



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 15, 2026 – 12:29 PM JST

PDB ID : 9WT8 / pdb_00009wt8
Title : Crystal structure of a multiheme cytochrome c selenoprotein (MccSep)
Authors : Mihara, H.; Yoshizawa, T.; Izu, Y.; Inoue, M.; Aono, R.; Zhang, W.;
Shibamoto, N.; Tobe, R.; Kurihara, T.; Matsumura, H.
Deposited on : 2025-09-16
Resolution : 1.75 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	:	1.8.5 (274361), CSD as541be (2020)
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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

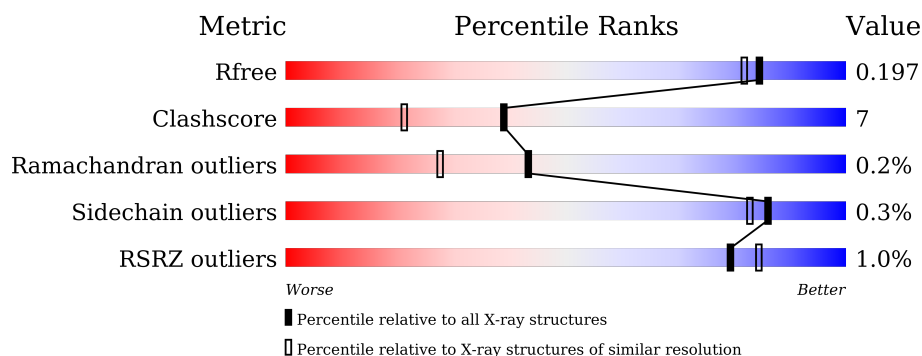
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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

Mol	Chain	Length	Quality of chain
1	A	450	0.1% 85% 8% 6%
1	B	450	0.1% 81% 13% 6%
1	C	450	2% 83% 11% 6%
1	D	450	0% 84% 10% 6%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	B	541	-	-	X	-
4	EDO	A	537	-	-	X	-
4	EDO	B	533	-	-	X	-
4	EDO	B	534	-	-	X	-
4	EDO	C	531	-	-	X	-
4	EDO	D	529	-	-	X	-
6	PGE	D	530	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 16025 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Cytochrome c, Multiheme cytochrome c selenoprotein (MccSep).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	422	Total	C	N	O	S	Se	0	19	0
			3382	2122	584	644	30	2			
1	B	422	Total	C	N	O	S	Se	0	18	0
			3376	2122	581	641	30	2			
1	C	422	Total	C	N	O	S	Se	0	15	0
			3370	2113	582	643	30	2			
1	D	422	Total	C	N	O	S	Se	0	13	0
			3346	2098	577	639	30	2			

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	325	SEC	-	linker	UNP Q748R4
A	326	PRO	-	linker	UNP Q748R4
A	327	THR	-	linker	UNP Q748R4
A	328	PRO	-	linker	UNP Q748R4
A	329	ASN	-	linker	UNP Q748R4
A	330	ARG	-	linker	UNP Q748R4
A	331	LEU	-	linker	UNP Q748R4
A	332	VAL	-	linker	UNP Q748R4
A	333	LEU	-	linker	UNP Q748R4
A	334	SER	-	linker	UNP Q748R4
A	335	VAL	-	linker	UNP Q748R4
A	336	ILE	-	linker	UNP Q748R4
A	337	ALA	-	linker	UNP Q748R4
A	338	LYS	-	linker	UNP Q748R4
A	339	THR	-	linker	UNP Q748R4
A	340	LYS	-	linker	UNP Q748R4
A	341	ASP	-	linker	UNP Q748R4
A	342	GLY	-	linker	UNP Q748R4
A	343	GLU	-	linker	UNP Q748R4
A	344	GLU	-	linker	UNP Q748R4
A	345	VAL	-	linker	UNP Q748R4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	346	PHE	-	linker	UNP Q748R4
A	347	ASN	-	linker	UNP Q748R4
A	348	GLN	-	linker	UNP Q748R4
A	349	GLU	-	linker	UNP Q748R4
A	350	LYS	-	linker	UNP Q748R4
A	351	ILE	-	linker	UNP Q748R4
A	352	TYR	-	linker	UNP Q748R4
B	325	SEC	-	linker	UNP Q748R4
B	326	PRO	-	linker	UNP Q748R4
B	327	THR	-	linker	UNP Q748R4
B	328	PRO	-	linker	UNP Q748R4
B	329	ASN	-	linker	UNP Q748R4
B	330	ARG	-	linker	UNP Q748R4
B	331	LEU	-	linker	UNP Q748R4
B	332	VAL	-	linker	UNP Q748R4
B	333	LEU	-	linker	UNP Q748R4
B	334	SER	-	linker	UNP Q748R4
B	335	VAL	-	linker	UNP Q748R4
B	336	ILE	-	linker	UNP Q748R4
B	337	ALA	-	linker	UNP Q748R4
B	338	LYS	-	linker	UNP Q748R4
B	339	THR	-	linker	UNP Q748R4
B	340	LYS	-	linker	UNP Q748R4
B	341	ASP	-	linker	UNP Q748R4
B	342	GLY	-	linker	UNP Q748R4
B	343	GLU	-	linker	UNP Q748R4
B	344	GLU	-	linker	UNP Q748R4
B	345	VAL	-	linker	UNP Q748R4
B	346	PHE	-	linker	UNP Q748R4
B	347	ASN	-	linker	UNP Q748R4
B	348	GLN	-	linker	UNP Q748R4
B	349	GLU	-	linker	UNP Q748R4
B	350	LYS	-	linker	UNP Q748R4
B	351	ILE	-	linker	UNP Q748R4
B	352	TYR	-	linker	UNP Q748R4
C	325	SEC	-	linker	UNP Q748R4
C	326	PRO	-	linker	UNP Q748R4
C	327	THR	-	linker	UNP Q748R4
C	328	PRO	-	linker	UNP Q748R4
C	329	ASN	-	linker	UNP Q748R4
C	330	ARG	-	linker	UNP Q748R4
C	331	LEU	-	linker	UNP Q748R4

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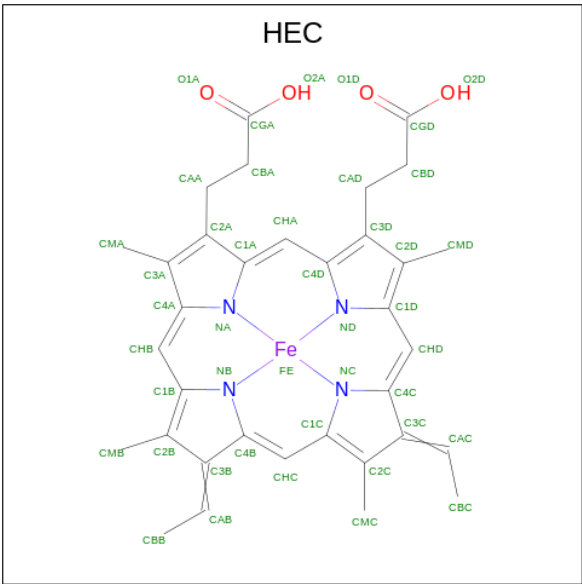
Chain	Residue	Modelled	Actual	Comment	Reference
C	332	VAL	-	linker	UNP Q748R4
C	333	LEU	-	linker	UNP Q748R4
C	334	SER	-	linker	UNP Q748R4
C	335	VAL	-	linker	UNP Q748R4
C	336	ILE	-	linker	UNP Q748R4
C	337	ALA	-	linker	UNP Q748R4
C	338	LYS	-	linker	UNP Q748R4
C	339	THR	-	linker	UNP Q748R4
C	340	LYS	-	linker	UNP Q748R4
C	341	ASP	-	linker	UNP Q748R4
C	342	GLY	-	linker	UNP Q748R4
C	343	GLU	-	linker	UNP Q748R4
C	344	GLU	-	linker	UNP Q748R4
C	345	VAL	-	linker	UNP Q748R4
C	346	PHE	-	linker	UNP Q748R4
C	347	ASN	-	linker	UNP Q748R4
C	348	GLN	-	linker	UNP Q748R4
C	349	GLU	-	linker	UNP Q748R4
C	350	LYS	-	linker	UNP Q748R4
C	351	ILE	-	linker	UNP Q748R4
C	352	TYR	-	linker	UNP Q748R4
D	325	SEC	-	linker	UNP Q748R4
D	326	PRO	-	linker	UNP Q748R4
D	327	THR	-	linker	UNP Q748R4
D	328	PRO	-	linker	UNP Q748R4
D	329	ASN	-	linker	UNP Q748R4
D	330	ARG	-	linker	UNP Q748R4
D	331	LEU	-	linker	UNP Q748R4
D	332	VAL	-	linker	UNP Q748R4
D	333	LEU	-	linker	UNP Q748R4
D	334	SER	-	linker	UNP Q748R4
D	335	VAL	-	linker	UNP Q748R4
D	336	ILE	-	linker	UNP Q748R4
D	337	ALA	-	linker	UNP Q748R4
D	338	LYS	-	linker	UNP Q748R4
D	339	THR	-	linker	UNP Q748R4
D	340	LYS	-	linker	UNP Q748R4
D	341	ASP	-	linker	UNP Q748R4
D	342	GLY	-	linker	UNP Q748R4
D	343	GLU	-	linker	UNP Q748R4
D	344	GLU	-	linker	UNP Q748R4
D	345	VAL	-	linker	UNP Q748R4

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Chain	Residue	Modelled	Actual	Comment	Reference
D	346	PHE	-	linker	UNP Q748R4
D	347	ASN	-	linker	UNP Q748R4
D	348	GLN	-	linker	UNP Q748R4
D	349	GLU	-	linker	UNP Q748R4
D	350	LYS	-	linker	UNP Q748R4
D	351	ILE	-	linker	UNP Q748R4
D	352	TYR	-	linker	UNP Q748R4

- Molecule 2 is HEME C (CCD ID: HEC) (formula: C₃₄H₃₄FeN₄O₄) (labeled as "Ligand of Interest" by depositor).



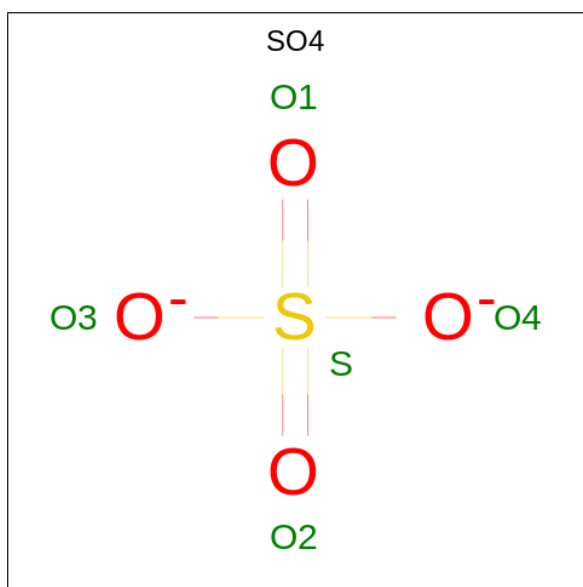
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0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

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

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



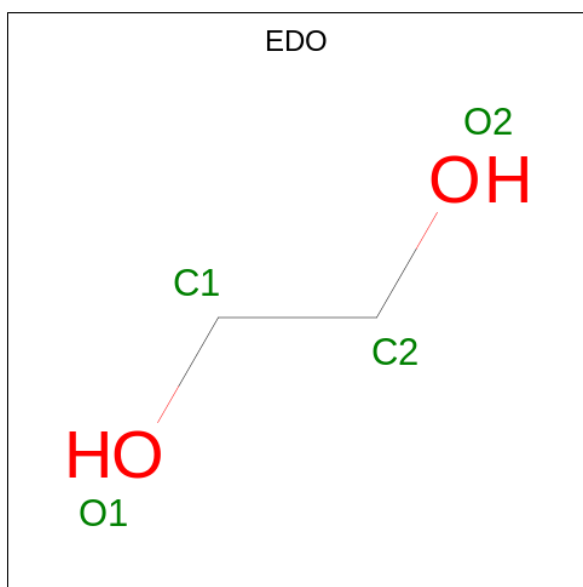
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total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

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

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		

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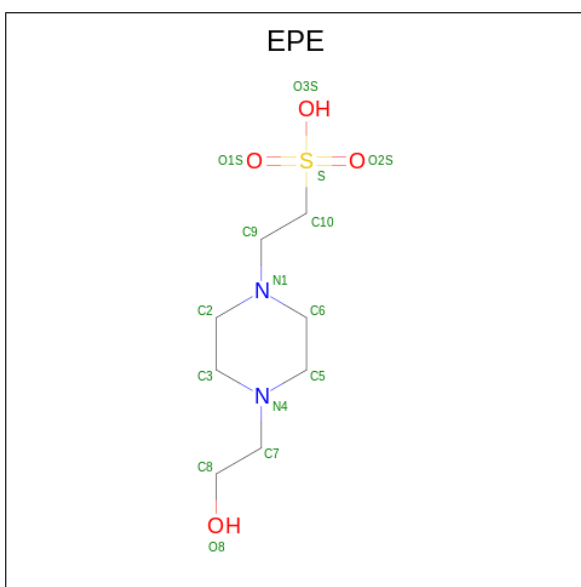
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0

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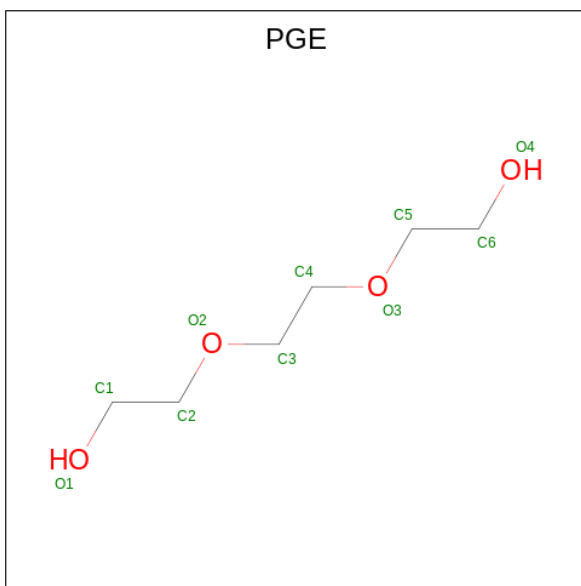
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 6 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			10	6	4		
6	D	1	Total	C	O	0	0
			10	6	4		

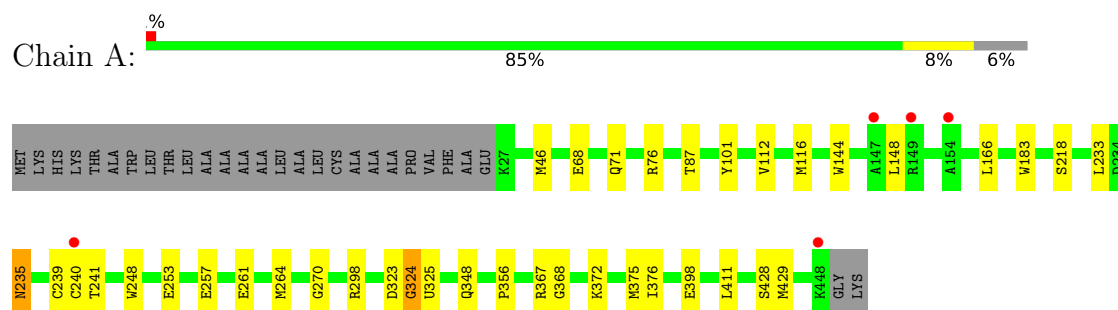
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	306	Total 306	O 306	0	0
7	B	291	Total 291	O 291	0	0
7	C	241	Total 241	O 241	0	0
7	D	303	Total 303	O 303	0	0

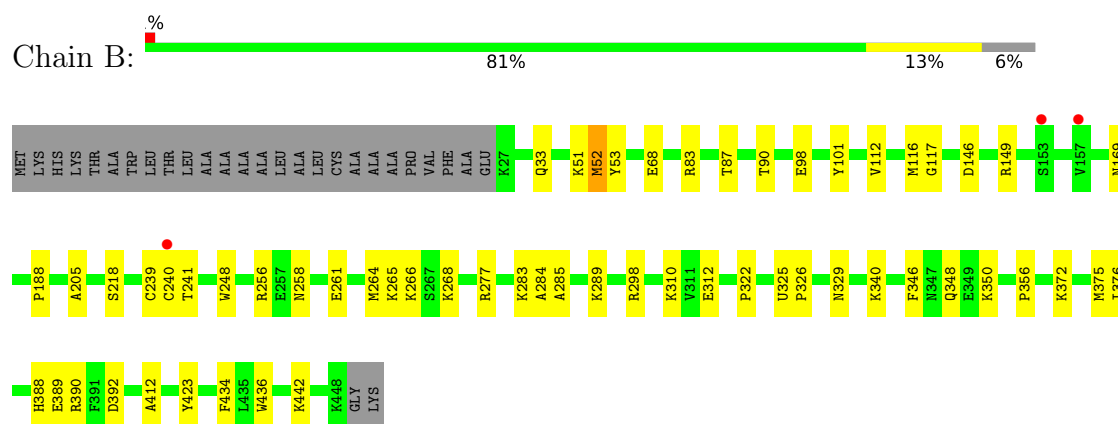
3 Residue-property plots [i](#)

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.

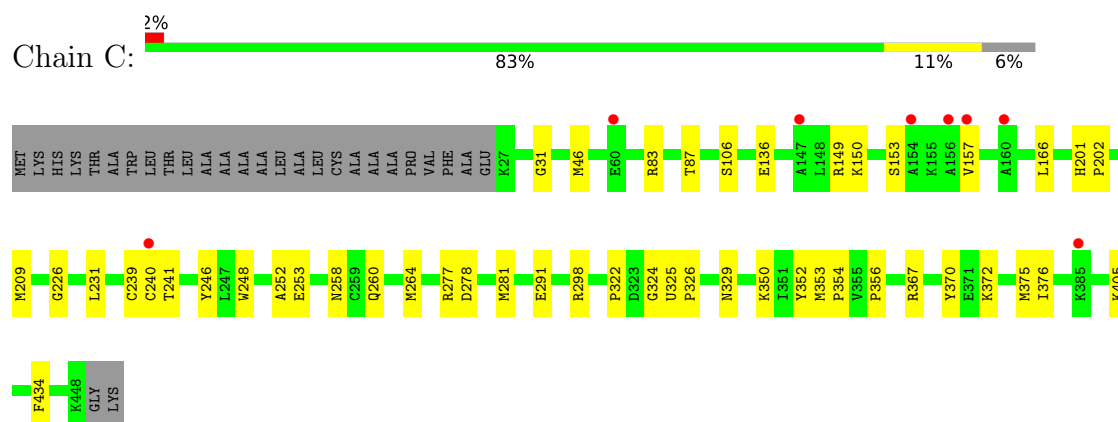
- Molecule 1: Cytochrome c, Multiheme cytochrome c selenoprotein (MccSep)



- Molecule 1: Cytochrome c, Multiheme cytochrome c selenoprotein (MccSep)



- Molecule 1: Cytochrome c, Multiheme cytochrome c selenoprotein (MccSep)



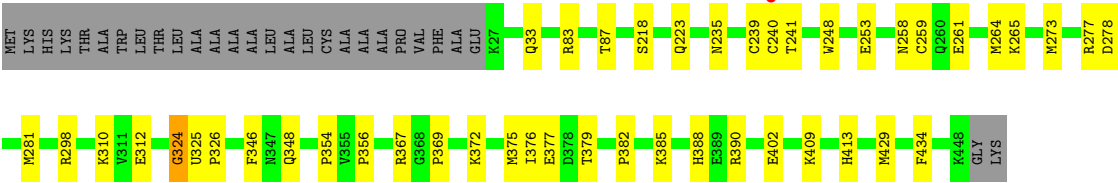
● Molecule 1: Cytochrome c,Multiheme cytochrome c selenoprotein (McCep)

Chain D:

84%

10%

6%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	83.03Å 123.54Å 116.52Å 90.00° 92.19° 90.00°	Depositor
Resolution (Å)	48.54 – 1.75 48.54 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.0 (48.54-1.75) 99.3 (48.54-1.75)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 1.75Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.167 , 0.198 0.166 , 0.197	Depositor DCC
R_{free} test set	11708 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	28.5	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 40.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.038 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	16025	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% 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 [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.33	0/3486	0.56	0/4702
1	B	0.33	0/3479	0.56	1/4695 (0.0%)
1	C	0.29	0/3456	0.53	0/4661
1	D	0.34	0/3435	0.55	0/4635
All	All	0.32	0/13856	0.55	1/18693 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	52	MET	CB-CA-C	-5.40	101.78	110.74

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3382	0	3312	37	0
1	B	3376	0	3298	57	0
1	C	3370	0	3283	40	0
1	D	3346	0	3259	43	0
2	A	215	0	150	6	0
2	B	215	0	150	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	215	0	150	4	0
2	D	215	0	150	5	0
3	A	25	0	0	0	0
3	B	40	0	0	3	0
3	C	40	0	0	3	0
3	D	30	0	0	1	0
4	A	112	0	168	19	0
4	B	108	0	162	32	0
4	C	76	0	114	19	0
4	D	84	0	126	12	0
5	B	15	0	17	0	0
6	B	10	0	14	2	0
6	D	10	0	14	7	0
7	A	306	0	0	8	0
7	B	291	0	0	12	0
7	C	241	0	0	1	0
7	D	303	0	0	5	0
All	All	16025	0	14367	200	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 (200) 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:B:239[B]:CYS:SG	1:B:240[B]:CYS:N	2.30	1.03
1:A:239[B]:CYS:SG	1:A:240[B]:CYS:N	2.28	1.03
1:D:239[B]:CYS:SG	1:D:240[B]:CYS:N	2.29	0.98
1:C:239[B]:CYS:SG	1:C:240[B]:CYS:N	2.38	0.95
2:A:502:HEC:HBC1	4:A:531:EDO:H22	1.54	0.88
1:D:310:LYS:HB3	6:D:530:PGE:H5	1.61	0.82
1:B:312:GLU:HG3	4:B:534:EDO:H22	1.61	0.81
1:C:298:ARG:HH12	4:C:502:EDO:H21	1.45	0.80
1:D:312:GLU:HG3	6:D:530:PGE:H6	1.64	0.77
1:A:239[B]:CYS:HG	1:A:240[B]:CYS:H	1.32	0.77
1:B:268:LYS:HA	4:B:531:EDO:H12	1.66	0.76
3:D:514:SO4:O4	7:D:601:HOH:O	2.03	0.76
1:A:46:MET:HB3	1:A:166:LEU:HD11	1.69	0.74
1:D:390:ARG:HB2	6:D:530:PGE:H4	1.69	0.74
1:B:284:ALA:HB1	4:B:537:EDO:H21	1.68	0.74
4:B:522:EDO:H11	1:D:298:ARG:HH12	1.53	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:390:ARG:HB2	6:B:539:PGE:H4	1.69	0.73
2:A:503:HEC:HAA1	4:A:517:EDO:H11	1.71	0.73
2:B:504:HEC:HAD2	4:B:532:EDO:H22	1.71	0.72
1:D:388:HIS:ND1	6:D:530:PGE:H62	2.05	0.72
1:A:323[A]:ASP:HA	4:A:526:EDO:H12	1.72	0.71
7:A:823:HOH:O	1:B:375[B]:MET:SD	2.49	0.70
1:A:367:ARG:HD3	4:C:502:EDO:H12	1.74	0.69
1:A:298:ARG:HH22	4:A:534:EDO:H21	1.58	0.69
2:A:503:HEC:HAD2	4:A:517:EDO:H22	1.77	0.67
1:C:258[B]:ASN:OD1	4:C:520:EDO:H21	1.94	0.67
1:C:149:ARG:HH21	1:C:150:LYS:HE2	1.61	0.66
1:A:253:GLU:HA	4:A:538:EDO:H12	1.79	0.65
1:C:201:HIS:HB2	1:C:209:MET:HB3	1.77	0.65
4:C:520:EDO:H11	7:D:683:HOH:O	1.97	0.65
7:B:814:HOH:O	4:C:531:EDO:H22	1.98	0.64
1:A:398:GLU:HG2	1:A:411:LEU:HD21	1.80	0.64
7:A:628:HOH:O	4:D:501:EDO:H22	1.97	0.63
1:B:68:GLU:HG2	4:B:521:EDO:H22	1.78	0.62
4:B:533:EDO:O2	7:B:601:HOH:O	2.00	0.62
4:D:529:EDO:O2	7:D:602:HOH:O	2.05	0.62
1:B:356:PRO:HG3	1:B:372:LYS:HD3	1.82	0.61
1:C:241:THR:HG21	1:D:248:TRP:CH2	2.35	0.61
1:C:46:MET:HB3	1:C:166:LEU:HD11	1.83	0.61
4:A:538:EDO:H11	7:D:820:HOH:O	2.01	0.60
1:A:240[B]:CYS:HA	1:A:324[B]:GLY:HA3	1.83	0.60
1:B:218:SER:H	4:B:533:EDO:H21	1.65	0.60
1:A:235:ASN:O	4:A:537:EDO:H11	2.02	0.60
1:D:253:GLU:HA	4:D:501:EDO:H21	1.83	0.60
1:B:265:LYS:HE2	2:B:504:HEC:O2D	2.02	0.59
1:B:310:LYS:HB3	4:B:534:EDO:H21	1.85	0.59
1:C:258[A]:ASN:ND2	4:C:523:EDO:O1	2.24	0.59
1:B:51:LYS:NZ	7:B:606:HOH:O	2.36	0.58
1:C:87:THR:HG22	2:C:504:HEC:HMB2	1.85	0.58
1:C:252:ALA:O	4:C:531:EDO:H11	2.02	0.58
1:B:375[B]:MET:HG3	1:B:376:ILE:N	2.19	0.58
1:C:291:GLU:HG2	4:C:525:EDO:H22	1.86	0.58
1:C:260:GLN:O	1:C:264:MET:HB2	2.04	0.57
1:D:356:PRO:HG3	1:D:372:LYS:HE3	1.85	0.57
1:B:356:PRO:CG	1:B:372:LYS:HD3	2.34	0.57
1:A:68:GLU:HG2	4:A:522:EDO:H11	1.86	0.57
1:A:248:TRP:CH2	1:B:241:THR:HG21	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:531:EDO:H21	1:D:379:THR:HG22	1.88	0.56
1:A:348[A]:GLN:HE22	4:A:514:EDO:H11	1.71	0.55
2:D:506:HEC:HBB1	4:D:518:EDO:H22	1.88	0.55
1:B:265:LYS:HA	4:B:531:EDO:H11	1.88	0.55
1:D:218:SER:H	4:D:529:EDO:H21	1.72	0.55
1:D:402:GLU:OE2	1:D:409:LYS:NZ	2.39	0.55
1:A:240[A]:CYS:HB3	1:A:325[A]:SEC:SE	2.57	0.54
1:C:370:TYR:HE1	4:C:527:EDO:H21	1.72	0.54
1:D:33:GLN:HG2	4:D:517:EDO:H12	1.89	0.54
1:B:83:ARG:HD3	1:B:326[A]:PRO:HG3	1.90	0.53
1:C:46:MET:HG3	1:C:136:GLU:CD	2.34	0.53
4:A:517:EDO:H21	7:A:717:HOH:O	2.09	0.53
1:A:233:LEU:HB3	4:A:537:EDO:C1	2.38	0.53
1:C:356:PRO:HB2	1:C:372:LYS:HG2	1.90	0.52
4:B:524:EDO:H12	1:D:367:ARG:HD3	1.91	0.52
1:C:253[A]:GLU:OE2	4:C:531:EDO:O2	2.28	0.52
1:A:241:THR:HG21	1:B:248:TRP:CH2	2.45	0.52
4:A:537:EDO:H22	7:A:611:HOH:O	2.10	0.51
1:D:240[A]:CYS:HB3	1:D:325[A]:SEC:SE	2.60	0.51
1:C:106:SER:OG	3:C:509:SO4:O1	2.28	0.51
1:A:71:GLN:HG2	7:A:845:HOH:O	2.10	0.51
1:A:240[B]:CYS:SG	1:A:325[B]:SEC:N	2.84	0.51
1:D:218:SER:H	4:D:529:EDO:C2	2.25	0.50
1:B:340:LYS:HG2	7:B:737:HOH:O	2.11	0.50
1:D:240[B]:CYS:SG	1:D:325[B]:SEC:N	2.85	0.50
2:D:509:HEC:HHA	2:D:509:HEC:CGD	2.42	0.50
1:C:277:ARG:HG2	1:C:434:PHE:CZ	2.47	0.49
4:A:516:EDO:H22	7:A:794:HOH:O	2.13	0.49
3:C:508:SO4:O2	4:C:527:EDO:O1	2.19	0.49
1:A:240[B]:CYS:HB3	1:A:323[B]:ASP:OD2	2.12	0.49
1:B:117:GLY:HA3	4:B:530:EDO:H11	1.93	0.49
1:B:289:LYS:NZ	4:B:534:EDO:O1	2.37	0.49
3:B:511:SO4:O4	7:B:602:HOH:O	2.19	0.49
1:C:248:TRP:CH2	1:D:241:THR:HG21	2.48	0.49
1:B:218:SER:H	4:B:533:EDO:C2	2.26	0.49
1:B:98:GLU:HG3	7:B:794:HOH:O	2.12	0.49
1:A:218:SER:H	4:A:524:EDO:C2	2.26	0.49
1:C:202:PRO:O	2:C:503:HEC:HBC2	2.13	0.49
1:B:52:MET:HB3	1:B:53:TYR:CD2	2.47	0.49
1:C:246:TYR:OH	4:C:520:EDO:H12	2.13	0.49
2:D:506:HEC:HBA1	4:D:522:EDO:H11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:LYS:HE2	1:B:389:GLU:OE1	2.13	0.48
1:B:423:TYR:HD2	1:B:436[B]:TRP:HZ3	1.60	0.48
1:C:322:PRO:HB2	1:C:329[A]:ASN:OD1	2.13	0.48
1:D:429:MET:HA	1:D:429:MET:HE3	1.95	0.48
1:B:346:PHE:CZ	1:B:348:GLN:HG3	2.47	0.48
1:B:325[B]:SEC:SE	1:B:326[B]:PRO:HA	2.63	0.48
4:B:524:EDO:O2	3:B:541:SO4:O4	2.32	0.48
1:D:87:THR:HG22	2:D:506:HEC:HMB2	1.94	0.48
1:D:388:HIS:HB3	6:D:530:PGE:O3	2.13	0.48
1:B:90:THR:HA	4:B:528:EDO:H12	1.96	0.48
1:B:240[B]:CYS:SG	1:B:325[B]:SEC:N	2.87	0.47
1:C:278:ASP:HB3	1:C:281:MET:HB2	1.96	0.47
1:C:367:ARG:NH1	3:C:513:SO4:O4	2.46	0.47
2:D:506:HEC:HMC3	2:D:506:HEC:HBC3	1.94	0.47
1:B:283:LYS:HE2	7:B:684:HOH:O	2.13	0.47
1:C:240[A]:CYS:HB3	1:C:325[A]:SEC:SE	2.64	0.47
4:B:530:EDO:H12	7:B:731:HOH:O	2.14	0.47
1:A:76[B]:ARG:NH1	1:A:76[B]:ARG:HB3	2.29	0.47
1:D:382:PRO:HG2	1:D:385:LYS:HB3	1.96	0.47
1:A:257[B]:GLU:OE1	1:A:261:GLU:HG2	2.13	0.47
4:B:532:EDO:H21	7:B:777:HOH:O	2.13	0.47
1:A:233:LEU:HB3	4:A:537:EDO:H12	1.95	0.47
1:B:205:ALA:H	4:B:538:EDO:H22	1.80	0.47
1:D:83:ARG:HD3	1:D:326[A]:PRO:HG3	1.97	0.47
4:C:531:EDO:H12	1:D:377:GLU:HB2	1.96	0.47
1:B:258[B]:ASN:OD1	4:B:533:EDO:H11	2.15	0.47
1:D:240[B]:CYS:HA	1:D:324[B]:GLY:HA3	1.97	0.47
1:D:375[B]:MET:HG3	1:D:376:ILE:N	2.29	0.47
1:B:87:THR:HG22	2:B:503:HEC:HMB2	1.96	0.46
1:B:392:ASP:H	4:B:523:EDO:H21	1.80	0.46
1:B:266:LYS:HD2	7:B:672:HOH:O	2.16	0.46
1:C:31:GLY:HA3	4:C:518:EDO:H11	1.96	0.46
1:B:372:LYS:NZ	7:B:603:HOH:O	2.26	0.46
1:A:368:GLY:C	1:A:372:LYS:HD3	2.40	0.46
1:A:183:TRP:CZ3	4:B:530:EDO:H21	2.51	0.46
1:D:264:MET:HE3	1:D:273:MET:HE2	1.97	0.46
2:C:507:HEC:CGD	2:C:507:HEC:HHA	2.46	0.46
1:B:112:VAL:O	1:B:116:MET:HG2	2.16	0.46
1:D:413:HIS:ND1	4:D:525:EDO:H11	2.31	0.46
1:C:375[B]:MET:HE3	1:C:375[B]:MET:HB2	1.86	0.45
1:C:350[A]:LYS:HE2	1:C:350[A]:LYS:HB3	1.73	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:265:LYS:NZ	7:D:610:HOH:O	2.45	0.45
1:B:277:ARG:HG2	1:B:434:PHE:CZ	2.51	0.45
1:B:388:HIS:HB3	6:B:539:PGE:H62	1.99	0.45
1:C:153:SER:O	1:C:157:VAL:HG23	2.17	0.45
1:B:423:TYR:HD2	1:B:436[B]:TRP:CZ3	2.35	0.44
1:A:112:VAL:O	1:A:116:MET:HG2	2.17	0.44
2:A:505:HEC:CGD	2:A:505:HEC:HHA	2.47	0.44
1:B:261[B]:GLU:HG2	4:B:525:EDO:H11	1.99	0.44
1:C:405:LYS:HG3	7:C:737:HOH:O	2.17	0.44
1:A:264:MET:HB3	1:A:270:GLY:O	2.17	0.44
1:D:258[A]:ASN:OD1	1:D:261[A]:GLU:HG3	2.15	0.44
2:C:505:HEC:O1D	4:C:523:EDO:H12	2.18	0.44
1:D:310:LYS:CB	6:D:530:PGE:H5	2.42	0.44
1:A:348[B]:GLN:HE22	4:A:514:EDO:H21	1.83	0.43
1:B:33:GLN:HG3	4:B:518:EDO:C1	2.48	0.43
1:B:169:ASN:HB2	7:B:826:HOH:O	2.18	0.43
1:C:370:TYR:CE1	4:C:527:EDO:H21	2.51	0.43
1:A:356:PRO:HB2	1:A:372:LYS:HG2	1.99	0.43
4:B:522:EDO:H11	1:D:298:ARG:NH1	2.27	0.43
1:C:352:TYR:HD1	4:C:516:EDO:H22	1.83	0.43
1:D:265:LYS:HG3	4:D:526:EDO:H12	2.00	0.43
1:C:434:PHE:HA	4:C:529:EDO:H21	2.00	0.43
1:D:325[B]:SEC:SE	1:D:326[B]:PRO:HA	2.69	0.43
1:D:346:PHE:CZ	1:D:348:GLN:HG3	2.54	0.43
1:B:392:ASP:H	4:B:523:EDO:C2	2.31	0.43
1:A:144:TRP:CE2	1:A:148:LEU:HD11	2.54	0.42
1:B:298:ARG:NH2	3:B:541:SO4:O2	2.52	0.42
1:C:83:ARG:HD3	1:C:326[A]:PRO:HG3	2.01	0.42
1:C:149:ARG:NH2	1:C:150:LYS:HE2	2.30	0.42
2:B:506:HEC:HHA	2:B:506:HEC:CGD	2.48	0.42
1:C:375[B]:MET:HG3	1:C:376:ILE:N	2.33	0.42
1:C:353:MET:HA	1:C:354:PRO:HD3	1.94	0.42
1:D:310:LYS:HG2	6:D:530:PGE:H42	2.01	0.42
1:D:369:PRO:HA	1:D:372:LYS:HD3	2.01	0.42
1:A:218:SER:H	4:A:524:EDO:H21	1.84	0.42
1:A:101:TYR:OH	4:B:514:EDO:H12	2.19	0.42
1:B:240[A]:CYS:HB3	1:B:325[A]:SEC:SE	2.69	0.42
1:B:256:ARG:HD2	4:B:517:EDO:O1	2.20	0.42
1:B:312:GLU:CG	4:B:534:EDO:H22	2.41	0.42
1:D:277:ARG:HG2	1:D:434:PHE:CZ	2.54	0.42
1:D:278:ASP:HB3	1:D:281:MET:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:LYS:HE3	1:B:442:LYS:CE	2.50	0.42
1:A:240[B]:CYS:SG	2:A:502:HEC:HBD1	2.60	0.42
1:B:188:PRO:HG2	4:B:529:EDO:H22	2.02	0.41
1:D:324[A]:GLY:HA3	1:D:354:PRO:HG2	2.02	0.41
1:D:375[B]:MET:HE3	1:D:375[B]:MET:HB2	1.86	0.41
4:A:515:EDO:H21	1:B:101:TYR:OH	2.21	0.41
1:A:372:LYS:NZ	7:A:618:HOH:O	2.53	0.41
1:B:412:ALA:HA	4:B:520:EDO:H21	2.02	0.41
1:B:146:ASP:OD1	1:B:149:ARG:NH1	2.53	0.41
1:A:429:MET:HE3	1:A:429:MET:HB3	1.88	0.41
1:B:322:PRO:HB2	1:B:329[A]:ASN:OD1	2.21	0.41
1:C:201:HIS:CB	1:C:209:MET:HB3	2.49	0.41
1:A:87:THR:HG22	2:A:502:HEC:HMB2	2.03	0.41
7:A:746:HOH:O	4:D:524:EDO:H22	2.21	0.41
1:C:231:LEU:HD13	1:D:223:GLN:HA	2.02	0.41
1:A:375[B]:MET:HG3	1:A:376:ILE:N	2.36	0.41
1:B:264:MET:O	4:B:531:EDO:H11	2.21	0.41
1:C:226:GLY:HA3	1:C:240[B]:CYS:O	2.21	0.40
1:D:258[B]:ASN:OD1	4:D:529:EDO:H11	2.21	0.40
1:B:285:ALA:HB3	1:B:436[B]:TRP:HZ2	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	438/450 (97%)	418 (95%)	18 (4%)	2 (0%)	24	11
1	B	436/450 (97%)	423 (97%)	13 (3%)	0	100	100
1	C	434/450 (96%)	417 (96%)	15 (4%)	2 (0%)	24	11
1	D	432/450 (96%)	416 (96%)	14 (3%)	2 (0%)	24	11
All	All	1740/1800 (97%)	1674 (96%)	60 (3%)	6 (0%)	43	21

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	324[A]	GLY
1	A	324[B]	GLY
1	C	324[A]	GLY
1	C	324[B]	GLY
1	D	324[A]	GLY
1	D	324[B]	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	370/369 (100%)	368 (100%)	2 (0%)	81	75
1	B	368/369 (100%)	368 (100%)	0	100	100
1	C	366/369 (99%)	366 (100%)	0	100	100
1	D	364/369 (99%)	362 (100%)	2 (0%)	81	75
All	All	1468/1476 (100%)	1464 (100%)	4 (0%)	86	83

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	235	ASN
1	A	428	SER
1	D	235	ASN
1	D	259	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	94	ASN
1	B	175	ASN
1	B	358	GLN
1	C	94	ASN
1	D	71	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

145 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	A	538	-	3,3,3	0.31	0	2,2,2	0.53	0
3	SO4	A	508	-	4,4,4	0.13	0	6,6,6	0.15	0
2	HEC	D	507	1	46,50,50	3.36	8 (17%)	60,82,82	1.60	7 (11%)
2	HEC	B	506	1	46,50,50	3.54	6 (13%)	60,82,82	1.75	9 (15%)
3	SO4	D	512	-	4,4,4	0.18	0	6,6,6	0.27	0
4	EDO	D	517	-	3,3,3	0.38	0	2,2,2	0.50	0
4	EDO	C	525	-	3,3,3	0.49	0	2,2,2	0.22	0
3	SO4	A	506	-	4,4,4	0.18	0	6,6,6	0.17	0
2	HEC	A	503	1	46,50,50	3.45	8 (17%)	60,82,82	1.62	7 (11%)
2	HEC	C	507	1	46,50,50	3.58	7 (15%)	60,82,82	1.79	12 (20%)
3	SO4	C	508	-	4,4,4	0.18	0	6,6,6	0.13	0
4	EDO	B	521	-	3,3,3	0.47	0	2,2,2	0.43	0
4	EDO	B	531	-	3,3,3	0.44	0	2,2,2	0.22	0
4	EDO	C	530	-	3,3,3	0.56	0	2,2,2	0.45	0
4	EDO	B	537	-	3,3,3	0.38	0	2,2,2	0.60	0
4	EDO	B	517	-	3,3,3	0.37	0	2,2,2	0.71	0
3	SO4	A	507	-	4,4,4	0.15	0	6,6,6	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	C	531	-	3,3,3	0.33	0	2,2,2	0.19	0
4	EDO	B	516	-	3,3,3	0.34	0	2,2,2	0.52	0
2	HEC	D	506	1	46,50,50	3.51	8 (17%)	60,82,82	1.57	9 (15%)
3	SO4	D	510	-	4,4,4	0.18	0	6,6,6	0.19	0
4	EDO	A	537	-	3,3,3	0.53	0	2,2,2	1.14	0
2	HEC	A	502	1	46,50,50	3.41	5 (10%)	60,82,82	1.52	8 (13%)
3	SO4	B	510	-	4,4,4	0.13	0	6,6,6	0.13	0
2	HEC	B	505	1	46,50,50	3.49	7 (15%)	60,82,82	1.55	7 (11%)
6	PGE	B	539	-	9,9,9	0.32	0	8,8,8	0.32	0
4	EDO	D	521	-	3,3,3	0.46	0	2,2,2	0.38	0
4	EDO	D	531	-	3,3,3	0.46	0	2,2,2	0.43	0
4	EDO	A	522	-	3,3,3	0.50	0	2,2,2	0.34	0
4	EDO	D	503	-	3,3,3	0.36	0	2,2,2	0.55	0
3	SO4	C	509	-	4,4,4	0.14	0	6,6,6	0.11	0
4	EDO	A	530	-	3,3,3	0.50	0	2,2,2	0.19	0
4	EDO	A	510	-	3,3,3	0.49	0	2,2,2	0.44	0
4	EDO	D	515	-	3,3,3	0.42	0	2,2,2	0.25	0
4	EDO	A	524	-	3,3,3	0.43	0	2,2,2	0.53	0
4	EDO	D	528	-	3,3,3	0.52	0	2,2,2	0.22	0
4	EDO	C	529	-	3,3,3	0.46	0	2,2,2	0.24	0
3	SO4	B	508	-	4,4,4	0.14	0	6,6,6	0.13	0
4	EDO	B	515	-	3,3,3	0.49	0	2,2,2	0.55	0
3	SO4	B	509	-	4,4,4	0.17	0	6,6,6	0.32	0
4	EDO	B	525	-	3,3,3	0.39	0	2,2,2	0.60	0
6	PGE	D	530	-	9,9,9	0.31	0	8,8,8	0.32	0
3	SO4	A	533	-	4,4,4	0.11	0	6,6,6	0.16	0
3	SO4	C	511	-	4,4,4	0.14	0	6,6,6	0.11	0
4	EDO	A	517	-	3,3,3	0.66	0	2,2,2	0.26	0
4	EDO	D	516	-	3,3,3	0.46	0	2,2,2	0.24	0
4	EDO	A	511	-	3,3,3	0.48	0	2,2,2	0.41	0
4	EDO	C	532	-	3,3,3	0.49	0	2,2,2	0.37	0
4	EDO	D	518	-	3,3,3	0.45	0	2,2,2	0.57	0
4	EDO	A	520	-	3,3,3	0.43	0	2,2,2	0.75	0
4	EDO	D	523	-	3,3,3	0.52	0	2,2,2	0.28	0
4	EDO	A	519	-	3,3,3	0.49	0	2,2,2	0.25	0
3	SO4	C	501	-	4,4,4	0.15	0	6,6,6	0.21	0
4	EDO	B	518	-	3,3,3	0.39	0	2,2,2	0.60	0
4	EDO	A	515	-	3,3,3	0.41	0	2,2,2	0.45	0
3	SO4	D	511	-	4,4,4	0.17	0	6,6,6	0.21	0
3	SO4	C	514	-	4,4,4	0.23	0	6,6,6	0.23	0
4	EDO	D	532	-	3,3,3	0.63	0	2,2,2	0.01	0
4	EDO	A	525	-	3,3,3	0.54	0	2,2,2	0.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	A	513	-	3,3,3	0.38	0	2,2,2	0.51	0
4	EDO	C	519	-	3,3,3	0.47	0	2,2,2	0.40	0
4	EDO	A	516	-	3,3,3	0.41	0	2,2,2	0.40	0
2	HEC	A	501	1	46,50,50	3.63	7 (15%)	60,82,82	1.49	8 (13%)
3	SO4	B	541	-	4,4,4	0.13	0	6,6,6	0.15	0
4	EDO	A	518	-	3,3,3	0.50	0	2,2,2	0.29	0
4	EDO	C	502	-	3,3,3	0.45	0	2,2,2	0.41	0
4	EDO	D	520	-	3,3,3	0.44	0	2,2,2	0.32	0
2	HEC	D	505	1	46,50,50	3.66	7 (15%)	60,82,82	1.60	10 (16%)
3	SO4	C	513	-	4,4,4	0.16	0	6,6,6	0.10	0
4	EDO	B	526	-	3,3,3	0.35	0	2,2,2	0.53	0
4	EDO	C	528	-	3,3,3	0.38	0	2,2,2	0.74	0
4	EDO	A	526	-	3,3,3	0.53	0	2,2,2	0.18	0
4	EDO	A	534	-	3,3,3	0.48	0	2,2,2	0.20	0
3	SO4	A	509	-	4,4,4	0.13	0	6,6,6	0.13	0
4	EDO	B	532	-	3,3,3	0.57	0	2,2,2	0.20	0
4	EDO	A	532	-	3,3,3	0.41	0	2,2,2	0.64	0
4	EDO	C	518	-	3,3,3	0.43	0	2,2,2	0.33	0
2	HEC	C	503	1	46,50,50	3.58	7 (15%)	60,82,82	1.44	7 (11%)
3	SO4	B	540	-	4,4,4	0.14	0	6,6,6	0.33	0
4	EDO	A	512	-	3,3,3	0.48	0	2,2,2	0.35	0
3	SO4	B	511	-	4,4,4	0.13	0	6,6,6	0.07	0
4	EDO	D	527	-	3,3,3	0.45	0	2,2,2	0.44	0
4	EDO	B	534	-	3,3,3	0.41	0	2,2,2	0.40	0
4	EDO	A	521	-	3,3,3	0.38	0	2,2,2	0.56	0
4	EDO	B	527	-	3,3,3	0.70	0	2,2,2	0.39	0
3	SO4	D	502	-	4,4,4	0.12	0	6,6,6	0.18	0
4	EDO	B	530	-	3,3,3	0.48	0	2,2,2	0.36	0
3	SO4	C	512	-	4,4,4	0.17	0	6,6,6	0.13	0
4	EDO	C	520	-	3,3,3	0.21	0	2,2,2	0.68	0
4	EDO	C	524	-	3,3,3	0.62	0	2,2,2	0.08	0
2	HEC	B	504	1	46,50,50	3.57	8 (17%)	60,82,82	1.62	10 (16%)
4	EDO	B	538	-	3,3,3	0.50	0	2,2,2	0.32	0
4	EDO	B	528	-	3,3,3	0.45	0	2,2,2	0.37	0
4	EDO	A	527	-	3,3,3	0.55	0	2,2,2	0.23	0
4	EDO	B	523	-	3,3,3	0.46	0	2,2,2	0.45	0
4	EDO	B	522	-	3,3,3	0.42	0	2,2,2	0.47	0
2	HEC	C	506	1	46,50,50	3.55	5 (10%)	60,82,82	1.48	6 (10%)
3	SO4	B	507	-	4,4,4	0.18	0	6,6,6	0.31	0
2	HEC	A	504	1	46,50,50	3.60	7 (15%)	60,82,82	1.57	7 (11%)
4	EDO	C	515	-	3,3,3	0.48	0	2,2,2	0.45	0
4	EDO	D	524	-	3,3,3	0.54	0	2,2,2	0.05	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEC	D	508	1	46,50,50	3.62	9 (19%)	60,82,82	1.59	8 (13%)
4	EDO	B	519	-	3,3,3	0.42	0	2,2,2	0.74	0
4	EDO	B	542	-	3,3,3	0.44	0	2,2,2	0.36	0
4	EDO	C	521	-	3,3,3	0.61	0	2,2,2	0.29	0
2	HEC	C	504	1	46,50,50	3.51	6 (13%)	60,82,82	1.57	9 (15%)
4	EDO	A	523	-	3,3,3	0.55	0	2,2,2	0.18	0
4	EDO	D	522	-	3,3,3	0.44	0	2,2,2	0.27	0
4	EDO	D	529	-	3,3,3	0.22	0	2,2,2	0.50	0
4	EDO	D	526	-	3,3,3	0.53	0	2,2,2	0.17	0
4	EDO	B	529	-	3,3,3	0.44	0	2,2,2	0.39	0
4	EDO	C	523	-	3,3,3	0.42	0	2,2,2	0.54	0
4	EDO	A	536	-	3,3,3	0.44	0	2,2,2	0.52	0
4	EDO	D	504	-	3,3,3	0.49	0	2,2,2	0.29	0
4	EDO	D	533	-	3,3,3	0.38	0	2,2,2	0.35	0
4	EDO	A	514	-	3,3,3	0.46	0	2,2,2	0.61	0
2	HEC	A	505	1	46,50,50	3.54	6 (13%)	60,82,82	1.78	12 (20%)
4	EDO	B	535	-	3,3,3	0.46	0	2,2,2	0.41	0
4	EDO	B	501	-	3,3,3	0.34	0	2,2,2	0.62	0
3	SO4	D	514	-	4,4,4	0.23	0	6,6,6	0.19	0
4	EDO	A	535	-	3,3,3	0.30	0	2,2,2	0.56	0
4	EDO	B	520	-	3,3,3	0.44	0	2,2,2	0.39	0
4	EDO	B	524	-	3,3,3	0.44	0	2,2,2	0.51	0
4	EDO	B	533	-	3,3,3	0.29	0	2,2,2	0.40	0
4	EDO	C	516	-	3,3,3	0.43	0	2,2,2	0.42	0
2	HEC	D	509	1	46,50,50	3.53	7 (15%)	60,82,82	1.68	10 (16%)
4	EDO	B	514	-	3,3,3	0.50	0	2,2,2	0.21	0
3	SO4	C	510	-	4,4,4	0.17	0	6,6,6	0.20	0
4	EDO	C	522	-	3,3,3	0.50	0	2,2,2	0.27	0
2	HEC	C	505	1	46,50,50	3.51	8 (17%)	60,82,82	1.45	8 (13%)
4	EDO	A	531	-	3,3,3	0.49	0	2,2,2	0.34	0
4	EDO	A	528	-	3,3,3	0.40	0	2,2,2	0.48	0
4	EDO	C	526	-	3,3,3	0.43	0	2,2,2	0.52	0
3	SO4	D	513	-	4,4,4	0.15	0	6,6,6	0.13	0
3	SO4	B	512	-	4,4,4	0.17	0	6,6,6	0.14	0
4	EDO	C	527	-	3,3,3	0.41	0	2,2,2	0.38	0
4	EDO	C	517	-	3,3,3	0.49	0	2,2,2	0.15	0
4	EDO	A	529	-	3,3,3	0.65	0	2,2,2	0.09	0
4	EDO	D	501	-	3,3,3	0.32	0	2,2,2	0.45	0
2	HEC	B	502	1	46,50,50	3.56	7 (15%)	60,82,82	1.53	8 (13%)
5	EPE	B	513	-	15,15,15	0.85	1 (6%)	18,20,20	2.04	6 (33%)
4	EDO	D	519	-	3,3,3	0.38	0	2,2,2	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	D	525	-	3,3,3	0.51	0	2,2,2	0.19	0
2	HEC	B	503	1	46,50,50	3.39	9 (19%)	60,82,82	1.58	6 (10%)
4	EDO	B	536	-	3,3,3	0.72	0	2,2,2	0.12	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
4	EDO	A	538	-	-	1/1/1/1	-
2	HEC	D	507	1	-	6/14/54/54	-
2	HEC	B	506	1	-	8/14/54/54	-
4	EDO	D	517	-	-	0/1/1/1	-
4	EDO	C	525	-	-	1/1/1/1	-
2	HEC	A	503	1	-	6/14/54/54	-
2	HEC	C	507	1	-	7/14/54/54	-
4	EDO	B	521	-	-	1/1/1/1	-
4	EDO	B	531	-	-	0/1/1/1	-
4	EDO	C	530	-	-	0/1/1/1	-
4	EDO	B	537	-	-	0/1/1/1	-
4	EDO	B	517	-	-	1/1/1/1	-
4	EDO	C	531	-	-	1/1/1/1	-
4	EDO	B	516	-	-	1/1/1/1	-
2	HEC	D	506	1	-	8/14/54/54	-
4	EDO	A	537	-	-	0/1/1/1	-
2	HEC	A	502	1	-	8/14/54/54	-
2	HEC	B	505	1	-	4/14/54/54	-
6	PGE	B	539	-	-	4/7/7/7	-
4	EDO	D	521	-	-	0/1/1/1	-
4	EDO	D	531	-	-	0/1/1/1	-
4	EDO	A	522	-	-	1/1/1/1	-
4	EDO	D	503	-	-	1/1/1/1	-
4	EDO	A	530	-	-	1/1/1/1	-
4	EDO	A	510	-	-	0/1/1/1	-
4	EDO	D	515	-	-	0/1/1/1	-
4	EDO	A	524	-	-	1/1/1/1	-
4	EDO	D	528	-	-	1/1/1/1	-
4	EDO	C	529	-	-	0/1/1/1	-
4	EDO	B	515	-	-	0/1/1/1	-
4	EDO	B	525	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PGE	D	530	-	-	4/7/7/7	-
4	EDO	A	517	-	-	1/1/1/1	-
4	EDO	D	516	-	-	0/1/1/1	-
4	EDO	A	511	-	-	0/1/1/1	-
4	EDO	C	532	-	-	1/1/1/1	-
4	EDO	D	518	-	-	1/1/1/1	-
4	EDO	A	520	-	-	1/1/1/1	-
4	EDO	D	523	-	-	0/1/1/1	-
4	EDO	A	519	-	-	0/1/1/1	-
4	EDO	B	518	-	-	0/1/1/1	-
4	EDO	A	515	-	-	1/1/1/1	-
4	EDO	D	532	-	-	1/1/1/1	-
4	EDO	A	525	-	-	1/1/1/1	-
4	EDO	A	513	-	-	0/1/1/1	-
4	EDO	C	519	-	-	1/1/1/1	-
4	EDO	A	516	-	-	0/1/1/1	-
2	HEC	A	501	1	-	7/14/54/54	-
4	EDO	A	518	-	-	0/1/1/1	-
4	EDO	C	502	-	-	1/1/1/1	-
4	EDO	D	520	-	-	0/1/1/1	-
2	HEC	D	505	1	-	6/14/54/54	-
4	EDO	B	526	-	-	1/1/1/1	-
4	EDO	C	528	-	-	1/1/1/1	-
4	EDO	A	526	-	-	1/1/1/1	-
4	EDO	A	534	-	-	0/1/1/1	-
4	EDO	B	532	-	-	1/1/1/1	-
4	EDO	A	532	-	-	1/1/1/1	-
4	EDO	C	518	-	-	0/1/1/1	-
2	HEC	C	503	1	-	6/14/54/54	-
4	EDO	A	512	-	-	1/1/1/1	-
4	EDO	D	527	-	-	1/1/1/1	-
4	EDO	B	534	-	-	1/1/1/1	-
4	EDO	A	521	-	-	1/1/1/1	-
4	EDO	B	527	-	-	0/1/1/1	-
4	EDO	B	530	-	-	0/1/1/1	-
4	EDO	C	520	-	-	0/1/1/1	-
4	EDO	C	524	-	-	0/1/1/1	-
2	HEC	B	504	1	-	6/14/54/54	-
4	EDO	B	538	-	-	0/1/1/1	-
4	EDO	B	528	-	-	0/1/1/1	-
4	EDO	A	527	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	B	523	-	-	0/1/1/1	-
4	EDO	B	522	-	-	0/1/1/1	-
2	HEC	C	506	1	-	4/14/54/54	-
4	EDO	C	515	-	-	0/1/1/1	-
2	HEC	A	504	1	-	4/14/54/54	-
4	EDO	D	524	-	-	0/1/1/1	-
2	HEC	D	508	1	-	4/14/54/54	-
4	EDO	B	519	-	-	0/1/1/1	-
4	EDO	B	542	-	-	1/1/1/1	-
4	EDO	C	521	-	-	0/1/1/1	-
2	HEC	C	504	1	-	8/14/54/54	-
4	EDO	A	523	-	-	1/1/1/1	-
4	EDO	D	522	-	-	0/1/1/1	-
4	EDO	D	529	-	-	0/1/1/1	-
4	EDO	D	526	-	-	0/1/1/1	-
4	EDO	B	529	-	-	0/1/1/1	-
4	EDO	C	523	-	-	1/1/1/1	-
4	EDO	A	536	-	-	0/1/1/1	-
4	EDO	D	504	-	-	0/1/1/1	-
4	EDO	D	533	-	-	1/1/1/1	-
4	EDO	A	514	-	-	1/1/1/1	-
2	HEC	A	505	1	-	9/14/54/54	-
4	EDO	B	535	-	-	1/1/1/1	-
4	EDO	B	501	-	-	0/1/1/1	-
4	EDO	A	535	-	-	1/1/1/1	-
4	EDO	B	520	-	-	0/1/1/1	-
4	EDO	B	524	-	-	0/1/1/1	-
4	EDO	B	533	-	-	0/1/1/1	-
4	EDO	C	516	-	-	1/1/1/1	-
2	HEC	D	509	1	-	9/14/54/54	-
4	EDO	B	514	-	-	0/1/1/1	-
4	EDO	C	522	-	-	0/1/1/1	-
2	HEC	C	505	1	-	6/14/54/54	-
4	EDO	A	531	-	-	0/1/1/1	-
4	EDO	A	528	-	-	0/1/1/1	-
4	EDO	C	526	-	-	1/1/1/1	-
4	EDO	C	527	-	-	1/1/1/1	-
4	EDO	C	517	-	-	0/1/1/1	-
4	EDO	A	529	-	-	1/1/1/1	-
4	EDO	D	501	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEC	B	502	1	-	6/14/54/54	-
5	EPE	B	513	-	-	4/9/19/19	0/1/1/1
4	EDO	D	519	-	-	0/1/1/1	-
4	EDO	D	525	-	-	1/1/1/1	-
2	HEC	B	503	1	-	8/14/54/54	-
4	EDO	B	536	-	-	1/1/1/1	-

All (143) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	504	HEC	CAC-C3C	17.15	1.56	1.34
2	A	501	HEC	CAC-C3C	16.80	1.56	1.34
2	D	509	HEC	CAC-C3C	16.65	1.56	1.34
2	C	505	HEC	CAC-C3C	16.65	1.56	1.34
2	D	508	HEC	CAC-C3C	16.61	1.56	1.34
2	B	505	HEC	CAC-C3C	16.57	1.56	1.34
2	B	506	HEC	CAC-C3C	16.50	1.56	1.34
2	D	505	HEC	CAB-C3B	16.43	1.55	1.34
2	D	505	HEC	CAC-C3C	16.42	1.55	1.34
2	A	504	HEC	CAB-C3B	16.33	1.55	1.34
2	C	503	HEC	CAC-C3C	16.31	1.55	1.34
2	C	506	HEC	CAB-C3B	16.30	1.55	1.34
2	C	504	HEC	CAC-C3C	16.25	1.55	1.34
2	A	505	HEC	CAC-C3C	16.22	1.55	1.34
2	B	502	HEC	CAC-C3C	16.11	1.55	1.34
2	C	507	HEC	CAC-C3C	16.02	1.55	1.34
2	A	504	HEC	CAC-C3C	16.01	1.55	1.34
2	D	506	HEC	CAC-C3C	15.96	1.55	1.34
2	C	507	HEC	CAB-C3B	15.95	1.55	1.34
2	A	502	HEC	CAC-C3C	15.93	1.55	1.34
2	D	507	HEC	CAC-C3C	15.89	1.55	1.34
2	A	501	HEC	CAB-C3B	15.75	1.55	1.34
2	A	503	HEC	CAC-C3C	15.68	1.54	1.34
2	B	502	HEC	CAB-C3B	15.65	1.54	1.34
2	D	508	HEC	CAB-C3B	15.62	1.54	1.34
2	C	503	HEC	CAB-C3B	15.58	1.54	1.34
2	A	505	HEC	CAB-C3B	15.50	1.54	1.34
2	C	506	HEC	CAC-C3C	15.37	1.54	1.34
2	B	503	HEC	CAC-C3C	15.23	1.54	1.34
2	D	506	HEC	CAB-C3B	15.10	1.54	1.34
2	A	503	HEC	CAB-C3B	15.07	1.54	1.34
2	C	504	HEC	CAB-C3B	15.01	1.54	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	509	HEC	CAB-C3B	15.01	1.54	1.34
2	B	506	HEC	CAB-C3B	14.88	1.53	1.34
2	B	503	HEC	CAB-C3B	14.80	1.53	1.34
2	B	504	HEC	CAB-C3B	14.75	1.53	1.34
2	C	505	HEC	CAB-C3B	14.65	1.53	1.34
2	B	505	HEC	CAB-C3B	14.60	1.53	1.34
2	A	502	HEC	CAB-C3B	14.31	1.53	1.34
2	D	507	HEC	CAB-C3B	13.80	1.52	1.34
2	C	503	HEC	CBC-CAC	-4.13	1.34	1.49
2	B	502	HEC	CBC-CAC	-4.01	1.34	1.49
2	D	505	HEC	CBC-CAC	-4.00	1.34	1.49
2	C	503	HEC	CBB-CAB	-3.95	1.34	1.49
2	A	501	HEC	CBC-CAC	-3.94	1.34	1.49
2	C	504	HEC	CBB-CAB	-3.86	1.35	1.49
2	C	507	HEC	CBC-CAC	-3.83	1.35	1.49
2	C	506	HEC	CBB-CAB	-3.82	1.35	1.49
2	C	506	HEC	CBC-CAC	-3.78	1.35	1.49
2	D	505	HEC	CBB-CAB	-3.78	1.35	1.49
2	C	504	HEC	CBC-CAC	-3.76	1.35	1.49
2	D	507	HEC	CBB-CAB	-3.76	1.35	1.49
2	D	506	HEC	CBB-CAB	-3.75	1.35	1.49
2	C	505	HEC	CBB-CAB	-3.74	1.35	1.49
2	B	503	HEC	CBB-CAB	-3.72	1.35	1.49
2	A	502	HEC	CBB-CAB	-3.71	1.35	1.49
2	D	506	HEC	CBC-CAC	-3.68	1.35	1.49
2	B	504	HEC	CBB-CAB	-3.66	1.35	1.49
2	B	502	HEC	CBB-CAB	-3.66	1.35	1.49
2	C	505	HEC	CBC-CAC	-3.61	1.36	1.49
2	A	502	HEC	CBC-CAC	-3.61	1.36	1.49
2	A	503	HEC	CBB-CAB	-3.61	1.36	1.49
2	D	508	HEC	CBB-CAB	-3.58	1.36	1.49
2	C	507	HEC	CBB-CAB	-3.57	1.36	1.49
2	A	501	HEC	CBB-CAB	-3.57	1.36	1.49
2	B	504	HEC	CBC-CAC	-3.55	1.36	1.49
2	B	506	HEC	CBC-CAC	-3.53	1.36	1.49
2	B	506	HEC	CBB-CAB	-3.49	1.36	1.49
2	B	503	HEC	CBC-CAC	-3.47	1.36	1.49
2	B	505	HEC	CBB-CAB	-3.47	1.36	1.49
2	A	503	HEC	CBC-CAC	-3.46	1.36	1.49
2	D	509	HEC	CBC-CAC	-3.44	1.36	1.49
2	A	505	HEC	CBB-CAB	-3.43	1.36	1.49
2	A	504	HEC	CBB-CAB	-3.40	1.36	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	508	HEC	CBC-CAC	-3.40	1.36	1.49
2	A	505	HEC	CBC-CAC	-3.38	1.36	1.49
2	D	507	HEC	CBC-CAC	-3.28	1.37	1.49
2	D	509	HEC	CBB-CAB	-3.25	1.37	1.49
2	A	504	HEC	CBC-CAC	-3.24	1.37	1.49
2	B	505	HEC	CBC-CAC	-3.17	1.37	1.49
5	B	513	EPE	C10-S	2.87	1.81	1.77
2	A	502	HEC	CMB-C2B	2.70	1.56	1.50
2	D	508	HEC	CMA-C3A	2.63	1.56	1.50
2	D	508	HEC	CMC-C2C	2.62	1.56	1.50
2	A	503	HEC	CMC-C2C	2.51	1.56	1.50
2	B	506	HEC	CMC-C2C	2.49	1.56	1.50
2	D	509	HEC	CMB-C2B	2.48	1.56	1.50
2	B	502	HEC	CMD-C2D	2.39	1.55	1.50
2	B	504	HEC	CMD-C2D	2.38	1.55	1.50
2	D	507	HEC	CMA-C3A	2.33	1.55	1.50
2	C	505	HEC	CMA-C3A	2.33	1.55	1.50
2	C	505	HEC	CMC-C2C	2.32	1.55	1.50
2	D	505	HEC	CMA-C3A	2.30	1.55	1.50
2	B	502	HEC	CMA-C3A	2.30	1.55	1.50
2	B	504	HEC	CMB-C2B	2.28	1.55	1.50
2	B	505	HEC	CMB-C2B	2.27	1.55	1.50
2	A	503	HEC	CMD-C2D	2.27	1.55	1.50
2	D	505	HEC	CMD-C2D	2.24	1.55	1.50
2	B	505	HEC	CMA-C3A	2.23	1.55	1.50
2	D	506	HEC	CMB-C2B	2.22	1.55	1.50
2	B	506	HEC	CMB-C2B	2.19	1.55	1.50
2	D	508	HEC	CMB-C2B	2.19	1.55	1.50
2	C	503	HEC	CMB-C2B	2.19	1.55	1.50
2	D	506	HEC	CMA-C3A	2.18	1.55	1.50
2	B	505	HEC	CMC-C2C	2.18	1.55	1.50
2	A	501	HEC	CMA-C3A	2.17	1.55	1.50
2	B	503	HEC	CMA-C3A	2.17	1.55	1.50
2	D	509	HEC	CMC-C2C	2.16	1.55	1.50
2	B	504	HEC	CMA-C3A	2.15	1.55	1.50
2	C	504	HEC	C3D-C2D	-2.14	1.33	1.38
2	D	507	HEC	CMB-C2B	2.14	1.55	1.50
2	A	505	HEC	CMC-C2C	2.14	1.55	1.50
2	C	504	HEC	CMA-C3A	2.14	1.55	1.50
2	A	504	HEC	CMB-C2B	2.13	1.55	1.50
2	D	507	HEC	C3B-C2B	-2.13	1.33	1.41
2	A	503	HEC	C3B-C2B	-2.12	1.33	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	507	HEC	CMD-C2D	2.11	1.55	1.50
2	A	505	HEC	CAD-C3D	2.11	1.56	1.51
2	D	505	HEC	CMC-C2C	2.11	1.55	1.50
2	B	504	HEC	C3B-C2B	-2.08	1.34	1.41
2	C	507	HEC	CMC-C2C	2.08	1.55	1.50
2	B	503	HEC	CMC-C2C	2.08	1.55	1.50
2	C	503	HEC	CMD-C2D	2.08	1.55	1.50
2	B	502	HEC	CMC-C2C	2.07	1.55	1.50
2	A	504	HEC	CMA-C3A	2.06	1.55	1.50
2	D	508	HEC	C3D-C2D	-2.06	1.33	1.38
2	B	503	HEC	C3C-C2C	-2.06	1.34	1.41
2	B	503	HEC	CMB-C2B	2.05	1.55	1.50
2	C	503	HEC	CMC-C2C	2.05	1.55	1.50
2	A	503	HEC	CMB-C2B	2.05	1.55	1.50
2	C	505	HEC	CMB-C2B	2.05	1.55	1.50
2	D	508	HEC	O2D-CGD	-2.05	1.23	1.30
2	B	503	HEC	C3B-C2B	-2.04	1.34	1.41
2	C	505	HEC	CMD-C2D	2.03	1.55	1.50
2	C	506	HEC	CMC-C2C	2.03	1.55	1.50
2	C	507	HEC	CAA-C2A	2.03	1.56	1.51
2	D	506	HEC	CMD-C2D	2.03	1.55	1.50
2	A	501	HEC	CMB-C2B	2.02	1.55	1.50
2	C	507	HEC	CMD-C2D	2.02	1.55	1.50
2	D	506	HEC	CMC-C2C	2.01	1.55	1.50
2	A	501	HEC	CMC-C2C	2.01	1.55	1.50
2	D	509	HEC	CMD-C2D	2.00	1.55	1.50
2	A	504	HEC	CAD-C3D	2.00	1.56	1.51

All (174) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	503	HEC	CBB-CAB-C3B	-7.63	113.84	127.86
2	B	506	HEC	CBB-CAB-C3B	-7.34	114.38	127.86
2	C	507	HEC	CBB-CAB-C3B	-7.32	114.41	127.86
2	A	505	HEC	CBB-CAB-C3B	-7.13	114.76	127.86
2	D	509	HEC	CBB-CAB-C3B	-6.85	115.27	127.86
2	D	507	HEC	CBB-CAB-C3B	-6.80	115.36	127.86
2	B	503	HEC	CBB-CAB-C3B	-6.77	115.42	127.86
2	B	504	HEC	CBB-CAB-C3B	-6.65	115.63	127.86
2	D	506	HEC	CBB-CAB-C3B	-6.55	115.82	127.86
2	C	504	HEC	CBB-CAB-C3B	-6.16	116.53	127.86
2	C	505	HEC	CBB-CAB-C3B	-5.80	117.19	127.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	504	HEC	CBB-CAB-C3B	-5.72	117.34	127.86
2	B	505	HEC	CBB-CAB-C3B	-5.71	117.37	127.86
2	D	508	HEC	CBC-CAC-C3C	-5.66	117.46	127.86
2	D	508	HEC	CBB-CAB-C3B	-5.54	117.67	127.86
2	B	505	HEC	CBC-CAC-C3C	-5.53	117.70	127.86
2	B	502	HEC	CBB-CAB-C3B	-5.48	117.79	127.86
2	C	507	HEC	CBC-CAC-C3C	-5.43	117.89	127.86
2	A	502	HEC	CBB-CAB-C3B	-5.41	117.92	127.86
2	B	503	HEC	CBC-CAC-C3C	-5.34	118.04	127.86
2	A	502	HEC	CBC-CAC-C3C	-5.29	118.13	127.86
2	D	507	HEC	CBC-CAC-C3C	-5.18	118.34	127.86
2	A	505	HEC	CBC-CAC-C3C	-5.17	118.35	127.86
2	D	509	HEC	CBC-CAC-C3C	-5.03	118.61	127.86
2	B	506	HEC	CBC-CAC-C3C	-4.98	118.71	127.86
2	B	504	HEC	CBC-CAC-C3C	-4.81	119.01	127.86
2	A	501	HEC	CBB-CAB-C3B	-4.80	119.04	127.86
2	C	506	HEC	CBC-CAC-C3C	-4.71	119.21	127.86
5	B	513	EPE	C5-N4-C3	4.66	119.31	108.83
2	D	505	HEC	CBB-CAB-C3B	-4.63	119.35	127.86
2	A	503	HEC	CBC-CAC-C3C	-4.46	119.67	127.86
2	A	504	HEC	CBC-CAC-C3C	-4.43	119.71	127.86
2	A	501	HEC	CBC-CAC-C3C	-4.23	120.08	127.86
2	C	504	HEC	CBC-CAC-C3C	-4.16	120.20	127.86
2	D	506	HEC	CBC-CAC-C3C	-4.12	120.30	127.86
2	C	506	HEC	CBB-CAB-C3B	-4.04	120.43	127.86
2	C	505	HEC	CBC-CAC-C3C	-3.84	120.80	127.86
2	D	505	HEC	CBC-CAC-C3C	-3.81	120.85	127.86
2	C	506	HEC	C4A-NA-C1A	3.75	109.02	105.35
2	A	504	HEC	C4C-NC-C1C	3.70	108.97	105.35
2	C	507	HEC	C4B-NB-C1B	3.63	108.90	105.35
5	B	513	EPE	C7-N4-C5	3.59	120.42	111.23
2	D	506	HEC	C4B-NB-C1B	3.55	108.83	105.35
2	C	503	HEC	CBC-CAC-C3C	-3.53	121.37	127.86
2	B	502	HEC	CBC-CAC-C3C	-3.45	121.52	127.86
2	C	504	HEC	C4B-NB-C1B	3.43	108.71	105.35
2	D	505	HEC	C4C-NC-C1C	3.43	108.70	105.35
2	C	503	HEC	CBB-CAB-C3B	-3.41	121.59	127.86
2	A	505	HEC	C4B-NB-C1B	3.35	108.63	105.35
2	A	501	HEC	C4C-NC-C1C	3.25	108.53	105.35
2	B	503	HEC	C4B-NB-C1B	3.21	108.50	105.35
2	D	506	HEC	C4D-ND-C1D	3.18	108.46	105.35
2	D	505	HEC	C4A-NA-C1A	3.12	108.41	105.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	509	HEC	CBA-CAA-C2A	-3.12	103.95	112.63
2	C	503	HEC	C4A-NA-C1A	3.12	108.40	105.35
2	C	507	HEC	C4D-ND-C1D	3.12	108.40	105.35
2	A	505	HEC	C4D-ND-C1D	3.12	108.40	105.35
2	B	506	HEC	C4B-NB-C1B	3.11	108.39	105.35
2	B	504	HEC	C4D-ND-C1D	3.10	108.38	105.35
5	B	513	EPE	C7-N4-C3	3.08	119.12	111.23
5	B	513	EPE	O3S-S-C10	3.07	110.74	105.77
2	C	507	HEC	CBA-CAA-C2A	-3.07	104.10	112.63
2	D	509	HEC	C4A-NA-C1A	3.06	108.35	105.35
2	B	506	HEC	C4A-NA-C1A	3.03	108.31	105.35
2	D	508	HEC	C4B-NB-C1B	3.03	108.31	105.35
2	B	502	HEC	C4A-NA-C1A	3.02	108.31	105.35
2	B	506	HEC	C4D-ND-C1D	3.02	108.31	105.35
2	C	506	HEC	C4B-NB-C1B	3.02	108.30	105.35
2	A	505	HEC	CBA-CAA-C2A	-3.01	104.27	112.63
2	C	506	HEC	C2A-C1A-NA	-3.01	107.40	110.32
2	A	502	HEC	C4B-NB-C1B	3.00	108.28	105.35
2	C	503	HEC	C4D-ND-C1D	3.00	108.28	105.35
5	B	513	EPE	C9-N1-C2	-2.98	103.61	111.23
2	D	508	HEC	C4C-NC-C1C	2.98	108.27	105.35
2	A	501	HEC	C4A-NA-C1A	2.98	108.26	105.35
2	A	503	HEC	CHC-C4B-NB	2.95	127.63	124.44
2	B	502	HEC	C4C-NC-C1C	2.92	108.20	105.35
2	D	505	HEC	CHB-C4A-NA	2.90	127.58	124.44
2	A	502	HEC	C4D-ND-C1D	2.83	108.12	105.35
2	B	504	HEC	C4A-NA-C1A	2.81	108.10	105.35
2	D	507	HEC	C4D-ND-C1D	2.81	108.09	105.35
2	C	505	HEC	C4D-ND-C1D	2.79	108.08	105.35
2	C	503	HEC	C2A-C1A-NA	-2.76	107.63	110.32
2	D	507	HEC	C4B-NB-C1B	2.76	108.06	105.35
2	D	505	HEC	C2A-C1A-NA	-2.76	107.64	110.32
2	B	505	HEC	C4C-NC-C1C	2.75	108.04	105.35
2	C	503	HEC	C4C-NC-C1C	2.73	108.02	105.35
2	A	503	HEC	C4D-ND-C1D	2.71	108.01	105.35
2	B	502	HEC	CAA-CBA-CGA	-2.71	107.77	113.60
2	C	504	HEC	C4C-NC-C1C	2.71	108.00	105.35
2	B	503	HEC	C4D-ND-C1D	2.68	107.97	105.35
2	A	504	HEC	C4A-NA-C1A	2.67	107.96	105.35
2	D	509	HEC	C4B-NB-C1B	2.66	107.96	105.35
2	B	503	HEC	CAD-CBD-CGD	-2.65	107.89	113.60
2	A	505	HEC	C4A-NA-C1A	2.65	107.94	105.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	507	HEC	CHC-C4B-NB	2.64	127.30	124.44
2	B	502	HEC	C2A-C1A-NA	-2.62	107.77	110.32
2	D	509	HEC	C4D-ND-C1D	2.62	107.92	105.35
2	A	504	HEC	C2A-C1A-NA	-2.61	107.78	110.32
2	B	506	HEC	CBA-CAA-C2A	-2.61	105.39	112.63
2	D	506	HEC	CBA-CAA-C2A	-2.58	105.45	112.63
2	C	505	HEC	C4A-NA-C1A	2.58	107.87	105.35
2	B	505	HEC	C4A-NA-C1A	2.53	107.82	105.35
2	D	505	HEC	C4D-ND-C1D	2.52	107.82	105.35
2	C	505	HEC	C4B-NB-C1B	2.50	107.79	105.35
2	A	503	HEC	C4B-NB-C1B	2.50	107.79	105.35
2	B	504	HEC	C4C-NC-C1C	2.49	107.79	105.35
2	D	507	HEC	C4C-NC-C1C	2.47	107.77	105.35
2	D	505	HEC	C3D-C4D-ND	-2.47	107.39	110.15
2	D	505	HEC	C4B-NB-C1B	2.47	107.76	105.35
2	B	506	HEC	O2A-CGA-CBA	2.47	121.95	114.03
2	D	509	HEC	C4C-NC-C1C	2.45	107.75	105.35
2	D	507	HEC	C3B-C4B-NB	-2.41	107.22	110.58
2	B	502	HEC	C4B-NB-C1B	2.41	107.71	105.35
2	A	501	HEC	CMC-C2C-C1C	-2.39	121.73	125.37
2	C	504	HEC	CAD-CBD-CGD	-2.38	108.48	113.60
2	A	505	HEC	O2A-CGA-CBA	2.36	121.62	114.03
2	A	503	HEC	C3B-C4B-NB	-2.34	107.32	110.58
2	D	507	HEC	C4A-NA-C1A	2.34	107.64	105.35
2	D	506	HEC	C3B-C4B-NB	-2.33	107.33	110.58
2	A	502	HEC	C3B-C4B-NB	-2.33	107.33	110.58
2	D	509	HEC	CHB-C4A-NA	2.32	126.95	124.44
2	B	504	HEC	C3D-C4D-ND	-2.32	107.56	110.15
2	B	505	HEC	CBA-CAA-C2A	-2.30	106.23	112.63
2	D	506	HEC	CAD-CBD-CGD	-2.30	108.66	113.60
2	A	505	HEC	CMD-C2D-C1D	-2.29	121.89	125.37
2	B	506	HEC	CHC-C4B-NB	2.28	126.91	124.44
2	C	507	HEC	O1D-CGD-CBD	-2.26	115.81	123.08
2	A	501	HEC	C2A-C1A-NA	-2.26	108.12	110.32
2	C	506	HEC	C4C-NC-C1C	2.26	107.56	105.35
2	B	505	HEC	C2A-C1A-NA	-2.25	108.14	110.32
5	B	513	EPE	O2S-S-C10	2.24	109.62	106.92
2	C	504	HEC	C3B-C4B-NB	-2.23	107.47	110.58
2	D	508	HEC	CBD-CAD-C3D	-2.22	106.45	112.63
2	B	504	HEC	C4B-NB-C1B	2.22	107.52	105.35
2	D	509	HEC	O2D-CGD-CBD	2.22	121.15	114.03
2	A	505	HEC	O2D-CGD-CBD	2.21	121.14	114.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	505	HEC	C2A-C1A-NA	-2.19	108.19	110.32
2	B	504	HEC	C2A-C1A-NA	-2.18	108.20	110.32
2	D	508	HEC	CMC-C2C-C1C	-2.18	122.05	125.37
2	B	506	HEC	O2D-CGD-CBD	2.18	121.02	114.03
2	B	503	HEC	CBA-CAA-C2A	-2.17	106.60	112.63
2	C	505	HEC	C3D-C4D-ND	-2.17	107.72	110.15
2	C	507	HEC	O2D-CGD-CBD	2.17	120.99	114.03
2	A	502	HEC	CHC-C4B-NB	2.16	126.78	124.44
2	D	506	HEC	CBD-CAD-C3D	-2.16	106.63	112.63
2	C	504	HEC	CBD-CAD-C3D	-2.16	106.63	112.63
2	B	504	HEC	CMC-C2C-C1C	-2.16	122.09	125.37
2	C	504	HEC	C4D-ND-C1D	2.15	107.45	105.35
2	D	508	HEC	C4A-NA-C1A	2.15	107.45	105.35
2	B	502	HEC	O1A-CGA-CBA	-2.15	116.19	123.08
2	D	506	HEC	C3D-C4D-ND	-2.15	107.75	110.15
2	D	505	HEC	CAD-CBD-CGD	-2.12	109.04	113.60
2	C	507	HEC	C3B-C4B-NB	-2.12	107.62	110.58
2	A	505	HEC	C3B-C4B-NB	-2.11	107.64	110.58
2	A	501	HEC	C3C-C4C-NC	-2.11	107.64	110.58
2	A	505	HEC	CHD-C1D-ND	2.10	127.71	123.85
2	D	509	HEC	O2A-CGA-CBA	2.10	120.77	114.03
2	C	503	HEC	C3C-C4C-NC	-2.08	107.68	110.58
2	A	502	HEC	CBA-CAA-C2A	-2.06	106.89	112.63
2	C	507	HEC	C4C-NC-C1C	2.06	107.36	105.35
2	A	502	HEC	CAD-CBD-CGD	-2.05	109.19	113.60
2	D	508	HEC	C2A-C1A-NA	-2.05	108.33	110.32
2	A	504	HEC	CBD-CAD-C3D	-2.05	106.94	112.63
2	C	505	HEC	CHD-C1D-ND	2.05	127.61	123.85
2	A	505	HEC	CHC-C4B-NB	2.03	126.64	124.44
2	B	505	HEC	C4B-NB-C1B	2.03	107.34	105.35
2	C	504	HEC	C2A-C1A-NA	-2.02	108.35	110.32
2	C	507	HEC	O2A-CGA-CBA	2.02	120.53	114.03
2	B	504	HEC	CHC-C4B-NB	2.02	126.63	124.44
2	C	507	HEC	CAA-CBA-CGA	2.02	117.95	113.60
2	A	503	HEC	C2A-C1A-NA	-2.02	108.36	110.32
2	A	501	HEC	CAA-CBA-CGA	-2.02	109.26	113.60
2	A	504	HEC	CMB-C2B-C1B	-2.01	122.31	125.37

There are no chirality outliers.

All (185) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	HEC	C2B-C3B-CAB-CBB
2	A	501	HEC	C4B-C3B-CAB-CBB
2	A	501	HEC	C2C-C3C-CAC-CBC
2	A	501	HEC	C4C-C3C-CAC-CBC
2	A	502	HEC	C2B-C3B-CAB-CBB
2	A	502	HEC	C4B-C3B-CAB-CBB
2	A	502	HEC	C2C-C3C-CAC-CBC
2	A	502	HEC	C4C-C3C-CAC-CBC
2	A	503	HEC	C2B-C3B-CAB-CBB
2	A	503	HEC	C4B-C3B-CAB-CBB
2	A	503	HEC	C2C-C3C-CAC-CBC
2	A	503	HEC	C4C-C3C-CAC-CBC
2	A	504	HEC	C2B-C3B-CAB-CBB
2	A	504	HEC	C4B-C3B-CAB-CBB
2	A	504	HEC	C2C-C3C-CAC-CBC
2	A	504	HEC	C4C-C3C-CAC-CBC
2	A	505	HEC	C2B-C3B-CAB-CBB
2	A	505	HEC	C4B-C3B-CAB-CBB
2	A	505	HEC	C2C-C3C-CAC-CBC
2	A	505	HEC	C4C-C3C-CAC-CBC
2	B	502	HEC	C2B-C3B-CAB-CBB
2	B	502	HEC	C4B-C3B-CAB-CBB
2	B	502	HEC	C2C-C3C-CAC-CBC
2	B	502	HEC	C4C-C3C-CAC-CBC
2	B	503	HEC	C2B-C3B-CAB-CBB
2	B	503	HEC	C4B-C3B-CAB-CBB
2	B	503	HEC	C2C-C3C-CAC-CBC
2	B	503	HEC	C4C-C3C-CAC-CBC
2	B	504	HEC	C2B-C3B-CAB-CBB
2	B	504	HEC	C4B-C3B-CAB-CBB
2	B	504	HEC	C2C-C3C-CAC-CBC
2	B	504	HEC	C4C-C3C-CAC-CBC
2	B	505	HEC	C2B-C3B-CAB-CBB
2	B	505	HEC	C4B-C3B-CAB-CBB
2	B	505	HEC	C2C-C3C-CAC-CBC
2	B	505	HEC	C4C-C3C-CAC-CBC
2	B	506	HEC	C2B-C3B-CAB-CBB
2	B	506	HEC	C4B-C3B-CAB-CBB
2	B	506	HEC	C2C-C3C-CAC-CBC
2	B	506	HEC	C4C-C3C-CAC-CBC
2	C	503	HEC	C2B-C3B-CAB-CBB
2	C	503	HEC	C4B-C3B-CAB-CBB
2	C	503	HEC	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
2	C	503	HEC	C4C-C3C-CAC-CBC
2	C	504	HEC	C2B-C3B-CAB-CBB
2	C	504	HEC	C4B-C3B-CAB-CBB
2	C	504	HEC	C2C-C3C-CAC-CBC
2	C	504	HEC	C4C-C3C-CAC-CBC
2	C	505	HEC	C2B-C3B-CAB-CBB
2	C	505	HEC	C4B-C3B-CAB-CBB
2	C	505	HEC	C2C-C3C-CAC-CBC
2	C	505	HEC	C4C-C3C-CAC-CBC
2	C	506	HEC	C2B-C3B-CAB-CBB
2	C	506	HEC	C4B-C3B-CAB-CBB
2	C	506	HEC	C2C-C3C-CAC-CBC
2	C	506	HEC	C4C-C3C-CAC-CBC
2	C	507	HEC	C2B-C3B-CAB-CBB
2	C	507	HEC	C4B-C3B-CAB-CBB
2	C	507	HEC	C2C-C3C-CAC-CBC
2	C	507	HEC	C4C-C3C-CAC-CBC
2	D	505	HEC	C2B-C3B-CAB-CBB
2	D	505	HEC	C4B-C3B-CAB-CBB
2	D	505	HEC	C2C-C3C-CAC-CBC
2	D	505	HEC	C4C-C3C-CAC-CBC
2	D	506	HEC	C2B-C3B-CAB-CBB
2	D	506	HEC	C4B-C3B-CAB-CBB
2	D	506	HEC	C2C-C3C-CAC-CBC
2	D	506	HEC	C4C-C3C-CAC-CBC
2	D	507	HEC	C2B-C3B-CAB-CBB
2	D	507	HEC	C4B-C3B-CAB-CBB
2	D	507	HEC	C2C-C3C-CAC-CBC
2	D	507	HEC	C4C-C3C-CAC-CBC
2	D	508	HEC	C2B-C3B-CAB-CBB
2	D	508	HEC	C4B-C3B-CAB-CBB
2	D	508	HEC	C2C-C3C-CAC-CBC
2	D	508	HEC	C4C-C3C-CAC-CBC
2	D	509	HEC	C2B-C3B-CAB-CBB
2	D	509	HEC	C4B-C3B-CAB-CBB
2	D	509	HEC	C2C-C3C-CAC-CBC
2	D	509	HEC	C4C-C3C-CAC-CBC
5	B	513	EPE	C9-C10-S-O1S
5	B	513	EPE	C9-C10-S-O3S
2	A	502	HEC	C2A-CAA-CBA-CGA
2	B	503	HEC	C2A-CAA-CBA-CGA
2	C	504	HEC	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
2	D	506	HEC	C2A-CAA-CBA-CGA
6	B	539	PGE	O2-C3-C4-O3
6	D	530	PGE	C4-C3-O2-C2
4	D	532	EDO	O1-C1-C2-O2
6	D	530	PGE	O2-C3-C4-O3
4	A	517	EDO	O1-C1-C2-O2
4	A	523	EDO	O1-C1-C2-O2
4	A	529	EDO	O1-C1-C2-O2
4	B	526	EDO	O1-C1-C2-O2
4	B	542	EDO	O1-C1-C2-O2
4	C	502	EDO	O1-C1-C2-O2
4	C	519	EDO	O1-C1-C2-O2
4	C	528	EDO	O1-C1-C2-O2
4	C	531	EDO	O1-C1-C2-O2
4	D	528	EDO	O1-C1-C2-O2
2	C	507	HEC	C3D-CAD-CBD-CGD
4	C	525	EDO	O1-C1-C2-O2
4	D	525	EDO	O1-C1-C2-O2
2	A	505	HEC	C3D-CAD-CBD-CGD
2	B	506	HEC	C3D-CAD-CBD-CGD
2	D	509	HEC	C3D-CAD-CBD-CGD
6	B	539	PGE	O3-C5-C6-O4
4	A	524	EDO	O1-C1-C2-O2
4	A	526	EDO	O1-C1-C2-O2
4	B	517	EDO	O1-C1-C2-O2
4	B	532	EDO	O1-C1-C2-O2
6	D	530	PGE	C6-C5-O3-C4
5	B	513	EPE	C8-C7-N4-C5
6	B	539	PGE	C3-C4-O3-C5
4	A	521	EDO	O1-C1-C2-O2
4	A	525	EDO	O1-C1-C2-O2
2	B	503	HEC	C3D-CAD-CBD-CGD
5	B	513	EPE	C9-C10-S-O2S
4	A	512	EDO	O1-C1-C2-O2
4	A	514	EDO	O1-C1-C2-O2
4	A	522	EDO	O1-C1-C2-O2
4	A	535	EDO	O1-C1-C2-O2
4	B	534	EDO	O1-C1-C2-O2
4	C	516	EDO	O1-C1-C2-O2
4	D	527	EDO	O1-C1-C2-O2
2	B	503	HEC	CAA-CBA-CGA-O1A
2	C	503	HEC	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
2	A	501	HEC	CAA-CBA-CGA-O1A
2	A	505	HEC	CAA-CBA-CGA-O1A
2	B	502	HEC	CAA-CBA-CGA-O1A
2	A	502	HEC	CAA-CBA-CGA-O1A
2	D	506	HEC	CAA-CBA-CGA-O1A
2	A	502	HEC	C3D-CAD-CBD-CGD
2	C	504	HEC	C3D-CAD-CBD-CGD
6	D	530	PGE	C3-C4-O3-C5
2	C	503	HEC	CAA-CBA-CGA-O2A
2	D	505	HEC	CAA-CBA-CGA-O1A
2	A	502	HEC	CAA-CBA-CGA-O2A
2	C	504	HEC	CAA-CBA-CGA-O1A
2	D	505	HEC	CAA-CBA-CGA-O2A
2	D	506	HEC	CAA-CBA-CGA-O2A
2	A	501	HEC	CAA-CBA-CGA-O2A
2	A	505	HEC	CAA-CBA-CGA-O2A
2	D	509	HEC	CAA-CBA-CGA-O2A
2	D	506	HEC	C3D-CAD-CBD-CGD
2	B	503	HEC	CAA-CBA-CGA-O2A
2	B	506	HEC	CAA-CBA-CGA-O2A
2	D	509	HEC	CAA-CBA-CGA-O1A
2	C	504	HEC	CAA-CBA-CGA-O2A
4	B	516	EDO	O1-C1-C2-O2
4	C	527	EDO	O1-C1-C2-O2
4	D	518	EDO	O1-C1-C2-O2
2	B	502	HEC	CAA-CBA-CGA-O2A
2	B	504	HEC	CAA-CBA-CGA-O2A
2	C	505	HEC	CAA-CBA-CGA-O2A
2	D	507	HEC	CAA-CBA-CGA-O2A
2	C	507	HEC	CAA-CBA-CGA-O1A
2	B	506	HEC	CAA-CBA-CGA-O1A
2	C	505	HEC	CAA-CBA-CGA-O1A
2	D	509	HEC	CAD-CBD-CGD-O1D
2	A	503	HEC	CAA-CBA-CGA-O2A
2	A	505	HEC	CAD-CBD-CGD-O1D
2	B	504	HEC	CAA-CBA-CGA-O1A
4	A	527	EDO	O1-C1-C2-O2
4	A	532	EDO	O1-C1-C2-O2
4	A	538	EDO	O1-C1-C2-O2
4	B	535	EDO	O1-C1-C2-O2
4	B	536	EDO	O1-C1-C2-O2
4	C	532	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	D	503	EDO	O1-C1-C2-O2
2	C	507	HEC	CAA-CBA-CGA-O2A
2	A	503	HEC	CAA-CBA-CGA-O1A
2	D	509	HEC	CAD-CBD-CGD-O2D
2	D	507	HEC	CAA-CBA-CGA-O1A
6	B	539	PGE	C4-C3-O2-C2
2	A	505	HEC	CAD-CBD-CGD-O2D
4	A	515	EDO	O1-C1-C2-O2
4	A	520	EDO	O1-C1-C2-O2
4	A	530	EDO	O1-C1-C2-O2
4	B	521	EDO	O1-C1-C2-O2
4	C	523	EDO	O1-C1-C2-O2
4	C	526	EDO	O1-C1-C2-O2
4	D	533	EDO	O1-C1-C2-O2
2	A	501	HEC	CAD-CBD-CGD-O2D
2	B	506	HEC	CAD-CBD-CGD-O1D

There are no ring outliers.

66 monomers are involved in 108 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	538	EDO	2	0
2	B	506	HEC	1	0
4	D	517	EDO	1	0
4	C	525	EDO	1	0
2	A	503	HEC	2	0
2	C	507	HEC	1	0
3	C	508	SO4	1	0
4	B	521	EDO	1	0
4	B	531	EDO	3	0
4	B	537	EDO	1	0
4	B	517	EDO	1	0
4	C	531	EDO	5	0
2	D	506	HEC	4	0
4	A	537	EDO	4	0
2	A	502	HEC	3	0
6	B	539	PGE	2	0
4	A	522	EDO	1	0
3	C	509	SO4	1	0
4	A	524	EDO	2	0
4	C	529	EDO	1	0
4	B	525	EDO	1	0

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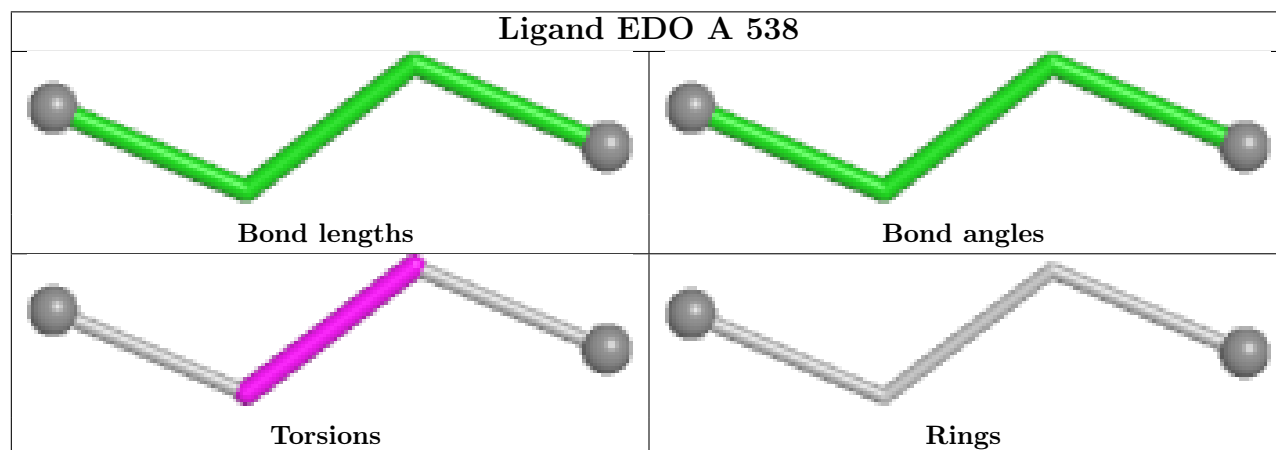
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	530	PGE	7	0
4	A	517	EDO	3	0
4	D	518	EDO	1	0
4	B	518	EDO	1	0
4	A	515	EDO	1	0
4	A	516	EDO	1	0
3	B	541	SO4	2	0
4	C	502	EDO	2	0
3	C	513	SO4	1	0
4	A	526	EDO	1	0
4	A	534	EDO	1	0
4	B	532	EDO	2	0
4	C	518	EDO	1	0
2	C	503	HEC	1	0
3	B	511	SO4	1	0
4	B	534	EDO	4	0
4	B	530	EDO	3	0
4	C	520	EDO	3	0
2	B	504	HEC	2	0
4	B	538	EDO	1	0
4	B	528	EDO	1	0
4	B	523	EDO	2	0
4	B	522	EDO	2	0
4	D	524	EDO	1	0
2	C	504	HEC	1	0
4	D	522	EDO	1	0
4	D	529	EDO	4	0
4	D	526	EDO	1	0
4	B	529	EDO	1	0
4	C	523	EDO	2	0
4	A	514	EDO	2	0
2	A	505	HEC	1	0
3	D	514	SO4	1	0
4	B	520	EDO	1	0
4	B	524	EDO	2	0
4	B	533	EDO	4	0
4	C	516	EDO	1	0
2	D	509	HEC	1	0
4	B	514	EDO	1	0
2	C	505	HEC	1	0
4	A	531	EDO	1	0
4	C	527	EDO	3	0

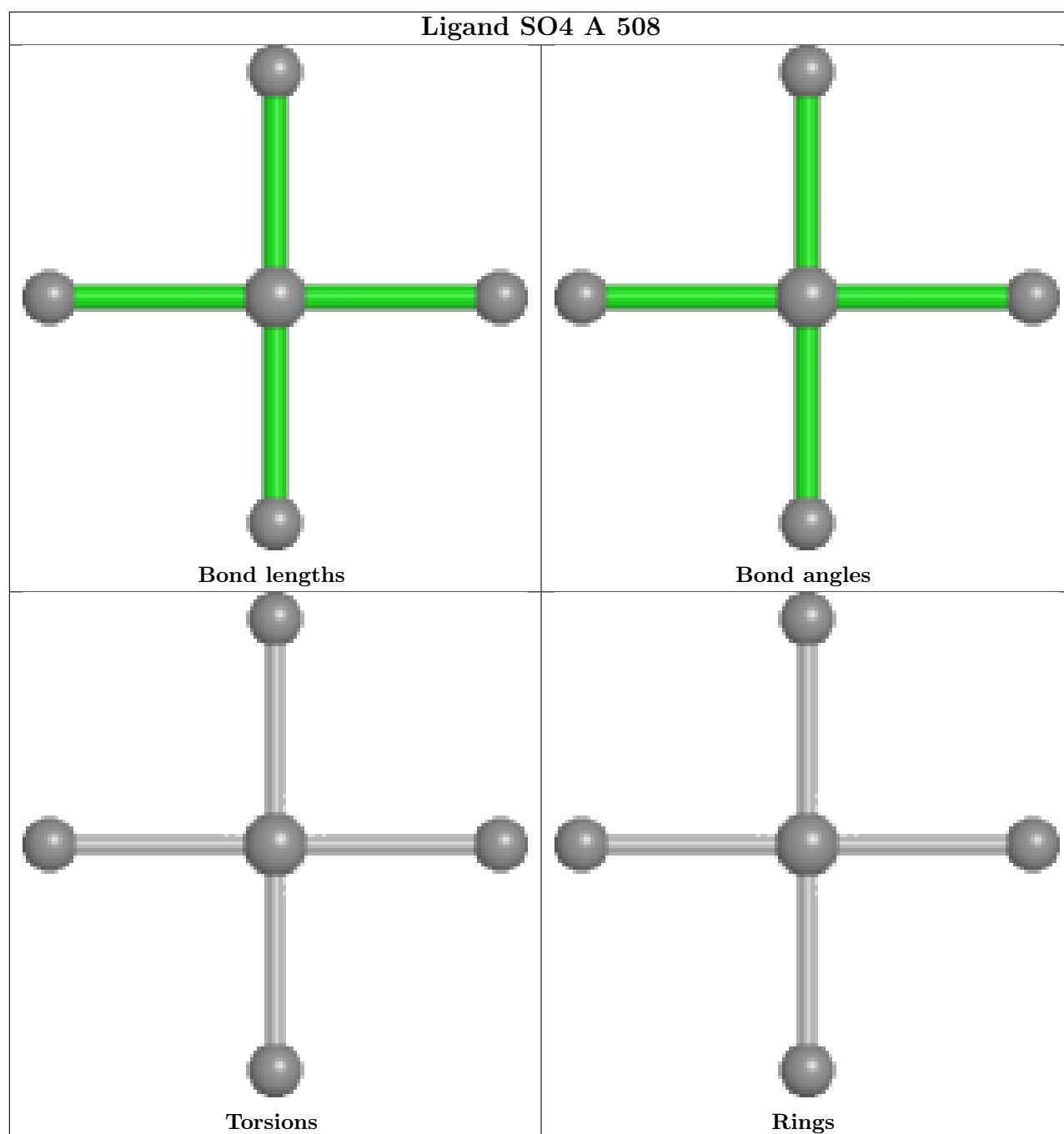
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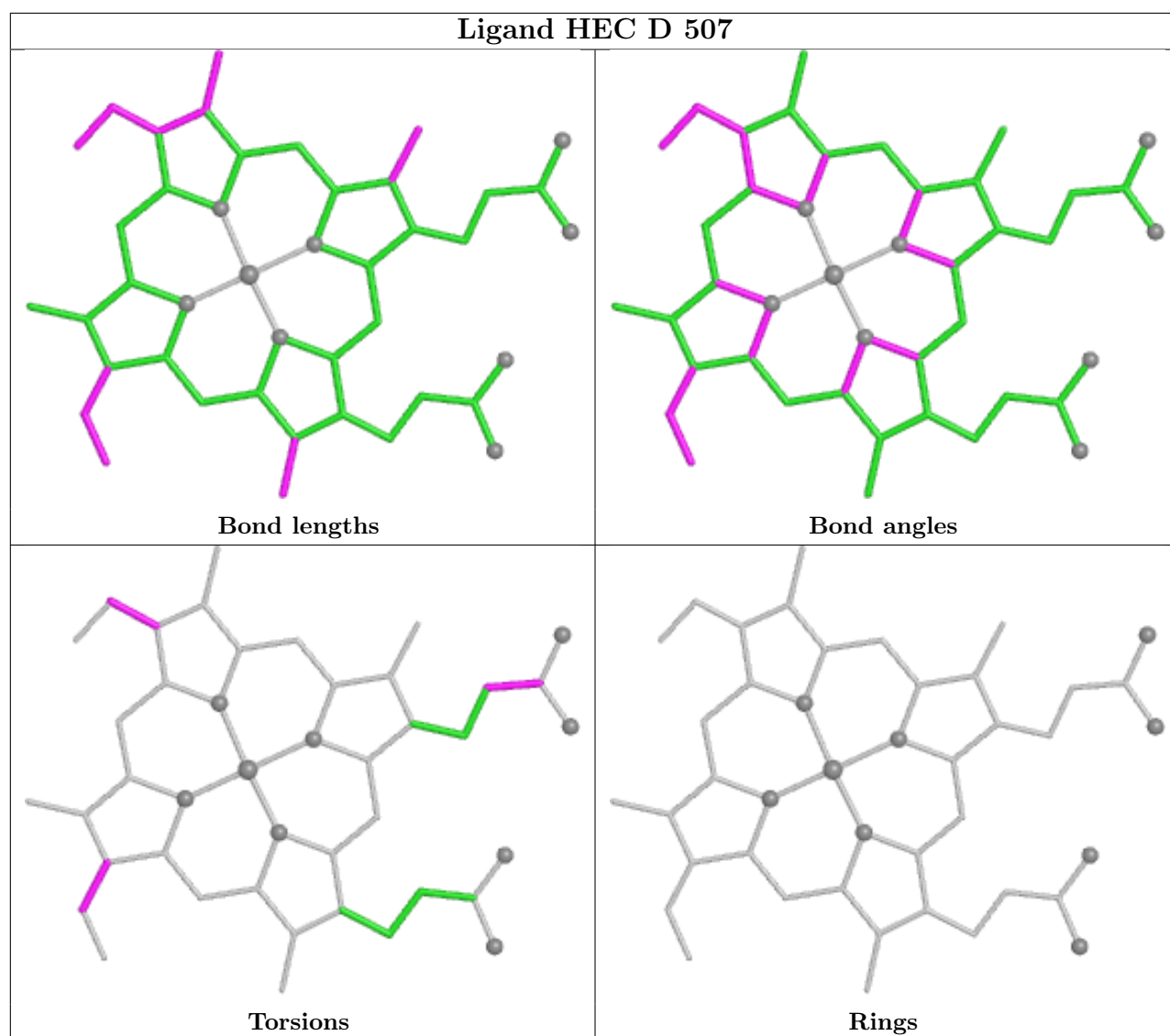
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	501	EDO	2	0
4	D	525	EDO	1	0
2	B	503	HEC	1	0

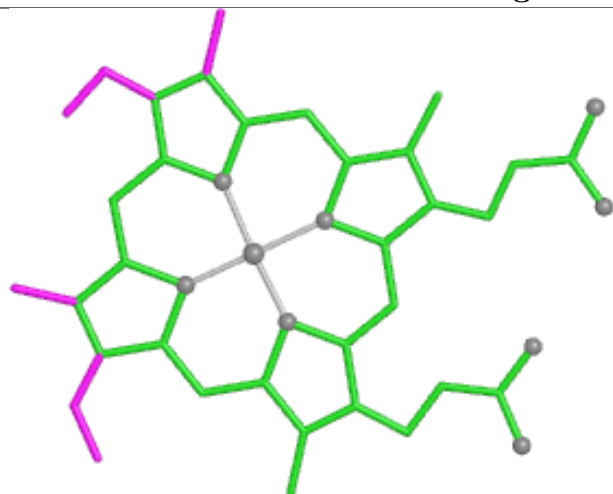
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



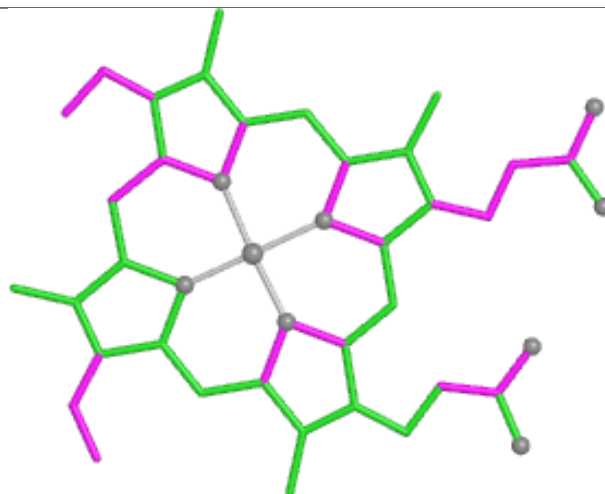




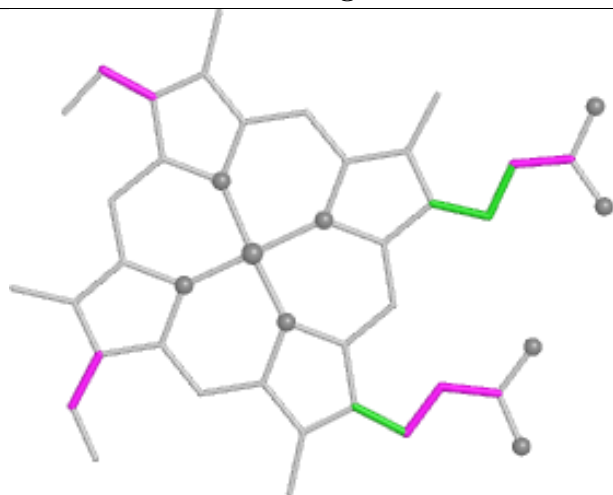
Ligand HEC B 506



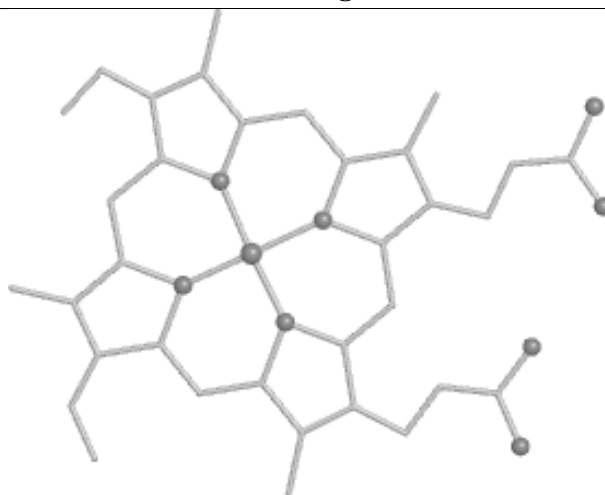
Bond lengths



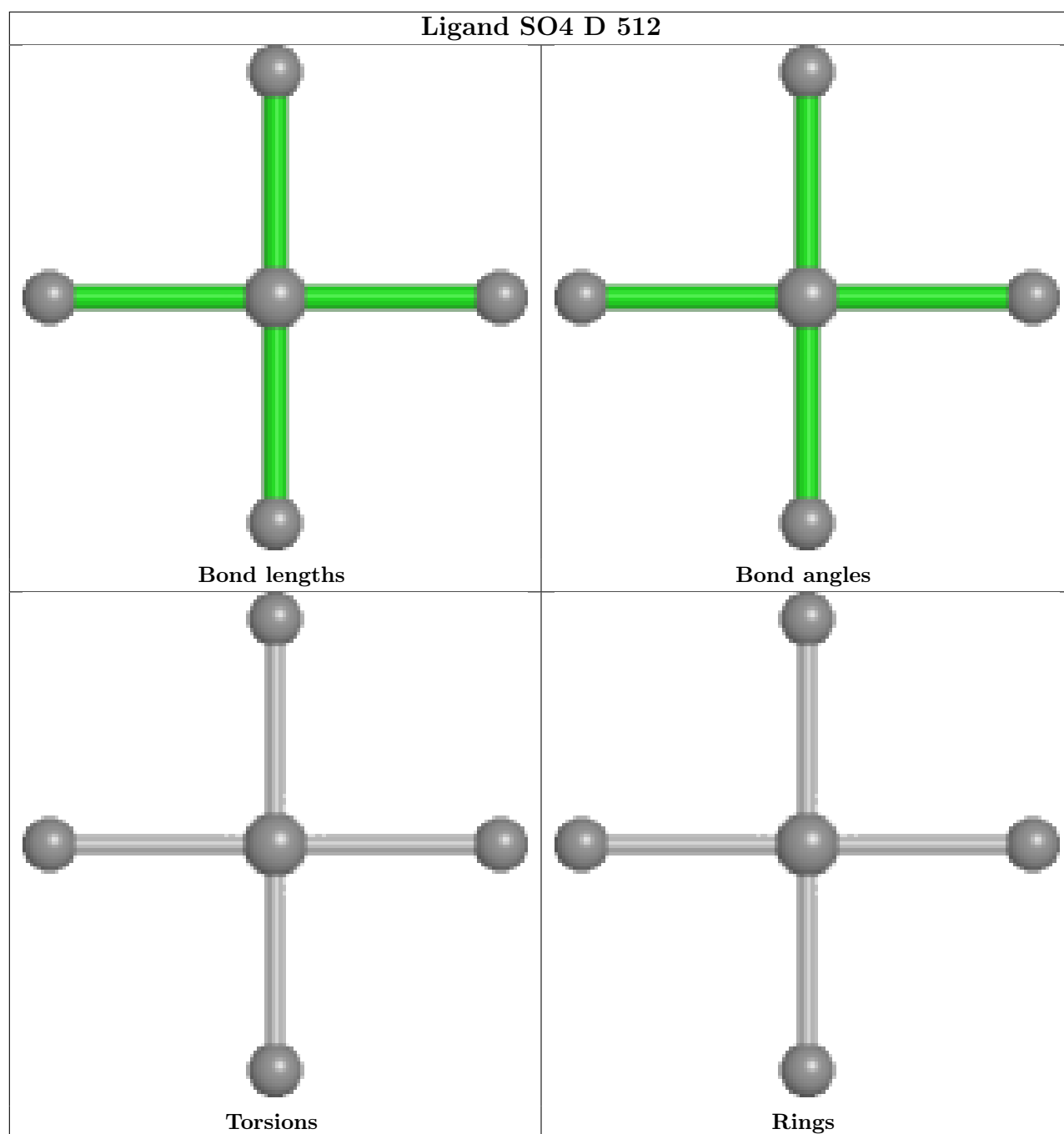
Bond angles

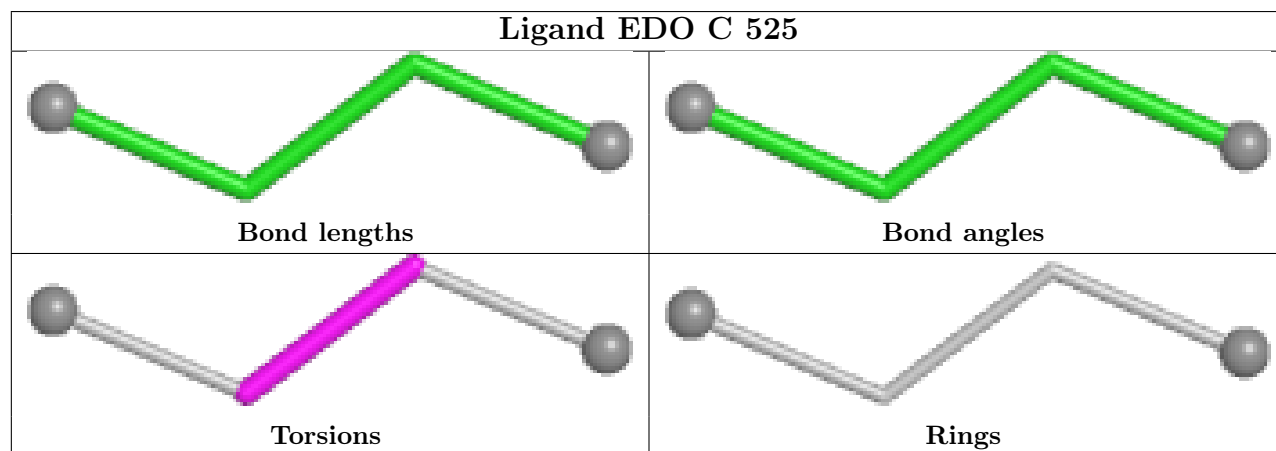
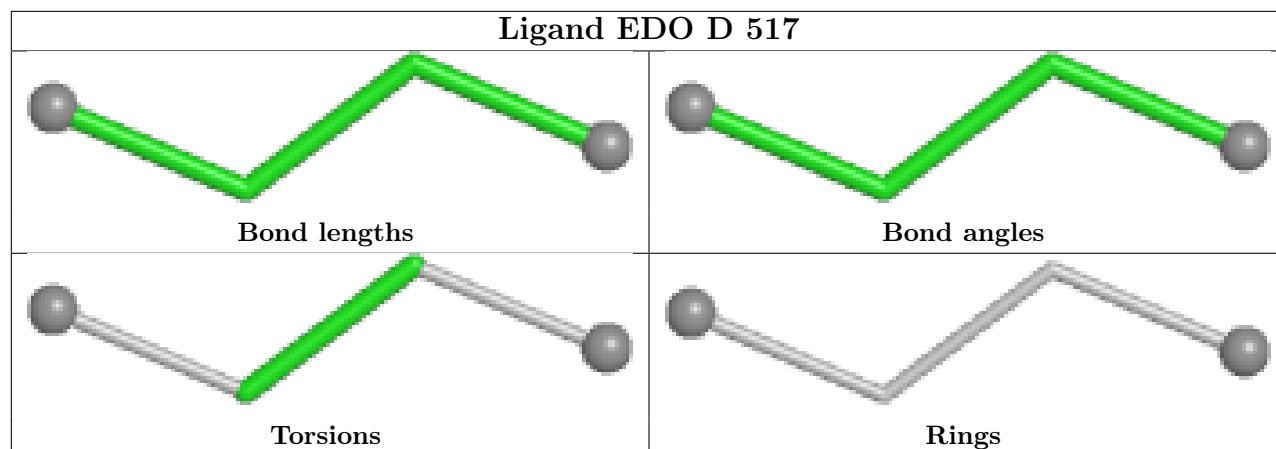


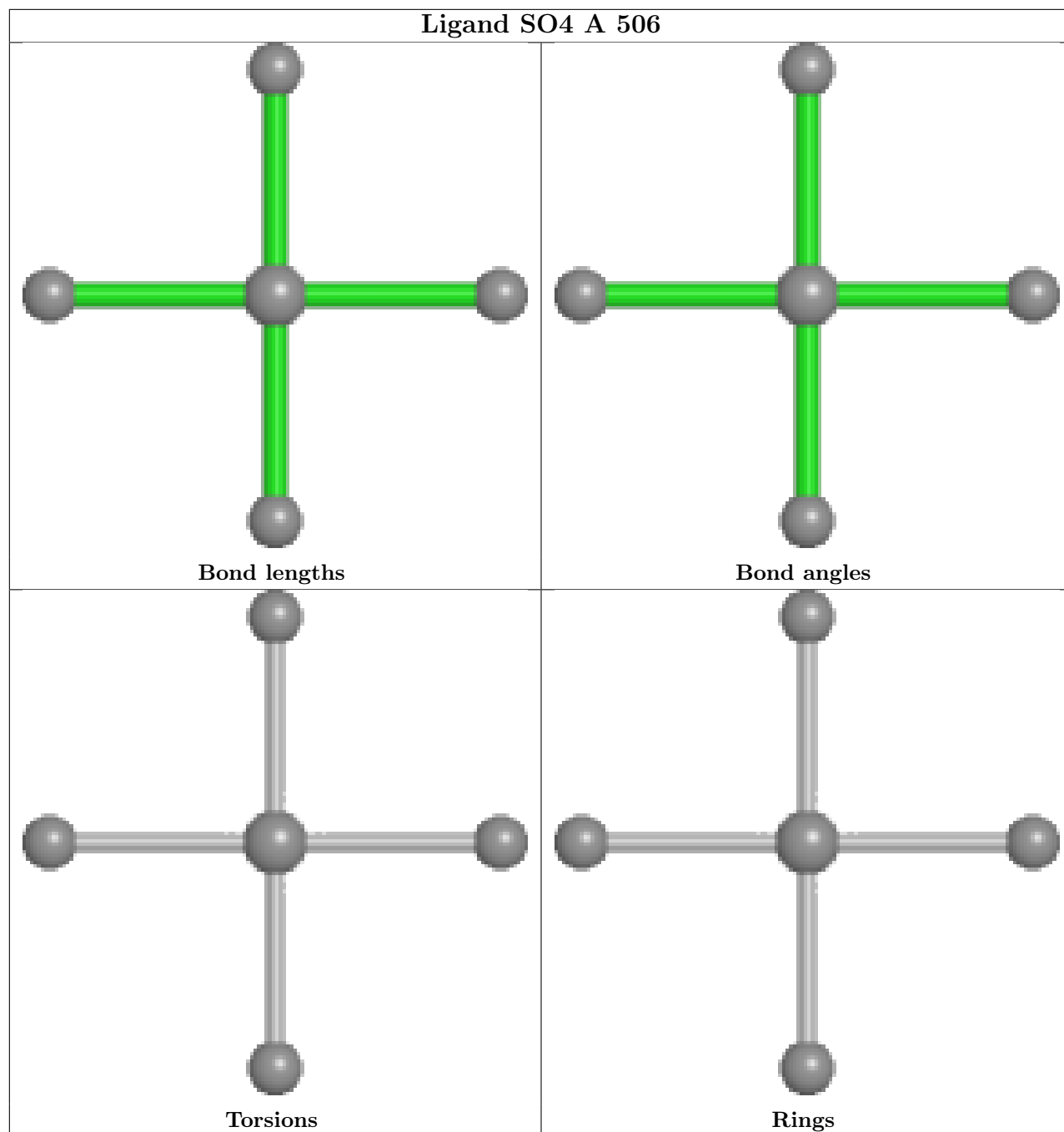
Torsions

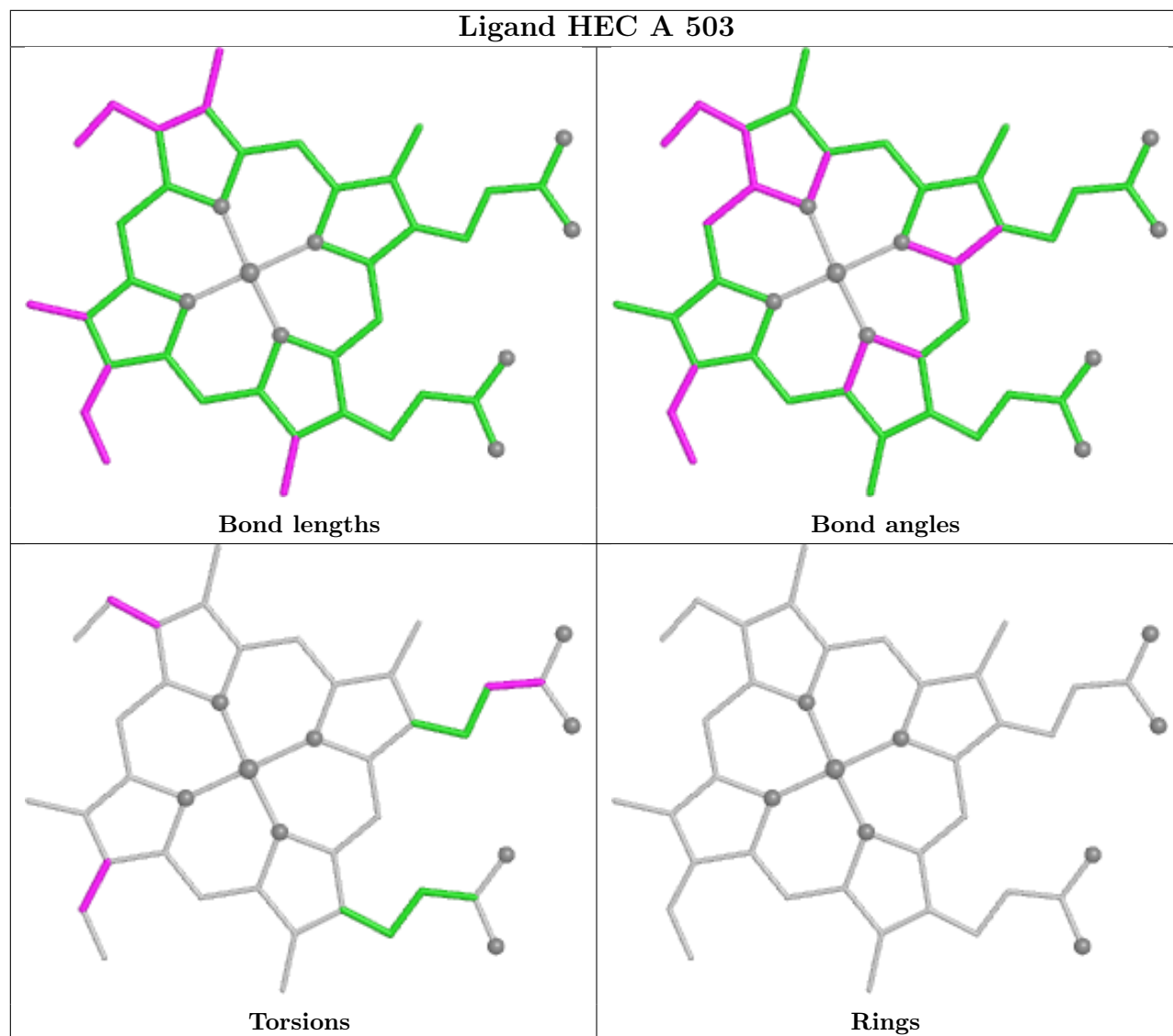


Rings

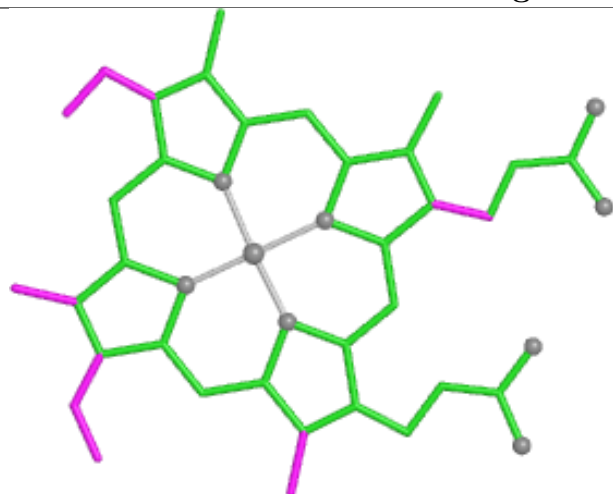




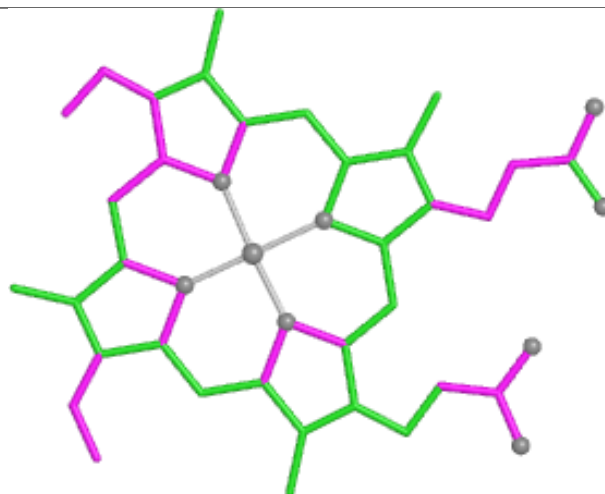




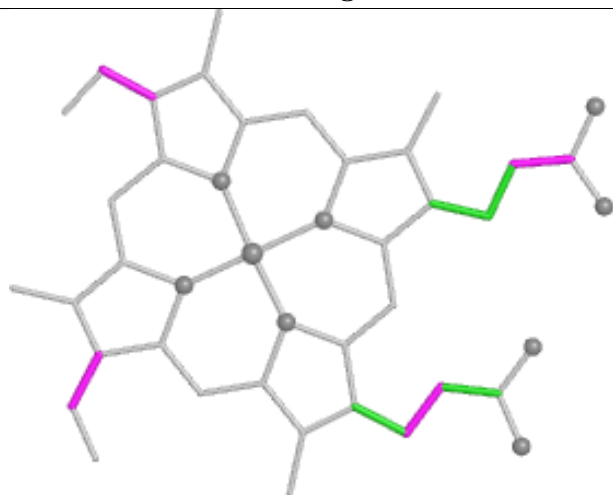
Ligand HEC C 507



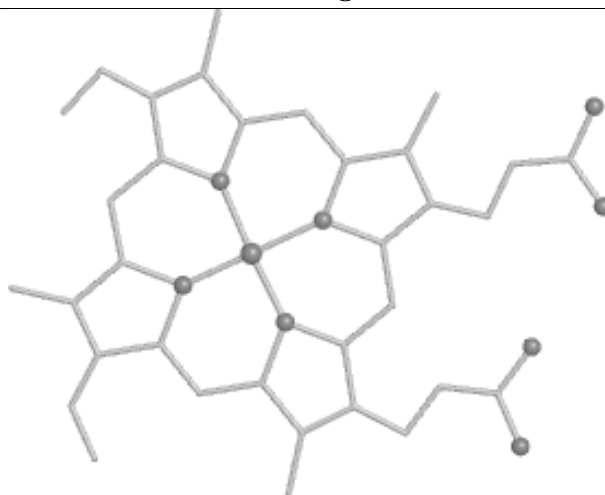
Bond lengths



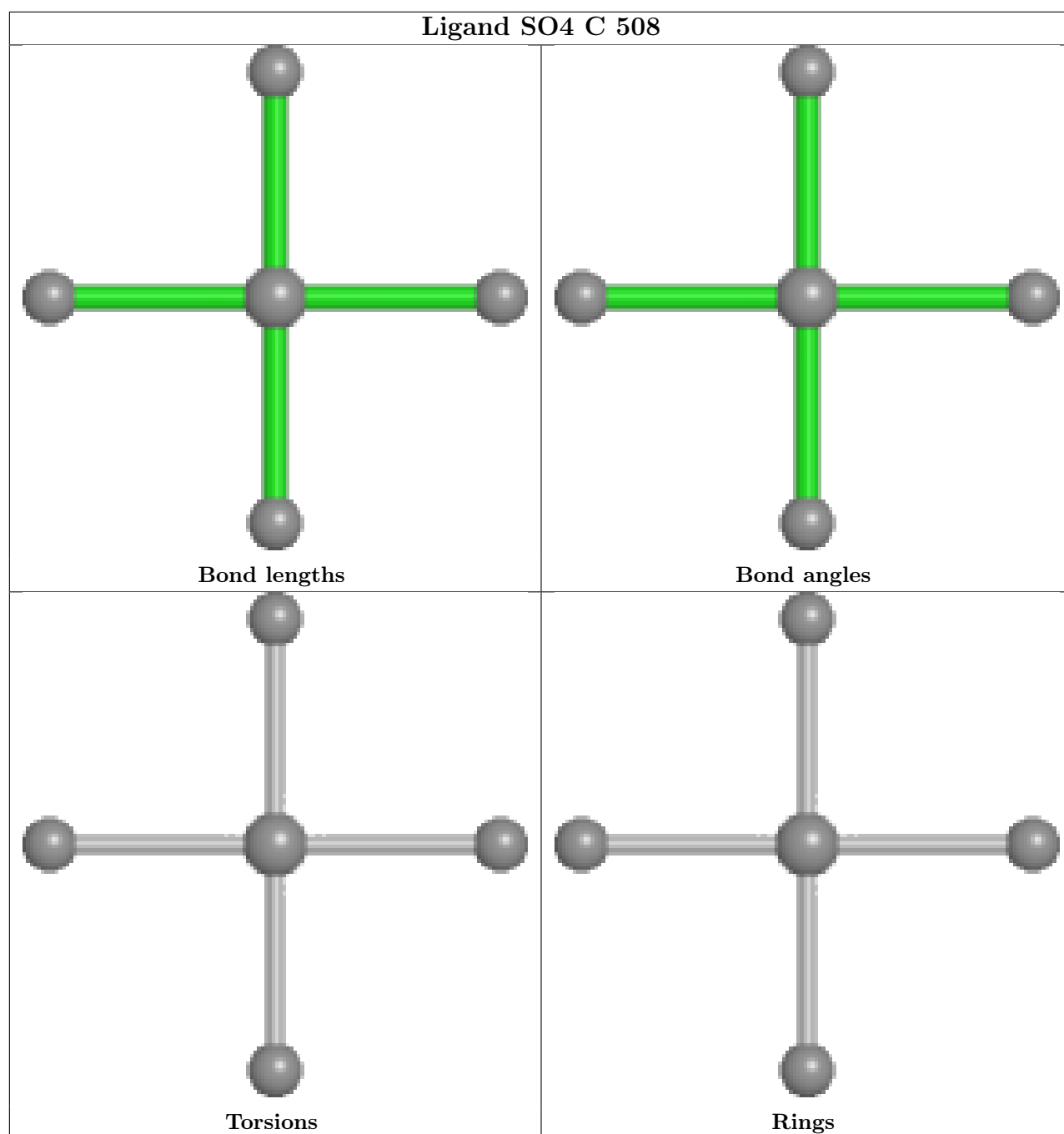
Bond angles

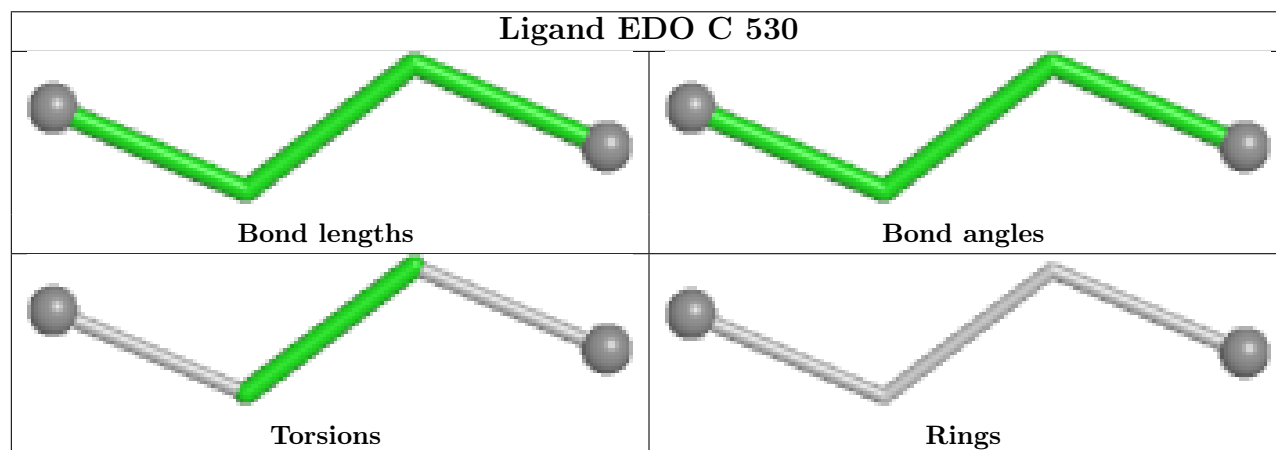
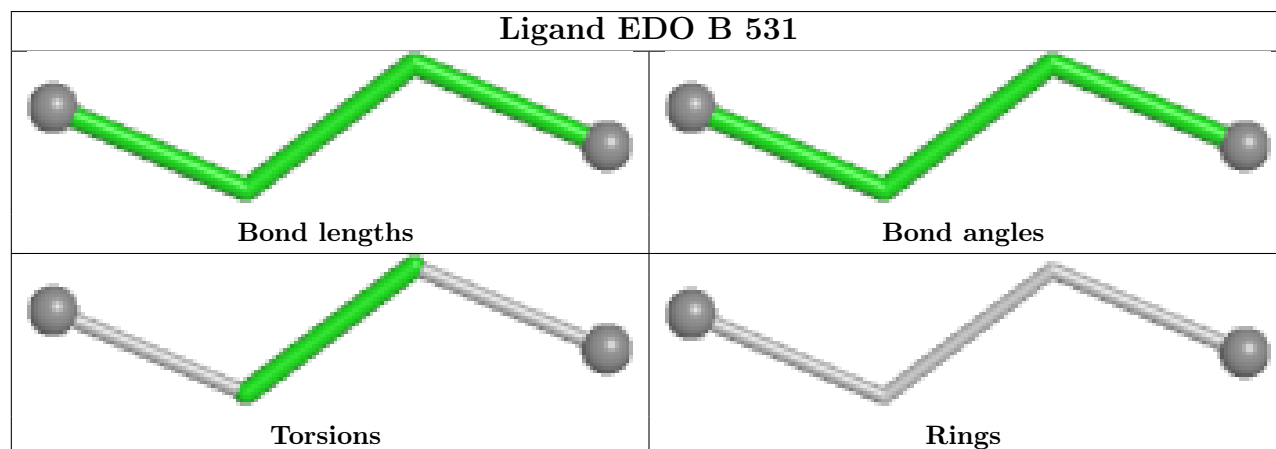
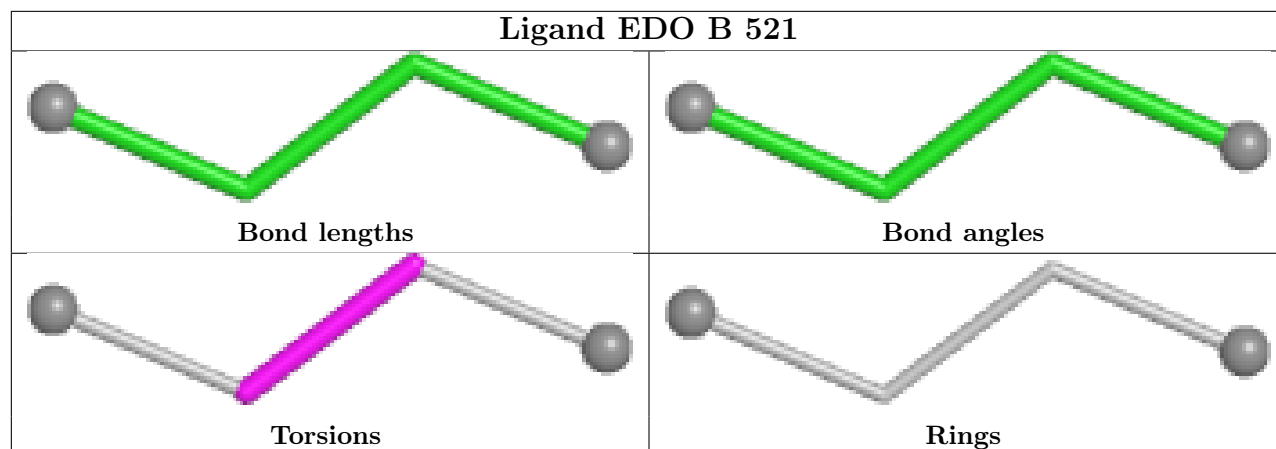


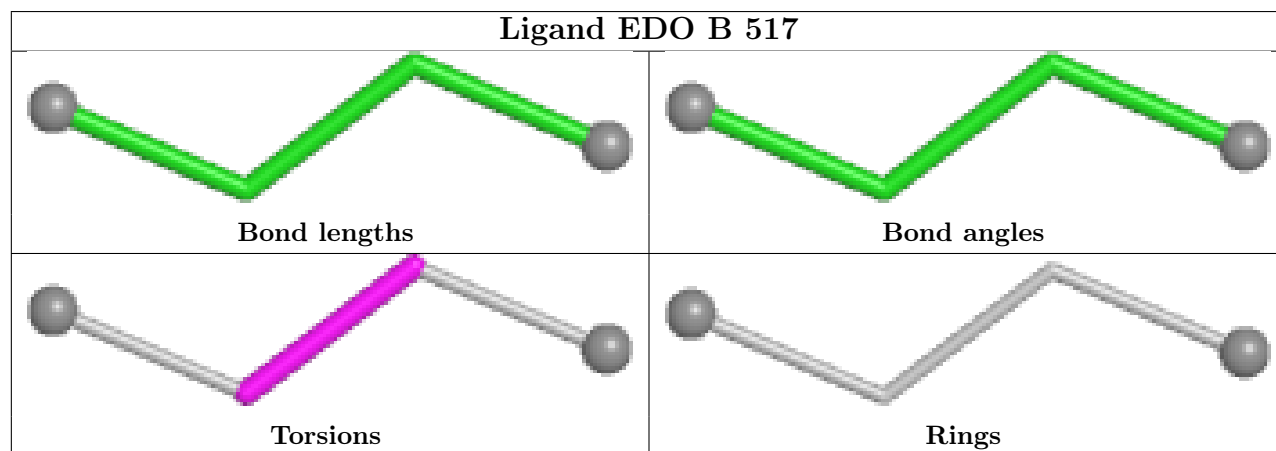
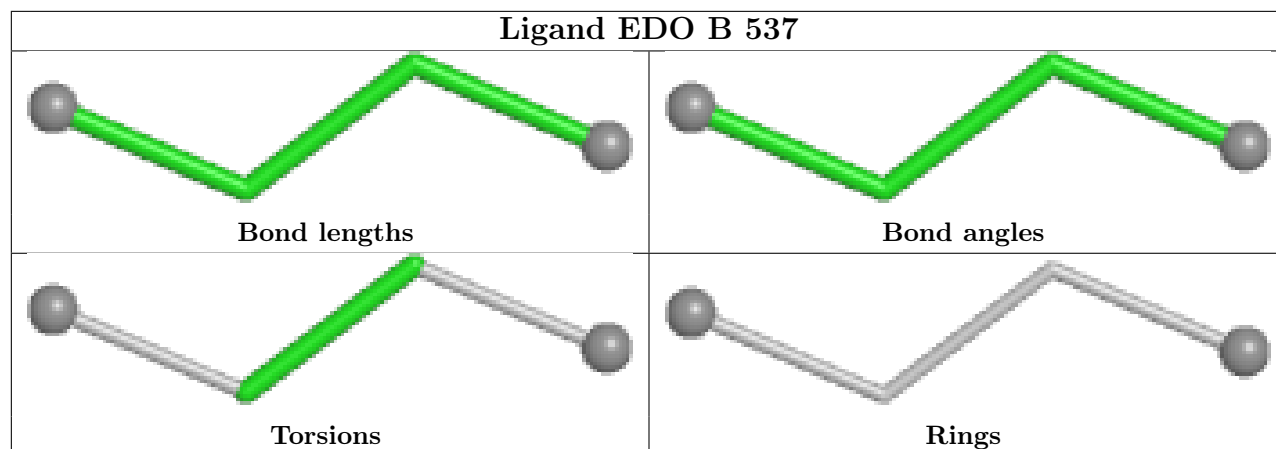
Torsions

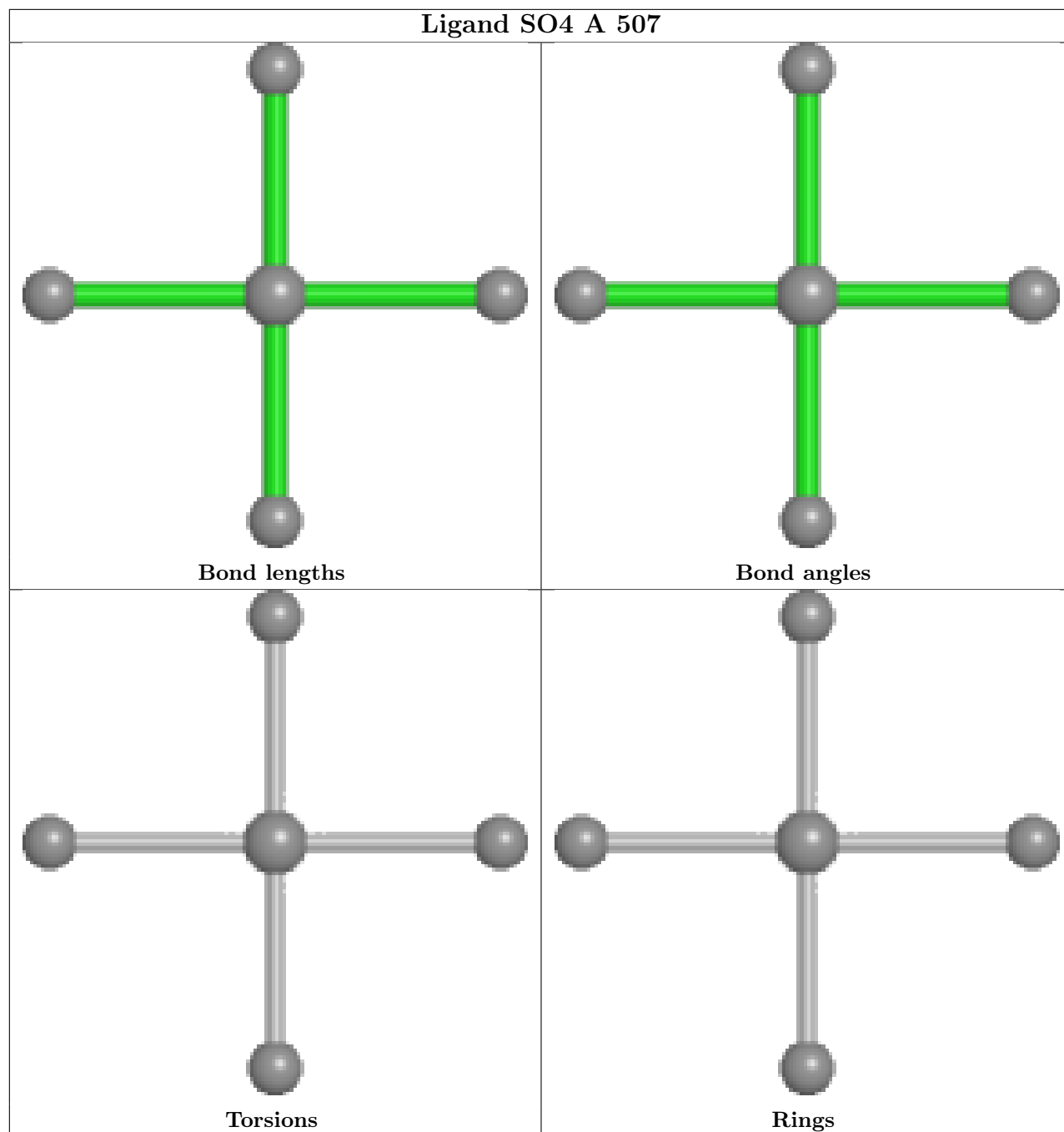


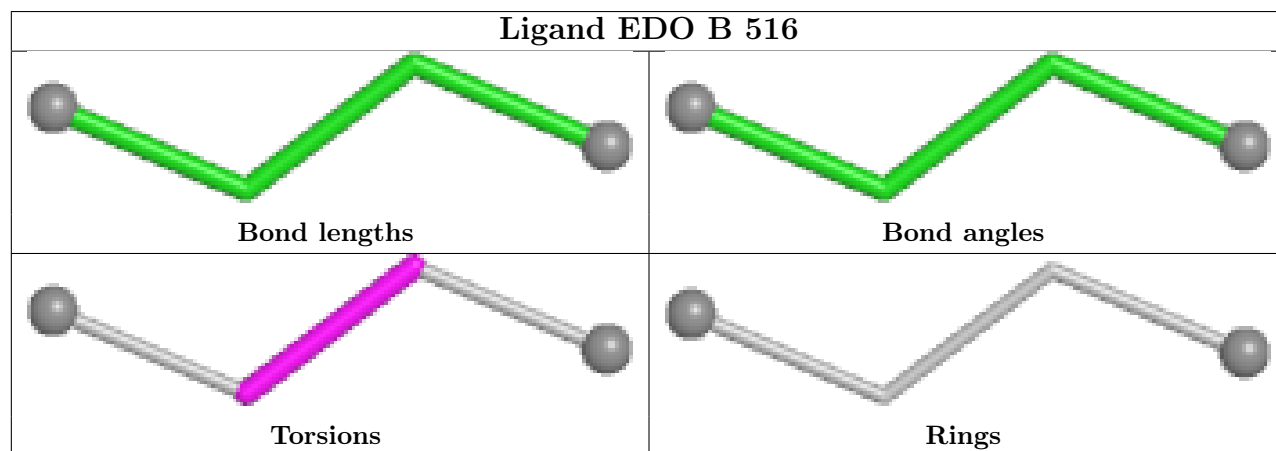
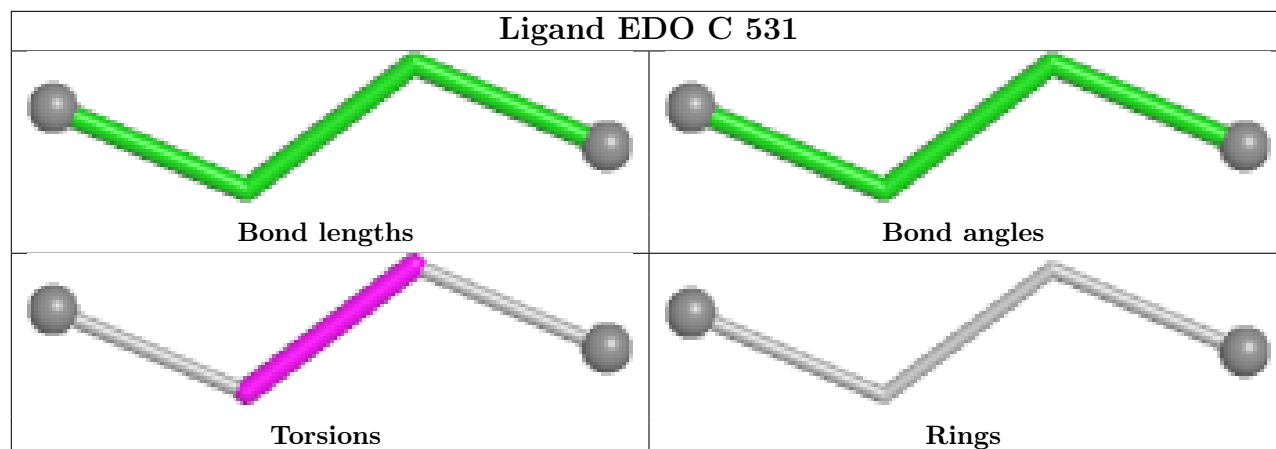
Rings

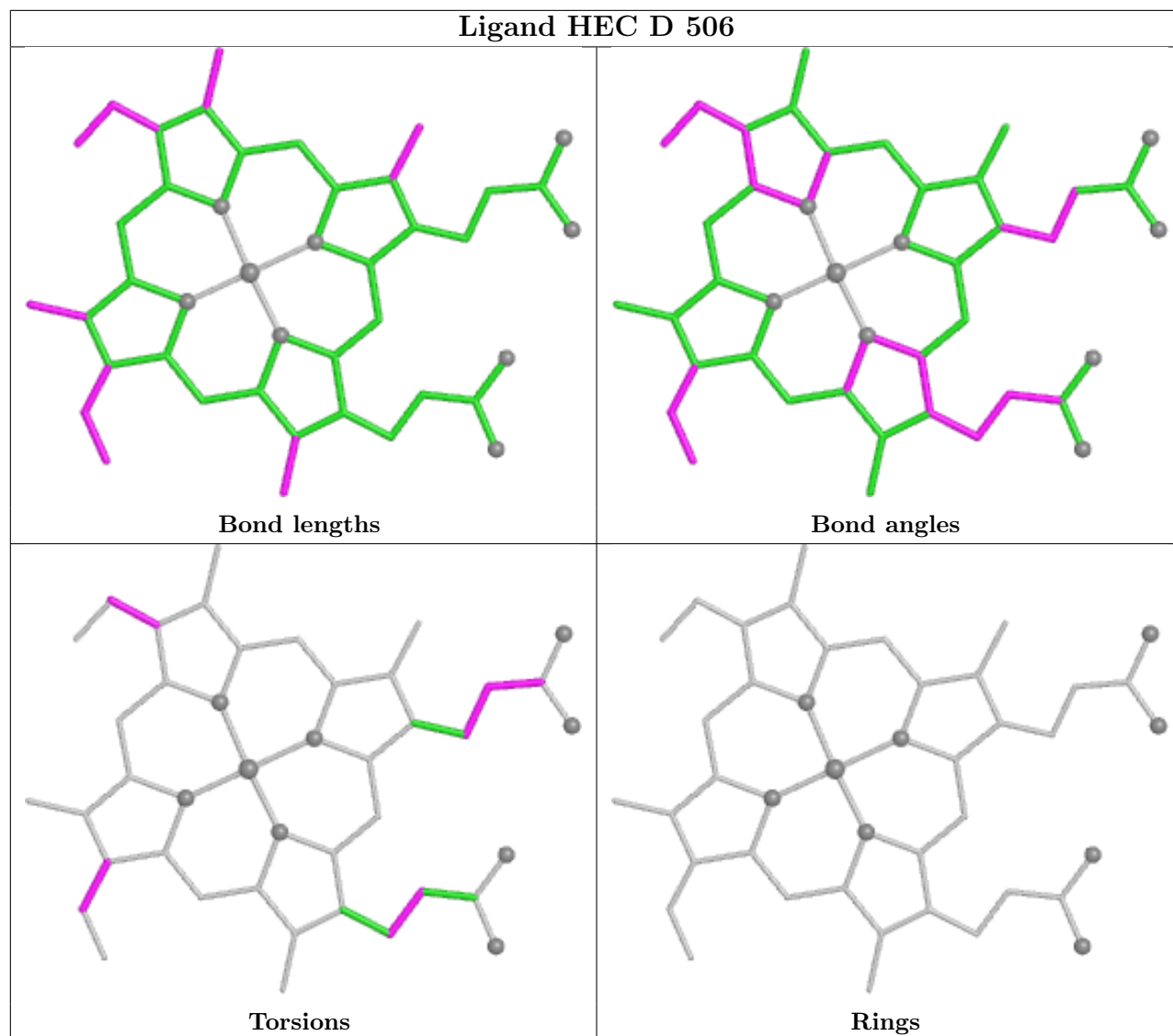


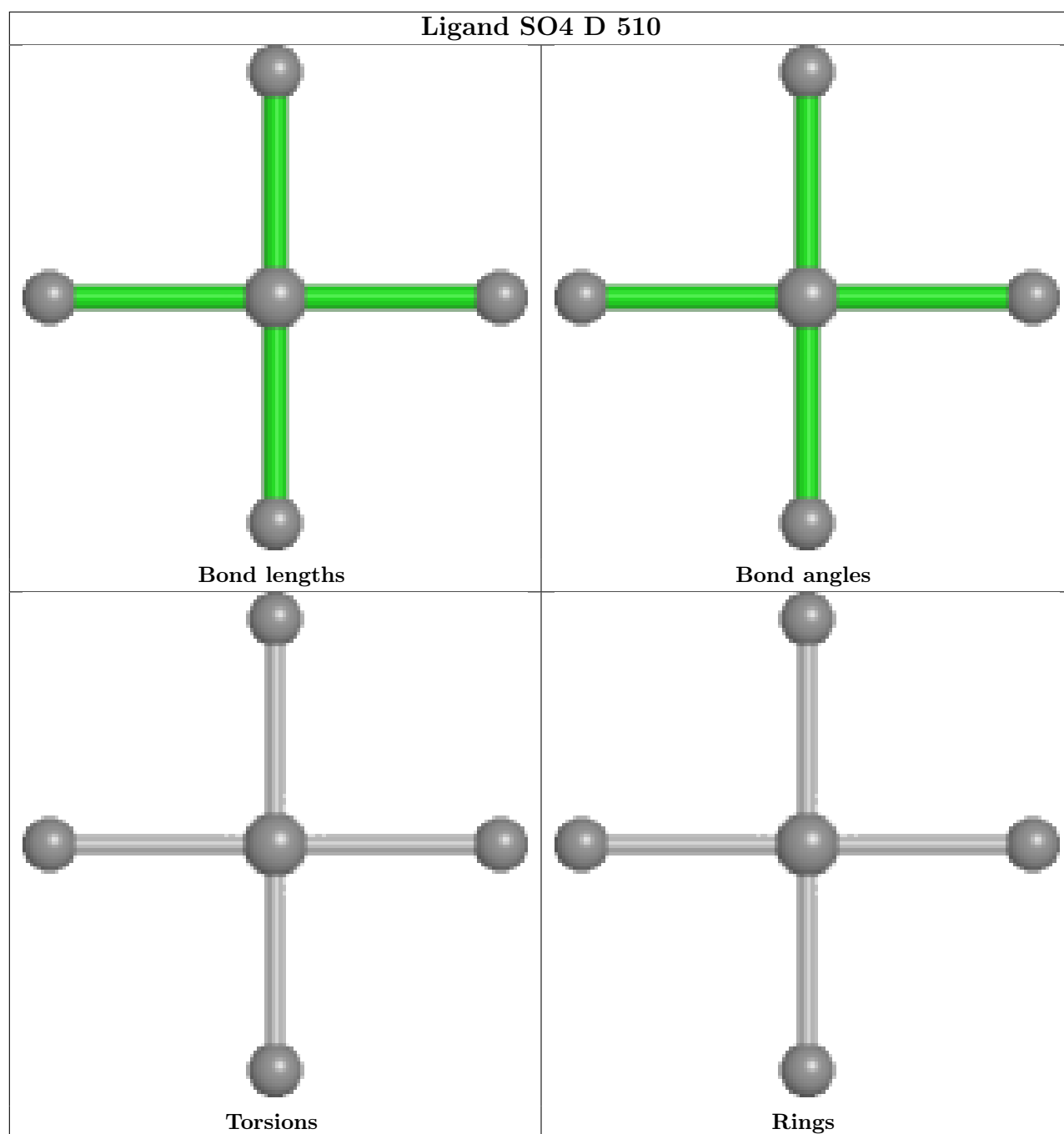


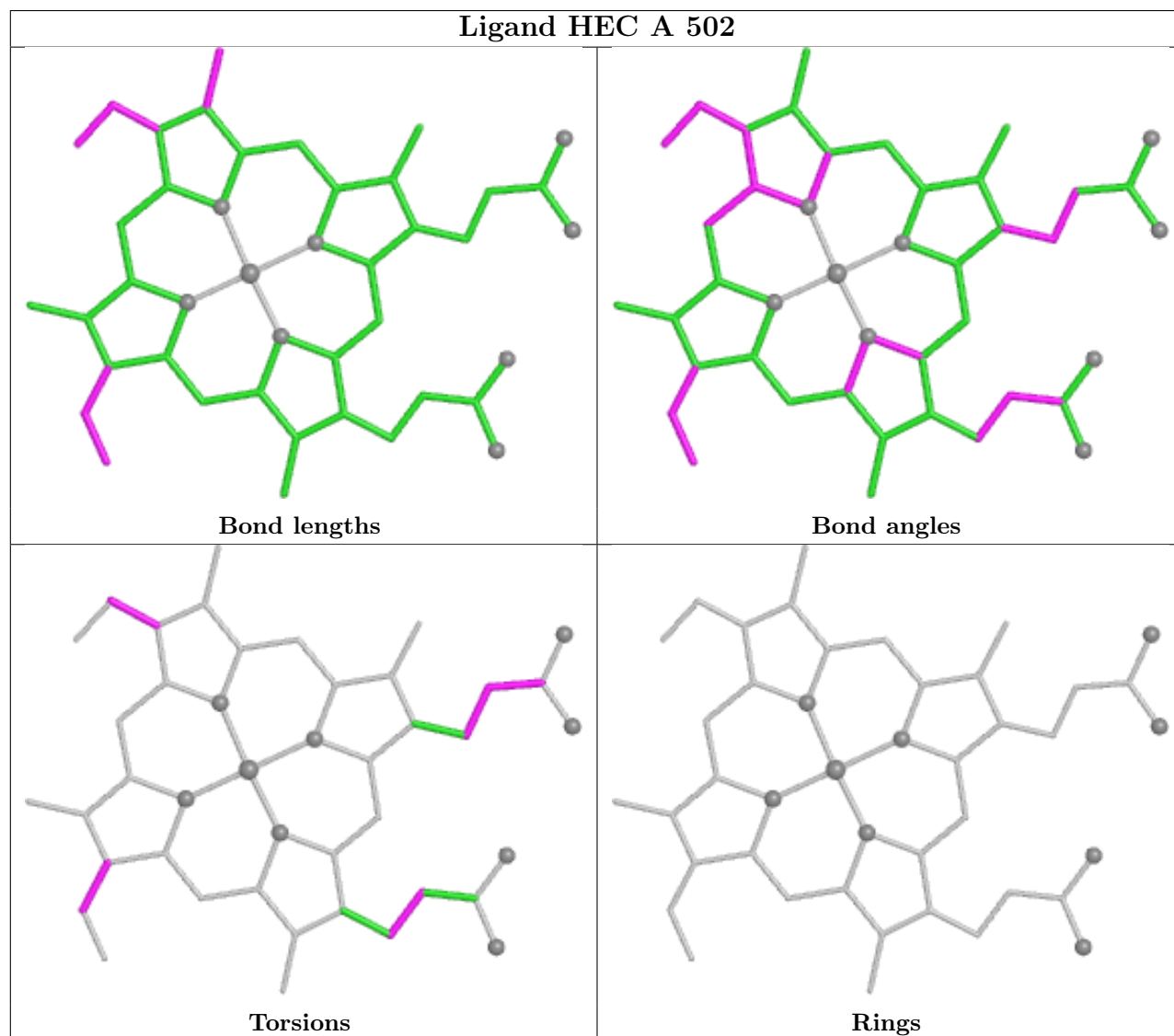
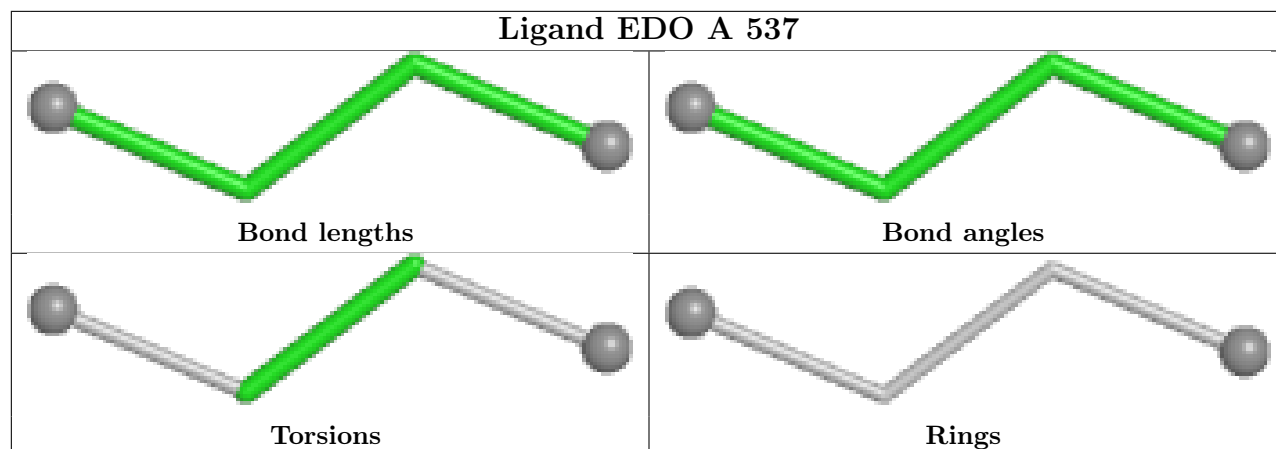


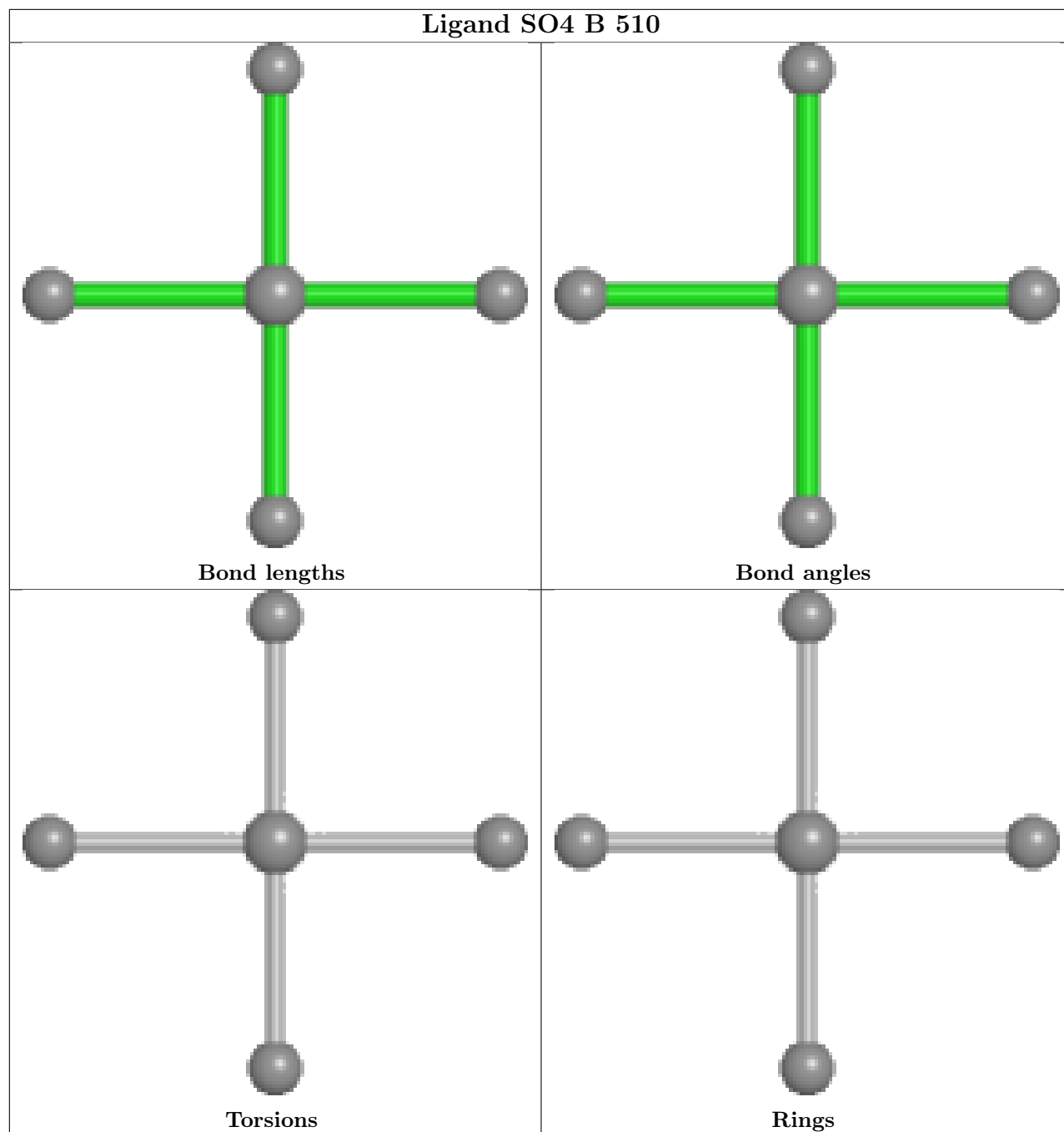




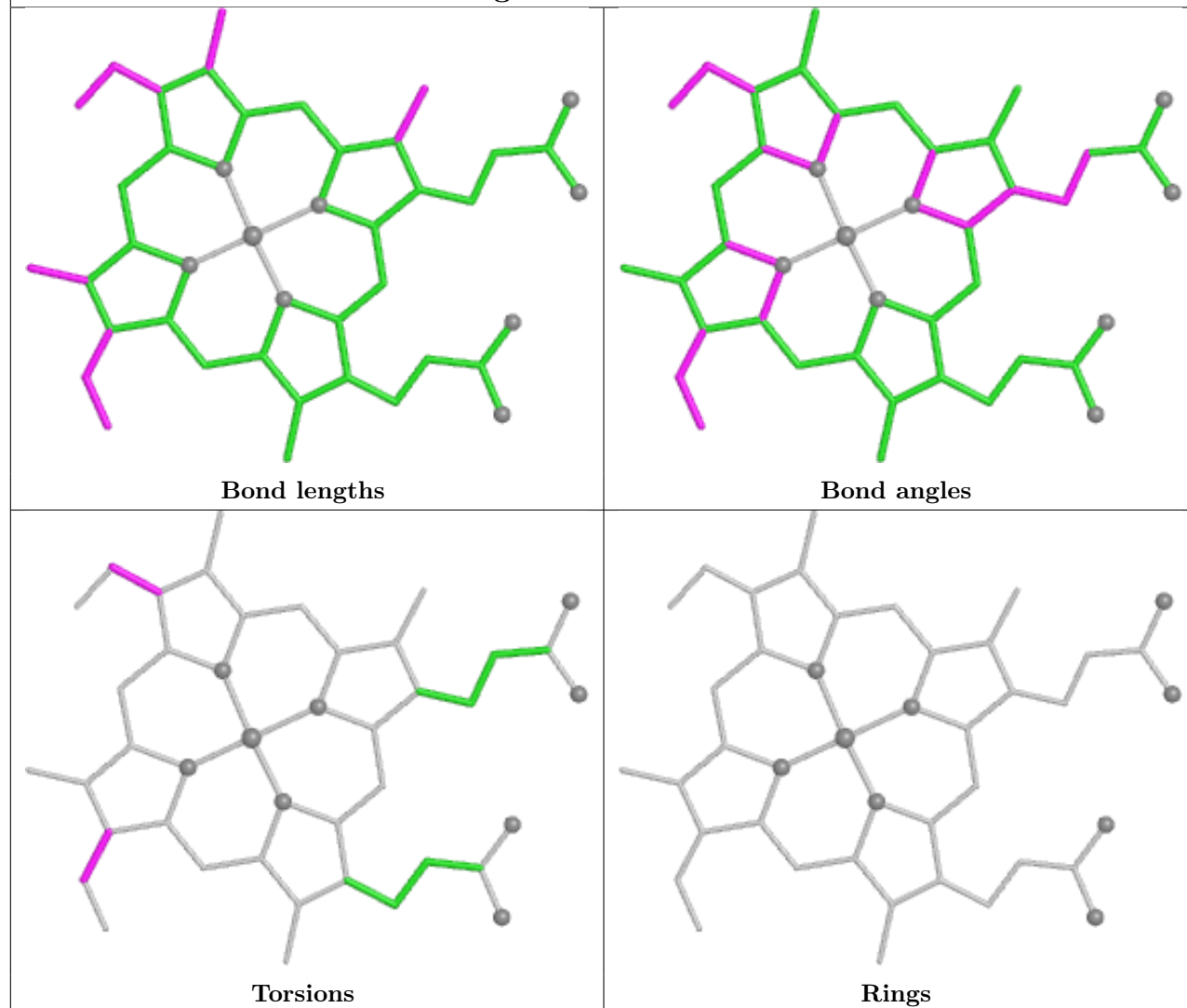




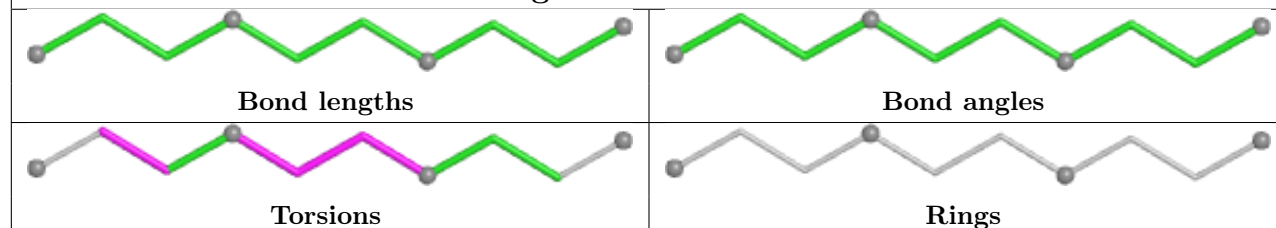


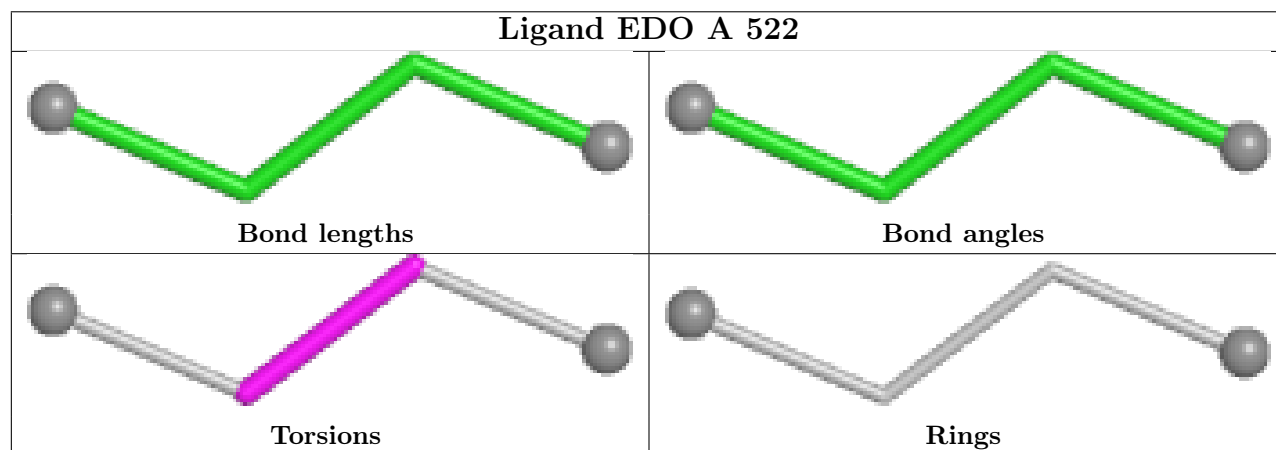
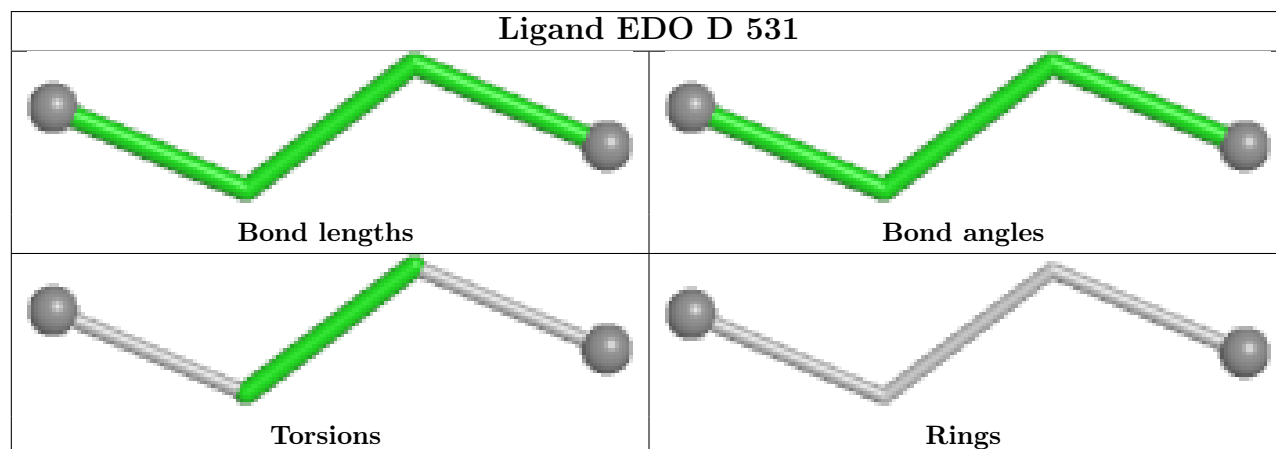
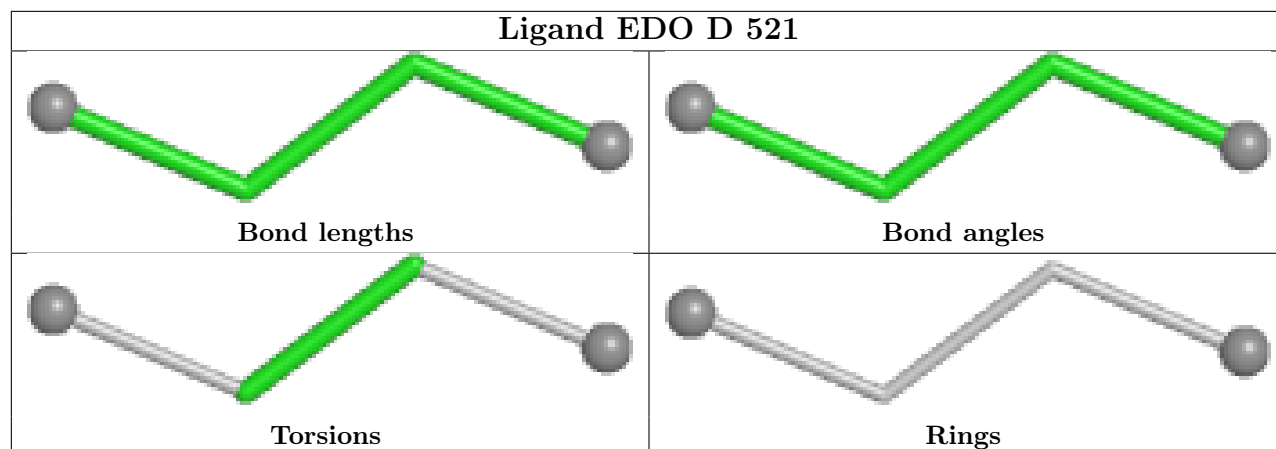


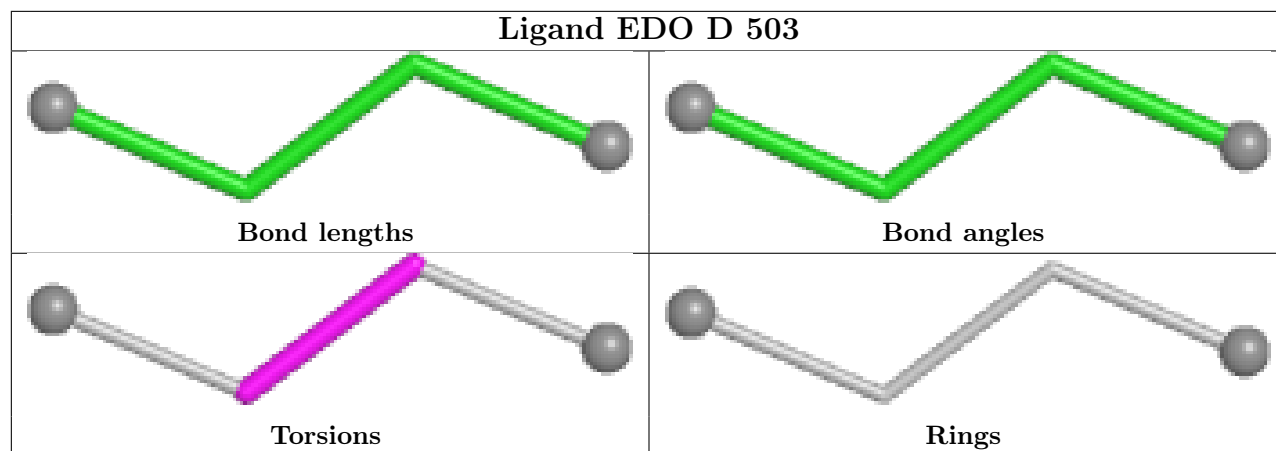
Ligand HEC B 505

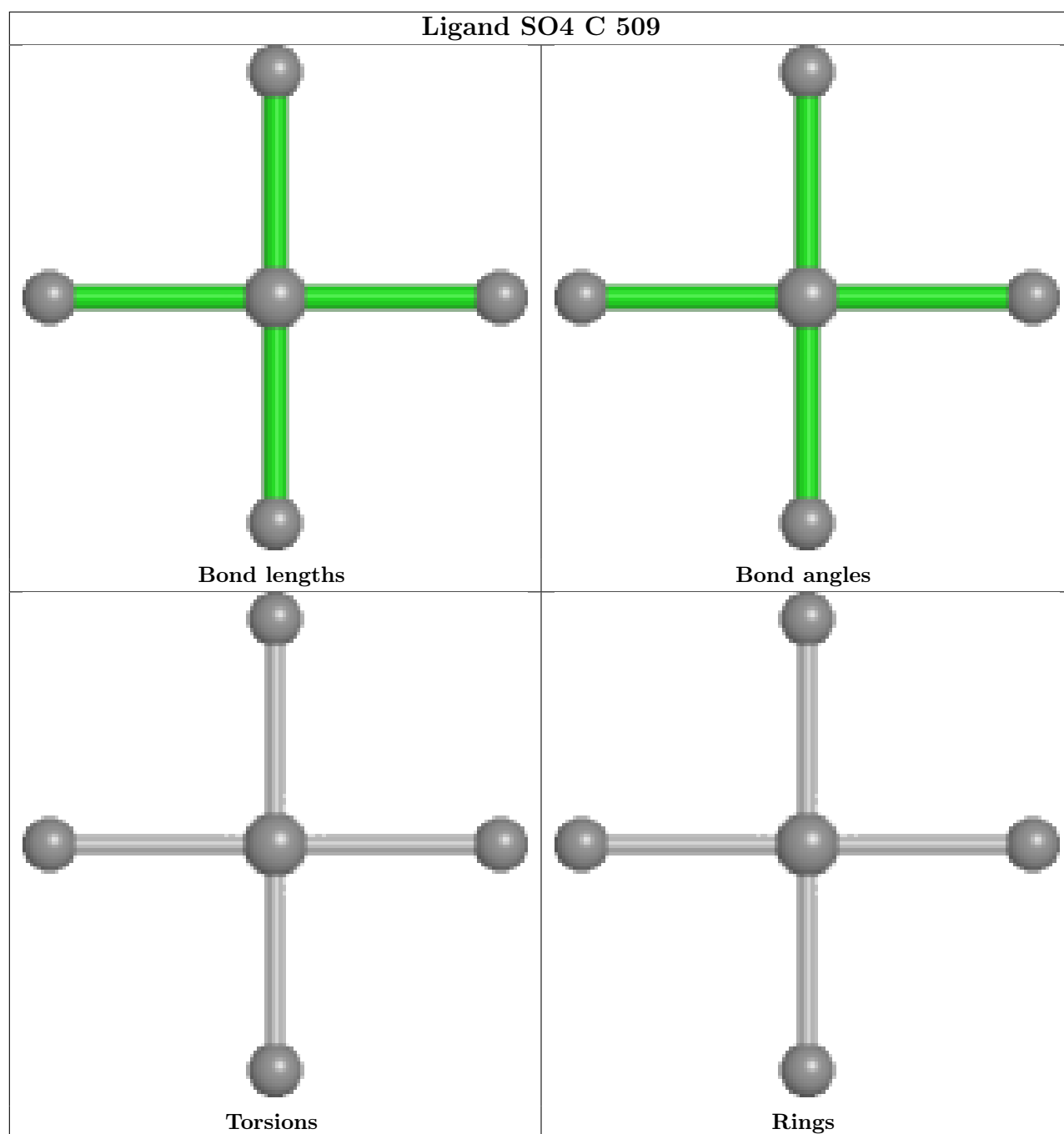


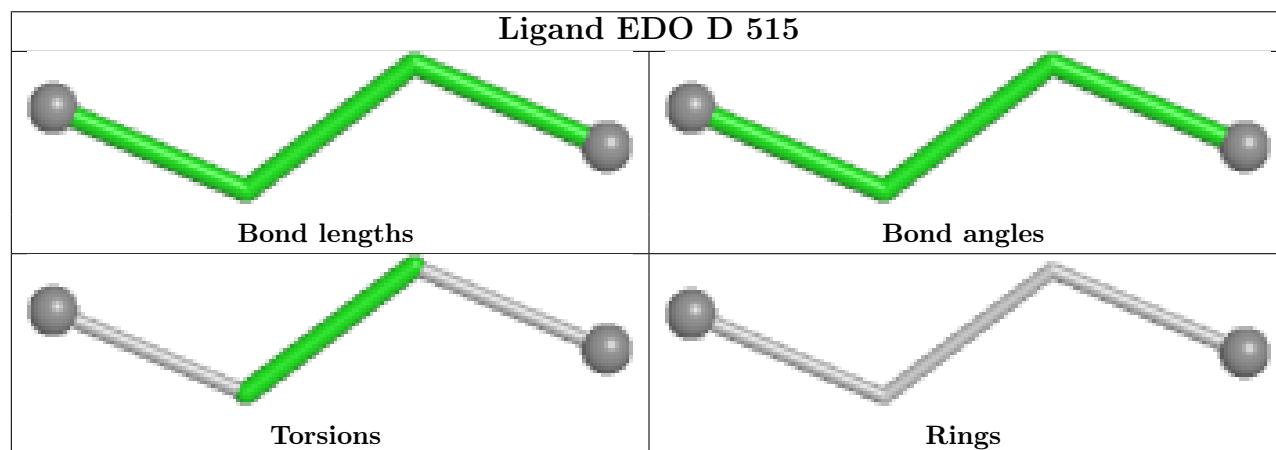
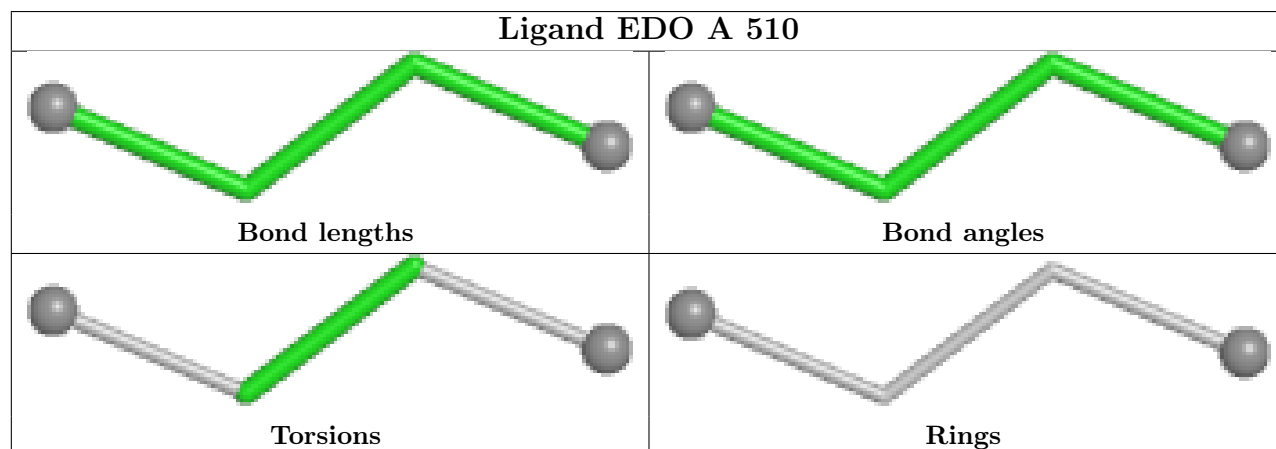
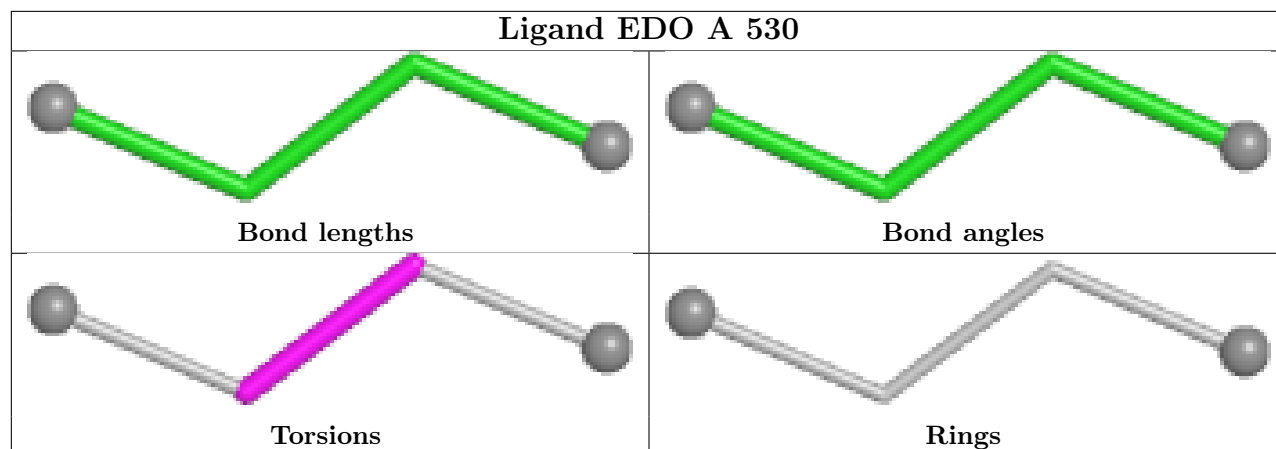
Ligand PGE B 539

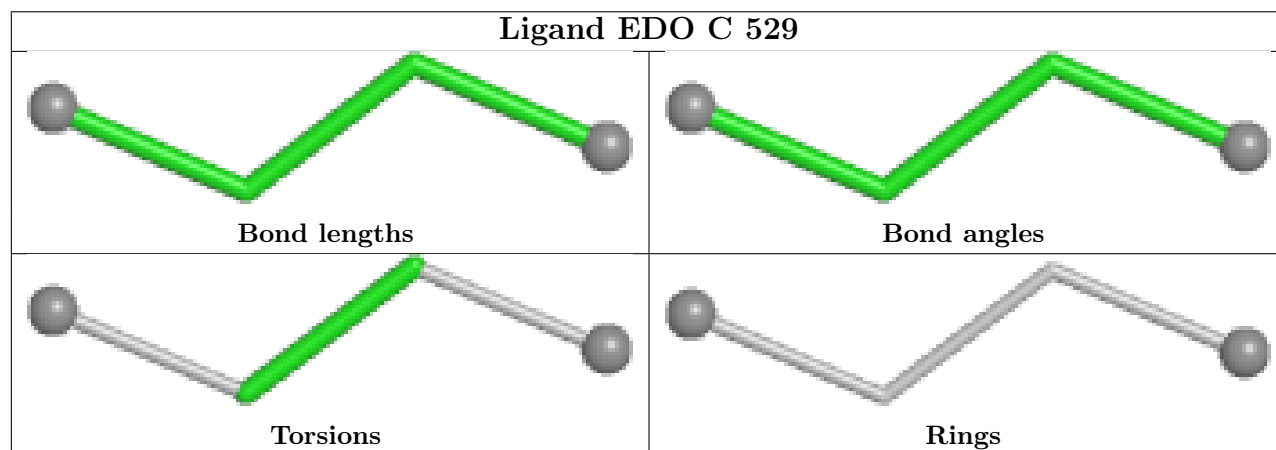
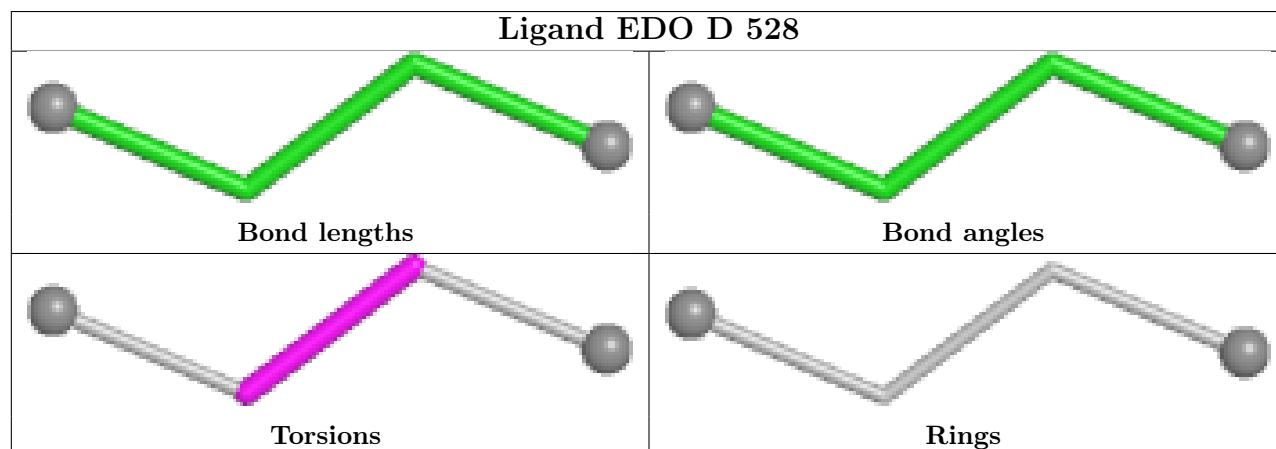
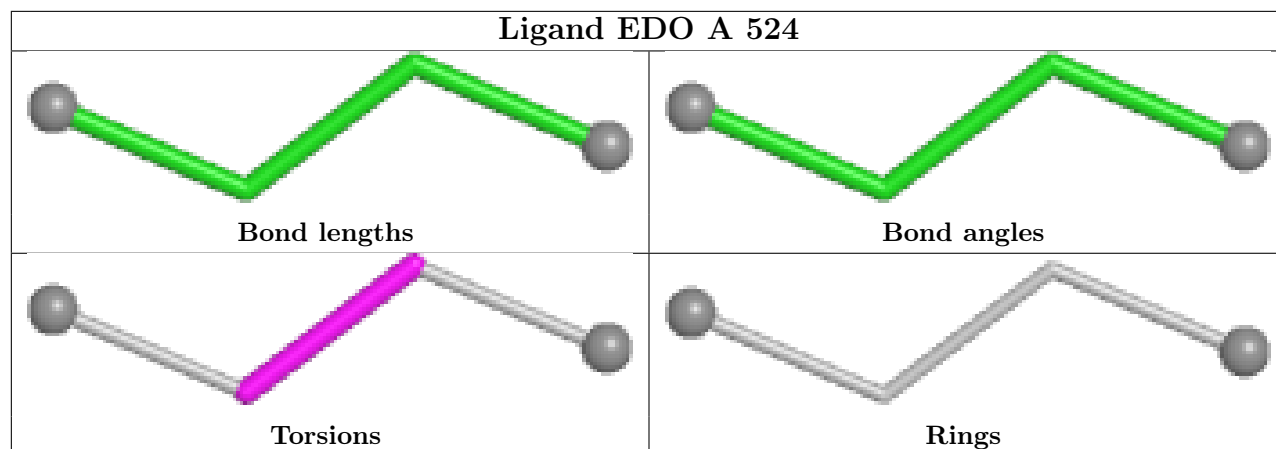


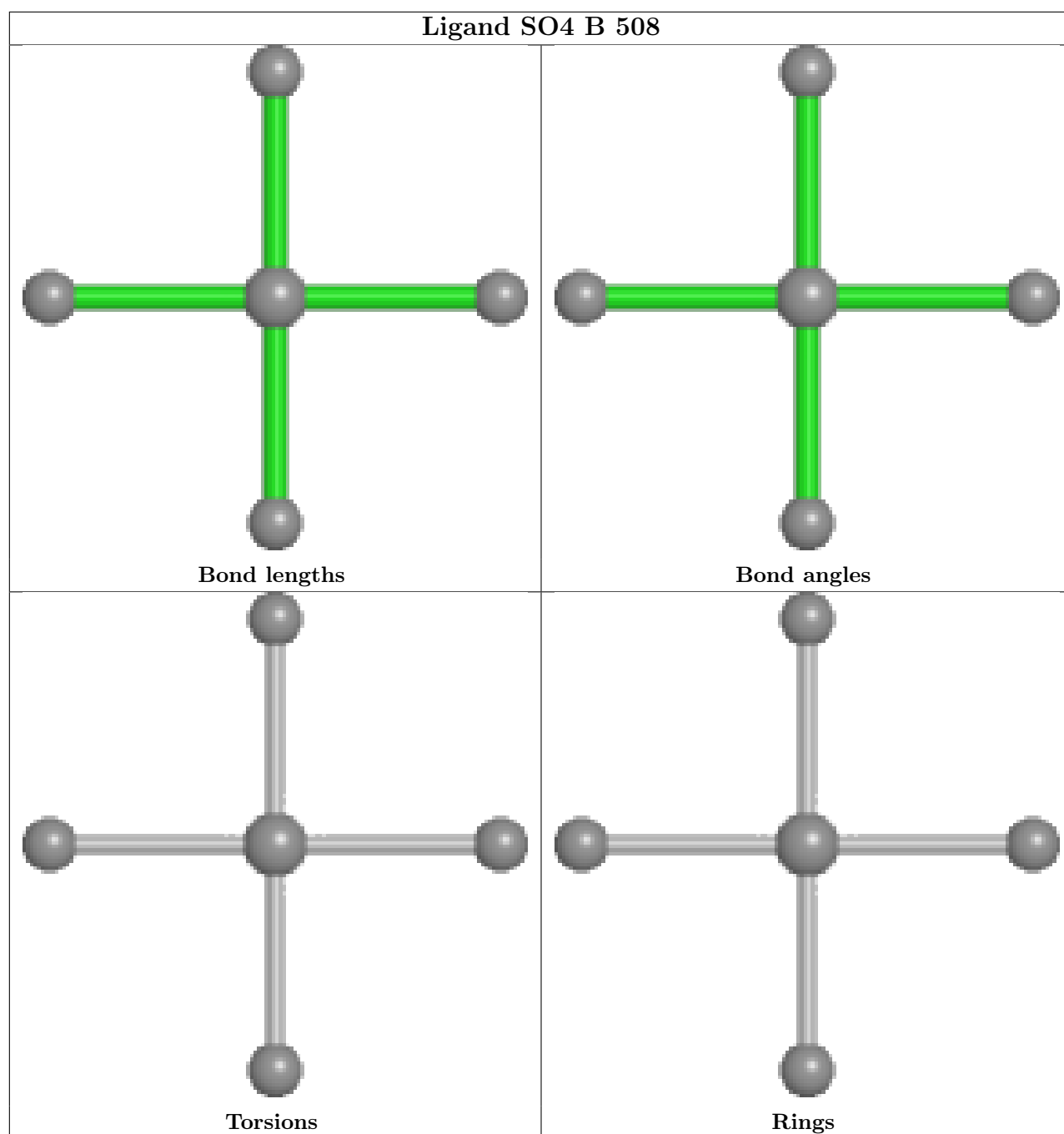


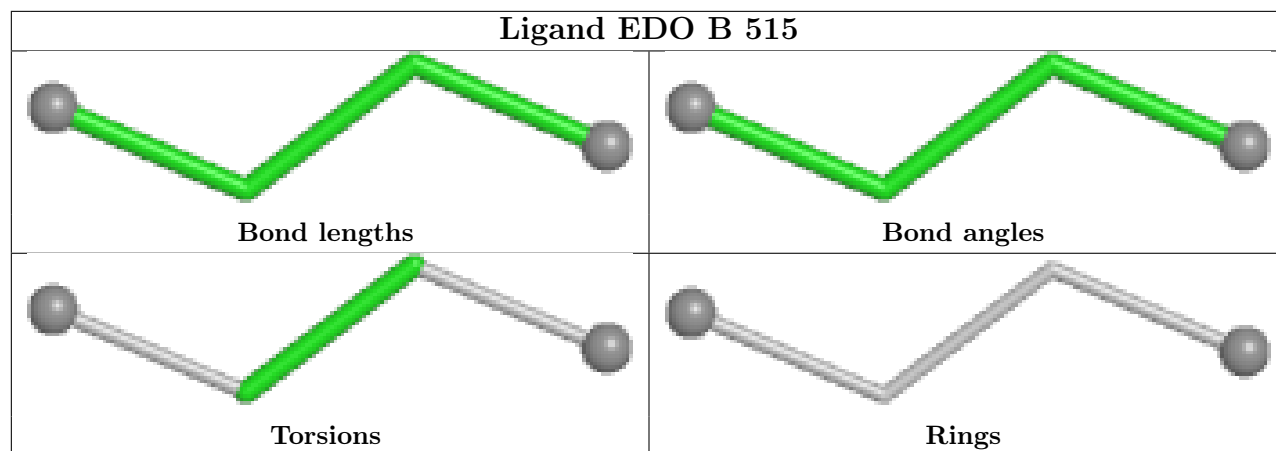


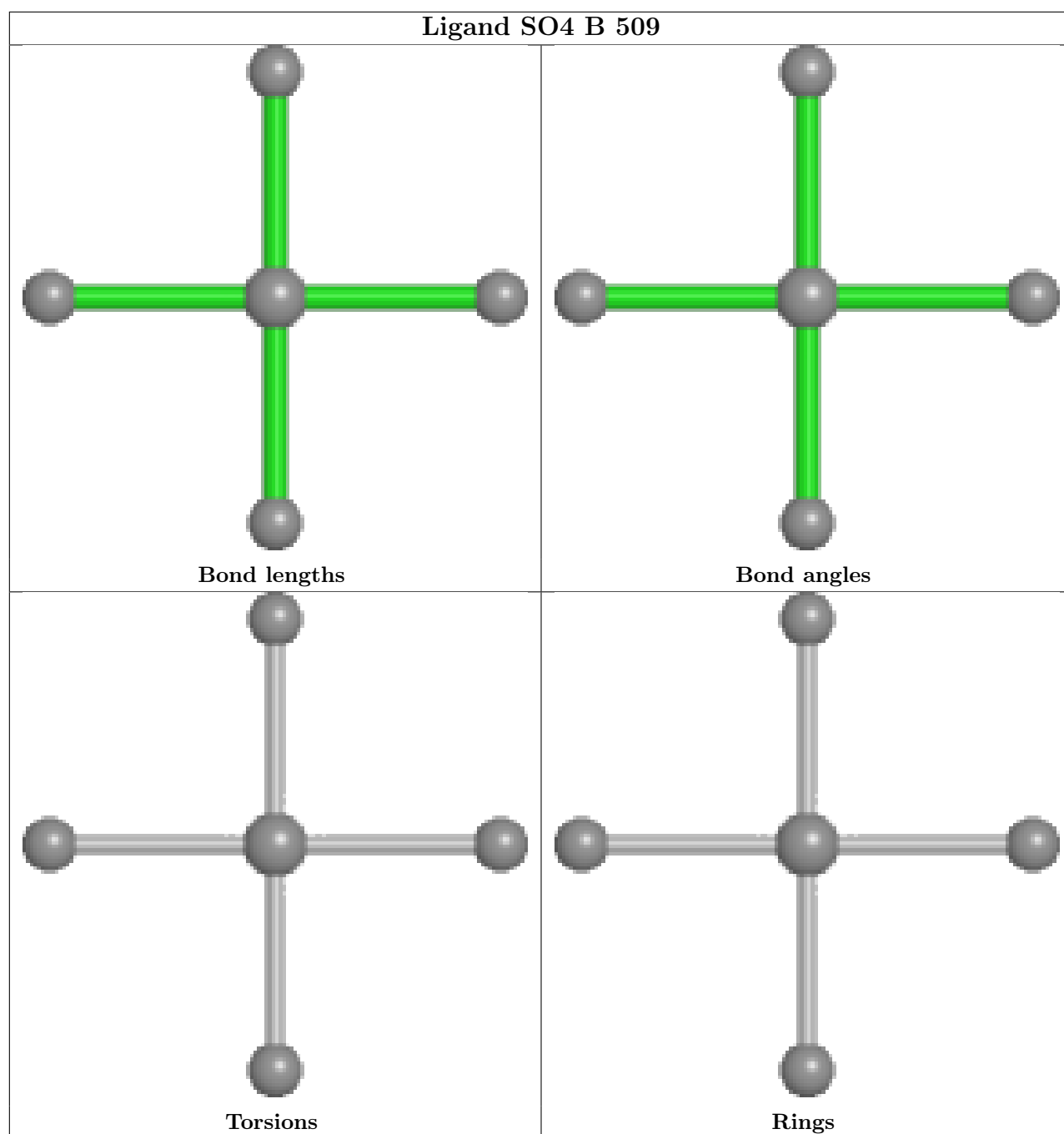


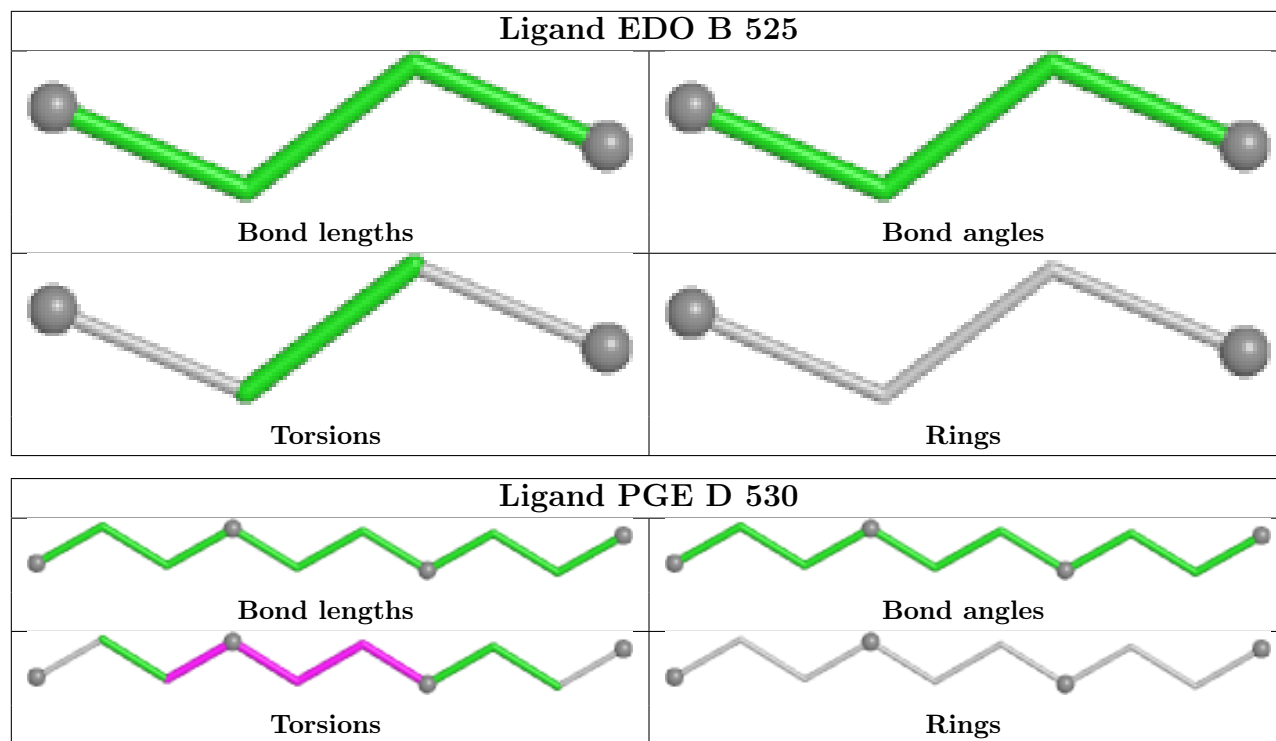


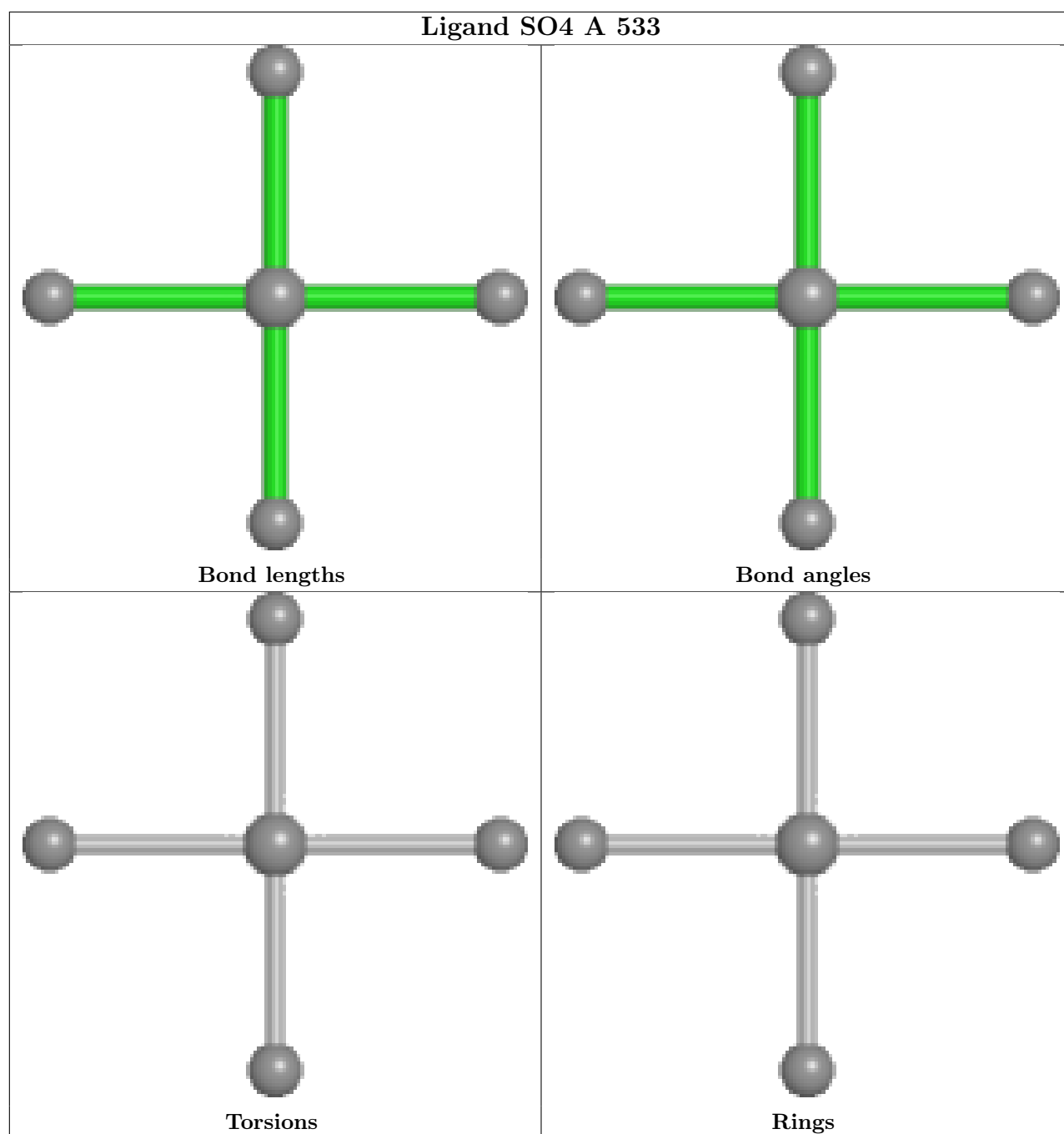


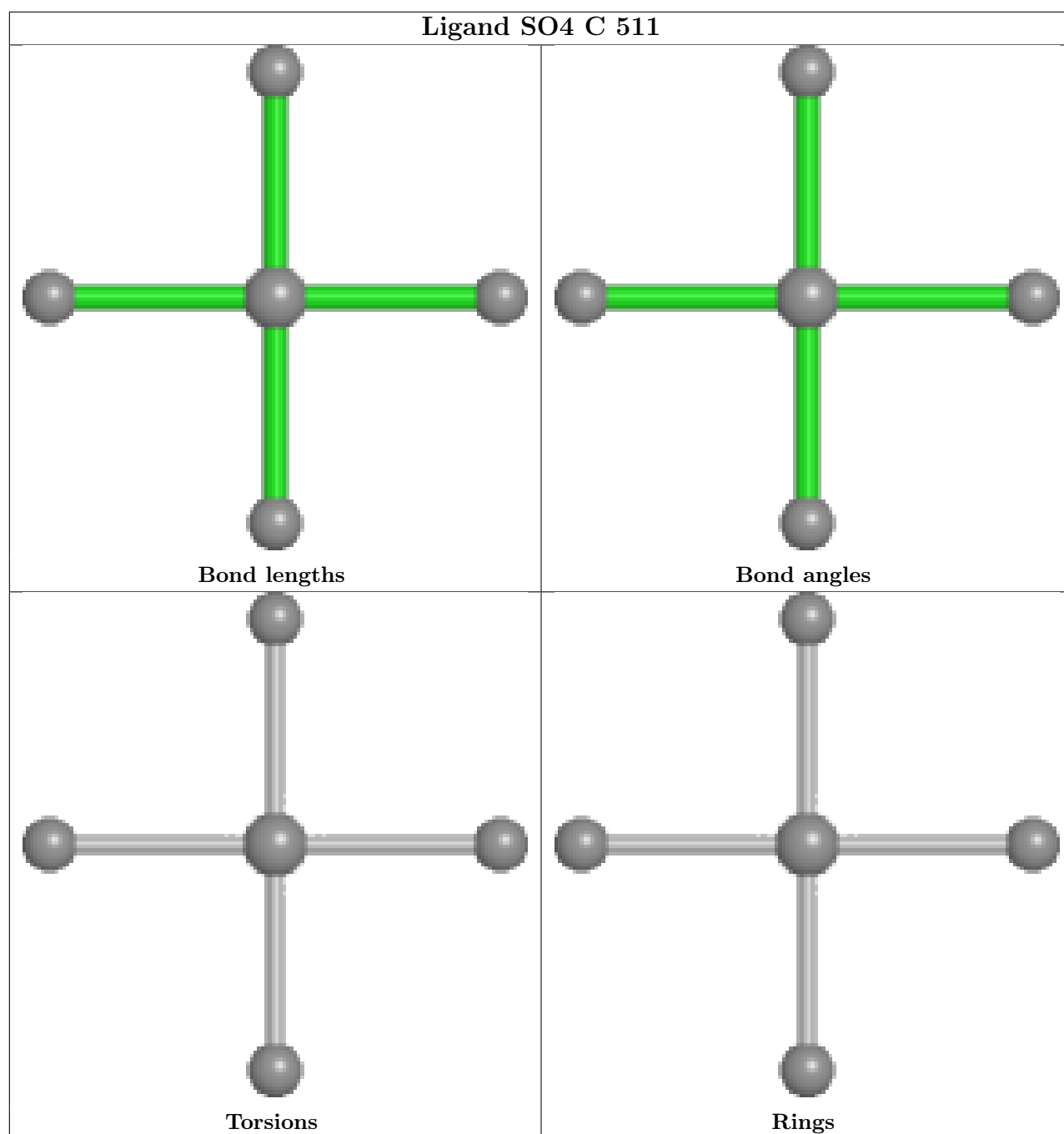


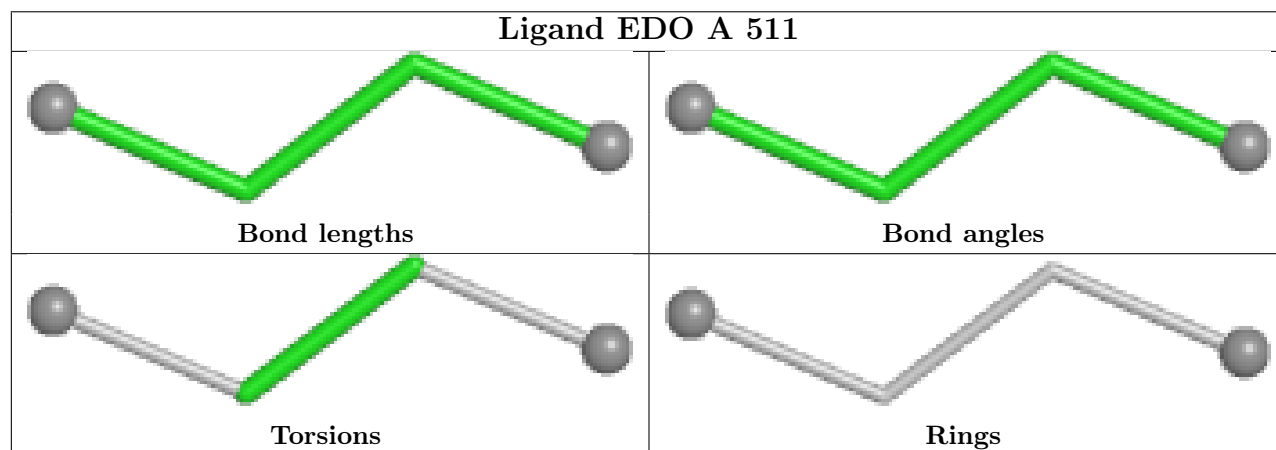
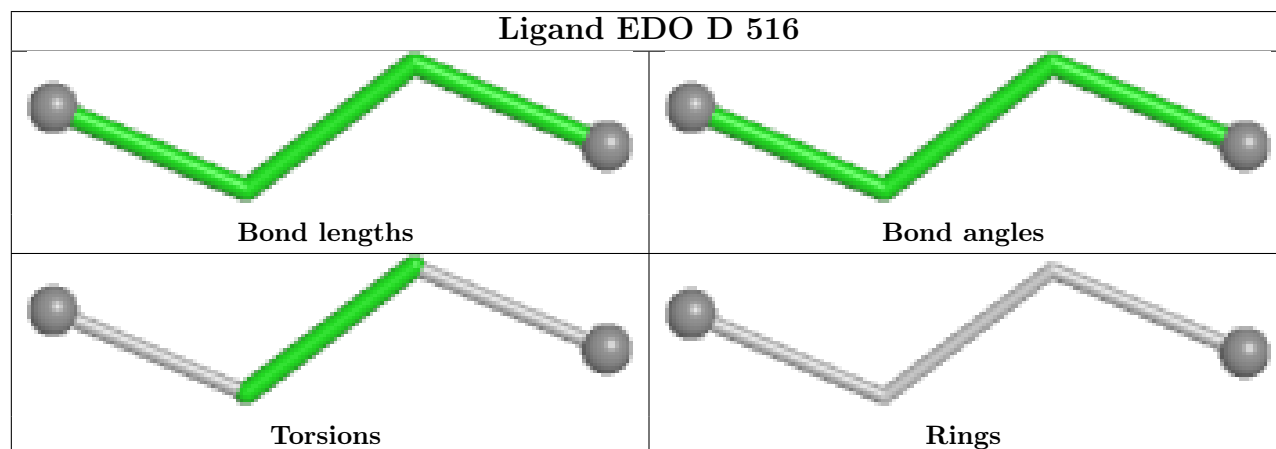
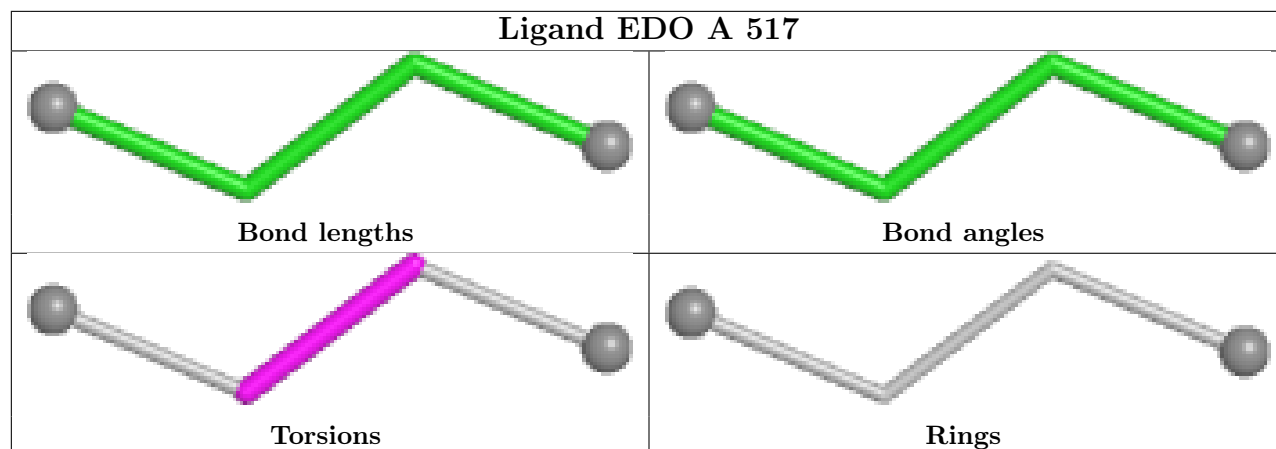


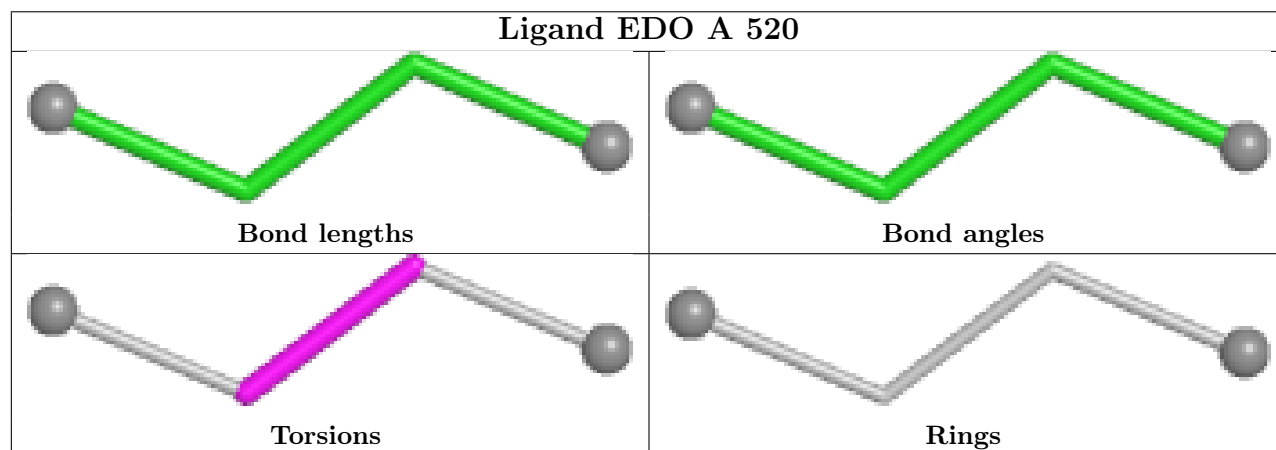
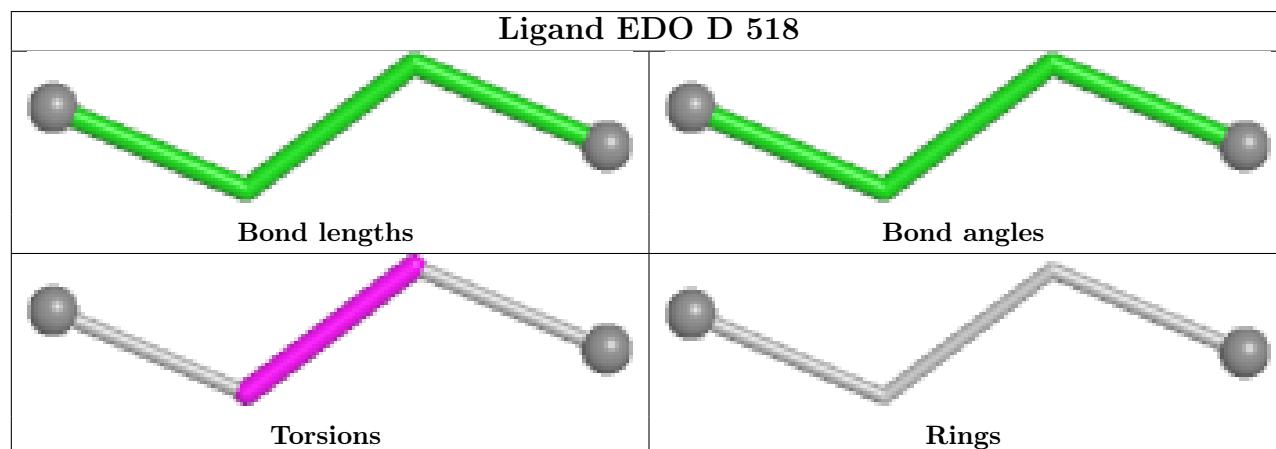
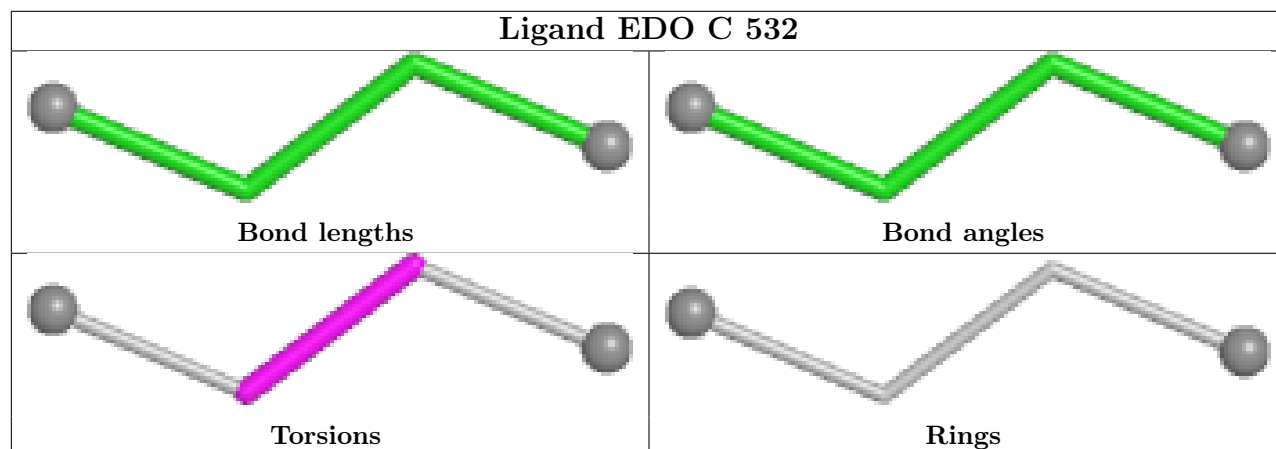


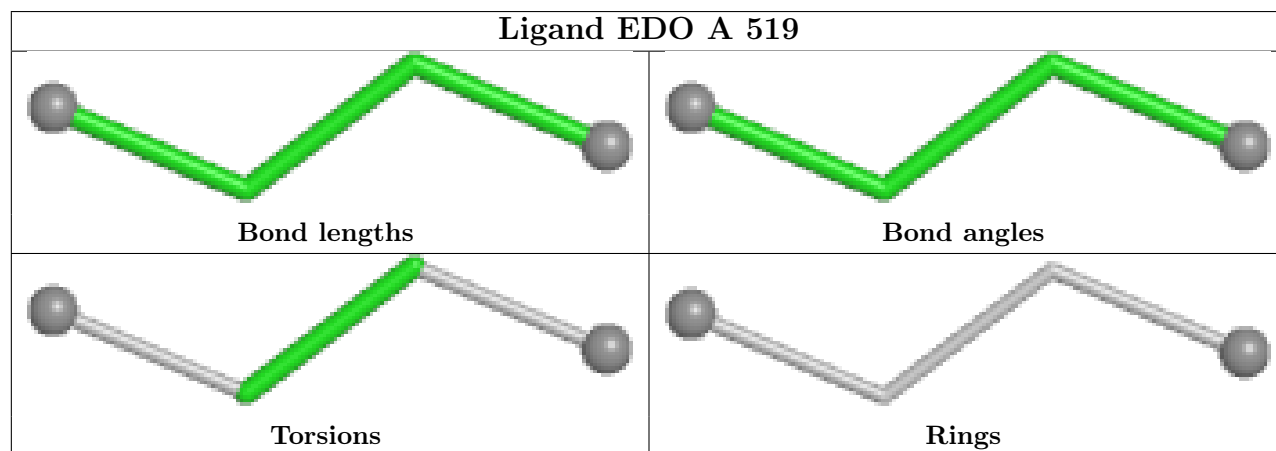
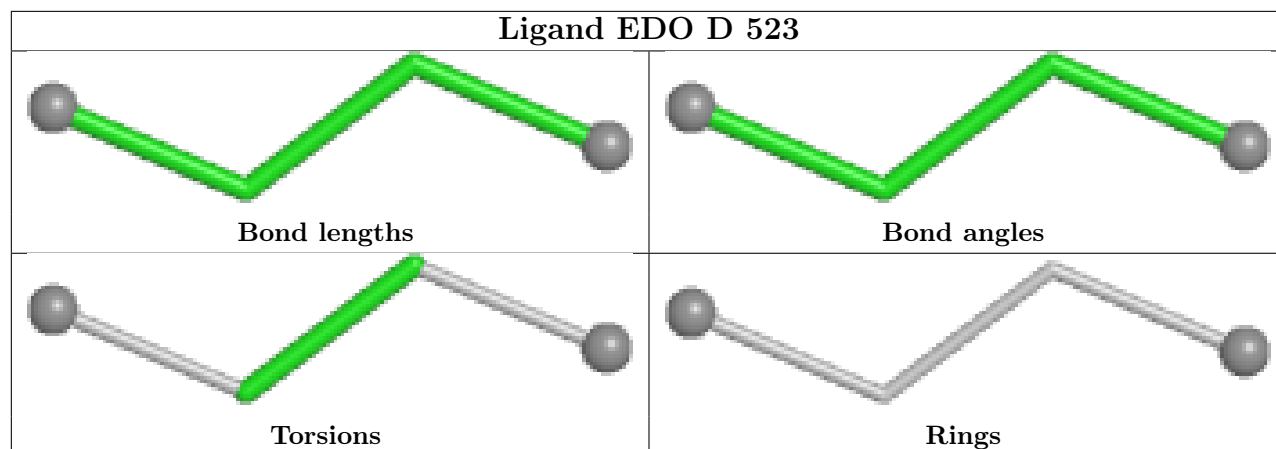


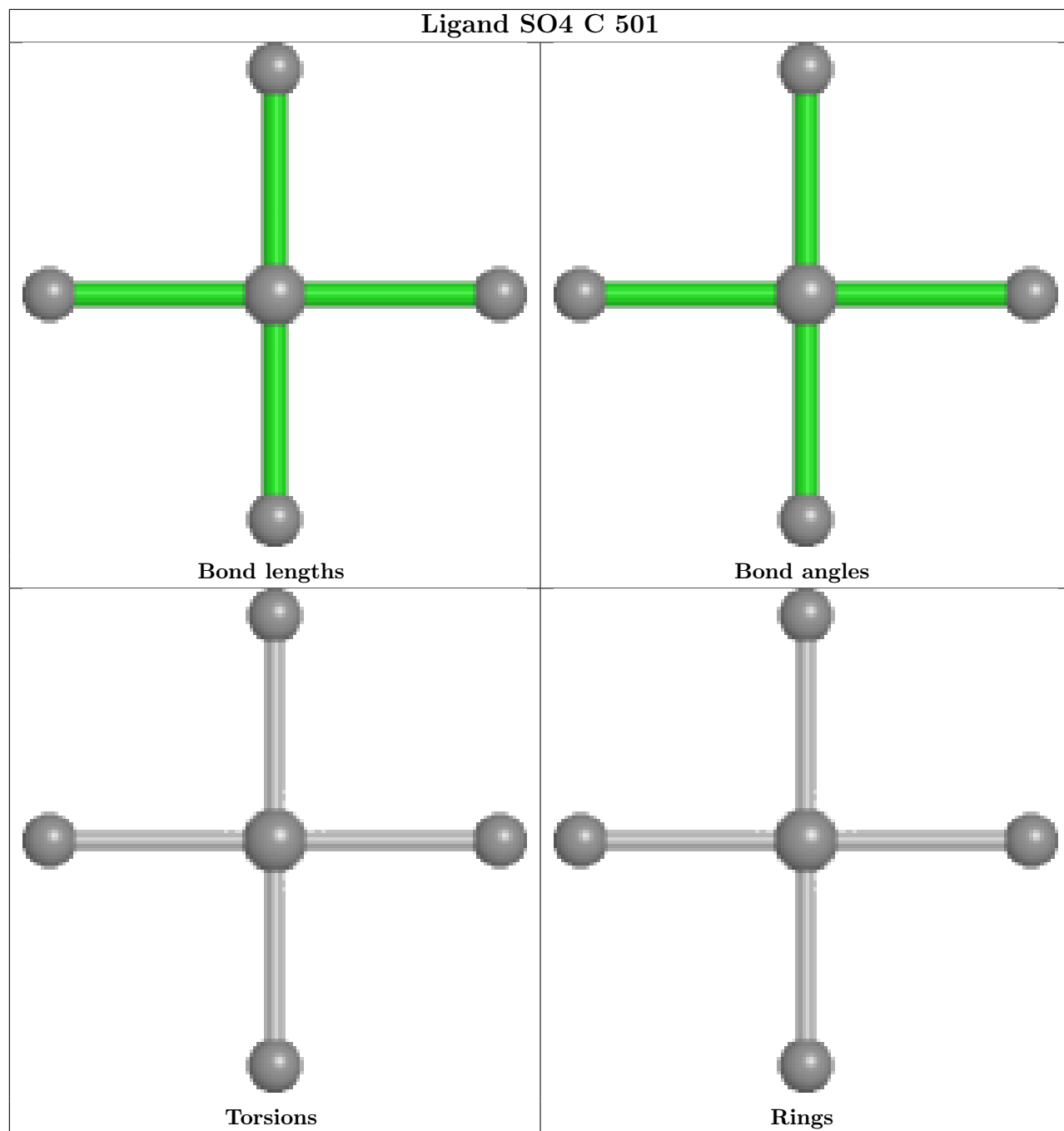


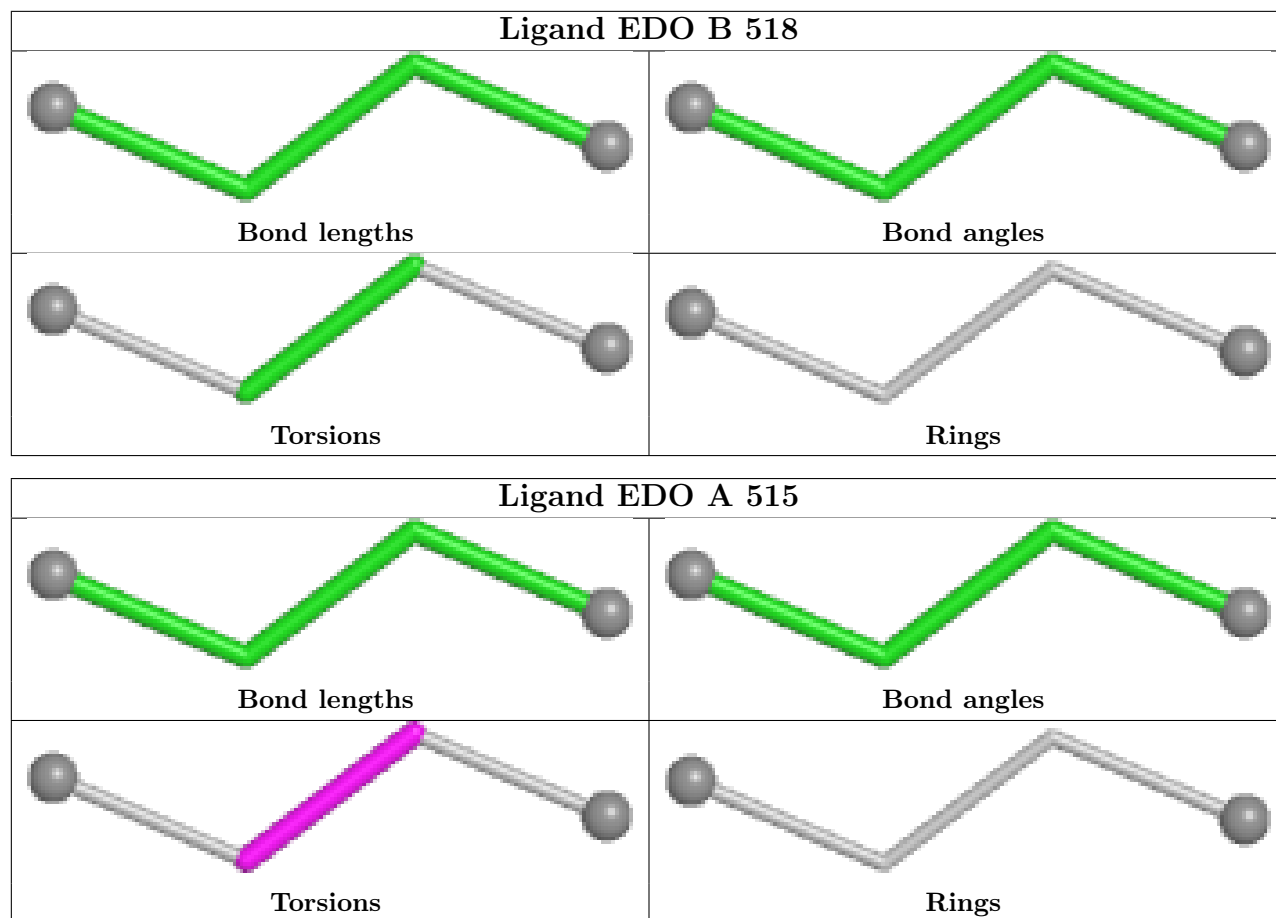


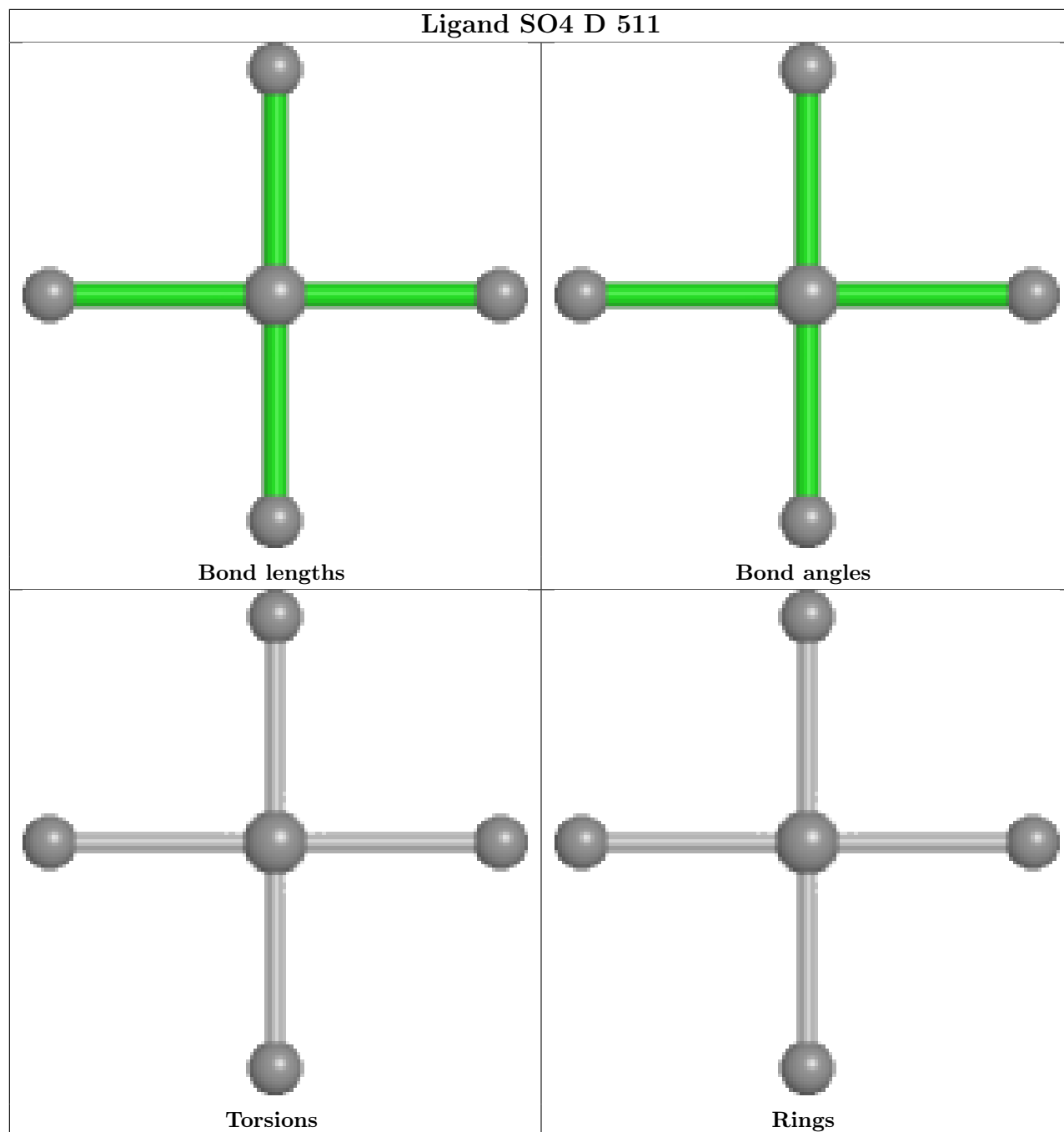


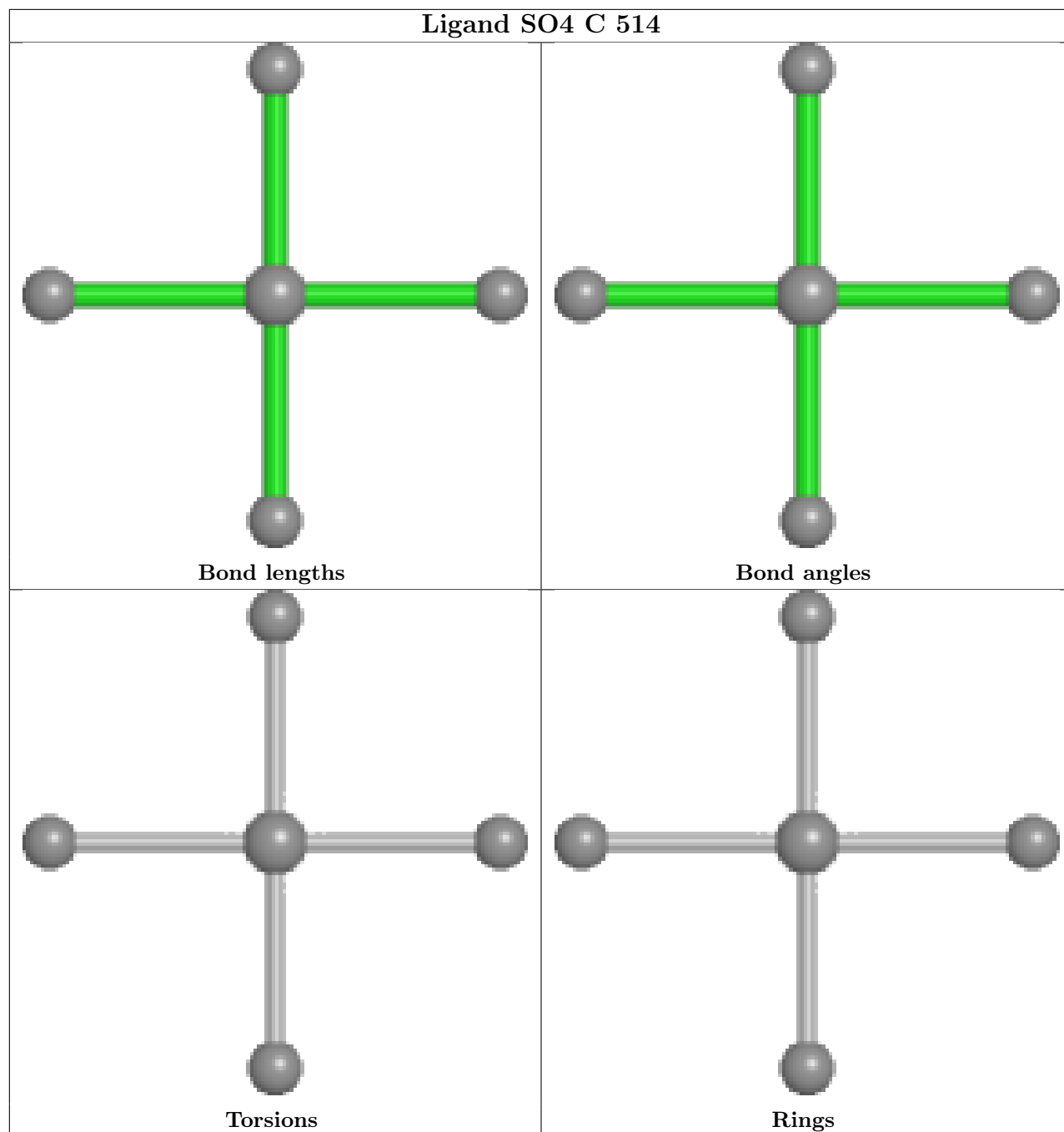


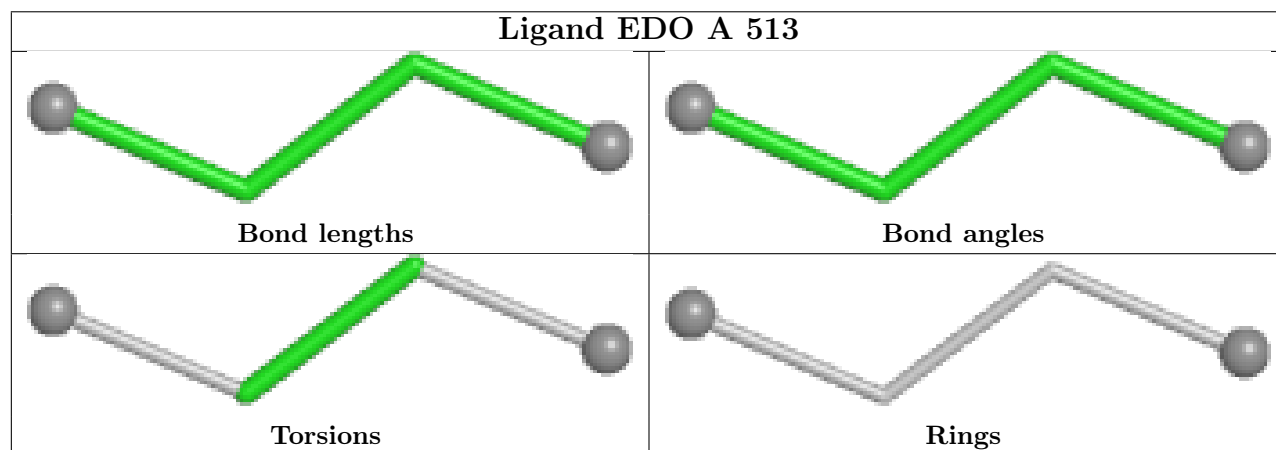
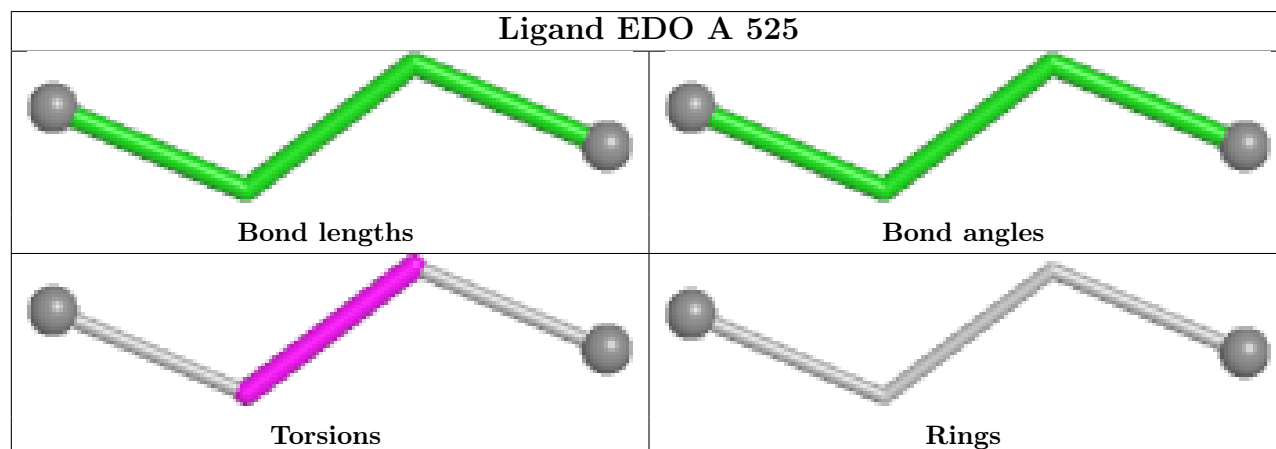
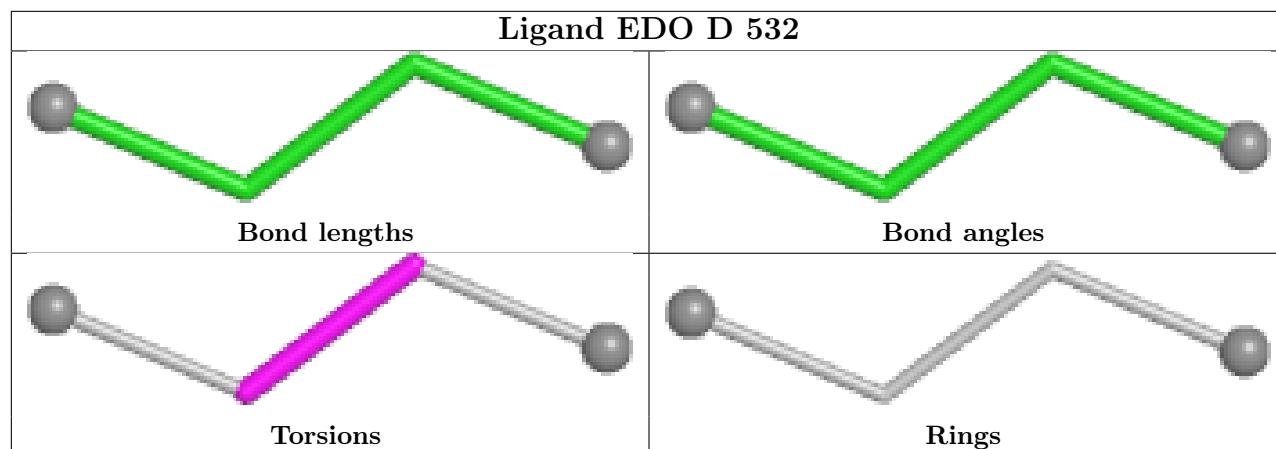


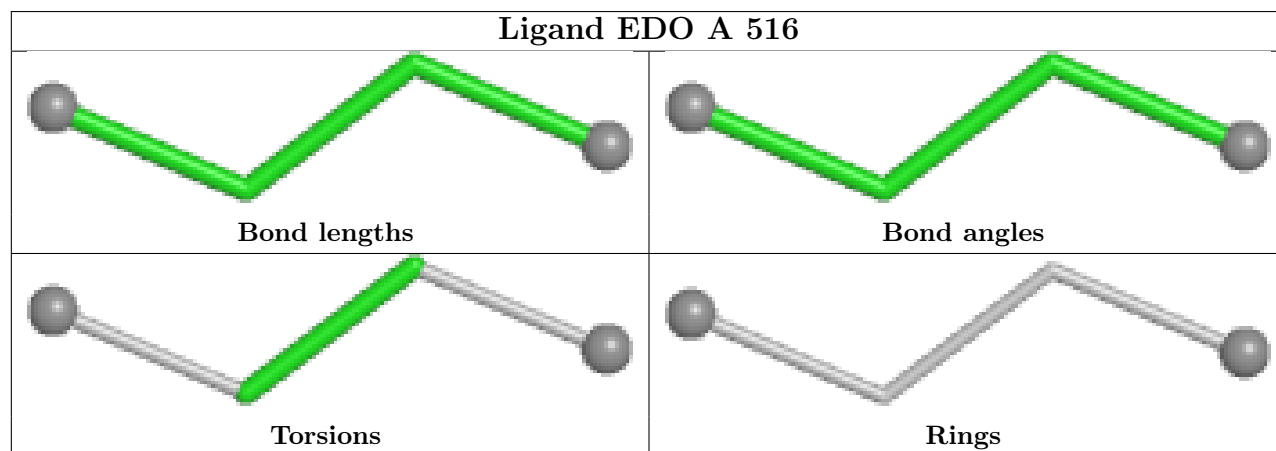
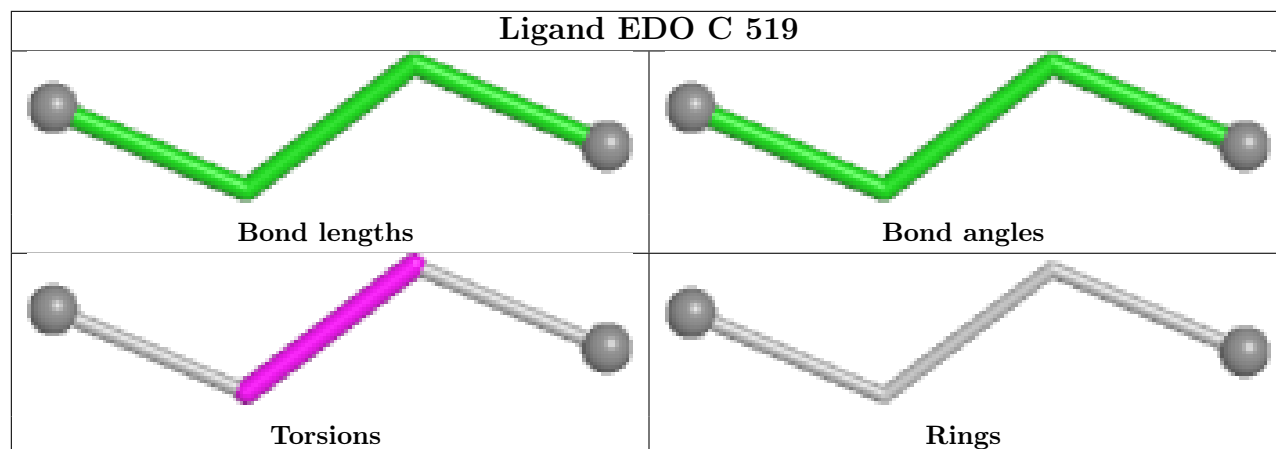


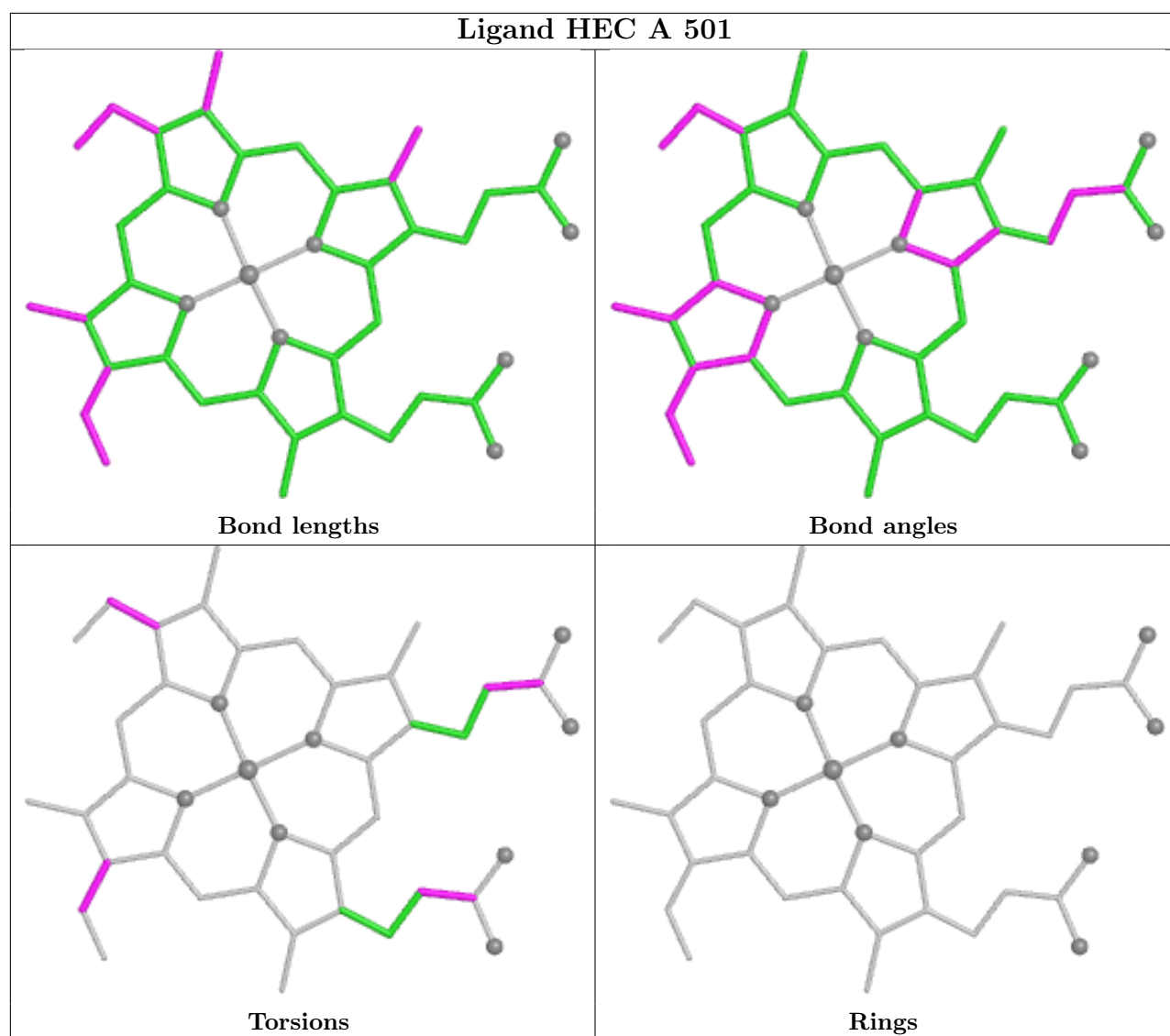


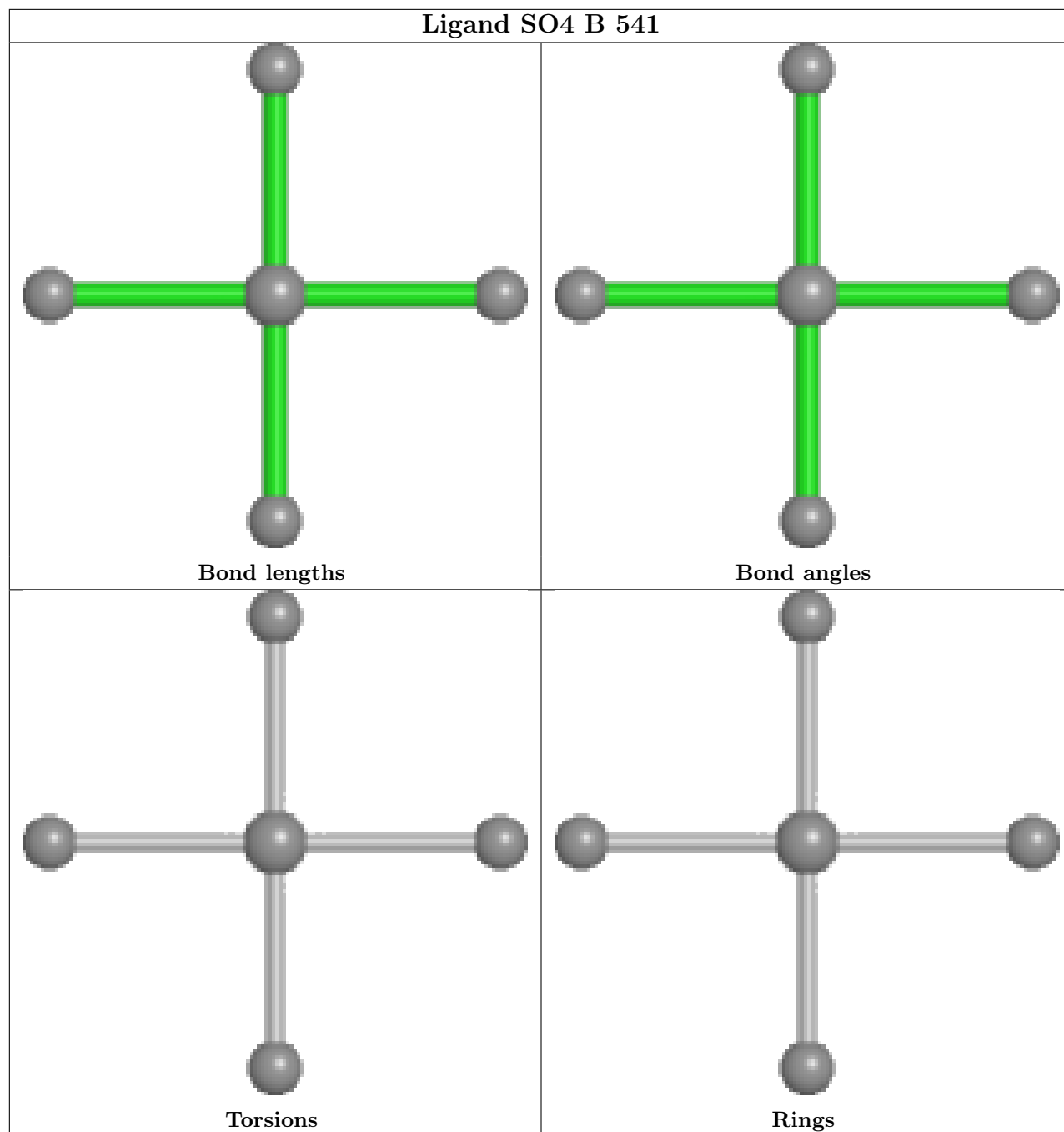


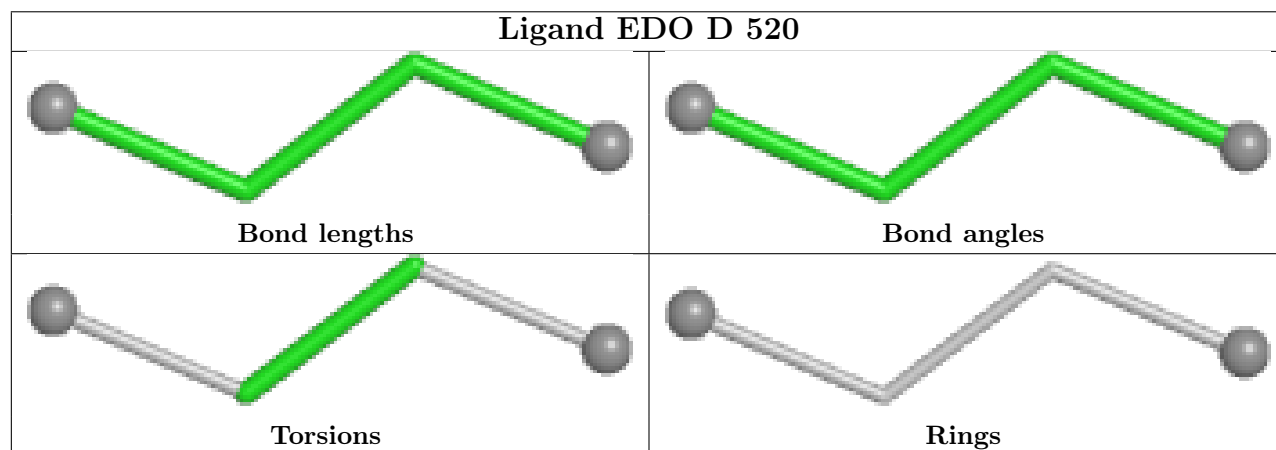
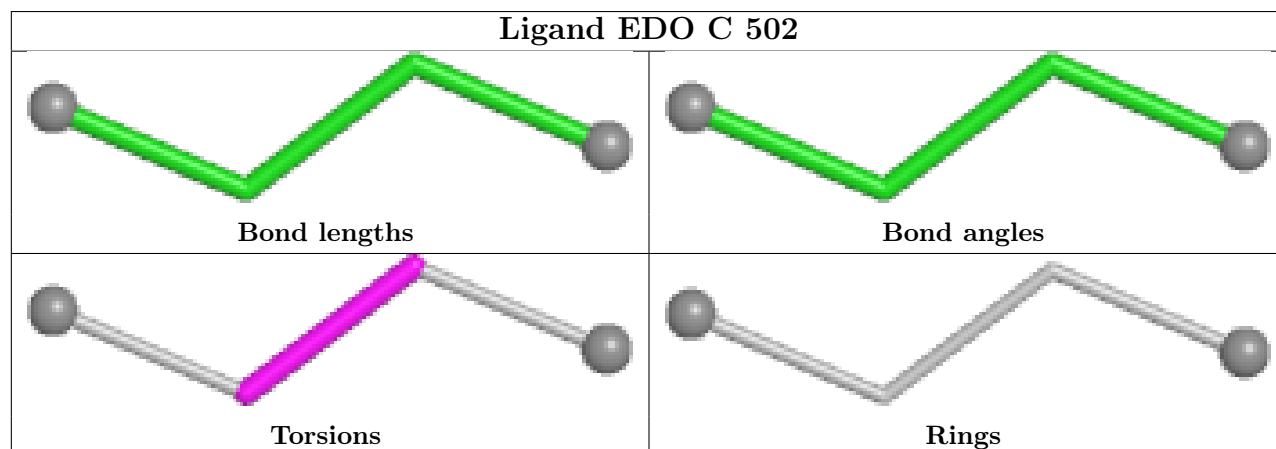
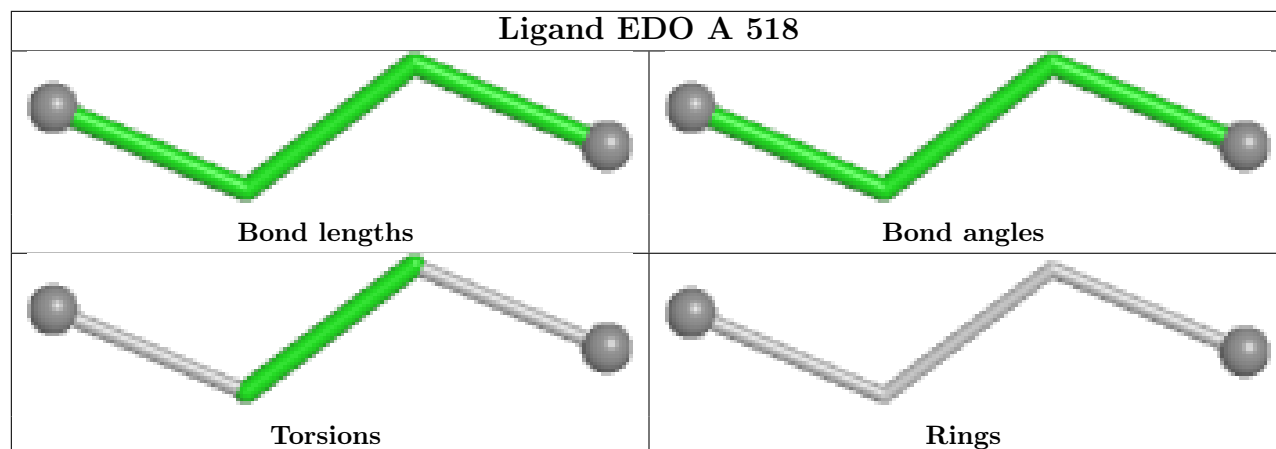


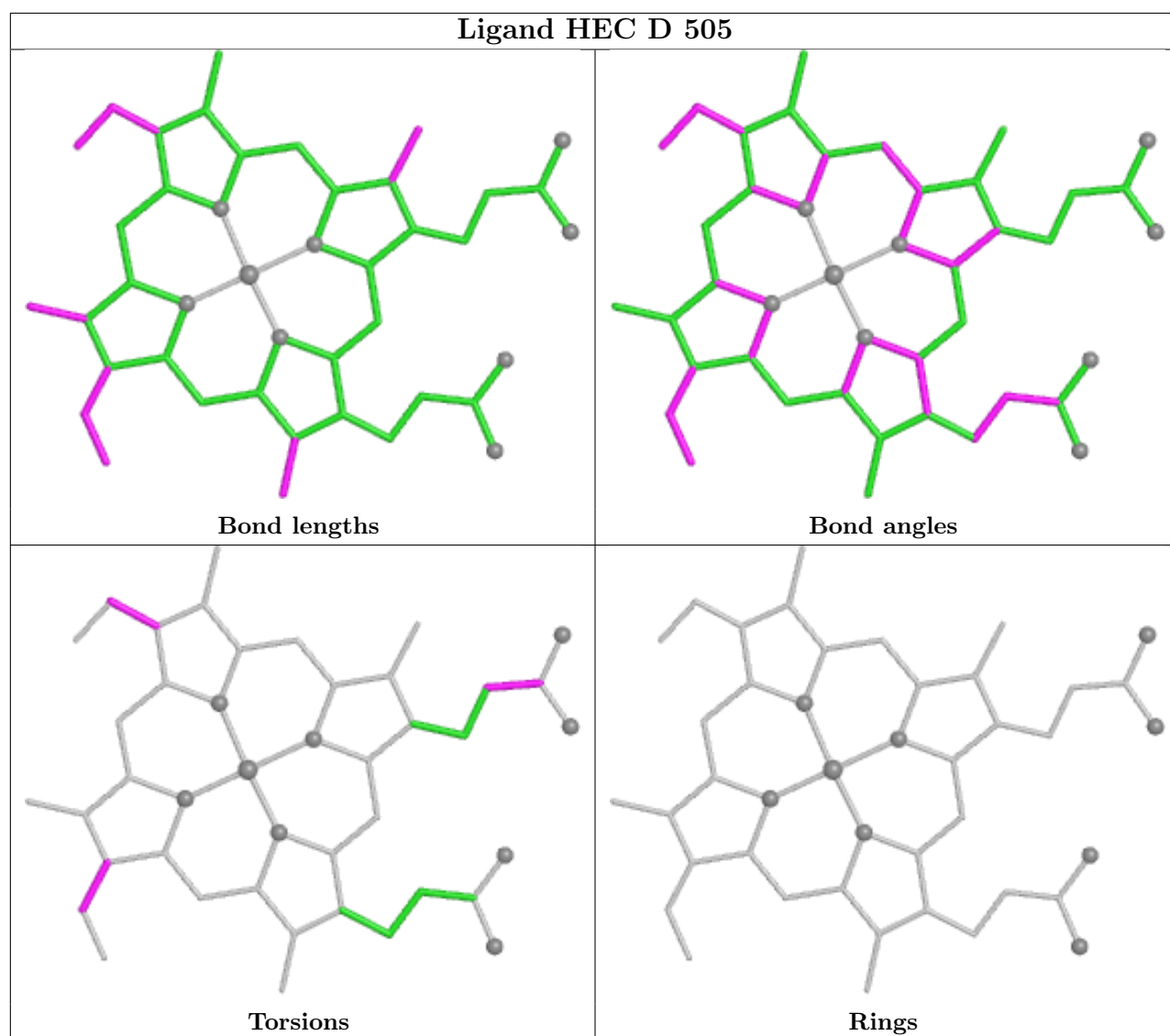


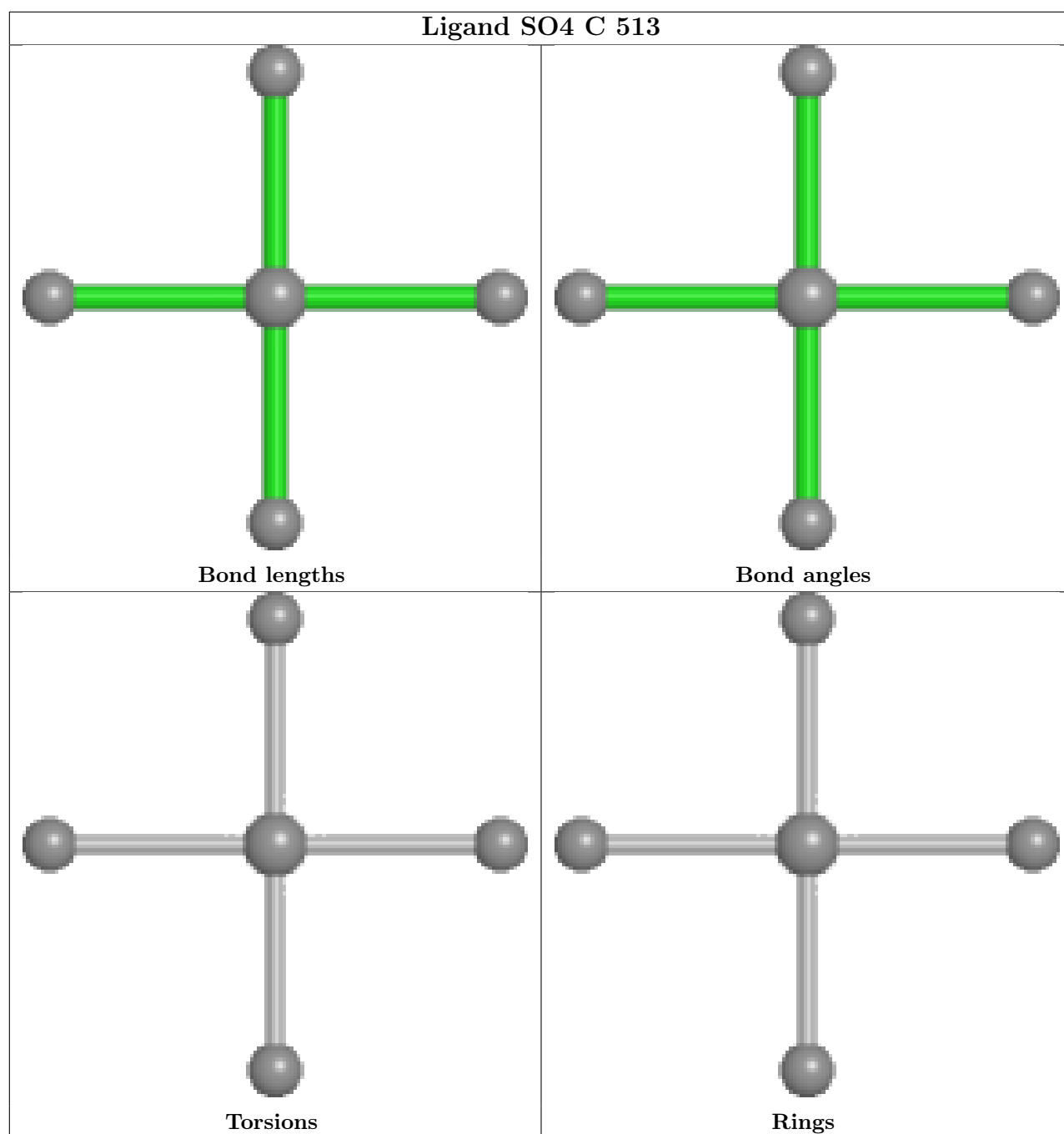


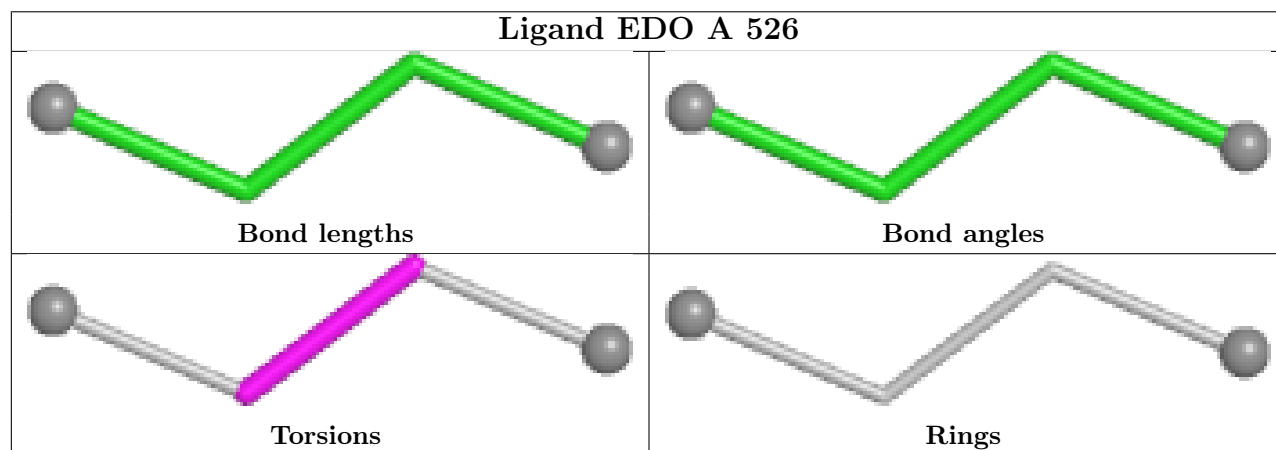
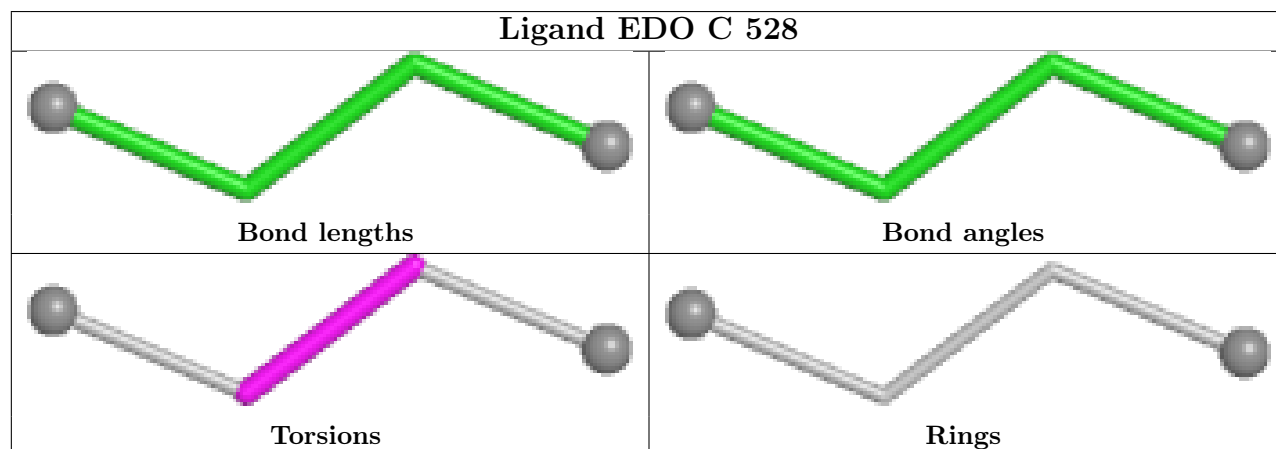
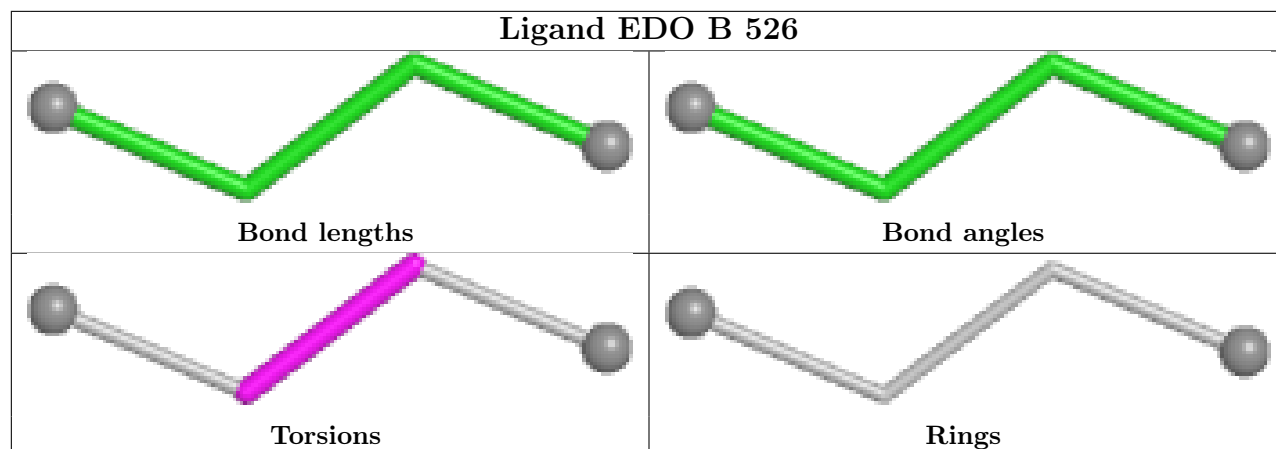


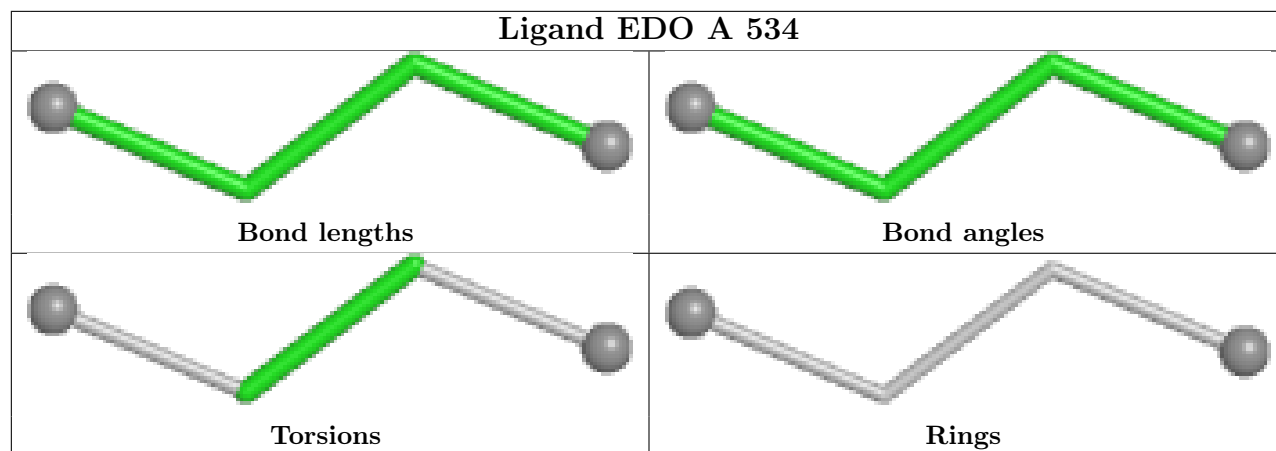


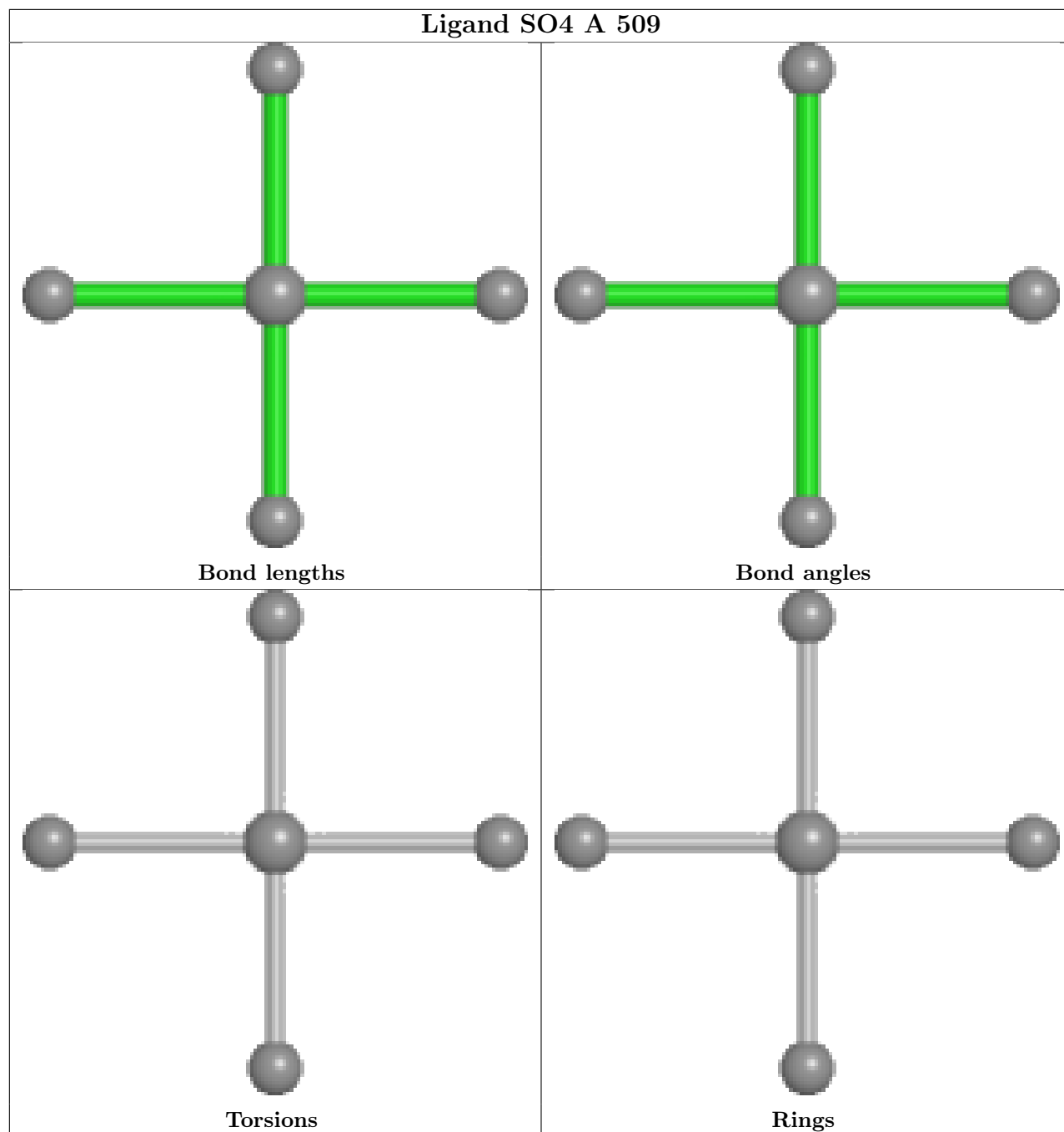


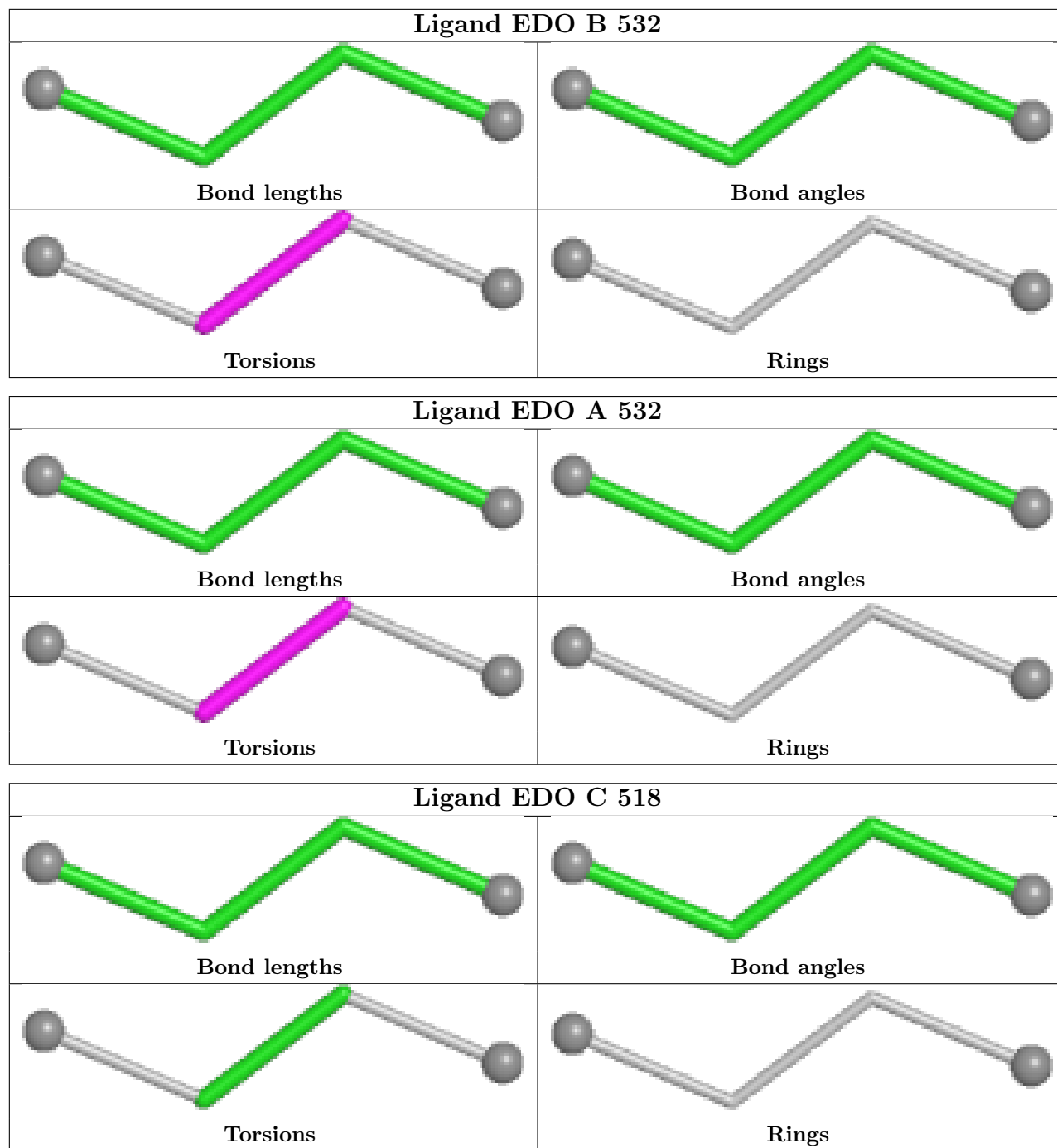




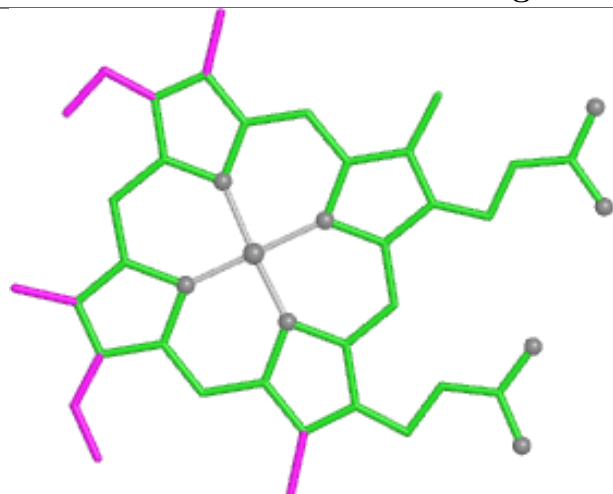




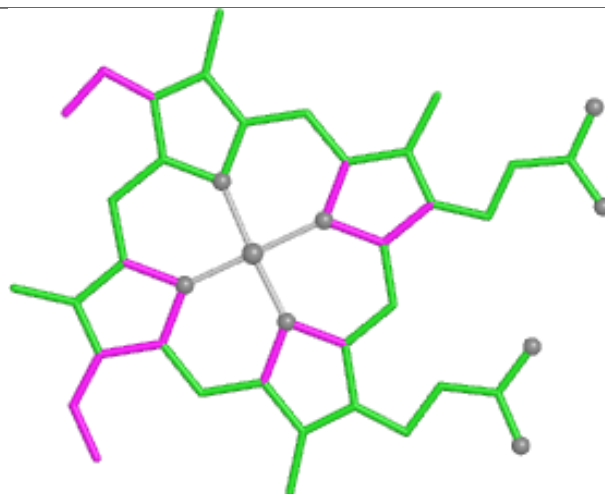




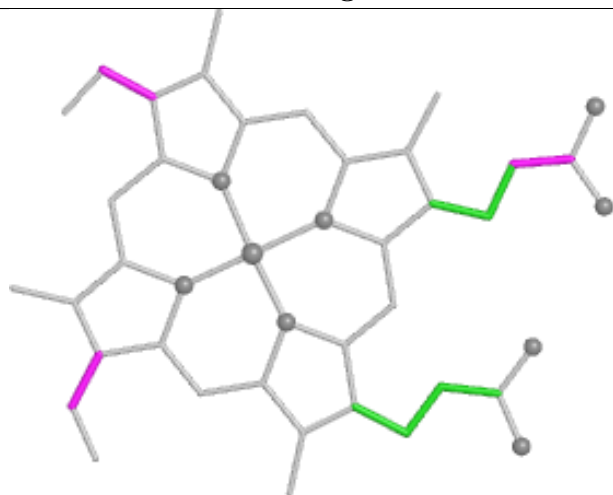
Ligand HEC C 503



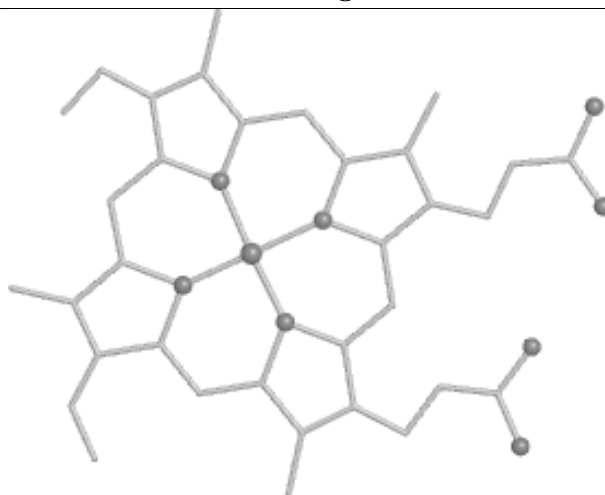
Bond lengths



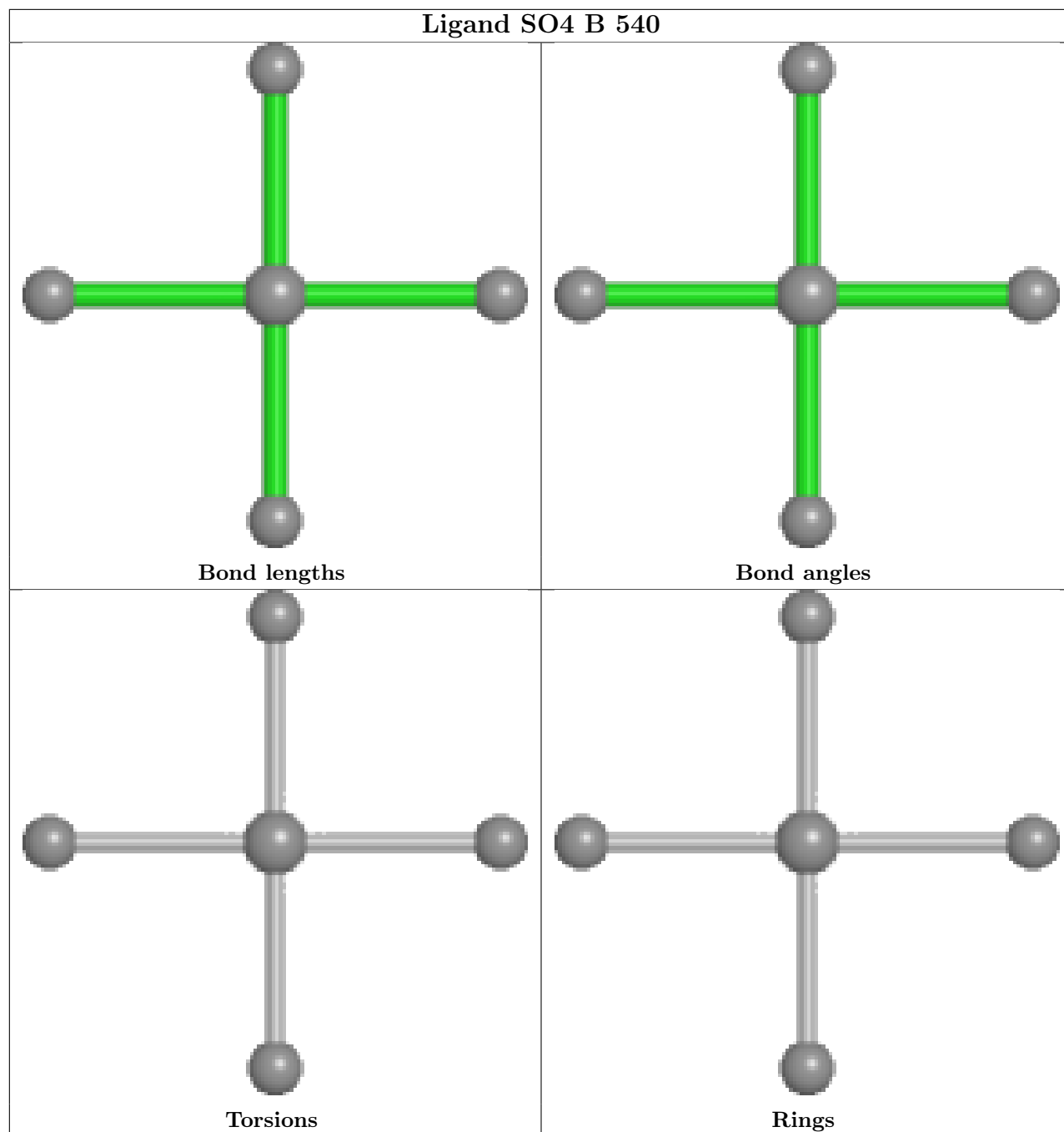
Bond angles

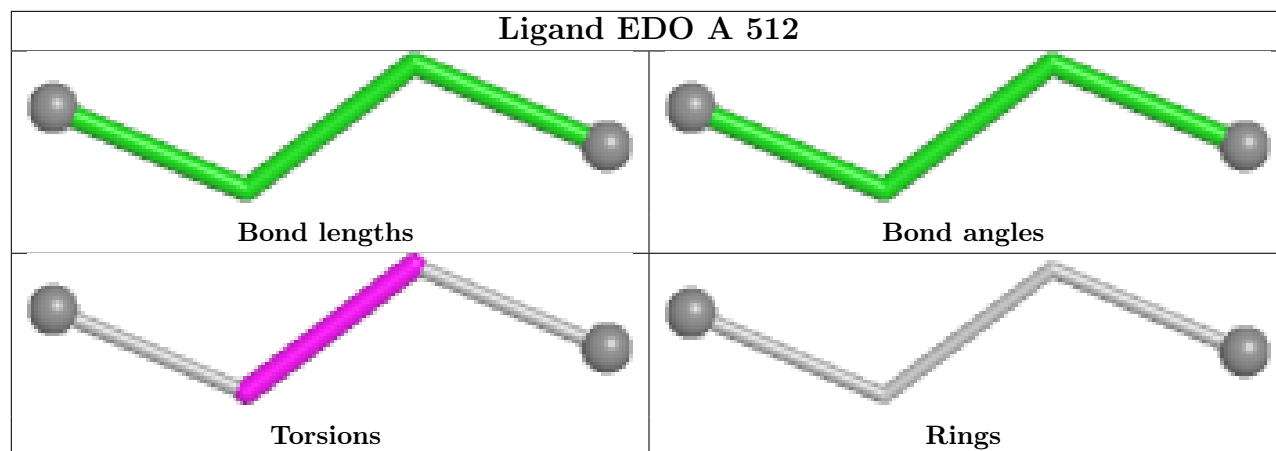


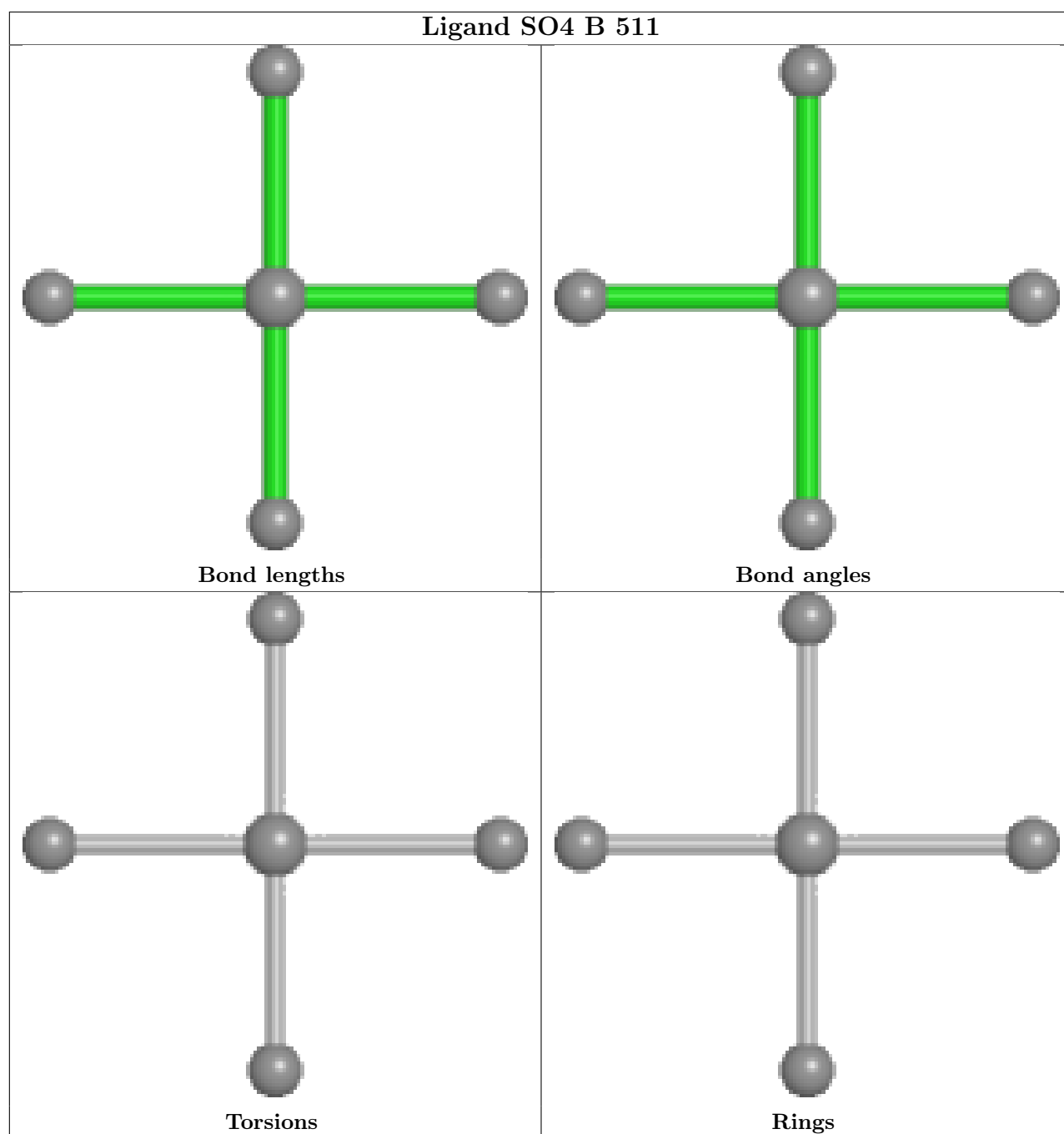
Torsions

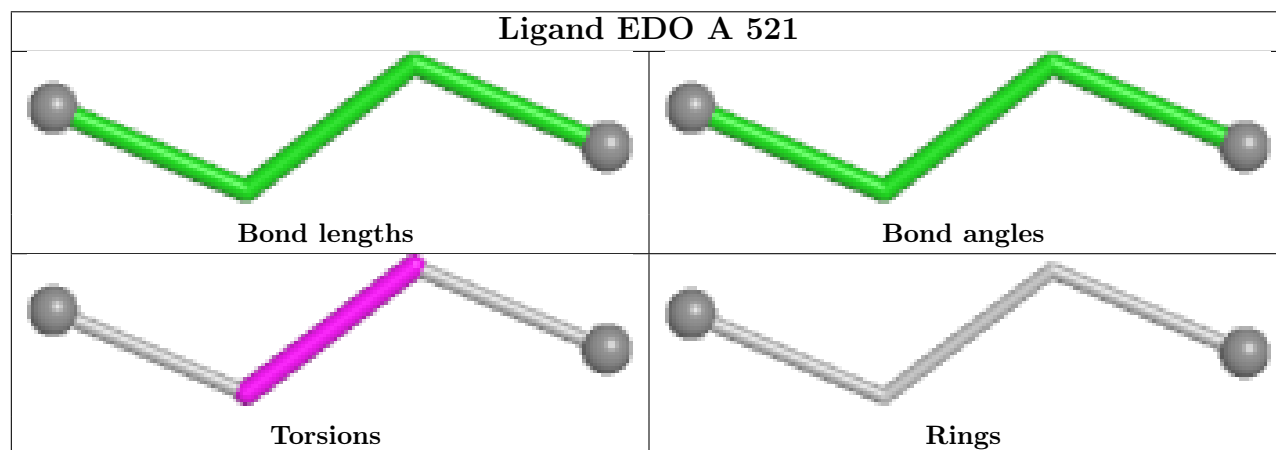
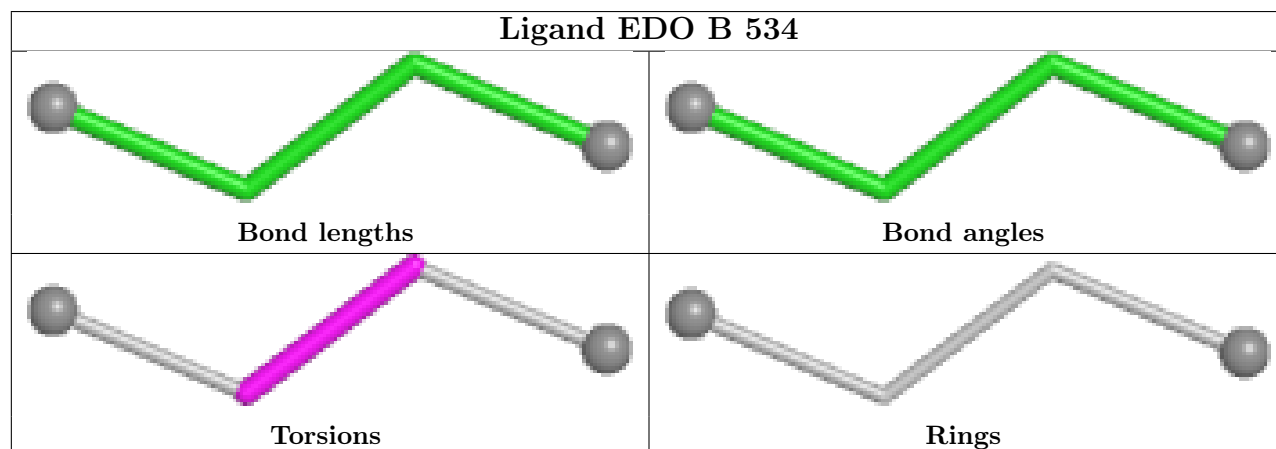
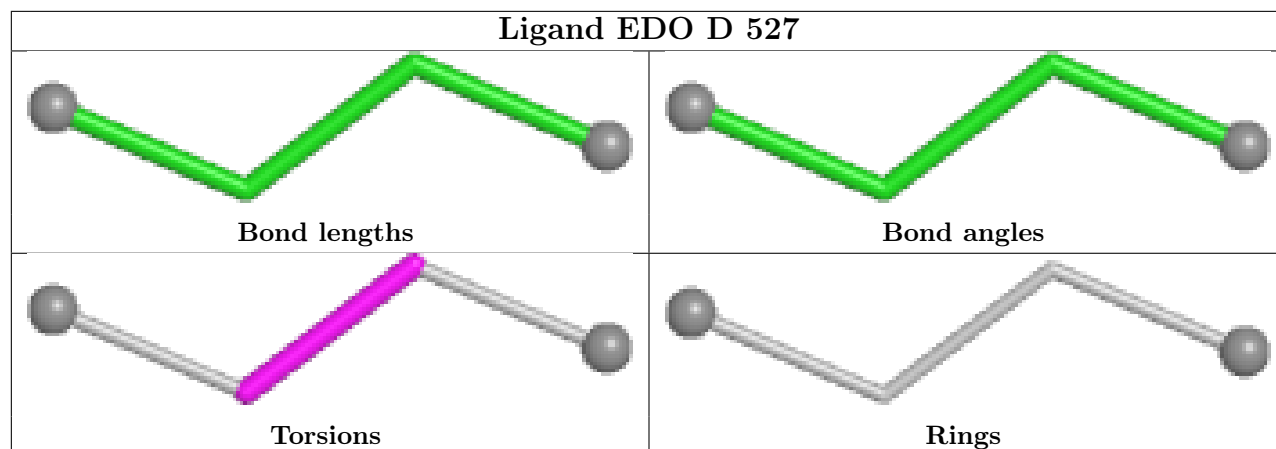


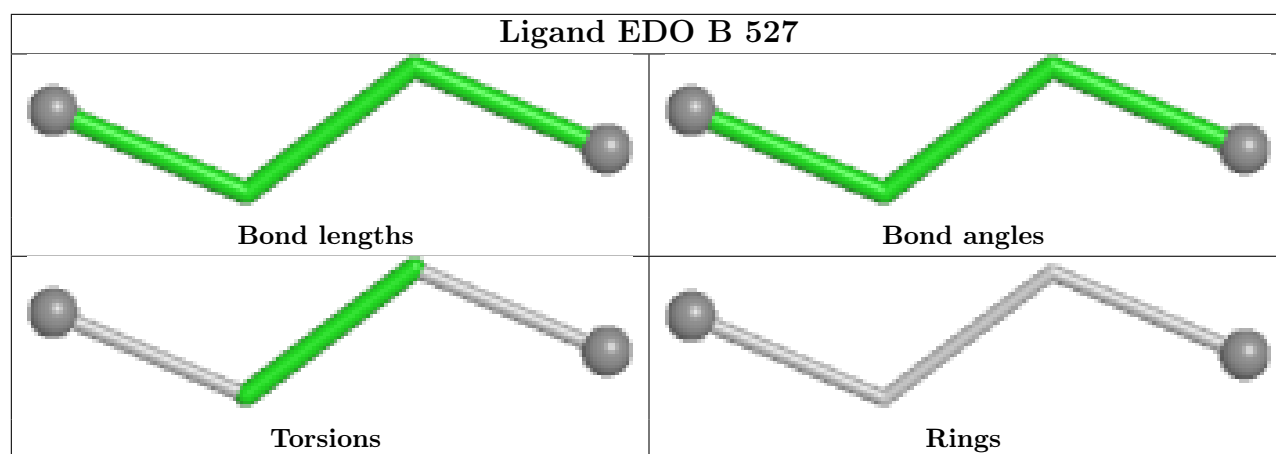
Rings

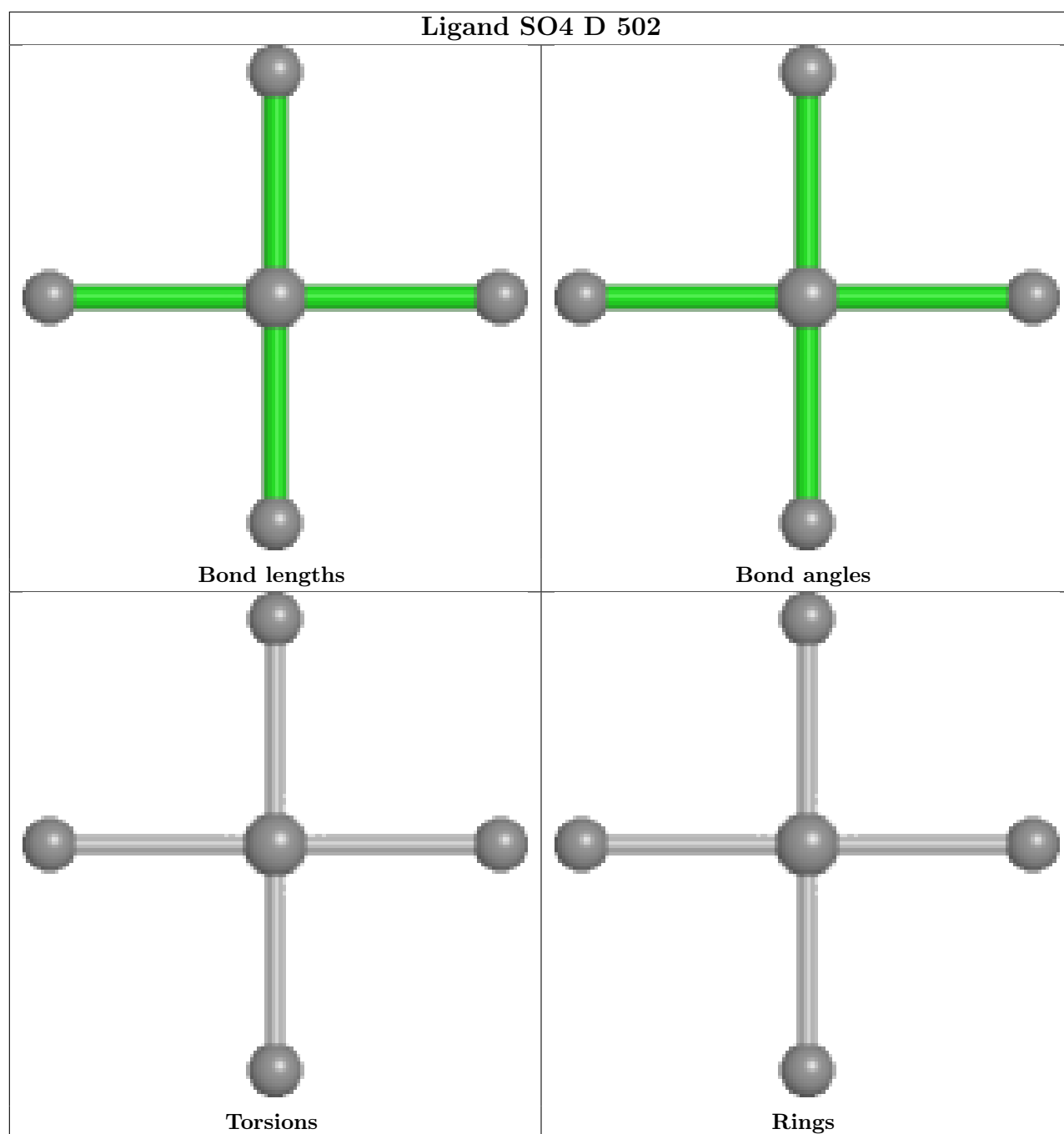


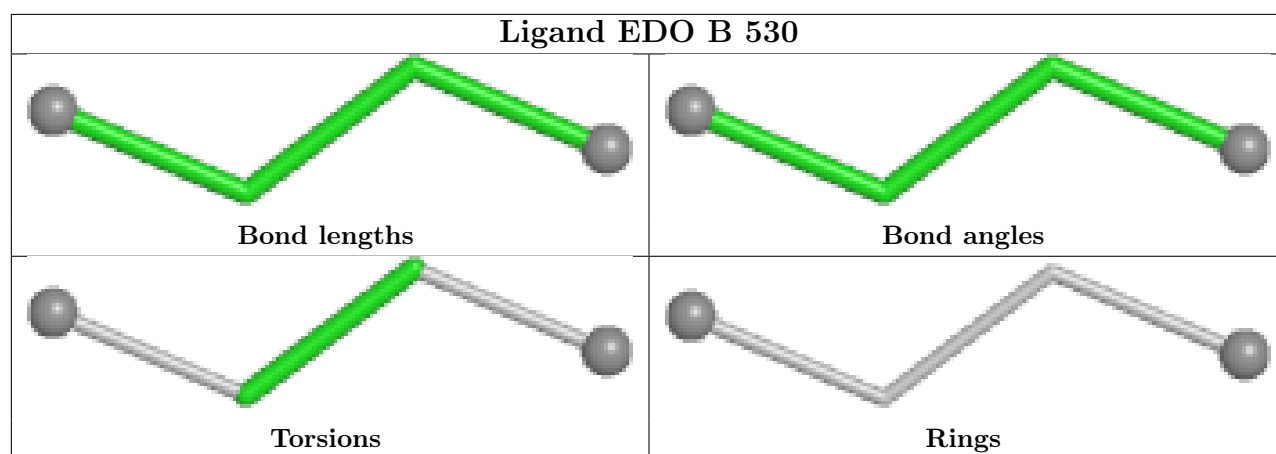


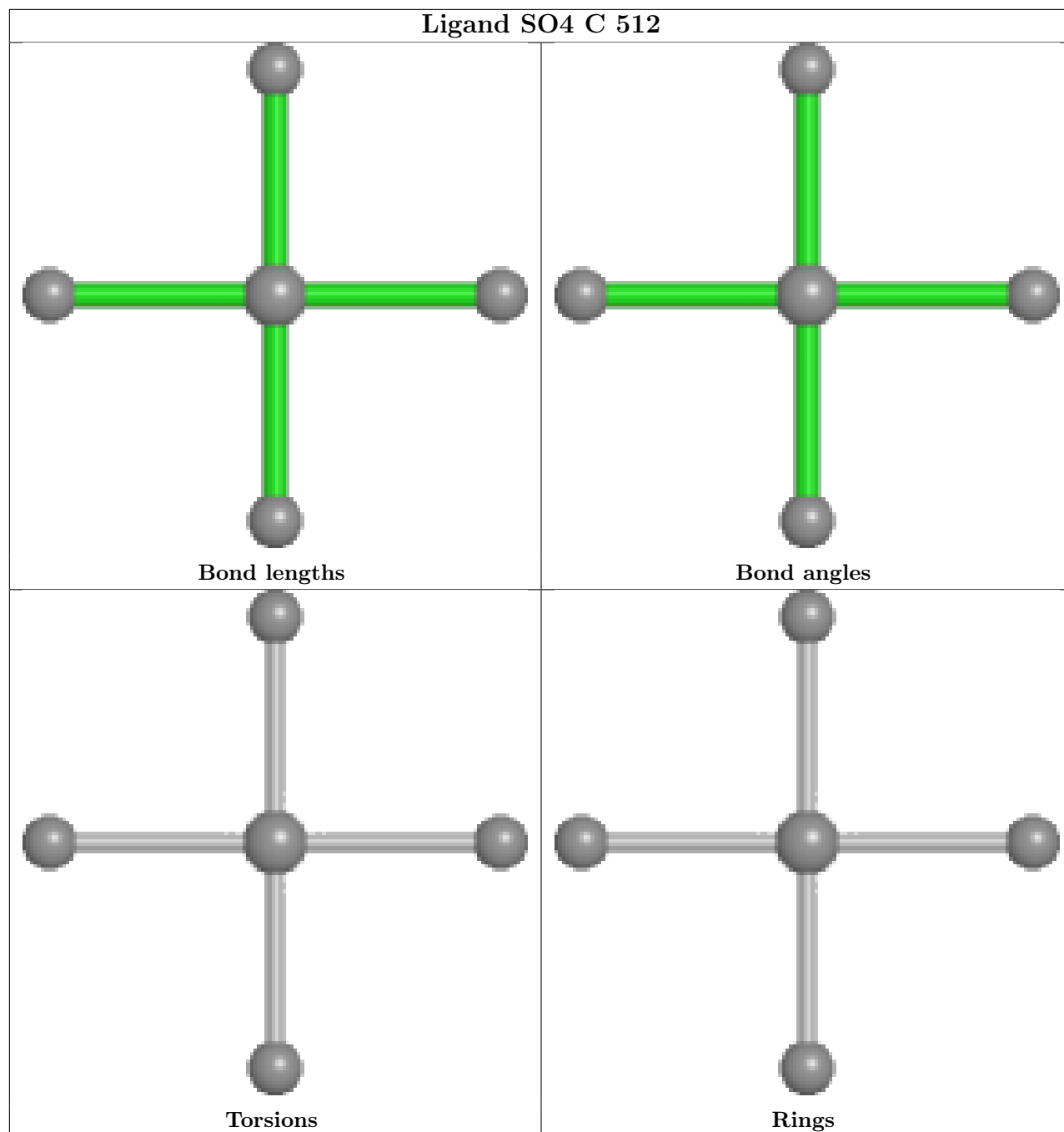


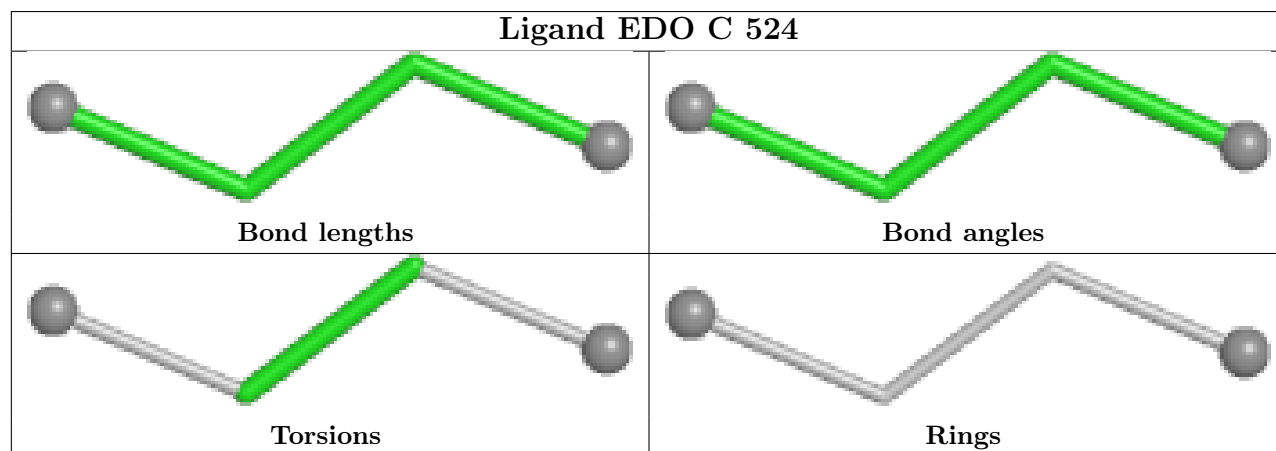
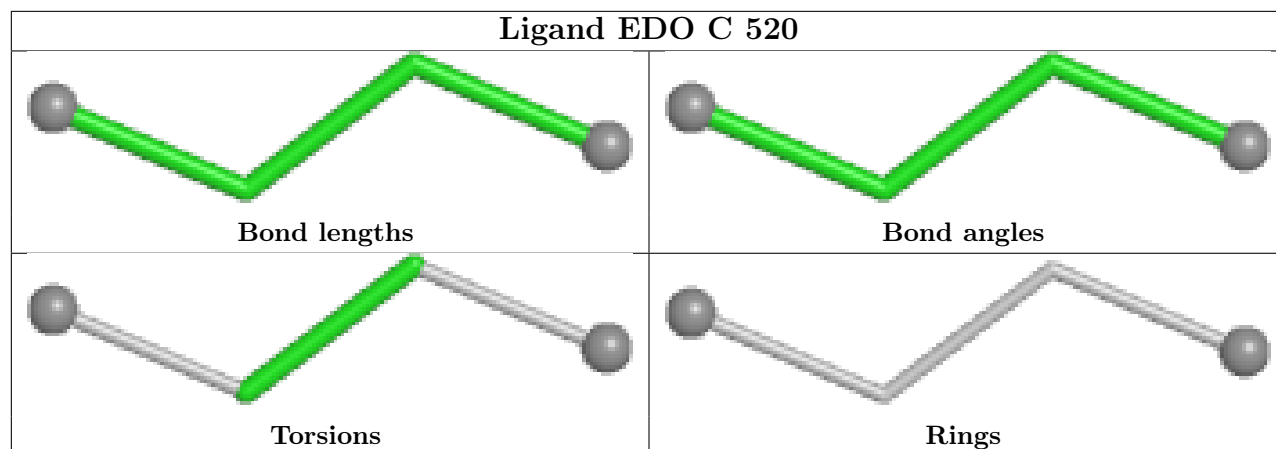




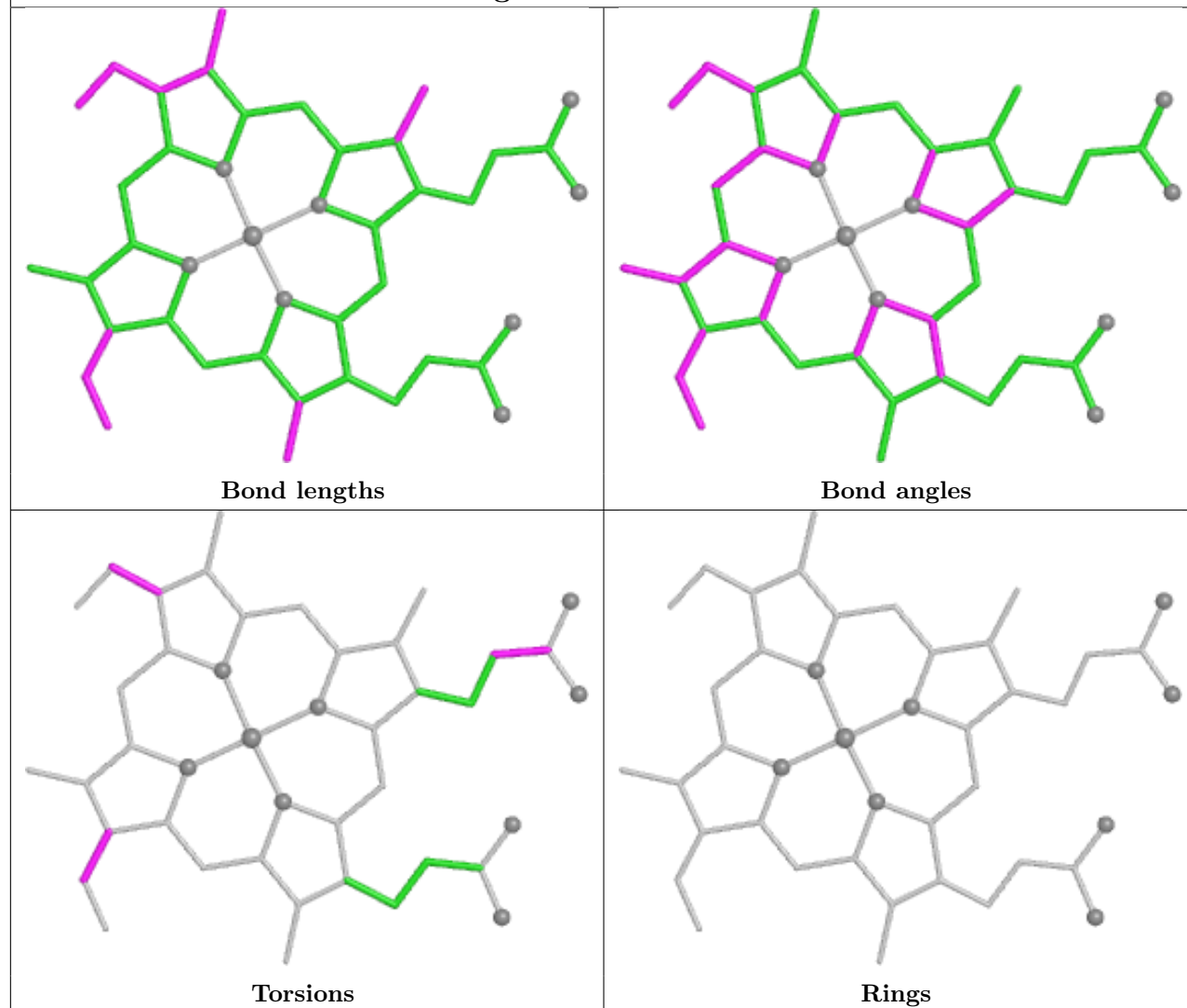




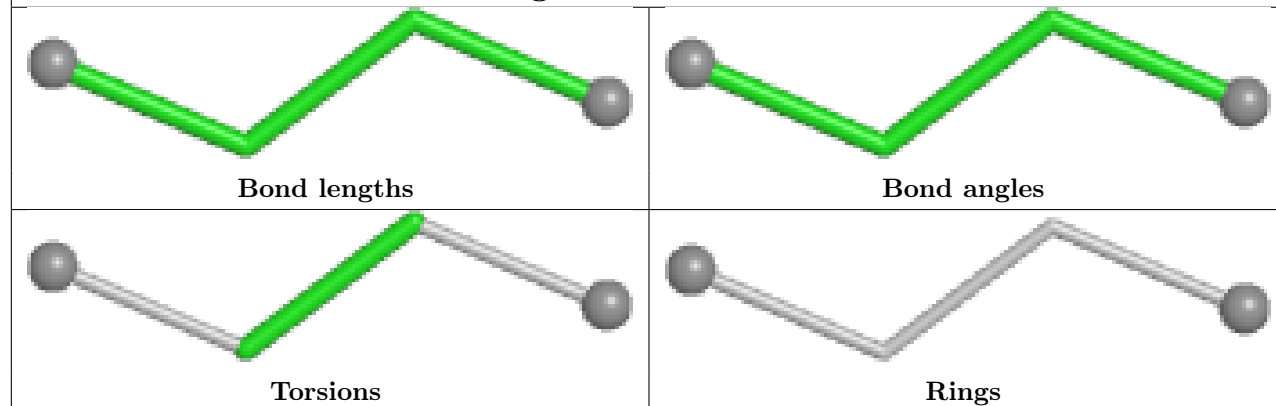


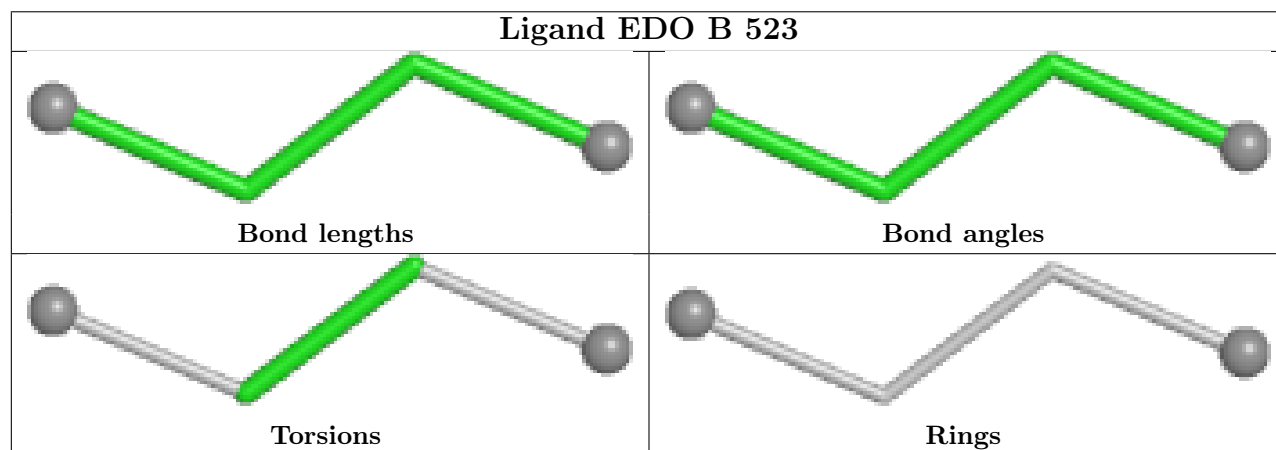
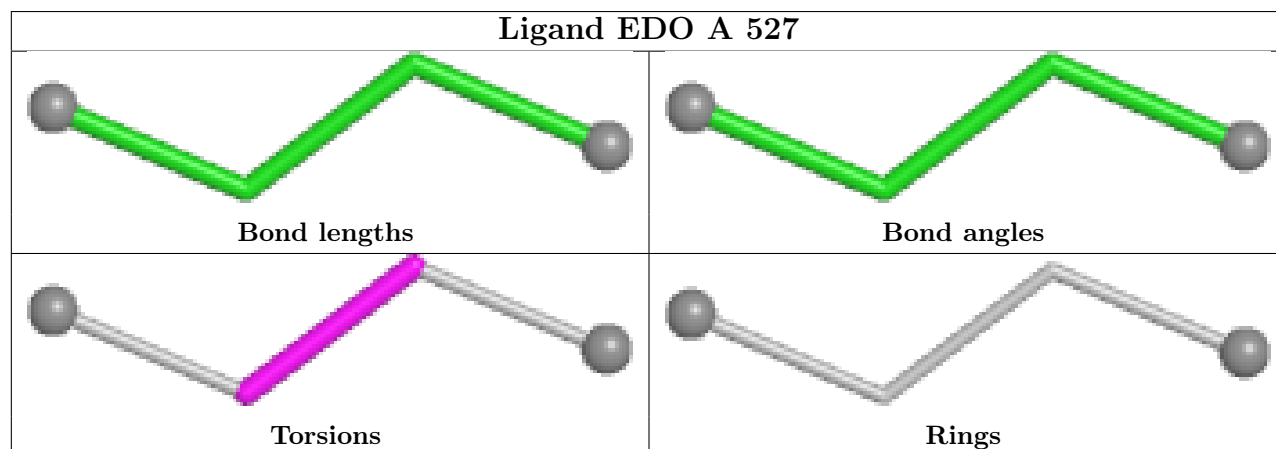
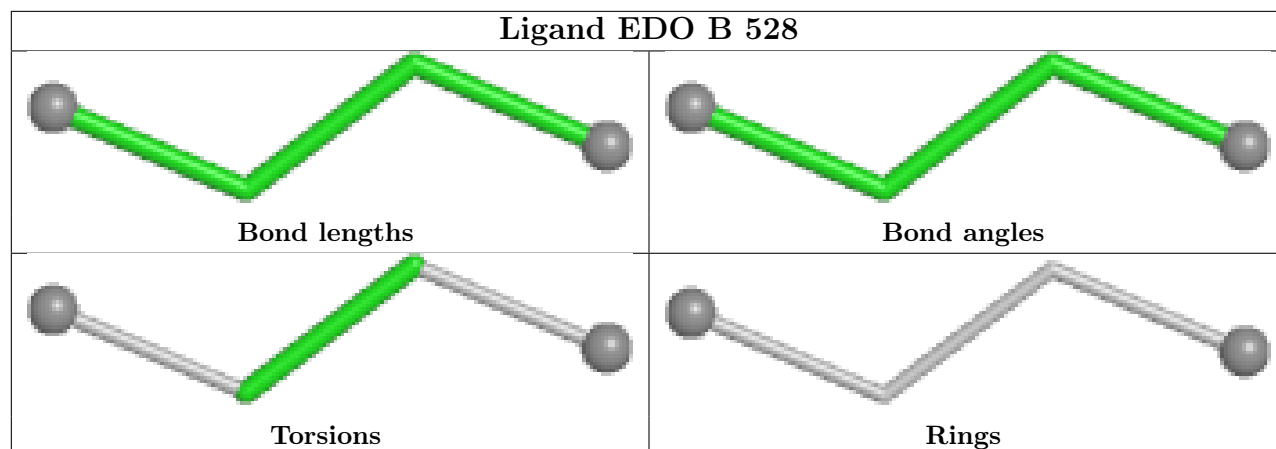


Ligand HEC B 504

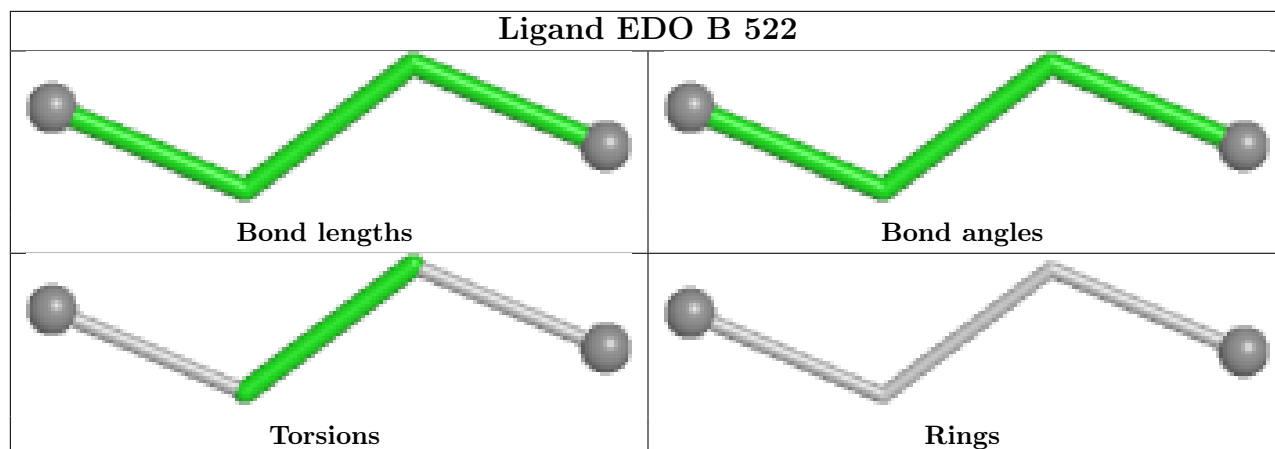


Ligand EDO B 538

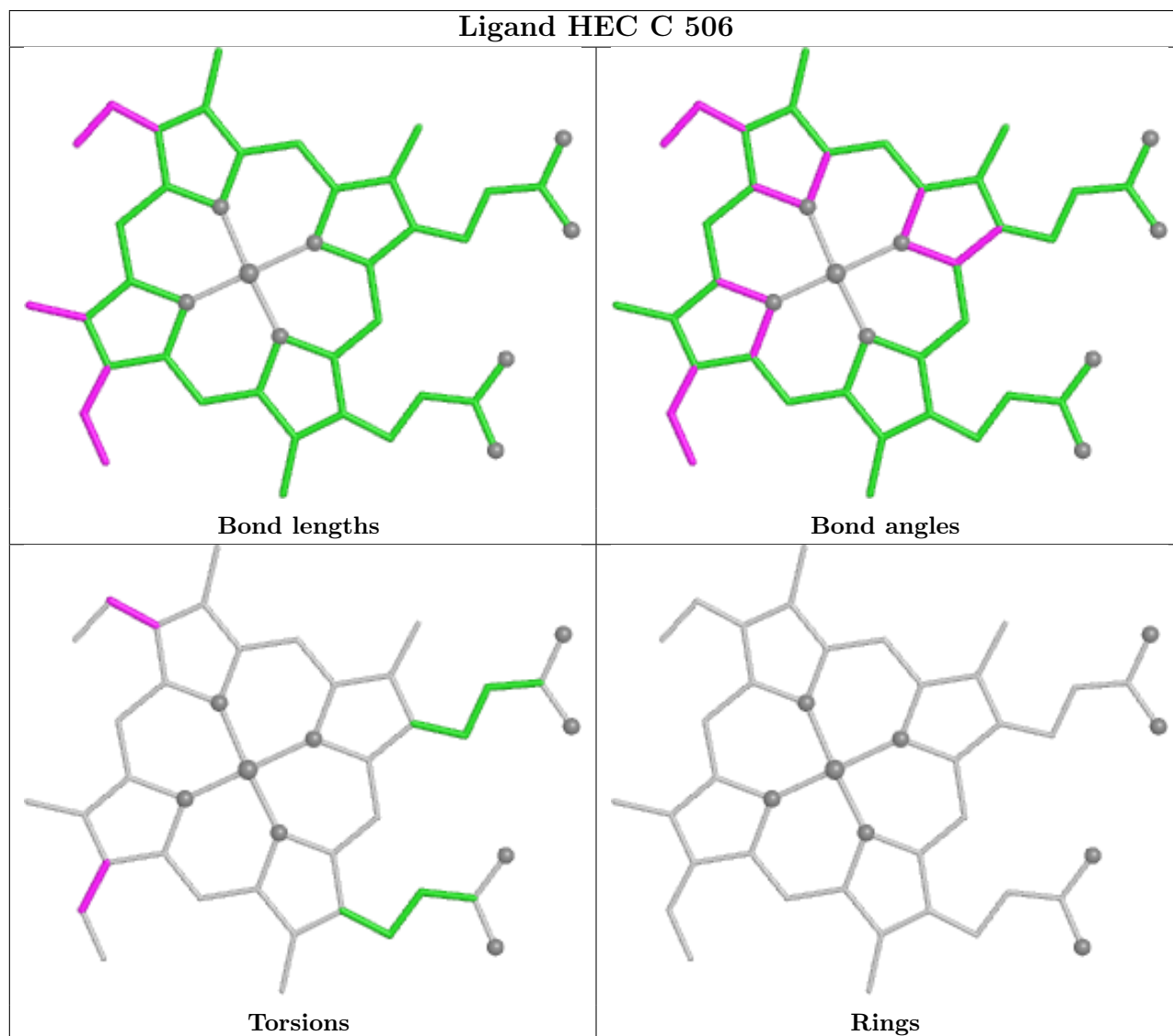


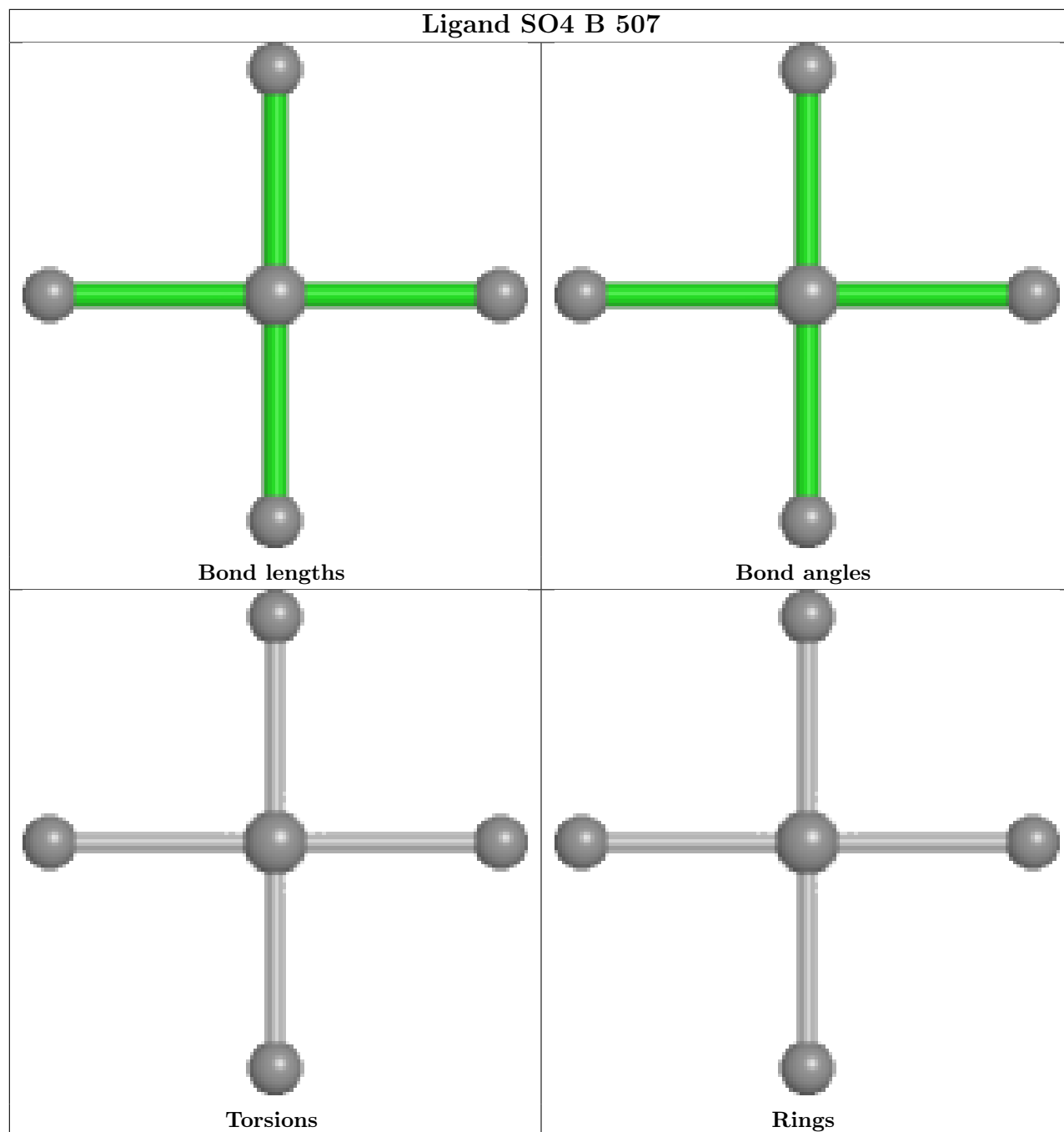


Ligand EDO B 522

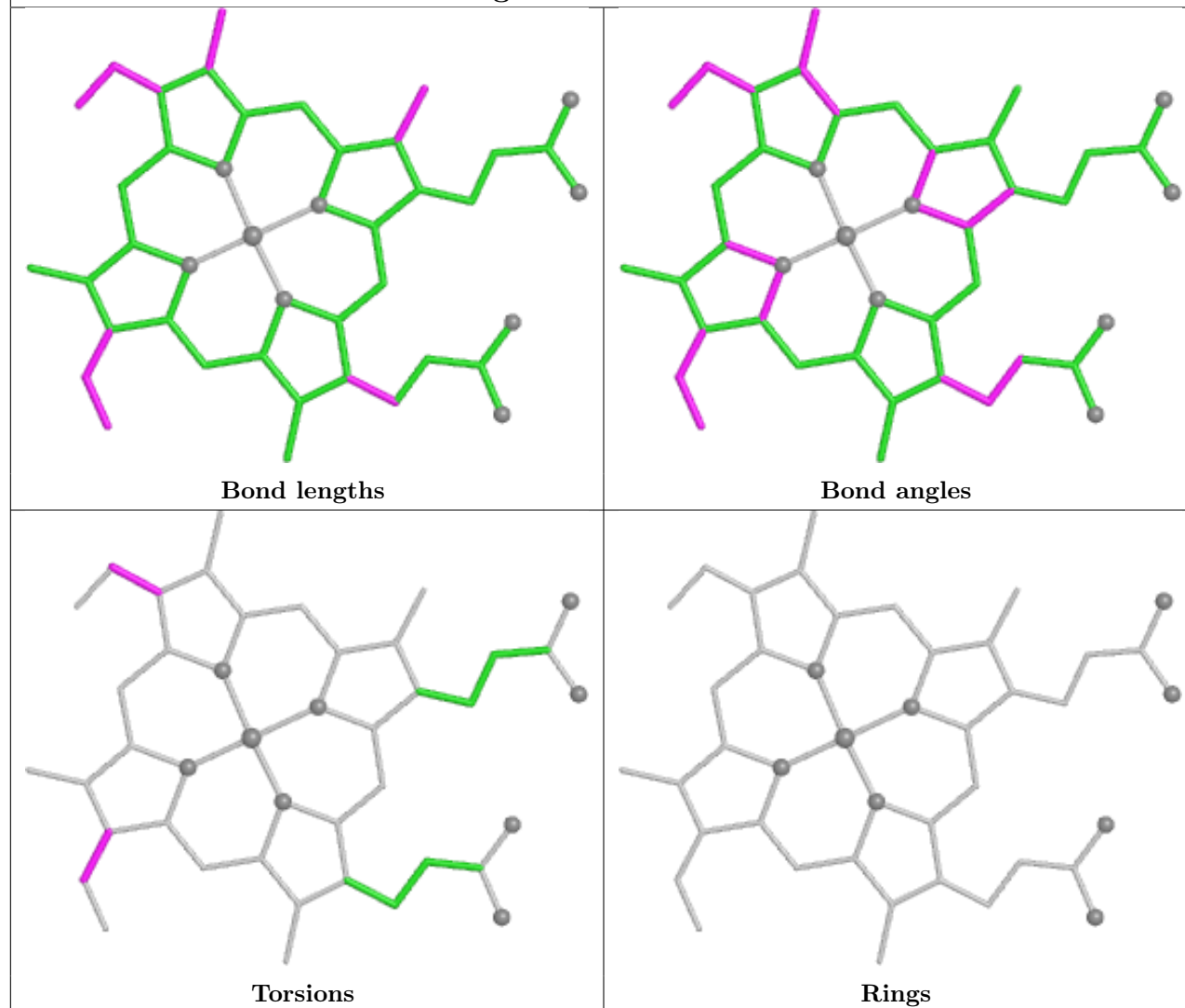


Ligand HEC C 506

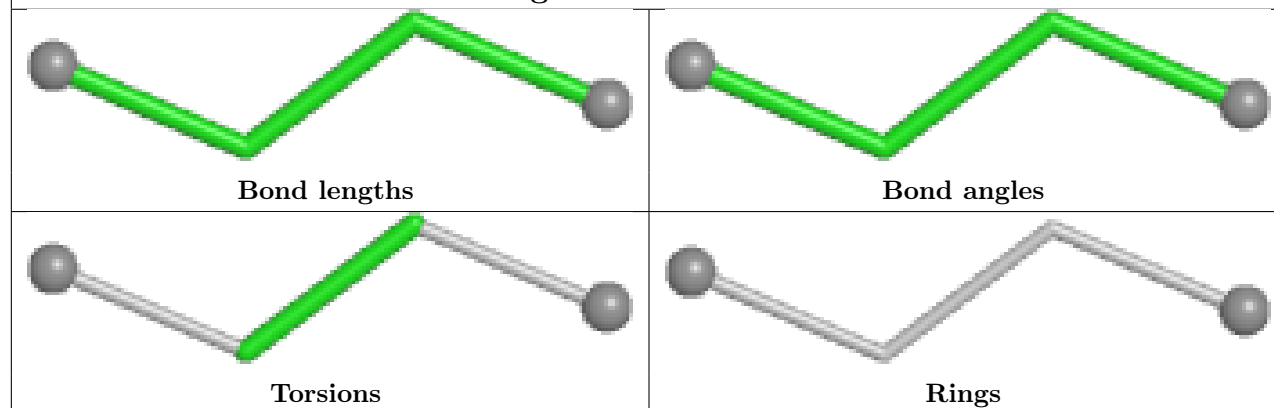


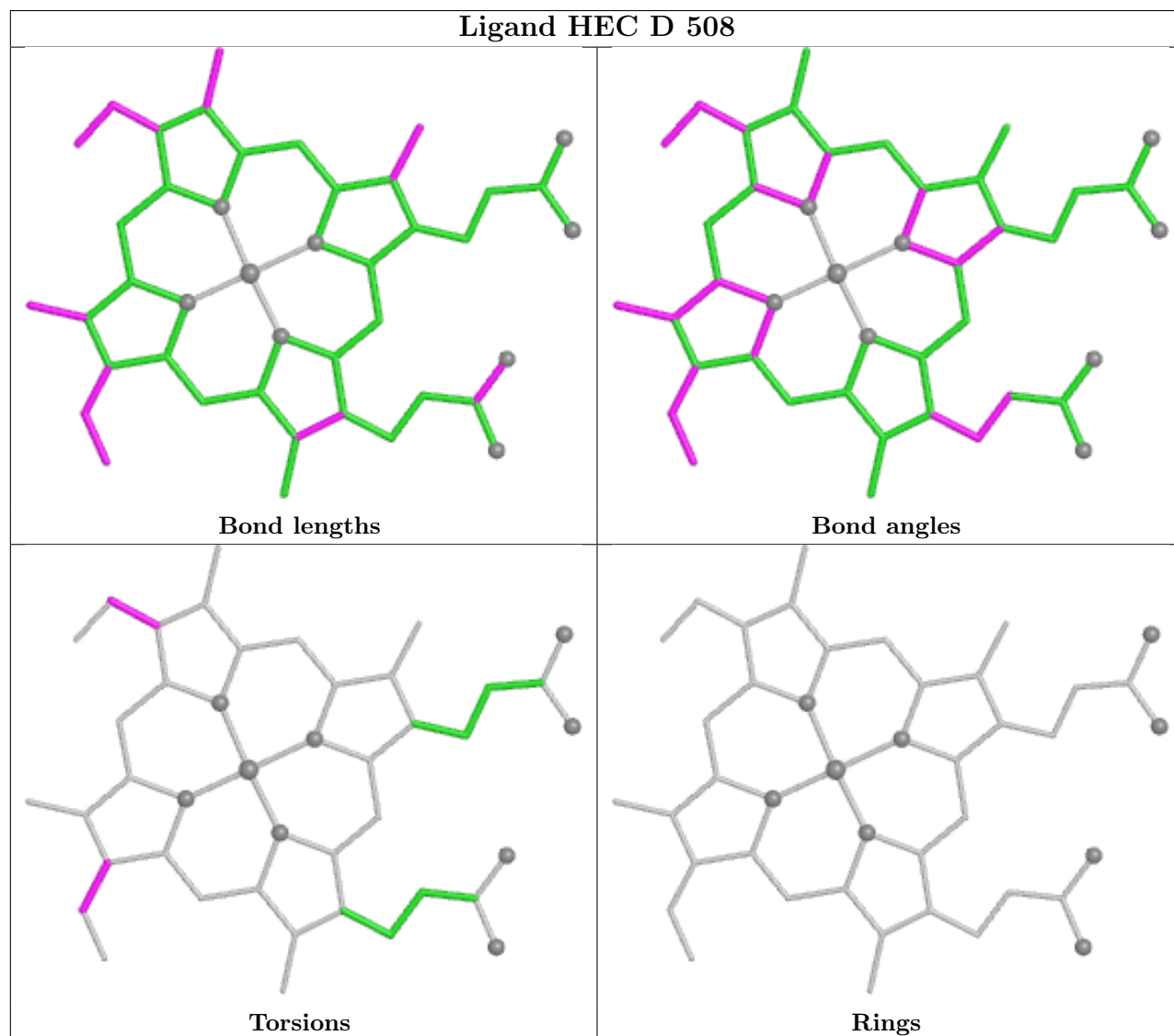
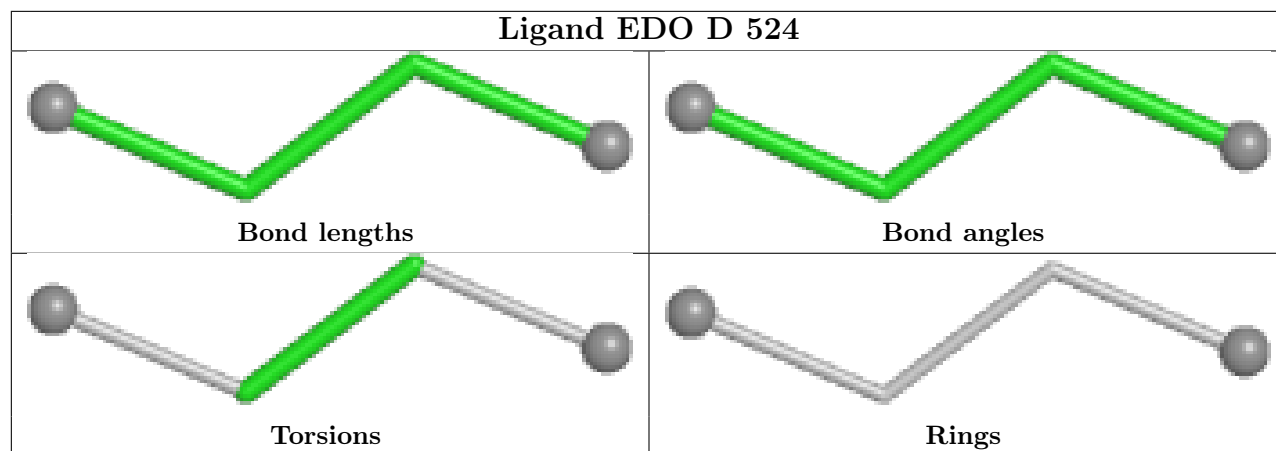


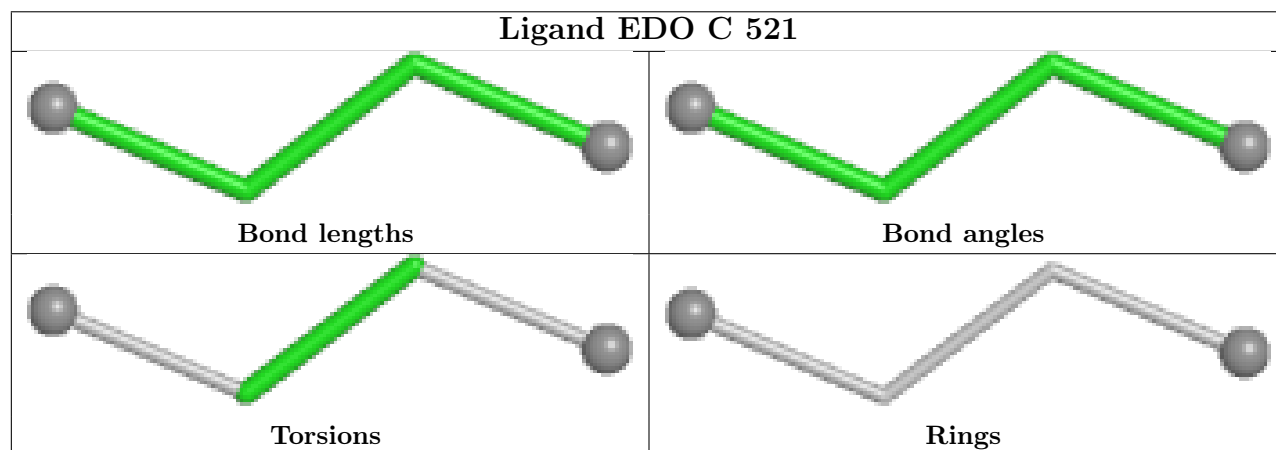
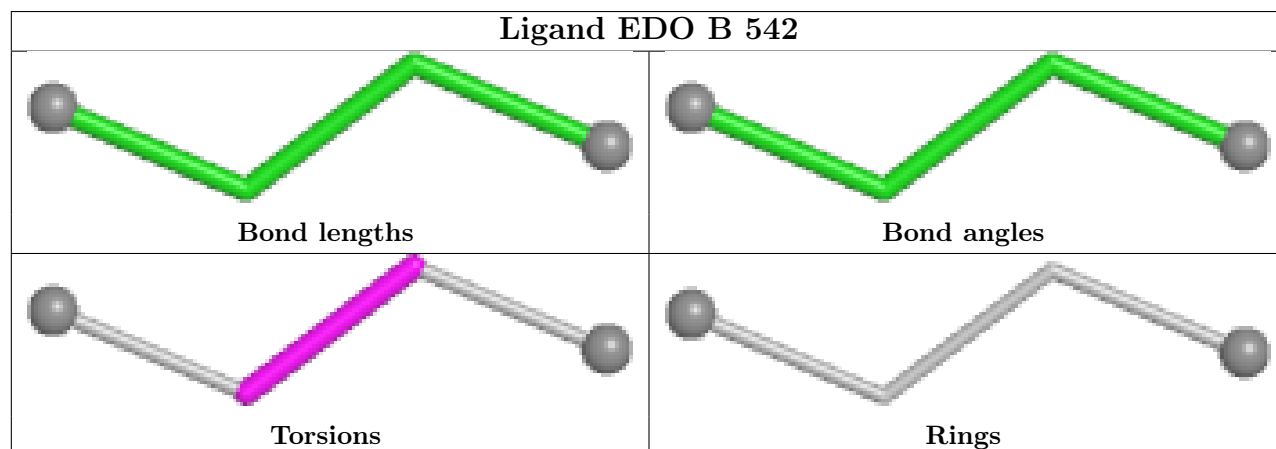
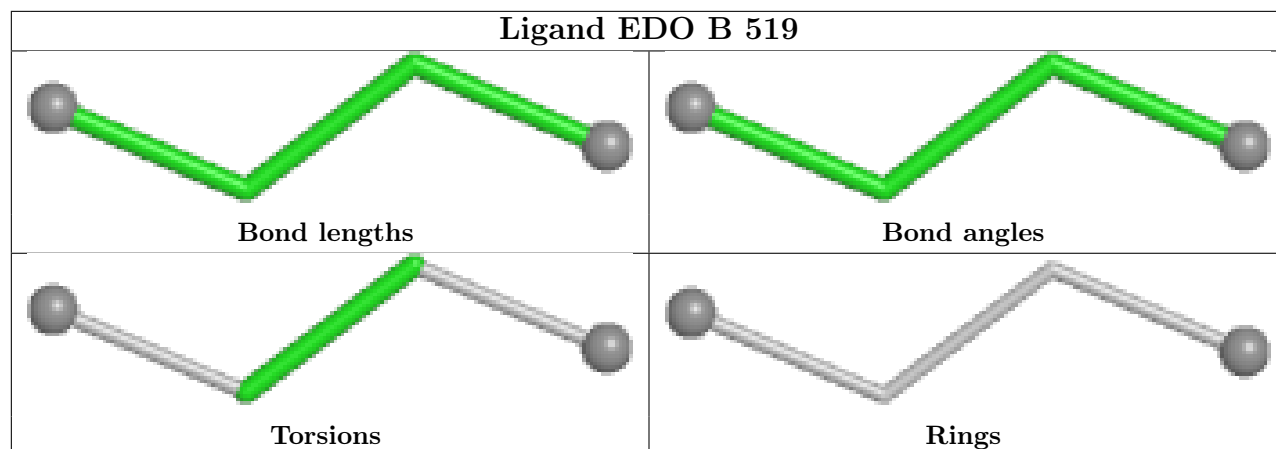
Ligand HEC A 504



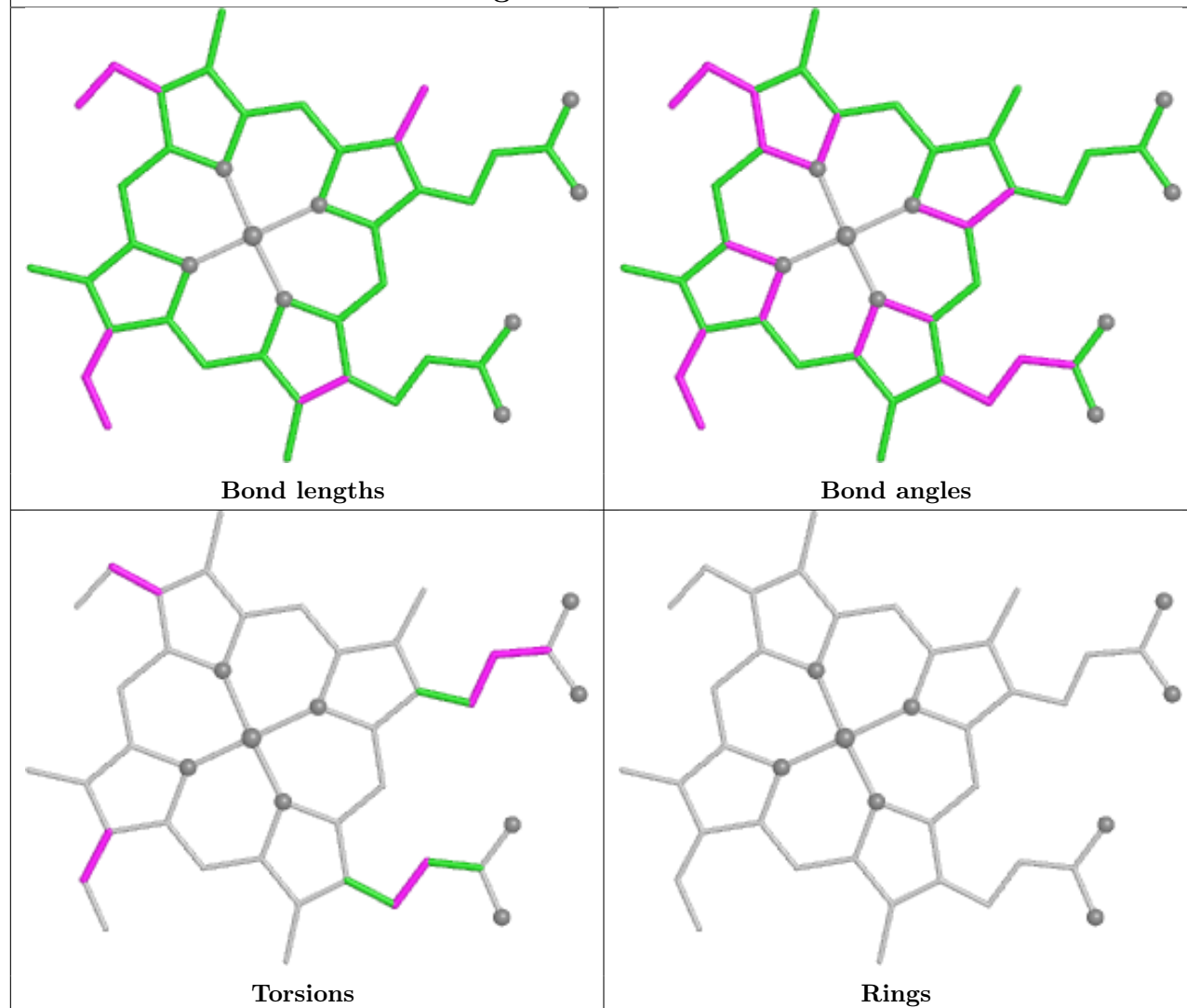
Ligand EDO C 515



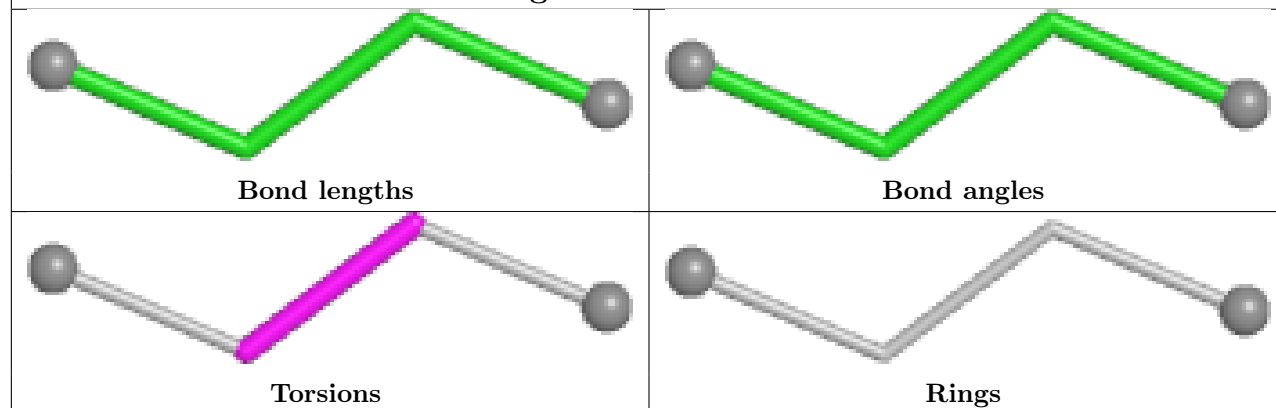


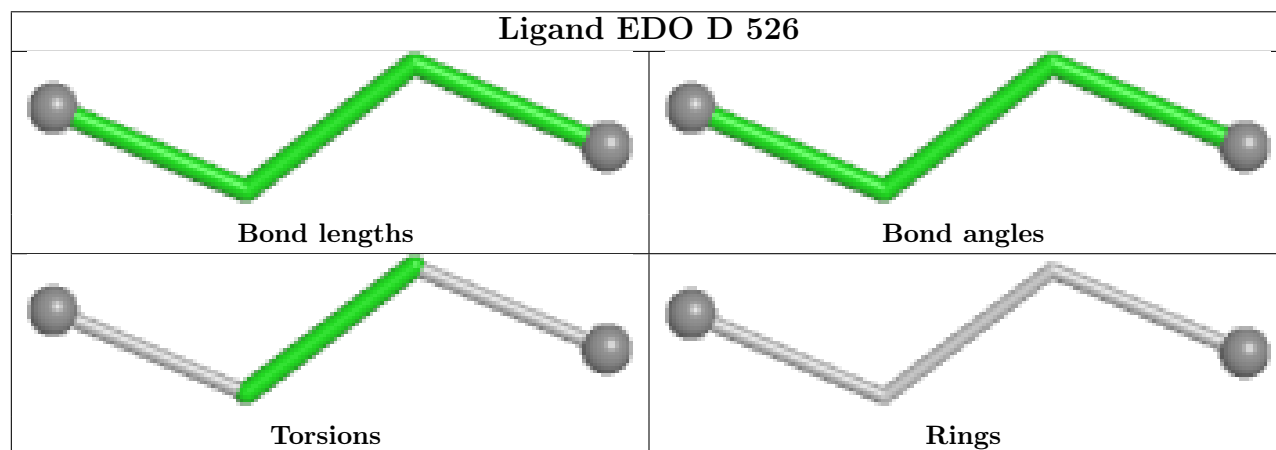
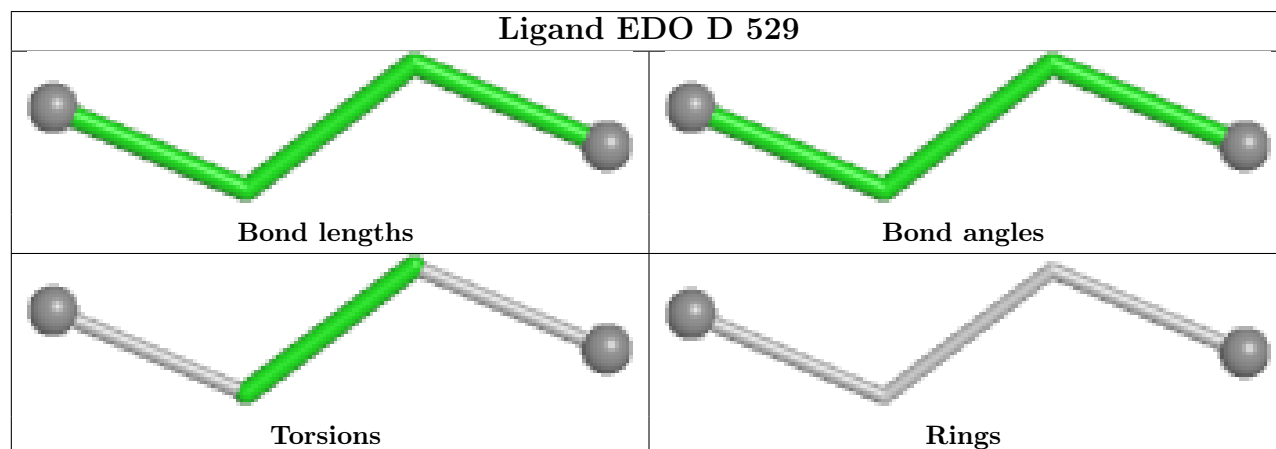
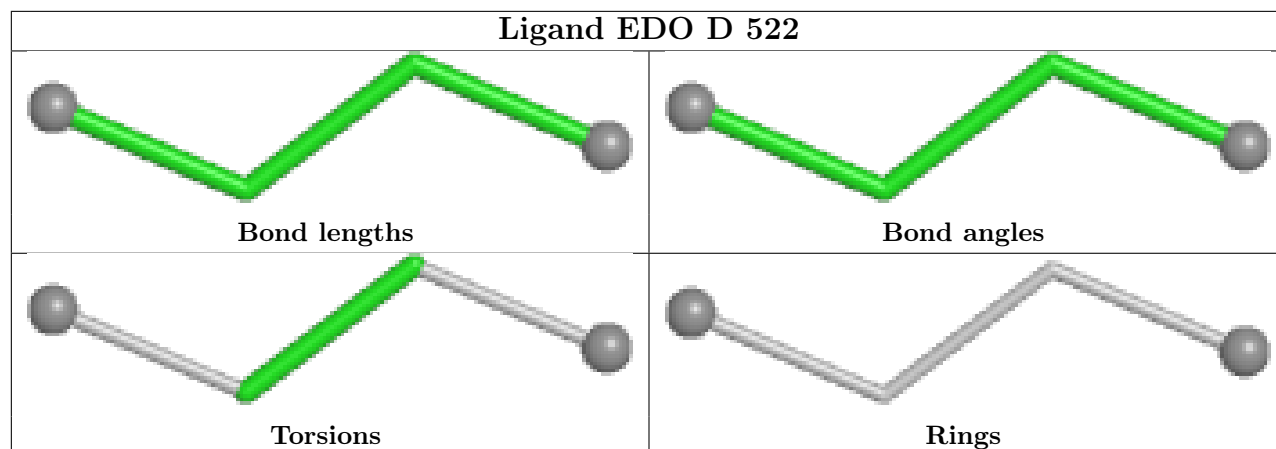


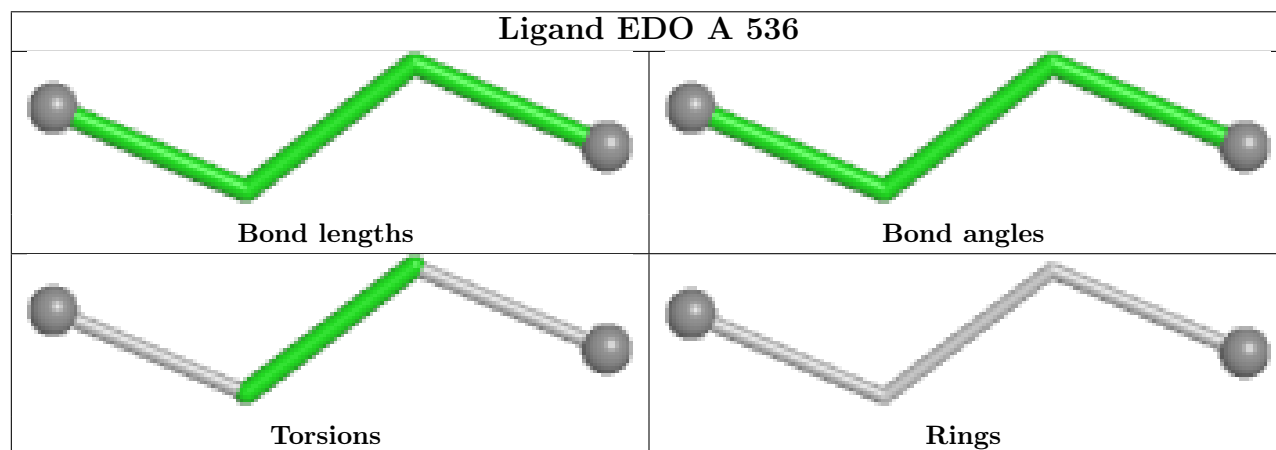
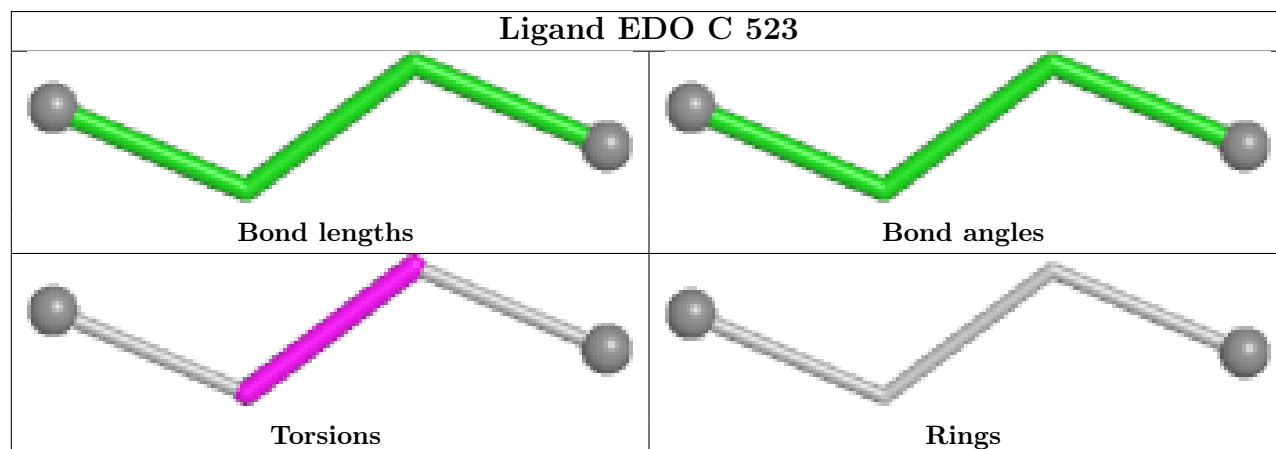
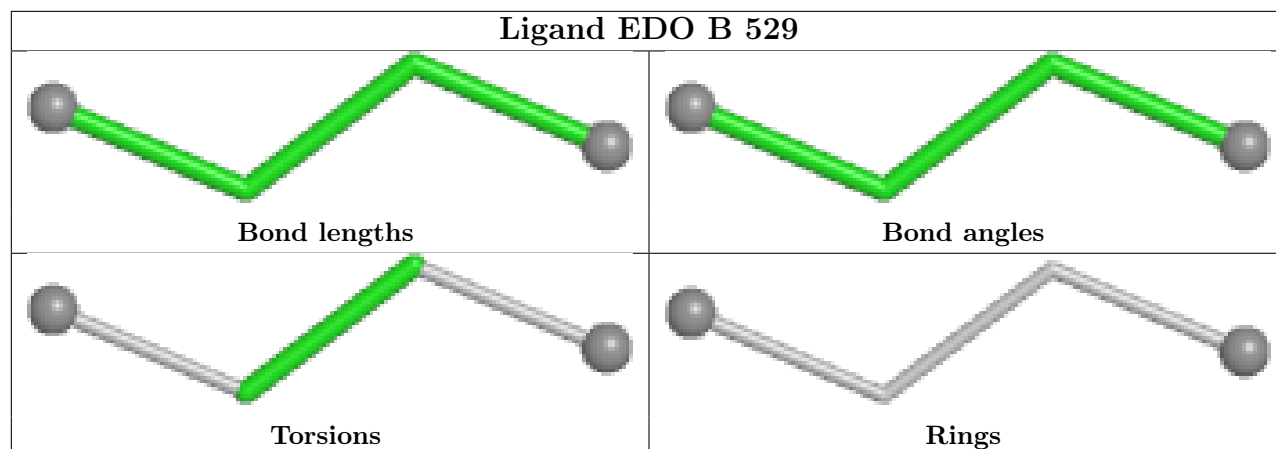
Ligand HEC C 504

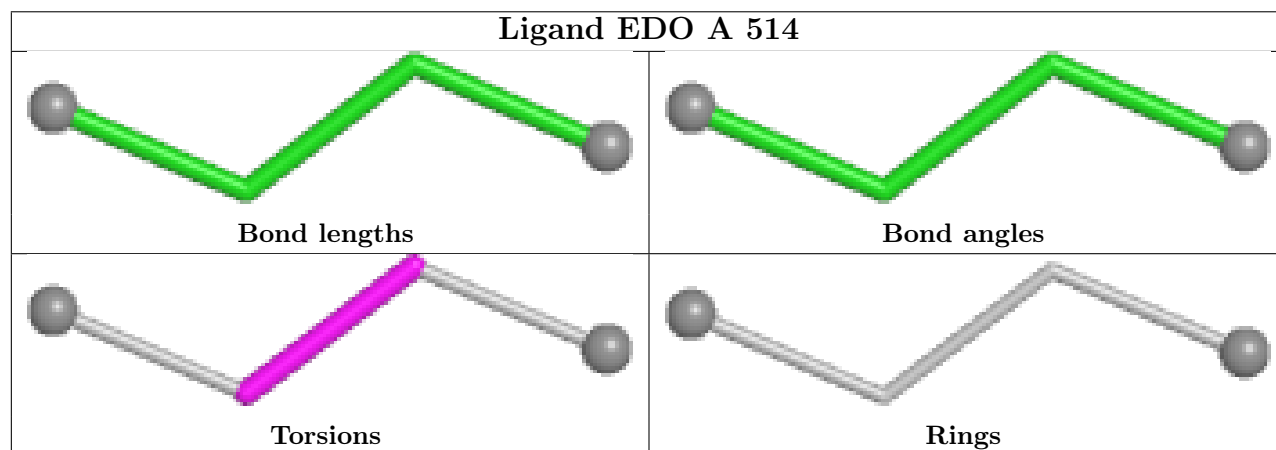
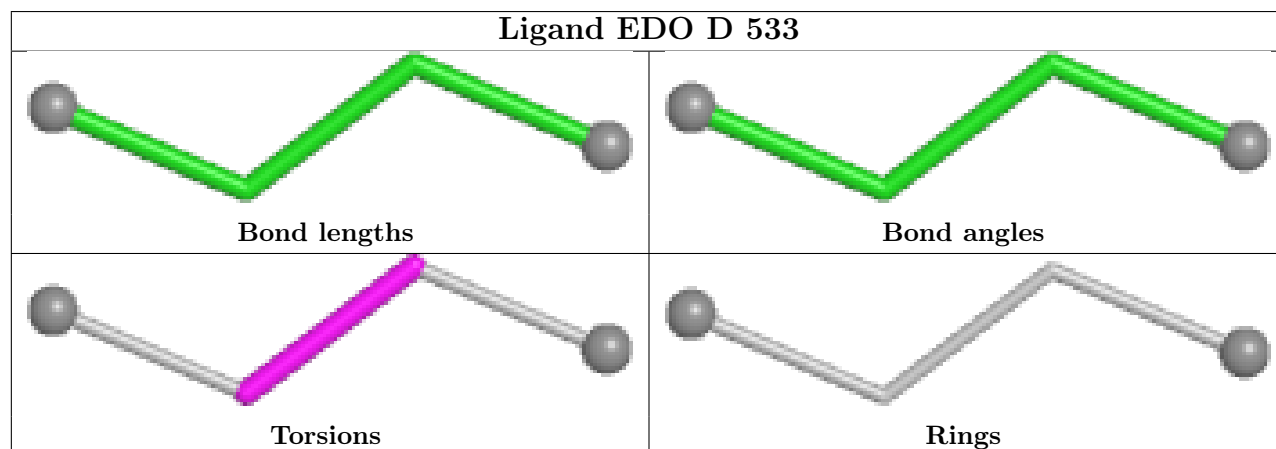
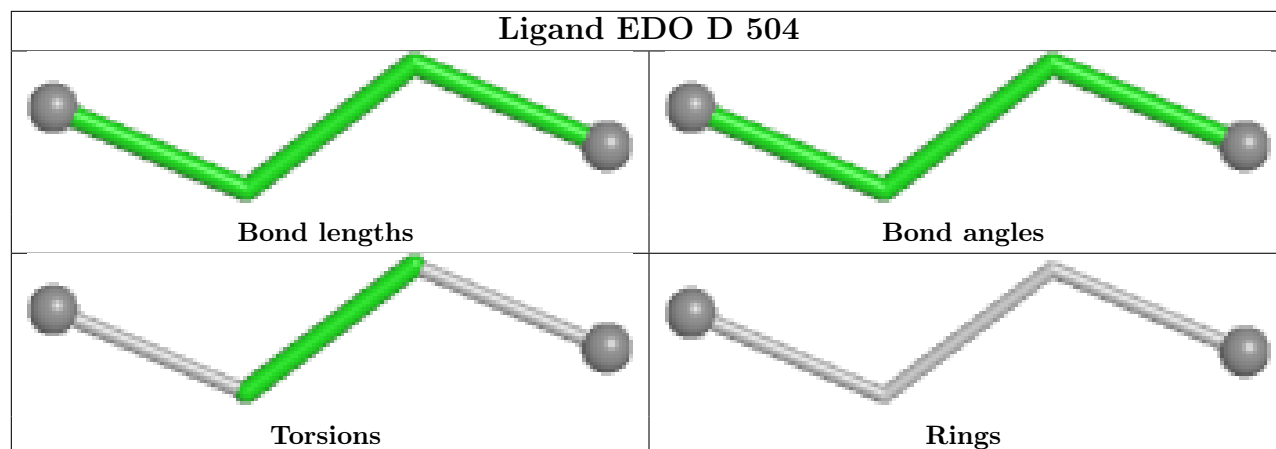


Ligand EDO A 523

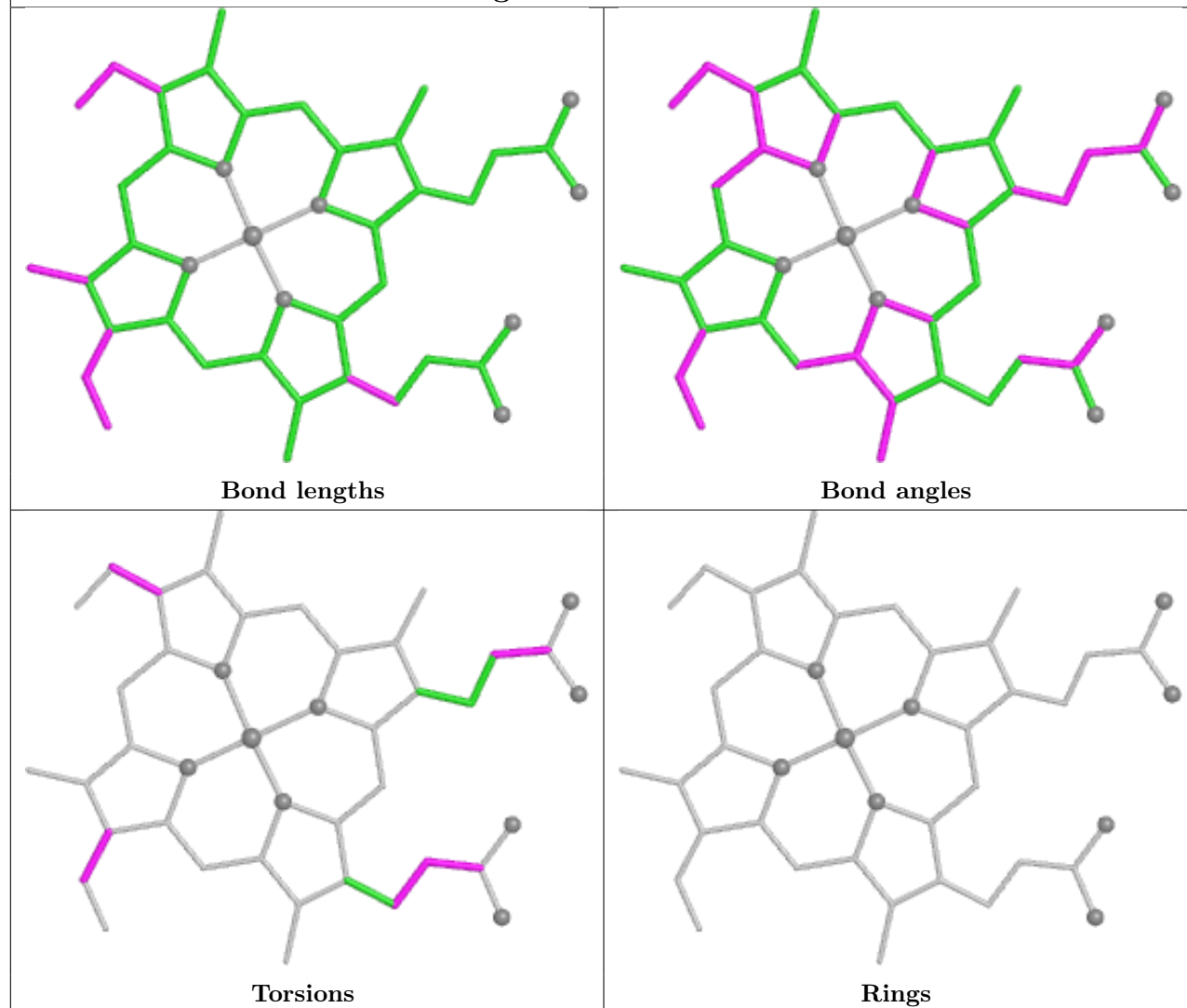




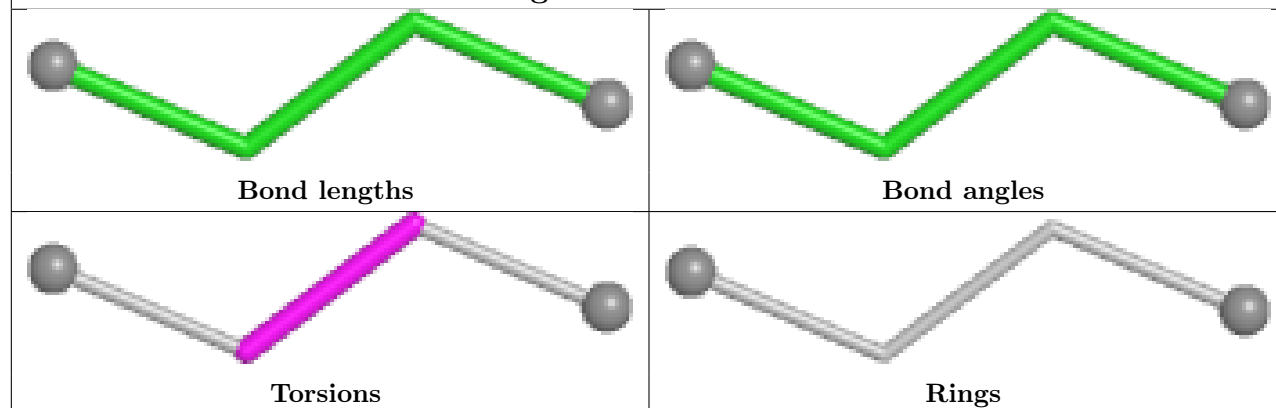


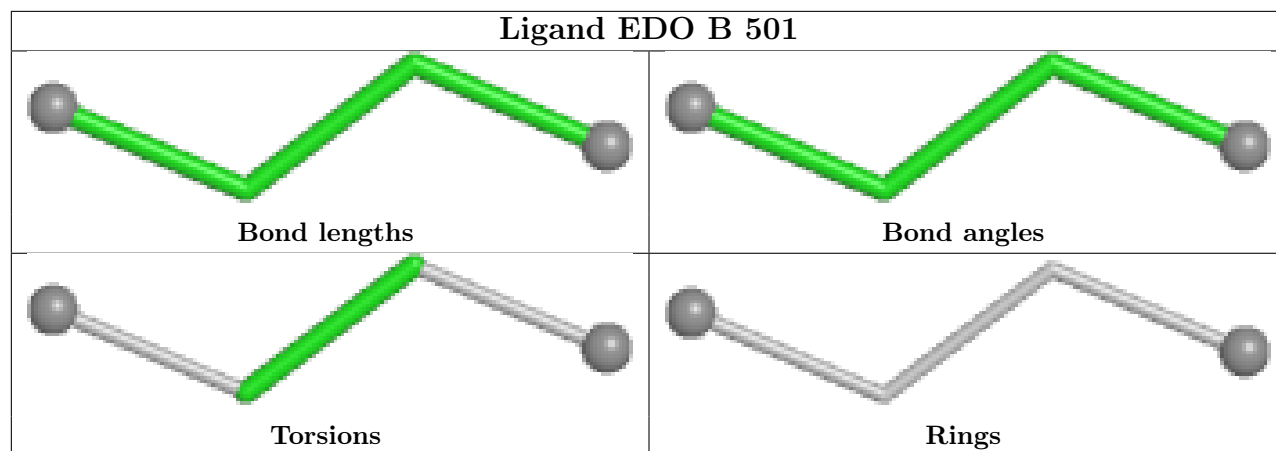


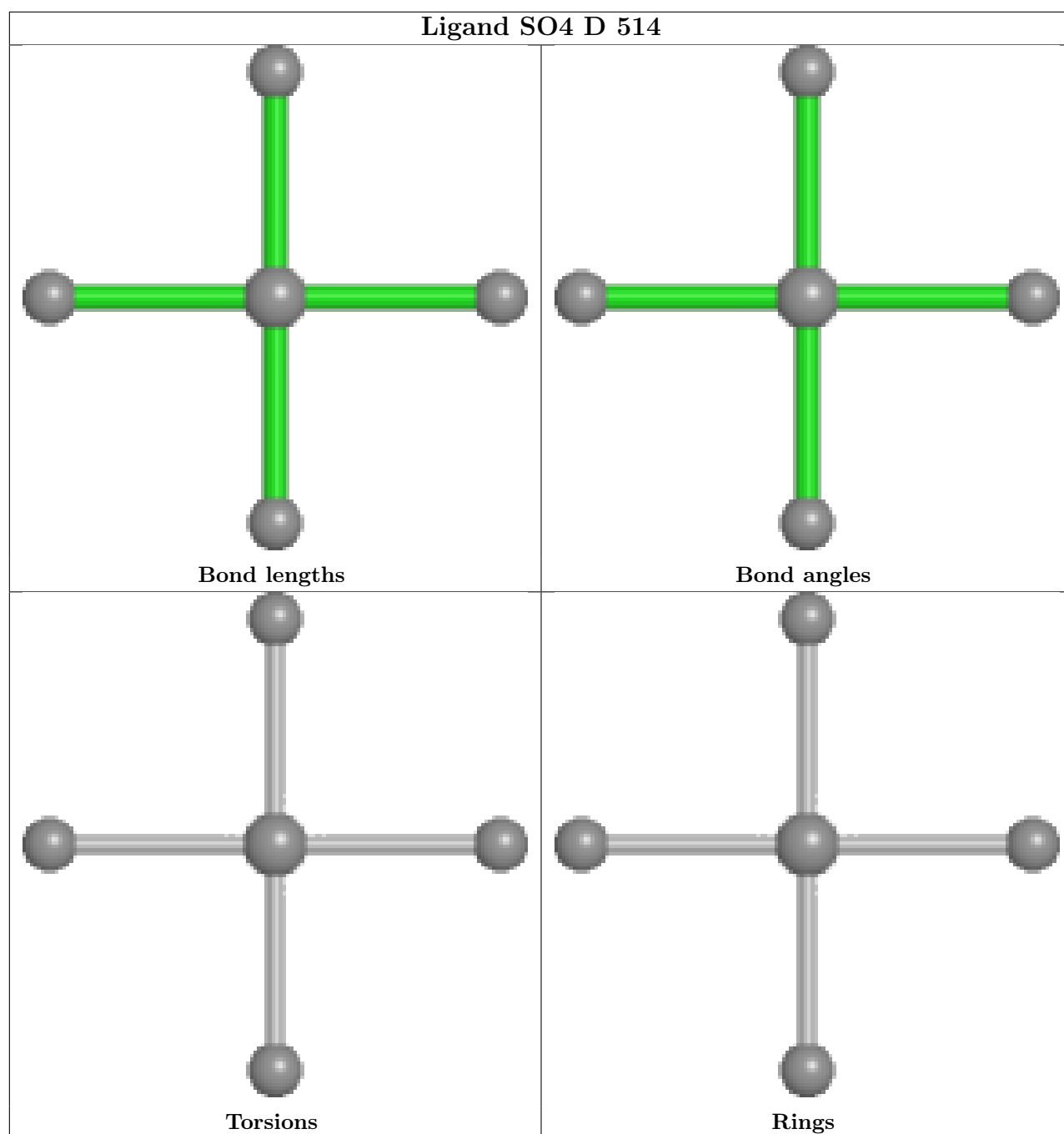
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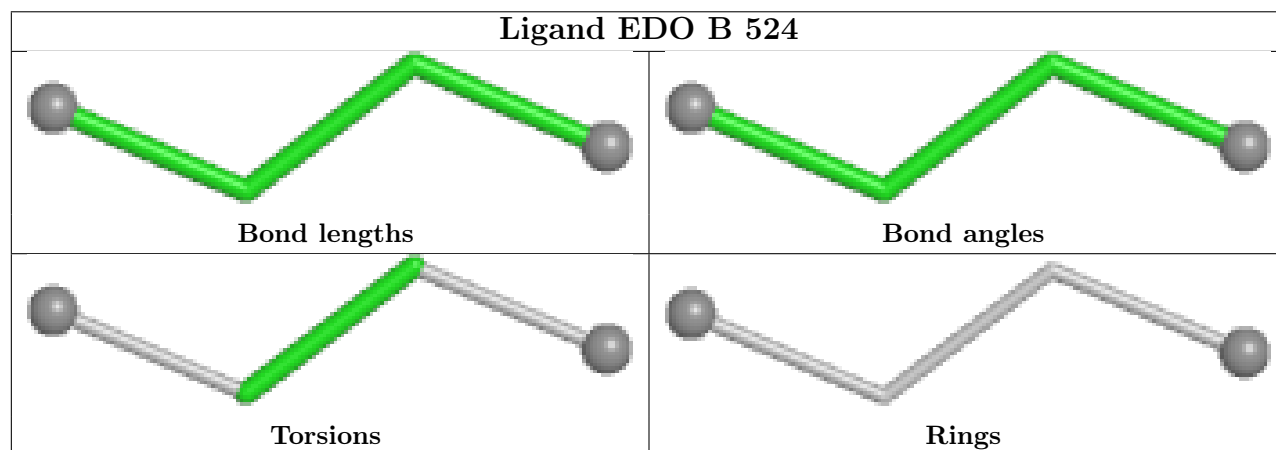
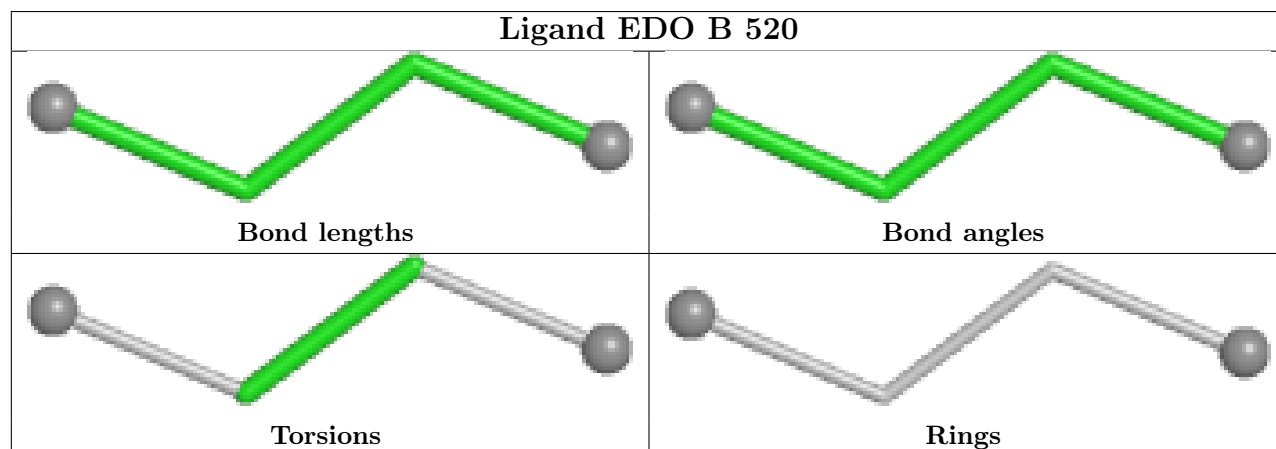
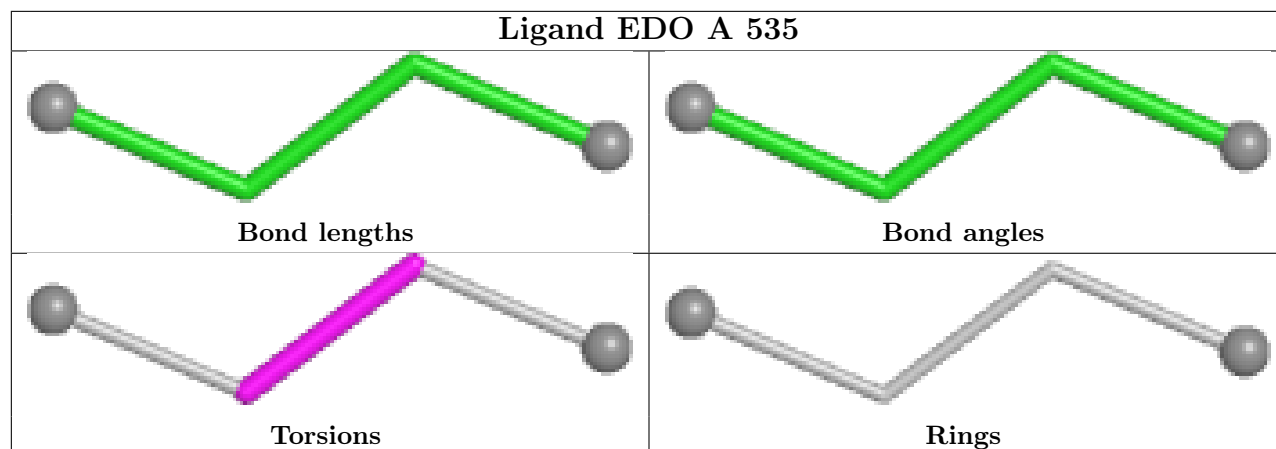


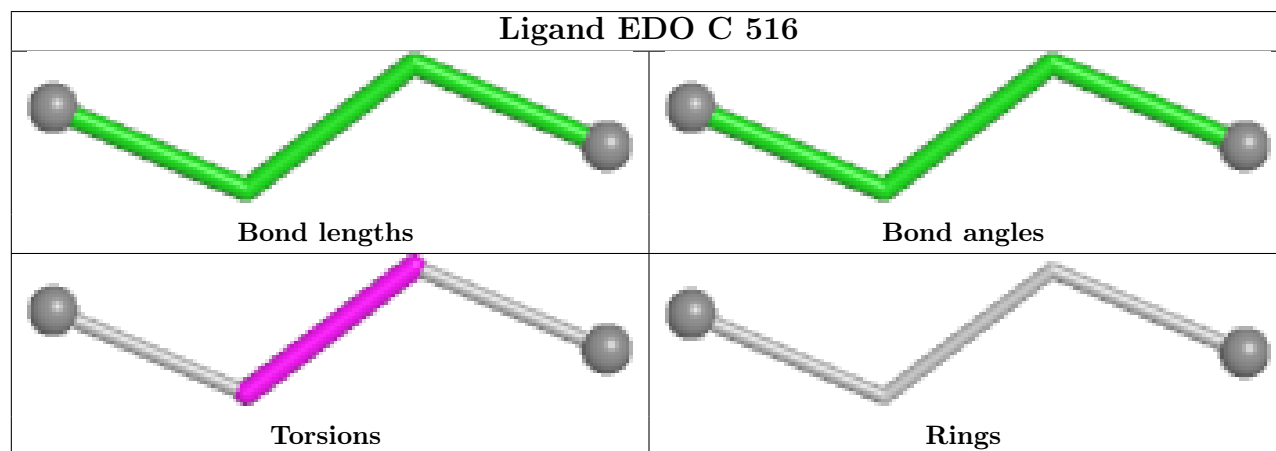
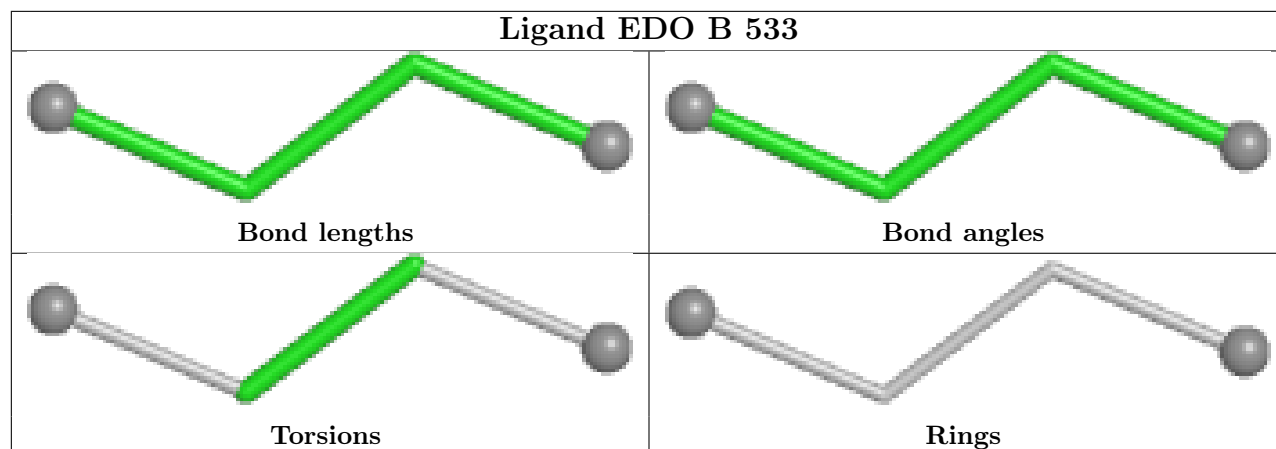
Ligand EDO B 535



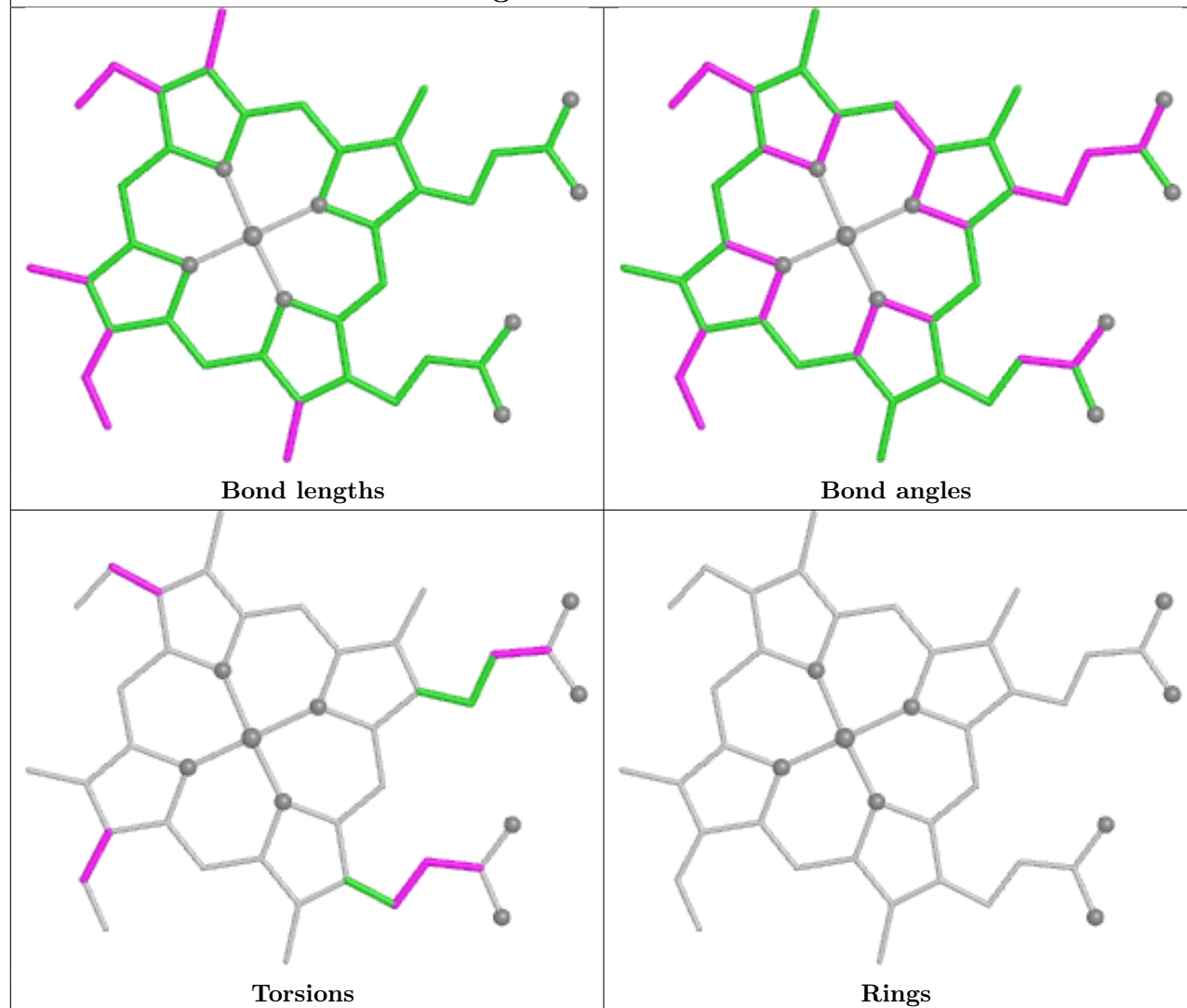




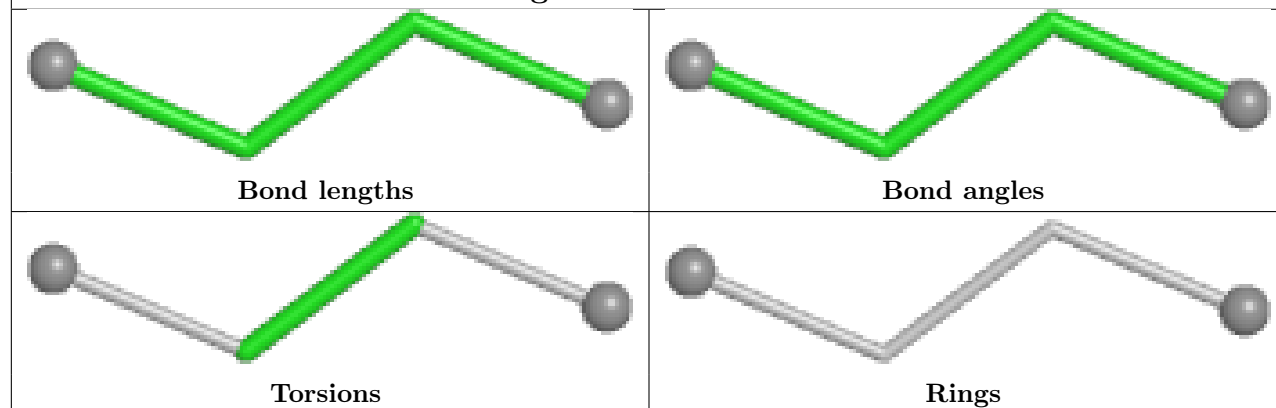


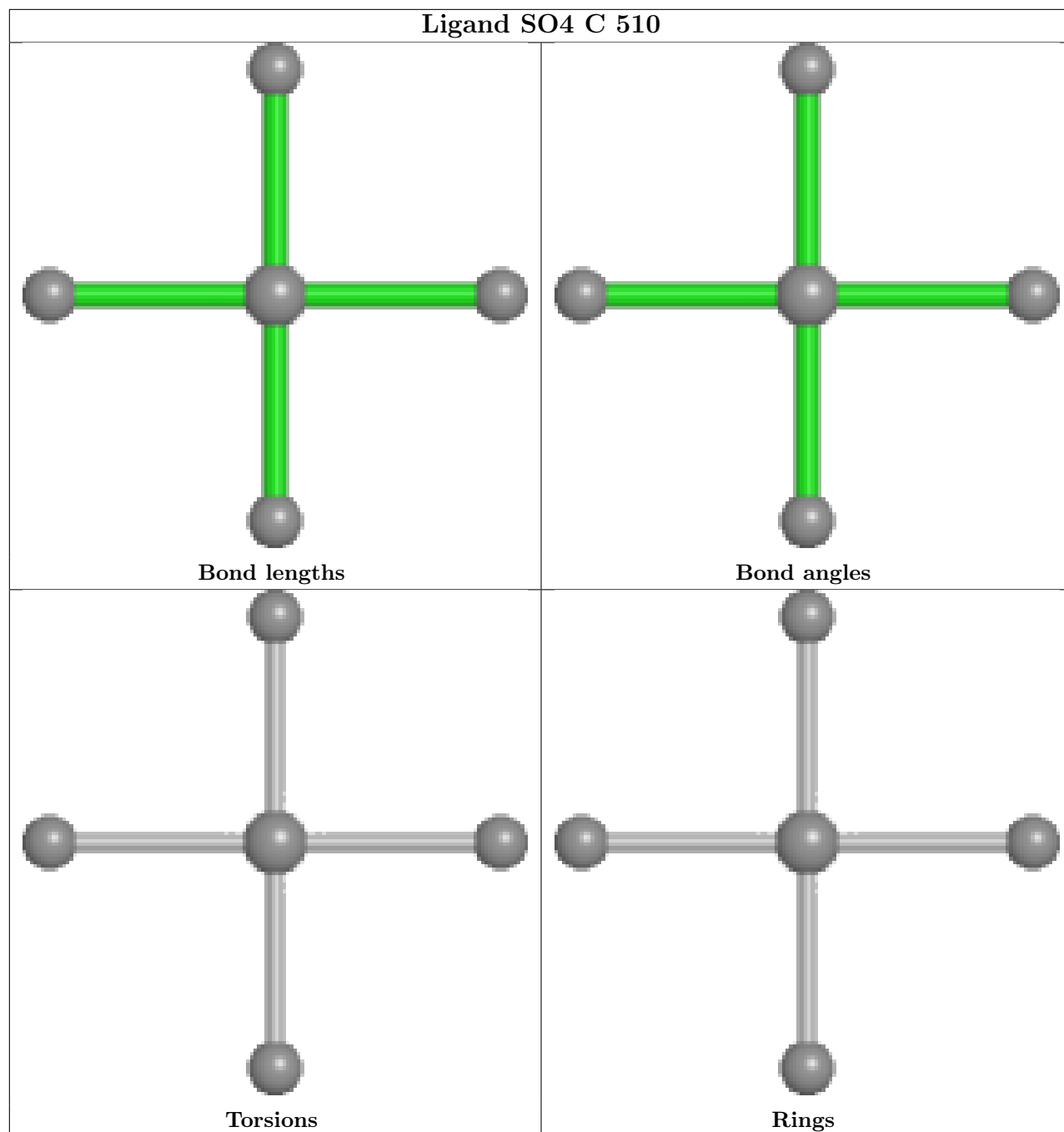


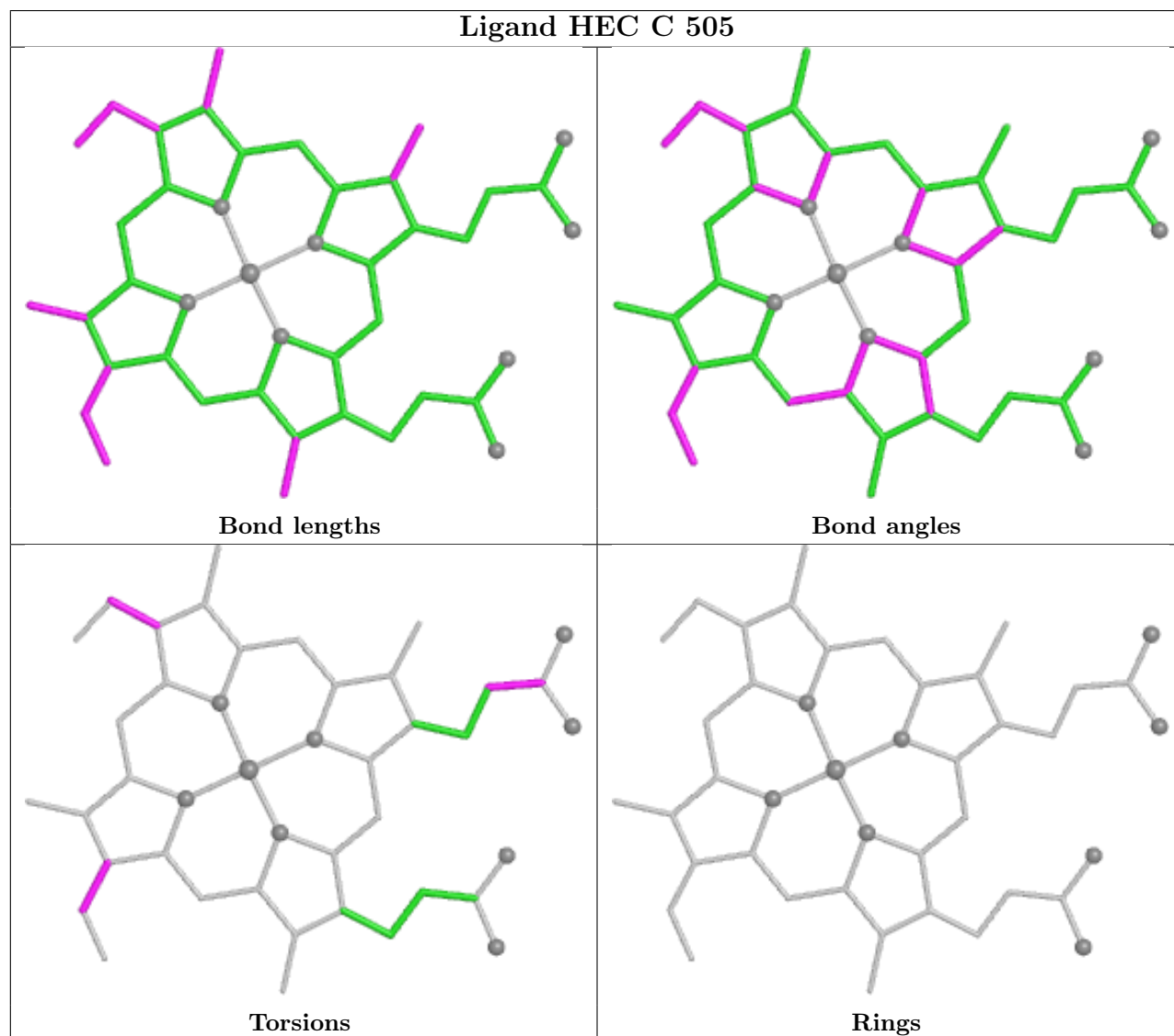
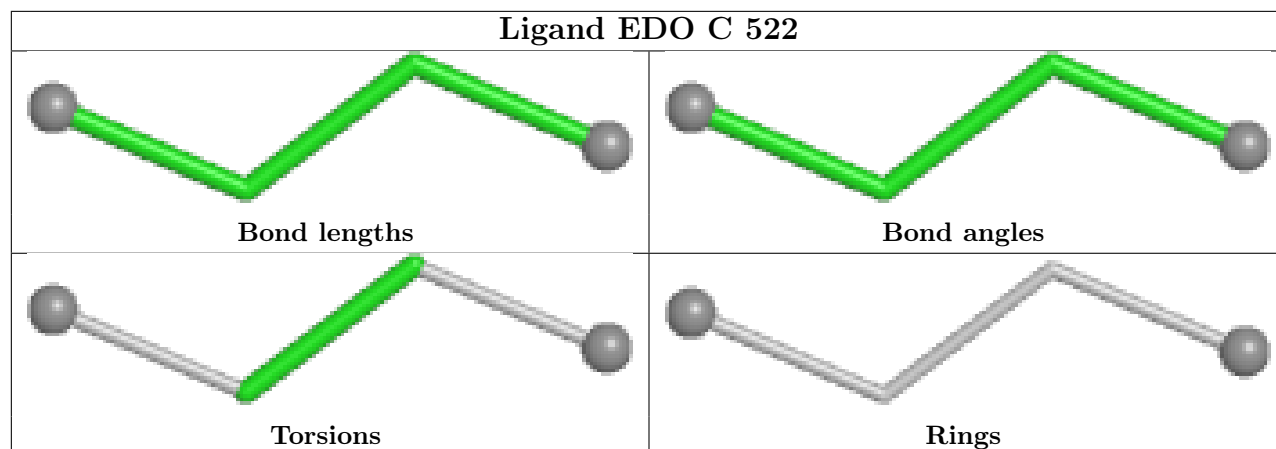
Ligand HEC D 509

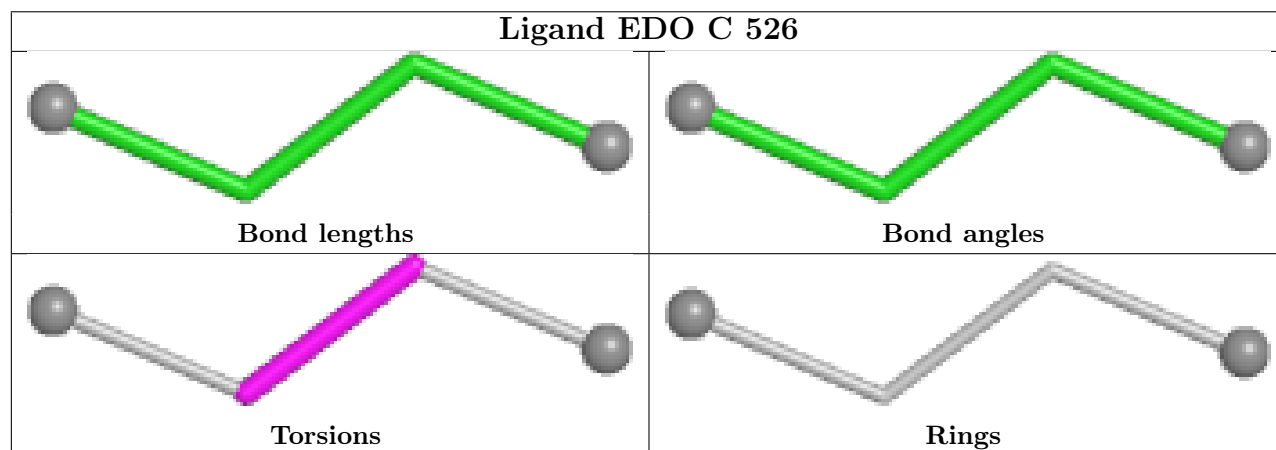
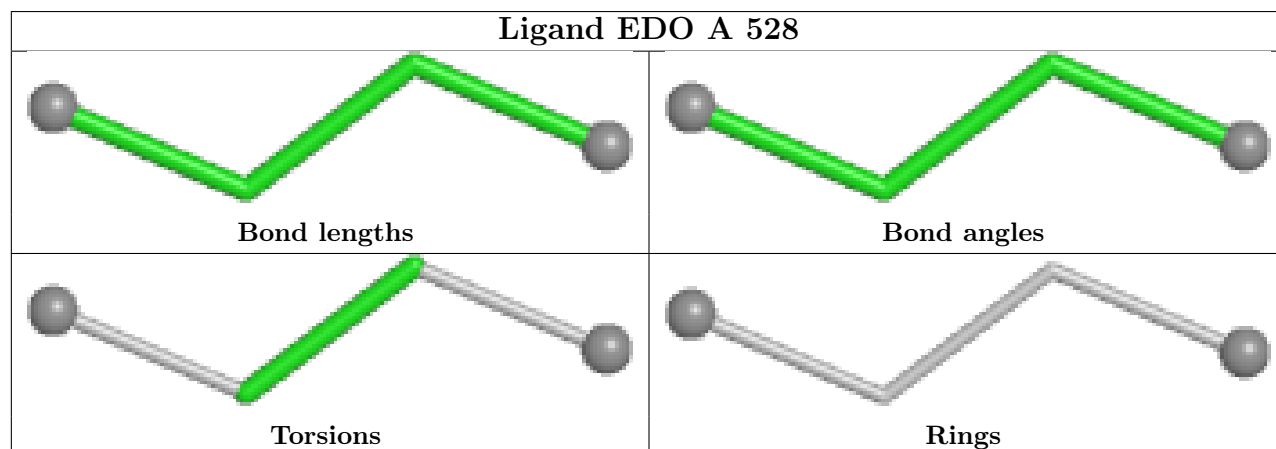
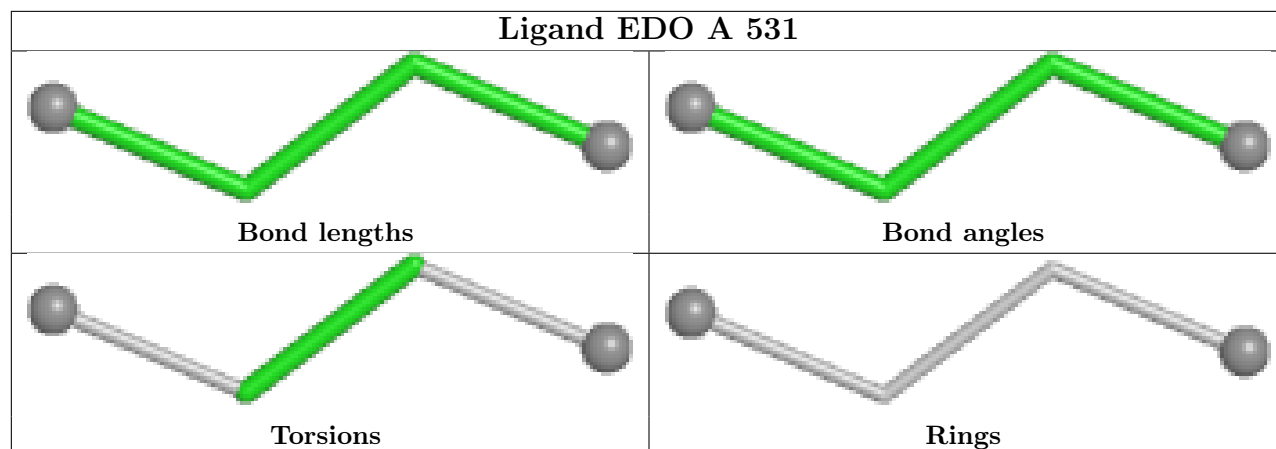


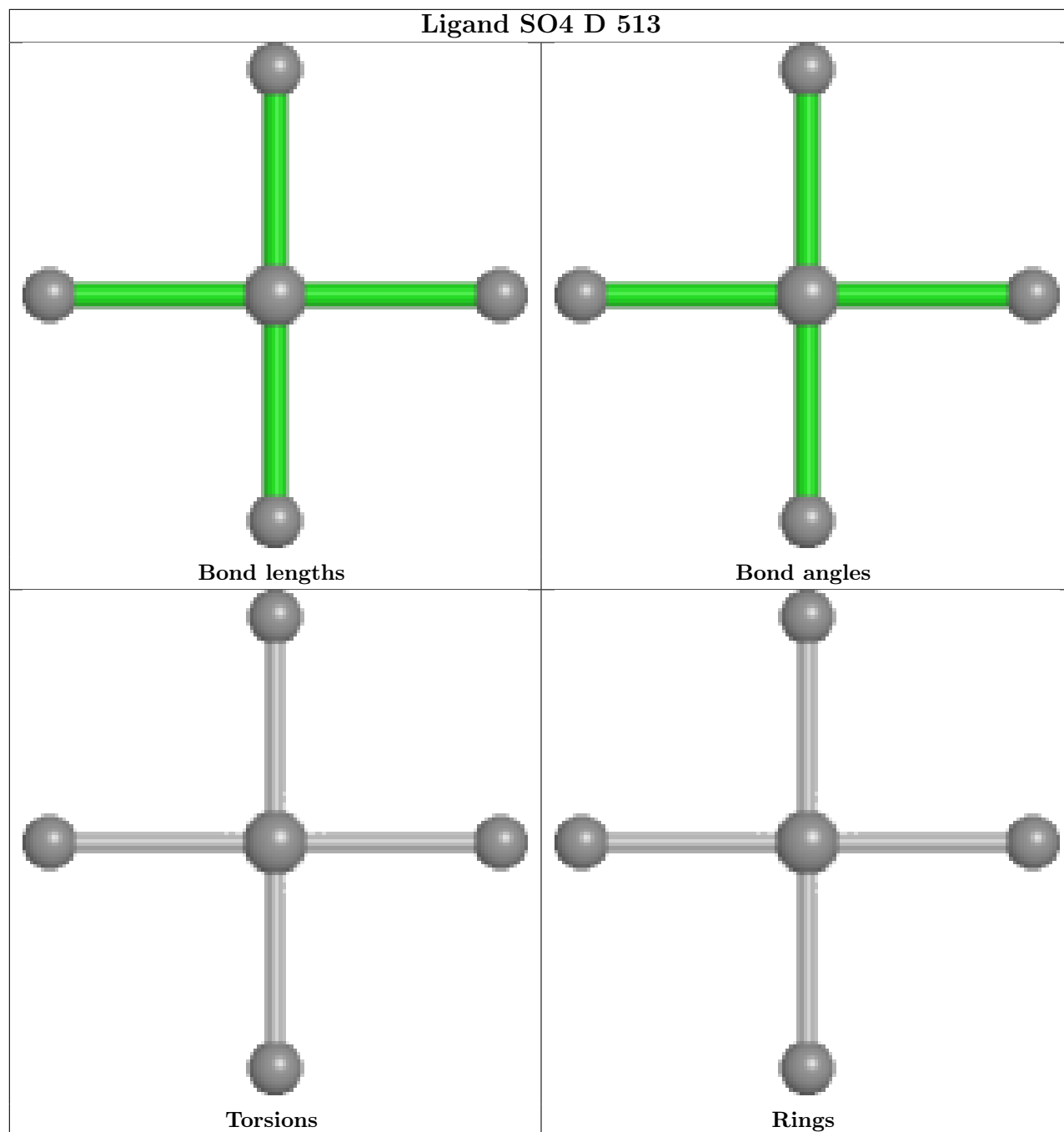
Ligand EDO B 514

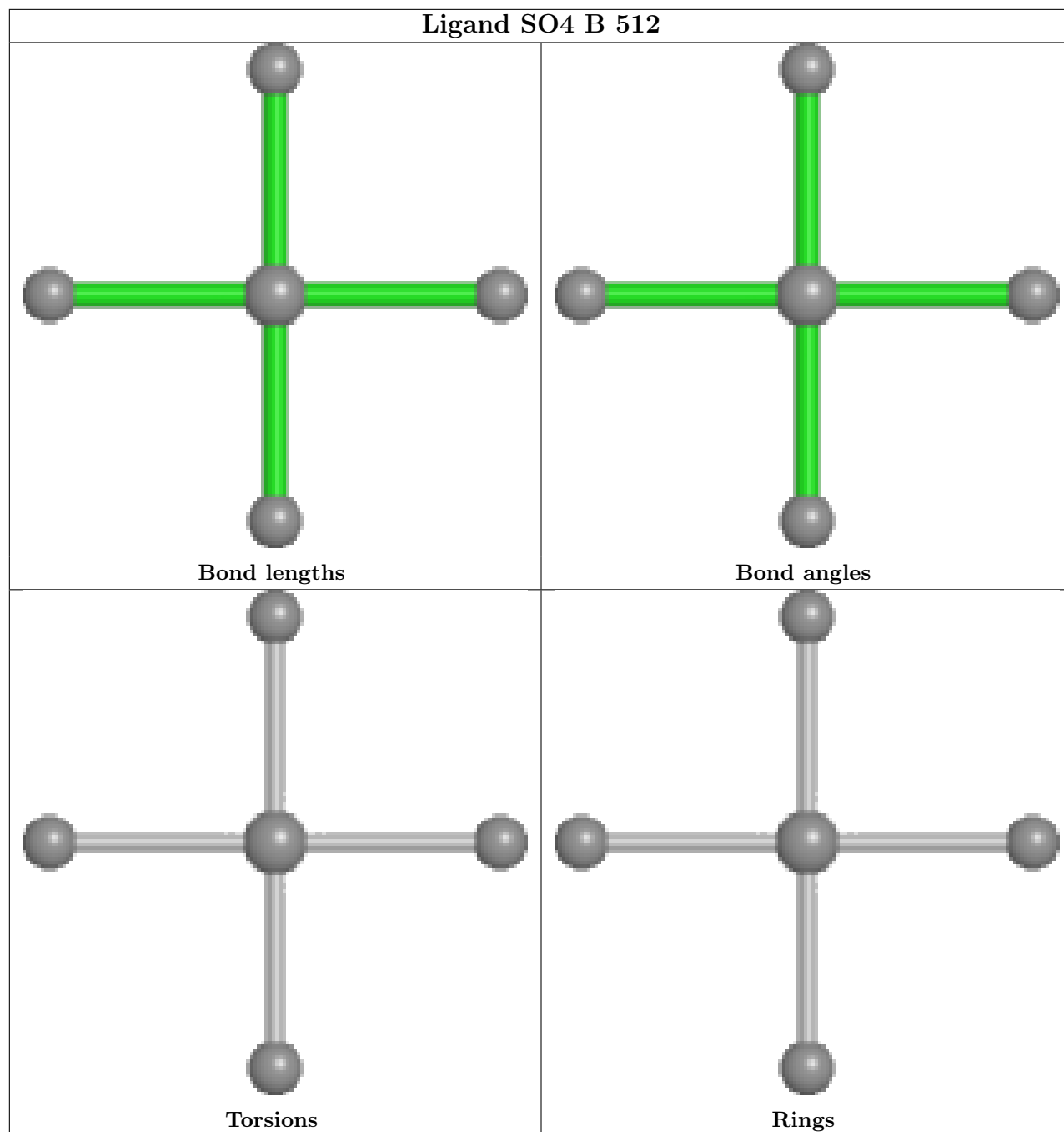


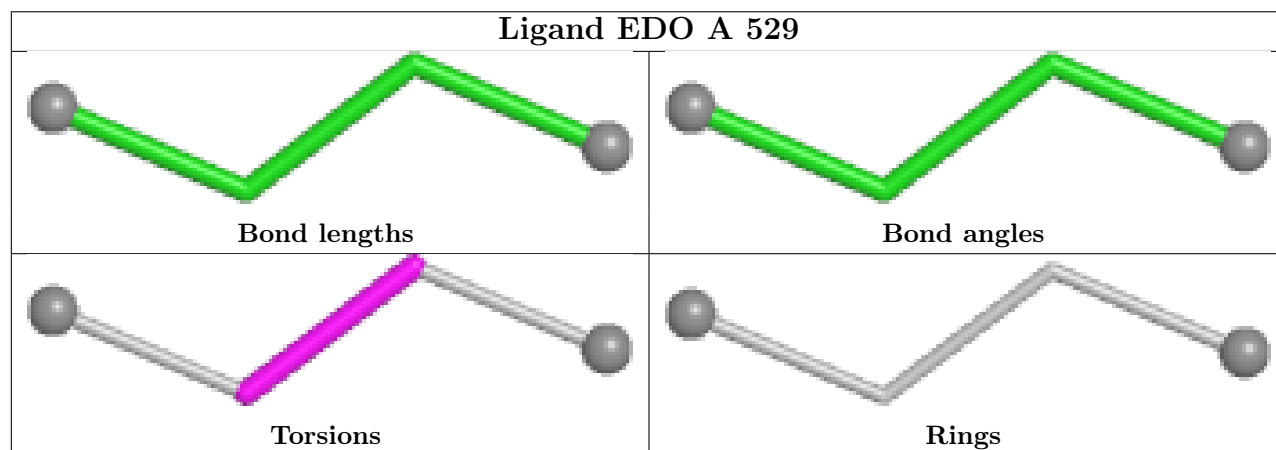
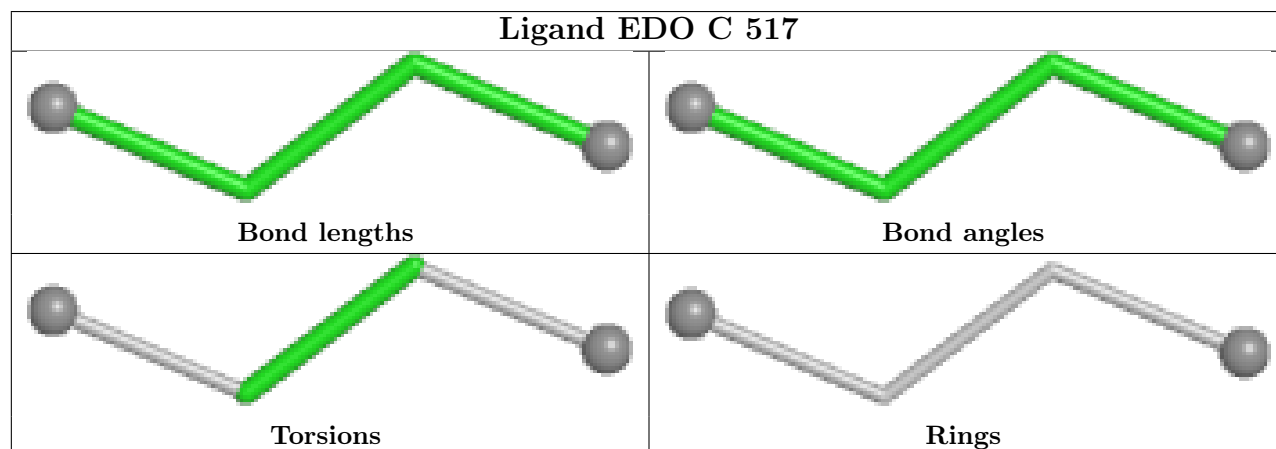
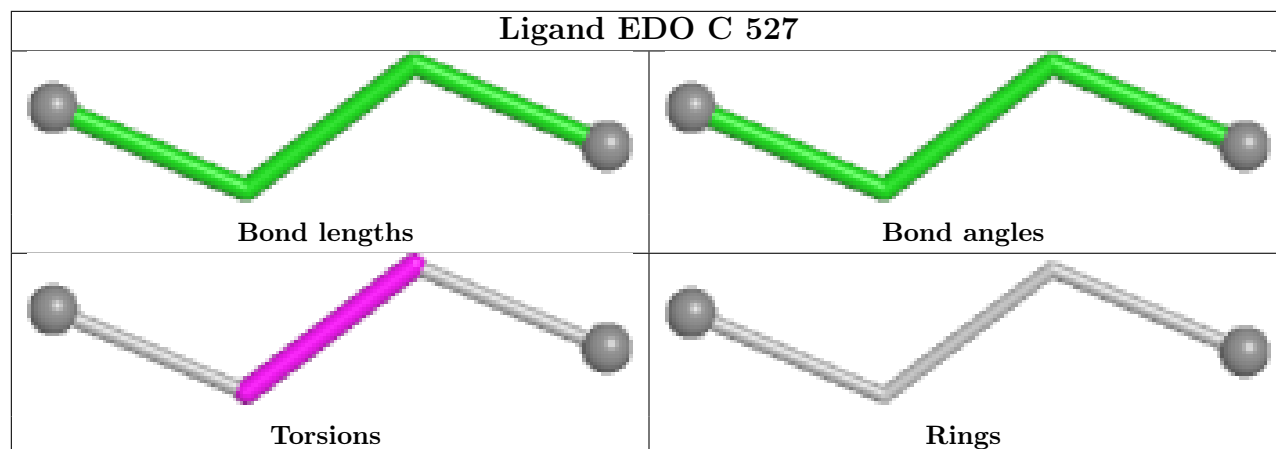


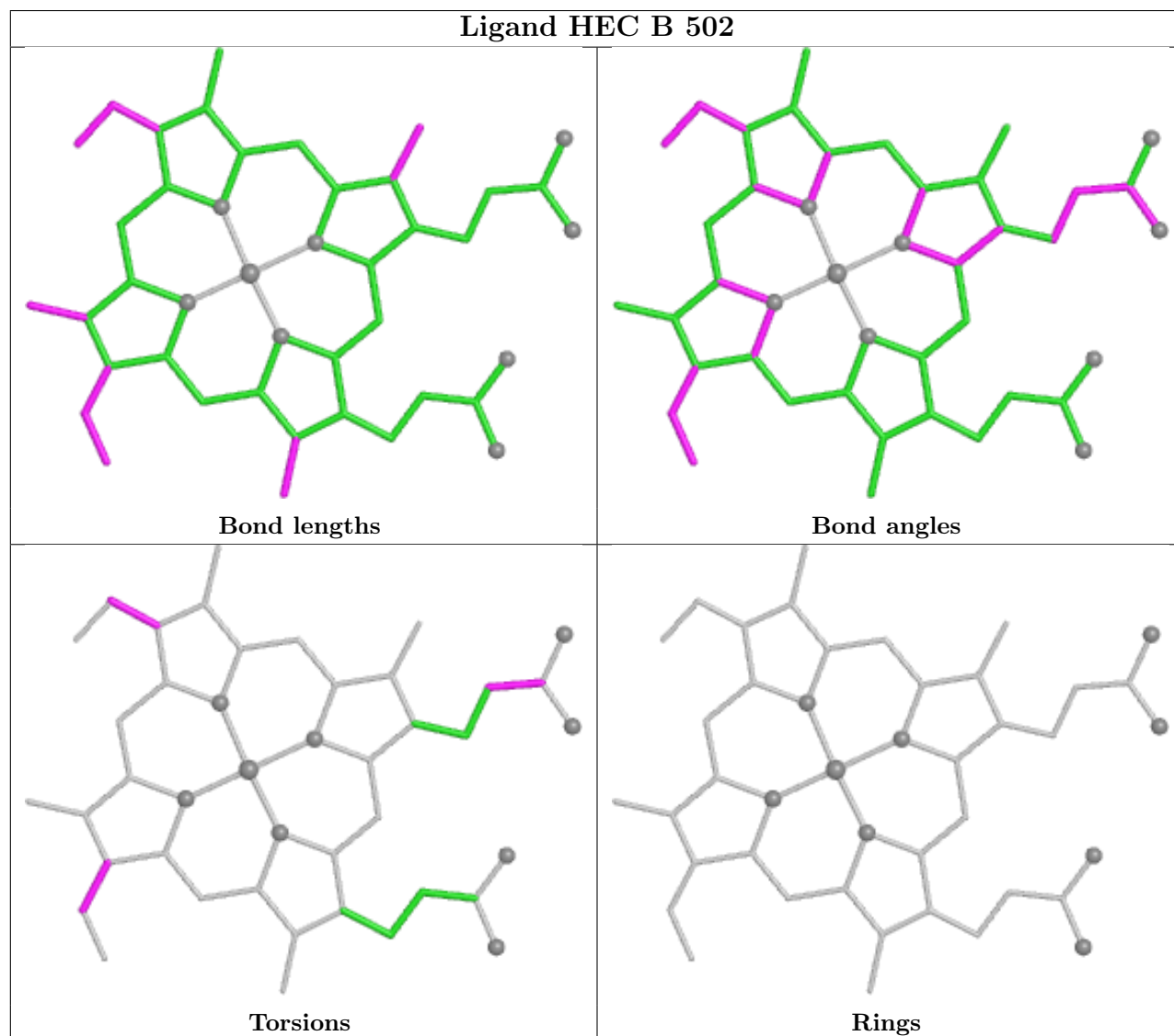
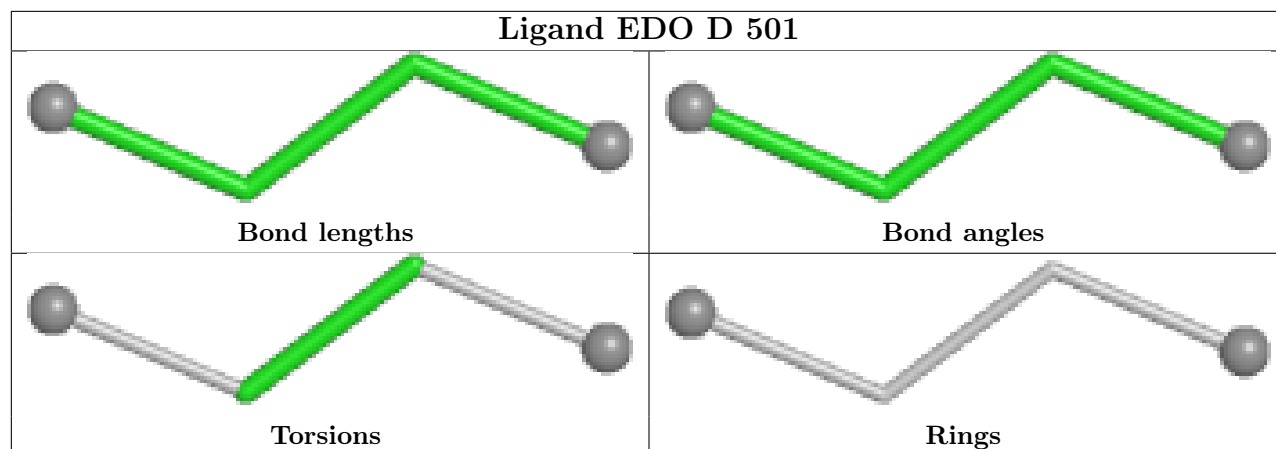


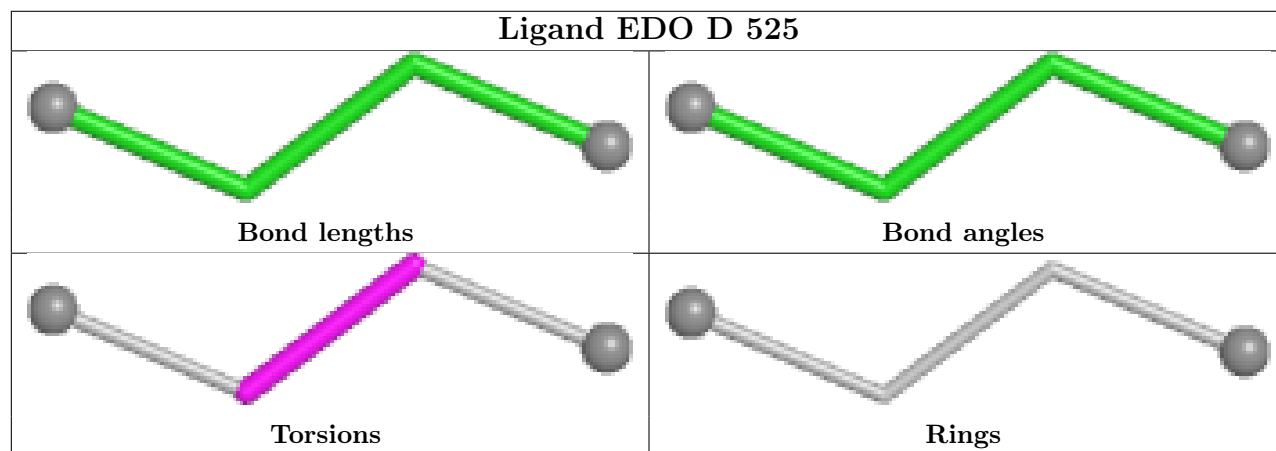
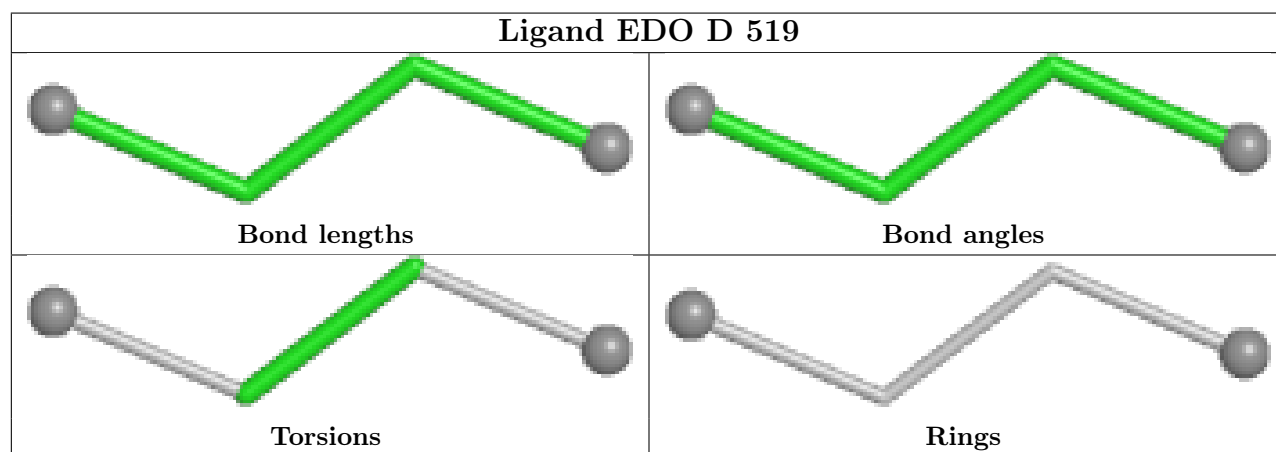
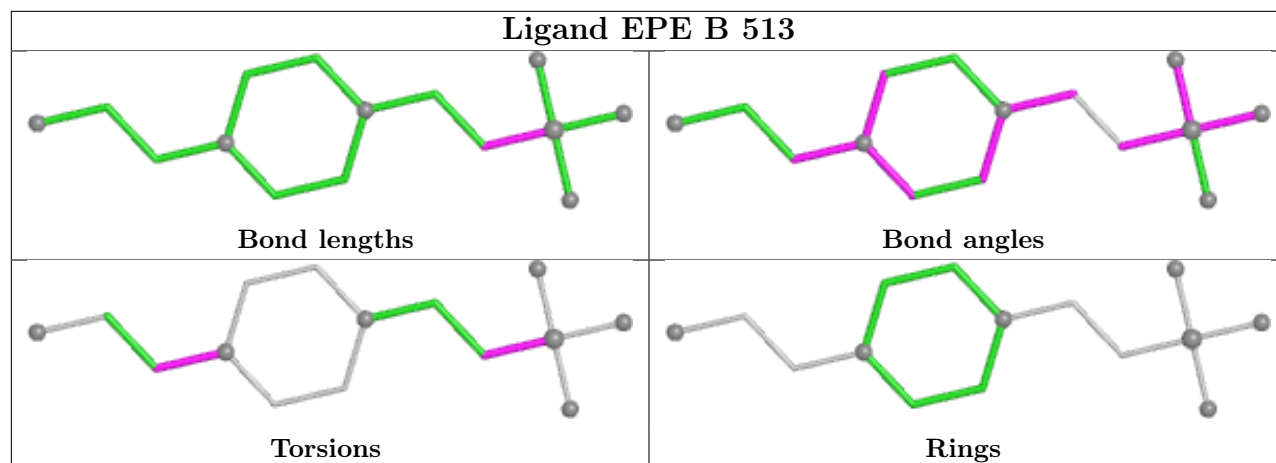


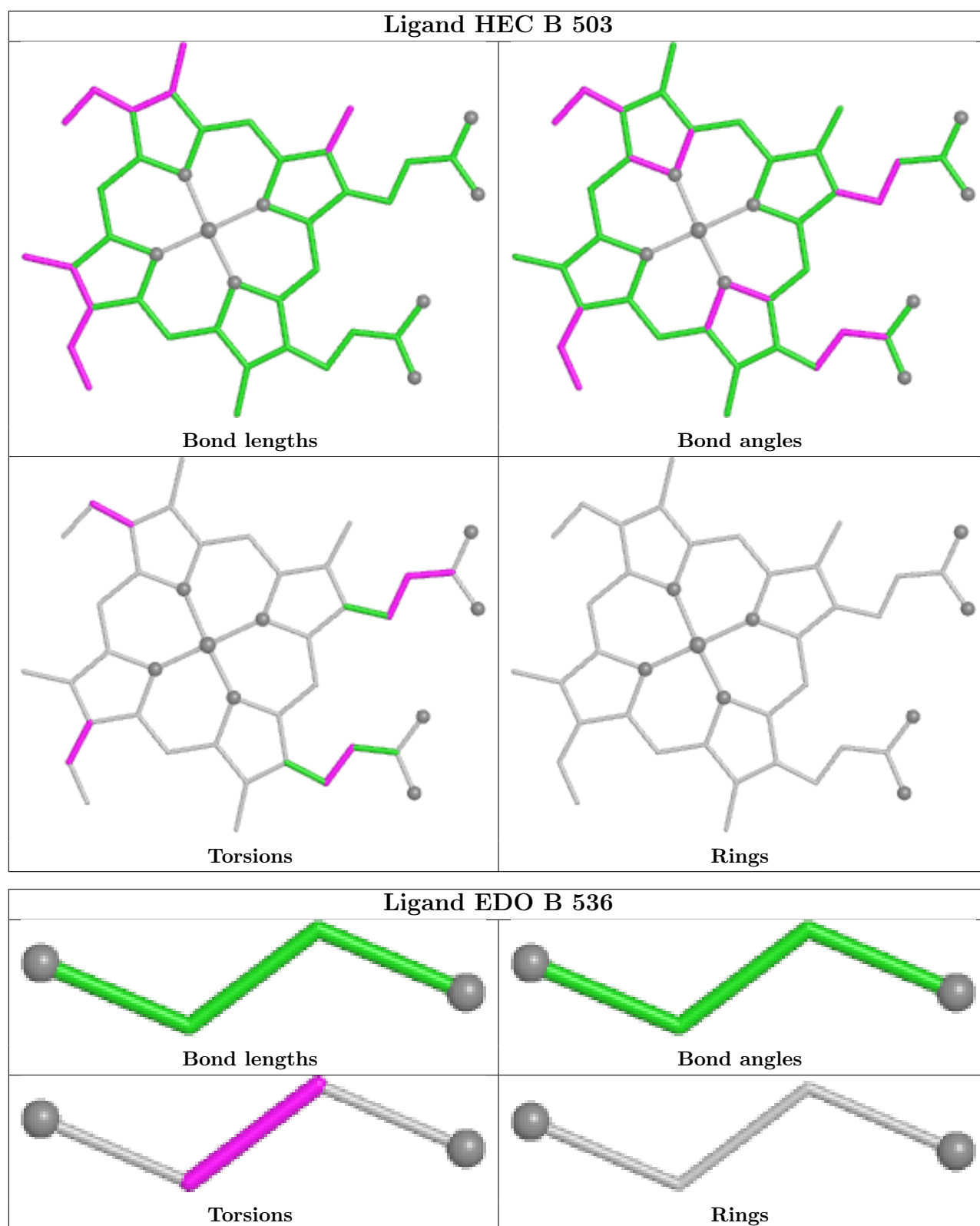












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	421/450 (93%)	0.02	5 (1%) 76 82	10, 30, 51, 68	18 (4%)
1	B	421/450 (93%)	-0.04	3 (0%) 84 88	14, 29, 48, 63	17 (4%)
1	C	421/450 (93%)	0.21	8 (1%) 66 73	14, 34, 53, 70	14 (3%)
1	D	421/450 (93%)	-0.03	1 (0%) 91 93	12, 30, 48, 71	12 (2%)
All	All	1684/1800 (93%)	0.04	17 (1%) 79 84	10, 31, 50, 71	61 (3%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	240[A]	CYS	3.9
1	C	156	ALA	3.0
1	C	157	VAL	2.9
1	B	240[A]	CYS	2.9
1	A	154	ALA	2.9
1	D	240[A]	CYS	2.8
1	B	157	VAL	2.7
1	C	154	ALA	2.6
1	A	240[A]	CYS	2.5
1	A	147	ALA	2.4
1	C	147	ALA	2.4
1	C	160	ALA	2.3
1	B	153	SER	2.3
1	C	60[A]	GLU	2.3
1	A	448	LYS	2.2
1	A	149	ARG	2.1
1	C	385[A]	LYS	2.0

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

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

6.3 Carbohydrates [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($\text{\AA}^2$)	Q<0.9
4	EDO	B	527	4/4	0.69	0.27	35,41,41,43	4
4	EDO	B	501	4/4	0.73	0.24	24,34,39,40	4
3	SO4	D	514	5/5	0.74	0.24	37,39,43,44	5
4	EDO	A	536	4/4	0.75	0.18	48,50,54,59	0
4	EDO	B	526	4/4	0.76	0.23	35,35,37,42	4
4	EDO	A	528	4/4	0.76	0.22	44,44,51,56	4
4	EDO	A	529	4/4	0.77	0.20	35,47,52,53	0
4	EDO	C	502	4/4	0.77	0.17	53,56,59,69	0
4	EDO	B	521	4/4	0.78	0.18	33,35,40,53	4
4	EDO	C	524	4/4	0.78	0.19	43,50,53,56	0
4	EDO	D	519	4/4	0.78	0.15	40,41,54,57	0
4	EDO	D	524	4/4	0.78	0.19	43,54,55,56	4
4	EDO	D	532	4/4	0.78	0.21	36,38,38,40	4
4	EDO	C	523	4/4	0.79	0.18	45,47,54,57	0
3	SO4	C	512	5/5	0.79	0.14	51,51,62,67	5
4	EDO	D	525	4/4	0.79	0.14	35,51,59,63	0
4	EDO	C	528	4/4	0.79	0.20	44,47,52,53	4
4	EDO	C	521	4/4	0.80	0.19	40,43,44,49	0
3	SO4	B	510	5/5	0.80	0.15	47,56,63,64	5
4	EDO	B	538	4/4	0.80	0.18	37,46,50,54	4
3	SO4	B	512	5/5	0.80	0.11	52,54,57,57	5
6	PGE	B	539	10/10	0.80	0.20	26,39,47,49	10
6	PGE	D	530	10/10	0.80	0.20	28,34,44,45	10
4	EDO	D	526	4/4	0.81	0.18	32,37,47,52	4
4	EDO	A	522	4/4	0.81	0.14	41,43,54,59	0
4	EDO	B	531	4/4	0.82	0.16	38,44,50,50	4
4	EDO	C	527	4/4	0.82	0.17	41,46,48,50	4
4	EDO	A	514	4/4	0.82	0.17	35,45,55,59	0
4	EDO	B	542	4/4	0.82	0.18	40,43,48,52	4
4	EDO	D	521	4/4	0.82	0.18	37,38,40,49	4
4	EDO	D	523	4/4	0.82	0.16	55,56,58,58	0
4	EDO	B	535	4/4	0.83	0.15	46,48,50,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	B	524	4/4	0.83	0.16	56,59,66,67	0
3	SO4	B	541	5/5	0.83	0.14	56,57,59,64	5
3	SO4	C	513	5/5	0.83	0.14	51,54,64,65	5
4	EDO	B	528	4/4	0.83	0.16	33,39,46,47	4
4	EDO	A	517	4/4	0.83	0.22	25,31,39,43	4
4	EDO	B	533	4/4	0.84	0.18	25,26,29,43	0
4	EDO	B	525	4/4	0.84	0.18	35,41,42,49	4
4	EDO	C	525	4/4	0.84	0.18	39,39,44,48	4
4	EDO	A	518	4/4	0.84	0.20	37,40,43,47	4
4	EDO	D	529	4/4	0.84	0.17	25,27,28,38	0
4	EDO	B	520	4/4	0.84	0.14	39,51,53,58	0
4	EDO	A	523	4/4	0.84	0.13	33,42,47,54	0
4	EDO	A	526	4/4	0.84	0.21	31,32,34,39	4
4	EDO	B	522	4/4	0.85	0.15	48,55,60,63	0
3	SO4	B	511	5/5	0.85	0.11	50,53,62,70	5
4	EDO	B	530	4/4	0.85	0.18	25,33,34,37	4
3	SO4	C	511	5/5	0.85	0.11	43,44,52,56	5
4	EDO	A	521	4/4	0.85	0.13	42,49,51,53	0
4	EDO	C	532	4/4	0.86	0.14	34,35,41,46	4
4	EDO	A	512	4/4	0.86	0.18	38,39,45,48	0
3	SO4	C	509	5/5	0.86	0.12	48,51,57,60	5
4	EDO	A	532	4/4	0.86	0.16	25,30,34,36	4
4	EDO	C	519	4/4	0.86	0.14	49,52,55,60	0
4	EDO	A	534	4/4	0.86	0.12	57,58,62,65	0
4	EDO	B	523	4/4	0.86	0.14	26,52,55,55	0
4	EDO	B	532	4/4	0.86	0.20	31,34,38,40	4
4	EDO	D	531	4/4	0.86	0.14	46,50,54,57	0
4	EDO	A	516	4/4	0.86	0.13	42,45,54,67	0
4	EDO	A	537	4/4	0.86	0.18	23,26,30,35	4
4	EDO	B	536	4/4	0.86	0.17	43,44,45,50	0
4	EDO	C	529	4/4	0.87	0.14	47,48,50,50	4
4	EDO	A	527	4/4	0.87	0.14	38,42,45,47	0
4	EDO	A	525	4/4	0.87	0.17	35,39,43,49	0
4	EDO	A	524	4/4	0.87	0.14	21,23,29,38	0
4	EDO	D	527	4/4	0.87	0.18	37,38,39,45	4
4	EDO	D	517	4/4	0.88	0.14	39,40,43,55	0
4	EDO	B	516	4/4	0.88	0.14	34,39,43,52	0
4	EDO	C	515	4/4	0.88	0.14	42,43,44,51	0
4	EDO	D	522	4/4	0.88	0.15	38,38,42,42	4
4	EDO	C	516	4/4	0.88	0.13	31,36,48,51	4
4	EDO	D	533	4/4	0.88	0.13	31,36,40,42	4
3	SO4	D	513	5/5	0.88	0.12	44,44,51,52	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	D	503	4/4	0.88	0.16	32,33,36,41	4
4	EDO	C	522	4/4	0.89	0.13	45,47,49,49	0
4	EDO	B	515	4/4	0.89	0.15	33,39,40,44	0
4	EDO	B	529	4/4	0.89	0.15	35,36,38,44	4
3	SO4	D	512	5/5	0.89	0.12	33,34,44,47	5
4	EDO	A	510	4/4	0.90	0.15	38,38,39,47	0
4	EDO	C	518	4/4	0.90	0.17	29,43,46,47	4
4	EDO	A	519	4/4	0.90	0.14	41,46,49,54	4
4	EDO	A	520	4/4	0.90	0.14	29,35,35,37	4
4	EDO	B	534	4/4	0.91	0.11	33,46,48,52	0
4	EDO	C	517	4/4	0.91	0.14	31,38,43,48	4
4	EDO	A	535	4/4	0.91	0.13	38,39,42,47	0
3	SO4	B	509	5/5	0.91	0.11	34,36,43,44	5
4	EDO	C	530	4/4	0.91	0.13	41,43,44,45	0
4	EDO	C	520	4/4	0.91	0.12	22,27,29,43	0
4	EDO	B	517	4/4	0.91	0.13	35,37,44,51	0
4	EDO	D	516	4/4	0.91	0.14	33,44,44,50	0
4	EDO	B	518	4/4	0.91	0.12	39,39,42,54	0
3	SO4	C	514	5/5	0.91	0.12	27,42,52,53	5
4	EDO	D	520	4/4	0.91	0.12	42,42,45,54	0
3	SO4	A	509	5/5	0.91	0.10	42,56,60,61	5
3	SO4	A	508	5/5	0.92	0.12	32,35,41,44	5
4	EDO	B	519	4/4	0.92	0.13	39,41,43,44	0
5	EPE	B	513	15/15	0.92	0.14	36,41,49,52	15
4	EDO	A	511	4/4	0.92	0.12	37,39,41,59	0
4	EDO	A	530	4/4	0.92	0.12	31,34,37,44	0
3	SO4	C	510	5/5	0.93	0.09	36,41,47,50	5
4	EDO	C	531	4/4	0.93	0.15	24,32,33,41	4
3	SO4	A	507	5/5	0.93	0.08	41,47,50,50	5
4	EDO	D	501	4/4	0.93	0.16	19,27,33,48	4
4	EDO	A	515	4/4	0.93	0.09	41,42,46,54	0
4	EDO	D	528	4/4	0.93	0.10	41,41,42,47	0
4	EDO	A	531	4/4	0.93	0.14	26,29,37,40	4
4	EDO	B	514	4/4	0.93	0.11	47,48,50,56	0
4	EDO	D	518	4/4	0.93	0.12	41,43,45,46	0
4	EDO	C	526	4/4	0.93	0.10	34,35,38,42	4
3	SO4	D	511	5/5	0.93	0.09	44,46,50,52	5
4	EDO	B	537	4/4	0.93	0.15	33,34,35,42	4
3	SO4	B	508	5/5	0.93	0.10	42,43,49,49	5
3	SO4	B	540	5/5	0.94	0.08	41,48,49,59	0
4	EDO	A	538	4/4	0.94	0.18	27,35,42,55	0
4	EDO	D	515	4/4	0.95	0.08	31,36,36,49	0

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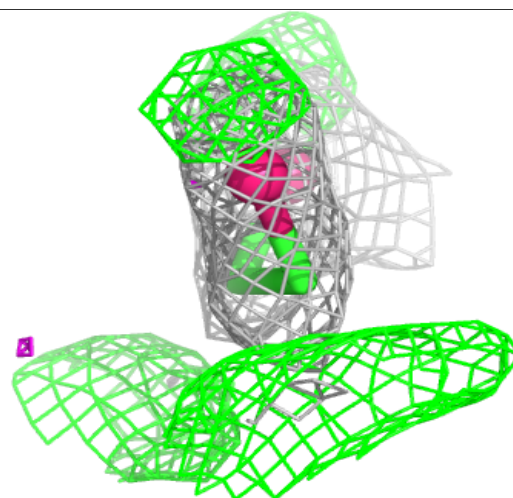
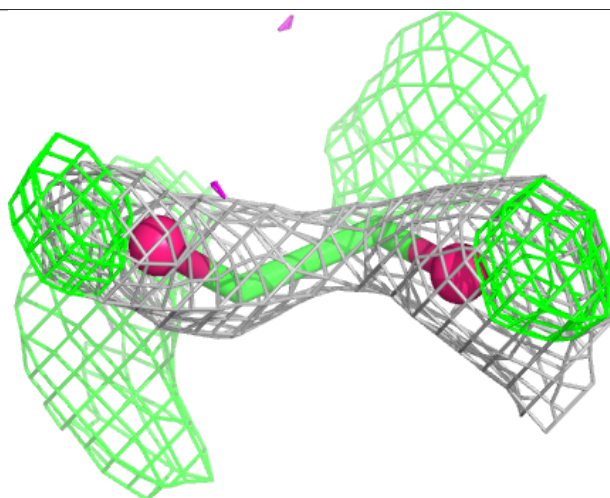
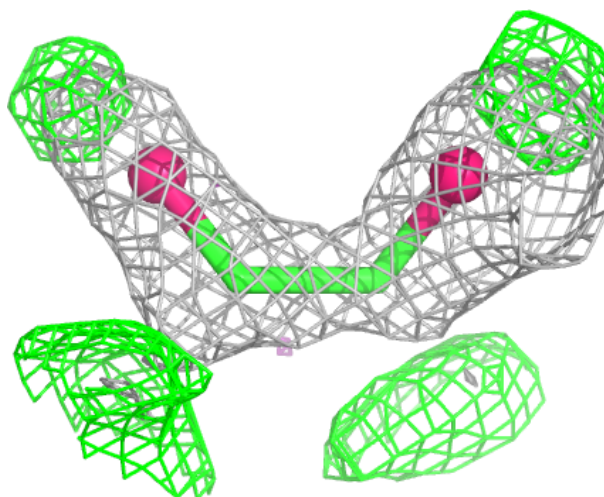
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	C	508	5/5	0.96	0.07	35,37,40,40	5
4	EDO	A	513	4/4	0.96	0.11	29,39,44,48	0
4	EDO	D	504	4/4	0.96	0.09	31,36,38,46	0
3	SO4	A	506	5/5	0.97	0.07	33,35,38,40	5
3	SO4	C	501	5/5	0.97	0.07	43,46,56,64	0
2	HEC	C	503	43/43	0.97	0.09	32,41,48,62	0
2	HEC	D	505	43/43	0.98	0.07	28,32,42,53	0
2	HEC	D	506	43/43	0.98	0.06	22,27,35,40	0
2	HEC	D	507	43/43	0.98	0.06	21,26,43,56	0
2	HEC	D	508	43/43	0.98	0.06	19,23,31,35	0
2	HEC	A	502	43/43	0.98	0.07	20,27,42,47	0
2	HEC	A	503	43/43	0.98	0.07	20,24,41,47	0
2	HEC	B	502	43/43	0.98	0.07	26,33,45,51	0
2	HEC	B	503	43/43	0.98	0.06	21,26,37,41	0
3	SO4	A	533	5/5	0.98	0.06	44,46,54,61	0
3	SO4	D	502	5/5	0.98	0.05	36,45,52,55	0
2	HEC	B	504	43/43	0.98	0.07	20,27,44,51	0
2	HEC	A	501	43/43	0.98	0.07	24,28,36,45	0
2	HEC	C	504	43/43	0.98	0.07	25,31,43,47	0
2	HEC	C	505	43/43	0.98	0.08	27,32,49,59	0
2	HEC	C	506	43/43	0.98	0.07	22,27,38,42	0
2	HEC	C	507	43/43	0.98	0.06	21,26,31,37	0
2	HEC	B	506	43/43	0.99	0.05	18,23,30,36	0
2	HEC	A	505	43/43	0.99	0.05	19,22,27,38	0
3	SO4	D	510	5/5	0.99	0.05	31,32,34,35	5
2	HEC	D	509	43/43	0.99	0.05	18,21,26,32	0
3	SO4	B	507	5/5	0.99	0.08	34,36,37,37	0
2	HEC	A	504	43/43	0.99	0.06	19,21,35,42	0
2	HEC	B	505	43/43	0.99	0.06	19,23,33,37	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.

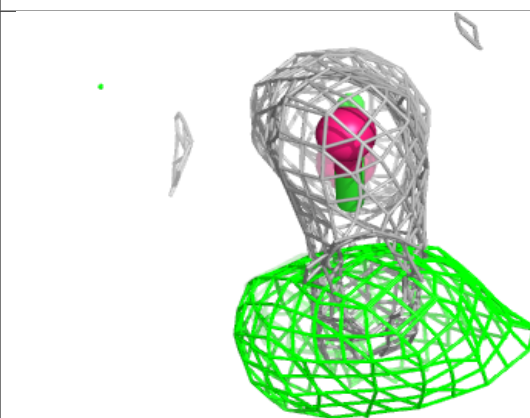
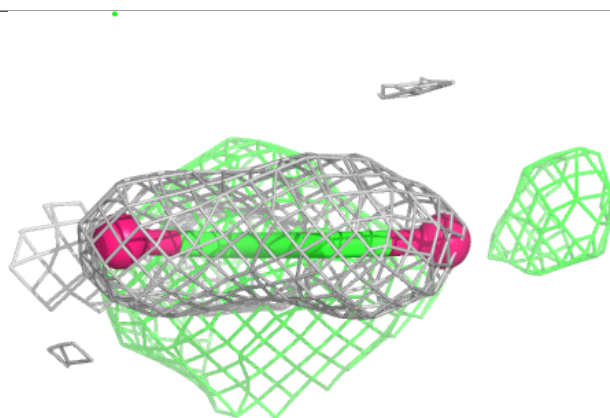
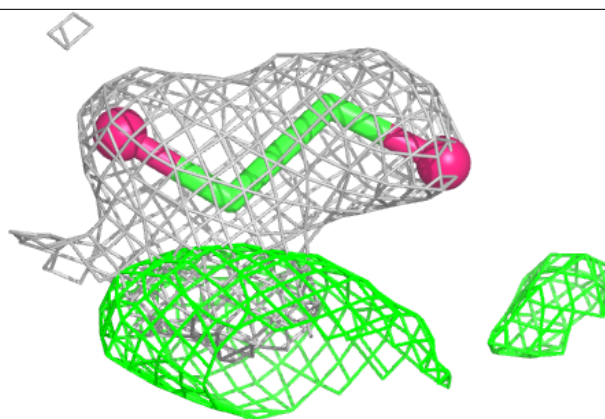
Electron density around EDO B 527:

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



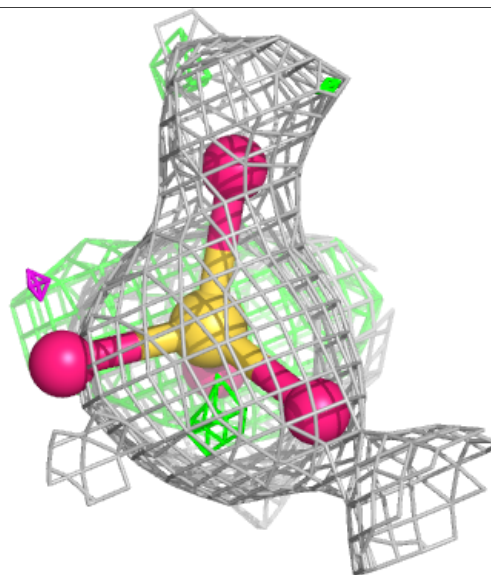
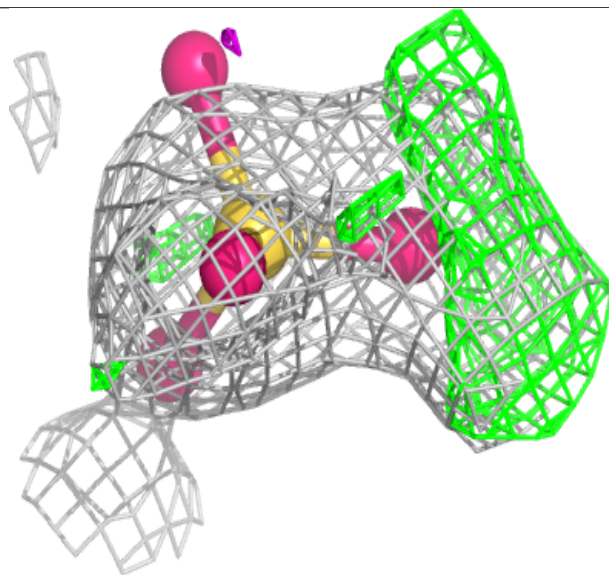
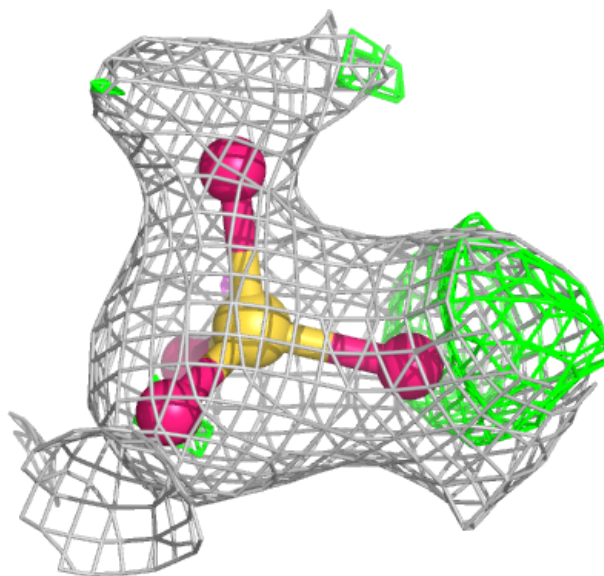
Electron density around EDO B 501:

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



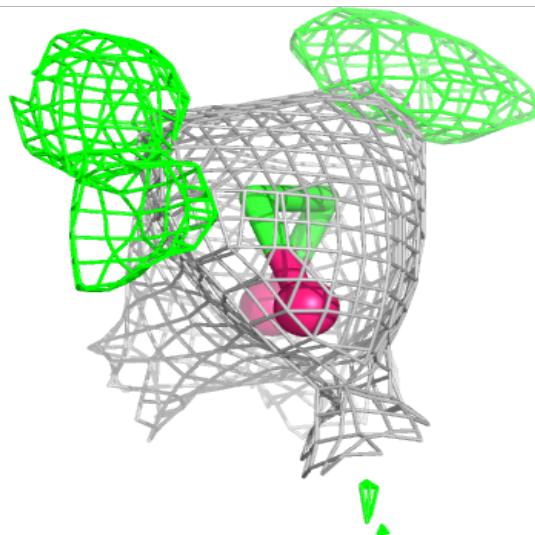
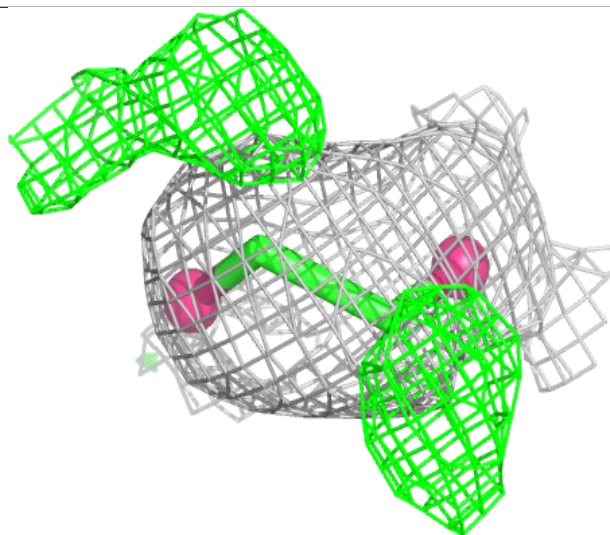
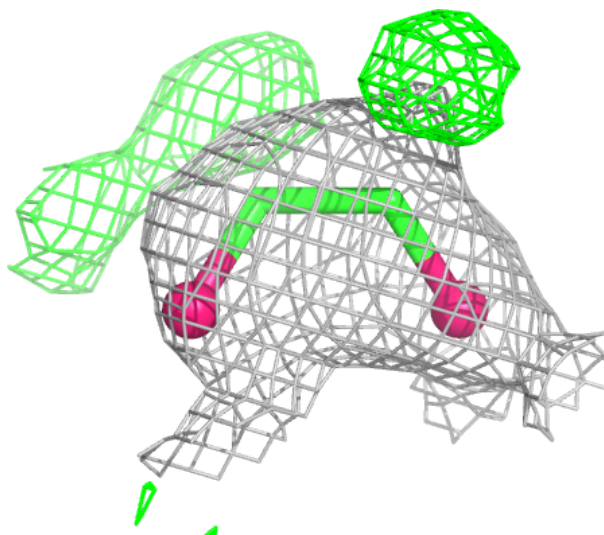
Electron density around SO4 D 514:

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



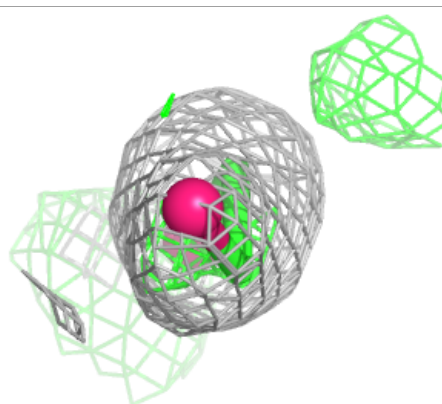
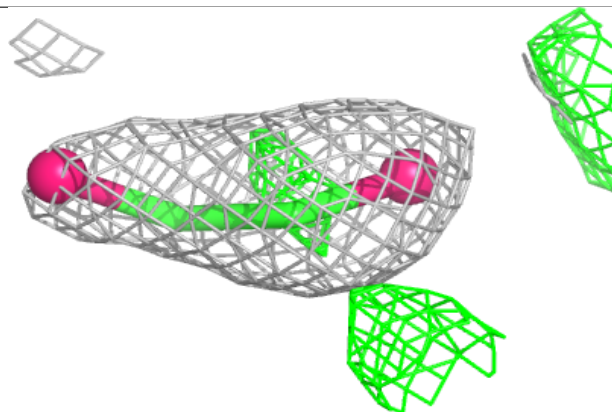
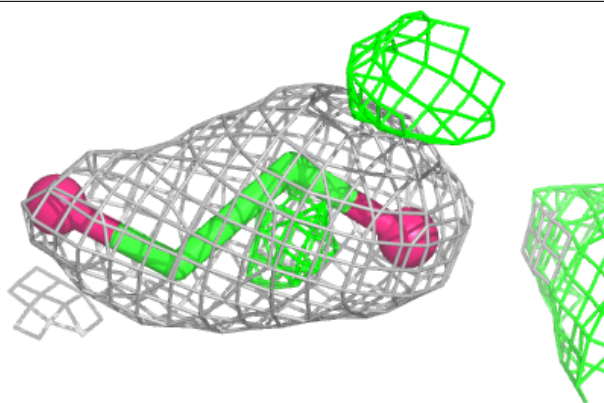
Electron density around EDO A 536:

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

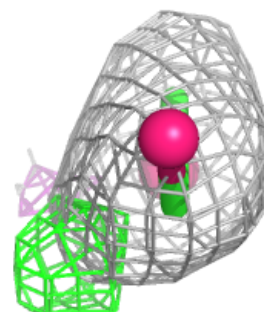
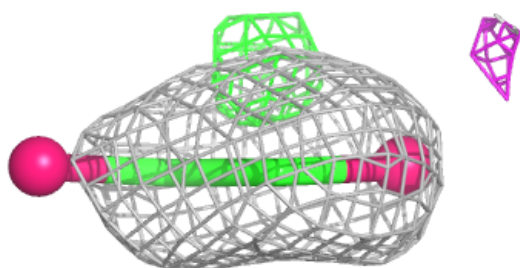
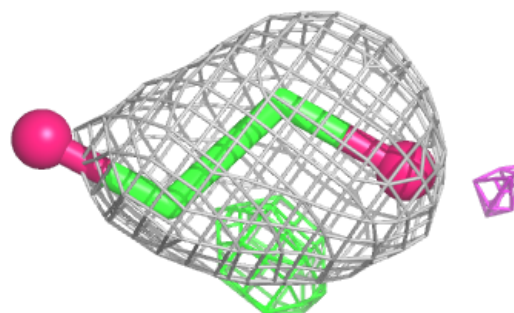


Electron density around EDO B 526:

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

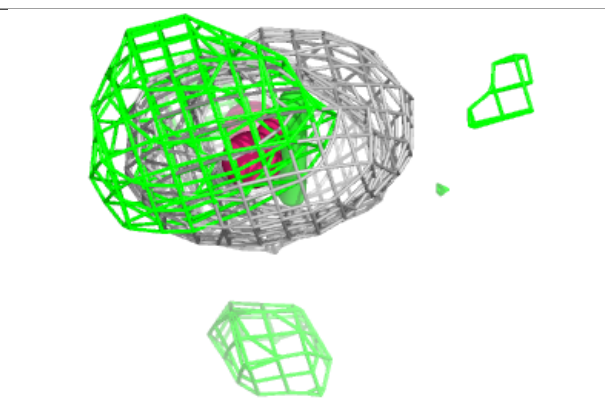
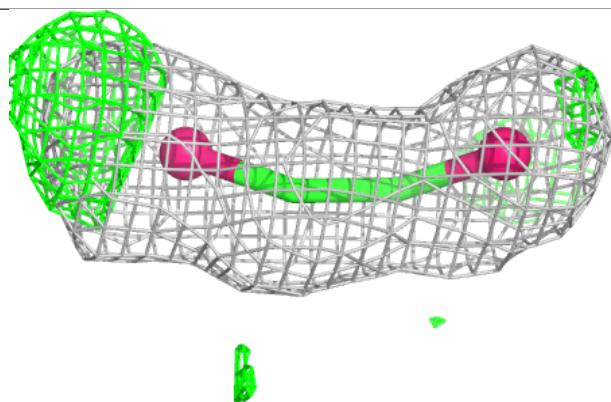
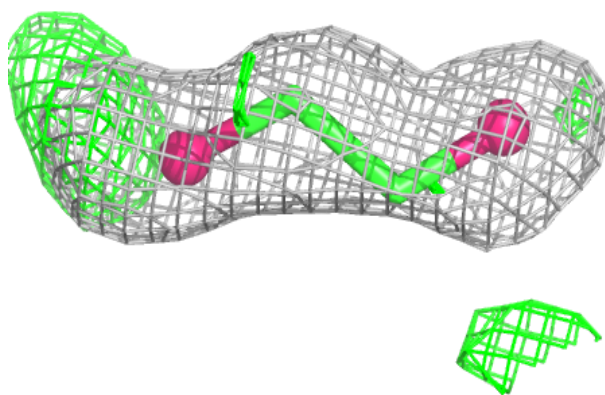
**Electron density around EDO A 528:**

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

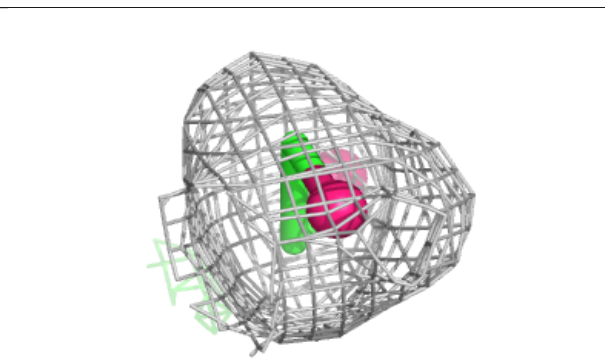
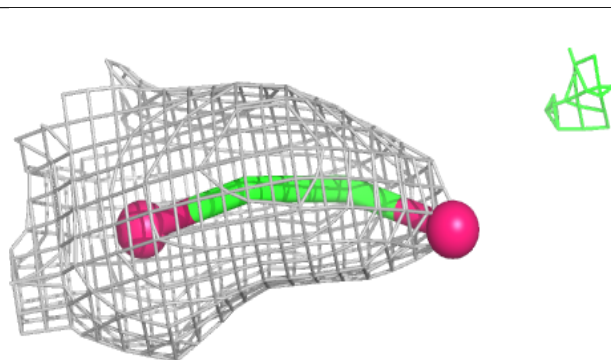
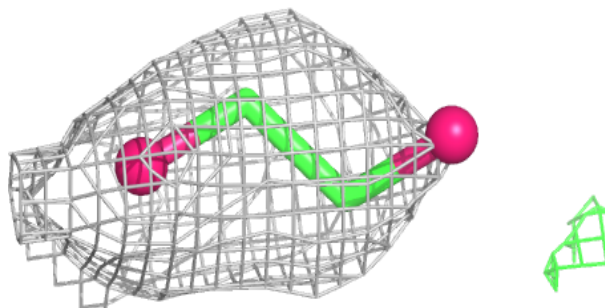


Electron density around EDO A 529:

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

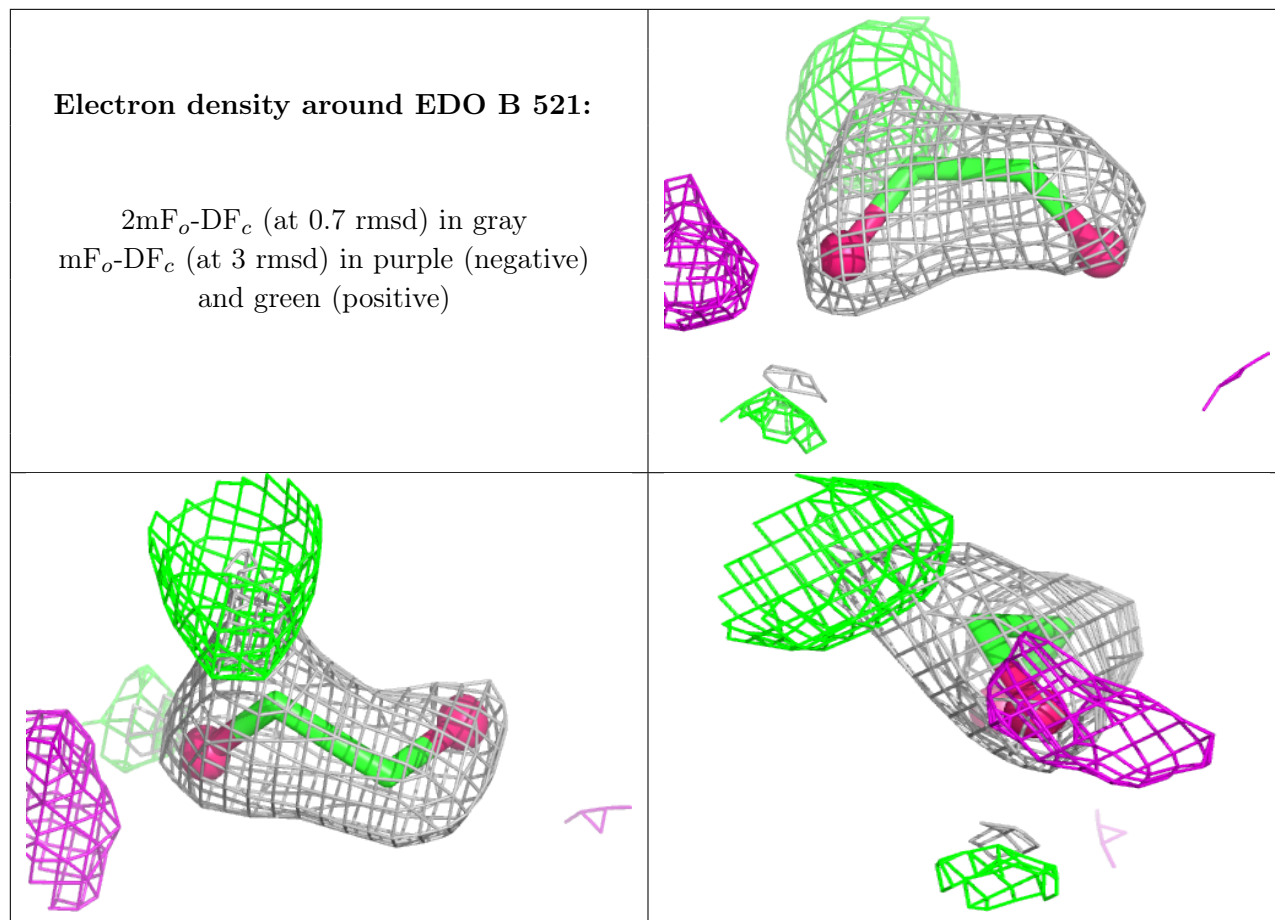
**Electron density around EDO C 502:**

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



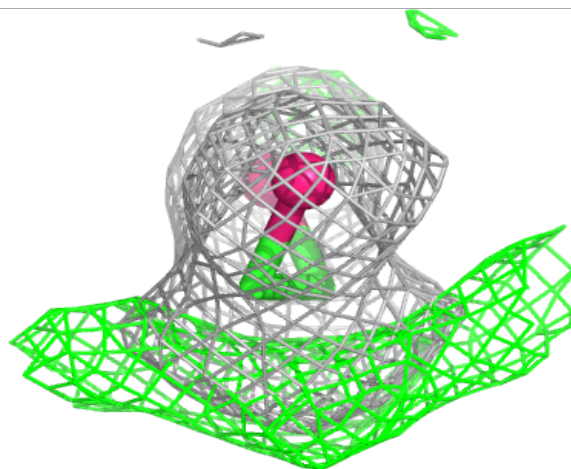
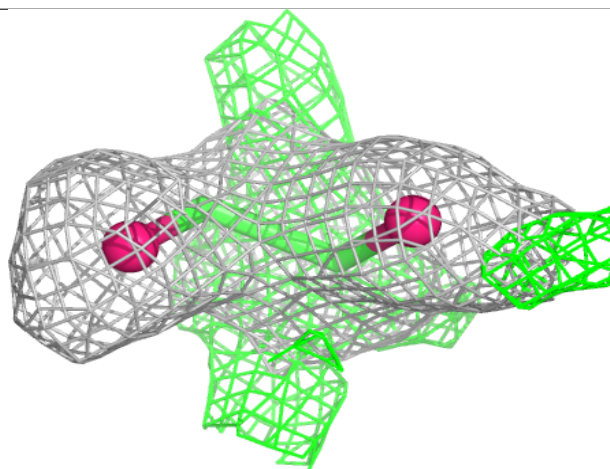
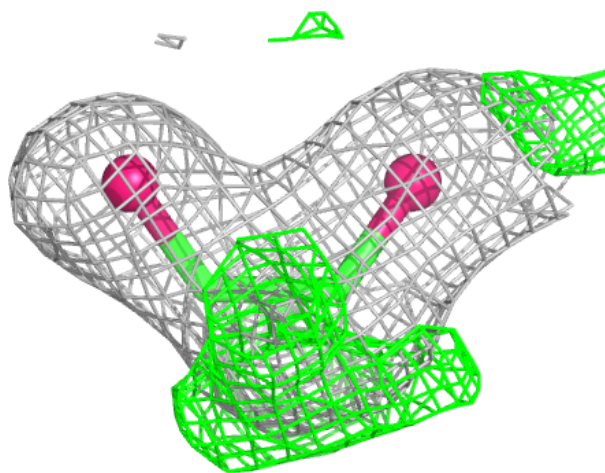
Electron density around EDO B 521:

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



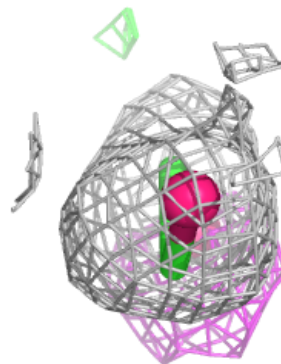
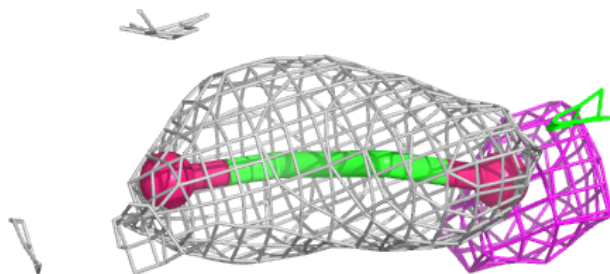
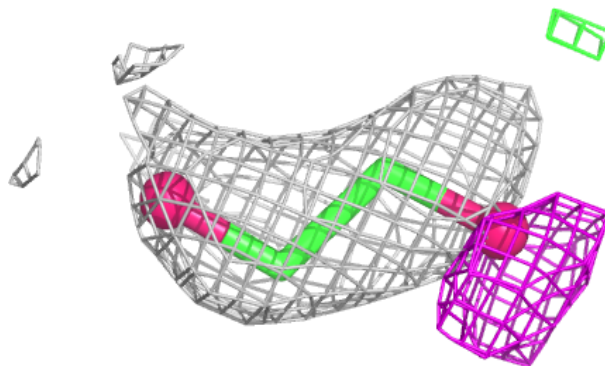
Electron density around EDO C 524:

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

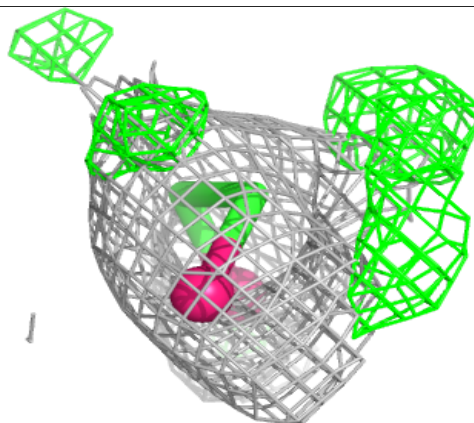
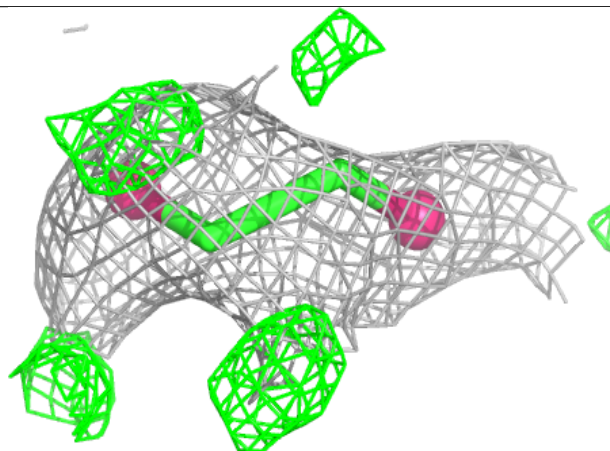
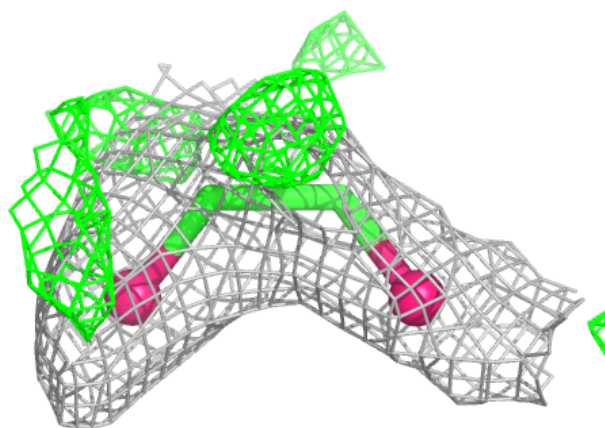


Electron density around EDO D 519:

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

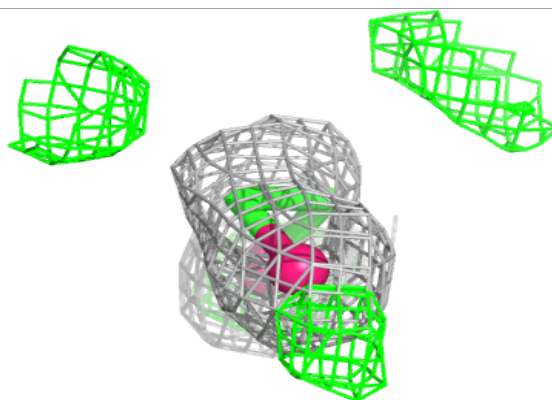
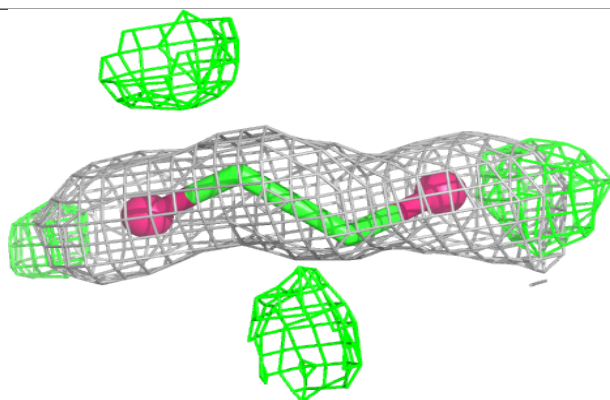
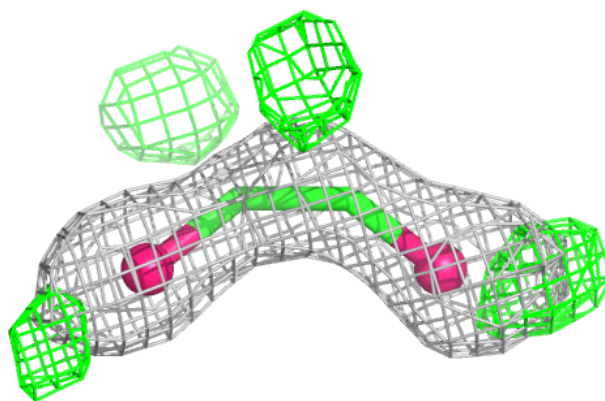
**Electron density around EDO D 524:**

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



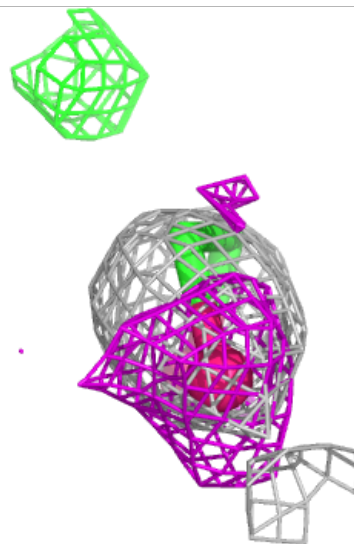
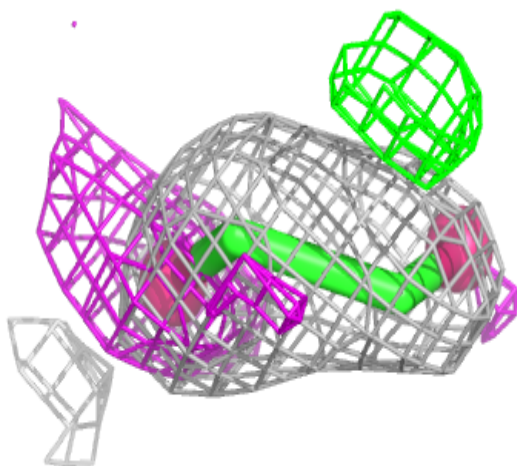
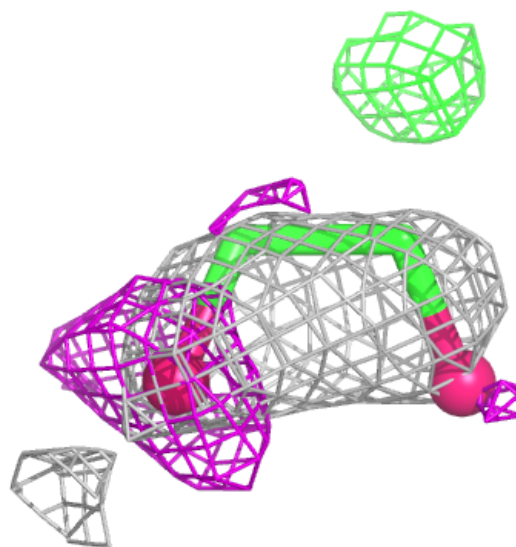
Electron density around EDO D 532:

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



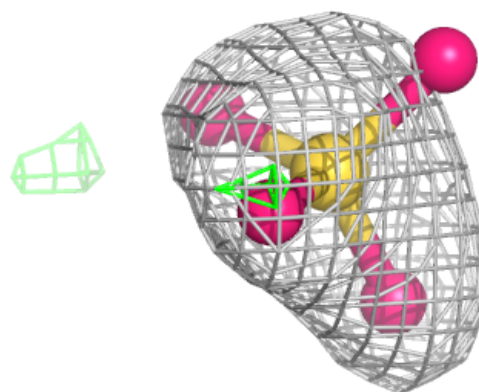
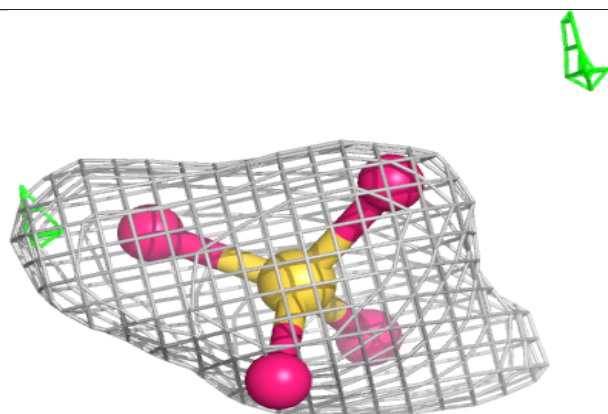
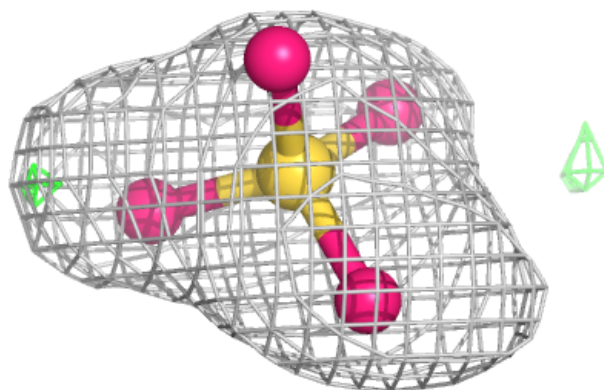
Electron density around EDO C 523:

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



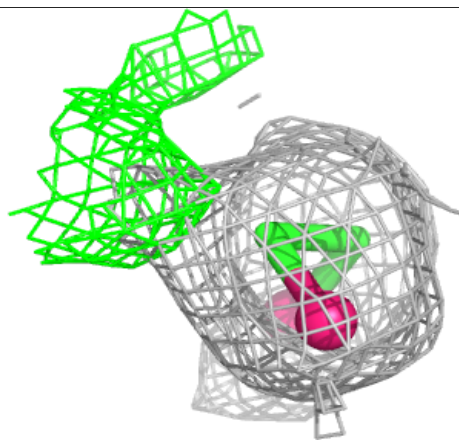
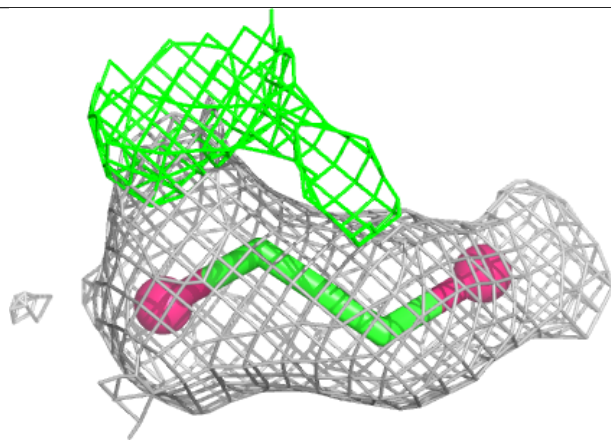
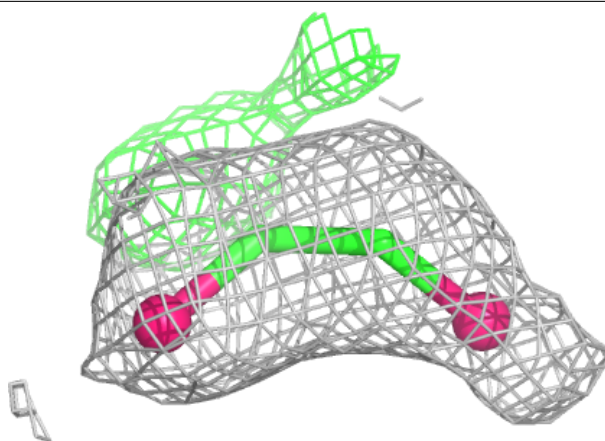
Electron density around SO4 C 512:

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



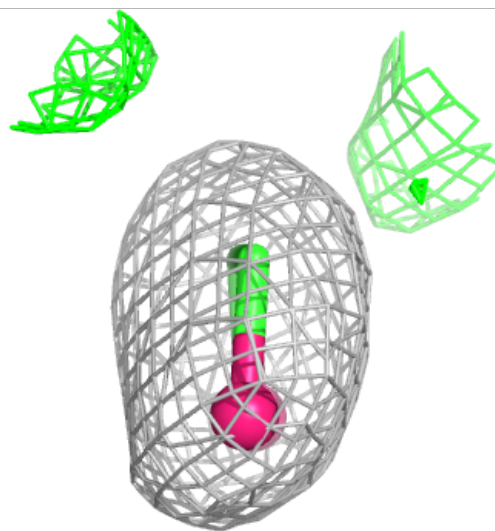
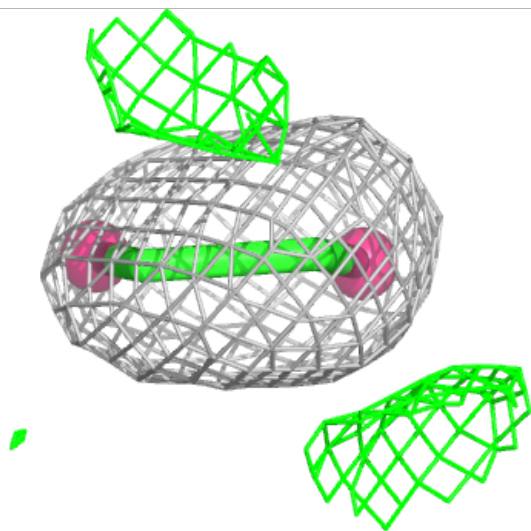
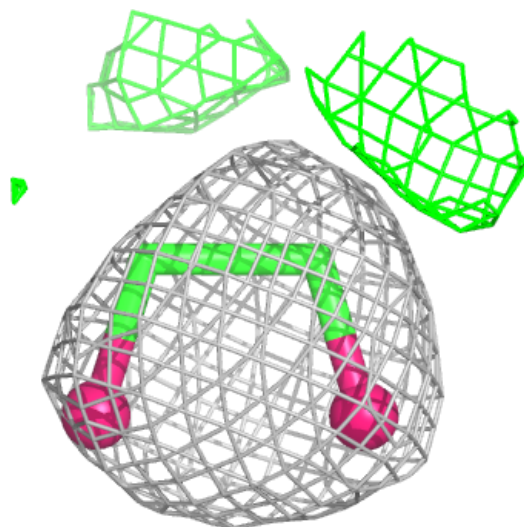
Electron density around EDO D 525:

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



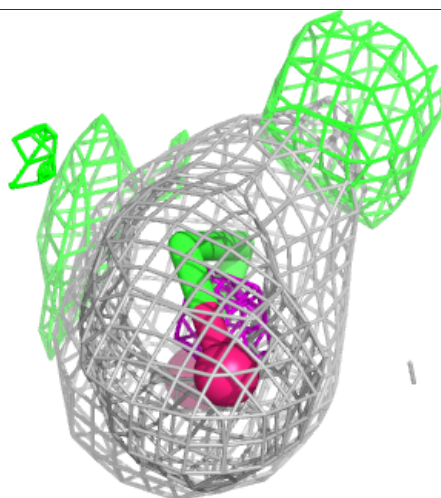
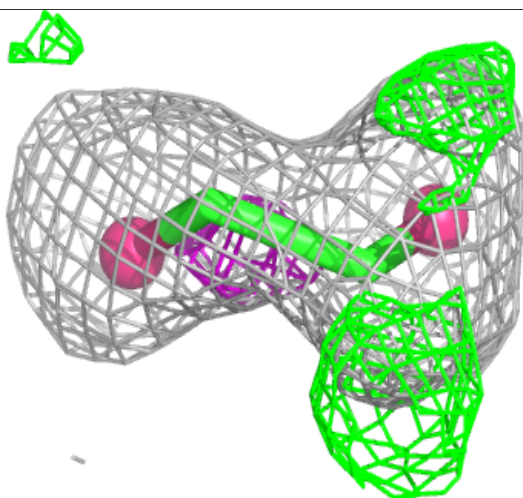
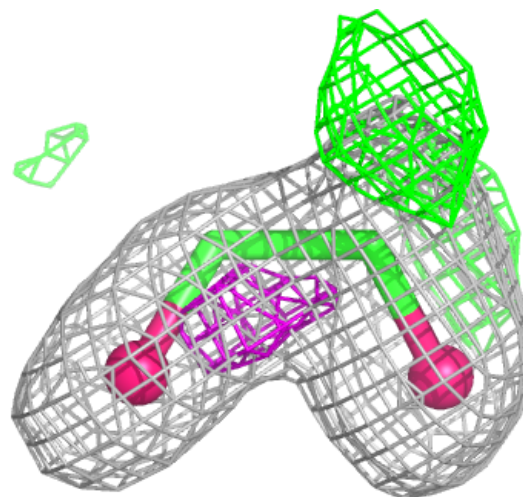
Electron density around EDO C 528:

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



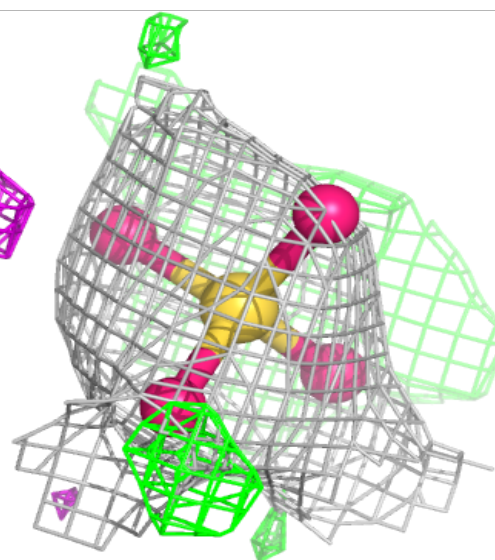
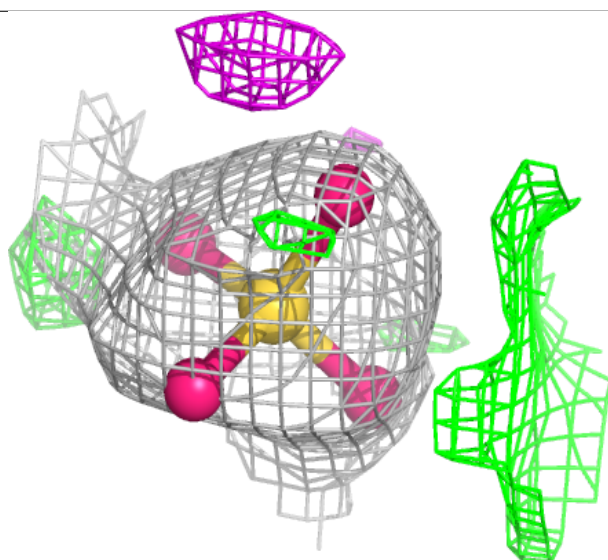
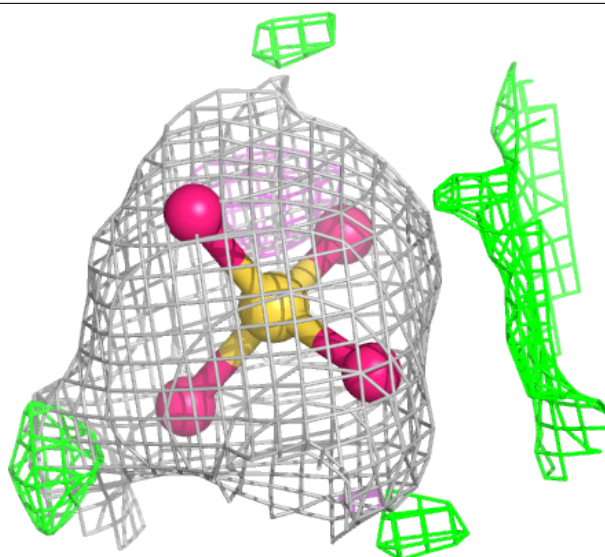
Electron density around EDO C 521:

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



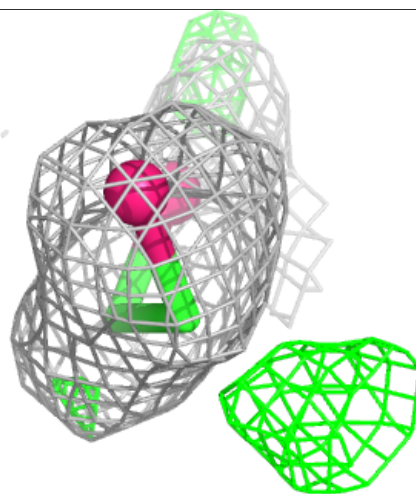
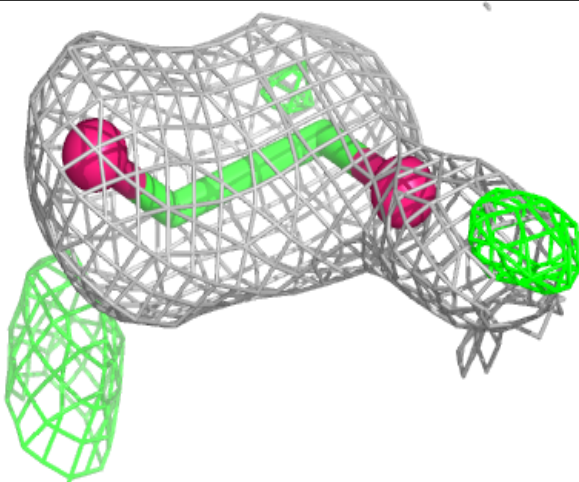
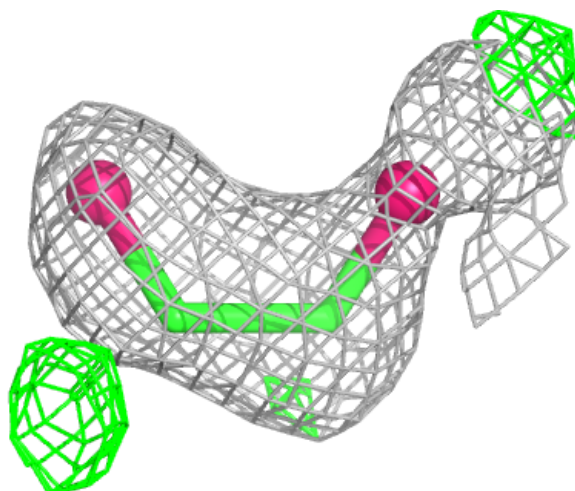
Electron density around SO4 B 510:

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



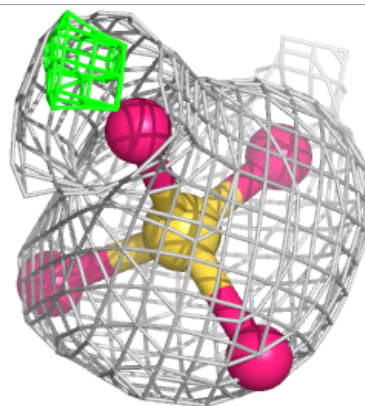
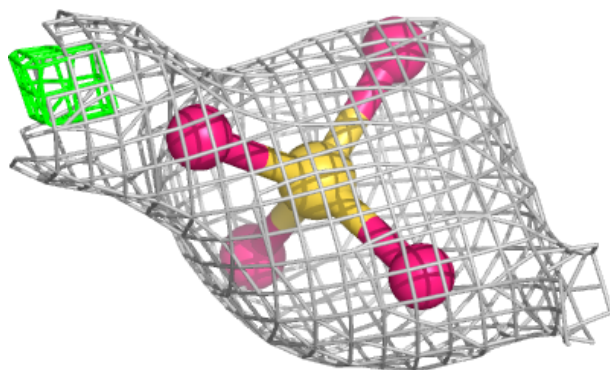
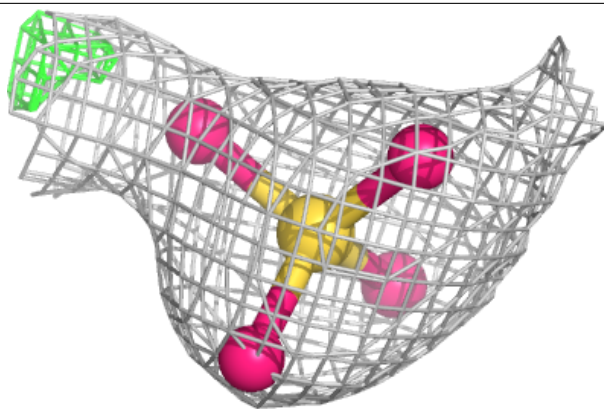
Electron density around EDO B 538:

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

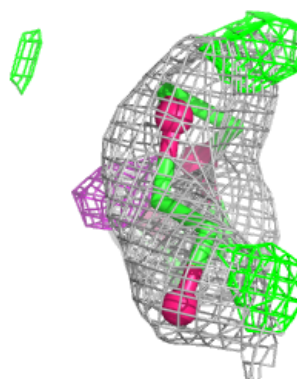
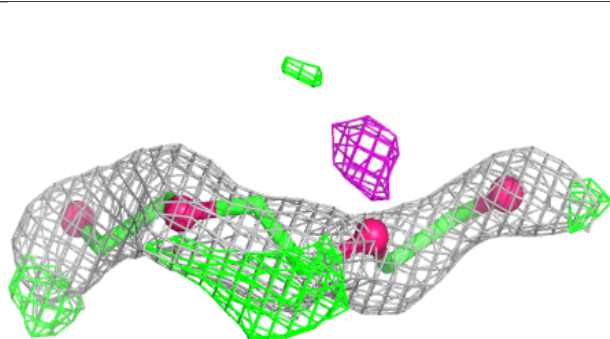
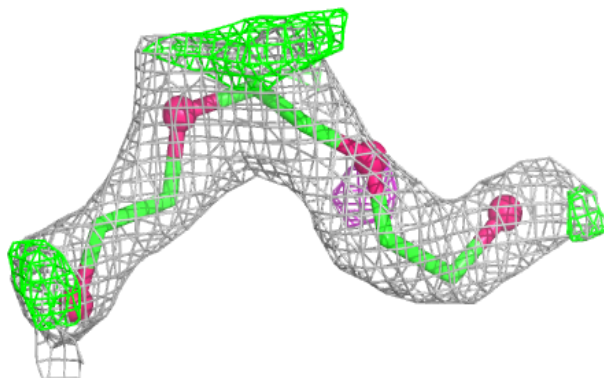


Electron density around SO4 B 512:

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

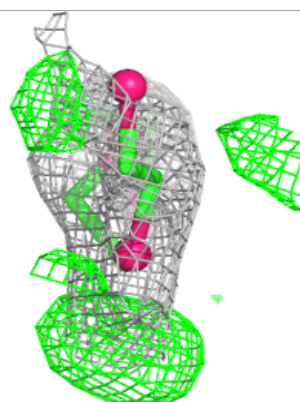
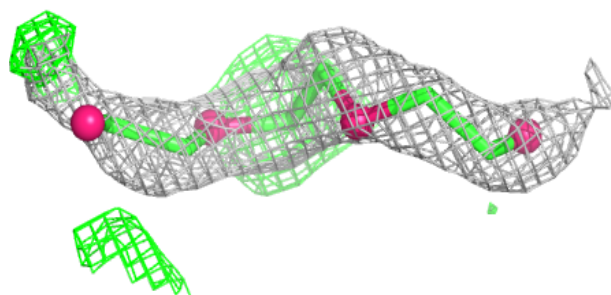
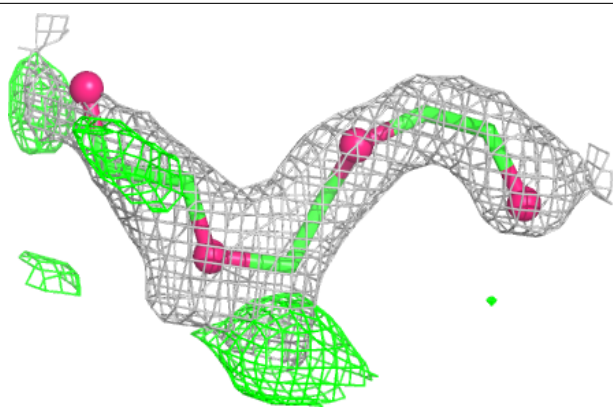
**Electron density around PGE B 539:**

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



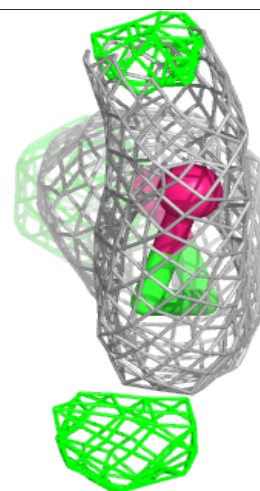
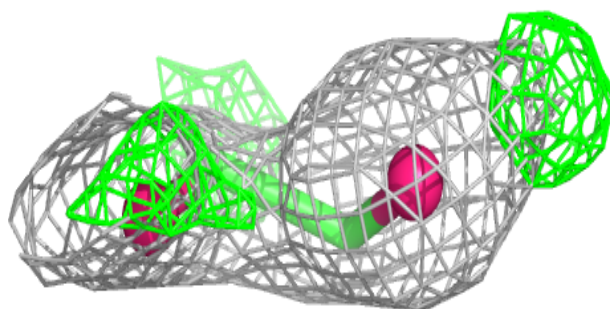
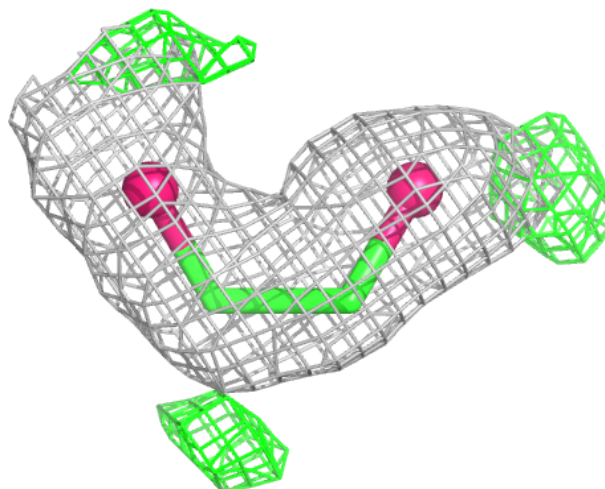
Electron density around PGE D 530:

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



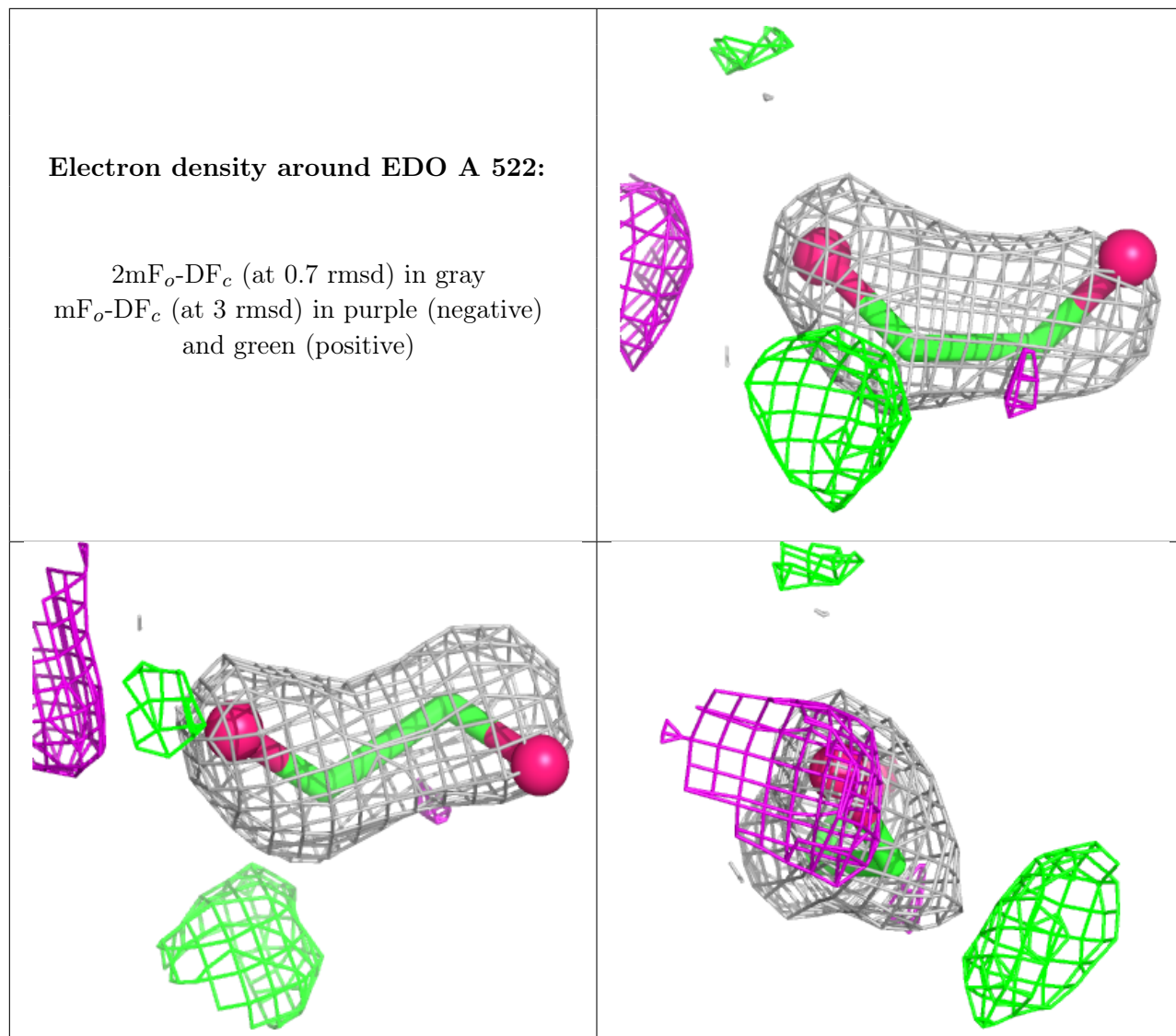
Electron density around EDO D 526:

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



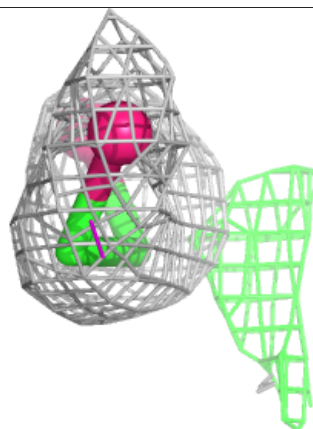
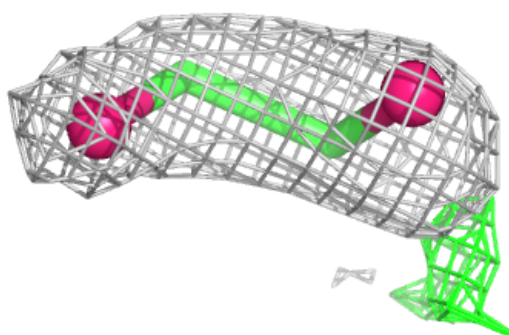
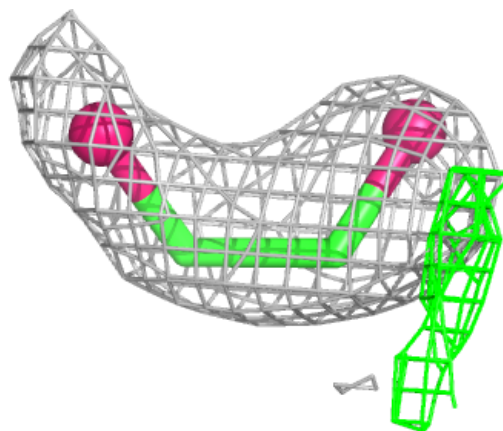
Electron density around EDO A 522:

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

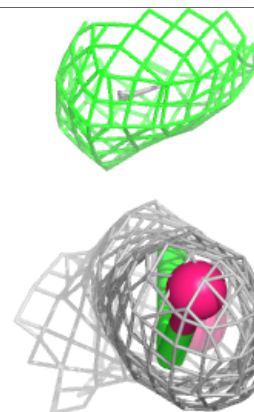
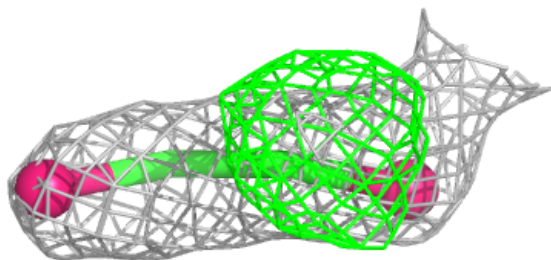
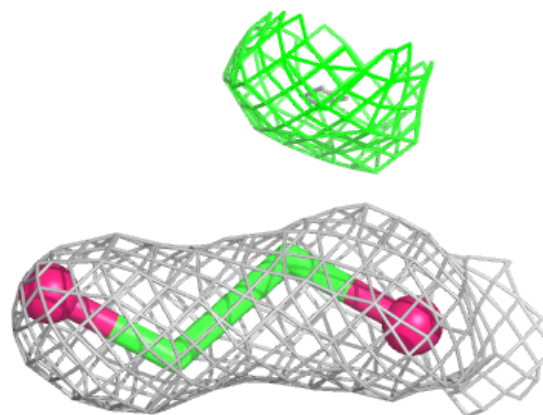


Electron density around EDO B 531:

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

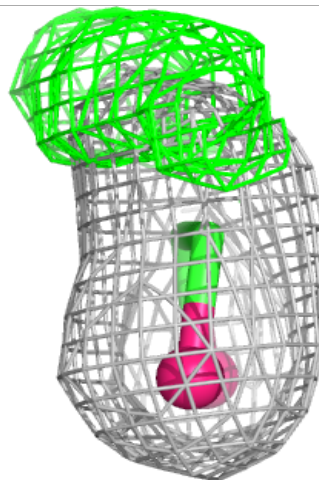
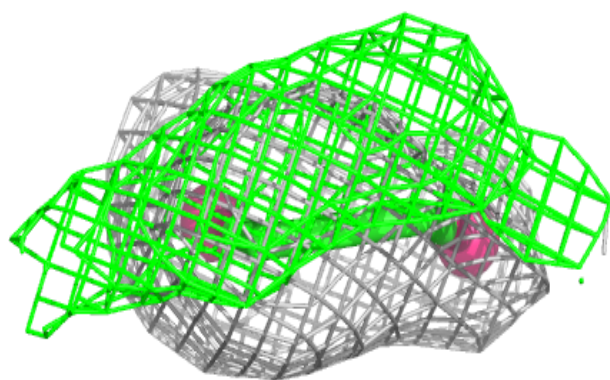
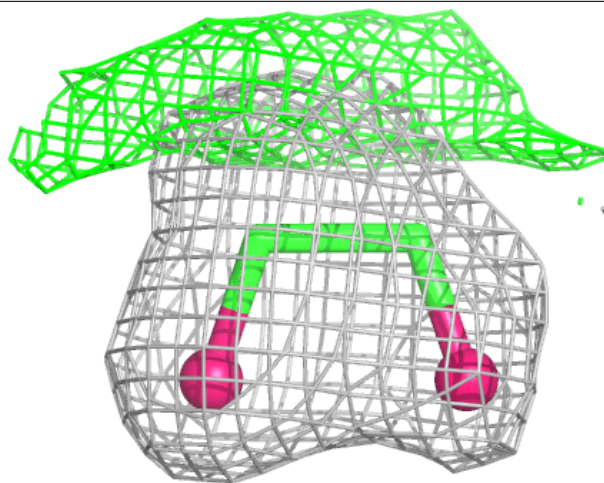
**Electron density around EDO C 527:**

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



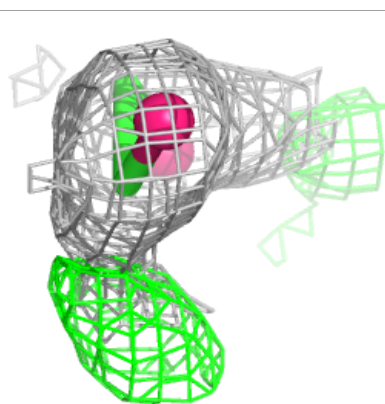
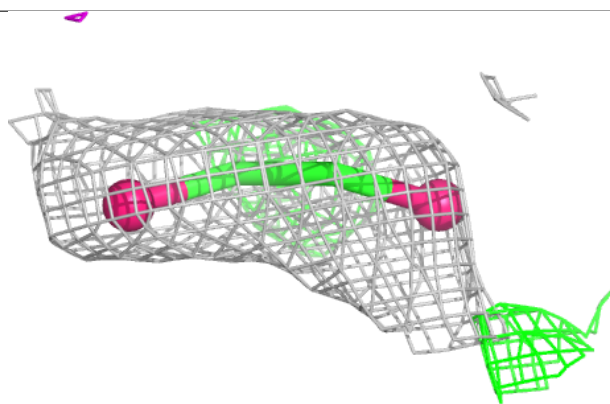
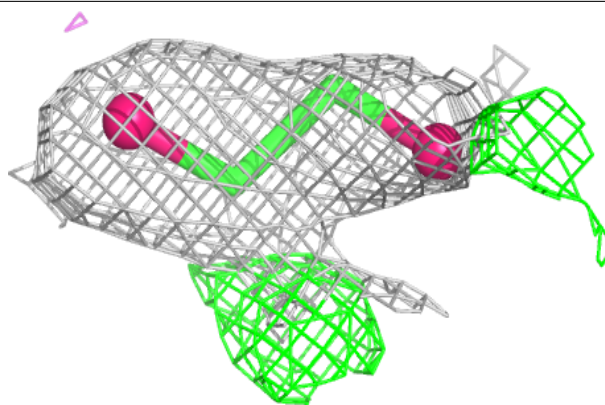
Electron density around EDO A 514:

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



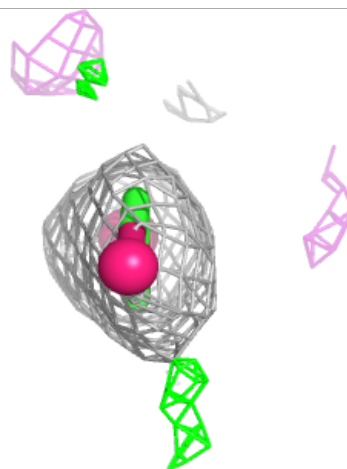
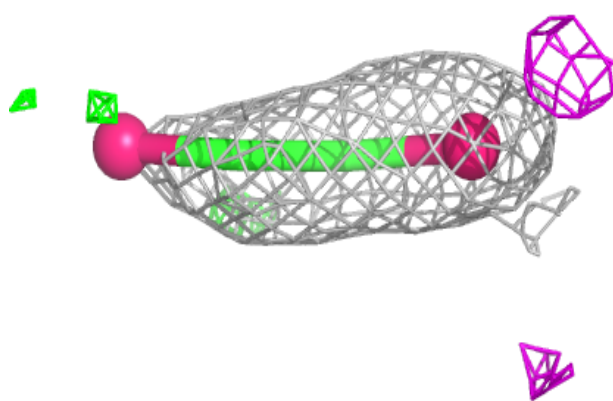
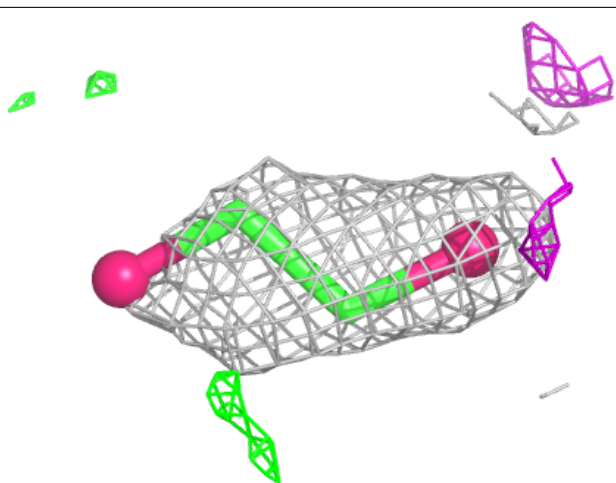
Electron density around EDO B 542:

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



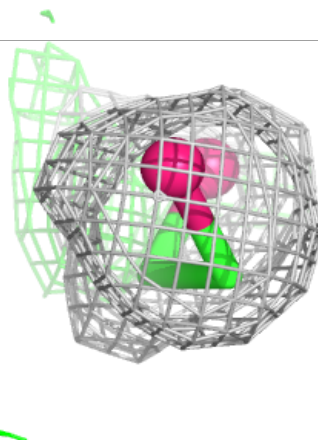
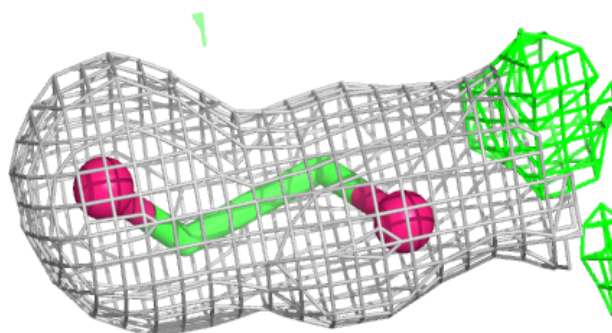
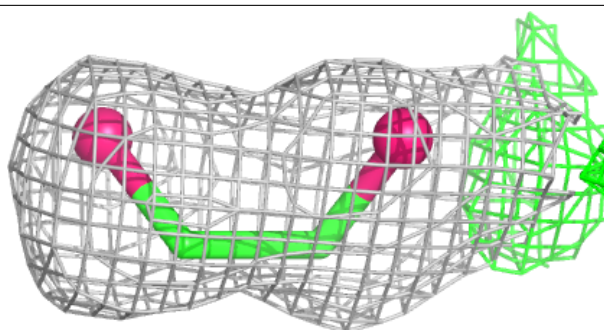
Electron density around EDO D 521:

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

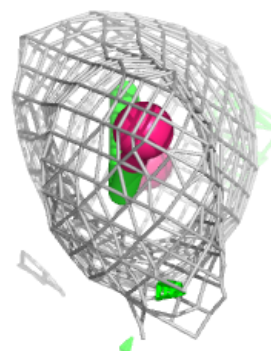
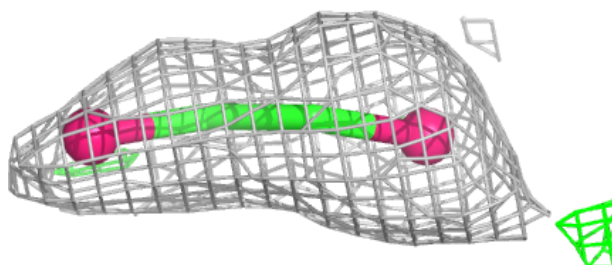
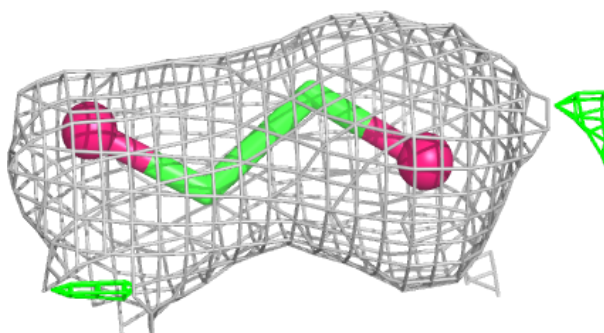


Electron density around EDO D 523:

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

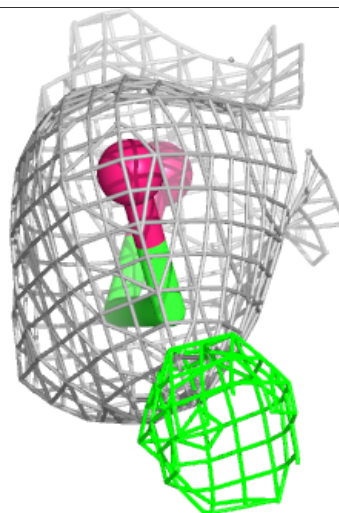
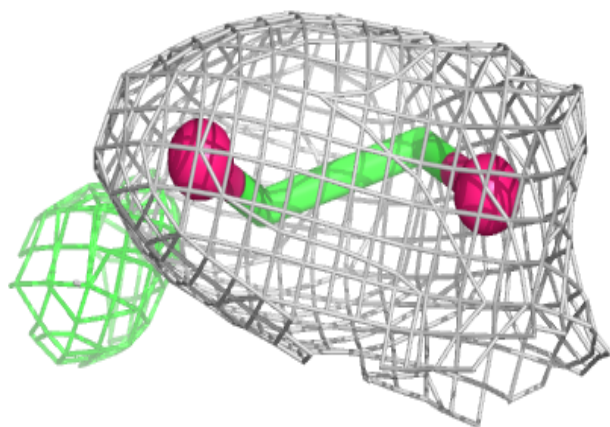
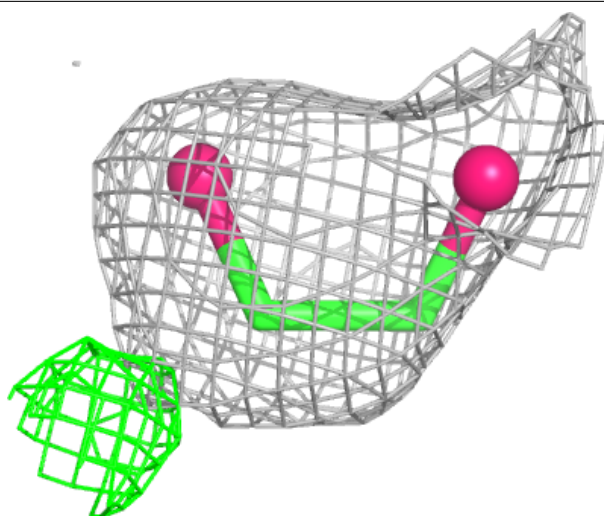
**Electron density around EDO B 535:**

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



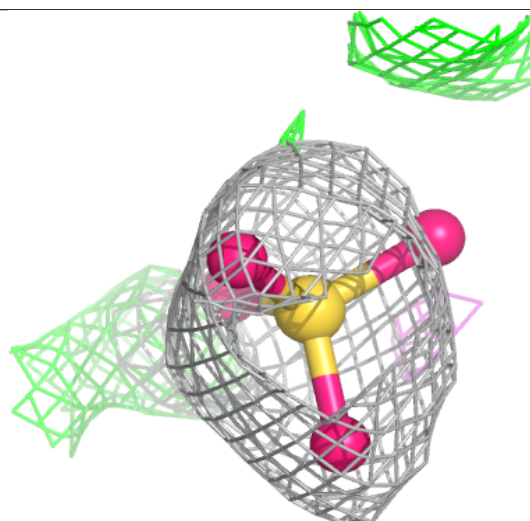
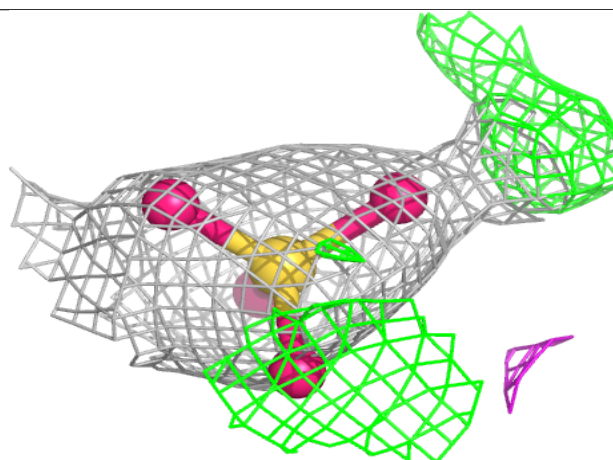
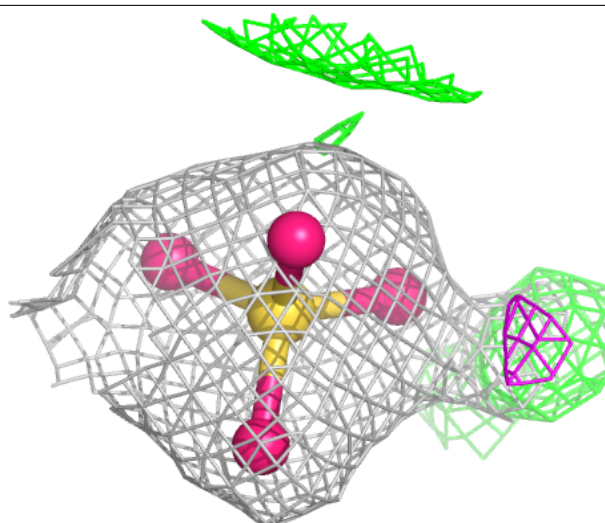
Electron density around EDO B 524:

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



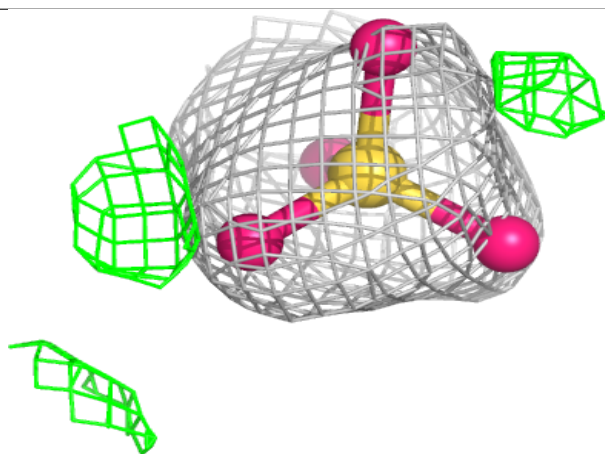
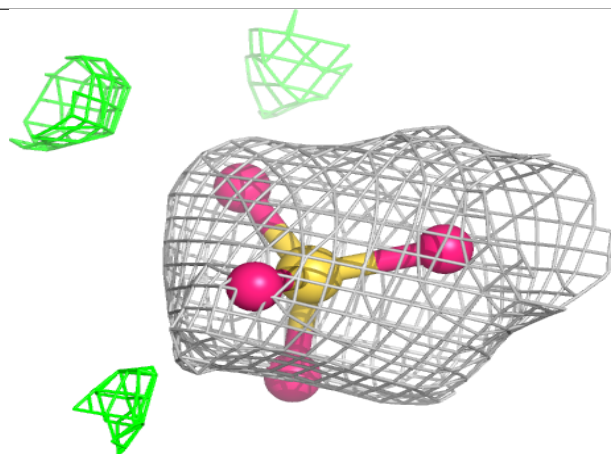
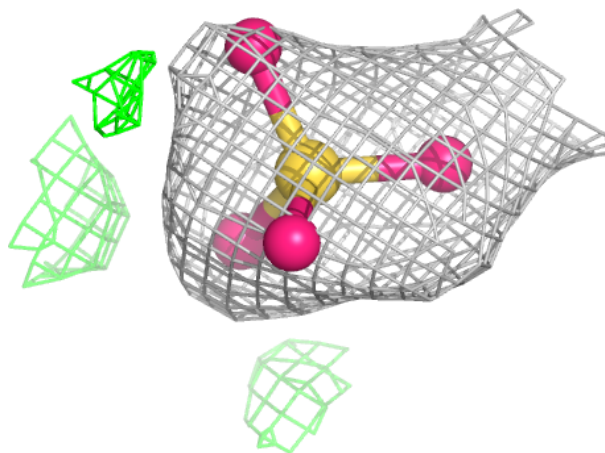
Electron density around SO4 B 541:

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



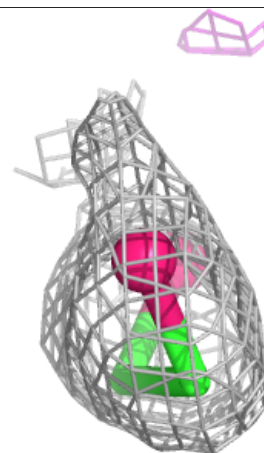
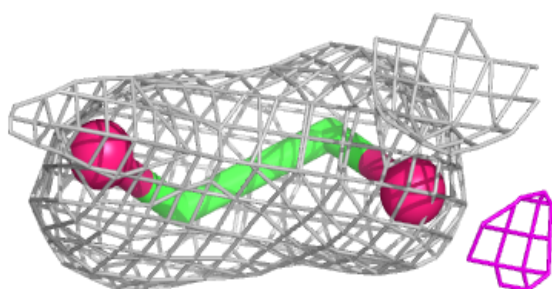
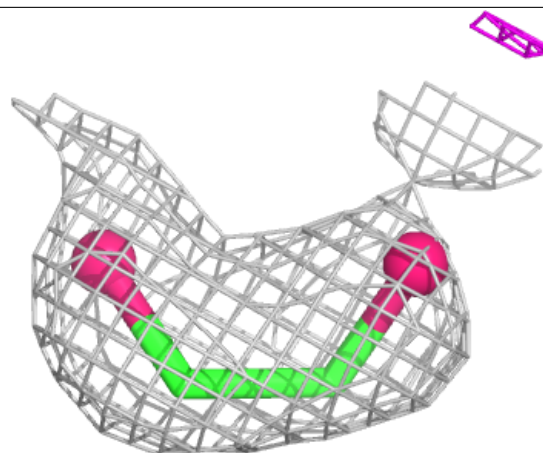
Electron density around SO4 C 513:

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

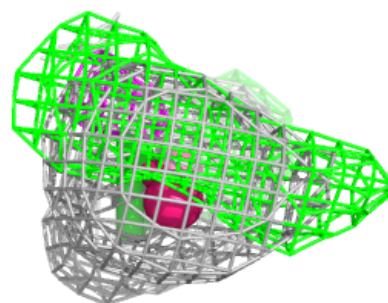
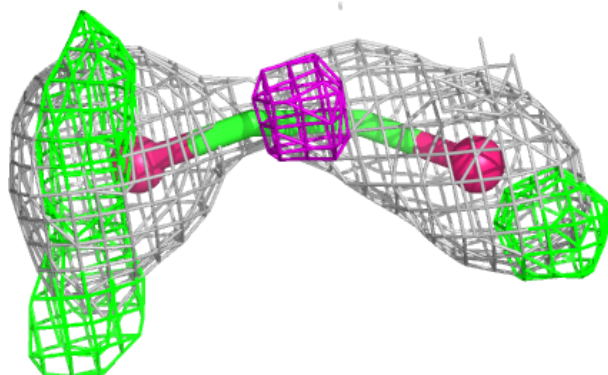
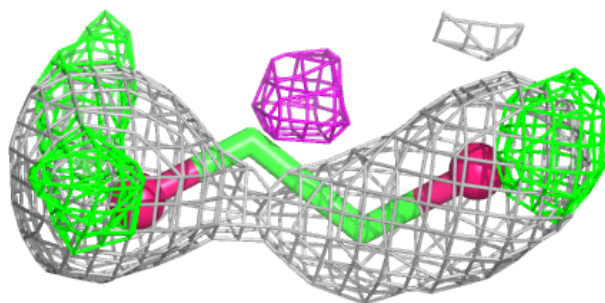


Electron density around EDO B 528:

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

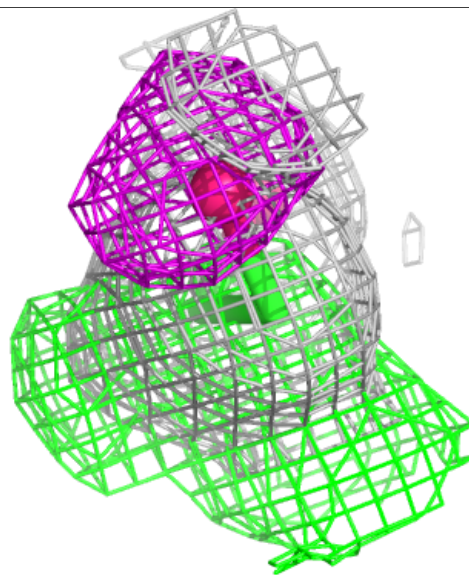
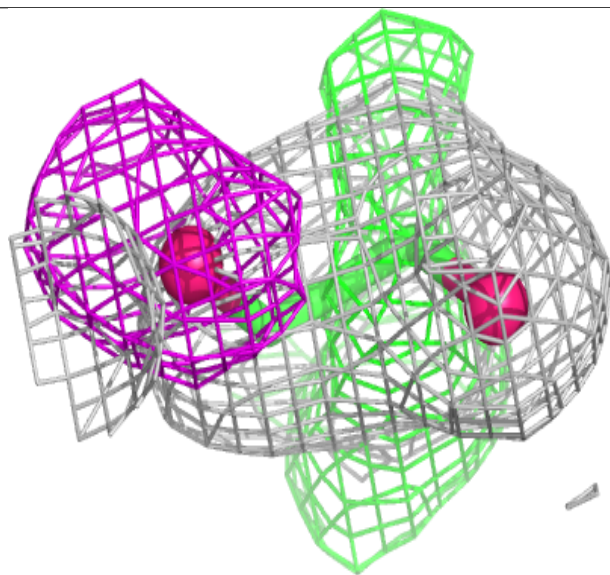
**Electron density around EDO A 517:**

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



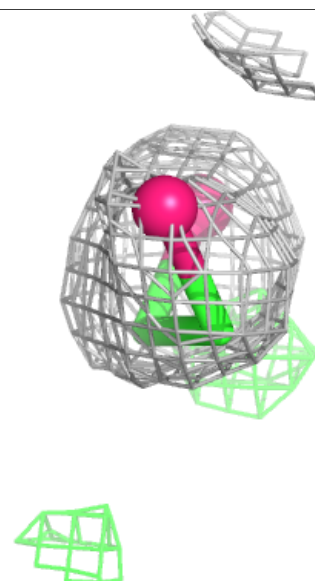
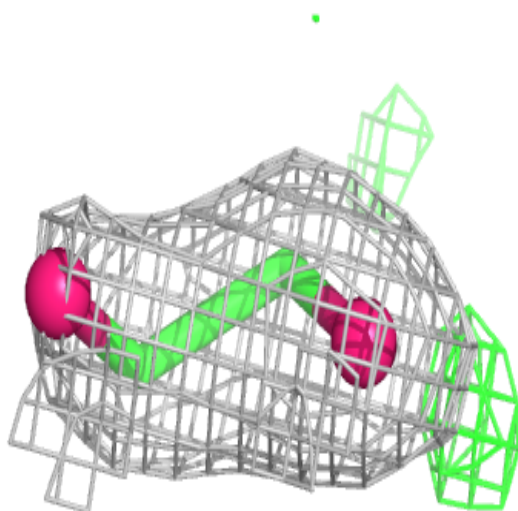
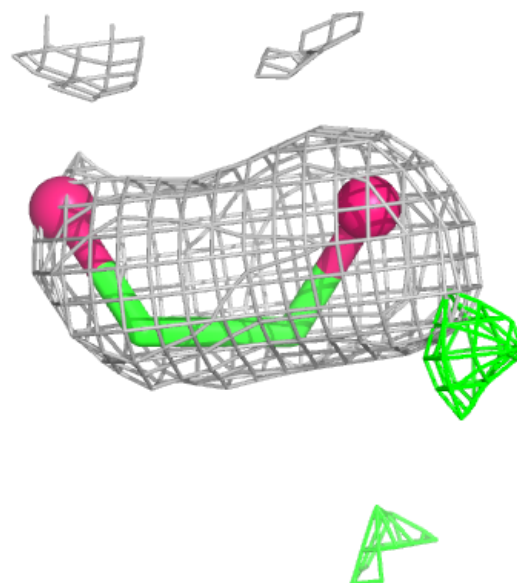
Electron density around EDO B 533:

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



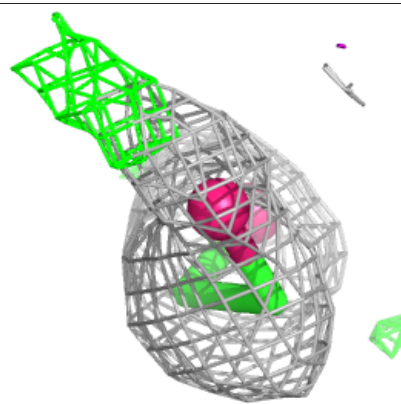
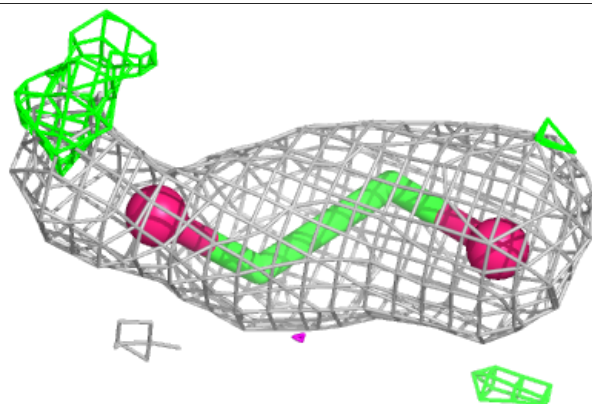
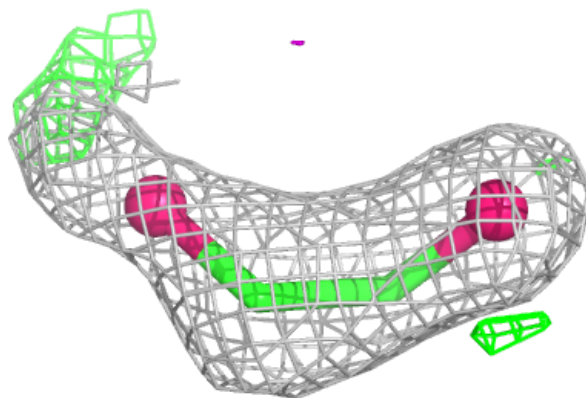
Electron density around EDO B 525:

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

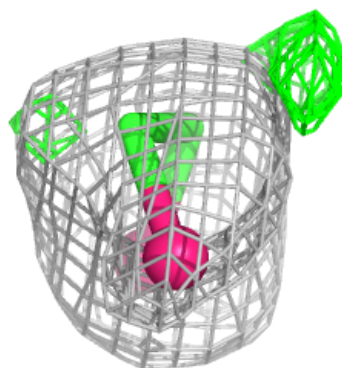
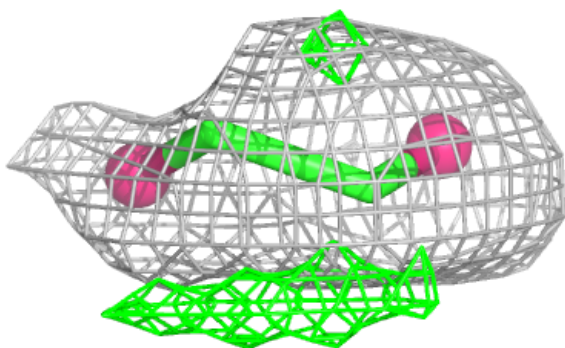
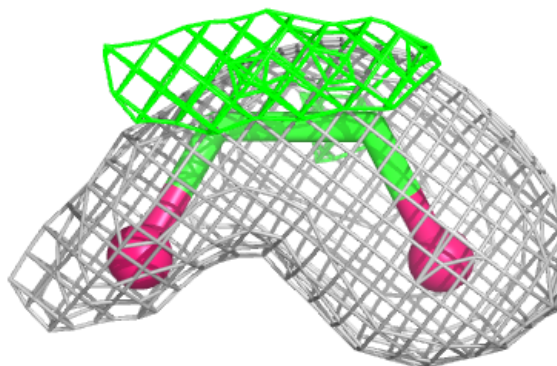


Electron density around EDO C 525:

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

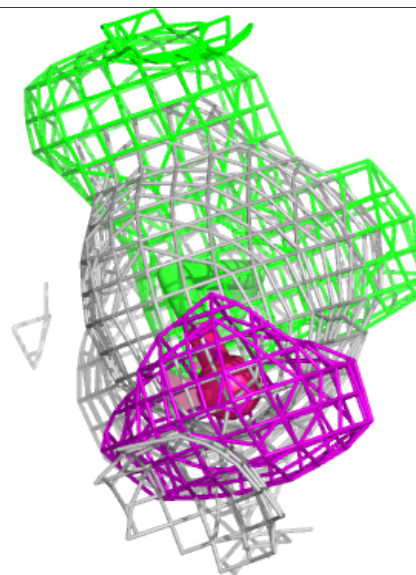
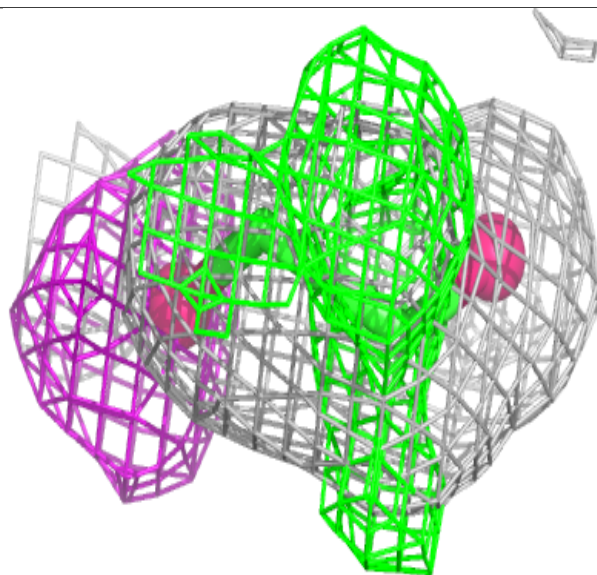
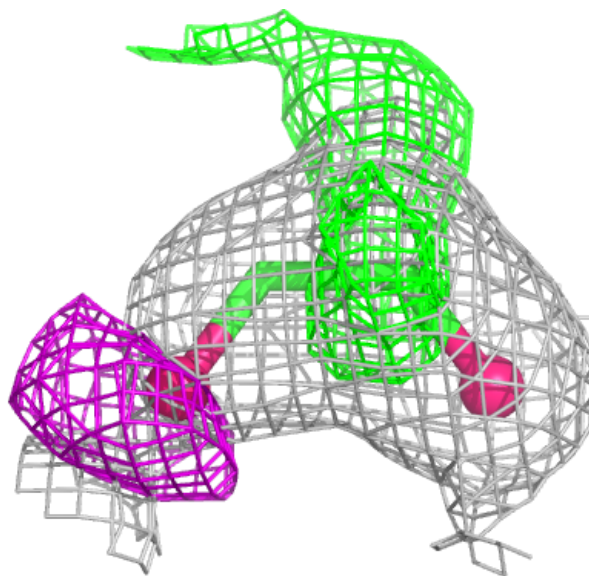
**Electron density around EDO A 518:**

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



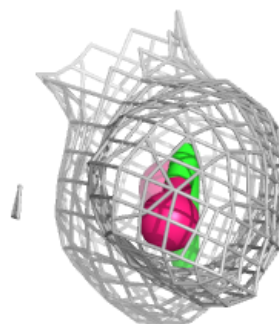
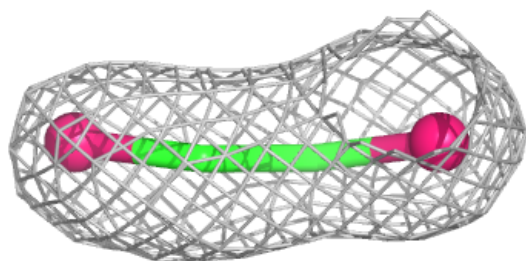
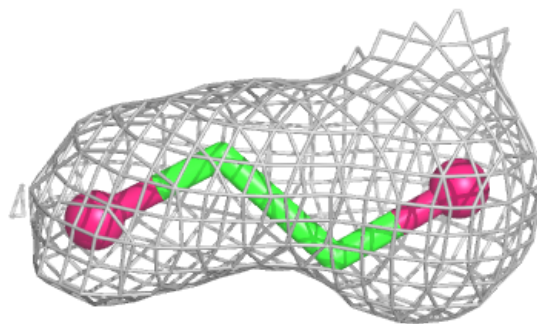
Electron density around EDO D 529:

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



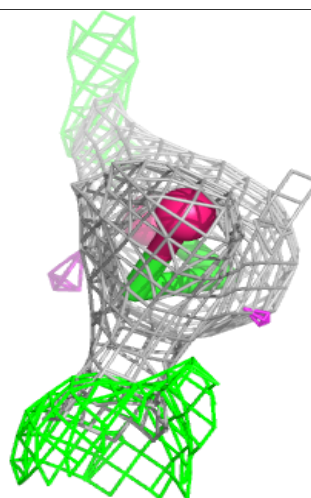
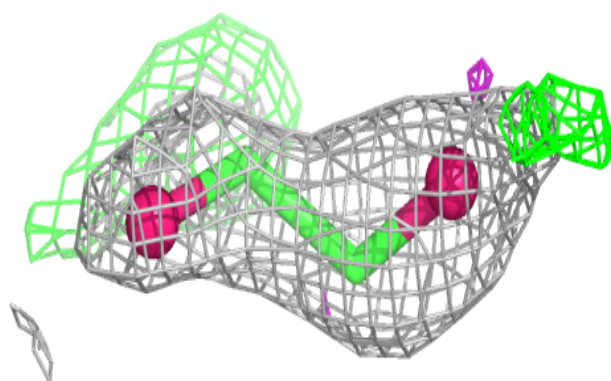
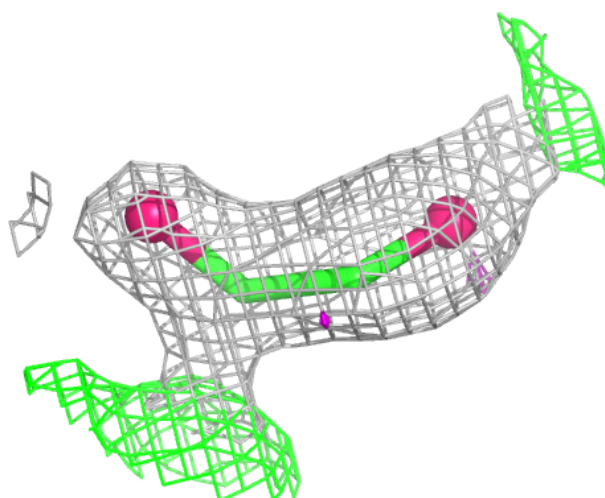
Electron density around EDO B 520:

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



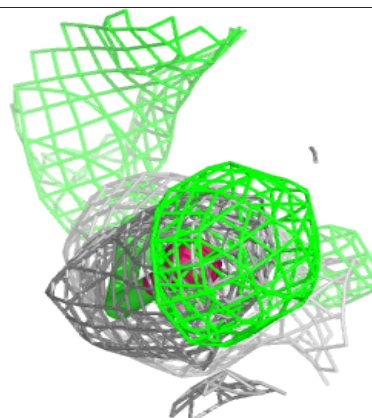
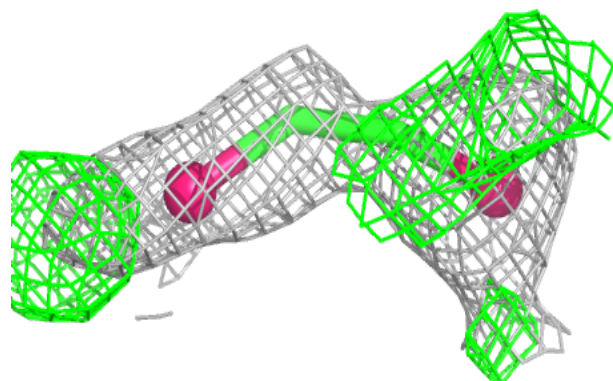
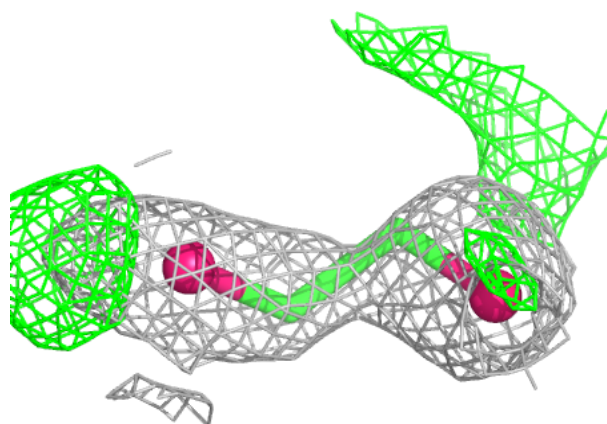
Electron density around EDO A 523:

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



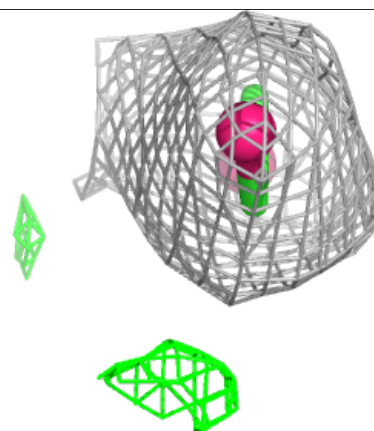
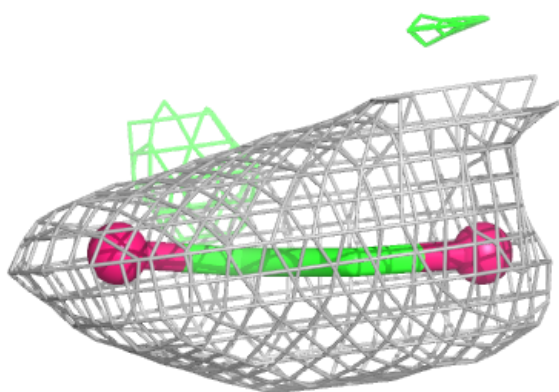
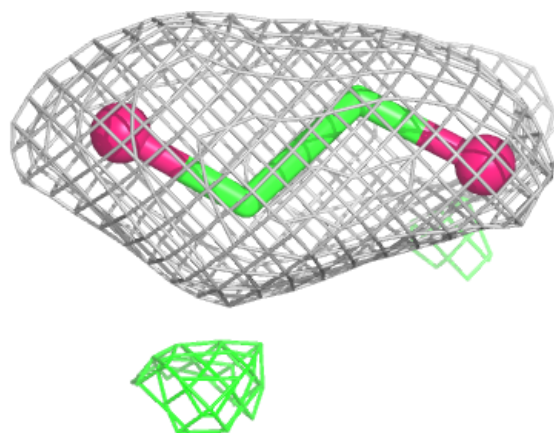
Electron density around EDO A 526:

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



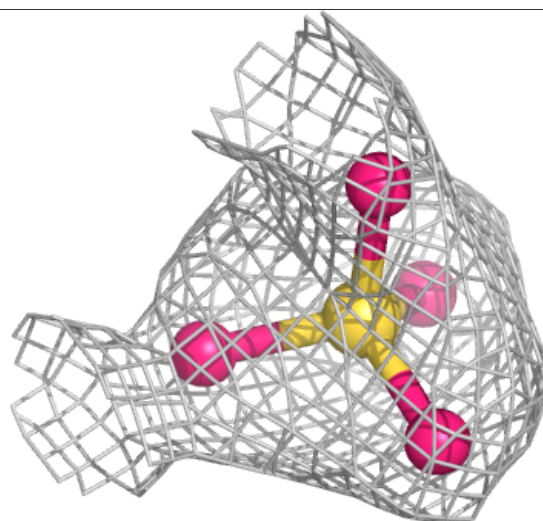
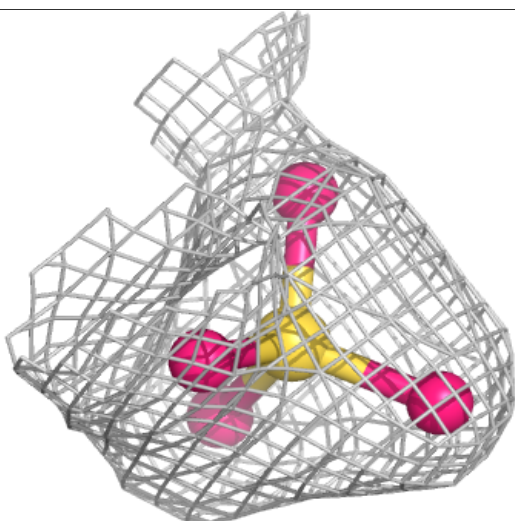
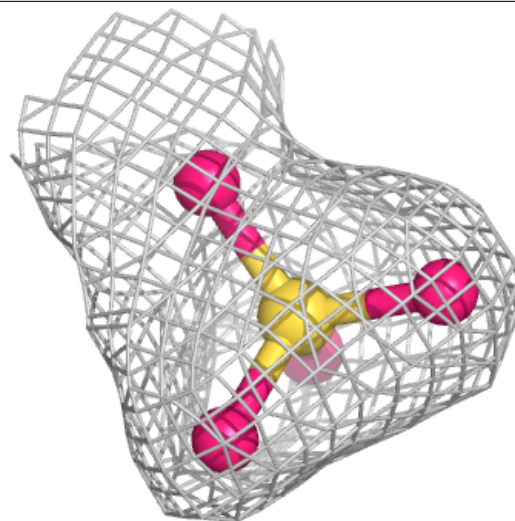
Electron density around EDO B 522:

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



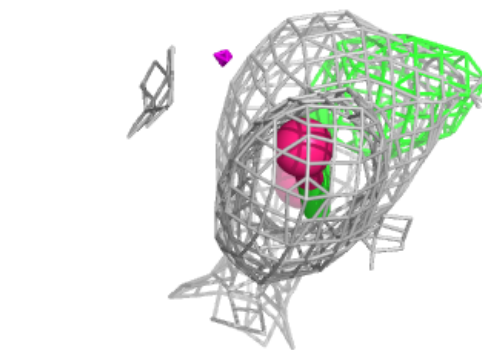
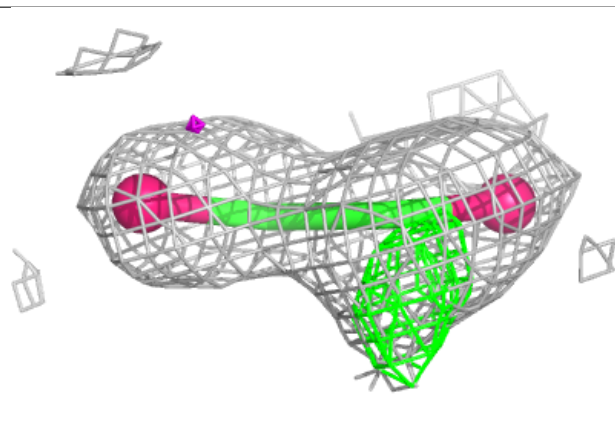
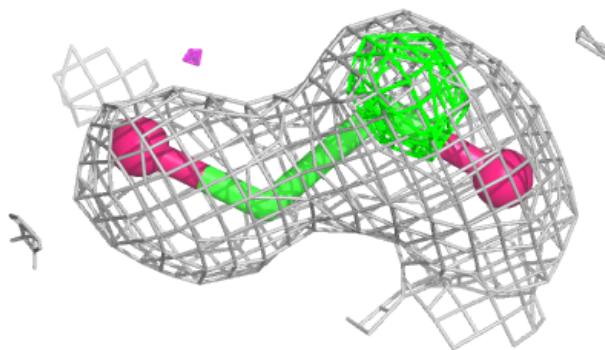
Electron density around SO4 B 511:

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



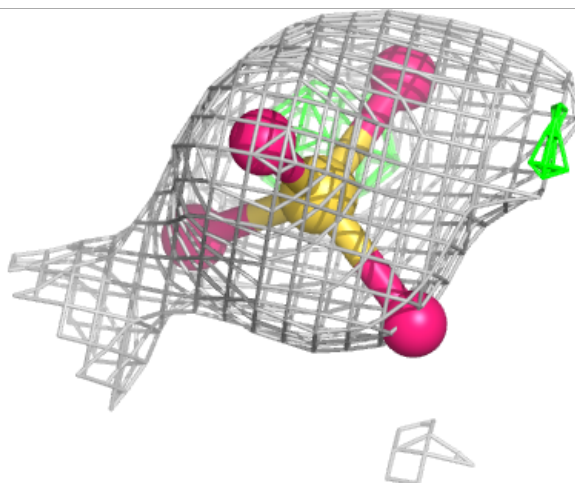
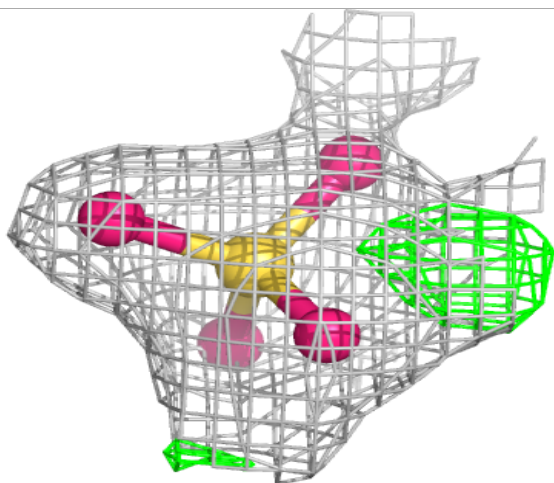
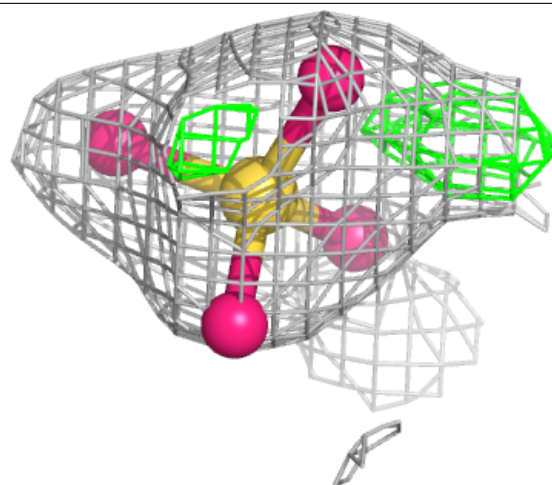
Electron density around EDO B 530:

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



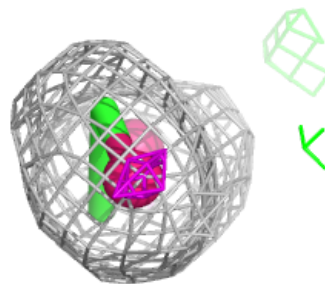
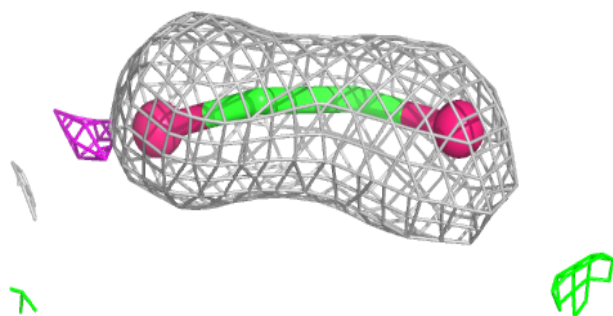
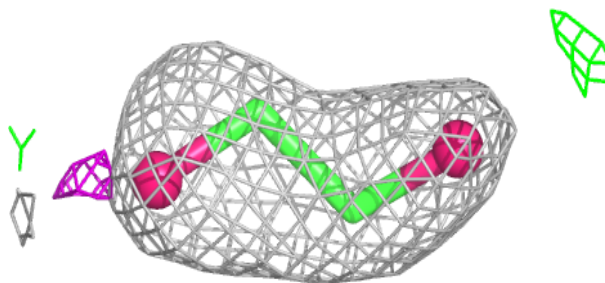
Electron density around SO4 C 511:

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

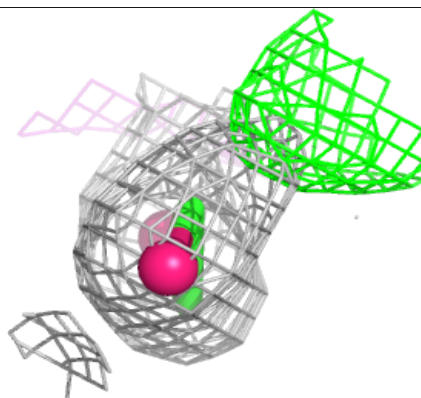
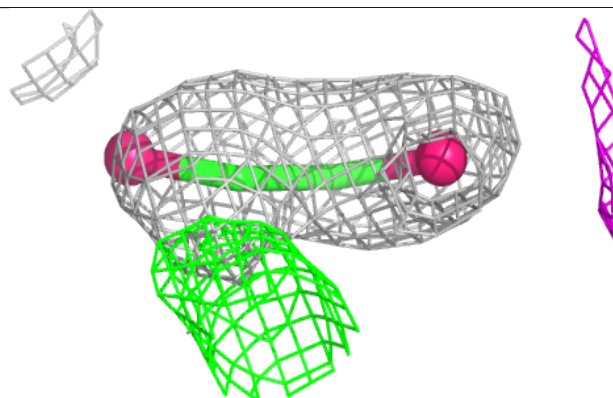
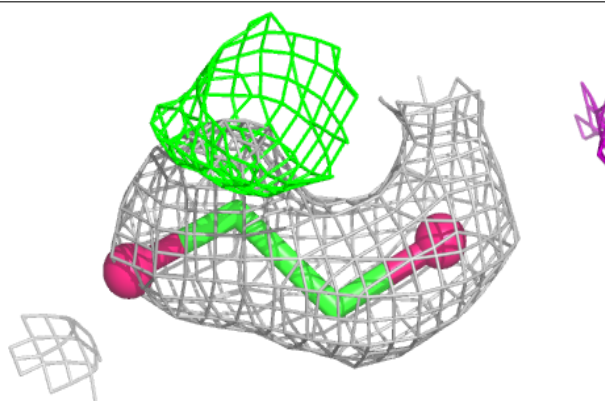


Electron density around EDO A 521:

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

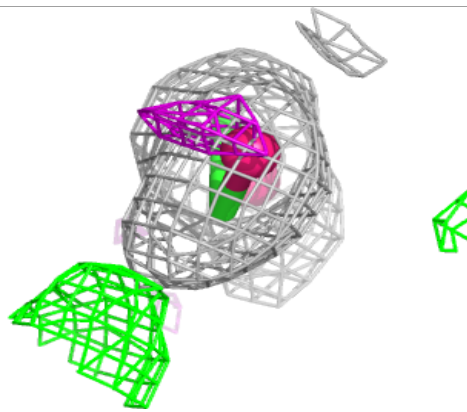
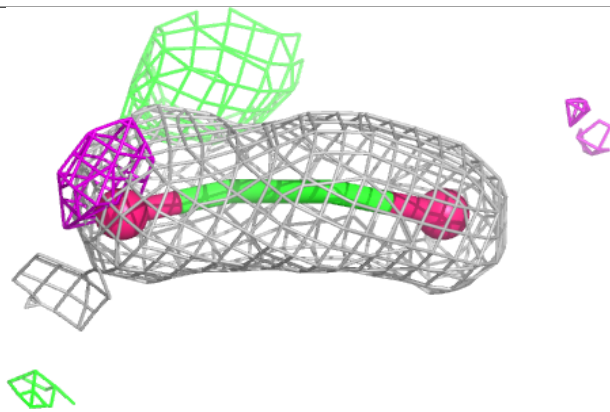
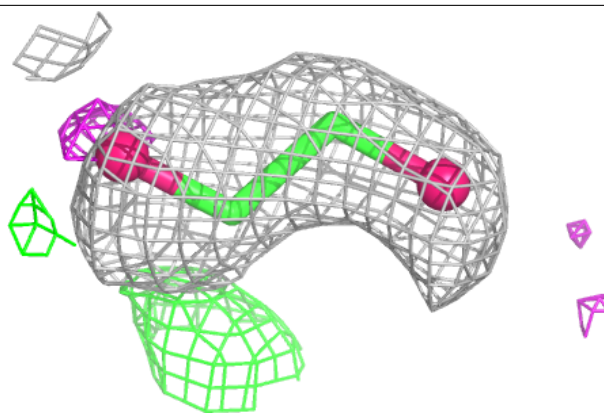
**Electron density around EDO C 532:**

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



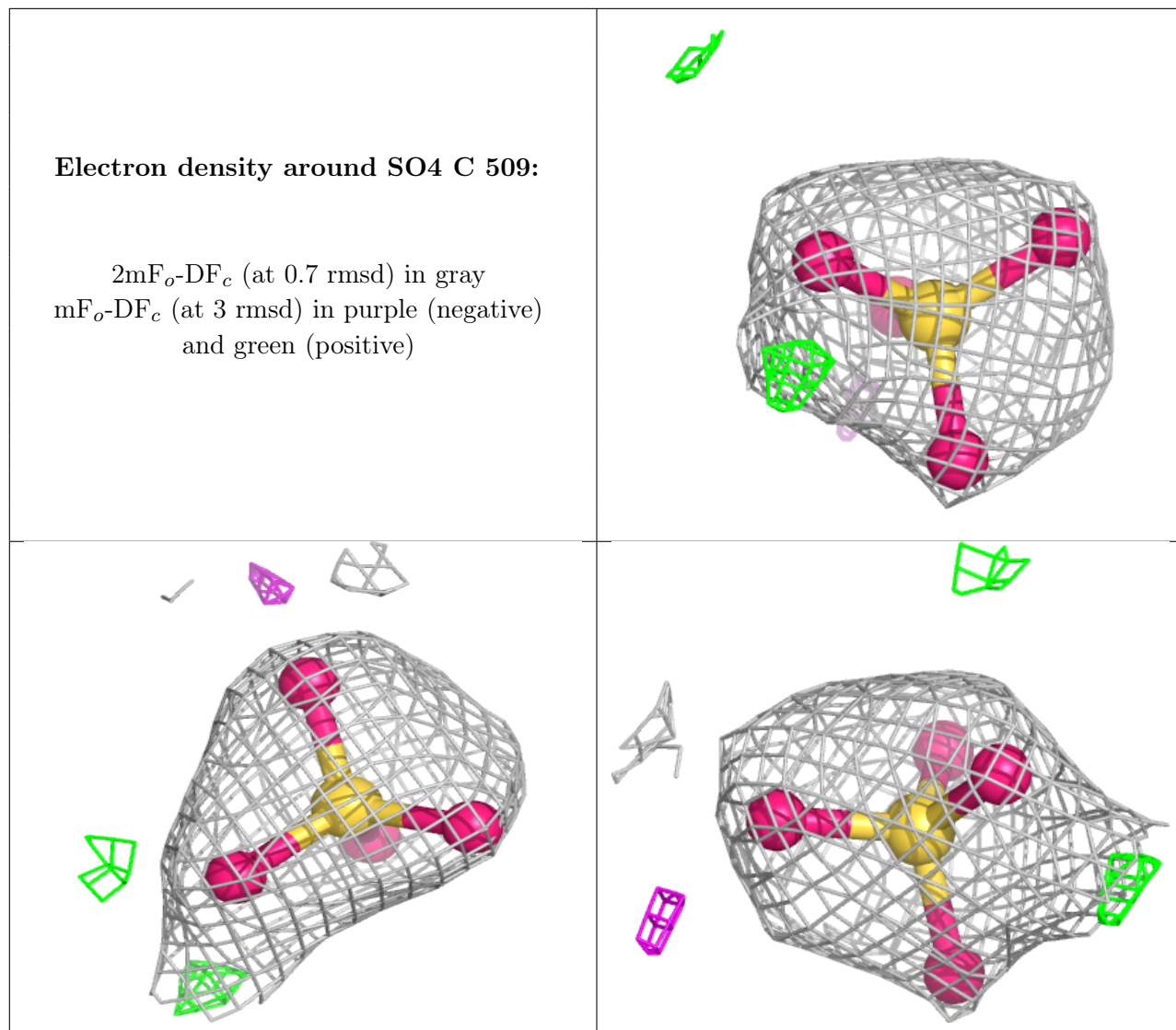
Electron density around EDO A 512:

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



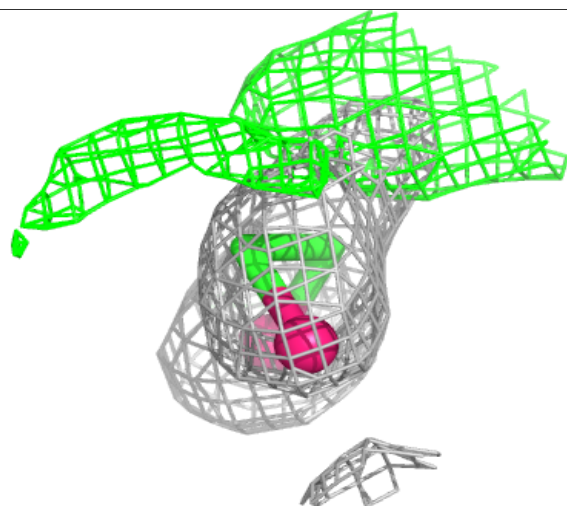
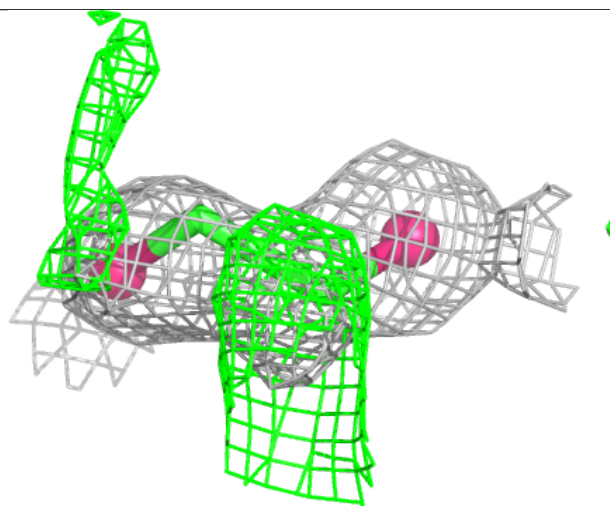
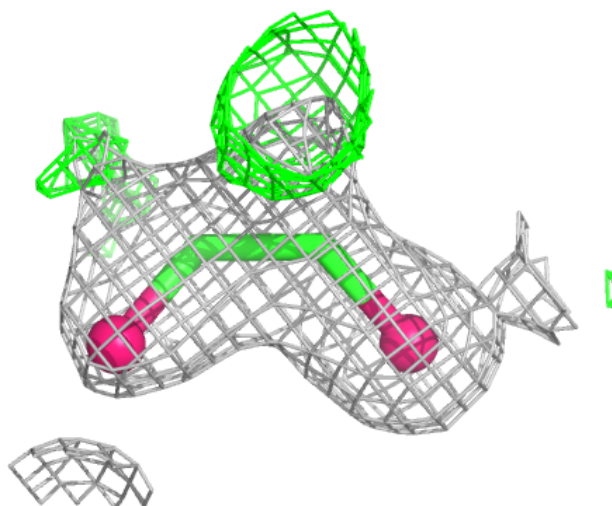
Electron density around SO4 C 509:

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



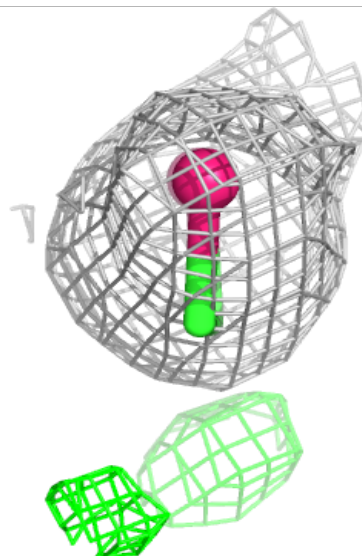
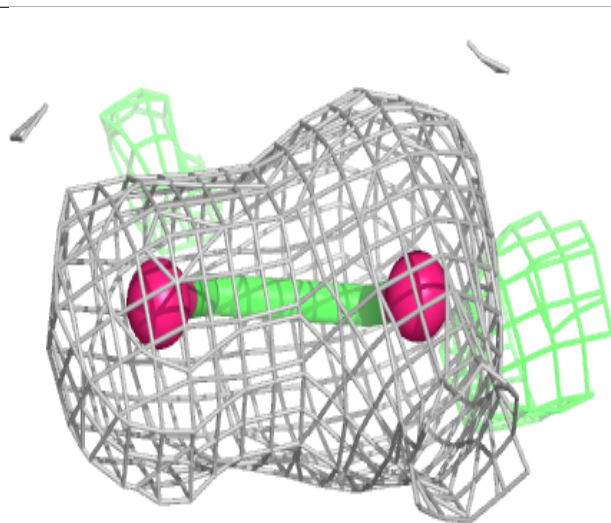
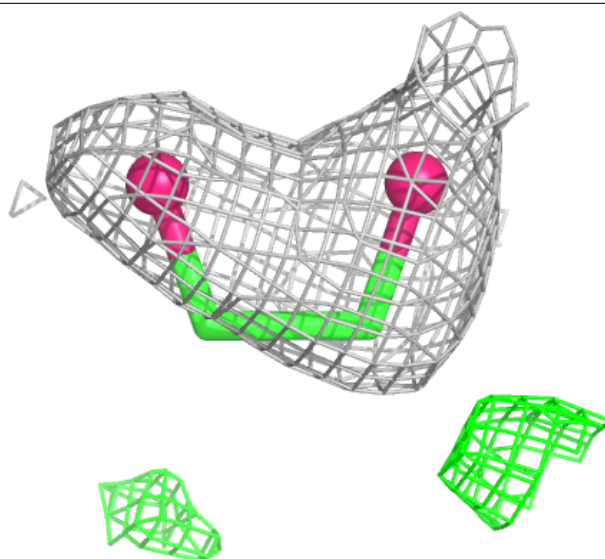
Electron density around EDO A 532:

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



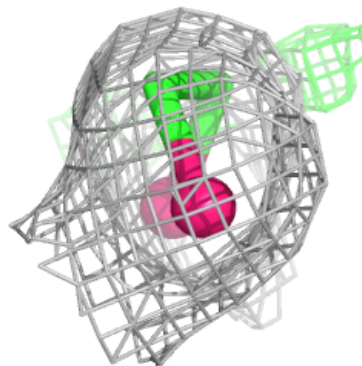
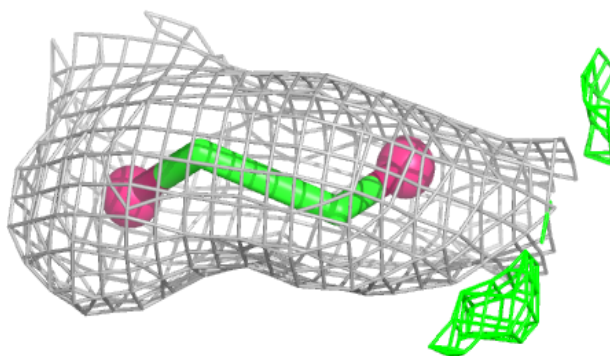
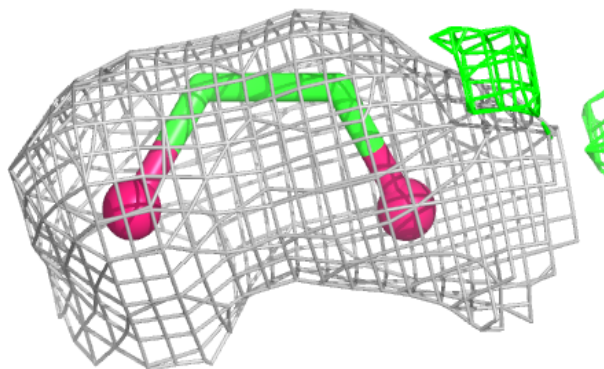
Electron density around EDO C 519:

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

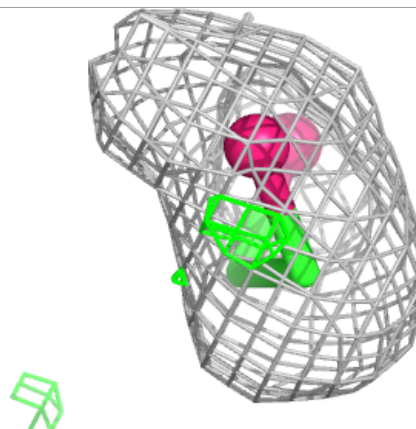
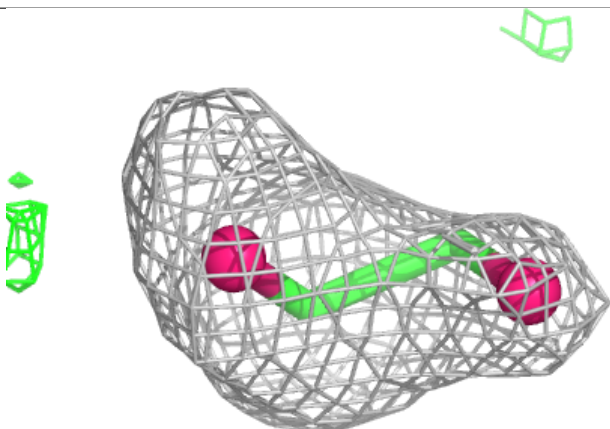
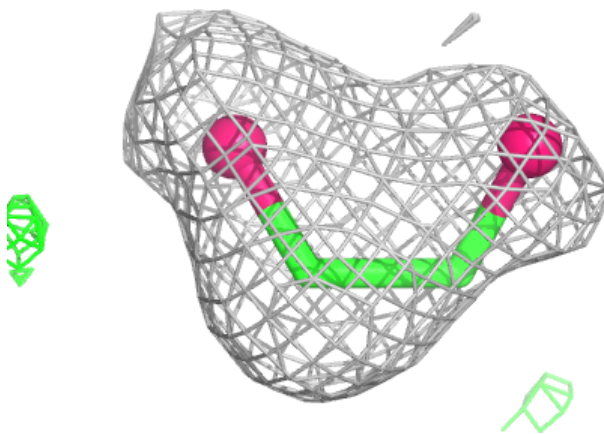


Electron density around EDO A 534:

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

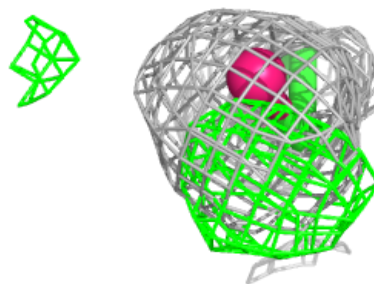
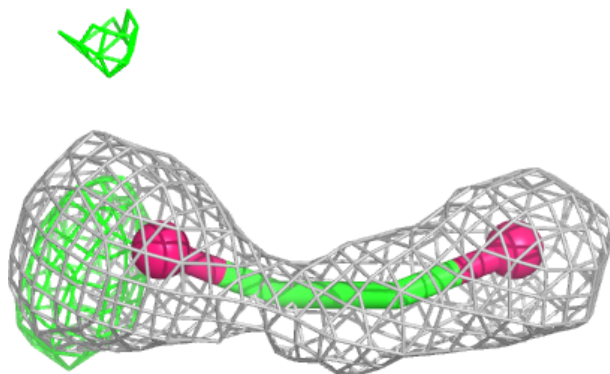
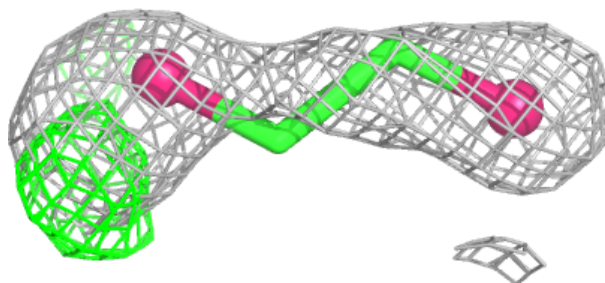
**Electron density around EDO B 523:**

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

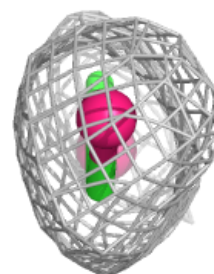
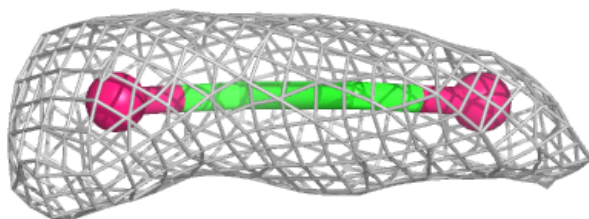
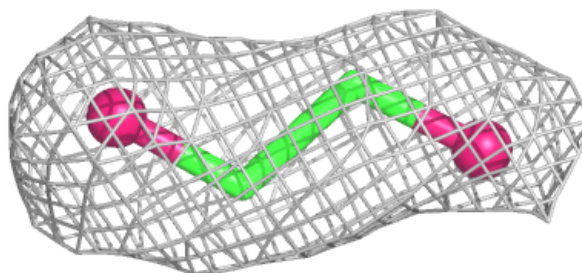


Electron density around EDO B 532:

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

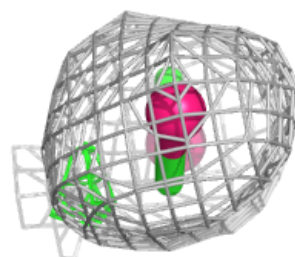
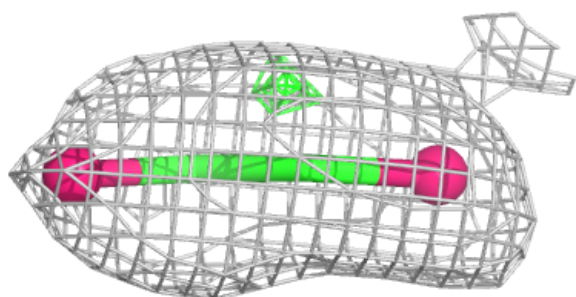
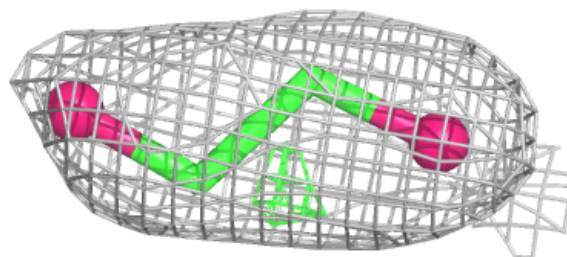
**Electron density around EDO D 531:**

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

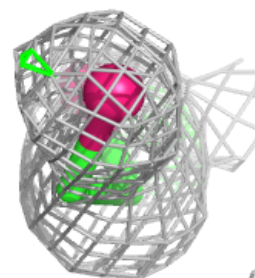
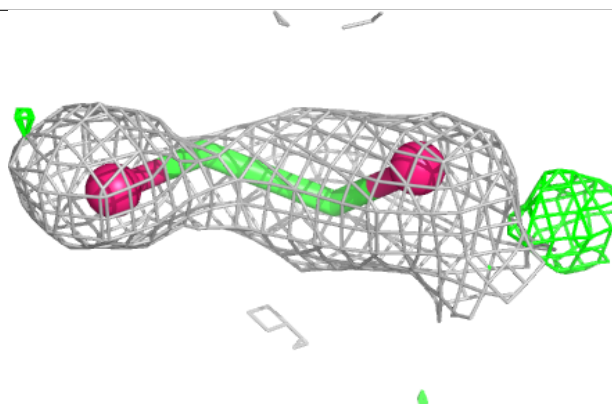
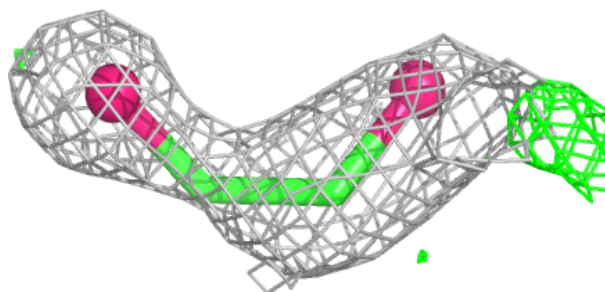


Electron density around EDO A 516:

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

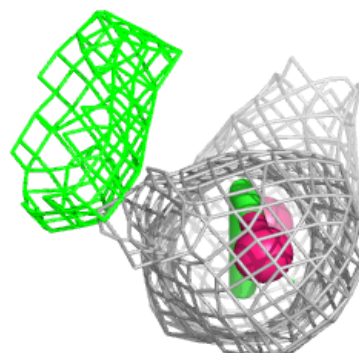
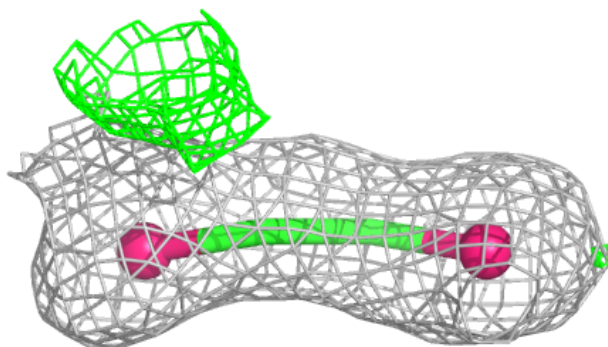
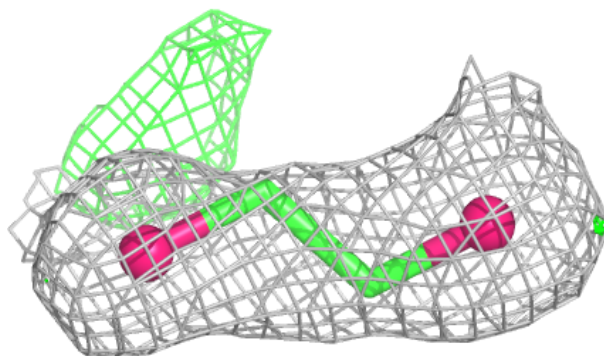
**Electron density around EDO A 537:**

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

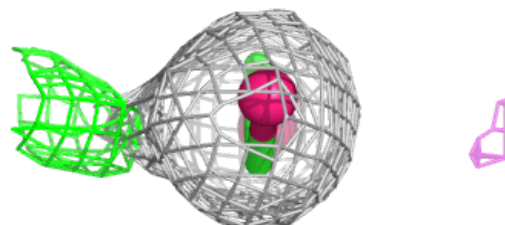
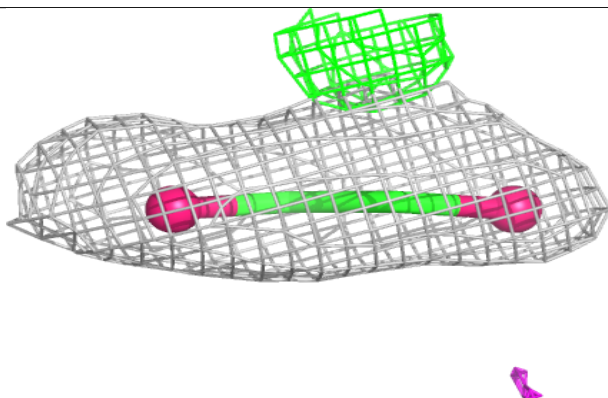
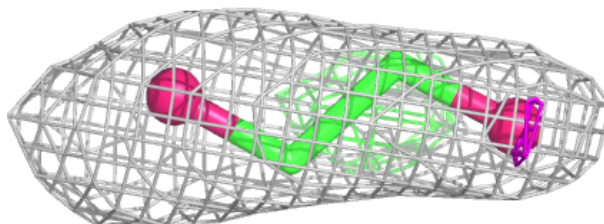


Electron density around EDO B 536:

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

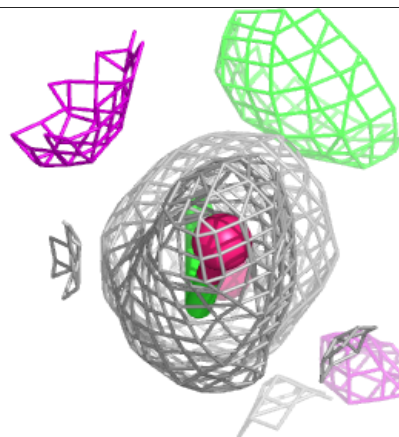
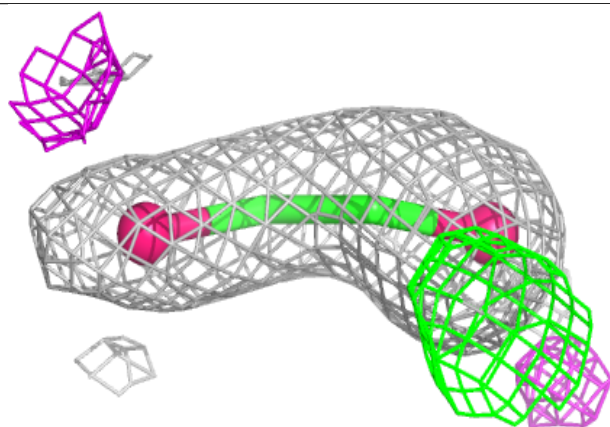
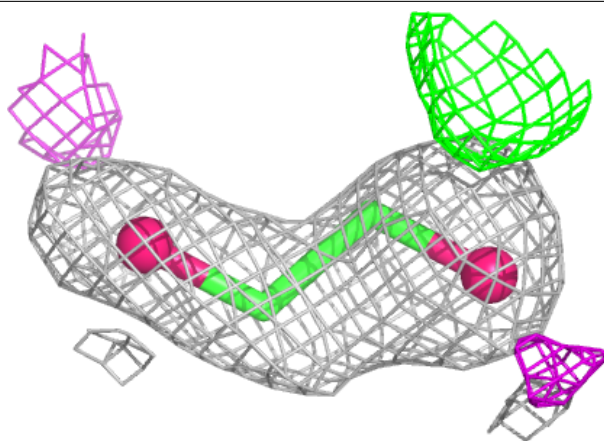
**Electron density around EDO C 529:**

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



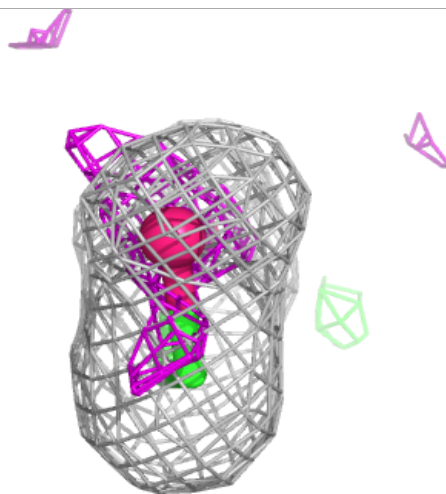
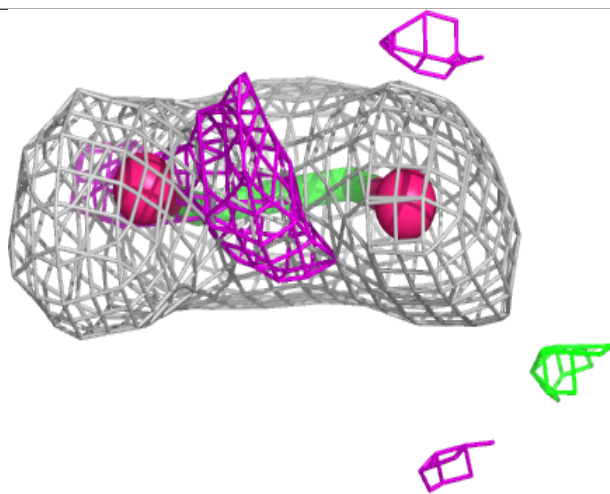
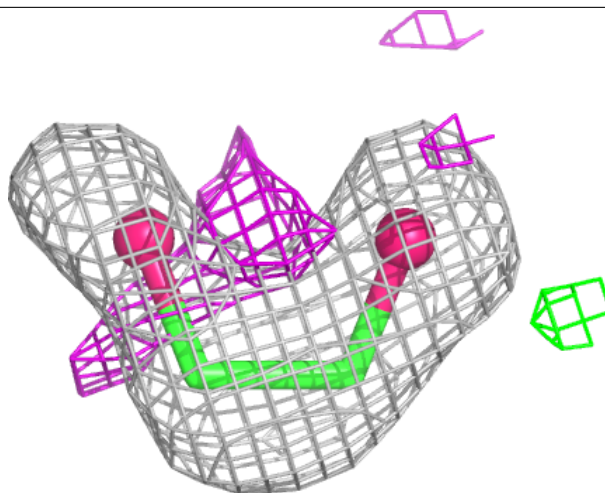
Electron density around EDO A 527:

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



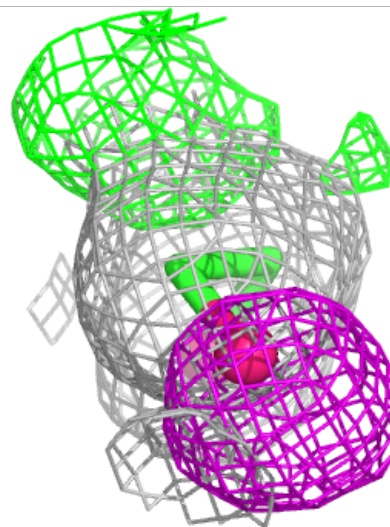
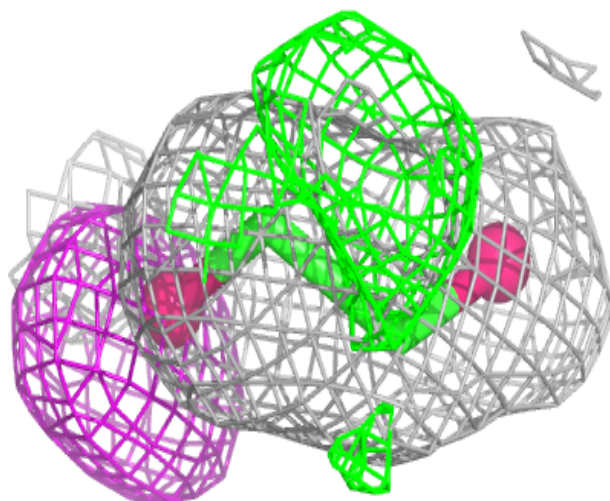
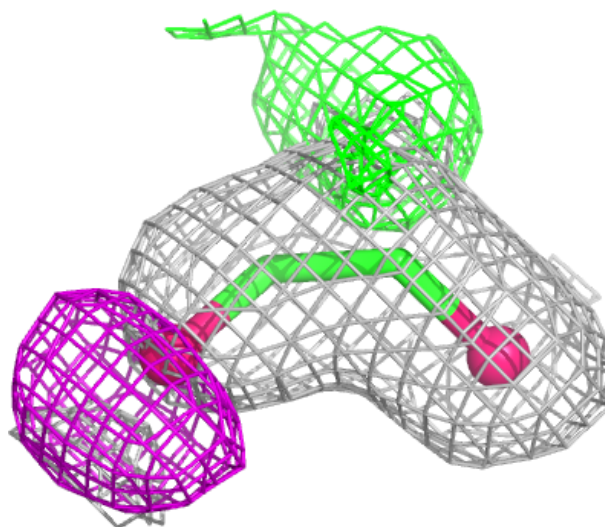
Electron density around EDO A 525:

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



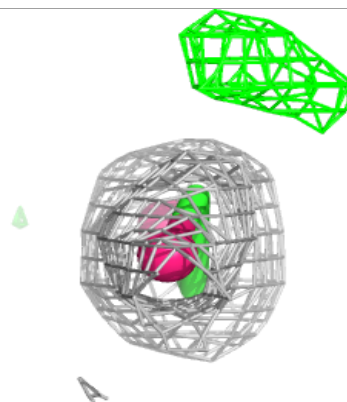
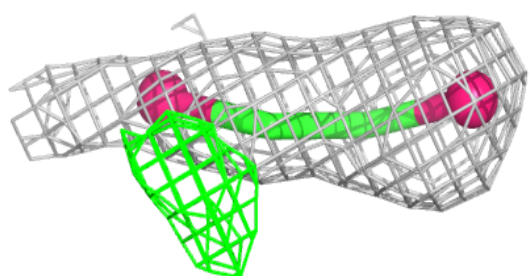
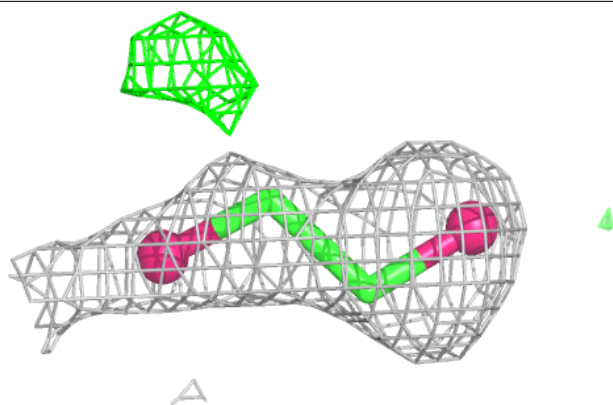
Electron density around EDO A 524:

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

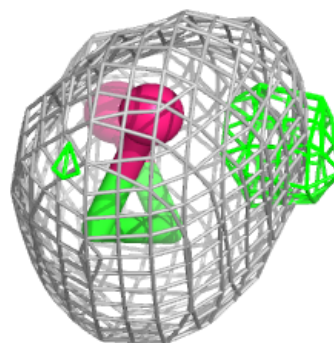
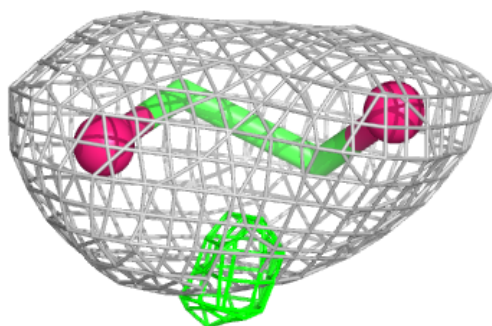
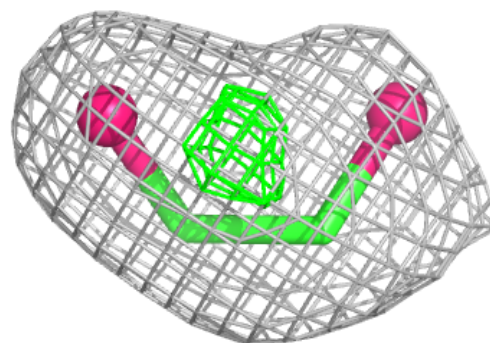


Electron density around EDO D 527:

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

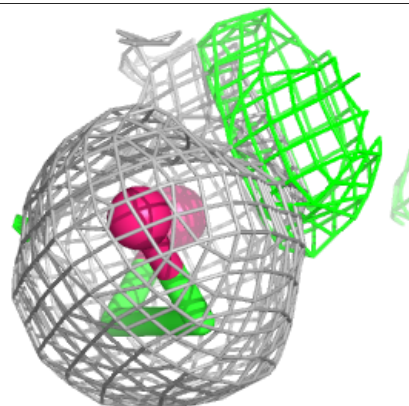
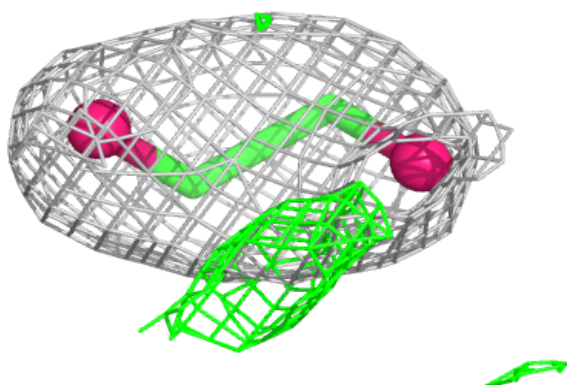
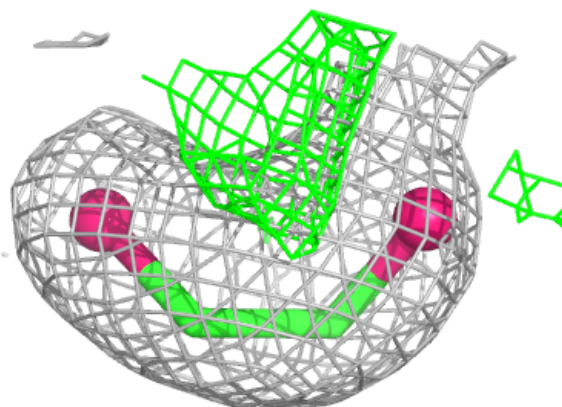
**Electron density around EDO D 517:**

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



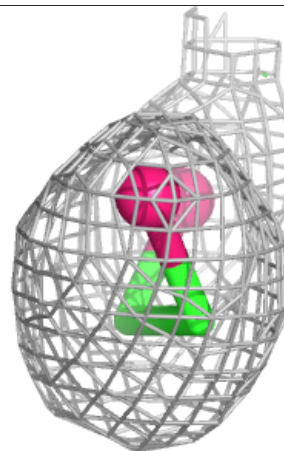
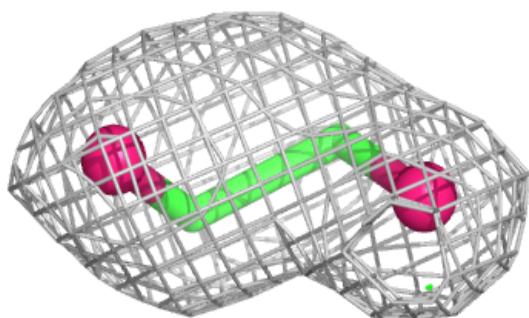
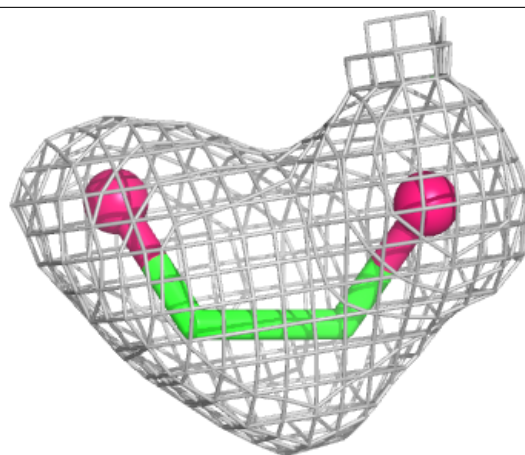
Electron density around EDO B 516:

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



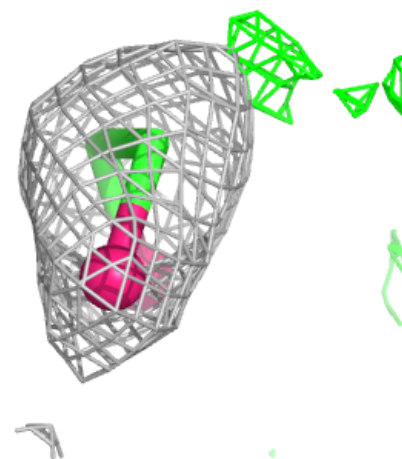
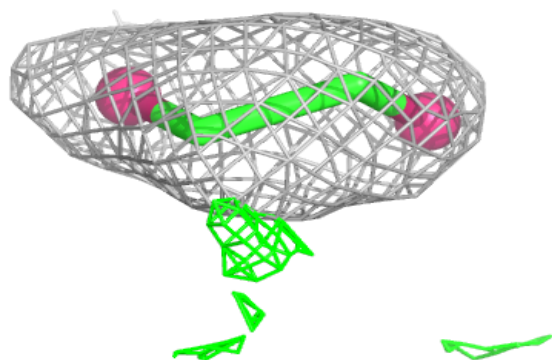
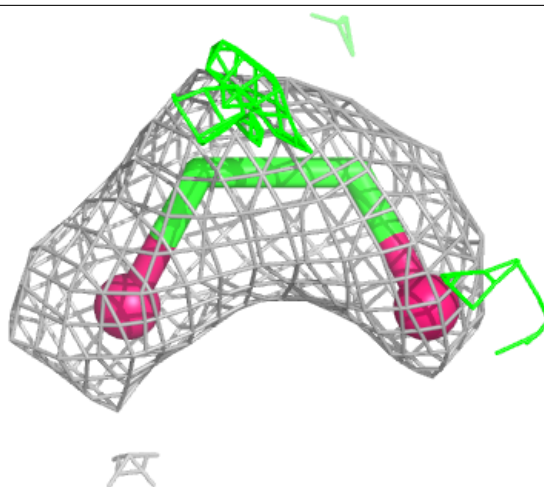
Electron density around EDO C 515:

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



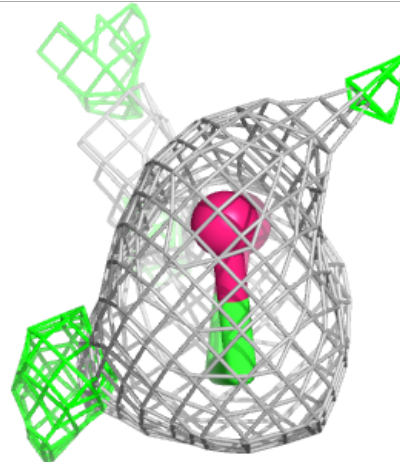
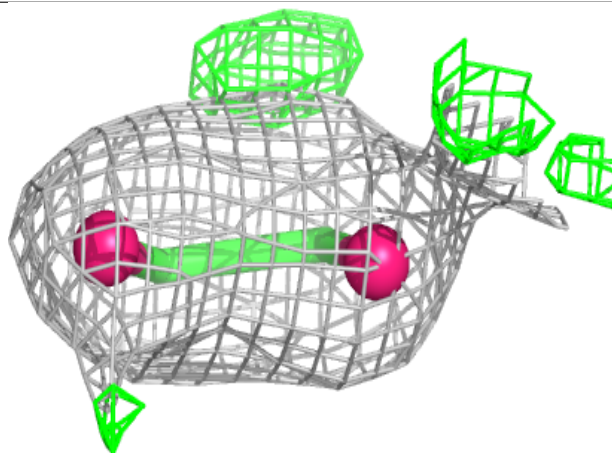
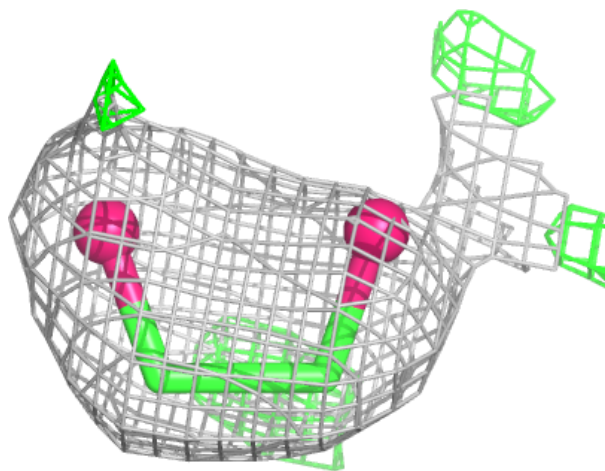
Electron density around EDO D 522:

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



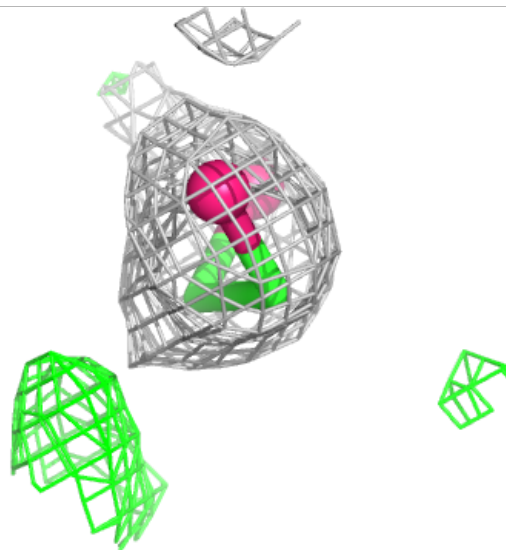
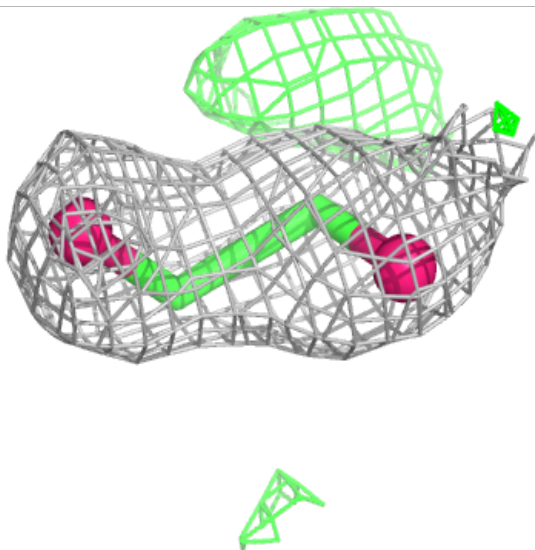
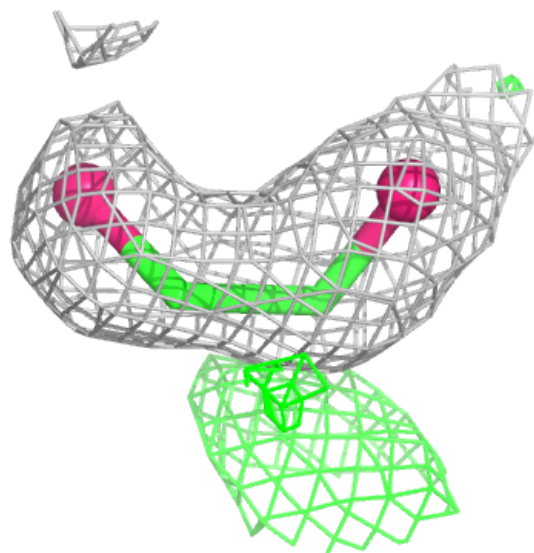
Electron density around EDO C 516:

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



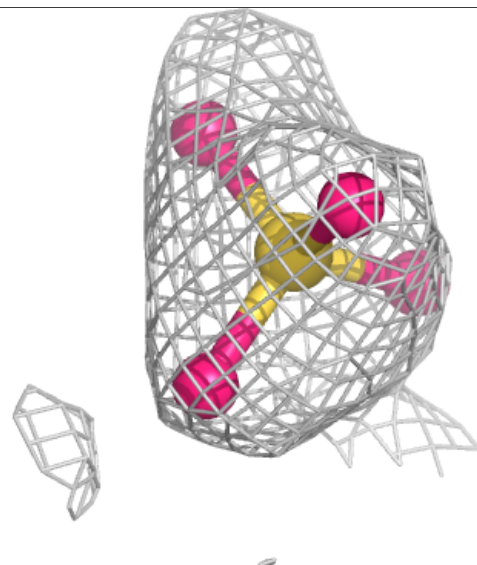
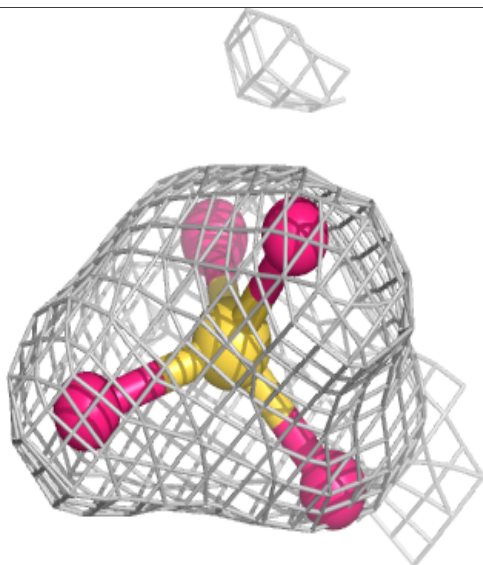
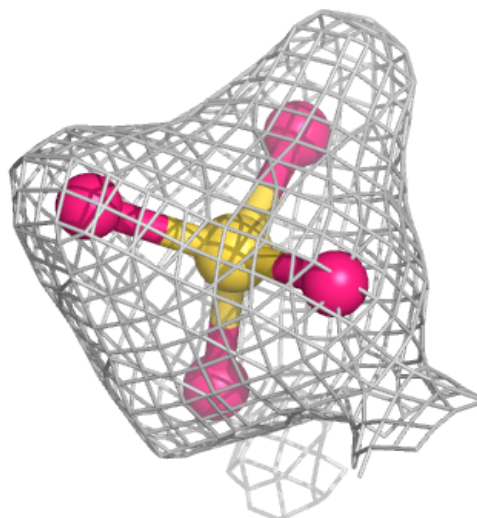
Electron density around EDO D 533:

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



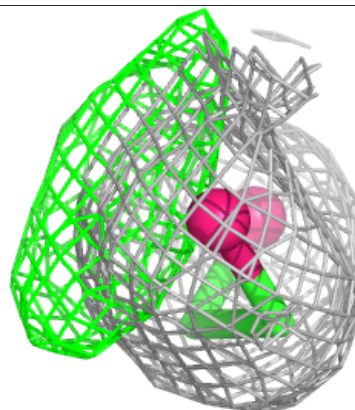
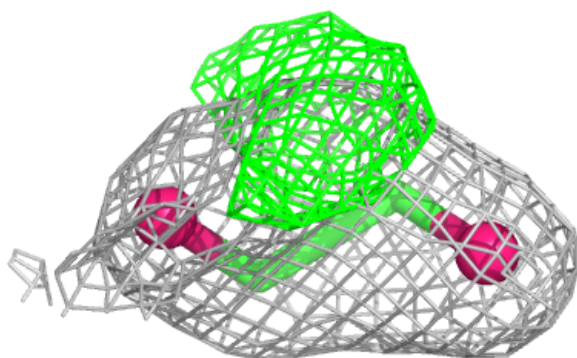
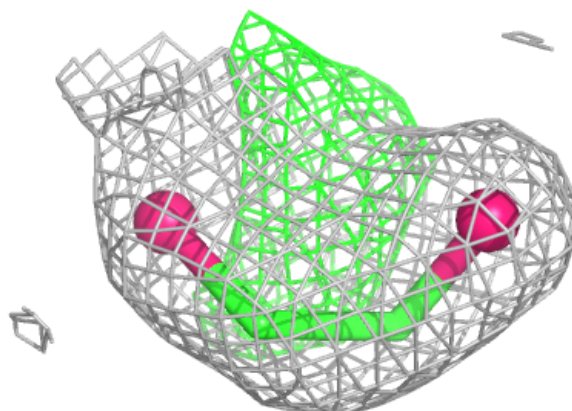
Electron density around SO4 D 513:

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

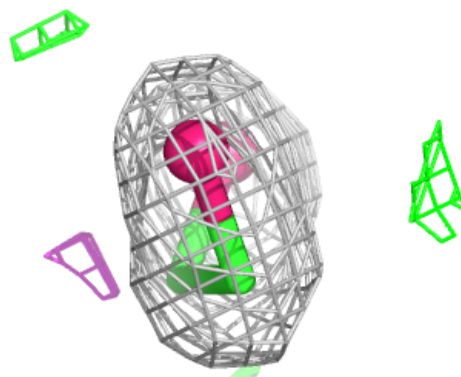
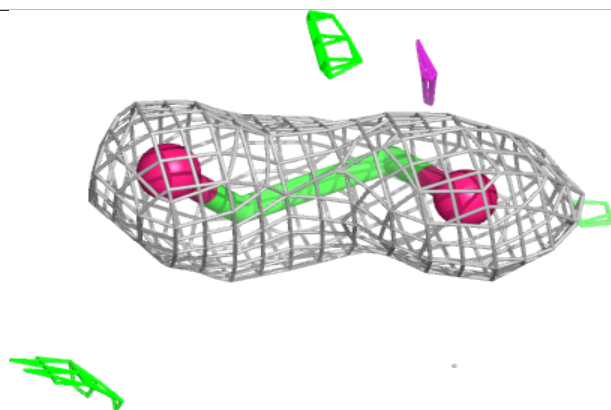
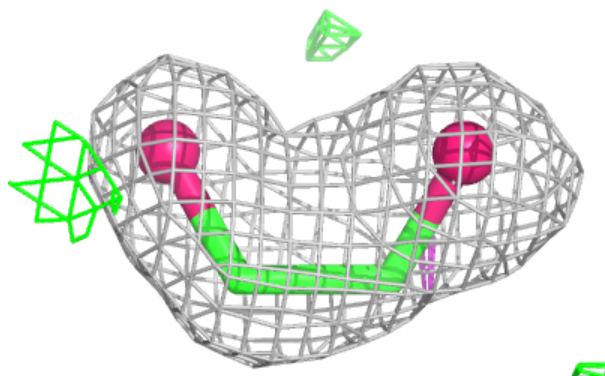


Electron density around EDO D 503:

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

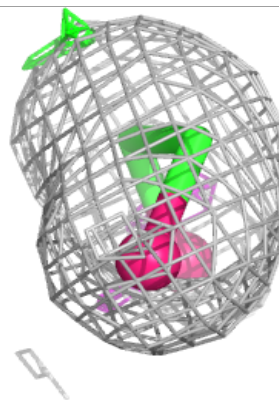
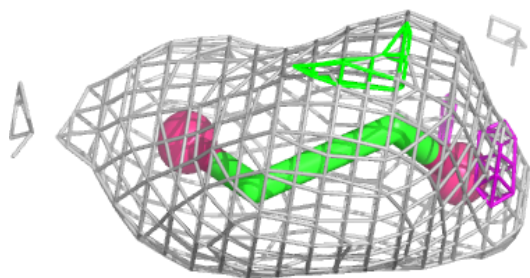
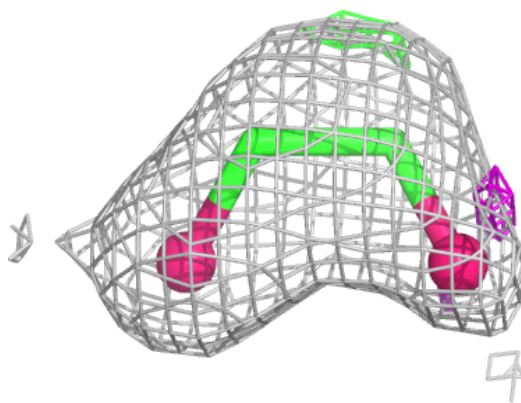
**Electron density around EDO C 522:**

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

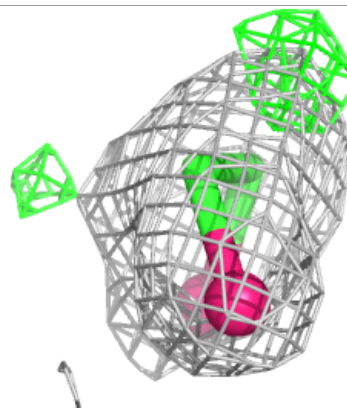
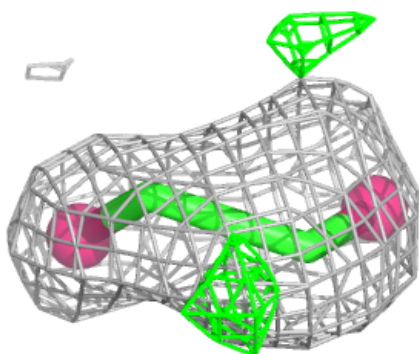
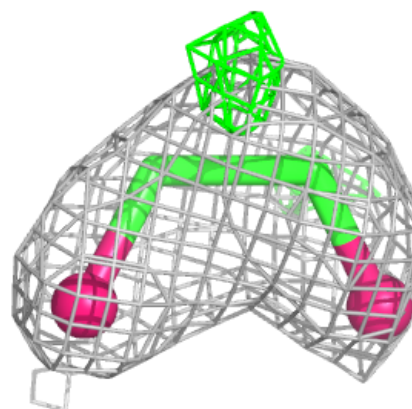


Electron density around EDO B 515:

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

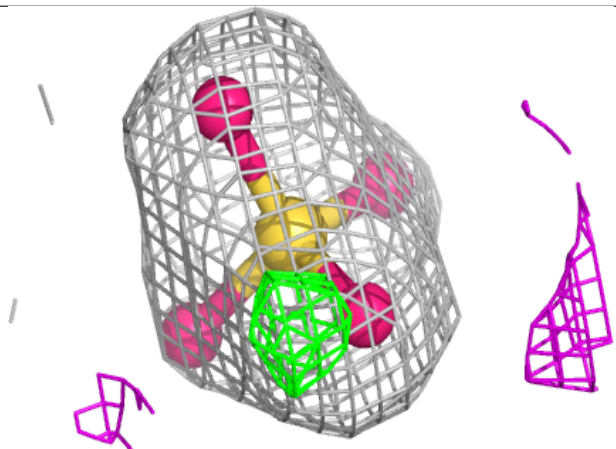
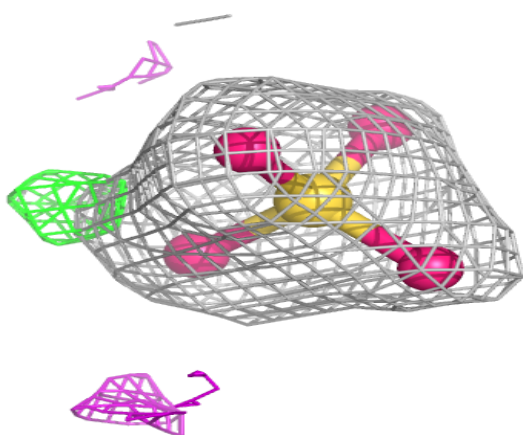
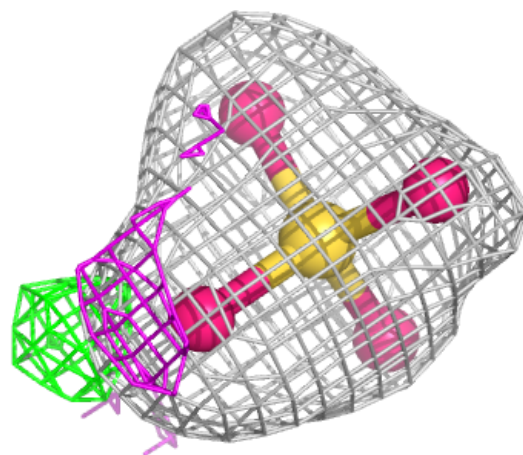
**Electron density around EDO B 529:**

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



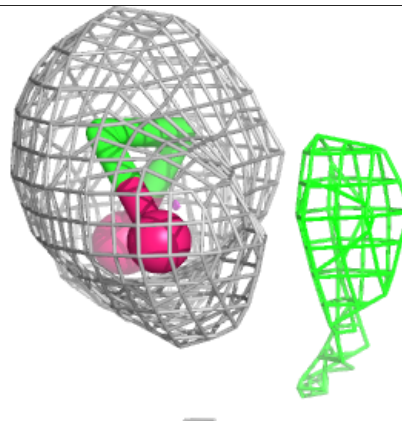
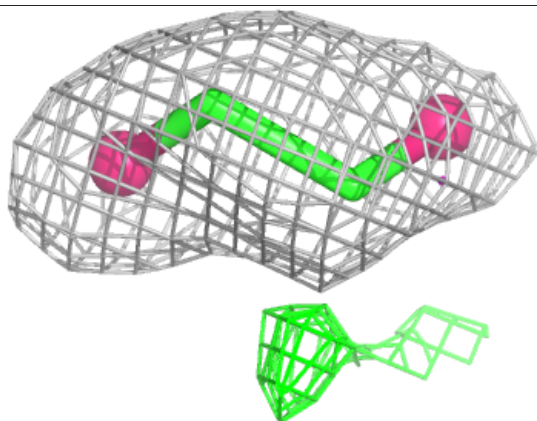
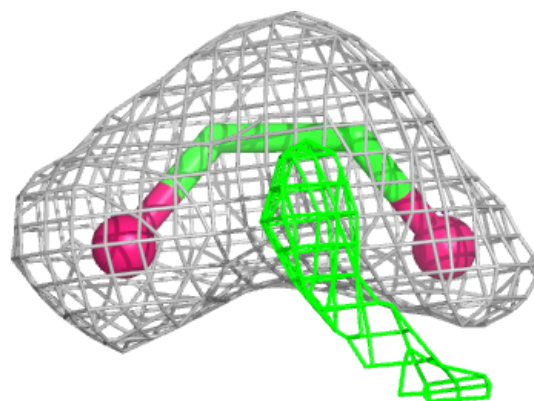
Electron density around SO4 D 512:

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

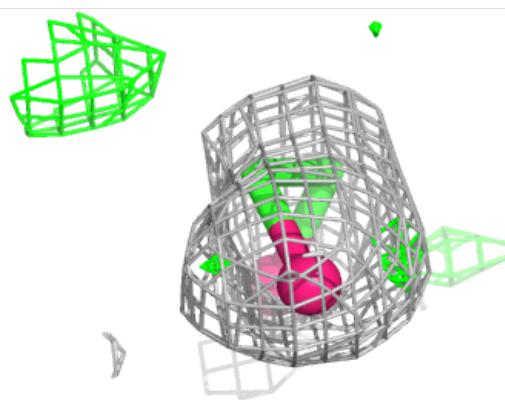
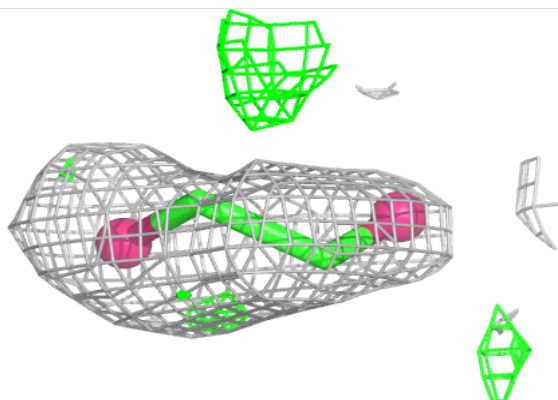
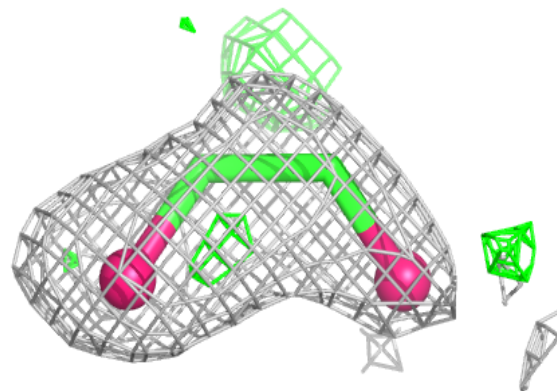


Electron density around EDO A 510:

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

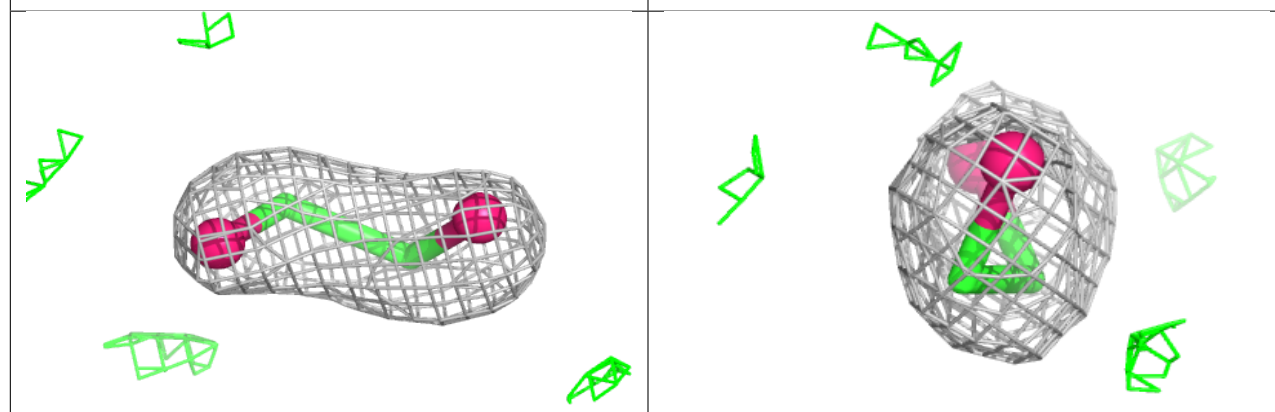
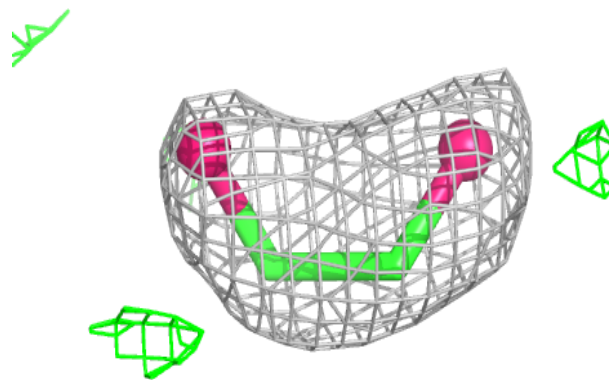
**Electron density around EDO C 518:**

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



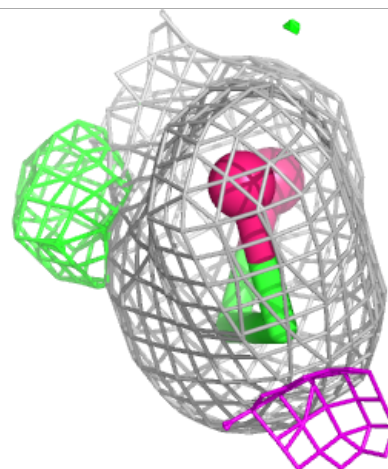
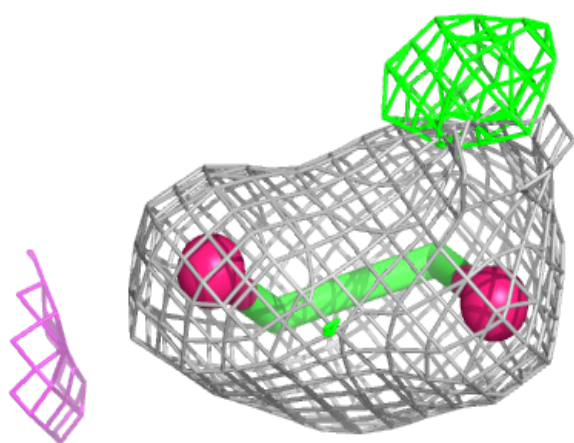
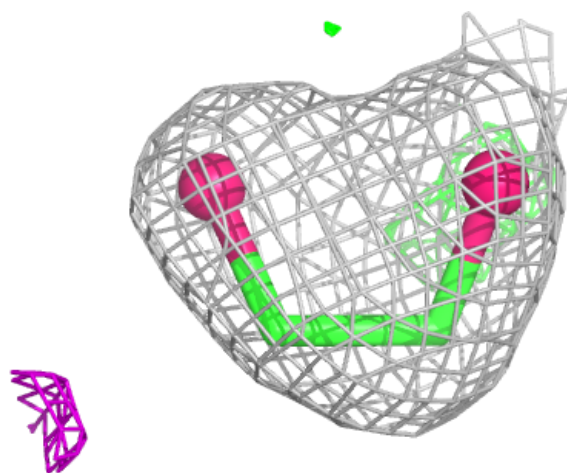
Electron density around EDO A 519:

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



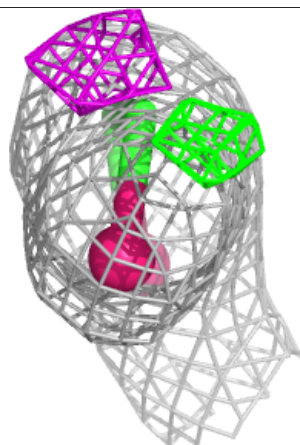
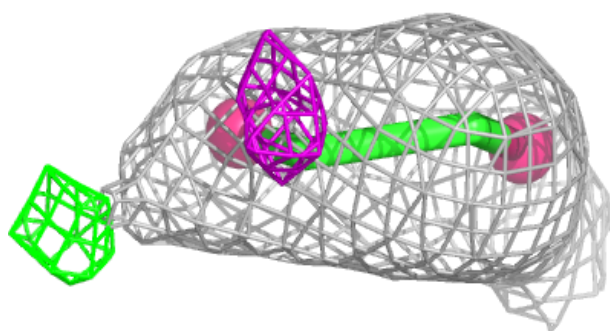
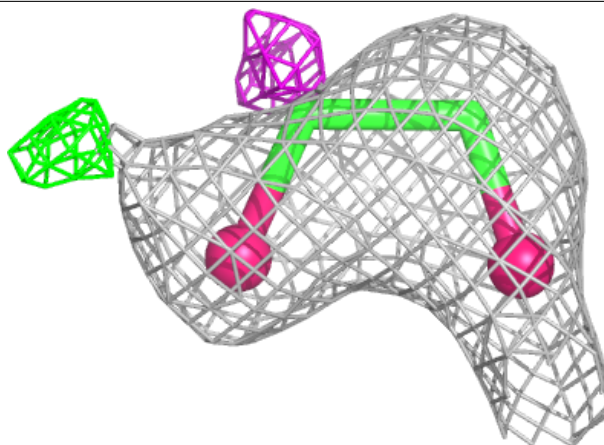
Electron density around EDO A 520:

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

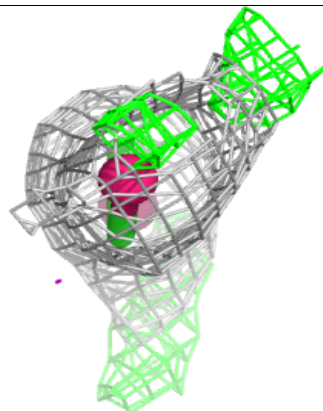
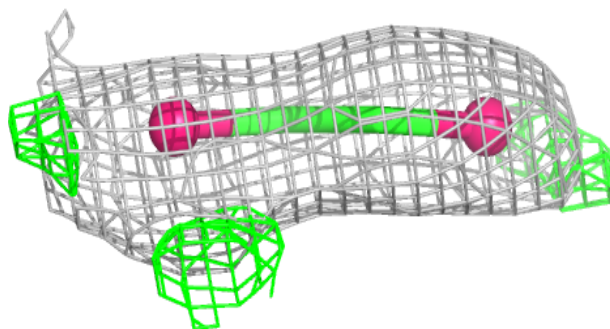
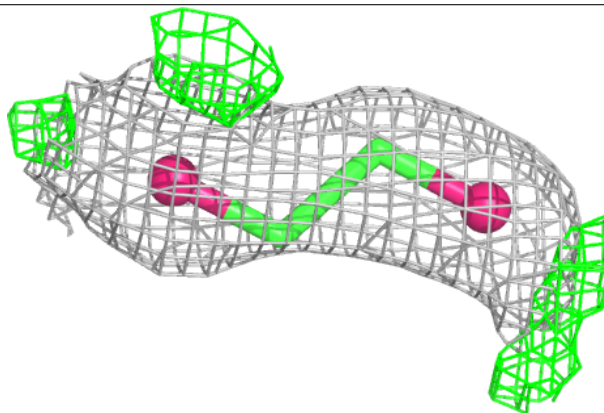


Electron density around EDO B 534:

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

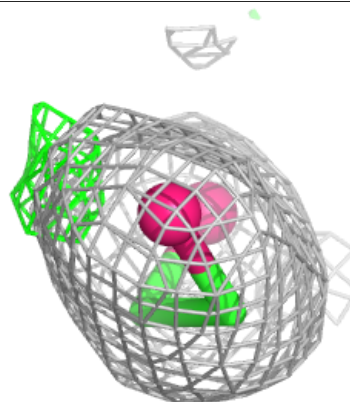
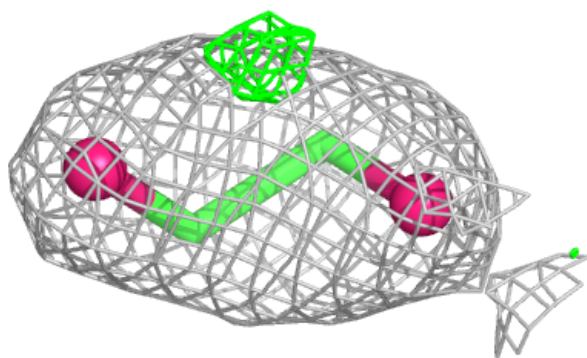
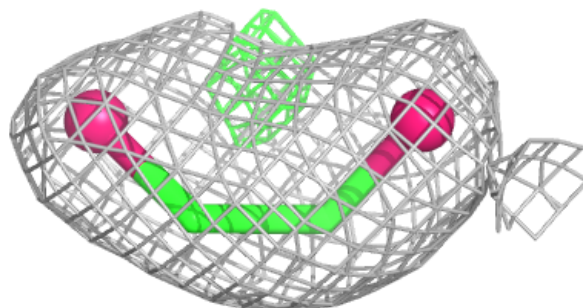
**Electron density around EDO C 517:**

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



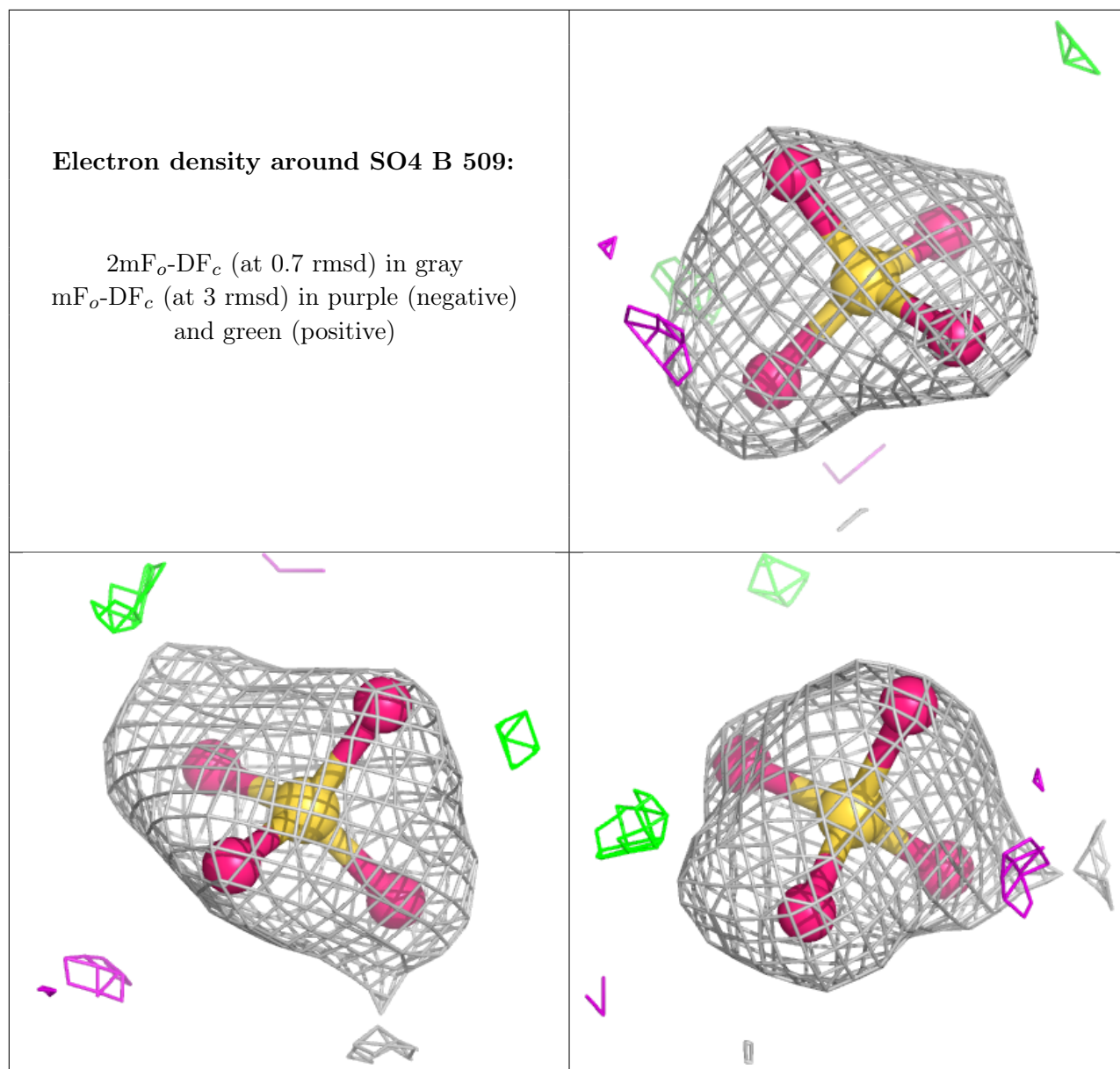
Electron density around EDO A 535:

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



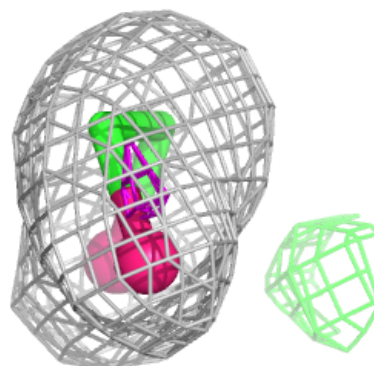
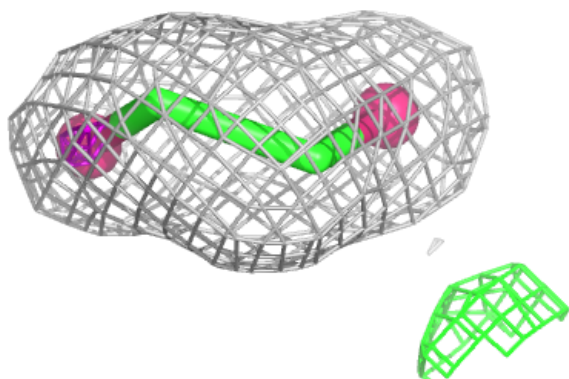
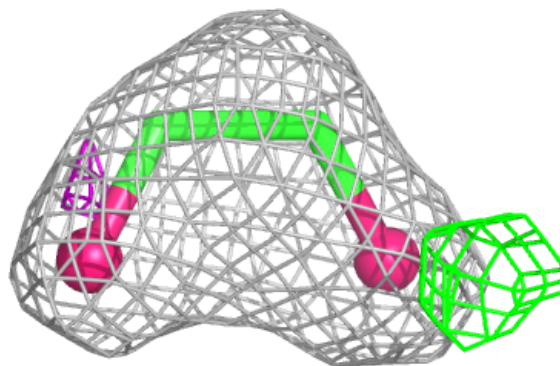
Electron density around SO4 B 509:

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



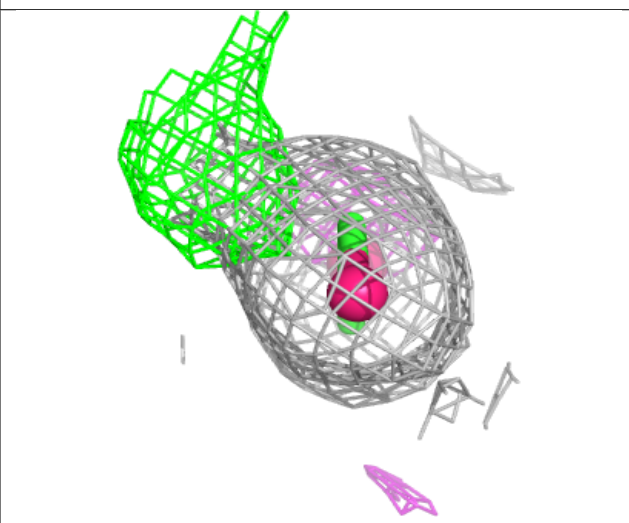
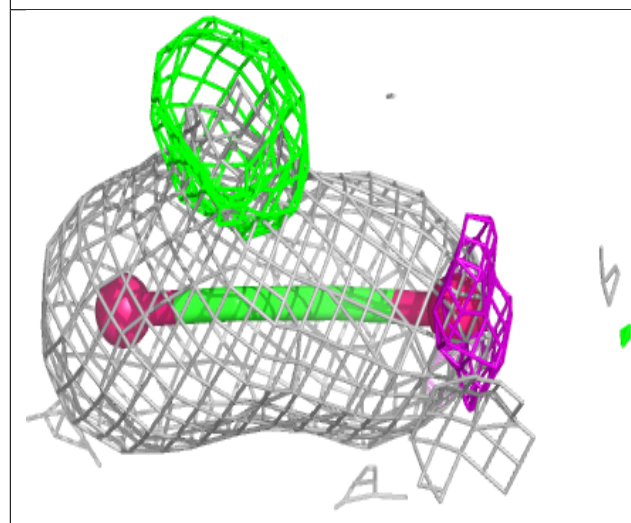
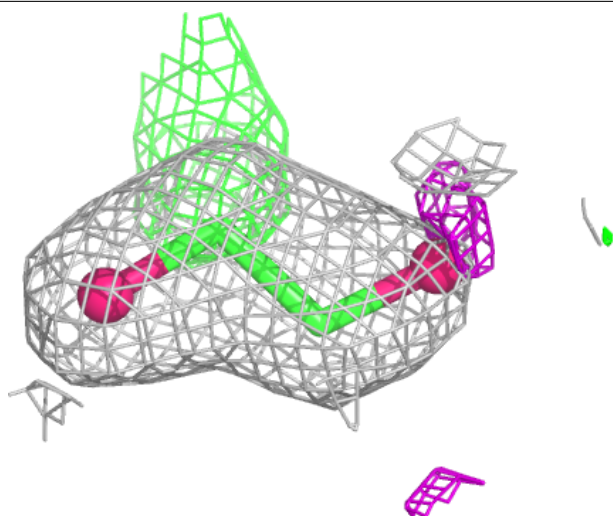
Electron density around EDO C 530:

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



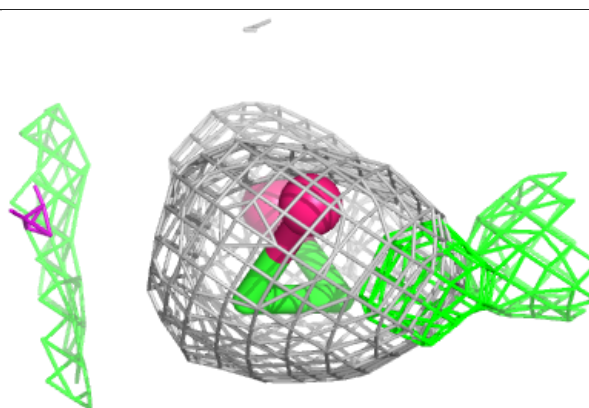
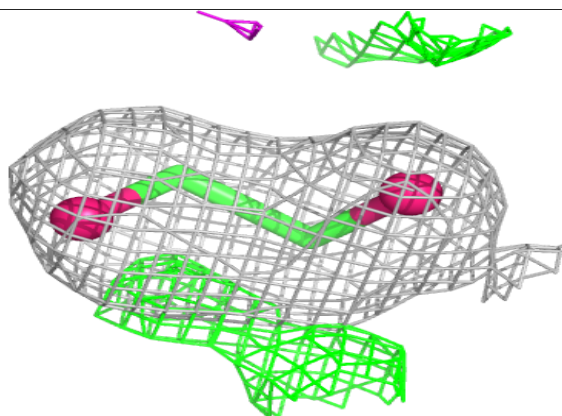
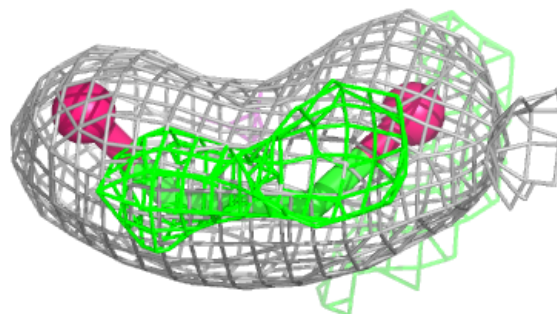
Electron density around EDO C 520:

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

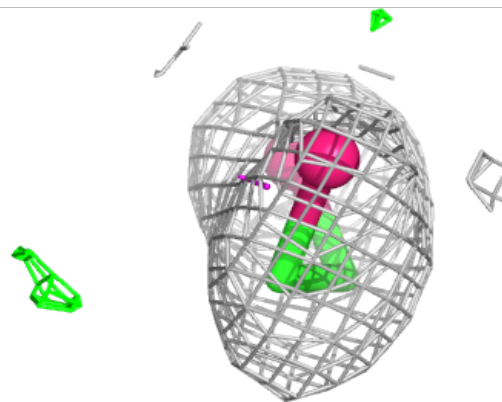
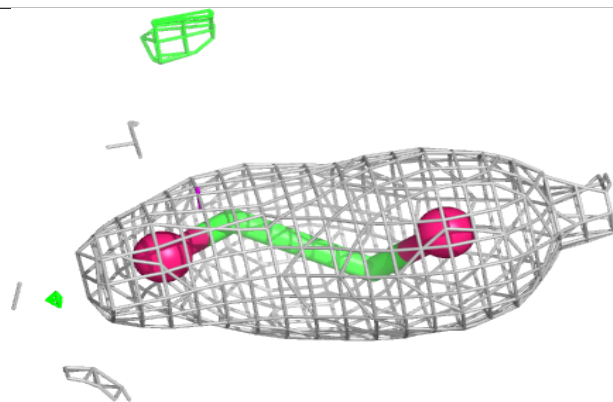
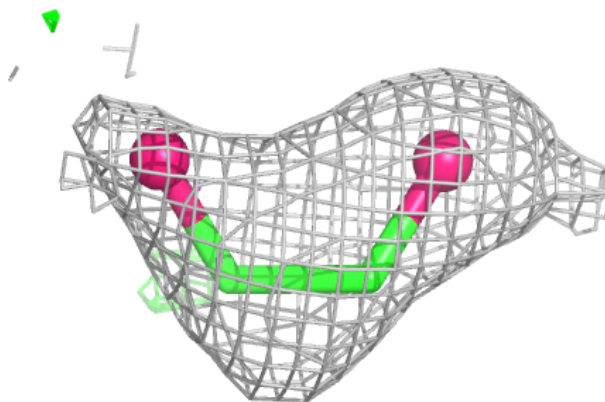


Electron density around EDO B 517:

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

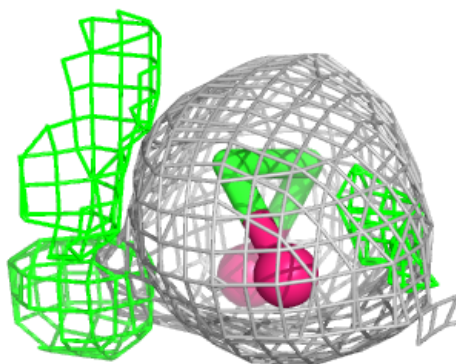
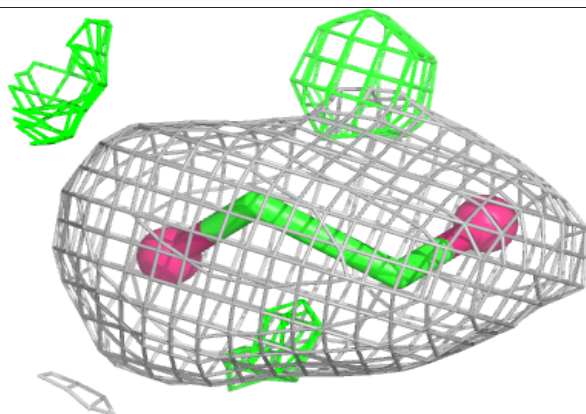
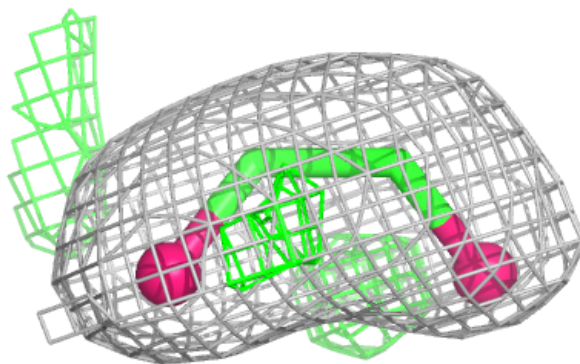
**Electron density around EDO D 516:**

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



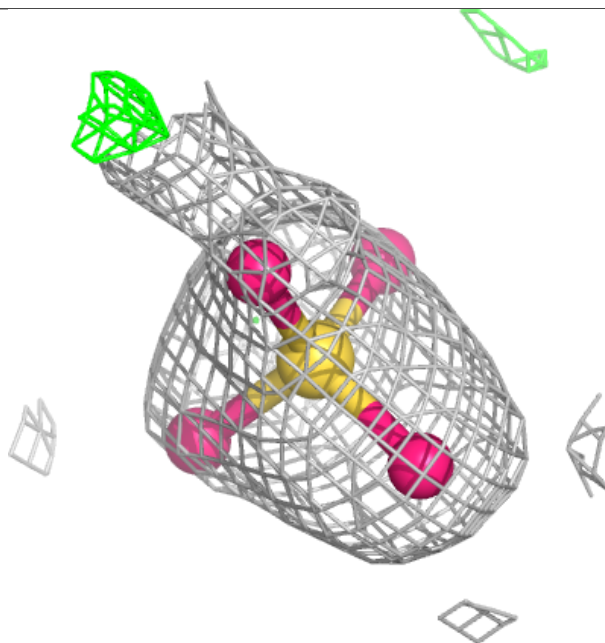
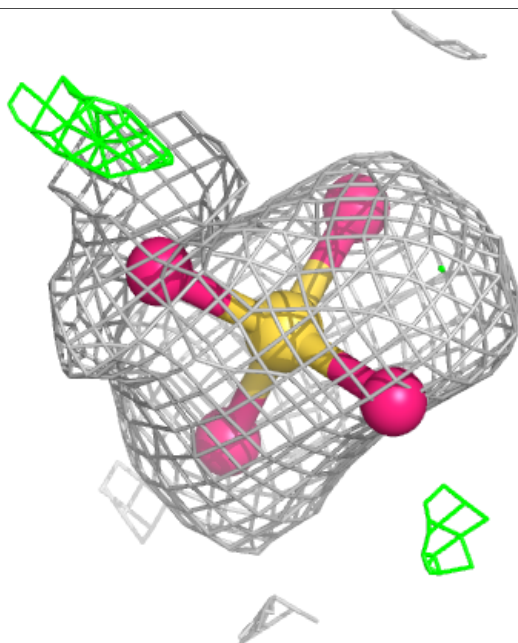
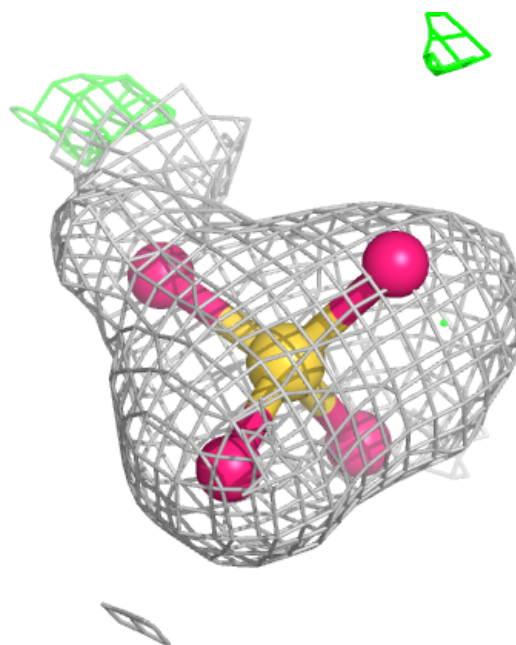
Electron density around EDO B 518:

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



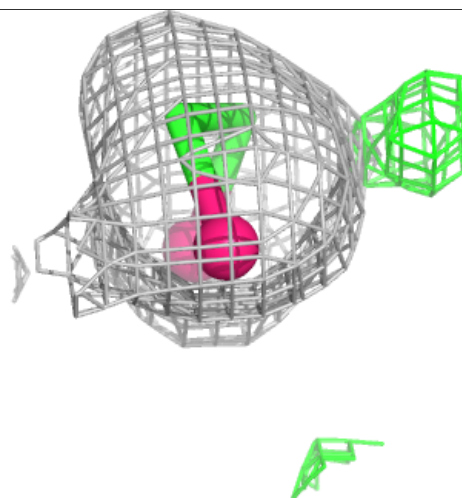
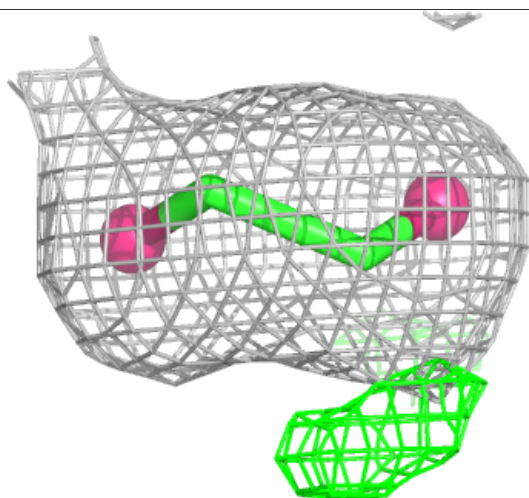
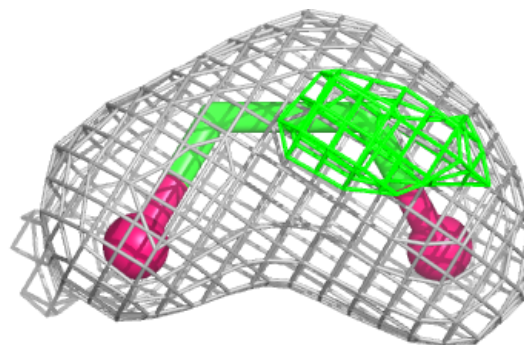
Electron density around SO4 C 514:

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



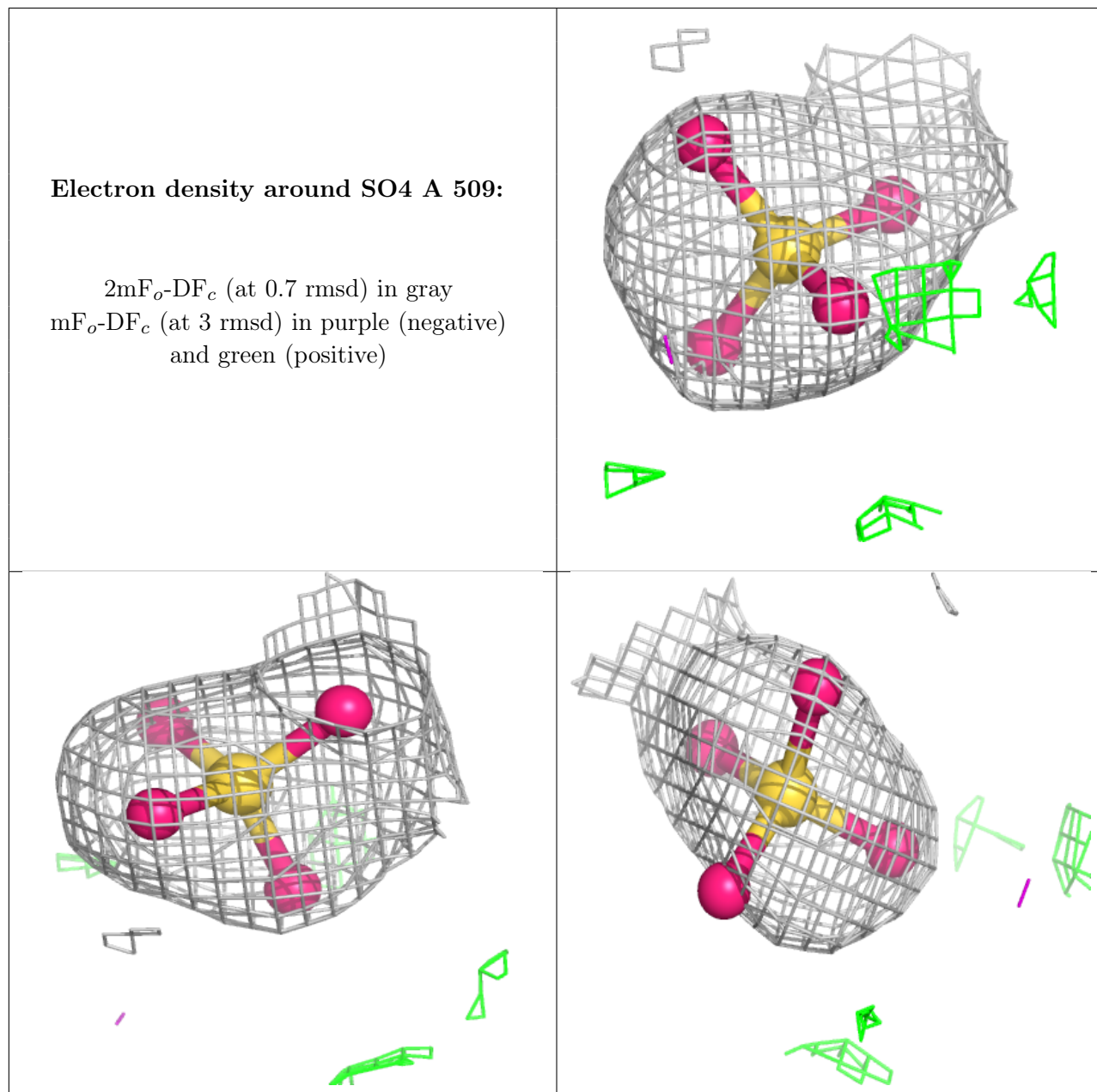
Electron density around EDO D 520:

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



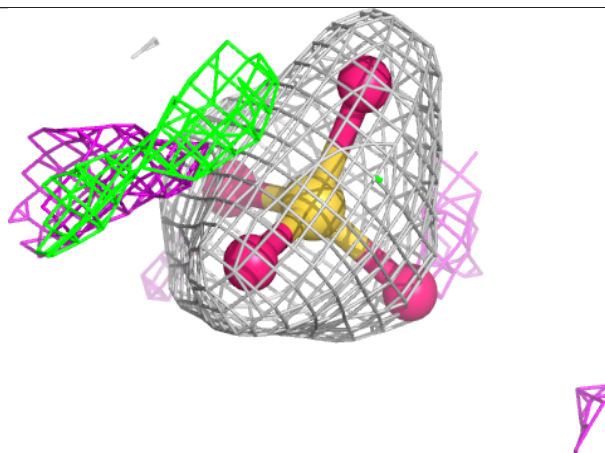
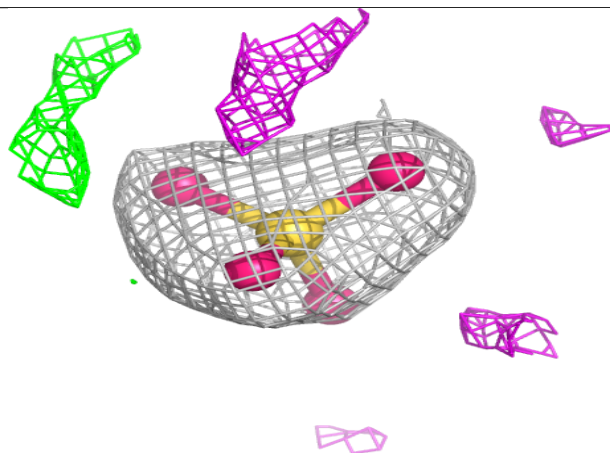
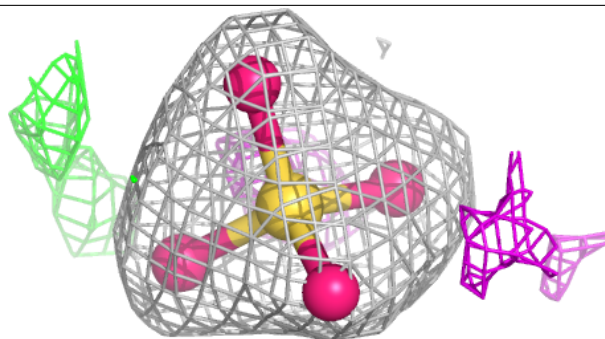
Electron density around SO4 A 509:

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



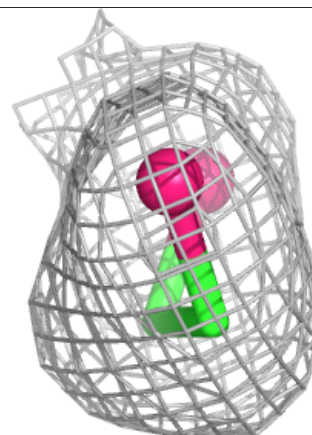
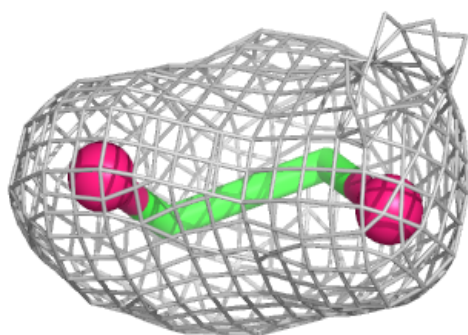
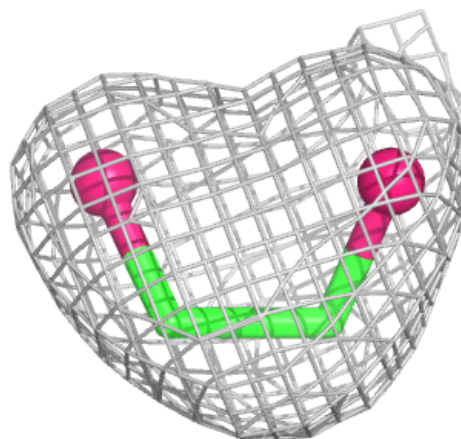
Electron density around SO4 A 508:

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

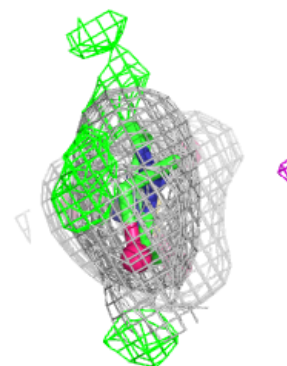
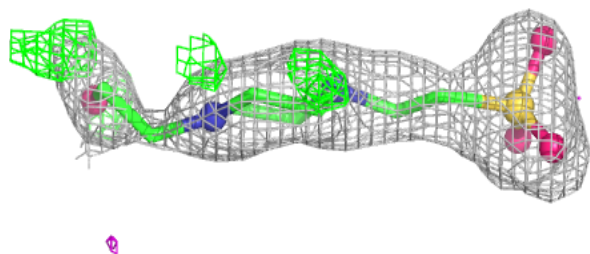
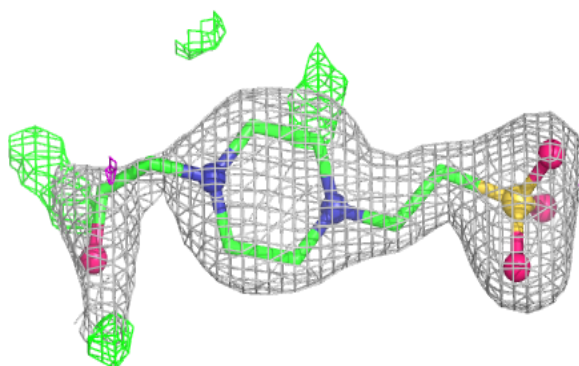


Electron density around EDO B 519:

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

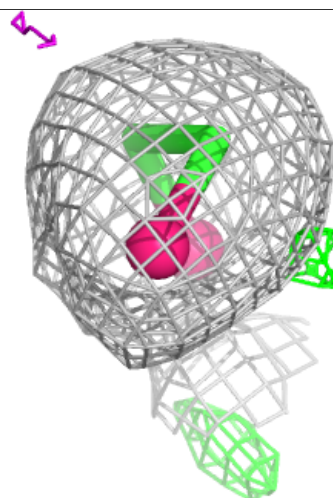
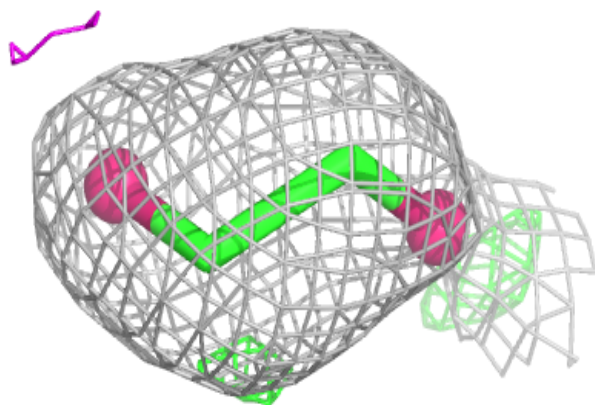
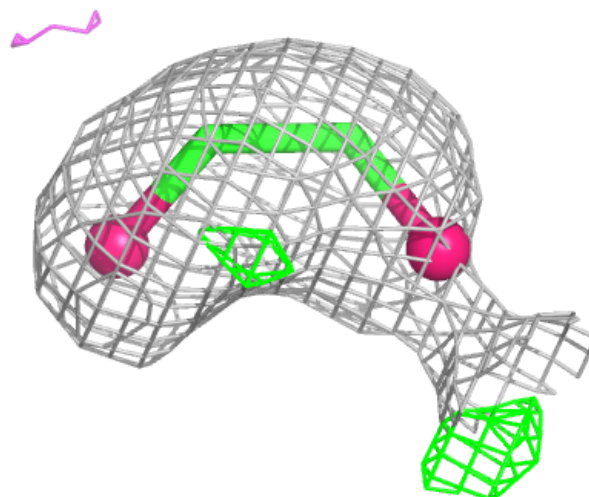
**Electron density around EPE B 513:**

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



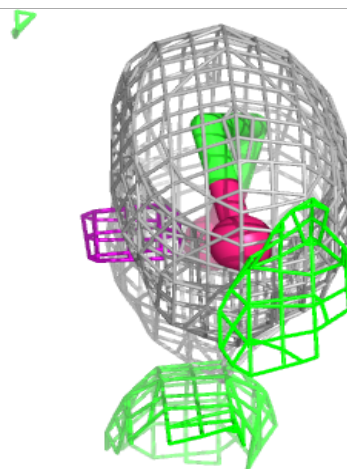
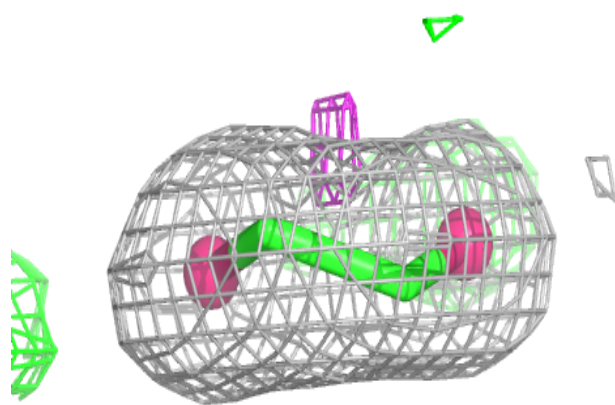
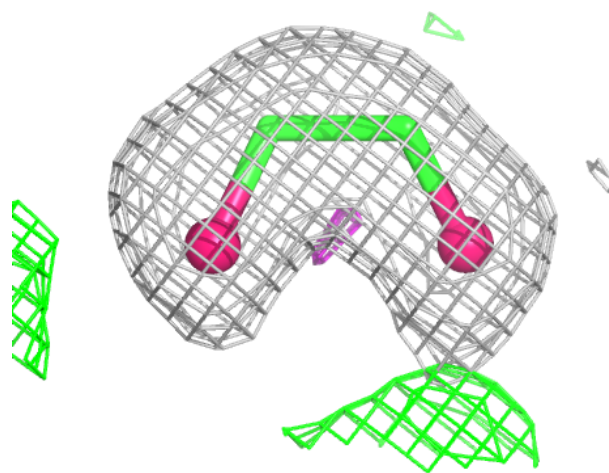
Electron density around EDO A 511:

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



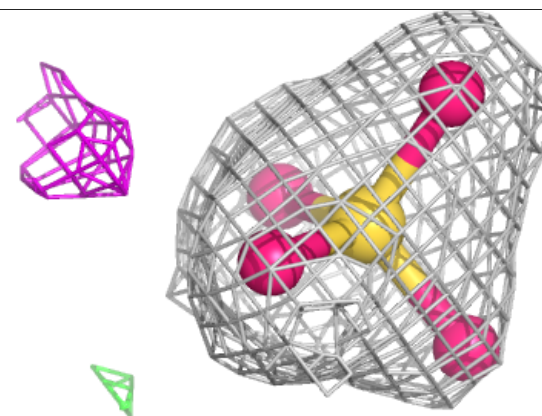
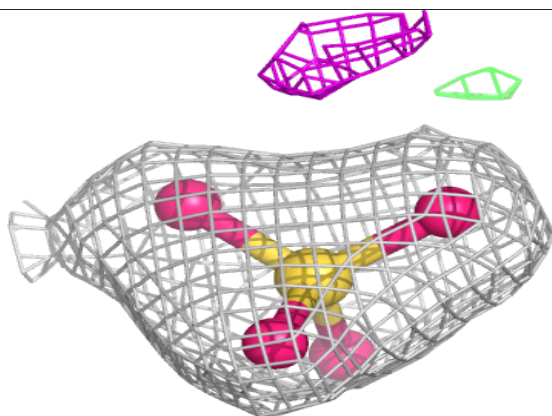
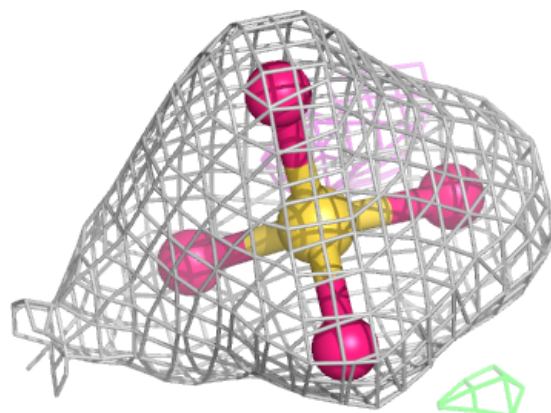
Electron density around EDO A 530:

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

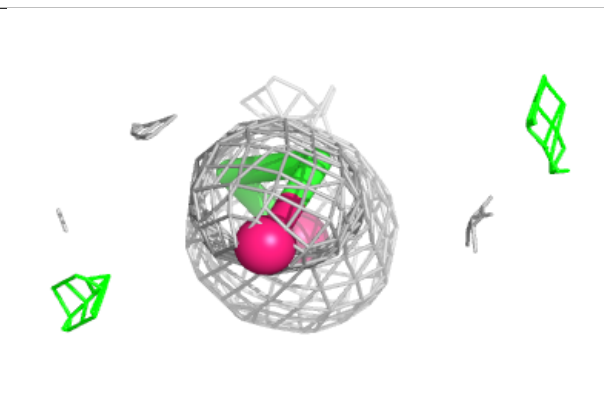
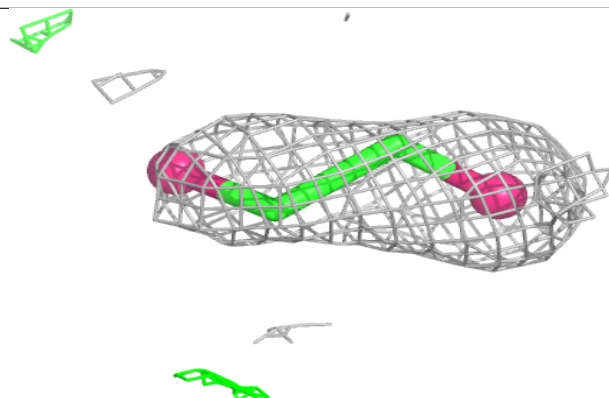
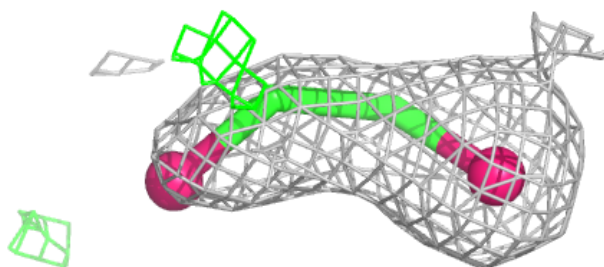


Electron density around SO4 C 510:

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

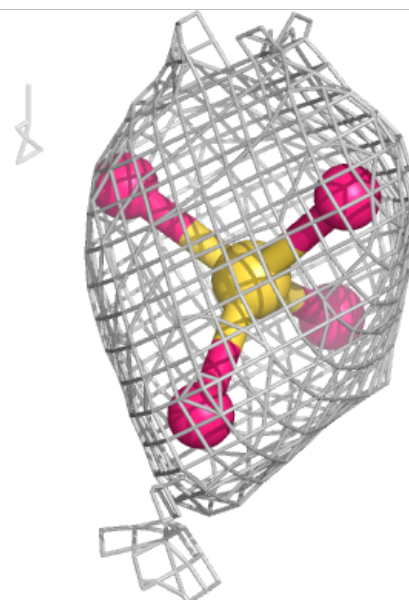
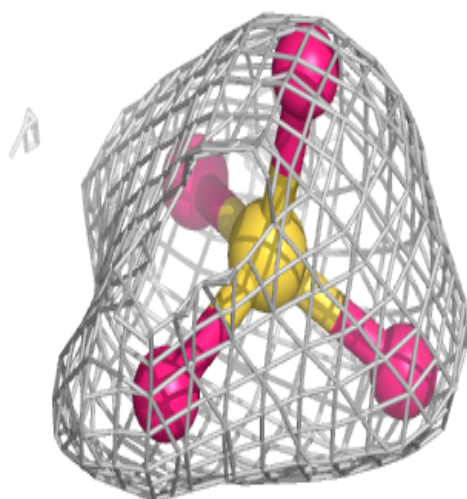
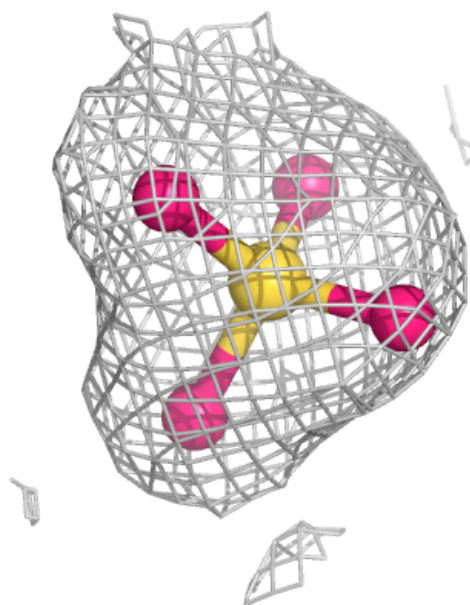
**Electron density around EDO C 531:**

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



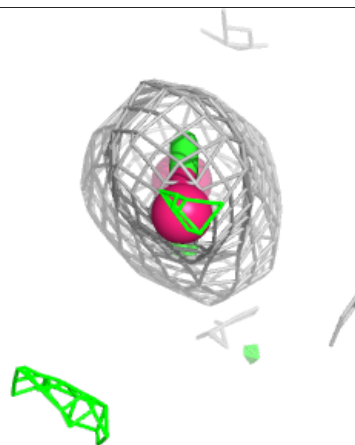
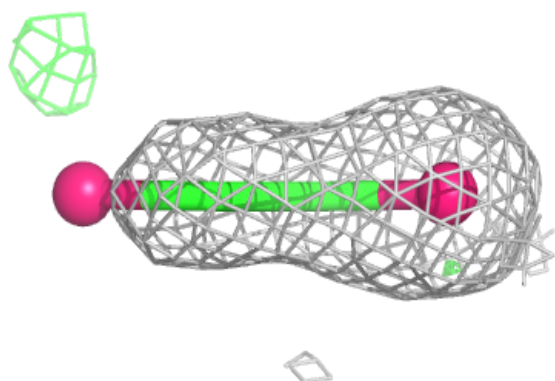
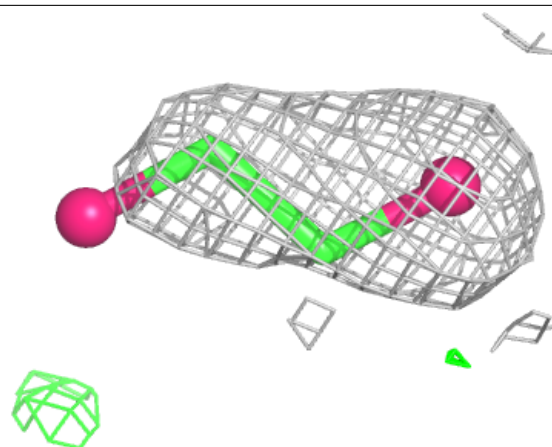
Electron density around SO4 A 507:

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



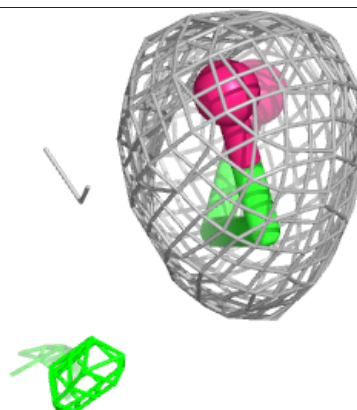
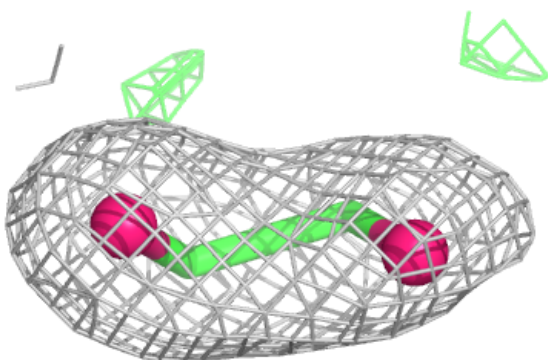
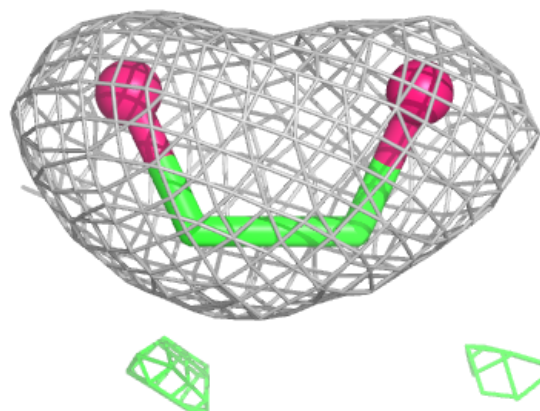
Electron density around EDO D 501:

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

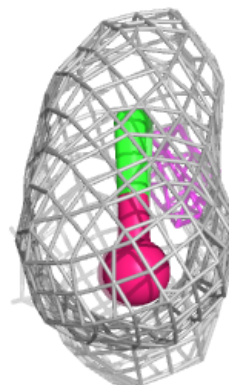
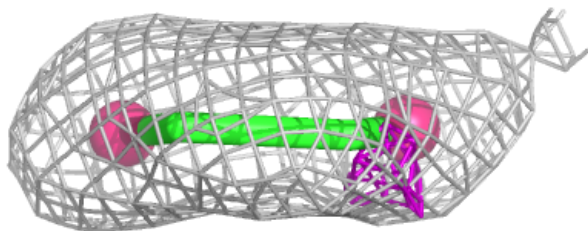
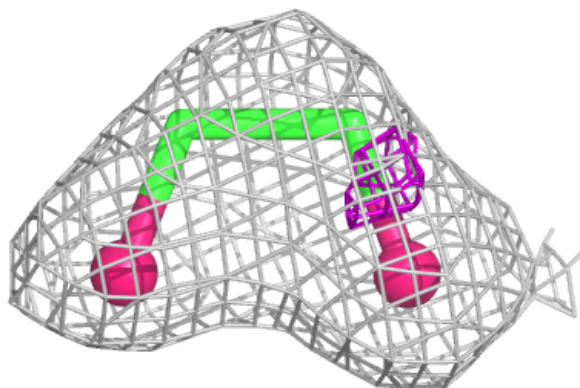


Electron density around EDO A 515:

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

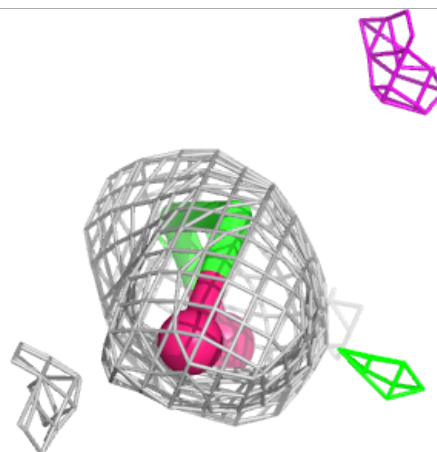
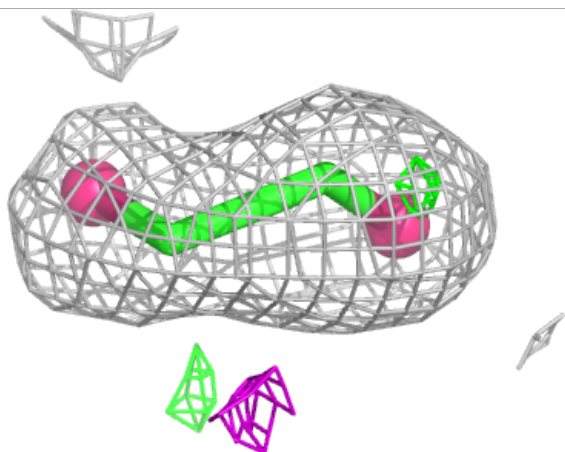
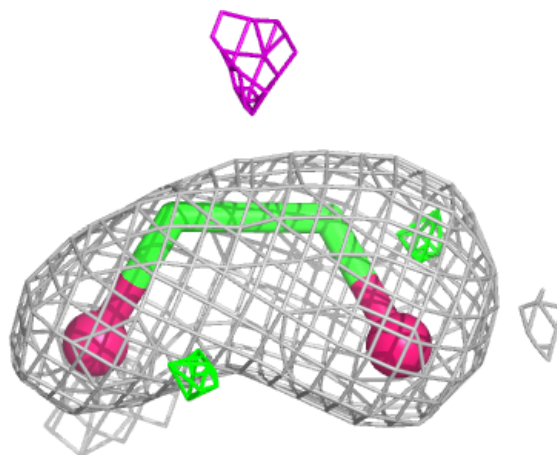
**Electron density around EDO D 528:**

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

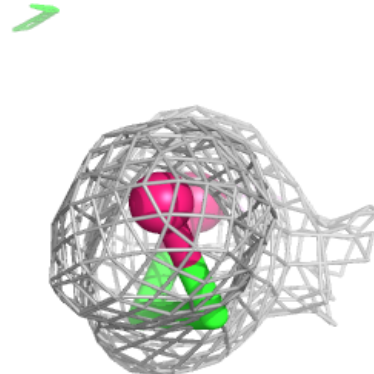
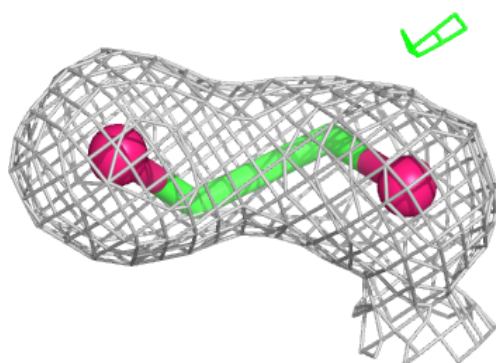
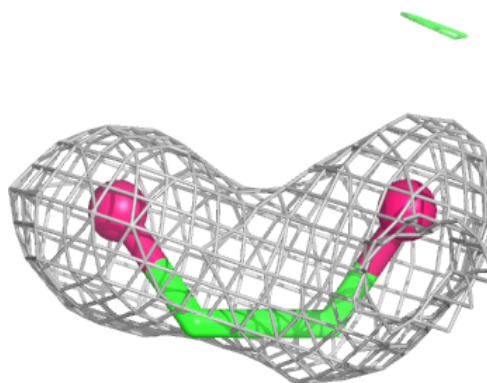


Electron density around EDO A 531:

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

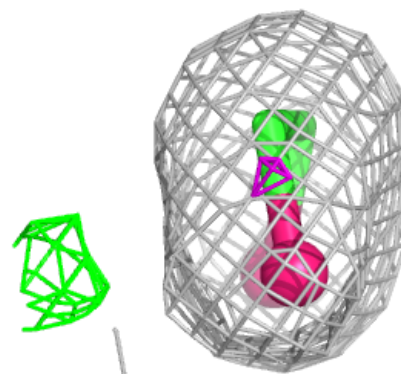
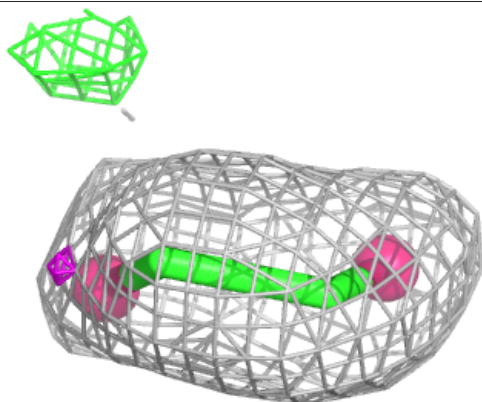
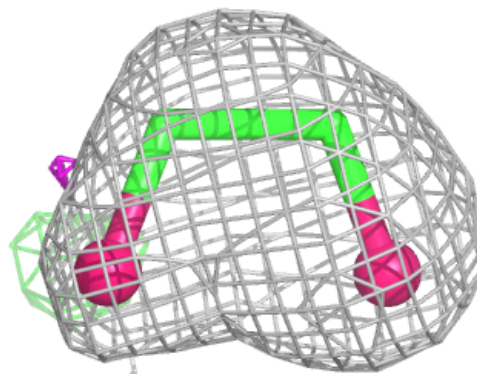
**Electron density around EDO B 514:**

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



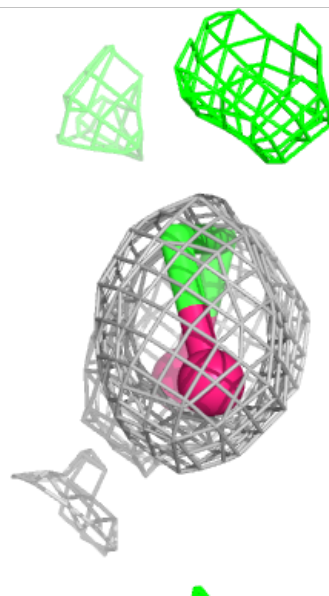
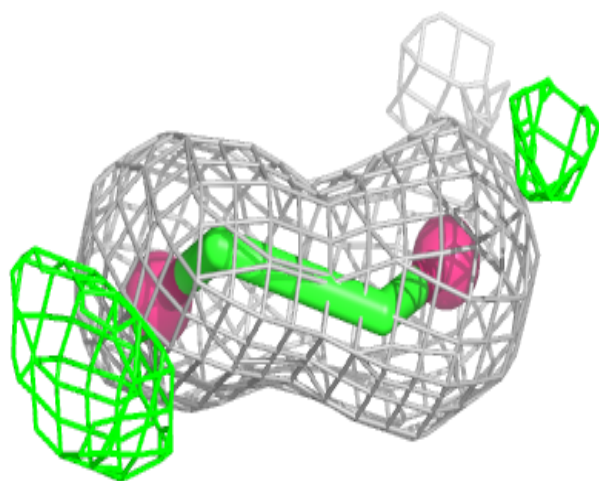
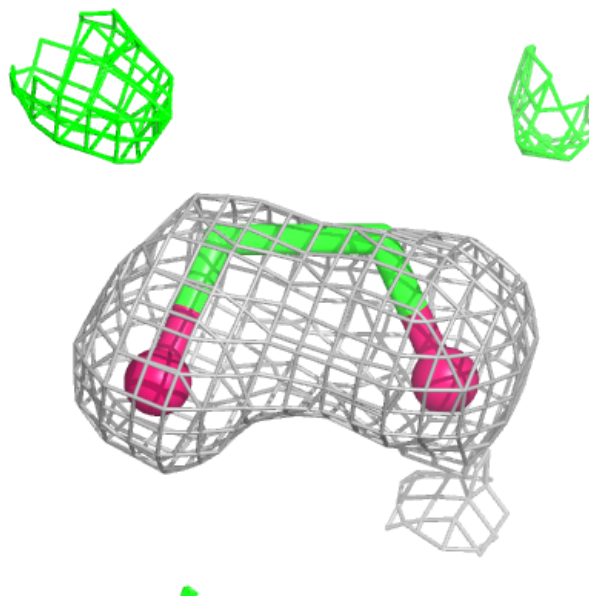
Electron density around EDO D 518:

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



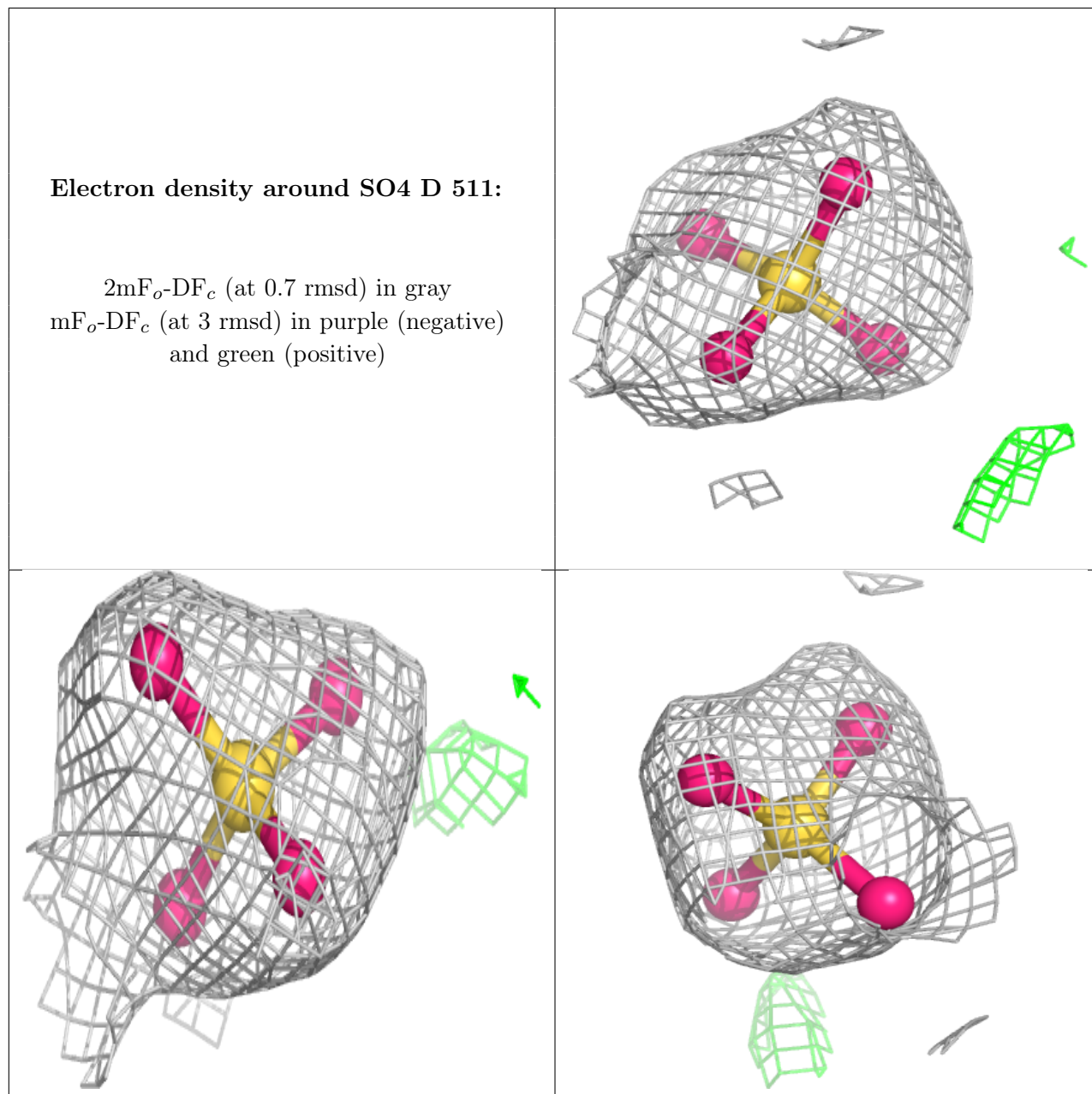
Electron density around EDO C 526:

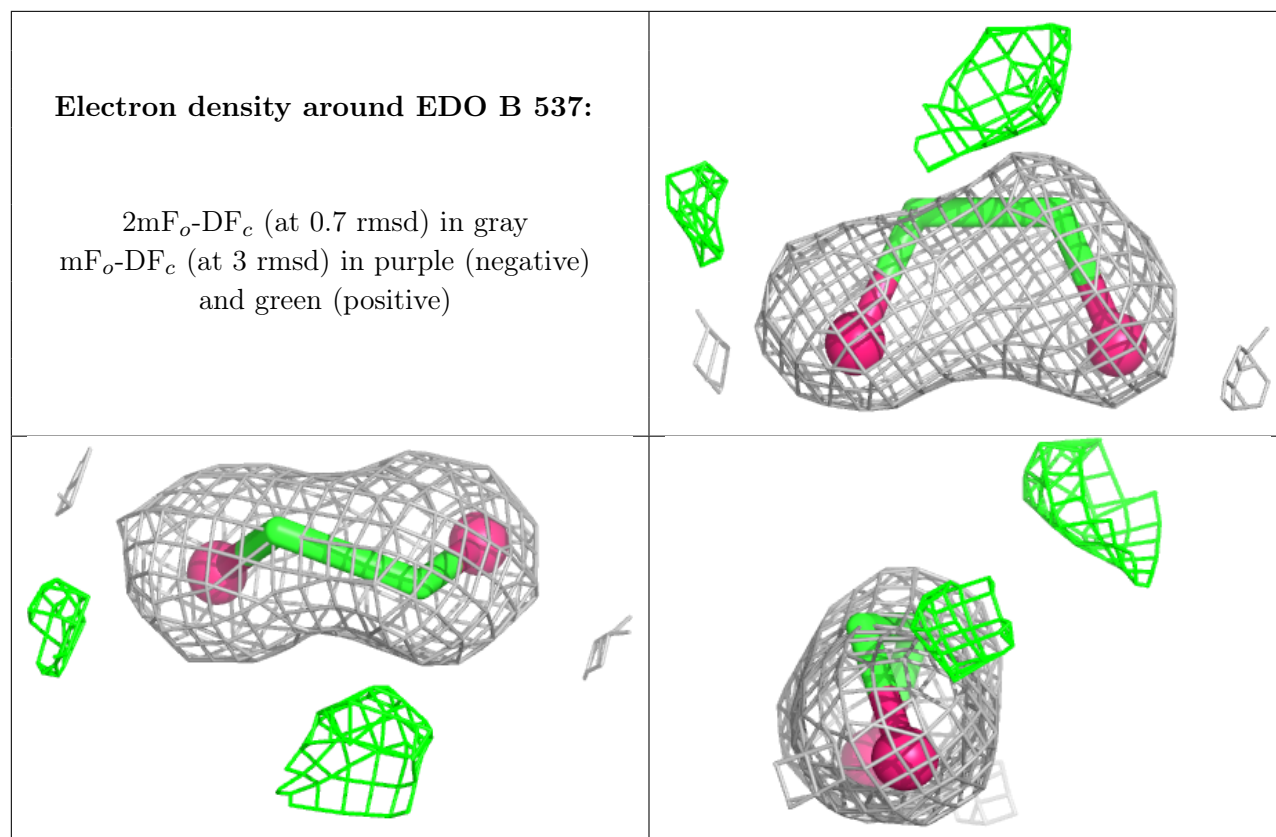
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around SO4 D 511:

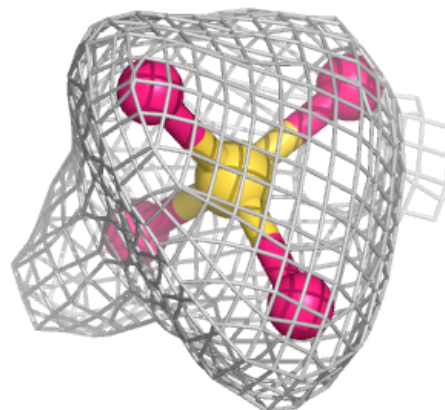
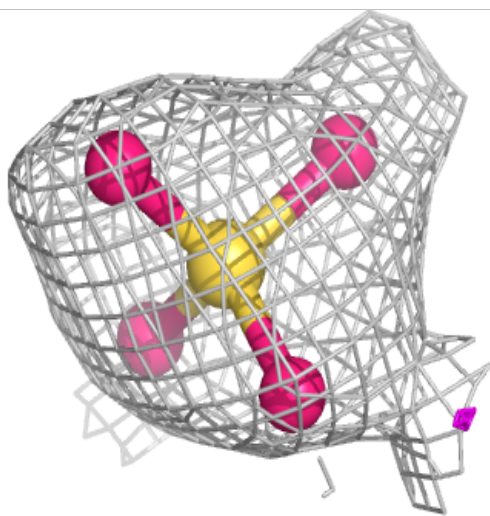
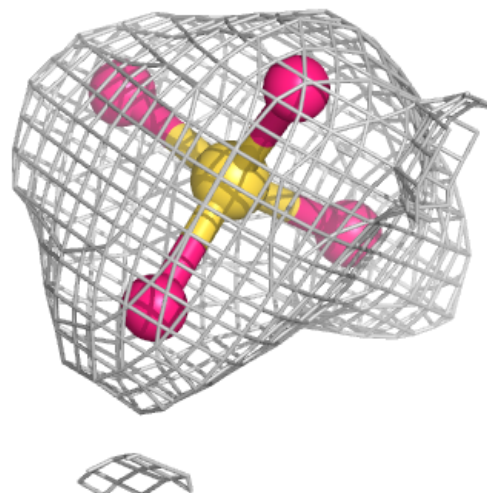
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





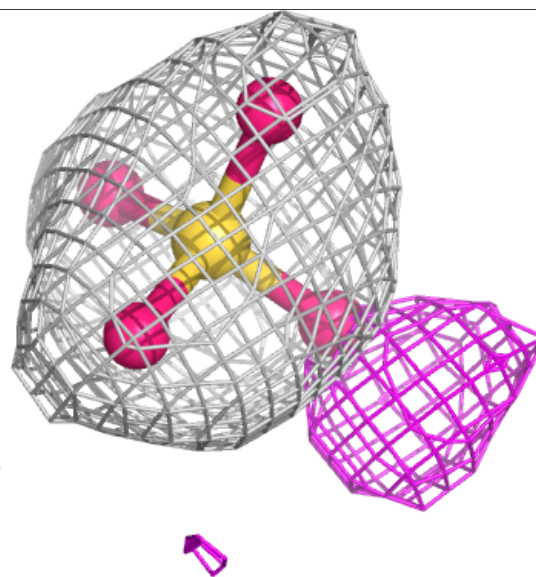
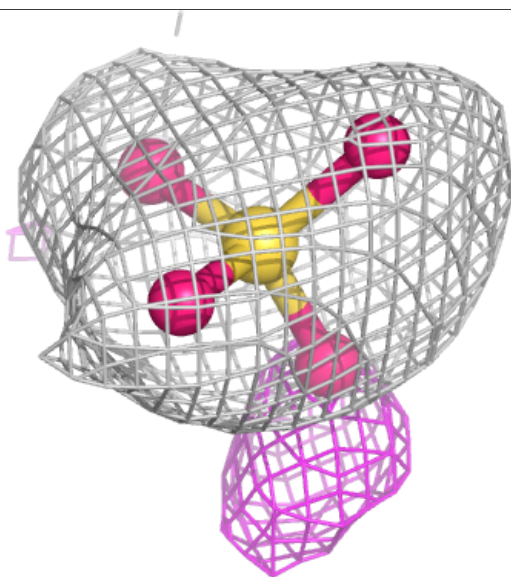
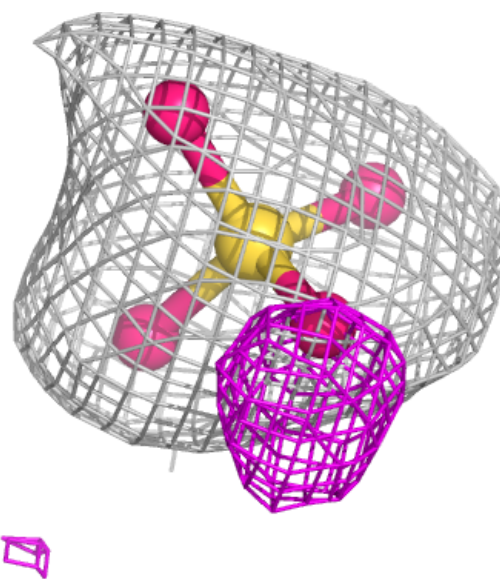
Electron density around SO4 B 508:

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



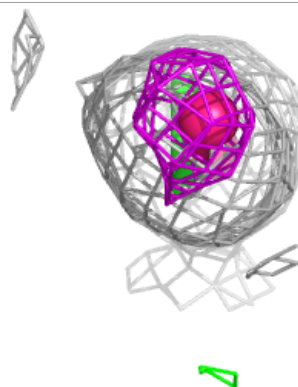
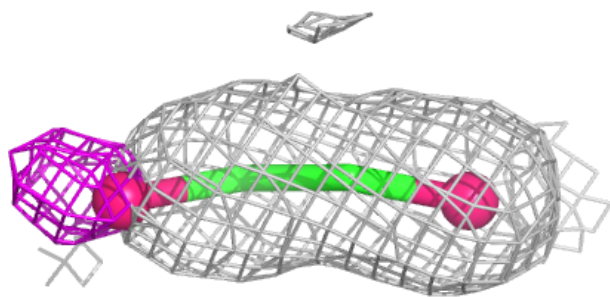
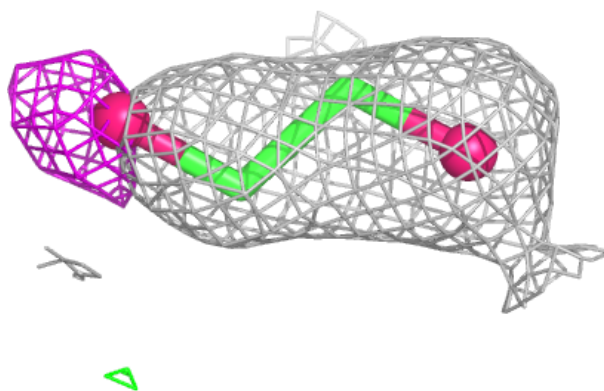
Electron density around SO4 B 540:

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



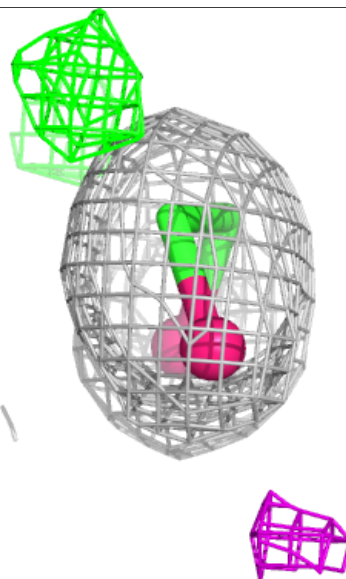
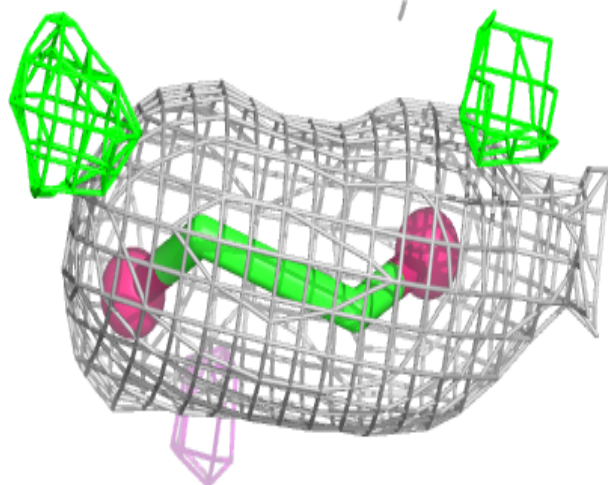
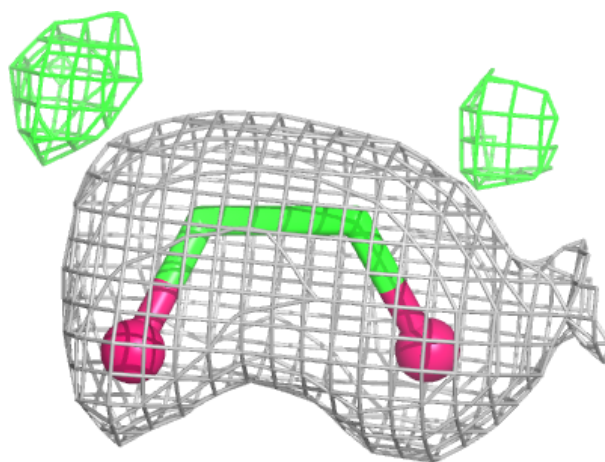
Electron density around EDO A 538:

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



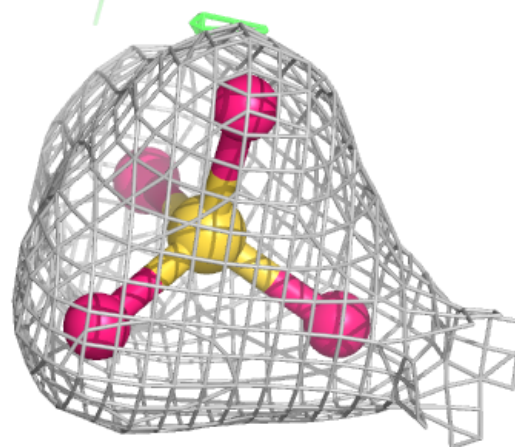
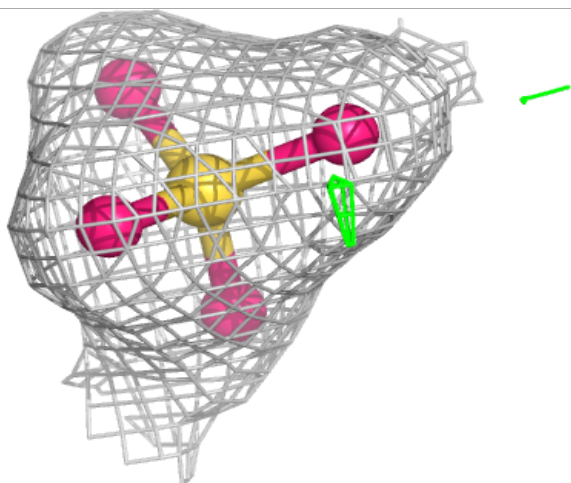
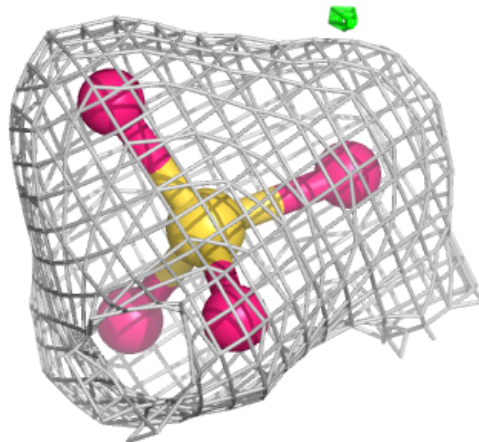
Electron density around EDO D 515:

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



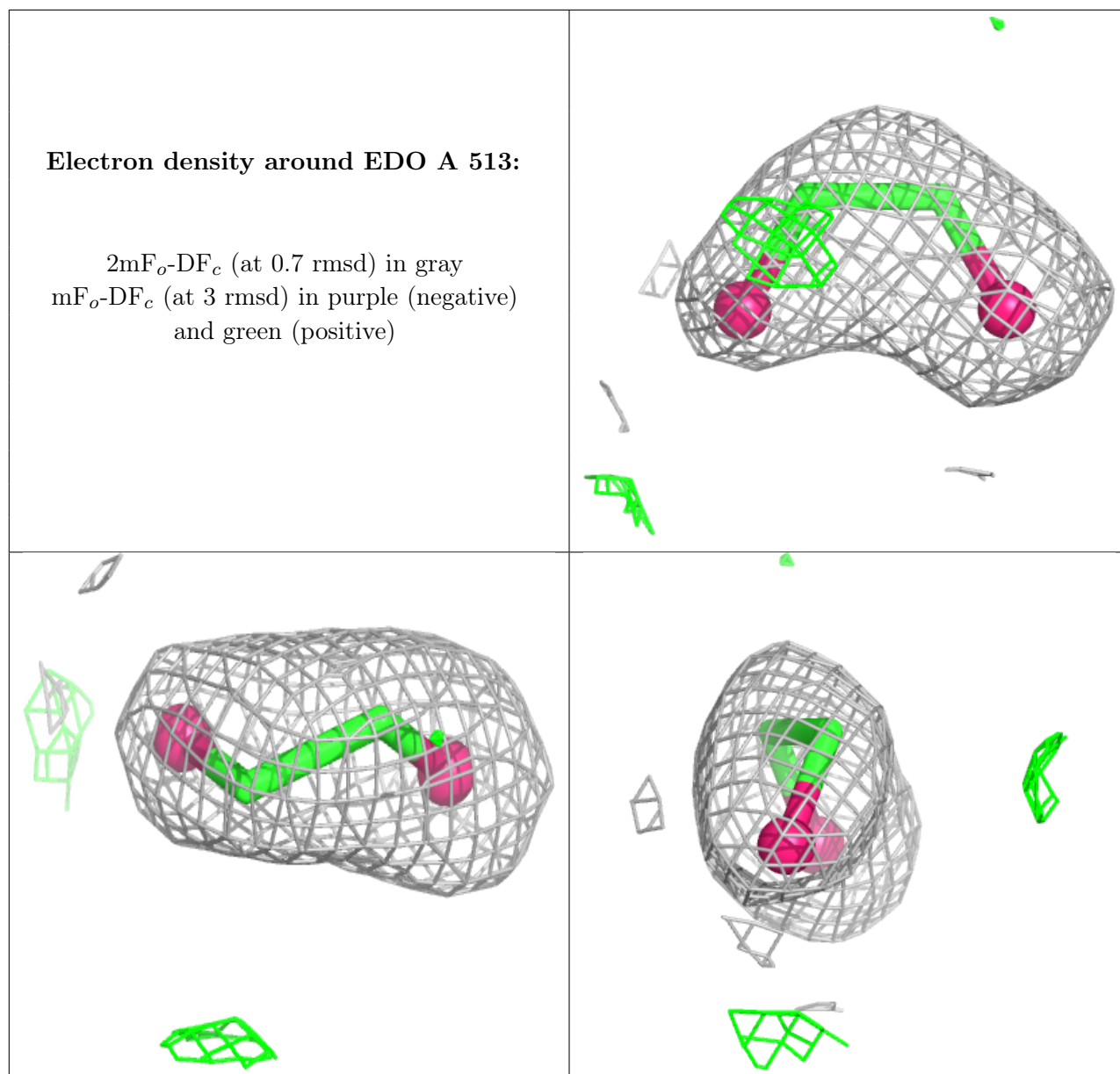
Electron density around SO4 C 508:

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



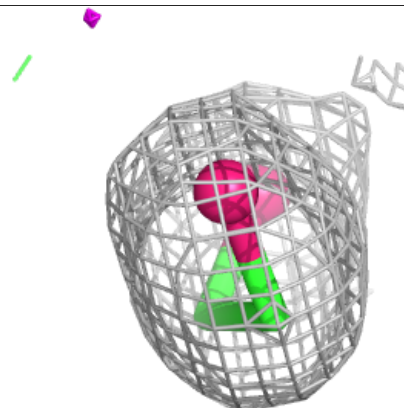
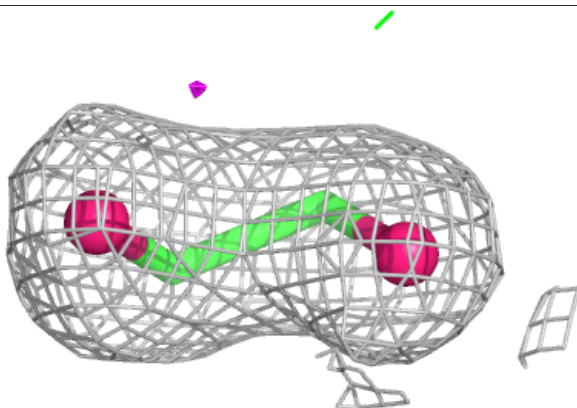
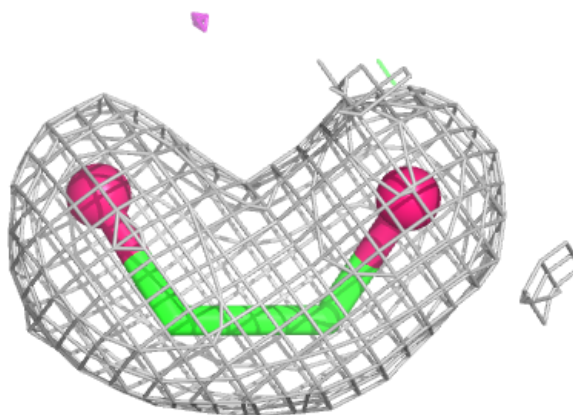
Electron density around EDO A 513:

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



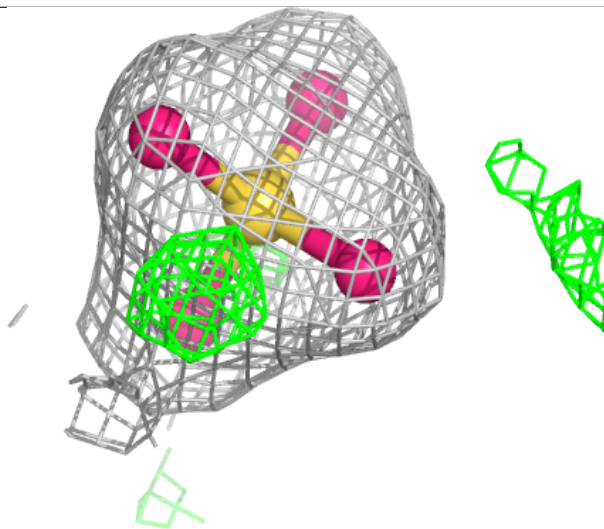
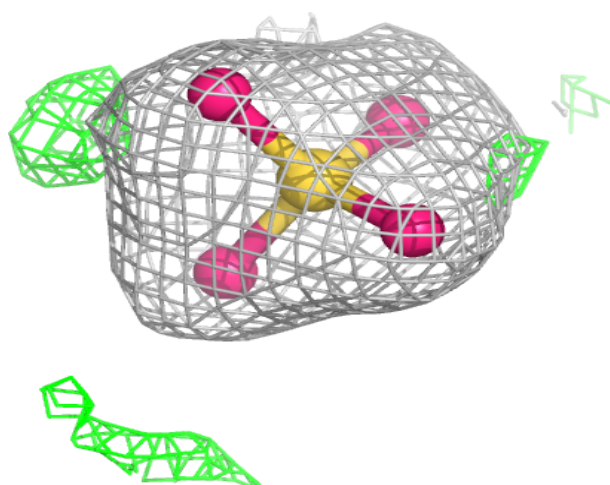
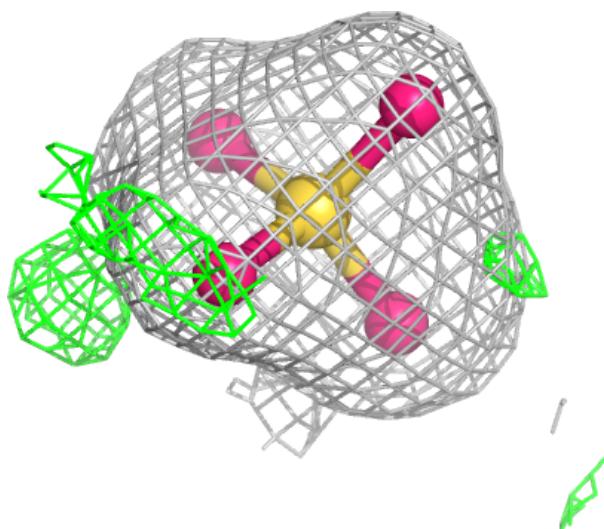
Electron density around EDO D 504:

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



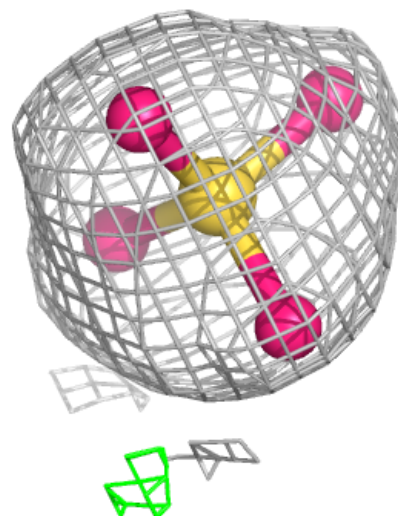
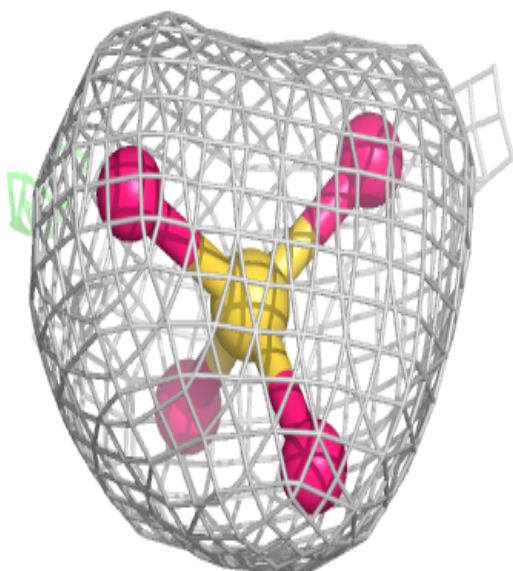
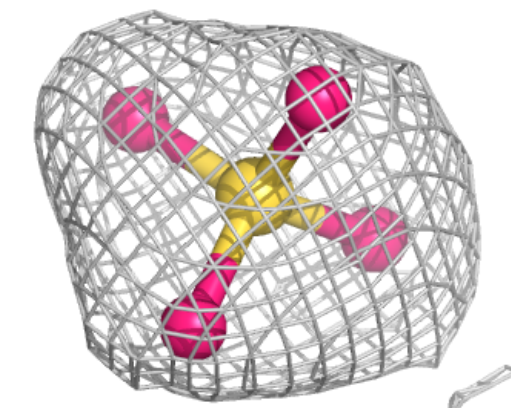
Electron density around SO4 A 506:

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



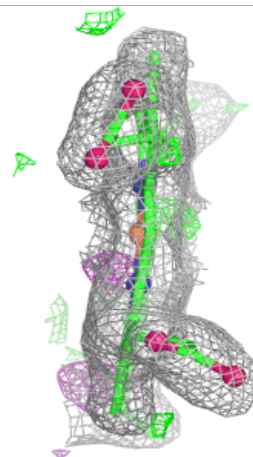
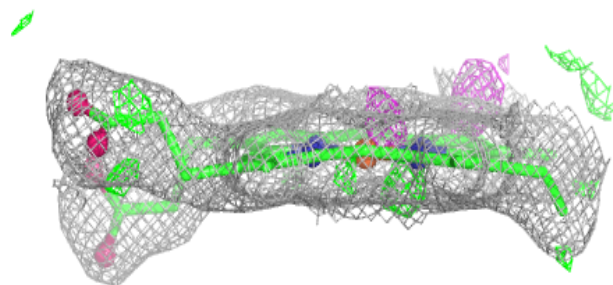
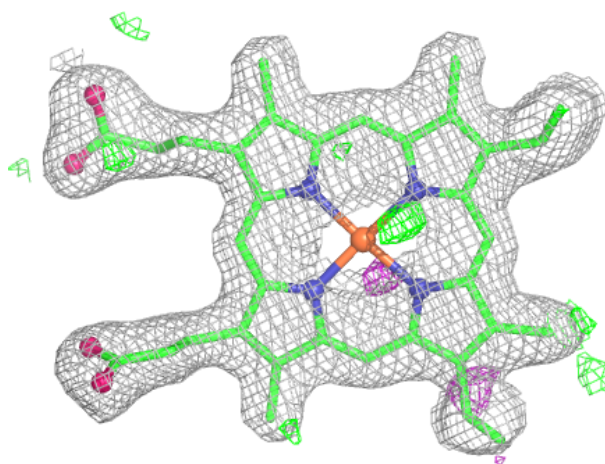
Electron density around SO4 C 501:

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



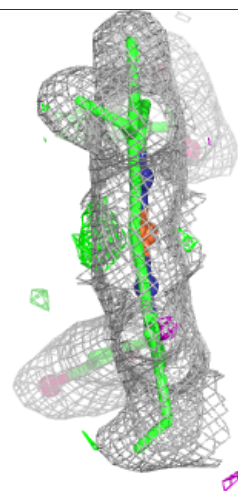
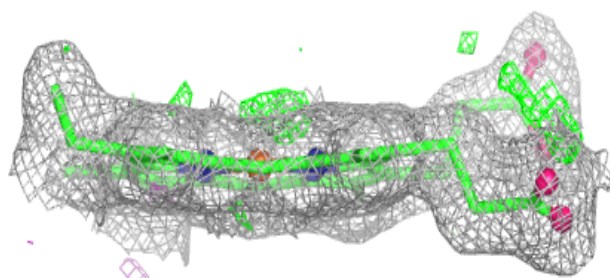
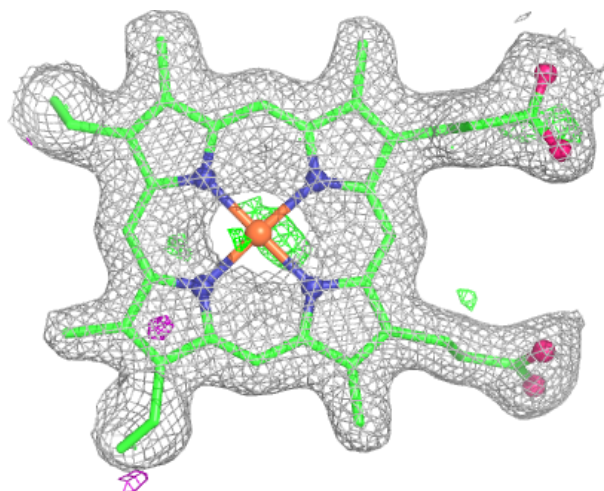
Electron density around HEC C 503:

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



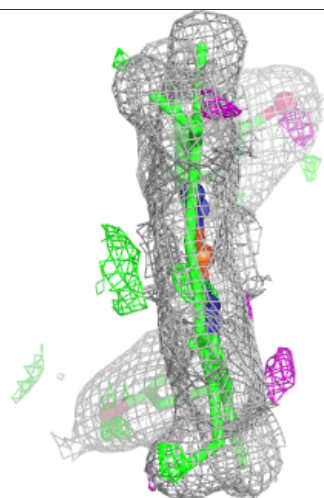
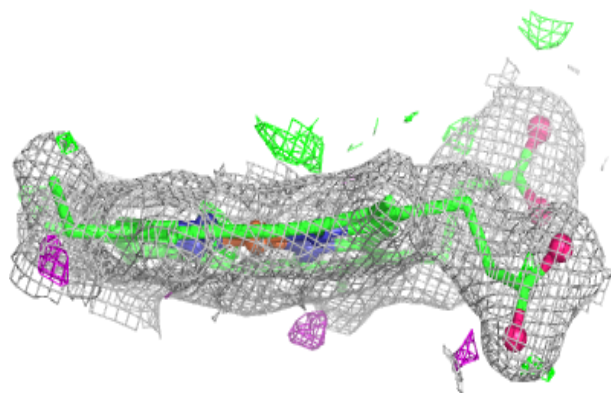
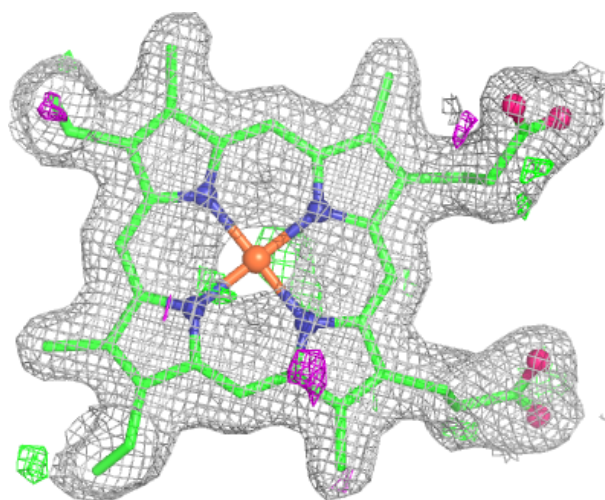
Electron density around HEC D 505:

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



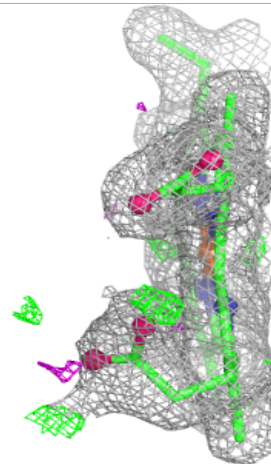
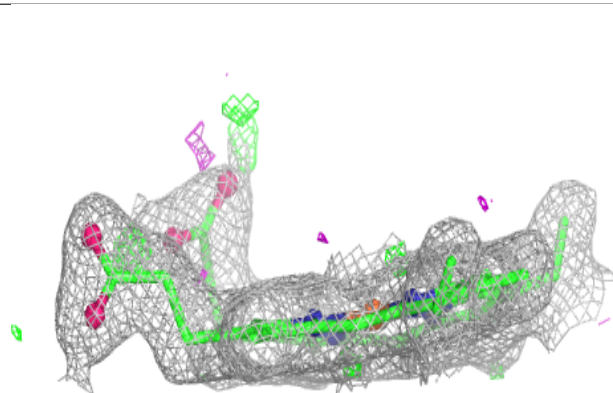
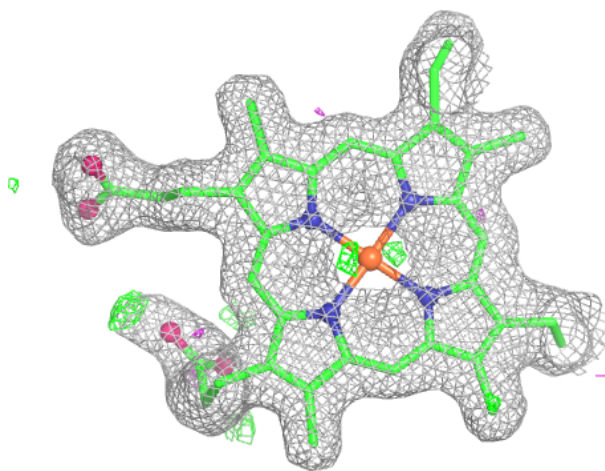
Electron density around HEC D 506:

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



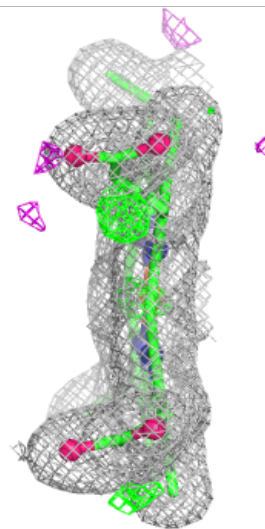
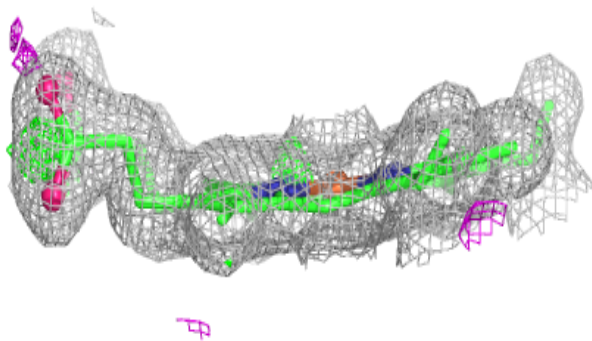
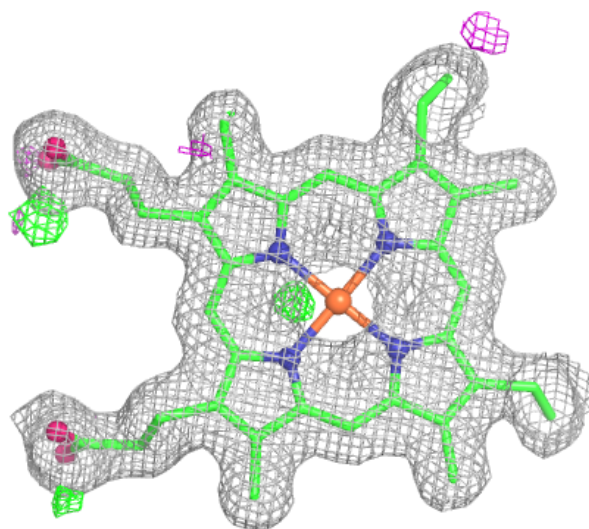
Electron density around HEC D 507:

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



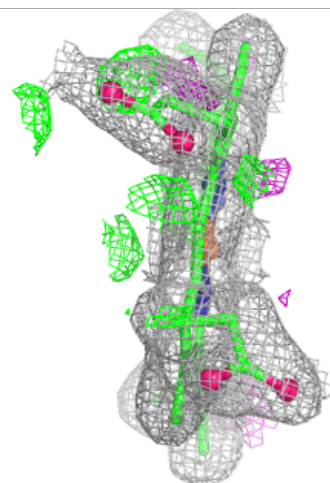
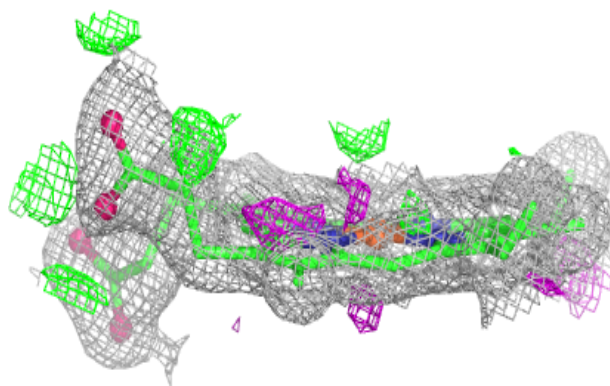
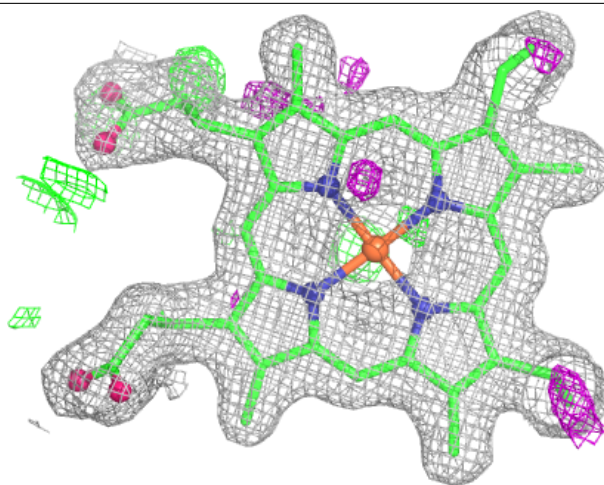
Electron density around HEC D 508:

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



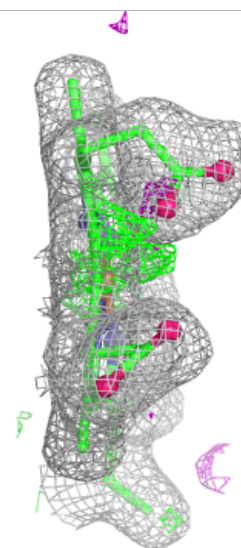
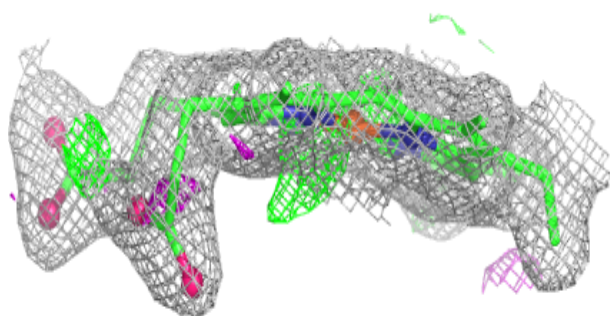
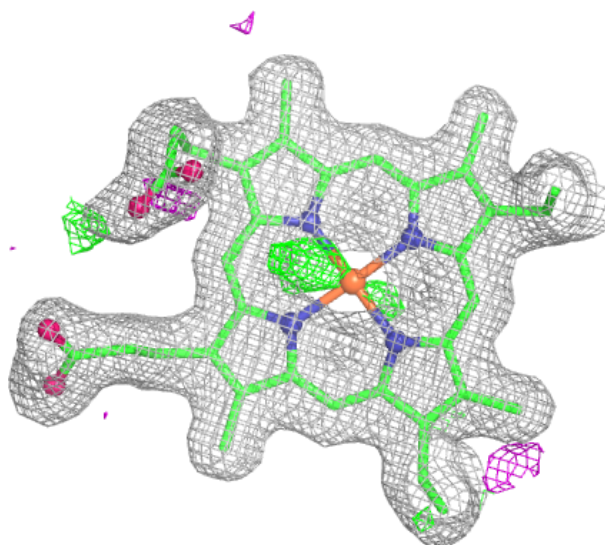
Electron density around HEC A 502:

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



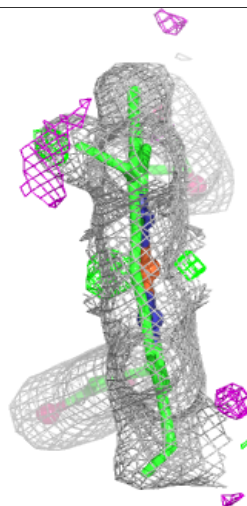
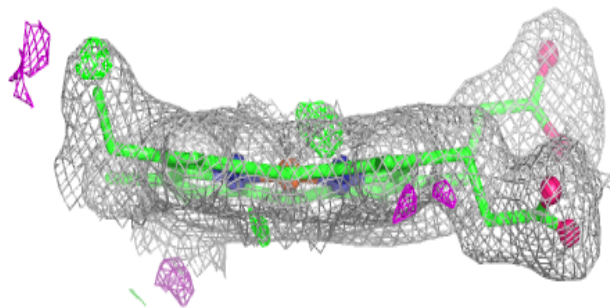
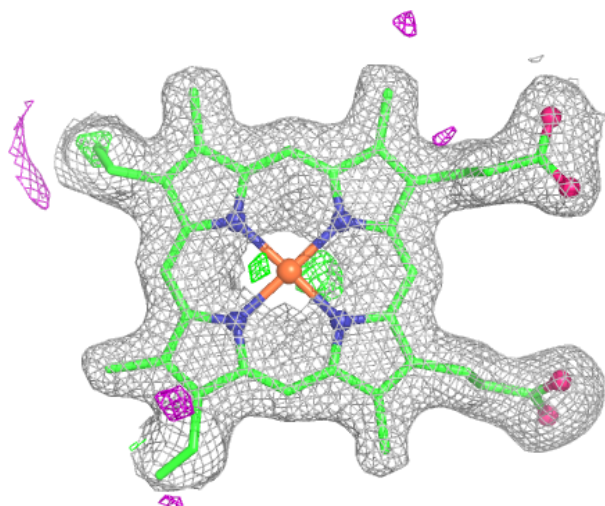
Electron density around HEC A 503:

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



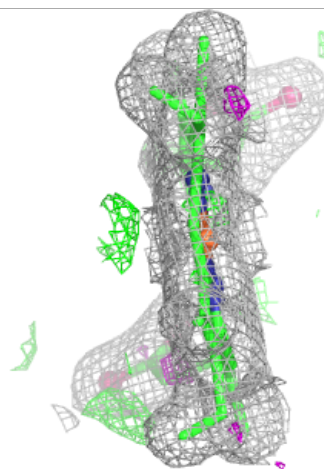
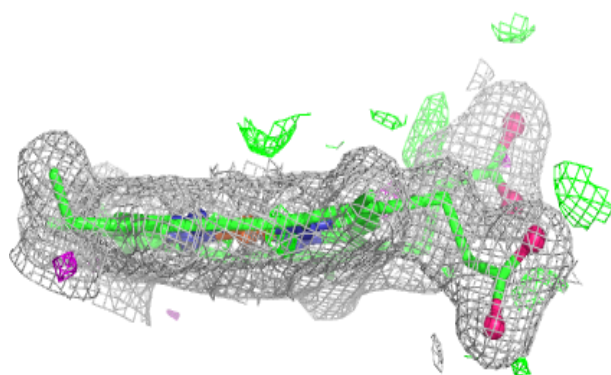
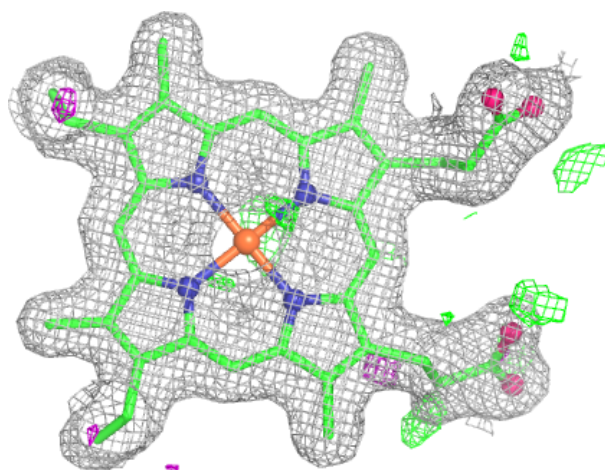
Electron density around HEC B 502:

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



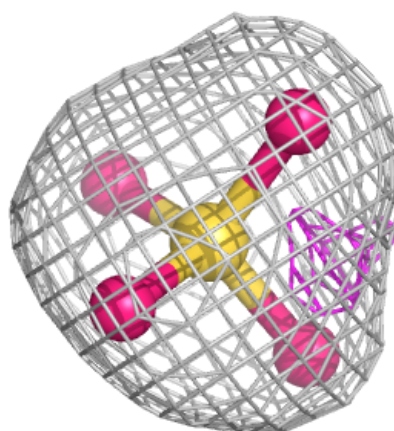
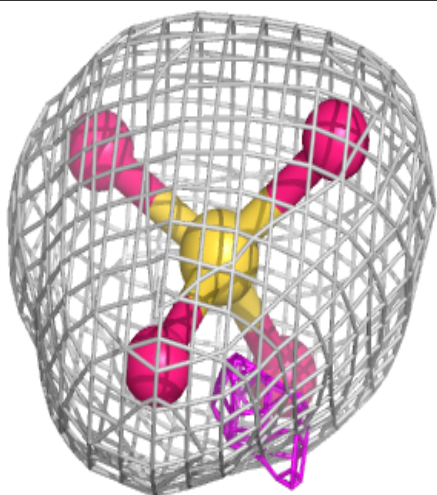
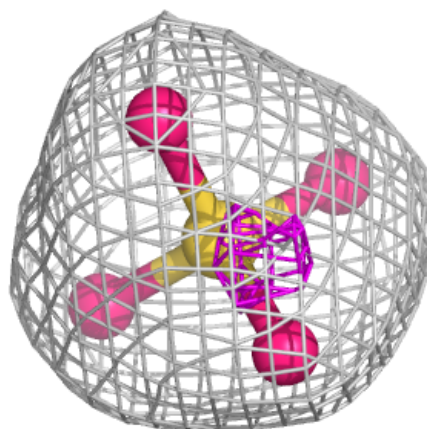
Electron density around HEC B 503:

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



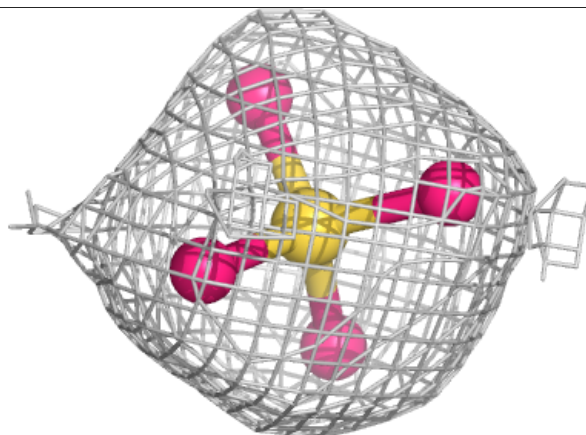
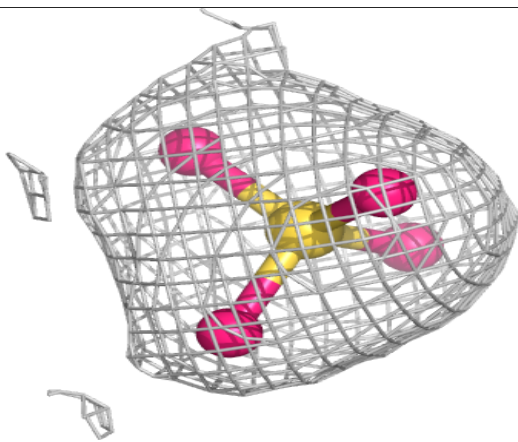
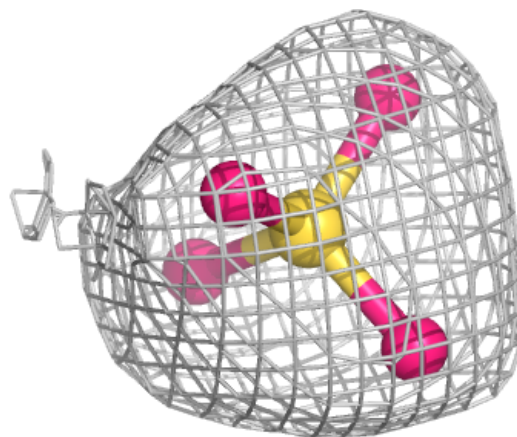
Electron density around SO4 A 533:

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



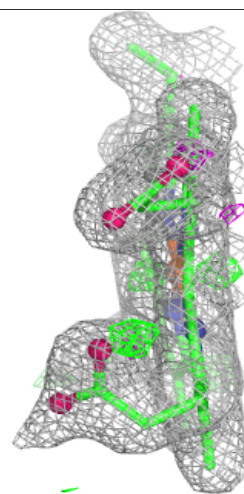
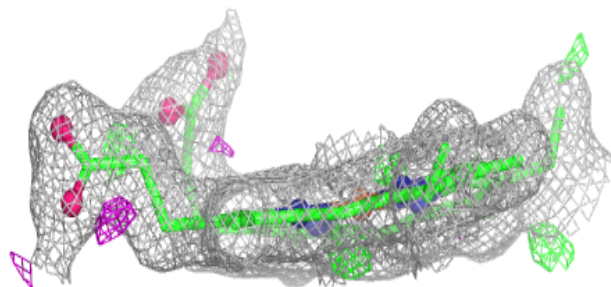
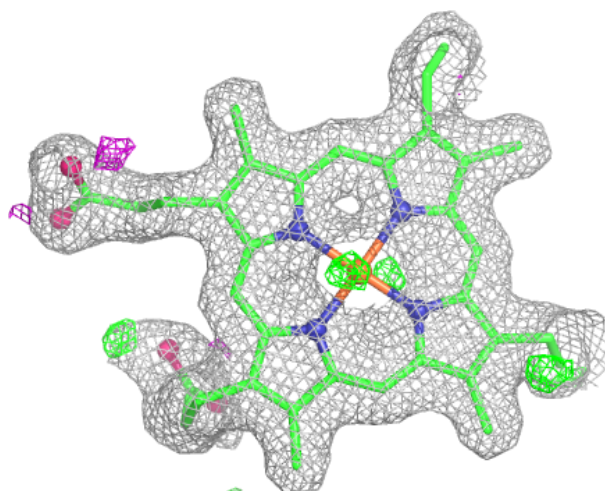
Electron density around SO4 D 502:

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



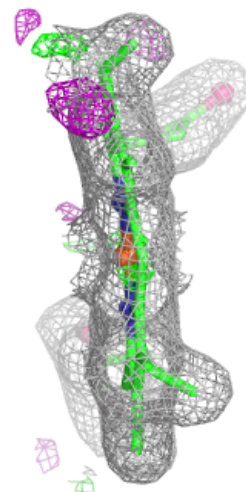
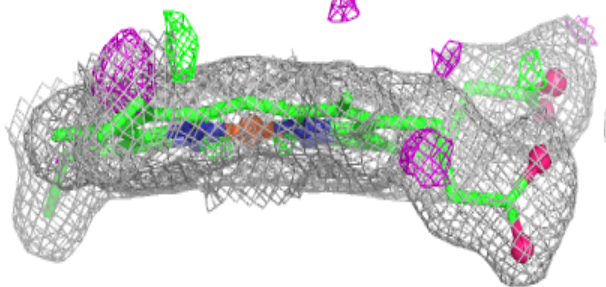
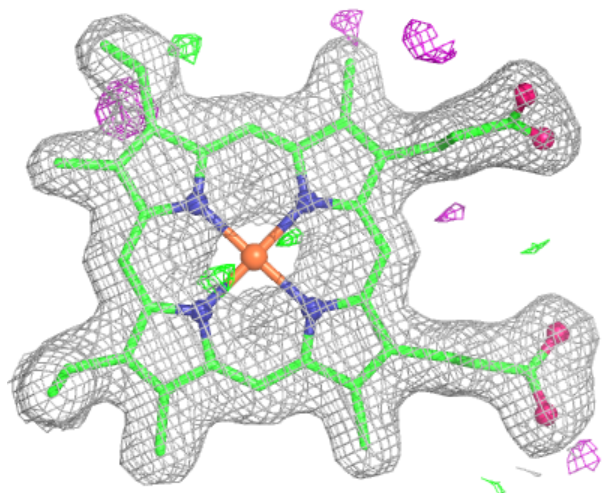
Electron density around HEC B 504:

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



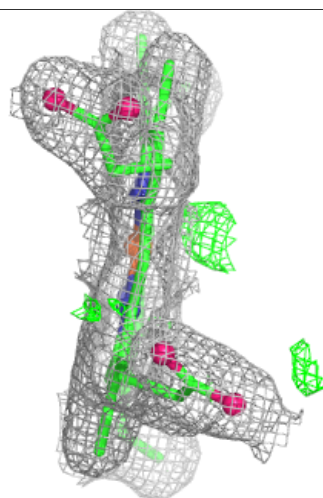
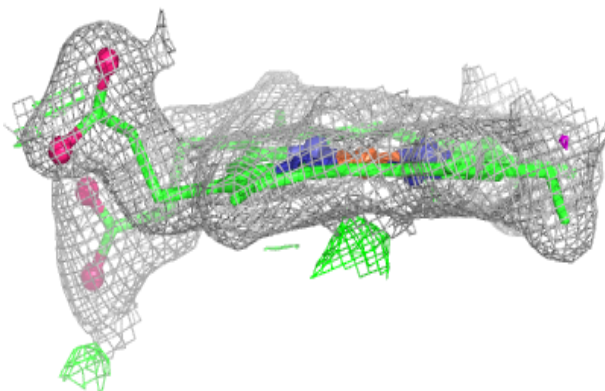
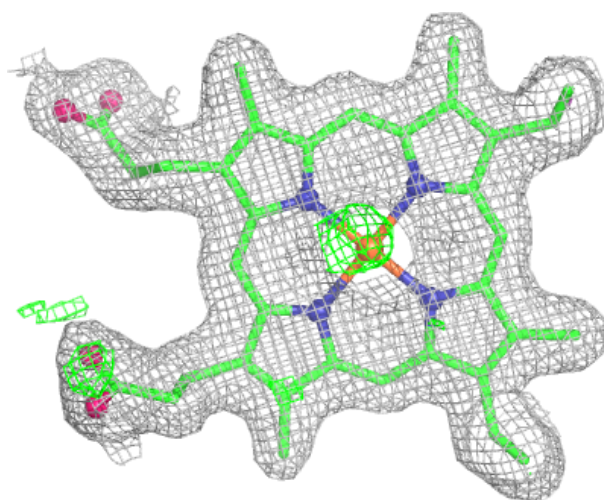
Electron density around HEC A 501:

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



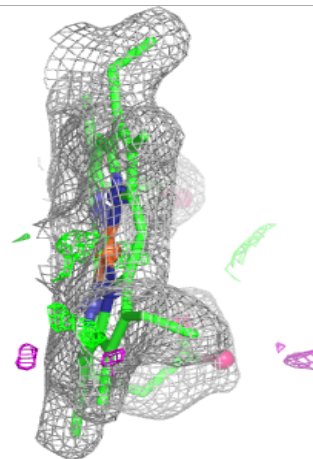
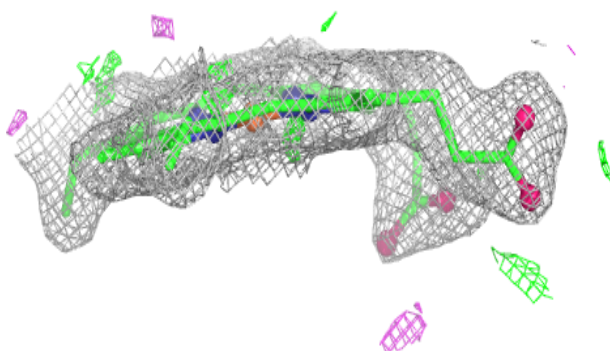
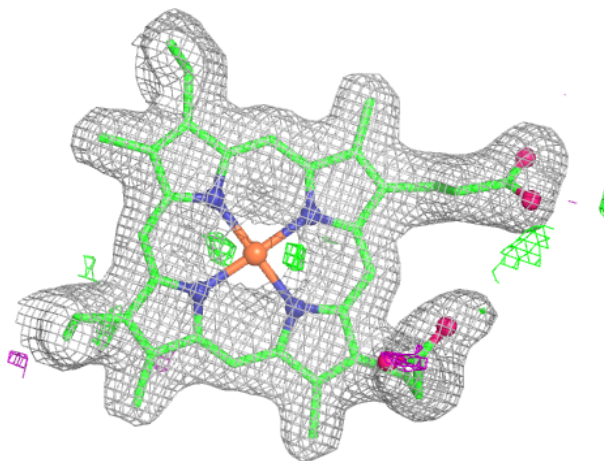
Electron density around HEC C 504:

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



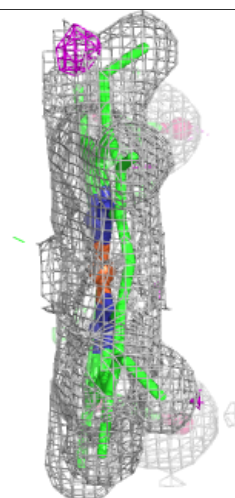
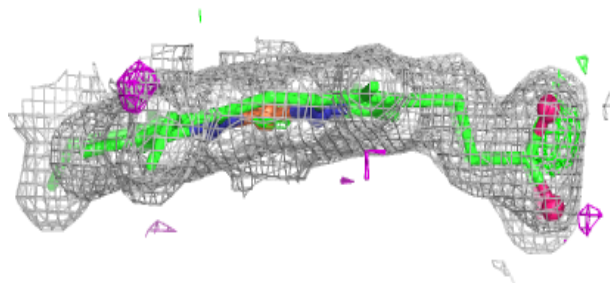
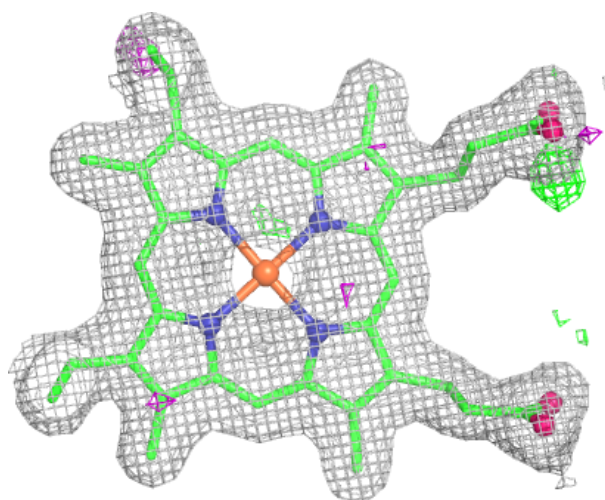
Electron density around HEC C 505:

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



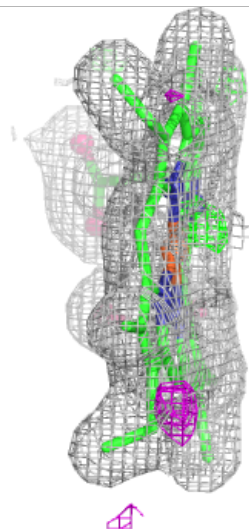
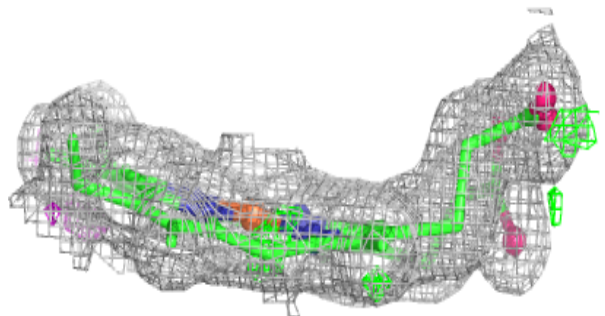
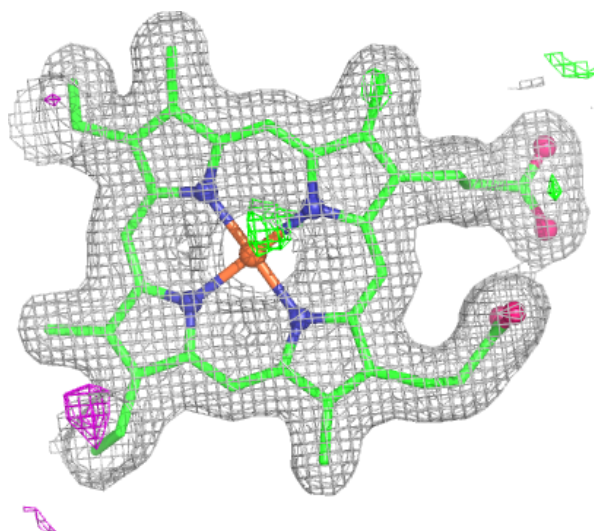
Electron density around HEC C 506:

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



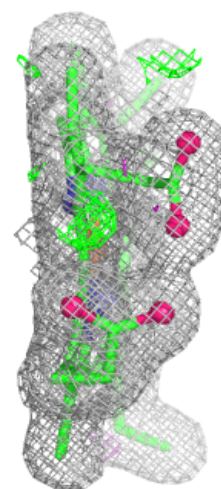
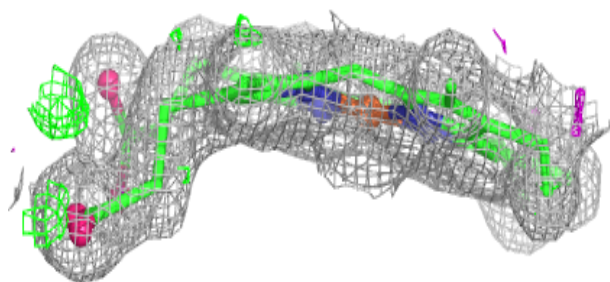
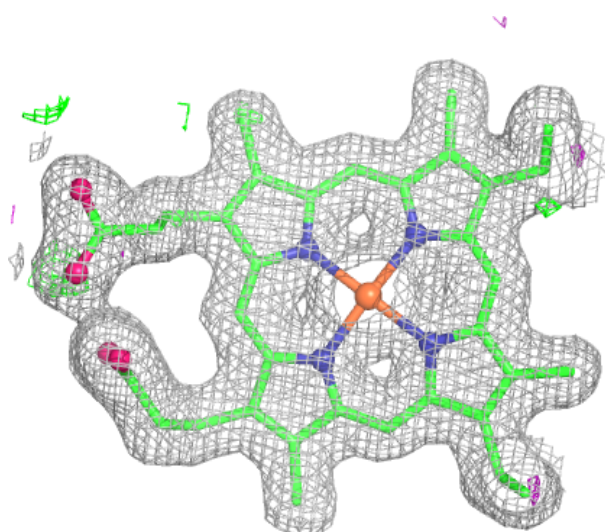
Electron density around HEC C 507:

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



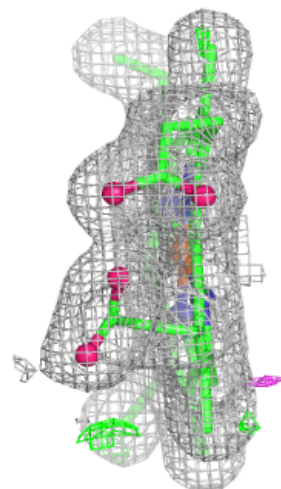
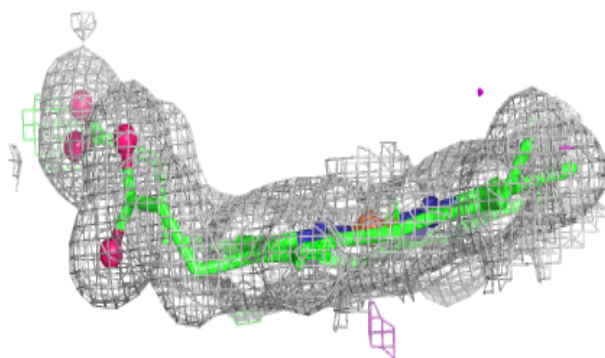
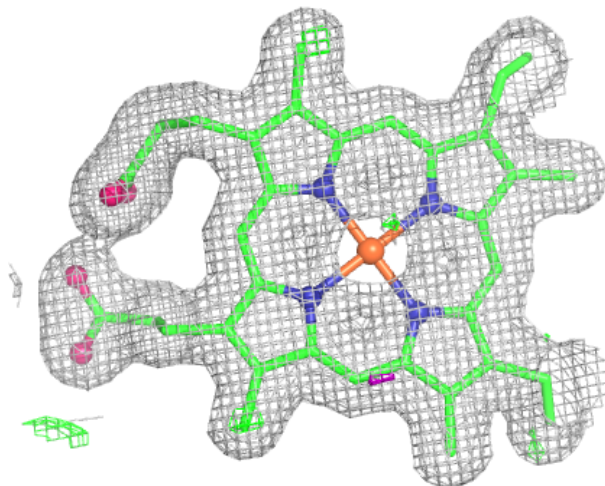
Electron density around HEC B 506:

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



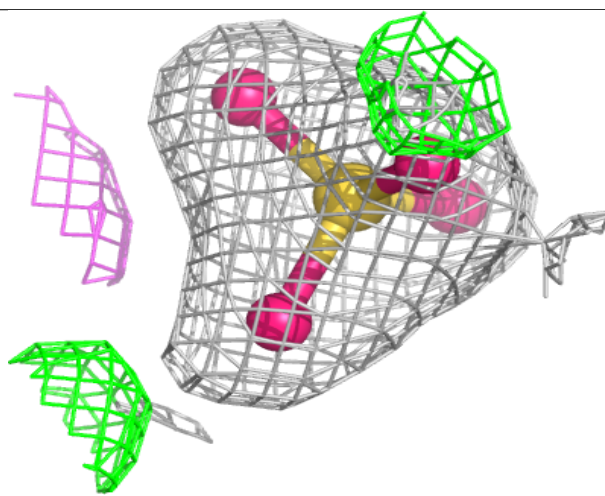
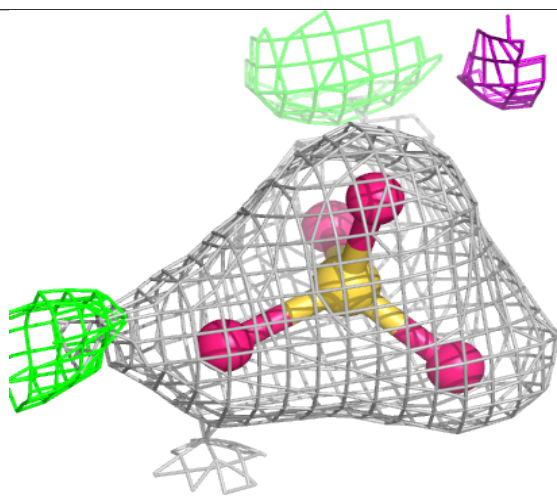
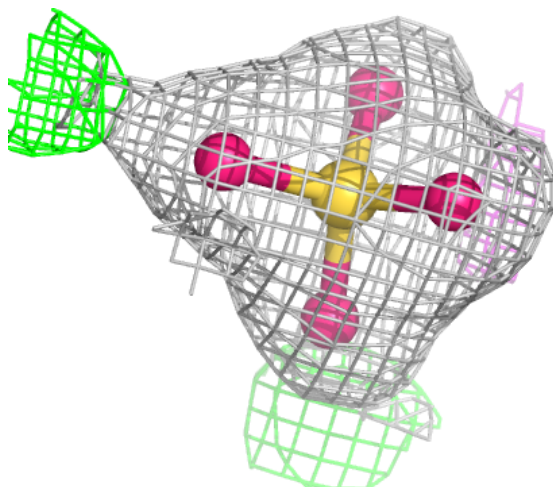
Electron density around HEC A 505:

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



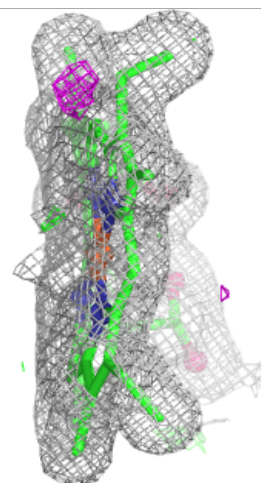
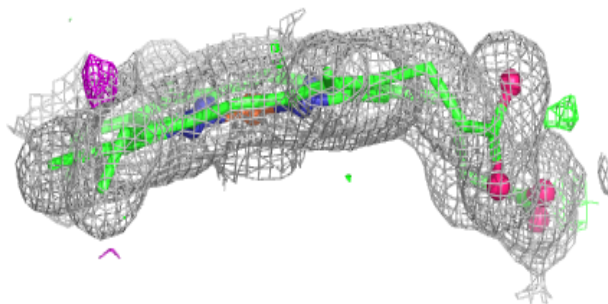
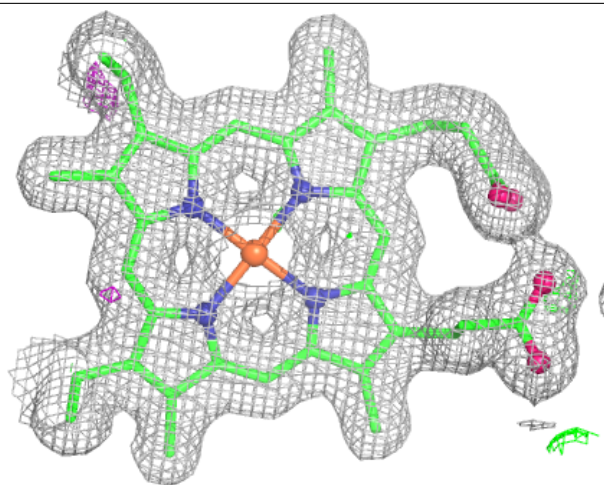
Electron density around SO4 D 510:

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



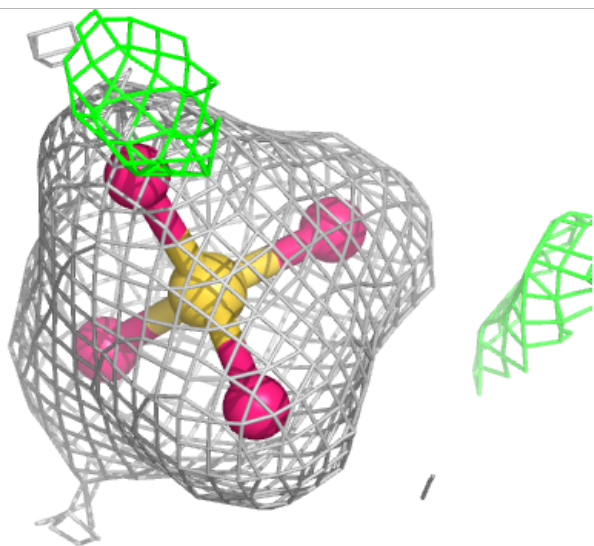
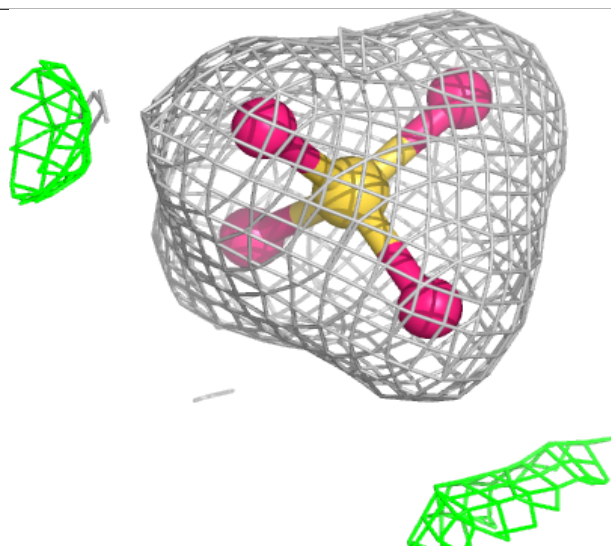
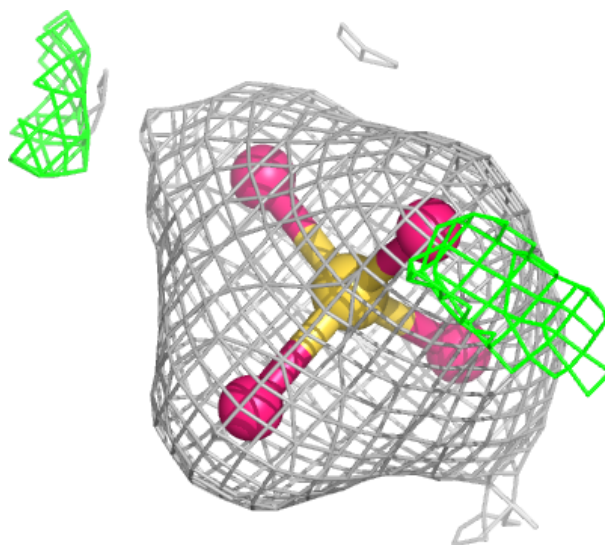
Electron density around HEC D 509:

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



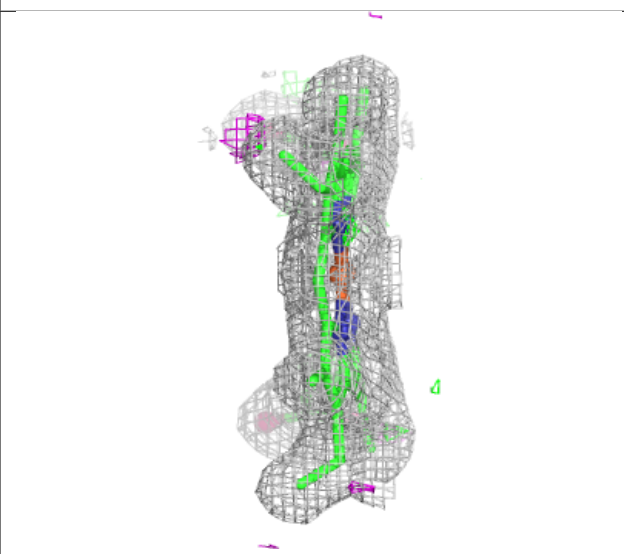
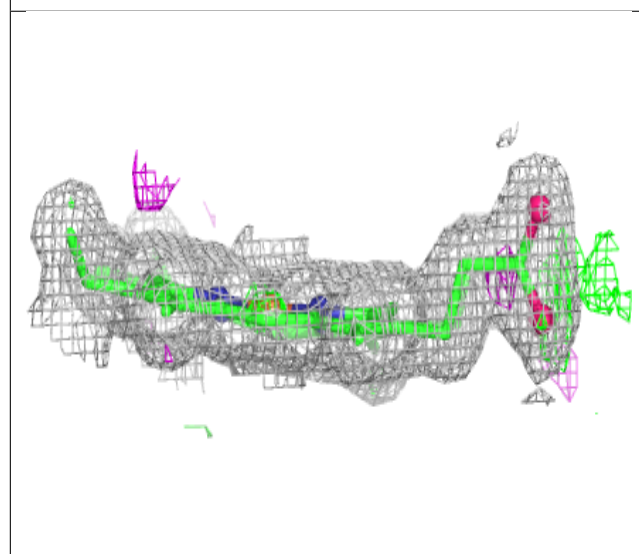
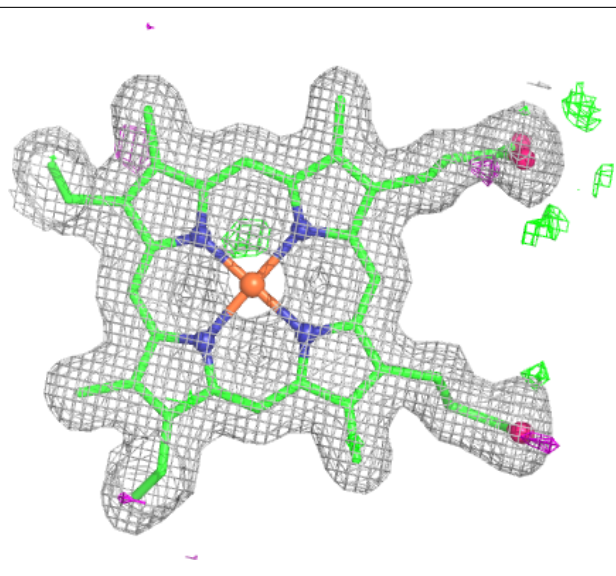
Electron density around SO4 B 507:

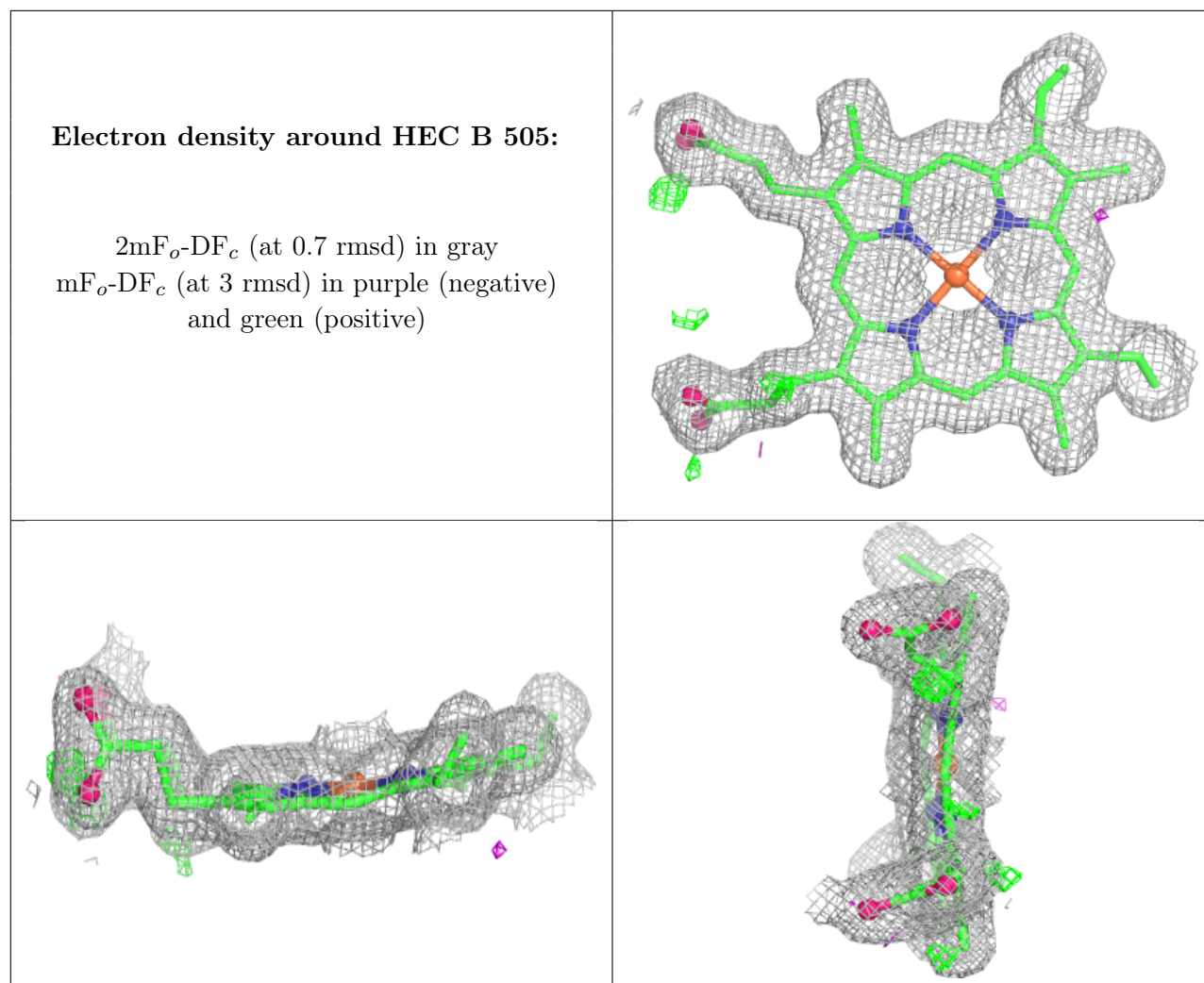
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEC A 504:

$2mF_o-DF_c$ (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.