



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 4, 2026 – 09:56 PM UTC

PDB ID : 9VDX / pdb_00009vdx
Title : Serial synchrotron crystallography structure of a photosynthetic reaction center using a goniometer-compatible chip-based platform
Authors : Ghosh, S.; Banacore, A.; Neutze, R.; Branden, G.
Deposited on : 2025-06-09
Resolution : 2.80 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

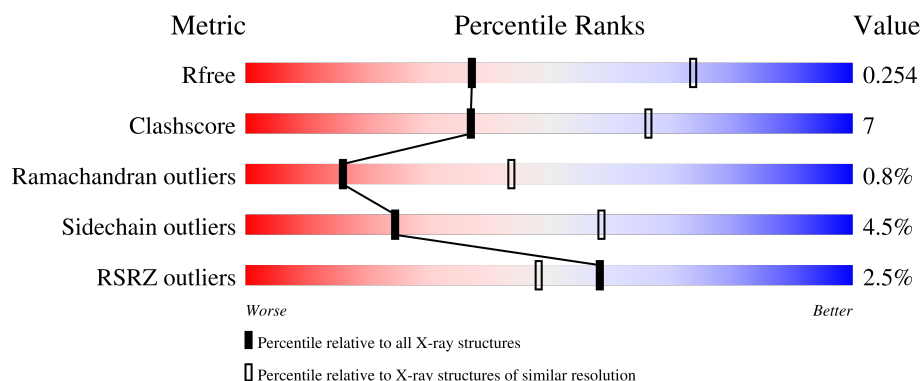
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	C	336	 2% 82% 16% ..
2	H	258	 6% 76% 21% .
3	L	273	 % 88% 12%
4	M	323	 % 82% 16% .

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
10	BCB	L	301	X	-	-	-
10	BCB	L	302	X	-	-	-
10	BCB	M	405	X	-	-	-
10	BCB	M	406	X	-	-	-
11	BPB	L	303	X	-	-	-
11	BPB	M	407	X	-	-	-

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 10352 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 Photosynthetic reaction center cytochrome c subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	332	Total	C	N	O	S	0	0	0
			2602	1640	466	478	18			

- Molecule 2 is a protein called Reaction center protein H chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	258	Total	C	N	O	S	0	0	0
			2018	1292	344	380	2			

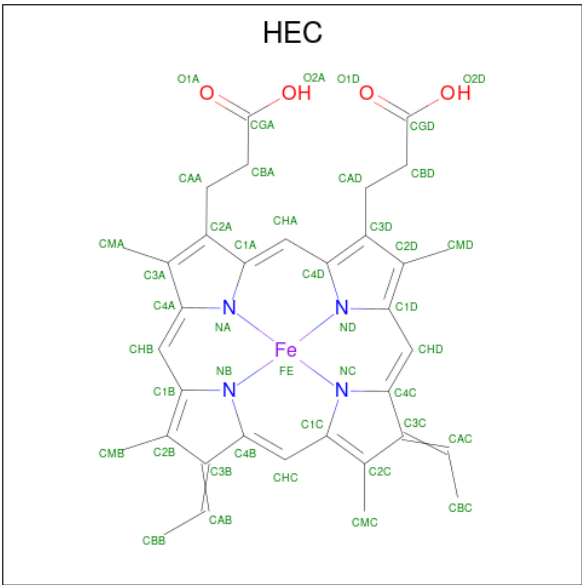
- Molecule 3 is a protein called Reaction center protein L chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	273	Total	C	N	O	S	0	1	0
			2172	1460	350	355	7			

- Molecule 4 is a protein called Reaction center protein M chain.

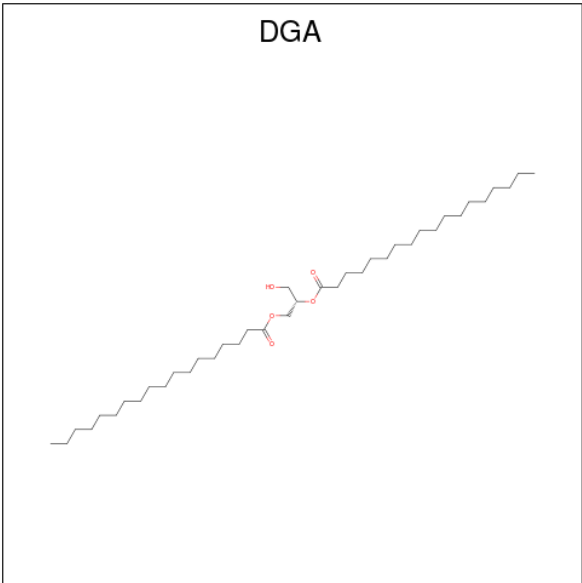
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	M	323	Total	C	N	O	S	0	0	0
			2555	1702	419	423	11			

- Molecule 5 is HEME C (CCD ID: HEC) (formula: C₃₄H₃₄FeN₄O₄) (labeled as "Ligand of Interest" by depositor).



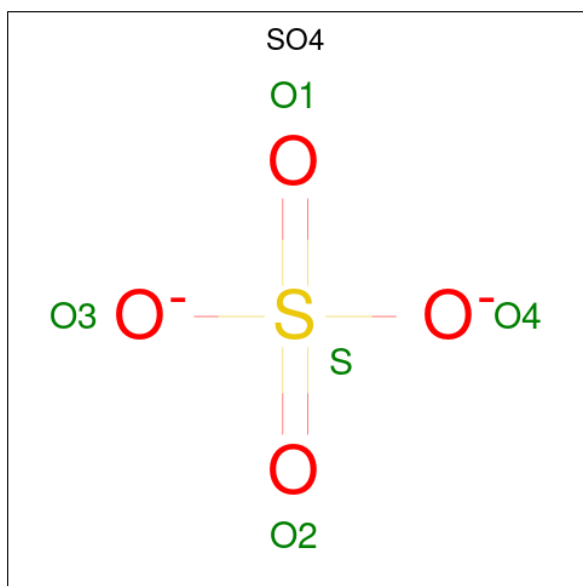
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 6 is DIACYL GLYCEROL (CCD ID: DGA) (formula: $C_{39}H_{76}O_5$) (labeled as "Lig- and of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			37	33	4		

- Molecule 7 is SULFATE ION (CCD ID: SO4) (formula: O₄S) (labeled as "Ligand of Interest" by depositor).



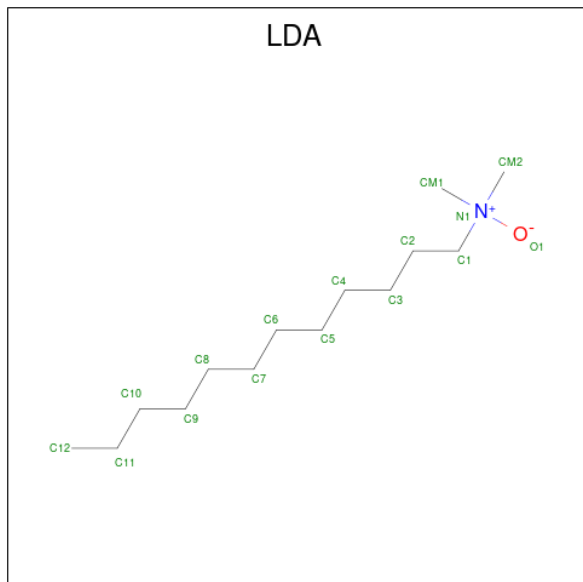
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		
7	H	1	Total	O	S	0	0
			5	4	1		
7	H	1	Total	O	S	0	0
			5	4	1		
7	H	1	Total	O	S	0	0
			5	4	1		
7	H	1	Total	O	S	0	0
			5	4	1		
7	M	1	Total	O	S	0	0
			5	4	1		
7	M	1	Total	O	S	0	0
			5	4	1		
7	M	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	M	1	Total	O	S	0	0
			5	4	1		
7	M	1	Total	O	S	0	0
			5	4	1		
7	M	1	Total	O	S	0	0
			5	4	1		
7	M	1	Total	O	S	0	0
			5	4	1		
7	M	1	Total	O	S	0	0
			5	4	1		

- Molecule 8 is LAURYL DIMETHYLAMINE-N-OXIDE (CCD ID: LDA) (formula: $C_{14}H_{31}NO$) (labeled as "Ligand of Interest" by depositor).



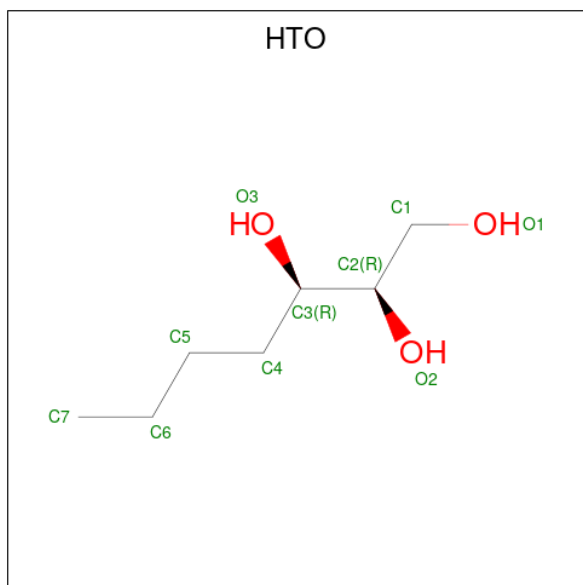
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	H	1	Total	C	N	O	0	0
			16	14	1	1		
8	H	1	Total	C	N	O	0	0
			16	14	1	1		
8	L	1	Total	C	N	O	0	0
			16	14	1	1		
8	L	1	Total	C	N	O	0	0
			16	14	1	1		
8	M	1	Total	C	N	O	0	0
			16	14	1	1		
8	M	1	Total	C	N	O	0	0
			16	14	1	1		

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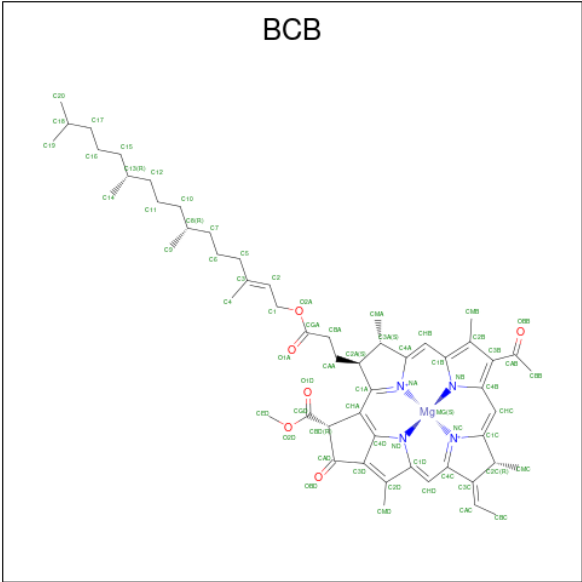
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	M	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 9 is HEPTANE-1,2,3-TRIOL (CCD ID: HTO) (formula: $C_7H_{16}O_3$) (labeled as "Ligand of Interest" by depositor).



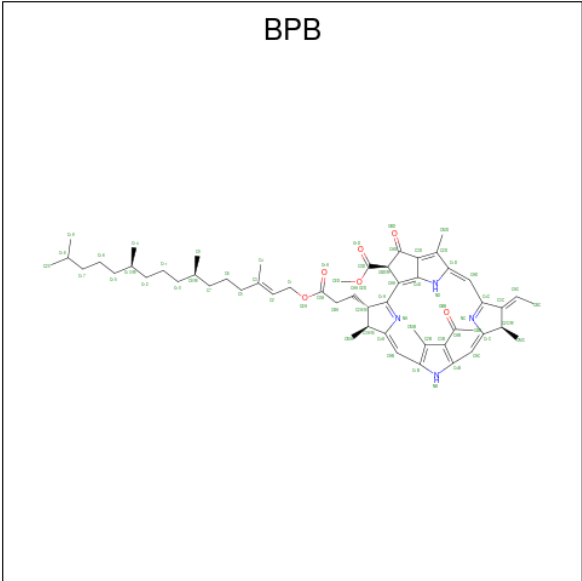
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	H	1	Total	C	O	0	0
			10	7	3		
9	L	1	Total	C	O	0	0
			10	7	3		
9	M	1	Total	C	O	0	0
			10	7	3		

- Molecule 10 is BACTERIOCHLOROPHYLL B (CCD ID: BCB) (formula: $C_{55}H_{72}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
10	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
10	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
10	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

- Molecule 11 is BACTERIOPHEOPHYTIN B (CCD ID: BPB) (formula: C₅₅H₇₄N₄O₆) (labeled as "Ligand of Interest" by depositor).

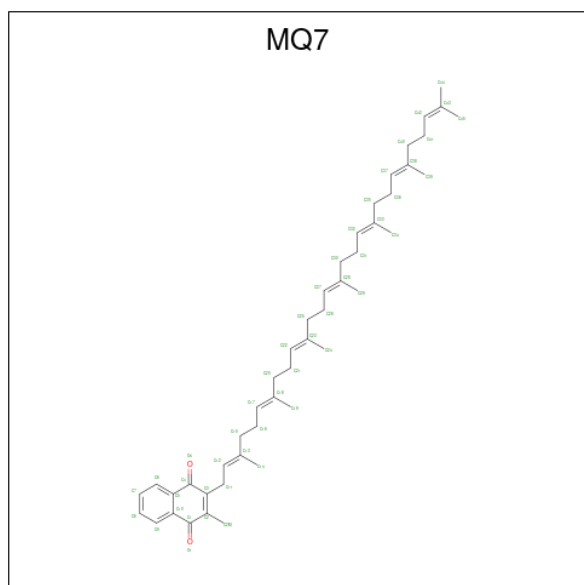


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	L	1	Total	C	N	O	0	0
			65	55	4	6		
11	M	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 12 is FE (II) ION (CCD ID: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

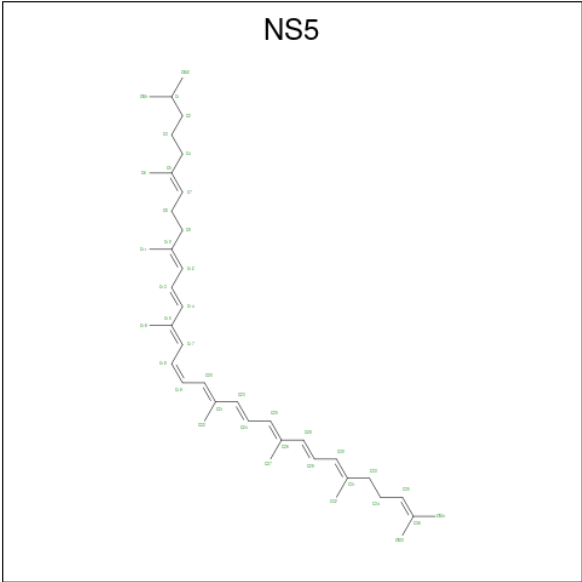
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	M	1	Total	Fe	0	0
			1	1		

- Molecule 13 is MENAQUINONE-7 (CCD ID: MQ7) (formula: C₄₆H₆₄O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	M	1	Total	C	O	0	0
			48	46	2		

- Molecule 14 is 15-cis-1,2-dihydroneurosporene (CCD ID: NS5) (formula: C₄₀H₆₀) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	M	1	Total C 40 40	0	0

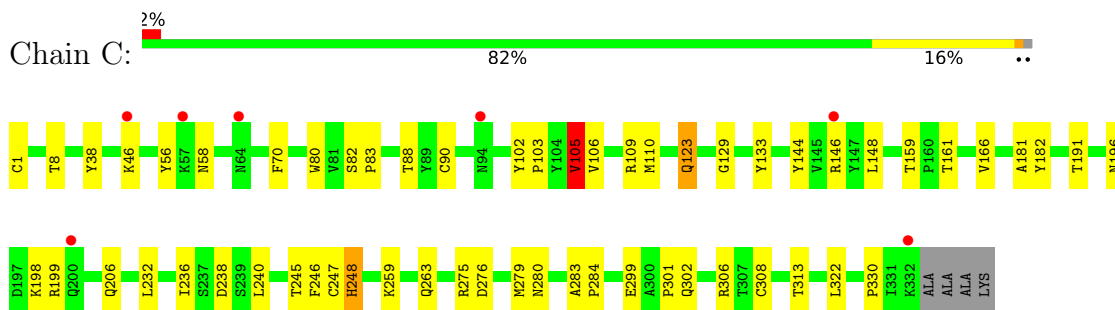
- Molecule 15 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	C	34	Total O 34 34	0	0
15	H	16	Total O 16 16	0	0
15	L	17	Total O 17 17	0	0
15	M	29	Total O 29 29	0	0

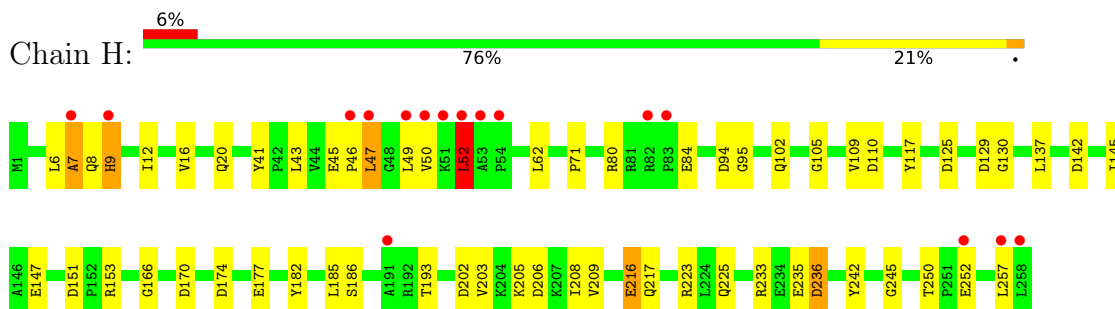
3 Residue-property plots [i](#)

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

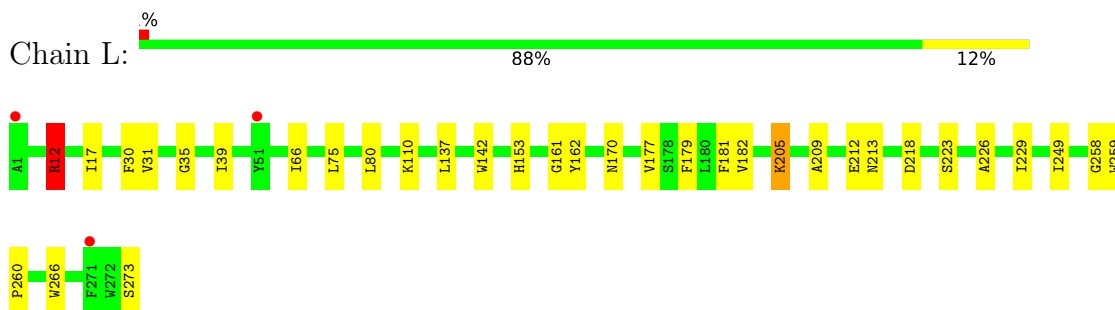
- Molecule 1: Photosynthetic reaction center cytochrome c subunit



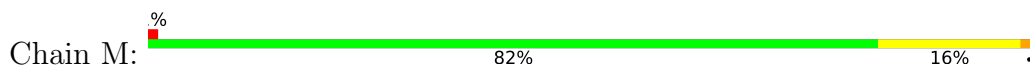
- Molecule 2: Reaction center protein H chain

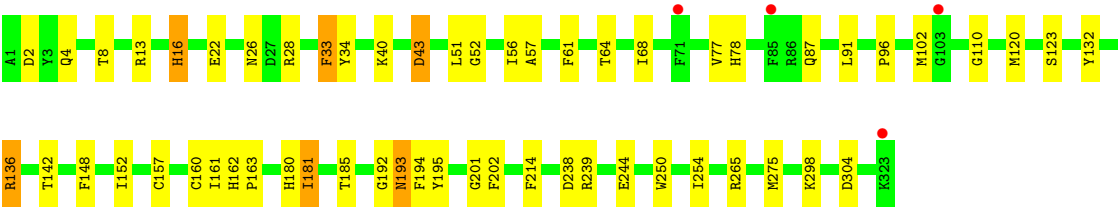


- Molecule 3: Reaction center protein L chain



- Molecule 4: Reaction center protein M chain





4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	223.80Å 223.80Å 113.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.80 – 2.80 36.80 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.6 (36.80-2.80) 99.6 (36.80-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.10 (at 1.43Å)	Xtriage
Refinement program	REFMAC 8.0.010	Depositor
R, R_{free}	0.215 , 0.253 0.215 , 0.254	Depositor DCC
R_{free} test set	23557 reflections (4.57%)	wwPDB-VP
Wilson B-factor (Å ²)	-31.7	Xtriage
Anisotropy	-0.632	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 53.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10352	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.75% 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, NS5, MQ7, FE2, FME, HEC, HTO, LDA, DGA, BCB, BPB

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	C	0.58	0/2669	1.09	1/3637 (0.0%)
2	H	0.58	0/2055	1.08	2/2807 (0.1%)
3	L	0.58	0/2267	1.03	1/3095 (0.0%)
4	M	0.58	0/2659	1.09	4/3637 (0.1%)
All	All	0.58	0/9650	1.07	8/13176 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	2
2	H	0	1
3	L	0	1
4	M	0	3
All	All	0	7

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	206	ASP	CA-CB-CG	6.82	119.42	112.60
4	M	16	HIS	CA-CB-CG	6.41	120.21	113.80
1	C	105	VAL	N-CA-CB	5.77	117.30	110.55
4	M	33	PHE	CA-CB-CG	5.50	119.30	113.80
4	M	43	ASP	CB-CA-C	5.43	118.49	109.53
3	L	153	HIS	CA-CB-CG	5.34	119.14	113.80
4	M	8	THR	CA-CB-OG1	-5.15	101.88	109.60
2	H	125	ASP	CA-CB-CG	5.04	117.64	112.60

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	199	ARG	Sidechain
1	C	248	HIS	Peptide
2	H	223	ARG	Sidechain
3	L	12	ARG	Sidechain
4	M	13	ARG	Sidechain
4	M	136	ARG	Sidechain
4	M	265	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2602	0	2581	45	0
2	H	2018	0	2020	29	0
3	L	2172	0	2097	24	0
4	M	2555	0	2452	31	0
5	C	172	0	122	18	0
6	C	37	0	58	2	0
7	C	15	0	0	0	0
7	H	20	0	0	1	0
7	M	40	0	0	1	0
8	H	32	0	62	2	0
8	L	32	0	62	0	0
8	M	48	0	93	0	0
9	H	10	0	16	0	0
9	L	10	0	16	0	0
9	M	10	0	16	0	0
10	L	132	0	144	9	0
10	M	132	0	144	9	0
11	L	65	0	74	3	0
11	M	65	0	74	5	0
12	M	1	0	0	0	0
13	M	48	0	64	1	0
14	M	40	0	60	2	0
15	C	34	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	H	16	0	0	0	0
15	L	17	0	0	0	0
15	M	29	0	0	0	0
All	All	10352	0	10155	144	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 7.

All (144) 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:C:247:CYS:SG	5:C:403:HEC:CAC	2.01	1.48
1:C:90:CYS:SG	5:C:401:HEC:CAC	2.06	1.44
1:C:308:CYS:SG	5:C:404:HEC:CAC	2.26	1.22
1:C:90:CYS:SG	5:C:401:HEC:CBC	2.47	1.02
1:C:308:CYS:SG	5:C:404:HEC:HAC	2.00	0.98
1:C:247:CYS:SG	5:C:403:HEC:C3C	2.64	0.85
1:C:90:CYS:SG	5:C:401:HEC:HAC	2.20	0.80
10:L:301:BCB:H193	13:M:404:MQ7:H292	1.63	0.79
1:C:90:CYS:SG	5:C:401:HEC:HBC3	2.25	0.75
11:M:407:BPB:HHC	11:M:407:BPB:HBBB	1.68	0.73
10:M:405:BCB:HBB2	10:M:405:BCB:HHC	1.70	0.73
4:M:52:GLY:O	4:M:56:ILE:HG12	1.89	0.72
1:C:90:CYS:SG	5:C:401:HEC:C3C	2.80	0.70
3:L:213:ASN:OD1	3:L:223:SER:OG	2.07	0.70
4:M:160:CYS:SG	14:M:408:NS5:H322	2.34	0.68
2:H:52:LEU:N	2:H:52:LEU:HD12	2.11	0.66
5:C:401:HEC:HBC3	5:C:401:HEC:HMC1	1.78	0.66
2:H:52:LEU:N	2:H:52:LEU:CD1	2.59	0.65
3:L:181:PHE:CD2	11:M:407:BPB:HBB	2.33	0.64
2:H:12:ILE:O	2:H:16:VAL:HG23	1.99	0.63
2:H:182:TYR:OH	2:H:235:GLU:OE1	2.14	0.63
1:C:308:CYS:SG	5:C:404:HEC:C3C	2.87	0.62
5:C:403:HEC:HBC1	5:C:404:HEC:HMA1	1.82	0.62
3:L:170:ASN:HB2	3:L:259:TRP:CD1	2.34	0.61
3:L:259:TRP:N	3:L:260:PRO:CD	2.63	0.61
10:L:301:BCB:HBB3	10:L:301:BCB:HMB3	1.82	0.61
2:H:52:LEU:HD12	2:H:52:LEU:H	1.65	0.61
10:L:301:BCB:HMB3	10:L:301:BCB:CBB	2.30	0.61
4:M:2:ASP:OD1	4:M:4:GLN:HB2	2.00	0.60
2:H:151:ASP:OD1	2:H:153:ARG:HB2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:TYR:CG	1:C:103:PRO:HD3	2.37	0.58
1:C:80:TRP:CD1	1:C:133:TYR:HB2	2.39	0.58
2:H:6:LEU:O	2:H:7:ALA:O	2.21	0.57
3:L:181:PHE:HB3	11:M:407:BPB:CBB	2.33	0.57
2:H:45:GLU:O	2:H:47:LEU:N	2.37	0.57
1:C:1:CYS:SG	6:C:405:DGA:HG12	2.44	0.57
1:C:246:PHE:CZ	1:C:263:GLN:HG2	2.40	0.56
11:M:407:BPB:HBBB	11:M:407:BPB:CHC	2.34	0.56
3:L:161:GLY:HA3	10:L:301:BCB:HAC1	1.87	0.56
2:H:102:GLN:HE22	3:L:12:ARG:HD3	1.70	0.56
2:H:151:ASP:OD2	2:H:153:ARG:NH2	2.24	0.56
11:L:303:BPB:HBBB	11:L:303:BPB:HMBB	1.87	0.55
1:C:144:TYR:CD1	1:C:306:ARG:HD3	2.42	0.55
10:M:405:BCB:HBB3	10:M:406:BCB:H62	1.87	0.55
10:L:301:BCB:HBD	10:L:301:BCB:HAA1	1.87	0.55
2:H:166:GLY:HA3	2:H:186:SER:O	2.06	0.55
4:M:181:ILE:HG12	10:M:405:BCB:CED	2.37	0.54
2:H:202:ASP:HB3	2:H:209:VAL:HB	1.88	0.54
10:M:406:BCB:HMB3	10:M:406:BCB:CBB	2.38	0.54
1:C:161:THR:OG1	3:L:273:SER:O	2.22	0.53
2:H:71:PRO:HA	3:L:205:LYS:HD3	1.90	0.53
11:L:303:BPB:HMBB	11:L:303:BPB:CBB	2.39	0.53
1:C:276:ASP:OD1	1:C:280:ASN:ND2	2.41	0.53
2:H:117:TYR:HB2	2:H:236:ASP:HB3	1.91	0.53
4:M:120:MET:O	4:M:123:SER:HB3	2.09	0.52
4:M:180:HIS:CE1	4:M:181:ILE:HD13	2.44	0.52
4:M:275:MET:HA	4:M:275:MET:HE2	1.92	0.52
1:C:56:TYR:HB3	5:C:401:HEC:O2A	2.09	0.52
10:L:301:BCB:HBB3	10:L:301:BCB:CMB	2.40	0.52
1:C:238:ASP:OD2	1:C:306:ARG:NH2	2.44	0.50
2:H:174:ASP:OD1	2:H:177:GLU:N	2.42	0.50
1:C:1:CYS:SG	6:C:405:DGA:CG3	2.99	0.50
2:H:242:TYR:O	2:H:245:GLY:N	2.45	0.50
4:M:148:PHE:CZ	4:M:152:ILE:HD11	2.48	0.49
1:C:275:ARG:HB3	1:C:279:MET:HE2	1.93	0.49
2:H:216:GLU:HG3	2:H:217:GLN:HG3	1.93	0.49
2:H:41:TYR:CE2	2:H:43:LEU:HD21	2.48	0.49
3:L:170:ASN:HB2	3:L:259:TRP:CG	2.46	0.49
1:C:301:PRO:HG2	5:C:402:HEC:HBD1	1.94	0.48
3:L:162:TYR:OH	4:M:185:THR:HG23	2.13	0.48
2:H:94:ASP:OD1	2:H:95:GLY:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:16:HIS:HB2	7:M:416:SO4:S	2.54	0.48
1:C:283:ALA:N	1:C:284:PRO:CD	2.76	0.48
5:C:401:HEC:HBB3	5:C:401:HEC:CMB	2.43	0.48
1:C:102:TYR:N	1:C:103:PRO:CD	2.77	0.48
10:L:302:BCB:HMB3	10:L:302:BCB:HBB2	1.96	0.48
1:C:322:LEU:HD21	1:C:330:PRO:HD3	1.96	0.47
1:C:259:LYS:NZ	4:M:304:ASP:OD1	2.43	0.47
3:L:209:ALA:O	3:L:212:GLU:HB2	2.14	0.47
2:H:8:GLN:O	2:H:9:HIS:HB2	2.14	0.47
11:L:303:BPB:HEDB	4:M:254:ILE:HG21	1.96	0.47
14:M:408:NS5:H29	14:M:408:NS5:H271	1.69	0.47
1:C:181:ALA:O	1:C:182:TYR:HB2	2.15	0.47
4:M:87:GLN:O	4:M:91:LEU:HG	2.15	0.47
3:L:179:PHE:HA	3:L:182:VAL:HG12	1.97	0.47
4:M:239:ARG:HD2	4:M:244:GLU:OE2	2.15	0.47
1:C:105:VAL:O	1:C:106:VAL:C	2.57	0.46
4:M:238:ASP:O	4:M:239:ARG:C	2.58	0.46
2:H:142:ASP:OD1	2:H:142:ASP:N	2.45	0.46
1:C:302:GLN:NE2	15:C:505:HOH:O	2.48	0.46
1:C:109:ARG:HH11	1:C:109:ARG:HG3	1.80	0.46
1:C:232:LEU:O	1:C:236:ILE:HG13	2.16	0.45
1:C:38:TYR:CD1	1:C:133:TYR:CD2	3.05	0.45
10:L:302:BCB:OBD	4:M:201:GLY:HA2	2.16	0.45
3:L:226:ALA:O	3:L:229:ILE:HG22	2.16	0.45
10:L:301:BCB:CBB	10:L:301:BCB:CMB	2.94	0.45
10:M:406:BCB:HMB3	10:M:406:BCB:HBB3	1.99	0.45
1:C:70:PHE:HE2	5:C:401:HEC:C2A	2.30	0.44
3:L:75:LEU:HA	3:L:142:TRP:CD1	2.52	0.44
4:M:57:ALA:O	4:M:61:PHE:CD2	2.70	0.44
2:H:203:VAL:HG22	2:H:208:ILE:HD12	1.99	0.44
3:L:137:LEU:HD23	3:L:137:LEU:HA	1.89	0.44
4:M:96:PRO:HD3	4:M:110:GLY:HA3	1.99	0.44
1:C:148:LEU:HG	1:C:299:GLU:HG3	1.99	0.44
2:H:145:ILE:CD1	2:H:151:ASP:HA	2.47	0.44
1:C:148:LEU:O	1:C:191:THR:HG21	2.18	0.44
4:M:64:THR:O	4:M:68:ILE:HG13	2.18	0.43
1:C:283:ALA:HB3	1:C:284:PRO:HD3	2.00	0.43
15:C:515:HOH:O	3:L:258:GLY:HA3	2.18	0.43
4:M:181:ILE:CD1	10:M:405:BCB:HED3	2.48	0.43
4:M:192:GLY:O	4:M:193:ASN:HB3	2.18	0.43
3:L:177:VAL:HG11	10:M:405:BCB:HMD3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:192:GLY:O	4:M:193:ASN:CB	2.66	0.43
1:C:109:ARG:HG3	1:C:109:ARG:NH1	2.34	0.43
1:C:110:MET:HG3	5:C:402:HEC:C4A	2.48	0.43
2:H:225:GLN:HA	2:H:225:GLN:OE1	2.18	0.43
4:M:34:TYR:CD1	4:M:34:TYR:N	2.88	0.42
10:M:405:BCB:HBB2	10:M:405:BCB:CHC	2.45	0.42
1:C:245:THR:HA	1:C:248:HIS:O	2.19	0.42
3:L:35:GLY:O	3:L:39:ILE:HG12	2.20	0.42
3:L:218:ASP:OD2	4:M:28:ARG:NH2	2.53	0.42
2:H:137:LEU:HB2	2:H:170:ASP:OD1	2.20	0.42
2:H:62:LEU:O	8:H:706:LDA:HM11	2.20	0.42
3:L:30:PHE:CE1	3:L:110:LYS:HE3	2.55	0.42
2:H:257:LEU:HD23	2:H:257:LEU:HA	1.93	0.41
4:M:157:CYS:HA	4:M:161:ILE:HB	2.02	0.41
1:C:206:GLN:NE2	15:C:510:HOH:O	2.53	0.41
1:C:82:SER:N	1:C:83:PRO:CD	2.82	0.41
1:C:196:ASN:ND2	1:C:198:LYS:HG2	2.35	0.41
7:H:705:SO4:O2	8:H:706:LDA:O1	2.38	0.41
1:C:123:GLN:NE2	1:C:123:GLN:H	2.18	0.41
3:L:181:PHE:HB3	11:M:407:BPB:HBBA	2.02	0.41
1:C:129:GLY:HA3	1:C:322:LEU:HD13	2.03	0.41
5:C:401:HEC:HBC3	5:C:401:HEC:CMC	2.48	0.41
2:H:105:GLY:HA3	2:H:110:ASP:OD2	2.21	0.41
4:M:132:TYR:CE1	4:M:142:THR:HG21	2.55	0.41
4:M:195:TYR:CZ	10:M:406:BCB:HMC2	2.56	0.41
4:M:250:TRP:O	4:M:254:ILE:HG12	2.21	0.41
1:C:196:ASN:OD1	1:C:196:ASN:N	2.53	0.40
2:H:20:GLN:HG2	4:M:202:PHE:CE2	2.57	0.40
4:M:77:VAL:O	4:M:78:HIS:C	2.65	0.40
4:M:162:HIS:HB3	4:M:163:PRO:HD3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	330/336 (98%)	317 (96%)	12 (4%)	1 (0%)	36	66
2	H	256/258 (99%)	236 (92%)	13 (5%)	7 (3%)	4	15
3	L	272/273 (100%)	261 (96%)	10 (4%)	1 (0%)	30	60
4	M	321/323 (99%)	309 (96%)	11 (3%)	1 (0%)	36	66
All	All	1179/1190 (99%)	1123 (95%)	46 (4%)	10 (1%)	16	44

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	7	ALA
1	C	58	ASN
2	H	9	HIS
2	H	50	VAL
2	H	52	LEU
4	M	193	ASN
2	H	46	PRO
2	H	130	GLY
2	H	147	GLU
3	L	31	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	C	281/282 (100%)	271 (96%)	10 (4%)	31	66
2	H	212/212 (100%)	197 (93%)	15 (7%)	13	39
3	L	219/218 (100%)	213 (97%)	6 (3%)	39	74
4	M	249/249 (100%)	237 (95%)	12 (5%)	23	56
All	All	961/961 (100%)	918 (96%)	43 (4%)	24	58

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	8	THR
1	C	46	LYS
1	C	88	THR
1	C	105	VAL
1	C	123	GLN
1	C	146	ARG
1	C	159	THR
1	C	166	VAL
1	C	240	LEU
1	C	313	THR
2	H	47	LEU
2	H	49	LEU
2	H	52	LEU
2	H	80	ARG
2	H	84	GLU
2	H	109	VAL
2	H	129	ASP
2	H	185	LEU
2	H	193	THR
2	H	205	LYS
2	H	216	GLU
2	H	233	ARG
2	H	236	ASP
2	H	250	THR
2	H	252	GLU
3	L	12	ARG
3	L	17	ILE
3	L	80	LEU
3	L	205	LYS
3	L	249	ILE
3	L	266	TRP
4	M	22	GLU
4	M	26	ASN
4	M	33	PHE
4	M	40	LYS
4	M	43	ASP
4	M	51	LEU
4	M	102	MET
4	M	136	ARG
4	M	181	ILE
4	M	194	PHE
4	M	214	PHE
4	M	298	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	24	HIS
1	C	64	ASN
1	C	123	GLN
1	C	302	GLN
2	H	92	GLN
2	H	102	GLN
2	H	220	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
2	FME	H	1	2	8,9,10	0.46	0	8,9,11	0.73	0

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	FME	H	1	2	-	4/7/9/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	1	FME	C-CA-CB-CG
2	H	1	FME	N-CA-CB-CG
2	H	1	FME	CB-CG-SD-CE
2	H	1	FME	CA-CB-CG-SD

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 39 ligands modelled in this entry, 1 is monoatomic - leaving 38 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	SO4	M	412	-	4,4,4	0.32	0	6,6,6	0.10	0
10	BCB	L	301	3	60,74,74	2.78	17 (28%)	59,115,115	2.54	22 (37%)
7	SO4	M	413	-	4,4,4	0.33	0	6,6,6	0.17	0
8	LDA	L	304	-	13,15,15	0.37	0	14,17,17	0.39	0
7	SO4	H	702	-	4,4,4	0.31	0	6,6,6	0.13	0
7	SO4	C	406	-	4,4,4	0.32	0	6,6,6	0.08	0
5	HEC	C	403	1	46,50,50	1.78	6 (13%)	58,82,82	2.46	10 (17%)
7	SO4	C	407	-	4,4,4	0.28	0	6,6,6	0.13	0
11	BPB	L	303	-	57,70,70	2.43	15 (26%)	55,101,101	2.25	15 (27%)
5	HEC	C	402	1	46,50,50	1.79	9 (19%)	58,82,82	1.66	9 (15%)
8	LDA	H	701	-	13,15,15	0.31	0	14,17,17	0.26	0
8	LDA	M	417	-	13,15,15	0.17	0	14,17,17	0.23	0
10	BCB	L	302	3	60,74,74	2.78	18 (30%)	59,115,115	3.04	21 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	BCB	M	405	4	60,74,74	2.79	21 (35%)	59,115,115	3.48	19 (32%)
5	HEC	C	404	1	46,50,50	1.76	4 (8%)	58,82,82	1.66	7 (12%)
8	LDA	M	418	-	13,15,15	0.37	0	14,17,17	0.41	0
6	DGA	C	405	-	36,36,43	1.38	2 (5%)	38,38,45	1.35	5 (13%)
8	LDA	M	401	-	13,15,15	0.26	0	14,17,17	0.38	0
8	LDA	H	706	-	13,15,15	0.37	0	14,17,17	0.71	1 (7%)
7	SO4	M	409	-	4,4,4	0.31	0	6,6,6	0.14	0
7	SO4	M	411	-	4,4,4	0.33	0	6,6,6	0.34	0
9	HTO	H	707	-	9,9,9	0.83	0	10,10,10	1.36	2 (20%)
13	MQ7	M	404	-	49,49,49	1.44	3 (6%)	61,63,63	1.54	11 (18%)
11	BPB	M	407	-	57,70,70	2.64	14 (24%)	55,101,101	2.21	14 (25%)
8	LDA	L	306	-	13,15,15	0.37	0	14,17,17	0.40	0
7	SO4	H	705	-	4,4,4	0.35	0	6,6,6	0.14	0
14	NS5	M	408	-	39,39,39	0.90	1 (2%)	46,46,46	2.00	11 (23%)
7	SO4	H	703	-	4,4,4	0.28	0	6,6,6	0.08	0
7	SO4	M	410	-	4,4,4	0.31	0	6,6,6	0.12	0
9	HTO	L	305	-	9,9,9	1.12	0	10,10,10	1.51	1 (10%)
7	SO4	M	415	-	4,4,4	0.34	0	6,6,6	0.07	0
5	HEC	C	401	1	46,50,50	1.86	8 (17%)	58,82,82	3.02	10 (17%)
7	SO4	M	416	-	4,4,4	0.33	0	6,6,6	0.05	0
10	BCB	M	406	4	60,74,74	2.63	17 (28%)	59,115,115	2.12	17 (28%)
7	SO4	H	704	-	4,4,4	0.31	0	6,6,6	0.14	0
9	HTO	M	402	-	9,9,9	1.27	1 (11%)	10,10,10	1.63	2 (20%)
7	SO4	C	408	-	4,4,4	0.30	0	6,6,6	0.05	0
7	SO4	M	414	-	4,4,4	0.33	0	6,6,6	0.10	0

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
10	BCB	L	301	3	3/3/21/26	6/37/137/137	-
8	LDA	L	304	-	-	5/13/13/13	-
11	BPB	L	303	-	1/1/18/23	9/37/105/105	0/5/6/6
5	HEC	C	403	1	-	6/14/54/54	-
5	HEC	C	402	1	-	7/14/54/54	-
8	LDA	H	701	-	-	6/13/13/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	LDA	M	417	-	-	5/13/13/13	-
10	BCB	M	405	4	3/3/21/26	10/37/137/137	-
10	BCB	L	302	3	3/3/21/26	8/37/137/137	-
5	HEC	C	404	1	-	6/14/54/54	-
8	LDA	M	418	-	-	7/13/13/13	-
6	DGA	C	405	-	-	13/37/37/45	-
8	LDA	M	401	-	-	4/13/13/13	-
8	LDA	H	706	-	-	8/13/13/13	-
9	HTO	H	707	-	-	6/10/10/10	-
13	MQ7	M	404	-	-	3/41/61/61	0/2/2/2
11	BPB	M	407	-	1/1/18/23	9/37/105/105	0/5/6/6
8	LDA	L	306	-	-	12/13/13/13	-
14	NS5	M	408	-	-	11/43/43/43	-
9	HTO	L	305	-	-	1/10/10/10	-
5	HEC	C	401	1	-	9/14/54/54	-
10	BCB	M	406	4	3/3/21/26	10/37/137/137	-
9	HTO	M	402	-	-	1/10/10/10	-

All (136) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	L	302	BCB	C1A-CHA	9.51	1.50	1.40
10	L	302	BCB	C1B-C2B	9.37	1.50	1.39
11	L	303	BPB	C1D-C2D	9.22	1.49	1.39
11	M	407	BPB	C1D-C2D	8.99	1.49	1.39
10	L	301	BCB	CHC-C1C	8.88	1.49	1.38
11	M	407	BPB	C1B-C2B	8.22	1.48	1.39
10	M	405	BCB	C1A-CHA	8.03	1.49	1.40
13	M	404	MQ7	C3-C2	7.55	1.48	1.35
10	L	301	BCB	C1B-C2B	7.39	1.48	1.39
10	M	406	BCB	CHC-C1C	7.12	1.47	1.38
5	C	404	HEC	CAC-C3C	7.05	1.57	1.35
10	L	301	BCB	C1A-CHA	7.01	1.48	1.40
10	M	406	BCB	C1B-C2B	6.94	1.47	1.39
10	M	406	BCB	C1A-CHA	6.79	1.47	1.40
10	M	405	BCB	C1B-C2B	6.75	1.47	1.39
10	L	301	BCB	C1D-C2D	6.74	1.47	1.39
11	L	303	BPB	C3D-C4D	-6.65	1.32	1.41
10	M	405	BCB	CHC-C1C	6.60	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	402	HEC	CAC-C3C	6.58	1.56	1.35
5	C	401	HEC	CAC-C3C	6.50	1.56	1.35
11	L	303	BPB	C1B-C2B	6.31	1.46	1.39
5	C	403	HEC	CAB-C3B	6.27	1.55	1.35
5	C	402	HEC	CAB-C3B	6.26	1.55	1.35
5	C	404	HEC	CAB-C3B	6.08	1.54	1.35
5	C	403	HEC	CAC-C3C	5.97	1.54	1.35
10	L	301	BCB	CHB-C1B	5.94	1.49	1.39
11	M	407	BPB	O2A-CGA	5.90	1.50	1.33
10	M	405	BCB	C1D-C2D	5.86	1.46	1.39
10	M	405	BCB	C3A-C2A	-5.83	1.49	1.54
10	M	405	BCB	CHC-C4B	5.78	1.49	1.39
10	M	406	BCB	C1D-C2D	5.76	1.46	1.39
10	M	405	BCB	CHB-C1B	5.73	1.48	1.39
5	C	401	HEC	CAB-C3B	5.66	1.53	1.35
11	M	407	BPB	C3D-C4D	-5.62	1.33	1.41
11	M	407	BPB	CBD-CGD	-5.52	1.45	1.52
10	M	406	BCB	CHC-C4B	5.45	1.48	1.39
6	C	405	DGA	OG2-CB1	5.32	1.49	1.34
10	M	406	BCB	CHB-C1B	5.23	1.48	1.39
10	L	301	BCB	O2D-CGD	5.21	1.46	1.33
10	L	302	BCB	CHC-C1C	5.09	1.44	1.38
10	L	302	BCB	C3B-C4B	5.09	1.49	1.41
11	L	303	BPB	C3D-C2D	4.92	1.48	1.39
10	L	302	BCB	CHB-C1B	4.91	1.47	1.39
6	C	405	DGA	OG1-CA1	4.84	1.47	1.33
10	L	301	BCB	CHC-C4B	4.75	1.47	1.39
10	M	406	BCB	O2D-CGD	4.75	1.44	1.33
10	M	406	BCB	OBD-CAD	4.72	1.28	1.22
10	L	302	BCB	C3D-C2D	4.71	1.47	1.39
10	L	302	BCB	C3B-C2B	4.69	1.47	1.39
10	M	406	BCB	C3B-C2B	4.68	1.47	1.39
10	L	302	BCB	CHC-C4B	4.66	1.47	1.39
10	M	405	BCB	C3B-C2B	4.64	1.47	1.39
10	M	405	BCB	O2D-CGD	4.52	1.44	1.33
10	L	301	BCB	C3B-C2B	4.52	1.47	1.39
10	L	301	BCB	CHA-CBD	-4.50	1.46	1.51
11	M	407	BPB	C3B-C2B	4.46	1.47	1.39
11	L	303	BPB	O2D-CGD	4.32	1.43	1.33
10	M	405	BCB	O2A-CGA	4.29	1.45	1.33
10	L	302	BCB	C1D-C2D	4.25	1.44	1.39
11	M	407	BPB	O2D-CGD	4.18	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	M	407	BPB	OBD-CAD	4.17	1.27	1.22
10	L	301	BCB	C3A-C2A	-4.15	1.51	1.54
11	M	407	BPB	C3D-C2D	4.14	1.46	1.39
10	M	406	BCB	C3D-C2D	3.99	1.46	1.39
10	L	302	BCB	O2D-CGD	3.94	1.42	1.33
11	L	303	BPB	CBD-CGD	-3.93	1.47	1.52
10	M	406	BCB	CHD-C1D	3.85	1.45	1.39
10	L	302	BCB	C3A-C2A	-3.84	1.51	1.54
11	M	407	BPB	C4C-NC	-3.82	1.25	1.37
10	L	301	BCB	O2A-CGA	3.82	1.44	1.33
10	M	406	BCB	C3B-C4B	3.81	1.47	1.41
10	M	405	BCB	OBD-CAD	3.77	1.27	1.22
10	L	302	BCB	CHB-C4A	-3.76	1.34	1.38
11	L	303	BPB	C4D-CHA	3.75	1.45	1.39
13	M	404	MQ7	C10-C5	3.74	1.46	1.40
11	M	407	BPB	C4D-CHA	3.73	1.45	1.39
11	L	303	BPB	O2A-CGA	3.71	1.44	1.33
10	M	405	BCB	C3B-C4B	3.69	1.47	1.41
11	L	303	BPB	C4C-NC	-3.58	1.26	1.37
10	M	405	BCB	CHA-CBD	-3.57	1.47	1.51
10	L	301	BCB	CHD-C1D	3.55	1.45	1.39
10	M	406	BCB	CHD-C4C	3.49	1.46	1.39
10	L	302	BCB	O2A-CGA	3.49	1.43	1.33
10	M	406	BCB	C3A-C2A	-3.48	1.51	1.54
10	L	301	BCB	OBD-CAD	3.46	1.26	1.22
10	L	301	BCB	C3D-C2D	3.44	1.45	1.39
10	L	302	BCB	CHD-C4C	3.42	1.45	1.39
10	L	301	BCB	CHD-C4C	3.39	1.45	1.39
10	M	405	BCB	CBD-CGD	-3.35	1.48	1.52
11	L	303	BPB	C3B-C2B	3.30	1.45	1.39
10	L	302	BCB	CHA-CBD	-3.30	1.47	1.51
11	L	303	BPB	CHA-CBD	-3.30	1.47	1.51
10	L	302	BCB	OBD-CAD	3.29	1.26	1.22
10	M	406	BCB	O2A-CGA	3.25	1.42	1.33
10	M	405	BCB	CHD-C4C	3.20	1.45	1.39
10	L	302	BCB	CHD-C1D	3.08	1.44	1.39
10	L	302	BCB	CBD-CGD	-3.00	1.48	1.52
10	L	301	BCB	C3B-C4B	2.99	1.46	1.41
10	M	405	BCB	CHD-C1D	2.99	1.44	1.39
10	M	405	BCB	CHB-C4A	-2.90	1.35	1.38
5	C	403	HEC	CMB-C2B	2.72	1.56	1.50
5	C	404	HEC	CBA-CGA	2.66	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	401	HEC	C1A-NA	-2.61	1.34	1.39
11	M	407	BPB	C3B-C4B	2.52	1.45	1.41
14	M	408	NS5	C24-C25	2.51	1.51	1.43
11	M	407	BPB	C4B-NB	-2.47	1.34	1.38
13	M	404	MQ7	O1-C1	2.44	1.28	1.23
5	C	401	HEC	C4B-NB	-2.42	1.35	1.39
9	M	402	HTO	C4-C3	2.40	1.56	1.52
11	L	303	BPB	C3B-C4B	2.38	1.45	1.41
5	C	401	HEC	O1D-CGD	2.37	1.29	1.22
5	C	402	HEC	CBA-CGA	2.36	1.56	1.50
10	M	405	BCB	C3D-C2D	2.35	1.43	1.39
5	C	401	HEC	C3B-C2B	-2.34	1.33	1.41
5	C	403	HEC	CBD-CGD	2.32	1.55	1.50
11	L	303	BPB	O2A-C1	-2.29	1.40	1.46
10	M	406	BCB	CHA-CBD	-2.29	1.49	1.51
5	C	403	HEC	C1D-C2D	2.24	1.48	1.43
10	L	301	BCB	CHB-C4A	-2.24	1.35	1.38
10	M	405	BCB	C3D-CAD	-2.23	1.43	1.47
5	C	404	HEC	CMB-C2B	2.22	1.55	1.50
5	C	402	HEC	O1D-CGD	2.21	1.29	1.22
5	C	402	HEC	C1C-NC	-2.21	1.35	1.39
11	M	407	BPB	C2-C3	2.20	1.38	1.33
11	L	303	BPB	C1D-ND	-2.19	1.34	1.38
5	C	402	HEC	C4B-NB	-2.18	1.35	1.39
5	C	401	HEC	C1C-NC	-2.15	1.35	1.39
5	C	402	HEC	C3D-C2D	-2.13	1.33	1.38
11	L	303	BPB	C1B-NB	-2.11	1.34	1.38
10	M	405	BCB	C1C-C2C	-2.11	1.46	1.51
10	M	406	BCB	CHB-C4A	-2.11	1.36	1.38
10	M	405	BCB	C3D-C4D	-2.10	1.38	1.41
5	C	401	HEC	CBD-CGD	2.10	1.55	1.50
5	C	402	HEC	O1A-CGA	2.07	1.28	1.22
5	C	402	HEC	C3B-C2B	-2.05	1.34	1.41
5	C	403	HEC	CBA-CGA	2.01	1.55	1.50

All (177) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	401	HEC	CBB-CAB-C3B	-18.82	89.83	127.43
10	M	405	BCB	O2D-CGD-CBD	16.49	129.06	110.95
5	C	403	HEC	CBB-CAB-C3B	-13.32	100.81	127.43
10	L	302	BCB	C1B-CHB-C4A	10.45	128.04	121.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	L	303	BPB	O2D-CGD-CBD	10.26	122.22	110.95
10	L	302	BCB	O2D-CGD-CBD	10.20	122.15	110.95
10	M	405	BCB	OBD-CAD-C3D	-9.56	112.97	127.89
5	C	403	HEC	CBC-CAC-C3C	8.97	145.36	127.43
5	C	401	HEC	CBC-CAC-C3C	-8.60	110.25	127.43
10	L	302	BCB	C4B-CHC-C1C	7.94	126.43	121.32
11	M	407	BPB	O2D-CGD-CBD	7.37	119.04	110.95
5	C	404	HEC	CBB-CAB-C3B	-7.12	113.19	127.43
10	L	301	BCB	O2D-CGD-CBD	7.09	118.73	110.95
10	M	405	BCB	C4B-CHC-C1C	6.83	125.72	121.32
5	C	402	HEC	CBC-CAC-C3C	-6.83	113.79	127.43
10	L	302	BCB	C3D-CAD-CBD	6.66	116.37	107.61
10	L	301	BCB	C4B-CHC-C1C	6.62	125.58	121.32
10	M	405	BCB	C3D-CAD-CBD	6.46	116.11	107.61
14	M	408	NS5	C19-C20-C21	-6.29	118.45	127.28
10	L	302	BCB	OBD-CAD-C3D	-6.17	118.26	127.89
10	M	406	BCB	C4B-CHC-C1C	5.85	125.09	121.32
5	C	404	HEC	CBC-CAC-C3C	-5.64	116.16	127.43
10	M	405	BCB	O1D-CGD-CBD	-5.58	116.26	124.72
6	C	405	DGA	OG2-CB1-CB2	5.37	123.09	111.48
10	L	301	BCB	C3D-CAD-CBD	5.33	114.62	107.61
10	L	302	BCB	CHA-C1A-C2A	-5.19	121.13	133.31
11	M	407	BPB	C1A-C2A-C3A	-5.16	97.93	102.84
10	M	405	BCB	C1B-CHB-C4A	5.09	124.60	121.32
10	L	301	BCB	CHA-C1A-C2A	-5.02	121.53	133.31
10	L	302	BCB	C3D-C4D-CHA	4.84	115.90	108.54
10	M	405	BCB	CHA-C1A-C2A	-4.79	122.05	133.31
10	M	405	BCB	O2D-CGD-O1D	-4.73	114.65	123.85
10	L	301	BCB	OBD-CAD-C3D	-4.67	120.61	127.89
11	M	407	BPB	C3D-C4D-ND	4.46	113.42	107.71
10	M	406	BCB	O2D-CGD-CBD	4.44	115.82	110.95
11	M	407	BPB	O2A-CGA-CBA	4.40	125.24	111.83
10	M	405	BCB	O2A-CGA-CBA	4.37	125.17	111.83
10	L	301	BCB	C1B-CHB-C4A	4.32	124.10	121.32
13	M	404	MQ7	C24-C23-C25	4.32	122.72	115.23
5	C	402	HEC	CBA-CAA-C2A	-4.31	100.62	112.53
10	L	301	BCB	CMD-C2D-C3D	-4.30	116.08	124.68
11	M	407	BPB	O1D-CGD-CBD	-4.28	118.23	124.72
11	L	303	BPB	C2B-C1B-NB	4.21	112.47	109.43
10	M	406	BCB	C3D-CAD-CBD	4.18	113.11	107.61
10	M	406	BCB	CHA-C1A-C2A	-4.17	123.52	133.31
11	L	303	BPB	C3D-C4D-ND	4.16	113.04	107.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	M	408	NS5	C13-C12-C10	-4.14	121.87	127.69
11	L	303	BPB	C1A-C2A-C3A	-4.11	98.92	102.84
10	L	301	BCB	C3D-C4D-CHA	4.06	114.71	108.54
10	M	405	BCB	C3D-C4D-CHA	4.05	114.69	108.54
14	M	408	NS5	C23-C21-C20	4.03	125.34	119.01
14	M	408	NS5	C18-C19-C20	3.99	131.68	123.52
10	L	302	BCB	O2D-CGD-O1D	-3.99	116.08	123.85
10	M	406	BCB	C3D-C4D-ND	3.93	119.24	112.94
10	M	406	BCB	OBB-CAB-C3B	3.93	126.55	119.99
11	M	407	BPB	CMA-C3A-C4A	-3.88	106.25	114.61
11	L	303	BPB	C2D-C1D-ND	3.86	112.22	109.43
11	L	303	BPB	O1D-CGD-CBD	-3.79	118.98	124.72
11	M	407	BPB	C2B-C1B-NB	3.78	112.16	109.43
10	M	406	BCB	C3D-C4D-CHA	3.73	114.21	108.54
10	M	406	BCB	CMB-C2B-C3B	3.73	132.13	124.68
10	L	301	BCB	CMB-C2B-C3B	3.70	132.07	124.68
10	M	405	BCB	CMD-C2D-C3D	-3.69	117.31	124.68
11	M	407	BPB	CBB-CAB-C3B	-3.67	109.34	120.34
5	C	401	HEC	C2A-C1A-NA	-3.61	106.84	110.32
11	M	407	BPB	OBB-CAB-C3B	3.56	125.94	119.99
13	M	404	MQ7	C2M-C2-C3	-3.55	118.61	124.45
14	M	408	NS5	C14-C15-C17	-3.53	113.45	119.01
13	M	404	MQ7	C39-C38-C40	3.51	121.31	115.23
10	L	302	BCB	CHD-C4C-C3C	-3.50	119.57	130.04
10	M	406	BCB	C1B-CHB-C4A	3.49	123.57	121.32
10	L	302	BCB	C3D-C4D-ND	3.48	118.52	112.94
10	M	405	BCB	OBD-CAD-CBD	3.46	130.91	125.82
10	M	406	BCB	C1A-CHA-C4D	3.42	124.69	118.98
10	M	405	BCB	CHC-C1C-C2C	-3.41	113.57	122.69
11	L	303	BPB	CMA-C3A-C4A	-3.37	107.36	114.61
10	L	301	BCB	C1A-CHA-C4D	3.32	124.52	118.98
10	M	405	BCB	C4D-ND-C1D	-3.31	102.71	105.22
10	L	301	BCB	C3D-C4D-ND	3.22	118.10	112.94
10	L	302	BCB	C4D-ND-C1D	-3.21	102.78	105.22
9	M	402	HTO	C4-C3-C2	3.21	121.46	113.73
5	C	402	HEC	CBB-CAB-C3B	-3.20	121.04	127.43
5	C	402	HEC	C2A-C1A-NA	-3.12	107.32	110.32
10	M	405	BCB	CMB-C2B-C3B	3.10	130.87	124.68
14	M	408	NS5	C6-C5-C4	3.07	120.56	115.23
10	M	406	BCB	CHD-C4C-C3C	-3.07	120.88	130.04
6	C	405	DGA	OG1-CA1-CA2	3.05	121.14	111.83
5	C	403	HEC	C2D-C1D-ND	-3.05	105.25	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	404	MQ7	C11-C3-C4	-3.01	115.41	118.58
5	C	401	HEC	CBA-CAA-C2A	-3.00	104.24	112.53
5	C	402	HEC	C1D-C2D-C3D	2.99	110.24	106.82
10	L	301	BCB	C1-C2-C3	-2.94	121.37	126.20
10	M	406	BCB	OBD-CAD-C3D	-2.94	123.30	127.89
11	M	407	BPB	C3B-C4B-NB	2.91	112.29	108.05
11	M	407	BPB	C5-C3-C2	2.90	127.69	121.17
10	L	301	BCB	CHD-C4C-C3C	-2.90	121.38	130.04
10	L	301	BCB	C4-C3-C5	2.88	120.23	115.23
6	C	405	DGA	OG2-CG2-CG1	2.88	112.84	106.21
10	L	301	BCB	CED-O2D-CGD	2.84	122.36	115.92
10	L	301	BCB	C4D-ND-C1D	-2.81	103.09	105.22
5	C	404	HEC	CAD-CBD-CGD	-2.81	106.22	113.67
11	M	407	BPB	O2A-C1-C2	2.78	118.81	108.11
10	M	405	BCB	O2A-CGA-O1A	-2.76	116.73	123.63
10	L	301	BCB	O2D-CGD-O1D	-2.76	118.48	123.85
9	H	707	HTO	C1-C2-C3	2.74	118.59	113.00
13	M	404	MQ7	C21-C22-C23	-2.68	121.50	127.62
14	M	408	NS5	C18-C17-C15	-2.67	123.53	127.28
10	M	405	BCB	C3D-C4D-ND	2.67	117.22	112.94
5	C	404	HEC	CMC-C2C-C1C	-2.65	121.39	125.42
9	L	305	HTO	C1-C2-C3	2.62	118.34	113.00
10	M	406	BCB	CMD-C2D-C3D	-2.62	119.45	124.68
5	C	403	HEC	CMB-C2B-C1B	-2.62	121.44	125.42
11	L	303	BPB	O2D-CGD-O1D	-2.60	118.78	123.85
5	C	403	HEC	C1D-C2D-C3D	2.59	109.79	106.82
10	M	405	BCB	C4-C3-C5	2.59	119.72	115.23
13	M	404	MQ7	C24-C23-C22	-2.59	116.98	123.63
10	L	302	BCB	C1A-CHA-C4D	2.57	123.27	118.98
10	M	406	BCB	CHC-C1C-C2C	-2.54	115.90	122.69
10	L	301	BCB	O2A-CGA-CBA	2.53	119.54	111.83
10	L	302	BCB	CMB-C2B-C3B	2.52	129.72	124.68
10	L	301	BCB	O2A-CGA-O1A	-2.52	117.33	123.63
10	L	302	BCB	CHC-C1C-C2C	-2.52	115.95	122.69
13	M	404	MQ7	C26-C27-C28	-2.51	121.89	127.62
10	L	301	BCB	CHC-C1C-C2C	-2.50	115.99	122.69
9	M	402	HTO	O1-C1-C2	2.50	116.41	111.16
10	L	301	BCB	C6-C7-C8	-2.49	107.68	115.97
11	L	303	BPB	C4D-ND-C1D	-2.48	105.90	108.87
5	C	403	HEC	C4B-NB-C1B	2.48	109.86	105.82
5	C	402	HEC	C2D-C1D-ND	-2.45	106.21	110.14
14	M	408	NS5	C30-C29-C28	-2.44	116.12	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	M	406	BCB	O2A-C1-C2	2.42	117.43	108.11
5	C	402	HEC	CHA-C1A-NA	2.42	127.08	124.45
5	C	401	HEC	C4C-NC-C1C	2.41	109.75	105.82
5	C	403	HEC	O2D-CGD-CBD	2.37	121.49	114.00
5	C	404	HEC	O1D-CGD-CBD	-2.37	115.58	123.09
5	C	401	HEC	CHD-C4C-NC	2.35	127.01	124.45
5	C	403	HEC	CHC-C4B-NB	2.35	127.01	124.45
8	H	706	LDA	CM2-N1-C1	2.34	115.14	110.23
10	L	302	BCB	C4-C3-C5	2.33	119.27	115.23
14	M	408	NS5	C32-C31-C33	2.32	119.26	115.23
10	M	406	BCB	CAA-C2A-C3A	-2.31	106.75	113.00
11	L	303	BPB	C1-C2-C3	-2.30	122.42	126.20
10	L	301	BCB	OBB-CAB-CBB	2.29	125.05	120.19
5	C	402	HEC	C4C-NC-C1C	2.28	109.54	105.82
13	M	404	MQ7	O1-C1-C2	2.23	123.38	120.45
6	C	405	DGA	CG1-OG1-CA1	2.20	125.14	117.12
5	C	404	HEC	CMB-C2B-C1B	-2.19	122.08	125.42
14	M	408	NS5	C6-C5-C7	-2.19	118.00	123.63
10	M	405	BCB	CHD-C4C-C3C	-2.19	123.49	130.04
10	L	302	BCB	C1-C2-C3	-2.19	122.61	126.20
10	M	406	BCB	C4D-ND-C1D	-2.19	103.56	105.22
9	H	707	HTO	O1-C1-C2	2.17	115.72	111.16
5	C	402	HEC	C4B-NB-C1B	2.17	109.36	105.82
11	L	303	BPB	CBA-CAA-C2A	-2.17	107.38	113.78
11	M	407	BPB	O1A-CGA-CBA	-2.17	115.30	123.78
11	L	303	BPB	CMB-C2B-C3B	2.16	129.01	124.68
5	C	404	HEC	C4C-NC-C1C	2.14	109.31	105.82
10	L	302	BCB	C6-C5-C3	-2.14	108.26	113.47
5	C	401	HEC	CBD-CAD-C3D	-2.14	106.63	112.53
14	M	408	NS5	C22-C21-C20	-2.11	119.40	122.82
11	M	407	BPB	OBB-CAB-CBB	2.11	124.67	120.19
5	C	403	HEC	C4D-ND-C1D	2.10	109.25	105.82
11	L	303	BPB	CED-O2D-CGD	2.10	120.67	115.92
13	M	404	MQ7	C35-C33-C32	-2.09	116.47	121.17
13	M	404	MQ7	C7-C8-C9	2.09	122.82	120.24
10	L	302	BCB	O2A-CGA-O1A	-2.09	118.40	123.63
13	M	404	MQ7	C40-C38-C37	-2.09	116.48	121.17
6	C	405	DGA	OG1-CA1-OA1	-2.08	118.42	123.63
5	C	403	HEC	O1D-CGD-CBD	-2.07	116.54	123.09
5	C	401	HEC	CHB-C4A-NA	2.05	126.68	124.45
5	C	401	HEC	C3D-C4D-ND	-2.04	107.88	110.15
5	C	401	HEC	C4A-NA-C1A	2.04	109.14	105.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	L	302	BCB	OBB-CAB-C3B	2.03	123.38	119.99
10	L	302	BCB	CAA-CBA-CGA	2.02	118.94	113.21
10	L	302	BCB	O1D-CGD-CBD	-2.01	121.68	124.72
11	L	303	BPB	C7-C6-C5	-2.00	107.92	113.26
11	L	303	BPB	CAA-C2A-C3A	2.00	118.41	113.00

All (14) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	L	301	BCB	ND
10	L	301	BCB	NC
10	L	301	BCB	NA
10	L	302	BCB	ND
10	L	302	BCB	NC
10	L	302	BCB	NA
10	M	405	BCB	ND
10	M	405	BCB	NC
10	M	405	BCB	NA
10	M	406	BCB	ND
10	M	406	BCB	NC
10	M	406	BCB	NA
11	L	303	BPB	C13
11	M	407	BPB	C13

All (162) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	401	HEC	C2B-C3B-CAB-CBB
5	C	401	HEC	C2C-C3C-CAC-CBC
5	C	401	HEC	C4C-C3C-CAC-CBC
5	C	402	HEC	C2B-C3B-CAB-CBB
5	C	402	HEC	C4B-C3B-CAB-CBB
5	C	402	HEC	C2C-C3C-CAC-CBC
5	C	402	HEC	C4C-C3C-CAC-CBC
5	C	403	HEC	C2B-C3B-CAB-CBB
5	C	403	HEC	C4B-C3B-CAB-CBB
5	C	403	HEC	C2C-C3C-CAC-CBC
5	C	403	HEC	C4C-C3C-CAC-CBC
5	C	404	HEC	C2B-C3B-CAB-CBB
5	C	404	HEC	C4B-C3B-CAB-CBB
5	C	404	HEC	C2C-C3C-CAC-CBC
5	C	404	HEC	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
8	H	706	LDA	C2-C1-N1-O1
8	H	706	LDA	C2-C1-N1-CM2
8	L	306	LDA	C2-C1-N1-O1
8	L	306	LDA	C2-C1-N1-CM1
8	L	306	LDA	C2-C1-N1-CM2
8	L	306	LDA	N1-C1-C2-C3
8	M	401	LDA	N1-C1-C2-C3
9	H	707	HTO	C1-C2-C3-O3
9	H	707	HTO	O2-C2-C3-O3
9	H	707	HTO	O2-C2-C3-C4
10	L	301	BCB	C2C-C3C-CAC-CBC
10	L	301	BCB	C4C-C3C-CAC-CBC
10	L	302	BCB	C2C-C3C-CAC-CBC
10	M	405	BCB	C2C-C3C-CAC-CBC
10	M	405	BCB	CBD-CGD-O2D-CED
10	M	405	BCB	O1D-CGD-O2D-CED
10	M	406	BCB	C2C-C3C-CAC-CBC
10	M	406	BCB	CAD-CBD-CGD-O1D
10	M	406	BCB	CAD-CBD-CGD-O2D
11	L	303	BPB	C11-C12-C13-C15
11	L	303	BPB	C2C-C3C-CAC-CBC
11	M	407	BPB	C2C-C3C-CAC-CBC
11	M	407	BPB	C4C-C3C-CAC-CBC
14	M	408	NS5	C3-C4-C5-C6
10	L	301	BCB	C4-C3-C5-C6
14	M	408	NS5	C3-C4-C5-C7
11	M	407	BPB	CBA-CGA-O2A-C1
11	L	303	BPB	CBD-CGD-O2D-CED
10	L	301	BCB	C2-C3-C5-C6
11	M	407	BPB	O1A-CGA-O2A-C1
11	M	407	BPB	C5-C6-C7-C8
14	M	408	NS5	C2-C3-C4-C5
14	M	408	NS5	C22-C21-C23-C24
8	M	417	LDA	C1-C2-C3-C4
10	M	406	BCB	C8-C10-C11-C12
10	M	406	BCB	C13-C15-C16-C17
11	L	303	BPB	O1D-CGD-O2D-CED
10	M	406	BCB	C2A-CAA-CBA-CGA
8	L	306	LDA	C7-C8-C9-C10
13	M	404	MQ7	C38-C40-C41-C42
14	M	408	NS5	C20-C21-C23-C24
10	L	302	BCB	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
10	L	302	BCB	C16-C17-C18-C19
8	H	706	LDA	C4-C5-C6-C7
8	H	706	LDA	C5-C6-C7-C8
8	M	417	LDA	C5-C6-C7-C8
10	M	405	BCB	C8-C10-C11-C12
6	C	405	DGA	CCB-CDB-CEB-CFB
8	M	417	LDA	C7-C8-C9-C10
5	C	401	HEC	C2A-CAA-CBA-CGA
11	L	303	BPB	C4-C3-C5-C6
8	M	418	LDA	C1-C2-C3-C4
8	H	701	LDA	C11-C10-C9-C8
8	H	701	LDA	C3-C4-C5-C6
8	M	401	LDA	C9-C10-C11-C12
14	M	408	NS5	C1-C2-C3-C4
6	C	405	DGA	CA6-CA7-CA8-CA9
8	H	701	LDA	C1-C2-C3-C4
10	L	301	BCB	C13-C15-C16-C17
6	C	405	DGA	CB2-CB3-CB4-CB5
8	M	418	LDA	C5-C6-C7-C8
6	C	405	DGA	CB1-CB2-CB3-CB4
5	C	401	HEC	C3D-CAD-CBD-CGD
11	L	303	BPB	C2-C3-C5-C6
8	M	417	LDA	C6-C7-C8-C9
6	C	405	DGA	CA7-CA8-CA9-CAA
8	L	304	LDA	C11-C10-C9-C8
8	M	401	LDA	C3-C4-C5-C6
8	H	701	LDA	N1-C1-C2-C3
8	L	304	LDA	C7-C8-C9-C10
8	L	304	LDA	C2-C3-C4-C5
8	L	306	LDA	C9-C10-C11-C12
9	H	707	HTO	C4-C5-C6-C7
11	L	303	BPB	C11-C12-C13-C14
8	L	306	LDA	C3-C4-C5-C6
6	C	405	DGA	CB9-CAB-CBB-CCB
8	M	418	LDA	C6-C7-C8-C9
8	L	306	LDA	C5-C6-C7-C8
11	L	303	BPB	C8-C10-C11-C12
6	C	405	DGA	CA4-CA5-CA6-CA7
10	M	406	BCB	C12-C13-C15-C16
5	C	402	HEC	C3D-CAD-CBD-CGD
8	M	417	LDA	C9-C10-C11-C12
8	M	401	LDA	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
6	C	405	DGA	CEB-CFB-CGB-CHB
8	H	706	LDA	C9-C10-C11-C12
10	M	406	BCB	C14-C13-C15-C16
8	M	418	LDA	C2-C3-C4-C5
8	H	706	LDA	C2-C1-N1-CM1
9	H	707	HTO	O1-C1-C2-O2
5	C	401	HEC	C4B-C3B-CAB-CBB
10	M	405	BCB	O1A-CGA-O2A-C1
10	M	405	BCB	CHA-CBD-CGD-O2D
8	H	706	LDA	C11-C10-C9-C8
8	L	306	LDA	C1-C2-C3-C4
14	M	408	NS5	CM1-C1-C2-C3
8	M	418	LDA	N1-C1-C2-C3
8	L	304	LDA	C3-C4-C5-C6
10	L	302	BCB	C2-C1-O2A-CGA
14	M	408	NS5	C31-C33-C34-C35
13	M	404	MQ7	C39-C38-C40-C41
11	M	407	BPB	C16-C17-C18-C20
10	L	302	BCB	C13-C15-C16-C17
14	M	408	NS5	CM2-C1-C2-C3
8	H	701	LDA	C7-C8-C9-C10
5	C	401	HEC	CAA-CBA-CGA-O1A
10	L	301	BCB	C15-C16-C17-C18
8	L	306	LDA	C11-C10-C9-C8
11	M	407	BPB	C4-C3-C5-C6
10	M	405	BCB	C14-C13-C15-C16
10	M	406	BCB	C11-C10-C8-C9
5	C	401	HEC	CAA-CBA-CGA-O2A
5	C	402	HEC	CAA-CBA-CGA-O1A
5	C	402	HEC	CAA-CBA-CGA-O2A
14	M	408	NS5	C7-C8-C9-C10
8	M	418	LDA	C9-C10-C11-C12
5	C	403	HEC	CAD-CBD-CGD-O2D
8	L	306	LDA	C6-C7-C8-C9
5	C	403	HEC	CAD-CBD-CGD-O1D
10	M	405	BCB	CHA-CBD-CGD-O1D
10	M	405	BCB	C10-C11-C12-C13
10	M	405	BCB	CBA-CGA-O2A-C1
10	L	302	BCB	C14-C13-C15-C16
8	H	706	LDA	C2-C3-C4-C5
9	L	305	HTO	C4-C5-C6-C7
6	C	405	DGA	OG1-CA1-CA2-CA3

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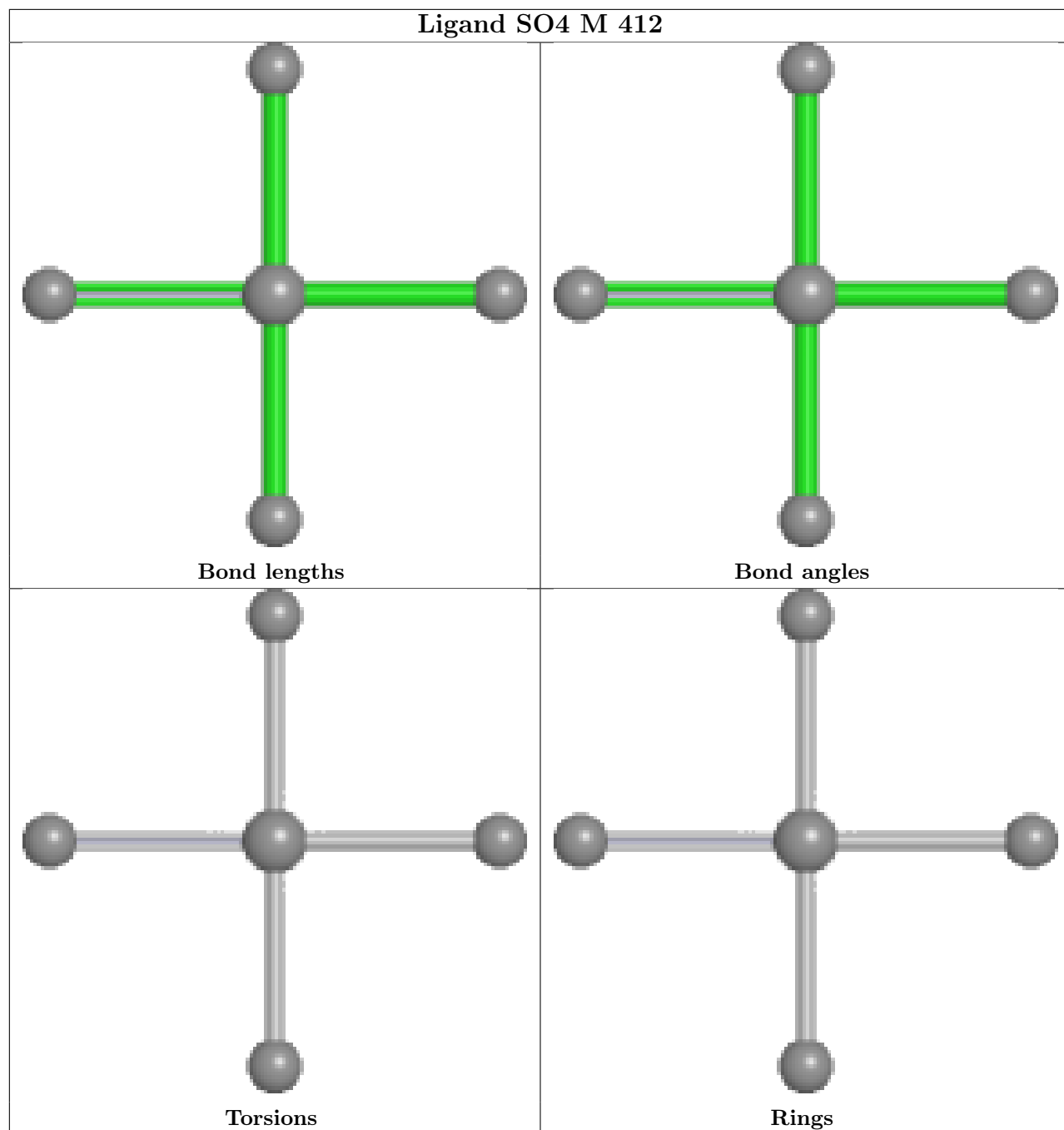
Mol	Chain	Res	Type	Atoms
6	C	405	DGA	CBB-CAB-CB9-CB8
10	L	302	BCB	C12-C13-C15-C16
8	H	701	LDA	C5-C6-C7-C8
11	M	407	BPB	C16-C17-C18-C19
8	L	306	LDA	C4-C5-C6-C7
13	M	404	MQ7	C37-C38-C40-C41
10	M	406	BCB	O2A-C1-C2-C3
11	L	303	BPB	O2A-C1-C2-C3
9	M	402	HTO	C3-C4-C5-C6
6	C	405	DGA	CBB-CCB-CDB-CEB
6	C	405	DGA	CAB-CBB-CCB-CDB
8	M	418	LDA	C11-C10-C9-C8
11	M	407	BPB	C2-C3-C5-C6
8	L	304	LDA	C2-C1-N1-O1
9	H	707	HTO	C3-C4-C5-C6
6	C	405	DGA	OA1-CA1-CA2-CA3
14	M	408	NS5	C33-C34-C35-C36
5	C	401	HEC	CAD-CBD-CGD-O2D
5	C	404	HEC	CAD-CBD-CGD-O2D
10	L	302	BCB	CAD-CBD-CGD-O2D
5	C	404	HEC	CAD-CBD-CGD-O1D

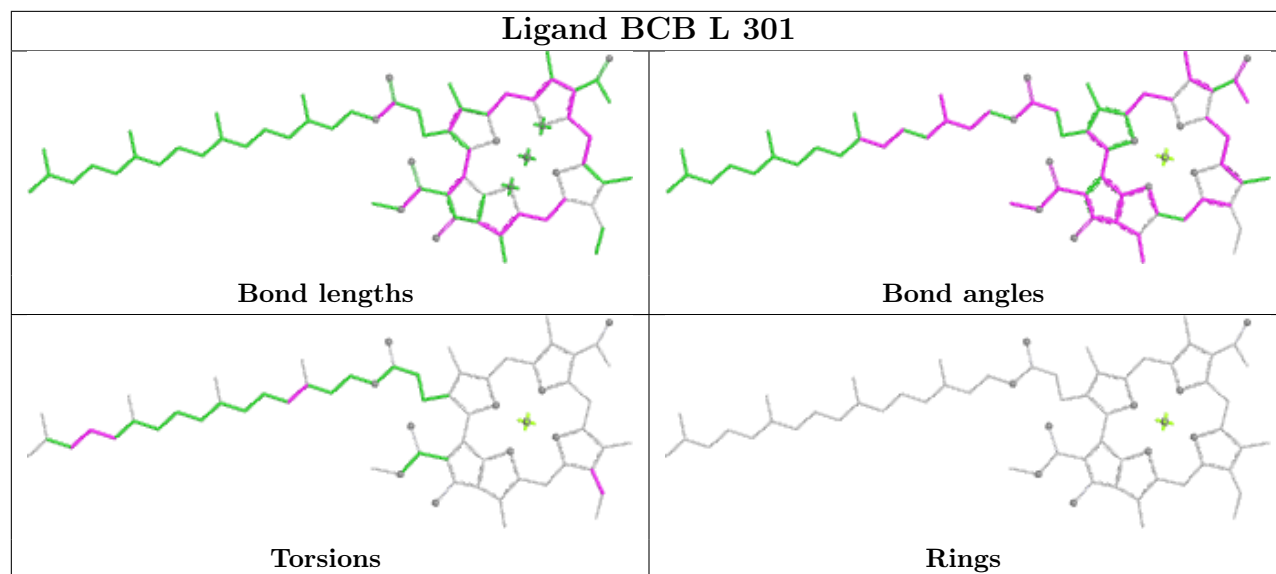
There are no ring outliers.

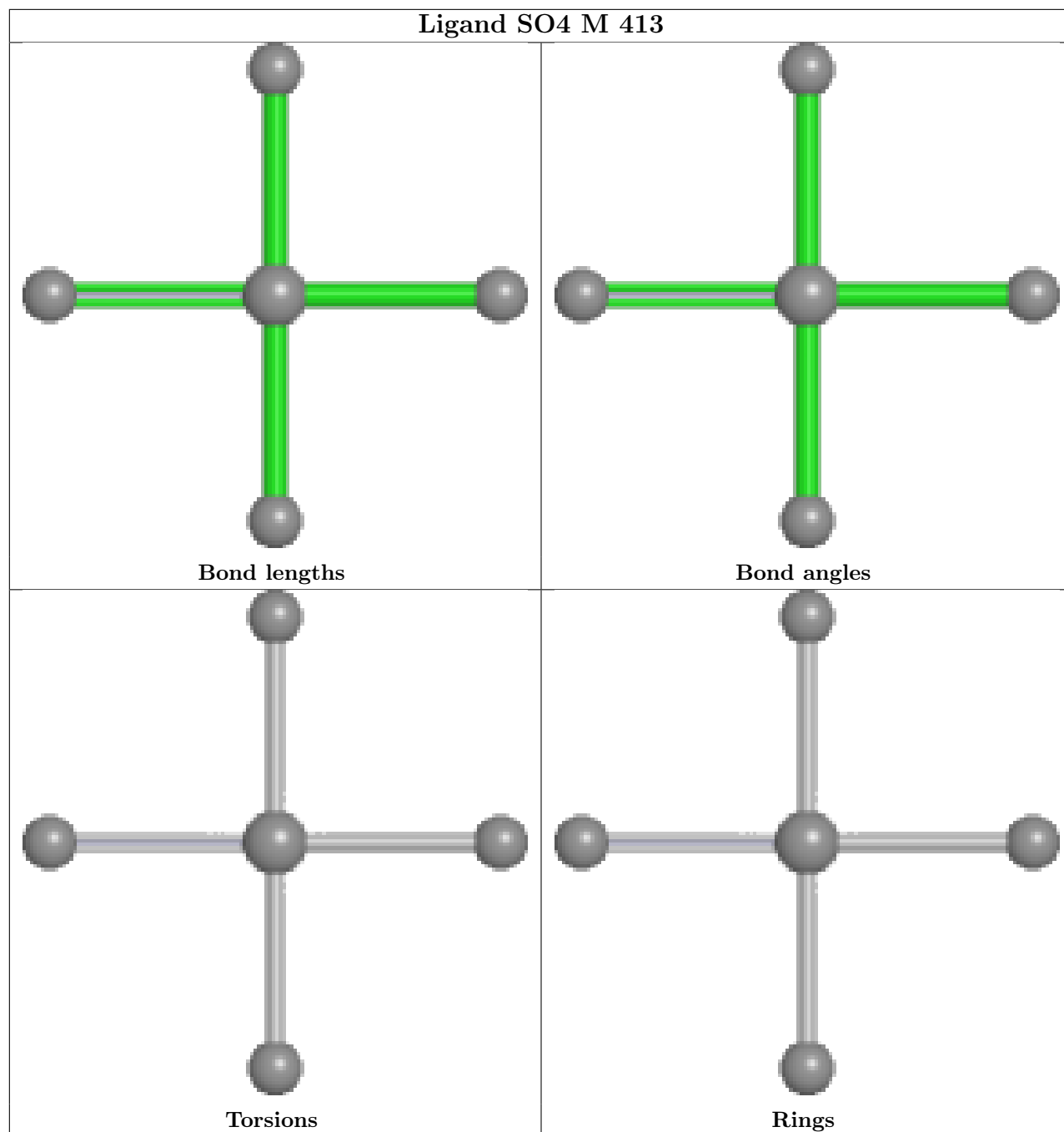
16 monomers are involved in 51 short contacts:

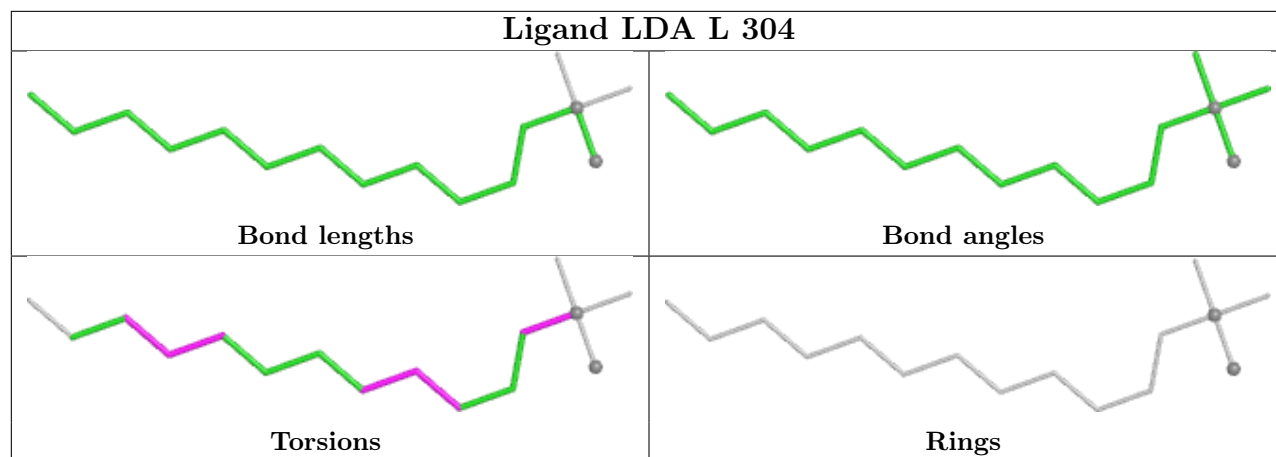
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	L	301	BCB	7	0
5	C	403	HEC	3	0
11	L	303	BPB	3	0
5	C	402	HEC	2	0
10	L	302	BCB	2	0
10	M	405	BCB	6	0
5	C	404	HEC	4	0
6	C	405	DGA	2	0
8	H	706	LDA	2	0
13	M	404	MQ7	1	0
11	M	407	BPB	5	0
7	H	705	SO4	1	0
14	M	408	NS5	2	0
5	C	401	HEC	10	0
7	M	416	SO4	1	0
10	M	406	BCB	4	0

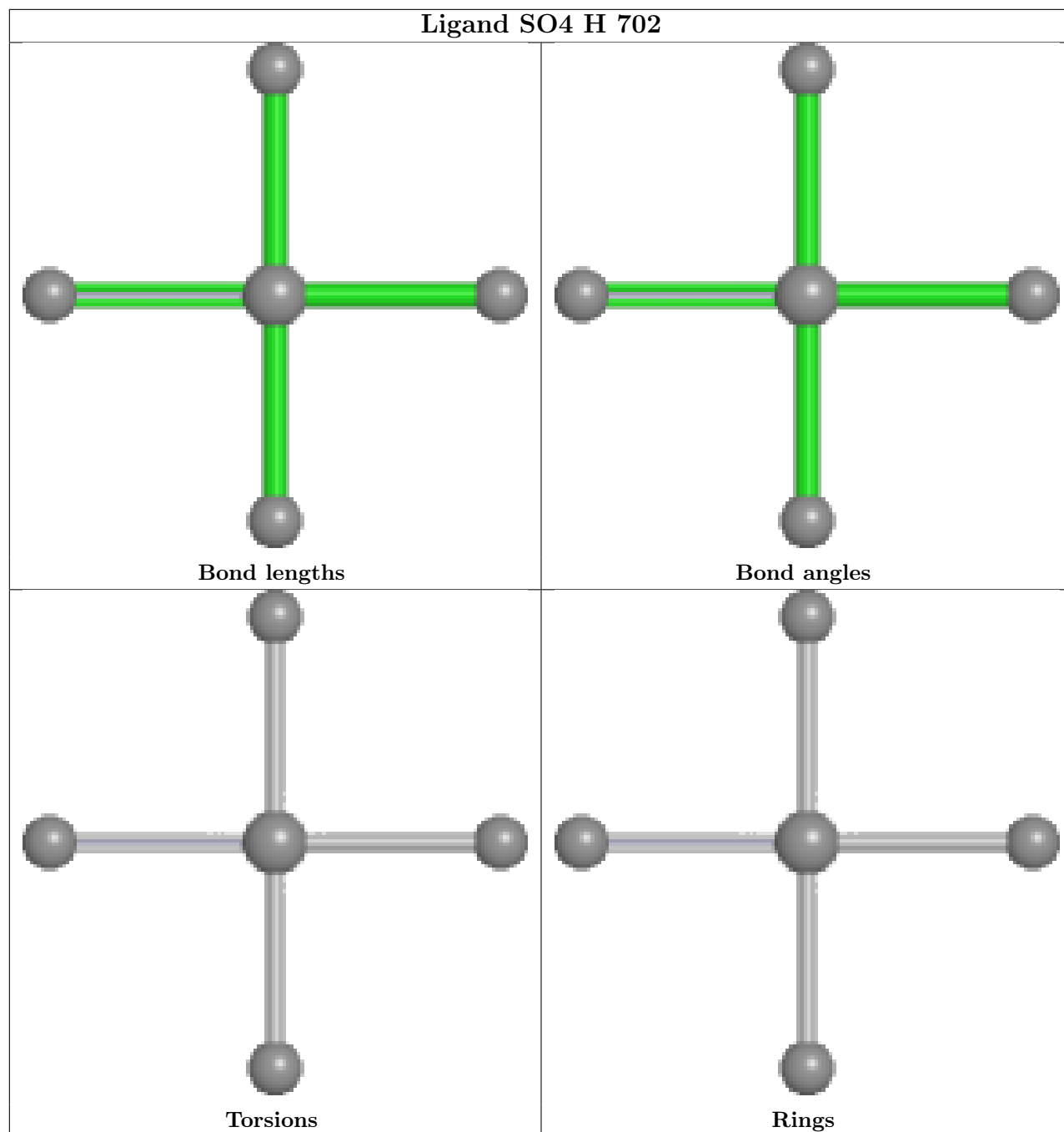
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

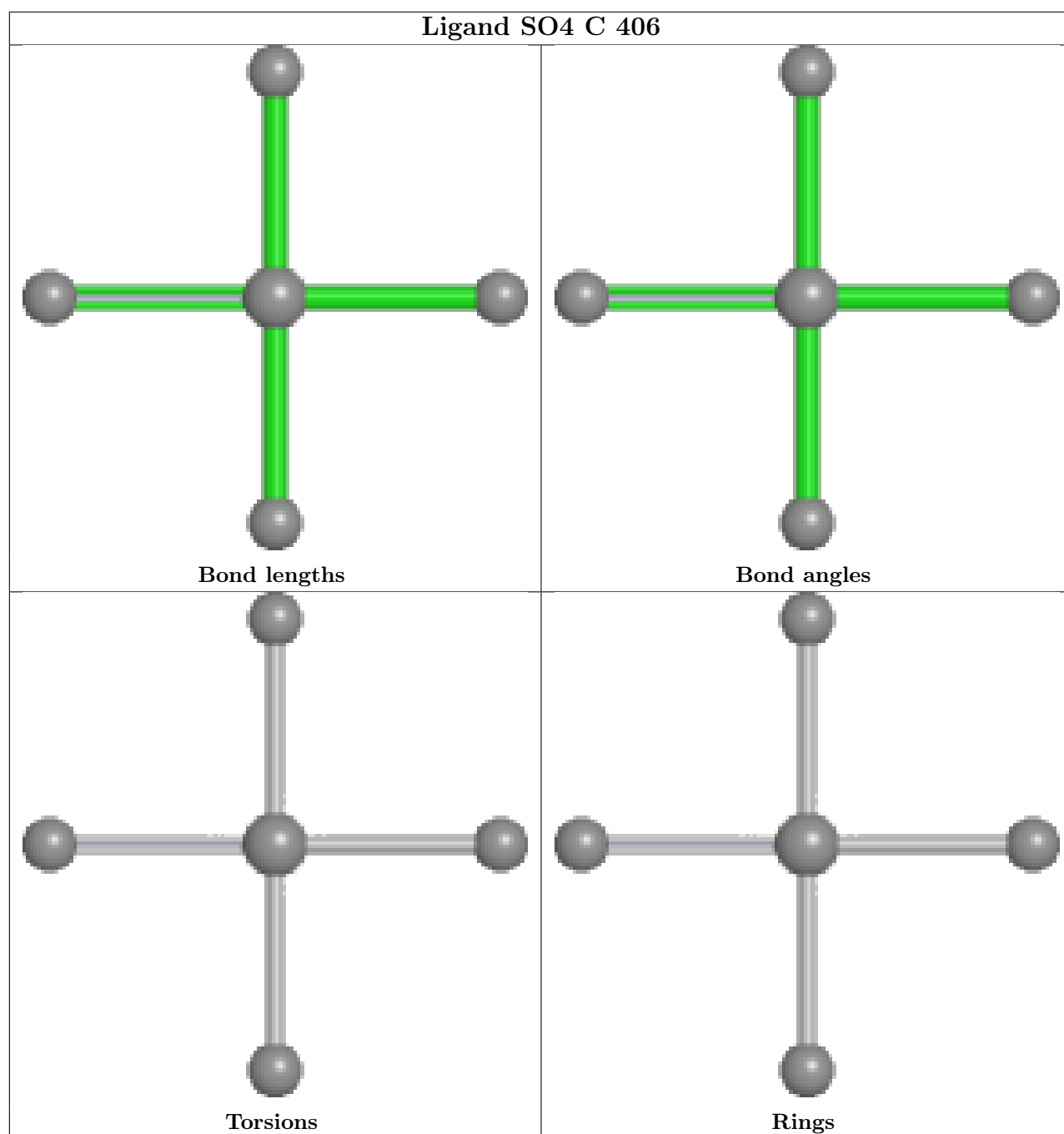




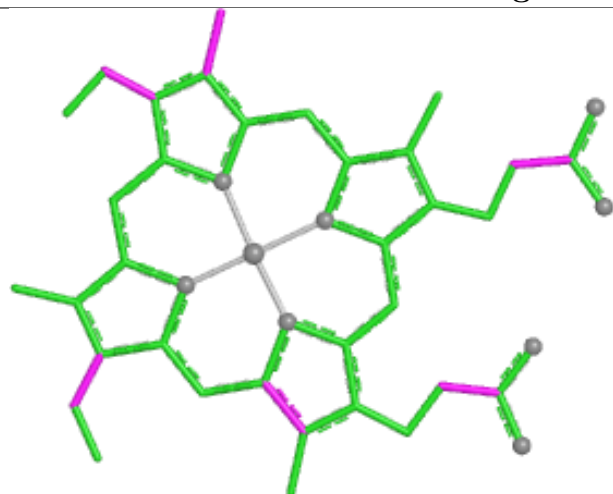




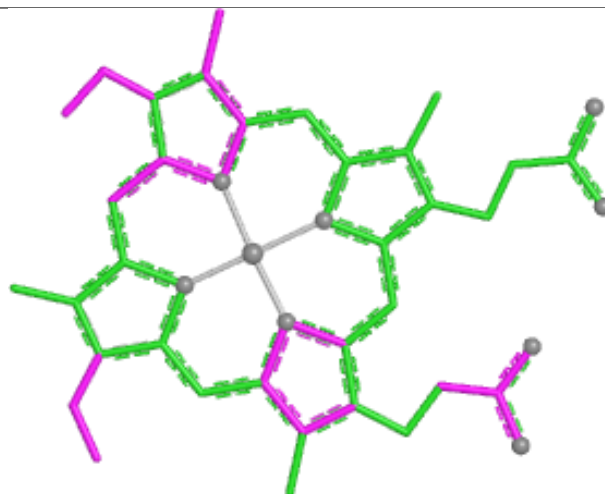




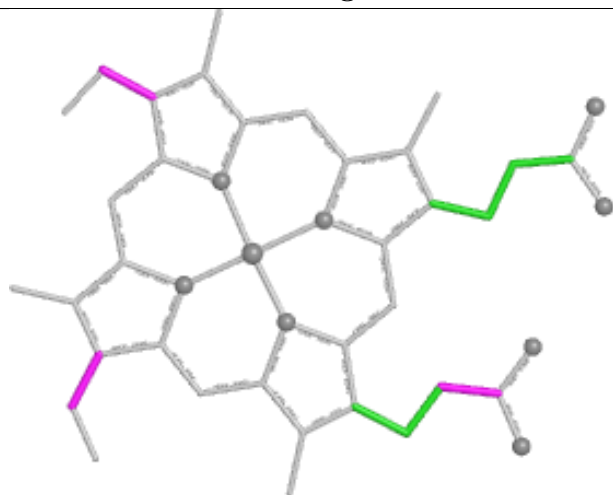
Ligand HEC C 403



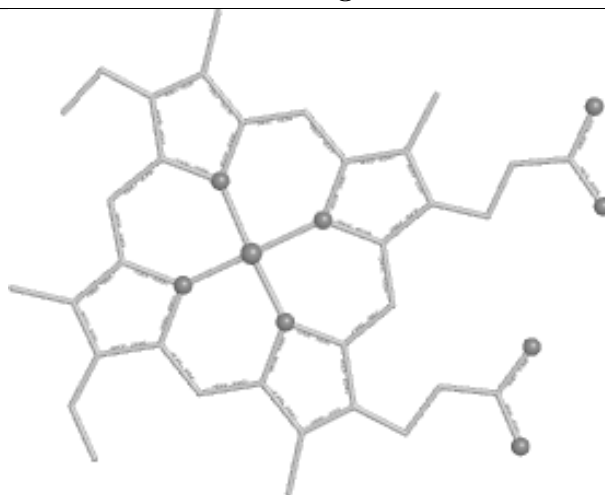
Bond lengths



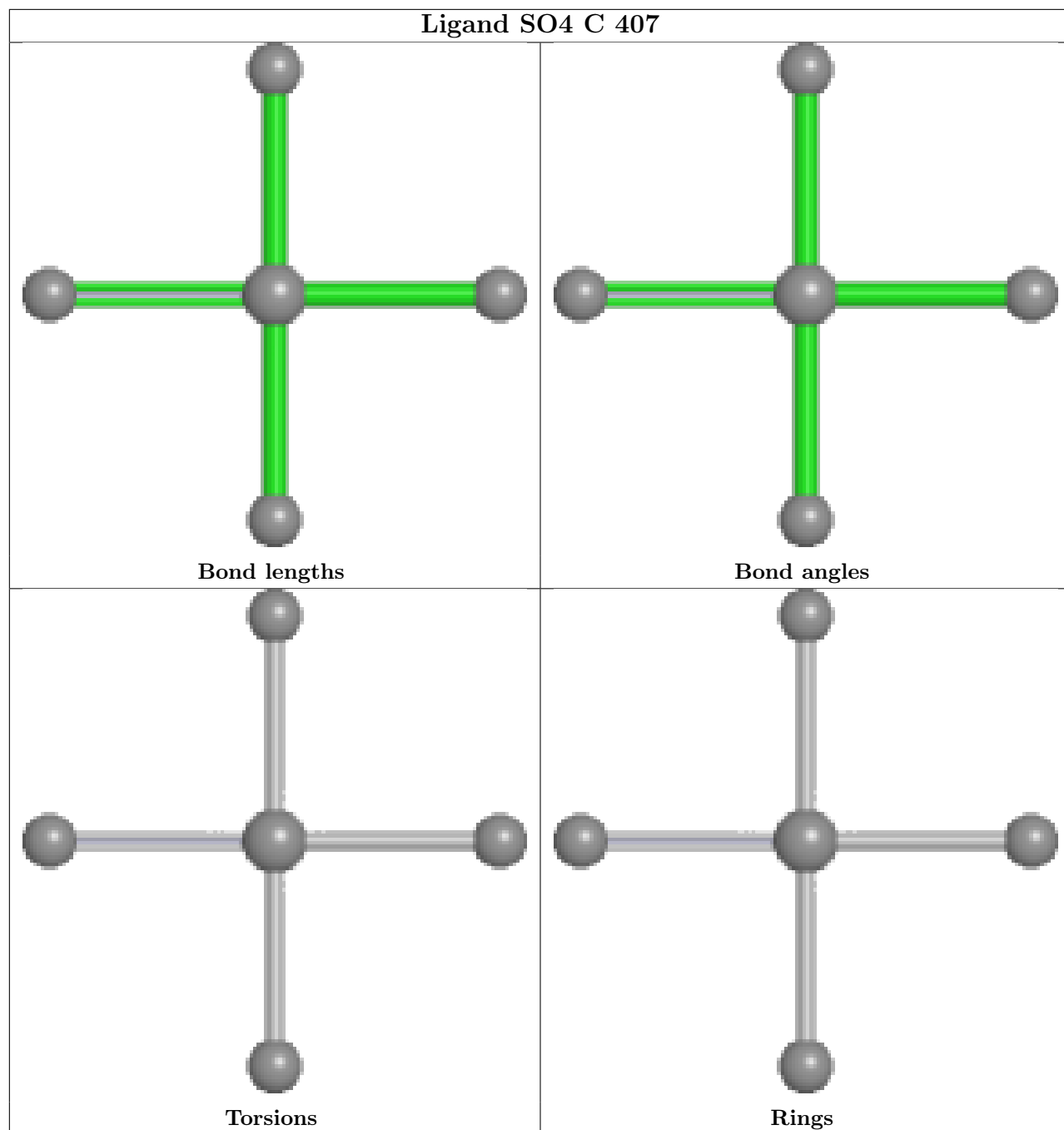
Bond angles



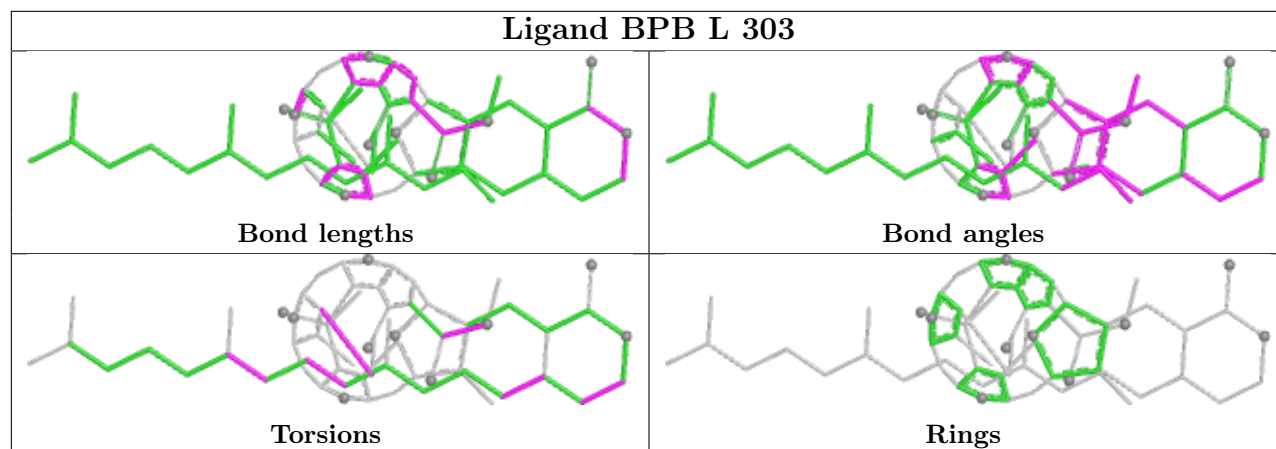
Torsions



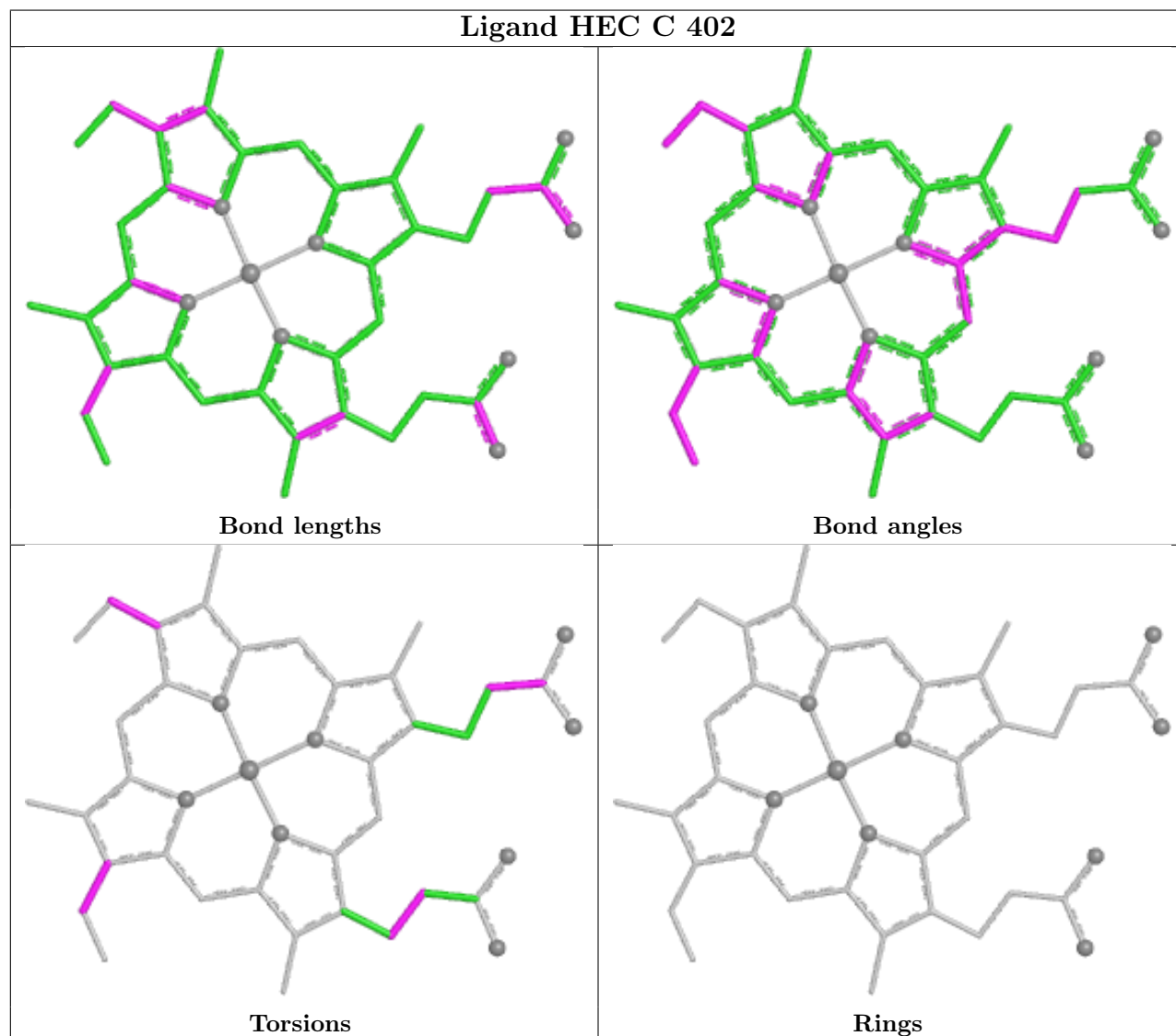
Rings

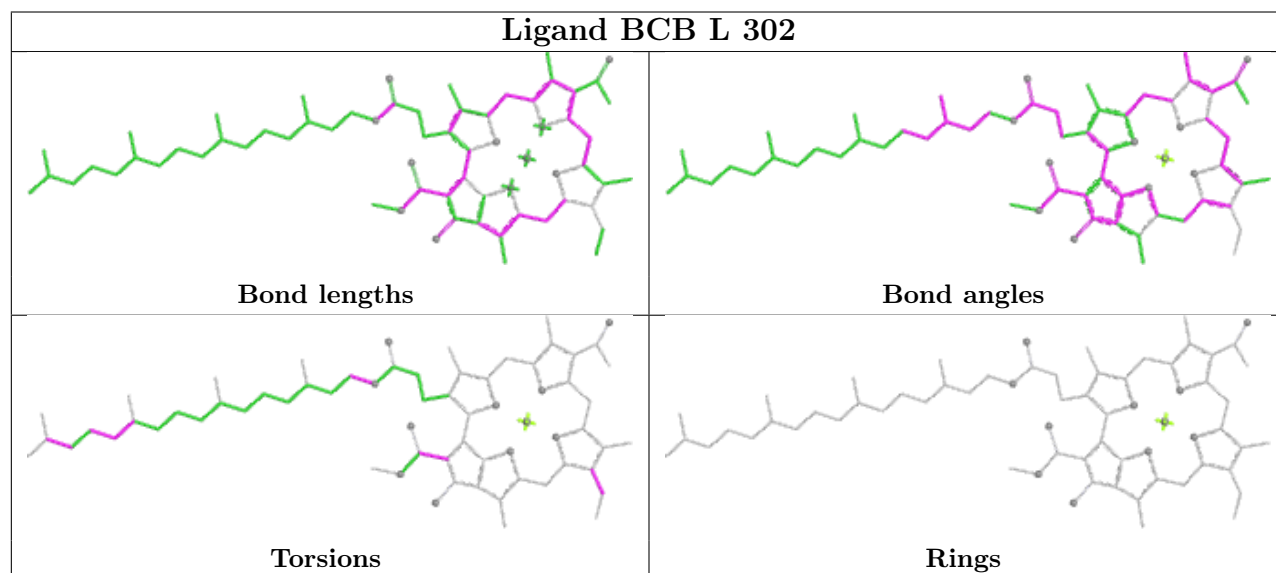
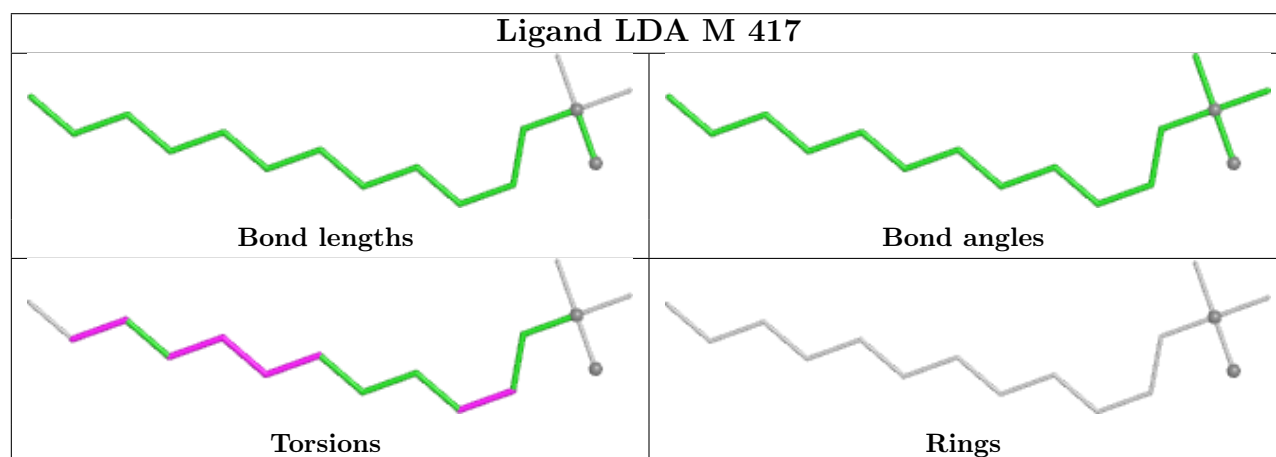
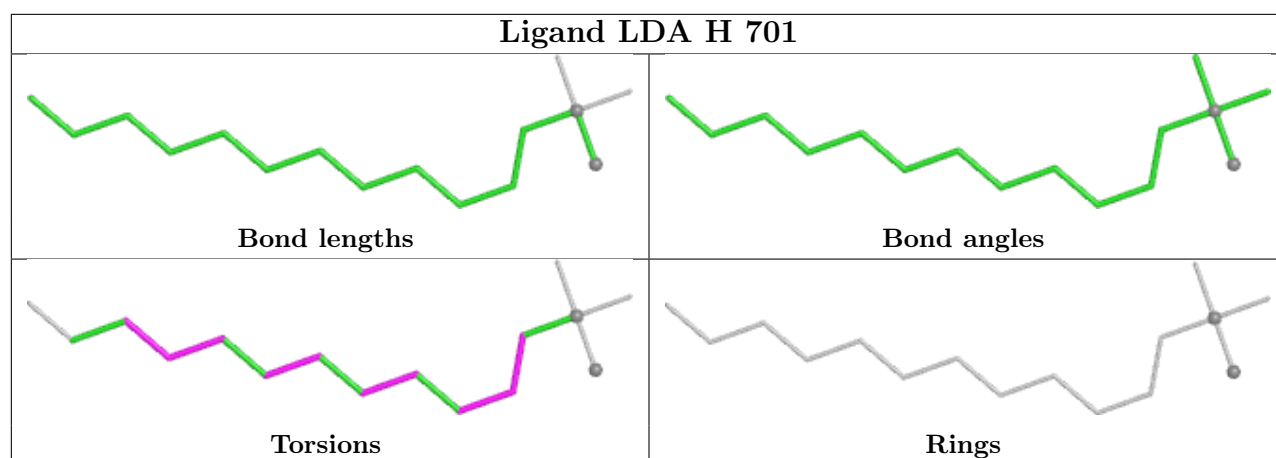


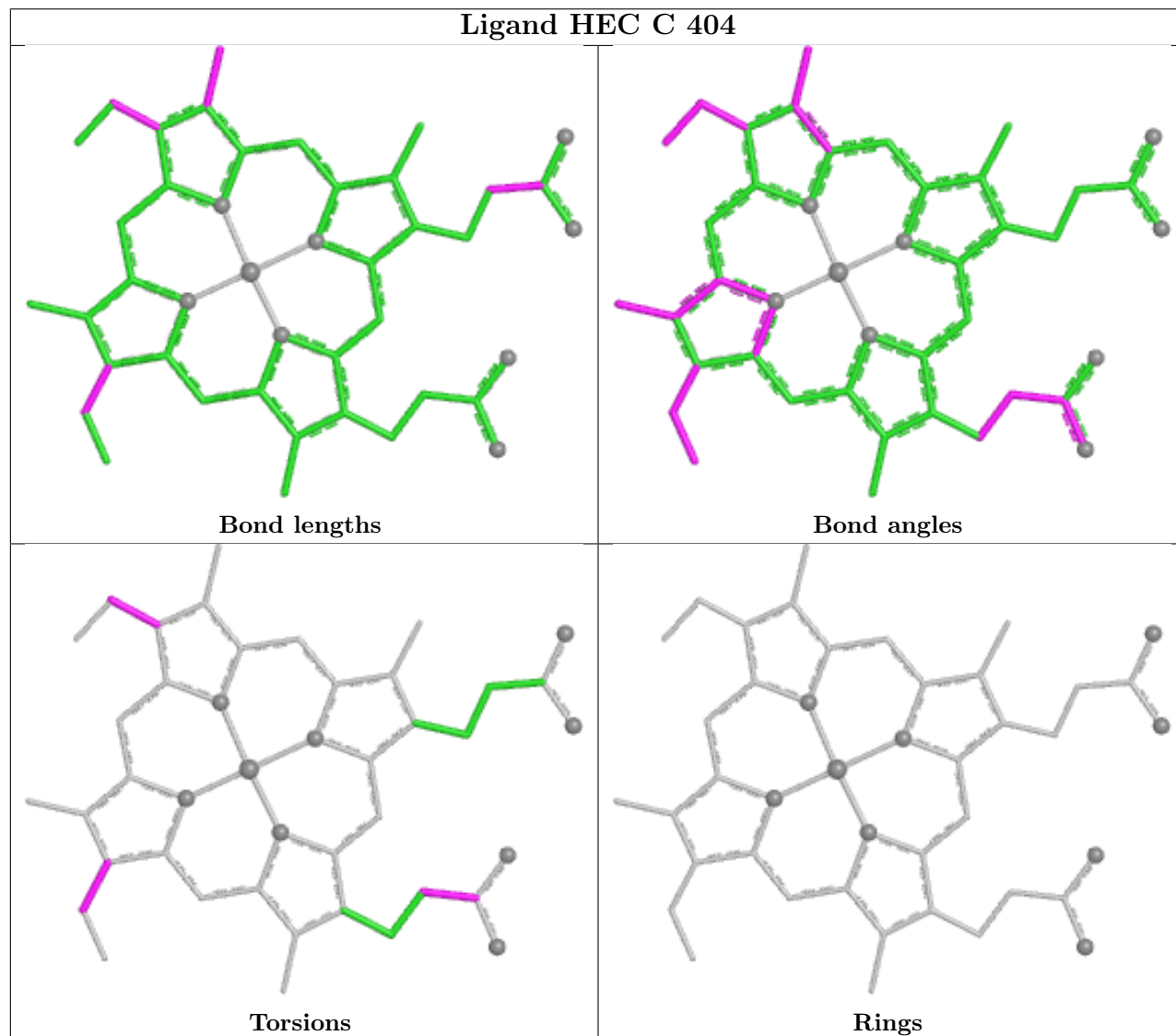
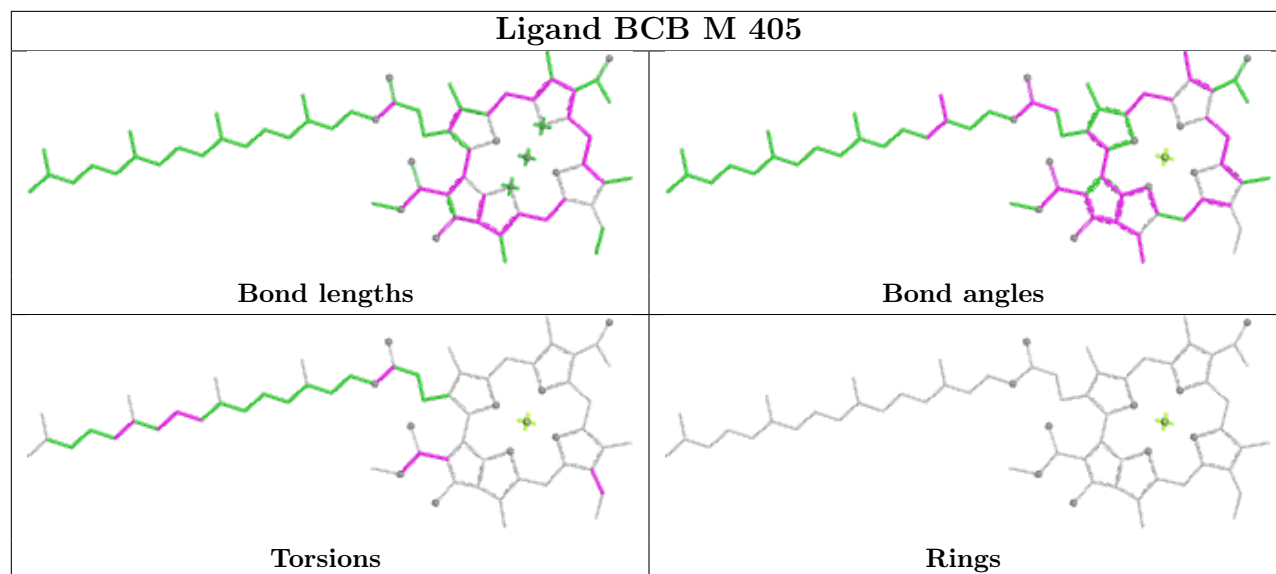
Ligand BPB L 303

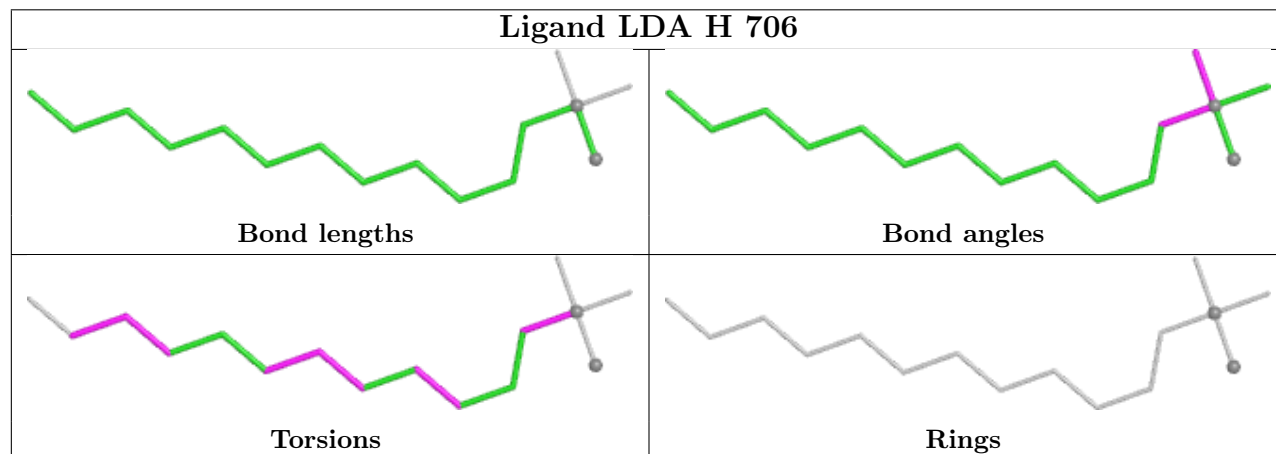
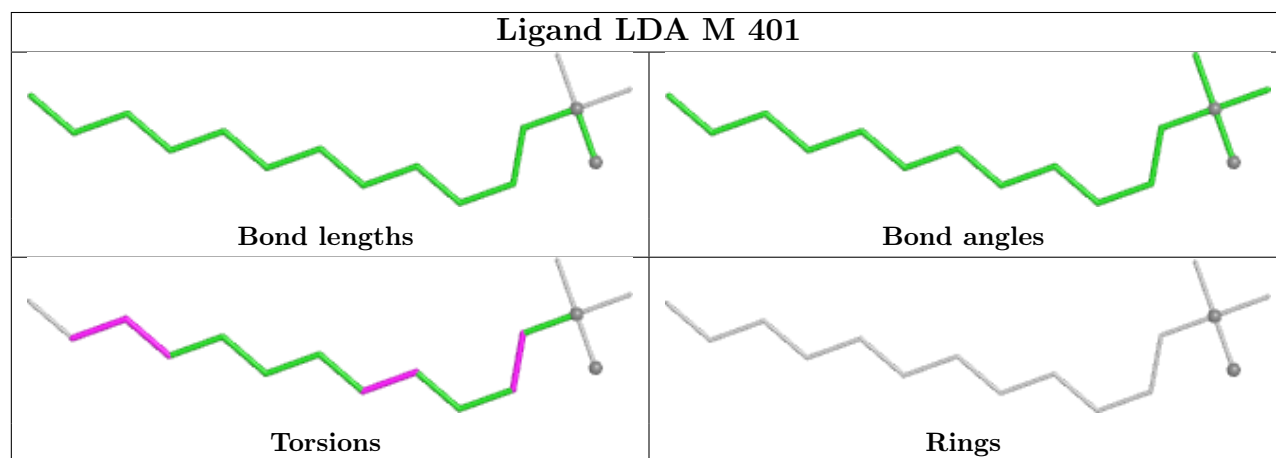
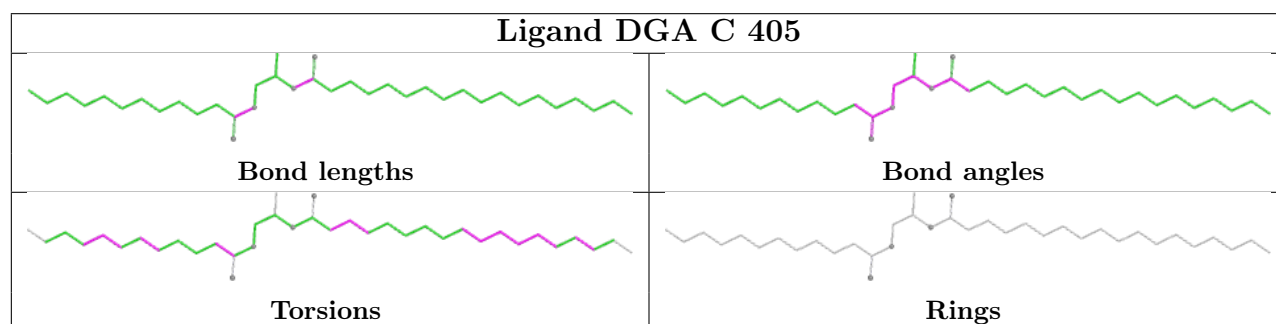
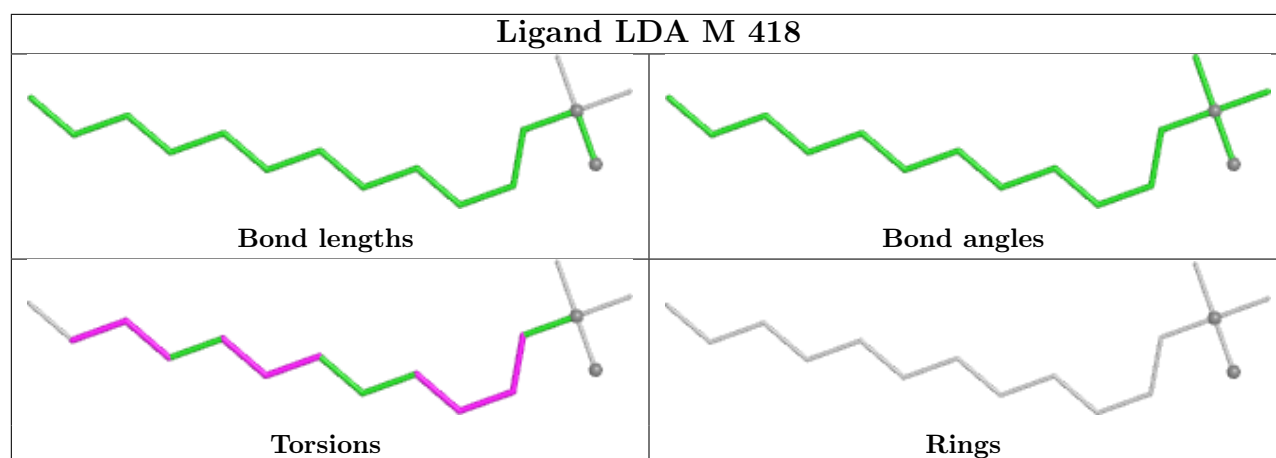


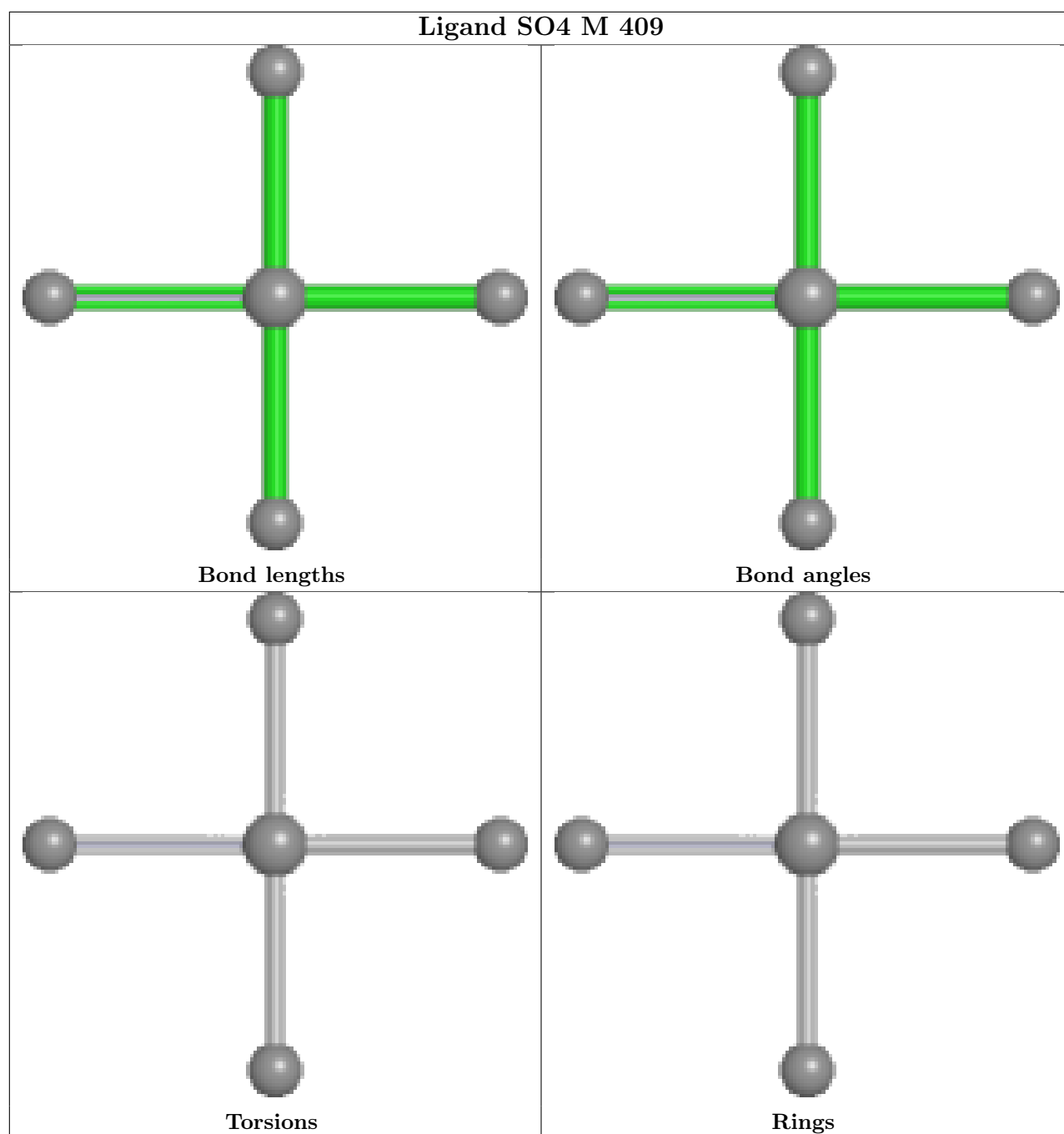
Ligand HEC C 402

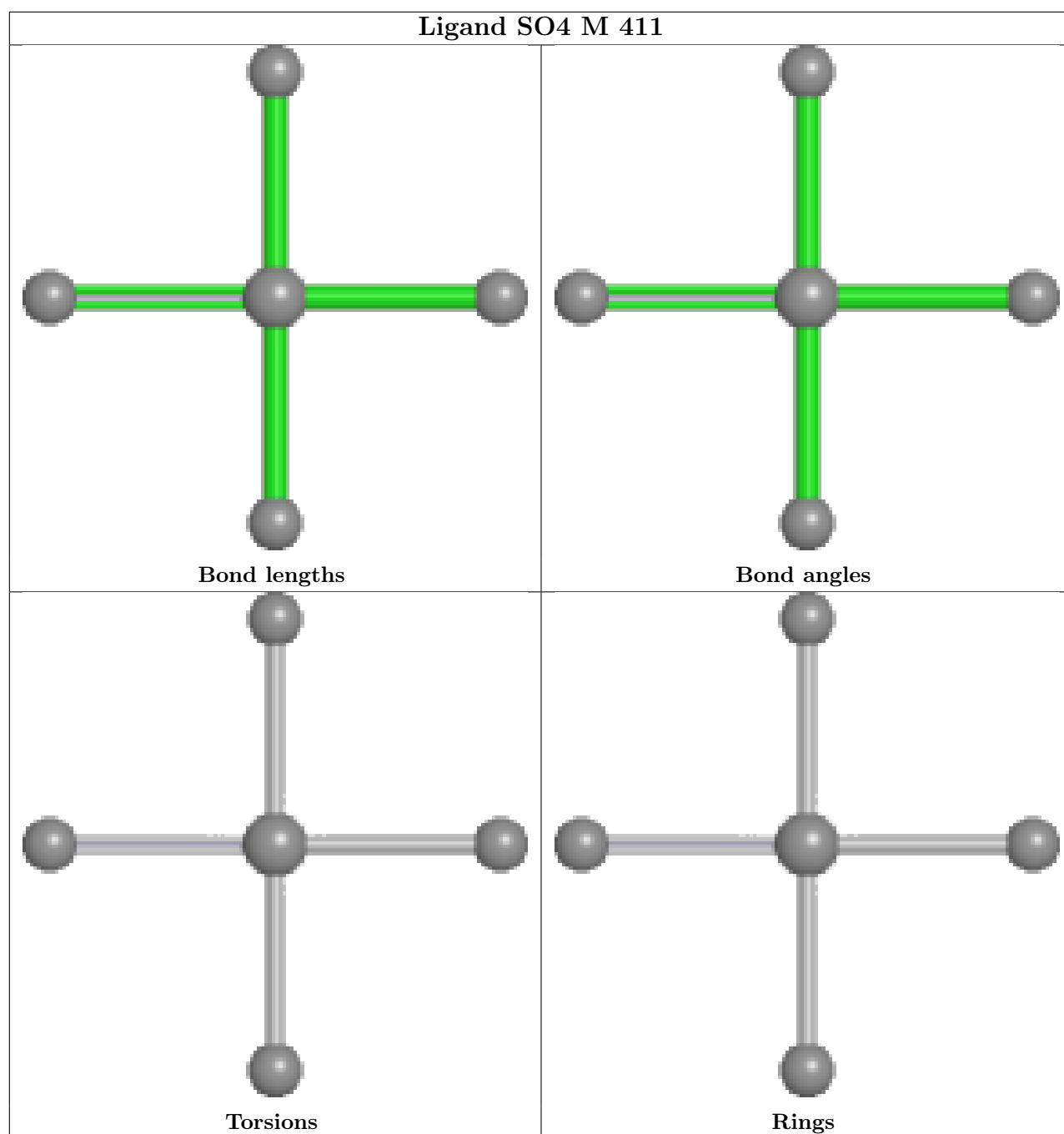


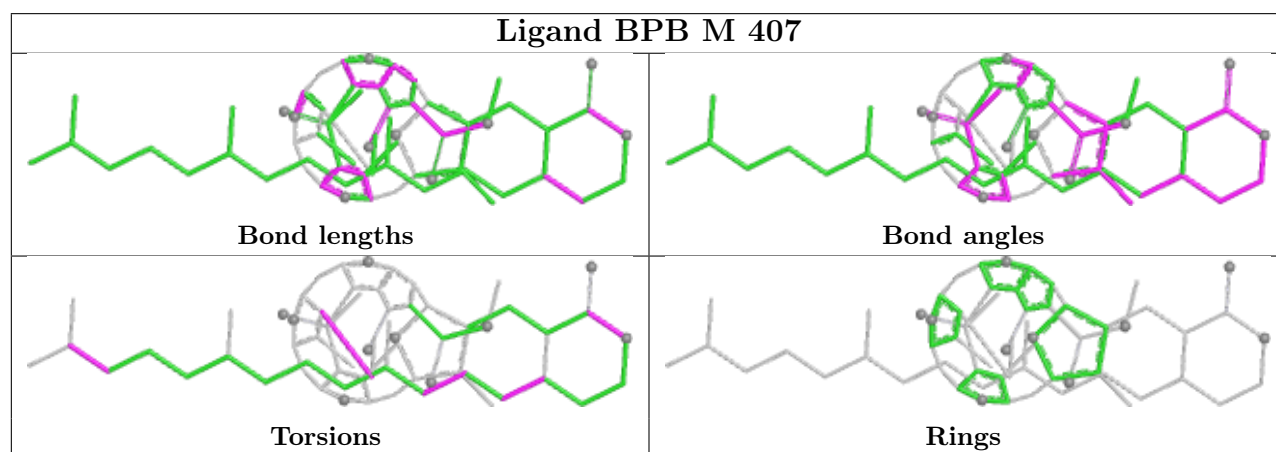
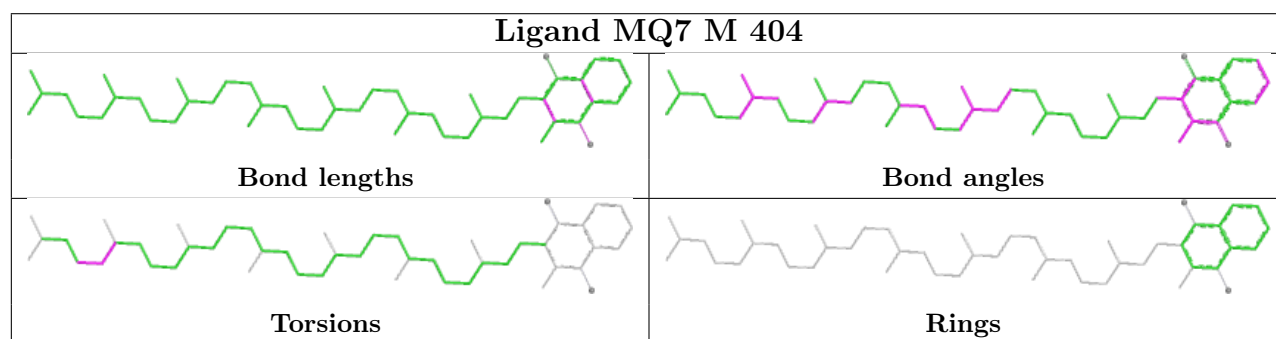
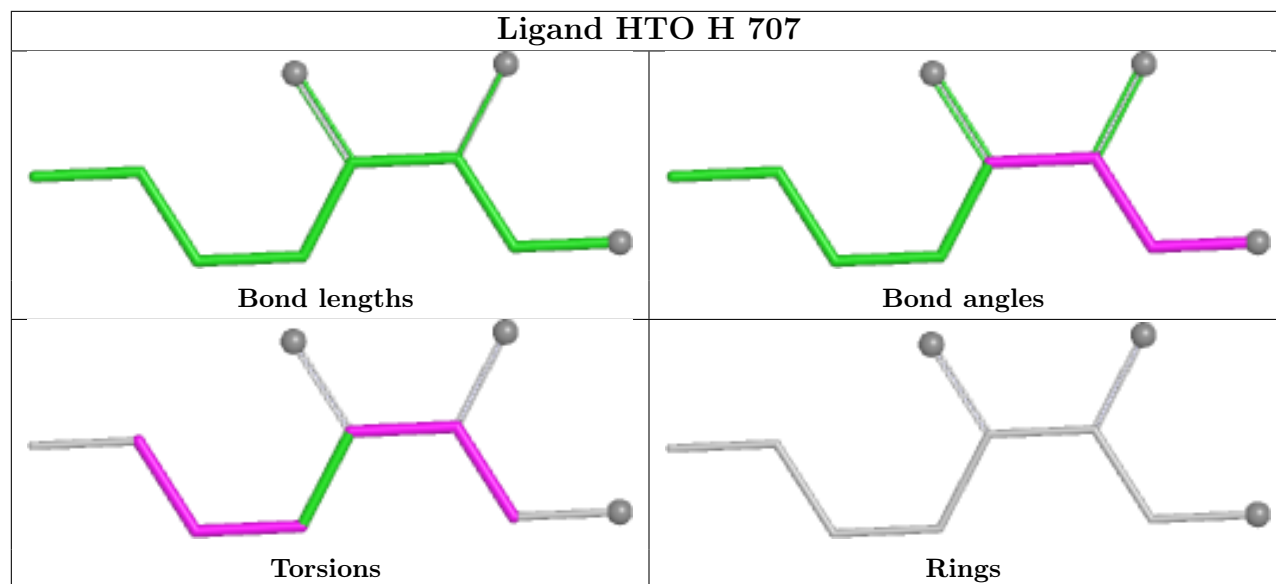


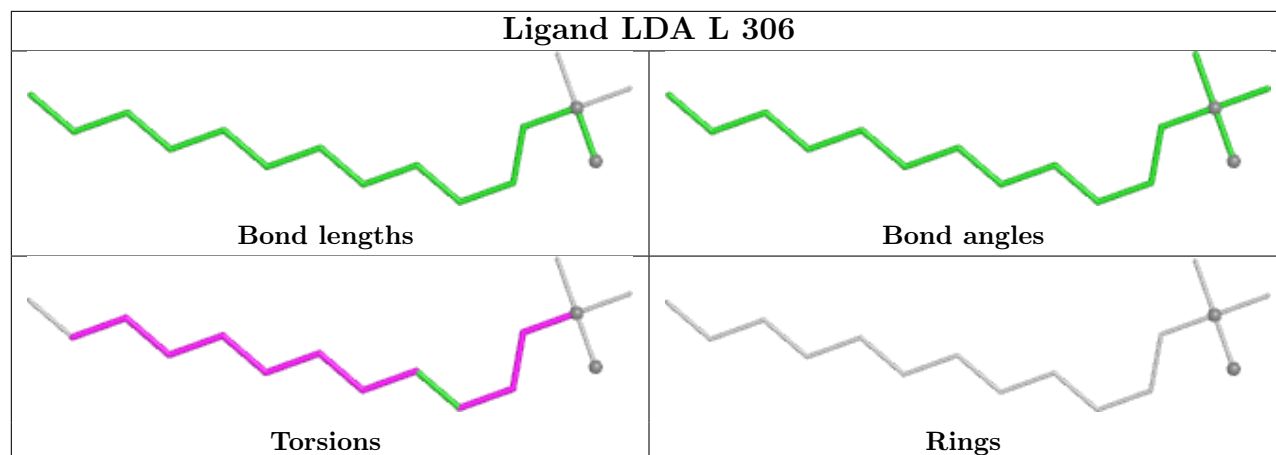


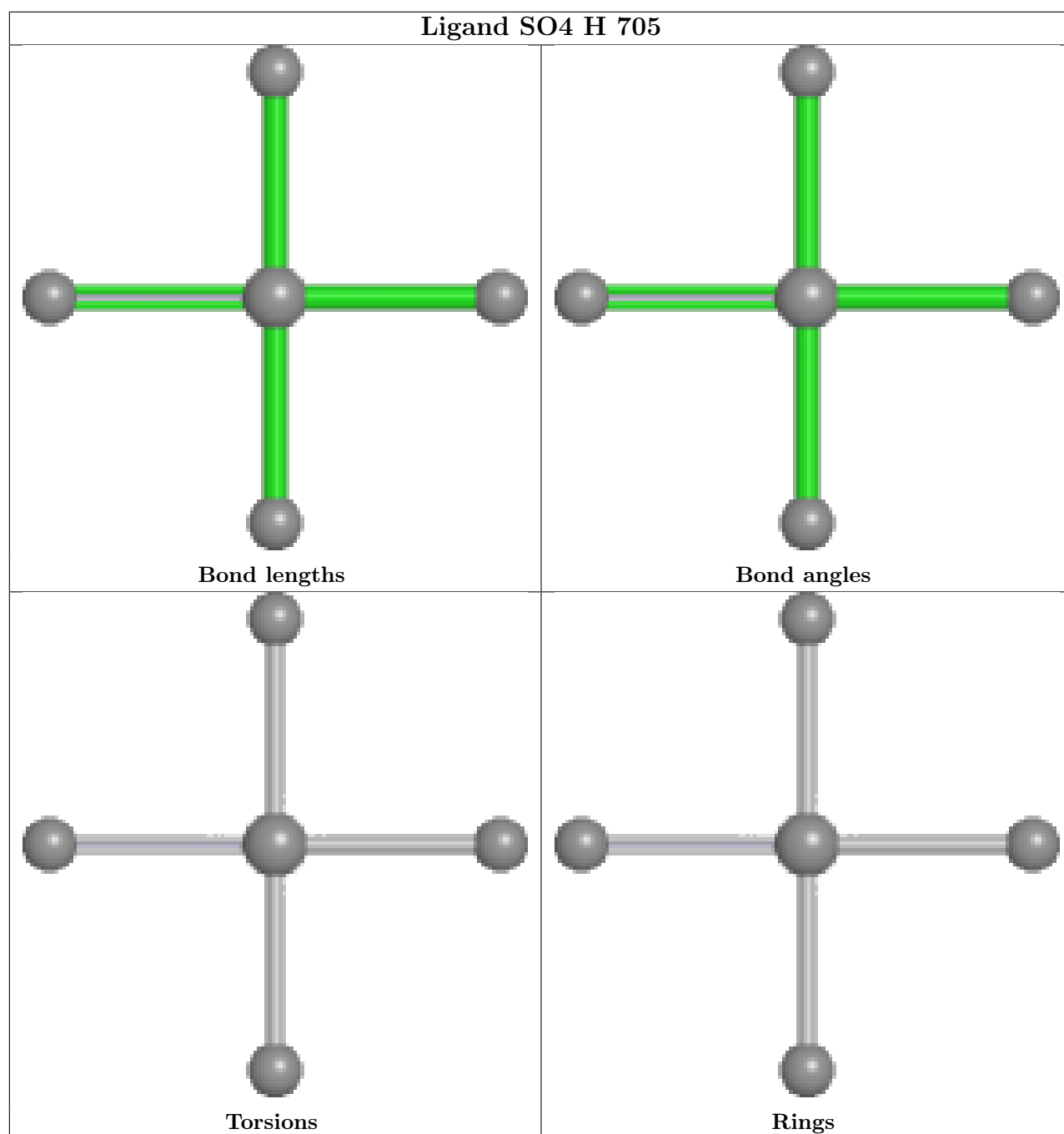


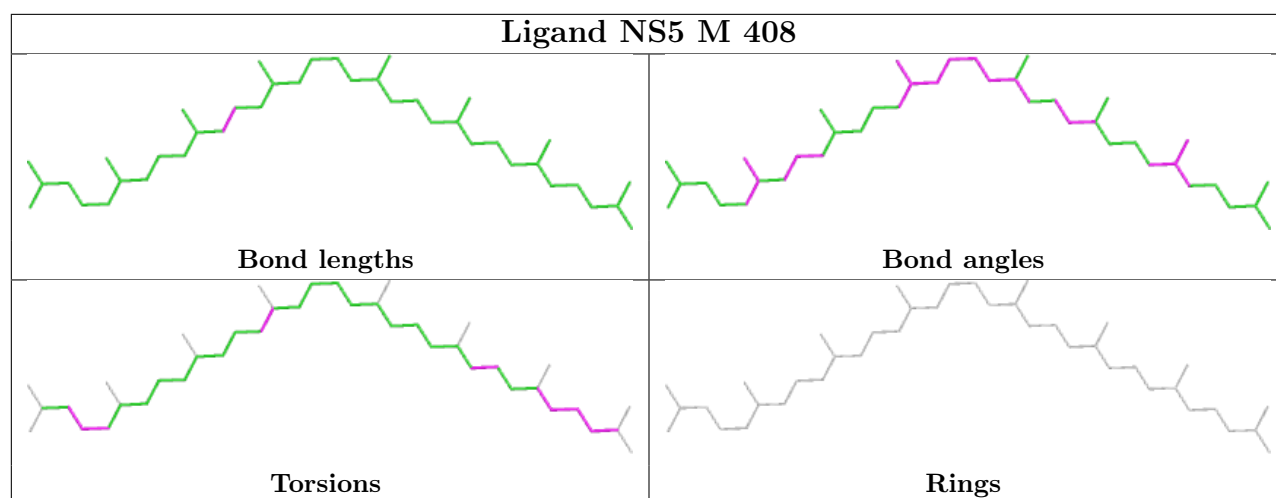


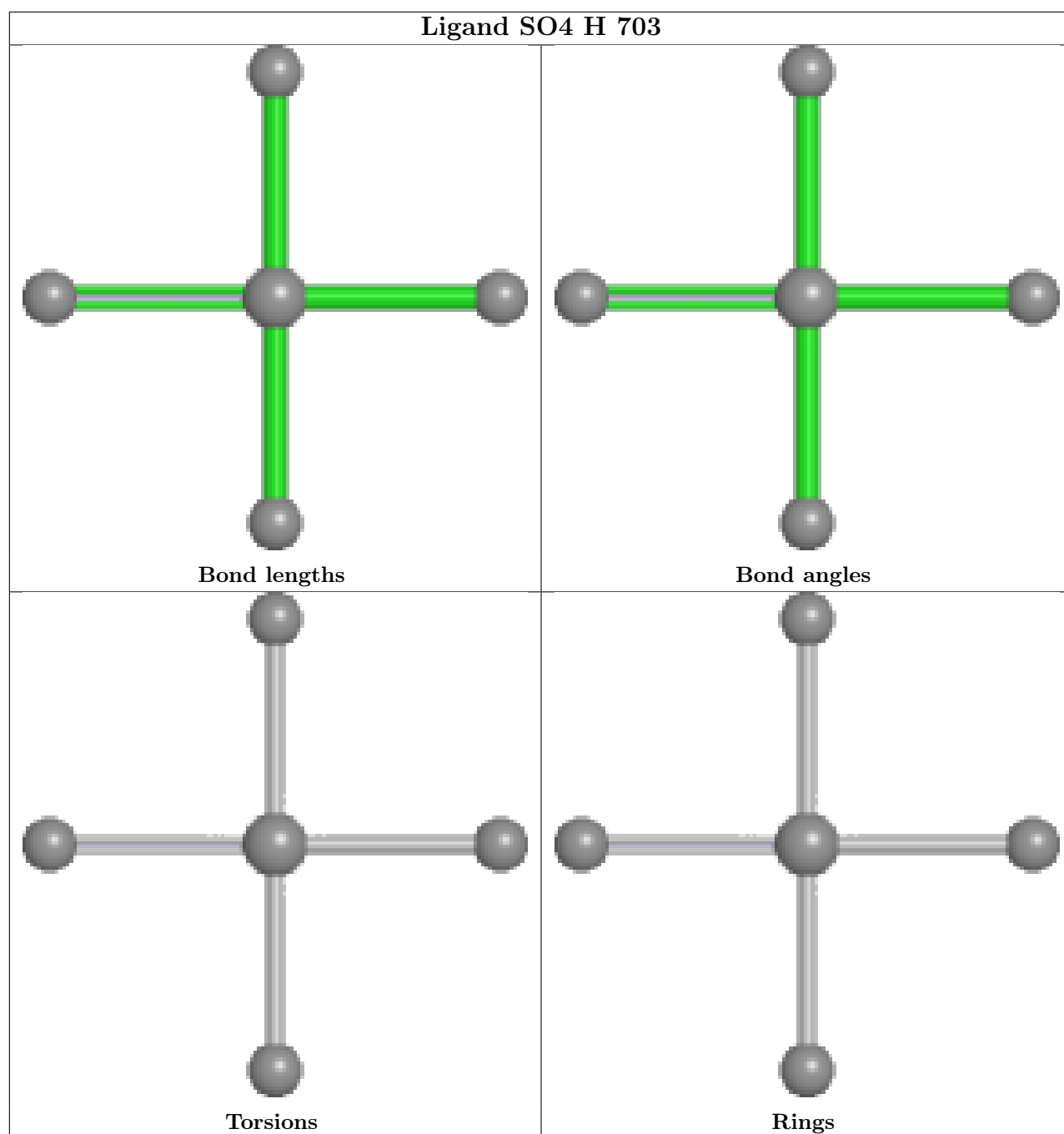


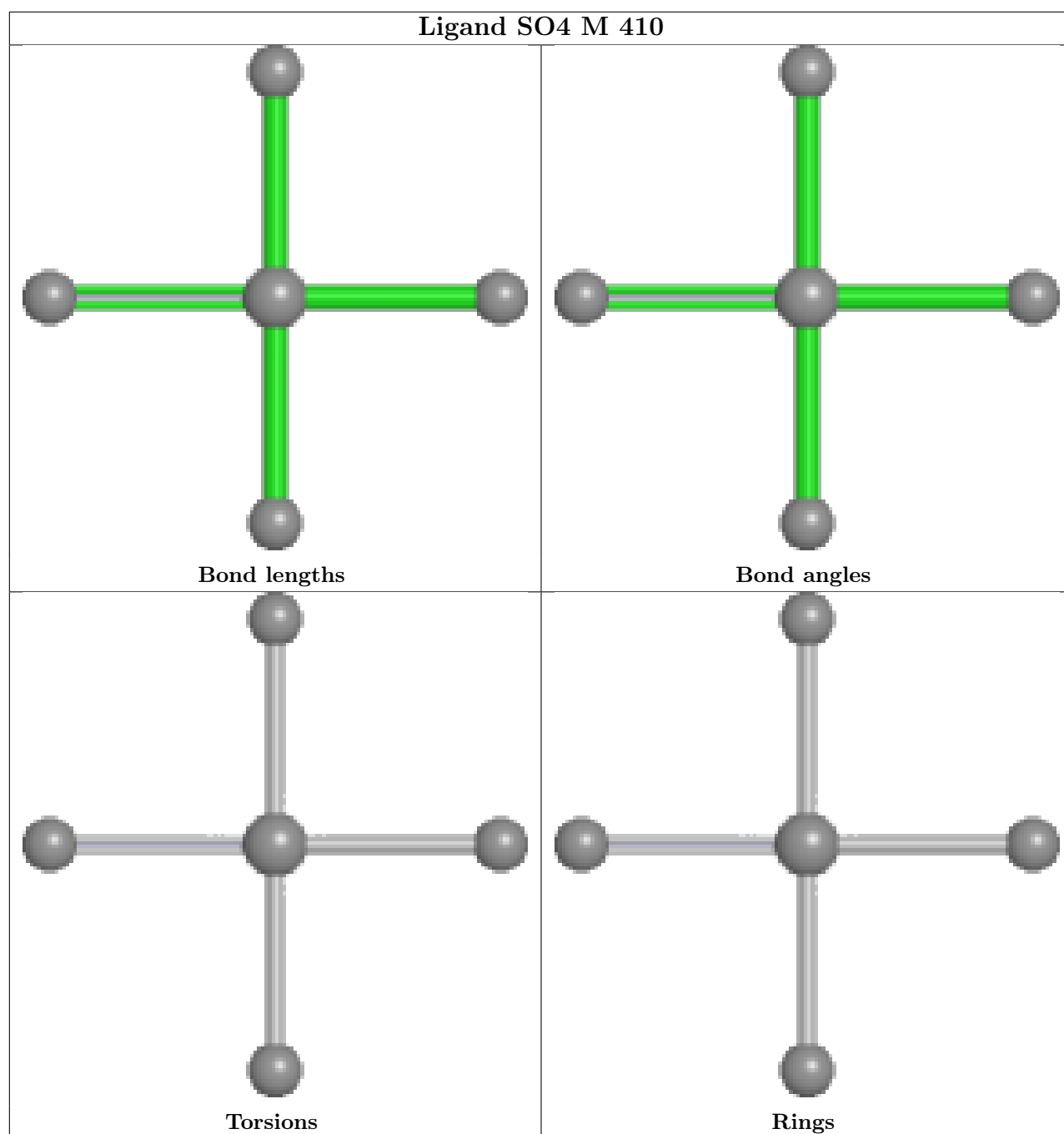


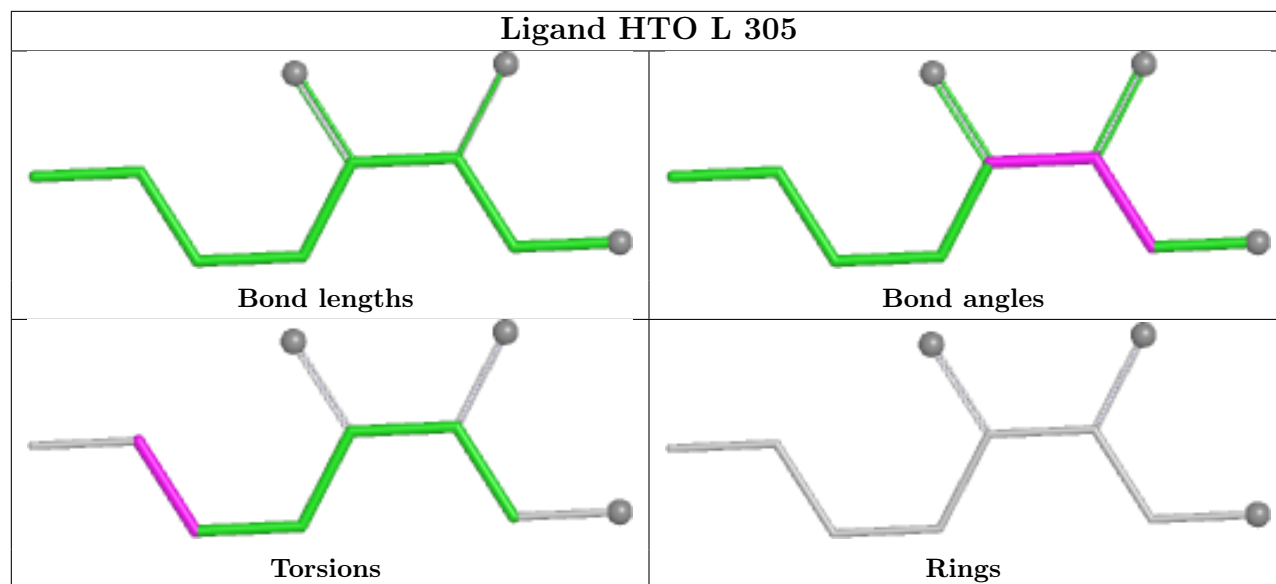


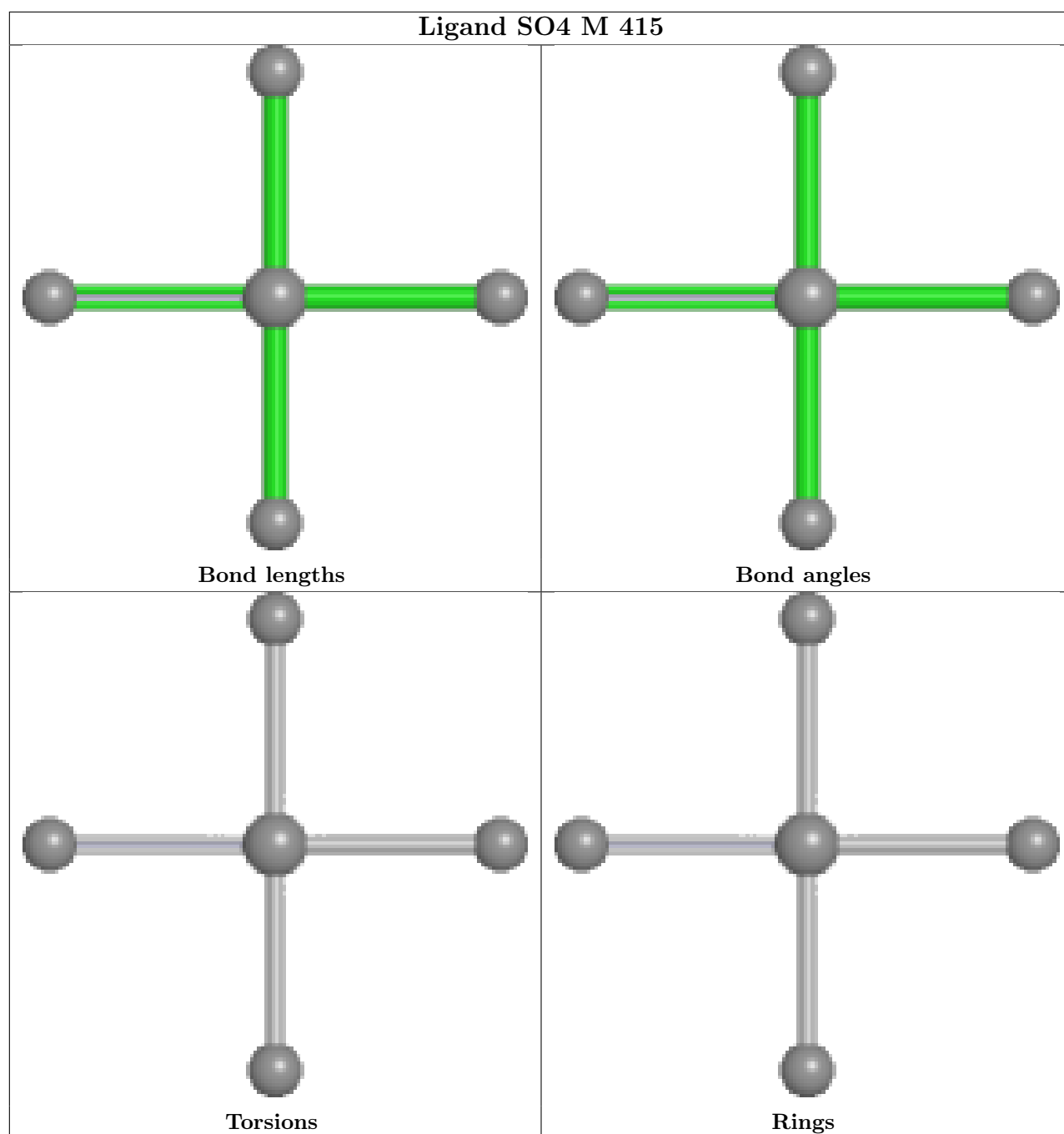




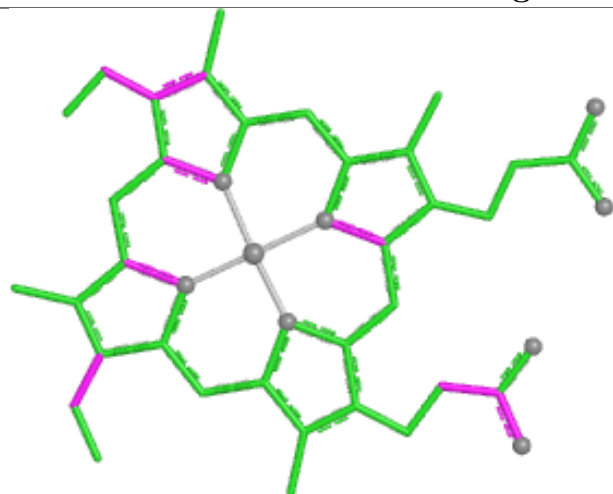




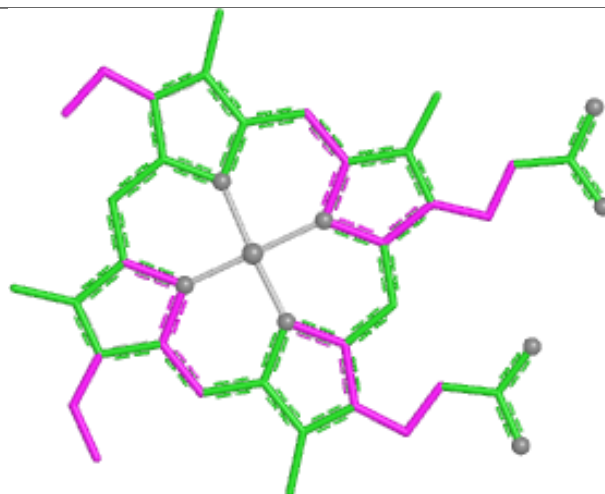




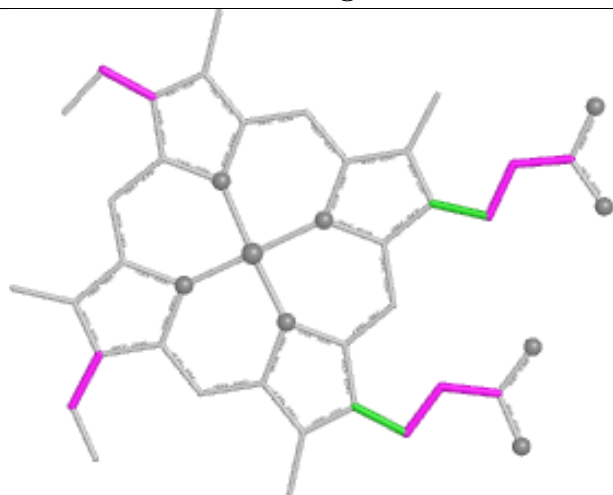
Ligand HEC C 401



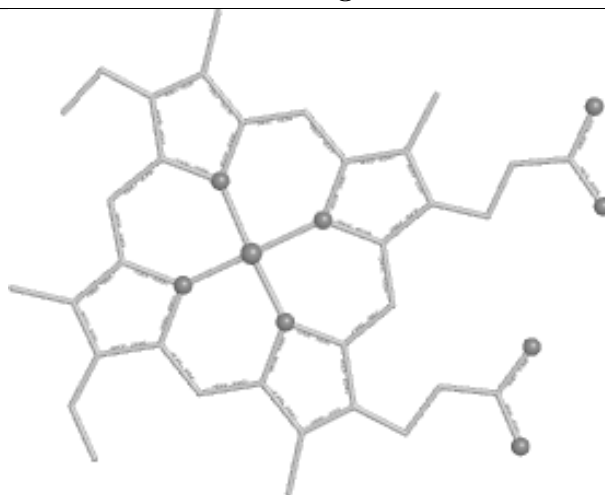
Bond lengths



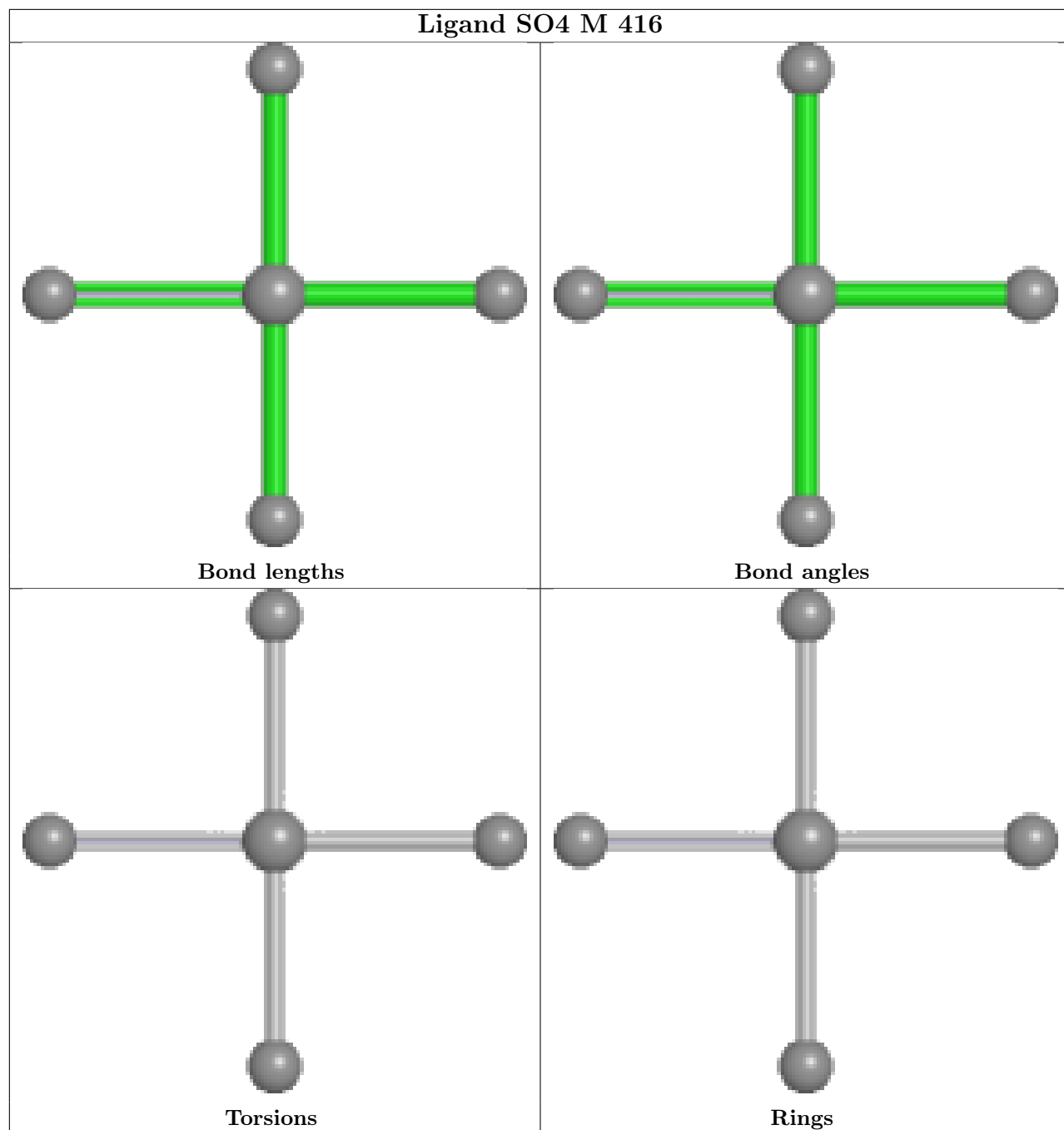
Bond angles

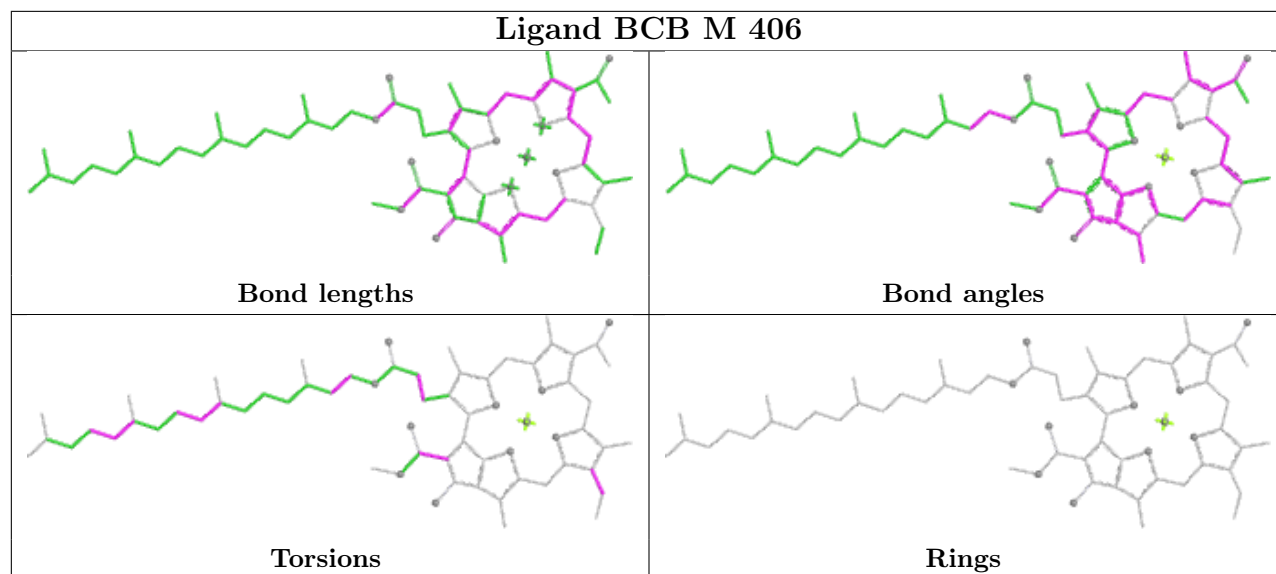


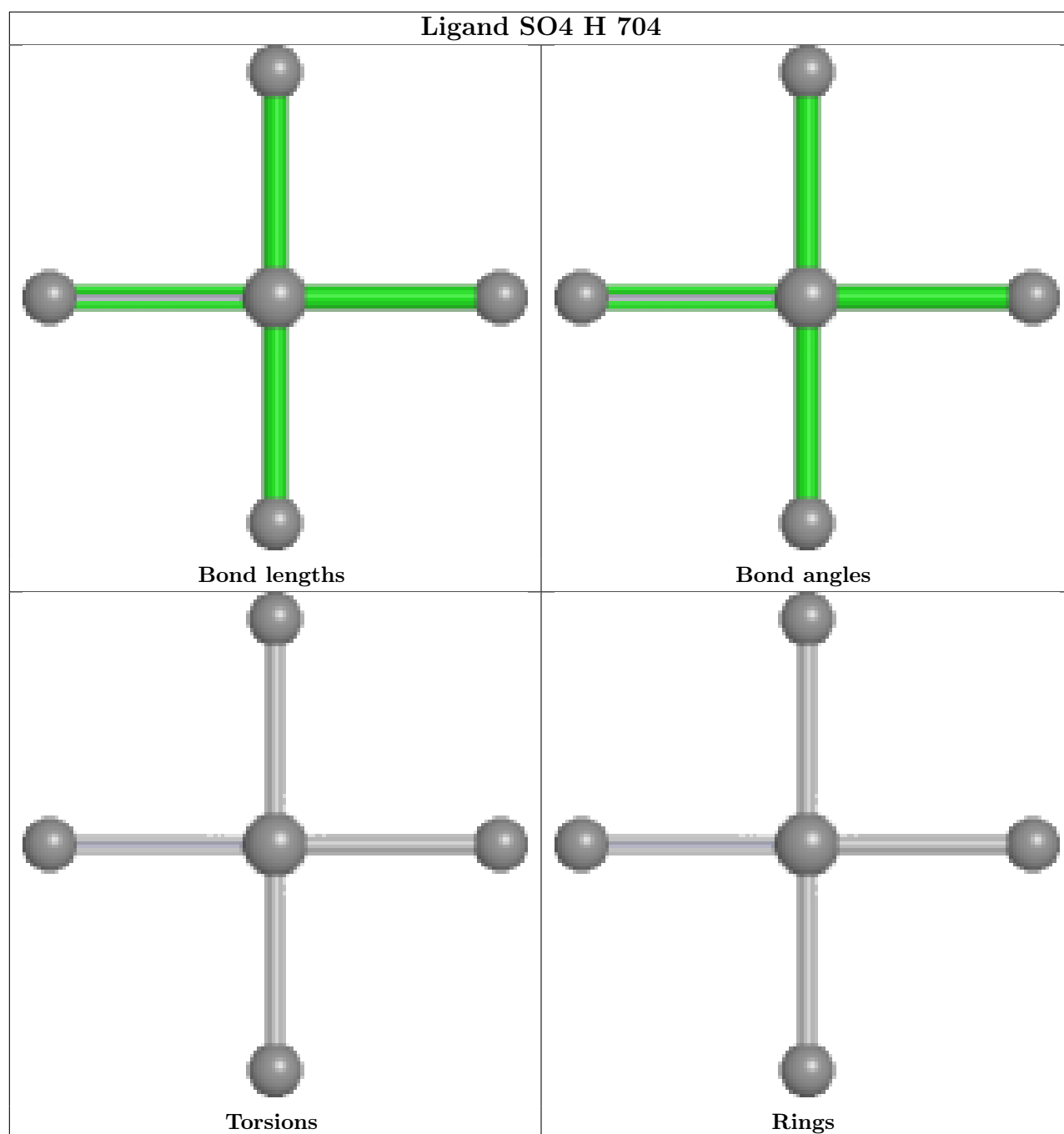
Torsions

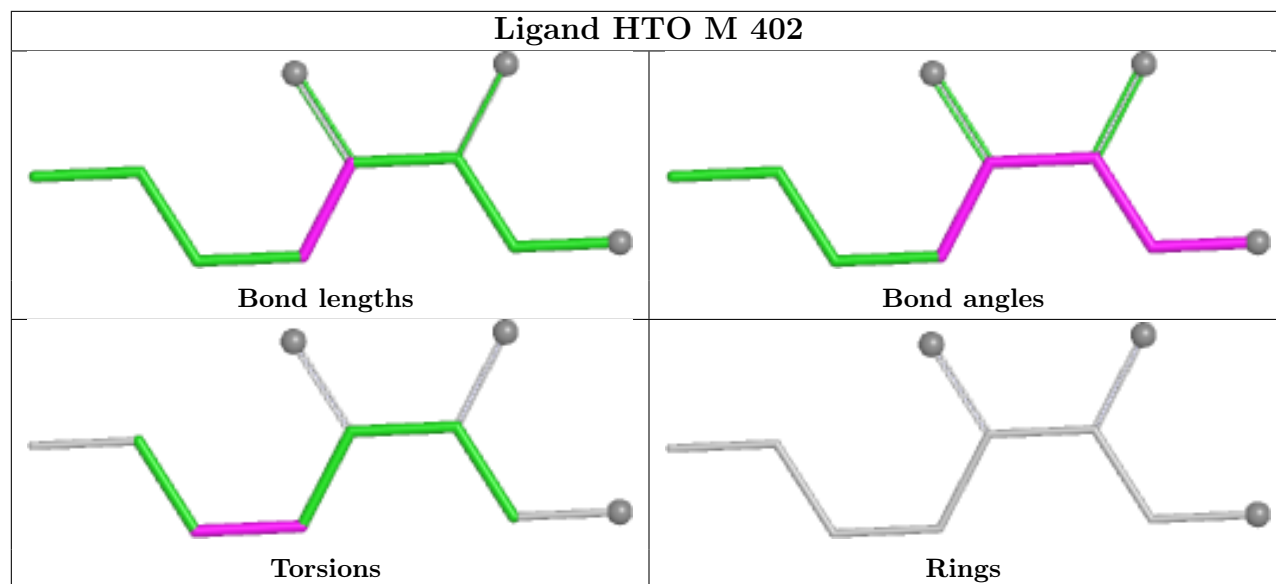


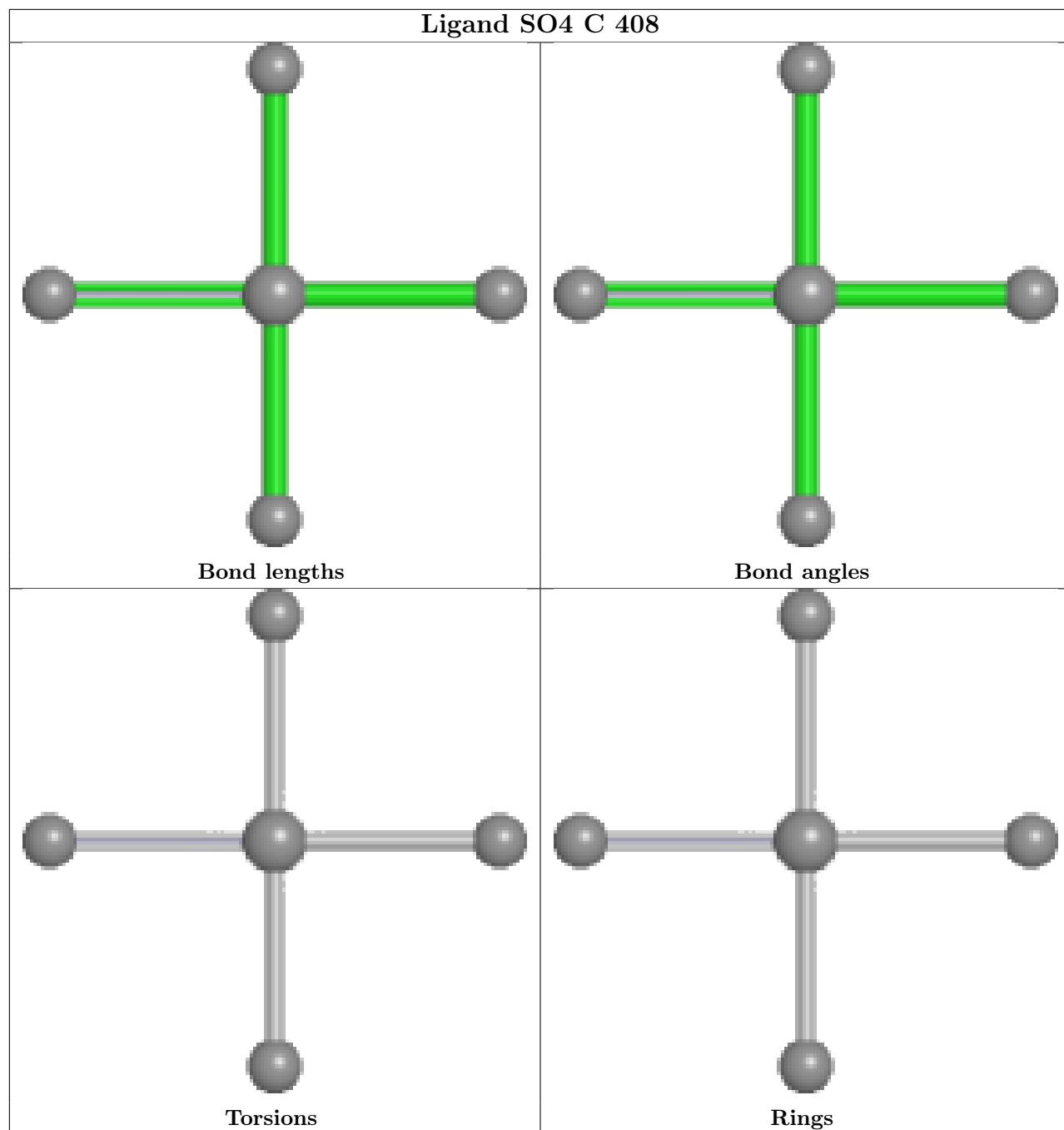
Rings

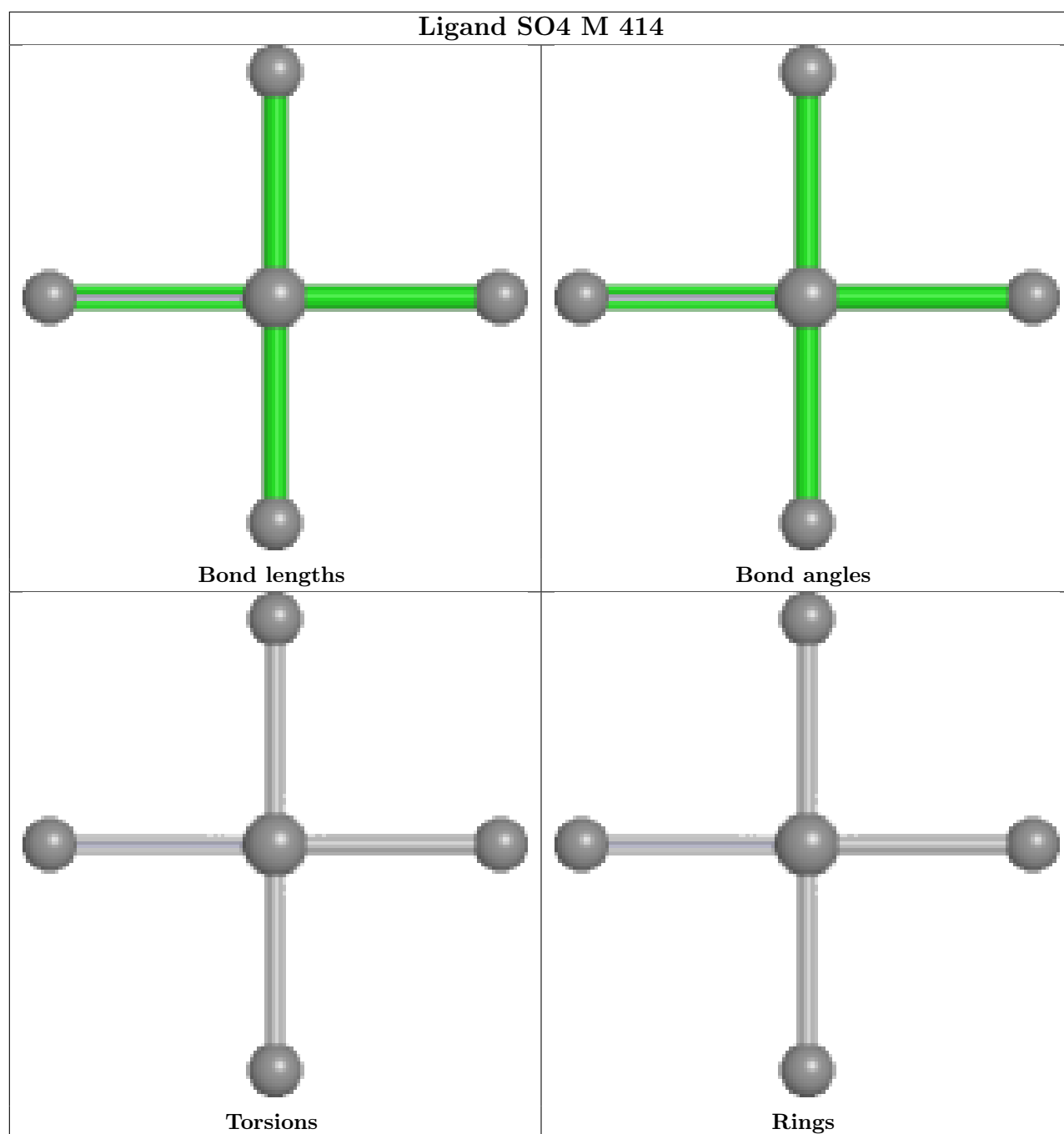












5.7 Other polymers [i](#)

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	C	332/336 (98%)	-0.01	7 (2%) 63 54	30, 48, 79, 107	0
2	H	257/258 (99%)	0.45	16 (6%) 26 20	31, 55, 105, 190	0
3	L	273/273 (100%)	-0.26	3 (1%) 78 70	26, 41, 72, 107	1 (0%)
4	M	323/323 (100%)	-0.10	4 (1%) 76 68	24, 44, 77, 97	0
All	All	1185/1190 (99%)	0.01	30 (2%) 58 48	24, 47, 82, 190	1 (0%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	54	PRO	7.7
2	H	53	ALA	6.7
2	H	50	VAL	6.6
2	H	52	LEU	5.7
2	H	49	LEU	4.4
2	H	46	PRO	4.2
1	C	57	LYS	3.9
4	M	85	PHE	3.8
3	L	1	ALA	3.5
3	L	271	PHE	3.4
2	H	252	GLU	3.4
2	H	258	LEU	3.2
2	H	47	LEU	3.1
2	H	51	LYS	3.1
1	C	332	LYS	3.0
3	L	51	TYR	2.8
4	M	71	PHE	2.8
2	H	82	ARG	2.7
2	H	257	LEU	2.7
2	H	7	ALA	2.6
1	C	94	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
2	H	191	ALA	2.4
1	C	200	GLN	2.4
4	M	103	GLY	2.3
2	H	9	HIS	2.2
1	C	64	ASN	2.2
1	C	146	ARG	2.2
2	H	83	PRO	2.2
4	M	323	LYS	2.1
1	C	46	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
2	FME	H	1	10/11	0.89	0.16	50,57,76,88	0

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
7	SO4	M	412	5/5	0.52	0.18	172,173,180,189	0
7	SO4	M	414	5/5	0.58	0.16	173,179,186,191	0
9	HTO	M	402	10/10	0.58	0.38	60,85,94,97	0
7	SO4	C	407	5/5	0.62	0.19	76,80,81,86	5
7	SO4	M	416	5/5	0.64	0.24	234,252,256,269	0
9	HTO	L	305	10/10	0.66	0.32	74,85,95,102	0
7	SO4	C	406	5/5	0.71	0.15	129,133,138,144	0
6	DGA	C	405	37/44	0.72	0.32	69,100,131,140	0

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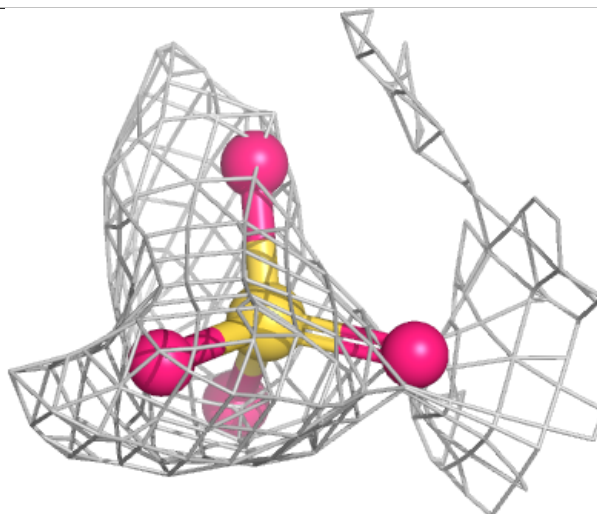
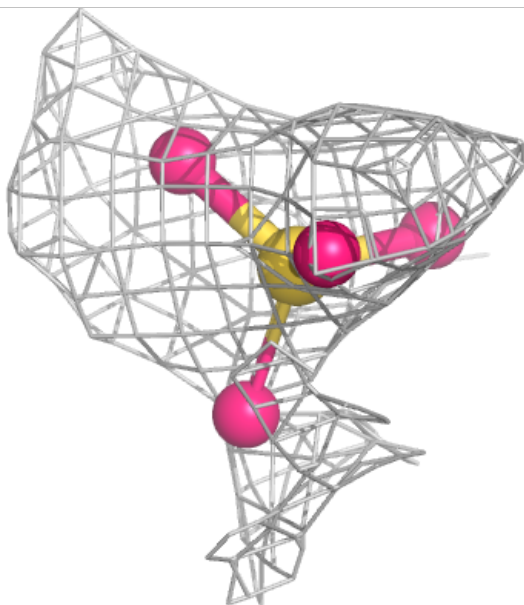
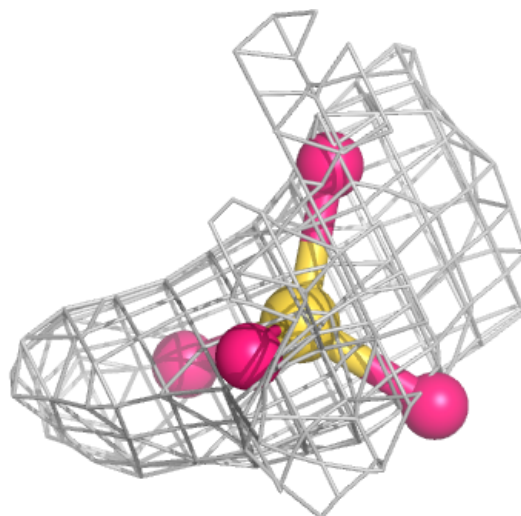
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	SO4	H	703	5/5	0.73	0.13	109,116,128,147	0
8	LDA	M	418	16/16	0.76	0.35	74,101,122,127	0
7	SO4	M	415	5/5	0.78	0.16	185,192,195,197	0
8	LDA	M	417	16/16	0.81	0.38	91,104,132,138	0
8	LDA	L	306	16/16	0.82	0.31	69,90,110,114	0
7	SO4	C	408	5/5	0.83	0.15	56,60,65,67	5
9	HTO	H	707	10/10	0.84	0.21	55,80,85,95	0
7	SO4	H	704	5/5	0.85	0.24	56,58,63,63	5
8	LDA	L	304	16/16	0.86	0.33	99,120,136,136	0
7	SO4	M	410	5/5	0.87	0.14	75,82,88,99	0
7	SO4	M	413	5/5	0.87	0.16	52,53,57,60	5
8	LDA	M	401	16/16	0.89	0.26	71,92,125,138	0
14	NS5	M	408	40/40	0.89	0.21	41,65,103,108	0
8	LDA	H	706	16/16	0.90	0.23	51,83,108,110	0
11	BPB	M	407	65/65	0.93	0.15	36,44,139,149	0
7	SO4	H	702	5/5	0.93	0.14	79,82,87,88	0
13	MQ7	M	404	48/48	0.94	0.12	30,37,74,88	0
10	BCB	M	405	66/66	0.95	0.14	28,36,129,137	0
8	LDA	H	701	16/16	0.96	0.12	36,50,61,64	0
10	BCB	M	406	66/66	0.96	0.09	22,28,48,51	0
7	SO4	M	411	5/5	0.96	0.08	47,49,56,68	0
10	BCB	L	301	66/66	0.96	0.09	22,31,45,51	0
10	BCB	L	302	66/66	0.96	0.10	27,31,59,68	0
7	SO4	M	409	5/5	0.97	0.08	59,61,66,67	0
5	HEC	C	401	43/43	0.97	0.09	40,51,73,78	0
11	BPB	L	303	65/65	0.97	0.07	22,29,40,44	0
5	HEC	C	402	43/43	0.98	0.07	33,46,55,61	0
5	HEC	C	403	43/43	0.98	0.08	26,35,44,48	0
5	HEC	C	404	43/43	0.98	0.08	30,39,56,81	0
7	SO4	H	705	5/5	0.99	0.08	47,48,49,49	5
12	FE2	M	403	1/1	1.00	0.01	35,35,35,35	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.

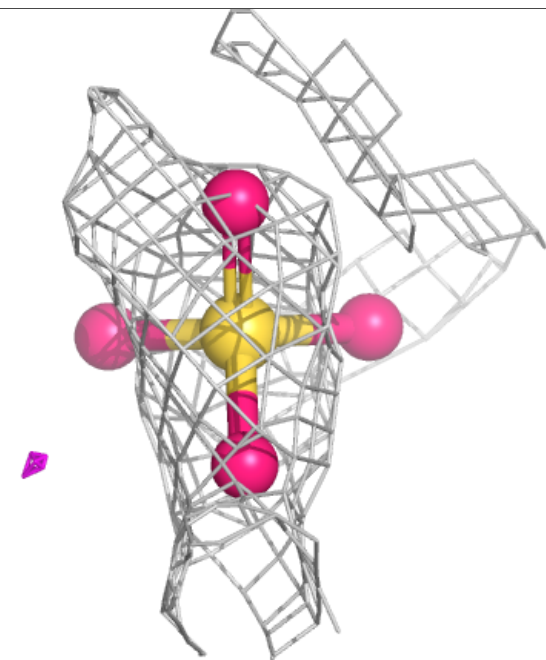
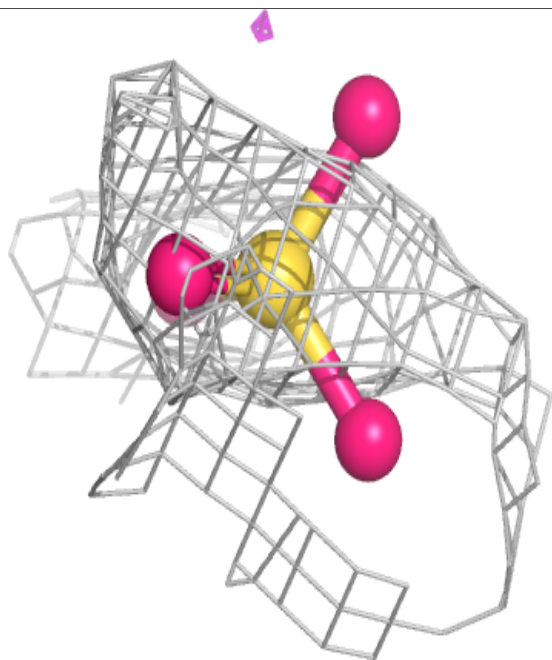
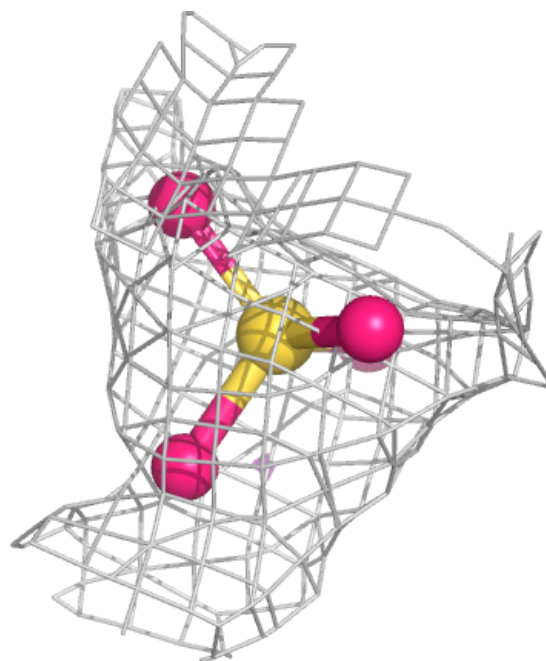
Electron density around SO4 M 412:

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



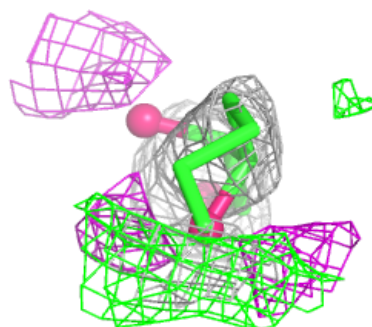
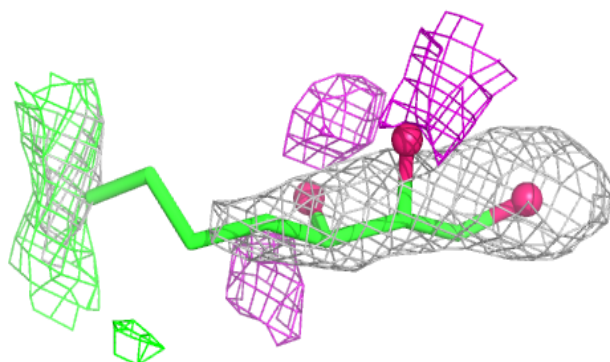
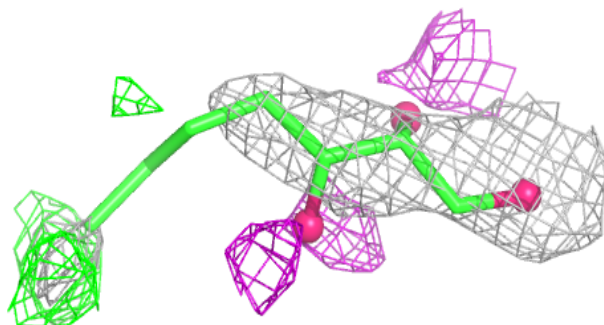
Electron density around SO4 M 414:

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

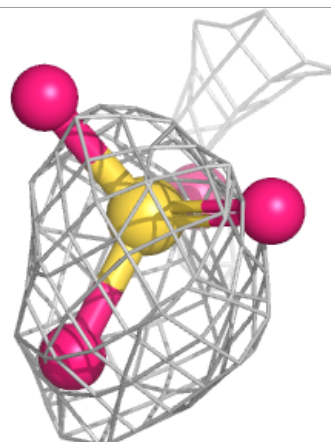
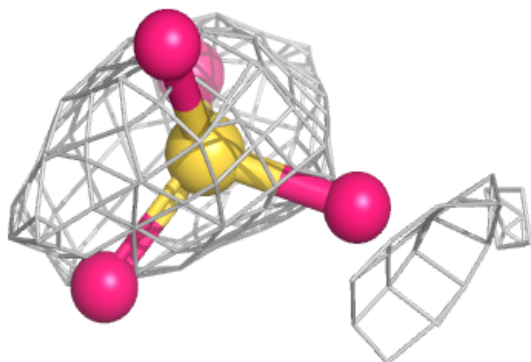
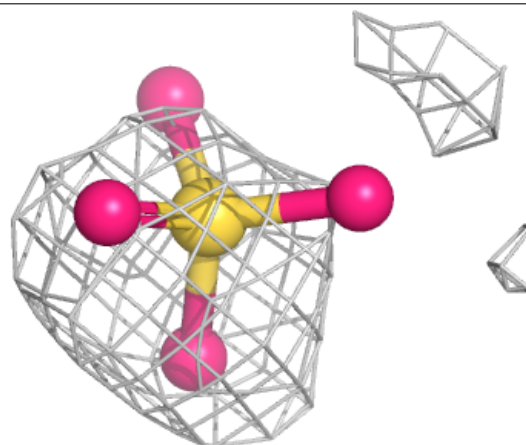


Electron density around HTO M 402:

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

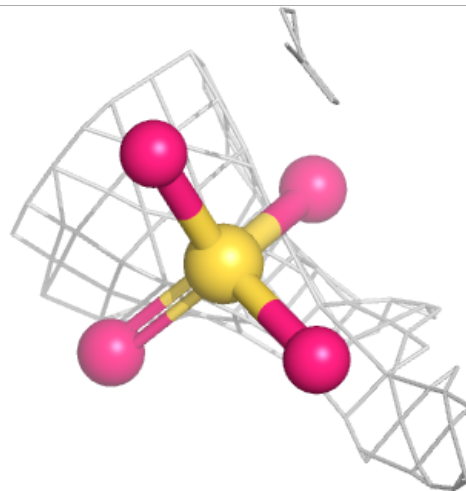
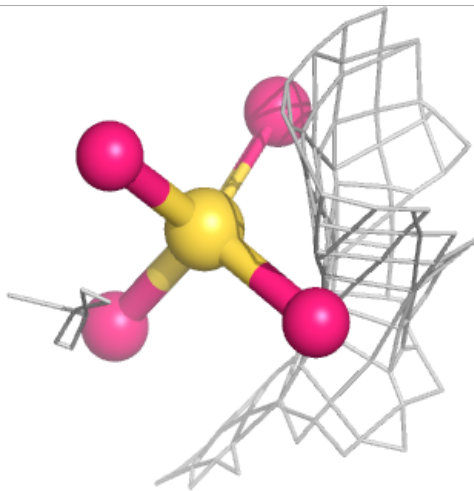
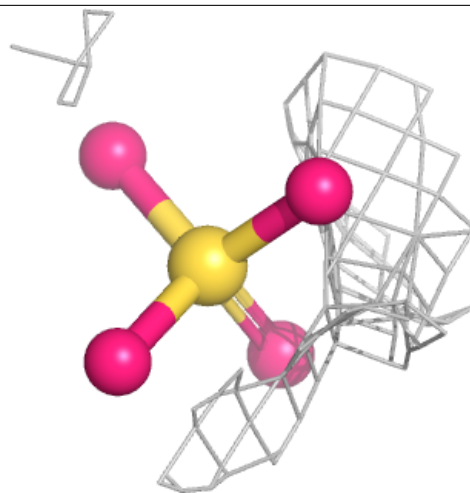
**Electron density around SO4 C 407:**

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



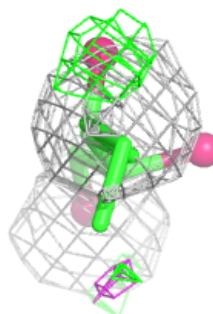
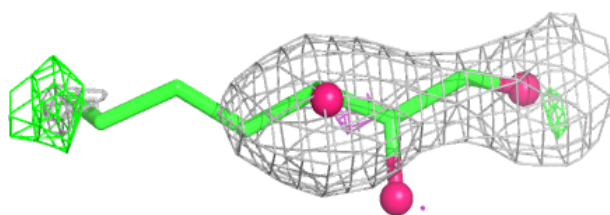
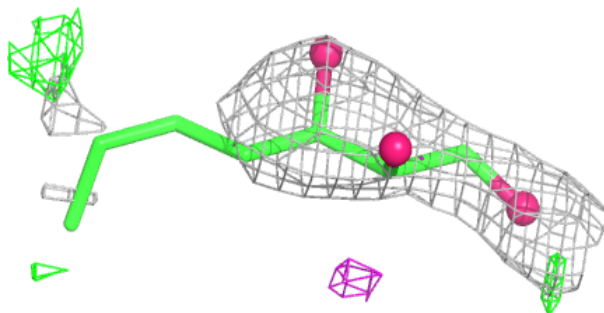
Electron density around SO4 M 416:

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



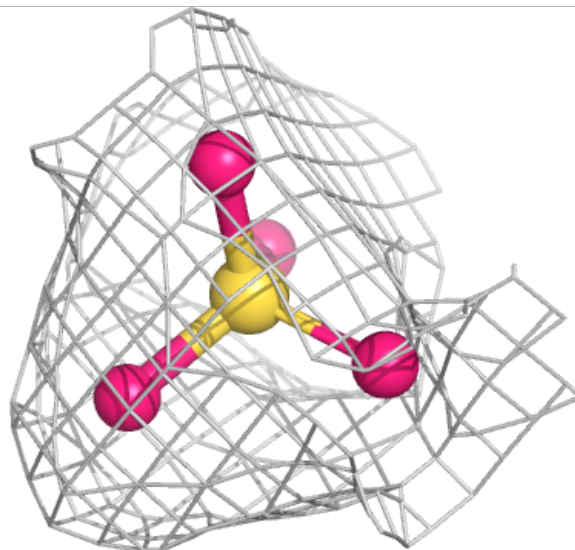
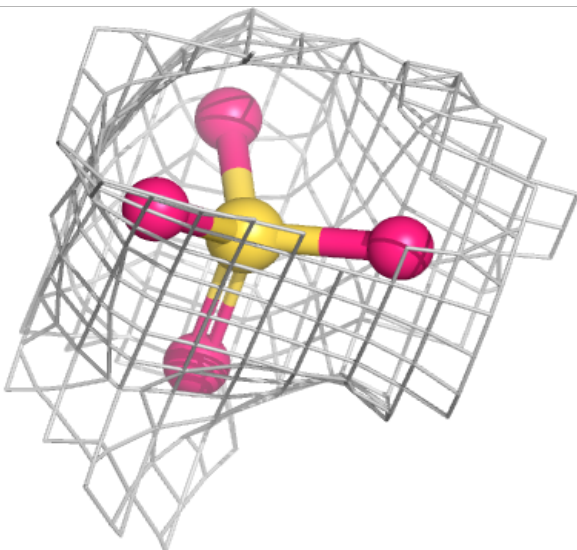
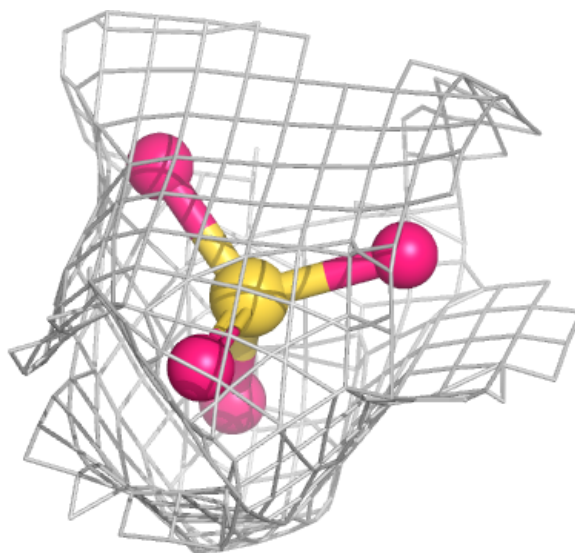
Electron density around HTO L 305:

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



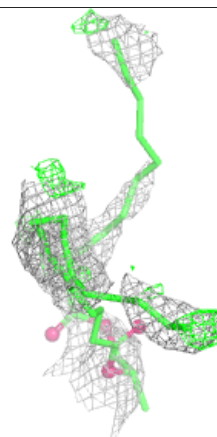
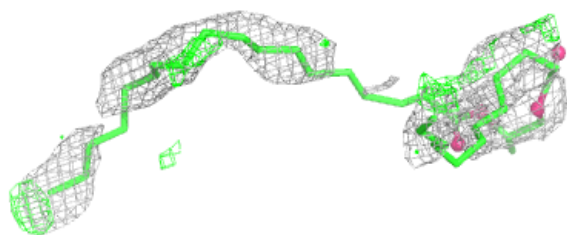
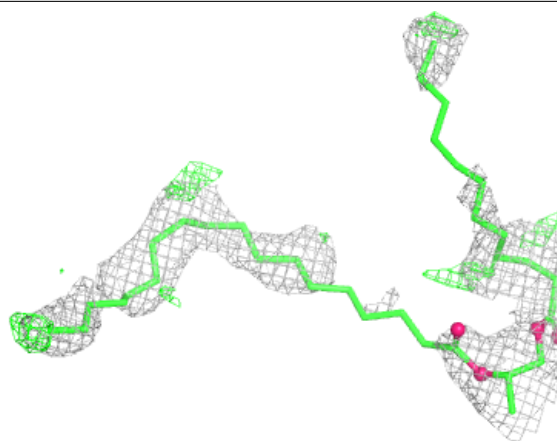
Electron density around SO4 C 406:

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



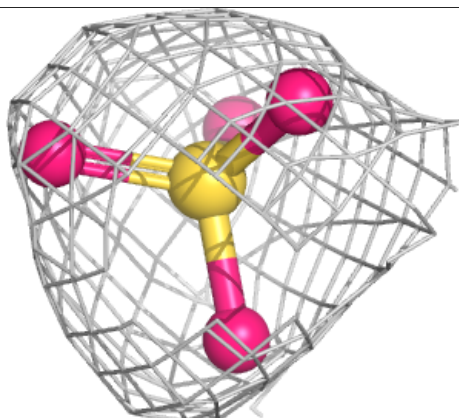
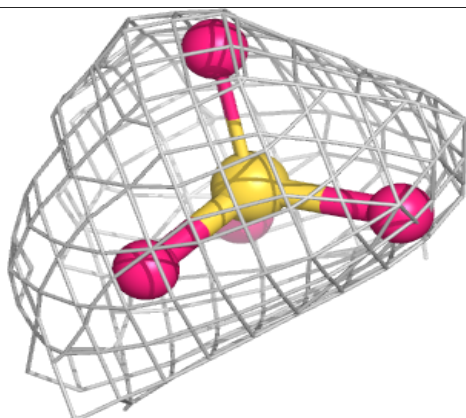
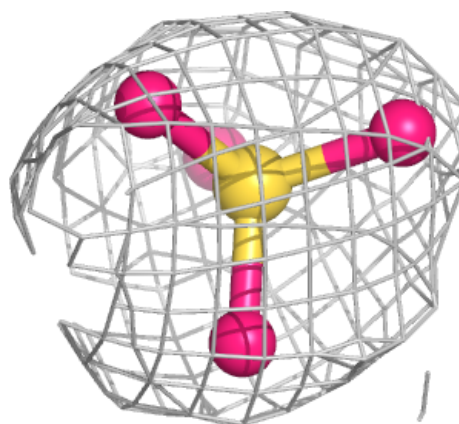
Electron density around DGA C 405:

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

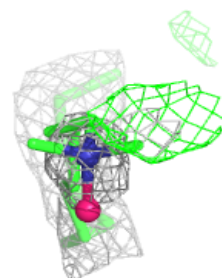
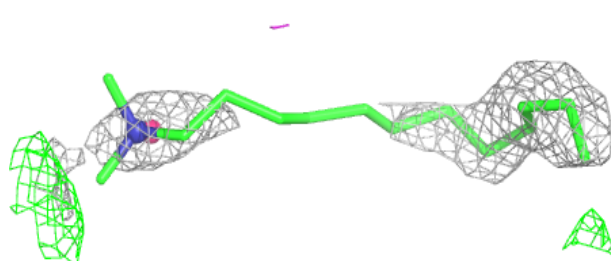
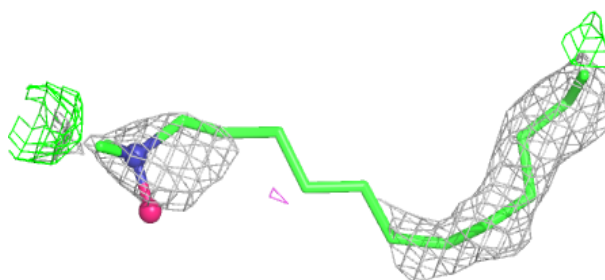


Electron density around SO4 H 703:

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

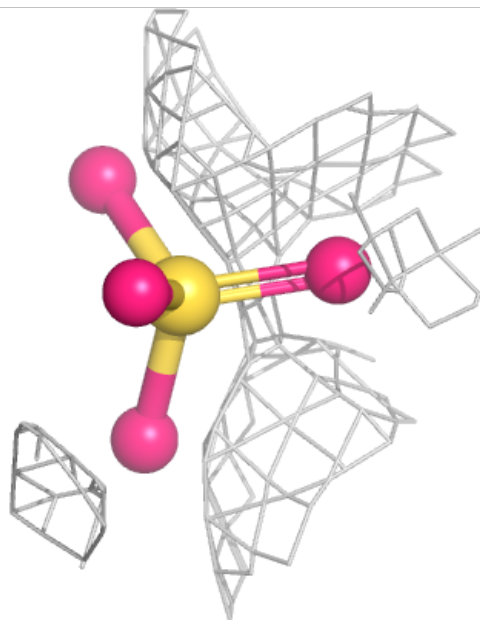
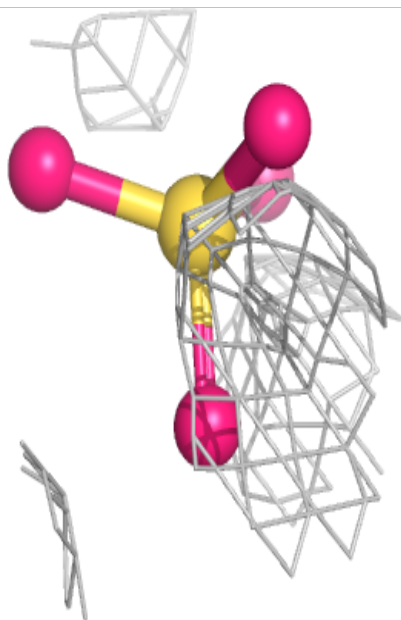
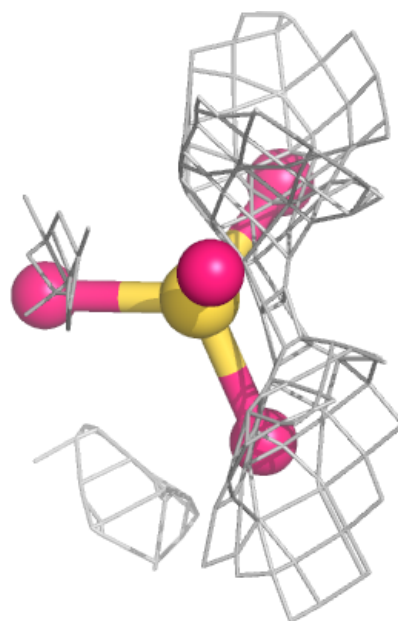
**Electron density around LDA M 418:**

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



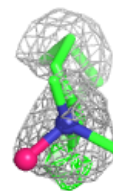
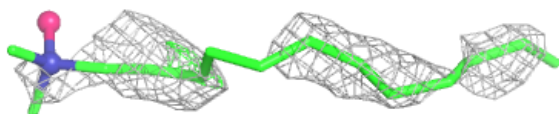
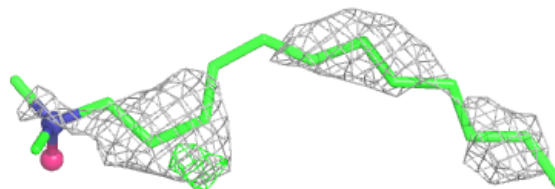
Electron density around SO4 M 415:

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

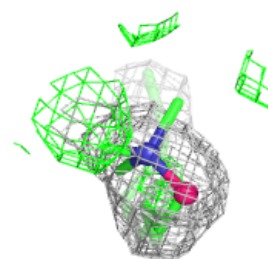
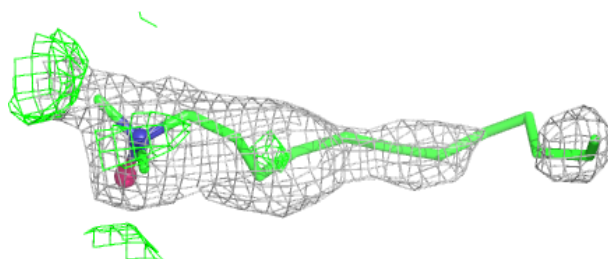
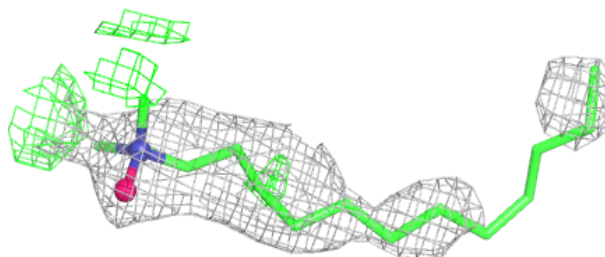


Electron density around LDA M 417:

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

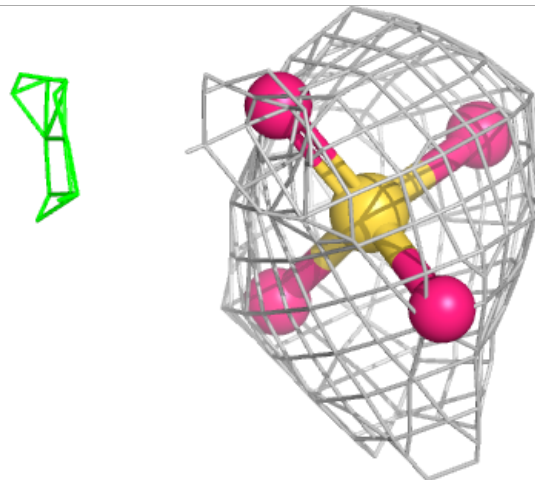
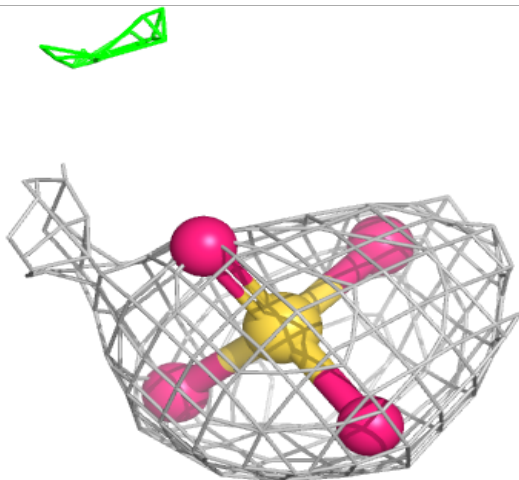
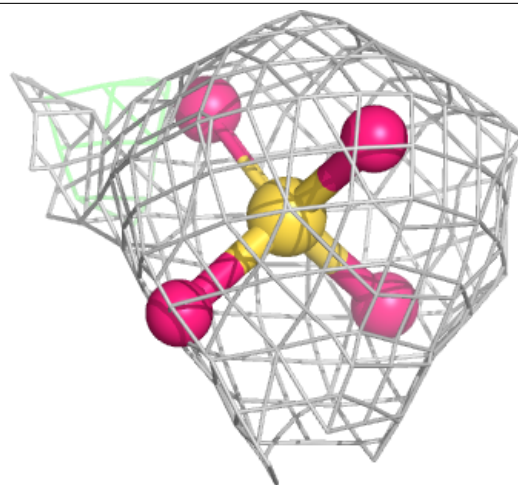
**Electron density around LDA L 306:**

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



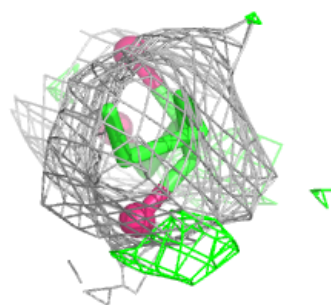
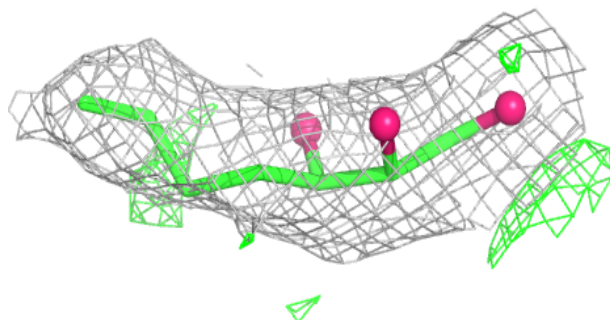
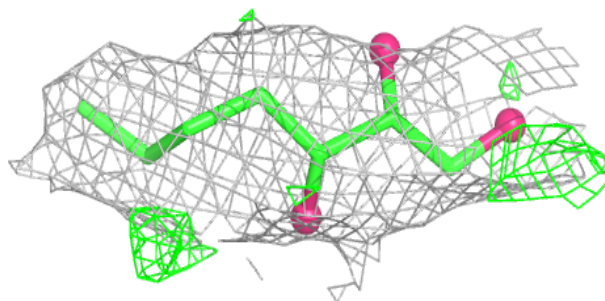
Electron density around SO4 C 408:

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

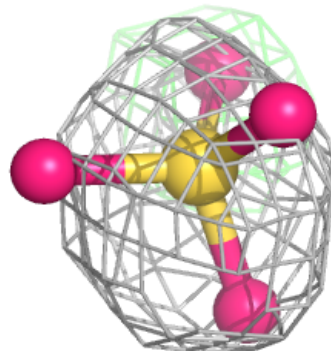
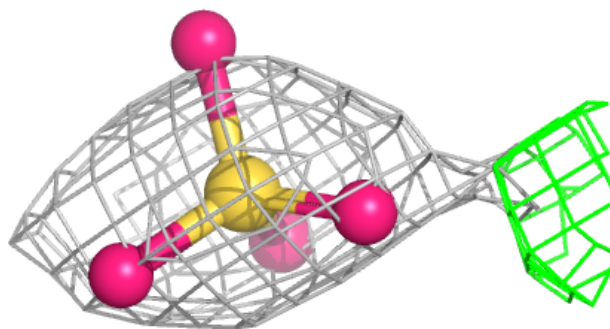
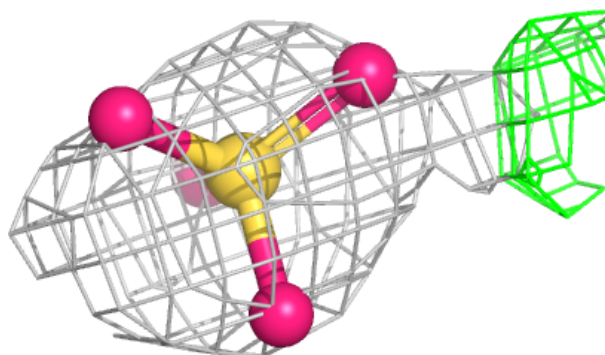


Electron density around HTO H 707:

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

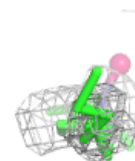
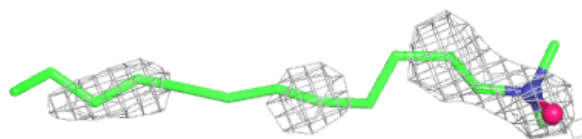
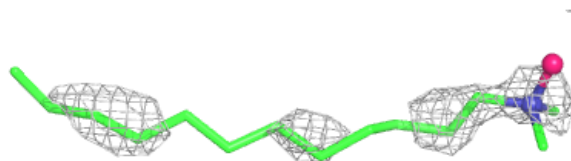
**Electron density around SO4 H 704:**

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



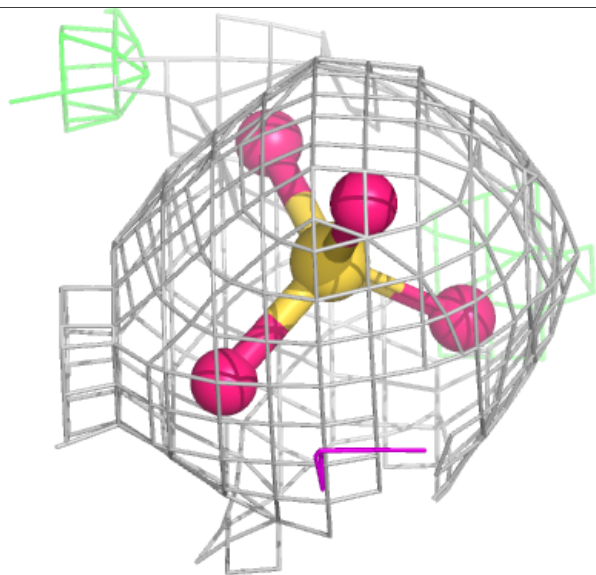
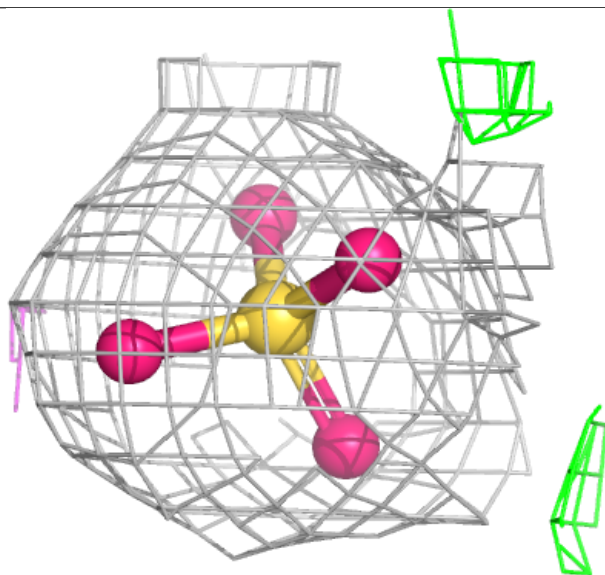
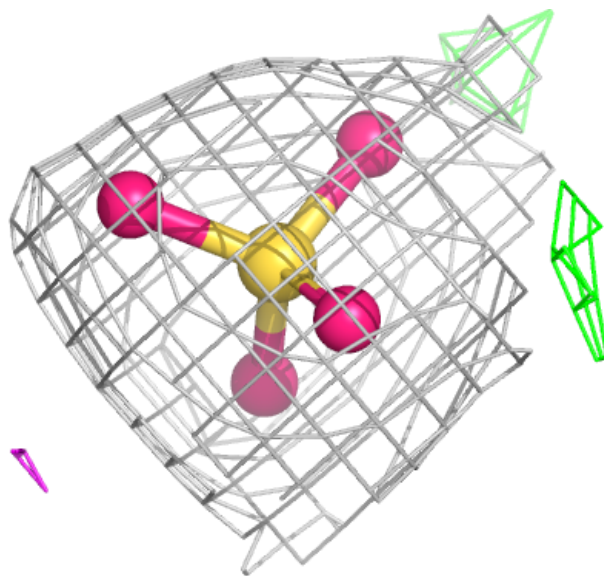
Electron density around LDA L 304:

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



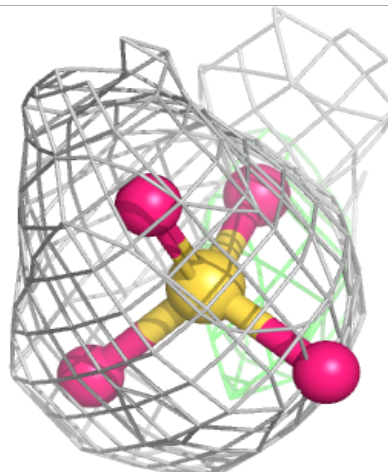
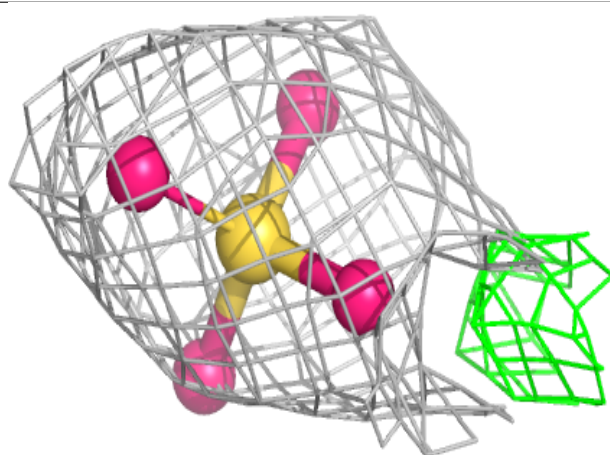
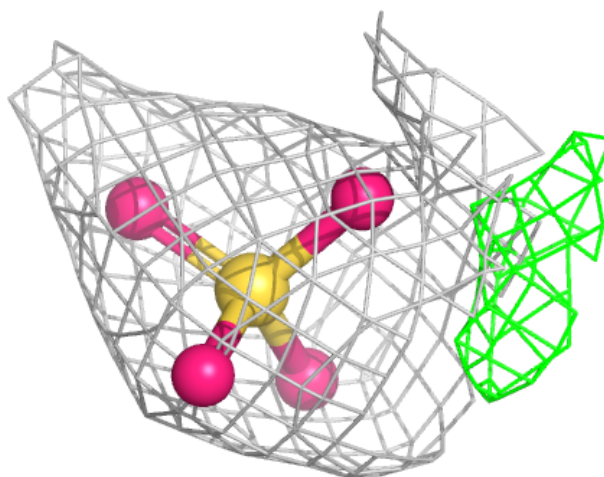
Electron density around SO4 M 410:

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



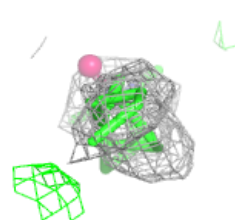
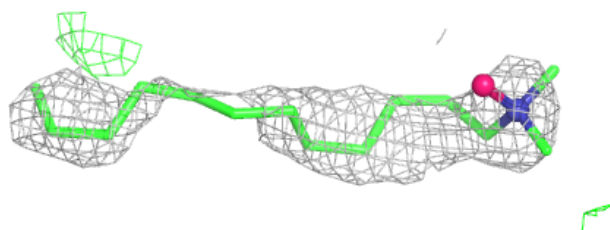
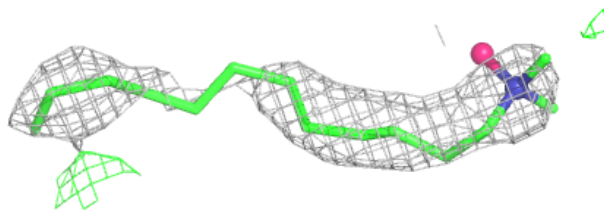
Electron density around SO4 M 413:

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

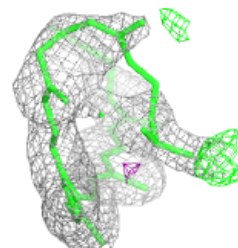
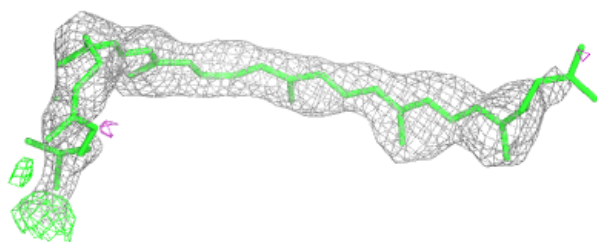
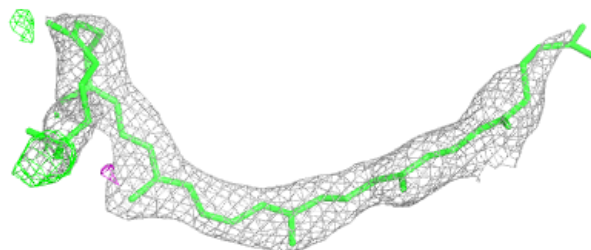


Electron density around LDA M 401:

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

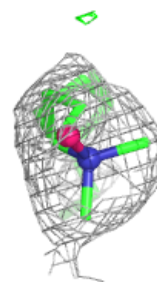
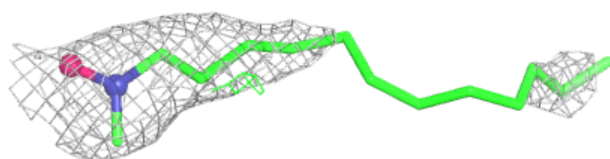
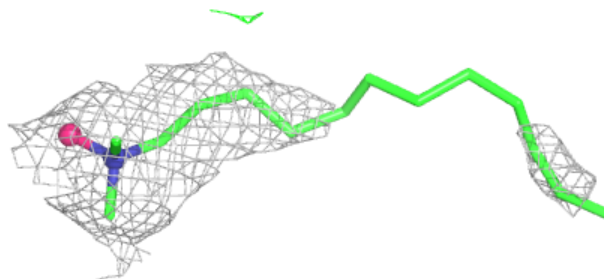
**Electron density around NS5 M 408:**

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

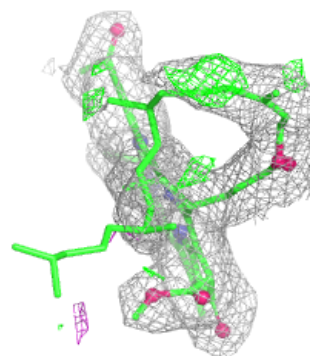
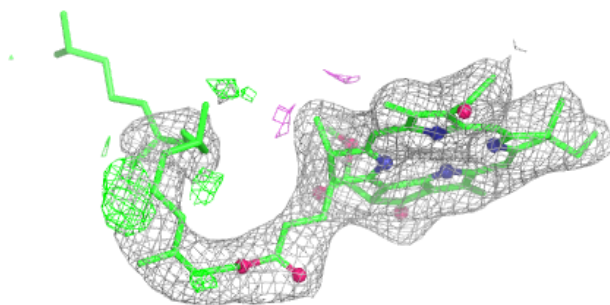
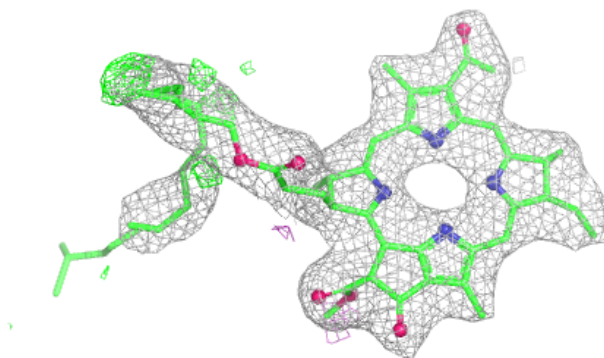


Electron density around LDA H 706:

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

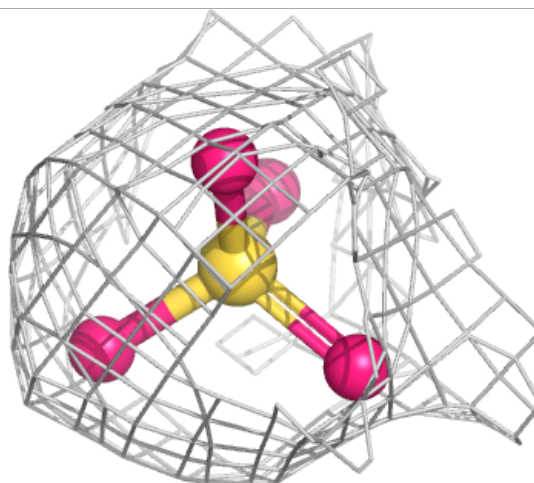
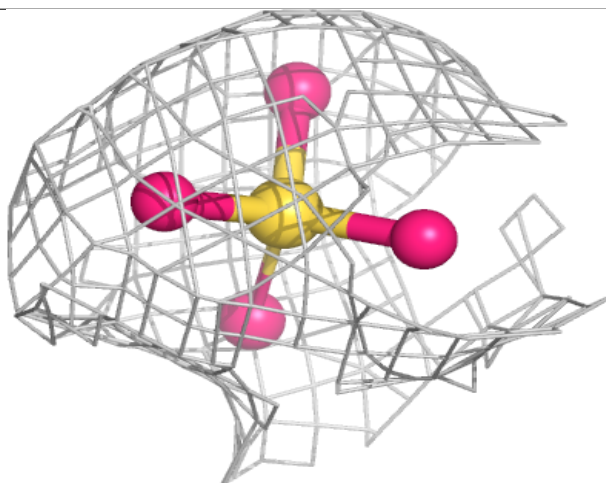
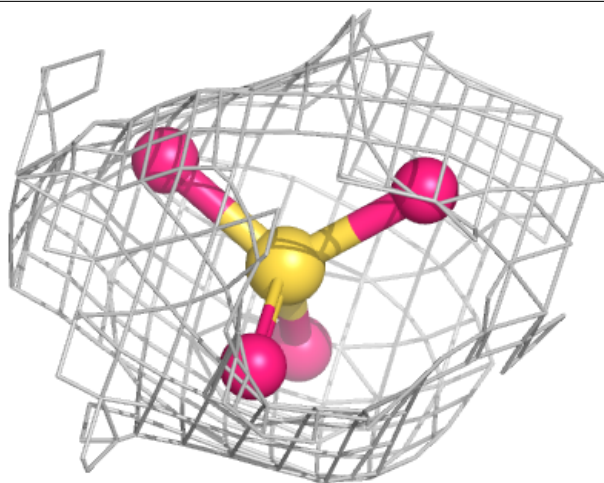
**Electron density around BPB M 407:**

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



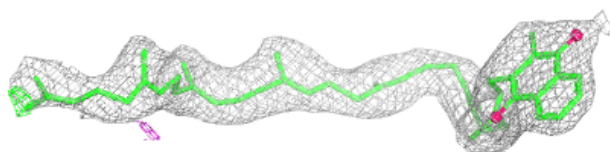
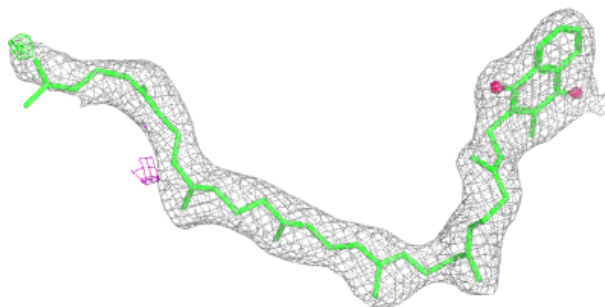
Electron density around SO4 H 702:

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

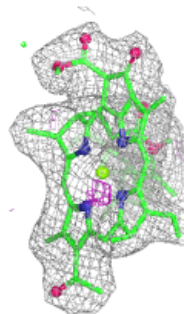
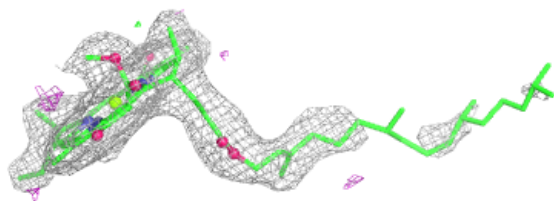
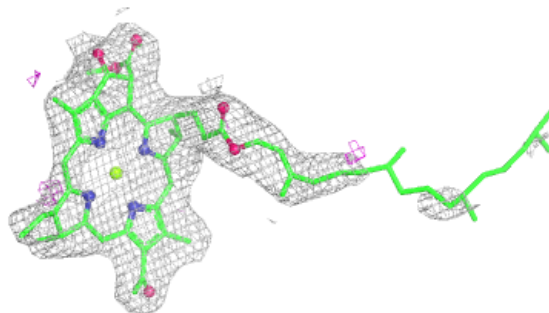


Electron density around MQ7 M 404:

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

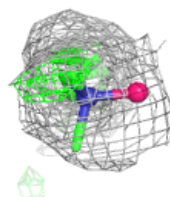
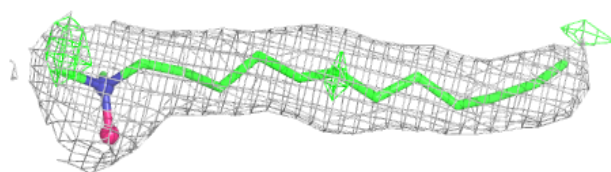
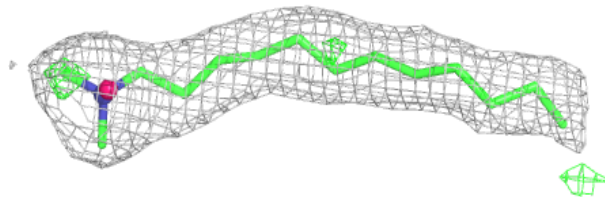
**Electron density around BCB M 405:**

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

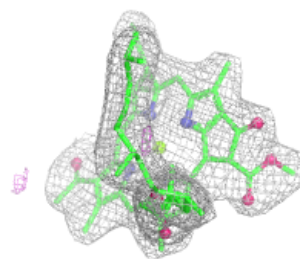
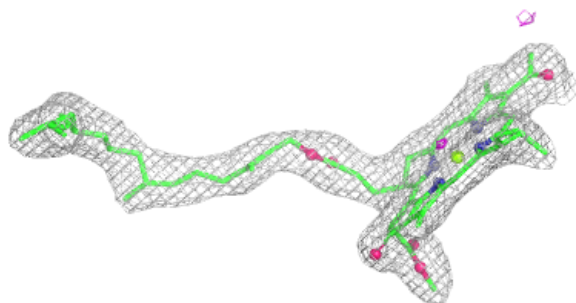
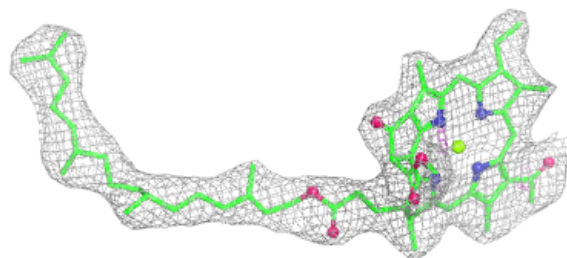


Electron density around LDA H 701:

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

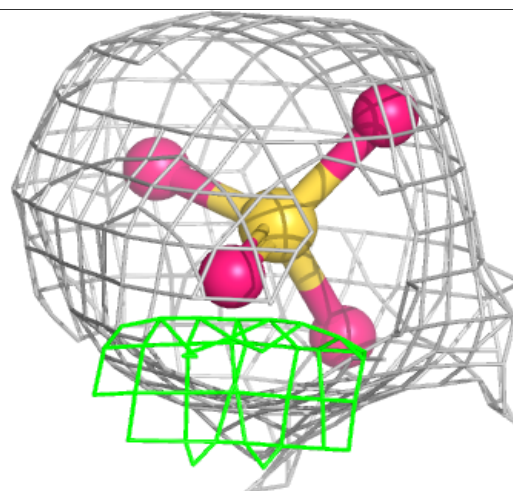
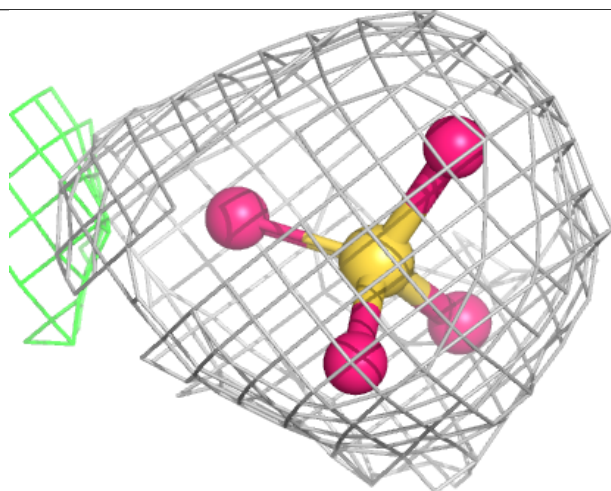
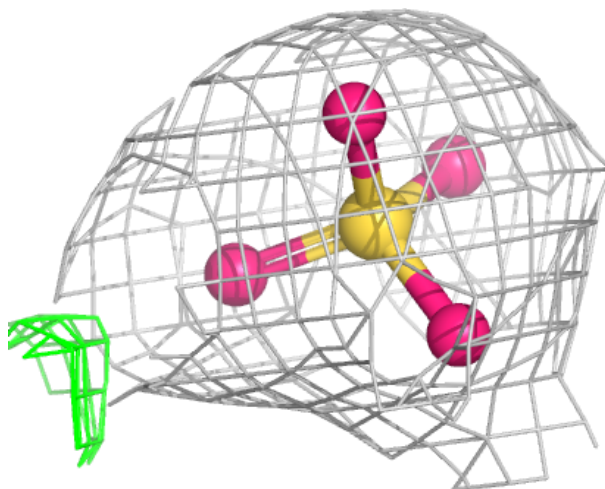
**Electron density around BCB M 406:**

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



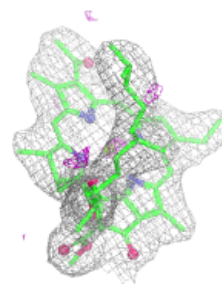
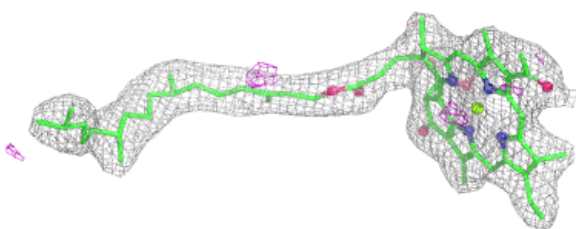
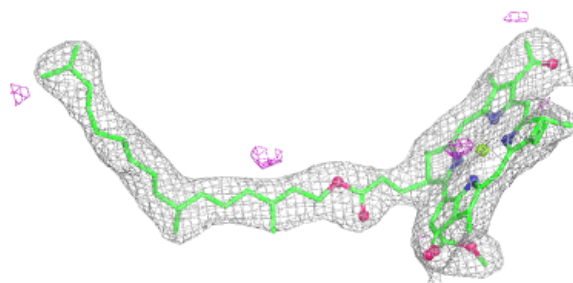
Electron density around SO4 M 411:

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

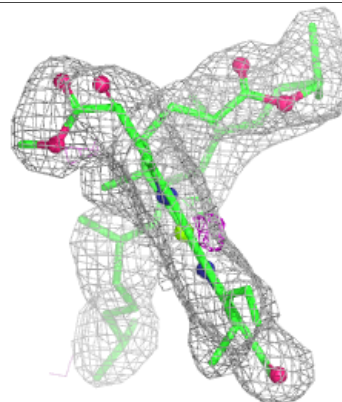
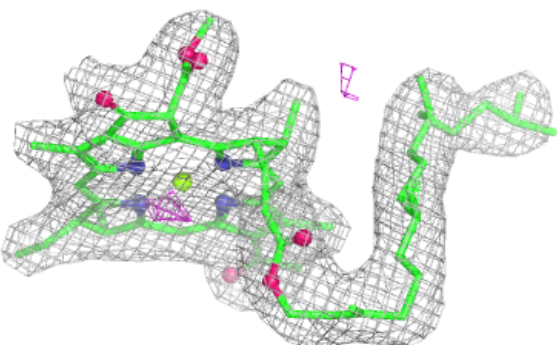
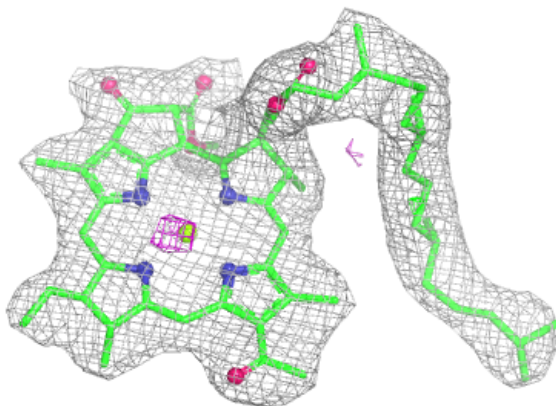


Electron density around BCB L 301:

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

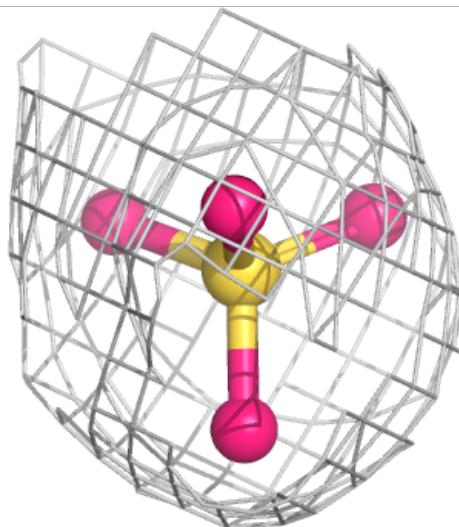
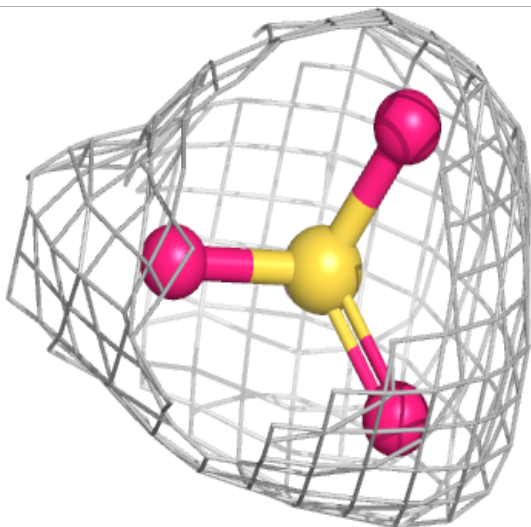
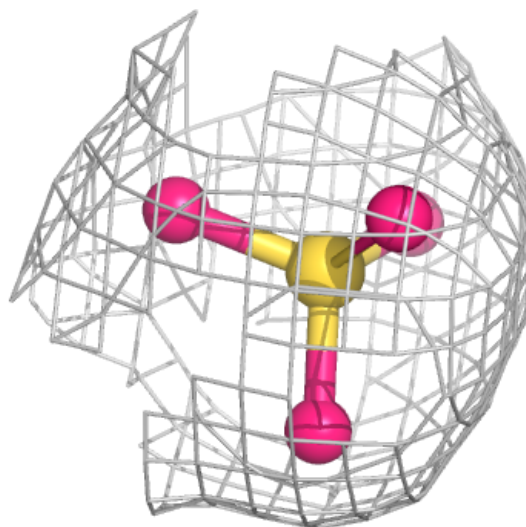
**Electron density around BCB L 302:**

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



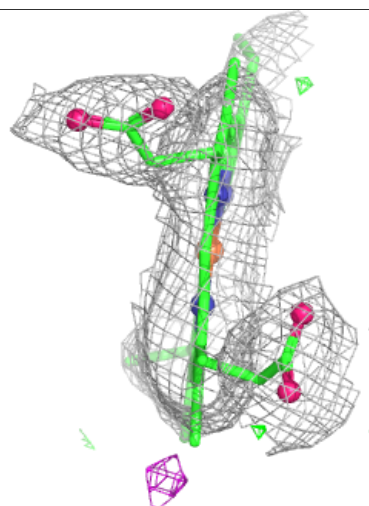
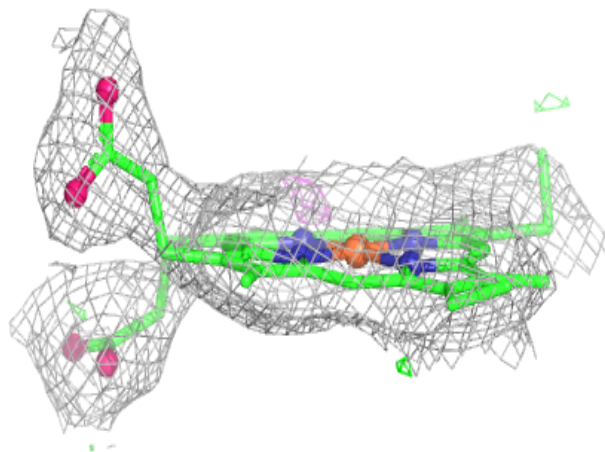
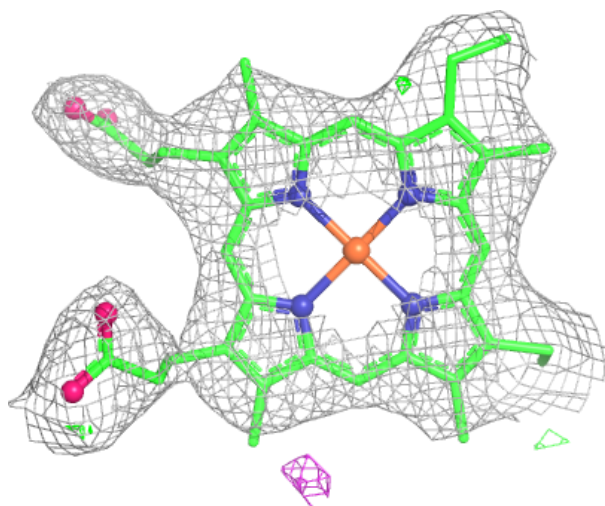
Electron density around SO4 M 409:

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



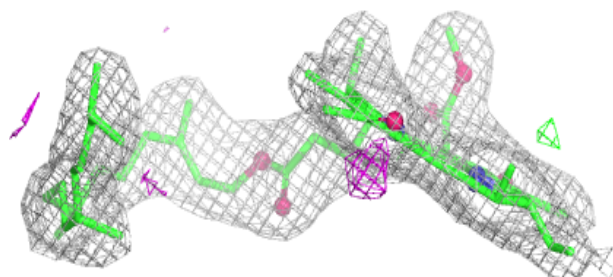
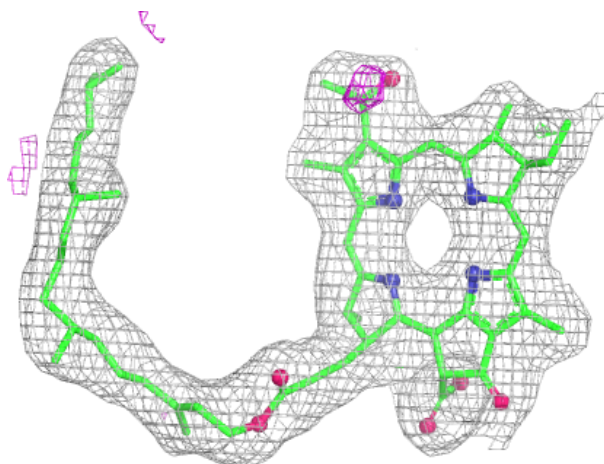
Electron density around HEC C 401:

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



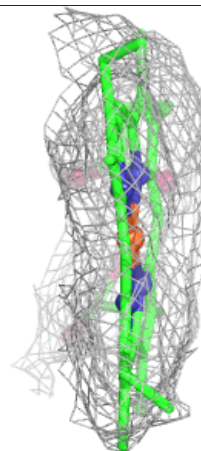
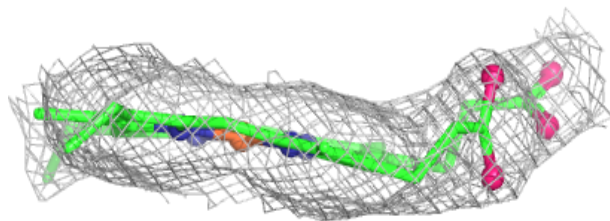
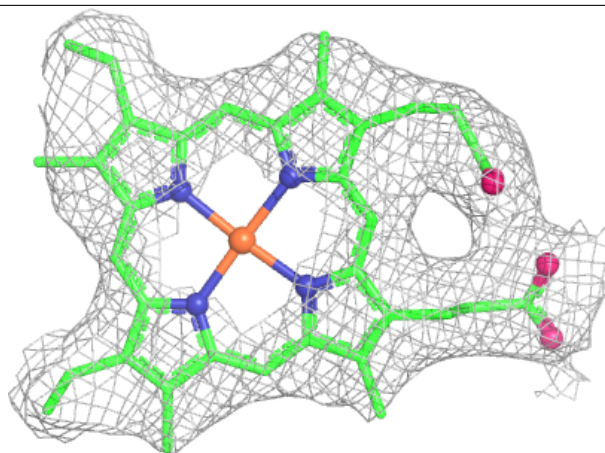
Electron density around BPB L 303:

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



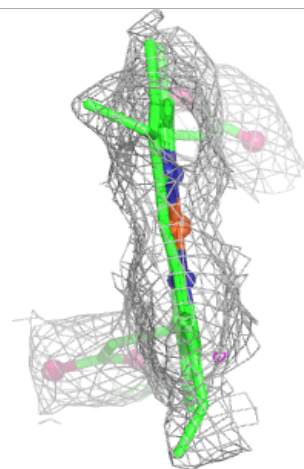
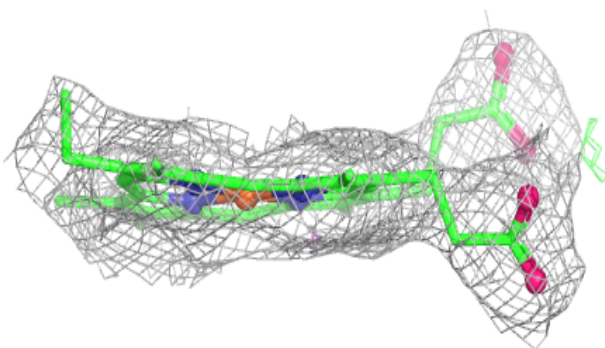
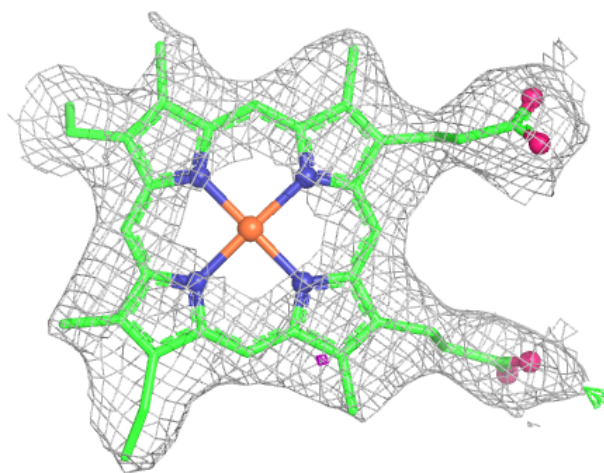
Electron density around HEC C 402:

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



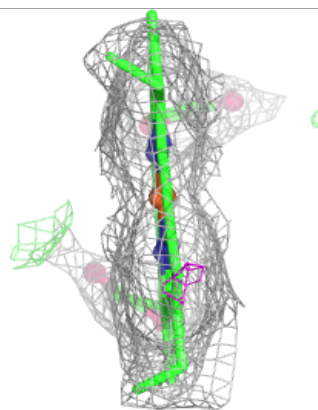
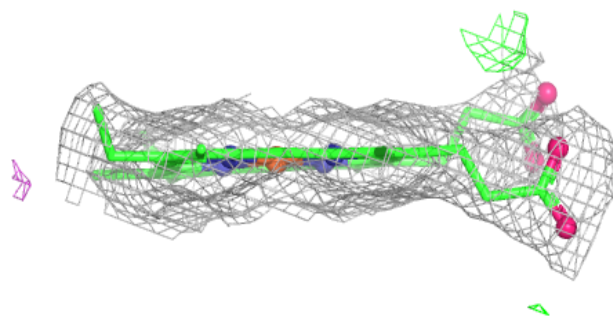
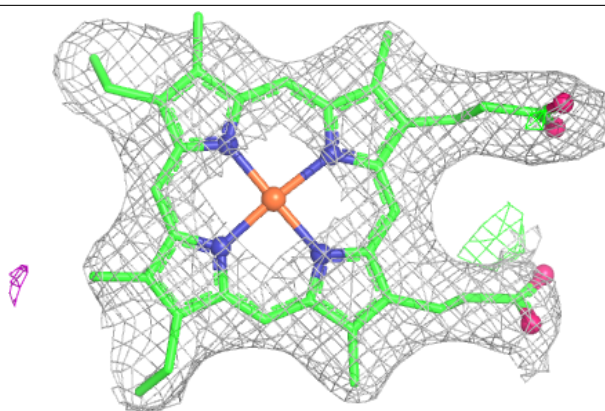
Electron density around HEC C 403:

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



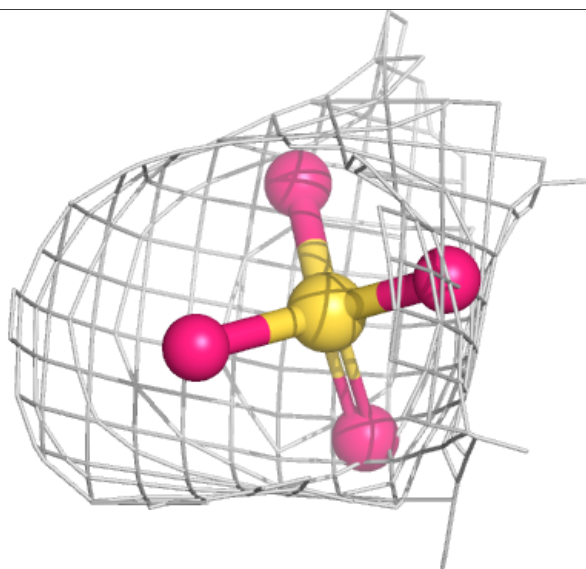
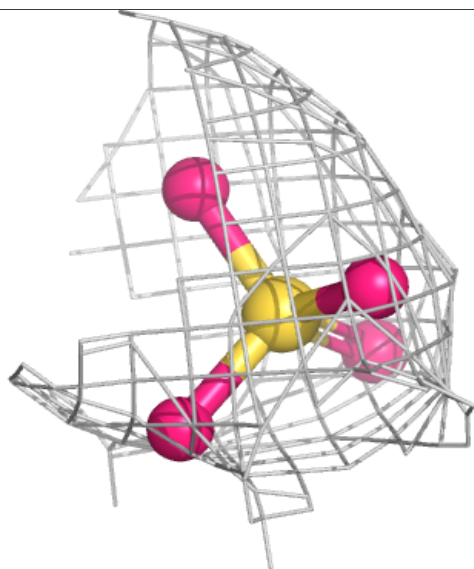
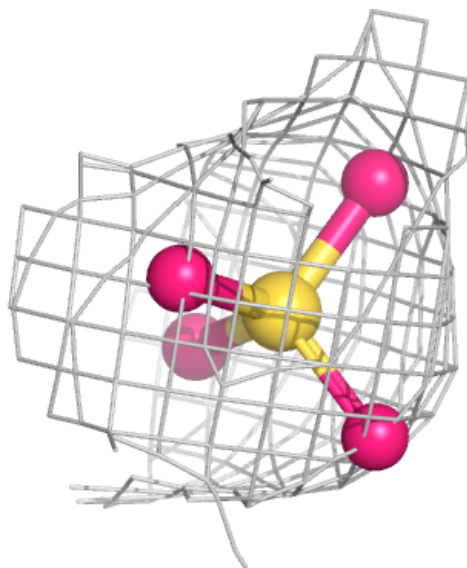
Electron density around HEC C 404:

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



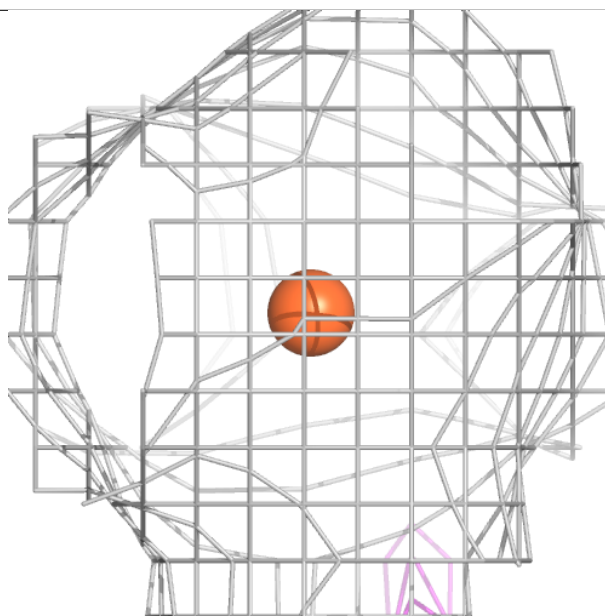
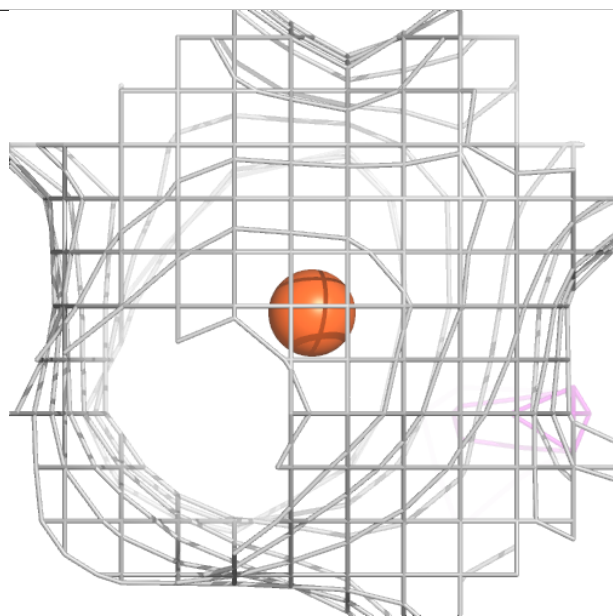
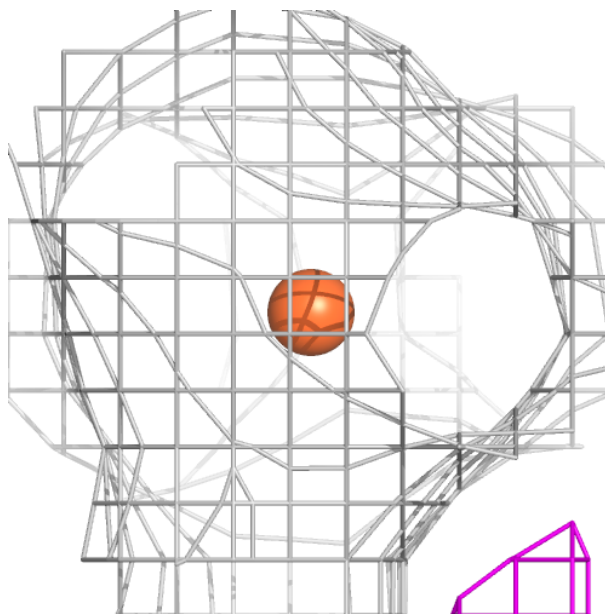
Electron density around SO4 H 705:

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



Electron density around FE2 M 403:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.