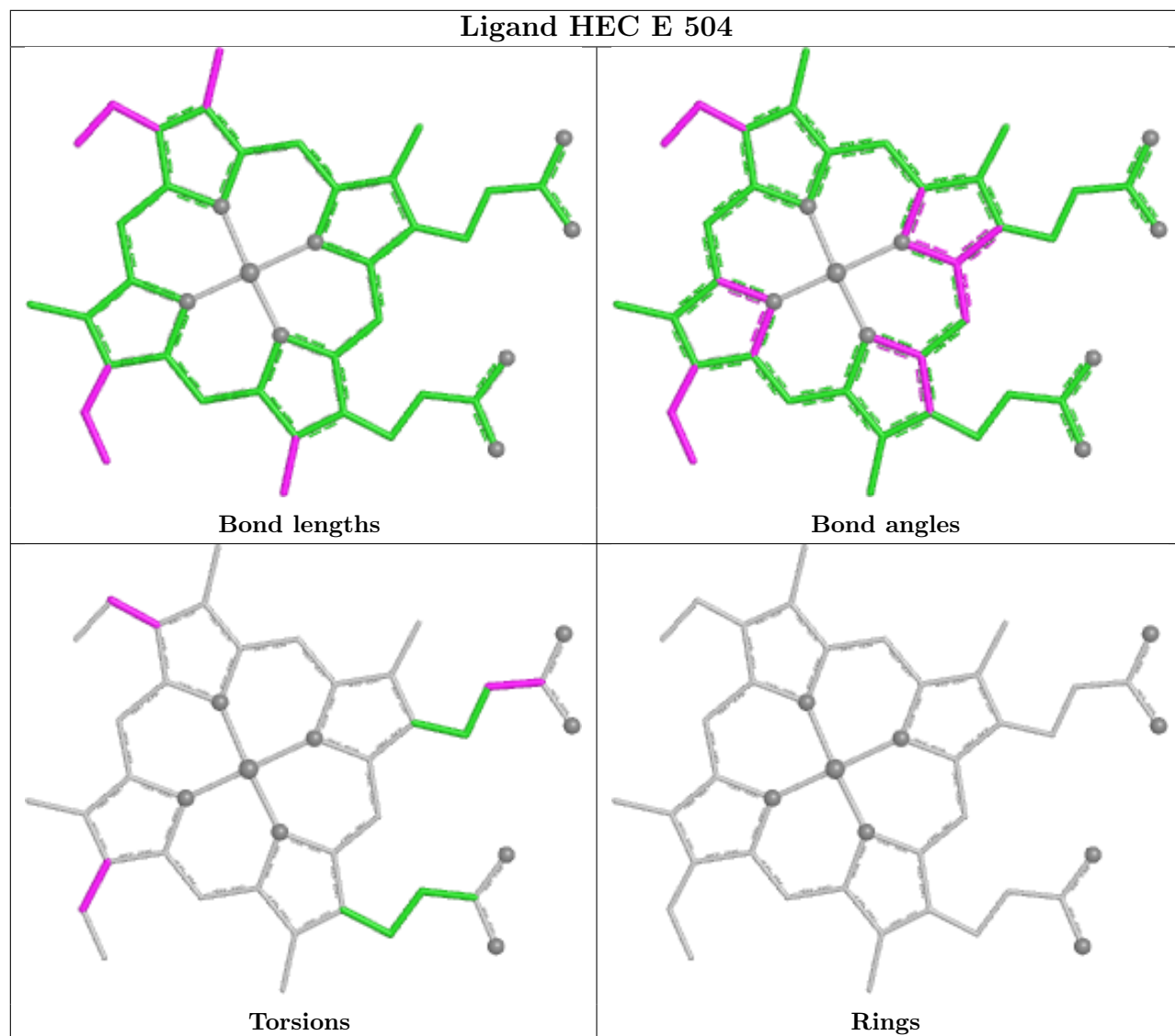


Torsions



Rings





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	443/482 (91%)	-0.53	2 (0%) 87 89	18, 28, 45, 64	0
1	B	444/482 (92%)	-0.51	7 (1%) 70 71	17, 28, 44, 91	0
1	C	442/482 (91%)	-0.07	11 (2%) 58 59	21, 39, 60, 97	0
1	D	444/482 (92%)	0.13	18 (4%) 41 42	21, 40, 63, 99	0
1	E	443/482 (91%)	0.20	12 (2%) 56 57	28, 43, 71, 93	0
1	F	441/482 (91%)	0.41	14 (3%) 50 51	32, 48, 72, 91	0
All	All	2657/2892 (91%)	-0.06	64 (2%) 59 61	17, 38, 64, 99	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	307	VAL	5.9
1	B	308	GLY	5.4
1	D	376	ALA	4.4
1	D	480	PRO	3.8
1	C	308	GLY	3.6
1	F	307	VAL	3.6
1	B	310	LYS	3.5
1	D	377	ALA	3.5
1	C	178	LYS	3.4
1	C	176	ASN	3.3
1	B	306	LYS	3.3
1	E	377	ALA	3.1
1	F	308	GLY	3.1
1	E	309	SER	3.0
1	D	330	GLN	3.0
1	F	438	ALA	2.9
1	C	330	GLN	2.9
1	E	480	PRO	2.9
1	E	370	MET	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	444	VAL	2.7
1	D	462	GLY	2.7
1	C	179	ASP	2.6
1	F	376	ALA	2.6
1	D	442	ALA	2.6
1	D	311	LYS	2.6
1	D	463	ALA	2.5
1	E	440	THR	2.5
1	B	309	SER	2.5
1	D	305	THR	2.5
1	F	309	SER	2.5
1	B	311	LYS	2.5
1	C	310	LYS	2.4
1	D	309	SER	2.4
1	D	466	LEU	2.4
1	F	440	THR	2.4
1	A	330	GLN	2.3
1	B	35	ILE	2.3
1	E	445	ASP	2.3
1	F	445	ASP	2.3
1	C	304	TYR	2.3
1	F	202	THR	2.2
1	F	142	GLN	2.2
1	F	385	MET	2.2
1	C	450	ILE	2.2
1	E	442	ALA	2.2
1	E	449	LYS	2.2
1	E	455	SER	2.2
1	C	203	LYS	2.1
1	E	388	GLN	2.1
1	D	308	GLY	2.1
1	B	304	TYR	2.1
1	D	179	ASP	2.1
1	E	387	ASP	2.1
1	C	306	LYS	2.1
1	D	379	LYS	2.1
1	A	480	PRO	2.1
1	F	267	ALA	2.1
1	D	378	GLY	2.1
1	C	373	LYS	2.1
1	D	375	GLN	2.1
1	F	271	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	454	LEU	2.0
1	E	452	LEU	2.0
1	F	378	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	C	506	5/5	0.91	0.14	29,30,37,37	5
3	SO4	E	506	5/5	0.93	0.10	35,37,40,45	5
3	SO4	F	506	5/5	0.93	0.10	45,46,52,54	5
3	SO4	D	506	5/5	0.95	0.09	30,35,38,43	5
2	HEC	E	505	43/43	0.96	0.09	31,39,49,54	0
2	HEC	F	501	43/43	0.96	0.10	36,43,50,76	0
2	HEC	F	503	43/43	0.96	0.08	29,38,41,43	0
2	HEC	F	504	43/43	0.96	0.08	29,35,39,40	0
2	HEC	F	505	43/43	0.96	0.09	30,35,44,58	0
3	SO4	A	506	5/5	0.96	0.09	20,23,30,31	5
2	HEC	C	502	43/43	0.96	0.08	30,34,43,51	0
2	HEC	D	503	43/43	0.96	0.09	22,31,37,49	0
2	HEC	D	505	43/43	0.96	0.09	24,32,43,53	0
2	HEC	E	503	43/43	0.96	0.09	26,35,44,51	0
2	HEC	D	502	43/43	0.97	0.07	20,32,37,42	0
2	HEC	A	503	43/43	0.97	0.07	16,20,24,29	0
2	HEC	D	504	43/43	0.97	0.07	15,28,35,38	0
2	HEC	A	504	43/43	0.97	0.07	14,18,23,26	0
2	HEC	E	501	43/43	0.97	0.08	28,36,44,46	0
2	HEC	E	502	43/43	0.97	0.07	26,31,38,40	0

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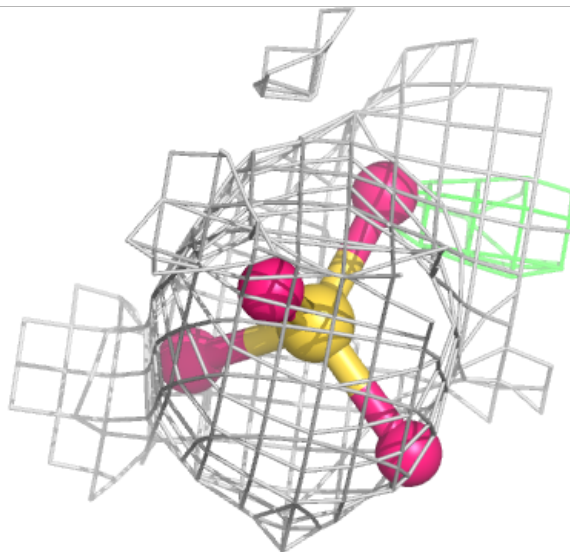
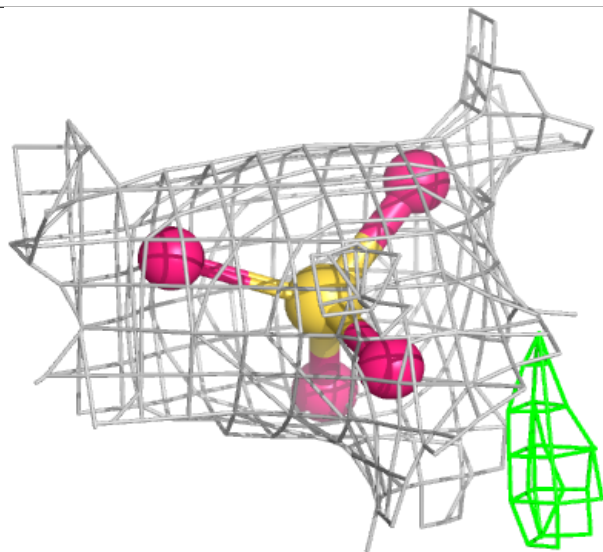
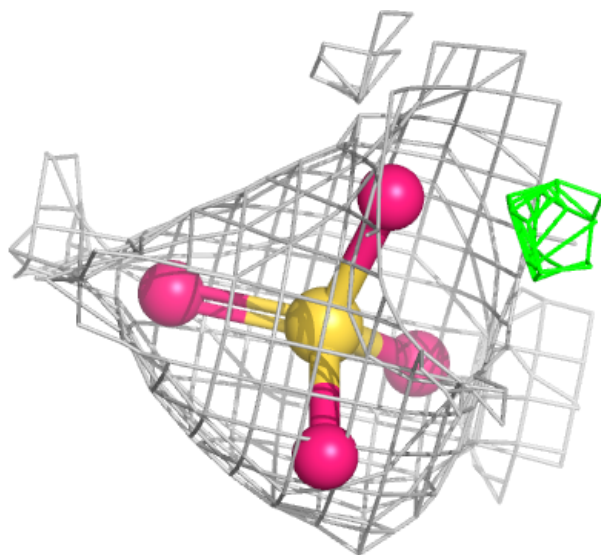
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	HEC	A	505	43/43	0.97	0.08	17,27,39,49	0
2	HEC	E	504	43/43	0.97	0.07	25,35,39,41	0
2	HEC	B	502	43/43	0.97	0.07	24,32,36,42	0
2	HEC	B	503	43/43	0.97	0.08	15,24,29,39	0
2	HEC	F	502	43/43	0.97	0.07	32,37,48,67	0
2	HEC	B	504	43/43	0.97	0.07	14,22,26,28	0
2	HEC	B	505	43/43	0.97	0.07	17,26,34,39	0
2	HEC	C	501	43/43	0.97	0.07	23,30,35,39	0
2	HEC	A	501	43/43	0.97	0.07	17,23,29,33	0
3	SO4	B	506	5/5	0.97	0.07	21,23,30,33	5
2	HEC	C	503	43/43	0.97	0.08	20,28,32,33	0
2	HEC	C	504	43/43	0.97	0.07	19,26,29,31	0
2	HEC	C	505	43/43	0.97	0.08	22,35,44,48	0
2	HEC	D	501	43/43	0.97	0.08	26,33,38,44	0
2	HEC	A	502	43/43	0.98	0.06	20,26,32,45	0
2	HEC	B	501	43/43	0.98	0.06	20,25,28,31	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

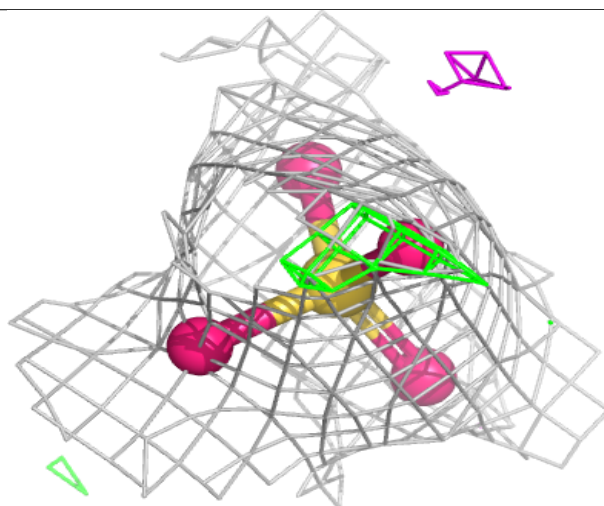
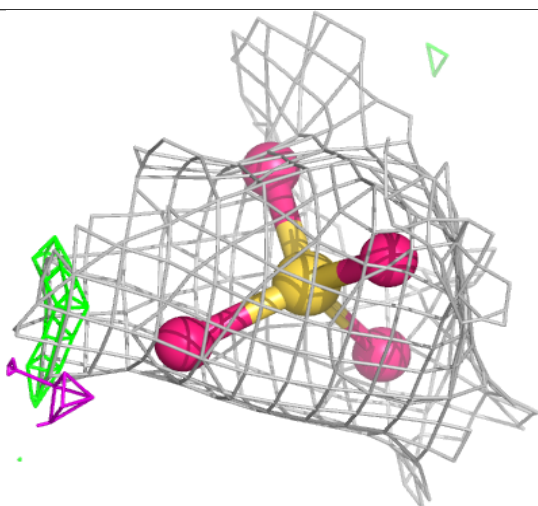
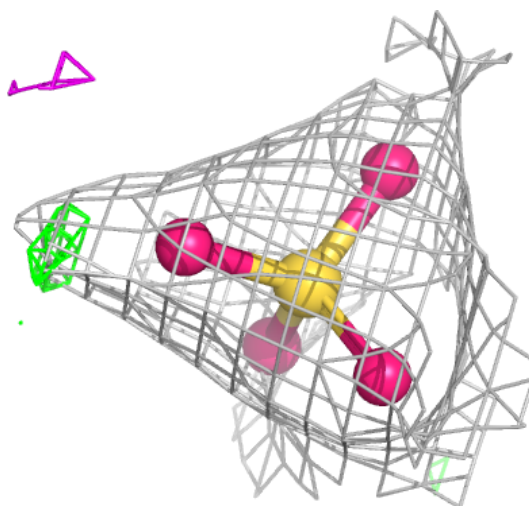
Electron density around SO4 C 506:

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



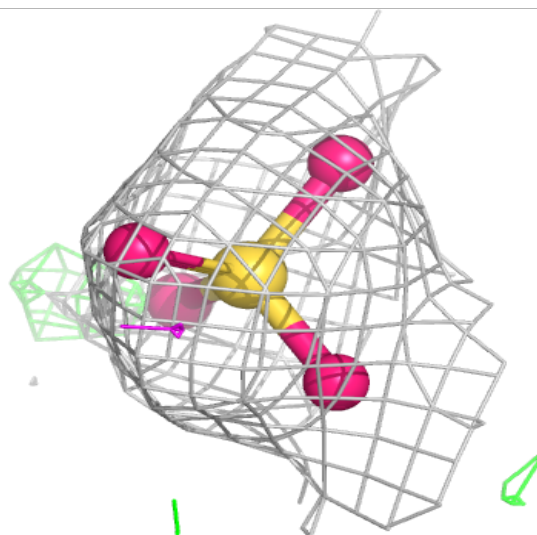
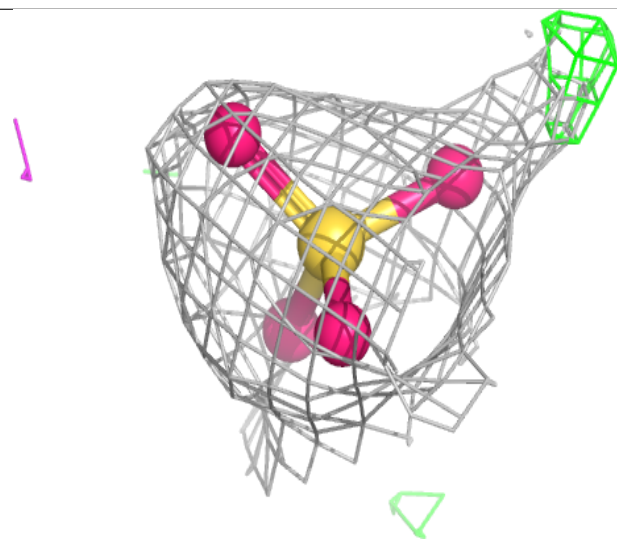
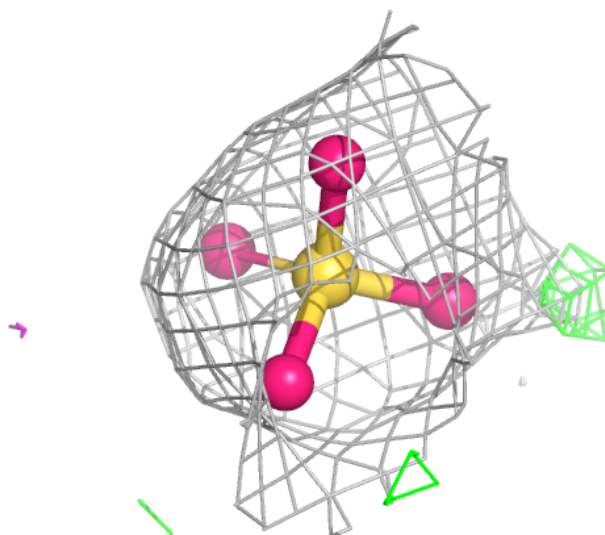
Electron density around SO4 E 506:

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and green (positive)



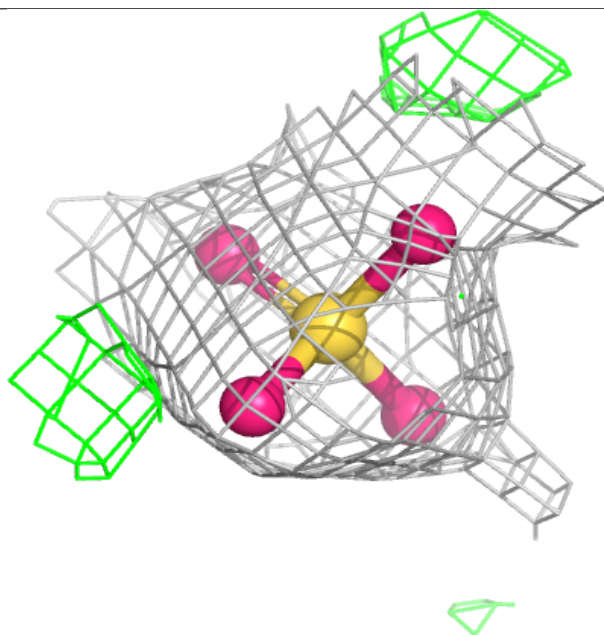
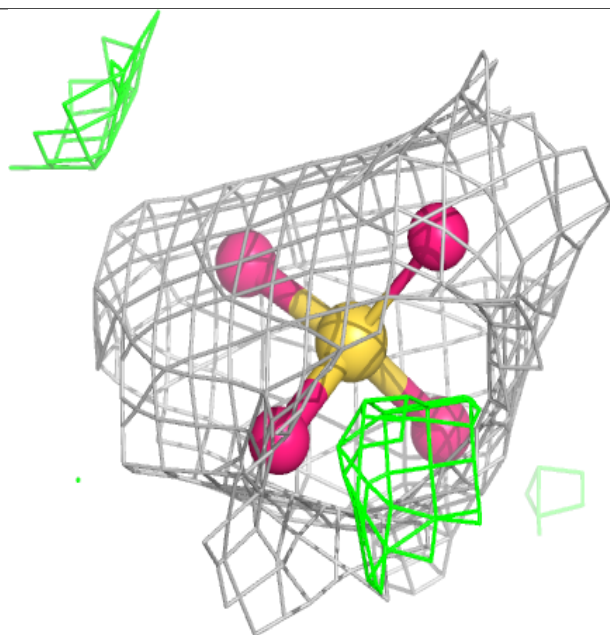
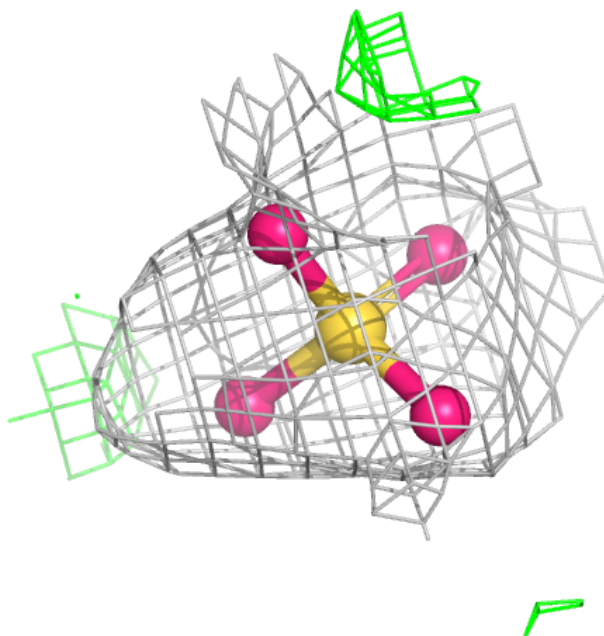
Electron density around SO4 F 506:

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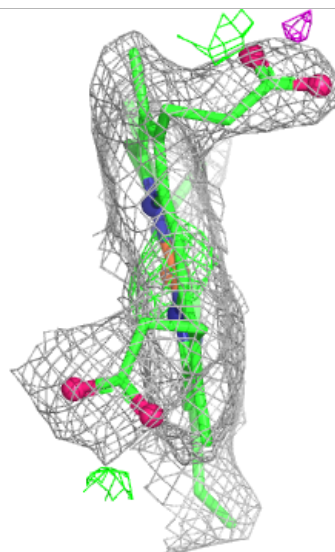
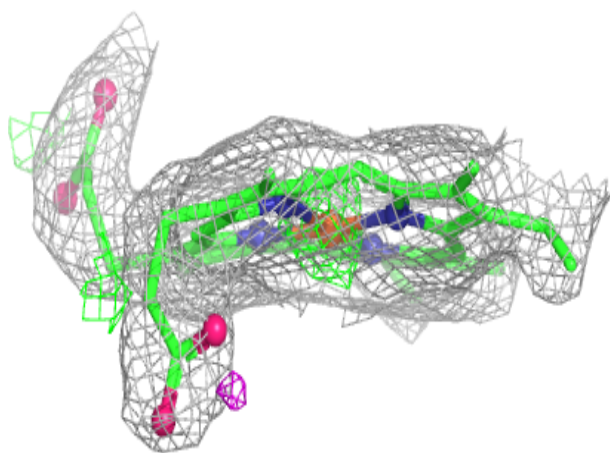
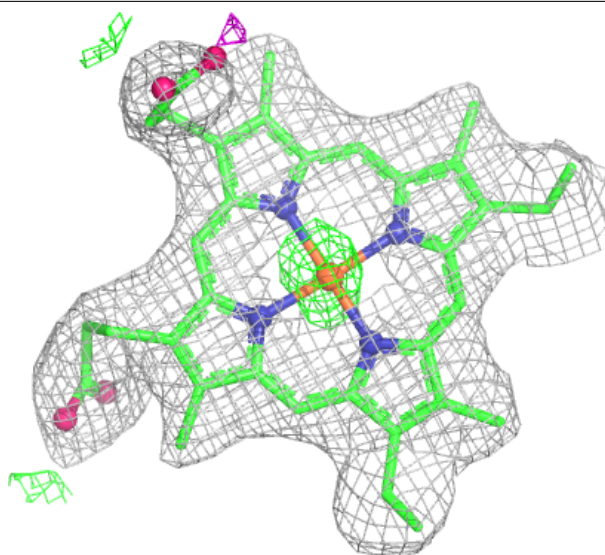
Electron density around SO4 D 506:

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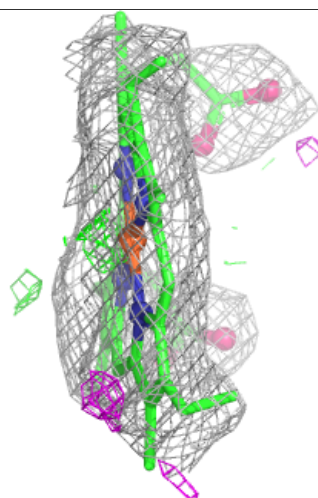
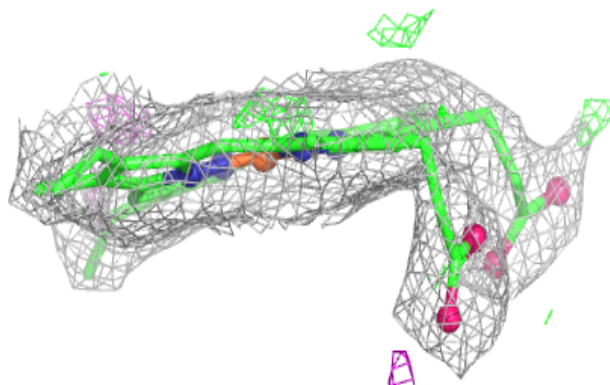
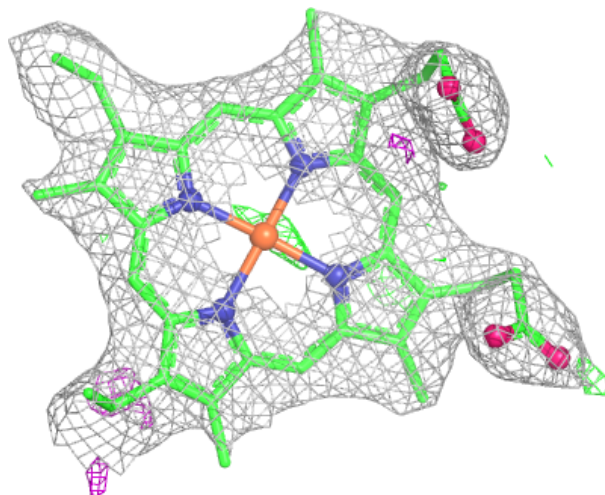
Electron density around HEC E 505:

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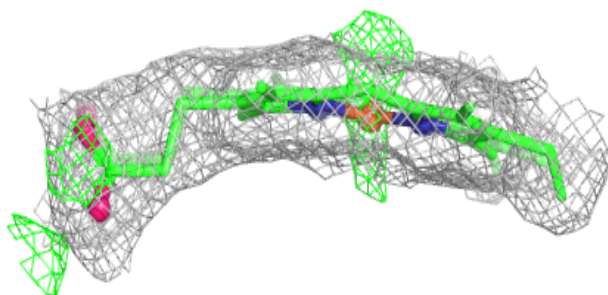
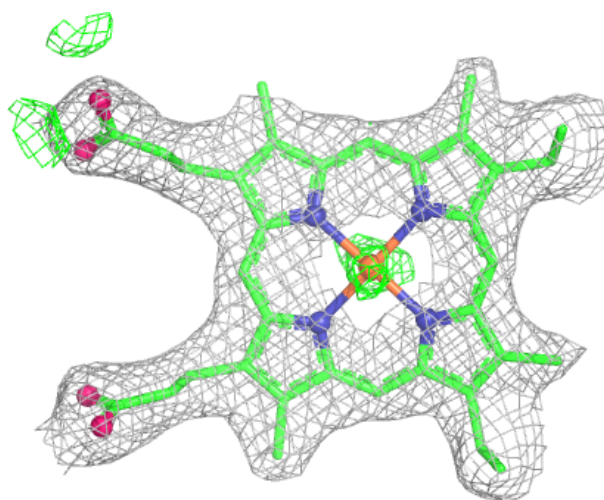
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and green (positive)



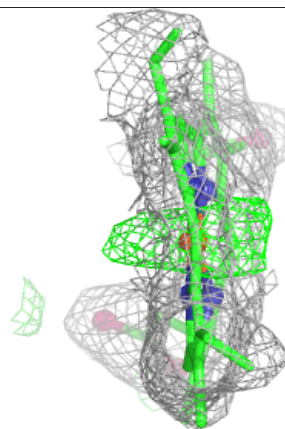
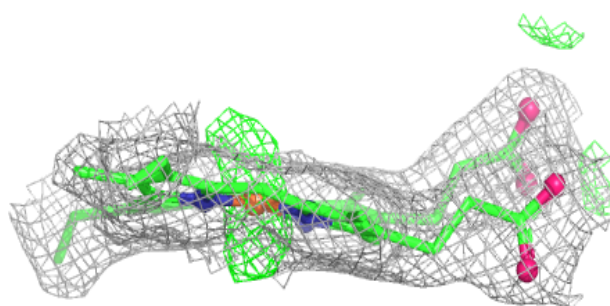
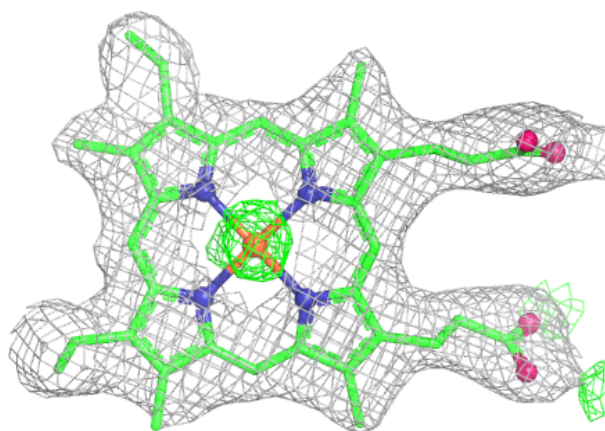
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and green (positive)



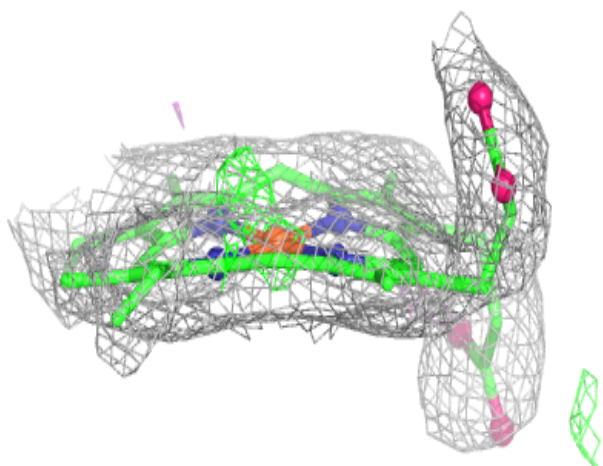
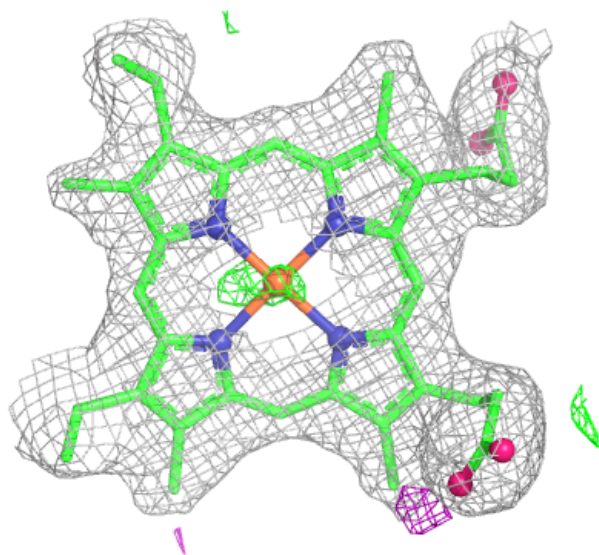
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and green (positive)



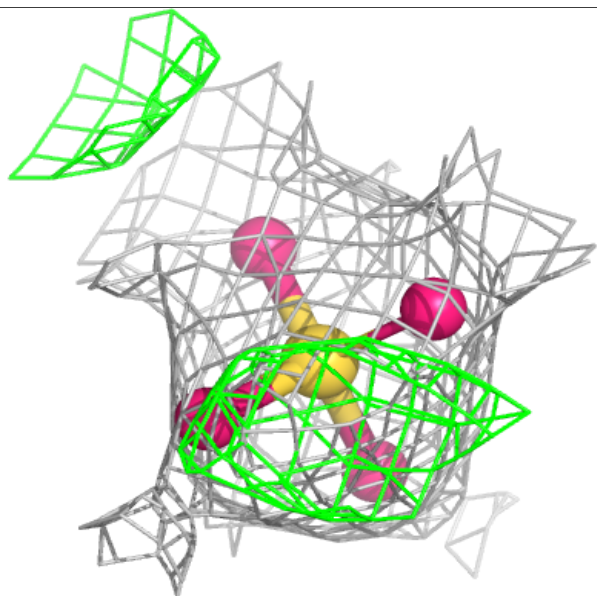
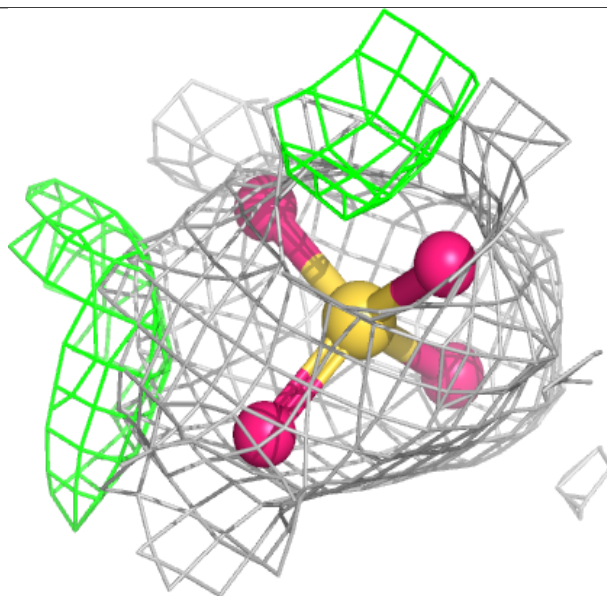
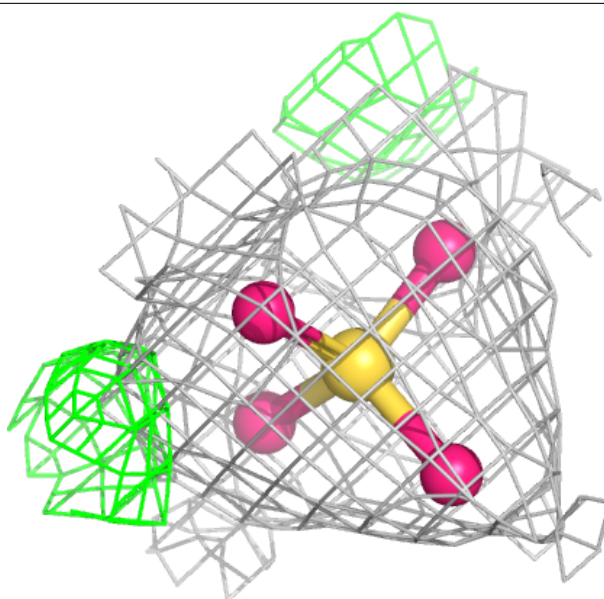
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and green (positive)



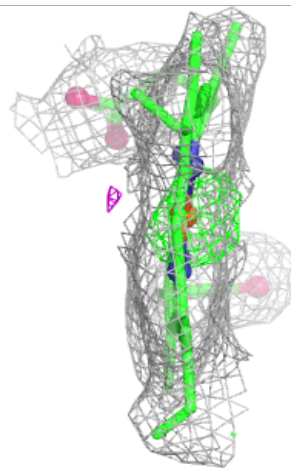
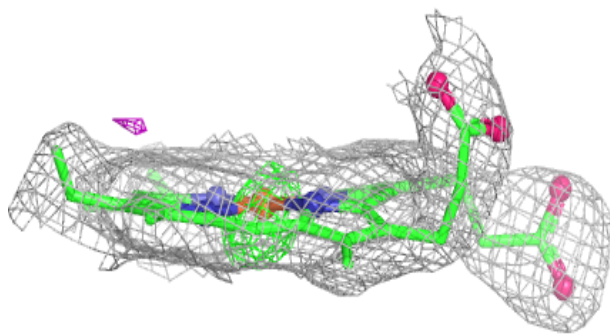
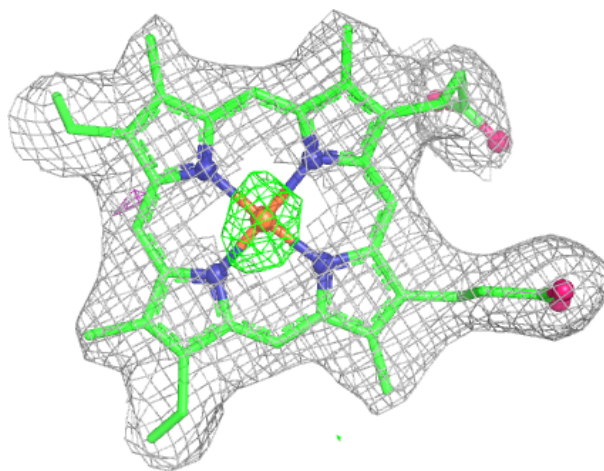
Electron density around SO4 A 506:

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and green (positive)



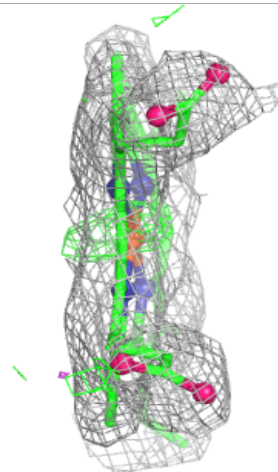
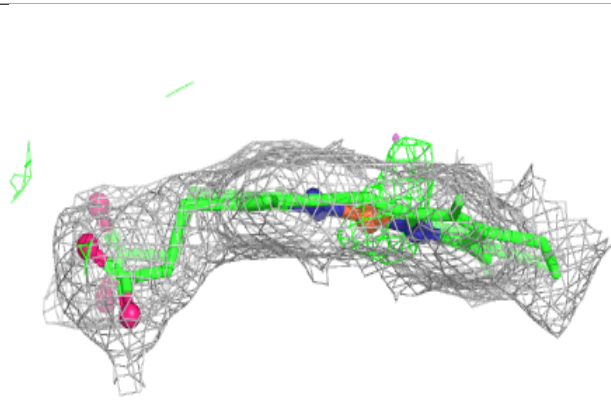
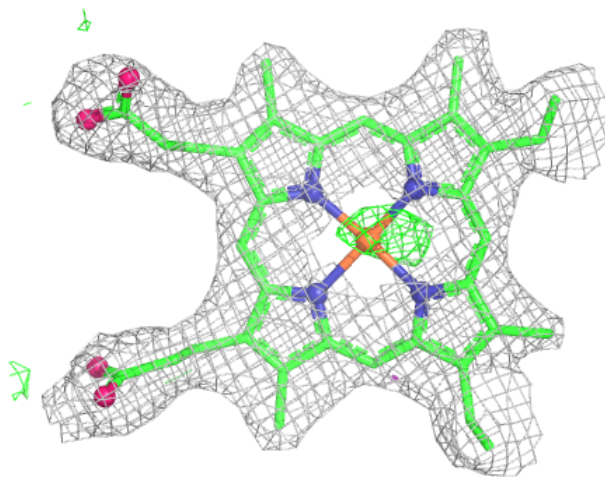
Electron density around HEC C 502:

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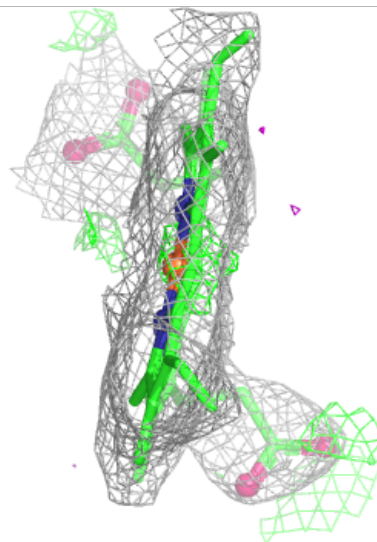
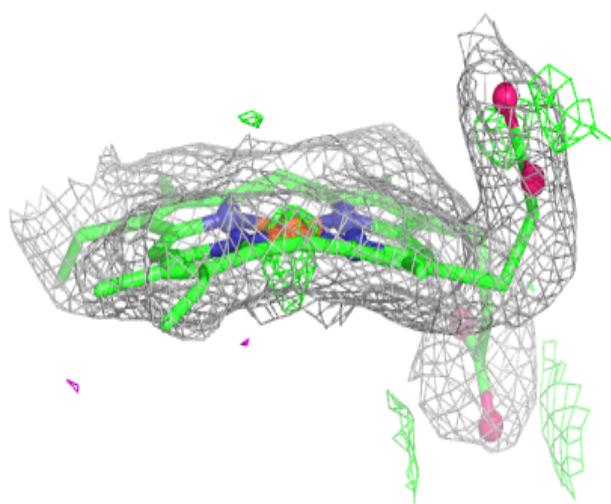
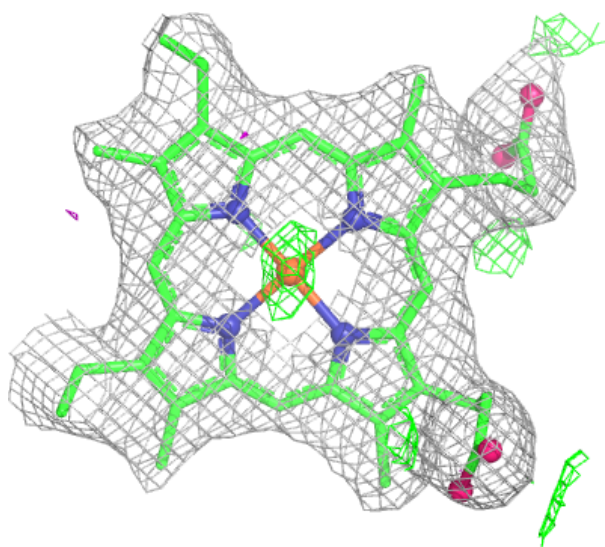
Electron density around HEC D 503:

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and green (positive)



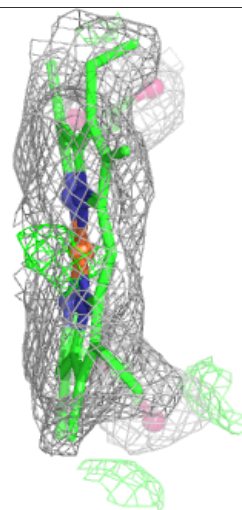
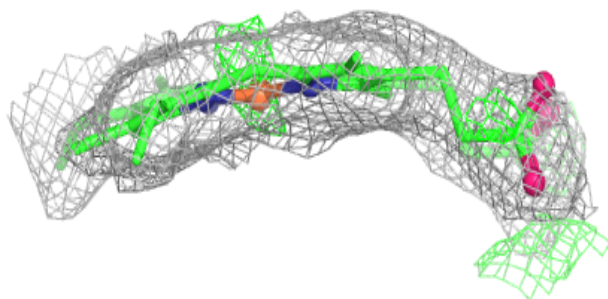
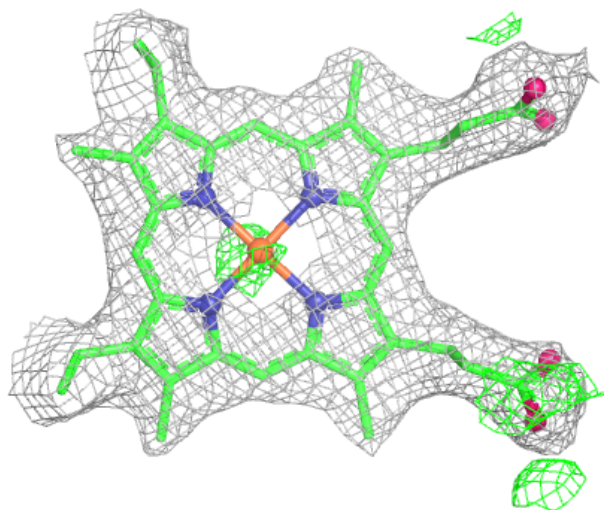
Electron density around HEC D 505:

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and green (positive)



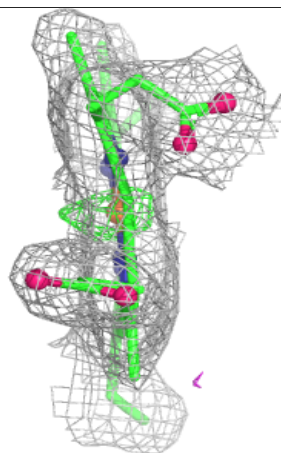
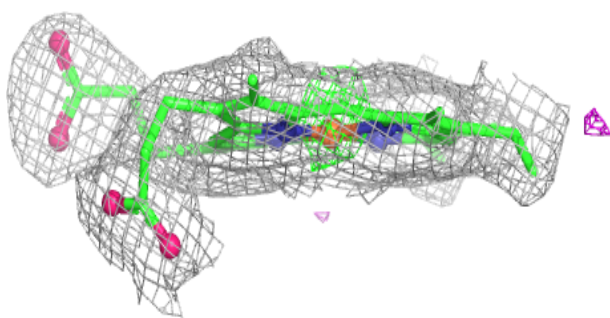
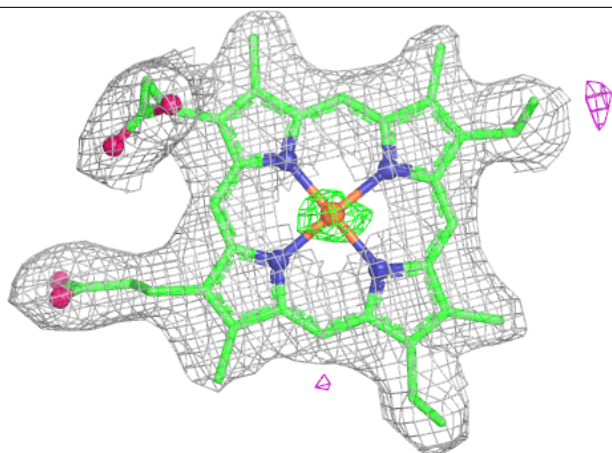
Electron density around HEC E 503:

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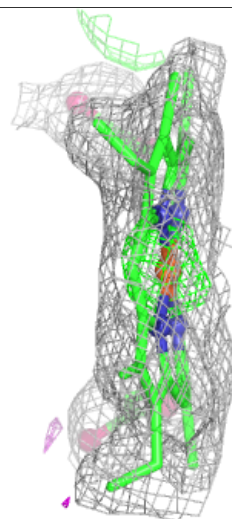
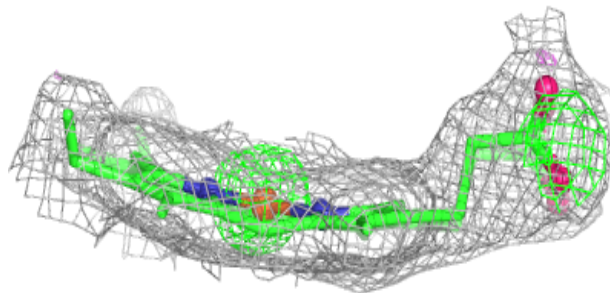
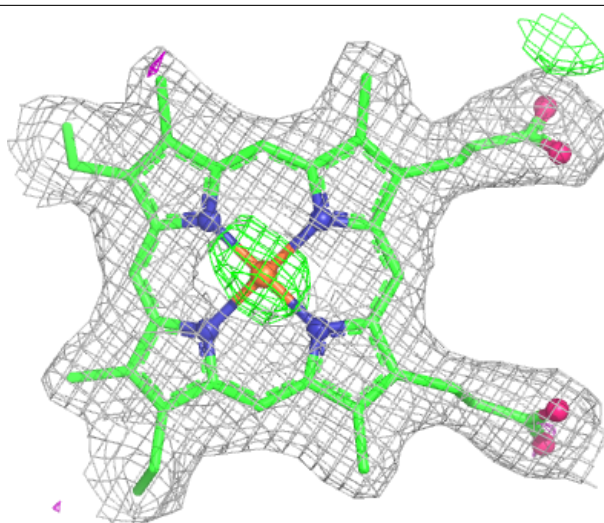
Electron density around HEC D 502:

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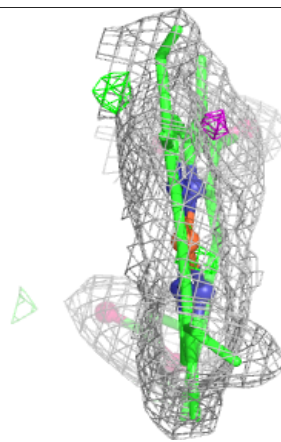
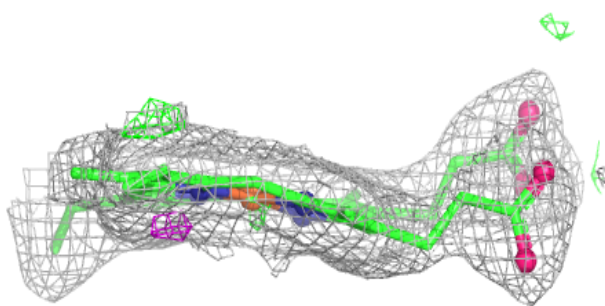
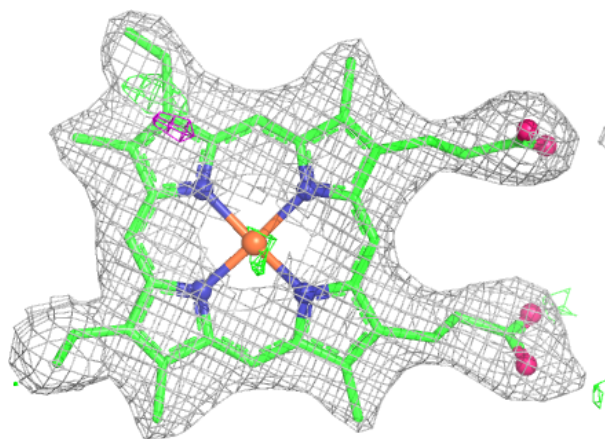
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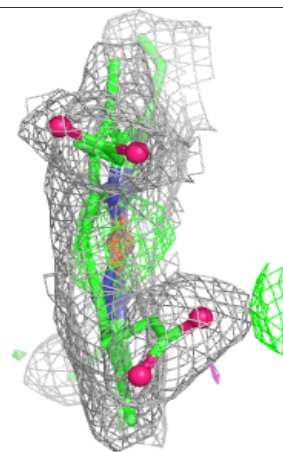
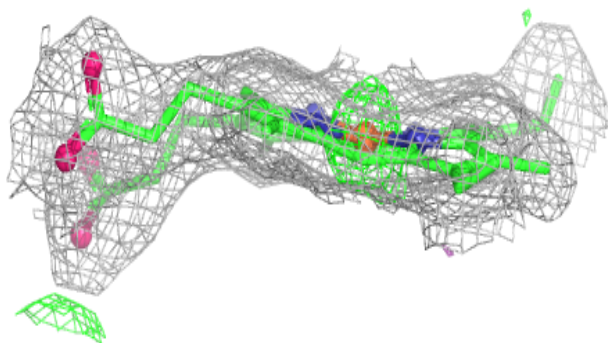
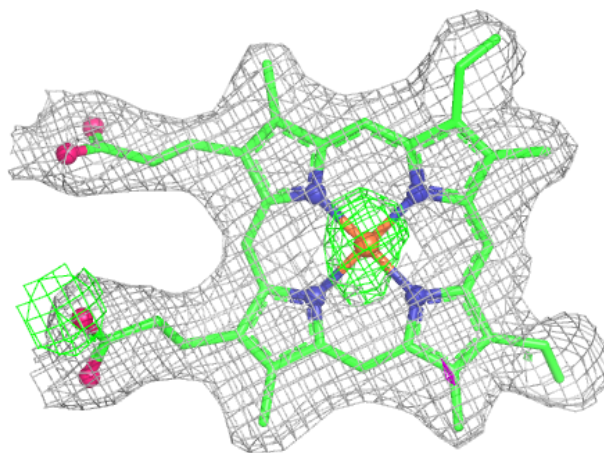
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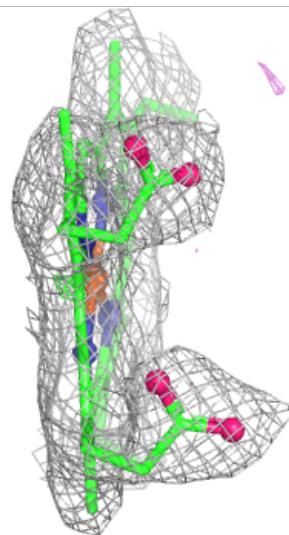
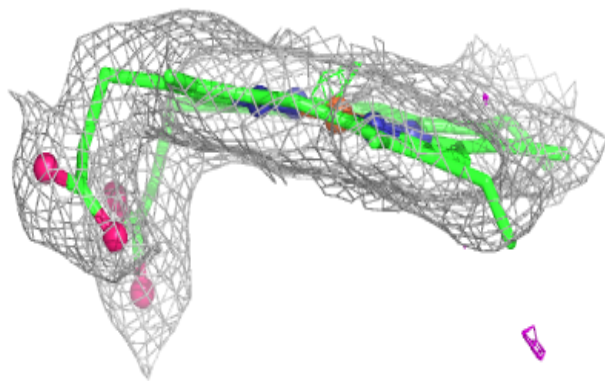
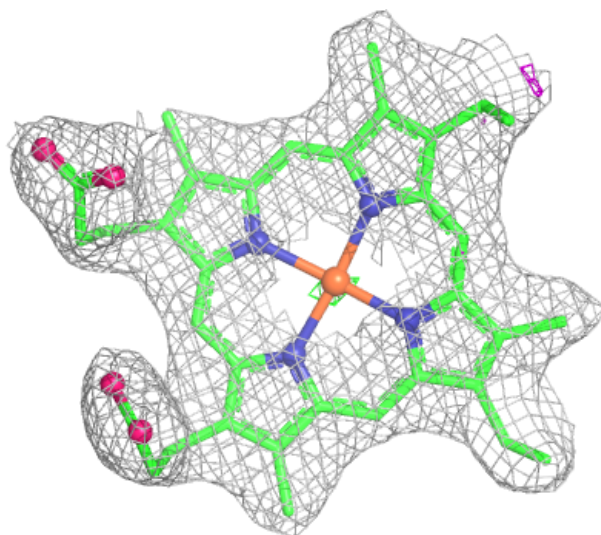
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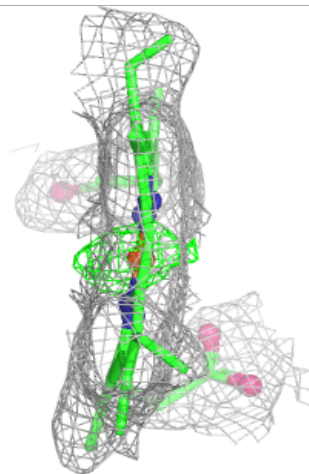
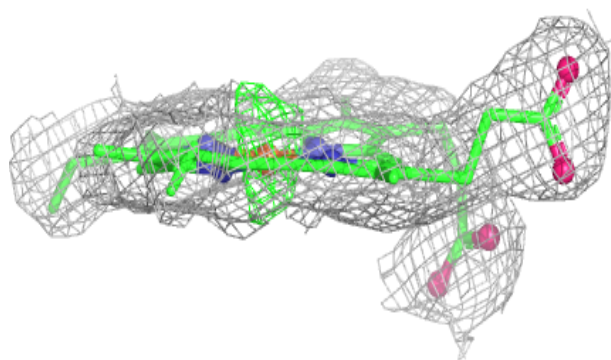
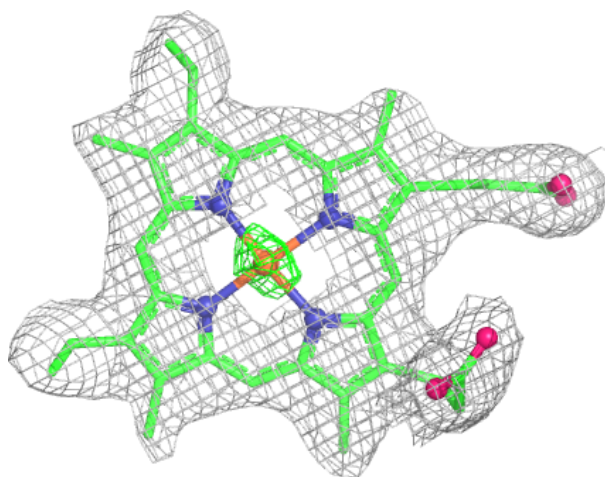
Electron density around HEC E 501:

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



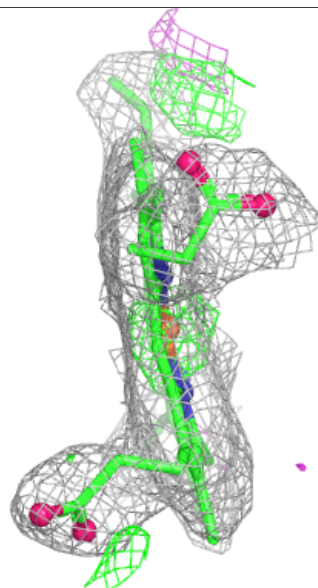
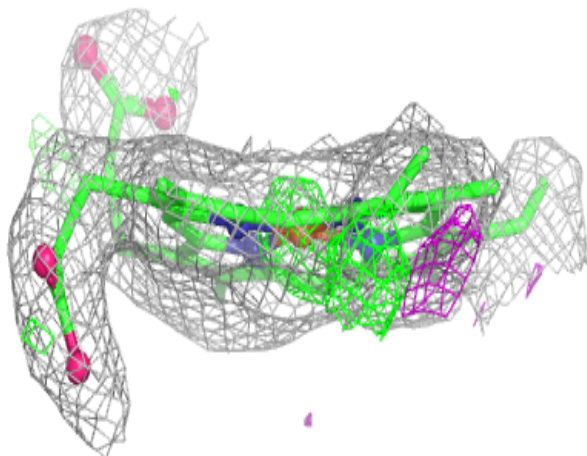
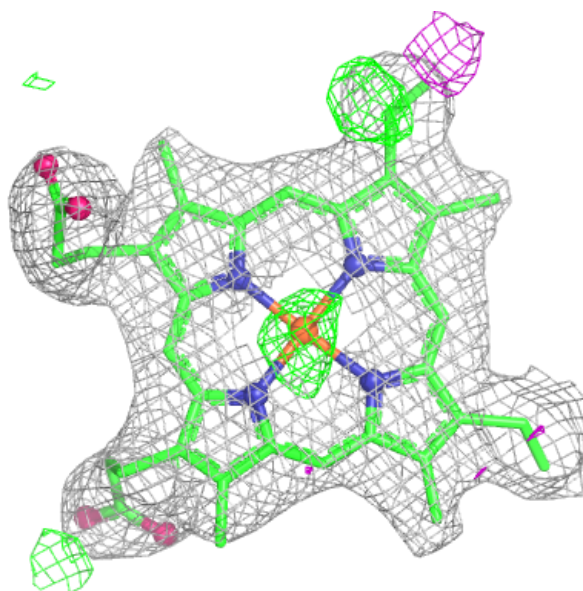
Electron density around HEC E 502:

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



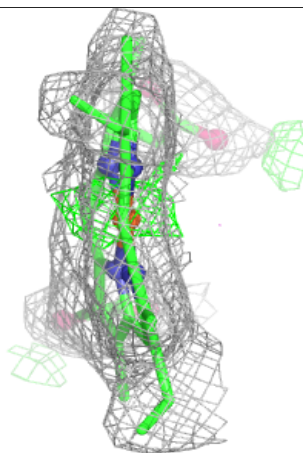
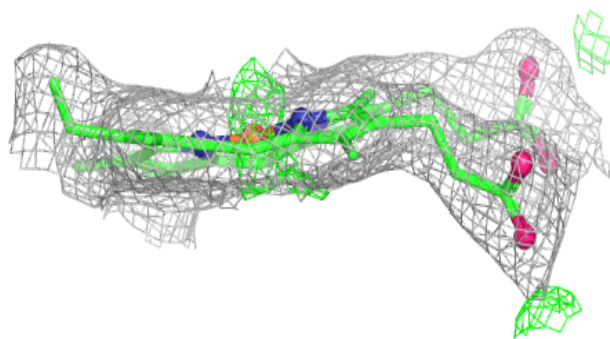
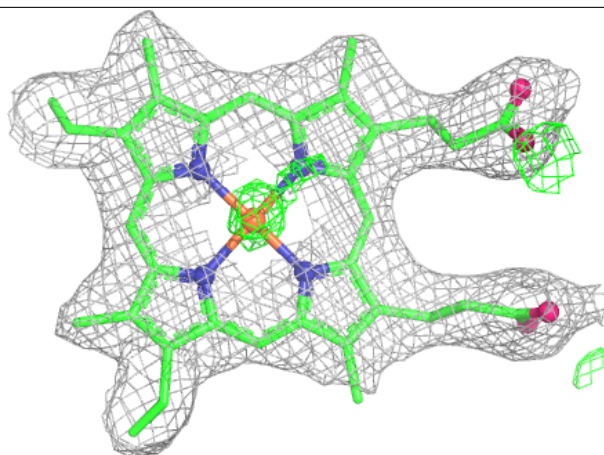
Electron density around HEC A 505:

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



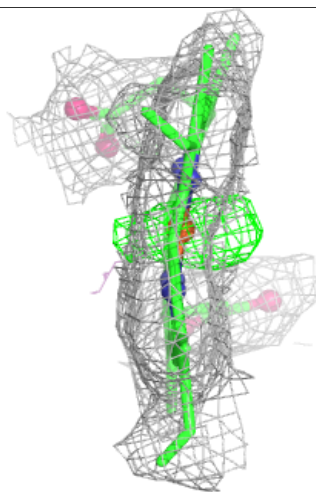
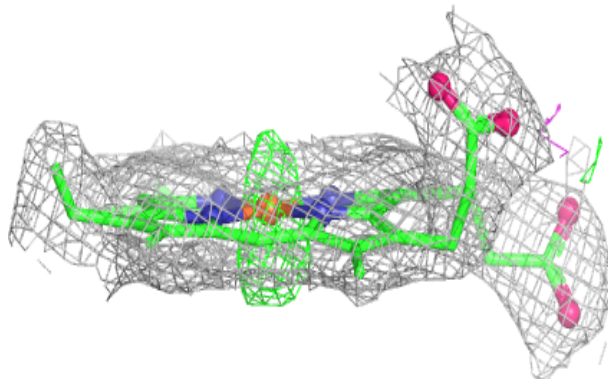
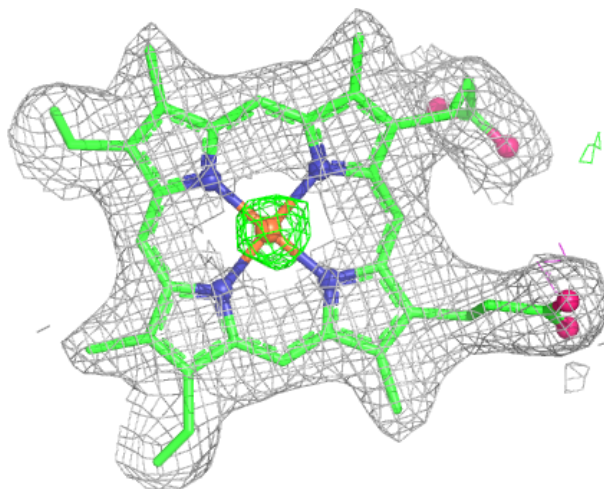
Electron density around HEC E 504:

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



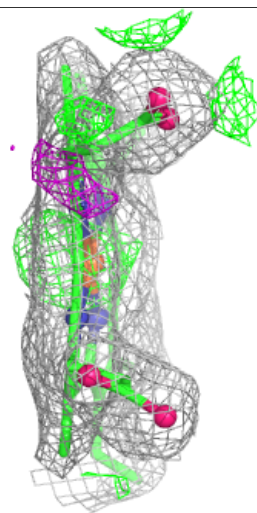
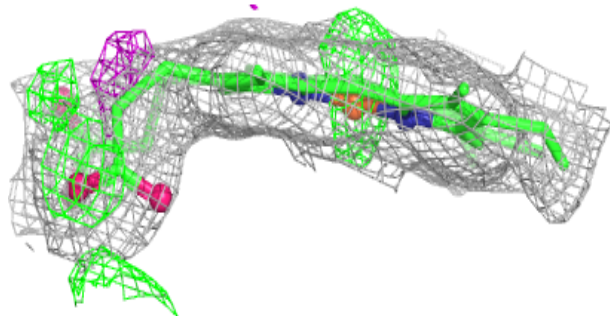
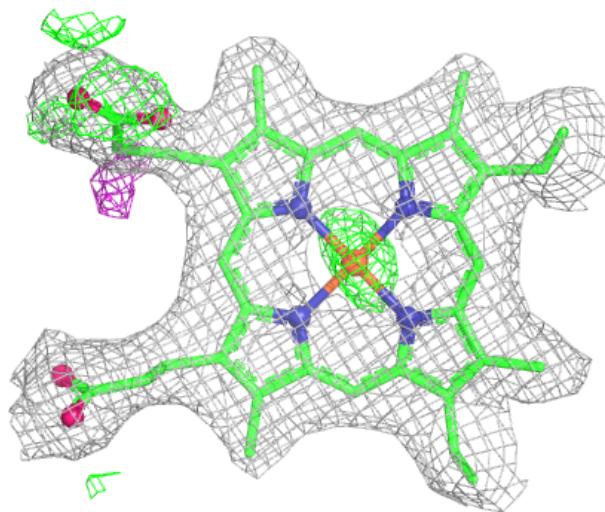
Electron density around HEC B 502:

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



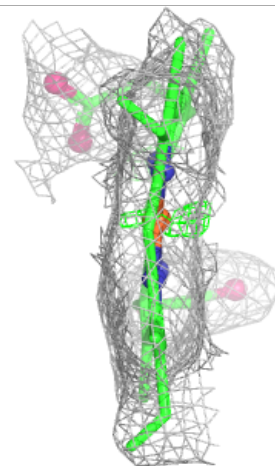
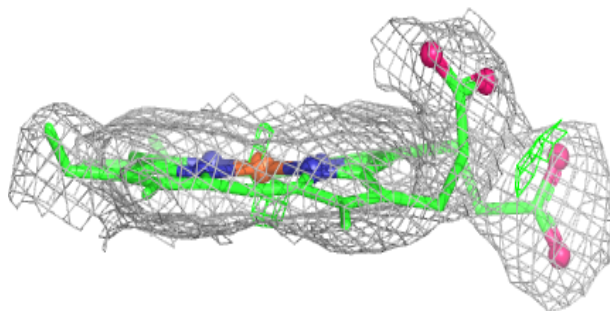
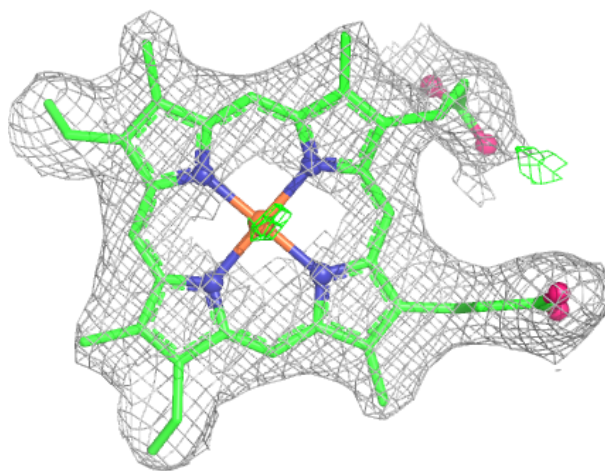
Electron density around HEC B 503:

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



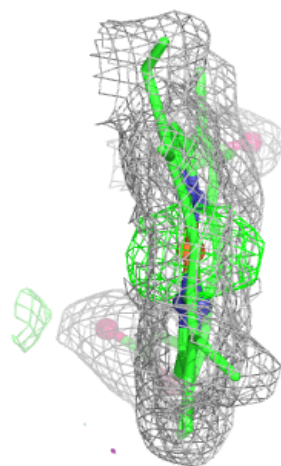
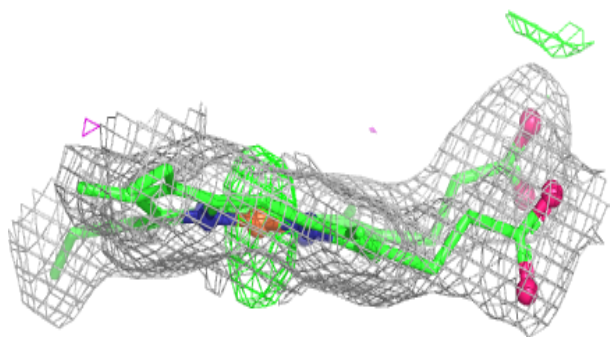
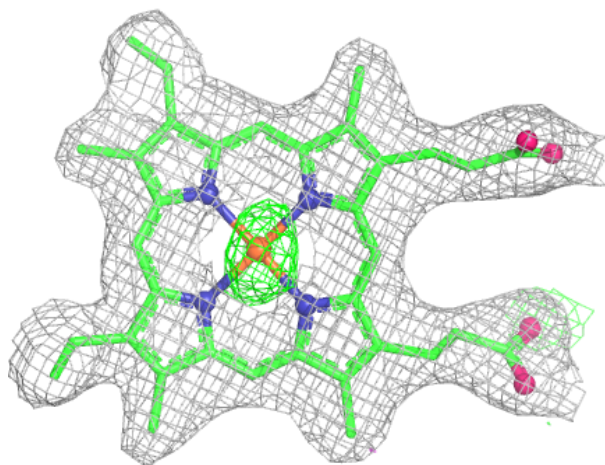
Electron density around HEC F 502:

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



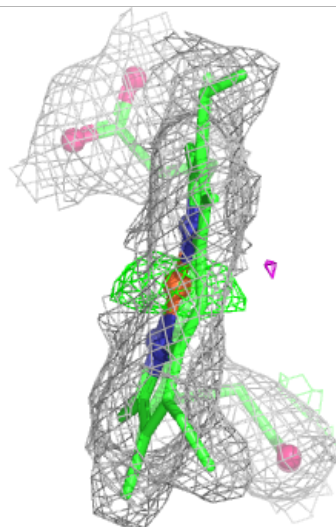
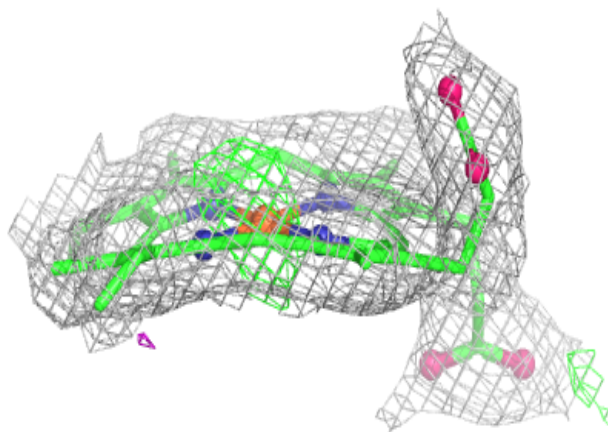
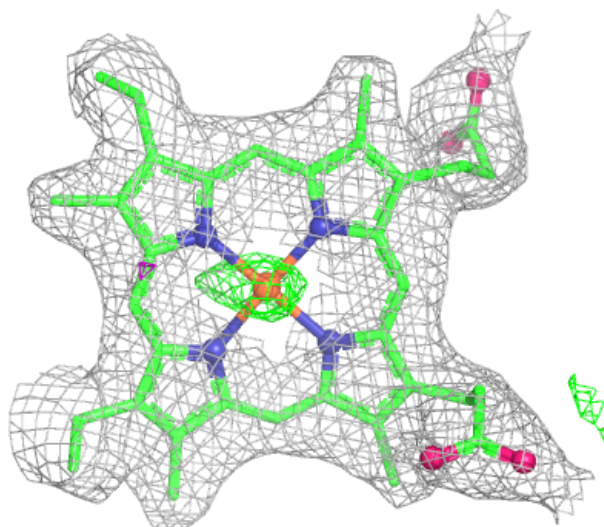
Electron density around HEC B 504:

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



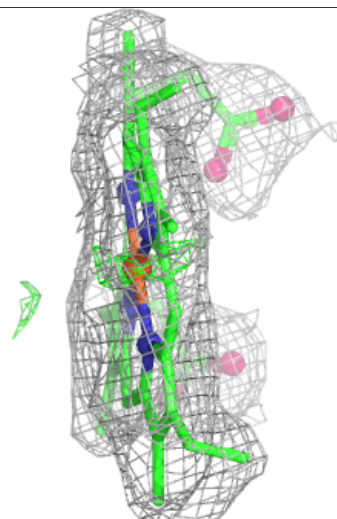
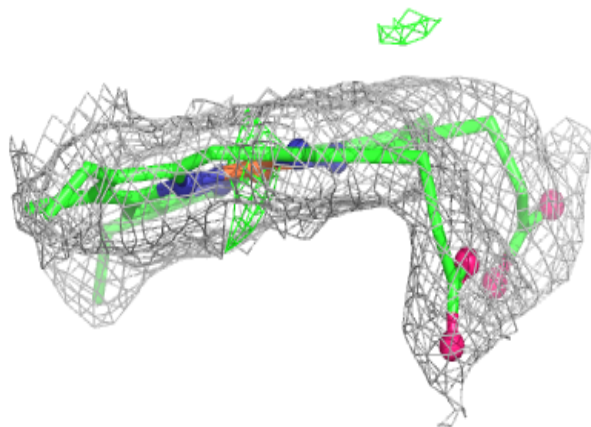
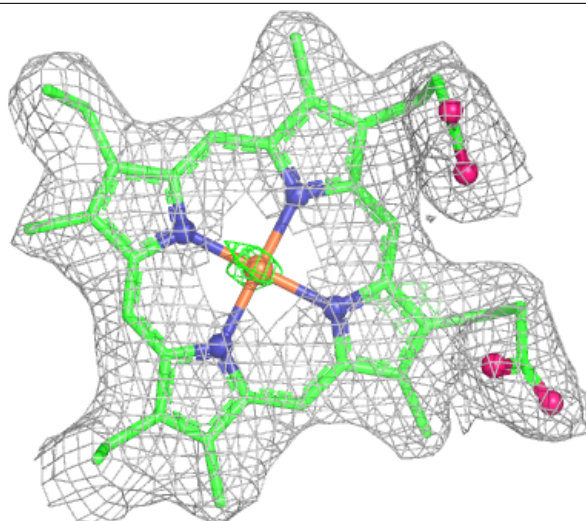
Electron density around HEC B 505:

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



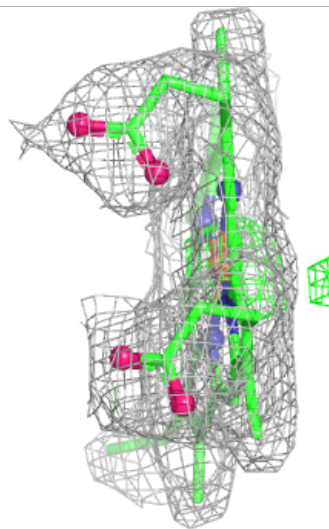
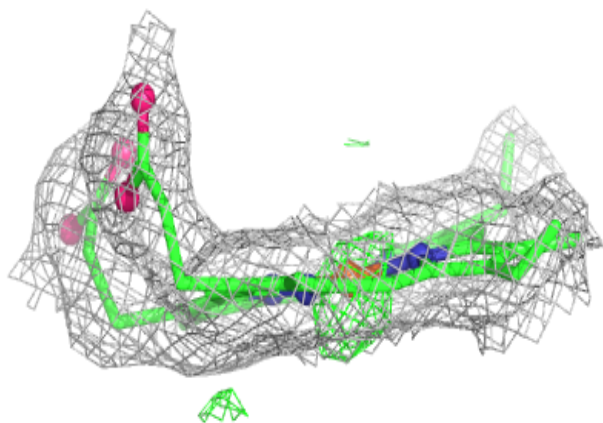
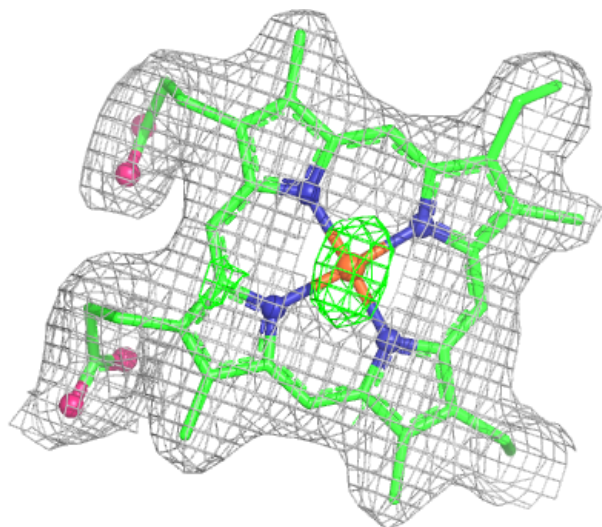
Electron density around HEC C 501:

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



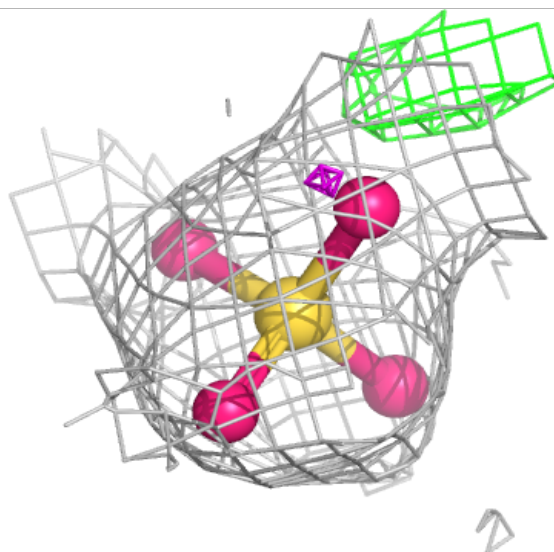
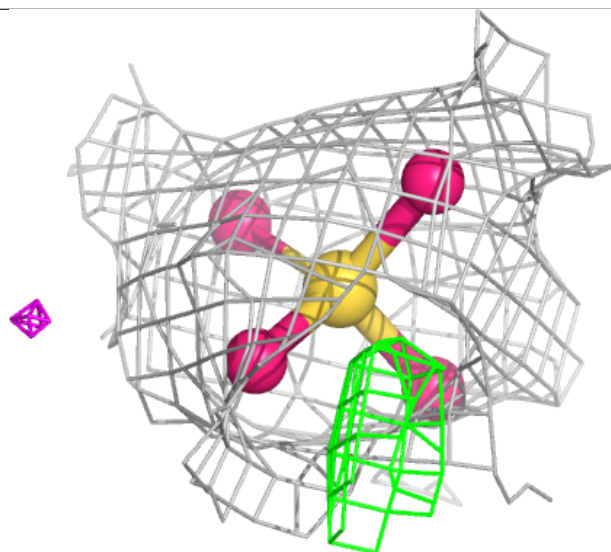
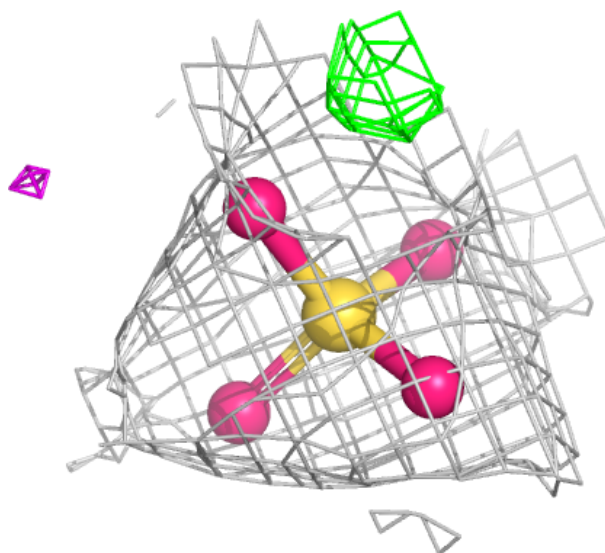
Electron density around HEC A 501:

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



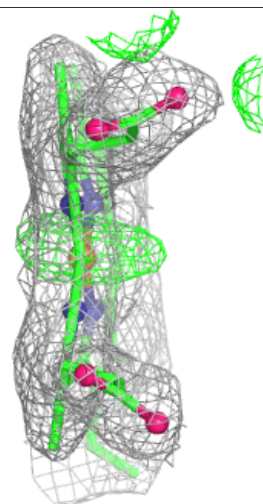
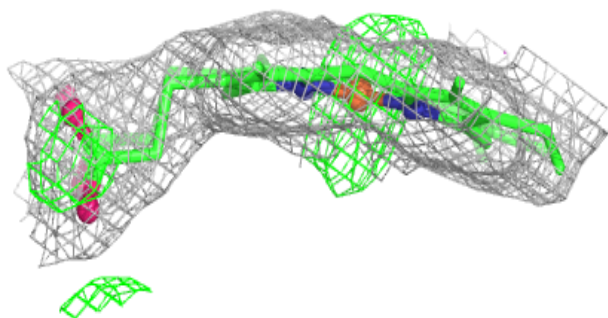
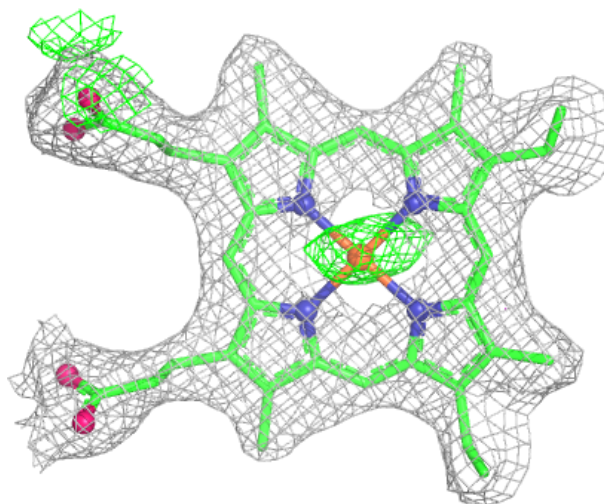
Electron density around SO4 B 506:

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



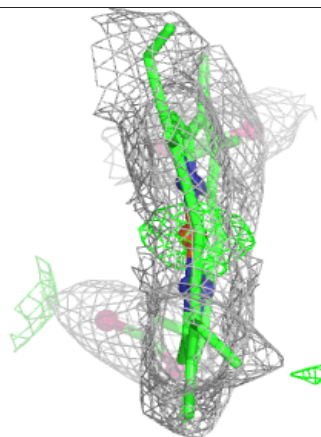
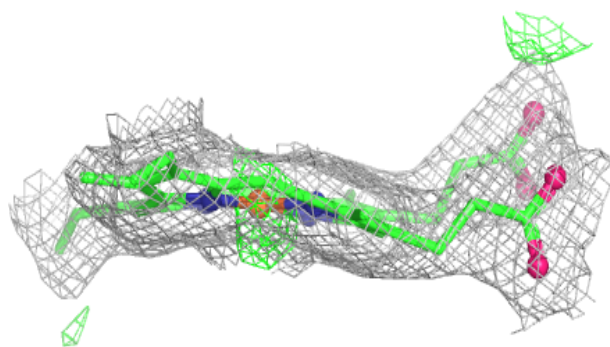
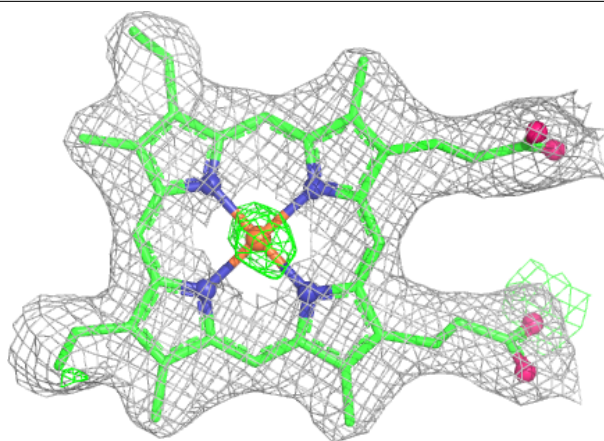
Electron density around HEC C 503:

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



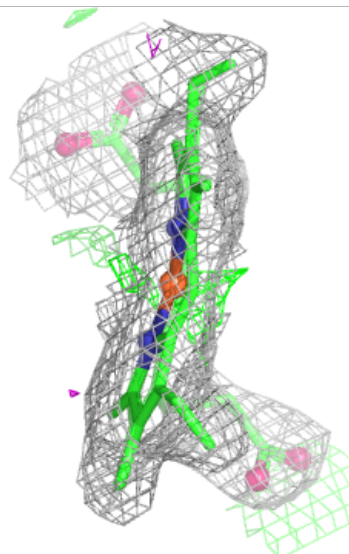
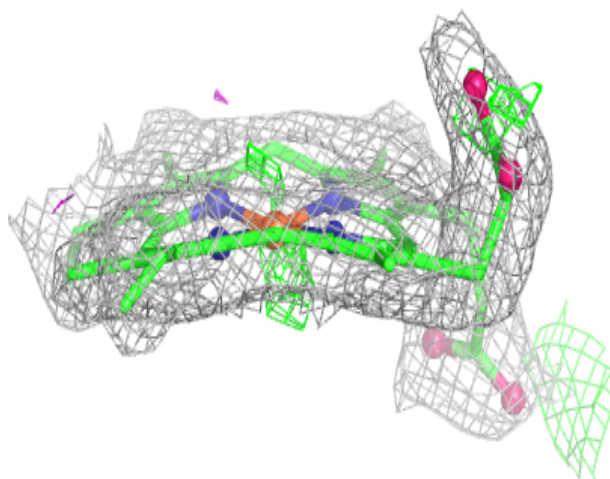
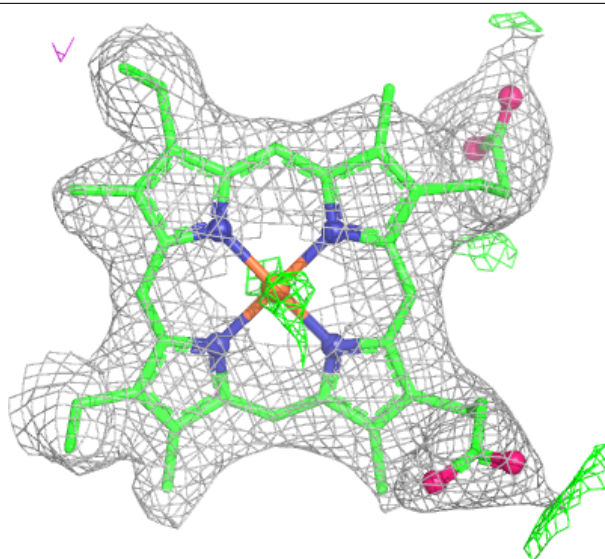
Electron density around HEC C 504:

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



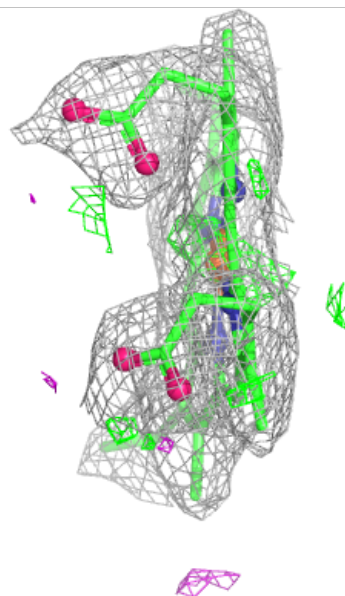
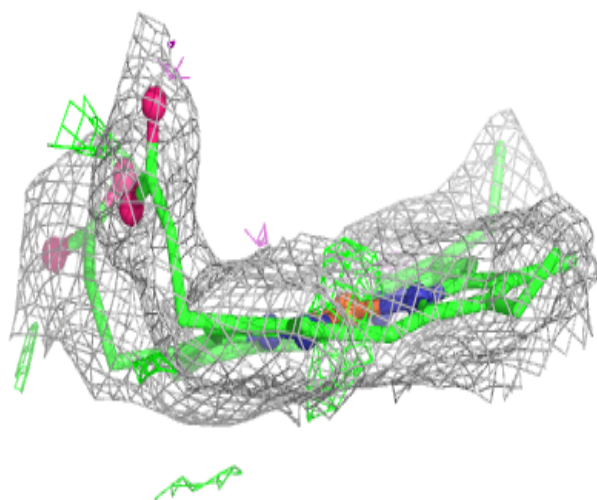
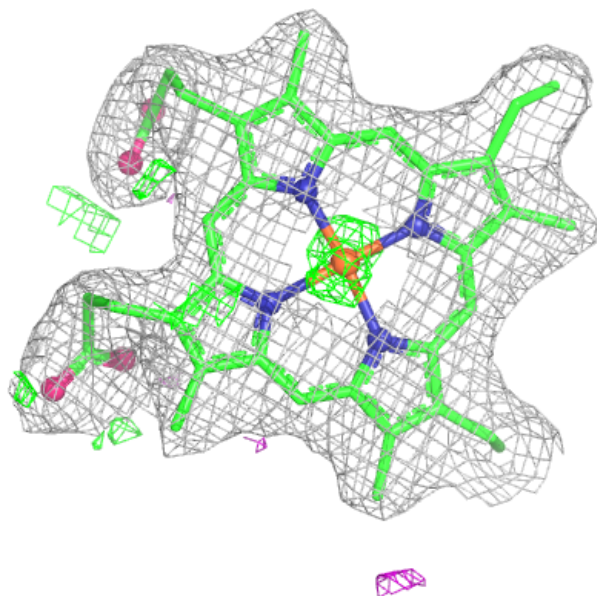
Electron density around HEC C 505:

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



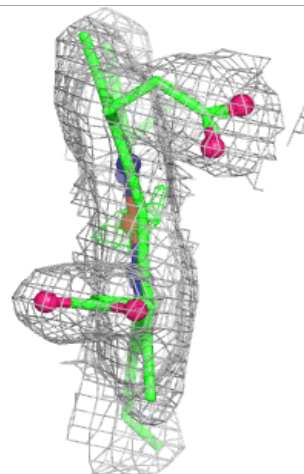
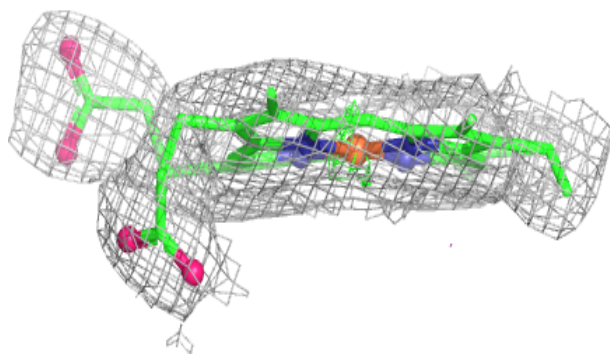
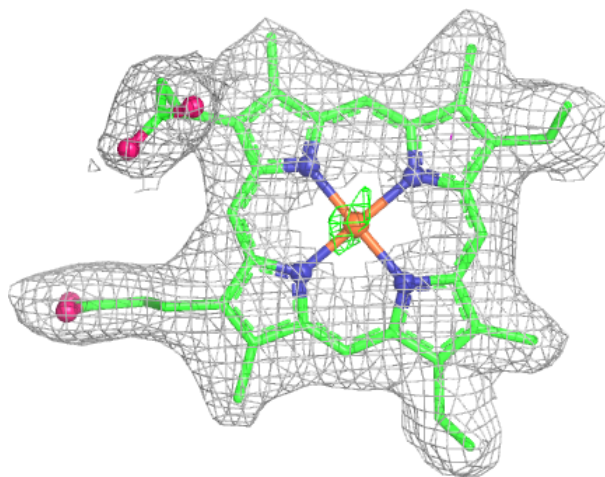
Electron density around HEC D 501:

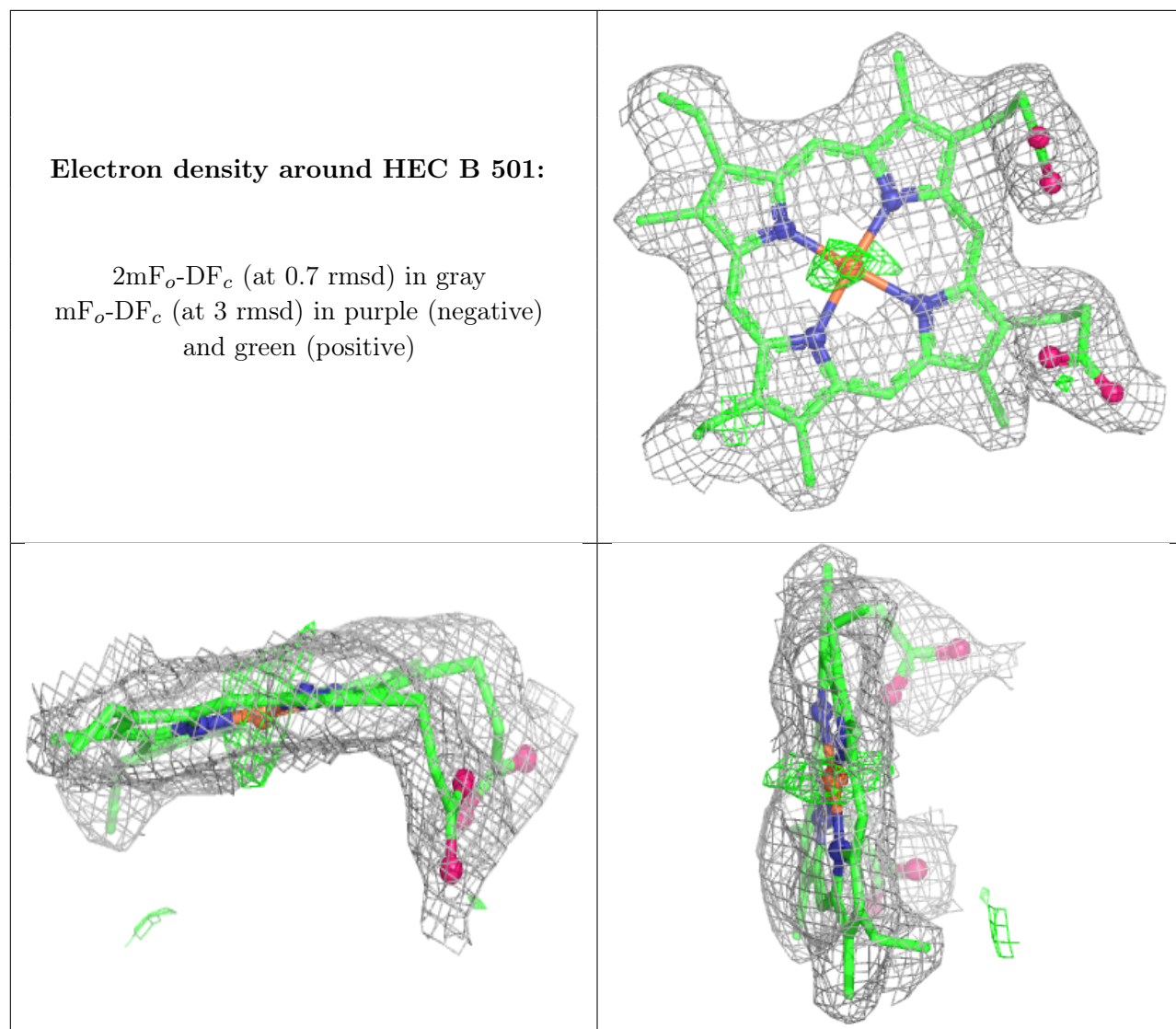
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEC A 502:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.